Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 03:31 AM UTC

PDB ID	:	5OY0 / pdb_00005oy0
Title	:	Structure of synechocystis photosystem I trimer at 2.5A resolution
Authors	:	Nelson, N.; Malavath, T.; Caspy, I.
Deposited on	:	2017-09-07
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

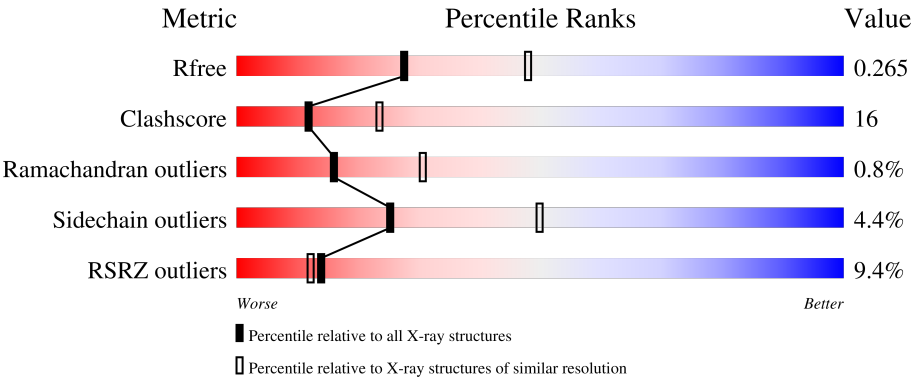
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



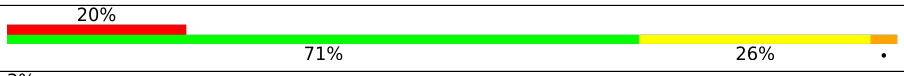
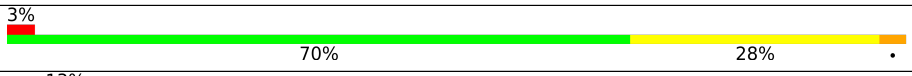
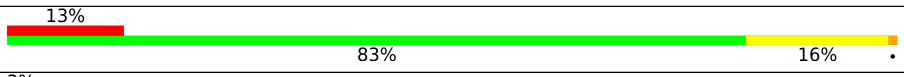
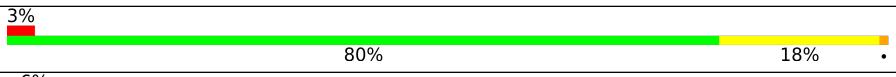
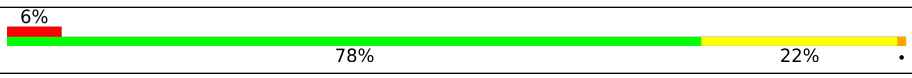
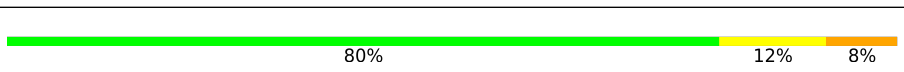
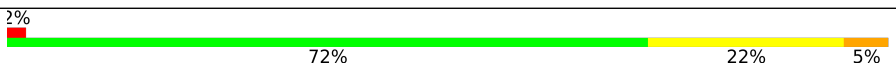
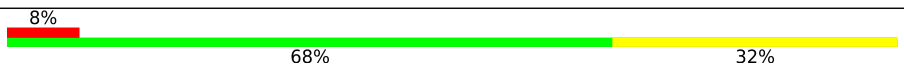
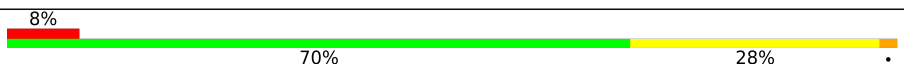
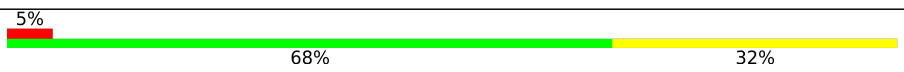
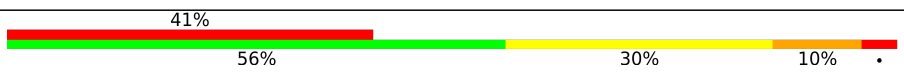
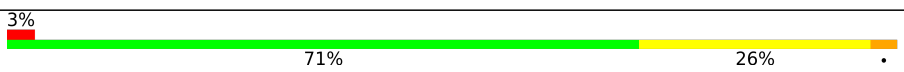
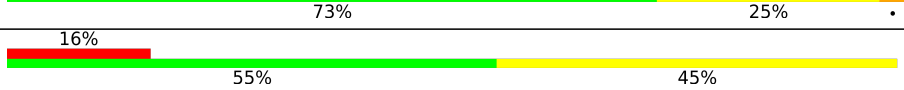
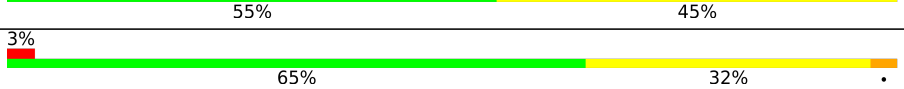
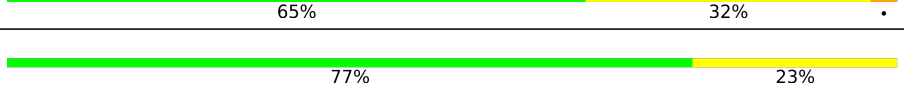
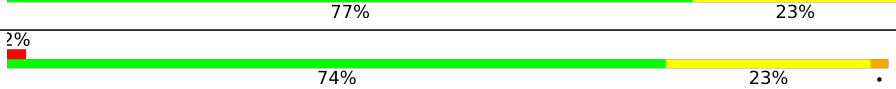
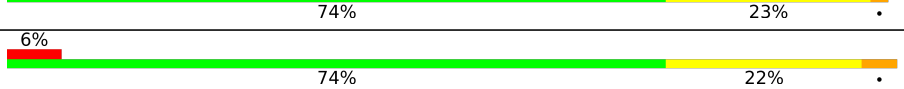
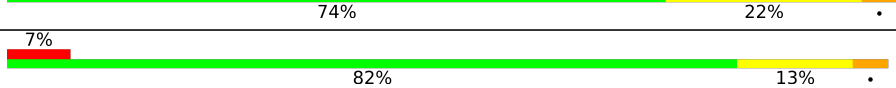
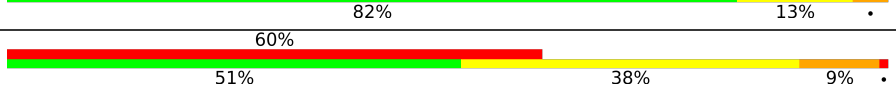
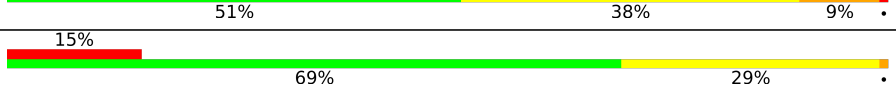
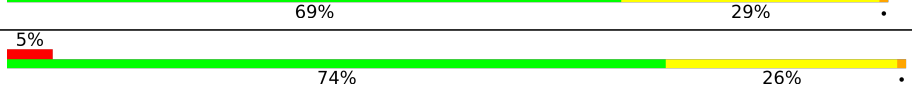
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	3% 78% 21%
1	a	751	15% 72% 27%
2	2	731	15% 75% 24%
2	B	731	3% 78% 21%
3	3	80	5% 66% 32%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	80	
4	D	141	
4	d	141	
5	5	69	
5	E	69	
6	6	143	
6	F	143	
6	f	143	
7	I	40	
7	i	40	
8	7	40	
8	J	40	
8	j	40	
9	K	80	
10	L	157	
10	l	157	
11	9	31	
11	M	31	
11	m	31	
12	b	729	
13	c	81	
14	e	68	
15	k	78	
16	1	744	
17	4	140	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	h	38	5% 55% 37% 8%
19	8	79	58% 67% 28% 5%
20	0	154	% 74% 25%

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
21	CLA	0	1501	X	-	-	-
21	CLA	0	1502	X	-	-	-
21	CLA	0	1503	X	-	-	-
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	-	-
21	CLA	1	1013	X	-	-	-
21	CLA	1	1102	X	-	-	-
21	CLA	1	1103	X	-	-	-
21	CLA	1	1104	X	-	-	-
21	CLA	1	1105	X	-	-	-
21	CLA	1	1106	X	-	-	-
21	CLA	1	1107	X	-	-	-
21	CLA	1	1108	X	-	-	-
21	CLA	1	1109	X	-	-	-
21	CLA	1	1110	X	-	-	-
21	CLA	1	1111	X	-	-	-
21	CLA	1	1112	X	-	-	-
21	CLA	1	1113	X	-	-	-
21	CLA	1	1114	X	-	-	-
21	CLA	1	1115	X	-	-	-
21	CLA	1	1116	X	-	-	-
21	CLA	1	1117	X	-	-	-
21	CLA	1	1118	X	-	-	-
21	CLA	1	1119	X	-	-	-
21	CLA	1	1120	X	-	-	-
21	CLA	1	1121	X	-	-	-
21	CLA	1	1122	X	-	-	-
21	CLA	1	1124	X	-	-	-
21	CLA	1	1125	X	-	-	-
21	CLA	1	1126	X	-	-	-
21	CLA	1	1127	X	-	-	-
21	CLA	1	1128	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	1129	X	-	-	-
21	CLA	1	1130	X	-	-	-
21	CLA	1	1131	X	-	-	-
21	CLA	1	1132	X	-	-	-
21	CLA	1	1133	X	-	-	-
21	CLA	1	1134	X	-	-	-
21	CLA	1	1136	X	-	-	-
21	CLA	1	1137	X	-	-	-
21	CLA	1	1138	X	-	-	-
21	CLA	1	1139	X	-	-	-
21	CLA	1	1140	X	-	-	-
21	CLA	1	1801	X	-	-	-
21	CLA	2	1021	X	-	-	-
21	CLA	2	1022	X	-	-	-
21	CLA	2	1023	X	-	-	-
21	CLA	2	1201	X	-	-	-
21	CLA	2	1202	X	-	-	-
21	CLA	2	1203	X	-	-	-
21	CLA	2	1204	X	-	-	-
21	CLA	2	1205	X	-	-	-
21	CLA	2	1206	X	-	-	-
21	CLA	2	1208	X	-	-	-
21	CLA	2	1211	X	-	-	-
21	CLA	2	1212	X	-	-	-
21	CLA	2	1213	X	-	-	-
21	CLA	2	1214	X	-	-	-
21	CLA	2	1215	X	-	-	-
21	CLA	2	1216	X	-	-	-
21	CLA	2	1217	X	-	-	-
21	CLA	2	1218	X	-	-	-
21	CLA	2	1220	X	-	-	-
21	CLA	2	1221	X	-	-	-
21	CLA	2	1222	X	-	-	-
21	CLA	2	1224	X	-	-	-
21	CLA	2	1225	X	-	-	-
21	CLA	2	1226	X	-	-	-
21	CLA	2	1227	X	-	-	-
21	CLA	2	1228	X	-	-	-
21	CLA	2	1229	X	-	-	-
21	CLA	2	1230	X	-	-	-
21	CLA	2	1231	X	-	-	-
21	CLA	2	1232	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	1234	X	-	-	-
21	CLA	2	1235	X	-	-	-
21	CLA	2	1236	X	-	-	-
21	CLA	2	1237	X	-	-	-
21	CLA	2	1238	X	-	-	-
21	CLA	2	1239	X	-	-	-
21	CLA	6	1301	X	-	-	-
21	CLA	6	1302	X	-	-	-
21	CLA	7	1302	X	-	-	-
21	CLA	7	1303	X	-	-	-
21	CLA	8	1401	X	-	-	-
21	CLA	8	1402	X	-	-	-
21	CLA	A	1011	X	-	-	-
21	CLA	A	1012	X	-	-	-
21	CLA	A	1013	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1130	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1801	X	-	-	-
21	CLA	B	1021	X	-	-	-
21	CLA	B	1022	X	-	-	-
21	CLA	B	1023	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	-	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1232	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	J	1302	X	-	-	-
21	CLA	J	1303	X	-	-	-
21	CLA	K	1401	X	-	-	-
21	CLA	L	1501	X	-	-	-
21	CLA	L	1502	X	-	-	-
21	CLA	a	1011	X	-	-	-
21	CLA	a	1012	X	-	-	-
21	CLA	a	1013	X	-	-	-
21	CLA	a	1102	X	-	-	-
21	CLA	a	1103	X	-	-	-
21	CLA	a	1104	X	-	-	-
21	CLA	a	1105	X	-	-	-
21	CLA	a	1106	X	-	-	-
21	CLA	a	1107	X	-	-	-
21	CLA	a	1108	X	-	-	-
21	CLA	a	1109	X	-	-	-
21	CLA	a	1110	X	-	-	-
21	CLA	a	1111	X	-	-	-
21	CLA	a	1112	X	-	-	-
21	CLA	a	1113	X	-	-	-
21	CLA	a	1114	X	-	-	-
21	CLA	a	1116	X	-	-	-
21	CLA	a	1117	X	-	-	-
21	CLA	a	1118	X	-	-	-
21	CLA	a	1119	X	-	-	-
21	CLA	a	1121	X	-	-	-
21	CLA	a	1122	X	-	-	-
21	CLA	a	1123	X	-	-	-
21	CLA	a	1124	X	-	-	-
21	CLA	a	1125	X	-	-	-
21	CLA	a	1126	X	-	-	-
21	CLA	a	1127	X	-	-	-
21	CLA	a	1128	X	-	-	-
21	CLA	a	1129	X	-	-	-
21	CLA	a	1130	X	-	-	-
21	CLA	a	1131	X	-	-	-
21	CLA	a	1132	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	a	1134	X	-	-	-
21	CLA	a	1135	X	-	-	-
21	CLA	a	1136	X	-	-	-
21	CLA	a	1137	X	-	-	-
21	CLA	a	1138	X	-	-	-
21	CLA	a	1139	X	-	-	-
21	CLA	a	1140	X	-	-	-
21	CLA	a	1801	X	-	-	-
21	CLA	b	1021	X	-	-	-
21	CLA	b	1022	X	-	-	-
21	CLA	b	1023	X	-	-	-
21	CLA	b	1201	X	-	-	-
21	CLA	b	1202	X	-	-	-
21	CLA	b	1203	X	-	-	-
21	CLA	b	1204	X	-	-	-
21	CLA	b	1205	X	-	-	-
21	CLA	b	1206	X	-	-	-
21	CLA	b	1208	X	-	-	-
21	CLA	b	1211	X	-	-	-
21	CLA	b	1213	X	-	-	-
21	CLA	b	1214	X	-	-	-
21	CLA	b	1215	X	-	-	-
21	CLA	b	1216	X	-	-	-
21	CLA	b	1217	X	-	-	-
21	CLA	b	1218	X	-	-	-
21	CLA	b	1219	X	-	-	-
21	CLA	b	1220	X	-	-	-
21	CLA	b	1221	X	-	-	-
21	CLA	b	1222	X	-	-	-
21	CLA	b	1223	X	-	-	-
21	CLA	b	1224	X	-	-	-
21	CLA	b	1225	X	-	-	-
21	CLA	b	1226	X	-	-	-
21	CLA	b	1227	X	-	-	-
21	CLA	b	1228	X	-	-	-
21	CLA	b	1229	X	-	-	-
21	CLA	b	1230	X	-	-	-
21	CLA	b	1231	X	-	-	-
21	CLA	b	1232	X	-	-	-
21	CLA	b	1234	X	-	-	-
21	CLA	b	1235	X	-	-	-
21	CLA	b	1236	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	b	1237	X	-	-	-
21	CLA	b	1238	X	-	-	-
21	CLA	b	1239	X	-	-	-
21	CLA	b	1240	X	-	-	-
21	CLA	f	1301	X	-	-	-
21	CLA	f	1302	X	-	-	-
21	CLA	j	1302	X	-	-	-
21	CLA	j	1303	X	-	-	-
21	CLA	k	1401	X	-	-	-
21	CLA	k	1402	X	-	-	-
21	CLA	l	1501	X	-	-	-
21	CLA	l	1502	X	-	-	-
21	CLA	l	1503	X	-	-	-
23	SF4	C	3003	-	-	X	-
34	ZEX	F	4016	X	-	-	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 77117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			
1	a	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			
2	2	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	3	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			
4	d	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			543	340	96	107			
5	5	69	Total	C	N	O	0	0	0
			543	340	96	107			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			
6	f	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			
6	6	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			
7	i	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	j	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	7	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	80	Total	C	N	O	S	0	1	0
			579	378	93	102	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			
10	l	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	m	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	9	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			

- Molecule 12 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	b	729	Total	C	N	O	S	0	0	0
			5770	3798	967	990	15			

- Molecule 13 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	c	81	Total	C	N	O	S	0	0	0
			608	374	104	118	12			

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	e	68	Total	C	N	O	0	0	0
			533	335	94	104			

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	k	78	Total	C	N	O	S	0	0	0
			559	366	90	98	5			

- Molecule 16 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1	744	Total	C	N	O	S	0	0	0
			5826	3814	993	992	27			

- Molecule 17 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	140	Total	C	N	O	S	0	0	0
			1094	692	189	210	3			

- Molecule 18 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	h	38	Total	C	N	O	S	0	0	0
			298	202	42	51	3			

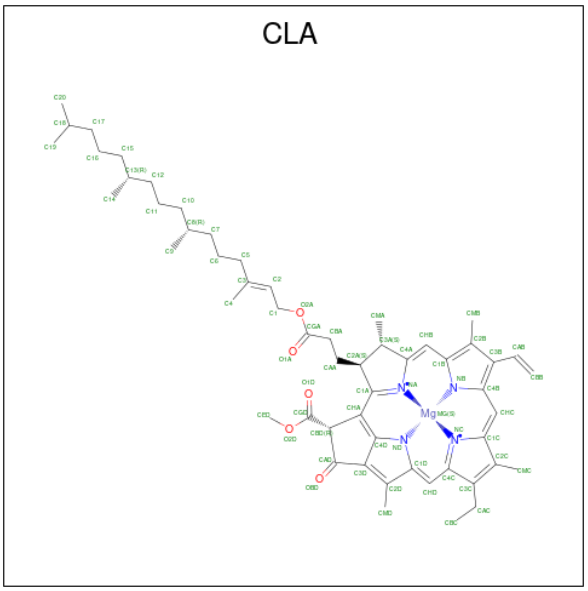
- Molecule 19 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	8	79	Total	C	N	O	S	0	0	0
			565	369	91	100	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	0	154	Total	C	N	O	S	0	0	0
			1156	753	188	213	2			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	f	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	f	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	j	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	j	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	k	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		

Continued on next page...

Continued from previous page...

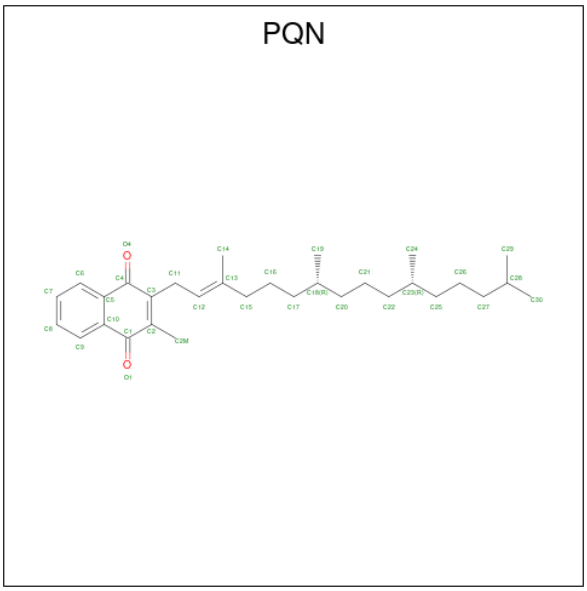
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

Continued on next page...

Continued from previous page...

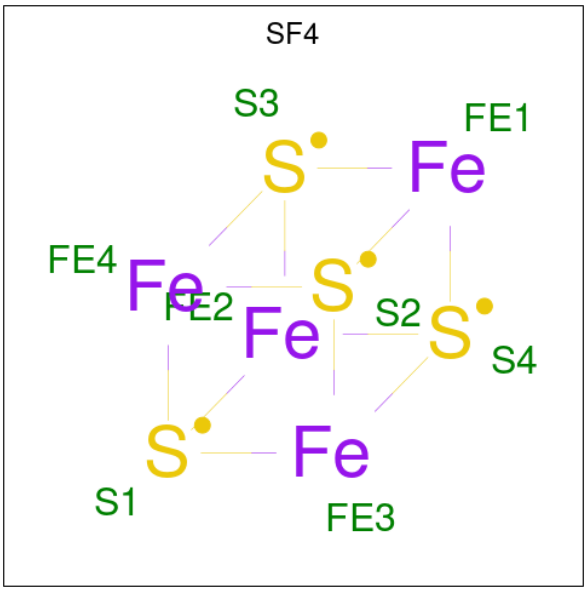
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



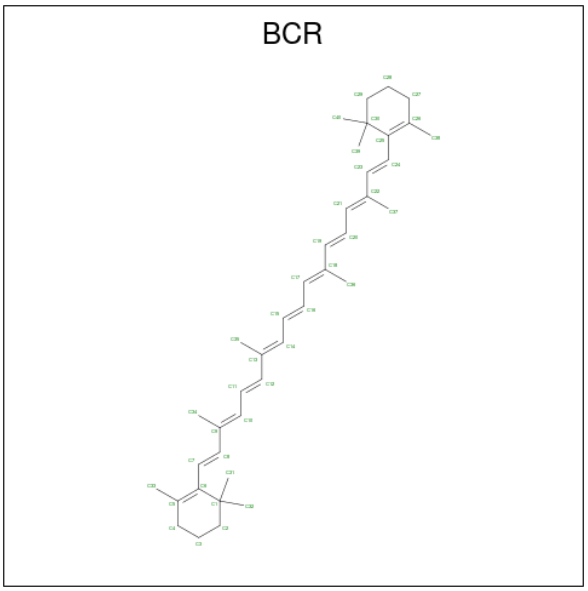
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 33 31 2	0	0
22	B	1	Total C O 33 31 2	0	0
22	a	1	Total C O 33 31 2	0	0
22	b	1	Total C O 33 31 2	0	0
22	1	1	Total C O 33 31 2	0	0
22	2	1	Total C O 33 31 2	0	0

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total Fe S 8 4 4	0	0
23	C	1	Total Fe S 8 4 4	0	0
23	C	1	Total Fe S 8 4 4	0	0
23	a	1	Total Fe S 8 4 4	0	0
23	c	1	Total Fe S 8 4 4	0	0
23	c	1	Total Fe S 8 4 4	0	0
23	1	1	Total Fe S 8 4 4	0	0
23	3	1	Total Fe S 8 4 4	0	0
23	3	1	Total Fe S 8 4 4	0	0

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	I	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	i	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

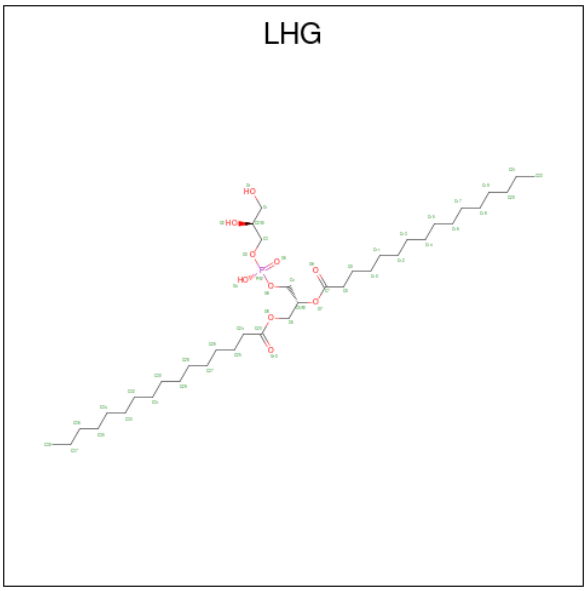
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	l	1	Total C 40 40	0	0
24	l	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	0	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	0	1	Total C 40 40	0	0
24	9	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



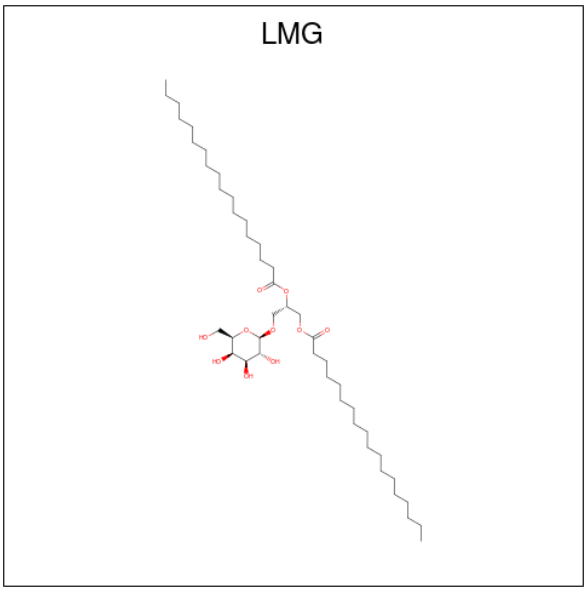
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	F	1	Total C O P 49 38 10 1	0	0
25	L	1	Total C O P 49 38 10 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	M	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	b	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	2	1	Total	C	O	P	0	0
			49	38	10	1		
25	6	1	Total	C	O	P	0	0
			12	5	6	1		
25	0	1	Total	C	O	P	0	0
			49	38	10	1		
25	0	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



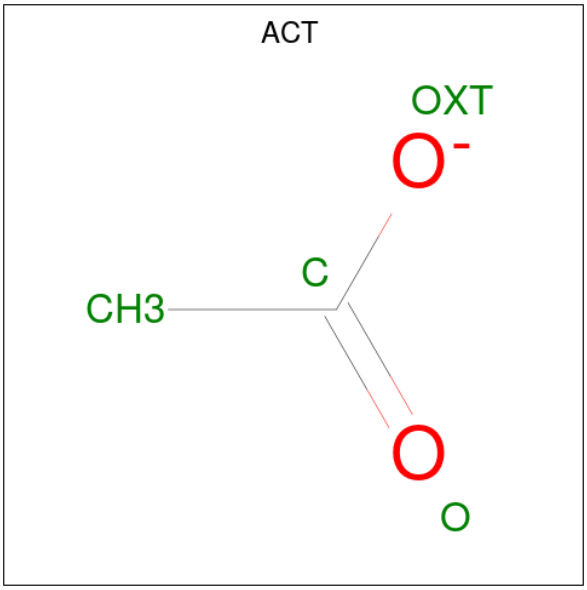
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 50 40 10	0	0
26	A	1	Total C O 48 38 10	0	0
26	A	1	Total C O 55 45 10	0	0
26	B	1	Total C O 55 45 10	0	0
26	B	1	Total C O 55 45 10	0	0
26	K	1	Total C O 55 45 10	0	0
26	a	1	Total C O 50 40 10	0	0
26	a	1	Total C O 55 45 10	0	0
26	b	1	Total C O 55 45 10	0	0
26	b	1	Total C O 55 45 10	0	0
26	b	1	Total C O 55 45 10	0	0
26	1	1	Total C O 50 40 10	0	0
26	1	1	Total C O 55 45 10	0	0
26	2	1	Total C O 55 45 10	0	0

Continued on next page...

Continued from previous page...

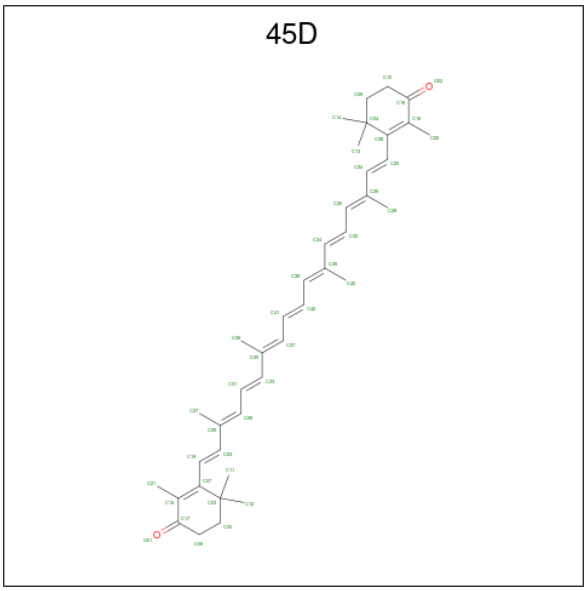
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	2	1	Total C O 55 45 10	0	0
26	0	1	Total C O 55 45 10	0	0

- Molecule 27 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 4 2 2	0	0
27	B	1	Total C O 4 2 2	0	0
27	B	1	Total C O 4 2 2	0	0
27	a	1	Total C O 4 2 2	0	0

- Molecule 28 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: $C_{40}H_{52}O_2$).

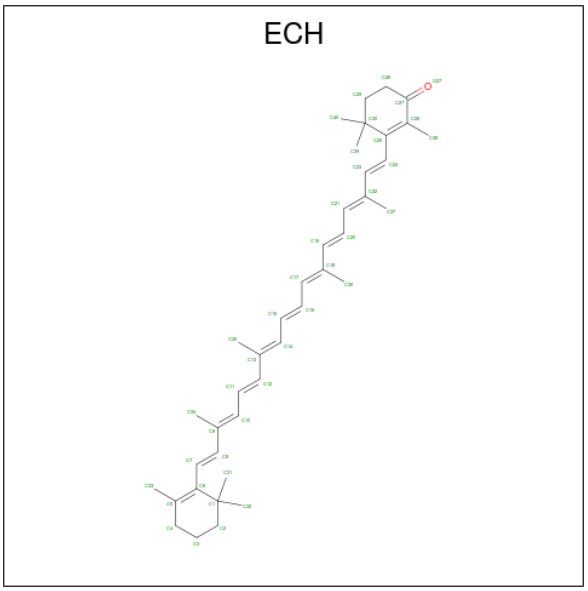


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C O 42 40 2	0	0
28	h	1	Total C O 42 40 2	0	0

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

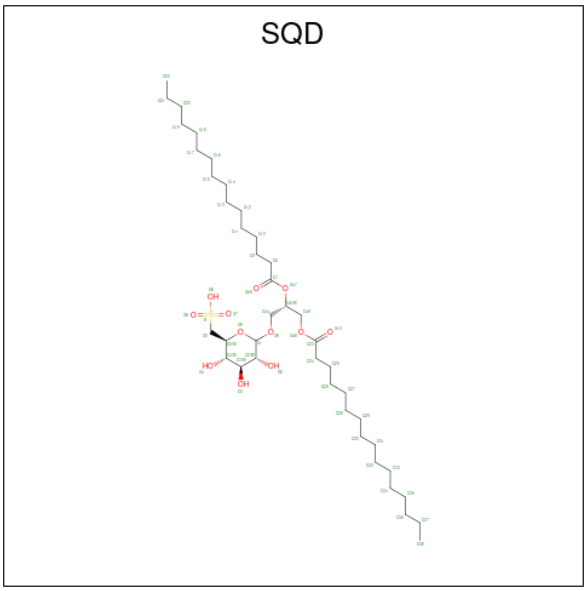
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total Cl 1 1	0	0
29	b	1	Total Cl 1 1	0	0
29	2	1	Total Cl 1 1	0	0

- Molecule 30 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C O 41 40 1	0	0
30	M	1	Total C O 41 40 1	0	0
30	b	1	Total C O 41 40 1	0	0
30	b	1	Total C O 41 40 1	0	0
30	i	1	Total C O 41 40 1	0	0
30	m	1	Total C O 41 40 1	0	0
30	2	1	Total C O 41 40 1	0	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	F	1	Total	C	O	S	0	0
			54	41	12	1		
31	L	1	Total	C	O	S	0	0
			51	38	12	1		
31	L	1	Total	C	O	S	0	0
			54	41	12	1		
31	b	1	Total	C	O	S	0	0
			54	41	12	1		
31	f	1	Total	C	O	S	0	0
			54	41	12	1		
31	0	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	1	Total	Ca	0	0
			1	1		
32	L	1	Total	Ca	0	0
			1	1		
32	b	1	Total	Ca	0	0
			1	1		
32	l	1	Total	Ca	0	0
			1	1		
32	2	1	Total	Ca	0	0
			1	1		

Continued on next page...

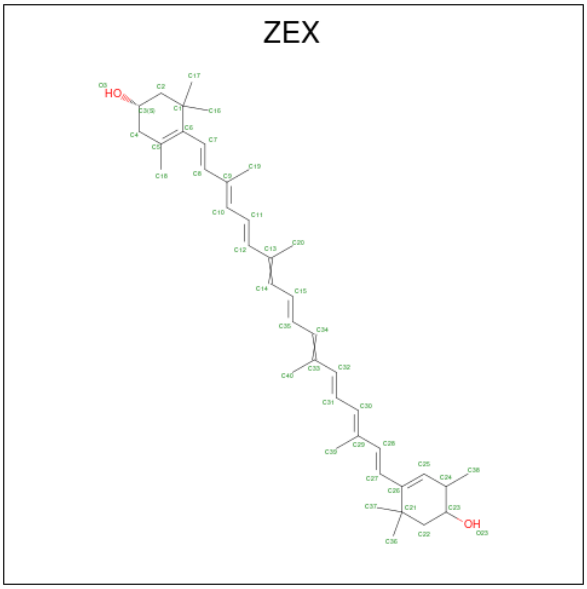
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total Ca 1 1	0	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

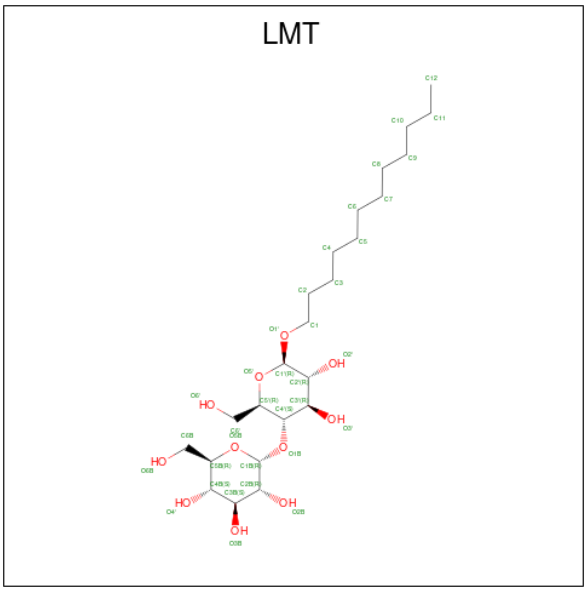
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Mg 1 1	0	0
33	b	1	Total Mg 1 1	0	0

- Molecule 34 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



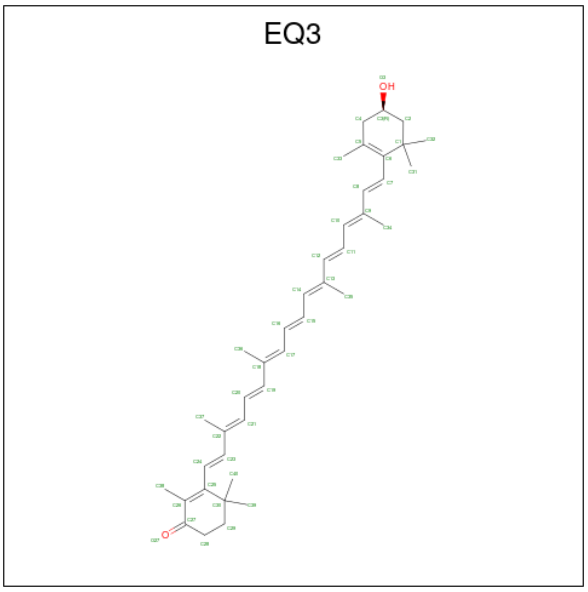
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total C O 42 40 2	0	0
34	J	1	Total C O 42 40 2	0	0
34	j	1	Total C O 42 40 2	0	0
34	7	1	Total C O 42 40 2	0	0

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



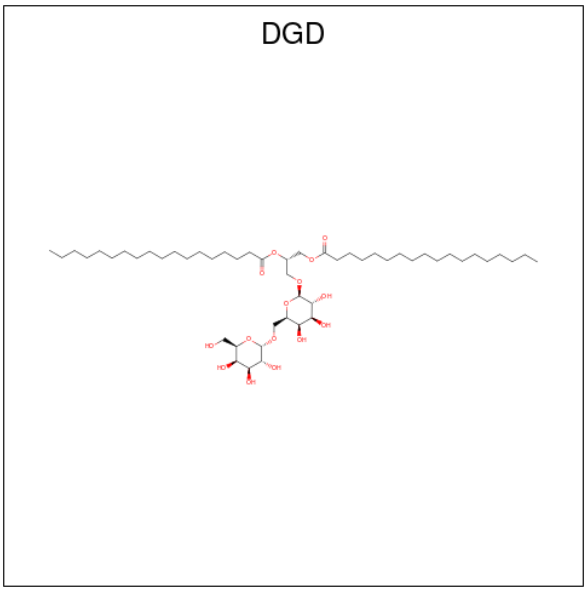
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	F	1	Total C O 35 24 11	0	0
35	L	1	Total C O 35 24 11	0	0
35	l	1	Total C O 35 24 11	0	0
35	1	1	Total C O 35 24 11	0	0
35	0	1	Total C O 35 24 11	0	0

- Molecule 36 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	I	1	Total	C	O	0	0
			42	40	2		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	L	1	Total	C	O	0	0
			66	51	15		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	186	Total O 186 186	0	0
38	B	114	Total O 114 114	0	0
38	C	48	Total O 48 48	0	0
38	D	57	Total O 57 57	0	0
38	E	16	Total O 16 16	0	0
38	F	8	Total O 8 8	0	0
38	I	6	Total O 6 6	0	0
38	J	4	Total O 4 4	0	0
38	K	9	Total O 9 9	0	0
38	L	46	Total O 46 46	0	0
38	M	3	Total O 3 3	0	0
38	a	39	Total O 39 39	0	0
38	b	141	Total O 141 141	0	0
38	c	13	Total O 13 13	0	0
38	d	15	Total O 15 15	0	0
38	e	4	Total O 4 4	0	0
38	f	10	Total O 10 10	0	0
38	i	7	Total O 7 7	0	0
38	j	5	Total O 5 5	0	0
38	l	20	Total O 20 20	0	0
38	m	8	Total O 8 8	0	0
38	1	37	Total O 37 37	0	0

Continued on next page...

Continued from previous page...

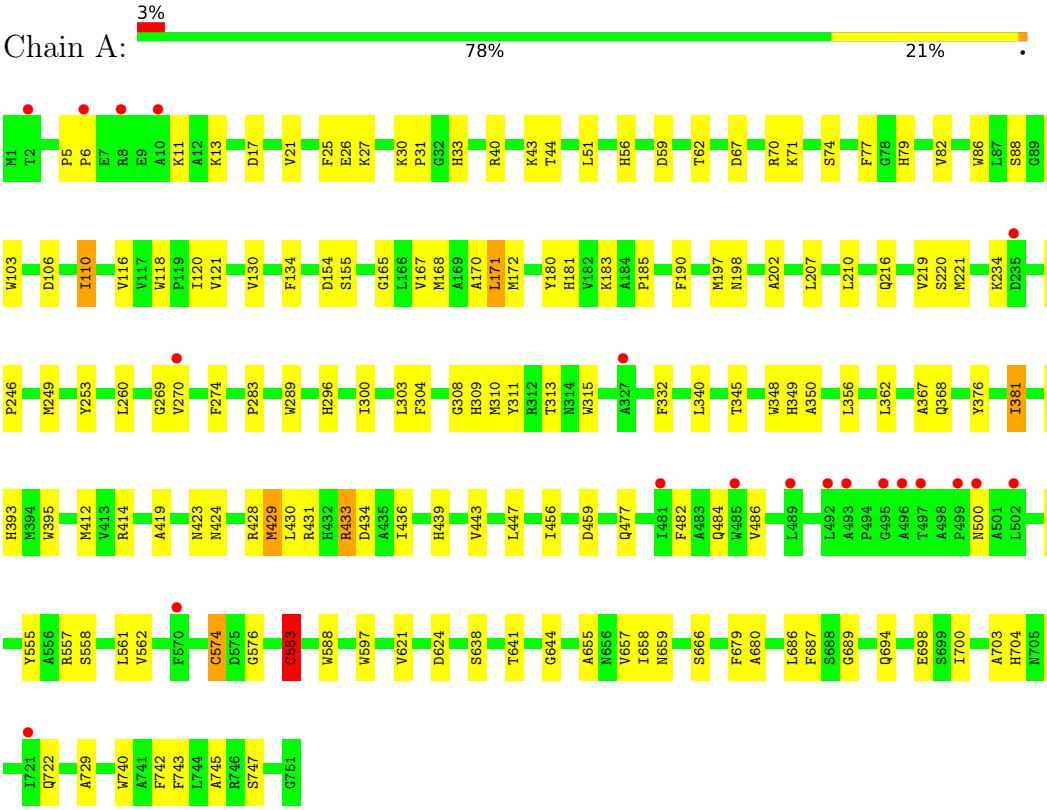
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	2	24	Total O 24 24	0	0
38	3	11	Total O 11 11	0	0
38	4	13	Total O 13 13	0	0
38	5	4	Total O 4 4	0	0
38	6	1	Total O 1 1	0	0
38	h	3	Total O 3 3	0	0
38	7	1	Total O 1 1	0	0
38	8	2	Total O 2 2	0	0
38	0	33	Total O 33 33	0	0
38	9	1	Total O 1 1	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

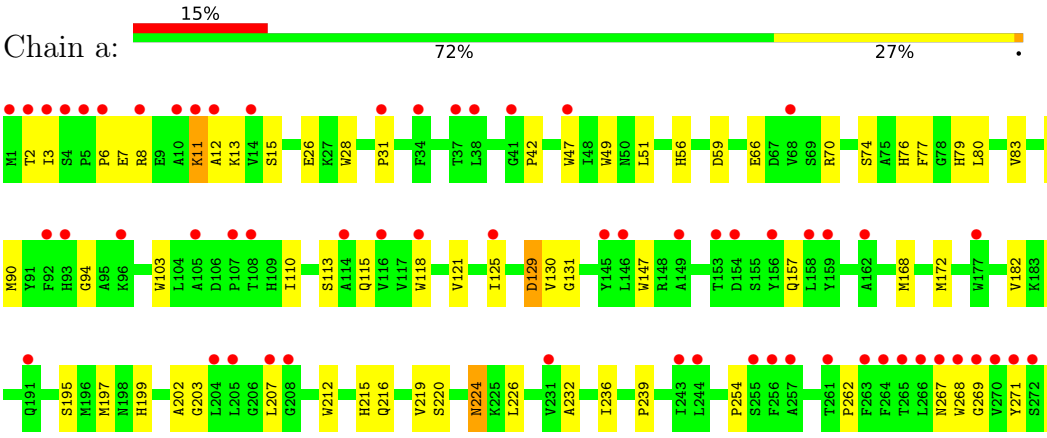
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

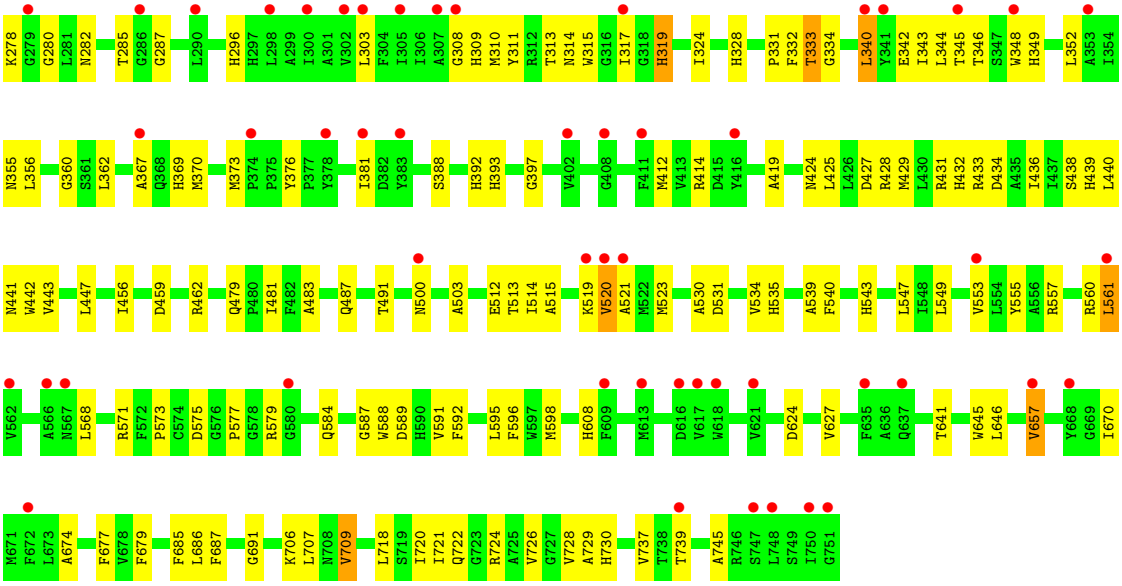
Chain A:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:

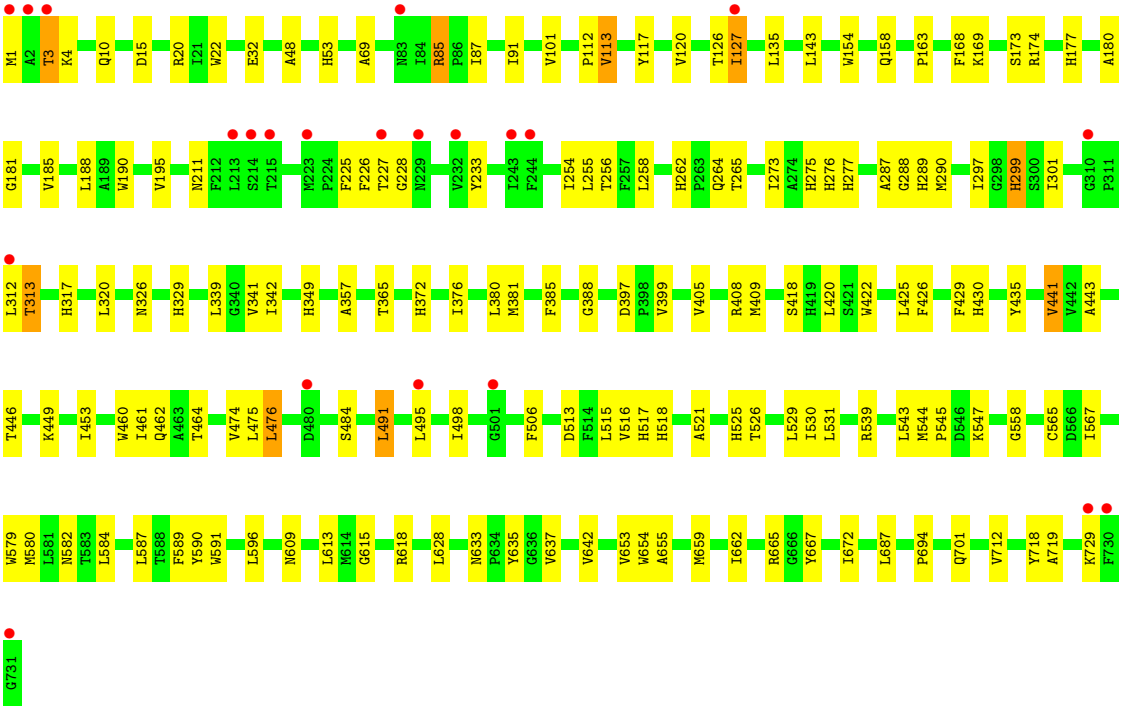




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

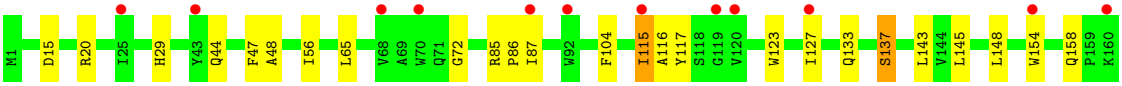


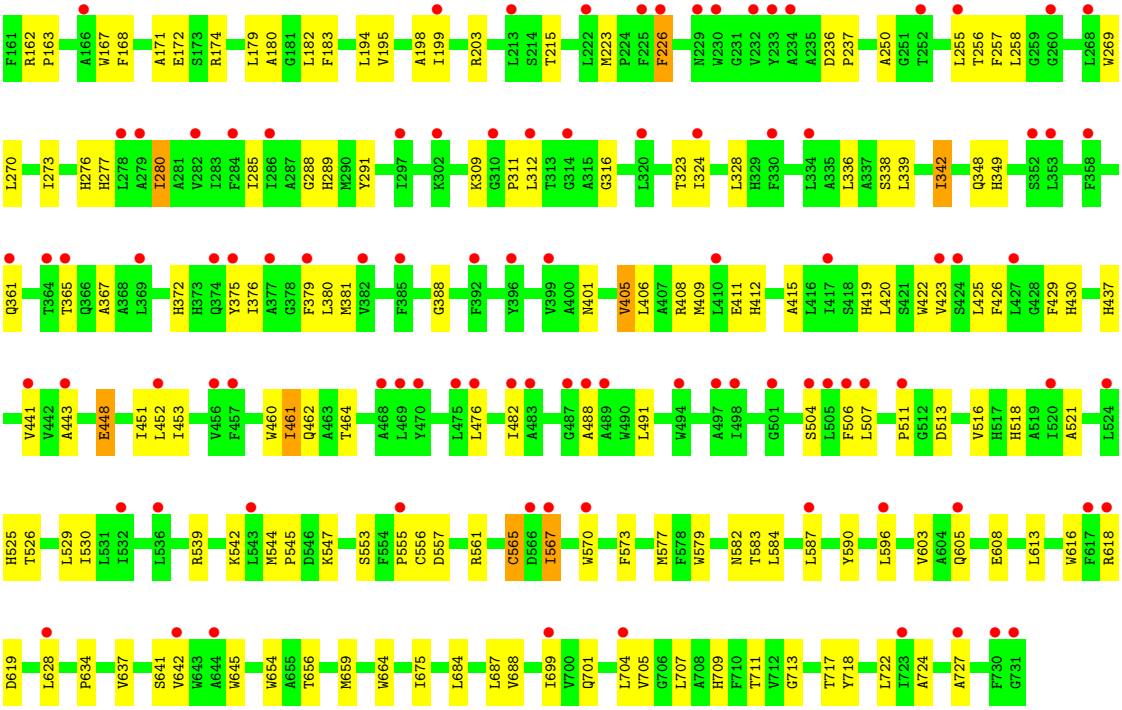


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:

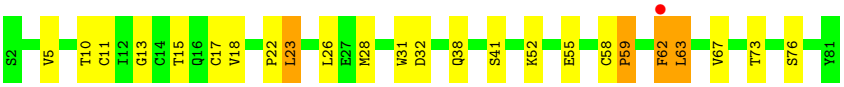






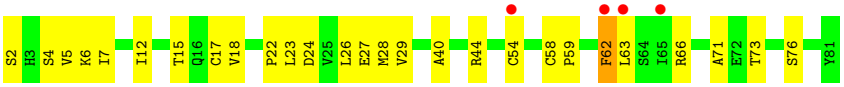
• Molecule 3: Photosystem I iron-sulfur center



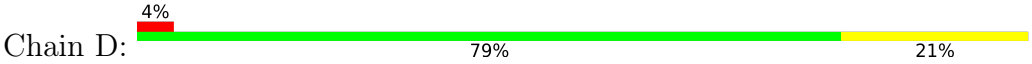


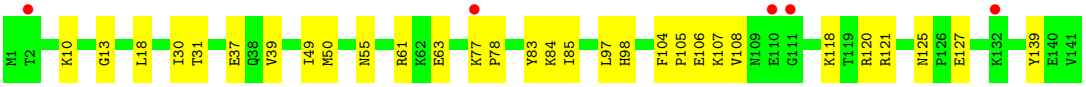
• Molecule 3: Photosystem I iron-sulfur center



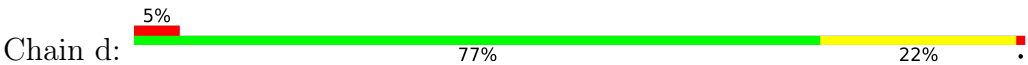


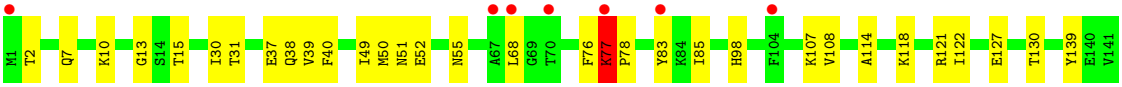
• Molecule 4: Photosystem I reaction center subunit II





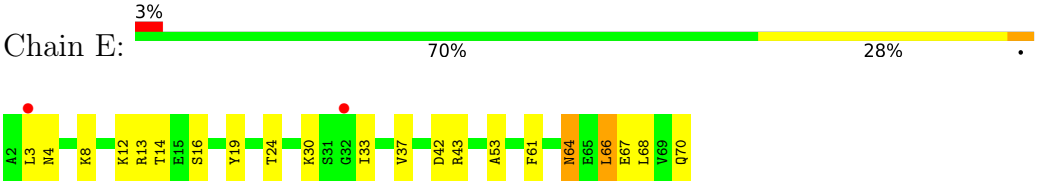
• Molecule 4: Photosystem I reaction center subunit II





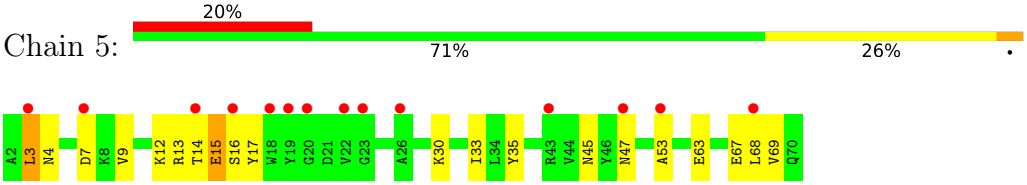
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



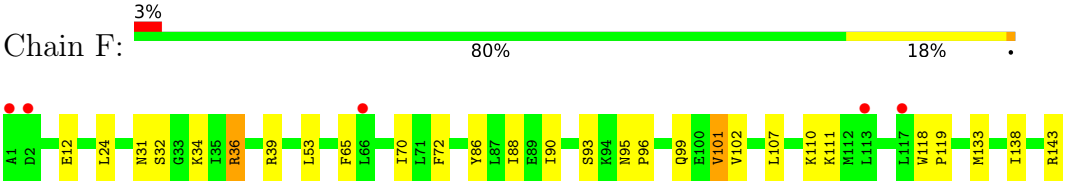
• Molecule 5: Photosystem I reaction center subunit IV

Chain 5:



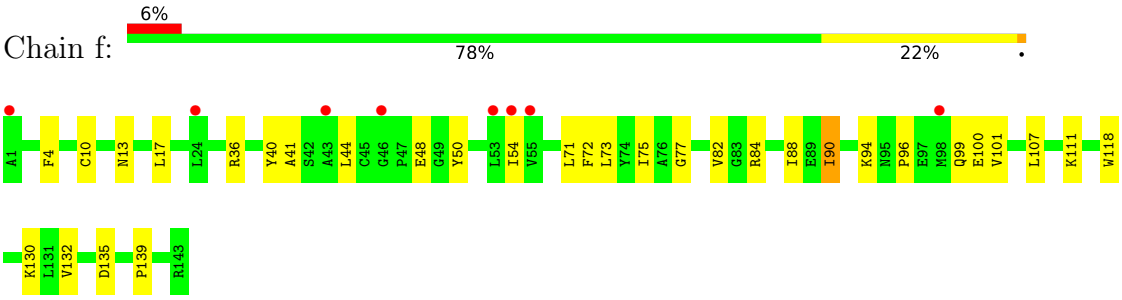
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



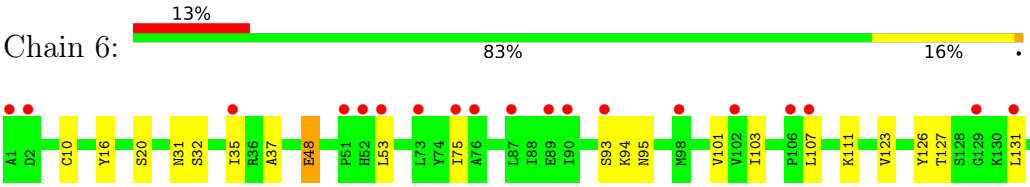
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



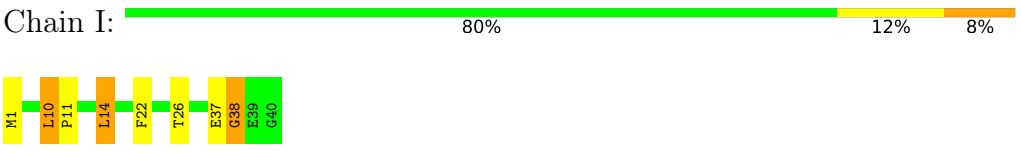
• Molecule 6: Photosystem I reaction center subunit III

Chain 6:



• Molecule 7: Photosystem I reaction center subunit VIII

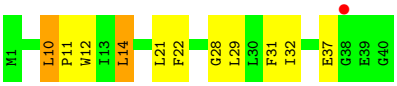
Chain I:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

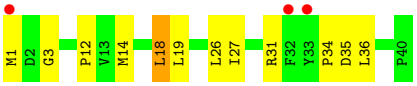




• Molecule 8: Photosystem I reaction center subunit IX

Chain J:





• Molecule 8: Photosystem I reaction center subunit IX

Chain j:

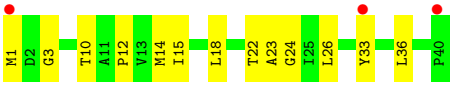




• Molecule 8: Photosystem I reaction center subunit IX

Chain 7:

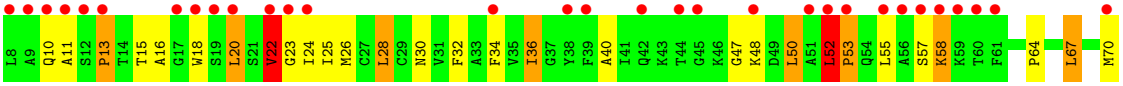


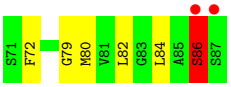


• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K:



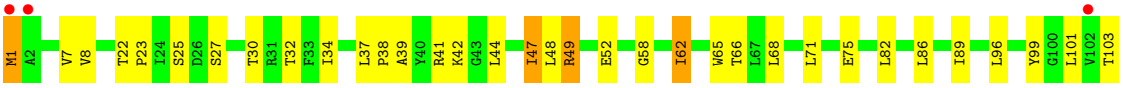


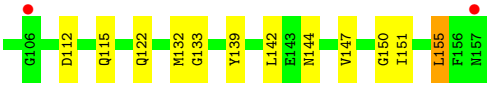


• Molecule 10: Photosystem I reaction center subunit XI

Chain L:

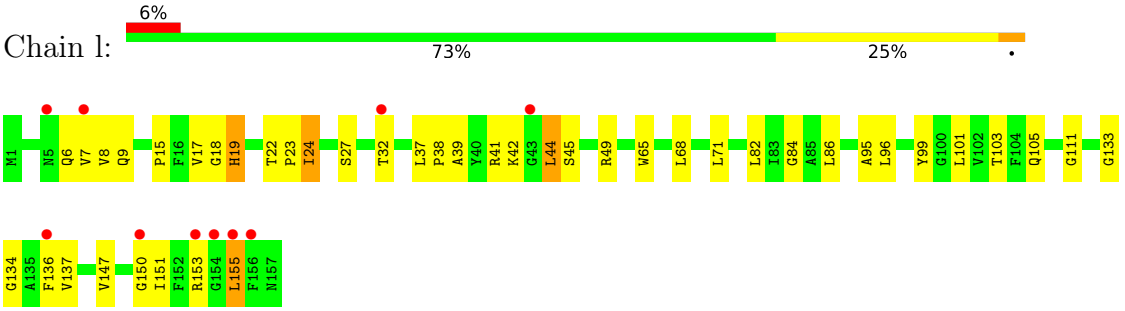






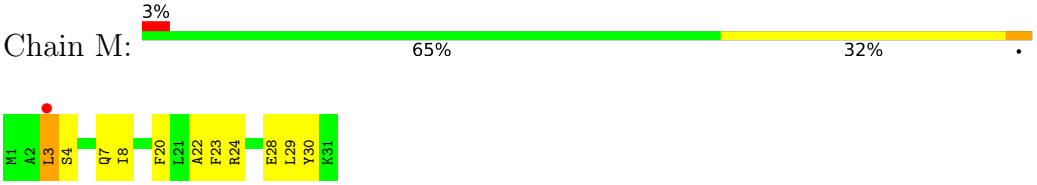
• Molecule 10: Photosystem I reaction center subunit XI

Chain l:



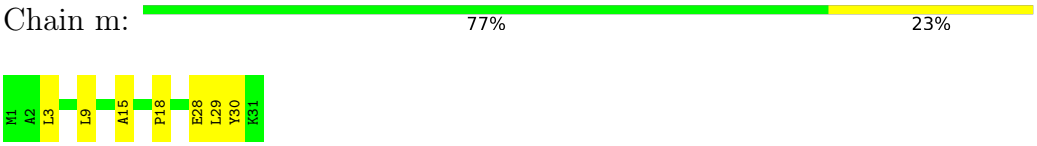
• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



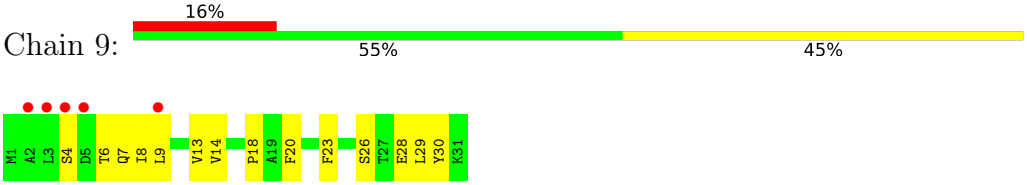
• Molecule 11: Photosystem I reaction center subunit XII

Chain m:



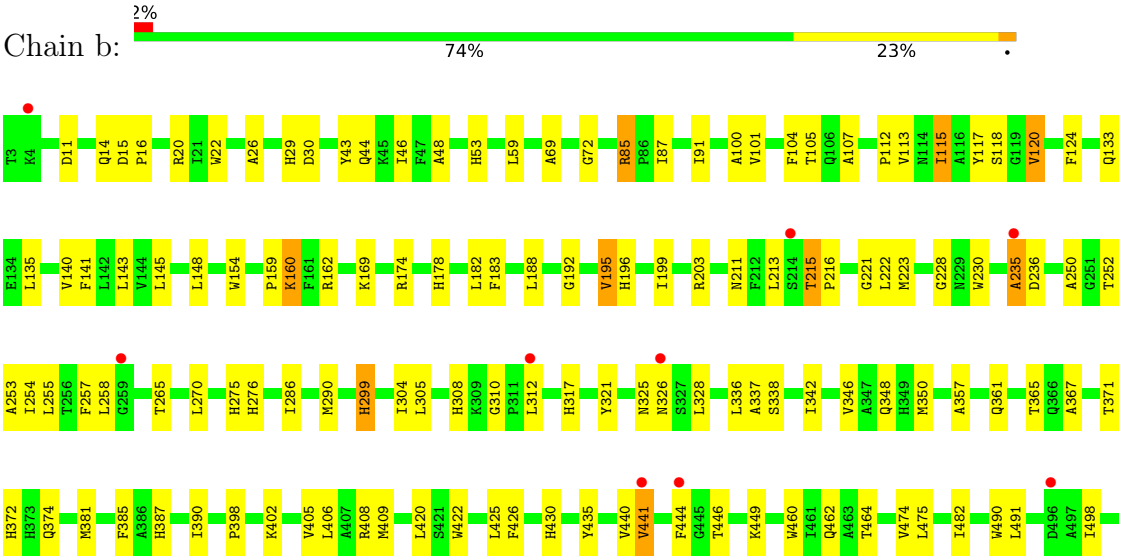
• Molecule 11: Photosystem I reaction center subunit XII

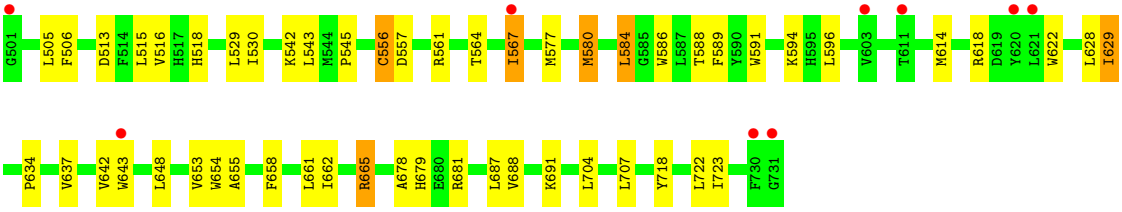
Chain 9:



• Molecule 12: Photosystem I P700 chlorophyll a apoprotein A2

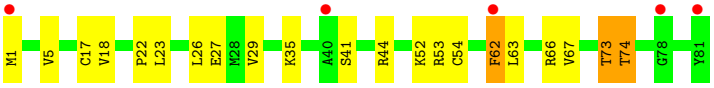
Chain b:



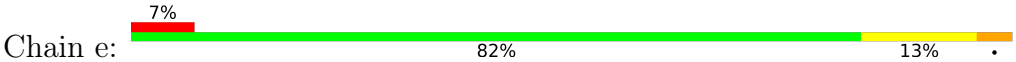


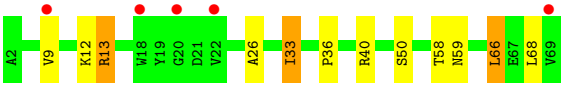
• Molecule 13: Photosystem I iron-sulfur center





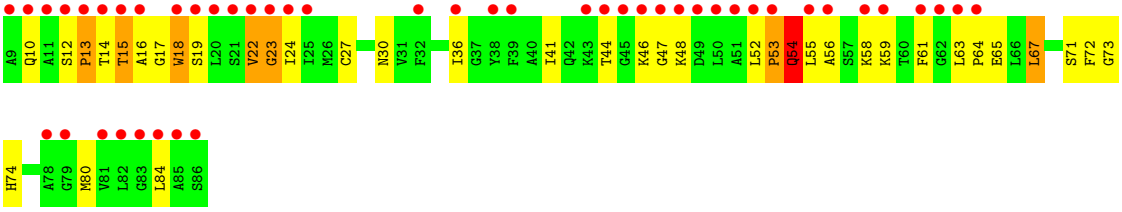
• Molecule 14: Photosystem I reaction center subunit IV





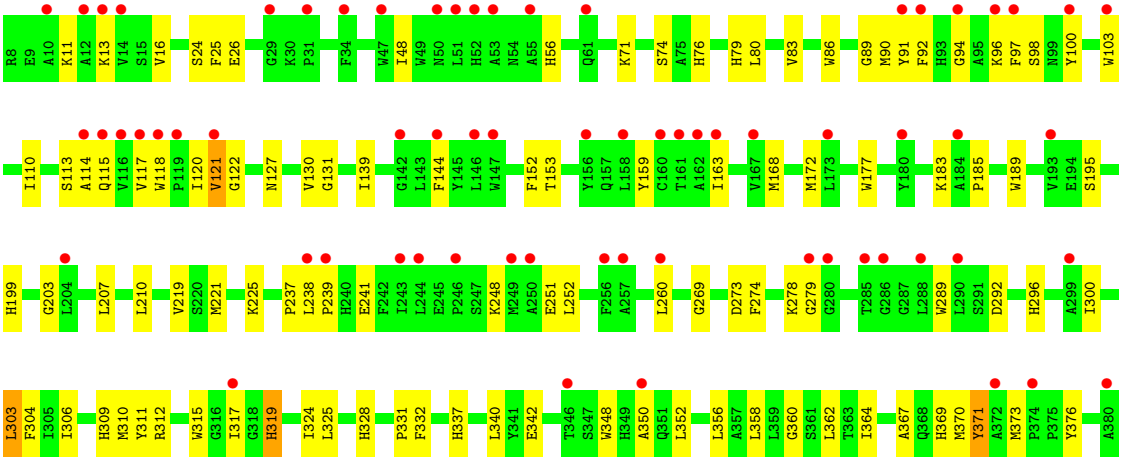
• Molecule 15: Photosystem I reaction center subunit PsaK 2

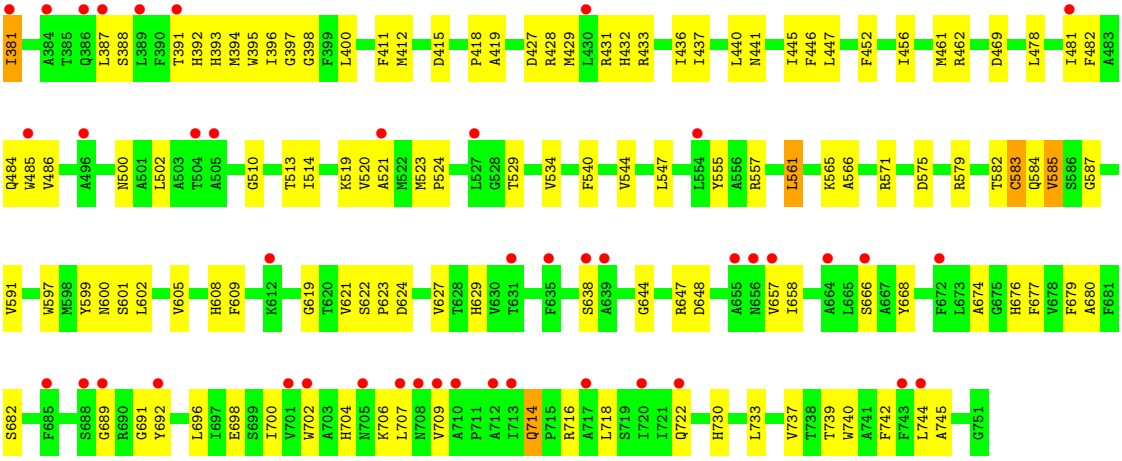




• Molecule 16: Photosystem I P700 chlorophyll a apoprotein A1

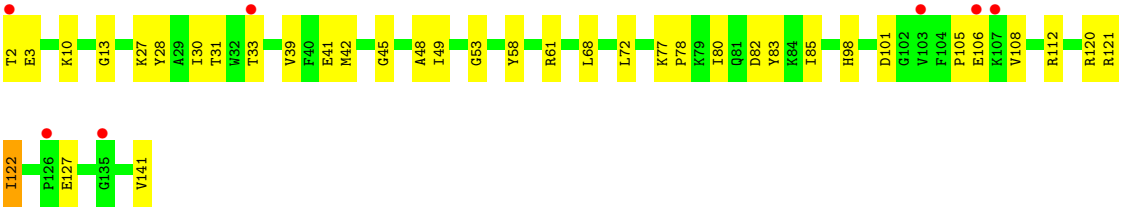






• Molecule 17: Photosystem I reaction center subunit II





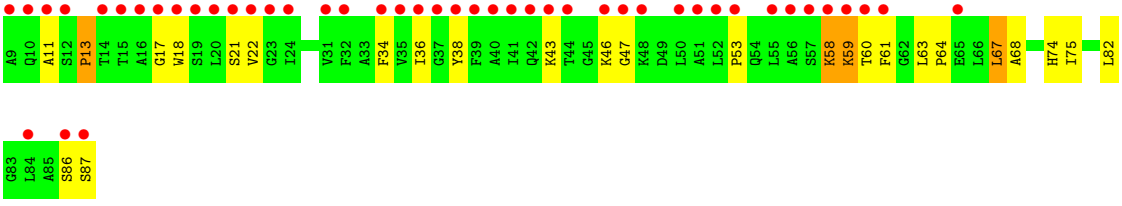
• Molecule 18: Photosystem I reaction center subunit VIII





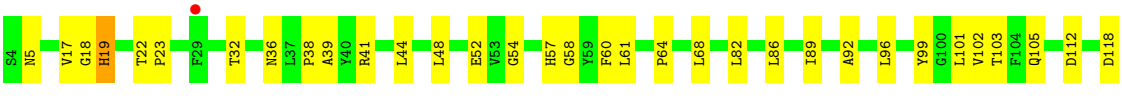
• Molecule 19: Photosystem I reaction center subunit PsaK 2





• Molecule 20: Photosystem I reaction center subunit XI






G131
M132
G133
G150
I151
F152
R153
G154
L155
F156
N157

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	212.17Å 137.62Å 225.09Å 90.00° 116.74° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.48-2.50) 99.4 (49.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.265	Depositor DCC
R_{free} test set	7916 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	77117	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ACT, DGD, 45D, PQN, SQD, MG, ZEX, SF4, LMG, EQ3, LMT, LHG, CA, CL, CLA, BCR, ECH

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	0.26	1/6078 (0.0%)	0.40	2/8284 (0.0%)
1	a	0.18	0/6078	0.33	0/8284
2	2	0.14	0/5994	0.32	0/8195
2	B	0.28	0/5994	0.42	3/8195 (0.0%)
3	3	0.12	0/610	0.35	0/826
3	C	0.25	0/610	0.48	0/826
4	D	0.17	0/1126	0.39	0/1517
4	d	0.13	0/1126	0.41	0/1517
5	5	0.10	0/552	0.29	0/745
5	E	0.15	0/552	0.36	0/745
6	6	0.12	0/1143	0.30	0/1553
6	F	0.14	0/1143	0.33	0/1553
6	f	0.15	0/1143	0.31	0/1553
7	I	0.16	0/322	0.35	0/438
7	i	0.14	0/322	0.37	0/438
8	7	0.12	0/328	0.26	0/443
8	J	0.15	0/328	0.35	0/443
8	j	0.12	0/328	0.28	0/443
9	K	0.17	0/590	0.45	0/797
10	L	0.16	0/1208	0.37	0/1640
10	l	0.14	0/1208	0.33	0/1640
11	9	0.14	0/241	0.41	0/326
11	M	0.15	0/241	0.29	0/326
11	m	0.17	0/241	0.29	0/326
12	b	0.24	0/5981	0.44	3/8178 (0.0%)
13	c	0.15	0/618	0.41	0/836
14	e	0.12	0/542	0.29	0/733
15	k	0.17	0/570	0.41	0/770
16	1	0.13	0/6024	0.30	0/8209
17	4	0.12	0/1118	0.33	0/1507
18	h	0.14	0/309	0.34	0/421
19	8	0.15	0/576	0.38	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
20	0	0.15	0/1186	0.33	0/1611
All	All	0.19	1/54430 (0.0%)	0.37	8/74096 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	CYS	C-O	-5.02	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	665	ARG	N-CA-C	18.12	131.03	111.28
2	B	665	ARG	N-CA-C	15.63	128.31	111.28
12	b	662	ILE	N-CA-C	9.46	119.42	110.53
1	A	576	GLY	CA-C-N	5.88	126.64	120.12
1	A	576	GLY	C-N-CA	5.88	126.64	120.12
2	B	558	GLY	CA-C-N	5.22	125.92	120.12
2	B	558	GLY	C-N-CA	5.22	125.92	120.12
12	b	661	LEU	N-CA-C	5.20	116.75	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	52	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5743	146	0
1	a	5878	0	5743	180	0
2	2	5783	0	5565	153	0
2	B	5783	0	5564	131	0
3	3	600	0	589	17	0
3	C	600	0	582	18	0
4	D	1102	0	1101	16	0
4	d	1102	0	1101	21	0
5	5	543	0	525	11	0
5	E	543	0	525	13	0
6	6	1113	0	1108	12	0
6	F	1113	0	1108	24	0
6	f	1113	0	1108	25	0
7	I	311	0	304	10	0
7	i	311	0	304	11	0
8	7	319	0	328	15	0
8	J	319	0	328	15	0
8	j	319	0	328	14	0
9	K	579	0	601	42	0
10	L	1178	0	1150	34	0
10	l	1178	0	1150	34	0
11	9	238	0	260	13	0
11	M	238	0	260	11	0
11	m	238	0	260	7	0
12	b	5770	0	5547	166	0
13	c	608	0	596	23	0
14	e	533	0	517	8	0
15	k	559	0	581	28	0
16	1	5826	0	5688	194	0
17	4	1094	0	1089	27	0
18	h	298	0	295	16	0
19	8	565	0	586	17	0
20	0	1156	0	1127	36	0
21	0	195	0	216	17	0
21	1	2642	0	2675	211	0
21	2	2363	0	2238	162	0
21	6	90	0	67	7	0
21	7	82	0	56	3	0
21	8	91	0	64	4	0
21	A	2831	0	3095	230	0
21	B	2662	0	2858	211	0
21	F	130	0	143	6	0
21	J	130	0	142	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	130	0	144	13	0
21	L	195	0	215	15	0
21	a	2718	0	2828	228	0
21	b	2694	0	2933	245	0
21	f	115	0	111	10	0
21	j	120	0	119	6	0
21	k	99	0	77	2	0
21	l	195	0	215	14	0
22	1	33	0	46	5	0
22	2	33	0	46	3	0
22	A	33	0	46	3	0
22	B	33	0	46	2	0
22	a	33	0	46	4	0
22	b	33	0	46	2	0
23	1	8	0	0	0	0
23	3	16	0	0	0	0
23	A	8	0	0	0	0
23	C	16	0	0	4	0
23	a	8	0	0	0	0
23	c	16	0	0	1	0
24	0	80	0	110	10	0
24	1	280	0	385	38	0
24	2	280	0	385	36	0
24	6	40	0	55	1	0
24	7	40	0	55	6	0
24	8	40	0	55	3	0
24	9	40	0	56	5	0
24	A	280	0	385	37	0
24	B	240	0	330	43	0
24	I	40	0	55	6	0
24	J	40	0	55	8	0
24	K	40	0	55	4	0
24	L	80	0	110	7	0
24	a	280	0	384	34	0
24	b	240	0	330	33	0
24	f	40	0	55	4	0
24	h	40	0	55	6	0
24	i	40	0	55	7	0
24	j	40	0	55	8	0
24	k	40	0	55	5	0
24	l	80	0	110	8	0
25	0	98	0	148	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	1	196	0	296	11	0
25	2	49	0	74	5	0
25	6	12	0	9	1	0
25	A	245	0	370	31	0
25	B	98	0	148	12	0
25	F	49	0	74	2	0
25	L	49	0	74	7	0
25	M	49	0	74	2	0
25	a	196	0	296	20	0
25	b	49	0	74	7	0
25	l	196	0	296	17	0
26	0	55	0	86	4	0
26	1	105	0	159	5	0
26	2	110	0	172	10	0
26	A	153	0	228	12	0
26	B	110	0	172	9	0
26	K	55	0	86	11	0
26	a	105	0	159	10	0
26	b	165	0	258	17	0
27	A	4	0	3	1	0
27	B	8	0	6	0	0
27	a	4	0	3	0	0
28	B	42	0	52	5	0
28	h	42	0	52	7	0
29	2	1	0	0	0	0
29	B	1	0	0	0	0
29	b	1	0	0	0	0
30	2	41	0	54	3	0
30	B	41	0	54	4	0
30	M	41	0	54	2	0
30	b	82	0	108	16	0
30	i	41	0	54	3	0
30	m	41	0	54	1	0
31	0	54	0	77	2	0
31	B	54	0	77	5	0
31	F	54	0	77	4	0
31	L	105	0	145	11	0
31	b	54	0	77	6	0
31	f	54	0	77	8	0
32	0	1	0	0	0	0
32	2	1	0	0	0	0
32	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	b	1	0	0	0	0
32	l	1	0	0	0	0
33	B	1	0	0	0	0
33	b	1	0	0	0	0
34	7	42	0	54	6	0
34	F	42	0	54	1	0
34	J	42	0	54	5	0
34	j	42	0	54	6	0
35	0	35	0	45	4	0
35	1	35	0	46	0	0
35	F	35	0	45	0	0
35	L	35	0	45	1	0
35	l	35	0	45	1	0
36	I	42	0	0	0	0
37	L	66	0	96	5	0
38	0	33	0	0	1	0
38	1	37	0	0	5	0
38	2	24	0	0	1	0
38	3	11	0	0	0	0
38	4	13	0	0	0	0
38	5	4	0	0	0	0
38	6	1	0	0	0	0
38	7	1	0	0	0	0
38	8	2	0	0	0	0
38	9	1	0	0	1	0
38	A	186	0	0	4	0
38	B	114	0	0	1	0
38	C	48	0	0	0	0
38	D	57	0	0	0	0
38	E	16	0	0	5	0
38	F	8	0	0	1	0
38	I	6	0	0	1	0
38	J	4	0	0	0	0
38	K	9	0	0	1	0
38	L	46	0	0	0	0
38	M	3	0	0	0	0
38	a	39	0	0	2	0
38	b	141	0	0	3	0
38	c	13	0	0	1	0
38	d	15	0	0	1	0
38	e	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	10	0	0	1	0
38	h	3	0	0	0	0
38	i	7	0	0	0	0
38	j	5	0	0	0	0
38	l	20	0	0	2	0
38	m	8	0	0	0	0
All	All	77117	0	78138	2440	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 16.

All (2440) 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)
21:A:1112:CLA:HAB	24:A:4002:BCR:H14C	1.41	1.03
21:1:1107:CLA:HBB1	24:1:4012:BCR:HC8	1.48	0.94
1:a:56:HIS:HB2	21:a:1128:CLA:HBA1	1.51	0.92
1:a:86:TRP:HA	21:a:1105:CLA:HBB2	1.53	0.90
21:1:1012:CLA:H42	24:2:4011:BCR:H362	1.57	0.86
21:a:1013:CLA:HMA2	21:a:1013:CLA:H2	1.57	0.86
12:b:580:MET:HG3	21:b:1222:CLA:HBC1	1.56	0.85
8:J:31:ARG:HD3	24:J:4013:BCR:H312	1.58	0.85
21:l:1501:CLA:H111	18:h:25:VAL:HG22	1.58	0.85
12:b:22:TRP:HE1	21:b:1238:CLA:HBB1	1.43	0.84
18:h:27:MET:HB3	24:0:4019:BCR:H12C	1.59	0.84
21:b:1203:CLA:H162	21:b:1225:CLA:HBB2	1.60	0.83
26:K:5009:LMG:H211	21:b:1212:CLA:H42	1.61	0.82
1:A:56:HIS:HB2	21:A:1128:CLA:HBA1	1.61	0.82
21:B:1209:CLA:H101	21:B:1217:CLA:H2	1.62	0.81
21:b:1212:CLA:H171	24:b:4004:BCR:H11C	1.62	0.81
1:a:269:GLY:H	15:k:13:PRO:HG3	1.42	0.81
21:a:1125:CLA:HED1	21:a:1133:CLA:HAB	1.62	0.80
16:1:76:HIS:HB3	21:1:1111:CLA:HED2	1.63	0.80
21:B:1234:CLA:H52	21:F:1302:CLA:HBB2	1.62	0.80
25:l:5001:LHG:HC91	18:h:29:LEU:HB3	1.62	0.80
21:a:1107:CLA:HBB1	24:a:4012:BCR:HC8	1.64	0.79
12:b:160:LYS:HE3	12:b:160:LYS:H	1.48	0.79
3:C:15:THR:HA	3:C:28:MET:HE3	1.65	0.79
16:1:86:TRP:HA	21:1:1105:CLA:HBB2	1.63	0.78
22:A:2001:PQN:H201	21:A:1101:CLA:H12	1.65	0.77
21:A:1107:CLA:HBB1	24:A:4012:BCR:HC8	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:41:ARG:O	10:L:49:ARG:NH2	2.18	0.77
16:1:118:TRP:HE1	24:1:4019:BCR:H332	1.50	0.77
21:b:1217:CLA:HBB1	24:b:4004:BCR:H14C	1.66	0.76
16:1:348:TRP:HB3	21:1:1103:CLA:HAC1	1.67	0.76
21:A:1110:CLA:H102	26:A:5008:LMG:H252	1.68	0.76
21:2:1222:CLA:HBA1	21:2:1223:CLA:HED2	1.66	0.76
24:2:4010:BCR:H21C	24:2:4018:BCR:H402	1.66	0.76
11:9:4:SER:HB3	11:9:7:GLN:HB2	1.66	0.76
21:1:1138:CLA:H43	21:2:1229:CLA:HAA2	1.68	0.76
21:A:1139:CLA:H41	8:J:18:LEU:HD23	1.66	0.76
1:A:315:TRP:HA	9:K:47:GLY:HA2	1.68	0.75
21:2:1022:CLA:H152	24:2:4017:BCR:H11C	1.69	0.75
21:a:1136:CLA:HBC1	26:a:5002:LMG:H391	1.67	0.75
21:a:1126:CLA:H161	24:a:4012:BCR:H14C	1.67	0.75
12:b:338:SER:HB3	21:b:1221:CLA:H42	1.69	0.74
1:A:362:LEU:HD11	21:A:1117:CLA:H71	1.69	0.74
21:A:1122:CLA:HBB2	25:A:5003:LHG:HC82	1.68	0.74
21:A:1103:CLA:H72	24:A:4003:BCR:H24C	1.70	0.74
5:E:12:LYS:HD2	5:E:67:GLU:HB2	1.69	0.74
2:2:15:ASP:HB3	2:2:20:ARG:HB2	1.69	0.73
1:a:706:LYS:NZ	6:f:135:ASP:OD1	2.22	0.73
21:A:1126:CLA:H52	28:B:4011:45D:H221	1.71	0.73
1:a:103:TRP:HA	1:a:110:ILE:HG21	1.70	0.73
2:2:642:VAL:HG22	21:2:1206:CLA:HAC1	1.71	0.72
21:A:1122:CLA:H43	24:A:4007:BCR:H19C	1.71	0.72
21:b:1224:CLA:HBC3	26:b:5002:LMG:H441	1.69	0.72
21:2:1237:CLA:H93	21:2:1237:CLA:HBB1	1.70	0.72
16:1:113:SER:HB2	16:1:130:VAL:HG11	1.72	0.72
21:A:1137:CLA:H122	24:A:4007:BCR:H23C	1.70	0.72
25:B:5004:LHG:H122	25:B:5004:LHG:H272	1.71	0.72
21:1:1103:CLA:H51	21:1:1111:CLA:H12	1.71	0.72
9:K:34:PHE:HE2	21:K:1402:CLA:H42	1.54	0.72
21:b:1232:CLA:H143	21:b:1236:CLA:H172	1.71	0.72
16:1:103:TRP:HA	16:1:110:ILE:HG21	1.72	0.72
34:7:4015:ZEX:H27	21:7:1303:CLA:HBC3	1.71	0.72
24:2:4011:BCR:H271	21:2:1229:CLA:HHB	1.71	0.72
21:A:1105:CLA:HHC	21:A:1105:CLA:HBB1	1.71	0.71
25:1:5003:LHG:H121	25:1:5003:LHG:H262	1.70	0.71
1:A:269:GLY:H	9:K:13:PRO:HG3	1.55	0.71
12:b:15:ASP:HB3	12:b:20:ARG:HB2	1.71	0.71
1:a:500:ASN:HB2	21:a:1134:CLA:HED2	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1101:CLA:HBD	21:1:1101:CLA:HBA2	1.72	0.71
1:A:40:ARG:HH21	1:A:43:LYS:HG3	1.54	0.71
1:A:103:TRP:HA	1:A:110:ILE:HG21	1.72	0.71
8:j:12:PRO:HB2	24:j:4013:BCR:H391	1.73	0.71
16:1:739:THR:HG23	21:1:1126:CLA:HBB2	1.73	0.71
24:2:4011:BCR:H282	24:2:4014:BCR:H14C	1.73	0.71
21:2:1204:CLA:H152	21:2:1205:CLA:H191	1.73	0.71
21:2:1228:CLA:HBD	25:6:5001:LHG:HC2	1.71	0.71
2:2:336:LEU:HD21	21:2:1226:CLA:HBB1	1.72	0.71
21:1:1130:CLA:H2	21:0:1502:CLA:H43	1.71	0.71
21:2:1023:CLA:H142	24:h:4018:BCR:H271	1.71	0.71
20:0:133:GLY:HA3	24:0:4022:BCR:H383	1.71	0.71
21:a:1128:CLA:H172	30:b:4011:ECH:H34A	1.73	0.71
21:B:1227:CLA:HBC1	24:B:4018:BCR:H21C	1.73	0.70
21:B:1232:CLA:HHC	21:B:1232:CLA:HBB1	1.72	0.70
21:b:1023:CLA:H143	24:b:4017:BCR:H362	1.71	0.70
2:2:718:TYR:HB2	21:2:1021:CLA:HED3	1.74	0.70
21:0:1501:CLA:HMB3	24:0:4022:BCR:H11C	1.74	0.70
3:C:58:CYS:HA	23:C:3003:SF4:S4	2.30	0.70
21:a:1120:CLA:H41	21:a:1121:CLA:H201	1.74	0.70
21:B:1226:CLA:H191	24:B:4017:BCR:H10C	1.74	0.70
6:f:100:GLU:OE2	38:f:8001:HOH:O	2.09	0.70
21:B:1238:CLA:H18	24:I:4018:BCR:H362	1.74	0.70
21:1:1103:CLA:H142	24:1:4003:BCR:H372	1.73	0.70
26:A:5004:LMG:H371	25:A:5006:LHG:H301	1.74	0.69
21:2:1227:CLA:HHC	21:2:1227:CLA:HBB1	1.73	0.69
21:A:1801:CLA:H12	25:L:5005:LHG:H162	1.73	0.69
12:b:679:HIS:ND1	38:b:8003:HOH:O	2.25	0.69
21:a:1112:CLA:HHC	24:a:4002:BCR:H14C	1.75	0.69
2:B:4:LYS:HE3	7:I:38:GLY:HA3	1.73	0.69
21:1:1138:CLA:HBB1	21:1:1138:CLA:HHC	1.75	0.69
21:a:1138:CLA:H43	21:b:1229:CLA:HAA2	1.75	0.69
16:1:315:TRP:HA	19:8:47:GLY:HA2	1.74	0.69
21:A:1101:CLA:HBB1	24:J:4013:BCR:H292	1.75	0.69
21:B:1201:CLA:HMA3	11:M:29:LEU:HD13	1.75	0.69
21:B:1205:CLA:H121	21:B:1224:CLA:H171	1.73	0.69
21:B:1220:CLA:HMB3	21:B:1240:CLA:HAB	1.73	0.69
16:1:13:LYS:HB2	21:1:1110:CLA:HED1	1.75	0.69
21:1:1136:CLA:HBC1	26:1:5002:LMG:H391	1.74	0.69
21:A:1112:CLA:C3B	24:A:4002:BCR:H12C	2.23	0.69
21:A:1138:CLA:H111	21:A:1138:CLA:HAB	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:LEU:O	6:F:36:ARG:NH2	2.26	0.69
12:b:154:TRP:CD1	11:m:28:GLU:HG3	2.28	0.69
16:1:210:LEU:HD11	24:1:4001:BCR:H10C	1.74	0.68
21:1:1107:CLA:HMA2	24:7:4013:BCR:H12C	1.73	0.68
1:a:332:PHE:HB2	25:a:5003:LHG:HC41	1.74	0.68
21:b:1212:CLA:HHC	21:b:1212:CLA:HBB1	1.75	0.68
21:a:1103:CLA:H51	21:a:1111:CLA:H12	1.74	0.68
21:l:1501:CLA:HAB	38:l:8019:HOH:O	1.92	0.68
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.74	0.68
2:B:312:LEU:HB2	25:B:5004:LHG:HC42	1.76	0.68
21:A:1138:CLA:H43	21:B:1229:CLA:HAA2	1.76	0.68
21:a:1104:CLA:H151	21:a:1127:CLA:HBB2	1.76	0.68
4:d:31:THR:O	4:d:83:TYR:HA	1.92	0.68
20:0:41:ARG:HB3	20:0:44:LEU:HD22	1.75	0.68
21:2:1224:CLA:HBC3	26:2:5002:LMG:H441	1.76	0.68
3:3:27:GLU:HG3	3:3:44:ARG:HH22	1.58	0.68
31:B:5008:SQD:H262	21:1:1801:CLA:H52	1.76	0.67
21:a:1121:CLA:HMC2	21:a:1121:CLA:H102	1.75	0.67
2:2:180:ALA:HB2	2:2:288:GLY:HA3	1.76	0.67
5:5:12:LYS:HD2	5:5:67:GLU:HG3	1.76	0.67
2:2:461:ILE:HD11	21:2:1234:CLA:H2	1.75	0.67
12:b:642:VAL:HG22	21:b:1206:CLA:HAC1	1.76	0.67
21:b:1220:CLA:HAB	21:b:1227:CLA:HMD2	1.76	0.67
1:a:456:ILE:HG22	21:a:1132:CLA:HBC2	1.77	0.67
21:1:1112:CLA:HBA2	24:1:4002:BCR:H342	1.77	0.67
1:A:86:TRP:HA	21:A:1105:CLA:HBB2	1.75	0.67
12:b:409:MET:HG3	24:b:4018:BCR:H402	1.75	0.67
16:1:83:VAL:HG12	21:1:1103:CLA:H92	1.76	0.67
21:1:1104:CLA:H151	21:1:1127:CLA:HBB2	1.77	0.67
21:A:1135:CLA:H193	25:A:5003:LHG:H262	1.74	0.67
21:A:1130:CLA:H42	10:L:34:ILE:HD11	1.75	0.67
24:L:4022:BCR:H282	24:l:4022:BCR:H292	1.75	0.67
1:a:691:GLY:HA3	12:b:567:ILE:HG12	1.76	0.67
12:b:16:PRO:HG3	13:c:74:THR:HG22	1.74	0.67
21:2:1220:CLA:HAB	21:2:1227:CLA:HMD2	1.76	0.67
8:7:12:PRO:HB2	24:7:4013:BCR:H391	1.76	0.67
4:d:118:LYS:NZ	4:d:139:TYR:O	2.26	0.67
21:1:1012:CLA:HBC2	2:2:582:ASN:HB2	1.77	0.67
1:A:348:TRP:HB3	21:A:1103:CLA:HAC1	1.77	0.66
1:A:433:ARG:HG3	1:A:555:TYR:CZ	2.29	0.66
21:a:1112:CLA:HBA2	24:a:4002:BCR:H342	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:1012:CLA:H42	30:b:4011:ECH:H36A	1.76	0.66
16:1:737:VAL:HG22	24:2:4011:BCR:HC21	1.76	0.66
2:2:518:HIS:HD2	34:7:4015:ZEX:H21	1.59	0.66
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.77	0.66
26:K:5009:LMG:H122	12:b:223:MET:HB2	1.77	0.66
21:1:1012:CLA:HAB	2:2:579:TRP:CH2	2.31	0.66
1:A:332:PHE:HB2	25:A:5003:LHG:HC41	1.77	0.66
21:a:1129:CLA:HAB	21:a:1137:CLA:CBB	2.24	0.66
21:1:1122:CLA:H43	24:1:4007:BCR:H19C	1.77	0.66
1:a:195:SER:O	1:a:199:HIS:ND1	2.19	0.66
1:a:315:TRP:HB3	15:k:64:PRO:HB3	1.77	0.66
10:l:133:GLY:HA3	24:l:4022:BCR:H383	1.78	0.66
21:B:1226:CLA:HMB3	21:B:1226:CLA:HBB1	1.77	0.66
9:K:79:GLY:O	38:K:8001:HOH:O	2.13	0.66
4:D:77:LYS:HB2	4:D:78:PRO:HD3	1.77	0.66
21:A:1135:CLA:H101	25:A:5006:LHG:H372	1.78	0.66
21:b:1210:CLA:H172	24:b:4005:BCR:H271	1.77	0.66
21:B:1212:CLA:HHC	21:B:1212:CLA:HBB1	1.76	0.66
6:F:86:TYR:O	6:F:90:ILE:HG13	1.96	0.66
12:b:72:GLY:HA2	12:b:87:ILE:HG13	1.78	0.66
1:a:584:GLN:HB3	1:a:589:ASP:HB3	1.78	0.65
13:c:5:VAL:HG22	13:c:67:VAL:HG22	1.77	0.65
2:B:117:TYR:HA	2:B:365:THR:HG22	1.78	0.65
21:B:1204:CLA:H152	26:0:5001:LMG:H242	1.78	0.65
9:K:30:ASN:HB3	9:K:70:MET:HE1	1.78	0.65
21:b:1235:CLA:H18	24:f:4016:BCR:H383	1.78	0.65
1:A:207:LEU:HD13	24:A:4003:BCR:H10C	1.78	0.65
21:1:1104:CLA:H43	21:1:1128:CLA:H51	1.79	0.65
1:A:433:ARG:HH21	1:A:555:TYR:HA	1.61	0.65
1:A:482:PHE:HB3	21:A:1135:CLA:H42	1.79	0.65
21:A:1130:CLA:H12	21:L:1502:CLA:H93	1.78	0.65
9:K:53:PRO:HG2	24:K:4001:BCR:H282	1.78	0.65
16:1:117:VAL:HB	16:1:127:ASN:HD21	1.62	0.65
21:B:1207:CLA:HBC3	24:I:4018:BCR:C21	2.27	0.65
21:b:1234:CLA:H52	21:f:1302:CLA:HBB2	1.77	0.65
12:b:312:LEU:HB2	25:b:5004:LHG:HC42	1.79	0.65
21:1:1137:CLA:HMC2	21:1:1130:CLA:HBC2	1.79	0.65
21:B:1219:CLA:HBD	21:B:1219:CLA:HBA1	1.78	0.65
8:J:12:PRO:HB2	24:J:4013:BCR:H381	1.78	0.65
10:L:62:ILE:HD11	10:L:82:LEU:HA	1.79	0.64
1:a:203:GLY:HA3	21:a:1111:CLA:HBB1	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:44:LEU:O	10:l:49:ARG:NH1	2.30	0.64
5:5:9:VAL:HG12	5:5:68:LEU:HA	1.78	0.64
21:A:1133:CLA:H142	21:K:1401:CLA:H172	1.77	0.64
21:B:1219:CLA:HBB1	21:B:1219:CLA:HHC	1.79	0.64
21:b:1237:CLA:H61	21:b:1238:CLA:H43	1.79	0.64
21:b:1227:CLA:HBA2	25:b:5004:LHG:H241	1.79	0.64
16:1:317:ILE:HD13	19:8:68:ALA:HB2	1.79	0.64
2:B:539:ARG:NH1	4:D:127:GLU:OE1	2.31	0.64
21:a:1013:CLA:H93	30:b:4011:ECH:H37B	1.77	0.64
16:1:79:HIS:CE1	21:1:1103:CLA:HMA2	2.33	0.64
21:A:1137:CLA:HMC2	21:A:1130:CLA:HBC2	1.80	0.64
16:1:398:GLY:HA3	16:1:602:LEU:HD11	1.78	0.64
21:1:1127:CLA:H51	24:1:4003:BCR:H23C	1.79	0.64
2:B:339:LEU:HD12	2:B:342:ILE:HD11	1.79	0.64
1:a:89:GLY:HA3	21:a:1105:CLA:HBB1	1.79	0.64
21:b:1208:CLA:O1A	31:b:5006:SQD:O2	2.14	0.64
1:A:304:PHE:HZ	21:A:1117:CLA:H121	1.61	0.64
17:4:77:LYS:HB2	17:4:78:PRO:HD3	1.79	0.64
21:B:1220:CLA:HAB	21:B:1227:CLA:HMD2	1.80	0.64
12:b:642:VAL:HG11	21:b:1205:CLA:HAC1	1.79	0.64
2:2:608:GLU:HG2	6:6:48:GLU:HG2	1.78	0.64
21:2:1228:CLA:HHC	21:2:1228:CLA:HBB1	1.80	0.64
25:A:5005:LHG:H191	12:b:141:PHE:HD1	1.63	0.64
5:E:64:ASN:OD1	5:E:64:ASN:N	2.28	0.64
25:0:5002:LHG:O3	25:0:5002:LHG:O1	2.16	0.64
1:A:207:LEU:HB3	24:A:4003:BCR:H12C	1.78	0.63
21:b:1207:CLA:HED2	10:l:65:TRP:CD1	2.33	0.63
21:b:1214:CLA:HBC3	21:b:1221:CLA:H193	1.80	0.63
2:2:488:ALA:HB3	2:2:491:LEU:HD13	1.80	0.63
21:2:1238:CLA:H18	24:h:4018:BCR:H362	1.80	0.63
21:B:1212:CLA:HMB1	30:B:4006:ECH:H35A	1.80	0.63
21:A:1123:CLA:H42	21:A:1127:CLA:H193	1.79	0.63
16:1:373:MET:HE1	21:1:1125:CLA:HAB	1.80	0.63
21:B:1023:CLA:H151	24:B:4017:BCR:H16C	1.79	0.63
15:k:71:SER:HA	24:k:4001:BCR:H11C	1.80	0.63
21:B:1216:CLA:HBB1	21:B:1221:CLA:H121	1.80	0.63
21:B:1227:CLA:H93	25:B:5004:LHG:H101	1.81	0.63
12:b:117:TYR:HA	12:b:365:THR:HG22	1.80	0.63
12:b:195:VAL:HG22	12:b:254:ILE:HB	1.79	0.63
21:2:1229:CLA:HBB1	21:2:1229:CLA:HHC	1.81	0.63
21:A:1013:CLA:HMA2	21:A:1013:CLA:H2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:ILE:HD11	21:B:1234:CLA:H2	1.80	0.63
12:b:350:MET:HE3	21:b:1215:CLA:HBA1	1.81	0.63
21:b:1023:CLA:H122	24:i:4018:BCR:H281	1.81	0.63
21:b:1220:CLA:HBA1	24:b:4018:BCR:H351	1.81	0.63
2:2:255:LEU:HD11	21:2:1212:CLA:HBC1	1.80	0.63
28:h:4020:45D:C32	21:0:1502:CLA:HAB	2.28	0.63
25:A:5007:LHG:H351	25:L:5005:LHG:H161	1.81	0.63
6:F:86:TYR:CE2	6:F:90:ILE:HD11	2.34	0.63
12:b:222:LEU:HD11	21:b:1212:CLA:HBA2	1.80	0.63
21:b:1226:CLA:H193	21:b:1239:CLA:HMA3	1.81	0.63
21:2:1210:CLA:H172	24:2:4005:BCR:H271	1.80	0.63
21:A:1132:CLA:HMA2	10:L:68:LEU:HB3	1.81	0.62
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.80	0.62
12:b:513:ASP:OD2	12:b:594:LYS:NZ	2.28	0.62
16:1:309:HIS:CD2	24:1:4001:BCR:H19C	2.34	0.62
21:2:1239:CLA:HBA2	24:2:4017:BCR:H352	1.80	0.62
17:4:30:ILE:HD11	17:4:83:TYR:HB2	1.81	0.62
3:C:13:GLY:O	3:C:38:GLN:NE2	2.29	0.62
31:L:5002:SQD:H361	7:i:22:PHE:HA	1.80	0.62
1:a:76:HIS:HB3	21:a:1111:CLA:HED2	1.81	0.62
12:b:69:ALA:HB2	12:b:135:LEU:HB2	1.81	0.62
4:d:10:LYS:HB2	4:d:49:ILE:HB	1.81	0.62
16:1:696:LEU:HD21	21:1:1013:CLA:HED2	1.81	0.62
2:B:420:LEU:HD13	2:B:529:LEU:HA	1.82	0.62
6:F:101:VAL:HG12	6:F:102:VAL:HG23	1.81	0.62
21:2:1225:CLA:H51	24:2:4005:BCR:H23C	1.81	0.62
1:A:79:HIS:CE1	21:A:1103:CLA:HMA2	2.35	0.62
21:2:1206:CLA:H142	26:2:5002:LMG:H222	1.81	0.62
26:A:5002:LMG:H322	26:A:5002:LMG:HC91	1.82	0.62
5:E:13:ARG:NH1	38:E:8001:HOH:O	2.31	0.62
31:L:5002:SQD:H382	21:b:1201:CLA:H172	1.82	0.62
24:2:4014:BCR:H10C	21:6:1301:CLA:C3B	2.29	0.62
9:K:50:LEU:HD22	9:K:52:LEU:HA	1.82	0.62
30:M:4021:ECH:H33B	35:0:6001:LMT:H81	1.82	0.62
1:A:33:HIS:NE2	21:A:1109:CLA:O1A	2.31	0.62
2:B:174:ARG:HB2	21:B:1210:CLA:HBC2	1.81	0.62
21:a:1122:CLA:H43	24:a:4008:BCR:H363	1.82	0.62
21:b:1209:CLA:HBB2	21:b:1217:CLA:H43	1.81	0.62
21:A:1115:CLA:H101	21:K:1401:CLA:HHD	1.82	0.62
8:J:1:MET:HG3	8:J:3:GLY:H	1.63	0.62
21:A:1119:CLA:H71	24:A:4008:BCR:H12C	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:1126:CLA:HBB1	21:a:1126:CLA:HMB3	1.81	0.62
21:b:1023:CLA:H43	21:b:1023:CLA:HMA3	1.81	0.62
2:2:375:TYR:HA	2:2:584:LEU:HD13	1.82	0.62
2:2:582:ASN:OD1	38:2:8001:HOH:O	2.16	0.62
16:1:575:ASP:OD2	16:1:579:ARG:NH2	2.33	0.61
24:2:4014:BCR:H12C	21:6:1301:CLA:CAB	2.30	0.61
3:3:58:CYS:O	5:5:47:ASN:ND2	2.33	0.61
34:J:4015:ZEX:H27	21:J:1303:CLA:HBC3	1.81	0.61
9:K:10:GLN:NE2	9:K:11:ALA:O	2.32	0.61
9:K:70:MET:HE2	9:K:70:MET:HA	1.82	0.61
2:2:44:GLN:OE1	2:2:162:ARG:NH2	2.31	0.61
21:2:1203:CLA:HMB2	21:2:1226:CLA:HBB2	1.82	0.61
16:1:571:ARG:NH1	21:1:1128:CLA:O1D	2.33	0.61
2:2:203:ARG:HD3	2:2:250:ALA:HB1	1.83	0.61
21:b:1023:CLA:H151	24:b:4017:BCR:H16C	1.83	0.61
21:A:1104:CLA:H42	25:A:5001:LHG:H261	1.81	0.61
1:a:571:ARG:NH1	21:a:1128:CLA:O1D	2.34	0.61
17:4:121:ARG:HD3	5:5:13:ARG:HH11	1.65	0.61
31:L:5001:SQD:H241	7:i:29:LEU:HB3	1.82	0.61
1:a:670:ILE:HG23	21:a:1012:CLA:H62	1.83	0.61
16:1:56:HIS:HB2	21:1:1128:CLA:HBA1	1.82	0.61
16:1:482:PHE:HB3	21:1:1135:CLA:H11	1.81	0.61
1:a:500:ASN:HB3	21:a:1115:CLA:HED2	1.82	0.61
16:1:584:GLN:HG3	2:2:664:TRP:HB2	1.83	0.61
21:B:1217:CLA:HBB1	24:B:4004:BCR:H14C	1.83	0.61
21:a:1129:CLA:HMA1	10:l:22:THR:HG21	1.83	0.61
2:2:237:PRO:HB3	2:2:256:THR:HG21	1.82	0.61
3:3:17:CYS:HB2	3:3:54:CYS:HB2	1.83	0.61
1:A:170:ALA:HB2	24:A:4019:BCR:H381	1.82	0.60
2:B:275:HIS:HB3	21:B:1214:CLA:HMB2	1.83	0.60
12:b:420:LEU:HD13	12:b:529:LEU:HA	1.83	0.60
21:A:1129:CLA:HMA1	10:L:22:THR:HG21	1.83	0.60
21:A:1130:CLA:H141	37:L:5004:DGD:HBN2	1.83	0.60
21:a:1118:CLA:H141	24:a:4002:BCR:H292	1.83	0.60
21:b:1023:CLA:H111	24:b:4017:BCR:H362	1.84	0.60
25:A:5005:LHG:H223	31:b:5006:SQD:H352	1.83	0.60
21:B:1214:CLA:HBD	21:B:1223:CLA:HAB	1.84	0.60
21:a:1123:CLA:HBA1	21:a:1127:CLA:H191	1.83	0.60
21:a:1101:CLA:HBB1	24:j:4013:BCR:H271	1.82	0.60
25:l:5003:LHG:HC92	11:9:20:PHE:HE1	1.67	0.60
16:1:433:ARG:HA	16:1:436:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1130:CLA:HBB1	21:1:1130:CLA:HMB3	1.84	0.60
2:2:545:PRO:HB3	6:6:142:PRO:HG2	1.83	0.60
21:A:1140:CLA:H143	21:A:1101:CLA:H192	1.84	0.60
21:B:1203:CLA:H43	26:B:5002:LMG:H321	1.81	0.60
21:b:1022:CLA:H162	21:b:1206:CLA:HMB2	1.82	0.60
21:1:1127:CLA:H2	24:1:4003:BCR:H392	1.83	0.60
6:6:141:SER:O	6:6:143:ARG:NH1	2.35	0.60
21:B:1215:CLA:H101	21:B:1221:CLA:H41	1.83	0.60
10:L:23:PRO:HB3	25:L:5005:LHG:HC5	1.82	0.60
21:a:1138:CLA:HED2	12:b:422:TRP:HB2	1.84	0.60
10:l:37:LEU:HD22	21:l:1502:CLA:HBD	1.83	0.60
18:h:10:LEU:O	18:h:14:LEU:HB2	2.01	0.60
21:A:1136:CLA:HBB2	21:A:1137:CLA:HBC3	1.83	0.60
16:1:622:SER:O	16:1:624:ASP:N	2.33	0.60
21:a:1132:CLA:H152	30:i:4020:ECH:H34B	1.82	0.60
19:8:59:LYS:HD2	24:8:4001:BCR:H383	1.84	0.60
21:A:1801:CLA:H121	31:b:5006:SQD:H262	1.84	0.59
37:L:5004:DGD:O5D	37:L:5004:DGD:O4D	2.09	0.59
37:L:5004:DGD:HB81	35:L:6001:LMT:H82	1.84	0.59
13:c:1:MET:N	38:c:8002:HOH:O	2.34	0.59
8:j:38:PHE:HA	34:j:4015:ZEX:H34	1.82	0.59
2:2:48:ALA:HB3	11:9:29:LEU:HD21	1.84	0.59
21:b:1227:CLA:HBC1	24:b:4018:BCR:H21C	1.84	0.59
21:1:1134:CLA:HHC	21:1:1134:CLA:HBB1	1.84	0.59
21:2:1023:CLA:H111	24:2:4017:BCR:H362	1.84	0.59
21:1:1126:CLA:HBB1	21:1:1126:CLA:HMB3	1.83	0.59
12:b:665:ARG:O	12:b:665:ARG:HG2	2.00	0.59
21:b:1220:CLA:HMA1	21:b:1240:CLA:HAB	1.83	0.59
21:2:1229:CLA:H203	24:6:4016:BCR:H17C	1.84	0.59
2:B:276:HIS:HB2	21:B:1214:CLA:C1B	2.33	0.59
16:1:26:GLU:HA	8:7:3:GLY:HA3	1.84	0.59
16:1:269:GLY:H	19:8:13:PRO:HG3	1.68	0.59
21:2:1215:CLA:HBB2	21:2:1221:CLA:H193	1.84	0.59
21:a:1135:CLA:H93	26:a:5004:LMG:H371	1.85	0.59
14:e:13:ARG:HH21	14:e:59:ASN:HD21	1.48	0.59
21:2:1201:CLA:H12	11:9:26:SER:HB3	1.84	0.59
6:6:107:LEU:O	6:6:111:LYS:HG2	2.03	0.59
21:A:1118:CLA:HAB	21:A:1118:CLA:H152	1.84	0.59
21:A:1135:CLA:H171	25:A:5003:LHG:H211	1.85	0.59
3:C:18:VAL:HG23	3:C:28:MET:HE2	1.84	0.59
6:F:138:ILE:O	38:F:8001:HOH:O	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:8:VAL:HG13	10:l:22:THR:HG22	1.83	0.59
2:2:104:PHE:CZ	2:2:642:VAL:HG23	2.37	0.59
21:A:1112:CLA:HBA2	24:A:4002:BCR:H342	1.85	0.59
21:A:1133:CLA:H203	24:A:4007:BCR:H21C	1.84	0.59
21:A:1134:CLA:H42	21:A:1134:CLA:H151	1.85	0.59
2:B:53:HIS:CE1	21:B:1202:CLA:HMA2	2.37	0.59
21:B:1215:CLA:HBB2	21:B:1221:CLA:H203	1.84	0.59
10:L:99:TYR:O	10:L:103:THR:HG23	2.03	0.59
1:a:707:LEU:HG	21:b:1228:CLA:HMA2	1.84	0.59
21:b:1235:CLA:HBB2	21:b:1236:CLA:HBC3	1.84	0.59
21:1:1138:CLA:HED2	2:2:422:TRP:HB2	1.83	0.59
2:2:87:ILE:HA	2:2:115:ILE:HA	1.85	0.59
24:A:4012:BCR:HC7	8:J:26:LEU:HD23	1.85	0.59
25:A:5007:LHG:HC11	12:b:160:LYS:HD2	1.84	0.59
24:B:4014:BCR:H12C	21:F:1301:CLA:CAB	2.32	0.59
12:b:275:HIS:HB3	21:b:1214:CLA:HMB2	1.85	0.59
21:B:1226:CLA:H142	26:B:5002:LMG:H211	1.84	0.59
22:B:2002:PQN:H292	24:L:4019:BCR:H343	1.84	0.59
25:M:5001:LHG:H112	25:M:5001:LHG:H241	1.85	0.59
21:a:1136:CLA:H202	21:a:1130:CLA:H121	1.85	0.59
12:b:580:MET:HE3	12:b:584:LEU:HD13	1.85	0.59
21:b:1022:CLA:HBB1	21:b:1022:CLA:HMB3	1.84	0.58
21:1:1118:CLA:H193	24:1:4002:BCR:H372	1.85	0.58
21:2:1023:CLA:H43	21:2:1023:CLA:HMA3	1.84	0.58
21:A:1130:CLA:O1A	10:L:25:SER:HA	2.03	0.58
2:B:312:LEU:HD11	21:B:1240:CLA:HED1	1.84	0.58
24:l:4022:BCR:H393	20:0:132:MET:HB3	1.85	0.58
16:1:740:TRP:NE1	21:1:1126:CLA:O1A	2.36	0.58
1:a:646:LEU:HD23	12:b:629:ILE:HD11	1.85	0.58
4:d:37:GLU:HG2	4:d:51:ASN:HA	1.83	0.58
20:0:44:LEU:HG	20:0:48:LEU:HD23	1.85	0.58
2:B:409:MET:HG3	24:B:4018:BCR:H402	1.84	0.58
1:a:333:THR:HG21	1:a:425:LEU:HD23	1.84	0.58
24:b:4014:BCR:H12C	21:f:1301:CLA:CAB	2.33	0.58
25:l:5002:LHG:H112	11:9:23:PHE:HE1	1.68	0.58
17:4:72:LEU:HB3	17:4:80:ILE:HB	1.84	0.58
10:l:153:ARG:NH2	18:h:2:ASP:OD1	2.36	0.58
21:2:1214:CLA:HBC3	21:2:1221:CLA:H192	1.85	0.58
21:B:1207:CLA:HED2	10:L:65:TRP:CD1	2.38	0.58
1:A:655:ALA:O	1:A:659:ASN:ND2	2.31	0.58
21:a:1013:CLA:HBA2	12:b:425:LEU:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:1117:CLA:H8	21:a:1117:CLA:HAB	1.86	0.58
16:1:666:SER:HB2	2:2:443:ALA:HB1	1.86	0.58
21:2:1227:CLA:HBA2	25:2:5004:LHG:H241	1.84	0.58
22:a:2001:PQN:H212	21:a:1101:CLA:H92	1.86	0.58
21:b:1240:CLA:H171	31:f:5001:SQD:H82	1.85	0.58
16:1:86:TRP:HE1	21:1:1106:CLA:HBA1	1.68	0.58
2:2:406:LEU:HG	21:2:1220:CLA:HBC1	1.86	0.58
24:2:4004:BCR:HC31	30:2:4006:ECH:H32A	1.85	0.58
1:A:477:GLN:H	26:A:5002:LMG:HC72	1.69	0.58
16:1:692:TYR:OH	21:1:1013:CLA:OBD	2.19	0.58
21:a:1117:CLA:H172	21:a:1125:CLA:H51	1.85	0.58
6:f:44:LEU:HD12	6:f:54:ILE:HD11	1.85	0.58
25:l:5002:LHG:H381	21:2:1206:CLA:H122	1.84	0.58
16:1:195:SER:O	16:1:199:HIS:ND1	2.25	0.58
21:A:1118:CLA:HMA2	9:K:67:LEU:HB3	1.86	0.57
21:A:1119:CLA:H8	24:A:4007:BCR:H11C	1.85	0.57
12:b:174:ARG:HB2	21:b:1210:CLA:HBC2	1.86	0.57
21:1:1140:CLA:H161	8:7:23:ALA:HB2	1.86	0.57
2:2:462:GLN:HG2	2:2:506:PHE:HD1	1.70	0.57
2:2:590:TYR:HA	2:2:616:TRP:HH2	1.69	0.57
12:b:286:ILE:HD11	21:b:1213:CLA:H121	1.86	0.57
16:1:412:MET:O	16:1:557:ARG:HD3	2.03	0.57
6:6:93:SER:O	6:6:95:ASN:N	2.34	0.57
21:B:1219:CLA:CBB	21:B:1240:CLA:HBB1	2.34	0.57
10:L:96:LEU:HG	24:L:4019:BCR:H24C	1.86	0.57
1:a:15:SER:HB2	1:a:186:LYS:HD2	1.85	0.57
21:b:1206:CLA:H92	24:b:4017:BCR:H341	1.86	0.57
2:B:712:VAL:HG22	26:B:5002:LMG:H432	1.87	0.57
2:2:336:LEU:HD21	21:2:1226:CLA:CBB	2.34	0.57
28:h:4020:45D:H133	21:0:1502:CLA:H52	1.86	0.57
24:A:4001:BCR:H11C	24:K:4001:BCR:H333	1.87	0.57
21:B:1022:CLA:H152	24:B:4017:BCR:H11C	1.84	0.57
21:B:1234:CLA:H93	21:B:1235:CLA:H42	1.86	0.57
1:a:77:PHE:CE1	21:a:1108:CLA:HBB1	2.39	0.57
16:1:456:ILE:HG22	21:1:1132:CLA:HBC2	1.86	0.57
2:2:420:LEU:HD13	2:2:529:LEU:HA	1.86	0.57
2:2:167:TRP:CE2	21:2:1210:CLA:HBC3	2.39	0.57
26:2:5005:LMG:H453	26:2:5005:LMG:H402	1.85	0.57
1:A:433:ARG:NH2	1:A:558:SER:O	2.38	0.57
21:B:1225:CLA:H8	24:B:4005:BCR:H21C	1.85	0.57
1:a:348:TRP:HB3	21:a:1103:CLA:HAC1	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:367:ALA:HB1	12:b:722:LEU:HD11	1.86	0.57
16:1:534:VAL:HG11	16:1:608:HIS:CG	2.40	0.57
2:2:72:GLY:HA2	2:2:87:ILE:HG13	1.86	0.57
2:2:415:ALA:O	2:2:419:HIS:ND1	2.31	0.57
2:2:577:MET:HG3	2:2:707:LEU:HD21	1.86	0.57
21:2:1208:CLA:H2	21:2:1209:CLA:C1D	2.35	0.57
21:a:1140:CLA:H143	21:a:1101:CLA:H192	1.87	0.57
21:1:1139:CLA:H2	8:7:15:ILE:HB	1.85	0.57
16:1:306:ILE:HG12	24:1:4001:BCR:H362	1.87	0.57
21:1:1111:CLA:HBA2	21:1:1123:CLA:H43	1.85	0.57
21:B:1208:CLA:H172	21:B:1211:CLA:H111	1.86	0.56
12:b:312:LEU:HD22	31:f:5001:SQD:H121	1.86	0.56
13:c:26:LEU:HA	13:c:41:SER:O	2.04	0.56
4:d:7:GLN:NE2	38:d:8001:HOH:O	2.31	0.56
16:1:716:ARG:NH2	5:5:45:ASN:O	2.38	0.56
21:1:1111:CLA:H203	24:1:4003:BCR:H11C	1.86	0.56
21:1:1140:CLA:H143	21:1:1101:CLA:H192	1.86	0.56
21:2:1216:CLA:CMD	21:2:1218:CLA:HAB	2.34	0.56
2:B:719:ALA:HB2	21:B:1224:CLA:HBB1	1.86	0.56
5:E:8:LYS:HD3	5:E:24:THR:HG22	1.88	0.56
10:L:47:ILE:HG12	10:L:122:GLN:HB3	1.87	0.56
1:a:59:ASP:OD2	1:a:349:HIS:NE2	2.24	0.56
1:a:212:TRP:NE1	21:a:1117:CLA:O1D	2.37	0.56
12:b:564:THR:HB	12:b:567:ILE:HG13	1.86	0.56
21:b:1204:CLA:H111	24:i:4018:BCR:HC31	1.87	0.56
21:b:1213:CLA:HED2	21:b:1213:CLA:H2A	1.86	0.56
16:1:332:PHE:O	16:1:428:ARG:NH1	2.38	0.56
16:1:561:LEU:HD22	16:1:579:ARG:HD2	1.87	0.56
19:8:47:GLY:HA3	19:8:64:PRO:HG3	1.87	0.56
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.88	0.56
30:b:4006:ECH:H21	30:b:4006:ECH:H36	1.87	0.56
21:b:1230:CLA:H122	6:f:71:LEU:HD11	1.87	0.56
21:2:1238:CLA:H51	21:2:1239:CLA:H121	1.88	0.56
20:0:153:ARG:HH12	35:0:6001:LMT:H6D	1.70	0.56
2:B:518:HIS:HD2	34:J:4015:ZEX:H21	1.70	0.56
21:L:1501:CLA:HBA1	24:L:4022:BCR:H363	1.85	0.56
12:b:255:LEU:HD11	21:b:1212:CLA:HBC1	1.87	0.56
16:1:440:LEU:HG	16:1:547:LEU:HB2	1.88	0.56
21:1:1013:CLA:HMD3	2:2:530:ILE:HG12	1.86	0.56
24:1:4001:BCR:H361	19:8:75:ILE:HD11	1.86	0.56
1:A:500:ASN:HB2	21:A:1134:CLA:HED2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:PRO:HG3	10:L:52:GLU:CD	2.31	0.56
1:a:332:PHE:O	1:a:428:ARG:NH1	2.39	0.56
16:1:25:PHE:HB2	8:7:1:MET:HG2	1.88	0.56
2:2:349:HIS:HB3	21:2:1214:CLA:HED2	1.88	0.56
21:2:1236:CLA:H43	24:2:4010:BCR:H10C	1.88	0.56
21:B:1213:CLA:HBD	21:B:1213:CLA:HBA1	1.88	0.56
21:B:1224:CLA:H161	26:B:5002:LMG:H272	1.86	0.56
21:b:1227:CLA:HED3	31:f:5001:SQD:H291	1.87	0.56
21:l:1501:CLA:H61	18:h:21:LEU:HD11	1.87	0.56
21:1:1101:CLA:HBB1	21:1:1101:CLA:HHC	1.87	0.56
2:2:86:PRO:O	2:2:116:ALA:N	2.34	0.56
1:A:367:ALA:HB2	1:A:393:HIS:HB2	1.86	0.56
12:b:372:HIS:HB2	21:b:1224:CLA:CHB	2.35	0.56
12:b:441:VAL:HG22	12:b:449:LYS:HE3	1.87	0.56
1:A:679:PHE:CG	21:A:1011:CLA:HMA2	2.41	0.56
21:A:1129:CLA:H8	21:L:1502:CLA:H141	1.87	0.56
21:a:1012:CLA:H143	30:b:4011:ECH:H19	1.87	0.56
21:b:1216:CLA:HBA1	21:b:1221:CLA:CAB	2.36	0.56
16:1:356:LEU:HD21	21:1:1128:CLA:HAB	1.88	0.56
21:A:1131:CLA:H91	21:B:1239:CLA:H93	1.89	0.56
21:B:1213:CLA:CHD	21:B:1214:CLA:HBB2	2.36	0.56
1:a:285:THR:HG23	1:a:287:GLY:H	1.71	0.56
21:A:1013:CLA:HBA2	2:B:425:LEU:HD12	1.88	0.55
21:A:1139:CLA:HAA1	21:A:1101:CLA:H43	1.88	0.55
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.87	0.55
1:a:355:ASN:ND2	21:a:1103:CLA:OBD	2.37	0.55
21:b:1229:CLA:HBB2	24:b:4014:BCR:HC21	1.87	0.55
16:1:481:ILE:HG23	26:1:5004:LMG:HC91	1.88	0.55
6:F:31:ASN:HA	6:F:34:LYS:HE3	1.87	0.55
1:a:726:VAL:O	1:a:730:HIS:ND1	2.38	0.55
21:a:1110:CLA:H41	21:a:1118:CLA:H42	1.89	0.55
21:a:1131:CLA:H101	22:b:2002:PQN:H212	1.88	0.55
12:b:304:ILE:O	12:b:308:HIS:ND1	2.39	0.55
21:2:1223:CLA:HBB1	21:2:1231:CLA:HMA2	1.88	0.55
1:A:376:TYR:CE2	21:A:1127:CLA:HED2	2.42	0.55
2:B:372:HIS:HB2	21:B:1224:CLA:CHB	2.36	0.55
2:B:441:VAL:HG22	2:B:449:LYS:HE3	1.87	0.55
21:B:1204:CLA:H71	24:I:4018:BCR:HC32	1.89	0.55
1:a:367:ALA:HB2	1:a:393:HIS:HB2	1.89	0.55
12:b:104:PHE:CZ	12:b:642:VAL:HG23	2.41	0.55
2:2:257:PHE:CD2	21:2:1214:CLA:HBB1	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ILE:HD13	21:A:1138:CLA:HMD1	1.87	0.55
2:B:461:ILE:O	2:B:464:THR:OG1	2.15	0.55
21:B:1214:CLA:H91	21:B:1231:CLA:H42	1.87	0.55
21:B:1216:CLA:H43	21:B:1223:CLA:H111	1.89	0.55
1:a:42:PRO:HB3	1:a:47:TRP:CD2	2.41	0.55
1:a:216:GLN:HA	1:a:220:SER:HB2	1.89	0.55
21:a:1129:CLA:HAB	21:a:1137:CLA:HBB2	1.87	0.55
12:b:460:TRP:HE1	12:b:474:VAL:HG21	1.71	0.55
21:2:1220:CLA:HAB	21:2:1227:CLA:CMD	2.37	0.55
21:A:1012:CLA:HBC2	2:B:582:ASN:HB2	1.87	0.55
12:b:276:HIS:HB2	21:b:1214:CLA:C1B	2.37	0.55
6:f:88:ILE:HG21	6:f:130:LYS:HZ1	1.71	0.55
16:1:296:HIS:HB2	21:1:1116:CLA:C1B	2.36	0.55
21:a:1124:CLA:H12	21:a:1135:CLA:HMA3	1.89	0.55
21:1:1121:CLA:H92	21:1:1121:CLA:H41	1.89	0.55
21:1:1129:CLA:HMA1	20:0:22:THR:HG21	1.86	0.55
2:B:173:SER:O	2:B:177:HIS:ND1	2.28	0.55
6:F:90:ILE:HG22	6:F:96:PRO:HA	1.87	0.55
11:M:4:SER:HB3	11:M:7:GLN:HG3	1.88	0.55
1:a:679:PHE:CG	21:a:1011:CLA:HMA2	2.42	0.55
21:1:1139:CLA:H11	6:6:103:ILE:HG13	1.88	0.55
21:A:1106:CLA:H71	24:A:4012:BCR:H372	1.89	0.55
21:A:1125:CLA:HED1	21:A:1133:CLA:HAB	1.89	0.55
12:b:648:LEU:HD23	21:b:1022:CLA:H11	1.89	0.55
21:b:1203:CLA:H191	26:b:5002:LMG:H271	1.89	0.55
2:2:123:TRP:O	2:2:127:ILE:HG12	2.06	0.55
2:2:154:TRP:CD1	11:9:28:GLU:HG3	2.41	0.55
21:A:1119:CLA:HBA1	21:A:1123:CLA:C3B	2.37	0.55
5:E:19:TYR:HB2	38:E:8006:HOH:O	2.07	0.55
31:L:5001:SQD:H301	31:L:5002:SQD:H191	1.88	0.55
1:a:157:GLN:NE2	21:a:1112:CLA:O1D	2.40	0.55
21:a:1122:CLA:HMB3	25:a:5003:LHG:HC2	1.89	0.55
12:b:14:GLN:HB2	13:c:1:MET:SD	2.47	0.55
12:b:178:HIS:HA	12:b:182:LEU:HB3	1.89	0.55
12:b:405:VAL:O	12:b:409:MET:HG2	2.07	0.55
2:B:226:PHE:HZ	21:B:1212:CLA:H52	1.71	0.55
21:a:1126:CLA:H152	21:a:1012:CLA:H202	1.88	0.55
2:B:3:THR:HG21	2:B:20:ARG:HD2	1.89	0.54
1:a:224:ASN:ND2	38:a:8003:HOH:O	2.38	0.54
1:a:268:TRP:O	1:a:271:TYR:HB2	2.08	0.54
12:b:402:LYS:HA	31:f:5001:SQD:H372	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:121:ARG:HD2	14:e:13:ARG:HD3	1.88	0.54
2:B:262:HIS:HE1	2:B:264:GLN:HB3	1.73	0.54
24:B:4014:BCR:H321	6:F:72:PHE:HB2	1.89	0.54
1:a:262:PRO:HA	1:a:267:ASN:HB3	1.90	0.54
21:a:1119:CLA:H142	24:a:4008:BCR:HC8	1.89	0.54
16:1:237:PRO:HG3	16:1:248:LYS:HE2	1.87	0.54
3:3:24:ASP:OD2	17:4:98:HIS:ND1	2.36	0.54
2:B:655:ALA:C	21:B:1023:CLA:HAB	2.33	0.54
9:K:80:MET:HE2	26:K:5009:LMG:H222	1.87	0.54
25:a:5005:LHG:H291	11:9:7:GLN:HG3	1.88	0.54
30:i:4020:ECH:C12	21:l:1502:CLA:HAB	2.37	0.54
2:2:518:HIS:CD2	34:7:4015:ZEX:H21	2.42	0.54
2:2:684:LEU:HB2	28:h:4020:45D:H102	1.90	0.54
20:0:92:ALA:HB1	24:0:4019:BCR:H401	1.90	0.54
1:A:260:LEU:HD11	21:A:1113:CLA:HBA2	1.90	0.54
9:K:32:PHE:O	9:K:36:ILE:HG23	2.07	0.54
1:a:26:GLU:HA	8:j:3:GLY:HA3	1.90	0.54
1:a:429:MET:HA	1:a:432:HIS:CE1	2.41	0.54
1:a:462:ARG:NE	38:a:8005:HOH:O	2.40	0.54
12:b:26:ALA:HB2	26:b:5002:LMG:H131	1.89	0.54
12:b:718:TYR:HB2	21:b:1021:CLA:HED2	1.90	0.54
21:b:1204:CLA:H71	24:i:4018:BCR:HC32	1.90	0.54
16:1:561:LEU:HD13	16:1:582:THR:HG22	1.90	0.54
21:1:1131:CLA:H111	21:2:1239:CLA:H71	1.89	0.54
21:2:1237:CLA:H61	21:2:1238:CLA:H43	1.90	0.54
17:4:33:THR:OG1	17:4:82:ASP:OD2	2.19	0.54
21:A:1134:CLA:H62	21:b:1211:CLA:H203	1.88	0.54
22:A:2001:PQN:H303	21:A:1101:CLA:H172	1.90	0.54
2:B:1:MET:N	7:I:37:GLU:OE1	2.40	0.54
6:F:93:SER:O	6:F:95:ASN:N	2.40	0.54
21:a:1132:CLA:HMA2	10:l:68:LEU:HB3	1.89	0.54
10:l:23:PRO:HA	10:l:27:SER:HB3	1.89	0.54
16:1:367:ALA:HB2	16:1:393:HIS:HB2	1.88	0.54
9:K:80:MET:HE3	21:K:1401:CLA:HBB2	1.89	0.54
31:L:5001:SQD:H262	31:L:5002:SQD:H302	1.90	0.54
12:b:53:HIS:CE1	21:b:1202:CLA:HMA2	2.43	0.54
21:b:1201:CLA:HMA3	11:m:29:LEU:HD13	1.88	0.54
2:2:654:TRP:CD2	21:2:1021:CLA:HMA2	2.43	0.54
21:B:1231:CLA:H111	21:B:1232:CLA:H2	1.90	0.54
8:7:24:GLY:HA3	21:7:1302:CLA:HBB1	1.88	0.54
2:2:557:ASP:OD2	2:2:561:ARG:NH2	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:15:THR:HA	3:3:28:MET:HE3	1.89	0.54
2:B:169:LYS:NZ	2:B:326:ASN:OD1	2.41	0.54
1:a:296:HIS:HB2	21:a:1116:CLA:C1B	2.37	0.54
21:a:1107:CLA:H12	24:a:4012:BCR:H17C	1.89	0.54
12:b:14:GLN:NE2	13:c:1:MET:SD	2.76	0.54
2:2:553:SER:HG	2:2:570:TRP:CG	2.25	0.54
1:A:296:HIS:HB2	21:A:1116:CLA:C1B	2.38	0.54
21:a:1129:CLA:HAA2	10:l:8:VAL:HG21	1.90	0.54
21:b:1215:CLA:H191	21:b:1231:CLA:H12	1.90	0.54
13:c:1:MET:HG3	13:c:73:THR:HG23	1.89	0.54
16:1:48:ILE:HD12	21:1:1139:CLA:HMB3	1.89	0.54
5:5:13:ARG:O	5:5:15:GLU:N	2.41	0.54
31:B:5008:SQD:H132	31:B:5008:SQD:H301	1.90	0.53
12:b:475:LEU:HD13	21:b:1231:CLA:HHD	1.89	0.53
21:1:1128:CLA:HBB1	21:1:1128:CLA:HMB3	1.90	0.53
2:2:408:ARG:O	2:2:412:HIS:ND1	2.41	0.53
1:A:118:TRP:HB3	24:J:4013:BCR:HC21	1.90	0.53
2:B:317:HIS:HB3	2:B:320:LEU:HD12	1.89	0.53
21:B:1203:CLA:H143	21:B:1225:CLA:HBB2	1.90	0.53
3:C:18:VAL:HG22	3:C:26:LEU:HB2	1.90	0.53
1:a:113:SER:HB2	1:a:130:VAL:HG11	1.90	0.53
1:a:561:LEU:HD22	1:a:579:ARG:HD2	1.90	0.53
1:a:729:ALA:HA	25:a:5001:LHG:H341	1.91	0.53
12:b:337:ALA:HB2	24:b:4010:BCR:H372	1.89	0.53
21:1:1103:CLA:HBA2	21:1:1111:CLA:HED1	1.90	0.53
24:B:4014:BCR:HC31	21:B:1230:CLA:HBA2	1.91	0.53
21:b:1228:CLA:H192	24:f:4016:BCR:H12C	1.90	0.53
2:2:488:ALA:HB2	21:2:1232:CLA:HED3	1.89	0.53
1:A:419:ALA:HA	4:D:39:VAL:HG11	1.91	0.53
21:A:1125:CLA:CAB	21:A:1133:CLA:HMA2	2.39	0.53
1:a:645:TRP:HB3	21:a:1011:CLA:H101	1.89	0.53
12:b:654:TRP:CD2	21:b:1021:CLA:HMA2	2.44	0.53
13:c:22:PRO:HG2	13:c:23:LEU:HD12	1.91	0.53
21:1:1135:CLA:HMB3	21:1:1135:CLA:HBB1	1.91	0.53
21:2:1203:CLA:H43	26:2:5002:LMG:H321	1.90	0.53
21:B:1222:CLA:H92	21:B:1236:CLA:H41	1.88	0.53
12:b:22:TRP:NE1	21:b:1238:CLA:HBB1	2.19	0.53
4:d:37:GLU:HA	4:d:50:MET:O	2.08	0.53
21:A:1121:CLA:HBD	21:A:1121:CLA:HBA1	1.89	0.53
8:J:36:LEU:HB3	34:J:4015:ZEX:H32	1.89	0.53
1:a:319:HIS:NE2	21:a:1121:CLA:OBD	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:258:LEU:H	2:2:258:LEU:HD23	1.74	0.53
21:2:1234:CLA:HMB1	21:2:1234:CLA:HBB1	1.91	0.53
21:A:1801:CLA:H111	25:A:5007:LHG:H131	1.91	0.53
2:B:313:THR:OG1	25:B:5004:LHG:O6	2.27	0.53
2:B:405:VAL:O	2:B:409:MET:HG2	2.09	0.53
7:I:26:THR:HG22	25:0:5002:LHG:H172	1.91	0.53
10:L:37:LEU:HD22	21:L:1502:CLA:HBD	1.91	0.53
1:a:373:MET:HE3	21:a:1125:CLA:HMC3	1.91	0.53
1:a:726:VAL:HG13	1:a:730:HIS:CE1	2.43	0.53
13:c:52:LYS:NZ	13:c:67:VAL:O	2.40	0.53
6:f:132:VAL:HG11	31:f:5001:SQD:H3	1.89	0.53
2:2:133:GLN:O	2:2:137:SER:OG	2.27	0.53
2:2:587:LEU:HD21	21:2:1234:CLA:HBB2	1.91	0.53
21:A:1107:CLA:HMA2	24:J:4013:BCR:H12C	1.91	0.53
21:B:1240:CLA:HBA1	21:B:1240:CLA:HED2	1.89	0.53
1:a:442:TRP:HH2	21:a:1136:CLA:H141	1.73	0.53
1:A:439:HIS:O	1:A:443:VAL:HG23	2.08	0.53
21:A:1119:CLA:H102	21:A:1122:CLA:H93	1.90	0.53
21:B:1220:CLA:HAB	21:B:1227:CLA:CMD	2.39	0.53
12:b:257:PHE:CE2	21:b:1214:CLA:HBB1	2.44	0.53
1:a:333:THR:OG1	25:a:5003:LHG:O4	2.24	0.53
21:a:1012:CLA:HBB1	21:a:1012:CLA:HMB3	1.91	0.53
12:b:658:PHE:HB3	21:b:1023:CLA:HMC2	1.90	0.53
21:1:1132:CLA:H51	28:h:4020:45D:H411	1.89	0.53
2:2:584:LEU:HD23	2:2:587:LEU:HD22	1.91	0.53
20:0:153:ARG:NH1	35:0:6001:LMT:H6D	2.24	0.53
11:9:14:VAL:O	11:9:18:PRO:HD2	2.09	0.53
21:A:1112:CLA:H52	21:A:1112:CLA:H13	1.91	0.52
21:b:1212:CLA:H202	24:b:4004:BCR:H353	1.89	0.52
15:k:23:GLY:HA2	15:k:27:CYS:HB3	1.90	0.52
1:A:574:CYS:HB3	1:A:583:CYS:HA	1.90	0.52
1:a:86:TRP:HE1	21:a:1106:CLA:HBA1	1.74	0.52
1:a:118:TRP:CE2	24:j:4013:BCR:HC41	2.45	0.52
21:b:1214:CLA:H91	21:b:1231:CLA:H42	1.92	0.52
21:1:1119:CLA:H41	24:1:4008:BCR:H16C	1.91	0.52
21:2:1208:CLA:H62	24:2:4005:BCR:H333	1.90	0.52
1:A:456:ILE:HG22	21:A:1132:CLA:HBC2	1.90	0.52
24:A:4007:BCR:H402	25:L:5005:LHG:H181	1.91	0.52
2:B:256:THR:HA	21:B:1213:CLA:HED1	1.90	0.52
3:C:26:LEU:HA	3:C:41:SER:O	2.08	0.52
5:E:8:LYS:HB2	5:E:70:GLN:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:587:GLY:O	1:a:591:VAL:HG23	2.10	0.52
21:b:1239:CLA:HBA2	24:b:4017:BCR:H352	1.91	0.52
16:1:168:MET:O	16:1:172:MET:HG2	2.09	0.52
2:2:557:ASP:CG	3:3:66:ARG:HH12	2.17	0.52
21:B:1213:CLA:H18	24:B:4004:BCR:H21C	1.91	0.52
21:a:1117:CLA:H8	21:a:1117:CLA:CAB	2.39	0.52
21:b:1023:CLA:H192	24:b:4017:BCR:H353	1.91	0.52
2:2:276:HIS:HB2	21:2:1214:CLA:CHB	2.40	0.52
24:9:4021:BCR:H403	24:9:4021:BCR:H23C	1.92	0.52
1:A:304:PHE:HE1	21:A:1119:CLA:HAB	1.74	0.52
2:B:127:ILE:HG21	21:B:1211:CLA:HMA3	1.90	0.52
21:J:1302:CLA:H93	21:J:1302:CLA:HBC3	1.91	0.52
1:a:331:PRO:HG2	21:a:1801:CLA:HED2	1.90	0.52
1:a:539:ALA:O	1:a:543:HIS:ND1	2.25	0.52
21:1:1119:CLA:H111	24:1:4007:BCR:H12C	1.91	0.52
21:1:1126:CLA:H161	24:1:4012:BCR:H14C	1.91	0.52
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.92	0.52
9:K:20:LEU:O	9:K:25:ILE:HG12	2.09	0.52
24:a:4001:BCR:H401	15:k:41:ILE:HD11	1.91	0.52
21:b:1234:CLA:H12	21:b:1235:CLA:CGA	2.40	0.52
2:2:236:ASP:OD1	2:2:236:ASP:N	2.43	0.52
1:A:315:TRP:HB3	9:K:64:PRO:HB3	1.92	0.52
1:a:262:PRO:HG2	1:a:271:TYR:CZ	2.45	0.52
12:b:101:VAL:O	12:b:105:THR:HG23	2.10	0.52
21:b:1222:CLA:H71	21:b:1234:CLA:H62	1.90	0.52
25:l:5003:LHG:H272	25:l:5003:LHG:H161	1.91	0.52
21:1:1118:CLA:H203	24:1:4003:BCR:H332	1.92	0.52
2:2:544:MET:SD	2:2:567:ILE:HG21	2.50	0.52
21:2:1238:CLA:HBB2	22:2:2002:PQN:H141	1.91	0.52
17:4:30:ILE:HG21	17:4:68:LEU:HD23	1.91	0.52
1:A:120:ILE:HG13	1:A:121:VAL:HG13	1.92	0.52
21:a:1134:CLA:HMB1	24:a:4008:BCR:H272	1.91	0.52
12:b:374:GLN:HB3	12:b:584:LEU:HD21	1.92	0.52
21:b:1217:CLA:HBB1	24:b:4004:BCR:C14	2.37	0.52
6:f:107:LEU:O	6:f:111:LYS:HG2	2.09	0.52
16:1:677:PHE:CG	24:2:4011:BCR:H363	2.45	0.52
21:2:1237:CLA:H192	20:0:61:LEU:HD21	1.91	0.52
21:2:1205:CLA:H2	21:2:1205:CLA:H111	1.92	0.52
1:A:21:VAL:O	1:A:181:HIS:ND1	2.42	0.52
21:A:1134:CLA:HBA1	21:A:1134:CLA:CHA	2.40	0.52
1:a:438:SER:HB2	12:b:678:ALA:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:371:THR:HG23	12:b:588:THR:HG21	1.92	0.52
21:b:1023:CLA:H122	24:i:4018:BCR:H393	1.92	0.52
2:2:637:VAL:HG13	2:2:641:SER:HB2	1.91	0.52
17:4:10:LYS:HB2	17:4:49:ILE:HB	1.92	0.52
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.91	0.52
21:B:1222:CLA:HMB2	21:B:1236:CLA:H3A	1.92	0.52
10:L:151:ILE:HD13	21:b:1207:CLA:H11	1.91	0.52
1:a:531:ASP:O	1:a:535:HIS:ND1	2.37	0.52
4:d:127:GLU:HB2	4:d:130:THR:HG23	1.91	0.52
16:1:388:SER:HB3	21:1:1126:CLA:HMA1	1.92	0.52
16:1:520:VAL:HG21	16:1:523:MET:HE3	1.91	0.52
21:1:1118:CLA:H151	24:1:4002:BCR:H24C	1.91	0.52
21:2:1201:CLA:H93	24:9:4021:BCR:H11C	1.91	0.52
17:4:72:LEU:HD22	17:4:80:ILE:HD12	1.92	0.52
1:A:484:GLN:HB3	26:A:5004:LMG:HC5	1.92	0.51
21:B:1213:CLA:H111	26:B:5005:LMG:H453	1.91	0.51
1:a:207:LEU:HD22	24:a:4002:BCR:H361	1.92	0.51
21:a:1119:CLA:H152	21:a:1129:CLA:HBC1	1.92	0.51
12:b:312:LEU:HB2	25:b:5004:LHG:HC62	1.92	0.51
31:b:5006:SQD:H82	31:b:5006:SQD:H241	1.92	0.51
21:b:1230:CLA:H91	21:f:1301:CLA:HMA1	1.91	0.51
2:2:349:HIS:ND1	21:2:1214:CLA:OBD	2.42	0.51
18:h:35:GLU:O	20:0:105:GLN:NE2	2.43	0.51
4:D:120:ARG:NH1	4:D:125:ASN:OD1	2.43	0.51
12:b:29:HIS:HB2	21:b:1226:CLA:HBA1	1.91	0.51
21:b:1235:CLA:HMA3	21:b:1236:CLA:HED2	1.93	0.51
13:c:62:PHE:CE2	4:d:122:ILE:HG21	2.46	0.51
7:i:10:LEU:O	7:i:14:LEU:HB2	2.11	0.51
16:1:74:SER:HB2	21:1:1109:CLA:HAC2	1.92	0.51
2:B:372:HIS:HB2	21:B:1224:CLA:C1B	2.40	0.51
2:B:408:ARG:HD3	21:B:1227:CLA:OBD	2.11	0.51
2:2:312:LEU:HB2	25:2:5004:LHG:HC42	1.91	0.51
2:2:518:HIS:CD2	34:7:4015:ZEX:H171	2.45	0.51
21:A:1110:CLA:H71	26:A:5008:LMG:H261	1.92	0.51
21:A:1112:CLA:C4B	24:A:4002:BCR:H12C	2.40	0.51
9:K:22:VAL:HG21	21:K:1402:CLA:H171	1.93	0.51
21:a:1102:CLA:HMC3	25:a:5001:LHG:H181	1.92	0.51
21:a:1139:CLA:H2	8:j:15:ILE:HB	1.93	0.51
21:a:1140:CLA:H161	8:j:23:ALA:HB2	1.92	0.51
12:b:48:ALA:HB3	11:m:29:LEU:HD21	1.92	0.51
12:b:506:PHE:HE1	21:b:1234:CLA:HED2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:1205:CLA:HAB	21:b:1206:CLA:O1A	2.10	0.51
21:1:1013:CLA:H2	21:1:1013:CLA:HMA3	1.90	0.51
21:A:1107:CLA:HBA1	21:A:1107:CLA:HBD	1.91	0.51
2:B:385:PHE:HB3	2:B:531:LEU:HB3	1.92	0.51
21:B:1021:CLA:O2D	21:B:1021:CLA:HAA2	2.11	0.51
21:B:1227:CLA:HHC	21:B:1227:CLA:HBB1	1.91	0.51
1:a:360:GLY:HA2	1:a:397:GLY:HA2	1.93	0.51
12:b:178:HIS:HE1	21:b:1202:CLA:H142	1.75	0.51
10:l:6:GLN:O	10:l:9:GLN:NE2	2.37	0.51
2:2:713:GLY:O	2:2:717:THR:HG22	2.11	0.51
18:h:31:PHE:CZ	20:0:102:VAL:HG21	2.45	0.51
21:B:1211:CLA:HMA2	30:B:4006:ECH:H29A	1.92	0.51
1:a:483:ALA:HA	21:a:1135:CLA:HBA1	1.93	0.51
21:a:1801:CLA:H41	2:2:148:LEU:HD23	1.93	0.51
21:b:1207:CLA:O2A	21:b:1207:CLA:H2A	2.09	0.51
16:1:278:LYS:HG2	16:1:502:LEU:HD12	1.93	0.51
16:1:523:MET:HE1	16:1:627:VAL:HG21	1.91	0.51
21:2:1222:CLA:H11	21:2:1236:CLA:HBD	1.91	0.51
1:A:74:SER:OG	1:A:180:TYR:HB2	2.11	0.51
1:A:216:GLN:HA	1:A:220:SER:HB2	1.92	0.51
21:B:1216:CLA:H43	24:B:4018:BCR:H363	1.91	0.51
21:B:1234:CLA:H111	25:B:5004:LHG:H382	1.93	0.51
1:a:28:TRP:CZ2	21:a:1102:CLA:H11	2.46	0.51
1:a:94:GLY:HA3	1:a:147:TRP:CH2	2.46	0.51
24:a:4003:BCR:H383	24:a:4003:BCR:H23C	1.93	0.51
21:2:1225:CLA:H122	30:2:4006:ECH:H37A	1.93	0.51
21:A:1013:CLA:O2A	2:B:425:LEU:HA	2.10	0.51
21:A:1102:CLA:H141	21:A:1107:CLA:H161	1.92	0.51
21:A:1801:CLA:H152	31:b:5006:SQD:H322	1.93	0.51
2:B:22:TRP:CG	2:B:701:GLN:HE22	2.29	0.51
2:B:718:TYR:HB2	21:B:1021:CLA:HED3	1.92	0.51
4:D:61:ARG:NH1	4:D:63:GLU:OE1	2.42	0.51
24:a:4001:BCR:H11C	24:k:4001:BCR:H333	1.92	0.51
21:1:1118:CLA:HMA2	19:8:67:LEU:HB3	1.93	0.51
2:2:342:ILE:HG21	21:2:1221:CLA:H42	1.91	0.51
3:3:73:THR:H	3:3:76:SER:HG	1.55	0.51
8:7:36:LEU:HB3	34:7:4015:ZEX:H32	1.93	0.51
20:0:36:ASN:HB3	21:0:1501:CLA:HAC1	1.93	0.51
21:A:1140:CLA:H162	24:A:4012:BCR:H11C	1.92	0.51
31:L:5001:SQD:H112	31:L:5002:SQD:H262	1.92	0.51
1:a:342:GLU:OE1	1:a:342:GLU:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:1112:CLA:H43	21:a:1112:CLA:H202	1.91	0.51
15:k:13:PRO:O	15:k:15:THR:N	2.41	0.51
10:l:96:LEU:HG	24:l:4019:BCR:H24C	1.92	0.51
16:1:120:ILE:HG12	16:1:121:VAL:HG13	1.92	0.51
2:2:426:PHE:O	2:2:430:HIS:ND1	2.31	0.51
2:2:521:ALA:O	2:2:525:HIS:ND1	2.42	0.51
2:B:381:MET:HE1	24:B:4010:BCR:H361	1.92	0.51
1:a:462:ARG:NH1	12:b:634:PRO:HA	2.25	0.51
16:1:400:LEU:HD21	21:1:1104:CLA:H142	1.92	0.51
21:1:1106:CLA:H8	24:1:4012:BCR:H372	1.92	0.51
19:8:74:HIS:CE1	24:8:4001:BCR:H14C	2.46	0.51
21:a:1104:CLA:O2D	21:a:1104:CLA:HBA2	2.11	0.50
12:b:188:LEU:HG	21:b:1212:CLA:CBB	2.40	0.50
12:b:195:VAL:HG21	21:b:1212:CLA:HBC3	1.93	0.50
21:b:1218:CLA:CGA	24:b:4004:BCR:H282	2.41	0.50
6:f:10:CYS:HB2	6:f:41:ALA:HA	1.91	0.50
16:1:428:ARG:O	16:1:432:HIS:ND1	2.37	0.50
2:2:285:ILE:O	2:2:289:HIS:ND1	2.44	0.50
25:A:5006:LHG:H132	11:m:9:LEU:HD13	1.94	0.50
2:B:545:PRO:HD2	3:C:62:PHE:CE1	2.46	0.50
21:B:1235:CLA:HMA3	21:B:1236:CLA:HED2	1.94	0.50
9:K:20:LEU:HA	9:K:24:ILE:HD12	1.92	0.50
1:a:596:PHE:HZ	1:a:686:LEU:HD21	1.75	0.50
12:b:160:LYS:H	12:b:160:LYS:CE	2.20	0.50
21:b:1240:CLA:H141	31:f:5001:SQD:H101	1.94	0.50
13:c:62:PHE:HZ	13:c:66:ARG:HH21	1.58	0.50
10:l:7:VAL:HG23	25:l:5003:LHG:HC12	1.94	0.50
16:1:94:GLY:O	16:1:98:SER:OG	2.29	0.50
11:M:23:PHE:HE1	25:0:5002:LHG:H121	1.76	0.50
1:a:310:MET:HE3	1:a:311:TYR:CZ	2.46	0.50
1:a:685:PHE:HA	22:a:2001:PQN:H9	1.94	0.50
25:a:5005:LHG:H252	25:a:5005:LHG:HC92	1.93	0.50
12:b:87:ILE:HA	12:b:115:ILE:HA	1.93	0.50
21:b:1225:CLA:H192	30:b:4006:ECH:H17	1.94	0.50
15:k:54:GLN:H	15:k:54:GLN:CD	2.20	0.50
21:1:1132:CLA:OBD	38:1:8001:HOH:O	2.19	0.50
1:A:447:LEU:HD21	21:A:1136:CLA:CAB	2.42	0.50
21:B:1224:CLA:CGA	21:B:1224:CLA:H3A	2.41	0.50
21:B:1229:CLA:HBB1	21:B:1229:CLA:HHC	1.92	0.50
1:a:429:MET:HE3	1:a:436:ILE:HD13	1.93	0.50
21:a:1013:CLA:HMD3	12:b:530:ILE:HG12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:216:PRO:HB3	21:b:1212:CLA:OBD	2.12	0.50
21:b:1203:CLA:H71	21:b:1226:CLA:H93	1.93	0.50
13:c:35:LYS:N	14:e:33:ILE:HD11	2.26	0.50
16:1:657:VAL:HG22	16:1:745:ALA:HB3	1.93	0.50
21:2:1223:CLA:HMA1	24:2:4010:BCR:HC21	1.93	0.50
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.94	0.50
21:B:1211:CLA:H122	21:B:1225:CLA:H193	1.93	0.50
21:a:1119:CLA:HMB1	21:a:1119:CLA:HBB1	1.92	0.50
12:b:107:ALA:O	38:b:8001:HOH:O	2.20	0.50
12:b:516:VAL:HG12	21:b:1021:CLA:H142	1.93	0.50
10:l:17:VAL:O	10:l:19:HIS:N	2.43	0.50
2:2:372:HIS:HB2	21:2:1224:CLA:C1B	2.42	0.50
1:A:729:ALA:HA	25:A:5001:LHG:H342	1.93	0.50
9:K:34:PHE:CE2	21:K:1402:CLA:H42	2.40	0.50
10:L:58:GLY:HA2	10:L:89:ILE:HD11	1.94	0.50
12:b:490:TRP:CG	21:b:1214:CLA:H42	2.47	0.50
15:k:30:ASN:HA	15:k:73:GLY:HA3	1.93	0.50
16:1:691:GLY:HA3	2:2:567:ILE:HG12	1.93	0.50
21:1:1115:CLA:C1D	21:1:1116:CLA:HBB2	2.42	0.50
2:2:56:ILE:HG12	24:9:4021:BCR:H343	1.94	0.50
2:2:195:VAL:HG21	21:2:1212:CLA:HBC3	1.92	0.50
21:2:1201:CLA:HMA3	11:9:29:LEU:HD13	1.94	0.50
21:2:1215:CLA:HBB2	21:2:1221:CLA:C19	2.41	0.50
20:0:64:PRO:HA	21:0:1503:CLA:HBB1	1.93	0.50
1:A:428:ARG:HD3	21:A:1129:CLA:OBD	2.12	0.50
21:A:1107:CLA:H12	24:A:4012:BCR:H17C	1.93	0.50
2:B:654:TRP:CG	21:B:1021:CLA:HMA2	2.47	0.50
21:a:1123:CLA:H42	21:a:1127:CLA:H193	1.93	0.50
12:b:104:PHE:HZ	12:b:642:VAL:HG23	1.77	0.50
21:b:1212:CLA:H201	21:b:1213:CLA:H91	1.93	0.50
16:1:500:ASN:HB3	21:1:1115:CLA:HED2	1.93	0.50
1:A:221:MET:HE1	1:A:274:PHE:HB2	1.93	0.50
21:A:1104:CLA:H61	21:A:1128:CLA:HBC3	1.94	0.50
25:a:5005:LHG:HC92	25:a:5005:LHG:H281	1.93	0.50
22:1:2001:PQN:H241	21:1:1101:CLA:HAA1	1.94	0.50
20:0:32:THR:O	20:0:36:ASN:ND2	2.36	0.50
1:A:447:LEU:HD21	21:A:1136:CLA:HAB	1.93	0.50
24:A:4001:BCR:H282	9:K:36:ILE:HD11	1.94	0.50
1:a:433:ARG:HG3	1:a:555:TYR:CZ	2.47	0.50
21:a:1118:CLA:HMA3	15:k:67:LEU:HB3	1.93	0.50
21:b:1226:CLA:H91	26:b:5002:LMG:H261	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:310:MET:O	16:1:319:HIS:N	2.44	0.50
1:A:118:TRP:CE3	24:J:4013:BCR:H323	2.46	0.49
1:A:689:GLY:HA3	2:B:565:CYS:HB2	1.93	0.49
21:A:1801:CLA:H13	25:A:5007:LHG:H151	1.93	0.49
21:A:1012:CLA:H152	28:B:4011:45D:H381	1.93	0.49
2:B:659:MET:HB2	21:B:1023:CLA:C1C	2.42	0.49
21:a:1121:CLA:H111	21:a:1121:CLA:HAC2	1.94	0.49
21:b:1225:CLA:HMB1	21:b:1225:CLA:HBB1	1.93	0.49
2:2:117:TYR:HA	2:2:365:THR:HG22	1.94	0.49
6:6:20:SER:HB2	6:6:37:ALA:HB1	1.94	0.49
21:A:1112:CLA:OBD	38:A:8002:HOH:O	2.19	0.49
21:B:1205:CLA:O1A	21:B:1224:CLA:HBD	2.11	0.49
21:B:1212:CLA:C4B	24:B:4004:BCR:HC21	2.42	0.49
5:E:13:ARG:O	5:E:14:THR:OG1	2.26	0.49
9:K:84:LEU:HD12	26:K:5009:LMG:H331	1.93	0.49
21:L:1501:CLA:C1B	21:L:1502:CLA:HED1	2.42	0.49
12:b:154:TRP:NE1	11:m:28:GLU:HG3	2.28	0.49
21:b:1226:CLA:H141	21:b:1239:CLA:HAA2	1.93	0.49
16:1:523:MET:HE1	16:1:627:VAL:HG11	1.94	0.49
16:1:706:LYS:HE2	21:2:1228:CLA:HED2	1.93	0.49
24:1:4012:BCR:H16C	21:1:1012:CLA:H201	1.93	0.49
21:2:1213:CLA:C1D	21:2:1214:CLA:HBB2	2.42	0.49
1:A:5:PRO:HG2	1:A:183:LYS:HE3	1.95	0.49
2:B:349:HIS:HB3	21:B:1214:CLA:HED2	1.94	0.49
21:B:1224:CLA:H193	26:B:5002:LMG:H251	1.94	0.49
5:E:16:SER:HB3	38:E:8006:HOH:O	2.11	0.49
26:K:5009:LMG:H172	26:K:5009:LMG:H311	1.92	0.49
16:1:373:MET:HE1	21:1:1125:CLA:CAB	2.42	0.49
16:1:486:VAL:HG21	21:1:1135:CLA:H12	1.94	0.49
21:A:1012:CLA:H11	2:B:613:LEU:HD12	1.94	0.49
2:B:181:GLY:HA3	21:B:1210:CLA:HBB1	1.94	0.49
21:B:1222:CLA:HMA3	24:B:4010:BCR:H14C	1.95	0.49
31:B:5008:SQD:H331	31:B:5008:SQD:H161	1.94	0.49
31:L:5002:SQD:H221	21:b:1204:CLA:H192	1.95	0.49
13:c:27:GLU:OE2	13:c:44:ARG:NH1	2.37	0.49
19:8:17:GLY:HA2	19:8:21:SER:HB3	1.94	0.49
20:0:38:PRO:HG3	20:0:52:GLU:OE2	2.12	0.49
21:B:1222:CLA:HHB	24:B:4010:BCR:H16C	1.94	0.49
4:D:118:LYS:NZ	4:D:139:TYR:O	2.35	0.49
12:b:11:ASP:O	13:c:1:MET:HE1	2.13	0.49
12:b:361:GLN:OE1	12:b:361:GLN:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:20:THR:HG23	24:j:4013:BCR:H351	1.93	0.49
10:l:96:LEU:HD21	24:l:4019:BCR:H383	1.94	0.49
1:A:198:ASN:HB3	21:A:1118:CLA:HMD2	1.94	0.49
2:B:225:PHE:HB2	2:B:233:TYR:HE2	1.78	0.49
21:a:1107:CLA:CHB	24:a:4012:BCR:H12C	2.43	0.49
12:b:381:MET:HE1	24:b:4010:BCR:H361	1.95	0.49
14:e:26:ALA:HB2	14:e:40:ARG:HE	1.78	0.49
16:1:431:ARG:NH1	17:4:13:GLY:O	2.43	0.49
2:2:688:VAL:HG13	20:0:99:TYR:CE1	2.48	0.49
24:2:4010:BCR:C21	24:2:4018:BCR:H402	2.41	0.49
1:A:658:ILE:HD12	2:B:618:ARG:HG3	1.95	0.49
21:A:1104:CLA:H101	21:A:1126:CLA:HBC1	1.95	0.49
24:A:4001:BCR:H23C	9:K:72:PHE:HB2	1.94	0.49
1:a:324:ILE:O	1:a:328:HIS:ND1	2.46	0.49
21:a:1122:CLA:HBA1	21:a:1122:CLA:CHA	2.41	0.49
16:1:597:TRP:CH2	21:2:1022:CLA:HAB	2.48	0.49
21:2:1222:CLA:H43	21:2:1235:CLA:HBA1	1.95	0.49
1:A:202:ALA:HB2	1:A:308:GLY:HA3	1.95	0.49
1:A:392:HIS:HB2	21:A:1126:CLA:CHB	2.43	0.49
1:a:219:VAL:HG13	1:a:239:PRO:HB3	1.95	0.49
21:a:1121:CLA:HBA1	21:a:1121:CLA:CHA	2.42	0.49
12:b:618:ARG:HA	12:b:622:TRP:HB3	1.94	0.49
16:1:657:VAL:HG21	16:1:742:PHE:HA	1.93	0.49
21:2:1203:CLA:H162	21:2:1225:CLA:HBB2	1.94	0.49
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.45	0.49
1:A:597:TRP:HE1	21:B:1023:CLA:C1D	2.25	0.49
31:L:5001:SQD:H332	21:b:1201:CLA:H102	1.94	0.49
21:a:1133:CLA:H62	21:a:1133:CLA:H41	1.47	0.49
21:b:1215:CLA:CGA	21:b:1215:CLA:H3A	2.41	0.49
21:b:1224:CLA:CGA	21:b:1224:CLA:H3A	2.41	0.49
16:1:16:VAL:HG12	16:1:185:PRO:HA	1.94	0.49
21:2:1205:CLA:CAD	21:2:1224:CLA:HBA1	2.43	0.49
1:A:381:ILE:HG13	1:A:519:LYS:HE3	1.94	0.49
1:a:110:ILE:HG13	1:a:131:GLY:HA3	1.94	0.49
21:a:1129:CLA:HBB2	21:a:1137:CLA:HMC2	1.95	0.49
24:b:4014:BCR:H321	6:f:72:PHE:HB2	1.95	0.49
6:f:88:ILE:HG21	6:f:130:LYS:NZ	2.26	0.49
16:1:90:MET:HE1	21:1:1106:CLA:HMA2	1.95	0.49
21:1:1132:CLA:H72	28:h:4020:45D:H381	1.94	0.49
6:6:126:TYR:HB2	6:6:131:LEU:HD23	1.95	0.49
1:A:482:PHE:HB3	21:A:1135:CLA:H11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1121:CLA:H112	21:A:1121:CLA:H93	1.72	0.48
2:B:526:THR:HG21	2:B:579:TRP:CE2	2.48	0.48
1:a:90:MET:HE1	21:a:1106:CLA:HMA2	1.94	0.48
1:a:523:MET:HE1	1:a:627:VAL:HG11	1.95	0.48
21:a:1011:CLA:H122	21:a:1011:CLA:H162	1.55	0.48
16:1:324:ILE:O	16:1:328:HIS:ND1	2.46	0.48
16:1:600:ASN:OD1	38:1:8002:HOH:O	2.20	0.48
20:0:150:GLY:HA2	20:0:155:LEU:HD22	1.95	0.48
2:B:388:GLY:HA2	24:B:4010:BCR:H393	1.95	0.48
2:B:654:TRP:CD2	21:B:1021:CLA:HMA2	2.47	0.48
9:K:86:SER:HA	26:K:5009:LMG:H391	1.94	0.48
10:L:150:GLY:HA2	10:L:155:LEU:HD22	1.94	0.48
21:a:1129:CLA:HBA1	10:l:22:THR:HB	1.95	0.48
12:b:254:ILE:HG13	12:b:255:LEU:HG	1.94	0.48
16:1:92:PHE:CZ	16:1:96:LYS:HD2	2.47	0.48
16:1:118:TRP:CE2	24:7:4013:BCR:HC41	2.48	0.48
21:1:1130:CLA:H61	21:1:1130:CLA:H41	1.56	0.48
8:7:12:PRO:HA	8:7:15:ILE:HG22	1.94	0.48
21:A:1102:CLA:H52	21:A:1109:CLA:H13	1.94	0.48
24:A:4001:BCR:C11	24:K:4001:BCR:H333	2.42	0.48
21:B:1220:CLA:NC	24:B:4018:BCR:H19C	2.27	0.48
10:L:133:GLY:C	24:L:4022:BCR:H23C	2.38	0.48
1:a:197:MET:HE3	21:a:1119:CLA:HMA2	1.95	0.48
1:a:577:PRO:HB3	12:b:556:CYS:SG	2.53	0.48
12:b:299:HIS:NE2	21:b:1219:CLA:OBD	2.46	0.48
16:1:98:SER:HB2	16:1:144:PHE:HZ	1.78	0.48
21:1:1109:CLA:H91	21:1:1109:CLA:H142	1.95	0.48
21:A:1116:CLA:H62	21:A:1116:CLA:H41	1.51	0.48
21:A:1118:CLA:H193	24:A:4002:BCR:H372	1.95	0.48
2:B:687:LEU:HD11	10:L:39:ALA:HB1	1.95	0.48
1:a:419:ALA:HA	4:d:39:VAL:HG11	1.96	0.48
1:a:677:PHE:CD2	30:b:4011:ECH:H36B	2.48	0.48
21:a:1117:CLA:H2	21:a:1127:CLA:H92	1.95	0.48
16:1:376:TYR:CE2	21:1:1127:CLA:HED2	2.48	0.48
2:2:223:MET:HA	2:2:226:PHE:HB2	1.96	0.48
2:2:628:LEU:HD12	2:2:724:ALA:HB3	1.96	0.48
19:8:11:ALA:HB1	19:8:87:SER:HA	1.94	0.48
1:a:8:ARG:HH11	21:a:1108:CLA:HBA1	1.79	0.48
21:a:1111:CLA:H203	24:a:4002:BCR:H351	1.94	0.48
12:b:230:TRP:CE3	26:b:5005:LMG:H391	2.48	0.48
12:b:614:MET:O	12:b:618:ARG:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:1208:CLA:HAB	31:b:5006:SQD:H142	1.96	0.48
22:b:2002:PQN:H291	24:l:4019:BCR:HC7	1.96	0.48
6:f:90:ILE:HD13	6:f:99:GLN:HB3	1.94	0.48
21:l:1501:CLA:HHC	38:l:8019:HOH:O	2.14	0.48
16:1:619:GLY:HA3	16:1:629:HIS:HA	1.96	0.48
2:2:544:MET:HE2	2:2:547:LYS:HA	1.95	0.48
3:3:4:SER:HB3	3:3:6:LYS:HE2	1.95	0.48
1:A:168:MET:HE2	21:A:1112:CLA:H151	1.95	0.48
22:A:2001:PQN:H262	21:A:1101:CLA:HMA1	1.96	0.48
2:B:32:GLU:OE1	2:B:329:HIS:NE2	2.38	0.48
2:B:87:ILE:HD13	2:B:113:VAL:HG21	1.95	0.48
2:B:518:HIS:CD2	34:J:4015:ZEX:H21	2.47	0.48
21:a:1138:CLA:H8	21:a:1138:CLA:HMC2	1.95	0.48
12:b:462:GLN:HG2	12:b:506:PHE:CD1	2.48	0.48
21:b:1203:CLA:H92	26:b:5002:LMG:H401	1.95	0.48
1:A:486:VAL:CG1	21:A:1135:CLA:HED1	2.44	0.48
21:A:1013:CLA:HMD3	2:B:530:ILE:HG12	1.94	0.48
2:B:580:MET:CG	21:B:1222:CLA:HBC1	2.43	0.48
21:B:1205:CLA:H142	21:B:1205:CLA:H111	1.70	0.48
21:B:1222:CLA:HBA2	21:B:1222:CLA:H3A	1.59	0.48
24:B:4014:BCR:C32	6:F:72:PHE:HB2	2.44	0.48
26:K:5009:LMG:H422	12:b:213:LEU:O	2.13	0.48
1:a:86:TRP:HB2	24:a:4012:BCR:H391	1.95	0.48
21:a:1111:CLA:H3A	21:a:1111:CLA:HBA1	1.50	0.48
12:b:30:ASP:HB2	21:b:1226:CLA:HAA2	1.96	0.48
12:b:328:LEU:HB3	21:b:1202:CLA:HAC1	1.95	0.48
21:b:1226:CLA:H143	26:b:5002:LMG:H221	1.95	0.48
15:k:17:GLY:C	15:k:18:TRP:HD1	2.21	0.48
21:l:1503:CLA:H111	21:l:1503:CLA:H151	1.42	0.48
2:2:405:VAL:O	2:2:409:MET:HG2	2.13	0.48
1:A:486:VAL:HG21	21:A:1135:CLA:H12	1.96	0.48
24:B:4018:BCR:HC7	25:B:5006:LHG:H223	1.96	0.48
10:L:27:SER:OG	10:L:30:THR:HG23	2.14	0.48
1:a:168:MET:HG3	24:a:4002:BCR:H322	1.95	0.48
1:a:657:VAL:HG22	1:a:745:ALA:HB3	1.95	0.48
16:1:304:PHE:HZ	21:1:1117:CLA:H121	1.78	0.48
21:1:1131:CLA:HMA1	24:h:4018:BCR:H292	1.95	0.48
2:2:85:ARG:NH2	2:2:117:TYR:OH	2.47	0.48
2:2:328:LEU:HD22	21:2:1202:CLA:H203	1.95	0.48
21:2:1205:CLA:O1A	21:2:1224:CLA:HBD	2.14	0.48
1:a:356:LEU:HD21	21:a:1128:CLA:CAB	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:739:THR:HG23	21:a:1126:CLA:HBB2	1.95	0.48
21:a:1126:CLA:H93	21:a:1126:CLA:H61	1.71	0.48
22:a:2001:PQN:H302	22:a:2001:PQN:H262	1.74	0.48
21:b:1225:CLA:H162	30:b:4006:ECH:H19	1.95	0.48
21:b:1238:CLA:H18	24:i:4018:BCR:H362	1.96	0.48
16:1:332:PHE:HB2	25:1:5003:LHG:HC41	1.95	0.48
21:1:1119:CLA:HMB1	21:1:1119:CLA:HBB1	1.96	0.48
21:1:1012:CLA:HAB	2:2:579:TRP:CZ2	2.47	0.48
21:2:1203:CLA:H192	21:2:1203:CLA:H93	1.96	0.48
1:A:310:MET:HE3	1:A:311:TYR:CZ	2.49	0.48
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.48	0.48
21:B:1217:CLA:H151	24:B:4005:BCR:H342	1.95	0.48
21:L:1503:CLA:H62	21:L:1503:CLA:H41	1.46	0.48
1:a:595:LEU:HD21	21:a:1128:CLA:HBC1	1.96	0.48
21:a:1120:CLA:HBB2	21:a:1121:CLA:H152	1.96	0.48
12:b:542:LYS:NZ	6:f:139:PRO:HB2	2.28	0.48
13:c:67:VAL:HG21	23:c:3002:SF4:S2	2.53	0.48
16:1:114:ALA:HB3	16:1:139:ILE:HG21	1.95	0.48
16:1:278:LYS:HA	16:1:502:LEU:HB2	1.96	0.48
16:1:352:LEU:HD21	21:1:1128:CLA:C2B	2.44	0.48
16:1:419:ALA:HA	17:4:39:VAL:HG11	1.95	0.48
21:1:1105:CLA:HMB2	24:1:4012:BCR:H23C	1.95	0.48
21:1:1118:CLA:H91	21:1:1118:CLA:H111	1.62	0.48
1:A:27:LYS:HA	1:A:30:LYS:HD2	1.96	0.47
1:A:430:LEU:O	1:A:433:ARG:HD2	2.14	0.47
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.32	0.47
21:B:1203:CLA:H162	21:B:1225:CLA:HBB2	1.96	0.47
1:a:362:LEU:HD21	21:a:1117:CLA:H71	1.96	0.47
21:b:1213:CLA:HBD	21:b:1213:CLA:HBA1	1.96	0.47
6:f:82:VAL:HG21	21:f:1301:CLA:OBD	2.14	0.47
21:l:1501:CLA:C2B	21:l:1502:CLA:HED1	2.43	0.47
21:1:1139:CLA:H101	8:7:14:MET:HE3	1.96	0.47
21:2:1201:CLA:H141	21:2:1201:CLA:H162	1.61	0.47
21:2:1229:CLA:HBB2	24:2:4014:BCR:HC21	1.96	0.47
19:8:38:TYR:HE1	19:8:61:PHE:HE2	1.60	0.47
2:B:273:ILE:O	2:B:277:HIS:ND1	2.39	0.47
21:a:1101:CLA:HBA2	21:a:1101:CLA:HBD	1.96	0.47
16:1:24:SER:O	21:1:1109:CLA:HHB	2.14	0.47
21:1:1102:CLA:HBB1	21:1:1102:CLA:HMB1	1.96	0.47
21:1:1104:CLA:H91	25:1:5001:LHG:H351	1.96	0.47
2:2:539:ARG:NH1	17:4:127:GLU:OE1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1107:CLA:HBB1	24:A:4012:BCR:C8	2.38	0.47
2:B:429:PHE:CZ	24:B:4014:BCR:H372	2.49	0.47
28:B:4011:45D:H191	21:B:1230:CLA:HMC2	1.96	0.47
9:K:36:ILE:O	9:K:40:ALA:HB3	2.14	0.47
1:a:282:ASN:HB3	1:a:285:THR:HG22	1.96	0.47
1:a:440:LEU:HG	1:a:547:LEU:HB2	1.96	0.47
21:a:1115:CLA:H71	21:k:1401:CLA:HMD2	1.97	0.47
26:a:5002:LMG:H342	26:a:5002:LMG:H371	1.71	0.47
21:b:1218:CLA:H2	21:b:1218:CLA:H61	1.62	0.47
21:b:1222:CLA:H191	21:b:1232:CLA:H112	1.95	0.47
13:c:62:PHE:HE2	4:d:122:ILE:HG21	1.79	0.47
15:k:74:HIS:CG	24:k:4001:BCR:H12C	2.49	0.47
16:1:462:ARG:NH1	2:2:634:PRO:HA	2.29	0.47
21:1:1122:CLA:HBB1	24:1:4007:BCR:H362	1.96	0.47
24:1:4012:BCR:HC7	8:7:26:LEU:HD23	1.96	0.47
21:2:1023:CLA:H122	24:h:4018:BCR:H281	1.95	0.47
20:0:5:ASN:OD1	20:0:5:ASN:N	2.46	0.47
1:A:82:VAL:HG22	21:A:1109:CLA:H161	1.96	0.47
1:A:315:TRP:HB2	21:A:1118:CLA:HED1	1.96	0.47
21:B:1210:CLA:H172	24:B:4005:BCR:H271	1.95	0.47
21:B:1207:CLA:H62	21:B:1207:CLA:H101	1.63	0.47
11:M:22:ALA:HB2	30:M:4021:ECH:H37B	1.97	0.47
21:a:1104:CLA:H61	21:a:1128:CLA:HBC3	1.96	0.47
12:b:704:LEU:HD11	26:b:5002:LMG:H362	1.97	0.47
21:b:1205:CLA:O1A	21:b:1224:CLA:HBD	2.14	0.47
7:i:37:GLU:HG2	10:l:105:GLN:OE1	2.14	0.47
1:A:99:ASN:ND2	1:A:110:ILE:HD11	2.30	0.47
1:A:283:PRO:HD3	1:A:289:TRP:CZ2	2.50	0.47
1:A:704:HIS:NE2	21:A:1139:CLA:HAC1	2.30	0.47
2:B:429:PHE:HZ	24:B:4014:BCR:H372	1.79	0.47
3:C:73:THR:H	3:C:76:SER:HG	1.60	0.47
25:a:5003:LHG:H202	25:a:5003:LHG:H371	1.96	0.47
26:a:5004:LMG:H262	26:a:5004:LMG:H361	1.96	0.47
12:b:691:LYS:HB2	21:b:1238:CLA:HED3	1.96	0.47
21:b:1216:CLA:H61	21:b:1216:CLA:H41	1.46	0.47
21:b:1227:CLA:H191	21:b:1236:CLA:H111	1.96	0.47
10:l:151:ILE:HG23	21:2:1207:CLA:HBA1	1.97	0.47
16:1:310:MET:HE3	16:1:311:TYR:CZ	2.49	0.47
16:1:446:PHE:HE2	21:1:1136:CLA:HBB1	1.80	0.47
2:2:29:HIS:ND1	21:2:1203:CLA:O1A	2.33	0.47
2:2:291:TYR:HE1	21:2:1216:CLA:HED1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HE1	21:A:1119:CLA:C1D	2.44	0.47
21:A:1140:CLA:H3A	21:A:1140:CLA:HBA1	1.59	0.47
21:b:1228:CLA:HBA1	21:b:1228:CLA:CHA	2.43	0.47
16:1:203:GLY:HA3	21:1:1111:CLA:HBB1	1.95	0.47
1:A:167:VAL:HG22	24:A:4019:BCR:H282	1.96	0.47
21:A:1111:CLA:HBA1	21:A:1111:CLA:H3A	1.72	0.47
21:A:1124:CLA:H43	25:A:5003:LHG:H381	1.96	0.47
21:A:1134:CLA:H51	21:K:1401:CLA:HAA1	1.95	0.47
21:B:1216:CLA:OBD	21:B:1219:CLA:HHD	2.15	0.47
5:E:14:THR:N	38:E:8006:HOH:O	2.47	0.47
1:a:427:ASP:O	1:a:431:ARG:HG3	2.14	0.47
21:a:1108:CLA:H92	21:a:1108:CLA:H61	1.68	0.47
21:b:1207:CLA:H62	21:b:1207:CLA:H101	1.55	0.47
16:1:238:LEU:HB2	16:1:241:GLU:HG3	1.96	0.47
16:1:337:HIS:CE1	25:1:5003:LHG:HC11	2.50	0.47
21:1:1117:CLA:CAB	21:1:1117:CLA:H62	2.44	0.47
21:1:1132:CLA:HMA2	20:0:68:LEU:HB3	1.97	0.47
2:2:704:LEU:HD11	26:2:5002:LMG:H362	1.97	0.47
21:2:1204:CLA:H71	24:h:4018:BCR:HC32	1.96	0.47
18:h:27:MET:HG2	24:0:4019:BCR:H10C	1.97	0.47
21:0:1501:CLA:CMB	24:0:4022:BCR:H11C	2.42	0.47
21:A:1129:CLA:HAB	21:A:1137:CLA:CBB	2.44	0.47
10:L:1:MET:SD	12:b:159:PRO:HB3	2.55	0.47
10:L:82:LEU:HD22	10:L:139:TYR:CD2	2.50	0.47
1:a:278:LYS:O	1:a:503:ALA:N	2.44	0.47
21:a:1112:CLA:CHC	24:a:4002:BCR:H14C	2.44	0.47
12:b:381:MET:HB2	21:b:1222:CLA:HBC3	1.96	0.47
30:b:4011:ECH:H15	30:b:4011:ECH:H35	1.56	0.47
21:b:1240:CLA:HBB1	21:b:1240:CLA:HMB3	1.95	0.47
8:j:21:PHE:HD1	21:j:1302:CLA:H152	1.79	0.47
15:k:22:VAL:O	15:k:24:ILE:N	2.47	0.47
16:1:484:GLN:HB3	26:1:5004:LMG:HC5	1.97	0.47
16:1:557:ARG:HD2	16:1:566:ALA:HB2	1.97	0.47
21:1:1133:CLA:H141	21:1:1133:CLA:H161	1.68	0.47
2:2:104:PHE:HZ	2:2:642:VAL:HG23	1.79	0.47
2:2:309:LYS:O	21:2:1240:CLA:HBC2	2.15	0.47
3:3:18:VAL:HG22	3:3:26:LEU:HB2	1.96	0.47
1:A:424:ASN:O	1:A:428:ARG:HG3	2.15	0.47
21:B:1202:CLA:HMB1	21:B:1202:CLA:HBB1	1.97	0.47
21:B:1205:CLA:H143	21:B:1205:CLA:H161	1.65	0.47
21:B:1217:CLA:H3A	21:B:1217:CLA:HBA2	1.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:4022:BCR:HC32	31:L:5001:SQD:H161	1.97	0.47
1:a:315:TRP:HA	15:k:47:GLY:HA2	1.96	0.47
21:a:1134:CLA:HBA1	21:a:1134:CLA:CHA	2.45	0.47
21:1:1013:CLA:H91	21:1:1013:CLA:H111	1.80	0.47
21:1:1101:CLA:CBB	24:7:4013:BCR:H271	2.45	0.47
2:2:172:GLU:HG3	2:2:291:TYR:HB3	1.96	0.47
21:2:1218:CLA:HBB1	21:2:1218:CLA:H8	1.97	0.47
21:A:1123:CLA:H141	21:A:1123:CLA:H161	1.66	0.47
1:a:560:ARG:NH2	4:d:15:THR:O	2.48	0.47
21:a:1013:CLA:H161	21:a:1013:CLA:H141	1.62	0.47
21:a:1105:CLA:HAB	24:a:4012:BCR:H382	1.97	0.47
12:b:687:LEU:HD11	10:l:39:ALA:HB1	1.97	0.47
26:b:5007:LMG:O4	26:b:5007:LMG:O5	2.28	0.47
16:1:97:PHE:HE1	21:1:1105:CLA:HED2	1.80	0.47
16:1:411:PHE:CD1	16:1:415:ASP:HB2	2.50	0.47
22:1:2001:PQN:H162	24:2:4014:BCR:H382	1.97	0.47
21:2:1202:CLA:H91	21:2:1202:CLA:H112	1.80	0.47
21:2:1206:CLA:H151	21:2:1206:CLA:H112	1.55	0.47
20:0:38:PRO:HG2	21:0:1502:CLA:HED2	1.96	0.47
1:A:99:ASN:HB3	1:A:134:PHE:CG	2.49	0.46
1:A:197:MET:HE1	21:A:1123:CLA:C4D	2.45	0.46
1:A:315:TRP:HB3	9:K:64:PRO:CB	2.45	0.46
21:A:1127:CLA:H102	21:A:1127:CLA:H62	1.82	0.46
2:B:188:LEU:HG	21:B:1212:CLA:CBB	2.45	0.46
2:B:299:HIS:NE2	21:B:1219:CLA:OBD	2.48	0.46
4:D:31:THR:HA	4:D:55:ASN:O	2.15	0.46
1:a:356:LEU:HD21	21:a:1128:CLA:HAB	1.96	0.46
1:a:442:TRP:HB2	21:b:1237:CLA:HED2	1.96	0.46
21:a:1105:CLA:CAD	24:a:4019:BCR:H14C	2.45	0.46
21:b:1023:CLA:H142	24:i:4018:BCR:H271	1.96	0.46
21:b:1219:CLA:H93	21:b:1219:CLA:H111	1.71	0.46
21:b:1227:CLA:H111	21:b:1227:CLA:H72	1.69	0.46
21:b:1231:CLA:C4B	24:b:4010:BCR:HC42	2.45	0.46
21:b:1235:CLA:CBB	21:b:1236:CLA:HBC3	2.45	0.46
2:2:174:ARG:HB3	21:2:1221:CLA:HMD1	1.96	0.46
2:2:705:VAL:HG13	2:2:709:HIS:CE1	2.50	0.46
1:A:31:PRO:HB2	1:A:51:LEU:HD11	1.97	0.46
1:A:154:ASP:OD1	1:A:155:SER:N	2.48	0.46
1:A:304:PHE:CZ	21:A:1117:CLA:H121	2.47	0.46
21:A:1121:CLA:H52	25:A:5007:LHG:H142	1.96	0.46
21:B:1214:CLA:H171	21:B:1214:CLA:HMC3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1239:CLA:HBA2	24:B:4017:BCR:H352	1.96	0.46
1:a:12:ALA:HB1	21:a:1110:CLA:HAA1	1.97	0.46
21:a:1136:CLA:H61	21:a:1136:CLA:H41	1.66	0.46
21:b:1227:CLA:H122	21:b:1227:CLA:H162	1.54	0.46
21:b:1229:CLA:H152	6:f:73:LEU:HD22	1.96	0.46
21:b:1230:CLA:H111	6:f:75:ILE:HD11	1.97	0.46
16:1:203:GLY:HA3	21:1:1111:CLA:CBB	2.46	0.46
16:1:679:PHE:CG	21:1:1011:CLA:HMA2	2.49	0.46
21:1:1125:CLA:HHB	21:1:1133:CLA:H43	1.98	0.46
21:1:1129:CLA:H3A	21:1:1129:CLA:HBA1	1.58	0.46
2:2:555:PRO:HB3	2:2:699:ILE:HD12	1.97	0.46
2:2:645:TRP:CE3	24:2:4017:BCR:HC41	2.50	0.46
1:A:395:TRP:CD1	21:A:1126:CLA:HAB	2.50	0.46
21:A:1109:CLA:HMA2	38:A:8048:HOH:O	2.15	0.46
21:A:1134:CLA:H61	21:A:1134:CLA:H41	1.66	0.46
25:A:5005:LHG:H291	25:A:5005:LHG:H121	1.97	0.46
21:A:1012:CLA:H42	28:B:4011:45D:H393	1.97	0.46
21:B:1220:CLA:HBA1	24:B:4018:BCR:H351	1.96	0.46
21:B:1222:CLA:CMA	24:B:4010:BCR:H14C	2.46	0.46
1:a:118:TRP:HB3	24:j:4013:BCR:HC21	1.97	0.46
21:a:1108:CLA:H12	21:a:1110:CLA:C3D	2.46	0.46
21:a:1111:CLA:HBA2	21:a:1123:CLA:H43	1.97	0.46
21:a:1116:CLA:H93	21:a:1134:CLA:HAA2	1.96	0.46
21:a:1135:CLA:H13	21:a:1135:CLA:H171	1.44	0.46
21:b:1201:CLA:H162	21:b:1201:CLA:H141	1.73	0.46
4:d:77:LYS:HB2	4:d:78:PRO:CD	2.45	0.46
16:1:319:HIS:CG	16:1:324:ILE:HD11	2.51	0.46
2:2:513:ASP:HA	2:2:516:VAL:HG22	1.97	0.46
21:2:1212:CLA:HMB1	30:2:4006:ECH:H35A	1.98	0.46
21:2:1221:CLA:H71	21:2:1223:CLA:H42	1.98	0.46
20:0:99:TYR:CZ	20:0:103:THR:HG21	2.50	0.46
21:A:1128:CLA:H162	21:A:1140:CLA:HMA3	1.97	0.46
21:B:1206:CLA:HMA2	21:B:1207:CLA:HAB	1.96	0.46
21:B:1229:CLA:HBB2	24:B:4014:BCR:HC21	1.97	0.46
10:L:32:THR:HG22	31:L:5001:SQD:H82	1.98	0.46
26:a:5004:LMG:HC72	26:a:5004:LMG:HC2	1.65	0.46
2:2:339:LEU:HD12	2:2:342:ILE:HD11	1.97	0.46
22:2:2002:PQN:H142	24:2:4017:BCR:H271	1.97	0.46
1:A:197:MET:HG2	1:A:311:TYR:CE2	2.51	0.46
1:A:414:ARG:HE	27:A:7001:ACT:H3	1.81	0.46
2:B:48:ALA:HB3	11:M:29:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:VAL:HG11	24:B:4005:BCR:H341	1.96	0.46
21:B:1205:CLA:H62	21:B:1205:CLA:H101	1.61	0.46
8:J:27:ILE:HD13	24:J:4013:BCR:H10C	1.97	0.46
1:a:319:HIS:CG	1:a:324:ILE:HD11	2.51	0.46
21:a:1128:CLA:HBB1	21:a:1128:CLA:HMB3	1.98	0.46
26:a:5002:LMG:H411	26:a:5002:LMG:H382	1.69	0.46
16:1:16:VAL:HG21	16:1:183:LYS:HD2	1.97	0.46
25:1:5007:LHG:H241	21:1:1801:CLA:HMD1	1.96	0.46
21:1:1134:CLA:H41	21:1:1134:CLA:H121	1.98	0.46
2:2:348:GLN:HG3	21:2:1222:CLA:HED1	1.98	0.46
18:h:20:TRP:C	18:h:23:PRO:HD2	2.40	0.46
1:A:638:SER:O	1:A:644:GLY:HA3	2.16	0.46
21:B:1206:CLA:H71	24:B:4017:BCR:H341	1.98	0.46
1:a:49:TRP:CG	1:a:722:GLN:HE22	2.33	0.46
1:a:296:HIS:HB2	21:a:1116:CLA:CHB	2.46	0.46
1:a:534:VAL:HG11	1:a:608:HIS:CG	2.51	0.46
21:a:1013:CLA:H3A	21:a:1013:CLA:CGA	2.46	0.46
21:a:1103:CLA:H62	21:a:1103:CLA:H41	1.51	0.46
25:a:5005:LHG:H111	25:a:5005:LHG:HC82	1.72	0.46
21:b:1213:CLA:H111	26:b:5005:LMG:H453	1.98	0.46
21:b:1215:CLA:HMB2	21:b:1215:CLA:H72	1.98	0.46
16:1:597:TRP:HE1	21:2:1023:CLA:C1D	2.28	0.46
21:2:1201:CLA:H193	21:2:1201:CLA:H161	1.85	0.46
3:3:2:SER:N	3:3:71:ALA:O	2.48	0.46
28:h:4020:45D:H401	28:h:4020:45D:H421	1.56	0.46
21:B:1218:CLA:H162	21:B:1218:CLA:H202	1.79	0.46
21:B:1219:CLA:H143	21:B:1219:CLA:H111	1.70	0.46
21:B:1227:CLA:HBA2	25:B:5004:LHG:H241	1.97	0.46
16:1:269:GLY:N	19:8:13:PRO:HG3	2.31	0.46
21:1:1121:CLA:H41	21:1:1121:CLA:H61	1.48	0.46
21:1:1140:CLA:H62	21:1:1140:CLA:H41	1.55	0.46
24:1:4001:BCR:H363	24:8:4001:BCR:H343	1.97	0.46
21:1:1139:CLA:H43	21:6:1301:CLA:HBC3	1.97	0.46
20:0:38:PRO:HG3	20:0:52:GLU:CD	2.41	0.46
21:B:1214:CLA:H62	21:B:1214:CLA:H41	1.70	0.46
21:B:1216:CLA:H3A	21:B:1216:CLA:HBA2	1.34	0.46
1:a:370:MET:HE1	21:a:1127:CLA:O1D	2.16	0.46
21:a:1011:CLA:CBB	21:b:1021:CLA:HAA1	2.46	0.46
12:b:188:LEU:HG	21:b:1212:CLA:HBB2	1.97	0.46
12:b:441:VAL:HG13	12:b:446:THR:O	2.15	0.46
12:b:482:ILE:HD11	21:b:1232:CLA:HAC1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:642:VAL:HG22	21:b:1206:CLA:HHD	1.98	0.46
13:c:17:CYS:SG	13:c:18:VAL:N	2.89	0.46
6:f:77:GLY:HA3	6:f:118:TRP:CZ2	2.51	0.46
16:1:110:ILE:HG13	16:1:131:GLY:HA3	1.97	0.46
16:1:115:GLN:N	38:1:8008:HOH:O	2.41	0.46
16:1:207:LEU:HD21	21:1:1118:CLA:HMC3	1.96	0.46
21:1:1124:CLA:HAB	24:1:4008:BCR:H311	1.98	0.46
2:2:426:PHE:CE2	21:2:1235:CLA:HAB	2.51	0.46
21:2:1204:CLA:H202	21:2:1204:CLA:H161	1.72	0.46
25:2:5004:LHG:H272	25:2:5004:LHG:H121	1.98	0.46
21:A:1101:CLA:HBD	21:A:1101:CLA:HBA2	1.98	0.46
21:A:1012:CLA:HAB	2:B:579:TRP:CZ2	2.51	0.46
30:B:4006:ECH:H36	30:B:4006:ECH:H20	1.52	0.46
9:K:48:LYS:HE2	9:K:48:LYS:HB3	1.61	0.46
1:a:568:LEU:HD21	13:c:53:ARG:NH2	2.31	0.46
21:a:1011:CLA:HAA2	21:a:1011:CLA:CGD	2.46	0.46
24:a:4019:BCR:H11C	24:j:4013:BCR:H333	1.97	0.46
12:b:643:TRP:CZ2	12:b:723:ILE:HG21	2.51	0.46
15:k:13:PRO:C	15:k:14:THR:HG1	2.24	0.46
21:1:1136:CLA:HAB	21:1:1137:CLA:HHD	1.97	0.46
21:1:1139:CLA:H42	8:7:15:ILE:HA	1.97	0.46
2:2:361:GLN:OE1	2:2:361:GLN:N	2.49	0.46
3:3:22:PRO:HG2	3:3:23:LEU:HD12	1.97	0.46
1:A:26:GLU:HA	8:J:3:GLY:HA3	1.97	0.46
2:B:342:ILE:HD13	21:B:1221:CLA:H42	1.98	0.46
21:B:1201:CLA:H141	21:B:1201:CLA:H162	1.65	0.46
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.97	0.46
4:D:31:THR:O	4:D:83:TYR:HA	2.16	0.46
21:L:1503:CLA:H162	21:L:1503:CLA:H203	1.68	0.46
1:a:70:ARG:HD3	1:a:184:ALA:HB1	1.98	0.46
1:a:340:LEU:HD21	21:a:1122:CLA:HBC3	1.98	0.46
21:a:1118:CLA:H142	21:a:1118:CLA:H112	1.71	0.46
12:b:203:ARG:HG2	12:b:250:ALA:HB1	1.98	0.46
12:b:426:PHE:O	12:b:430:HIS:ND1	2.30	0.46
12:b:591:TRP:CD1	21:b:1234:CLA:HBC2	2.51	0.46
12:b:654:TRP:CG	21:b:1021:CLA:HMA2	2.51	0.46
21:b:1203:CLA:HHB	21:b:1226:CLA:CBB	2.46	0.46
21:b:1212:CLA:H201	21:b:1213:CLA:H112	1.97	0.46
13:c:29:VAL:HG21	4:d:114:ALA:HB2	1.97	0.46
16:1:189:TRP:CD1	21:1:1110:CLA:HED2	2.51	0.46
21:1:1122:CLA:HMB2	24:1:4007:BCR:H362	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1125:CLA:HMB1	21:1:1133:CLA:H43	1.98	0.46
6:6:75:ILE:HG23	21:6:1301:CLA:HAA1	1.97	0.46
21:A:1801:CLA:H172	12:b:148:LEU:HD11	1.98	0.45
21:B:1225:CLA:H61	21:B:1225:CLA:H41	1.65	0.45
21:B:1235:CLA:CMA	21:B:1236:CLA:HED2	2.45	0.45
10:L:112:ASP:HB3	10:L:115:GLN:HB2	1.98	0.45
10:L:144:ASN:O	10:L:147:VAL:HG12	2.16	0.45
21:L:1503:CLA:H93	21:L:1503:CLA:H111	1.73	0.45
1:a:31:PRO:HB3	21:a:1101:CLA:HAC1	1.99	0.45
1:a:434:ASP:OD1	1:a:555:TYR:OH	2.34	0.45
12:b:44:GLN:OE1	12:b:162:ARG:NH2	2.48	0.45
21:b:1227:CLA:HBC2	24:b:4018:BCR:H383	1.98	0.45
16:1:437:ILE:HG13	16:1:555:TYR:HE2	1.80	0.45
16:1:679:PHE:HE2	21:1:1012:CLA:HMD3	1.81	0.45
16:1:698:GLU:CD	2:2:542:LYS:HB2	2.41	0.45
21:1:1134:CLA:H41	21:1:1134:CLA:H61	1.56	0.45
21:1:1012:CLA:H41	21:1:1012:CLA:H61	1.38	0.45
2:2:448:GLU:H	2:2:448:GLU:CD	2.23	0.45
1:A:86:TRP:HE1	21:A:1106:CLA:HBA1	1.80	0.45
1:A:296:HIS:HB2	21:A:1116:CLA:CHB	2.47	0.45
2:B:3:THR:H	7:I:37:GLU:HA	1.81	0.45
2:B:633:ASN:HB3	2:B:635:TYR:H	1.80	0.45
21:B:1211:CLA:H72	21:B:1211:CLA:H112	1.41	0.45
21:J:1302:CLA:HED2	21:J:1302:CLA:H2A	1.97	0.45
1:a:59:ASP:HB2	1:a:414:ARG:NH1	2.31	0.45
1:a:118:TRP:CD1	24:j:4013:BCR:HC41	2.52	0.45
1:a:309:HIS:NE2	24:a:4001:BCR:H17C	2.30	0.45
1:a:512:GLU:OE1	1:a:512:GLU:N	2.45	0.45
21:a:1013:CLA:O2A	12:b:425:LEU:HA	2.17	0.45
21:a:1107:CLA:HMB2	24:a:4012:BCR:H10C	1.99	0.45
21:a:1135:CLA:H121	25:a:5003:LHG:H382	1.98	0.45
21:a:1136:CLA:HHC	21:a:1136:CLA:HBB1	1.98	0.45
12:b:385:PHE:CE2	24:b:4010:BCR:H373	2.51	0.45
21:b:1220:CLA:HBB1	25:b:5004:LHG:H122	1.98	0.45
21:b:1225:CLA:H3A	21:b:1225:CLA:HBA2	1.34	0.45
15:k:74:HIS:ND1	24:k:4001:BCR:H12C	2.32	0.45
21:1:1111:CLA:H142	21:1:1111:CLA:H111	1.76	0.45
24:1:4002:BCR:H362	24:1:4003:BCR:HC8	1.98	0.45
1:A:657:VAL:HG21	1:A:742:PHE:HA	1.98	0.45
21:A:1122:CLA:H92	24:A:4007:BCR:C14	2.47	0.45
21:A:1137:CLA:HBB1	21:A:1137:CLA:HHC	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:TRP:HE1	2:B:474:VAL:HG21	1.80	0.45
4:D:104:PHE:HB3	4:D:106:GLU:OE1	2.16	0.45
1:a:520:VAL:HG21	1:a:523:MET:HE3	1.98	0.45
21:a:1139:CLA:H101	8:j:14:MET:HE3	1.97	0.45
21:a:1130:CLA:HBA2	10:l:24:ILE:HG22	1.97	0.45
12:b:235:ALA:HB3	12:b:253:ALA:HB2	1.97	0.45
21:b:1212:CLA:H142	21:b:1212:CLA:H112	1.81	0.45
21:b:1222:CLA:H62	21:b:1222:CLA:H41	1.74	0.45
16:1:177:TRP:HB2	21:1:1109:CLA:HMC2	1.98	0.45
16:1:689:GLY:HA3	2:2:565:CYS:HB2	1.98	0.45
21:1:1135:CLA:H62	21:1:1135:CLA:H41	1.52	0.45
21:2:1229:CLA:CBB	24:2:4014:BCR:HC21	2.46	0.45
1:A:106:ASP:O	1:A:110:ILE:HG22	2.16	0.45
2:B:495:LEU:HA	2:B:498:ILE:HG22	1.98	0.45
21:B:1201:CLA:C4D	25:0:5002:LHG:H321	2.47	0.45
21:B:1204:CLA:HMA1	21:B:1205:CLA:HHB	1.98	0.45
21:B:1240:CLA:H201	31:F:5001:SQD:H241	1.98	0.45
21:a:1102:CLA:H193	24:a:4012:BCR:H23C	1.99	0.45
12:b:440:VAL:HG21	21:b:1230:CLA:HAC2	1.97	0.45
21:b:1231:CLA:H161	21:b:1231:CLA:H141	1.67	0.45
25:l:5003:LHG:H301	25:l:5003:LHG:H331	1.72	0.45
16:1:482:PHE:HB3	21:1:1135:CLA:H42	1.99	0.45
21:1:1125:CLA:CED	21:1:1133:CLA:HAB	2.46	0.45
2:2:717:THR:HG23	21:2:1021:CLA:O1D	2.16	0.45
25:2:5004:LHG:H372	25:2:5004:LHG:H342	1.70	0.45
1:A:309:HIS:NE2	24:A:4001:BCR:H363	2.32	0.45
7:I:10:LEU:O	7:I:14:LEU:HB2	2.17	0.45
21:L:1503:CLA:H43	7:i:12:TRP:HH2	1.81	0.45
21:a:1102:CLA:H172	24:a:4012:BCR:H272	1.99	0.45
22:a:2001:PQN:H201	21:a:1101:CLA:H12	1.99	0.45
12:b:460:TRP:O	12:b:464:THR:HG23	2.16	0.45
16:1:638:SER:O	16:1:644:GLY:HA3	2.17	0.45
2:2:276:HIS:HB2	21:2:1214:CLA:C1B	2.47	0.45
2:2:367:ALA:HB1	2:2:722:LEU:HD11	1.98	0.45
2:2:687:LEU:HD11	20:0:39:ALA:HB1	1.98	0.45
21:2:1023:CLA:H151	24:2:4017:BCR:H16C	1.97	0.45
18:h:22:PHE:O	18:h:26:THR:OG1	2.34	0.45
1:A:706:LYS:NZ	6:F:133:MET:O	2.48	0.45
21:A:1105:CLA:H143	21:A:1105:CLA:H161	1.75	0.45
21:A:1133:CLA:H162	21:A:1133:CLA:H193	1.63	0.45
2:B:158:GLN:HB3	31:B:5008:SQD:H5	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:PHE:CE2	24:B:4010:BCR:H373	2.51	0.45
21:B:1225:CLA:HBA2	21:B:1225:CLA:H3A	1.33	0.45
31:F:5001:SQD:H121	31:F:5001:SQD:H152	1.61	0.45
1:a:268:TRP:CZ2	21:a:1115:CLA:HBB1	2.52	0.45
1:a:573:PRO:HG2	14:e:50:SER:HB3	1.99	0.45
21:a:1125:CLA:H111	21:a:1125:CLA:H152	1.63	0.45
21:b:1203:CLA:H112	21:b:1203:CLA:H72	1.81	0.45
21:b:1213:CLA:H102	26:b:5005:LMG:H271	1.98	0.45
21:b:1235:CLA:H202	21:b:1235:CLA:H161	1.75	0.45
10:l:41:ARG:O	10:l:49:ARG:NH2	2.50	0.45
25:l:5001:LHG:H212	21:2:1204:CLA:H162	1.97	0.45
25:l:5003:LHG:H122	25:l:5003:LHG:HC91	1.40	0.45
21:1:1103:CLA:HED2	21:1:1128:CLA:HBB2	1.98	0.45
21:1:1116:CLA:CGA	21:1:1116:CLA:H3A	2.47	0.45
1:A:412:MET:O	1:A:557:ARG:HD3	2.17	0.45
21:A:1013:CLA:H161	21:A:1013:CLA:H141	1.65	0.45
21:A:1103:CLA:H203	21:A:1103:CLA:H161	1.71	0.45
21:A:1122:CLA:H41	21:A:1135:CLA:H201	1.99	0.45
21:A:1101:CLA:H112	21:A:1101:CLA:H152	1.50	0.45
2:B:460:TRP:CH2	25:F:5002:LHG:H352	2.52	0.45
21:B:1203:CLA:H72	21:B:1203:CLA:H111	1.60	0.45
21:B:1206:CLA:H102	21:B:1224:CLA:H192	1.98	0.45
1:a:203:GLY:HA3	21:a:1111:CLA:CBB	2.47	0.45
1:a:313:THR:OG1	1:a:314:ASN:N	2.49	0.45
1:a:514:ILE:HG22	1:a:521:ALA:HB3	1.99	0.45
21:a:1013:CLA:H193	21:a:1101:CLA:H18	1.98	0.45
25:a:5007:LHG:H331	25:a:5007:LHG:H301	1.46	0.45
21:b:1230:CLA:H91	21:f:1301:CLA:CMA	2.46	0.45
2:2:183:PHE:CE2	21:2:1210:CLA:H72	2.52	0.45
2:2:452:LEU:HB3	2:2:511:PRO:HG3	1.99	0.45
2:2:460:TRP:O	2:2:464:THR:HG23	2.16	0.45
3:3:62:PHE:CD2	17:4:122:ILE:HG21	2.51	0.45
20:0:153:ARG:HB2	20:0:155:LEU:HD13	1.98	0.45
21:0:1503:CLA:H141	21:0:1503:CLA:H161	1.64	0.45
25:A:5001:LHG:H142	25:A:5001:LHG:H111	1.56	0.45
21:B:1222:CLA:C1B	24:B:4010:BCR:H363	2.47	0.45
21:B:1207:CLA:HED2	10:L:65:TRP:NE1	2.32	0.45
1:a:376:TYR:CE2	21:a:1127:CLA:HED2	2.51	0.45
1:a:424:ASN:OD1	1:a:424:ASN:N	2.49	0.45
21:a:1120:CLA:HED2	21:a:1120:CLA:H2A	1.99	0.45
12:b:100:ALA:O	12:b:104:PHE:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:82:LEU:O	10:l:86:LEU:HG	2.16	0.45
16:1:433:ARG:NH1	17:4:45:GLY:HA3	2.32	0.45
16:1:452:PHE:CZ	16:1:456:ILE:HD11	2.52	0.45
16:1:714:GLN:HG2	16:1:716:ARG:NH1	2.32	0.45
2:2:526:THR:O	2:2:530:ILE:HG13	2.17	0.45
21:2:1023:CLA:H61	21:2:1023:CLA:H41	1.74	0.45
11:9:18:PRO:HB2	24:9:4021:BCR:H351	1.99	0.45
1:A:356:LEU:HD21	21:A:1128:CLA:HAB	1.98	0.45
9:K:28:LEU:HD22	26:K:5009:LMG:H273	1.98	0.45
10:L:7:VAL:HG23	25:L:5005:LHG:HC2	1.98	0.45
21:a:1108:CLA:H51	21:a:1110:CLA:H91	1.99	0.45
21:a:1120:CLA:H62	21:a:1120:CLA:H92	1.69	0.45
21:a:1133:CLA:H112	24:a:4008:BCR:H362	1.97	0.45
12:b:543:LEU:O	12:b:561:ARG:NH2	2.48	0.45
8:j:12:PRO:HA	8:j:15:ILE:HG22	1.98	0.45
8:j:40:PRO:HD2	34:j:4015:ZEX:H381	1.99	0.45
16:1:303:LEU:HD22	21:1:1119:CLA:HMC3	1.99	0.45
16:1:331:PRO:HB3	20:0:5:ASN:O	2.17	0.45
21:1:1125:CLA:CAB	21:1:1133:CLA:HMA2	2.47	0.45
21:1:1127:CLA:H41	21:1:1127:CLA:H61	1.52	0.45
21:A:1118:CLA:HBA2	21:A:1118:CLA:H3A	1.79	0.45
21:A:1136:CLA:H71	21:A:1136:CLA:H112	1.73	0.45
21:A:1139:CLA:H112	21:A:1139:CLA:H152	1.81	0.45
25:B:5006:LHG:H332	25:B:5006:LHG:H361	1.86	0.45
21:B:1230:CLA:H91	21:B:1230:CLA:H111	1.71	0.45
21:L:1501:CLA:CBA	24:L:4022:BCR:H363	2.47	0.45
21:a:1124:CLA:H62	21:a:1124:CLA:H93	1.71	0.45
21:b:1021:CLA:H3A	21:b:1021:CLA:HBA2	1.69	0.45
21:b:1023:CLA:H201	21:b:1239:CLA:H62	1.99	0.45
16:1:159:TYR:O	16:1:163:ILE:HG12	2.16	0.45
21:1:1138:CLA:HBC1	22:1:2001:PQN:H191	1.99	0.45
21:1:1101:CLA:H112	21:1:1101:CLA:H152	1.63	0.45
20:0:57:HIS:HA	20:0:60:PHE:CD2	2.52	0.45
1:A:118:TRP:HE1	24:A:4019:BCR:HC41	1.81	0.44
2:B:301:ILE:HG21	21:B:1221:CLA:HAC1	1.99	0.44
21:B:1204:CLA:H93	21:B:1204:CLA:H61	1.75	0.44
21:B:1216:CLA:HBA1	21:B:1221:CLA:HAB	1.99	0.44
6:F:36:ARG:HG3	8:J:35:ASP:HB3	1.98	0.44
21:K:1402:CLA:H18	21:K:1402:CLA:H152	1.47	0.44
21:a:1139:CLA:H202	21:f:1301:CLA:HED3	1.99	0.44
21:b:1205:CLA:CGA	21:b:1205:CLA:C1A	2.94	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:1212:CLA:C4B	24:b:4004:BCR:HC21	2.47	0.44
21:b:1218:CLA:H61	21:b:1218:CLA:H93	1.71	0.44
21:b:1235:CLA:CMA	21:b:1236:CLA:HED2	2.46	0.44
4:d:85:ILE:HB	4:d:98:HIS:HB3	1.99	0.44
10:l:32:THR:HG21	25:l:5002:LHG:H102	2.00	0.44
21:1:1116:CLA:H203	21:1:1116:CLA:H161	1.76	0.44
21:1:1117:CLA:H111	21:1:1117:CLA:H72	1.76	0.44
2:2:504:SER:HA	2:2:507:LEU:HD21	1.98	0.44
21:2:1021:CLA:H112	21:2:1021:CLA:H152	1.69	0.44
24:A:4019:BCR:H15C	24:A:4019:BCR:H351	1.74	0.44
2:B:426:PHE:O	2:B:430:HIS:ND1	2.47	0.44
9:K:22:VAL:HB	21:K:1402:CLA:H203	2.00	0.44
1:a:11:LYS:HB3	15:k:48:LYS:NZ	2.33	0.44
21:a:1130:CLA:HMA2	12:b:681:ARG:C	2.42	0.44
21:b:1231:CLA:H18	21:b:1232:CLA:CAD	2.48	0.44
14:e:9:VAL:HB	14:e:66:LEU:HB3	2.00	0.44
21:l:1501:CLA:C1B	21:l:1502:CLA:HED1	2.47	0.44
16:1:601:SER:O	16:1:605:VAL:HG23	2.17	0.44
21:1:1116:CLA:H92	21:1:1116:CLA:H61	1.81	0.44
2:2:372:HIS:O	2:2:376:ILE:HG12	2.17	0.44
21:2:1225:CLA:H202	24:2:4005:BCR:H352	1.99	0.44
20:0:17:VAL:O	20:0:19:HIS:N	2.50	0.44
21:0:1501:CLA:HBB2	24:0:4022:BCR:H321	1.99	0.44
1:A:315:TRP:CD1	9:K:64:PRO:HG3	2.52	0.44
1:A:384:ALA:HA	1:A:747:SER:HB2	1.98	0.44
2:B:289:HIS:CE1	24:B:4004:BCR:H363	2.52	0.44
2:B:435:TYR:CZ	2:B:515:LEU:HB3	2.53	0.44
21:B:1206:CLA:H202	21:B:1206:CLA:H161	1.84	0.44
21:B:1209:CLA:H11	21:B:1209:CLA:H51	1.81	0.44
21:B:1238:CLA:HBB2	22:B:2002:PQN:H141	1.99	0.44
26:B:5005:LMG:H182	26:B:5005:LMG:H211	1.80	0.44
21:B:1207:CLA:H151	24:0:4022:BCR:H362	2.00	0.44
1:a:571:ARG:HH21	25:a:5001:LHG:HC31	1.82	0.44
12:b:545:PRO:HD2	13:c:62:PHE:CE1	2.52	0.44
21:b:1208:CLA:H112	21:b:1208:CLA:H71	1.32	0.44
30:i:4020:ECH:H35	30:i:4020:ECH:H15	1.43	0.44
16:1:427:ASP:O	16:1:431:ARG:HG3	2.17	0.44
21:1:1011:CLA:H62	21:1:1011:CLA:H102	1.81	0.44
2:2:199:ILE:HG12	2:2:270:LEU:HB3	1.99	0.44
21:2:1237:CLA:H41	21:2:1237:CLA:H62	1.37	0.44
21:2:1219:CLA:HBD	21:2:1219:CLA:HBA2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:3:LEU:HD11	5:5:63:GLU:HG2	2.00	0.44
1:A:350:ALA:HB1	24:A:4007:BCR:H312	2.00	0.44
1:A:433:ARG:HG2	1:A:434:ASP:N	2.32	0.44
2:B:513:ASP:O	2:B:517:HIS:ND1	2.49	0.44
8:J:31:ARG:HD3	24:J:4013:BCR:C31	2.39	0.44
21:J:1302:CLA:H111	21:J:1302:CLA:H72	1.76	0.44
21:J:1303:CLA:H122	21:J:1303:CLA:H162	1.46	0.44
1:a:344:LEU:HB3	21:a:1123:CLA:HBC3	1.99	0.44
21:a:1102:CLA:HMC3	21:a:1101:CLA:HAB	1.99	0.44
21:a:1103:CLA:H3A	21:a:1103:CLA:HBA1	1.57	0.44
21:a:1105:CLA:CAB	24:a:4012:BCR:H382	2.47	0.44
21:a:1129:CLA:HBA2	21:a:1129:CLA:H3A	1.35	0.44
12:b:43:TYR:CE1	12:b:328:LEU:HD21	2.52	0.44
12:b:577:MET:HG3	12:b:707:LEU:HD21	2.00	0.44
4:d:13:GLY:HA2	10:l:15:PRO:O	2.17	0.44
4:d:30:ILE:HG21	4:d:68:LEU:HD23	1.98	0.44
21:j:1302:CLA:H142	21:j:1302:CLA:H112	1.79	0.44
16:1:446:PHE:CE2	21:1:1136:CLA:HBB1	2.52	0.44
21:1:1011:CLA:HAA1	21:2:1021:CLA:CBB	2.48	0.44
2:2:618:ARG:NH1	2:2:619:ASP:OD1	2.50	0.44
21:2:1203:CLA:H162	21:2:1203:CLA:H143	1.75	0.44
3:3:12:ILE:HD11	3:3:59:PRO:HG2	2.00	0.44
17:4:120:ARG:NH1	17:4:141:VAL:O	2.44	0.44
21:A:1129:CLA:H91	25:A:5003:LHG:H301	2.00	0.44
21:A:1801:CLA:H161	21:A:1801:CLA:H122	1.53	0.44
25:A:5005:LHG:H302	12:b:140:VAL:HG11	2.00	0.44
2:B:341:VAL:HG21	21:B:1223:CLA:H51	1.98	0.44
2:B:521:ALA:O	2:B:525:HIS:ND1	2.31	0.44
21:B:1201:CLA:H193	21:B:1201:CLA:H161	1.71	0.44
21:B:1212:CLA:H62	21:B:1212:CLA:H41	1.65	0.44
21:B:1230:CLA:H143	21:B:1230:CLA:H161	1.77	0.44
9:K:22:VAL:HG23	9:K:23:GLY:H	1.83	0.44
21:a:1111:CLA:H121	21:a:1111:CLA:H161	1.54	0.44
12:b:91:ILE:HB	12:b:112:PRO:HB2	1.99	0.44
12:b:321:TYR:O	12:b:325:ASN:HB2	2.18	0.44
21:b:1214:CLA:H143	21:b:1214:CLA:H162	1.81	0.44
10:l:95:ALA:HB1	24:l:4019:BCR:C19	2.48	0.44
16:1:369:HIS:HB3	21:1:1116:CLA:HED2	1.99	0.44
24:2:4014:BCR:H10C	21:6:1301:CLA:C2B	2.47	0.44
17:4:101:ASP:OD2	17:4:112:ARG:NE	2.40	0.44
1:A:67:ASP:O	1:A:71:LYS:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1105:CLA:H62	21:A:1107:CLA:H72	2.00	0.44
21:A:1124:CLA:H142	21:A:1124:CLA:H111	1.85	0.44
2:B:422:TRP:HZ3	21:B:1236:CLA:HBC2	1.82	0.44
2:B:589:PHE:CE2	21:B:1021:CLA:H61	2.51	0.44
21:B:1202:CLA:HBA1	21:B:1202:CLA:H3A	1.61	0.44
30:B:4006:ECH:H8	30:B:4006:ECH:H11	1.78	0.44
4:D:10:LYS:HB2	4:D:49:ILE:HB	1.99	0.44
4:D:37:GLU:HA	4:D:50:MET:O	2.17	0.44
10:L:66:THR:HG21	10:L:142:LEU:HD13	1.98	0.44
21:a:1122:CLA:H41	21:a:1122:CLA:H61	1.42	0.44
21:b:1209:CLA:H62	21:b:1209:CLA:H41	1.69	0.44
14:e:12:LYS:HB3	14:e:12:LYS:HE2	1.87	0.44
16:1:279:GLY:HA2	21:1:1116:CLA:O1A	2.17	0.44
16:1:647:ARG:NE	16:1:648:ASP:OD1	2.48	0.44
21:2:1205:CLA:H102	21:2:1205:CLA:H62	1.39	0.44
21:2:1222:CLA:HBA2	21:2:1222:CLA:H3A	1.68	0.44
21:2:1222:CLA:HAA2	21:2:1223:CLA:OBD	2.17	0.44
21:2:1228:CLA:HBA2	21:2:1228:CLA:H3A	1.60	0.44
1:A:740:TRP:HD1	21:A:1126:CLA:HMB2	1.83	0.44
2:B:580:MET:SD	2:B:584:LEU:HD12	2.58	0.44
21:B:1215:CLA:H62	21:B:1215:CLA:H41	1.67	0.44
21:B:1207:CLA:H191	26:0:5001:LMG:H442	1.98	0.44
9:K:47:GLY:HA3	9:K:64:PRO:HG2	2.00	0.44
10:L:44:LEU:HG	10:L:48:LEU:HD23	2.00	0.44
21:a:1102:CLA:H111	21:a:1102:CLA:H142	1.67	0.44
21:a:1111:CLA:H41	21:a:1111:CLA:H61	1.58	0.44
21:a:1133:CLA:H102	21:a:1133:CLA:H13	1.74	0.44
21:a:1133:CLA:HMD2	21:a:1134:CLA:HBB1	1.99	0.44
21:b:1238:CLA:H62	21:b:1238:CLA:H102	1.63	0.44
25:l:5003:LHG:H331	25:l:5003:LHG:H361	1.42	0.44
2:2:258:LEU:HD11	2:2:269:TRP:CE2	2.53	0.44
2:2:642:VAL:HG22	21:2:1206:CLA:HHD	1.99	0.44
21:2:1203:CLA:H152	21:2:1203:CLA:CHB	2.48	0.44
21:2:1206:CLA:H142	26:2:5002:LMG:H212	2.00	0.44
20:0:58:GLY:HA2	20:0:89:ILE:HD11	2.00	0.44
1:A:77:PHE:HD1	1:A:172:MET:HE3	1.82	0.44
1:A:86:TRP:HA	21:A:1105:CLA:CBB	2.46	0.44
21:A:1140:CLA:H72	21:A:1140:CLA:H112	1.68	0.44
26:A:5008:LMG:HC8	26:A:5008:LMG:H111	1.63	0.44
26:A:5008:LMG:H351	26:A:5008:LMG:H382	1.64	0.44
21:A:1012:CLA:HED2	21:B:1021:CLA:H71	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1206:CLA:H142	26:B:5002:LMG:H222	1.99	0.44
21:B:1240:CLA:H102	21:B:1240:CLA:H62	1.55	0.44
21:b:1204:CLA:HED2	7:i:11:PRO:HB3	1.99	0.44
21:b:1216:CLA:H3A	21:b:1216:CLA:HBA2	1.51	0.44
21:b:1228:CLA:H12	24:f:4016:BCR:H341	2.00	0.44
35:l:6001:LMT:H62	24:9:4021:BCR:H292	1.99	0.44
16:1:700:ILE:HD13	21:1:1138:CLA:HMD1	2.00	0.44
21:1:1106:CLA:H162	21:1:1106:CLA:H141	1.64	0.44
21:2:1225:CLA:H92	24:2:4005:BCR:H21C	2.00	0.44
6:6:32:SER:HA	6:6:35:ILE:HG22	2.00	0.44
21:6:1302:CLA:HBB1	21:6:1302:CLA:HMB3	1.98	0.44
20:0:96:LEU:HG	24:0:4019:BCR:H24C	2.00	0.44
1:A:482:PHE:CE2	21:A:1136:CLA:H42	2.53	0.44
21:A:1137:CLA:H101	24:A:4008:BCR:H373	2.00	0.44
21:A:1140:CLA:H162	21:A:1140:CLA:H141	1.67	0.44
21:F:1301:CLA:H141	21:F:1301:CLA:H161	1.61	0.44
10:L:132:MET:HB3	24:0:4022:BCR:H393	2.00	0.44
21:a:1121:CLA:H152	21:a:1121:CLA:H112	1.29	0.44
21:a:1139:CLA:H152	21:a:1139:CLA:H111	1.59	0.44
16:1:296:HIS:CE1	16:1:300:ILE:HG13	2.53	0.44
16:1:362:LEU:HD11	21:1:1117:CLA:H93	1.99	0.44
21:1:1126:CLA:H62	21:1:1126:CLA:H41	1.89	0.44
2:2:437:HIS:CE1	2:2:451:ILE:HG13	2.53	0.44
22:2:2002:PQN:H241	22:2:2002:PQN:H261	1.74	0.44
20:0:23:PRO:HB3	31:0:5005:SQD:H441	1.98	0.44
25:0:5004:LHG:H351	21:0:1503:CLA:C1D	2.48	0.44
1:A:25:PHE:HB2	8:J:1:MET:HG2	2.00	0.43
21:A:1126:CLA:H62	21:A:1126:CLA:H41	1.60	0.43
2:B:420:LEU:HG	21:B:1236:CLA:CBB	2.47	0.43
11:M:20:PHE:CZ	11:M:24:ARG:HD2	2.53	0.43
1:a:388:SER:HB3	21:a:1126:CLA:HMA1	2.00	0.43
21:a:1102:CLA:H72	21:a:1102:CLA:H112	1.76	0.43
12:b:290:MET:HE1	21:b:1216:CLA:CAD	2.48	0.43
21:b:1209:CLA:CBB	21:b:1209:CLA:H71	2.47	0.43
21:b:1209:CLA:H193	21:b:1209:CLA:H161	1.77	0.43
21:b:1211:CLA:H62	21:b:1211:CLA:H2	1.70	0.43
16:1:304:PHE:HE1	21:1:1119:CLA:HAB	1.83	0.43
21:1:1139:CLA:H41	8:7:18:LEU:HD23	1.98	0.43
2:2:85:ARG:HH12	2:2:727:ALA:HA	1.82	0.43
21:2:1203:CLA:H111	21:2:1203:CLA:H151	1.65	0.43
21:A:1125:CLA:C3B	21:A:1133:CLA:HMA2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1023:CLA:H192	24:B:4017:BCR:H353	1.99	0.43
21:B:1206:CLA:H112	21:B:1206:CLA:H151	1.64	0.43
21:F:1301:CLA:H151	21:F:1301:CLA:H112	1.75	0.43
34:J:4015:ZEX:H401	34:J:4015:ZEX:H31	1.77	0.43
25:L:5005:LHG:H302	25:L:5005:LHG:H131	2.01	0.43
1:a:369:HIS:ND1	21:a:1116:CLA:OBD	2.51	0.43
1:a:515:ALA:HA	1:a:521:ALA:H	1.83	0.43
21:a:1129:CLA:HBB2	21:a:1137:CLA:CMC	2.48	0.43
12:b:85:ARG:HD3	12:b:85:ARG:HA	1.70	0.43
12:b:169:LYS:NZ	12:b:326:ASN:OD1	2.46	0.43
30:b:4011:ECH:H7	30:b:4011:ECH:H10	1.77	0.43
21:b:1222:CLA:H3A	21:b:1222:CLA:HBA2	1.70	0.43
15:k:44:THR:HG22	15:k:61:PHE:HB3	2.00	0.43
15:k:63:LEU:N	15:k:64:PRO:HD2	2.34	0.43
16:1:71:LYS:HA	21:1:1109:CLA:HMD2	2.01	0.43
16:1:189:TRP:CZ2	21:1:1111:CLA:HAC2	2.53	0.43
21:1:1131:CLA:HAA1	28:h:4020:45D:C38	2.48	0.43
2:2:194:LEU:HA	2:2:198:ALA:HB3	2.00	0.43
20:0:54:GLY:O	20:0:131:GLY:HA2	2.18	0.43
21:A:1110:CLA:H172	26:A:5008:LMG:H191	2.00	0.43
2:B:464:THR:O	2:B:476:LEU:HB2	2.19	0.43
2:B:539:ARG:NH2	6:F:143:ARG:O	2.51	0.43
25:M:5001:LHG:HC81	25:M:5001:LHG:HC5	1.70	0.43
21:a:1103:CLA:H162	24:a:4003:BCR:H362	2.00	0.43
21:a:1104:CLA:H41	21:a:1104:CLA:H62	1.59	0.43
21:a:1106:CLA:H51	21:a:1106:CLA:H8	1.67	0.43
21:a:1110:CLA:H142	21:a:1110:CLA:H111	1.75	0.43
21:a:1120:CLA:CHA	21:a:1120:CLA:HBA1	2.49	0.43
12:b:580:MET:HE3	12:b:584:LEU:CD1	2.47	0.43
21:b:1203:CLA:H43	26:b:5002:LMG:H321	1.99	0.43
21:b:1227:CLA:C4D	25:b:5004:LHG:H242	2.46	0.43
21:l:1501:CLA:H62	21:l:1501:CLA:H92	1.73	0.43
16:1:485:TRP:HB2	26:1:5004:LMG:O7	2.18	0.43
16:1:702:TRP:CH2	21:2:1228:CLA:HED1	2.53	0.43
21:1:1105:CLA:C4D	24:1:4019:BCR:H14C	2.47	0.43
21:1:1111:CLA:HBA1	21:1:1111:CLA:H3A	1.61	0.43
21:1:1126:CLA:H161	21:1:1126:CLA:H202	1.72	0.43
22:1:2001:PQN:H201	21:1:1101:CLA:H12	2.00	0.43
21:2:1205:CLA:H143	21:2:1205:CLA:H161	1.76	0.43
3:3:7:ILE:HG12	3:3:40:ALA:HB3	2.00	0.43
20:0:112:ASP:OD1	20:0:112:ASP:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1137:CLA:H143	21:A:1137:CLA:H112	1.74	0.43
2:B:376:ILE:O	2:B:380:LEU:HG	2.17	0.43
21:B:1215:CLA:H122	21:B:1215:CLA:H162	1.67	0.43
21:B:1216:CLA:H171	21:B:1216:CLA:H101	1.99	0.43
21:B:1222:CLA:C2B	24:B:4010:BCR:H363	2.48	0.43
1:a:80:LEU:HD23	1:a:80:LEU:HA	1.80	0.43
1:a:168:MET:O	1:a:172:MET:HG2	2.18	0.43
1:a:202:ALA:HB2	1:a:308:GLY:HA3	2.00	0.43
1:a:267:ASN:OD1	15:k:13:PRO:HG2	2.19	0.43
1:a:709:VAL:HG13	6:f:84:ARG:HG3	2.00	0.43
21:b:1021:CLA:H202	21:b:1021:CLA:H161	1.83	0.43
6:f:48:GLU:HG2	6:f:50:TYR:H	1.83	0.43
16:1:462:ARG:NH1	38:1:8010:HOH:O	2.45	0.43
21:1:1111:CLA:H203	24:1:4003:BCR:C11	2.48	0.43
21:1:1136:CLA:H91	21:0:1502:CLA:H201	2.01	0.43
26:1:5004:LMG:O8	26:1:5004:LMG:O2	2.23	0.43
21:1:1012:CLA:HMA3	21:2:1021:CLA:H202	1.99	0.43
2:2:338:SER:HA	21:2:1223:CLA:H41	2.01	0.43
19:8:59:LYS:HB2	19:8:59:LYS:HE2	1.78	0.43
21:A:1102:CLA:H203	21:A:1107:CLA:H92	2.00	0.43
2:B:516:VAL:HG21	2:B:590:TYR:HB2	2.00	0.43
21:B:1205:CLA:CGA	21:B:1205:CLA:C1A	2.97	0.43
25:F:5002:LHG:H211	21:F:1302:CLA:C1B	2.48	0.43
9:K:80:MET:HE3	21:K:1401:CLA:CBB	2.48	0.43
1:a:42:PRO:HB3	1:a:47:TRP:CE3	2.54	0.43
1:a:549:LEU:O	1:a:553:VAL:HG23	2.19	0.43
21:b:1216:CLA:HMB2	21:b:1221:CLA:H61	2.00	0.43
21:b:1223:CLA:H13	24:b:4010:BCR:H351	1.99	0.43
15:k:14:THR:O	15:k:15:THR:OG1	2.32	0.43
16:1:587:GLY:O	16:1:591:VAL:HG23	2.18	0.43
17:4:2:THR:OG1	17:4:3:GLU:N	2.51	0.43
5:5:13:ARG:HB3	5:5:16:SER:HB2	1.99	0.43
21:0:1501:CLA:HBA2	21:0:1501:CLA:H3A	1.48	0.43
1:A:219:VAL:HG13	1:A:239:PRO:HB3	2.00	0.43
21:A:1129:CLA:H11	21:A:1129:CLA:H52	1.81	0.43
21:A:1129:CLA:H102	21:L:1502:CLA:H151	1.99	0.43
21:A:1135:CLA:HBB1	21:A:1135:CLA:HMB3	2.00	0.43
25:A:5007:LHG:H281	25:A:5007:LHG:H312	1.62	0.43
2:B:287:ALA:HB2	21:B:1216:CLA:HBC2	2.01	0.43
21:B:1237:CLA:HMB1	21:B:1237:CLA:HBB1	2.00	0.43
21:B:1205:CLA:HBA1	21:B:1224:CLA:OBD	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1216:CLA:HMB2	21:B:1221:CLA:H92	2.00	0.43
21:a:1115:CLA:H202	21:a:1115:CLA:H161	1.71	0.43
21:a:1118:CLA:H162	21:a:1118:CLA:H121	1.42	0.43
25:a:5003:LHG:H302	25:a:5003:LHG:H272	1.74	0.43
12:b:586:TRP:NE1	38:b:8007:HOH:O	2.51	0.43
12:b:688:VAL:HG13	10:l:99:TYR:CE1	2.54	0.43
16:1:733:LEU:HA	25:1:5001:LHG:H383	2.00	0.43
21:A:1110:CLA:H51	21:A:1118:CLA:H41	2.00	0.43
26:A:5002:LMG:HC5	37:L:5004:DGD:HA32	1.99	0.43
26:A:5004:LMG:H111	25:A:5005:LHG:HC2	2.00	0.43
2:B:694:PRO:HB3	21:B:1238:CLA:C1C	2.49	0.43
21:B:1203:CLA:H61	21:B:1203:CLA:H41	1.38	0.43
21:B:1211:CLA:H202	21:B:1211:CLA:H161	1.78	0.43
10:L:82:LEU:O	10:L:86:LEU:HG	2.19	0.43
31:L:5001:SQD:H292	31:L:5002:SQD:H182	2.00	0.43
21:a:1106:CLA:H3A	21:a:1106:CLA:HBA2	1.52	0.43
21:a:1124:CLA:HAB	24:a:4008:BCR:H311	2.01	0.43
25:a:5007:LHG:H182	25:a:5007:LHG:H151	1.86	0.43
12:b:236:ASP:OD1	12:b:252:THR:OG1	2.31	0.43
12:b:350:MET:HG2	21:b:1215:CLA:O1A	2.18	0.43
21:b:1203:CLA:H172	21:b:1203:CLA:H111	2.00	0.43
21:b:1219:CLA:HHC	21:b:1219:CLA:HBB1	2.00	0.43
21:b:1222:CLA:H2	21:b:1234:CLA:HMA2	2.01	0.43
16:1:441:ASN:O	16:1:445:ILE:HG13	2.19	0.43
21:1:1107:CLA:HBD	21:1:1107:CLA:HBA1	2.00	0.43
21:1:1012:CLA:H93	21:1:1012:CLA:H112	1.81	0.43
21:2:1225:CLA:H3A	21:2:1225:CLA:HBA2	1.37	0.43
3:3:5:VAL:HG11	3:3:26:LEU:HD21	2.01	0.43
1:A:391:THR:HG21	1:A:743:PHE:CE2	2.54	0.43
21:A:1106:CLA:HBB1	21:A:1107:CLA:O1A	2.18	0.43
21:A:1118:CLA:H141	24:A:4002:BCR:H383	2.00	0.43
21:A:1119:CLA:HBA1	21:A:1123:CLA:CAB	2.49	0.43
21:A:1119:CLA:HMB1	21:A:1119:CLA:HBB1	2.01	0.43
21:A:1125:CLA:CED	21:A:1133:CLA:HAB	2.49	0.43
25:A:5001:LHG:H382	25:A:5001:LHG:H352	1.78	0.43
2:B:672:ILE:HG12	24:B:4017:BCR:H282	2.00	0.43
21:B:1228:CLA:O1A	31:F:5001:SQD:O4	2.34	0.43
3:C:59:PRO:HD2	23:C:3003:SF4:S4	2.59	0.43
21:a:1012:CLA:H61	21:a:1012:CLA:H41	1.43	0.43
21:b:1215:CLA:H62	21:b:1215:CLA:H41	1.58	0.43
26:b:5007:LMG:H151	26:b:5007:LMG:H181	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:350:ALA:HB1	24:1:4007:BCR:H312	2.00	0.43
16:1:478:LEU:HB2	16:1:529:THR:HG23	1.99	0.43
21:1:1119:CLA:H72	24:1:4008:BCR:H14C	2.00	0.43
21:1:1139:CLA:H91	21:1:1139:CLA:H112	1.87	0.43
2:2:659:MET:HA	21:2:1023:CLA:C2C	2.49	0.43
21:A:1116:CLA:H3A	21:A:1116:CLA:HBA2	1.70	0.43
21:B:1213:CLA:H143	21:B:1213:CLA:H161	1.74	0.43
21:B:1207:CLA:HBA1	20:0:151:ILE:HG23	2.00	0.43
6:F:90:ILE:CG2	6:F:99:GLN:HB2	2.49	0.43
9:K:25:ILE:CD1	26:K:5009:LMG:H221	2.49	0.43
1:a:344:LEU:HD23	1:a:344:LEU:HA	1.81	0.43
1:a:575:ASP:OD2	1:a:579:ARG:NH2	2.51	0.43
21:a:1110:CLA:H3A	21:a:1110:CLA:HBA2	1.50	0.43
21:a:1135:CLA:H41	21:a:1135:CLA:H61	1.49	0.43
21:b:1023:CLA:H143	21:b:1023:CLA:H111	1.78	0.43
21:1:1109:CLA:H62	21:1:1109:CLA:H41	1.70	0.43
21:1:1134:CLA:H141	21:1:1134:CLA:H161	1.75	0.43
2:2:409:MET:HE2	24:2:4018:BCR:H271	2.01	0.43
21:2:1202:CLA:HBA1	21:2:1202:CLA:H3A	1.54	0.43
5:5:17:TYR:CE2	5:5:45:ASN:HA	2.53	0.43
6:6:10:CYS:HB3	6:6:16:TYR:CD2	2.54	0.43
24:7:4013:BCR:H15C	24:7:4013:BCR:H351	1.85	0.43
21:A:1107:CLA:H91	21:A:1107:CLA:H111	1.72	0.43
21:B:1234:CLA:H111	21:B:1234:CLA:H91	1.74	0.43
25:B:5006:LHG:H171	25:B:5006:LHG:H142	1.87	0.43
38:B:8036:HOH:O	31:F:5001:SQD:H382	2.18	0.43
3:C:52:LYS:HD2	3:C:55:GLU:OE1	2.19	0.43
3:C:55:GLU:HB3	3:C:63:LEU:HD13	2.01	0.43
6:F:39:ARG:NH1	8:J:34:PRO:O	2.47	0.43
7:I:22:PHE:HA	25:0:5002:LHG:H211	2.01	0.43
21:L:1502:CLA:HMA1	21:L:1503:CLA:HBC1	2.01	0.43
1:a:2:THR:HB	1:a:3:ILE:H	1.71	0.43
12:b:257:PHE:CD2	21:b:1214:CLA:HBB1	2.53	0.43
21:b:1022:CLA:H152	24:b:4017:BCR:H11C	1.99	0.43
21:b:1214:CLA:H41	21:b:1214:CLA:H62	1.67	0.43
21:b:1223:CLA:H122	24:b:4018:BCR:H373	2.00	0.43
4:d:77:LYS:HG3	4:d:78:PRO:HD2	2.01	0.43
21:f:1302:CLA:H93	21:f:1302:CLA:H62	1.84	0.43
7:i:10:LEU:HD12	7:i:10:LEU:HA	1.88	0.43
7:i:14:LEU:HD12	7:i:14:LEU:HA	1.87	0.43
8:j:28:GLU:HG3	21:j:1302:CLA:CHD	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:38:PRO:HG3	21:l:1502:CLA:HED2	2.00	0.43
10:l:44:LEU:HD12	10:l:44:LEU:HA	1.89	0.43
16:1:80:LEU:HA	16:1:80:LEU:HD23	1.73	0.43
16:1:342:GLU:OE1	16:1:342:GLU:N	2.43	0.43
2:2:376:ILE:O	2:2:380:LEU:HG	2.19	0.43
3:3:62:PHE:CE2	17:4:122:ILE:HG21	2.54	0.43
21:0:1502:CLA:HMA3	21:0:1503:CLA:HBC1	2.00	0.43
1:A:168:MET:O	1:A:172:MET:HG2	2.19	0.42
1:A:381:ILE:HD11	1:A:519:LYS:O	2.19	0.42
21:A:1801:CLA:C2D	25:A:5007:LHG:H241	2.49	0.42
2:B:462:GLN:HG2	2:B:506:PHE:CD1	2.54	0.42
2:B:653:VAL:HG22	21:B:1239:CLA:HMB2	2.00	0.42
8:J:18:LEU:O	8:J:18:LEU:HD12	2.18	0.42
21:L:1501:CLA:H42	7:i:21:LEU:HD21	2.01	0.42
37:L:5004:DGD:HAW1	37:L:5004:DGD:HB52	2.01	0.42
1:a:355:ASN:HB3	21:a:1123:CLA:O1A	2.19	0.42
1:a:381:ILE:HG23	1:a:519:LYS:HD2	2.01	0.42
1:a:709:VAL:HG22	6:f:84:ARG:HE	1.84	0.42
21:a:1124:CLA:H42	21:a:1136:CLA:HBA1	2.01	0.42
12:b:348:GLN:HG3	21:b:1222:CLA:HED1	1.99	0.42
21:b:1211:CLA:H13	21:b:1211:CLA:H193	2.00	0.42
21:b:1216:CLA:H93	21:b:1216:CLA:H111	1.77	0.42
4:d:31:THR:HA	4:d:55:ASN:O	2.19	0.42
21:k:1402:CLA:HAC2	24:k:4001:BCR:H332	2.01	0.42
10:l:150:GLY:HA2	10:l:155:LEU:HB2	2.01	0.42
16:1:364:ILE:HG23	16:1:394:MET:SD	2.59	0.42
16:1:433:ARG:HG3	16:1:555:TYR:CZ	2.54	0.42
25:1:5005:LHG:H202	21:8:1401:CLA:HBA1	2.00	0.42
25:1:5007:LHG:H172	25:1:5007:LHG:H141	1.88	0.42
21:1:1102:CLA:HMC2	21:1:1104:CLA:HED2	2.00	0.42
21:2:1217:CLA:H41	21:2:1217:CLA:H61	1.40	0.42
21:2:1238:CLA:H161	24:h:4018:BCR:H20C	2.01	0.42
1:A:551:LYS:HE3	2:B:667:TYR:CE1	2.54	0.42
21:B:1228:CLA:CAB	21:B:1229:CLA:H202	2.48	0.42
21:B:1235:CLA:H202	21:B:1235:CLA:H162	1.68	0.42
1:a:13:LYS:HG3	1:a:314:ASN:HD21	1.84	0.42
1:a:280:GLY:N	1:a:503:ALA:HB3	2.34	0.42
21:a:1129:CLA:HHC	21:a:1137:CLA:CBB	2.49	0.42
21:a:1136:CLA:HBB2	21:a:1137:CLA:HBC3	2.00	0.42
21:a:1140:CLA:H141	21:a:1140:CLA:H162	1.86	0.42
26:a:5002:LMG:H422	25:l:5004:LHG:H191	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:22:TRP:HE1	21:b:1238:CLA:CBB	2.23	0.42
12:b:342:ILE:HG12	21:b:1221:CLA:H43	2.01	0.42
12:b:518:HIS:HD2	34:j:4015:ZEX:H21	1.85	0.42
21:b:1226:CLA:HHC	21:b:1226:CLA:HBB1	2.00	0.42
21:b:1234:CLA:H11	21:b:1234:CLA:H51	1.89	0.42
21:j:1302:CLA:H122	21:j:1302:CLA:H162	1.80	0.42
16:1:561:LEU:HD23	16:1:561:LEU:HA	1.85	0.42
21:1:1119:CLA:H202	24:1:4007:BCR:H332	2.01	0.42
21:1:1136:CLA:HAB	21:1:1137:CLA:CHD	2.48	0.42
2:2:381:MET:HE1	24:2:4010:BCR:H361	2.01	0.42
2:2:656:THR:O	2:2:659:MET:HB3	2.20	0.42
1:A:17:ASP:OD2	1:A:70:ARG:NH2	2.38	0.42
1:A:313:THR:OG1	21:A:1118:CLA:HED2	2.18	0.42
21:A:1112:CLA:H193	21:A:1112:CLA:H162	1.85	0.42
2:B:163:PRO:HB2	2:B:168:PHE:CE2	2.54	0.42
21:a:1115:CLA:H92	21:a:1115:CLA:H62	1.91	0.42
24:a:4001:BCR:H272	15:k:72:PHE:CE2	2.54	0.42
12:b:557:ASP:OD2	12:b:561:ARG:NH2	2.41	0.42
12:b:681:ARG:HD2	10:l:19:HIS:CD2	2.55	0.42
21:b:1205:CLA:H62	21:b:1205:CLA:H102	1.56	0.42
21:b:1220:CLA:H192	24:b:4018:BCR:H312	2.02	0.42
21:b:1228:CLA:H193	21:b:1228:CLA:H52	2.01	0.42
26:b:5005:LMG:O8	26:b:5005:LMG:H122	2.19	0.42
21:1:1119:CLA:OBD	21:1:1121:CLA:HMD3	2.19	0.42
21:1:1125:CLA:HED1	21:1:1133:CLA:HAB	2.00	0.42
2:2:158:GLN:O	2:2:162:ARG:HG3	2.19	0.42
2:2:179:LEU:HD21	21:2:1216:CLA:C3B	2.49	0.42
2:2:324:ILE:HD12	21:2:1221:CLA:HMC2	2.01	0.42
2:2:461:ILE:O	2:2:464:THR:OG1	2.25	0.42
21:2:1210:CLA:HBC2	21:2:1210:CLA:HMC1	2.01	0.42
21:2:1239:CLA:H202	21:2:1239:CLA:H161	1.80	0.42
17:4:85:ILE:HB	17:4:98:HIS:HB3	2.01	0.42
21:0:1501:CLA:H202	21:0:1501:CLA:H161	1.77	0.42
1:A:666:SER:HB2	2:B:443:ALA:HB1	2.02	0.42
2:B:453:ILE:HD13	6:F:53:LEU:HB2	2.01	0.42
21:B:1213:CLA:HED2	21:B:1213:CLA:H2A	2.01	0.42
21:B:1219:CLA:H161	21:B:1219:CLA:H141	1.68	0.42
1:a:226:LEU:HD12	1:a:236:ILE:HG23	2.01	0.42
21:a:1011:CLA:HAA2	21:a:1011:CLA:O2D	2.19	0.42
21:a:1127:CLA:H102	21:a:1127:CLA:H62	1.64	0.42
21:a:1131:CLA:HMA1	24:i:4018:BCR:H292	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:5005:LHG:H171	2:2:137:SER:HB3	2.01	0.42
12:b:26:ALA:HA	21:b:1226:CLA:H42	2.01	0.42
12:b:118:SER:HB2	21:b:1225:CLA:HMA2	2.02	0.42
13:c:17:CYS:HB2	13:c:54:CYS:HB2	2.01	0.42
13:c:63:LEU:H	13:c:63:LEU:HG	1.59	0.42
31:f:5001:SQD:H242	31:f:5001:SQD:H462	1.67	0.42
16:1:658:ILE:HB	2:2:618:ARG:HB3	2.01	0.42
21:1:1124:CLA:H93	21:1:1124:CLA:H62	1.72	0.42
2:2:280:ILE:HD13	2:2:280:ILE:HA	1.81	0.42
2:2:420:LEU:HA	2:2:423:VAL:HG22	2.01	0.42
21:2:1202:CLA:H171	21:2:1202:CLA:HMD2	2.02	0.42
21:2:1203:CLA:H61	21:2:1203:CLA:H41	1.66	0.42
26:0:5001:LMG:H262	26:0:5001:LMG:H232	1.77	0.42
1:A:110:ILE:HG12	1:A:130:VAL:O	2.20	0.42
2:B:276:HIS:HB2	21:B:1214:CLA:CHB	2.49	0.42
28:B:4011:45D:H421	28:B:4011:45D:H401	1.94	0.42
21:B:1217:CLA:H141	21:B:1217:CLA:H161	1.83	0.42
21:B:1239:CLA:H112	21:B:1239:CLA:H91	1.64	0.42
6:F:107:LEU:O	6:F:111:LYS:HG2	2.19	0.42
1:a:677:PHE:HB2	21:a:1012:CLA:O1A	2.20	0.42
1:a:737:VAL:HG22	30:b:4011:ECH:H32B	2.02	0.42
25:a:5007:LHG:O10	25:a:5007:LHG:H271	2.20	0.42
12:b:120:VAL:HG13	12:b:124:PHE:CE2	2.55	0.42
12:b:435:TYR:CZ	12:b:515:LEU:HB3	2.55	0.42
12:b:655:ALA:O	12:b:658:PHE:HB2	2.19	0.42
21:b:1208:CLA:H61	21:b:1208:CLA:H41	1.42	0.42
8:j:21:PHE:CD1	21:j:1302:CLA:H152	2.54	0.42
16:1:114:ALA:HB1	38:1:8008:HOH:O	2.18	0.42
16:1:278:LYS:HD2	16:1:289:TRP:CG	2.54	0.42
21:1:1011:CLA:H203	21:2:1022:CLA:C1B	2.50	0.42
21:1:1115:CLA:H72	21:8:1401:CLA:HMD3	2.02	0.42
2:2:701:GLN:HG3	26:2:5002:LMG:H122	2.01	0.42
21:2:1201:CLA:O1A	11:9:30:TYR:HB2	2.19	0.42
21:2:1204:CLA:HHB	21:2:1205:CLA:HHB	2.02	0.42
21:2:1221:CLA:H161	21:2:1221:CLA:H141	1.76	0.42
1:A:74:SER:HB3	21:A:1109:CLA:HHD	2.01	0.42
1:A:429:MET:SD	21:A:1129:CLA:HBC3	2.59	0.42
21:A:1103:CLA:H111	24:A:4003:BCR:H372	2.01	0.42
21:A:1134:CLA:O1A	21:K:1401:CLA:H51	2.19	0.42
21:A:1101:CLA:H8	21:A:1101:CLA:H52	1.84	0.42
21:B:1203:CLA:H143	21:B:1203:CLA:H162	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1204:CLA:HED2	7:I:11:PRO:HB3	2.00	0.42
9:K:53:PRO:CG	24:K:4001:BCR:H282	2.47	0.42
1:a:215:HIS:CD2	1:a:219:VAL:HB	2.55	0.42
1:a:584:GLN:HG2	1:a:724:ARG:NH1	2.35	0.42
21:a:1101:CLA:H41	21:a:1101:CLA:H61	1.68	0.42
12:b:372:HIS:HB2	21:b:1224:CLA:C1B	2.50	0.42
21:b:1214:CLA:O1D	21:b:1215:CLA:HHB	2.20	0.42
21:b:1223:CLA:H62	21:b:1223:CLA:H41	1.84	0.42
16:1:89:GLY:HA3	21:1:1105:CLA:HBB1	2.01	0.42
21:1:1115:CLA:CHD	21:1:1116:CLA:HBB2	2.50	0.42
21:1:1123:CLA:H51	21:1:1123:CLA:HBD	2.01	0.42
2:2:163:PRO:HB2	2:2:168:PHE:CE2	2.55	0.42
21:2:1236:CLA:H43	24:2:4010:BCR:H12C	2.00	0.42
1:A:185:PRO:HG2	1:A:190:PHE:CZ	2.55	0.42
21:A:1013:CLA:HMA2	21:A:1013:CLA:C2	2.49	0.42
21:A:1131:CLA:HMA1	24:I:4018:BCR:H292	2.00	0.42
21:A:1138:CLA:H141	21:A:1138:CLA:H162	1.84	0.42
21:A:1138:CLA:HED2	2:B:418:SER:O	2.20	0.42
21:K:1401:CLA:HBB1	21:K:1401:CLA:HMB1	2.00	0.42
1:a:439:HIS:O	1:a:443:VAL:HG23	2.20	0.42
1:a:598:MET:CG	21:a:1124:CLA:HBC1	2.49	0.42
1:a:687:PHE:HB2	21:a:1013:CLA:HBC2	2.02	0.42
21:a:1133:CLA:H111	21:a:1133:CLA:H91	1.65	0.42
12:b:387:HIS:HA	12:b:390:ILE:HD12	2.01	0.42
12:b:491:LEU:HA	12:b:491:LEU:HD12	1.81	0.42
13:c:66:ARG:HD3	13:c:66:ARG:HA	1.95	0.42
21:1:1126:CLA:H111	21:1:1126:CLA:H143	1.79	0.42
1:A:249:MET:O	1:A:253:TYR:N	2.45	0.42
1:A:269:GLY:N	9:K:13:PRO:HG3	2.29	0.42
21:A:1113:CLA:H62	21:A:1113:CLA:H102	1.43	0.42
2:B:484:SER:HA	2:B:491:LEU:HD21	2.01	0.42
21:B:1234:CLA:H18	25:B:5004:LHG:H312	2.01	0.42
1:a:77:PHE:HE1	21:a:1108:CLA:HBB1	1.83	0.42
1:a:392:HIS:HB2	21:a:1126:CLA:CHB	2.49	0.42
1:a:720:ILE:O	1:a:724:ARG:HG3	2.19	0.42
21:a:1139:CLA:H61	21:a:1139:CLA:H41	1.83	0.42
21:b:1216:CLA:H12	21:b:1221:CLA:CBB	2.50	0.42
21:b:1225:CLA:H61	21:b:1225:CLA:H41	1.83	0.42
25:l:5001:LHG:H132	18:h:30:LEU:HD21	2.00	0.42
25:l:5002:LHG:H112	11:9:23:PHE:CE1	2.53	0.42
16:1:668:TYR:OH	16:1:744:LEU:HD23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:379:PHE:HZ	2:2:711:THR:HG21	1.83	0.42
1:A:207:LEU:HD21	21:A:1118:CLA:HMC3	2.02	0.42
21:A:1108:CLA:H12	21:A:1110:CLA:C3D	2.50	0.42
21:A:1124:CLA:HAB	24:A:4008:BCR:H311	2.01	0.42
25:A:5005:LHG:H372	25:L:5005:LHG:H222	2.02	0.42
2:B:180:ALA:HB1	21:B:1217:CLA:HAC2	2.01	0.42
2:B:441:VAL:HG13	2:B:446:THR:O	2.19	0.42
5:E:61:PHE:HB2	5:E:66:LEU:HD21	2.01	0.42
6:F:118:TRP:CG	6:F:119:PRO:HD3	2.55	0.42
34:F:4016:ZEX:H401	34:F:4016:ZEX:H31	1.81	0.42
9:K:22:VAL:O	9:K:26:MET:N	2.53	0.42
1:a:125:ILE:HG21	12:b:444:PHE:HA	2.02	0.42
1:a:274:PHE:HE1	21:a:1113:CLA:HAC2	1.84	0.42
1:a:487:GLN:O	1:a:491:THR:HG23	2.20	0.42
21:a:1117:CLA:CAB	21:a:1117:CLA:H62	2.50	0.42
21:b:1222:CLA:H161	21:b:1222:CLA:H141	1.84	0.42
21:b:1226:CLA:H122	26:b:5002:LMG:H412	2.01	0.42
15:k:12:SER:HA	15:k:13:PRO:HD3	1.92	0.42
16:1:394:MET:HE3	16:1:602:LEU:HD22	2.02	0.42
16:1:447:LEU:HB3	16:1:540:PHE:HB2	2.01	0.42
21:1:1102:CLA:H61	21:1:1102:CLA:H2	1.76	0.42
21:2:1202:CLA:H142	21:2:1202:CLA:H111	1.76	0.42
21:2:1211:CLA:CBB	21:2:1225:CLA:H121	2.50	0.42
17:4:27:LYS:HD3	17:4:58:TYR:HB3	2.02	0.42
18:h:10:LEU:HD12	18:h:10:LEU:HA	1.88	0.42
21:0:1503:CLA:H41	21:0:1503:CLA:H62	1.43	0.42
21:A:1011:CLA:HBA2	21:A:1011:CLA:H3A	1.70	0.42
21:A:1131:CLA:H93	21:A:1131:CLA:H112	1.86	0.42
21:A:1137:CLA:C12	24:A:4007:BCR:H23C	2.46	0.42
24:A:4001:BCR:C23	9:K:72:PHE:HB2	2.49	0.42
2:B:225:PHE:HB2	2:B:233:TYR:CE2	2.55	0.42
2:B:609:ASN:O	2:B:615:GLY:HA3	2.20	0.42
21:B:1234:CLA:H142	21:B:1234:CLA:H112	1.71	0.42
9:K:34:PHE:CE2	9:K:70:MET:HE3	2.55	0.42
9:K:58:LYS:H	9:K:58:LYS:HD2	1.83	0.42
1:a:718:LEU:HD11	21:a:1140:CLA:HMD2	2.02	0.42
21:a:1109:CLA:H93	21:a:1101:CLA:CBB	2.49	0.42
21:b:1211:CLA:H142	30:b:4006:ECH:C12	2.50	0.42
21:l:1502:CLA:H91	21:l:1502:CLA:H112	1.81	0.42
16:1:219:VAL:HG13	16:1:239:PRO:HB3	2.02	0.42
16:1:325:LEU:O	16:1:337:HIS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:429:MET:HA	16:1:432:HIS:CE1	2.55	0.42
16:1:561:LEU:O	17:4:61:ARG:NH2	2.52	0.42
2:2:269:TRP:O	2:2:273:ILE:HG13	2.19	0.42
2:2:420:LEU:HG	21:2:1236:CLA:CBB	2.50	0.42
21:2:1023:CLA:H192	24:2:4017:BCR:H353	2.02	0.42
31:0:5005:SQD:H301	31:0:5005:SQD:H331	1.74	0.42
1:A:332:PHE:CE2	21:A:1801:CLA:HED2	2.55	0.41
1:A:431:ARG:HD2	4:D:13:GLY:O	2.20	0.41
1:A:459:ASP:OD1	1:A:641:THR:HB	2.19	0.41
2:B:154:TRP:CD1	11:M:28:GLU:HG3	2.55	0.41
2:B:580:MET:HG3	21:B:1222:CLA:HBC1	2.02	0.41
21:B:1201:CLA:O1A	11:M:30:TYR:HB2	2.19	0.41
21:B:1221:CLA:HMA2	21:B:1221:CLA:H2	2.01	0.41
21:B:1227:CLA:HBC2	24:B:4018:BCR:H383	2.01	0.41
21:B:1235:CLA:H41	21:B:1235:CLA:H62	1.61	0.41
21:B:1230:CLA:HBA2	21:B:1230:CLA:H3A	1.91	0.41
3:C:18:VAL:HG11	4:D:105:PRO:C	2.45	0.41
6:F:36:ARG:NH1	8:J:35:ASP:OD2	2.53	0.41
10:L:38:PRO:HG2	21:L:1502:CLA:HED2	2.02	0.41
21:a:1140:CLA:H142	21:a:1140:CLA:H112	1.75	0.41
12:b:653:VAL:HG22	21:b:1239:CLA:HMB2	2.01	0.41
21:b:1203:CLA:C16	21:b:1225:CLA:HBB2	2.41	0.41
21:b:1205:CLA:H143	21:b:1205:CLA:H161	1.73	0.41
21:b:1217:CLA:H3A	21:b:1217:CLA:HBA2	1.33	0.41
15:k:13:PRO:C	15:k:15:THR:H	2.27	0.41
25:l:5001:LHG:H211	21:2:1201:CLA:H142	2.01	0.41
21:1:1102:CLA:HBD	21:1:1109:CLA:H2	2.01	0.41
21:1:1127:CLA:H102	21:1:1127:CLA:H62	1.72	0.41
2:2:291:TYR:CE1	21:2:1216:CLA:HED1	2.55	0.41
2:2:583:THR:O	2:2:587:LEU:HD13	2.20	0.41
21:2:1208:CLA:H61	21:2:1208:CLA:H41	1.67	0.41
17:4:33:THR:HA	17:4:53:GLY:O	2.20	0.41
8:7:10:THR:O	8:7:14:MET:HG2	2.20	0.41
1:A:708:ASN:O	6:F:88:ILE:HD11	2.20	0.41
21:A:1107:CLA:H112	21:A:1107:CLA:H151	1.70	0.41
25:A:5006:LHG:H121	25:A:5006:LHG:HC91	1.91	0.41
2:B:474:VAL:HG12	2:B:475:LEU:HG	2.02	0.41
2:B:589:PHE:HE2	21:B:1021:CLA:H61	1.86	0.41
21:B:1227:CLA:H3A	21:B:1227:CLA:HBA1	1.70	0.41
1:a:340:LEU:HD12	1:a:343:ILE:HD11	2.02	0.41
1:a:530:ALA:O	1:a:534:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:498:ILE:HG13	12:b:505:LEU:HG	2.02	0.41
21:b:1237:CLA:H62	21:b:1237:CLA:H41	1.36	0.41
21:b:1207:CLA:H42	10:l:84:GLY:HA2	2.02	0.41
30:b:4006:ECH:H35	30:b:4006:ECH:H15	1.84	0.41
7:i:28:GLY:O	7:i:32:ILE:HG13	2.20	0.41
15:k:52:LEU:HB3	15:k:53:PRO:HD2	2.02	0.41
10:l:99:TYR:CZ	10:l:103:THR:HG21	2.55	0.41
16:1:510:GLY:HA2	16:1:524:PRO:HG3	2.01	0.41
21:1:1101:CLA:HBA2	21:1:1101:CLA:CBD	2.45	0.41
2:2:422:TRP:CD1	21:2:1229:CLA:HED2	2.55	0.41
2:2:675:ILE:HD13	21:2:1237:CLA:HMD1	2.01	0.41
26:2:5005:LMG:HC92	26:2:5005:LMG:H321	2.01	0.41
3:3:62:PHE:HZ	3:3:66:ARG:HH21	1.68	0.41
17:4:31:THR:O	17:4:83:TYR:HA	2.21	0.41
8:7:33:TYR:CD1	34:7:4015:ZEX:H361	2.55	0.41
20:0:118:ASP:OD2	38:0:8001:HOH:O	2.22	0.41
1:A:381:ILE:HG13	1:A:519:LYS:HB2	2.01	0.41
21:A:1110:CLA:H93	21:A:1110:CLA:H61	1.70	0.41
21:A:1115:CLA:H51	21:A:1115:CLA:H11	1.90	0.41
21:A:1133:CLA:H62	21:A:1133:CLA:H41	1.50	0.41
21:B:1237:CLA:H62	21:B:1237:CLA:H41	1.46	0.41
31:B:5008:SQD:H371	31:B:5008:SQD:H341	1.92	0.41
1:a:79:HIS:HD2	21:a:1103:CLA:HMB3	1.84	0.41
1:a:412:MET:O	1:a:557:ARG:HD3	2.21	0.41
1:a:459:ASP:OD1	1:a:641:THR:HB	2.20	0.41
21:b:1209:CLA:HBA2	21:b:1209:CLA:H3A	1.46	0.41
21:b:1222:CLA:H92	21:b:1222:CLA:H61	1.77	0.41
16:1:74:SER:HB2	21:1:1109:CLA:HHD	2.01	0.41
16:1:221:MET:HE1	16:1:274:PHE:HB2	2.02	0.41
1:A:90:MET:HE1	21:A:1106:CLA:HMA2	2.01	0.41
1:A:304:PHE:CE1	21:A:1119:CLA:HAB	2.55	0.41
21:A:1011:CLA:CBB	21:B:1021:CLA:HAA1	2.51	0.41
21:A:1104:CLA:HMA2	21:A:1128:CLA:C3B	2.50	0.41
21:A:1135:CLA:H202	21:A:1137:CLA:H92	2.02	0.41
21:A:1139:CLA:H101	8:J:14:MET:HE3	2.02	0.41
2:B:397:ASP:OD1	2:B:399:VAL:HG22	2.21	0.41
2:B:591:TRP:CD1	21:B:1234:CLA:HBC2	2.55	0.41
21:B:1210:CLA:H92	21:B:1210:CLA:H61	1.75	0.41
21:B:1213:CLA:H203	21:B:1213:CLA:H162	1.73	0.41
21:B:1234:CLA:H201	25:B:5004:LHG:H281	2.03	0.41
7:I:22:PHE:CE1	7:I:26:THR:HG21	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:86:TRP:CD1	21:a:1104:CLA:HBC1	2.55	0.41
1:a:707:LEU:HD13	24:f:4016:BCR:H321	2.01	0.41
21:a:1011:CLA:HBA2	21:a:1011:CLA:H3A	1.71	0.41
21:a:1126:CLA:O1D	21:a:1127:CLA:HHB	2.20	0.41
21:a:1131:CLA:H141	21:a:1131:CLA:H162	1.74	0.41
26:a:5002:LMG:H161	21:a:1132:CLA:HMB3	2.02	0.41
21:b:1203:CLA:HBA1	21:b:1226:CLA:HMB1	2.02	0.41
21:b:1222:CLA:CMA	24:b:4010:BCR:H14C	2.51	0.41
21:b:1235:CLA:C4A	21:b:1235:CLA:HBA2	2.50	0.41
24:b:4010:BCR:H24C	24:b:4010:BCR:H21C	1.91	0.41
10:l:45:SER:O	10:l:49:ARG:HG3	2.21	0.41
21:1:1013:CLA:HBA1	2:2:425:LEU:HD12	2.02	0.41
21:1:1131:CLA:H101	21:1:1131:CLA:H62	1.76	0.41
21:2:1205:CLA:H92	24:2:4017:BCR:H342	2.01	0.41
5:5:33:ILE:HG22	5:5:35:TYR:H	1.86	0.41
21:A:1013:CLA:H3A	21:A:1013:CLA:CGA	2.51	0.41
2:B:101:VAL:HG22	7:I:1:MET:HE2	2.02	0.41
2:B:290:MET:HA	21:B:1218:CLA:HHD	2.02	0.41
21:B:1207:CLA:HBB1	21:B:1207:CLA:HHC	2.01	0.41
5:E:43:ARG:NH1	38:E:8008:HOH:O	2.53	0.41
11:M:3:LEU:HD12	11:M:3:LEU:HA	1.85	0.41
11:M:20:PHE:CE2	11:M:24:ARG:HD2	2.55	0.41
21:a:1132:CLA:C9	21:l:1503:CLA:HAB	2.51	0.41
12:b:704:LEU:HD23	26:b:5002:LMG:H121	2.02	0.41
4:d:40:PHE:HB3	4:d:76:PHE:HZ	1.85	0.41
6:f:96:PRO:O	6:f:100:GLU:HG3	2.20	0.41
34:j:4015:ZEX:H11	34:j:4015:ZEX:H191	1.93	0.41
25:l:5002:LHG:H182	18:h:26:THR:HG23	2.03	0.41
16:1:395:TRP:HZ3	16:1:599:TYR:HA	1.85	0.41
16:1:461:MET:HE3	16:1:469:ASP:HB3	2.02	0.41
21:1:1134:CLA:H41	21:1:1134:CLA:H102	2.03	0.41
17:4:105:PRO:HA	17:4:112:ARG:HH12	1.85	0.41
20:0:82:LEU:O	20:0:86:LEU:HG	2.20	0.41
25:0:5004:LHG:H262	35:0:6001:LMT:H42	2.01	0.41
1:A:59:ASP:OD2	1:A:349:HIS:NE2	2.42	0.41
1:A:332:PHE:CD1	10:L:7:VAL:HG11	2.54	0.41
1:A:680:ALA:HB3	21:A:1013:CLA:HBB2	2.03	0.41
1:A:687:PHE:HB2	21:A:1013:CLA:HBC2	2.02	0.41
21:A:1105:CLA:H151	21:A:1105:CLA:H112	1.58	0.41
21:A:1115:CLA:H142	21:A:1115:CLA:H112	1.79	0.41
21:A:1801:CLA:H122	21:A:1801:CLA:H8	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1230:CLA:HED2	21:B:1230:CLA:H2A	2.01	0.41
1:a:203:GLY:O	1:a:207:LEU:HB2	2.19	0.41
21:a:1119:CLA:H41	21:a:1119:CLA:H62	1.84	0.41
21:a:1135:CLA:H111	21:a:1135:CLA:H142	1.74	0.41
25:a:5003:LHG:H291	25:a:5003:LHG:H322	1.57	0.41
21:a:1132:CLA:H61	21:a:1132:CLA:H92	1.83	0.41
12:b:589:PHE:CE2	21:b:1021:CLA:H61	2.55	0.41
21:b:1237:CLA:HHD	24:b:4017:BCR:H383	2.01	0.41
15:k:47:GLY:HA3	15:k:64:PRO:HG3	2.01	0.41
10:l:134:GLY:HA2	10:l:137:VAL:HG12	2.02	0.41
16:1:289:TRP:HB2	16:1:292:ASP:OD2	2.21	0.41
21:1:1120:CLA:HMD1	24:1:4001:BCR:H24C	2.01	0.41
21:2:1204:CLA:H161	21:2:1204:CLA:H143	1.79	0.41
21:2:1227:CLA:CBB	25:2:5004:LHG:H311	2.51	0.41
17:4:42:MET:HE2	17:4:48:ALA:HB2	2.03	0.41
19:8:58:LYS:H	19:8:58:LYS:HG2	1.50	0.41
1:A:315:TRP:NE1	9:K:48:LYS:HB2	2.36	0.41
21:A:1103:CLA:HBA1	21:A:1103:CLA:H3A	1.52	0.41
21:A:1109:CLA:H93	21:A:1101:CLA:CBB	2.51	0.41
21:A:1113:CLA:H41	21:A:1113:CLA:H61	1.53	0.41
2:B:289:HIS:NE2	24:B:4004:BCR:H363	2.35	0.41
4:D:30:ILE:HA	4:D:84:LYS:O	2.20	0.41
4:D:85:ILE:HB	4:D:98:HIS:HB3	2.02	0.41
6:F:110:LYS:HE2	6:F:110:LYS:HB3	1.89	0.41
9:K:80:MET:CE	26:K:5009:LMG:H222	2.51	0.41
1:a:83:VAL:HG12	21:a:1103:CLA:H92	2.02	0.41
1:a:588:TRP:NE1	21:a:1128:CLA:HMD3	2.36	0.41
21:a:1116:CLA:HBA2	21:a:1116:CLA:H3A	1.60	0.41
21:a:1125:CLA:CED	21:a:1133:CLA:HAB	2.40	0.41
21:a:1135:CLA:H203	21:a:1135:CLA:H162	1.75	0.41
24:a:4001:BCR:H23C	24:a:4001:BCR:H383	2.01	0.41
12:b:346:VAL:O	12:b:350:MET:HG3	2.21	0.41
21:b:1239:CLA:H202	21:b:1239:CLA:H161	1.83	0.41
4:d:77:LYS:H	4:d:77:LYS:HG2	1.29	0.41
15:k:18:TRP:CG	15:k:19:SER:H	2.39	0.41
16:1:80:LEU:HD13	21:1:1111:CLA:H52	2.01	0.41
16:1:540:PHE:O	16:1:544:VAL:HG23	2.21	0.41
21:1:1129:CLA:HBB2	21:1:1137:CLA:CMC	2.51	0.41
21:1:1139:CLA:H152	21:1:1139:CLA:H111	1.57	0.41
24:1:4012:BCR:H362	21:1:1012:CLA:H191	2.02	0.41
19:8:63:LEU:N	19:8:64:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1011:CLA:H102	21:A:1011:CLA:H62	1.68	0.41
21:A:1013:CLA:H91	21:A:1013:CLA:H111	1.67	0.41
21:A:1105:CLA:O1A	21:A:1107:CLA:HBA2	2.20	0.41
21:A:1135:CLA:H141	21:A:1135:CLA:H161	1.81	0.41
21:A:1801:CLA:H62	21:A:1801:CLA:H2	1.83	0.41
21:B:1213:CLA:CGA	21:B:1213:CLA:C1A	2.99	0.41
21:B:1216:CLA:HAA2	21:B:1220:CLA:OBD	2.21	0.41
21:B:1226:CLA:H193	21:B:1226:CLA:H161	1.81	0.41
6:F:99:GLN:HA	6:F:102:VAL:O	2.21	0.41
9:K:25:ILE:HD13	26:K:5009:LMG:H221	2.02	0.41
21:a:1125:CLA:H151	21:a:1133:CLA:H121	2.02	0.41
21:b:1211:CLA:H141	21:b:1211:CLA:H161	1.80	0.41
7:i:31:PHE:HB2	24:l:4019:BCR:H14C	2.03	0.41
11:m:15:ALA:C	11:m:18:PRO:HD2	2.46	0.41
16:1:364:ILE:HG13	16:1:397:GLY:HA3	2.03	0.41
16:1:381:ILE:HG23	16:1:519:LYS:HE3	2.02	0.41
16:1:520:VAL:HG12	16:1:619:GLY:O	2.21	0.41
16:1:565:LYS:HE2	16:1:585:VAL:HG13	2.03	0.41
16:1:676:HIS:HB3	21:1:1012:CLA:HBD	2.01	0.41
21:1:1013:CLA:H11	2:2:429:PHE:N	2.35	0.41
21:1:1123:CLA:CBB	24:1:4007:BCR:H341	2.51	0.41
21:1:1126:CLA:H62	21:1:1126:CLA:H93	1.87	0.41
24:1:4002:BCR:H291	21:8:1402:CLA:HMC3	2.01	0.41
21:1:1012:CLA:H11	2:2:613:LEU:HD12	2.03	0.41
2:2:171:ALA:HA	21:2:1221:CLA:HMD3	2.03	0.41
2:2:316:GLY:O	2:2:405:VAL:HG22	2.21	0.41
24:2:4011:BCR:H23C	21:2:1230:CLA:HMC1	2.02	0.41
1:A:88:SER:HB3	1:A:165:GLY:HA3	2.03	0.41
1:A:428:ARG:NH2	38:A:8001:HOH:O	2.19	0.41
1:A:429:MET:HE2	1:A:436:ILE:HD11	2.03	0.41
1:A:694:GLN:O	1:A:698:GLU:HG3	2.20	0.41
1:A:703:ALA:HB2	2:B:418:SER:OG	2.21	0.41
21:A:1120:CLA:H121	21:A:1120:CLA:H161	1.89	0.41
21:A:1136:CLA:H193	21:A:1136:CLA:H162	1.63	0.41
21:A:1140:CLA:H171	21:A:1101:CLA:H203	2.03	0.41
21:A:1801:CLA:HBA1	21:A:1801:CLA:H3A	1.75	0.41
2:B:265:THR:HB	2:B:357:ALA:HA	2.03	0.41
2:B:642:VAL:HG21	21:B:1205:CLA:HAC1	2.03	0.41
21:B:1023:CLA:H143	24:B:4017:BCR:H362	2.01	0.41
21:B:1209:CLA:H3A	21:B:1209:CLA:HBA2	1.41	0.41
21:B:1223:CLA:H121	24:B:4018:BCR:C20	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1236:CLA:H12	24:B:4010:BCR:C14	2.50	0.41
21:B:1240:CLA:HED3	21:B:1240:CLA:H101	2.02	0.41
3:C:31:TRP:CG	3:C:32:ASP:H	2.39	0.41
6:F:90:ILE:HG23	6:F:99:GLN:HB2	2.03	0.41
9:K:67:LEU:HD12	9:K:67:LEU:HA	1.93	0.41
21:K:1401:CLA:H203	21:K:1401:CLA:H161	1.84	0.41
10:L:99:TYR:CZ	10:L:103:THR:HG21	2.55	0.41
11:M:4:SER:O	11:M:8:ILE:HG12	2.21	0.41
1:a:56:HIS:CE1	21:a:1103:CLA:HBB2	2.56	0.41
21:a:1109:CLA:HMB1	21:a:1109:CLA:HBB1	2.03	0.41
21:a:1123:CLA:CAD	21:a:1123:CLA:H71	2.51	0.41
21:a:1140:CLA:H93	21:a:1140:CLA:H61	1.86	0.41
24:a:4008:BCR:H393	24:a:4008:BCR:H281	1.88	0.41
12:b:46:ILE:HG21	21:b:1202:CLA:H202	2.02	0.41
12:b:59:LEU:HD12	30:m:4021:ECH:H37A	2.02	0.41
12:b:183:PHE:CZ	21:b:1210:CLA:H61	2.56	0.41
12:b:305:LEU:O	12:b:317:HIS:HB2	2.20	0.41
12:b:310:GLY:HA3	25:b:5004:LHG:O4	2.21	0.41
21:b:1210:CLA:H191	21:b:1225:CLA:H2	2.03	0.41
21:b:1217:CLA:C3B	21:b:1217:CLA:H42	2.51	0.41
21:b:1221:CLA:H161	21:b:1221:CLA:H203	1.73	0.41
21:b:1232:CLA:H192	21:b:1232:CLA:H162	1.75	0.41
21:b:1240:CLA:H71	21:b:1240:CLA:H111	1.83	0.41
21:b:1201:CLA:O1A	11:m:30:TYR:HB2	2.20	0.41
6:f:13:ASN:O	6:f:17:LEU:HG	2.21	0.41
6:f:36:ARG:HD2	6:f:40:TYR:CE2	2.56	0.41
21:l:1503:CLA:HBA1	21:l:1503:CLA:H3A	1.82	0.41
16:1:100:TYR:OH	16:1:152:PHE:O	2.31	0.41
16:1:418:PRO:HG3	17:4:41:GLU:HB2	2.02	0.41
16:1:514:ILE:HG22	16:1:521:ALA:HB3	2.02	0.41
16:1:583:CYS:HB2	2:2:664:TRP:HB3	2.03	0.41
21:1:1103:CLA:H3A	21:1:1103:CLA:HBA1	1.42	0.41
2:2:123:TRP:CZ2	21:2:1210:CLA:H201	2.56	0.41
2:2:182:LEU:HD11	21:2:1210:CLA:H43	2.03	0.41
2:2:375:TYR:HA	2:2:584:LEU:CD1	2.51	0.41
2:2:388:GLY:HA2	24:2:4010:BCR:H393	2.03	0.41
21:2:1202:CLA:H2	21:2:1202:CLA:H61	1.82	0.41
21:2:1218:CLA:H141	21:2:1218:CLA:H162	1.81	0.41
21:2:1218:CLA:H193	21:2:1218:CLA:H161	1.93	0.41
18:h:7:ALA:HA	18:h:9:TYR:CE2	2.56	0.41
21:A:1106:CLA:H141	21:A:1106:CLA:H162	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1135:CLA:H142	21:A:1135:CLA:H112	1.92	0.41
2:B:195:VAL:HG21	21:B:1212:CLA:HBC2	2.03	0.41
21:B:1220:CLA:H92	21:B:1220:CLA:H61	1.84	0.41
21:B:1228:CLA:HAB	21:B:1229:CLA:H202	2.03	0.41
7:I:38:GLY:N	38:I:8002:HOH:O	2.54	0.41
24:I:4018:BCR:H343	26:0:5001:LMG:H273	2.02	0.41
1:a:129:ASP:N	1:a:129:ASP:OD1	2.51	0.41
1:a:441:ASN:ND2	21:b:1023:CLA:HED2	2.36	0.41
1:a:674:ALA:HB1	30:b:4011:ECH:C15	2.51	0.41
1:a:721:ILE:HG22	25:a:5001:LHG:HC41	2.03	0.41
21:a:1119:CLA:H52	21:a:1119:CLA:H8	1.91	0.41
21:a:1122:CLA:H141	25:a:5003:LHG:H172	2.02	0.41
21:b:1219:CLA:H41	21:b:1219:CLA:H61	1.53	0.41
21:b:1222:CLA:H13	21:b:1232:CLA:HBB2	2.02	0.41
21:b:1222:CLA:H143	21:b:1222:CLA:H112	1.61	0.41
21:f:1302:CLA:H203	21:f:1302:CLA:H162	1.70	0.41
8:j:21:PHE:CZ	8:j:25:ILE:HD11	2.55	0.41
21:j:1302:CLA:H122	21:j:1302:CLA:H202	2.03	0.41
16:1:120:ILE:O	16:1:122:GLY:N	2.54	0.41
16:1:370:MET:HE1	21:1:1127:CLA:O1D	2.21	0.41
16:1:680:ALA:HB2	21:1:1012:CLA:C3D	2.51	0.41
16:1:702:TRP:HH2	21:2:1228:CLA:HED1	1.86	0.41
16:1:704:HIS:NE2	21:1:1139:CLA:HAC1	2.36	0.41
16:1:707:LEU:HG	21:2:1228:CLA:HMA2	2.03	0.41
16:1:718:LEU:HD22	16:1:722:GLN:NE2	2.36	0.41
25:1:5007:LHG:H242	21:1:1801:CLA:HBC2	2.02	0.41
2:2:605:GLN:OE1	2:2:619:ASP:HB3	2.21	0.41
26:2:5005:LMG:H352	26:2:5005:LMG:H322	1.78	0.41
19:8:87:SER:HB2	21:8:1401:CLA:H2A	2.02	0.41
21:0:1503:CLA:H92	21:0:1503:CLA:H61	1.87	0.41
1:A:244:LEU:O	1:A:246:PRO:HD3	2.20	0.40
21:A:1137:CLA:C1C	25:A:5003:LHG:H162	2.51	0.40
2:B:426:PHE:HD1	2:B:430:HIS:CE1	2.39	0.40
21:B:1225:CLA:ND	24:B:4005:BCR:H282	2.36	0.40
25:B:5004:LHG:H351	25:B:5004:LHG:H321	1.63	0.40
1:a:345:THR:HG23	1:a:346:THR:HG23	2.03	0.40
26:a:5002:LMG:H291	26:a:5002:LMG:H322	1.89	0.40
21:b:1022:CLA:H122	24:b:4017:BCR:H11C	2.03	0.40
30:b:4011:ECH:H23	21:b:1230:CLA:HMC1	2.03	0.40
21:b:1213:CLA:H61	21:b:1213:CLA:H41	1.83	0.40
15:k:59:LYS:HE2	15:k:63:LEU:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:91:TYR:CE2	24:1:4002:BCR:HC42	2.56	0.40
16:1:311:TYR:HA	16:1:319:HIS:H	1.85	0.40
16:1:312:ARG:NH1	19:8:43:LYS:HE2	2.35	0.40
16:1:358:LEU:HD12	21:1:1125:CLA:H62	2.02	0.40
21:1:1113:CLA:C3B	24:1:4001:BCR:H333	2.52	0.40
21:1:1124:CLA:H12	21:1:1135:CLA:HMA3	2.03	0.40
22:1:2001:PQN:H302	22:1:2001:PQN:H262	1.89	0.40
2:2:257:PHE:CE2	21:2:1214:CLA:HBB1	2.56	0.40
21:2:1215:CLA:H13	21:2:1221:CLA:H172	2.03	0.40
21:6:1301:CLA:C3B	8:7:22:THR:HG21	2.51	0.40
25:0:5002:LHG:H181	25:0:5002:LHG:H152	1.79	0.40
21:A:1118:CLA:H112	26:A:5008:LMG:H441	2.03	0.40
21:A:1124:CLA:H52	21:A:1133:CLA:HBB2	2.03	0.40
21:A:1128:CLA:H142	21:A:1128:CLA:H111	1.84	0.40
21:B:1209:CLA:H71	21:B:1217:CLA:O1A	2.21	0.40
3:C:10:THR:HG23	4:D:121:ARG:HG2	2.03	0.40
21:a:1109:CLA:H62	21:a:1109:CLA:H41	1.92	0.40
21:a:1118:CLA:H93	21:a:1118:CLA:H62	1.88	0.40
21:a:1128:CLA:H41	21:a:1128:CLA:H61	1.69	0.40
12:b:230:TRP:CH2	26:b:5005:LMG:H401	2.56	0.40
21:b:1204:CLA:HMA1	21:b:1205:CLA:CHB	2.50	0.40
21:b:1207:CLA:H91	21:b:1207:CLA:H111	1.83	0.40
21:b:1213:CLA:H52	21:b:1213:CLA:C1C	2.51	0.40
21:b:1223:CLA:H112	21:b:1223:CLA:H72	1.91	0.40
21:b:1235:CLA:H62	21:b:1235:CLA:H41	1.61	0.40
21:b:1235:CLA:HBC2	34:j:4015:ZEX:H7	2.02	0.40
21:b:1230:CLA:HBA2	21:b:1230:CLA:H3A	1.84	0.40
16:1:278:LYS:HA	16:1:502:LEU:HD12	2.03	0.40
21:1:1101:CLA:H141	21:1:1101:CLA:H162	1.88	0.40
2:2:408:ARG:HA	2:2:411:GLU:HB2	2.04	0.40
21:2:1237:CLA:H111	21:2:1237:CLA:H91	1.83	0.40
24:2:4018:BCR:H23C	24:2:4018:BCR:H20C	1.90	0.40
5:5:4:ASN:N	5:5:7:ASP:OD2	2.36	0.40
24:7:4013:BCR:H352	21:7:1302:CLA:HMC2	2.03	0.40
11:9:13:VAL:HG23	38:9:8001:HOH:O	2.22	0.40
1:A:171:LEU:HD11	21:A:1114:CLA:H143	2.02	0.40
1:A:482:PHE:O	1:A:486:VAL:HG23	2.21	0.40
1:A:588:TRP:NE1	21:A:1128:CLA:HMD3	2.36	0.40
21:A:1128:CLA:H61	21:A:1128:CLA:H41	1.49	0.40
25:A:5005:LHG:H192	25:A:5005:LHG:H162	1.83	0.40
2:B:276:HIS:HD2	2:B:277:HIS:CE1	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1206:CLA:H111	24:I:4018:BCR:H341	2.02	0.40
21:B:1234:CLA:HBB1	21:B:1234:CLA:HMB1	2.03	0.40
3:C:11:CYS:SG	23:C:3003:SF4:S2	3.14	0.40
1:a:59:ASP:HB2	1:a:414:ARG:HH11	1.85	0.40
21:a:1126:CLA:H142	21:a:1126:CLA:H111	1.75	0.40
12:b:211:ASN:O	12:b:215:THR:HG22	2.21	0.40
12:b:336:LEU:HD21	21:b:1226:CLA:CBB	2.51	0.40
12:b:398:PRO:O	31:f:5001:SQD:H381	2.22	0.40
12:b:408:ARG:HH12	21:b:1240:CLA:H191	1.86	0.40
24:b:4014:BCR:C32	6:f:72:PHE:HB2	2.52	0.40
14:e:13:ARG:NH2	14:e:59:ASN:HD21	2.16	0.40
21:f:1302:CLA:H143	21:f:1302:CLA:H111	1.74	0.40
25:l:5001:LHG:H223	18:h:22:PHE:CZ	2.57	0.40
16:1:80:LEU:HD11	21:1:1111:CLA:H2	2.03	0.40
16:1:310:MET:HE1	21:1:1119:CLA:C1D	2.52	0.40
16:1:392:HIS:O	16:1:396:ILE:HG12	2.21	0.40
16:1:674:ALA:HB1	24:2:4011:BCR:H351	2.04	0.40
25:1:5007:LHG:HC2	20:0:5:ASN:HB3	2.04	0.40
21:1:1128:CLA:H142	21:1:1128:CLA:H111	1.75	0.40
2:2:277:HIS:HE1	21:2:1215:CLA:ND	2.19	0.40
2:2:452:LEU:O	6:6:53:LEU:N	2.38	0.40
21:2:1213:CLA:HAA2	26:2:5005:LMG:H332	2.02	0.40
1:A:392:HIS:HB2	21:A:1126:CLA:C1B	2.51	0.40
1:A:686:LEU:HB3	2:B:662:ILE:HG12	2.03	0.40
1:A:740:TRP:CD1	21:A:1126:CLA:HMB2	2.57	0.40
21:A:1120:CLA:H11	21:A:1120:CLA:H52	1.83	0.40
21:A:1801:CLA:H92	21:A:1801:CLA:H61	1.77	0.40
25:A:5007:LHG:HC81	25:A:5007:LHG:HC5	1.60	0.40
2:B:85:ARG:HD3	2:B:85:ARG:HA	1.63	0.40
2:B:544:MET:HE2	2:B:547:LYS:HA	2.04	0.40
21:B:1023:CLA:H112	24:B:4017:BCR:H362	2.04	0.40
21:B:1224:CLA:C19	26:B:5002:LMG:H251	2.52	0.40
3:C:59:PRO:CD	23:C:3003:SF4:S4	3.09	0.40
1:a:31:PRO:HB2	1:a:51:LEU:HD11	2.03	0.40
1:a:66:GLU:HB2	1:a:187:LEU:HB2	2.03	0.40
1:a:479:GLN:O	26:a:5002:LMG:H321	2.21	0.40
1:a:592:PHE:CE1	1:a:728:VAL:HB	2.57	0.40
21:a:1119:CLA:H202	24:a:4007:BCR:HC41	2.02	0.40
12:b:199:ILE:HG12	12:b:270:LEU:HB3	2.03	0.40
12:b:265:THR:HB	12:b:357:ALA:HA	2.04	0.40
12:b:312:LEU:CB	25:b:5004:LHG:HC62	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:542:LYS:HZ3	6:f:139:PRO:HB2	1.87	0.40
21:f:1301:CLA:H3A	21:f:1301:CLA:HBA1	1.88	0.40
8:j:33:TYR:CD1	34:j:4015:ZEX:H361	2.56	0.40
15:k:52:LEU:O	15:k:53:PRO:C	2.64	0.40
16:1:76:HIS:ND1	21:1:1111:CLA:OBD	2.41	0.40
16:1:360:GLY:HA2	16:1:397:GLY:HA2	2.03	0.40
16:1:371:TYR:CD1	16:1:609:PHE:HE1	2.40	0.40
1:A:26:GLU:HG3	38:A:8048:HOH:O	2.22	0.40
1:A:44:THR:OG1	5:E:53:ALA:O	2.40	0.40
1:A:59:ASP:HB2	1:A:414:ARG:NH1	2.37	0.40
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.96	0.40
1:A:368:GLN:HG3	21:A:1124:CLA:HED2	2.03	0.40
1:A:722:GLN:NE2	25:A:5001:LHG:HC81	2.36	0.40
21:A:1124:CLA:H93	21:A:1124:CLA:H61	1.85	0.40
2:B:420:LEU:HB3	2:B:529:LEU:HD13	2.04	0.40
5:E:3:LEU:HD13	5:E:37:VAL:HG11	2.03	0.40
6:F:70:ILE:HD11	21:F:1302:CLA:H51	2.02	0.40
10:L:8:VAL:HG13	10:L:22:THR:HG22	2.03	0.40
21:L:1501:CLA:H62	21:L:1501:CLA:H102	1.80	0.40
1:a:254:PRO:HD2	1:a:273:ASP:OD2	2.21	0.40
1:a:352:LEU:HD21	21:a:1128:CLA:C2B	2.51	0.40
24:a:4019:BCR:H11C	24:j:4013:BCR:C33	2.52	0.40
12:b:192:GLY:O	12:b:196:HIS:HB2	2.22	0.40
30:b:4011:ECH:H23	21:b:1230:CLA:CMC	2.52	0.40
6:f:4:PHE:CE2	6:f:54:ILE:HD13	2.57	0.40
16:1:387:LEU:O	16:1:391:THR:HG23	2.20	0.40
16:1:682:SER:HB3	16:1:730:HIS:HB2	2.03	0.40
21:1:1103:CLA:H203	21:1:1103:CLA:H161	1.69	0.40
21:1:1121:CLA:H92	21:1:1121:CLA:H61	1.84	0.40
21:1:1121:CLA:CHA	21:1:1121:CLA:HBA1	2.52	0.40
21:1:1140:CLA:O1A	25:1:5001:LHG:H171	2.21	0.40
21:1:1101:CLA:H92	21:1:1101:CLA:H61	1.84	0.40
2:2:323:THR:OG1	2:2:401:ASN:OD1	2.27	0.40
21:2:1203:CLA:H111	21:2:1203:CLA:H72	1.62	0.40
17:4:27:LYS:HG2	17:4:28:TYR:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	749/751 (100%)	719 (96%)	28 (4%)	2 (0%)	36 55
1	a	749/751 (100%)	712 (95%)	31 (4%)	6 (1%)	16 31
2	2	729/731 (100%)	694 (95%)	33 (4%)	2 (0%)	36 55
2	B	729/731 (100%)	697 (96%)	28 (4%)	4 (0%)	24 43
3	3	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	9 18
3	C	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4 7
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100 100
4	d	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18 34
5	5	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	3 5
5	E	67/69 (97%)	61 (91%)	6 (9%)	0	100 100
6	6	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	18 34
6	F	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	18 34
6	f	141/143 (99%)	134 (95%)	7 (5%)	0	100 100
7	I	38/40 (95%)	36 (95%)	1 (3%)	1 (3%)	4 7
7	i	38/40 (95%)	37 (97%)	1 (3%)	0	100 100
8	7	38/40 (95%)	38 (100%)	0	0	100 100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100 100
8	j	38/40 (95%)	38 (100%)	0	0	100 100
9	K	79/80 (99%)	66 (84%)	6 (8%)	7 (9%)	0 0
10	L	155/157 (99%)	148 (96%)	7 (4%)	0	100 100
10	l	155/157 (99%)	150 (97%)	3 (2%)	2 (1%)	9 18
11	9	29/31 (94%)	27 (93%)	2 (7%)	0	100 100
11	M	29/31 (94%)	29 (100%)	0	0	100 100
11	m	29/31 (94%)	29 (100%)	0	0	100 100
12	b	727/729 (100%)	701 (96%)	22 (3%)	4 (1%)	21 38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	c	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	9 18
14	e	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	8 16
15	k	76/78 (97%)	60 (79%)	7 (9%)	9 (12%)	0 0
16	1	742/744 (100%)	706 (95%)	34 (5%)	2 (0%)	36 55
17	4	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
18	h	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4 6
19	8	77/79 (98%)	64 (83%)	9 (12%)	4 (5%)	1 1
20	0	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18 34
All	All	6706/6771 (99%)	6374 (95%)	277 (4%)	55 (1%)	16 31

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
9	K	16	ALA
9	K	52	LEU
13	c	62	PHE
15	k	13	PRO
15	k	18	TRP
19	8	53	PRO
1	A	6	PRO
2	B	228	GLY
9	K	22	VAL
1	a	6	PRO
1	a	182	VAL
12	b	235	ALA
15	k	23	GLY
10	l	18	GLY
2	2	556	CYS
3	3	62	PHE
5	5	14	THR
5	5	53	ALA
19	8	18	TRP
1	A	574	CYS
7	I	38	GLY
9	K	86	SER
15	k	15	THR
15	k	56	ALA
2	2	311	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	0	18	GLY
2	B	3	THR
1	a	115	GLN
12	b	221	GLY
12	b	556	CYS
15	k	54	GLN
18	h	37	GLU
19	8	86	SER
2	B	211	ASN
2	B	227	THR
4	d	77	LYS
15	k	55	LEU
6	F	65	PHE
9	K	13	PRO
9	K	57	SER
1	a	232	ALA
15	k	16	ALA
10	l	111	GLY
6	6	94	LYS
9	K	53	PRO
1	a	121	VAL
15	k	53	PRO
16	1	121	VAL
16	1	623	PRO
19	8	13	PRO
12	b	228	GLY
3	C	59	PRO
14	e	36	PRO
1	a	334	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/603 (100%)	581 (96%)	22 (4%)	31 58
1	a	603/603 (100%)	586 (97%)	17 (3%)	38 66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	2	583/583 (100%)	561 (96%)	22 (4%)	29 56
2	B	583/583 (100%)	562 (96%)	21 (4%)	31 58
3	3	68/68 (100%)	66 (97%)	2 (3%)	37 65
3	C	68/68 (100%)	65 (96%)	3 (4%)	25 50
4	D	116/116 (100%)	112 (97%)	4 (3%)	32 60
4	d	116/116 (100%)	110 (95%)	6 (5%)	21 42
5	5	58/58 (100%)	54 (93%)	4 (7%)	14 30
5	E	58/58 (100%)	51 (88%)	7 (12%)	5 10
6	6	119/119 (100%)	114 (96%)	5 (4%)	26 52
6	F	119/119 (100%)	115 (97%)	4 (3%)	32 60
6	f	119/119 (100%)	116 (98%)	3 (2%)	42 69
7	I	32/32 (100%)	30 (94%)	2 (6%)	16 34
7	i	32/32 (100%)	30 (94%)	2 (6%)	16 34
8	7	35/35 (100%)	35 (100%)	0	100 100
8	J	35/35 (100%)	33 (94%)	2 (6%)	18 39
8	j	35/35 (100%)	34 (97%)	1 (3%)	37 65
9	K	60/60 (100%)	47 (78%)	13 (22%)	1 2
10	L	118/118 (100%)	109 (92%)	9 (8%)	12 26
10	l	118/118 (100%)	109 (92%)	9 (8%)	12 26
11	9	25/25 (100%)	22 (88%)	3 (12%)	5 10
11	M	25/25 (100%)	24 (96%)	1 (4%)	28 54
11	m	25/25 (100%)	24 (96%)	1 (4%)	28 54
12	b	582/582 (100%)	561 (96%)	21 (4%)	31 58
13	c	69/69 (100%)	67 (97%)	2 (3%)	37 65
14	e	57/57 (100%)	52 (91%)	5 (9%)	9 20
15	k	57/58 (98%)	47 (82%)	10 (18%)	2 3
16	1	596/596 (100%)	577 (97%)	19 (3%)	34 62
17	4	115/115 (100%)	112 (97%)	3 (3%)	40 68
18	h	31/31 (100%)	28 (90%)	3 (10%)	8 17
19	8	58/59 (98%)	49 (84%)	9 (16%)	2 5
20	0	116/116 (100%)	113 (97%)	3 (3%)	40 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5434/5436 (100%)	5196 (96%)	238 (4%)	25 50

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	13	LYS
1	A	62	THR
1	A	110	ILE
1	A	116	VAL
1	A	171	LEU
1	A	210	LEU
1	A	234	LYS
1	A	270	VAL
1	A	303	LEU
1	A	340	LEU
1	A	345	THR
1	A	381	ILE
1	A	429	MET
1	A	433	ARG
1	A	520	VAL
1	A	561	LEU
1	A	562	VAL
1	A	583	CYS
1	A	621	VAL
1	A	624	ASP
1	A	709	VAL
2	B	10	GLN
2	B	85	ARG
2	B	113	VAL
2	B	120	VAL
2	B	126	THR
2	B	127	ILE
2	B	143	LEU
2	B	258	LEU
2	B	297	ILE
2	B	299	HIS
2	B	313	THR
2	B	441	VAL
2	B	476	LEU
2	B	491	LEU
2	B	543	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	567	ILE
2	B	587	LEU
2	B	596	LEU
2	B	628	LEU
2	B	637	VAL
2	B	729	LYS
3	C	17	CYS
3	C	23	LEU
3	C	63	LEU
4	D	18	LEU
4	D	97	LEU
4	D	107	LYS
4	D	108	VAL
5	E	4	ASN
5	E	30	LYS
5	E	33	ILE
5	E	42	ASP
5	E	64	ASN
5	E	66	LEU
5	E	68	LEU
6	F	12	GLU
6	F	32	SER
6	F	36	ARG
6	F	101	VAL
7	I	10	LEU
7	I	14	LEU
8	J	18	LEU
8	J	19	LEU
9	K	15	THR
9	K	18	TRP
9	K	20	LEU
9	K	22	VAL
9	K	28	LEU
9	K	36	ILE
9	K	50	LEU
9	K	52	LEU
9	K	55	LEU
9	K	58	LYS
9	K	67	LEU
9	K	82	LEU
9	K	86	SER
10	L	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	L	42	LYS
10	L	47	ILE
10	L	49	ARG
10	L	62	ILE
10	L	71	LEU
10	L	75	GLU
10	L	101	LEU
10	L	155	LEU
11	M	3	LEU
1	a	7	GLU
1	a	11	LYS
1	a	74	SER
1	a	129	ASP
1	a	224	ASN
1	a	303	LEU
1	a	317	ILE
1	a	319	HIS
1	a	333	THR
1	a	340	LEU
1	a	481	ILE
1	a	513	THR
1	a	520	VAL
1	a	561	LEU
1	a	624	ASP
1	a	657	VAL
1	a	709	VAL
12	b	85	ARG
12	b	113	VAL
12	b	115	ILE
12	b	120	VAL
12	b	133	GLN
12	b	143	LEU
12	b	145	LEU
12	b	160	LYS
12	b	195	VAL
12	b	215	THR
12	b	258	LEU
12	b	299	HIS
12	b	406	LEU
12	b	441	VAL
12	b	567	ILE
12	b	580	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	b	584	LEU
12	b	596	LEU
12	b	628	LEU
12	b	629	ILE
12	b	637	VAL
13	c	73	THR
13	c	74	THR
4	d	2	THR
4	d	38	GLN
4	d	52	GLU
4	d	77	LYS
4	d	107	LYS
4	d	108	VAL
14	e	13	ARG
14	e	33	ILE
14	e	58	THR
14	e	66	LEU
14	e	68	LEU
6	f	90	ILE
6	f	94	LYS
6	f	101	VAL
7	i	10	LEU
7	i	14	LEU
8	j	26	LEU
15	k	10	GLN
15	k	22	VAL
15	k	36	ILE
15	k	46	LYS
15	k	54	GLN
15	k	58	LYS
15	k	65	GLU
15	k	67	LEU
15	k	80	MET
15	k	84	LEU
10	l	19	HIS
10	l	24	ILE
10	l	42	LYS
10	l	44	LEU
10	l	71	LEU
10	l	101	LEU
10	l	136	PHE
10	l	147	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	l	155	LEU
11	m	3	LEU
16	1	11	LYS
16	1	153	THR
16	1	225	LYS
16	1	251	GLU
16	1	252	LEU
16	1	260	LEU
16	1	273	ASP
16	1	303	LEU
16	1	319	HIS
16	1	340	LEU
16	1	371	TYR
16	1	381	ILE
16	1	513	THR
16	1	561	LEU
16	1	583	CYS
16	1	585	VAL
16	1	621	VAL
16	1	709	VAL
16	1	714	GLN
2	2	47	PHE
2	2	65	LEU
2	2	115	ILE
2	2	137	SER
2	2	143	LEU
2	2	145	LEU
2	2	215	THR
2	2	226	PHE
2	2	280	ILE
2	2	342	ILE
2	2	405	VAL
2	2	441	VAL
2	2	448	GLU
2	2	453	ILE
2	2	461	ILE
2	2	476	LEU
2	2	482	ILE
2	2	565	CYS
2	2	567	ILE
2	2	573	PHE
2	2	596	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	603	VAL
3	3	29	VAL
3	3	63	LEU
17	4	106	GLU
17	4	108	VAL
17	4	122	ILE
5	5	3	LEU
5	5	15	GLU
5	5	30	LYS
5	5	69	VAL
6	6	31	ASN
6	6	48	GLU
6	6	101	VAL
6	6	123	VAL
6	6	127	THR
18	h	10	LEU
18	h	26	THR
18	h	35	GLU
19	8	22	VAL
19	8	34	PHE
19	8	36	ILE
19	8	46	LYS
19	8	58	LYS
19	8	59	LYS
19	8	60	THR
19	8	67	LEU
19	8	82	LEU
20	0	19	HIS
20	0	101	LEU
20	0	155	LEU
11	9	6	THR
11	9	8	ILE
11	9	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	192	ASN
1	A	240	HIS
2	B	14	GLN
2	B	53	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	83	ASN
2	B	276	HIS
2	B	478	ASN
2	B	627	GLN
4	D	51	ASN
6	F	61	HIS
7	I	33	HIS
1	a	54	ASN
1	a	79	HIS
1	a	138	GLN
1	a	567	ASN
12	b	41	ASN
12	b	53	HIS
12	b	158	GLN
12	b	277	HIS
12	b	582	ASN
12	b	602	ASN
14	e	4	ASN
16	1	50	ASN
16	1	56	HIS
16	1	79	HIS
16	1	135	HIS
16	1	181	HIS
16	1	722	GLN
2	2	158	GLN
2	2	206	HIS
2	2	277	HIS
2	2	518	HIS
2	2	627	GLN
2	2	686	ASN
17	4	7	GLN
20	0	122	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 443 ligands modelled in this entry, 11 are monoatomic - leaving 432 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	2	1221	-	69,73,73	1.36	9 (13%)	82,113,113	1.85	15 (18%)
21	CLA	J	1303	-	69,73,73	1.35	9 (13%)	82,113,113	1.84	15 (18%)
21	CLA	a	1112	-	69,73,73	1.35	9 (13%)	82,113,113	1.87	15 (18%)
21	CLA	2	1215	-	64,68,73	1.40	9 (14%)	76,107,113	1.88	16 (21%)
26	LMG	K	5009	-	55,55,55	1.31	7 (12%)	63,63,63	1.27	5 (7%)
21	CLA	K	1401	38	69,73,73	1.35	8 (11%)	82,113,113	1.82	17 (20%)
21	CLA	7	1303	-	45,49,73	1.67	9 (20%)	54,84,113	2.09	13 (24%)
24	BCR	1	4007	-	41,41,41	0.66	0	56,56,56	3.35	10 (17%)
24	BCR	7	4013	-	41,41,41	0.73	0	56,56,56	3.38	16 (28%)
30	ECH	B	4006	-	42,42,42	0.87	2 (4%)	55,58,58	2.54	14 (25%)
25	LHG	F	5002	-	48,48,48	0.37	0	51,54,54	0.97	2 (3%)
24	BCR	I	4018	-	41,41,41	0.61	0	56,56,56	3.17	14 (25%)
24	BCR	1	4019	-	41,41,41	0.69	0	56,56,56	3.44	8 (14%)
21	CLA	F	1302	6	69,73,73	1.35	9 (13%)	82,113,113	1.81	15 (18%)
21	CLA	2	1214	-	63,67,73	1.41	9 (14%)	74,105,113	1.80	15 (20%)
27	ACT	B	7002	-	3,3,3	1.45	1 (33%)	3,3,3	1.33	0
21	CLA	2	1206	2	69,73,73	1.35	9 (13%)	82,113,113	1.86	16 (19%)
21	CLA	B	1238	38	69,73,73	1.35	8 (11%)	82,113,113	1.69	13 (15%)
24	BCR	B	4018	-	41,41,41	0.73	0	56,56,56	3.54	12 (21%)
21	CLA	a	1124	-	59,63,73	1.42	9 (15%)	70,101,113	1.95	14 (20%)
21	CLA	2	1023	-	69,73,73	1.37	9 (13%)	82,113,113	1.91	14 (17%)
21	CLA	1	1104	-	69,73,73	1.34	9 (13%)	82,113,113	1.80	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	a	1012	38	69,73,73	1.35	9 (13%)	82,113,113	1.78	13 (15%)
21	CLA	A	1137	-	69,73,73	1.35	9 (13%)	82,113,113	1.73	14 (17%)
21	CLA	a	1120	-	59,63,73	1.46	9 (15%)	70,101,113	1.94	14 (20%)
30	ECH	M	4021	-	42,42,42	0.67	0	55,58,58	1.69	12 (21%)
21	CLA	a	1122	-	69,73,73	1.34	9 (13%)	82,113,113	1.83	14 (17%)
24	BCR	f	4016	-	41,41,41	0.74	0	56,56,56	3.36	14 (25%)
21	CLA	A	1135	-	69,73,73	1.34	9 (13%)	82,113,113	1.78	16 (19%)
26	LMG	A	5004	-	48,48,55	1.09	4 (8%)	56,56,63	1.11	3 (5%)
21	CLA	b	1209	-	69,73,73	1.35	8 (11%)	82,113,113	1.89	17 (20%)
21	CLA	2	1239	-	69,73,73	1.34	9 (13%)	82,113,113	1.81	16 (19%)
25	LHG	L	5005	-	48,48,48	0.40	0	51,54,54	0.96	2 (3%)
21	CLA	1	1139	-	69,73,73	1.35	9 (13%)	82,113,113	1.85	14 (17%)
21	CLA	1	1136	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	16 (19%)
21	CLA	A	1121	-	69,73,73	1.32	8 (11%)	82,113,113	1.84	14 (17%)
21	CLA	1	1129	-	54,58,73	1.52	8 (14%)	64,95,113	2.00	17 (26%)
21	CLA	A	1125	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	16 (19%)
26	LMG	A	5002	-	50,50,55	1.18	6 (12%)	58,58,63	1.18	4 (6%)
21	CLA	B	1226	-	69,73,73	1.35	9 (13%)	82,113,113	1.75	15 (18%)
21	CLA	A	1127	-	69,73,73	1.37	9 (13%)	82,113,113	1.66	13 (15%)
21	CLA	A	1105	-	69,73,73	1.36	8 (11%)	82,113,113	1.72	15 (18%)
23	SF4	C	3002	3	0,12,12	-	-	-		
30	ECH	b	4006	-	42,42,42	0.75	1 (2%)	55,58,58	2.29	16 (29%)
21	CLA	A	1132	-	69,73,73	1.35	9 (13%)	82,113,113	1.74	15 (18%)
21	CLA	a	1126	-	69,73,73	1.35	9 (13%)	82,113,113	1.90	14 (17%)
21	CLA	1	1105	-	54,58,73	1.53	9 (16%)	64,95,113	1.99	15 (23%)
21	CLA	B	1232	-	54,58,73	1.53	9 (16%)	64,95,113	2.04	15 (23%)
25	LHG	l	5001	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
21	CLA	B	1230	-	69,73,73	1.34	9 (13%)	82,113,113	1.81	14 (17%)
21	CLA	b	1202	-	69,73,73	1.34	9 (13%)	82,113,113	1.88	15 (18%)
28	45D	h	4020	21	43,43,43	3.52	17 (39%)	54,60,60	3.43	23 (42%)
21	CLA	A	1131	-	69,73,73	1.34	9 (13%)	82,113,113	1.76	13 (15%)
21	CLA	1	1137	-	55,59,73	1.51	9 (16%)	64,96,113	2.01	15 (23%)
21	CLA	A	1101	-	69,73,73	1.35	9 (13%)	82,113,113	1.87	17 (20%)
24	BCR	L	4019	-	41,41,41	0.70	0	56,56,56	2.93	14 (25%)
21	CLA	1	1135	-	56,60,73	1.50	8 (14%)	65,97,113	1.93	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LHG	a	5005	-	48,48,48	0.39	0	51,54,54	1.12	3 (5%)
21	CLA	1	1109	-	69,73,73	1.35	9 (13%)	82,113,113	1.86	12 (14%)
21	CLA	j	1303	-	59,63,73	1.47	9 (15%)	70,101,113	1.90	14 (20%)
21	CLA	b	1227	-	69,73,73	1.33	9 (13%)	82,113,113	1.77	15 (18%)
21	CLA	A	1120	-	69,73,73	1.34	8 (11%)	82,113,113	1.81	15 (18%)
24	BCR	B	4014	-	41,41,41	0.72	0	56,56,56	3.22	12 (21%)
21	CLA	B	1208	-	69,73,73	1.36	8 (11%)	82,113,113	1.78	15 (18%)
21	CLA	a	1140	-	69,73,73	1.36	9 (13%)	82,113,113	1.81	16 (19%)
21	CLA	b	1235	-	69,73,73	1.33	8 (11%)	82,113,113	1.80	14 (17%)
21	CLA	1	1122	-	64,68,73	1.41	9 (14%)	76,107,113	1.86	13 (17%)
21	CLA	A	1106	1	69,73,73	1.33	8 (11%)	82,113,113	1.78	15 (18%)
35	LMT	0	6001	-	36,36,36	1.10	4 (11%)	47,47,47	1.19	3 (6%)
24	BCR	A	4002	-	41,41,41	0.68	0	56,56,56	3.23	16 (28%)
21	CLA	B	1218	-	69,73,73	1.35	9 (13%)	82,113,113	1.79	14 (17%)
25	LHG	0	5004	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
21	CLA	b	1022	-	69,73,73	1.35	8 (11%)	82,113,113	1.77	14 (17%)
26	LMG	1	5002	-	50,50,55	1.16	5 (10%)	58,58,63	1.07	2 (3%)
24	BCR	K	4001	-	41,41,41	0.59	0	56,56,56	3.26	15 (26%)
21	CLA	a	1106	-	69,73,73	1.33	9 (13%)	82,113,113	1.87	14 (17%)
21	CLA	2	1230	-	51,55,73	1.57	9 (17%)	60,91,113	2.11	16 (26%)
25	LHG	1	5007	-	48,48,48	0.40	0	51,54,54	1.03	4 (7%)
21	CLA	b	1218	-	69,73,73	1.35	9 (13%)	82,113,113	1.75	13 (15%)
36	EQ3	I	4020	-	43,43,43	4.14	23 (53%)	55,60,60	2.27	21 (38%)
24	BCR	B	4017	-	41,41,41	0.67	0	56,56,56	3.34	13 (23%)
21	CLA	2	1207	-	60,64,73	1.43	9 (15%)	71,102,113	1.91	16 (22%)
24	BCR	a	4019	-	41,41,41	0.72	0	56,56,56	3.55	10 (17%)
24	BCR	b	4005	-	41,41,41	0.66	0	56,56,56	3.23	12 (21%)
21	CLA	b	1213	-	69,73,73	1.34	9 (13%)	82,113,113	1.86	16 (19%)
21	CLA	K	1402	-	69,73,73	1.33	9 (13%)	82,113,113	1.80	14 (17%)
25	LHG	1	5003	21	48,48,48	0.40	0	51,54,54	1.10	4 (7%)
21	CLA	2	1235	-	57,61,73	1.48	9 (15%)	67,98,113	1.96	13 (19%)
21	CLA	A	1108	-	57,61,73	1.47	9 (15%)	67,98,113	1.99	15 (22%)
21	CLA	A	1138	-	69,73,73	1.34	9 (13%)	82,113,113	1.82	15 (18%)
21	CLA	f	1302	-	69,73,73	1.35	9 (13%)	82,113,113	1.77	15 (18%)
25	LHG	1	5001	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	1107	1	69,73,73	1.35	8 (11%)	82,113,113	1.80	12 (14%)
24	BCR	2	4014	-	41,41,41	0.73	0	56,56,56	3.42	12 (21%)
21	CLA	1	1103	-	69,73,73	1.33	9 (13%)	82,113,113	1.82	11 (13%)
24	BCR	0	4022	-	41,41,41	0.72	0	56,56,56	3.35	15 (26%)
21	CLA	B	1206	2	69,73,73	1.35	9 (13%)	82,113,113	1.84	15 (18%)
21	CLA	7	1302	8	45,49,73	1.67	9 (20%)	54,84,113	2.16	13 (24%)
26	LMG	b	5002	-	55,55,55	1.28	6 (10%)	63,63,63	1.19	6 (9%)
21	CLA	k	1401	-	54,58,73	1.54	9 (16%)	64,95,113	2.00	14 (21%)
21	CLA	A	1122	-	64,68,73	1.40	9 (14%)	76,107,113	1.78	14 (18%)
21	CLA	A	1114	38	69,73,73	1.35	8 (11%)	82,113,113	1.73	15 (18%)
21	CLA	1	1114	-	49,53,73	1.60	9 (18%)	58,89,113	1.95	12 (20%)
21	CLA	2	1218	-	69,73,73	1.35	9 (13%)	82,113,113	1.79	15 (18%)
21	CLA	B	1209	-	69,73,73	1.36	9 (13%)	82,113,113	1.86	16 (19%)
21	CLA	a	1135	-	69,73,73	1.34	8 (11%)	82,113,113	1.74	15 (18%)
21	CLA	b	1206	12	69,73,73	1.36	9 (13%)	82,113,113	1.77	15 (18%)
21	CLA	1	1107	-	55,59,73	1.52	8 (14%)	64,96,113	2.00	15 (23%)
21	CLA	B	1225	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	12 (14%)
21	CLA	B	1212	-	59,63,73	1.45	9 (15%)	70,101,113	1.92	15 (21%)
21	CLA	B	1227	-	59,63,73	1.46	9 (15%)	70,101,113	1.91	14 (20%)
21	CLA	1	1101	-	69,73,73	1.36	9 (13%)	82,113,113	1.86	16 (19%)
23	SF4	C	3003	3	0,12,12	-	-	-		
21	CLA	b	1230	-	69,73,73	1.32	9 (13%)	82,113,113	1.88	14 (17%)
21	CLA	2	1213	-	54,58,73	1.52	9 (16%)	64,95,113	2.07	13 (20%)
26	LMG	a	5002	-	50,50,55	1.17	5 (10%)	58,58,63	1.10	3 (5%)
21	CLA	A	1115	-	69,73,73	1.34	8 (11%)	82,113,113	1.77	14 (17%)
21	CLA	1	1115	-	69,73,73	1.34	8 (11%)	82,113,113	1.78	14 (17%)
21	CLA	B	1221	-	69,73,73	1.34	9 (13%)	82,113,113	1.81	15 (18%)
21	CLA	B	1240	-	69,73,73	1.35	9 (13%)	82,113,113	1.81	16 (19%)
24	BCR	b	4018	-	41,41,41	0.71	0	56,56,56	3.42	8 (14%)
21	CLA	a	1132	-	69,73,73	1.34	8 (11%)	82,113,113	1.77	14 (17%)
24	BCR	b	4010	-	41,41,41	0.66	0	56,56,56	3.16	7 (12%)
21	CLA	B	1215	-	69,73,73	1.34	9 (13%)	82,113,113	1.81	16 (19%)
21	CLA	B	1201	-	69,73,73	1.33	9 (13%)	82,113,113	1.71	14 (17%)
21	CLA	2	1202	-	69,73,73	1.35	9 (13%)	82,113,113	1.81	15 (18%)
24	BCR	A	4001	-	41,41,41	0.70	0	56,56,56	3.15	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	1202	-	69,73,73	1.35	9 (13%)	82,113,113	1.79	15 (18%)
24	BCR	h	4018	-	41,41,41	0.71	0	56,56,56	3.41	11 (19%)
30	ECH	m	4021	-	42,42,42	0.66	0	55,58,58	1.70	11 (20%)
21	CLA	B	1022	38	69,73,73	1.37	8 (11%)	82,113,113	1.70	14 (17%)
21	CLA	A	1103	-	69,73,73	1.32	8 (11%)	82,113,113	1.79	12 (14%)
26	LMG	a	5004	-	55,55,55	1.28	7 (12%)	63,63,63	1.23	4 (6%)
21	CLA	A	1013	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	14 (17%)
25	LHG	A	5005	-	48,48,48	0.41	0	51,54,54	1.11	4 (7%)
21	CLA	2	1229	-	69,73,73	1.34	8 (11%)	82,113,113	1.84	15 (18%)
21	CLA	2	1209	-	49,53,73	1.62	9 (18%)	58,89,113	2.05	12 (20%)
25	LHG	1	5005	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
21	CLA	l	1501	10	69,73,73	1.34	9 (13%)	82,113,113	1.80	15 (18%)
24	BCR	L	4022	-	41,41,41	0.62	0	56,56,56	3.15	11 (19%)
21	CLA	A	1123	38	69,73,73	1.36	9 (13%)	82,113,113	1.79	13 (15%)
21	CLA	a	1128	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	16 (19%)
34	ZEX	J	4015	-	43,43,43	6.08	4 (9%)	51,60,60	6.76	10 (19%)
24	BCR	A	4008	-	41,41,41	0.66	0	56,56,56	2.99	9 (16%)
24	BCR	a	4001	-	41,41,41	0.72	0	56,56,56	3.53	13 (23%)
21	CLA	8	1401	-	49,53,73	1.61	9 (18%)	58,89,113	2.03	11 (18%)
21	CLA	F	1301	38	69,73,73	1.35	9 (13%)	82,113,113	1.73	14 (17%)
21	CLA	2	1227	-	49,53,73	1.60	9 (18%)	58,89,113	2.00	13 (22%)
21	CLA	B	1023	-	69,73,73	1.37	9 (13%)	82,113,113	1.85	14 (17%)
21	CLA	b	1220	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	14 (17%)
35	LMT	l	6001	-	36,36,36	1.08	4 (11%)	47,47,47	1.22	3 (6%)
24	BCR	j	4013	-	41,41,41	0.75	0	56,56,56	3.34	16 (28%)
24	BCR	a	4008	-	41,41,41	0.67	0	56,56,56	3.36	11 (19%)
21	CLA	A	1104	-	69,73,73	1.36	9 (13%)	82,113,113	1.76	14 (17%)
25	LHG	A	5001	-	48,48,48	0.41	0	51,54,54	1.12	3 (5%)
24	BCR	2	4010	-	41,41,41	0.75	0	56,56,56	3.72	15 (26%)
21	CLA	2	1201	-	69,73,73	1.35	9 (13%)	82,113,113	1.90	15 (18%)
24	BCR	2	4011	-	41,41,41	0.69	0	56,56,56	3.03	10 (17%)
21	CLA	b	1204	-	69,73,73	1.35	9 (13%)	82,113,113	1.71	13 (15%)
24	BCR	9	4021	-	41,41,41	0.69	0	56,56,56	3.32	18 (32%)
21	CLA	B	1204	-	69,73,73	1.36	8 (11%)	82,113,113	1.72	15 (18%)
21	CLA	b	1207	-	69,73,73	1.33	9 (13%)	82,113,113	1.77	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	b	4014	-	41,41,41	0.72	0	56,56,56	3.29	11 (19%)
21	CLA	A	1118	-	69,73,73	1.36	9 (13%)	82,113,113	1.70	13 (15%)
21	CLA	2	1022	38	69,73,73	1.36	9 (13%)	82,113,113	1.82	16 (19%)
23	SF4	A	3001	2,1	0,12,12	-	-	-		
25	LHG	l	5004	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
21	CLA	l	1503	-	69,73,73	1.32	8 (11%)	82,113,113	1.75	13 (15%)
23	SF4	3	3002	-	0,12,12	-	-	-		
21	CLA	A	1139	38	69,73,73	1.34	9 (13%)	82,113,113	1.82	12 (14%)
21	CLA	L	1502	-	69,73,73	1.32	8 (11%)	82,113,113	1.81	13 (15%)
24	BCR	l	4022	-	41,41,41	0.70	0	56,56,56	3.31	13 (23%)
21	CLA	2	1228	-	49,53,73	1.58	9 (18%)	58,89,113	2.15	14 (24%)
21	CLA	a	1127	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	16 (19%)
21	CLA	1	1124	-	60,64,73	1.45	9 (15%)	71,102,113	1.86	14 (19%)
21	CLA	1	1123	-	69,73,73	1.36	9 (13%)	82,113,113	1.77	11 (13%)
25	LHG	b	5004	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
21	CLA	a	1114	-	56,60,73	1.50	9 (16%)	65,97,113	2.01	15 (23%)
24	BCR	6	4016	-	41,41,41	0.71	0	56,56,56	3.50	12 (21%)
24	BCR	0	4019	-	41,41,41	0.68	0	56,56,56	3.18	11 (19%)
24	BCR	a	4002	-	41,41,41	0.67	0	56,56,56	3.61	14 (25%)
21	CLA	B	1228	-	69,73,73	1.34	9 (13%)	82,113,113	1.76	14 (17%)
24	BCR	k	4001	-	41,41,41	0.69	0	56,56,56	3.25	9 (16%)
21	CLA	f	1301	38	54,58,73	1.54	8 (14%)	64,95,113	1.90	15 (23%)
21	CLA	A	1130	-	64,68,73	1.41	9 (14%)	76,107,113	1.89	16 (21%)
21	CLA	2	1204	-	69,73,73	1.35	8 (11%)	82,113,113	1.83	14 (17%)
21	CLA	A	1117	-	69,73,73	1.36	9 (13%)	82,113,113	1.76	13 (15%)
21	CLA	L	1503	38	69,73,73	1.34	9 (13%)	82,113,113	1.80	16 (19%)
24	BCR	b	4017	-	41,41,41	0.65	0	56,56,56	3.36	12 (21%)
27	ACT	A	7001	-	3,3,3	1.62	1 (33%)	3,3,3	1.44	0
21	CLA	1	1013	-	69,73,73	1.37	9 (13%)	82,113,113	1.84	14 (17%)
21	CLA	A	1129	-	62,66,73	1.41	9 (14%)	73,104,113	1.89	15 (20%)
21	CLA	1	1117	-	69,73,73	1.35	9 (13%)	82,113,113	1.74	14 (17%)
21	CLA	a	1101	-	69,73,73	1.36	9 (13%)	82,113,113	1.91	17 (20%)
21	CLA	a	1105	-	62,66,73	1.43	9 (14%)	73,104,113	1.89	16 (21%)
31	SQD	L	5001	-	49,51,54	0.79	0	59,62,65	0.87	3 (5%)
21	CLA	0	1501	20	69,73,73	1.33	9 (13%)	82,113,113	1.74	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	1801	25	69,73,73	1.34	9 (13%)	82,113,113	1.84	15 (18%)
21	CLA	2	1232	-	49,53,73	1.60	9 (18%)	58,89,113	2.03	12 (20%)
24	BCR	2	4018	-	41,41,41	0.76	0	56,56,56	3.32	19 (33%)
21	CLA	a	1011	-	69,73,73	1.39	9 (13%)	82,113,113	1.85	14 (17%)
24	BCR	1	4003	-	41,41,41	0.71	0	56,56,56	3.35	10 (17%)
21	CLA	B	1216	38	69,73,73	1.36	9 (13%)	82,113,113	1.78	16 (19%)
31	SQD	0	5005	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
26	LMG	2	5002	-	55,55,55	1.28	6 (10%)	63,63,63	1.09	2 (3%)
21	CLA	2	1224	-	59,63,73	1.44	9 (15%)	70,101,113	1.93	13 (18%)
21	CLA	1	1012	38	69,73,73	1.34	9 (13%)	82,113,113	1.89	15 (18%)
21	CLA	A	1136	-	69,73,73	1.36	9 (13%)	82,113,113	1.74	14 (17%)
23	SF4	c	3003	13	0,12,12	-	-	-		
22	PQN	A	2001	-	34,34,34	0.42	0	43,45,45	1.24	5 (11%)
21	CLA	B	1222	38	59,63,73	1.43	9 (15%)	70,101,113	1.93	13 (18%)
21	CLA	B	1214	-	69,73,73	1.34	9 (13%)	82,113,113	1.75	14 (17%)
21	CLA	A	1128	-	69,73,73	1.36	8 (11%)	82,113,113	1.78	15 (18%)
22	PQN	1	2001	-	34,34,34	0.45	0	43,45,45	1.11	4 (9%)
24	BCR	A	4007	-	41,41,41	0.64	0	56,56,56	2.98	13 (23%)
21	CLA	1	1128	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	15 (18%)
24	BCR	8	4001	-	41,41,41	0.67	0	56,56,56	3.32	10 (17%)
23	SF4	1	3001	2,16	0,12,12	-	-	-		
25	LHG	A	5003	21	48,48,48	0.41	0	51,54,54	1.03	4 (7%)
21	CLA	2	1219	-	57,61,73	1.48	9 (15%)	67,98,113	2.02	16 (23%)
21	CLA	1	1801	25	60,64,73	1.45	9 (15%)	71,102,113	2.00	16 (22%)
21	CLA	A	1102	21	69,73,73	1.35	9 (13%)	82,113,113	1.82	16 (19%)
21	CLA	2	1220	-	49,53,73	1.61	9 (18%)	58,89,113	2.02	13 (22%)
21	CLA	a	1138	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	12 (14%)
21	CLA	b	1221	38	69,73,73	1.35	9 (13%)	82,113,113	1.87	15 (18%)
31	SQD	L	5002	-	52,54,54	0.79	0	62,65,65	0.83	2 (3%)
21	CLA	b	1215	-	69,73,73	1.35	9 (13%)	82,113,113	1.83	16 (19%)
21	CLA	b	1238	38	69,73,73	1.37	9 (13%)	82,113,113	1.73	14 (17%)
21	CLA	1	1110	-	54,58,73	1.53	9 (16%)	64,95,113	2.00	15 (23%)
21	CLA	a	1013	-	69,73,73	1.33	9 (13%)	82,113,113	1.83	14 (17%)
21	CLA	A	1119	38	69,73,73	1.33	8 (11%)	82,113,113	1.69	13 (15%)
24	BCR	a	4012	-	41,41,41	0.70	0	56,56,56	3.20	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	1213	-	69,73,73	1.37	9 (13%)	82,113,113	1.82	16 (19%)
30	ECH	b	4011	-	42,42,42	0.80	1 (2%)	55,58,58	2.46	17 (30%)
21	CLA	a	1103	-	69,73,73	1.32	8 (11%)	82,113,113	1.79	13 (15%)
21	CLA	2	1222	-	54,58,73	1.52	9 (16%)	64,95,113	2.04	17 (26%)
21	CLA	B	1231	38	69,73,73	1.34	9 (13%)	82,113,113	1.85	16 (19%)
21	CLA	b	1240	-	69,73,73	1.37	9 (13%)	82,113,113	1.83	13 (15%)
21	CLA	a	1119	-	69,73,73	1.34	8 (11%)	82,113,113	1.74	13 (15%)
21	CLA	b	1023	-	69,73,73	1.35	9 (13%)	82,113,113	1.92	15 (18%)
21	CLA	a	1139	38	69,73,73	1.35	9 (13%)	82,113,113	1.83	15 (18%)
24	BCR	i	4018	-	41,41,41	0.71	0	56,56,56	3.46	11 (19%)
27	ACT	B	7001	-	3,3,3	1.42	1 (33%)	3,3,3	1.52	0
21	CLA	b	1226	-	69,73,73	1.36	8 (11%)	82,113,113	1.74	13 (15%)
21	CLA	b	1239	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	14 (17%)
21	CLA	b	1237	38	69,73,73	1.33	8 (11%)	82,113,113	1.76	13 (15%)
21	CLA	A	1116	-	69,73,73	1.34	9 (13%)	82,113,113	1.75	13 (15%)
21	CLA	b	1232	-	69,73,73	1.34	9 (13%)	82,113,113	1.79	14 (17%)
21	CLA	a	1118	-	69,73,73	1.36	9 (13%)	82,113,113	1.73	15 (18%)
28	45D	B	4011	-	43,43,43	3.45	15 (34%)	54,60,60	2.27	18 (33%)
21	CLA	1	1108	-	50,54,73	1.58	9 (18%)	59,90,113	2.00	12 (20%)
21	CLA	2	1238	38	69,73,73	1.35	9 (13%)	82,113,113	1.77	16 (19%)
23	SF4	a	3001	1,12	0,12,12	-	-	-		
25	LHG	A	5007	-	48,48,48	0.40	0	51,54,54	1.12	3 (5%)
21	CLA	a	1117	-	69,73,73	1.36	9 (13%)	82,113,113	1.76	13 (15%)
21	CLA	2	1205	-	69,73,73	1.34	9 (13%)	82,113,113	1.88	14 (17%)
21	CLA	A	1109	21	69,73,73	1.35	9 (13%)	82,113,113	1.79	15 (18%)
21	CLA	b	1216	38	69,73,73	1.34	9 (13%)	82,113,113	1.79	14 (17%)
21	CLA	j	1302	-	69,73,73	1.35	9 (13%)	82,113,113	1.87	15 (18%)
24	BCR	l	4019	-	41,41,41	0.65	0	56,56,56	2.96	12 (21%)
26	LMG	0	5001	-	55,55,55	1.28	6 (10%)	63,63,63	1.29	6 (9%)
21	CLA	0	1502	28	69,73,73	1.36	8 (11%)	82,113,113	1.82	14 (17%)
21	CLA	2	1231	38	50,54,73	1.57	9 (18%)	59,90,113	2.00	13 (22%)
21	CLA	a	1137	-	54,58,73	1.54	9 (16%)	64,95,113	1.99	15 (23%)
25	LHG	B	5006	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
37	DGD	L	5004	-	67,67,67	1.19	7 (10%)	81,81,81	1.02	2 (2%)
21	CLA	b	1234	-	57,61,73	1.50	9 (15%)	67,98,113	1.92	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	1102	-	59,63,73	1.45	9 (15%)	70,101,113	1.98	15 (21%)
24	BCR	b	4004	-	41,41,41	0.69	0	56,56,56	3.39	14 (25%)
24	BCR	B	4010	-	41,41,41	0.67	0	56,56,56	3.27	11 (19%)
21	CLA	B	1210	-	69,73,73	1.37	9 (13%)	82,113,113	1.80	16 (19%)
21	CLA	b	1214	-	69,73,73	1.34	9 (13%)	82,113,113	1.75	14 (17%)
24	BCR	B	4005	-	41,41,41	0.69	0	56,56,56	3.29	9 (16%)
25	LHG	2	5004	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
21	CLA	B	1203	-	69,73,73	1.35	9 (13%)	82,113,113	1.75	11 (13%)
31	SQD	B	5008	-	52,54,54	0.79	0	62,65,65	0.85	2 (3%)
22	PQN	a	2001	-	34,34,34	0.48	0	43,45,45	1.05	2 (4%)
26	LMG	1	5004	-	55,55,55	1.28	6 (10%)	63,63,63	1.05	2 (3%)
21	CLA	1	1131	-	69,73,73	1.33	8 (11%)	82,113,113	1.76	13 (15%)
27	ACT	a	7001	-	3,3,3	1.39	1 (33%)	3,3,3	1.37	0
31	SQD	F	5001	-	52,54,54	0.79	0	62,65,65	0.85	2 (3%)
24	BCR	a	4007	-	41,41,41	0.67	0	56,56,56	3.18	12 (21%)
21	CLA	b	1203	-	69,73,73	1.34	9 (13%)	82,113,113	1.76	13 (15%)
21	CLA	a	1801	25	59,63,73	1.47	9 (15%)	70,101,113	1.93	13 (18%)
21	CLA	2	1216	-	54,58,73	1.51	9 (16%)	64,95,113	2.04	12 (18%)
21	CLA	b	1225	-	69,73,73	1.34	8 (11%)	82,113,113	1.68	12 (14%)
21	CLA	1	1125	-	69,73,73	1.37	9 (13%)	82,113,113	1.84	14 (17%)
24	BCR	1	4001	-	41,41,41	0.72	0	56,56,56	3.35	10 (17%)
21	CLA	1	1140	-	69,73,73	1.36	8 (11%)	82,113,113	1.79	15 (18%)
21	CLA	b	1210	-	69,73,73	1.34	9 (13%)	82,113,113	1.76	14 (17%)
21	CLA	A	1113	-	69,73,73	1.37	9 (13%)	82,113,113	1.79	16 (19%)
21	CLA	b	1205	-	69,73,73	1.33	8 (11%)	82,113,113	1.78	14 (17%)
21	CLA	1	1113	-	47,52,73	1.64	9 (19%)	55,87,113	2.09	13 (23%)
21	CLA	B	1236	-	54,58,73	1.53	9 (16%)	64,95,113	1.90	13 (20%)
21	CLA	B	1239	-	69,73,73	1.36	9 (13%)	82,113,113	1.81	14 (17%)
21	CLA	B	1021	-	69,73,73	1.36	9 (13%)	82,113,113	1.84	12 (14%)
25	LHG	M	5001	-	48,48,48	0.42	0	51,54,54	1.12	3 (5%)
21	CLA	A	1011	-	69,73,73	1.39	9 (13%)	82,113,113	2.05	19 (23%)
21	CLA	2	1225	-	69,73,73	1.34	8 (11%)	82,113,113	1.75	14 (17%)
21	CLA	b	1201	-	69,73,73	1.35	9 (13%)	82,113,113	1.75	15 (18%)
21	CLA	a	1115	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	14 (17%)
35	LMT	1	6001	-	36,36,36	1.13	4 (11%)	47,47,47	0.99	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	a	1104	-	69,73,73	1.34	9 (13%)	82,113,113	1.78	14 (17%)
25	LHG	a	5001	-	48,48,48	0.41	0	51,54,54	1.12	3 (5%)
21	CLA	a	1110	-	63,67,73	1.41	9 (14%)	74,105,113	1.89	14 (18%)
21	CLA	b	1211	-	69,73,73	1.33	9 (13%)	82,113,113	1.81	11 (13%)
24	BCR	1	4008	-	41,41,41	0.63	0	56,56,56	3.27	10 (17%)
21	CLA	A	1126	-	69,73,73	1.35	9 (13%)	82,113,113	1.78	12 (14%)
24	BCR	A	4012	-	41,41,41	0.72	0	56,56,56	3.20	9 (16%)
21	CLA	2	1210	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	15 (18%)
21	CLA	A	1134	1	69,73,73	1.35	9 (13%)	82,113,113	1.80	14 (17%)
21	CLA	b	1231	38	69,73,73	1.34	9 (13%)	82,113,113	1.89	14 (17%)
21	CLA	2	1203	-	69,73,73	1.34	9 (13%)	82,113,113	1.78	15 (18%)
22	PQN	B	2002	-	34,34,34	0.92	2 (5%)	43,45,45	1.28	3 (6%)
21	CLA	a	1136	-	69,73,73	1.35	9 (13%)	82,113,113	1.97	19 (23%)
24	BCR	A	4003	-	41,41,41	0.70	0	56,56,56	3.25	12 (21%)
21	CLA	A	1111	-	69,73,73	1.34	9 (13%)	82,113,113	1.81	16 (19%)
26	LMG	B	5005	-	55,55,55	1.27	6 (10%)	63,63,63	1.10	3 (4%)
24	BCR	B	4004	-	41,41,41	0.70	0	56,56,56	3.28	11 (19%)
30	ECH	2	4006	-	42,42,42	0.76	1 (2%)	55,58,58	2.56	17 (30%)
21	CLA	1	1130	-	59,63,73	1.45	9 (15%)	70,101,113	1.84	12 (17%)
24	BCR	2	4017	-	41,41,41	0.67	0	56,56,56	3.30	11 (19%)
21	CLA	a	1133	-	69,73,73	1.34	9 (13%)	82,113,113	1.78	16 (19%)
21	CLA	2	1208	-	64,68,73	1.41	9 (14%)	76,107,113	1.82	15 (19%)
21	CLA	A	1124	38	69,73,73	1.34	9 (13%)	82,113,113	1.80	14 (17%)
21	CLA	B	1211	-	69,73,73	1.36	9 (13%)	82,113,113	1.78	13 (15%)
25	LHG	A	5006	-	48,48,48	0.40	0	51,54,54	1.04	4 (7%)
21	CLA	2	1236	-	54,58,73	1.52	9 (16%)	64,95,113	1.94	14 (21%)
24	BCR	a	4003	-	41,41,41	0.74	0	56,56,56	3.40	11 (19%)
31	SQD	f	5001	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
21	CLA	a	1111	-	69,73,73	1.34	9 (13%)	82,113,113	1.75	17 (20%)
21	CLA	1	1127	-	69,73,73	1.37	9 (13%)	82,113,113	1.71	13 (15%)
21	CLA	1	1116	-	69,73,73	1.35	9 (13%)	82,113,113	1.84	16 (19%)
21	CLA	a	1108	-	61,65,73	1.45	9 (14%)	72,103,113	1.95	15 (20%)
21	CLA	b	1228	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	14 (17%)
21	CLA	1	1132	-	69,73,73	1.34	8 (11%)	82,113,113	1.81	15 (18%)
21	CLA	B	1219	-	69,73,73	1.34	8 (11%)	82,113,113	1.80	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	1	4002	-	41,41,41	0.66	0	56,56,56	3.35	13 (23%)
21	CLA	1	1111	-	69,73,73	1.36	9 (13%)	82,113,113	1.76	15 (18%)
21	CLA	1	1126	-	69,73,73	1.36	9 (13%)	82,113,113	1.84	14 (17%)
24	BCR	1	4012	-	41,41,41	0.69	0	56,56,56	3.31	9 (16%)
21	CLA	1	1121	-	59,63,73	1.46	9 (15%)	70,101,113	1.90	13 (18%)
22	PQN	2	2002	-	34,34,34	0.40	0	43,45,45	1.29	4 (9%)
21	CLA	1	1134	16	69,73,73	1.34	9 (13%)	82,113,113	1.83	15 (18%)
21	CLA	b	1219	-	64,68,73	1.40	8 (12%)	76,107,113	1.86	16 (21%)
26	LMG	2	5005	-	55,55,55	1.28	6 (10%)	63,63,63	1.08	2 (3%)
24	BCR	2	4004	-	41,41,41	0.70	0	56,56,56	3.36	11 (19%)
21	CLA	l	1502	-	69,73,73	1.34	8 (11%)	82,113,113	1.81	15 (18%)
21	CLA	B	1234	-	69,73,73	1.36	9 (13%)	82,113,113	1.80	14 (17%)
24	BCR	J	4013	-	41,41,41	0.71	0	56,56,56	3.30	10 (17%)
21	CLA	a	1102	-	69,73,73	1.34	9 (13%)	82,113,113	1.87	14 (17%)
21	CLA	b	1223	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	14 (17%)
21	CLA	B	1207	-	69,73,73	1.37	9 (13%)	82,113,113	1.89	16 (19%)
21	CLA	B	1224	-	69,73,73	1.34	9 (13%)	82,113,113	1.79	13 (15%)
21	CLA	k	1402	-	53,57,73	1.53	9 (16%)	61,93,113	2.20	15 (24%)
21	CLA	2	1211	-	54,58,73	1.54	9 (16%)	64,95,113	2.02	14 (21%)
21	CLA	1	1011	-	69,73,73	1.38	9 (13%)	82,113,113	1.85	14 (17%)
21	CLA	2	1226	-	59,63,73	1.46	9 (15%)	70,101,113	1.91	15 (21%)
21	CLA	0	1503	38	69,73,73	1.35	8 (11%)	82,113,113	1.75	14 (17%)
21	CLA	a	1107	1	54,58,73	1.53	9 (16%)	64,95,113	2.03	16 (25%)
21	CLA	6	1301	38	51,55,73	1.57	9 (17%)	60,91,113	1.96	14 (23%)
26	LMG	b	5007	-	55,55,55	1.28	7 (12%)	63,63,63	1.16	3 (4%)
25	LHG	a	5007	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
21	CLA	b	1021	-	69,73,73	1.38	10 (14%)	82,113,113	1.74	12 (14%)
21	CLA	8	1402	-	50,54,73	1.58	9 (18%)	59,90,113	2.00	11 (18%)
21	CLA	b	1222	38	69,73,73	1.32	8 (11%)	82,113,113	1.83	15 (18%)
25	LHG	a	5003	21	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
25	LHG	l	5003	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
21	CLA	a	1109	-	69,73,73	1.34	9 (13%)	82,113,113	1.89	14 (17%)
21	CLA	B	1220	-	61,65,73	1.44	9 (14%)	72,103,113	1.89	15 (20%)
21	CLA	a	1113	-	54,58,73	1.54	9 (16%)	64,95,113	2.00	13 (20%)
24	BCR	2	4005	-	41,41,41	0.74	0	56,56,56	3.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	SF4	c	3002	-	0,12,12	-	-	-		
22	PQN	b	2002	-	34,34,34	0.80	3 (8%)	43,45,45	1.26	5 (11%)
21	CLA	1	1138	-	64,68,73	1.41	9 (14%)	76,107,113	1.85	15 (19%)
21	CLA	2	1234	-	54,58,73	1.55	9 (16%)	64,95,113	2.01	16 (25%)
21	CLA	A	1110	-	69,73,73	1.34	9 (13%)	82,113,113	1.75	13 (15%)
21	CLA	6	1302	6	47,51,73	1.66	9 (19%)	55,86,113	2.27	17 (30%)
21	CLA	2	1240	-	45,49,73	1.65	9 (20%)	54,84,113	2.17	13 (24%)
23	SF4	3	3003	-	0,12,12	-	-	-		
25	LHG	l	5002	-	48,48,48	0.39	0	51,54,54	1.10	4 (7%)
34	ZEX	7	4015	-	43,43,43	6.07	4 (9%)	51,60,60	6.76	10 (19%)
21	CLA	a	1123	-	69,73,73	1.36	9 (13%)	82,113,113	1.80	13 (15%)
21	CLA	A	1012	38	69,73,73	1.36	9 (13%)	82,113,113	1.85	16 (19%)
21	CLA	B	1205	-	69,73,73	1.32	9 (13%)	82,113,113	1.80	11 (13%)
35	LMT	F	6001	-	36,36,36	1.12	5 (13%)	47,47,47	1.00	2 (4%)
21	CLA	1	1120	-	69,73,73	1.35	9 (13%)	82,113,113	1.82	15 (18%)
21	CLA	a	1134	1	53,57,73	1.54	9 (16%)	61,93,113	2.12	14 (22%)
21	CLA	1	1112	-	54,58,73	1.53	9 (16%)	64,95,113	2.09	15 (23%)
24	BCR	A	4019	-	41,41,41	0.72	0	56,56,56	3.68	15 (26%)
21	CLA	1	1106	16	69,73,73	1.34	9 (13%)	82,113,113	1.80	14 (17%)
21	CLA	2	1021	-	69,73,73	1.36	10 (14%)	82,113,113	1.81	12 (14%)
21	CLA	b	1236	-	69,73,73	1.35	9 (13%)	82,113,113	1.78	12 (14%)
21	CLA	L	1501	10	69,73,73	1.36	9 (13%)	82,113,113	1.71	11 (13%)
21	CLA	B	1237	38	69,73,73	1.33	8 (11%)	82,113,113	1.77	13 (15%)
31	SQD	b	5006	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
21	CLA	b	1212	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	14 (17%)
21	CLA	a	1125	-	69,73,73	1.35	9 (13%)	82,113,113	1.86	16 (19%)
21	CLA	1	1119	38	69,73,73	1.35	9 (13%)	82,113,113	1.85	15 (18%)
30	ECH	i	4020	-	42,42,42	0.77	1 (2%)	55,58,58	2.43	16 (29%)
21	CLA	b	1217	-	55,59,73	1.51	9 (16%)	64,96,113	1.97	15 (23%)
21	CLA	B	1223	-	69,73,73	1.35	9 (13%)	82,113,113	1.80	14 (17%)
21	CLA	B	1217	-	69,73,73	1.36	9 (13%)	82,113,113	1.89	18 (21%)
21	CLA	a	1129	-	56,60,73	1.49	9 (16%)	65,97,113	1.96	17 (26%)
25	LHG	B	5004	-	48,48,48	0.37	0	51,54,54	1.14	3 (5%)
26	LMG	A	5008	-	55,55,55	1.28	6 (10%)	63,63,63	1.05	2 (3%)
35	LMT	L	6001	-	36,36,36	1.12	3 (8%)	47,47,47	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	1133	-	69,73,73	1.34	8 (11%)	82,113,113	1.71	13 (15%)
34	ZEX	F	4016	-	43,43,43	6.14	3 (6%)	51,60,60	7.01	10 (19%)
21	CLA	a	1116	-	64,68,73	1.40	9 (14%)	76,107,113	1.87	15 (19%)
21	CLA	1	1133	-	69,73,73	1.36	9 (13%)	82,113,113	1.82	14 (17%)
21	CLA	J	1302	8	69,73,73	1.36	9 (13%)	82,113,113	1.90	14 (17%)
26	LMG	b	5005	-	55,55,55	1.28	6 (10%)	63,63,63	1.31	5 (7%)
21	CLA	b	1208	-	64,68,73	1.39	8 (12%)	76,107,113	1.78	14 (18%)
21	CLA	1	1118	-	69,73,73	1.35	9 (13%)	82,113,113	1.77	13 (15%)
21	CLA	a	1131	-	69,73,73	1.34	9 (13%)	82,113,113	1.73	13 (15%)
21	CLA	2	1237	38	69,73,73	1.33	8 (11%)	82,113,113	1.78	14 (17%)
21	CLA	B	1229	-	69,73,73	1.33	9 (13%)	82,113,113	1.87	15 (18%)
21	CLA	2	1212	-	45,49,73	1.66	9 (20%)	54,84,113	2.19	14 (25%)
21	CLA	A	1140	-	69,73,73	1.33	9 (13%)	82,113,113	1.82	15 (18%)
21	CLA	A	1112	-	69,73,73	1.35	9 (13%)	82,113,113	1.84	15 (18%)
21	CLA	b	1224	-	69,73,73	1.35	9 (13%)	82,113,113	1.78	14 (17%)
21	CLA	a	1121	-	69,73,73	1.36	9 (13%)	82,113,113	1.79	14 (17%)
34	ZEX	j	4015	-	43,43,43	6.06	3 (6%)	51,60,60	6.88	12 (23%)
21	CLA	a	1130	-	69,73,73	1.35	9 (13%)	82,113,113	1.75	14 (17%)
21	CLA	B	1235	-	69,73,73	1.33	9 (13%)	82,113,113	1.89	12 (14%)
25	LHG	6	5001	-	11,11,48	0.48	0	12,14,54	0.53	0
21	CLA	b	1229	-	69,73,73	1.34	8 (11%)	82,113,113	1.83	16 (19%)
26	LMG	B	5002	-	55,55,55	1.29	6 (10%)	63,63,63	1.07	5 (7%)
21	CLA	2	1223	-	59,63,73	1.46	9 (15%)	70,101,113	1.94	13 (18%)
21	CLA	2	1217	-	56,60,73	1.51	9 (16%)	65,97,113	1.96	15 (23%)
25	LHG	0	5002	-	48,48,48	0.39	0	51,54,54	1.05	2 (3%)

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
21	CLA	2	1221	-	1/1/15/20	15/39/115/115	-
21	CLA	J	1303	-	1/1/15/20	22/39/115/115	-
21	CLA	a	1112	-	1/1/15/20	17/39/115/115	-
21	CLA	2	1215	-	1/1/14/20	12/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	K	5009	-	-	17/50/70/70	0/1/1/1
21	CLA	K	1401	38	1/1/15/20	15/39/115/115	-
21	CLA	7	1303	-	1/1/10/20	4/10/86/115	-
24	BCR	1	4007	-	-	14/29/63/63	0/2/2/2
24	BCR	7	4013	-	-	11/29/63/63	0/2/2/2
30	ECH	B	4006	-	-	7/29/66/66	0/2/2/2
25	LHG	F	5002	-	-	40/53/53/53	-
24	BCR	I	4018	-	-	9/29/63/63	0/2/2/2
24	BCR	1	4019	-	-	12/29/63/63	0/2/2/2
21	CLA	F	1302	6	1/1/15/20	21/39/115/115	-
21	CLA	2	1214	-	1/1/13/20	14/32/108/115	-
21	CLA	2	1206	2	1/1/15/20	14/39/115/115	-
21	CLA	B	1238	38	1/1/15/20	8/39/115/115	-
24	BCR	B	4018	-	-	11/29/63/63	0/2/2/2
21	CLA	a	1124	-	1/1/13/20	8/27/103/115	-
21	CLA	2	1023	-	1/1/15/20	14/39/115/115	-
21	CLA	1	1104	-	1/1/15/20	15/39/115/115	-
21	CLA	a	1012	38	1/1/15/20	18/39/115/115	-
21	CLA	A	1137	-	1/1/15/20	14/39/115/115	-
21	CLA	a	1120	-	-	11/27/103/115	-
30	ECH	M	4021	-	-	7/29/66/66	0/2/2/2
21	CLA	a	1122	-	1/1/15/20	21/39/115/115	-
24	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1135	-	-	15/39/115/115	-
26	LMG	A	5004	-	-	18/43/63/70	0/1/1/1
21	CLA	b	1209	-	-	19/39/115/115	-
21	CLA	2	1239	-	1/1/15/20	13/39/115/115	-
25	LHG	L	5005	-	-	23/53/53/53	-
21	CLA	1	1139	-	1/1/15/20	14/39/115/115	-
21	CLA	1	1136	-	1/1/15/20	17/39/115/115	-
21	CLA	A	1121	-	1/1/15/20	18/39/115/115	-
21	CLA	1	1129	-	1/1/12/20	7/21/97/115	-
21	CLA	A	1125	-	-	18/39/115/115	-
26	LMG	A	5002	-	-	22/45/65/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1226	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1127	-	1/1/15/20	15/39/115/115	-
21	CLA	A	1105	-	1/1/15/20	14/39/115/115	-
23	SF4	C	3002	3	-	-	0/6/5/5
30	ECH	b	4006	-	-	7/29/66/66	0/2/2/2
21	CLA	A	1132	-	1/1/15/20	13/39/115/115	-
21	CLA	a	1126	-	1/1/15/20	19/39/115/115	-
21	CLA	1	1105	-	1/1/12/20	5/21/97/115	-
21	CLA	B	1232	-	1/1/12/20	4/21/97/115	-
25	LHG	l	5001	-	-	31/53/53/53	-
21	CLA	B	1230	-	1/1/15/20	21/39/115/115	-
21	CLA	b	1202	-	1/1/15/20	17/39/115/115	-
28	45D	h	4020	21	-	15/29/69/69	0/2/2/2
21	CLA	A	1131	-	1/1/15/20	17/39/115/115	-
21	CLA	1	1137	-	1/1/12/20	8/23/99/115	-
21	CLA	A	1101	-	-	7/39/115/115	-
24	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
21	CLA	1	1135	-	-	12/24/100/115	-
25	LHG	a	5005	-	-	30/53/53/53	-
21	CLA	1	1109	-	1/1/15/20	18/39/115/115	-
21	CLA	j	1303	-	1/1/13/20	12/27/103/115	-
21	CLA	b	1227	-	1/1/15/20	11/39/115/115	-
21	CLA	A	1120	-	1/1/15/20	17/39/115/115	-
24	BCR	B	4014	-	-	8/29/63/63	0/2/2/2
21	CLA	B	1208	-	1/1/15/20	15/39/115/115	-
21	CLA	a	1140	-	1/1/15/20	12/39/115/115	-
21	CLA	b	1235	-	1/1/15/20	17/39/115/115	-
21	CLA	1	1122	-	1/1/14/20	14/33/109/115	-
21	CLA	A	1106	1	1/1/15/20	19/39/115/115	-
35	LMT	0	6001	-	-	12/21/61/61	0/2/2/2
24	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
21	CLA	B	1218	-	1/1/15/20	18/39/115/115	-
25	LHG	0	5004	-	-	31/53/53/53	-
21	CLA	b	1022	-	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	1	5002	-	-	20/45/65/70	0/1/1/1
24	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1106	-	1/1/15/20	19/39/115/115	-
21	CLA	2	1230	-	1/1/11/20	13/18/94/115	-
25	LHG	1	5007	-	-	30/53/53/53	-
21	CLA	b	1218	-	1/1/15/20	17/39/115/115	-
36	EQ3	I	4020	-	-	7/29/68/68	0/2/2/2
24	BCR	B	4017	-	-	10/29/63/63	0/2/2/2
21	CLA	2	1207	-	-	10/29/105/115	-
24	BCR	a	4019	-	-	9/29/63/63	0/2/2/2
24	BCR	b	4005	-	-	11/29/63/63	0/2/2/2
21	CLA	b	1213	-	1/1/15/20	16/39/115/115	-
21	CLA	K	1402	-	-	15/39/115/115	-
25	LHG	1	5003	21	-	30/53/53/53	-
21	CLA	2	1235	-	1/1/12/20	9/25/101/115	-
21	CLA	A	1108	-	1/1/12/20	9/25/101/115	-
21	CLA	A	1138	-	1/1/15/20	12/39/115/115	-
21	CLA	f	1302	-	1/1/15/20	22/39/115/115	-
25	LHG	1	5001	-	-	26/53/53/53	-
21	CLA	A	1107	1	1/1/15/20	19/39/115/115	-
24	BCR	2	4014	-	-	6/29/63/63	0/2/2/2
21	CLA	1	1103	-	1/1/15/20	25/39/115/115	-
24	BCR	0	4022	-	-	9/29/63/63	0/2/2/2
21	CLA	B	1206	2	1/1/15/20	17/39/115/115	-
21	CLA	7	1302	8	1/1/10/20	4/10/86/115	-
26	LMG	b	5002	-	-	12/50/70/70	0/1/1/1
21	CLA	k	1401	-	1/1/12/20	2/21/97/115	-
21	CLA	A	1122	-	1/1/14/20	11/33/109/115	-
21	CLA	A	1114	38	1/1/15/20	18/39/115/115	-
21	CLA	1	1114	-	1/1/11/20	3/15/91/115	-
21	CLA	2	1218	-	1/1/15/20	18/39/115/115	-
21	CLA	B	1209	-	-	19/39/115/115	-
21	CLA	a	1135	-	1/1/15/20	21/39/115/115	-
21	CLA	b	1206	12	1/1/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1107	-	1/1/12/20	9/23/99/115	-
21	CLA	B	1225	-	1/1/15/20	13/39/115/115	-
21	CLA	B	1212	-	1/1/13/20	10/27/103/115	-
21	CLA	B	1227	-	-	11/27/103/115	-
21	CLA	1	1101	-	-	11/39/115/115	-
23	SF4	C	3003	3	-	-	0/6/5/5
21	CLA	b	1230	-	1/1/15/20	21/39/115/115	-
21	CLA	2	1213	-	1/1/12/20	7/21/97/115	-
26	LMG	a	5002	-	-	18/45/65/70	0/1/1/1
21	CLA	A	1115	-	1/1/15/20	9/39/115/115	-
21	CLA	1	1115	-	1/1/15/20	10/39/115/115	-
21	CLA	B	1221	-	1/1/15/20	12/39/115/115	-
21	CLA	B	1240	-	1/1/15/20	18/39/115/115	-
24	BCR	b	4018	-	-	10/29/63/63	0/2/2/2
21	CLA	a	1132	-	1/1/15/20	13/39/115/115	-
24	BCR	b	4010	-	-	9/29/63/63	0/2/2/2
21	CLA	B	1215	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1201	-	1/1/15/20	14/39/115/115	-
21	CLA	2	1202	-	1/1/15/20	19/39/115/115	-
24	BCR	A	4001	-	-	5/29/63/63	0/2/2/2
21	CLA	B	1202	-	1/1/15/20	15/39/115/115	-
24	BCR	h	4018	-	-	13/29/63/63	0/2/2/2
30	ECH	m	4021	-	-	7/29/66/66	0/2/2/2
21	CLA	B	1022	38	1/1/15/20	7/39/115/115	-
21	CLA	A	1103	-	1/1/15/20	16/39/115/115	-
26	LMG	a	5004	-	-	15/50/70/70	0/1/1/1
21	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
25	LHG	A	5005	-	-	35/53/53/53	-
21	CLA	2	1229	-	1/1/15/20	20/39/115/115	-
21	CLA	2	1209	-	-	6/15/91/115	-
25	LHG	1	5005	-	-	35/53/53/53	-
21	CLA	l	1501	10	1/1/15/20	20/39/115/115	-
24	BCR	L	4022	-	-	8/29/63/63	0/2/2/2
21	CLA	A	1123	38	1/1/15/20	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	1128	-	1/1/15/20	24/39/115/115	-
34	ZEX	J	4015	-	-	3/29/67/67	0/2/2/2
24	BCR	A	4008	-	-	5/29/63/63	0/2/2/2
24	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
21	CLA	8	1401	-	1/1/11/20	6/15/91/115	-
21	CLA	F	1301	38	1/1/15/20	15/39/115/115	-
21	CLA	2	1227	-	1/1/11/20	2/15/91/115	-
21	CLA	B	1023	-	1/1/15/20	5/39/115/115	-
21	CLA	b	1220	-	1/1/15/20	12/39/115/115	-
35	LMT	l	6001	-	-	5/21/61/61	0/2/2/2
24	BCR	j	4013	-	-	9/29/63/63	0/2/2/2
24	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
21	CLA	A	1104	-	1/1/15/20	16/39/115/115	-
25	LHG	A	5001	-	-	34/53/53/53	-
24	BCR	2	4010	-	-	12/29/63/63	0/2/2/2
21	CLA	2	1201	-	1/1/15/20	10/39/115/115	-
24	BCR	2	4011	-	-	15/29/63/63	0/2/2/2
21	CLA	b	1204	-	1/1/15/20	12/39/115/115	-
24	BCR	9	4021	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1204	-	1/1/15/20	13/39/115/115	-
21	CLA	b	1207	-	-	11/39/115/115	-
24	BCR	b	4014	-	-	9/29/63/63	0/2/2/2
21	CLA	A	1118	-	1/1/15/20	15/39/115/115	-
21	CLA	2	1022	38	1/1/15/20	7/39/115/115	-
23	SF4	A	3001	2,1	-	-	0/6/5/5
25	LHG	l	5004	-	-	27/53/53/53	-
21	CLA	l	1503	-	1/1/15/20	21/39/115/115	-
23	SF4	3	3002	-	-	-	0/6/5/5
21	CLA	A	1139	38	1/1/15/20	15/39/115/115	-
21	CLA	L	1502	-	1/1/15/20	13/39/115/115	-
24	BCR	l	4022	-	-	14/29/63/63	0/2/2/2
21	CLA	2	1228	-	1/1/11/20	9/15/91/115	-
21	CLA	a	1127	-	1/1/15/20	19/39/115/115	-
21	CLA	1	1124	-	1/1/13/20	10/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1123	-	-	15/39/115/115	-
25	LHG	b	5004	-	-	22/53/53/53	-
21	CLA	a	1114	-	1/1/12/20	8/24/100/115	-
24	BCR	6	4016	-	-	14/29/63/63	0/2/2/2
24	BCR	0	4019	-	-	10/29/63/63	0/2/2/2
24	BCR	a	4002	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1228	-	1/1/15/20	15/39/115/115	-
24	BCR	k	4001	-	-	10/29/63/63	0/2/2/2
21	CLA	f	1301	38	1/1/12/20	5/21/97/115	-
21	CLA	A	1130	-	1/1/14/20	6/33/109/115	-
21	CLA	2	1204	-	1/1/15/20	11/39/115/115	-
21	CLA	A	1117	-	1/1/15/20	13/39/115/115	-
21	CLA	L	1503	38	-	17/39/115/115	-
24	BCR	b	4017	-	-	9/29/63/63	0/2/2/2
21	CLA	1	1013	-	1/1/15/20	17/39/115/115	-
21	CLA	1	1117	-	1/1/15/20	14/39/115/115	-
21	CLA	A	1129	-	-	11/31/107/115	-
21	CLA	a	1101	-	-	9/39/115/115	-
21	CLA	a	1105	-	1/1/13/20	9/31/107/115	-
31	SQD	L	5001	-	-	21/46/66/69	0/1/1/1
21	CLA	0	1501	20	1/1/15/20	15/39/115/115	-
21	CLA	A	1801	25	1/1/15/20	18/39/115/115	-
21	CLA	2	1232	-	1/1/11/20	6/15/91/115	-
24	BCR	2	4018	-	-	14/29/63/63	0/2/2/2
21	CLA	a	1011	-	1/1/15/20	17/39/115/115	-
24	BCR	1	4003	-	-	11/29/63/63	0/2/2/2
21	CLA	B	1216	38	1/1/15/20	23/39/115/115	-
31	SQD	0	5005	-	-	27/49/69/69	0/1/1/1
26	LMG	2	5002	-	-	11/50/70/70	0/1/1/1
21	CLA	2	1224	-	1/1/13/20	15/27/103/115	-
21	CLA	1	1012	38	1/1/15/20	16/39/115/115	-
21	CLA	A	1136	-	1/1/15/20	17/39/115/115	-
23	SF4	c	3003	13	-	-	0/6/5/5
22	PQN	A	2001	-	-	10/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1222	38	1/1/13/20	7/27/103/115	-
21	CLA	B	1214	-	1/1/15/20	19/39/115/115	-
21	CLA	A	1128	-	1/1/15/20	15/39/115/115	-
22	PQN	1	2001	-	-	3/23/43/43	0/2/2/2
24	BCR	A	4007	-	-	8/29/63/63	0/2/2/2
21	CLA	1	1128	-	1/1/15/20	18/39/115/115	-
24	BCR	8	4001	-	-	8/29/63/63	0/2/2/2
23	SF4	1	3001	2,16	-	-	0/6/5/5
25	LHG	A	5003	21	-	26/53/53/53	-
21	CLA	2	1219	-	-	11/25/101/115	-
21	CLA	1	1801	25	1/1/13/20	9/29/105/115	-
21	CLA	A	1102	21	1/1/15/20	15/39/115/115	-
21	CLA	2	1220	-	1/1/11/20	6/15/91/115	-
21	CLA	a	1138	-	1/1/15/20	11/39/115/115	-
21	CLA	b	1221	38	1/1/15/20	13/39/115/115	-
31	SQD	L	5002	-	-	18/49/69/69	0/1/1/1
21	CLA	b	1215	-	1/1/15/20	16/39/115/115	-
21	CLA	b	1238	38	1/1/15/20	5/39/115/115	-
21	CLA	1	1110	-	1/1/12/20	8/21/97/115	-
21	CLA	a	1013	-	1/1/15/20	10/39/115/115	-
21	CLA	A	1119	38	1/1/15/20	16/39/115/115	-
24	BCR	a	4012	-	-	7/29/63/63	0/2/2/2
21	CLA	B	1213	-	1/1/15/20	14/39/115/115	-
30	ECH	b	4011	-	-	11/29/66/66	0/2/2/2
21	CLA	a	1103	-	1/1/15/20	20/39/115/115	-
21	CLA	2	1222	-	1/1/12/20	6/21/97/115	-
21	CLA	B	1231	38	-	19/39/115/115	-
21	CLA	b	1240	-	1/1/15/20	20/39/115/115	-
21	CLA	a	1119	-	1/1/15/20	14/39/115/115	-
21	CLA	b	1023	-	1/1/15/20	10/39/115/115	-
21	CLA	a	1139	38	1/1/15/20	12/39/115/115	-
24	BCR	i	4018	-	-	11/29/63/63	0/2/2/2
21	CLA	b	1226	-	1/1/15/20	13/39/115/115	-
21	CLA	b	1239	-	1/1/15/20	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	1237	38	1/1/15/20	12/39/115/115	-
21	CLA	A	1116	-	1/1/15/20	23/39/115/115	-
21	CLA	b	1232	-	1/1/15/20	17/39/115/115	-
21	CLA	a	1118	-	1/1/15/20	19/39/115/115	-
28	45D	B	4011	-	-	11/29/69/69	0/2/2/2
21	CLA	1	1108	-	1/1/11/20	10/17/93/115	-
21	CLA	2	1238	38	1/1/15/20	11/39/115/115	-
23	SF4	a	3001	1,12	-	-	0/6/5/5
25	LHG	A	5007	-	-	29/53/53/53	-
21	CLA	a	1117	-	1/1/15/20	18/39/115/115	-
21	CLA	2	1205	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1109	21	1/1/15/20	17/39/115/115	-
21	CLA	b	1216	38	1/1/15/20	23/39/115/115	-
21	CLA	j	1302	-	1/1/15/20	16/39/115/115	-
24	BCR	l	4019	-	-	6/29/63/63	0/2/2/2
26	LMG	0	5001	-	-	25/50/70/70	0/1/1/1
21	CLA	0	1502	28	1/1/15/20	12/39/115/115	-
21	CLA	2	1231	38	1/1/11/20	4/17/93/115	-
21	CLA	a	1137	-	1/1/12/20	5/21/97/115	-
25	LHG	B	5006	-	-	34/53/53/53	-
37	DGD	L	5004	-	-	23/55/95/95	0/2/2/2
21	CLA	b	1234	-	1/1/12/20	4/25/101/115	-
21	CLA	1	1102	-	1/1/13/20	10/27/103/115	-
24	BCR	b	4004	-	-	13/29/63/63	0/2/2/2
24	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
21	CLA	B	1210	-	-	18/39/115/115	-
21	CLA	b	1214	-	1/1/15/20	18/39/115/115	-
24	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
25	LHG	2	5004	-	-	25/53/53/53	-
21	CLA	B	1203	-	1/1/15/20	15/39/115/115	-
31	SQD	B	5008	-	-	23/49/69/69	0/1/1/1
22	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
26	LMG	1	5004	-	-	19/50/70/70	0/1/1/1
21	CLA	1	1131	-	1/1/15/20	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	F	5001	-	-	23/49/69/69	0/1/1/1
24	BCR	a	4007	-	-	9/29/63/63	0/2/2/2
21	CLA	b	1203	-	1/1/15/20	15/39/115/115	-
21	CLA	a	1801	25	1/1/13/20	14/27/103/115	-
21	CLA	2	1216	-	1/1/12/20	7/21/97/115	-
21	CLA	b	1225	-	1/1/15/20	11/39/115/115	-
21	CLA	1	1125	-	1/1/15/20	15/39/115/115	-
24	BCR	1	4001	-	-	8/29/63/63	0/2/2/2
21	CLA	1	1140	-	1/1/15/20	16/39/115/115	-
21	CLA	b	1210	-	-	21/39/115/115	-
21	CLA	A	1113	-	1/1/15/20	21/39/115/115	-
21	CLA	b	1205	-	1/1/15/20	10/39/115/115	-
21	CLA	1	1113	-	1/1/10/20	7/14/90/115	-
21	CLA	B	1236	-	1/1/12/20	5/21/97/115	-
21	CLA	B	1239	-	1/1/15/20	17/39/115/115	-
21	CLA	B	1021	-	1/1/15/20	8/39/115/115	-
25	LHG	M	5001	-	-	30/53/53/53	-
21	CLA	A	1011	-	1/1/15/20	10/39/115/115	-
21	CLA	2	1225	-	1/1/15/20	16/39/115/115	-
21	CLA	b	1201	-	1/1/15/20	12/39/115/115	-
21	CLA	a	1115	-	-	10/39/115/115	-
35	LMT	1	6001	-	-	8/21/61/61	0/2/2/2
21	CLA	a	1104	-	1/1/15/20	23/39/115/115	-
25	LHG	a	5001	-	-	26/53/53/53	-
21	CLA	a	1110	-	1/1/13/20	19/32/108/115	-
21	CLA	b	1211	-	1/1/15/20	17/39/115/115	-
24	BCR	1	4008	-	-	7/29/63/63	0/2/2/2
21	CLA	A	1126	-	1/1/15/20	16/39/115/115	-
24	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
21	CLA	2	1210	-	-	22/39/115/115	-
21	CLA	A	1134	1	1/1/15/20	15/39/115/115	-
21	CLA	b	1231	38	1/1/15/20	21/39/115/115	-
21	CLA	2	1203	-	1/1/15/20	18/39/115/115	-
22	PQN	B	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
21	CLA	a	1136	-	1/1/15/20	17/39/115/115	-
24	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
21	CLA	A	1111	-	1/1/15/20	11/39/115/115	-
26	LMG	B	5005	-	-	11/50/70/70	0/1/1/1
24	BCR	B	4004	-	-	15/29/63/63	0/2/2/2
30	ECH	2	4006	-	-	11/29/66/66	0/2/2/2
21	CLA	1	1130	-	1/1/13/20	9/27/103/115	-
24	BCR	2	4017	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1133	-	-	17/39/115/115	-
21	CLA	2	1208	-	1/1/14/20	12/33/109/115	-
21	CLA	A	1124	38	1/1/15/20	10/39/115/115	-
21	CLA	B	1211	-	1/1/15/20	18/39/115/115	-
25	LHG	A	5006	-	-	28/53/53/53	-
21	CLA	2	1236	-	1/1/12/20	8/21/97/115	-
24	BCR	a	4003	-	-	10/29/63/63	0/2/2/2
31	SQD	f	5001	-	-	19/49/69/69	0/1/1/1
21	CLA	a	1111	-	1/1/15/20	17/39/115/115	-
21	CLA	1	1127	-	1/1/15/20	21/39/115/115	-
21	CLA	1	1116	-	1/1/15/20	19/39/115/115	-
21	CLA	a	1108	-	1/1/13/20	13/30/106/115	-
21	CLA	b	1228	-	1/1/15/20	15/39/115/115	-
21	CLA	1	1132	-	1/1/15/20	11/39/115/115	-
21	CLA	B	1219	-	-	16/39/115/115	-
24	BCR	1	4002	-	-	14/29/63/63	0/2/2/2
21	CLA	1	1111	-	1/1/15/20	13/39/115/115	-
21	CLA	1	1126	-	1/1/15/20	18/39/115/115	-
24	BCR	1	4012	-	-	13/29/63/63	0/2/2/2
21	CLA	1	1121	-	1/1/13/20	12/27/103/115	-
22	PQN	2	2002	-	-	7/23/43/43	0/2/2/2
21	CLA	1	1134	16	1/1/15/20	21/39/115/115	-
21	CLA	b	1219	-	1/1/14/20	18/33/109/115	-
26	LMG	2	5005	-	-	18/50/70/70	0/1/1/1
24	BCR	2	4004	-	-	13/29/63/63	0/2/2/2
21	CLA	l	1502	-	1/1/15/20	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1234	-	-	11/39/115/115	-
24	BCR	J	4013	-	-	13/29/63/63	0/2/2/2
21	CLA	a	1102	-	1/1/15/20	11/39/115/115	-
21	CLA	b	1223	-	1/1/15/20	9/39/115/115	-
21	CLA	B	1207	-	-	11/39/115/115	-
21	CLA	B	1224	-	1/1/15/20	20/39/115/115	-
21	CLA	k	1402	-	1/1/11/20	13/20/96/115	-
21	CLA	2	1211	-	1/1/12/20	10/21/97/115	-
21	CLA	1	1011	-	1/1/15/20	11/39/115/115	-
21	CLA	2	1226	-	1/1/13/20	12/27/103/115	-
21	CLA	0	1503	38	1/1/15/20	18/39/115/115	-
21	CLA	a	1107	1	1/1/12/20	6/21/97/115	-
21	CLA	6	1301	38	1/1/11/20	5/18/94/115	-
26	LMG	b	5007	-	-	18/50/70/70	0/1/1/1
25	LHG	a	5007	-	-	33/53/53/53	-
21	CLA	b	1021	-	1/1/15/20	22/39/115/115	-
21	CLA	8	1402	-	1/1/11/20	7/17/93/115	-
21	CLA	b	1222	38	1/1/15/20	15/39/115/115	-
25	LHG	a	5003	21	-	39/53/53/53	-
25	LHG	l	5003	-	-	33/53/53/53	-
21	CLA	a	1109	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1220	-	1/1/13/20	13/30/106/115	-
21	CLA	a	1113	-	1/1/12/20	9/21/97/115	-
24	BCR	2	4005	-	-	11/29/63/63	0/2/2/2
23	SF4	c	3002	-	-	-	0/6/5/5
22	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
21	CLA	1	1138	-	1/1/14/20	10/33/109/115	-
21	CLA	2	1234	-	1/1/12/20	7/21/97/115	-
21	CLA	A	1110	-	1/1/15/20	19/39/115/115	-
21	CLA	6	1302	6	1/1/10/20	4/13/89/115	-
21	CLA	2	1240	-	-	4/10/86/115	-
25	LHG	l	5002	-	-	30/53/53/53	-
23	SF4	3	3003	-	-	-	0/6/5/5
34	ZEX	7	4015	-	-	7/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	1123	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1012	38	1/1/15/20	20/39/115/115	-
21	CLA	B	1205	-	1/1/15/20	14/39/115/115	-
35	LMT	F	6001	-	-	8/21/61/61	0/2/2/2
21	CLA	1	1120	-	1/1/15/20	18/39/115/115	-
21	CLA	a	1134	1	1/1/11/20	9/20/96/115	-
21	CLA	1	1112	-	1/1/12/20	9/21/97/115	-
24	BCR	A	4019	-	-	9/29/63/63	0/2/2/2
21	CLA	1	1106	16	1/1/15/20	17/39/115/115	-
21	CLA	2	1021	-	1/1/15/20	12/39/115/115	-
21	CLA	b	1236	-	1/1/15/20	14/39/115/115	-
21	CLA	L	1501	10	1/1/15/20	16/39/115/115	-
21	CLA	B	1237	38	1/1/15/20	12/39/115/115	-
31	SQD	b	5006	-	-	27/49/69/69	0/1/1/1
21	CLA	b	1212	-	-	15/39/115/115	-
21	CLA	a	1125	-	1/1/15/20	12/39/115/115	-
21	CLA	1	1119	38	1/1/15/20	13/39/115/115	-
30	ECH	i	4020	-	-	10/29/66/66	0/2/2/2
21	CLA	b	1217	-	1/1/12/20	13/23/99/115	-
21	CLA	B	1223	-	1/1/15/20	10/39/115/115	-
21	CLA	B	1217	-	1/1/15/20	15/39/115/115	-
21	CLA	a	1129	-	1/1/12/20	9/24/100/115	-
25	LHG	B	5004	-	-	28/53/53/53	-
26	LMG	A	5008	-	-	24/50/70/70	0/1/1/1
35	LMT	L	6001	-	-	9/21/61/61	0/2/2/2
21	CLA	A	1133	-	1/1/15/20	13/39/115/115	-
34	ZEX	F	4016	-	1/1/12/27	7/29/67/67	0/2/2/2
21	CLA	a	1116	-	1/1/14/20	10/33/109/115	-
21	CLA	1	1133	-	1/1/15/20	20/39/115/115	-
21	CLA	J	1302	8	1/1/15/20	14/39/115/115	-
26	LMG	b	5005	-	-	18/50/70/70	0/1/1/1
21	CLA	b	1208	-	1/1/14/20	13/33/109/115	-
21	CLA	1	1118	-	1/1/15/20	12/39/115/115	-
21	CLA	a	1131	-	1/1/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	1237	38	1/1/15/20	15/39/115/115	-
21	CLA	B	1229	-	1/1/15/20	16/39/115/115	-
21	CLA	2	1212	-	1/1/10/20	6/10/86/115	-
21	CLA	A	1140	-	1/1/15/20	19/39/115/115	-
21	CLA	A	1112	-	1/1/15/20	19/39/115/115	-
21	CLA	b	1224	-	1/1/15/20	12/39/115/115	-
21	CLA	a	1121	-	1/1/15/20	20/39/115/115	-
34	ZEX	j	4015	-	-	7/29/67/67	0/2/2/2
21	CLA	a	1130	-	1/1/15/20	15/39/115/115	-
21	CLA	B	1235	-	1/1/15/20	11/39/115/115	-
25	LHG	6	5001	-	-	4/12/12/53	-
21	CLA	b	1229	-	1/1/15/20	12/39/115/115	-
26	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
21	CLA	2	1223	-	-	7/27/103/115	-
21	CLA	2	1217	-	1/1/12/20	13/24/100/115	-
25	LHG	0	5002	-	-	23/53/53/53	-

All (2723) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	4016	ZEX	C38-C24	39.93	2.55	1.53
34	J	4015	ZEX	C38-C24	39.48	2.54	1.53
34	j	4015	ZEX	C38-C24	39.41	2.54	1.53
34	7	4015	ZEX	C38-C24	39.40	2.54	1.53
28	h	4020	45D	C08-C16	13.47	1.54	1.35
36	I	4020	EQ3	C25-C26	13.39	1.54	1.35
28	B	4011	45D	C08-C16	12.95	1.53	1.35
28	h	4020	45D	C07-C15	12.67	1.53	1.35
28	B	4011	45D	C07-C15	11.93	1.52	1.35
36	I	4020	EQ3	C5-C6	11.19	1.53	1.34
36	I	4020	EQ3	C4-C3	11.18	1.71	1.52
36	I	4020	EQ3	C2-C3	-6.52	1.43	1.52
21	B	1238	CLA	MG-NA	6.49	2.21	2.06
21	B	1210	CLA	MG-NA	6.47	2.21	2.06
21	a	1101	CLA	MG-NA	6.47	2.21	2.06
21	B	1213	CLA	MG-NA	6.46	2.21	2.06
21	1	1127	CLA	MG-NA	6.46	2.21	2.06
21	b	1238	CLA	MG-NA	6.45	2.21	2.06
21	a	1120	CLA	MG-NA	6.45	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1240	CLA	MG-NA	6.44	2.21	2.06
21	1	1121	CLA	MG-NA	6.44	2.21	2.06
21	A	1123	CLA	MG-NA	6.43	2.21	2.06
21	1	1124	CLA	MG-NA	6.43	2.21	2.06
21	2	1218	CLA	MG-NA	6.43	2.21	2.06
21	1	1123	CLA	MG-NA	6.43	2.21	2.06
21	A	1113	CLA	MG-NA	6.43	2.21	2.06
21	a	1108	CLA	MG-NA	6.42	2.21	2.06
21	A	1127	CLA	MG-NA	6.42	2.21	2.06
21	a	1123	CLA	MG-NA	6.42	2.21	2.06
21	2	1209	CLA	MG-NA	6.42	2.21	2.06
21	A	1105	CLA	MG-NA	6.41	2.21	2.06
21	2	1219	CLA	MG-NA	6.41	2.21	2.06
21	a	1121	CLA	MG-NA	6.41	2.21	2.06
21	B	1209	CLA	MG-NA	6.41	2.21	2.06
21	A	1136	CLA	MG-NA	6.41	2.21	2.06
21	j	1303	CLA	MG-NA	6.41	2.21	2.06
21	B	1239	CLA	MG-NA	6.41	2.21	2.06
21	A	1122	CLA	MG-NA	6.40	2.21	2.06
21	b	1226	CLA	MG-NA	6.40	2.21	2.06
21	1	1128	CLA	MG-NA	6.40	2.21	2.06
21	1	1101	CLA	MG-NA	6.39	2.21	2.06
21	B	1207	CLA	MG-NA	6.39	2.21	2.06
21	1	1114	CLA	MG-NA	6.39	2.21	2.06
21	1	1125	CLA	MG-NA	6.39	2.21	2.06
21	b	1240	CLA	MG-NA	6.39	2.21	2.06
21	A	1012	CLA	MG-NA	6.39	2.21	2.06
21	a	1136	CLA	MG-NA	6.38	2.21	2.06
21	1	1105	CLA	MG-NA	6.38	2.21	2.06
21	8	1401	CLA	MG-NA	6.38	2.21	2.06
21	2	1234	CLA	MG-NA	6.38	2.21	2.06
21	A	1114	CLA	MG-NA	6.38	2.21	2.06
21	b	1218	CLA	MG-NA	6.38	2.21	2.06
21	B	1022	CLA	MG-NA	6.37	2.21	2.06
21	1	1111	CLA	MG-NA	6.37	2.21	2.06
21	1	1120	CLA	MG-NA	6.37	2.21	2.06
21	A	1118	CLA	MG-NA	6.37	2.21	2.06
21	a	1114	CLA	MG-NA	6.37	2.21	2.06
21	a	1137	CLA	MG-NA	6.36	2.21	2.06
21	a	1133	CLA	MG-NA	6.36	2.21	2.06
21	b	1217	CLA	MG-NA	6.36	2.21	2.06
21	f	1301	CLA	MG-NA	6.35	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1212	CLA	MG-NA	6.35	2.21	2.06
21	2	1214	CLA	MG-NA	6.35	2.21	2.06
21	F	1302	CLA	MG-NA	6.35	2.21	2.06
21	2	1211	CLA	MG-NA	6.35	2.21	2.06
21	k	1401	CLA	MG-NA	6.35	2.21	2.06
21	2	1240	CLA	MG-NA	6.35	2.21	2.06
21	1	1135	CLA	MG-NA	6.34	2.21	2.06
21	B	1234	CLA	MG-NA	6.34	2.21	2.06
21	A	1117	CLA	MG-NA	6.34	2.21	2.06
21	b	1239	CLA	MG-NA	6.34	2.21	2.06
21	a	1117	CLA	MG-NA	6.34	2.21	2.06
21	1	1113	CLA	MG-NA	6.34	2.21	2.06
21	B	1218	CLA	MG-NA	6.34	2.21	2.06
21	2	1238	CLA	MG-NA	6.33	2.21	2.06
21	B	1216	CLA	MG-NA	6.33	2.21	2.06
21	a	1105	CLA	MG-NA	6.33	2.21	2.06
21	6	1301	CLA	MG-NA	6.33	2.21	2.06
21	F	1301	CLA	MG-NA	6.33	2.21	2.06
21	B	1204	CLA	MG-NA	6.32	2.21	2.06
21	a	1113	CLA	MG-NA	6.32	2.21	2.06
21	8	1402	CLA	MG-NA	6.32	2.21	2.06
21	A	1131	CLA	MG-NA	6.32	2.21	2.06
21	a	1134	CLA	MG-NA	6.32	2.21	2.06
21	2	1220	CLA	MG-NA	6.32	2.21	2.06
21	1	1139	CLA	MG-NA	6.32	2.21	2.06
21	2	1239	CLA	MG-NA	6.31	2.21	2.06
21	b	1228	CLA	MG-NA	6.31	2.21	2.06
21	B	1220	CLA	MG-NA	6.31	2.21	2.06
21	A	1134	CLA	MG-NA	6.31	2.21	2.06
21	f	1302	CLA	MG-NA	6.31	2.21	2.06
21	B	1232	CLA	MG-NA	6.31	2.21	2.06
21	a	1140	CLA	MG-NA	6.31	2.21	2.06
21	1	1129	CLA	MG-NA	6.31	2.21	2.06
21	A	1101	CLA	MG-NA	6.31	2.21	2.06
21	6	1302	CLA	MG-NA	6.31	2.21	2.06
21	7	1303	CLA	MG-NA	6.31	2.21	2.06
21	b	1221	CLA	MG-NA	6.30	2.21	2.06
21	a	1135	CLA	MG-NA	6.30	2.21	2.06
21	a	1139	CLA	MG-NA	6.30	2.21	2.06
21	2	1236	CLA	MG-NA	6.30	2.21	2.06
21	A	1130	CLA	MG-NA	6.30	2.21	2.06
21	B	1223	CLA	MG-NA	6.30	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1230	CLA	MG-NA	6.29	2.21	2.06
21	L	1501	CLA	MG-NA	6.29	2.21	2.06
21	a	1801	CLA	MG-NA	6.29	2.21	2.06
21	a	1130	CLA	MG-NA	6.29	2.21	2.06
21	2	1217	CLA	MG-NA	6.29	2.21	2.06
21	A	1125	CLA	MG-NA	6.29	2.21	2.06
21	1	1112	CLA	MG-NA	6.29	2.21	2.06
21	b	1209	CLA	MG-NA	6.29	2.21	2.06
21	1	1108	CLA	MG-NA	6.29	2.21	2.06
21	B	1214	CLA	MG-NA	6.29	2.21	2.06
21	2	1226	CLA	MG-NA	6.29	2.21	2.06
21	a	1110	CLA	MG-NA	6.29	2.21	2.06
21	b	1236	CLA	MG-NA	6.29	2.21	2.06
21	1	1137	CLA	MG-NA	6.29	2.21	2.06
21	7	1302	CLA	MG-NA	6.29	2.21	2.06
21	K	1402	CLA	MG-NA	6.29	2.21	2.06
21	b	1214	CLA	MG-NA	6.29	2.21	2.06
21	a	1127	CLA	MG-NA	6.29	2.21	2.06
21	A	1120	CLA	MG-NA	6.28	2.21	2.06
21	a	1118	CLA	MG-NA	6.28	2.21	2.06
21	1	1130	CLA	MG-NA	6.28	2.21	2.06
21	1	1136	CLA	MG-NA	6.28	2.21	2.06
21	a	1115	CLA	MG-NA	6.28	2.21	2.06
21	1	1138	CLA	MG-NA	6.28	2.21	2.06
21	B	1219	CLA	MG-NA	6.28	2.21	2.06
21	2	1225	CLA	MG-NA	6.28	2.21	2.06
21	B	1225	CLA	MG-NA	6.28	2.21	2.06
21	2	1208	CLA	MG-NA	6.28	2.21	2.06
21	2	1212	CLA	MG-NA	6.28	2.21	2.06
21	1	1102	CLA	MG-NA	6.27	2.21	2.06
21	1	1117	CLA	MG-NA	6.27	2.21	2.06
21	A	1112	CLA	MG-NA	6.27	2.21	2.06
21	A	1135	CLA	MG-NA	6.27	2.21	2.06
21	a	1107	CLA	MG-NA	6.27	2.21	2.06
21	A	1128	CLA	MG-NA	6.27	2.21	2.06
21	1	1801	CLA	MG-NA	6.27	2.21	2.06
21	b	1220	CLA	MG-NA	6.27	2.21	2.06
21	b	1219	CLA	MG-NA	6.27	2.21	2.06
21	b	1234	CLA	MG-NA	6.27	2.21	2.06
21	L	1503	CLA	MG-NA	6.26	2.21	2.06
21	2	1210	CLA	MG-NA	6.26	2.21	2.06
21	B	1212	CLA	MG-NA	6.26	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1138	CLA	MG-NA	6.26	2.21	2.06
21	b	1232	CLA	MG-NA	6.26	2.21	2.06
21	2	1227	CLA	MG-NA	6.26	2.21	2.06
21	1	1109	CLA	MG-NA	6.26	2.21	2.06
21	a	1125	CLA	MG-NA	6.26	2.21	2.06
21	1	1122	CLA	MG-NA	6.26	2.21	2.06
21	a	1129	CLA	MG-NA	6.26	2.21	2.06
21	2	1203	CLA	MG-NA	6.26	2.21	2.06
21	2	1221	CLA	MG-NA	6.25	2.21	2.06
21	2	1222	CLA	MG-NA	6.25	2.21	2.06
21	0	1503	CLA	MG-NA	6.25	2.21	2.06
21	j	1302	CLA	MG-NA	6.25	2.21	2.06
21	B	1237	CLA	MG-NA	6.25	2.21	2.06
21	B	1208	CLA	MG-NA	6.25	2.21	2.06
21	J	1303	CLA	MG-NA	6.24	2.21	2.06
21	B	1203	CLA	MG-NA	6.24	2.21	2.06
21	2	1223	CLA	MG-NA	6.24	2.21	2.06
21	A	1116	CLA	MG-NA	6.24	2.21	2.06
21	B	1217	CLA	MG-NA	6.24	2.21	2.06
21	1	1115	CLA	MG-NA	6.24	2.21	2.06
21	b	1223	CLA	MG-NA	6.24	2.21	2.06
21	a	1012	CLA	MG-NA	6.24	2.21	2.06
21	a	1122	CLA	MG-NA	6.23	2.21	2.06
21	a	1116	CLA	MG-NA	6.23	2.21	2.06
21	1	1134	CLA	MG-NA	6.23	2.21	2.06
21	2	1232	CLA	MG-NA	6.23	2.21	2.06
21	2	1215	CLA	MG-NA	6.23	2.21	2.06
21	A	1140	CLA	MG-NA	6.23	2.21	2.06
21	1	1118	CLA	MG-NA	6.23	2.21	2.06
21	1	1140	CLA	MG-NA	6.22	2.21	2.06
21	B	1211	CLA	MG-NA	6.22	2.21	2.06
21	A	1137	CLA	MG-NA	6.22	2.21	2.06
21	b	1210	CLA	MG-NA	6.22	2.21	2.06
21	A	1115	CLA	MG-NA	6.22	2.21	2.06
21	a	1112	CLA	MG-NA	6.22	2.21	2.06
21	1	1126	CLA	MG-NA	6.22	2.21	2.06
21	1	1110	CLA	MG-NA	6.21	2.21	2.06
21	b	1206	CLA	MG-NA	6.21	2.21	2.06
21	B	1236	CLA	MG-NA	6.21	2.21	2.06
21	1	1116	CLA	MG-NA	6.21	2.21	2.06
21	A	1104	CLA	MG-NA	6.21	2.21	2.06
21	B	1227	CLA	MG-NA	6.21	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1131	CLA	MG-NA	6.21	2.21	2.06
21	b	1225	CLA	MG-NA	6.21	2.21	2.06
21	1	1107	CLA	MG-NA	6.21	2.21	2.06
21	b	1213	CLA	MG-NA	6.21	2.21	2.06
21	a	1132	CLA	MG-NA	6.21	2.21	2.06
21	l	1502	CLA	MG-NA	6.20	2.21	2.06
21	A	1133	CLA	MG-NA	6.20	2.21	2.06
21	b	1229	CLA	MG-NA	6.20	2.21	2.06
21	k	1402	CLA	MG-NA	6.20	2.21	2.06
21	b	1208	CLA	MG-NA	6.20	2.21	2.06
21	1	1104	CLA	MG-NA	6.20	2.21	2.06
21	2	1207	CLA	MG-NA	6.20	2.21	2.06
21	b	1207	CLA	MG-NA	6.20	2.21	2.06
21	J	1302	CLA	MG-NA	6.20	2.21	2.06
21	b	1022	CLA	MG-NA	6.20	2.21	2.06
21	2	1202	CLA	MG-NA	6.20	2.21	2.06
21	a	1111	CLA	MG-NA	6.19	2.21	2.06
21	a	1119	CLA	MG-NA	6.19	2.21	2.06
21	b	1203	CLA	MG-NA	6.19	2.21	2.06
21	A	1102	CLA	MG-NA	6.19	2.21	2.06
21	a	1109	CLA	MG-NA	6.19	2.21	2.06
21	2	1229	CLA	MG-NA	6.19	2.21	2.06
21	A	1109	CLA	MG-NA	6.19	2.21	2.06
21	K	1401	CLA	MG-NA	6.19	2.21	2.06
21	1	1106	CLA	MG-NA	6.18	2.21	2.06
21	A	1132	CLA	MG-NA	6.18	2.21	2.06
21	1	1133	CLA	MG-NA	6.18	2.21	2.06
21	A	1129	CLA	MG-NA	6.18	2.20	2.06
21	A	1111	CLA	MG-NA	6.18	2.20	2.06
21	1	1011	CLA	MG-NA	6.18	2.20	2.06
21	B	1201	CLA	MG-NA	6.17	2.20	2.06
21	l	1501	CLA	MG-NA	6.17	2.20	2.06
21	0	1501	CLA	MG-NA	6.17	2.20	2.06
21	B	1228	CLA	MG-NA	6.17	2.20	2.06
21	2	1204	CLA	MG-NA	6.16	2.20	2.06
21	a	1128	CLA	MG-NA	6.16	2.20	2.06
21	2	1022	CLA	MG-NA	6.16	2.20	2.06
21	2	1206	CLA	MG-NA	6.16	2.20	2.06
21	2	1235	CLA	MG-NA	6.16	2.20	2.06
21	A	1801	CLA	MG-NA	6.16	2.20	2.06
21	b	1021	CLA	MG-NA	6.16	2.20	2.06
21	2	1231	CLA	MG-NA	6.16	2.20	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1104	CLA	MG-NA	6.16	2.20	2.06
21	A	1107	CLA	MG-NA	6.16	2.20	2.06
21	b	1204	CLA	MG-NA	6.16	2.20	2.06
21	B	1202	CLA	MG-NA	6.15	2.20	2.06
21	1	1132	CLA	MG-NA	6.15	2.20	2.06
21	a	1102	CLA	MG-NA	6.15	2.20	2.06
21	2	1237	CLA	MG-NA	6.15	2.20	2.06
21	0	1502	CLA	MG-NA	6.15	2.20	2.06
21	A	1121	CLA	MG-NA	6.15	2.20	2.06
21	1	1131	CLA	MG-NA	6.15	2.20	2.06
21	b	1215	CLA	MG-NA	6.14	2.20	2.06
21	2	1213	CLA	MG-NA	6.14	2.20	2.06
21	B	1226	CLA	MG-NA	6.13	2.20	2.06
21	b	1201	CLA	MG-NA	6.13	2.20	2.06
21	1	1013	CLA	MG-NA	6.13	2.20	2.06
21	a	1124	CLA	MG-NA	6.13	2.20	2.06
21	A	1110	CLA	MG-NA	6.12	2.20	2.06
21	B	1206	CLA	MG-NA	6.12	2.20	2.06
21	b	1211	CLA	MG-NA	6.12	2.20	2.06
21	a	1011	CLA	MG-NA	6.12	2.20	2.06
21	b	1227	CLA	MG-NA	6.11	2.20	2.06
21	A	1108	CLA	MG-NA	6.11	2.20	2.06
21	B	1224	CLA	MG-NA	6.11	2.20	2.06
21	B	1205	CLA	MG-NA	6.10	2.20	2.06
21	1	1012	CLA	MG-NA	6.10	2.20	2.06
21	2	1205	CLA	MG-NA	6.10	2.20	2.06
21	A	1139	CLA	MG-NA	6.10	2.20	2.06
21	A	1138	CLA	MG-NA	6.10	2.20	2.06
21	B	1215	CLA	MG-NA	6.10	2.20	2.06
21	B	1221	CLA	MG-NA	6.10	2.20	2.06
21	B	1230	CLA	MG-NA	6.10	2.20	2.06
21	2	1201	CLA	MG-NA	6.10	2.20	2.06
21	2	1021	CLA	MG-NA	6.10	2.20	2.06
21	B	1229	CLA	MG-NA	6.09	2.20	2.06
21	a	1126	CLA	MG-NA	6.09	2.20	2.06
21	a	1106	CLA	MG-NA	6.08	2.20	2.06
21	2	1023	CLA	MG-NA	6.08	2.20	2.06
21	B	1231	CLA	MG-NA	6.08	2.20	2.06
21	2	1224	CLA	MG-NA	6.08	2.20	2.06
21	A	1126	CLA	MG-NA	6.07	2.20	2.06
21	B	1222	CLA	MG-NA	6.06	2.20	2.06
21	2	1228	CLA	MG-NA	6.06	2.20	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1237	CLA	MG-NA	6.05	2.20	2.06
21	b	1230	CLA	MG-NA	6.05	2.20	2.06
21	b	1224	CLA	MG-NA	6.05	2.20	2.06
21	b	1235	CLA	MG-NA	6.05	2.20	2.06
21	B	1021	CLA	MG-NA	6.04	2.20	2.06
21	b	1216	CLA	MG-NA	6.04	2.20	2.06
21	2	1216	CLA	MG-NA	6.04	2.20	2.06
21	b	1231	CLA	MG-NA	6.04	2.20	2.06
21	1	1119	CLA	MG-NA	6.04	2.20	2.06
21	A	1124	CLA	MG-NA	6.04	2.20	2.06
21	A	1119	CLA	MG-NA	6.02	2.20	2.06
21	b	1205	CLA	MG-NA	6.02	2.20	2.06
21	A	1011	CLA	MG-NA	6.01	2.20	2.06
21	L	1502	CLA	MG-NA	6.01	2.20	2.06
21	b	1023	CLA	MG-NA	6.00	2.20	2.06
21	B	1023	CLA	MG-NA	5.98	2.20	2.06
21	b	1222	CLA	MG-NA	5.98	2.20	2.06
21	A	1013	CLA	MG-NA	5.98	2.20	2.06
21	a	1103	CLA	MG-NA	5.96	2.20	2.06
21	l	1503	CLA	MG-NA	5.93	2.20	2.06
21	A	1106	CLA	MG-NA	5.93	2.20	2.06
21	B	1235	CLA	MG-NA	5.93	2.20	2.06
21	1	1103	CLA	MG-NA	5.92	2.20	2.06
21	b	1202	CLA	MG-NA	5.91	2.20	2.06
21	A	1103	CLA	MG-NA	5.83	2.20	2.06
21	a	1013	CLA	MG-NA	5.81	2.20	2.06
36	I	4020	EQ3	C1-C6	-5.07	1.47	1.53
28	B	4011	45D	C23-C25	4.80	1.56	1.46
28	h	4020	45D	C23-C25	4.69	1.56	1.46
36	I	4020	EQ3	C11-C10	4.61	1.57	1.43
36	I	4020	EQ3	C15-C14	4.59	1.57	1.43
36	I	4020	EQ3	C4-C5	-4.59	1.43	1.51
28	B	4011	45D	C24-C26	4.51	1.55	1.46
21	B	1202	CLA	CBB-CAB	4.48	1.51	1.30
21	A	1117	CLA	CBB-CAB	4.47	1.51	1.30
21	b	1202	CLA	CBB-CAB	4.47	1.51	1.30
21	j	1302	CLA	CBB-CAB	4.45	1.51	1.30
21	2	1234	CLA	CBB-CAB	4.45	1.51	1.30
21	A	1127	CLA	CBB-CAB	4.44	1.51	1.30
21	A	1013	CLA	CBB-CAB	4.44	1.51	1.30
21	1	1132	CLA	CBB-CAB	4.44	1.51	1.30
21	6	1302	CLA	CBB-CAB	4.44	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1113	CLA	CBB-CAB	4.44	1.51	1.30
21	a	1117	CLA	CBB-CAB	4.44	1.51	1.30
21	B	1213	CLA	CBB-CAB	4.43	1.51	1.30
21	l	1501	CLA	CBB-CAB	4.43	1.51	1.30
21	B	1234	CLA	CBB-CAB	4.43	1.51	1.30
21	A	1123	CLA	CBB-CAB	4.43	1.51	1.30
21	b	1234	CLA	CBB-CAB	4.43	1.51	1.30
21	B	1228	CLA	CBB-CAB	4.43	1.51	1.30
21	6	1301	CLA	CBB-CAB	4.43	1.51	1.30
21	L	1501	CLA	CBB-CAB	4.43	1.51	1.30
21	2	1230	CLA	CBB-CAB	4.43	1.51	1.30
21	l	1503	CLA	CBB-CAB	4.43	1.51	1.30
21	2	1023	CLA	CBB-CAB	4.43	1.51	1.30
21	A	1109	CLA	CBB-CAB	4.43	1.51	1.30
21	B	1206	CLA	CBB-CAB	4.43	1.51	1.30
21	b	1222	CLA	CBB-CAB	4.42	1.51	1.30
21	8	1402	CLA	CBB-CAB	4.42	1.51	1.30
21	2	1212	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1131	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1128	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1801	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1121	CLA	CBB-CAB	4.42	1.51	1.30
21	k	1401	CLA	CBB-CAB	4.42	1.51	1.30
21	K	1401	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1102	CLA	CBB-CAB	4.42	1.51	1.30
21	B	1224	CLA	CBB-CAB	4.42	1.51	1.30
21	1	1103	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1138	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1118	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1104	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1126	CLA	CBB-CAB	4.42	1.51	1.30
21	a	1102	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1119	CLA	CBB-CAB	4.42	1.51	1.30
21	b	1224	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1130	CLA	CBB-CAB	4.42	1.51	1.30
21	1	1134	CLA	CBB-CAB	4.42	1.51	1.30
21	1	1125	CLA	CBB-CAB	4.42	1.51	1.30
21	2	1209	CLA	CBB-CAB	4.42	1.51	1.30
21	2	1216	CLA	CBB-CAB	4.42	1.51	1.30
21	1	1113	CLA	CBB-CAB	4.42	1.51	1.30
21	1	1118	CLA	CBB-CAB	4.42	1.51	1.30
21	B	1023	CLA	CBB-CAB	4.42	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1114	CLA	CBB-CAB	4.42	1.51	1.30
21	2	1206	CLA	CBB-CAB	4.42	1.51	1.30
21	8	1401	CLA	CBB-CAB	4.42	1.51	1.30
21	b	1231	CLA	CBB-CAB	4.42	1.51	1.30
21	A	1104	CLA	CBB-CAB	4.41	1.51	1.30
21	b	1215	CLA	CBB-CAB	4.41	1.51	1.30
21	a	1132	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1101	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1232	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1119	CLA	CBB-CAB	4.41	1.51	1.30
21	B	1210	CLA	CBB-CAB	4.41	1.51	1.30
21	K	1402	CLA	CBB-CAB	4.41	1.51	1.30
21	B	1236	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1204	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1236	CLA	CBB-CAB	4.41	1.51	1.30
21	B	1220	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1222	CLA	CBB-CAB	4.41	1.51	1.30
21	b	1236	CLA	CBB-CAB	4.41	1.51	1.30
21	b	1240	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1106	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1109	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1120	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1128	CLA	CBB-CAB	4.41	1.51	1.30
21	B	1222	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1801	CLA	CBB-CAB	4.41	1.51	1.30
21	j	1303	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1210	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1224	CLA	CBB-CAB	4.41	1.51	1.30
21	a	1012	CLA	CBB-CAB	4.41	1.51	1.30
21	a	1114	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1122	CLA	CBB-CAB	4.41	1.51	1.30
21	A	1103	CLA	CBB-CAB	4.41	1.51	1.30
21	A	1132	CLA	CBB-CAB	4.41	1.51	1.30
21	7	1303	CLA	CBB-CAB	4.41	1.51	1.30
21	1	1013	CLA	CBB-CAB	4.41	1.51	1.30
21	J	1302	CLA	CBB-CAB	4.41	1.51	1.30
21	L	1503	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1202	CLA	CBB-CAB	4.41	1.51	1.30
21	2	1239	CLA	CBB-CAB	4.41	1.51	1.30
21	A	1134	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1230	CLA	CBB-CAB	4.40	1.51	1.30
21	1	1104	CLA	CBB-CAB	4.40	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1013	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1201	CLA	CBB-CAB	4.40	1.51	1.30
21	1	1117	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1123	CLA	CBB-CAB	4.40	1.51	1.30
21	A	1111	CLA	CBB-CAB	4.40	1.51	1.30
21	1	1102	CLA	CBB-CAB	4.40	1.51	1.30
21	A	1106	CLA	CBB-CAB	4.40	1.51	1.30
21	1	1130	CLA	CBB-CAB	4.40	1.51	1.30
21	2	1235	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1206	CLA	CBB-CAB	4.40	1.51	1.30
21	2	1203	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1109	CLA	CBB-CAB	4.40	1.51	1.30
21	2	1213	CLA	CBB-CAB	4.40	1.51	1.30
21	F	1301	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1218	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1211	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1130	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1124	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1125	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1226	CLA	CBB-CAB	4.40	1.51	1.30
21	k	1402	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1230	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1120	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1022	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1221	CLA	CBB-CAB	4.40	1.51	1.30
21	l	1502	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1217	CLA	CBB-CAB	4.40	1.51	1.30
21	B	1231	CLA	CBB-CAB	4.40	1.51	1.30
21	b	1021	CLA	CBB-CAB	4.40	1.51	1.30
21	a	1108	CLA	CBB-CAB	4.40	1.51	1.30
21	1	1115	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1125	CLA	CBB-CAB	4.39	1.51	1.30
21	b	1207	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1012	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1012	CLA	CBB-CAB	4.39	1.51	1.30
21	a	1112	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1217	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1123	CLA	CBB-CAB	4.39	1.51	1.30
21	b	1211	CLA	CBB-CAB	4.39	1.51	1.30
21	b	1218	CLA	CBB-CAB	4.39	1.51	1.30
21	J	1303	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1113	CLA	CBB-CAB	4.39	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1201	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1238	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1128	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1209	CLA	CBB-CAB	4.39	1.51	1.30
21	b	1223	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1135	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1221	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1221	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1231	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1108	CLA	CBB-CAB	4.39	1.51	1.30
21	a	1134	CLA	CBB-CAB	4.39	1.51	1.30
21	a	1136	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1021	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1216	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1107	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1801	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1011	CLA	CBB-CAB	4.39	1.51	1.30
21	0	1503	CLA	CBB-CAB	4.39	1.51	1.30
21	b	1239	CLA	CBB-CAB	4.39	1.51	1.30
21	1	1139	CLA	CBB-CAB	4.39	1.51	1.30
28	B	4011	45D	C33-C35	4.39	1.55	1.46
21	2	1219	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1022	CLA	CBB-CAB	4.39	1.51	1.30
21	B	1203	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1208	CLA	CBB-CAB	4.39	1.51	1.30
21	A	1105	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1215	CLA	CBB-CAB	4.39	1.51	1.30
21	a	1122	CLA	CBB-CAB	4.39	1.51	1.30
21	a	1115	CLA	CBB-CAB	4.39	1.51	1.30
21	f	1301	CLA	CBB-CAB	4.39	1.51	1.30
21	2	1211	CLA	CBB-CAB	4.38	1.51	1.30
21	1	1108	CLA	CBB-CAB	4.38	1.51	1.30
21	b	1023	CLA	CBB-CAB	4.38	1.51	1.30
21	f	1302	CLA	CBB-CAB	4.38	1.51	1.30
21	1	1140	CLA	CBB-CAB	4.38	1.51	1.30
21	A	1118	CLA	CBB-CAB	4.38	1.51	1.30
21	2	1218	CLA	CBB-CAB	4.38	1.51	1.30
21	a	1131	CLA	CBB-CAB	4.38	1.51	1.30
21	b	1227	CLA	CBB-CAB	4.38	1.51	1.30
21	b	1205	CLA	CBB-CAB	4.38	1.51	1.30
21	1	1126	CLA	CBB-CAB	4.38	1.51	1.30
21	2	1240	CLA	CBB-CAB	4.38	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1232	CLA	CBB-CAB	4.38	1.51	1.30
21	A	1124	CLA	CBB-CAB	4.38	1.51	1.30
21	A	1135	CLA	CBB-CAB	4.38	1.51	1.30
21	A	1122	CLA	CBB-CAB	4.38	1.51	1.30
21	1	1124	CLA	CBB-CAB	4.38	1.51	1.30
21	b	1203	CLA	CBB-CAB	4.38	1.51	1.30
21	a	1105	CLA	CBB-CAB	4.38	1.51	1.30
21	a	1138	CLA	CBB-CAB	4.38	1.51	1.30
21	a	1140	CLA	CBB-CAB	4.38	1.51	1.30
21	7	1302	CLA	CBB-CAB	4.38	1.51	1.30
21	A	1120	CLA	CBB-CAB	4.37	1.51	1.30
21	A	1137	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1107	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1215	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1201	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1235	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1219	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1208	CLA	CBB-CAB	4.37	1.51	1.30
21	0	1502	CLA	CBB-CAB	4.37	1.51	1.30
21	2	1238	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1103	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1139	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1228	CLA	CBB-CAB	4.37	1.51	1.30
21	2	1223	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1011	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1133	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1223	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1127	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1119	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1216	CLA	CBB-CAB	4.37	1.51	1.30
21	1	1105	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1204	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1204	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1210	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1208	CLA	CBB-CAB	4.37	1.51	1.30
21	b	1213	CLA	CBB-CAB	4.37	1.51	1.30
21	1	1133	CLA	CBB-CAB	4.37	1.51	1.30
21	A	1139	CLA	CBB-CAB	4.37	1.51	1.30
21	B	1239	CLA	CBB-CAB	4.37	1.51	1.30
21	a	1111	CLA	CBB-CAB	4.37	1.51	1.30
21	A	1115	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1126	CLA	CBB-CAB	4.36	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1101	CLA	CBB-CAB	4.36	1.51	1.30
21	2	1021	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1114	CLA	CBB-CAB	4.36	1.51	1.30
21	2	1225	CLA	CBB-CAB	4.36	1.51	1.30
21	B	1207	CLA	CBB-CAB	4.36	1.51	1.30
21	a	1106	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1011	CLA	CBB-CAB	4.36	1.51	1.30
21	b	1232	CLA	CBB-CAB	4.36	1.51	1.30
21	L	1502	CLA	CBB-CAB	4.36	1.51	1.30
21	1	1129	CLA	CBB-CAB	4.36	1.51	1.30
21	A	1121	CLA	CBB-CAB	4.36	1.51	1.30
21	a	1129	CLA	CBB-CAB	4.36	1.51	1.30
21	1	1110	CLA	CBB-CAB	4.36	1.51	1.30
21	B	1022	CLA	CBB-CAB	4.35	1.51	1.30
21	1	1111	CLA	CBB-CAB	4.35	1.51	1.30
21	a	1116	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1129	CLA	CBB-CAB	4.35	1.51	1.30
21	1	1137	CLA	CBB-CAB	4.35	1.51	1.30
21	a	1135	CLA	CBB-CAB	4.35	1.51	1.30
21	A	1110	CLA	CBB-CAB	4.35	1.51	1.30
21	2	1214	CLA	CBB-CAB	4.35	1.51	1.30
21	0	1501	CLA	CBB-CAB	4.35	1.51	1.30
21	b	1226	CLA	CBB-CAB	4.34	1.51	1.30
21	b	1220	CLA	CBB-CAB	4.34	1.51	1.30
21	b	1237	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1107	CLA	CBB-CAB	4.34	1.51	1.30
21	1	1127	CLA	CBB-CAB	4.34	1.51	1.30
21	1	1131	CLA	CBB-CAB	4.34	1.51	1.30
21	B	1219	CLA	CBB-CAB	4.34	1.51	1.30
21	2	1227	CLA	CBB-CAB	4.34	1.51	1.30
21	B	1229	CLA	CBB-CAB	4.34	1.51	1.30
21	A	1140	CLA	CBB-CAB	4.34	1.51	1.30
21	1	1121	CLA	CBB-CAB	4.34	1.51	1.30
21	F	1302	CLA	CBB-CAB	4.34	1.51	1.30
21	1	1112	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1225	CLA	CBB-CAB	4.33	1.51	1.30
21	B	1227	CLA	CBB-CAB	4.33	1.51	1.30
21	2	1228	CLA	CBB-CAB	4.33	1.51	1.30
21	A	1136	CLA	CBB-CAB	4.32	1.51	1.30
21	a	1110	CLA	CBB-CAB	4.32	1.51	1.30
21	a	1137	CLA	CBB-CAB	4.32	1.51	1.30
21	1	1116	CLA	CBB-CAB	4.32	1.51	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1205	CLA	CBB-CAB	4.32	1.51	1.30
21	b	1209	CLA	CBB-CAB	4.32	1.51	1.30
21	b	1229	CLA	CBB-CAB	4.32	1.51	1.30
21	2	1207	CLA	CBB-CAB	4.32	1.51	1.30
21	B	1214	CLA	CBB-CAB	4.32	1.51	1.30
21	A	1112	CLA	CBB-CAB	4.32	1.51	1.30
21	b	1217	CLA	CBB-CAB	4.31	1.51	1.30
21	b	1225	CLA	CBB-CAB	4.31	1.51	1.30
21	2	1220	CLA	CBB-CAB	4.31	1.51	1.30
21	B	1205	CLA	CBB-CAB	4.31	1.51	1.30
21	B	1240	CLA	CBB-CAB	4.31	1.51	1.30
21	2	1229	CLA	CBB-CAB	4.30	1.51	1.30
21	B	1212	CLA	CBB-CAB	4.29	1.51	1.30
21	A	1133	CLA	CBB-CAB	4.29	1.51	1.30
21	b	1235	CLA	CBB-CAB	4.29	1.51	1.30
21	A	1116	CLA	CBB-CAB	4.29	1.51	1.30
21	1	1136	CLA	CBB-CAB	4.28	1.51	1.30
21	b	1238	CLA	CBB-CAB	4.28	1.51	1.30
21	1	1138	CLA	CBB-CAB	4.28	1.51	1.30
21	b	1212	CLA	CBB-CAB	4.27	1.50	1.30
21	b	1214	CLA	CBB-CAB	4.27	1.50	1.30
21	2	1226	CLA	CBB-CAB	4.26	1.50	1.30
28	h	4020	45D	C33-C35	4.26	1.55	1.46
28	B	4011	45D	C34-C36	4.26	1.55	1.46
21	A	1101	CLA	CBB-CAB	4.22	1.50	1.30
21	B	1237	CLA	CBB-CAB	4.22	1.50	1.30
21	2	1237	CLA	CBB-CAB	4.21	1.50	1.30
28	h	4020	45D	C24-C26	4.10	1.54	1.46
28	h	4020	45D	C34-C36	4.07	1.54	1.46
36	I	4020	EQ3	C7-C6	4.04	1.58	1.45
21	a	1011	CLA	MG-ND	-3.98	1.97	2.05
21	A	1011	CLA	MG-ND	-3.98	1.97	2.05
36	I	4020	EQ3	C23-C22	3.96	1.54	1.46
21	1	1011	CLA	MG-ND	-3.89	1.98	2.05
21	b	1021	CLA	MG-ND	-3.89	1.98	2.05
21	2	1023	CLA	MG-ND	-3.88	1.98	2.05
21	1	1013	CLA	MG-ND	-3.87	1.98	2.05
21	b	1206	CLA	MG-ND	-3.83	1.98	2.05
21	B	1023	CLA	MG-ND	-3.82	1.98	2.05
28	B	4011	45D	C42-C38	3.81	1.55	1.43
21	2	1021	CLA	MG-ND	-3.79	1.98	2.05
26	K	5009	LMG	C43-C42	-3.78	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	4020	EQ3	C12-C13	3.78	1.54	1.46
21	A	1104	CLA	MG-ND	-3.77	1.98	2.05
28	B	4011	45D	C41-C37	3.77	1.54	1.43
26	b	5002	LMG	C40-C39	-3.76	1.33	1.51
26	K	5009	LMG	C37-C36	-3.75	1.33	1.51
26	B	5002	LMG	C40-C39	-3.74	1.33	1.51
28	h	4020	45D	C42-C38	3.74	1.54	1.43
36	I	4020	EQ3	C19-C18	3.73	1.53	1.46
21	2	1226	CLA	MG-ND	-3.73	1.98	2.05
21	a	1103	CLA	MG-ND	-3.73	1.98	2.05
21	B	1226	CLA	MG-ND	-3.73	1.98	2.05
21	B	1021	CLA	MG-ND	-3.73	1.98	2.05
26	B	5002	LMG	C25-C24	-3.73	1.33	1.51
26	b	5002	LMG	C43-C42	-3.73	1.33	1.51
26	b	5005	LMG	C40-C39	-3.73	1.33	1.51
21	2	1221	CLA	MG-ND	-3.73	1.98	2.05
26	K	5009	LMG	C22-C21	-3.72	1.33	1.51
26	2	5005	LMG	C37-C36	-3.72	1.33	1.51
26	B	5002	LMG	C43-C42	-3.72	1.33	1.51
21	b	1223	CLA	MG-ND	-3.72	1.98	2.05
26	B	5002	LMG	C19-C18	-3.72	1.33	1.51
26	2	5002	LMG	C40-C39	-3.72	1.33	1.51
21	b	1221	CLA	MG-ND	-3.72	1.98	2.05
26	b	5005	LMG	C37-C36	-3.72	1.33	1.51
21	B	1207	CLA	MG-ND	-3.71	1.98	2.05
26	K	5009	LMG	C40-C39	-3.71	1.33	1.51
21	J	1302	CLA	MG-ND	-3.71	1.98	2.05
26	b	5002	LMG	C37-C36	-3.71	1.33	1.51
26	B	5002	LMG	C37-C36	-3.70	1.33	1.51
26	K	5009	LMG	C19-C18	-3.70	1.33	1.51
26	1	5004	LMG	C19-C18	-3.70	1.33	1.51
26	2	5005	LMG	C40-C39	-3.70	1.33	1.51
26	2	5005	LMG	C22-C21	-3.70	1.33	1.51
26	2	5002	LMG	C37-C36	-3.70	1.33	1.51
26	2	5002	LMG	C19-C18	-3.70	1.33	1.51
26	b	5007	LMG	C19-C18	-3.70	1.33	1.51
21	B	1215	CLA	MG-ND	-3.69	1.98	2.05
26	a	5004	LMG	C40-C39	-3.69	1.33	1.51
26	0	5001	LMG	C19-C18	-3.69	1.33	1.51
26	2	5002	LMG	C43-C42	-3.69	1.33	1.51
26	1	5004	LMG	C22-C21	-3.69	1.33	1.51
26	b	5002	LMG	C19-C18	-3.69	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	1501	CLA	MG-ND	-3.69	1.98	2.05
21	B	1213	CLA	MG-ND	-3.69	1.98	2.05
21	a	1140	CLA	MG-ND	-3.69	1.98	2.05
21	6	1302	CLA	MG-ND	-3.68	1.98	2.05
26	A	5002	LMG	C37-C36	-3.68	1.33	1.51
26	B	5005	LMG	C37-C36	-3.68	1.33	1.51
21	B	1221	CLA	MG-ND	-3.68	1.98	2.05
26	b	5005	LMG	C19-C18	-3.68	1.33	1.51
26	a	5004	LMG	C43-C42	-3.68	1.33	1.51
37	L	5004	DGD	CAB-C9B	-3.67	1.33	1.51
21	a	1013	CLA	MG-ND	-3.67	1.98	2.05
26	B	5005	LMG	C40-C39	-3.67	1.33	1.51
26	A	5008	LMG	C25-C24	-3.67	1.33	1.51
26	0	5001	LMG	C22-C21	-3.67	1.33	1.51
21	a	1128	CLA	MG-ND	-3.67	1.98	2.05
26	1	5004	LMG	C25-C24	-3.67	1.33	1.51
26	B	5005	LMG	C22-C21	-3.67	1.33	1.51
26	0	5001	LMG	C25-C24	-3.67	1.33	1.51
26	a	5004	LMG	C25-C24	-3.67	1.33	1.51
26	a	5002	LMG	C37-C36	-3.67	1.33	1.51
26	A	5004	LMG	C25-C24	-3.67	1.33	1.51
26	A	5002	LMG	C40-C39	-3.67	1.33	1.51
26	a	5004	LMG	C37-C36	-3.66	1.33	1.51
26	2	5005	LMG	C19-C18	-3.66	1.33	1.51
26	2	5005	LMG	C25-C24	-3.66	1.33	1.51
28	B	4011	45D	C32-C30	3.66	1.54	1.43
26	B	5005	LMG	C19-C18	-3.66	1.33	1.51
21	1	1118	CLA	MG-ND	-3.66	1.98	2.05
26	A	5008	LMG	C40-C39	-3.66	1.33	1.51
26	B	5005	LMG	C25-C24	-3.66	1.33	1.51
21	2	1022	CLA	MG-ND	-3.66	1.98	2.05
26	b	5007	LMG	C40-C39	-3.66	1.33	1.51
26	A	5008	LMG	C22-C21	-3.65	1.33	1.51
21	1	1112	CLA	MG-ND	-3.65	1.98	2.05
26	1	5002	LMG	C37-C36	-3.65	1.33	1.51
26	A	5008	LMG	C19-C18	-3.65	1.33	1.51
26	1	5002	LMG	C40-C39	-3.65	1.33	1.51
21	2	1209	CLA	MG-ND	-3.65	1.98	2.05
26	b	5005	LMG	C22-C21	-3.65	1.33	1.51
26	1	5002	LMG	C19-C18	-3.65	1.33	1.51
21	1	1123	CLA	MG-ND	-3.65	1.98	2.05
26	A	5008	LMG	C43-C42	-3.65	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	5002	LMG	C25-C24	-3.65	1.33	1.51
37	L	5004	DGD	CDB-CCB	-3.65	1.33	1.51
21	B	1208	CLA	MG-ND	-3.65	1.98	2.05
26	0	5001	LMG	C43-C42	-3.64	1.33	1.51
21	A	1128	CLA	MG-ND	-3.64	1.98	2.05
21	2	1220	CLA	MG-ND	-3.64	1.98	2.05
26	b	5007	LMG	C37-C36	-3.64	1.33	1.51
37	L	5004	DGD	CDA-CCA	-3.64	1.33	1.51
26	2	5002	LMG	C22-C21	-3.64	1.33	1.51
26	B	5002	LMG	C22-C21	-3.64	1.33	1.51
21	B	1022	CLA	MG-ND	-3.64	1.98	2.05
26	a	5004	LMG	C19-C18	-3.64	1.33	1.51
26	1	5004	LMG	C40-C39	-3.64	1.33	1.51
26	1	5004	LMG	C43-C42	-3.64	1.33	1.51
26	K	5009	LMG	C25-C24	-3.64	1.33	1.51
26	b	5007	LMG	C43-C42	-3.64	1.33	1.51
26	a	5002	LMG	C40-C39	-3.64	1.33	1.51
26	A	5008	LMG	C37-C36	-3.63	1.33	1.51
21	2	1228	CLA	MG-ND	-3.63	1.98	2.05
26	b	5002	LMG	C22-C21	-3.63	1.33	1.51
21	a	1118	CLA	MG-ND	-3.63	1.98	2.05
26	b	5005	LMG	C25-C24	-3.63	1.33	1.51
21	a	1012	CLA	MG-ND	-3.63	1.98	2.05
21	2	1227	CLA	MG-ND	-3.63	1.98	2.05
21	B	1211	CLA	MG-ND	-3.63	1.98	2.05
21	2	1208	CLA	MG-ND	-3.63	1.98	2.05
26	1	5002	LMG	C43-C42	-3.63	1.33	1.51
26	A	5004	LMG	C22-C21	-3.63	1.33	1.51
26	b	5007	LMG	C22-C21	-3.63	1.33	1.51
26	a	5002	LMG	C19-C18	-3.63	1.33	1.51
26	b	5007	LMG	C25-C24	-3.62	1.33	1.51
26	a	5002	LMG	C43-C42	-3.62	1.33	1.51
26	2	5002	LMG	C25-C24	-3.62	1.33	1.51
26	a	5004	LMG	C22-C21	-3.62	1.33	1.51
37	L	5004	DGD	CGA-CFA	-3.62	1.33	1.51
37	L	5004	DGD	CAA-C9A	-3.62	1.33	1.51
21	a	1104	CLA	MG-ND	-3.62	1.98	2.05
21	A	1118	CLA	MG-ND	-3.62	1.98	2.05
21	2	1202	CLA	MG-ND	-3.62	1.98	2.05
26	0	5001	LMG	C37-C36	-3.61	1.33	1.51
21	1	1140	CLA	MG-ND	-3.61	1.98	2.05
26	2	5005	LMG	C43-C42	-3.61	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1013	CLA	MG-ND	-3.61	1.98	2.05
21	1	1133	CLA	MG-ND	-3.61	1.98	2.05
21	b	1215	CLA	MG-ND	-3.61	1.98	2.05
21	b	1220	CLA	MG-ND	-3.61	1.98	2.05
37	L	5004	DGD	CGB-CFB	-3.61	1.33	1.51
21	1	1107	CLA	MG-ND	-3.61	1.98	2.05
26	A	5002	LMG	C19-C18	-3.61	1.33	1.51
26	1	5004	LMG	C37-C36	-3.61	1.33	1.51
21	B	1210	CLA	MG-ND	-3.60	1.98	2.05
26	0	5001	LMG	C40-C39	-3.60	1.33	1.51
21	A	1106	CLA	MG-ND	-3.60	1.98	2.05
21	1	1129	CLA	MG-ND	-3.60	1.98	2.05
21	A	1102	CLA	MG-ND	-3.60	1.98	2.05
21	a	1137	CLA	MG-ND	-3.60	1.98	2.05
26	A	5002	LMG	C43-C42	-3.60	1.33	1.51
26	b	5005	LMG	C43-C42	-3.59	1.33	1.51
21	a	1112	CLA	MG-ND	-3.59	1.98	2.05
21	2	1232	CLA	MG-ND	-3.59	1.98	2.05
21	2	1211	CLA	MG-ND	-3.59	1.98	2.05
21	2	1217	CLA	MG-ND	-3.59	1.98	2.05
21	A	1130	CLA	MG-ND	-3.58	1.98	2.05
21	A	1012	CLA	MG-ND	-3.58	1.98	2.05
21	B	1203	CLA	MG-ND	-3.58	1.98	2.05
21	b	1023	CLA	MG-ND	-3.58	1.98	2.05
21	A	1119	CLA	MG-ND	-3.58	1.98	2.05
28	B	4011	45D	C31-C29	3.58	1.54	1.43
21	1	1127	CLA	MG-ND	-3.58	1.98	2.05
21	1	1111	CLA	MG-ND	-3.57	1.98	2.05
26	A	5004	LMG	C19-C18	-3.57	1.34	1.51
26	B	5005	LMG	C43-C42	-3.57	1.34	1.51
21	b	1237	CLA	MG-ND	-3.57	1.98	2.05
21	A	1101	CLA	MG-ND	-3.57	1.98	2.05
21	A	1137	CLA	MG-ND	-3.57	1.98	2.05
21	k	1401	CLA	MG-ND	-3.57	1.98	2.05
21	B	1217	CLA	MG-ND	-3.57	1.98	2.05
21	a	1123	CLA	MG-ND	-3.57	1.98	2.05
21	B	1202	CLA	MG-ND	-3.56	1.98	2.05
21	A	1801	CLA	MG-ND	-3.56	1.98	2.05
21	a	1109	CLA	MG-ND	-3.56	1.98	2.05
21	1	1110	CLA	MG-ND	-3.56	1.98	2.05
21	B	1224	CLA	MG-ND	-3.56	1.98	2.05
21	2	1215	CLA	MG-ND	-3.56	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	1302	CLA	MG-ND	-3.56	1.98	2.05
21	b	1234	CLA	MG-ND	-3.56	1.98	2.05
21	B	1206	CLA	MG-ND	-3.56	1.98	2.05
21	2	1207	CLA	MG-ND	-3.56	1.98	2.05
21	2	1206	CLA	MG-ND	-3.55	1.98	2.05
28	h	4020	45D	C41-C37	3.55	1.54	1.43
21	1	1119	CLA	MG-ND	-3.55	1.98	2.05
21	B	1220	CLA	MG-ND	-3.55	1.98	2.05
21	2	1201	CLA	MG-ND	-3.55	1.98	2.05
21	L	1502	CLA	MG-ND	-3.54	1.98	2.05
21	a	1110	CLA	MG-ND	-3.54	1.98	2.05
21	b	1202	CLA	MG-ND	-3.54	1.98	2.05
21	b	1216	CLA	MG-ND	-3.54	1.98	2.05
21	A	1115	CLA	MG-ND	-3.53	1.98	2.05
21	2	1230	CLA	MG-ND	-3.53	1.98	2.05
21	1	1113	CLA	MG-ND	-3.53	1.98	2.05
21	1	1128	CLA	MG-ND	-3.53	1.98	2.05
21	1	1116	CLA	MG-ND	-3.53	1.98	2.05
21	2	1223	CLA	MG-ND	-3.53	1.98	2.05
21	A	1133	CLA	MG-ND	-3.53	1.98	2.05
21	A	1134	CLA	MG-ND	-3.53	1.98	2.05
21	a	1119	CLA	MG-ND	-3.53	1.98	2.05
21	1	1103	CLA	MG-ND	-3.53	1.98	2.05
21	2	1214	CLA	MG-ND	-3.53	1.98	2.05
21	b	1240	CLA	MG-ND	-3.53	1.98	2.05
21	1	1012	CLA	MG-ND	-3.53	1.98	2.05
21	b	1238	CLA	MG-ND	-3.52	1.98	2.05
21	A	1110	CLA	MG-ND	-3.52	1.98	2.05
21	b	1204	CLA	MG-ND	-3.52	1.98	2.05
21	2	1205	CLA	MG-ND	-3.52	1.98	2.05
21	A	1125	CLA	MG-ND	-3.52	1.98	2.05
21	b	1219	CLA	MG-ND	-3.52	1.98	2.05
21	a	1138	CLA	MG-ND	-3.52	1.98	2.05
21	b	1224	CLA	MG-ND	-3.52	1.98	2.05
21	a	1113	CLA	MG-ND	-3.52	1.98	2.05
21	1	1126	CLA	MG-ND	-3.51	1.98	2.05
21	8	1401	CLA	MG-ND	-3.51	1.98	2.05
21	A	1113	CLA	MG-ND	-3.51	1.98	2.05
21	a	1121	CLA	MG-ND	-3.51	1.98	2.05
21	1	1117	CLA	MG-ND	-3.51	1.98	2.05
21	J	1303	CLA	MG-ND	-3.50	1.98	2.05
21	B	1216	CLA	MG-ND	-3.50	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1231	CLA	MG-ND	-3.50	1.98	2.05
21	b	1208	CLA	MG-ND	-3.50	1.98	2.05
21	1	1104	CLA	MG-ND	-3.50	1.98	2.05
21	a	1106	CLA	MG-ND	-3.50	1.98	2.05
21	1	1101	CLA	MG-ND	-3.50	1.98	2.05
21	1	1122	CLA	MG-ND	-3.50	1.98	2.05
21	B	1209	CLA	MG-ND	-3.50	1.98	2.05
28	h	4020	45D	C31-C29	3.50	1.54	1.43
21	b	1231	CLA	MG-ND	-3.49	1.98	2.05
21	2	1231	CLA	MG-ND	-3.49	1.98	2.05
21	1	1125	CLA	MG-ND	-3.49	1.98	2.05
21	1	1132	CLA	MG-ND	-3.49	1.98	2.05
21	1	1121	CLA	MG-ND	-3.49	1.98	2.05
21	7	1302	CLA	MG-ND	-3.49	1.98	2.05
21	b	1201	CLA	MG-ND	-3.48	1.98	2.05
21	A	1132	CLA	MG-ND	-3.48	1.98	2.05
21	a	1107	CLA	MG-ND	-3.48	1.98	2.05
21	1	1114	CLA	MG-ND	-3.48	1.98	2.05
21	b	1209	CLA	MG-ND	-3.48	1.98	2.05
21	7	1303	CLA	MG-ND	-3.48	1.98	2.05
21	8	1402	CLA	MG-ND	-3.48	1.98	2.05
21	B	1201	CLA	MG-ND	-3.48	1.98	2.05
21	B	1235	CLA	MG-ND	-3.48	1.98	2.05
21	a	1115	CLA	MG-ND	-3.48	1.98	2.05
21	A	1135	CLA	MG-ND	-3.48	1.98	2.05
21	a	1130	CLA	MG-ND	-3.48	1.98	2.05
21	a	1132	CLA	MG-ND	-3.48	1.98	2.05
21	1	1138	CLA	MG-ND	-3.48	1.98	2.05
21	a	1125	CLA	MG-ND	-3.47	1.98	2.05
21	a	1102	CLA	MG-ND	-3.47	1.98	2.05
21	b	1218	CLA	MG-ND	-3.47	1.98	2.05
21	A	1112	CLA	MG-ND	-3.47	1.98	2.05
21	1	1130	CLA	MG-ND	-3.47	1.98	2.05
21	a	1114	CLA	MG-ND	-3.47	1.98	2.05
21	B	1236	CLA	MG-ND	-3.47	1.98	2.05
21	f	1302	CLA	MG-ND	-3.47	1.98	2.05
21	a	1116	CLA	MG-ND	-3.47	1.98	2.05
21	a	1111	CLA	MG-ND	-3.47	1.98	2.05
21	b	1205	CLA	MG-ND	-3.46	1.98	2.05
21	b	1228	CLA	MG-ND	-3.46	1.98	2.05
21	B	1214	CLA	MG-ND	-3.46	1.98	2.05
21	A	1123	CLA	MG-ND	-3.46	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1203	CLA	MG-ND	-3.46	1.98	2.05
21	a	1131	CLA	MG-ND	-3.46	1.98	2.05
21	a	1139	CLA	MG-ND	-3.46	1.98	2.05
21	B	1234	CLA	MG-ND	-3.46	1.98	2.05
21	1	1108	CLA	MG-ND	-3.46	1.98	2.05
21	b	1022	CLA	MG-ND	-3.45	1.98	2.05
21	a	1135	CLA	MG-ND	-3.45	1.98	2.05
21	A	1105	CLA	MG-ND	-3.45	1.98	2.05
21	1	1106	CLA	MG-ND	-3.45	1.98	2.05
21	a	1117	CLA	MG-ND	-3.45	1.98	2.05
21	f	1301	CLA	MG-ND	-3.45	1.99	2.05
21	a	1105	CLA	MG-ND	-3.45	1.99	2.05
21	A	1116	CLA	MG-ND	-3.45	1.99	2.05
21	1	1120	CLA	MG-ND	-3.45	1.99	2.05
21	b	1239	CLA	MG-ND	-3.44	1.99	2.05
21	K	1401	CLA	MG-ND	-3.44	1.99	2.05
21	b	1227	CLA	MG-ND	-3.44	1.99	2.05
21	2	1213	CLA	MG-ND	-3.44	1.99	2.05
21	B	1223	CLA	MG-ND	-3.44	1.99	2.05
21	2	1212	CLA	MG-ND	-3.44	1.99	2.05
21	b	1212	CLA	MG-ND	-3.44	1.99	2.05
21	A	1103	CLA	MG-ND	-3.44	1.99	2.05
21	A	1107	CLA	MG-ND	-3.44	1.99	2.05
21	1	1801	CLA	MG-ND	-3.44	1.99	2.05
21	1	1102	CLA	MG-ND	-3.43	1.99	2.05
21	a	1801	CLA	MG-ND	-3.43	1.99	2.05
21	b	1214	CLA	MG-ND	-3.43	1.99	2.05
21	b	1217	CLA	MG-ND	-3.43	1.99	2.05
21	1	1109	CLA	MG-ND	-3.43	1.99	2.05
21	2	1235	CLA	MG-ND	-3.43	1.99	2.05
21	A	1126	CLA	MG-ND	-3.43	1.99	2.05
21	a	1122	CLA	MG-ND	-3.43	1.99	2.05
21	2	1224	CLA	MG-ND	-3.43	1.99	2.05
21	a	1108	CLA	MG-ND	-3.43	1.99	2.05
21	a	1129	CLA	MG-ND	-3.43	1.99	2.05
21	B	1218	CLA	MG-ND	-3.43	1.99	2.05
21	a	1101	CLA	MG-ND	-3.42	1.99	2.05
21	B	1228	CLA	MG-ND	-3.42	1.99	2.05
21	B	1232	CLA	MG-ND	-3.42	1.99	2.05
21	A	1127	CLA	MG-ND	-3.42	1.99	2.05
21	a	1134	CLA	MG-ND	-3.42	1.99	2.05
21	6	1301	CLA	MG-ND	-3.42	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1216	CLA	MG-ND	-3.41	1.99	2.05
21	b	1235	CLA	MG-ND	-3.41	1.99	2.05
21	2	1238	CLA	MG-ND	-3.41	1.99	2.05
21	l	1502	CLA	MG-ND	-3.41	1.99	2.05
21	j	1302	CLA	MG-ND	-3.41	1.99	2.05
21	2	1218	CLA	MG-ND	-3.41	1.99	2.05
21	k	1402	CLA	MG-ND	-3.41	1.99	2.05
21	2	1219	CLA	MG-ND	-3.41	1.99	2.05
21	A	1122	CLA	MG-ND	-3.41	1.99	2.05
36	I	4020	EQ3	C35-C13	3.41	1.57	1.50
21	1	1139	CLA	MG-ND	-3.40	1.99	2.05
21	A	1138	CLA	MG-ND	-3.40	1.99	2.05
21	2	1234	CLA	MG-ND	-3.40	1.99	2.05
21	a	1126	CLA	MG-ND	-3.40	1.99	2.05
21	b	1236	CLA	MG-ND	-3.40	1.99	2.05
21	1	1124	CLA	MG-ND	-3.40	1.99	2.05
21	2	1204	CLA	MG-ND	-3.40	1.99	2.05
21	a	1136	CLA	MG-ND	-3.40	1.99	2.05
21	K	1402	CLA	MG-ND	-3.40	1.99	2.05
21	2	1237	CLA	MG-ND	-3.40	1.99	2.05
21	j	1303	CLA	MG-ND	-3.39	1.99	2.05
21	A	1139	CLA	MG-ND	-3.39	1.99	2.05
21	b	1210	CLA	MG-ND	-3.39	1.99	2.05
21	2	1222	CLA	MG-ND	-3.39	1.99	2.05
36	I	4020	EQ3	C38-C26	3.39	1.57	1.50
21	B	1222	CLA	MG-ND	-3.38	1.99	2.05
21	0	1503	CLA	MG-ND	-3.38	1.99	2.05
21	a	1127	CLA	MG-ND	-3.38	1.99	2.05
21	A	1111	CLA	MG-ND	-3.38	1.99	2.05
21	B	1240	CLA	MG-ND	-3.38	1.99	2.05
21	2	1210	CLA	MG-ND	-3.37	1.99	2.05
21	0	1502	CLA	MG-ND	-3.37	1.99	2.05
21	B	1219	CLA	MG-ND	-3.37	1.99	2.05
21	B	1229	CLA	MG-ND	-3.37	1.99	2.05
21	F	1301	CLA	MG-ND	-3.37	1.99	2.05
21	A	1120	CLA	MG-ND	-3.36	1.99	2.05
21	l	1501	CLA	MG-ND	-3.36	1.99	2.05
21	1	1137	CLA	MG-ND	-3.36	1.99	2.05
21	A	1117	CLA	MG-ND	-3.36	1.99	2.05
21	b	1226	CLA	MG-ND	-3.35	1.99	2.05
21	A	1129	CLA	MG-ND	-3.35	1.99	2.05
21	A	1109	CLA	MG-ND	-3.35	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1140	CLA	MG-ND	-3.34	1.99	2.05
21	2	1236	CLA	MG-ND	-3.34	1.99	2.05
28	h	4020	45D	C20-C08	3.33	1.56	1.45
21	2	1229	CLA	MG-ND	-3.33	1.99	2.05
21	2	1225	CLA	MG-ND	-3.33	1.99	2.05
21	B	1204	CLA	MG-ND	-3.33	1.99	2.05
21	A	1124	CLA	MG-ND	-3.33	1.99	2.05
36	I	4020	EQ3	O3-C3	-3.32	1.33	1.43
21	a	1120	CLA	MG-ND	-3.32	1.99	2.05
21	1	1135	CLA	MG-ND	-3.32	1.99	2.05
21	B	1230	CLA	MG-ND	-3.32	1.99	2.05
21	B	1227	CLA	MG-ND	-3.31	1.99	2.05
21	b	1207	CLA	MG-ND	-3.31	1.99	2.05
21	B	1237	CLA	MG-ND	-3.30	1.99	2.05
21	1	1115	CLA	MG-ND	-3.30	1.99	2.05
21	A	1136	CLA	MG-ND	-3.30	1.99	2.05
21	B	1239	CLA	MG-ND	-3.30	1.99	2.05
21	1	1105	CLA	MG-ND	-3.30	1.99	2.05
28	B	4011	45D	C20-C08	3.30	1.56	1.45
21	A	1114	CLA	MG-ND	-3.30	1.99	2.05
21	B	1212	CLA	MG-ND	-3.30	1.99	2.05
21	A	1108	CLA	MG-ND	-3.29	1.99	2.05
21	b	1213	CLA	MG-ND	-3.29	1.99	2.05
21	b	1229	CLA	MG-ND	-3.29	1.99	2.05
21	b	1230	CLA	MG-ND	-3.28	1.99	2.05
21	A	1131	CLA	MG-ND	-3.28	1.99	2.05
21	B	1205	CLA	MG-ND	-3.28	1.99	2.05
21	b	1232	CLA	MG-ND	-3.27	1.99	2.05
21	1	1131	CLA	MG-ND	-3.27	1.99	2.05
21	b	1225	CLA	MG-ND	-3.26	1.99	2.05
21	0	1501	CLA	MG-ND	-3.26	1.99	2.05
21	1	1134	CLA	MG-ND	-3.25	1.99	2.05
36	I	4020	EQ3	C2-C1	3.25	1.64	1.54
21	1	1136	CLA	MG-ND	-3.24	1.99	2.05
21	b	1211	CLA	MG-ND	-3.24	1.99	2.05
21	2	1203	CLA	MG-ND	-3.24	1.99	2.05
30	b	4006	ECH	C1-C6	-3.22	1.49	1.53
21	a	1124	CLA	MG-ND	-3.22	1.99	2.05
21	l	1503	CLA	MG-ND	-3.21	1.99	2.05
21	B	1225	CLA	MG-ND	-3.21	1.99	2.05
21	2	1239	CLA	MG-ND	-3.19	1.99	2.05
21	2	1240	CLA	MG-ND	-3.19	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1222	CLA	MG-ND	-3.15	1.99	2.05
21	L	1503	CLA	MG-ND	-3.15	1.99	2.05
21	a	1133	CLA	MG-ND	-3.14	1.99	2.05
28	h	4020	45D	C19-C07	3.12	1.55	1.45
21	A	1121	CLA	MG-ND	-3.10	1.99	2.05
21	B	1238	CLA	MG-ND	-3.09	1.99	2.05
28	h	4020	45D	C32-C30	3.07	1.52	1.43
28	B	4011	45D	C19-C07	3.05	1.55	1.45
36	I	4020	EQ3	C24-C25	3.00	1.55	1.45
36	I	4020	EQ3	C16-C17	2.95	1.52	1.43
36	I	4020	EQ3	C33-C5	2.93	1.55	1.50
26	A	5004	LMG	C37-C36	-2.92	1.33	1.51
21	B	1022	CLA	C1C-C2C	2.88	1.50	1.44
30	B	4006	ECH	C1-C6	-2.87	1.50	1.53
21	A	1101	CLA	C1C-C2C	2.87	1.50	1.44
21	1	1125	CLA	C1C-C2C	2.82	1.50	1.44
21	B	1023	CLA	C1C-C2C	2.82	1.50	1.44
21	A	1136	CLA	C1C-C2C	2.81	1.50	1.44
21	A	1127	CLA	C1C-C2C	2.80	1.50	1.44
21	1	1126	CLA	C1C-C2C	2.79	1.50	1.44
21	B	1225	CLA	C1C-C2C	2.78	1.50	1.44
21	1	1136	CLA	C1C-C2C	2.78	1.50	1.44
21	B	1216	CLA	C1C-C2C	2.77	1.50	1.44
36	I	4020	EQ3	C20-C21	2.77	1.51	1.43
21	1	1801	CLA	C1C-C2C	2.77	1.50	1.44
21	B	1229	CLA	C1C-C2C	2.77	1.50	1.44
21	2	1234	CLA	C1C-C2C	2.76	1.50	1.44
21	f	1301	CLA	C1C-C2C	2.76	1.50	1.44
21	B	1227	CLA	C1C-C2C	2.76	1.50	1.44
21	1	1127	CLA	C1C-C2C	2.75	1.50	1.44
21	B	1202	CLA	C1C-C2C	2.75	1.50	1.44
21	0	1502	CLA	C1C-C2C	2.74	1.50	1.44
21	a	1118	CLA	C1C-C2C	2.74	1.50	1.44
21	B	1212	CLA	C1C-C2C	2.74	1.50	1.44
21	1	1011	CLA	C1C-C2C	2.74	1.50	1.44
21	A	1132	CLA	C1C-C2C	2.74	1.50	1.44
21	2	1022	CLA	C1C-C2C	2.74	1.50	1.44
21	2	1240	CLA	C1C-C2C	2.73	1.50	1.44
21	b	1234	CLA	C1C-C2C	2.73	1.50	1.44
21	b	1214	CLA	C1C-C2C	2.73	1.50	1.44
21	a	1011	CLA	C1C-C2C	2.72	1.50	1.44
21	2	1236	CLA	C1C-C2C	2.72	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1117	CLA	C1C-C2C	2.72	1.50	1.44
36	I	4020	EQ3	C40-C30	2.72	1.58	1.53
21	b	1021	CLA	C1C-C2C	2.72	1.50	1.44
21	1	1131	CLA	C1C-C2C	2.72	1.50	1.44
21	2	1229	CLA	C1C-C2C	2.71	1.50	1.44
21	A	1126	CLA	C1C-C2C	2.71	1.50	1.44
21	A	1102	CLA	C1C-C2C	2.71	1.50	1.44
21	a	1126	CLA	C1C-C2C	2.71	1.50	1.44
21	b	1229	CLA	C1C-C2C	2.71	1.50	1.44
21	2	1216	CLA	C1C-C2C	2.71	1.50	1.44
21	j	1303	CLA	C1C-C2C	2.71	1.50	1.44
21	1	1012	CLA	C1C-C2C	2.70	1.50	1.44
21	B	1234	CLA	C1C-C2C	2.70	1.50	1.44
21	a	1127	CLA	C1C-C2C	2.70	1.50	1.44
21	A	1120	CLA	C1C-C2C	2.70	1.50	1.44
21	B	1236	CLA	C1C-C2C	2.70	1.50	1.44
21	B	1235	CLA	C1C-C2C	2.70	1.50	1.44
21	a	1101	CLA	C1C-C2C	2.70	1.50	1.44
21	1	1105	CLA	C1C-C2C	2.70	1.50	1.44
21	2	1208	CLA	C1C-C2C	2.70	1.50	1.44
21	B	1239	CLA	C1C-C2C	2.69	1.50	1.44
21	1	1013	CLA	C1C-C2C	2.69	1.50	1.44
21	2	1215	CLA	C1C-C2C	2.69	1.50	1.44
21	1	1132	CLA	C1C-C2C	2.68	1.50	1.44
30	i	4020	ECH	C1-C6	-2.68	1.50	1.53
21	B	1238	CLA	C1C-C2C	2.68	1.50	1.44
21	b	1240	CLA	C1C-C2C	2.68	1.50	1.44
21	2	1023	CLA	C1C-C2C	2.68	1.50	1.44
21	1	1138	CLA	C1C-C2C	2.68	1.50	1.44
21	A	1108	CLA	C1C-C2C	2.68	1.50	1.44
21	a	1012	CLA	C1C-C2C	2.68	1.50	1.44
21	a	1116	CLA	C1C-C2C	2.67	1.49	1.44
21	2	1235	CLA	C1C-C2C	2.67	1.49	1.44
21	b	1022	CLA	C1C-C2C	2.67	1.49	1.44
21	A	1118	CLA	C1C-C2C	2.67	1.49	1.44
21	l	1502	CLA	C1C-C2C	2.67	1.49	1.44
21	A	1104	CLA	C1C-C2C	2.67	1.49	1.44
21	b	1218	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1211	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1228	CLA	C1C-C2C	2.67	1.49	1.44
21	6	1302	CLA	C1C-C2C	2.67	1.49	1.44
21	A	1113	CLA	C1C-C2C	2.66	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1212	CLA	C1C-C2C	2.66	1.49	1.44
21	a	1108	CLA	C1C-C2C	2.66	1.49	1.44
21	b	1202	CLA	C1C-C2C	2.66	1.49	1.44
21	a	1129	CLA	C1C-C2C	2.66	1.49	1.44
21	B	1220	CLA	C1C-C2C	2.66	1.49	1.44
21	A	1110	CLA	C1C-C2C	2.65	1.49	1.44
21	1	1116	CLA	C1C-C2C	2.65	1.49	1.44
22	B	2002	PQN	C9-C10	-2.65	1.35	1.39
21	2	1203	CLA	C1C-C2C	2.65	1.49	1.44
21	F	1301	CLA	MG-NC	2.65	2.12	2.06
21	1	1107	CLA	C1C-C2C	2.64	1.49	1.44
21	1	1129	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1110	CLA	C1C-C2C	2.64	1.49	1.44
21	l	1503	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1139	CLA	C1C-C2C	2.64	1.49	1.44
21	b	1219	CLA	C1C-C2C	2.64	1.49	1.44
21	B	1207	CLA	C1C-NC	-2.64	1.33	1.37
21	B	1223	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1134	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1013	CLA	C1C-C2C	2.64	1.49	1.44
21	1	1113	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1123	CLA	MG-NC	2.63	2.12	2.06
21	2	1217	CLA	MG-NC	2.63	2.12	2.06
21	1	1108	CLA	C1C-C2C	2.63	1.49	1.44
21	B	1207	CLA	C1C-C2C	2.63	1.49	1.44
21	1	1101	CLA	C1C-C2C	2.63	1.49	1.44
21	J	1302	CLA	C1C-C2C	2.63	1.49	1.44
21	a	1130	CLA	C1C-C2C	2.63	1.49	1.44
21	J	1303	CLA	C1C-C2C	2.63	1.49	1.44
21	A	1116	CLA	C1C-C2C	2.63	1.49	1.44
21	2	1202	CLA	C1C-C2C	2.63	1.49	1.44
21	B	1210	CLA	MG-NC	2.63	2.12	2.06
21	b	1232	CLA	C1C-C2C	2.63	1.49	1.44
21	7	1302	CLA	C1C-C2C	2.63	1.49	1.44
21	a	1113	CLA	C1C-C2C	2.63	1.49	1.44
21	b	1023	CLA	C1C-C2C	2.62	1.49	1.44
21	2	1230	CLA	C1C-C2C	2.62	1.49	1.44
21	B	1230	CLA	C1C-C2C	2.62	1.49	1.44
21	1	1110	CLA	C1C-C2C	2.62	1.49	1.44
21	a	1131	CLA	C1C-C2C	2.62	1.49	1.44
21	b	1207	CLA	C1C-C2C	2.62	1.49	1.44
21	k	1402	CLA	C1C-C2C	2.62	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1137	CLA	C1C-NC	-2.62	1.33	1.37
21	2	1201	CLA	C1C-C2C	2.62	1.49	1.44
21	2	1223	CLA	C1C-C2C	2.61	1.49	1.44
21	A	1126	CLA	MG-NC	2.61	2.12	2.06
21	1	1120	CLA	C1C-C2C	2.61	1.49	1.44
28	B	4011	45D	O02-C18	-2.61	1.17	1.23
21	B	1213	CLA	C1C-C2C	2.61	1.49	1.44
21	B	1240	CLA	C1C-C2C	2.61	1.49	1.44
21	a	1138	CLA	C1C-C2C	2.61	1.49	1.44
21	2	1220	CLA	C1C-C2C	2.61	1.49	1.44
21	B	1215	CLA	C1C-C2C	2.61	1.49	1.44
21	b	1217	CLA	C1C-C2C	2.61	1.49	1.44
21	a	1121	CLA	C1C-C2C	2.61	1.49	1.44
21	2	1211	CLA	C1C-C2C	2.60	1.49	1.44
21	a	1125	CLA	C1C-C2C	2.60	1.49	1.44
21	A	1105	CLA	C1C-C2C	2.60	1.49	1.44
21	B	1219	CLA	C1C-C2C	2.60	1.49	1.44
21	b	1215	CLA	C1C-C2C	2.60	1.49	1.44
21	b	1240	CLA	MG-NC	2.60	2.12	2.06
21	1	1135	CLA	MG-NC	2.60	2.12	2.06
21	a	1119	CLA	C1C-C2C	2.60	1.49	1.44
21	1	1123	CLA	MG-NC	2.60	2.12	2.06
21	A	1011	CLA	C1C-C2C	2.60	1.49	1.44
21	B	1208	CLA	C1C-C2C	2.60	1.49	1.44
21	1	1109	CLA	C1C-C2C	2.60	1.49	1.44
21	0	1501	CLA	C1C-C2C	2.59	1.49	1.44
21	a	1136	CLA	C1C-C2C	2.59	1.49	1.44
21	2	1207	CLA	C1C-C2C	2.59	1.49	1.44
21	a	1140	CLA	C1C-C2C	2.59	1.49	1.44
21	a	1117	CLA	C1C-C2C	2.59	1.49	1.44
21	2	1217	CLA	C1C-C2C	2.59	1.49	1.44
21	2	1213	CLA	C1C-C2C	2.59	1.49	1.44
21	b	1239	CLA	C1C-C2C	2.58	1.49	1.44
21	1	1137	CLA	C1C-C2C	2.58	1.49	1.44
21	2	1210	CLA	C1C-C2C	2.58	1.49	1.44
21	A	1140	CLA	C1C-C2C	2.58	1.49	1.44
21	2	1218	CLA	C1C-C2C	2.58	1.49	1.44
21	8	1402	CLA	C1C-C2C	2.58	1.49	1.44
21	0	1502	CLA	MG-NC	2.58	2.12	2.06
21	2	1228	CLA	C1C-C2C	2.58	1.49	1.44
21	2	1204	CLA	C1C-C2C	2.57	1.49	1.44
21	2	1222	CLA	C1C-C2C	2.57	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	k	1401	CLA	C1C-C2C	2.57	1.49	1.44
21	1	1106	CLA	C1C-C2C	2.57	1.49	1.44
21	A	1125	CLA	C1C-C2C	2.57	1.49	1.44
21	B	1217	CLA	C1C-C2C	2.57	1.49	1.44
21	a	1115	CLA	C1C-C2C	2.57	1.49	1.44
21	2	1221	CLA	MG-NC	2.57	2.12	2.06
21	b	1220	CLA	C1C-C2C	2.57	1.49	1.44
21	2	1227	CLA	C1C-C2C	2.57	1.49	1.44
21	b	1231	CLA	C1C-C2C	2.57	1.49	1.44
21	B	1224	CLA	C1C-C2C	2.56	1.49	1.44
21	B	1021	CLA	C1C-C2C	2.56	1.49	1.44
21	a	1104	CLA	C1C-C2C	2.56	1.49	1.44
21	a	1112	CLA	C1C-C2C	2.56	1.49	1.44
21	B	1209	CLA	C1C-C2C	2.56	1.49	1.44
35	0	6001	LMT	O3'-C3'	-2.56	1.36	1.43
21	1	1139	CLA	C1C-C2C	2.56	1.49	1.44
21	a	1123	CLA	C1C-C2C	2.56	1.49	1.44
21	1	1140	CLA	C1C-C2C	2.56	1.49	1.44
21	A	1106	CLA	C1C-C2C	2.56	1.49	1.44
21	1	1114	CLA	C1C-C2C	2.56	1.49	1.44
21	b	1228	CLA	C1C-C2C	2.56	1.49	1.44
21	A	1133	CLA	C1C-C2C	2.56	1.49	1.44
21	L	1503	CLA	C1C-C2C	2.56	1.49	1.44
21	a	1135	CLA	C1C-C2C	2.56	1.49	1.44
21	b	1216	CLA	C1C-C2C	2.56	1.49	1.44
21	A	1129	CLA	C1C-C2C	2.55	1.49	1.44
21	b	1211	CLA	C1C-C2C	2.55	1.49	1.44
21	1	1135	CLA	C1C-C2C	2.55	1.49	1.44
21	2	1209	CLA	C1C-C2C	2.55	1.49	1.44
21	8	1401	CLA	C1C-C2C	2.55	1.49	1.44
21	L	1501	CLA	C1C-C2C	2.55	1.49	1.44
21	B	1211	CLA	MG-NC	2.55	2.12	2.06
21	2	1212	CLA	C1C-C2C	2.55	1.49	1.44
21	A	1801	CLA	C1C-C2C	2.55	1.49	1.44
21	a	1137	CLA	C1C-C2C	2.55	1.49	1.44
21	1	1118	CLA	C1C-C2C	2.55	1.49	1.44
21	j	1302	CLA	C1C-C2C	2.55	1.49	1.44
21	2	1232	CLA	C1C-C2C	2.55	1.49	1.44
21	7	1303	CLA	MG-NC	2.55	2.12	2.06
21	2	1206	CLA	C1C-C2C	2.55	1.49	1.44
21	b	1235	CLA	C1C-C2C	2.55	1.49	1.44
21	B	1240	CLA	MG-NC	2.55	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1204	CLA	C1C-C2C	2.54	1.49	1.44
21	b	1224	CLA	C1C-C2C	2.54	1.49	1.44
21	f	1302	CLA	C1C-C2C	2.54	1.49	1.44
21	b	1209	CLA	C1C-C2C	2.54	1.49	1.44
21	a	1111	CLA	C1C-C2C	2.54	1.49	1.44
21	2	1225	CLA	C1C-C2C	2.54	1.49	1.44
21	a	1132	CLA	C1C-C2C	2.54	1.49	1.44
21	2	1231	CLA	C1C-C2C	2.54	1.49	1.44
21	A	1134	CLA	C1C-C2C	2.54	1.49	1.44
21	a	1133	CLA	C1C-C2C	2.54	1.49	1.44
21	A	1136	CLA	MG-NC	2.54	2.12	2.06
21	b	1230	CLA	C1C-C2C	2.54	1.49	1.44
21	j	1303	CLA	MG-NC	2.54	2.12	2.06
35	F	6001	LMT	O3'-C3'	-2.53	1.36	1.43
21	B	1203	CLA	MG-NC	2.53	2.12	2.06
21	a	1106	CLA	C1C-C2C	2.53	1.49	1.44
21	A	1013	CLA	C1C-C2C	2.53	1.49	1.44
21	A	1107	CLA	C1C-C2C	2.53	1.49	1.44
21	A	1114	CLA	C1C-C2C	2.53	1.49	1.44
35	l	6001	LMT	O3'-C3'	-2.53	1.36	1.43
21	b	1223	CLA	C1C-C2C	2.53	1.49	1.44
21	1	1112	CLA	C1C-C2C	2.53	1.49	1.44
21	B	1232	CLA	C1C-C2C	2.53	1.49	1.44
21	2	1229	CLA	C1C-NC	-2.53	1.33	1.37
21	A	1131	CLA	C1C-C2C	2.52	1.49	1.44
21	B	1221	CLA	C1C-C2C	2.52	1.49	1.44
21	2	1219	CLA	C1C-C2C	2.52	1.49	1.44
21	8	1401	CLA	MG-NC	2.52	2.12	2.06
21	6	1301	CLA	C1C-C2C	2.52	1.49	1.44
21	A	1111	CLA	C1C-C2C	2.52	1.49	1.44
21	A	1119	CLA	C1C-C2C	2.52	1.49	1.44
21	B	1231	CLA	C1C-C2C	2.52	1.49	1.44
21	b	1208	CLA	C1C-C2C	2.52	1.49	1.44
21	F	1301	CLA	C1C-C2C	2.52	1.49	1.44
21	a	1801	CLA	MG-NC	2.52	2.12	2.06
21	A	1012	CLA	MG-NC	2.51	2.12	2.06
21	2	1214	CLA	MG-NC	2.51	2.12	2.06
21	K	1401	CLA	C1C-C2C	2.51	1.49	1.44
21	1	1124	CLA	C1C-C2C	2.51	1.49	1.44
21	b	1203	CLA	C1C-C2C	2.51	1.49	1.44
21	1	1127	CLA	MG-NC	2.51	2.12	2.06
21	1	1137	CLA	C1C-NC	-2.51	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1213	CLA	C1C-C2C	2.51	1.49	1.44
21	2	1221	CLA	C1C-C2C	2.51	1.49	1.44
21	a	1114	CLA	MG-NC	2.51	2.12	2.06
21	a	1114	CLA	C1C-C2C	2.51	1.49	1.44
21	b	1210	CLA	C1C-C2C	2.51	1.49	1.44
21	b	1210	CLA	MG-NC	2.51	2.12	2.06
35	L	6001	LMT	O3'-C3'	-2.51	1.36	1.43
21	b	1225	CLA	C1C-C2C	2.50	1.49	1.44
21	J	1303	CLA	MG-NC	2.50	2.12	2.06
21	1	1115	CLA	C1C-C2C	2.50	1.49	1.44
21	2	1237	CLA	C1C-C2C	2.50	1.49	1.44
21	2	1240	CLA	MG-NC	2.50	2.12	2.06
21	1	1121	CLA	C1C-C2C	2.50	1.49	1.44
34	J	4015	ZEX	C27-C26	2.50	1.49	1.46
21	1	1111	CLA	C1C-C2C	2.50	1.49	1.44
21	A	1129	CLA	MG-NC	2.50	2.12	2.06
21	A	1130	CLA	C1C-C2C	2.50	1.49	1.44
21	a	1801	CLA	C1C-C2C	2.50	1.49	1.44
21	k	1401	CLA	MG-NC	2.50	2.12	2.06
21	1	1130	CLA	C1C-C2C	2.50	1.49	1.44
21	0	1503	CLA	C1C-C2C	2.50	1.49	1.44
21	A	1012	CLA	C1C-C2C	2.49	1.49	1.44
21	A	1112	CLA	MG-NC	2.49	2.12	2.06
21	B	1206	CLA	C1C-C2C	2.49	1.49	1.44
21	a	1105	CLA	C1C-C2C	2.49	1.49	1.44
21	1	1133	CLA	C1C-C2C	2.49	1.49	1.44
21	A	1112	CLA	C1C-C2C	2.49	1.49	1.44
21	F	1302	CLA	C1C-C2C	2.49	1.49	1.44
21	a	1120	CLA	C1C-C2C	2.49	1.49	1.44
28	h	4020	45D	C17-C15	2.49	1.53	1.47
21	f	1301	CLA	MG-NC	2.49	2.12	2.06
21	1	1121	CLA	MG-NC	2.49	2.12	2.06
21	2	1220	CLA	MG-NC	2.49	2.12	2.06
21	b	1217	CLA	MG-NC	2.49	2.12	2.06
21	1	1104	CLA	C1C-C2C	2.49	1.49	1.44
21	b	1238	CLA	MG-NC	2.49	2.12	2.06
21	A	1125	CLA	C1C-NC	-2.49	1.34	1.37
21	b	1227	CLA	C1C-C2C	2.49	1.49	1.44
21	1	1113	CLA	MG-NC	2.49	2.12	2.06
22	B	2002	PQN	C10-C5	-2.49	1.36	1.40
21	F	1302	CLA	MG-NC	2.48	2.12	2.06
21	a	1128	CLA	C1C-C2C	2.48	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1224	CLA	MG-NC	2.48	2.12	2.06
21	b	1226	CLA	C1C-C2C	2.48	1.49	1.44
21	1	1134	CLA	C1C-C2C	2.48	1.49	1.44
21	1	1112	CLA	MG-NC	2.48	2.12	2.06
21	2	1021	CLA	C1C-C2C	2.48	1.49	1.44
21	A	1139	CLA	C1C-C2C	2.48	1.49	1.44
21	2	1209	CLA	MG-NC	2.47	2.12	2.06
21	2	1238	CLA	C1C-C2C	2.47	1.49	1.44
21	2	1210	CLA	C1C-NC	-2.47	1.34	1.37
21	b	1221	CLA	MG-NC	2.47	2.12	2.06
36	I	4020	EQ3	C28-C27	2.47	1.54	1.50
21	A	1137	CLA	C1C-C2C	2.47	1.49	1.44
21	b	1234	CLA	C1C-NC	-2.47	1.34	1.37
21	a	1107	CLA	C1C-C2C	2.47	1.49	1.44
21	A	1113	CLA	MG-NC	2.47	2.12	2.06
21	1	1136	CLA	MG-NC	2.47	2.12	2.06
21	2	1224	CLA	C1C-C2C	2.47	1.49	1.44
21	1	1120	CLA	MG-NC	2.47	2.12	2.06
21	a	1122	CLA	C1C-C2C	2.47	1.49	1.44
21	1	1105	CLA	MG-NC	2.47	2.12	2.06
21	2	1214	CLA	C1C-C2C	2.47	1.49	1.44
21	b	1232	CLA	MG-NC	2.47	2.12	2.06
21	l	1501	CLA	MG-NC	2.47	2.12	2.06
21	a	1120	CLA	MG-NC	2.46	2.12	2.06
21	a	1102	CLA	MG-NC	2.46	2.12	2.06
21	1	1140	CLA	MG-NC	2.46	2.12	2.06
21	B	1218	CLA	C1C-C2C	2.46	1.49	1.44
21	1	1119	CLA	C1C-C2C	2.46	1.49	1.44
21	B	1205	CLA	MG-NC	2.46	2.12	2.06
21	A	1132	CLA	MG-NC	2.46	2.12	2.06
21	B	1234	CLA	MG-NC	2.46	2.12	2.06
21	B	1214	CLA	C1C-C2C	2.46	1.49	1.44
21	b	1220	CLA	C1C-NC	-2.46	1.34	1.37
21	b	1222	CLA	C1C-C2C	2.46	1.49	1.44
21	1	1109	CLA	MG-NC	2.46	2.12	2.06
21	2	1204	CLA	C1C-NC	-2.46	1.34	1.37
21	J	1302	CLA	C1C-NC	-2.46	1.34	1.37
21	2	1210	CLA	MG-NC	2.46	2.12	2.06
21	L	1502	CLA	C1C-C2C	2.46	1.49	1.44
21	a	1135	CLA	MG-NC	2.45	2.12	2.06
21	B	1210	CLA	C1C-C2C	2.45	1.49	1.44
21	A	1123	CLA	MG-NC	2.45	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1217	CLA	MG-NC	2.45	2.12	2.06
21	a	1107	CLA	C1C-NC	-2.45	1.34	1.37
21	2	1230	CLA	MG-NC	2.45	2.12	2.06
21	l	1501	CLA	C1C-C2C	2.45	1.49	1.44
21	a	1105	CLA	MG-NC	2.45	2.12	2.06
21	a	1125	CLA	C1C-NC	-2.45	1.34	1.37
21	K	1402	CLA	C1C-C2C	2.45	1.49	1.44
21	a	1132	CLA	MG-NC	2.45	2.12	2.06
21	2	1219	CLA	MG-NC	2.45	2.12	2.06
21	b	1204	CLA	C1C-C2C	2.45	1.49	1.44
21	b	1201	CLA	C1C-C2C	2.45	1.49	1.44
21	a	1111	CLA	MG-NC	2.45	2.12	2.06
21	a	1124	CLA	C1C-C2C	2.45	1.49	1.44
21	1	1122	CLA	C1C-C2C	2.45	1.49	1.44
21	a	1138	CLA	MG-NC	2.44	2.12	2.06
21	1	1116	CLA	MG-NC	2.44	2.12	2.06
21	a	1139	CLA	MG-NC	2.44	2.12	2.06
21	2	1239	CLA	C1C-NC	-2.44	1.34	1.37
21	a	1102	CLA	C1C-C2C	2.44	1.49	1.44
21	A	1115	CLA	C1C-C2C	2.44	1.49	1.44
21	1	1103	CLA	C1C-NC	-2.44	1.34	1.37
21	A	1109	CLA	C1C-C2C	2.44	1.49	1.44
21	6	1301	CLA	MG-NC	2.44	2.12	2.06
21	A	1124	CLA	MG-NC	2.44	2.12	2.06
21	L	1503	CLA	MG-NC	2.44	2.12	2.06
21	a	1113	CLA	MG-NC	2.44	2.12	2.06
21	B	1209	CLA	MG-NC	2.44	2.12	2.06
21	A	1103	CLA	C1C-NC	-2.44	1.34	1.37
27	A	7001	ACT	CH3-C	2.44	1.58	1.49
21	a	1121	CLA	MG-NC	2.44	2.12	2.06
21	7	1303	CLA	C1C-C2C	2.44	1.49	1.44
21	1	1124	CLA	MG-NC	2.44	2.12	2.06
21	a	1012	CLA	C1C-NC	-2.43	1.34	1.37
21	1	1117	CLA	C1C-C2C	2.43	1.49	1.44
21	L	1501	CLA	MG-NC	2.43	2.12	2.06
21	B	1213	CLA	MG-NC	2.43	2.12	2.06
21	2	1211	CLA	MG-NC	2.43	2.12	2.06
21	1	1125	CLA	MG-NC	2.43	2.12	2.06
21	1	1122	CLA	C1C-NC	-2.43	1.34	1.37
21	a	1111	CLA	C1C-NC	-2.43	1.34	1.37
21	1	1123	CLA	C1C-C2C	2.43	1.49	1.44
21	a	1112	CLA	MG-NC	2.43	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1219	CLA	C1C-NC	-2.43	1.34	1.37
21	f	1302	CLA	MG-NC	2.43	2.12	2.06
21	b	1212	CLA	C1C-NC	-2.43	1.34	1.37
21	b	1236	CLA	C1C-C2C	2.43	1.49	1.44
21	A	1138	CLA	C1C-C2C	2.43	1.49	1.44
21	b	1205	CLA	MG-NC	2.43	2.12	2.06
21	A	1127	CLA	MG-NC	2.43	2.12	2.06
21	B	1220	CLA	C1C-NC	-2.43	1.34	1.37
21	b	1218	CLA	MG-NC	2.42	2.12	2.06
21	B	1221	CLA	MG-NC	2.42	2.12	2.06
21	b	1205	CLA	C1C-C2C	2.42	1.49	1.44
21	b	1214	CLA	MG-NC	2.42	2.12	2.06
21	1	1118	CLA	C1C-NC	-2.42	1.34	1.37
21	A	1124	CLA	C1C-C2C	2.42	1.49	1.44
21	B	1022	CLA	MG-NC	2.42	2.12	2.06
21	A	1122	CLA	C1C-NC	-2.42	1.34	1.37
34	7	4015	ZEX	C1-C6	-2.42	1.50	1.53
21	B	1227	CLA	C1C-NC	-2.42	1.34	1.37
21	b	1219	CLA	MG-NC	2.42	2.12	2.06
21	1	1111	CLA	MG-NC	2.42	2.12	2.06
21	A	1107	CLA	MG-NC	2.42	2.12	2.06
21	1	1138	CLA	MG-NC	2.41	2.12	2.06
21	J	1302	CLA	MG-NC	2.41	2.12	2.06
21	8	1402	CLA	MG-NC	2.41	2.12	2.06
21	B	1232	CLA	C1C-NC	-2.41	1.34	1.37
21	a	1108	CLA	MG-NC	2.41	2.12	2.06
35	1	6001	LMT	O3'-C3'	-2.41	1.37	1.43
21	B	1214	CLA	MG-NC	2.41	2.12	2.06
21	b	1237	CLA	MG-NC	2.41	2.12	2.06
21	A	1122	CLA	C1C-C2C	2.41	1.49	1.44
21	a	1130	CLA	MG-NC	2.41	2.12	2.06
21	A	1116	CLA	C1C-NC	-2.41	1.34	1.37
21	2	1228	CLA	C1C-NC	-2.41	1.34	1.37
21	1	1114	CLA	MG-NC	2.41	2.12	2.06
21	B	1216	CLA	MG-NC	2.41	2.12	2.06
21	b	1203	CLA	MG-NC	2.41	2.12	2.06
21	A	1111	CLA	C1C-NC	-2.41	1.34	1.37
21	b	1223	CLA	MG-NC	2.41	2.12	2.06
21	2	1206	CLA	MG-NC	2.41	2.12	2.06
22	b	2002	PQN	C10-C5	-2.41	1.36	1.40
21	B	1203	CLA	C1C-C2C	2.41	1.49	1.44
21	0	1502	CLA	C1C-NC	-2.41	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1234	CLA	MG-NC	2.41	2.12	2.06
21	0	1501	CLA	MG-NC	2.40	2.12	2.06
21	2	1226	CLA	C1B-NB	-2.40	1.34	1.37
21	2	1236	CLA	MG-NC	2.40	2.12	2.06
21	B	1222	CLA	C1C-NC	-2.40	1.34	1.37
21	1	1119	CLA	C1C-NC	-2.40	1.34	1.37
21	7	1302	CLA	MG-NC	2.40	2.12	2.06
21	b	1225	CLA	MG-NC	2.40	2.12	2.06
21	1	1139	CLA	MG-NC	2.40	2.12	2.06
21	2	1216	CLA	MG-NC	2.40	2.12	2.06
21	B	1230	CLA	C1C-NC	-2.40	1.34	1.37
21	a	1137	CLA	MG-NC	2.40	2.12	2.06
21	2	1226	CLA	C1C-C2C	2.40	1.49	1.44
21	B	1236	CLA	C1C-NC	-2.40	1.34	1.37
21	1	1011	CLA	MG-NC	2.40	2.12	2.06
21	1	1133	CLA	C1C-NC	-2.40	1.34	1.37
21	2	1239	CLA	C1C-C2C	2.40	1.49	1.44
21	b	1236	CLA	C1C-NC	-2.40	1.34	1.37
21	1	1128	CLA	MG-NC	2.40	2.12	2.06
21	A	1135	CLA	MG-NC	2.39	2.12	2.06
21	1	1102	CLA	C1C-C2C	2.39	1.49	1.44
34	7	4015	ZEX	C27-C26	2.39	1.49	1.46
21	2	1222	CLA	MG-NC	2.39	2.12	2.06
21	A	1121	CLA	C1C-C2C	2.39	1.49	1.44
21	b	1206	CLA	MG-NC	2.39	2.11	2.06
21	B	1223	CLA	C1C-NC	-2.39	1.34	1.37
21	a	1122	CLA	MG-NC	2.39	2.11	2.06
21	A	1138	CLA	C1C-NC	-2.39	1.34	1.37
21	0	1503	CLA	C1C-NC	-2.39	1.34	1.37
21	b	1238	CLA	C1C-C2C	2.39	1.49	1.44
21	B	1218	CLA	C1C-NC	-2.39	1.34	1.37
21	b	1238	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1223	CLA	MG-NC	2.39	2.11	2.06
21	K	1402	CLA	MG-NC	2.39	2.11	2.06
21	b	1237	CLA	C1C-C2C	2.39	1.49	1.44
21	a	1130	CLA	C1C-NC	-2.39	1.34	1.37
21	b	1023	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1022	CLA	MG-NC	2.39	2.11	2.06
21	B	1215	CLA	MG-NC	2.39	2.11	2.06
21	2	1224	CLA	MG-NC	2.38	2.11	2.06
21	1	1101	CLA	C1C-NC	-2.38	1.34	1.37
21	1	1012	CLA	MG-NC	2.38	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	1401	CLA	MG-NC	2.38	2.11	2.06
21	A	1114	CLA	MG-NC	2.38	2.11	2.06
21	2	1218	CLA	MG-NC	2.38	2.11	2.06
21	1	1108	CLA	MG-NC	2.38	2.11	2.06
21	b	1228	CLA	MG-NC	2.38	2.11	2.06
21	L	1502	CLA	MG-NC	2.38	2.11	2.06
21	1	1107	CLA	MG-NC	2.38	2.11	2.06
21	b	1216	CLA	C1C-NC	-2.38	1.34	1.37
21	j	1302	CLA	MG-NC	2.38	2.11	2.06
21	a	1140	CLA	C1C-NC	-2.38	1.34	1.37
21	2	1207	CLA	C1C-NC	-2.38	1.34	1.37
21	L	1501	CLA	C1C-NC	-2.38	1.34	1.37
21	A	1128	CLA	MG-NC	2.38	2.11	2.06
21	b	1237	CLA	C1C-NC	-2.38	1.34	1.37
21	A	1135	CLA	C1C-C2C	2.38	1.49	1.44
21	B	1226	CLA	C1B-NB	-2.38	1.34	1.37
21	A	1105	CLA	MG-NC	2.38	2.11	2.06
21	A	1106	CLA	C1C-NC	-2.37	1.34	1.37
21	a	1115	CLA	C1C-NC	-2.37	1.34	1.37
21	B	1225	CLA	MG-NC	2.37	2.11	2.06
21	1	1801	CLA	MG-NC	2.37	2.11	2.06
21	a	1136	CLA	MG-NC	2.37	2.11	2.06
21	B	1204	CLA	MG-NC	2.37	2.11	2.06
21	A	1108	CLA	C1C-NC	-2.37	1.34	1.37
21	1	1011	CLA	C1B-NB	-2.37	1.34	1.37
21	b	1207	CLA	C1C-NC	-2.37	1.34	1.37
21	a	1128	CLA	MG-NC	2.37	2.11	2.06
21	a	1112	CLA	C1C-NC	-2.37	1.34	1.37
21	a	1137	CLA	C1C-NC	-2.37	1.34	1.37
21	1	1106	CLA	MG-NC	2.37	2.11	2.06
21	a	1118	CLA	MG-NC	2.37	2.11	2.06
21	2	1232	CLA	MG-NC	2.37	2.11	2.06
21	6	1302	CLA	MG-NC	2.37	2.11	2.06
21	A	1104	CLA	MG-NC	2.37	2.11	2.06
21	1	1102	CLA	MG-NC	2.37	2.11	2.06
21	A	1116	CLA	MG-NC	2.37	2.11	2.06
21	2	1220	CLA	C1C-NC	-2.37	1.34	1.37
21	2	1230	CLA	C1C-NC	-2.37	1.34	1.37
21	1	1013	CLA	C1B-NB	-2.37	1.34	1.37
21	b	1209	CLA	MG-NC	2.37	2.11	2.06
21	a	1107	CLA	MG-NC	2.37	2.11	2.06
26	1	5002	LMG	C22-C21	-2.37	1.33	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1223	CLA	C1C-NC	-2.37	1.34	1.37
21	B	1223	CLA	MG-NC	2.37	2.11	2.06
21	a	1101	CLA	MG-NC	2.36	2.11	2.06
21	B	1222	CLA	C1B-NB	-2.36	1.34	1.37
21	1	1127	CLA	C1C-NC	-2.36	1.34	1.37
21	a	1109	CLA	C1C-C2C	2.36	1.49	1.44
21	1	1117	CLA	MG-NC	2.36	2.11	2.06
21	a	1012	CLA	MG-NC	2.36	2.11	2.06
21	a	1120	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1226	CLA	MG-NC	2.36	2.11	2.06
28	h	4020	45D	O02-C18	-2.36	1.18	1.23
21	2	1208	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1227	CLA	C1C-NC	-2.36	1.34	1.37
21	A	1121	CLA	C1C-NC	-2.36	1.34	1.37
21	B	1204	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1225	CLA	MG-NC	2.36	2.11	2.06
21	a	1126	CLA	C1C-NC	-2.36	1.34	1.37
21	b	1202	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1224	CLA	C1B-NB	-2.36	1.34	1.37
21	2	1203	CLA	MG-NC	2.36	2.11	2.06
21	B	1209	CLA	C1C-NC	-2.36	1.34	1.37
21	a	1124	CLA	MG-NC	2.36	2.11	2.06
21	K	1401	CLA	C1C-NC	-2.35	1.34	1.37
21	b	1206	CLA	C1C-C2C	2.35	1.49	1.44
21	b	1236	CLA	MG-NC	2.35	2.11	2.06
21	B	1229	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1236	CLA	C1C-NC	-2.35	1.34	1.37
21	A	1131	CLA	C1C-NC	-2.35	1.34	1.37
21	a	1103	CLA	C1C-NC	-2.35	1.34	1.37
21	0	1503	CLA	MG-NC	2.35	2.11	2.06
26	a	5002	LMG	C22-C21	-2.35	1.33	1.50
21	B	1227	CLA	MG-NC	2.35	2.11	2.06
21	a	1110	CLA	MG-NC	2.35	2.11	2.06
21	2	1237	CLA	MG-NC	2.35	2.11	2.06
21	A	1139	CLA	C1C-NC	-2.35	1.34	1.37
21	a	1127	CLA	C1C-NC	-2.35	1.34	1.37
21	7	1303	CLA	C1C-NC	-2.35	1.34	1.37
21	A	1118	CLA	MG-NC	2.35	2.11	2.06
21	1	1101	CLA	MG-NC	2.35	2.11	2.06
21	B	1208	CLA	MG-NC	2.35	2.11	2.06
21	b	1201	CLA	MG-NC	2.35	2.11	2.06
26	A	5002	LMG	C22-C21	-2.35	1.33	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1117	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1235	CLA	MG-NC	2.35	2.11	2.06
21	f	1302	CLA	C1C-NC	-2.35	1.34	1.37
21	A	1011	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1116	CLA	MG-NC	2.34	2.11	2.06
21	a	1109	CLA	MG-NC	2.34	2.11	2.06
21	2	1206	CLA	C1B-NB	-2.34	1.34	1.37
21	b	1223	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1011	CLA	C1B-NB	-2.34	1.34	1.37
21	1	1119	CLA	C1B-NB	-2.34	1.34	1.37
21	1	1118	CLA	MG-NC	2.34	2.11	2.06
21	1	1134	CLA	C1C-NC	-2.34	1.34	1.37
21	1	1140	CLA	C1B-NB	-2.34	1.34	1.37
21	6	1302	CLA	C4B-NB	-2.34	1.34	1.37
21	B	1237	CLA	MG-NC	2.34	2.11	2.06
21	1	1129	CLA	C1B-NB	-2.34	1.34	1.37
21	A	1128	CLA	C1C-C2C	2.34	1.49	1.44
21	2	1215	CLA	C1B-NB	-2.34	1.34	1.37
21	A	1123	CLA	C1C-C2C	2.34	1.49	1.44
28	B	4011	45D	C17-C15	2.34	1.52	1.47
21	j	1302	CLA	C1C-NC	-2.34	1.34	1.37
21	2	1021	CLA	C1B-NB	-2.34	1.34	1.37
21	1	1126	CLA	MG-NC	2.34	2.11	2.06
21	a	1133	CLA	MG-NC	2.34	2.11	2.06
21	B	1206	CLA	C1B-NB	-2.34	1.34	1.37
21	1	1115	CLA	MG-NC	2.34	2.11	2.06
21	b	1224	CLA	C1C-NC	-2.34	1.34	1.37
21	A	1115	CLA	C1C-NC	-2.34	1.34	1.37
21	B	1228	CLA	MG-NC	2.33	2.11	2.06
21	A	1107	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1239	CLA	MG-NC	2.33	2.11	2.06
21	A	1128	CLA	C1B-NB	-2.33	1.34	1.37
21	1	1115	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1231	CLA	MG-NC	2.33	2.11	2.06
28	h	4020	45D	C18-C16	2.33	1.52	1.47
21	A	1109	CLA	C1C-NC	-2.33	1.34	1.37
21	A	1124	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1212	CLA	C1C-NC	-2.33	1.34	1.37
21	1	1133	CLA	MG-NC	2.33	2.11	2.06
21	B	1206	CLA	C4B-NB	-2.33	1.34	1.37
21	b	1204	CLA	MG-NC	2.33	2.11	2.06
21	B	1206	CLA	MG-NC	2.33	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1115	CLA	MG-NC	2.33	2.11	2.06
21	a	1011	CLA	MG-NC	2.33	2.11	2.06
21	b	1226	CLA	C1B-NB	-2.33	1.34	1.37
21	2	1206	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1220	CLA	MG-NC	2.33	2.11	2.06
21	a	1106	CLA	MG-NC	2.33	2.11	2.06
21	A	1105	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1023	CLA	C1C-NC	-2.33	1.34	1.37
21	2	1231	CLA	MG-NC	2.33	2.11	2.06
21	a	1109	CLA	C1B-NB	-2.33	1.34	1.37
21	B	1226	CLA	MG-NC	2.33	2.11	2.06
21	1	1122	CLA	MG-NC	2.33	2.11	2.06
21	k	1402	CLA	MG-NC	2.33	2.11	2.06
21	A	1105	CLA	C1B-NB	-2.33	1.34	1.37
21	b	1022	CLA	C4B-NB	-2.33	1.34	1.37
21	1	1108	CLA	C1C-NC	-2.33	1.34	1.37
21	b	1238	CLA	C4B-NB	-2.32	1.34	1.37
21	0	1502	CLA	C4B-NB	-2.32	1.34	1.37
21	A	1117	CLA	MG-NC	2.32	2.11	2.06
21	a	1102	CLA	C1C-NC	-2.32	1.34	1.37
21	2	1219	CLA	C1C-NC	-2.32	1.34	1.37
21	B	1210	CLA	C1B-NB	-2.32	1.34	1.37
21	b	1227	CLA	MG-NC	2.32	2.11	2.06
21	1	1132	CLA	MG-NC	2.32	2.11	2.06
21	a	1117	CLA	MG-NC	2.32	2.11	2.06
21	B	1226	CLA	C1C-NC	-2.32	1.34	1.37
21	b	1209	CLA	C1C-NC	-2.32	1.34	1.37
21	1	1138	CLA	C1C-NC	-2.32	1.34	1.37
21	2	1231	CLA	C1C-NC	-2.32	1.34	1.37
21	2	1201	CLA	C1B-NB	-2.32	1.34	1.37
21	B	1207	CLA	C1A-CHA	2.32	1.52	1.43
21	a	1122	CLA	C1C-NC	-2.32	1.34	1.37
21	a	1127	CLA	MG-NC	2.32	2.11	2.06
21	b	1207	CLA	MG-NC	2.32	2.11	2.06
21	1	1013	CLA	C1A-CHA	2.32	1.52	1.43
21	2	1239	CLA	MG-NC	2.32	2.11	2.06
21	b	1223	CLA	C1B-NB	-2.32	1.34	1.37
21	2	1022	CLA	C1C-NC	-2.32	1.34	1.37
21	A	1115	CLA	MG-NC	2.32	2.11	2.06
21	a	1012	CLA	C4B-NB	-2.32	1.34	1.37
21	2	1022	CLA	C1B-NB	-2.32	1.34	1.37
21	A	1106	CLA	C4B-NB	-2.32	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1022	CLA	MG-NC	2.32	2.11	2.06
21	6	1302	CLA	C1A-CHA	2.32	1.52	1.43
21	B	1237	CLA	C1C-C2C	2.32	1.49	1.44
21	b	1211	CLA	MG-NC	2.32	2.11	2.06
21	b	1239	CLA	MG-NC	2.32	2.11	2.06
21	2	1201	CLA	MG-NC	2.32	2.11	2.06
21	a	1136	CLA	C1C-NC	-2.32	1.34	1.37
21	a	1103	CLA	C1C-C2C	2.32	1.49	1.44
21	2	1202	CLA	MG-NC	2.32	2.11	2.06
21	1	1103	CLA	C1B-NB	-2.32	1.34	1.37
21	2	1202	CLA	C1C-NC	-2.31	1.34	1.37
21	b	1231	CLA	MG-NC	2.31	2.11	2.06
21	a	1801	CLA	C1C-NC	-2.31	1.34	1.37
21	a	1117	CLA	C1C-NC	-2.31	1.34	1.37
21	2	1209	CLA	C1C-NC	-2.31	1.34	1.37
21	a	1128	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1129	CLA	C1B-NB	-2.31	1.34	1.37
21	B	1023	CLA	C1B-NB	-2.31	1.34	1.37
21	L	1501	CLA	C1B-NB	-2.31	1.34	1.37
21	b	1023	CLA	C1B-NB	-2.31	1.34	1.37
21	1	1119	CLA	C4B-NB	-2.31	1.34	1.37
21	B	1214	CLA	C1C-NC	-2.31	1.34	1.37
21	b	1229	CLA	C1C-NC	-2.31	1.34	1.37
21	1	1120	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1108	CLA	MG-NC	2.31	2.11	2.06
21	2	1023	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1101	CLA	C1B-NB	-2.31	1.34	1.37
21	a	1103	CLA	C1B-NB	-2.31	1.34	1.37
21	b	1237	CLA	C1B-NB	-2.31	1.34	1.37
21	B	1218	CLA	MG-NC	2.31	2.11	2.06
21	2	1212	CLA	MG-NC	2.31	2.11	2.06
21	a	1012	CLA	C1B-NB	-2.31	1.34	1.37
21	B	1238	CLA	MG-NC	2.31	2.11	2.06
21	a	1125	CLA	MG-NC	2.31	2.11	2.06
21	2	1215	CLA	MG-NC	2.31	2.11	2.06
21	A	1801	CLA	MG-NC	2.31	2.11	2.06
21	b	1206	CLA	C1B-NB	-2.31	1.34	1.37
21	1	1110	CLA	MG-NC	2.31	2.11	2.06
21	1	1140	CLA	C1C-NC	-2.31	1.34	1.37
21	B	1235	CLA	MG-NC	2.31	2.11	2.06
21	B	1207	CLA	MG-NC	2.31	2.11	2.06
21	b	1022	CLA	C1C-NC	-2.31	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1225	CLA	C1C-NC	-2.31	1.34	1.37
21	B	1215	CLA	C1B-NB	-2.31	1.34	1.37
21	1	1132	CLA	C1B-NB	-2.31	1.34	1.37
21	2	1231	CLA	C1B-NB	-2.31	1.34	1.37
21	A	1101	CLA	MG-NC	2.31	2.11	2.06
21	l	1503	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1115	CLA	C1B-NB	-2.31	1.34	1.37
21	a	1126	CLA	MG-NC	2.30	2.11	2.06
21	b	1234	CLA	MG-NC	2.30	2.11	2.06
21	A	1011	CLA	C1B-NB	-2.30	1.34	1.37
21	2	1021	CLA	C1C-NC	-2.30	1.34	1.37
21	A	1102	CLA	MG-NC	2.30	2.11	2.06
21	1	1128	CLA	C1B-NB	-2.30	1.34	1.37
21	a	1129	CLA	C1C-NC	-2.30	1.34	1.37
21	B	1201	CLA	MG-NC	2.30	2.11	2.06
21	2	1205	CLA	C1C-C2C	2.30	1.49	1.44
21	B	1205	CLA	C1C-NC	-2.30	1.34	1.37
21	F	1301	CLA	C1B-NB	-2.30	1.34	1.37
21	B	1236	CLA	MG-NC	2.30	2.11	2.06
21	B	1201	CLA	C1C-C2C	2.30	1.49	1.44
21	1	1111	CLA	C1C-NC	-2.30	1.34	1.37
21	2	1225	CLA	C1C-NC	-2.30	1.34	1.37
21	8	1401	CLA	C1C-NC	-2.30	1.34	1.37
21	b	1204	CLA	C1C-NC	-2.30	1.34	1.37
21	2	1213	CLA	C1C-NC	-2.30	1.34	1.37
21	b	1222	CLA	C1B-NB	-2.30	1.34	1.37
21	a	1134	CLA	MG-NC	2.30	2.11	2.06
21	L	1503	CLA	C1C-NC	-2.30	1.34	1.37
21	A	1013	CLA	C1B-NB	-2.30	1.34	1.37
21	B	1222	CLA	C4B-NB	-2.30	1.34	1.37
21	2	1211	CLA	C1B-NB	-2.30	1.34	1.37
21	2	1228	CLA	C1B-NB	-2.30	1.34	1.37
21	B	1235	CLA	C1C-NC	-2.30	1.34	1.37
21	b	1232	CLA	C1B-NB	-2.30	1.34	1.37
21	b	1239	CLA	C1C-NC	-2.30	1.34	1.37
21	A	1118	CLA	C4B-NB	-2.30	1.34	1.37
21	a	1124	CLA	C1B-NB	-2.30	1.34	1.37
21	a	1131	CLA	MG-NC	2.30	2.11	2.06
21	a	1105	CLA	C1C-NC	-2.30	1.34	1.37
21	2	1235	CLA	C1C-NC	-2.30	1.34	1.37
21	A	1122	CLA	C4B-NB	-2.30	1.34	1.37
21	1	1136	CLA	C1B-NB	-2.30	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1137	CLA	C1B-NB	-2.30	1.34	1.37
21	a	1134	CLA	C1B-NB	-2.30	1.34	1.37
21	b	1231	CLA	C1C-NC	-2.29	1.34	1.37
21	B	1239	CLA	C1B-NB	-2.29	1.34	1.37
21	2	1238	CLA	MG-NC	2.29	2.11	2.06
21	6	1302	CLA	C1B-NB	-2.29	1.34	1.37
21	B	1224	CLA	MG-NC	2.29	2.11	2.06
21	B	1238	CLA	C1B-NB	-2.29	1.34	1.37
21	2	1237	CLA	C4B-NB	-2.29	1.34	1.37
21	A	1122	CLA	MG-NC	2.29	2.11	2.06
21	A	1110	CLA	C1C-NC	-2.29	1.34	1.37
21	A	1121	CLA	MG-NC	2.29	2.11	2.06
21	2	1237	CLA	C1B-NB	-2.29	1.34	1.37
21	2	1227	CLA	MG-NC	2.29	2.11	2.06
21	1	1118	CLA	C1B-NB	-2.29	1.34	1.37
21	1	1122	CLA	C1B-NB	-2.29	1.34	1.37
21	B	1216	CLA	C1C-NC	-2.29	1.34	1.37
21	a	1110	CLA	C1C-NC	-2.29	1.34	1.37
21	b	1213	CLA	MG-NC	2.29	2.11	2.06
21	A	1138	CLA	C4B-NB	-2.29	1.34	1.37
21	2	1205	CLA	C1C-NC	-2.29	1.34	1.37
21	7	1302	CLA	C1C-NC	-2.29	1.34	1.37
21	A	1128	CLA	C4B-NB	-2.29	1.34	1.37
21	B	1230	CLA	C1B-NB	-2.29	1.34	1.37
21	1	1104	CLA	MG-NC	2.29	2.11	2.06
21	1	1137	CLA	MG-NC	2.29	2.11	2.06
21	1	1110	CLA	C1C-NC	-2.29	1.34	1.37
21	2	1212	CLA	C1C-NC	-2.29	1.34	1.37
21	f	1301	CLA	C1B-NB	-2.29	1.34	1.37
21	1	1104	CLA	C1B-NB	-2.29	1.34	1.37
21	B	1206	CLA	C1C-NC	-2.29	1.34	1.37
21	B	1219	CLA	MG-NC	2.29	2.11	2.06
21	b	1235	CLA	MG-NC	2.29	2.11	2.06
21	1	1121	CLA	C1B-NB	-2.29	1.34	1.37
21	2	1021	CLA	C4B-NB	-2.29	1.34	1.37
21	a	1113	CLA	C1C-NC	-2.29	1.34	1.37
21	b	1228	CLA	C1C-NC	-2.29	1.34	1.37
21	2	1208	CLA	MG-NC	2.29	2.11	2.06
21	b	1238	CLA	C1B-NB	-2.29	1.34	1.37
21	B	1217	CLA	C1C-NC	-2.29	1.34	1.37
21	A	1111	CLA	MG-NC	2.29	2.11	2.06
21	1	1129	CLA	MG-NC	2.29	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	1402	CLA	C1C-NC	-2.29	1.34	1.37
21	A	1134	CLA	C1B-NB	-2.29	1.34	1.37
21	a	1136	CLA	C1B-NB	-2.29	1.34	1.37
21	2	1211	CLA	C4B-NB	-2.29	1.34	1.37
21	a	1140	CLA	MG-NC	2.28	2.11	2.06
21	B	1213	CLA	C1C-NC	-2.28	1.34	1.37
21	a	1105	CLA	C4B-NB	-2.28	1.34	1.37
21	1	1117	CLA	C1B-NB	-2.28	1.34	1.37
21	2	1230	CLA	C1B-NB	-2.28	1.34	1.37
21	1	1103	CLA	C1C-C2C	2.28	1.49	1.44
21	B	1218	CLA	C1B-NB	-2.28	1.34	1.37
21	B	1238	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1124	CLA	C1B-NB	-2.28	1.34	1.37
21	B	1210	CLA	C4B-NB	-2.28	1.34	1.37
21	b	1201	CLA	C4B-NB	-2.28	1.34	1.37
21	B	1215	CLA	C1C-NC	-2.28	1.34	1.37
21	B	1234	CLA	C1C-NC	-2.28	1.34	1.37
21	1	1115	CLA	C1B-NB	-2.28	1.34	1.37
21	2	1227	CLA	C1B-NB	-2.28	1.34	1.37
21	a	1109	CLA	C1C-NC	-2.28	1.34	1.37
21	b	1206	CLA	C1C-NC	-2.28	1.34	1.37
21	B	1201	CLA	C1C-NC	-2.28	1.34	1.37
21	b	1201	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1109	CLA	C1B-NB	-2.28	1.34	1.37
21	B	1208	CLA	C1B-NB	-2.28	1.34	1.37
21	2	1203	CLA	C1B-NB	-2.28	1.34	1.37
21	A	1139	CLA	MG-NC	2.28	2.11	2.06
21	A	1110	CLA	C1B-NB	-2.28	1.34	1.37
21	1	1103	CLA	C4B-NB	-2.28	1.34	1.37
21	1	1134	CLA	MG-NC	2.28	2.11	2.06
21	2	1211	CLA	C1C-NC	-2.28	1.34	1.37
21	1	1128	CLA	C1C-C2C	2.28	1.49	1.44
21	B	1230	CLA	MG-NC	2.28	2.11	2.06
21	A	1109	CLA	MG-NC	2.28	2.11	2.06
21	1	1130	CLA	MG-NC	2.28	2.11	2.06
21	A	1119	CLA	C4B-NB	-2.28	1.34	1.37
21	6	1301	CLA	C1B-NB	-2.28	1.34	1.37
21	a	1117	CLA	C1B-NB	-2.28	1.34	1.37
21	a	1116	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1130	CLA	C4B-NB	-2.28	1.34	1.37
21	B	1221	CLA	C1B-NB	-2.28	1.34	1.37
21	1	1126	CLA	C4B-NB	-2.28	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1133	CLA	C1B-NB	-2.28	1.34	1.37
21	1	1131	CLA	MG-NC	2.28	2.11	2.06
21	a	1101	CLA	C1B-NB	-2.28	1.34	1.37
21	2	1216	CLA	C1B-NB	-2.28	1.34	1.37
21	1	1122	CLA	C4B-NB	-2.28	1.34	1.37
21	b	1222	CLA	C4B-NB	-2.28	1.34	1.37
21	2	1023	CLA	C4B-NB	-2.28	1.34	1.37
21	b	1213	CLA	C1C-NC	-2.28	1.34	1.37
21	a	1104	CLA	MG-NC	2.28	2.11	2.06
21	A	1123	CLA	C1A-CHA	2.27	1.52	1.43
21	A	1011	CLA	C4B-NB	-2.27	1.34	1.37
21	A	1109	CLA	C4B-NB	-2.27	1.34	1.37
21	A	1120	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1226	CLA	C4B-NB	-2.27	1.34	1.37
21	l	1501	CLA	C1B-NB	-2.27	1.34	1.37
21	b	1021	CLA	MG-NC	2.27	2.11	2.06
21	8	1401	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1239	CLA	C1C-NC	-2.27	1.34	1.37
21	b	1208	CLA	C4B-NB	-2.27	1.34	1.37
21	A	1123	CLA	C4B-NB	-2.27	1.34	1.37
21	2	1221	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1208	CLA	C1C-NC	-2.27	1.34	1.37
21	B	1224	CLA	C1C-NC	-2.27	1.34	1.37
21	2	1234	CLA	C1C-NC	-2.27	1.34	1.37
22	b	2002	PQN	C9-C10	-2.27	1.36	1.39
21	A	1012	CLA	C4B-NB	-2.27	1.34	1.37
21	B	1205	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1234	CLA	C1B-NB	-2.27	1.34	1.37
21	a	1129	CLA	C1B-NB	-2.27	1.34	1.37
21	2	1222	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1225	CLA	C1C-NC	-2.27	1.34	1.37
21	A	1801	CLA	C4B-NB	-2.27	1.34	1.37
21	B	1237	CLA	C4B-NB	-2.27	1.34	1.37
21	k	1401	CLA	C1B-NB	-2.27	1.34	1.37
21	1	1102	CLA	C1B-NB	-2.27	1.34	1.37
21	b	1216	CLA	MG-NC	2.27	2.11	2.06
21	B	1237	CLA	C1C-NC	-2.27	1.34	1.37
21	1	1130	CLA	C1C-NC	-2.27	1.34	1.37
21	B	1231	CLA	C4B-NB	-2.27	1.34	1.37
21	a	1120	CLA	C1B-NB	-2.27	1.34	1.37
21	b	1209	CLA	C4B-NB	-2.27	1.34	1.37
21	1	1112	CLA	C1B-NB	-2.27	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1122	CLA	C1B-NB	-2.27	1.34	1.37
21	a	1122	CLA	C1B-NB	-2.27	1.34	1.37
21	1	1012	CLA	C1B-NB	-2.27	1.34	1.37
21	B	1218	CLA	C4B-NB	-2.27	1.34	1.37
21	a	1114	CLA	C1B-NB	-2.27	1.34	1.37
21	a	1134	CLA	C1C-NC	-2.27	1.34	1.37
21	a	1013	CLA	C1B-NB	-2.27	1.34	1.37
21	a	1119	CLA	C1B-NB	-2.27	1.34	1.37
21	b	1225	CLA	C1B-NB	-2.27	1.34	1.37
26	A	5002	LMG	O1-C1	2.27	1.44	1.40
21	A	1134	CLA	MG-NC	2.27	2.11	2.06
21	B	1212	CLA	MG-NC	2.27	2.11	2.06
21	B	1215	CLA	C4B-NB	-2.26	1.34	1.37
21	L	1502	CLA	C1B-NB	-2.26	1.34	1.37
21	b	1021	CLA	C1B-NB	-2.26	1.34	1.37
21	1	1107	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1220	CLA	C1B-NB	-2.26	1.34	1.37
21	F	1301	CLA	C1C-NC	-2.26	1.34	1.37
21	2	1203	CLA	C1C-NC	-2.26	1.34	1.37
21	b	1227	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1213	CLA	C4B-NB	-2.26	1.34	1.37
21	8	1402	CLA	C1C-NC	-2.26	1.34	1.37
21	A	1132	CLA	C1B-NB	-2.26	1.34	1.37
21	a	1137	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1225	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1224	CLA	C1C-NC	-2.26	1.34	1.37
21	B	1228	CLA	C4B-NB	-2.26	1.34	1.37
21	2	1206	CLA	C4B-NB	-2.26	1.34	1.37
21	2	1212	CLA	C1B-NB	-2.26	1.34	1.37
21	F	1302	CLA	C1C-NC	-2.26	1.34	1.37
21	a	1133	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1218	CLA	C1B-NB	-2.26	1.34	1.37
21	1	1104	CLA	C1C-NC	-2.26	1.34	1.37
21	B	1223	CLA	C1B-NB	-2.26	1.34	1.37
21	1	1011	CLA	C4B-NB	-2.26	1.34	1.37
21	1	1139	CLA	C1B-NB	-2.26	1.34	1.37
21	2	1224	CLA	C4B-NB	-2.26	1.34	1.37
21	A	1125	CLA	MG-NC	2.26	2.11	2.06
21	A	1107	CLA	C4B-NB	-2.26	1.34	1.37
21	a	1113	CLA	C1B-NB	-2.26	1.34	1.37
21	a	1140	CLA	C4B-NB	-2.26	1.34	1.37
21	2	1210	CLA	C4B-NB	-2.26	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1118	CLA	C1C-NC	-2.26	1.34	1.37
21	A	1112	CLA	C4B-NB	-2.26	1.34	1.37
21	K	1401	CLA	C1B-NB	-2.26	1.34	1.37
21	a	1136	CLA	C1A-CHA	2.26	1.52	1.43
21	b	1215	CLA	C1C-NC	-2.26	1.34	1.37
21	b	1221	CLA	C1C-NC	-2.26	1.34	1.37
21	A	1139	CLA	C4B-NB	-2.26	1.34	1.37
21	1	1801	CLA	C1B-NB	-2.26	1.34	1.37
21	A	1119	CLA	C1B-NB	-2.26	1.34	1.37
21	A	1801	CLA	C1B-NB	-2.26	1.34	1.37
21	B	1021	CLA	C1B-NB	-2.26	1.34	1.37
21	1	1102	CLA	C4B-NB	-2.26	1.34	1.37
21	l	1503	CLA	MG-NC	2.26	2.11	2.06
21	b	1219	CLA	C1C-NC	-2.26	1.34	1.37
21	l	1501	CLA	C1C-NC	-2.26	1.34	1.37
21	a	1109	CLA	C4B-NB	-2.26	1.34	1.37
21	b	1227	CLA	C4B-NB	-2.26	1.34	1.37
21	7	1302	CLA	C1B-NB	-2.26	1.34	1.37
21	B	1213	CLA	C1B-NB	-2.26	1.34	1.37
21	b	1208	CLA	C1C-NC	-2.26	1.34	1.37
21	1	1012	CLA	C1C-NC	-2.26	1.34	1.37
21	b	1215	CLA	C1B-NB	-2.26	1.34	1.37
21	B	1210	CLA	C1C-NC	-2.26	1.34	1.37
21	A	1115	CLA	C4B-NB	-2.25	1.34	1.37
21	B	1208	CLA	C4B-NB	-2.25	1.34	1.37
21	a	1106	CLA	C1B-NB	-2.25	1.34	1.37
21	a	1106	CLA	C4B-NB	-2.25	1.34	1.37
21	1	1113	CLA	C4B-NB	-2.25	1.34	1.37
30	2	4006	ECH	C1-C6	-2.25	1.50	1.53
21	a	1131	CLA	C1C-NC	-2.25	1.34	1.37
21	B	1023	CLA	MG-NC	2.25	2.11	2.06
21	A	1140	CLA	C1C-NC	-2.25	1.34	1.37
21	2	1236	CLA	C1B-NB	-2.25	1.34	1.37
21	7	1303	CLA	C4B-NB	-2.25	1.34	1.37
21	a	1138	CLA	C1C-NC	-2.25	1.34	1.37
21	a	1128	CLA	C1B-NB	-2.25	1.34	1.37
21	b	1023	CLA	C4B-NB	-2.25	1.34	1.37
21	b	1208	CLA	MG-NC	2.25	2.11	2.06
21	b	1240	CLA	C1C-NC	-2.25	1.34	1.37
21	2	1204	CLA	MG-NC	2.25	2.11	2.06
21	A	1118	CLA	C1B-NB	-2.25	1.34	1.37
21	B	1228	CLA	C1C-NC	-2.25	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1112	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1101	CLA	C1B-NB	-2.25	1.34	1.37
21	2	1239	CLA	C1B-NB	-2.25	1.34	1.37
21	B	1021	CLA	MG-NC	2.25	2.11	2.06
21	a	1119	CLA	MG-NC	2.25	2.11	2.06
21	1	1013	CLA	C1C-NC	-2.25	1.34	1.37
21	a	1119	CLA	C4B-NB	-2.25	1.34	1.37
21	a	1123	CLA	C1B-NB	-2.25	1.34	1.37
21	b	1215	CLA	C4B-NB	-2.25	1.34	1.37
21	1	1128	CLA	C4B-NB	-2.25	1.34	1.37
21	a	1121	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1126	CLA	C1C-NC	-2.25	1.34	1.37
21	a	1139	CLA	C1B-NB	-2.25	1.34	1.37
21	b	1229	CLA	C1B-NB	-2.25	1.34	1.37
21	1	1111	CLA	C1B-NB	-2.25	1.34	1.37
21	1	1105	CLA	C1C-NC	-2.25	1.34	1.37
21	2	1237	CLA	C1C-NC	-2.25	1.34	1.37
21	A	1011	CLA	MG-NC	2.25	2.11	2.06
21	a	1011	CLA	C4B-NB	-2.25	1.34	1.37
21	b	1021	CLA	C4B-NB	-2.25	1.34	1.37
21	b	1217	CLA	C1B-NB	-2.25	1.34	1.37
21	l	1501	CLA	C4B-NB	-2.25	1.34	1.37
21	B	1232	CLA	MG-NC	2.25	2.11	2.06
21	A	1104	CLA	C1B-NB	-2.25	1.34	1.37
21	a	1112	CLA	C1B-NB	-2.25	1.34	1.37
21	1	1130	CLA	C1B-NB	-2.25	1.34	1.37
21	a	1129	CLA	MG-NC	2.25	2.11	2.06
21	b	1204	CLA	C1B-NB	-2.25	1.34	1.37
21	b	1207	CLA	C1B-NB	-2.25	1.34	1.37
21	b	1216	CLA	C1B-NB	-2.25	1.34	1.37
21	1	1106	CLA	C1B-NB	-2.25	1.34	1.37
21	1	1125	CLA	C4B-NB	-2.25	1.34	1.37
21	2	1234	CLA	C4B-NB	-2.25	1.34	1.37
21	A	1126	CLA	C1C-NC	-2.25	1.34	1.37
21	A	1127	CLA	C1B-NB	-2.25	1.34	1.37
21	a	1105	CLA	C1B-NB	-2.25	1.34	1.37
21	a	1119	CLA	C1C-NC	-2.24	1.34	1.37
36	I	4020	EQ3	C27-C26	2.24	1.52	1.47
21	B	1023	CLA	C4B-NB	-2.24	1.34	1.37
21	a	1801	CLA	C1B-NB	-2.24	1.34	1.37
21	2	1210	CLA	C1B-NB	-2.24	1.34	1.37
21	L	1501	CLA	C4B-NB	-2.24	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1211	CLA	C1B-NB	-2.24	1.34	1.37
21	b	1224	CLA	C1B-NB	-2.24	1.34	1.37
21	b	1224	CLA	C4B-NB	-2.24	1.34	1.37
21	B	1240	CLA	C1C-NC	-2.24	1.34	1.37
21	1	1129	CLA	C1C-NC	-2.24	1.34	1.37
21	A	1106	CLA	C1B-NB	-2.24	1.34	1.37
21	b	1231	CLA	C4B-NB	-2.24	1.34	1.37
21	A	1114	CLA	C1C-NC	-2.24	1.34	1.37
21	B	1211	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1213	CLA	C1B-NB	-2.24	1.34	1.37
21	B	1229	CLA	MG-NC	2.24	2.11	2.06
21	1	1113	CLA	C1B-NB	-2.24	1.34	1.37
21	0	1501	CLA	C4B-NB	-2.24	1.34	1.37
21	A	1104	CLA	C4B-NB	-2.24	1.34	1.37
21	A	1108	CLA	C1B-NB	-2.24	1.34	1.37
21	B	1228	CLA	C1B-NB	-2.24	1.34	1.37
21	a	1112	CLA	C4B-NB	-2.24	1.34	1.37
21	1	1114	CLA	C1B-NB	-2.24	1.34	1.37
21	2	1201	CLA	C4B-NB	-2.24	1.34	1.37
21	0	1503	CLA	C4B-NB	-2.24	1.34	1.37
21	a	1011	CLA	C1C-NC	-2.24	1.34	1.37
21	a	1133	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1221	CLA	C1C-C2C	2.24	1.49	1.44
21	A	1124	CLA	C4B-NB	-2.24	1.34	1.37
21	b	1225	CLA	C4B-NB	-2.24	1.34	1.37
21	1	1106	CLA	C4B-NB	-2.24	1.34	1.37
21	2	1021	CLA	MG-NC	2.24	2.11	2.06
21	A	1103	CLA	C1C-C2C	2.24	1.49	1.44
30	b	4011	ECH	C1-C6	-2.24	1.50	1.53
21	a	1111	CLA	C4B-NB	-2.24	1.34	1.37
21	a	1140	CLA	C1B-NB	-2.24	1.34	1.37
21	b	1218	CLA	C1B-NB	-2.24	1.34	1.37
21	1	1110	CLA	C1B-NB	-2.24	1.34	1.37
21	2	1202	CLA	C1B-NB	-2.24	1.34	1.37
21	B	1216	CLA	C1B-NB	-2.24	1.34	1.37
21	a	1801	CLA	C4B-NB	-2.24	1.34	1.37
21	6	1301	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1022	CLA	C1B-NB	-2.24	1.34	1.37
21	A	1119	CLA	C1C-NC	-2.24	1.34	1.37
35	0	6001	LMT	O2B-C2B	-2.24	1.37	1.43
21	1	1013	CLA	MG-NC	2.24	2.11	2.06
21	B	1227	CLA	C1B-NB	-2.24	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	1302	CLA	C1B-NB	-2.24	1.34	1.37
21	l	1503	CLA	C1B-NB	-2.24	1.34	1.37
21	1	1109	CLA	C1B-NB	-2.24	1.34	1.37
21	l	1502	CLA	MG-NC	2.24	2.11	2.06
21	B	1202	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1214	CLA	C1B-NB	-2.24	1.34	1.37
21	2	1023	CLA	C1A-CHA	2.24	1.52	1.43
21	B	1209	CLA	C1B-NB	-2.23	1.34	1.37
21	k	1402	CLA	C1B-NB	-2.23	1.34	1.37
21	2	1214	CLA	C1B-NB	-2.23	1.34	1.37
21	A	1112	CLA	C1C-NC	-2.23	1.34	1.37
21	b	1230	CLA	C1C-NC	-2.23	1.34	1.37
21	1	1102	CLA	C1C-NC	-2.23	1.34	1.37
21	1	1125	CLA	C1C-NC	-2.23	1.34	1.37
21	B	1021	CLA	C4B-NB	-2.23	1.34	1.37
21	1	1801	CLA	C4B-NB	-2.23	1.34	1.37
21	2	1023	CLA	C1B-NB	-2.23	1.34	1.37
21	2	1238	CLA	C1B-NB	-2.23	1.34	1.37
21	a	1126	CLA	C4B-NB	-2.23	1.34	1.37
21	a	1129	CLA	C4B-NB	-2.23	1.34	1.37
21	1	1107	CLA	C4B-NB	-2.23	1.34	1.37
21	B	1231	CLA	C1B-NB	-2.23	1.34	1.37
21	B	1235	CLA	C1B-NB	-2.23	1.34	1.37
21	a	1128	CLA	C4B-NB	-2.23	1.34	1.37
21	B	1214	CLA	C4B-NB	-2.23	1.34	1.37
21	B	1231	CLA	C1C-NC	-2.23	1.34	1.37
21	b	1237	CLA	C4B-NB	-2.23	1.34	1.37
21	2	1219	CLA	C1B-NB	-2.23	1.34	1.37
21	A	1120	CLA	MG-NC	2.23	2.11	2.06
21	j	1302	CLA	C4B-NB	-2.23	1.34	1.37
21	1	1131	CLA	C1B-NB	-2.23	1.34	1.37
21	0	1501	CLA	C1B-NB	-2.23	1.34	1.37
21	a	1120	CLA	C4B-NB	-2.23	1.34	1.37
21	0	1503	CLA	C1B-NB	-2.23	1.34	1.37
21	k	1401	CLA	C1C-NC	-2.23	1.34	1.37
21	2	1213	CLA	MG-NC	2.23	2.11	2.06
21	a	1121	CLA	C1B-NB	-2.23	1.34	1.37
21	b	1240	CLA	C1B-NB	-2.23	1.34	1.37
21	1	1013	CLA	C4B-NB	-2.23	1.34	1.37
21	1	1137	CLA	C1B-NB	-2.23	1.34	1.37
21	2	1205	CLA	MG-NC	2.23	2.11	2.06
21	a	1118	CLA	C1B-NB	-2.23	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1132	CLA	C4B-NB	-2.23	1.34	1.37
21	b	1210	CLA	C1B-NB	-2.23	1.34	1.37
21	b	1228	CLA	C1B-NB	-2.23	1.34	1.37
21	l	1502	CLA	C1B-NB	-2.23	1.34	1.37
21	1	1137	CLA	C4B-NB	-2.23	1.34	1.37
21	A	1103	CLA	C4B-NB	-2.23	1.34	1.37
21	L	1502	CLA	C4B-NB	-2.23	1.34	1.37
21	A	1117	CLA	C1C-NC	-2.23	1.34	1.37
21	b	1220	CLA	MG-NC	2.23	2.11	2.06
21	a	1132	CLA	C1B-NB	-2.23	1.34	1.37
21	2	1222	CLA	C4B-NB	-2.23	1.34	1.37
21	A	1130	CLA	C1C-NC	-2.23	1.34	1.37
21	B	1211	CLA	C4B-NB	-2.23	1.34	1.37
21	1	1116	CLA	C4B-NB	-2.23	1.34	1.37
21	b	1215	CLA	MG-NC	2.23	2.11	2.06
21	A	1138	CLA	MG-NC	2.22	2.11	2.06
21	f	1301	CLA	C1C-NC	-2.22	1.34	1.37
21	2	1238	CLA	C1C-NC	-2.22	1.34	1.37
21	k	1401	CLA	C4B-NB	-2.22	1.34	1.37
21	2	1231	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1107	CLA	C1C-NC	-2.22	1.34	1.37
21	B	1022	CLA	C1B-NB	-2.22	1.34	1.37
21	B	1220	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1130	CLA	C4B-NB	-2.22	1.34	1.37
21	2	1226	CLA	C4B-NB	-2.22	1.34	1.37
21	A	1112	CLA	C1A-CHA	2.22	1.52	1.43
21	B	1234	CLA	C4B-NB	-2.22	1.34	1.37
21	a	1111	CLA	C1B-NB	-2.22	1.34	1.37
21	a	1126	CLA	C1B-NB	-2.22	1.34	1.37
21	f	1301	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1104	CLA	C4B-NB	-2.22	1.34	1.37
21	2	1209	CLA	C1B-NB	-2.22	1.34	1.37
21	8	1402	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1135	CLA	C1B-NB	-2.22	1.34	1.37
21	2	1234	CLA	C1B-NB	-2.22	1.34	1.37
21	1	1113	CLA	C1C-NC	-2.22	1.34	1.37
21	a	1110	CLA	C1B-NB	-2.22	1.34	1.37
21	1	1011	CLA	C1C-NC	-2.22	1.34	1.37
21	A	1102	CLA	C1B-NB	-2.22	1.34	1.37
21	A	1125	CLA	C4B-NB	-2.22	1.34	1.37
21	F	1301	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1117	CLA	C4B-NB	-2.22	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1022	CLA	C4B-NB	-2.22	1.34	1.37
21	2	1216	CLA	C4B-NB	-2.22	1.34	1.37
21	J	1302	CLA	C1A-CHA	2.22	1.52	1.43
21	a	1135	CLA	C1C-NC	-2.22	1.34	1.37
21	A	1121	CLA	C1B-NB	-2.22	1.34	1.37
21	A	1126	CLA	C1B-NB	-2.22	1.34	1.37
21	B	1203	CLA	C1B-NB	-2.22	1.34	1.37
21	B	1217	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1127	CLA	C4B-NB	-2.22	1.34	1.37
21	2	1223	CLA	C1B-NB	-2.22	1.34	1.37
21	2	1207	CLA	MG-NC	2.22	2.11	2.06
21	A	1127	CLA	C1C-NC	-2.22	1.34	1.37
21	A	1107	CLA	C1B-NB	-2.22	1.34	1.37
21	A	1113	CLA	C4B-NB	-2.22	1.34	1.37
21	L	1502	CLA	C1C-NC	-2.22	1.34	1.37
21	1	1119	CLA	MG-NC	2.22	2.11	2.06
21	1	1111	CLA	C4B-NB	-2.22	1.34	1.37
21	1	1118	CLA	C4B-NB	-2.22	1.34	1.37
21	0	1501	CLA	C1C-NC	-2.22	1.34	1.37
21	B	1021	CLA	C1C-NC	-2.22	1.34	1.37
21	b	1205	CLA	C1B-NB	-2.22	1.34	1.37
21	b	1221	CLA	C1B-NB	-2.22	1.34	1.37
21	2	1205	CLA	C4B-NB	-2.22	1.34	1.37
21	b	1230	CLA	MG-NC	2.22	2.11	2.06
21	b	1023	CLA	C1A-CHA	2.22	1.52	1.43
21	k	1402	CLA	C1C-NC	-2.22	1.34	1.37
21	B	1204	CLA	C4B-NB	-2.22	1.34	1.37
21	b	1212	CLA	C1B-NB	-2.22	1.34	1.37
21	1	1126	CLA	C1B-NB	-2.22	1.34	1.37
21	b	1205	CLA	C1C-NC	-2.22	1.34	1.37
21	B	1222	CLA	MG-NC	2.22	2.11	2.06
21	A	1102	CLA	C1C-NC	-2.22	1.34	1.37
21	1	1116	CLA	C1C-NC	-2.22	1.34	1.37
21	2	1214	CLA	C1C-NC	-2.22	1.34	1.37
21	1	1011	CLA	C1A-CHA	2.22	1.52	1.43
21	B	1219	CLA	C1B-NB	-2.22	1.35	1.37
21	B	1221	CLA	C4B-NB	-2.22	1.35	1.37
21	a	1102	CLA	C1B-NB	-2.22	1.35	1.37
21	b	1206	CLA	C4B-NB	-2.22	1.35	1.37
21	2	1232	CLA	C1A-CHA	2.22	1.52	1.43
21	a	1123	CLA	C1A-CHA	2.21	1.52	1.43
21	A	1111	CLA	C1B-NB	-2.21	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1204	CLA	C1B-NB	-2.21	1.35	1.37
21	B	1202	CLA	C1B-NB	-2.21	1.35	1.37
21	b	1235	CLA	C4B-NB	-2.21	1.35	1.37
21	j	1302	CLA	C1B-NB	-2.21	1.35	1.37
21	1	1109	CLA	C4B-NB	-2.21	1.35	1.37
21	a	1103	CLA	MG-NC	2.21	2.11	2.06
21	A	1131	CLA	C4B-NB	-2.21	1.35	1.37
21	a	1108	CLA	C1B-NB	-2.21	1.35	1.37
21	b	1221	CLA	C4B-NB	-2.21	1.35	1.37
21	f	1302	CLA	C1B-NB	-2.21	1.35	1.37
21	j	1303	CLA	C1C-NC	-2.21	1.34	1.37
21	A	1137	CLA	C4B-NB	-2.21	1.35	1.37
21	2	1215	CLA	C4B-NB	-2.21	1.35	1.37
21	b	1229	CLA	MG-NC	2.21	2.11	2.06
21	1	1103	CLA	MG-NC	2.21	2.11	2.06
21	A	1120	CLA	C4B-NB	-2.21	1.35	1.37
21	B	1224	CLA	C1B-NB	-2.21	1.35	1.37
21	a	1138	CLA	C4B-NB	-2.21	1.35	1.37
21	1	1114	CLA	C4B-NB	-2.21	1.35	1.37
21	A	1130	CLA	MG-NC	2.21	2.11	2.06
21	1	1108	CLA	C1B-NB	-2.21	1.35	1.37
21	2	1220	CLA	C4B-NB	-2.21	1.35	1.37
21	7	1303	CLA	C1B-NB	-2.21	1.35	1.37
21	b	1220	CLA	C1A-CHA	2.21	1.52	1.43
21	A	1117	CLA	C1B-NB	-2.21	1.35	1.37
21	1	1133	CLA	C4B-NB	-2.21	1.35	1.37
21	A	1013	CLA	C1C-NC	-2.21	1.34	1.37
21	B	1205	CLA	C1C-C2C	2.21	1.49	1.44
21	B	1212	CLA	C1B-NB	-2.21	1.35	1.37
21	b	1235	CLA	C1B-NB	-2.21	1.35	1.37
21	1	1127	CLA	C1B-NB	-2.21	1.35	1.37
21	2	1240	CLA	C1B-NB	-2.21	1.35	1.37
21	6	1301	CLA	C4B-NB	-2.21	1.35	1.37
21	A	1123	CLA	C1C-NC	-2.21	1.34	1.37
21	2	1229	CLA	MG-NC	2.21	2.11	2.06
21	A	1139	CLA	C1B-NB	-2.21	1.35	1.37
21	F	1302	CLA	C1B-NB	-2.21	1.35	1.37
21	a	1138	CLA	C1B-NB	-2.21	1.35	1.37
21	1	1129	CLA	C4B-NB	-2.21	1.35	1.37
21	A	1801	CLA	C1C-NC	-2.21	1.34	1.37
21	2	1232	CLA	C1C-NC	-2.21	1.34	1.37
21	B	1202	CLA	MG-NC	2.21	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1237	CLA	C1B-NB	-2.21	1.35	1.37
21	a	1118	CLA	C4B-NB	-2.21	1.35	1.37
21	2	1232	CLA	C1B-NB	-2.21	1.35	1.37
21	a	1124	CLA	C1C-NC	-2.21	1.34	1.37
21	2	1201	CLA	C1C-NC	-2.21	1.34	1.37
21	a	1113	CLA	C4B-NB	-2.21	1.35	1.37
21	a	1114	CLA	C4B-NB	-2.21	1.35	1.37
21	2	1240	CLA	C1C-NC	-2.21	1.34	1.37
21	B	1220	CLA	C1B-NB	-2.21	1.35	1.37
21	B	1232	CLA	C1B-NB	-2.21	1.35	1.37
21	a	1104	CLA	C1C-NC	-2.21	1.34	1.37
21	1	1120	CLA	C1A-CHA	2.21	1.52	1.43
21	a	1138	CLA	C1A-CHA	2.20	1.52	1.43
21	A	1127	CLA	C4B-NB	-2.20	1.35	1.37
21	1	1138	CLA	C4B-NB	-2.20	1.35	1.37
21	2	1213	CLA	C1B-NB	-2.20	1.35	1.37
21	B	1224	CLA	C4B-NB	-2.20	1.35	1.37
21	a	1114	CLA	C1C-NC	-2.20	1.34	1.37
21	A	1133	CLA	C1B-NB	-2.20	1.35	1.37
21	K	1401	CLA	C4B-NB	-2.20	1.35	1.37
21	b	1202	CLA	C1B-NB	-2.20	1.35	1.37
21	2	1235	CLA	C1B-NB	-2.20	1.35	1.37
21	A	1114	CLA	C1B-NB	-2.20	1.35	1.37
21	J	1303	CLA	C1B-NB	-2.20	1.35	1.37
21	1	1112	CLA	C4B-NB	-2.20	1.35	1.37
21	2	1214	CLA	C4B-NB	-2.20	1.35	1.37
21	k	1402	CLA	C4B-NB	-2.20	1.35	1.37
21	a	1124	CLA	C4B-NB	-2.20	1.35	1.37
21	b	1220	CLA	C1B-NB	-2.20	1.35	1.37
21	1	1105	CLA	C1B-NB	-2.20	1.35	1.37
21	1	1134	CLA	C1B-NB	-2.20	1.35	1.37
21	2	1235	CLA	C4B-NB	-2.20	1.35	1.37
21	2	1215	CLA	C1C-NC	-2.20	1.34	1.37
21	A	1012	CLA	C1B-NB	-2.20	1.35	1.37
21	a	1013	CLA	C4B-NB	-2.20	1.35	1.37
21	a	1139	CLA	C1C-NC	-2.20	1.34	1.37
21	a	1011	CLA	C1A-CHA	2.20	1.52	1.43
21	a	1013	CLA	C1C-NC	-2.20	1.34	1.37
21	B	1213	CLA	C1A-CHA	2.20	1.52	1.43
21	a	1125	CLA	C1B-NB	-2.20	1.35	1.37
21	a	1127	CLA	C1B-NB	-2.20	1.35	1.37
21	b	1209	CLA	C1B-NB	-2.20	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1211	CLA	C4B-NB	-2.20	1.35	1.37
21	1	1114	CLA	C1C-NC	-2.20	1.34	1.37
21	B	1217	CLA	C1A-CHA	2.20	1.52	1.43
21	A	1135	CLA	C1C-NC	-2.20	1.34	1.37
21	1	1801	CLA	C1C-NC	-2.20	1.34	1.37
21	1	1120	CLA	C1B-NB	-2.20	1.35	1.37
35	F	6001	LMT	O3B-C3B	-2.20	1.37	1.43
35	0	6001	LMT	O2'-C2'	-2.20	1.37	1.43
21	2	1209	CLA	C1A-CHA	2.20	1.52	1.43
21	J	1303	CLA	C1C-NC	-2.20	1.34	1.37
21	b	1203	CLA	C1B-NB	-2.20	1.35	1.37
21	2	1217	CLA	C1B-NB	-2.20	1.35	1.37
21	2	1230	CLA	C4B-NB	-2.20	1.35	1.37
21	0	1502	CLA	C1B-NB	-2.20	1.35	1.37
26	a	5004	LMG	O1-C1	2.20	1.43	1.40
21	a	1117	CLA	C4B-NB	-2.19	1.35	1.37
21	1	1120	CLA	C4B-NB	-2.19	1.35	1.37
21	1	1124	CLA	C1B-NB	-2.19	1.35	1.37
21	2	1203	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1234	CLA	C4B-NB	-2.19	1.35	1.37
21	1	1012	CLA	C4B-NB	-2.19	1.35	1.37
21	2	1240	CLA	C4B-NB	-2.19	1.35	1.37
21	a	1123	CLA	C1C-NC	-2.19	1.34	1.37
21	b	1232	CLA	C1C-NC	-2.19	1.34	1.37
21	A	1132	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1229	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1230	CLA	C1B-NB	-2.19	1.35	1.37
21	b	1204	CLA	C4B-NB	-2.19	1.35	1.37
21	2	1201	CLA	C1A-CHA	2.19	1.52	1.43
21	a	1103	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1239	CLA	C1B-NB	-2.19	1.35	1.37
21	A	1013	CLA	C4B-NB	-2.19	1.35	1.37
21	A	1133	CLA	C4B-NB	-2.19	1.35	1.37
21	B	1235	CLA	C4B-NB	-2.19	1.35	1.37
21	a	1108	CLA	C1C-NC	-2.19	1.34	1.37
21	1	1112	CLA	C1A-CHA	2.19	1.52	1.43
21	B	1214	CLA	C1B-NB	-2.19	1.35	1.37
21	a	1107	CLA	C1B-NB	-2.19	1.35	1.37
21	b	1220	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1232	CLA	C4B-NB	-2.19	1.35	1.37
21	1	1115	CLA	C4B-NB	-2.19	1.35	1.37
21	A	1130	CLA	C1B-NB	-2.19	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1116	CLA	C1B-NB	-2.19	1.35	1.37
21	A	1128	CLA	C1C-NC	-2.19	1.34	1.37
21	1	1106	CLA	C1C-NC	-2.19	1.34	1.37
21	A	1125	CLA	C1B-NB	-2.19	1.35	1.37
21	B	1201	CLA	C4B-NB	-2.19	1.35	1.37
21	J	1303	CLA	C4B-NB	-2.19	1.35	1.37
21	1	1138	CLA	C1B-NB	-2.19	1.35	1.37
21	k	1401	CLA	C1A-CHA	2.19	1.52	1.43
21	F	1302	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1210	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1218	CLA	C4B-NB	-2.19	1.35	1.37
21	2	1205	CLA	C1B-NB	-2.19	1.35	1.37
35	F	6001	LMT	O2B-C2B	-2.19	1.37	1.43
21	B	1223	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1236	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1212	CLA	MG-NC	2.19	2.11	2.06
21	B	1212	CLA	C4B-NB	-2.19	1.35	1.37
21	b	1235	CLA	C1C-NC	-2.19	1.34	1.37
21	1	1131	CLA	C1C-NC	-2.19	1.34	1.37
21	2	1226	CLA	C1C-NC	-2.19	1.34	1.37
21	1	1102	CLA	C1A-CHA	2.19	1.52	1.43
21	b	1203	CLA	C1C-NC	-2.19	1.34	1.37
21	B	1229	CLA	C1B-NB	-2.19	1.35	1.37
21	a	1115	CLA	C4B-NB	-2.18	1.35	1.37
21	1	1124	CLA	C4B-NB	-2.18	1.35	1.37
21	1	1125	CLA	C1B-NB	-2.18	1.35	1.37
21	2	1236	CLA	C4B-NB	-2.18	1.35	1.37
21	2	1206	CLA	C1A-CHA	2.18	1.52	1.43
21	1	1121	CLA	C1C-NC	-2.18	1.34	1.37
21	a	1127	CLA	C4B-NB	-2.18	1.35	1.37
21	2	1217	CLA	C4B-NB	-2.18	1.35	1.37
21	A	1104	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1113	CLA	C1C-NC	-2.18	1.34	1.37
21	b	1217	CLA	C1C-NC	-2.18	1.34	1.37
21	a	1130	CLA	C4B-NB	-2.18	1.35	1.37
21	2	1208	CLA	C1B-NB	-2.18	1.35	1.37
21	2	1218	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1102	CLA	C4B-NB	-2.18	1.35	1.37
21	a	1135	CLA	C1B-NB	-2.18	1.35	1.37
21	b	1219	CLA	C4B-NB	-2.18	1.35	1.37
21	1	1123	CLA	C4B-NB	-2.18	1.35	1.37
21	1	1012	CLA	C1A-CHA	2.18	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1205	CLA	C4B-NB	-2.18	1.35	1.37
21	B	1211	CLA	C1B-NB	-2.18	1.35	1.37
21	B	1213	CLA	C4B-NB	-2.18	1.35	1.37
21	1	1135	CLA	C4B-NB	-2.18	1.35	1.37
21	2	1204	CLA	C1B-NB	-2.18	1.35	1.37
21	2	1232	CLA	C4B-NB	-2.18	1.35	1.37
21	2	1207	CLA	C1A-CHA	2.18	1.52	1.43
21	a	1132	CLA	C1C-NC	-2.18	1.34	1.37
21	7	1303	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1123	CLA	C1B-NB	-2.18	1.35	1.37
21	B	1022	CLA	C4B-NB	-2.18	1.35	1.37
21	b	1205	CLA	C4B-NB	-2.18	1.35	1.37
21	B	1236	CLA	C1B-NB	-2.18	1.35	1.37
21	K	1402	CLA	C1B-NB	-2.18	1.35	1.37
21	2	1238	CLA	C4B-NB	-2.18	1.35	1.37
21	b	1227	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1138	CLA	C1B-NB	-2.18	1.35	1.37
21	B	1227	CLA	C4B-NB	-2.18	1.35	1.37
21	B	1239	CLA	C1A-CHA	2.18	1.52	1.43
21	L	1501	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1113	CLA	C1B-NB	-2.18	1.35	1.37
21	A	1129	CLA	C4B-NB	-2.18	1.35	1.37
21	A	1140	CLA	C1B-NB	-2.18	1.35	1.37
21	b	1223	CLA	C4B-NB	-2.18	1.35	1.37
21	b	1236	CLA	C1B-NB	-2.18	1.35	1.37
35	F	6001	LMT	O2'-C2'	-2.18	1.37	1.43
21	A	1119	CLA	MG-NC	2.18	2.11	2.06
21	b	1240	CLA	C1A-CHA	2.18	1.52	1.43
28	B	4011	45D	O01-C17	-2.18	1.18	1.23
21	a	1112	CLA	C1A-CHA	2.18	1.52	1.43
21	1	1139	CLA	C4B-NB	-2.18	1.35	1.37
21	b	1226	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1012	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1116	CLA	C4B-NB	-2.18	1.35	1.37
21	a	1115	CLA	C1B-NB	-2.18	1.35	1.37
21	B	1022	CLA	C1C-NC	-2.18	1.34	1.37
21	b	1214	CLA	C1C-NC	-2.18	1.34	1.37
21	l	1502	CLA	C1C-NC	-2.18	1.34	1.37
21	6	1302	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1112	CLA	C1B-NB	-2.18	1.35	1.37
21	a	1106	CLA	C1C-NC	-2.17	1.34	1.37
21	B	1201	CLA	C1B-NB	-2.17	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1225	CLA	C1B-NB	-2.17	1.35	1.37
21	b	1208	CLA	C1B-NB	-2.17	1.35	1.37
21	2	1207	CLA	C1B-NB	-2.17	1.35	1.37
21	b	1234	CLA	C1B-NB	-2.17	1.35	1.37
21	1	1105	CLA	C4B-NB	-2.17	1.35	1.37
21	8	1401	CLA	C4B-NB	-2.17	1.35	1.37
21	2	1212	CLA	C1A-CHA	2.17	1.52	1.43
21	A	1110	CLA	MG-NC	2.17	2.11	2.06
21	j	1303	CLA	C1B-NB	-2.17	1.35	1.37
21	B	1203	CLA	C4B-NB	-2.17	1.35	1.37
21	b	1203	CLA	C4B-NB	-2.17	1.35	1.37
21	j	1303	CLA	C4B-NB	-2.17	1.35	1.37
21	2	1221	CLA	C4B-NB	-2.17	1.35	1.37
21	b	1210	CLA	C1C-NC	-2.17	1.34	1.37
21	a	1134	CLA	C4B-NB	-2.17	1.35	1.37
21	l	1502	CLA	C4B-NB	-2.17	1.35	1.37
21	2	1229	CLA	C1B-NB	-2.17	1.35	1.37
21	B	1221	CLA	C1C-NC	-2.17	1.34	1.37
21	b	1201	CLA	C1B-NB	-2.17	1.35	1.37
21	7	1302	CLA	C4B-NB	-2.17	1.35	1.37
21	A	1117	CLA	C4B-NB	-2.17	1.35	1.37
21	a	1102	CLA	C4B-NB	-2.17	1.35	1.37
21	2	1209	CLA	C4B-NB	-2.17	1.35	1.37
21	j	1302	CLA	C1A-CHA	2.17	1.52	1.43
21	2	1217	CLA	C1C-NC	-2.17	1.34	1.37
21	b	1219	CLA	C1B-NB	-2.17	1.35	1.37
21	2	1204	CLA	C4B-NB	-2.17	1.35	1.37
21	8	1402	CLA	C1B-NB	-2.17	1.35	1.37
21	B	1206	CLA	C1A-CHA	2.16	1.52	1.43
21	a	1102	CLA	C1A-CHA	2.16	1.52	1.43
21	A	1101	CLA	C1C-NC	-2.16	1.34	1.37
21	b	1021	CLA	C1C-NC	-2.16	1.34	1.37
21	A	1105	CLA	C4B-NB	-2.16	1.35	1.37
21	b	1213	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1123	CLA	C1C-NC	-2.16	1.34	1.37
21	B	1217	CLA	C1B-NB	-2.16	1.35	1.37
21	7	1302	CLA	C1A-CHA	2.16	1.52	1.43
21	B	1240	CLA	C1B-NB	-2.16	1.35	1.37
21	1	1111	CLA	C1A-CHA	2.16	1.52	1.43
21	1	1108	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1123	CLA	C1B-NB	-2.16	1.35	1.37
21	a	1125	CLA	C4B-NB	-2.16	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1230	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1110	CLA	C4B-NB	-2.16	1.35	1.37
21	2	1219	CLA	C4B-NB	-2.16	1.35	1.37
21	a	1131	CLA	C1B-NB	-2.16	1.35	1.37
21	b	1231	CLA	C1B-NB	-2.16	1.35	1.37
21	A	1131	CLA	MG-NC	2.16	2.11	2.06
34	F	4016	ZEX	C24-C25	-2.16	1.47	1.50
21	A	1103	CLA	C1B-NB	-2.16	1.35	1.37
21	2	1208	CLA	C4B-NB	-2.16	1.35	1.37
21	J	1302	CLA	C4B-NB	-2.16	1.35	1.37
21	a	1104	CLA	C1B-NB	-2.16	1.35	1.37
21	2	1212	CLA	C4B-NB	-2.16	1.35	1.37
21	a	1109	CLA	C1A-CHA	2.16	1.52	1.43
21	a	1108	CLA	C1A-CHA	2.16	1.52	1.43
21	A	1140	CLA	MG-NC	2.16	2.11	2.06
21	b	1202	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1132	CLA	C4B-NB	-2.16	1.35	1.37
21	b	1226	CLA	MG-NC	2.16	2.11	2.06
21	a	1139	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1134	CLA	C4B-NB	-2.16	1.35	1.37
21	1	1110	CLA	C1A-CHA	2.16	1.52	1.43
21	B	1202	CLA	C4B-NB	-2.16	1.35	1.37
21	2	1228	CLA	C1A-CHA	2.16	1.52	1.43
21	a	1136	CLA	C4B-NB	-2.16	1.35	1.37
21	b	1216	CLA	C4B-NB	-2.16	1.35	1.37
21	A	1121	CLA	C4B-NB	-2.15	1.35	1.37
21	2	1218	CLA	C4B-NB	-2.15	1.35	1.37
21	1	1135	CLA	C1C-NC	-2.15	1.34	1.37
21	a	1801	CLA	C1A-CHA	2.15	1.52	1.43
21	a	1012	CLA	C1A-CHA	2.15	1.52	1.43
21	b	1218	CLA	C1A-CHA	2.15	1.52	1.43
21	a	1118	CLA	C1C-NC	-2.15	1.34	1.37
21	1	1138	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1211	CLA	C1A-CHA	2.15	1.52	1.43
21	a	1107	CLA	C4B-NB	-2.15	1.35	1.37
21	b	1240	CLA	C4B-NB	-2.15	1.35	1.37
21	l	1503	CLA	C4B-NB	-2.15	1.35	1.37
21	a	1104	CLA	C4B-NB	-2.15	1.35	1.37
21	a	1122	CLA	C4B-NB	-2.15	1.35	1.37
21	b	1239	CLA	C4B-NB	-2.15	1.35	1.37
21	1	1113	CLA	C1A-CHA	2.15	1.52	1.43
21	a	1122	CLA	C1A-CHA	2.15	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1134	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1210	CLA	C1A-CHA	2.15	1.52	1.43
21	b	1217	CLA	C1A-CHA	2.15	1.52	1.43
21	A	1131	CLA	C1B-NB	-2.15	1.35	1.37
21	a	1125	CLA	C1A-CHA	2.15	1.51	1.43
21	B	1209	CLA	C4B-NB	-2.15	1.35	1.37
21	2	1239	CLA	C1A-CHA	2.15	1.51	1.43
21	1	1121	CLA	C4B-NB	-2.15	1.35	1.37
21	b	1202	CLA	MG-NC	2.15	2.11	2.06
21	a	1121	CLA	C4B-NB	-2.15	1.35	1.37
21	a	1130	CLA	C1B-NB	-2.15	1.35	1.37
21	b	1206	CLA	C1A-CHA	2.15	1.51	1.43
21	B	1222	CLA	C1C-C2C	2.15	1.48	1.44
21	A	1108	CLA	C4B-NB	-2.15	1.35	1.37
21	b	1214	CLA	C4B-NB	-2.15	1.35	1.37
21	A	1106	CLA	MG-NC	2.15	2.11	2.06
21	A	1136	CLA	C1B-NB	-2.14	1.35	1.37
21	b	1211	CLA	C1C-NC	-2.14	1.34	1.37
21	B	1209	CLA	C1A-CHA	2.14	1.51	1.43
34	J	4015	ZEX	C1-C6	-2.14	1.51	1.53
21	2	1227	CLA	C1A-CHA	2.14	1.51	1.43
21	a	1101	CLA	C1C-NC	-2.14	1.34	1.37
21	2	1220	CLA	C1A-CHA	2.14	1.51	1.43
21	B	1230	CLA	C4B-NB	-2.14	1.35	1.37
21	1	1136	CLA	C4B-NB	-2.14	1.35	1.37
30	B	4006	ECH	C25-C26	-2.14	1.32	1.35
21	A	1135	CLA	C1B-NB	-2.14	1.35	1.37
21	K	1402	CLA	C4B-NB	-2.14	1.35	1.37
21	B	1232	CLA	C4B-NB	-2.14	1.35	1.37
21	1	1139	CLA	C1C-NC	-2.14	1.34	1.37
21	B	1214	CLA	C1A-CHA	2.14	1.51	1.43
21	A	1111	CLA	C4B-NB	-2.14	1.35	1.37
21	a	1116	CLA	C1B-NB	-2.14	1.35	1.37
21	a	1137	CLA	C4B-NB	-2.14	1.35	1.37
21	b	1228	CLA	C1A-CHA	2.14	1.51	1.43
21	A	1116	CLA	C1B-NB	-2.14	1.35	1.37
21	A	1135	CLA	C4B-NB	-2.14	1.35	1.37
21	a	1123	CLA	C4B-NB	-2.14	1.35	1.37
21	a	1133	CLA	C4B-NB	-2.14	1.35	1.37
21	A	1132	CLA	C1C-NC	-2.14	1.34	1.37
21	a	1116	CLA	C1A-CHA	2.14	1.51	1.43
21	A	1126	CLA	C4B-NB	-2.14	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	1503	CLA	C1B-NB	-2.14	1.35	1.37
21	L	1503	CLA	C4B-NB	-2.14	1.35	1.37
21	a	1124	CLA	C1A-CHA	2.14	1.51	1.43
21	a	1108	CLA	C4B-NB	-2.14	1.35	1.37
21	2	1239	CLA	C4B-NB	-2.14	1.35	1.37
34	j	4015	ZEX	C24-C25	-2.14	1.47	1.50
21	B	1226	CLA	C1C-C2C	2.14	1.48	1.44
21	B	1216	CLA	C1A-CHA	2.14	1.51	1.43
21	1	1122	CLA	C1A-CHA	2.14	1.51	1.43
21	2	1202	CLA	C1A-CHA	2.14	1.51	1.43
21	A	1134	CLA	C1C-NC	-2.14	1.34	1.37
34	J	4015	ZEX	C24-C25	-2.14	1.47	1.50
21	a	1131	CLA	C4B-NB	-2.13	1.35	1.37
21	b	1207	CLA	C1A-CHA	2.13	1.51	1.43
21	B	1240	CLA	C4B-NB	-2.13	1.35	1.37
21	1	1128	CLA	C1C-NC	-2.13	1.34	1.37
21	A	1138	CLA	C1A-CHA	2.13	1.51	1.43
21	a	1121	CLA	C1A-CHA	2.13	1.51	1.43
21	2	1202	CLA	C4B-NB	-2.13	1.35	1.37
27	B	7002	ACT	CH3-C	2.13	1.57	1.49
21	b	1228	CLA	C4B-NB	-2.13	1.35	1.37
21	A	1120	CLA	C1C-NC	-2.13	1.34	1.37
21	2	1228	CLA	MG-NC	2.13	2.11	2.06
22	b	2002	PQN	C6-C5	-2.13	1.36	1.39
21	1	1125	CLA	C1A-CHA	2.13	1.51	1.43
21	a	1120	CLA	C1A-CHA	2.13	1.51	1.43
21	J	1303	CLA	C1A-CHA	2.13	1.51	1.43
21	2	1225	CLA	C4B-NB	-2.13	1.35	1.37
21	2	1228	CLA	C4B-NB	-2.13	1.35	1.37
21	A	1012	CLA	C1C-NC	-2.13	1.34	1.37
21	1	1121	CLA	C1A-CHA	2.13	1.51	1.43
21	1	1123	CLA	C1A-CHA	2.13	1.51	1.43
21	f	1302	CLA	C4B-NB	-2.13	1.35	1.37
21	k	1402	CLA	C1A-CHA	2.12	1.51	1.43
21	a	1110	CLA	C1A-CHA	2.12	1.51	1.43
21	B	1023	CLA	C1A-CHA	2.12	1.51	1.43
21	b	1230	CLA	C1A-CHA	2.12	1.51	1.43
21	1	1109	CLA	C1A-CHA	2.12	1.51	1.43
21	B	1220	CLA	C1A-CHA	2.12	1.51	1.43
21	A	1140	CLA	C4B-NB	-2.12	1.35	1.37
21	2	1213	CLA	C1A-CHA	2.12	1.51	1.43
21	b	1222	CLA	MG-NC	2.12	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1217	CLA	C1A-CHA	2.12	1.51	1.43
21	a	1110	CLA	C4B-NB	-2.12	1.35	1.37
21	a	1111	CLA	C1A-CHA	2.12	1.51	1.43
21	A	1129	CLA	C1C-NC	-2.12	1.34	1.37
21	b	1210	CLA	C1A-CHA	2.12	1.51	1.43
21	2	1223	CLA	C1A-CHA	2.12	1.51	1.43
21	2	1221	CLA	C1A-CHA	2.12	1.51	1.43
21	1	1101	CLA	C4B-NB	-2.12	1.35	1.37
21	2	1215	CLA	C1A-CHA	2.12	1.51	1.43
21	A	1137	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1132	CLA	C1C-NC	-2.11	1.34	1.37
21	B	1207	CLA	C1B-NB	-2.11	1.35	1.37
21	a	1116	CLA	C4B-NB	-2.11	1.35	1.37
21	1	1139	CLA	C1A-CHA	2.11	1.51	1.43
21	A	1134	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1127	CLA	C1A-CHA	2.11	1.51	1.43
21	b	1226	CLA	C4B-NB	-2.11	1.35	1.37
21	2	1223	CLA	C4B-NB	-2.11	1.35	1.37
21	2	1229	CLA	C4B-NB	-2.11	1.35	1.37
21	b	1222	CLA	C1C-NC	-2.11	1.34	1.37
21	B	1232	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1140	CLA	C4B-NB	-2.11	1.35	1.37
34	F	4016	ZEX	C1-C6	-2.10	1.51	1.53
21	2	1023	CLA	MG-NC	2.10	2.11	2.06
21	a	1130	CLA	C1A-CHA	2.10	1.51	1.43
21	1	1101	CLA	C1A-CHA	2.10	1.51	1.43
21	B	1215	CLA	C1A-CHA	2.10	1.51	1.43
21	a	1101	CLA	C1A-CHA	2.10	1.51	1.43
21	A	1136	CLA	C1C-NC	-2.10	1.34	1.37
21	2	1207	CLA	C4B-NB	-2.10	1.35	1.37
21	a	1135	CLA	C4B-NB	-2.10	1.35	1.37
21	a	1013	CLA	MG-NC	2.10	2.11	2.06
21	2	1231	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1227	CLA	C4B-NB	-2.10	1.35	1.37
21	a	1101	CLA	C4B-NB	-2.10	1.35	1.37
21	b	1217	CLA	C4B-NB	-2.10	1.35	1.37
21	1	1133	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1221	CLA	C1C-NC	-2.10	1.34	1.37
21	2	1021	CLA	C3D-C4D	-2.10	1.39	1.44
21	l	1501	CLA	C1A-CHA	2.10	1.51	1.43
21	b	1212	CLA	C4B-NB	-2.10	1.35	1.37
21	B	1021	CLA	C1A-CHA	2.10	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1203	CLA	C1C-NC	-2.10	1.34	1.37
21	B	1223	CLA	C1A-CHA	2.10	1.51	1.43
21	b	1213	CLA	C1A-CHA	2.10	1.51	1.43
21	B	1203	CLA	C1A-CHA	2.10	1.51	1.43
21	a	1139	CLA	C1A-CHA	2.10	1.51	1.43
21	1	1118	CLA	C1A-CHA	2.10	1.51	1.43
35	L	6001	LMT	O2'-C2'	-2.10	1.37	1.43
21	A	1101	CLA	C4B-NB	-2.10	1.35	1.37
21	8	1402	CLA	C1A-CHA	2.09	1.51	1.43
35	1	6001	LMT	O2'-C2'	-2.09	1.37	1.43
21	F	1302	CLA	C1A-CHA	2.09	1.51	1.43
21	F	1301	CLA	C1A-CHA	2.09	1.51	1.43
21	1	1801	CLA	C1A-CHA	2.09	1.51	1.43
35	l	6001	LMT	O2B-C2B	-2.09	1.37	1.43
26	K	5009	LMG	O1-C1	2.09	1.43	1.40
21	b	1218	CLA	C1C-NC	-2.09	1.34	1.37
21	b	1224	CLA	C1A-CHA	2.09	1.51	1.43
21	B	1216	CLA	C4B-NB	-2.09	1.35	1.37
21	B	1218	CLA	C1A-CHA	2.09	1.51	1.43
21	A	1011	CLA	C3D-C4D	-2.09	1.39	1.44
21	A	1134	CLA	C4B-NB	-2.09	1.35	1.37
21	B	1207	CLA	C4B-NB	-2.09	1.35	1.37
21	a	1104	CLA	C1A-CHA	2.09	1.51	1.43
21	A	1102	CLA	C1A-CHA	2.09	1.51	1.43
21	A	1013	CLA	C1A-CHA	2.09	1.51	1.43
21	A	1133	CLA	MG-NC	2.09	2.11	2.06
21	A	1114	CLA	C4B-NB	-2.09	1.35	1.37
21	B	1229	CLA	C4B-NB	-2.09	1.35	1.37
21	b	1201	CLA	C1A-CHA	2.09	1.51	1.43
35	1	6001	LMT	O3B-C3B	-2.09	1.37	1.43
21	B	1225	CLA	C4B-NB	-2.09	1.35	1.37
21	1	1104	CLA	C1A-CHA	2.09	1.51	1.43
21	a	1137	CLA	C1A-CHA	2.08	1.51	1.43
21	a	1117	CLA	C1A-CHA	2.08	1.51	1.43
21	2	1235	CLA	C1A-CHA	2.08	1.51	1.43
21	2	1203	CLA	C1A-CHA	2.08	1.51	1.43
21	2	1230	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1136	CLA	C4B-NB	-2.08	1.35	1.37
21	A	1122	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1136	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1228	CLA	C1A-CHA	2.08	1.51	1.43
21	2	1234	CLA	C1A-CHA	2.08	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1216	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1240	CLA	C1A-CHA	2.08	1.51	1.43
34	7	4015	ZEX	C24-C25	-2.08	1.47	1.50
21	A	1139	CLA	C1A-CHA	2.08	1.51	1.43
21	b	1212	CLA	C1A-CHA	2.08	1.51	1.43
21	a	1114	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1111	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1110	CLA	C4B-NB	-2.08	1.35	1.37
21	2	1021	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1130	CLA	C1A-CHA	2.08	1.51	1.43
28	h	4020	45D	O01-C17	-2.08	1.18	1.23
21	b	1221	CLA	C1A-CHA	2.08	1.51	1.43
21	B	1201	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1126	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1109	CLA	C1C-NC	-2.08	1.34	1.37
21	A	1108	CLA	C1A-CHA	2.08	1.51	1.43
21	b	1231	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1136	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1124	CLA	C1C-NC	-2.08	1.34	1.37
21	A	1801	CLA	C1A-CHA	2.08	1.51	1.43
21	B	1222	CLA	C1A-CHA	2.08	1.51	1.43
21	a	1106	CLA	C1A-CHA	2.08	1.51	1.43
21	a	1127	CLA	C1A-CHA	2.08	1.51	1.43
35	0	6001	LMT	O3B-C3B	-2.08	1.37	1.43
21	a	1126	CLA	C1A-CHA	2.08	1.51	1.43
21	8	1401	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1104	CLA	C1A-CHA	2.07	1.51	1.43
21	f	1302	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1216	CLA	C1A-CHA	2.07	1.51	1.43
21	B	1236	CLA	C4B-NB	-2.07	1.35	1.37
21	B	1212	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1232	CLA	C1A-CHA	2.07	1.51	1.43
35	1	6001	LMT	O2B-C2B	-2.07	1.37	1.43
21	2	1222	CLA	C1C-NC	-2.07	1.34	1.37
21	2	1211	CLA	C1A-CHA	2.07	1.51	1.43
21	K	1402	CLA	C1A-CHA	2.07	1.51	1.43
21	1	1134	CLA	C1A-CHA	2.06	1.51	1.43
21	j	1303	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1127	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1130	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1113	CLA	C1A-CHA	2.06	1.51	1.43
21	2	1240	CLA	C1A-CHA	2.06	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1124	CLA	C1A-CHA	2.06	1.51	1.43
21	B	1238	CLA	C4B-NB	-2.06	1.35	1.37
21	1	1131	CLA	C4B-NB	-2.06	1.35	1.37
21	B	1231	CLA	C1A-CHA	2.06	1.51	1.43
21	1	1103	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1131	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1013	CLA	C1A-CHA	2.06	1.51	1.43
21	b	1223	CLA	C1A-CHA	2.06	1.51	1.43
21	1	1114	CLA	C1A-CHA	2.06	1.51	1.43
21	2	1218	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1118	CLA	C1A-CHA	2.06	1.51	1.43
21	1	1105	CLA	C1A-CHA	2.05	1.51	1.43
35	L	6001	LMT	O2B-C2B	-2.05	1.37	1.43
21	B	1221	CLA	C1A-CHA	2.05	1.51	1.43
21	B	1239	CLA	C4B-NB	-2.05	1.35	1.37
35	l	6001	LMT	O2'-C2'	-2.05	1.37	1.43
21	2	1210	CLA	C1A-CHA	2.05	1.51	1.43
21	B	1219	CLA	C4B-NB	-2.05	1.35	1.37
21	A	1133	CLA	C1C-NC	-2.05	1.34	1.37
21	2	1226	CLA	C1A-CHA	2.05	1.51	1.43
21	B	1226	CLA	C3D-C4D	-2.05	1.39	1.44
21	2	1214	CLA	C1A-CHA	2.05	1.51	1.43
21	A	1140	CLA	C1A-CHA	2.04	1.51	1.43
21	b	1203	CLA	C1A-CHA	2.04	1.51	1.43
21	b	1021	CLA	C1A-CHA	2.04	1.51	1.43
21	B	1235	CLA	C1A-CHA	2.04	1.51	1.43
21	1	1116	CLA	C1A-CHA	2.04	1.51	1.43
21	B	1229	CLA	C1A-CHA	2.04	1.51	1.43
21	2	1224	CLA	C1A-CHA	2.04	1.51	1.43
21	1	1108	CLA	C1A-CHA	2.04	1.51	1.43
21	A	1129	CLA	C1A-CHA	2.04	1.51	1.43
21	b	1021	CLA	C3D-C4D	-2.04	1.39	1.44
21	a	1107	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1101	CLA	C1A-CHA	2.03	1.51	1.43
21	a	1128	CLA	C1A-CHA	2.03	1.51	1.43
21	2	1205	CLA	C1A-CHA	2.03	1.51	1.43
34	j	4015	ZEX	C27-C26	2.03	1.48	1.46
21	B	1202	CLA	C1A-CHA	2.03	1.51	1.43
21	a	1133	CLA	C1A-CHA	2.03	1.51	1.43
21	0	1501	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1116	CLA	C1A-CHA	2.03	1.51	1.43
21	B	1234	CLA	C1A-CHA	2.03	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	6001	LMT	O1'-C1'	-2.03	1.36	1.40
28	h	4020	45D	C23-C19	2.03	1.39	1.33
21	6	1301	CLA	C1A-CHA	2.03	1.51	1.43
21	B	1225	CLA	C1A-CHA	2.03	1.51	1.43
21	2	1219	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1109	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1103	CLA	MG-NC	2.03	2.11	2.06
21	A	1135	CLA	C1A-CHA	2.03	1.51	1.43
21	a	1118	CLA	C1A-CHA	2.03	1.51	1.43
21	b	1239	CLA	C1A-CHA	2.03	1.51	1.43
21	1	1137	CLA	C1A-CHA	2.03	1.51	1.43
26	b	5007	LMG	O1-C1	2.02	1.43	1.40
21	b	1207	CLA	C4B-NB	-2.02	1.35	1.37
21	b	1211	CLA	C1A-CHA	2.02	1.51	1.43
21	B	1236	CLA	C1A-CHA	2.02	1.51	1.43
21	2	1236	CLA	C1A-CHA	2.02	1.51	1.43
27	B	7001	ACT	CH3-C	2.02	1.57	1.49
21	2	1216	CLA	C1A-CHA	2.02	1.51	1.43
21	b	1215	CLA	C1A-CHA	2.02	1.51	1.43
21	L	1503	CLA	C1A-CHA	2.02	1.51	1.43
21	A	1113	CLA	C1A-CHA	2.02	1.51	1.43
21	A	1137	CLA	MG-NC	2.02	2.11	2.06
21	1	1128	CLA	C1A-CHA	2.02	1.51	1.43
35	l	6001	LMT	O3B-C3B	-2.02	1.38	1.43
21	B	1227	CLA	C1A-CHA	2.02	1.51	1.43
21	B	1230	CLA	C1A-CHA	2.02	1.51	1.43
27	a	7001	ACT	CH3-C	2.02	1.57	1.49
21	A	1013	CLA	MG-NC	2.02	2.11	2.06
21	1	1119	CLA	C1A-CHA	2.02	1.51	1.43
21	1	1117	CLA	C1A-CHA	2.02	1.51	1.43
21	1	1106	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1126	CLA	C1A-CHA	2.01	1.51	1.43
21	a	1140	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1125	CLA	C3D-C4D	-2.01	1.39	1.44
21	b	1238	CLA	C1A-CHA	2.01	1.51	1.43
37	L	5004	DGD	O5D-C1E	2.01	1.43	1.40
21	a	1105	CLA	C1A-CHA	2.01	1.51	1.43
21	2	1222	CLA	C1A-CHA	2.01	1.51	1.43
21	B	1205	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1117	CLA	C1A-CHA	2.01	1.51	1.43
21	a	1115	CLA	C1A-CHA	2.01	1.51	1.43
21	2	1022	CLA	C1A-CHA	2.01	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1224	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1124	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1214	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1131	CLA	C1A-CHA	2.01	1.51	1.43
21	2	1208	CLA	C1A-CHA	2.01	1.51	1.43
21	A	1110	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1227	CLA	C1A-CHA	2.01	1.51	1.43
21	1	1136	CLA	C1A-CHA	2.00	1.51	1.43
21	b	1202	CLA	C1A-CHA	2.00	1.51	1.43
21	b	1023	CLA	MG-NC	2.00	2.11	2.06
21	b	1236	CLA	C1A-CHA	2.00	1.51	1.43
21	2	1238	CLA	C3D-C4D	-2.00	1.39	1.44
21	b	1204	CLA	C3D-C4D	-2.00	1.39	1.44
21	a	1129	CLA	C1A-CHA	2.00	1.51	1.43
21	b	1234	CLA	C3D-C4D	-2.00	1.39	1.44
21	A	1132	CLA	C1A-CHA	2.00	1.51	1.43

All (5167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	4016	ZEX	C38-C24-C25	-46.83	31.10	110.76
34	J	4015	ZEX	C38-C24-C25	-46.55	31.58	110.76
34	j	4015	ZEX	C38-C24-C25	-46.54	31.59	110.76
34	7	4015	ZEX	C38-C24-C25	-46.47	31.71	110.76
24	a	4019	BCR	C16-C15-C14	16.67	157.64	123.52
24	b	4018	BCR	C16-C15-C14	16.24	156.75	123.52
24	a	4002	BCR	C16-C15-C14	15.53	155.29	123.52
24	1	4019	BCR	C16-C15-C14	15.42	155.06	123.52
24	i	4018	BCR	C16-C15-C14	14.92	154.06	123.52
24	a	4001	BCR	C16-C15-C14	14.81	153.83	123.52
24	A	4019	BCR	C16-C15-C14	14.62	153.42	123.52
24	2	4018	BCR	C11-C10-C9	14.47	147.57	127.28
24	b	4010	BCR	C21-C20-C19	14.40	164.93	123.20
24	h	4018	BCR	C16-C15-C14	14.36	152.91	123.52
24	A	4019	BCR	C11-C10-C9	14.33	147.38	127.28
24	2	4010	BCR	C21-C20-C19	14.29	164.61	123.20
24	2	4005	BCR	C16-C15-C14	14.28	152.73	123.52
24	2	4014	BCR	C21-C20-C19	14.25	164.48	123.20
24	9	4021	BCR	C16-C15-C14	14.23	152.63	123.52
24	1	4002	BCR	C21-C20-C19	14.21	164.37	123.20
24	1	4007	BCR	C16-C15-C14	14.10	152.36	123.52
24	B	4018	BCR	C16-C15-C14	14.08	152.32	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	4010	BCR	C16-C15-C14	14.08	152.32	123.52
24	a	4008	BCR	C16-C15-C14	14.06	152.28	123.52
24	0	4022	BCR	C21-C20-C19	14.04	163.88	123.20
24	1	4003	BCR	C21-C20-C19	14.03	163.86	123.20
24	B	4018	BCR	C21-C20-C19	13.92	163.53	123.20
24	1	4001	BCR	C16-C15-C14	13.83	151.83	123.52
24	j	4013	BCR	C21-C20-C19	13.83	163.28	123.20
24	b	4014	BCR	C21-C20-C19	13.79	163.16	123.20
24	A	4003	BCR	C21-C20-C19	13.75	163.04	123.20
24	B	4005	BCR	C16-C15-C14	13.73	151.62	123.52
24	2	4004	BCR	C21-C20-C19	13.71	162.92	123.20
24	8	4001	BCR	C21-C20-C19	13.70	162.90	123.20
24	8	4001	BCR	C16-C15-C14	13.70	151.55	123.52
34	F	4016	ZEX	C21-C26-C25	-13.63	112.30	122.84
24	1	4002	BCR	C16-C15-C14	13.62	151.38	123.52
24	a	4003	BCR	C16-C15-C14	13.61	151.38	123.52
24	l	4022	BCR	C21-C20-C19	13.56	162.49	123.20
24	A	4012	BCR	C21-C20-C19	13.50	162.33	123.20
24	1	4012	BCR	C16-C15-C14	13.49	151.11	123.52
24	7	4013	BCR	C21-C20-C19	13.47	162.22	123.20
24	A	4001	BCR	C21-C20-C19	13.46	162.20	123.20
24	2	4010	BCR	C11-C10-C9	13.46	146.15	127.28
24	B	4014	BCR	C21-C20-C19	13.45	162.17	123.20
24	1	4008	BCR	C16-C15-C14	13.38	150.90	123.52
24	6	4016	BCR	C21-C20-C19	13.36	161.91	123.20
24	b	4017	BCR	C16-C15-C14	13.35	150.83	123.52
24	B	4017	BCR	C11-C10-C9	13.34	145.98	127.28
24	B	4010	BCR	C21-C20-C19	13.28	161.68	123.20
24	B	4004	BCR	C21-C20-C19	13.27	161.66	123.20
24	f	4016	BCR	C21-C20-C19	13.26	161.62	123.20
24	2	4014	BCR	C11-C10-C9	13.21	145.81	127.28
24	6	4016	BCR	C11-C10-C9	13.21	145.81	127.28
24	0	4022	BCR	C11-C10-C9	13.21	145.81	127.28
24	2	4017	BCR	C11-C10-C9	13.20	145.79	127.28
24	1	4019	BCR	C21-C20-C19	13.17	161.36	123.20
24	a	4007	BCR	C21-C20-C19	13.14	161.27	123.20
24	1	4003	BCR	C16-C15-C14	13.14	150.40	123.52
24	k	4001	BCR	C16-C15-C14	13.05	150.21	123.52
24	B	4004	BCR	C16-C15-C14	13.04	150.20	123.52
24	1	4012	BCR	C21-C20-C19	12.99	160.85	123.20
24	b	4017	BCR	C11-C10-C9	12.99	145.50	127.28
24	B	4017	BCR	C16-C15-C14	12.98	150.07	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	4004	BCR	C21-C20-C19	12.96	160.77	123.20
24	a	4001	BCR	C21-C20-C19	12.95	160.72	123.20
24	2	4004	BCR	C16-C15-C14	12.91	149.93	123.52
24	b	4004	BCR	C11-C10-C9	12.89	145.36	127.28
24	1	4008	BCR	C21-C20-C19	12.84	160.39	123.20
24	K	4001	BCR	C16-C15-C14	12.79	149.68	123.52
24	a	4012	BCR	C16-C15-C14	12.69	149.49	123.52
24	l	4022	BCR	C11-C10-C9	12.68	145.06	127.28
24	A	4019	BCR	C21-C20-C19	12.66	159.90	123.20
24	a	4003	BCR	C21-C20-C19	12.64	159.81	123.20
24	a	4019	BCR	C11-C10-C9	12.64	145.00	127.28
24	a	4002	BCR	C11-C10-C9	12.61	144.96	127.28
24	6	4016	BCR	C16-C15-C14	12.56	149.22	123.52
24	k	4001	BCR	C21-C20-C19	12.52	159.47	123.20
24	J	4013	BCR	C16-C15-C14	12.42	148.94	123.52
24	a	4002	BCR	C21-C20-C19	12.41	159.17	123.20
24	9	4021	BCR	C11-C10-C9	12.38	144.64	127.28
24	A	4008	BCR	C21-C20-C19	12.37	159.04	123.20
24	J	4013	BCR	C11-C10-C9	12.28	144.50	127.28
24	1	4007	BCR	C21-C20-C19	12.27	158.76	123.20
24	0	4019	BCR	C16-C15-C14	12.26	148.60	123.52
24	J	4013	BCR	C21-C20-C19	12.25	158.71	123.20
24	i	4018	BCR	C11-C10-C9	12.25	144.46	127.28
24	1	4001	BCR	C11-C10-C9	12.25	144.46	127.28
24	7	4013	BCR	C16-C15-C14	12.24	148.56	123.52
24	b	4014	BCR	C11-C10-C9	12.23	144.43	127.28
24	1	4001	BCR	C21-C20-C19	12.19	158.52	123.20
24	A	4002	BCR	C21-C20-C19	12.16	158.45	123.20
24	L	4022	BCR	C21-C20-C19	12.16	158.44	123.20
24	2	4005	BCR	C11-C10-C9	12.16	144.33	127.28
24	l	4019	BCR	C21-C20-C19	12.15	158.41	123.20
24	f	4016	BCR	C11-C10-C9	12.13	144.28	127.28
24	7	4013	BCR	C11-C10-C9	12.12	144.28	127.28
24	2	4017	BCR	C16-C15-C14	12.12	148.32	123.52
24	2	4005	BCR	C21-C20-C19	12.12	158.31	123.20
24	b	4005	BCR	C16-C15-C14	12.10	148.28	123.52
24	B	4014	BCR	C11-C10-C9	12.04	144.17	127.28
24	b	4010	BCR	C16-C15-C14	12.03	148.14	123.52
24	b	4005	BCR	C11-C10-C9	11.97	144.06	127.28
24	K	4001	BCR	C21-C20-C19	11.96	157.84	123.20
24	B	4010	BCR	C16-C15-C14	11.90	147.86	123.52
24	a	4012	BCR	C21-C20-C19	11.88	157.62	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4010	BCR	C11-C10-C9	11.86	143.91	127.28
24	b	4018	BCR	C21-C20-C19	11.86	157.56	123.20
24	2	4011	BCR	C21-C20-C19	11.82	157.46	123.20
24	2	4018	BCR	C16-C15-C14	11.81	147.68	123.52
24	0	4019	BCR	C21-C20-C19	11.80	157.40	123.20
24	a	4008	BCR	C11-C10-C9	11.79	143.81	127.28
24	a	4001	BCR	C11-C10-C9	11.78	143.80	127.28
24	B	4018	BCR	C11-C10-C9	11.78	143.80	127.28
24	h	4018	BCR	C11-C10-C9	11.77	143.78	127.28
24	j	4013	BCR	C11-C10-C9	11.75	143.76	127.28
24	A	4001	BCR	C16-C15-C14	11.75	147.56	123.52
24	b	4004	BCR	C16-C15-C14	11.73	147.53	123.52
24	I	4018	BCR	C16-C15-C14	11.73	147.53	123.52
21	b	1023	CLA	C4A-NA-C1A	11.72	112.03	106.68
24	a	4003	BCR	C11-C10-C9	11.69	143.67	127.28
24	2	4004	BCR	C11-C10-C9	11.62	143.58	127.28
24	B	4005	BCR	C21-C20-C19	11.55	156.68	123.20
24	L	4019	BCR	C21-C20-C19	11.52	156.58	123.20
24	l	4022	BCR	C16-C15-C14	11.49	147.04	123.52
24	A	4007	BCR	C21-C20-C19	11.49	156.49	123.20
24	A	4002	BCR	C16-C15-C14	11.47	147.00	123.52
24	a	4007	BCR	C16-C15-C14	11.47	147.00	123.52
24	j	4013	BCR	C16-C15-C14	11.47	146.98	123.52
24	L	4022	BCR	C16-C15-C14	11.46	146.97	123.52
24	L	4022	BCR	C11-C10-C9	11.45	143.34	127.28
21	A	1011	CLA	C4A-NA-C1A	11.44	111.90	106.68
24	I	4018	BCR	C11-C10-C9	11.43	143.31	127.28
21	a	1011	CLA	C4A-NA-C1A	11.43	111.89	106.68
21	2	1023	CLA	C4A-NA-C1A	11.43	111.89	106.68
24	A	4003	BCR	C16-C15-C14	11.41	146.86	123.52
24	a	4008	BCR	C21-C20-C19	11.36	156.13	123.20
24	A	4012	BCR	C16-C15-C14	11.33	146.71	123.52
24	f	4016	BCR	C16-C15-C14	11.32	146.68	123.52
24	2	4014	BCR	C16-C15-C14	11.32	146.67	123.52
24	A	4003	BCR	C11-C10-C9	11.26	143.06	127.28
21	6	1302	CLA	C4A-NA-C1A	11.23	111.80	106.68
21	a	1109	CLA	C4A-NA-C1A	11.19	111.78	106.68
24	h	4018	BCR	C20-C19-C18	11.18	157.01	126.36
21	a	1126	CLA	C4A-NA-C1A	11.17	111.77	106.68
24	b	4014	BCR	C16-C15-C14	11.16	146.35	123.52
24	1	4003	BCR	C11-C10-C9	11.15	142.91	127.28
21	2	1201	CLA	C4A-NA-C1A	11.14	111.76	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	4018	BCR	C20-C19-C18	11.12	156.86	126.36
24	b	4005	BCR	C21-C20-C19	11.11	155.38	123.20
21	1	1012	CLA	C4A-NA-C1A	11.09	111.74	106.68
21	1	1013	CLA	C4A-NA-C1A	11.08	111.74	106.68
24	k	4001	BCR	C11-C10-C9	11.06	142.79	127.28
21	J	1302	CLA	C4A-NA-C1A	11.02	111.71	106.68
24	1	4007	BCR	C11-C10-C9	11.00	142.70	127.28
21	B	1235	CLA	C4A-NA-C1A	10.99	111.69	106.68
21	B	1021	CLA	C4A-NA-C1A	10.98	111.69	106.68
21	1	1011	CLA	C4A-NA-C1A	10.97	111.68	106.68
24	1	4012	BCR	C11-C10-C9	10.97	142.66	127.28
24	a	4019	BCR	C21-C20-C19	10.90	154.78	123.20
21	b	1202	CLA	C4A-NA-C1A	10.86	111.63	106.68
24	A	4002	BCR	C11-C10-C9	10.84	142.48	127.28
21	b	1230	CLA	C4A-NA-C1A	10.83	111.62	106.68
24	A	4007	BCR	C16-C15-C14	10.82	145.67	123.52
24	i	4018	BCR	C20-C19-C18	10.79	155.95	126.36
24	B	4004	BCR	C11-C10-C9	10.76	142.37	127.28
21	a	1102	CLA	C4A-NA-C1A	10.76	111.59	106.68
21	A	1112	CLA	C4A-NA-C1A	10.76	111.59	106.68
21	B	1023	CLA	C4A-NA-C1A	10.76	111.59	106.68
24	1	4019	BCR	C11-C10-C9	10.76	142.36	127.28
24	K	4001	BCR	C11-C10-C9	10.75	142.36	127.28
21	1	1103	CLA	C4A-NA-C1A	10.72	111.57	106.68
24	A	4012	BCR	C11-C10-C9	10.71	142.30	127.28
24	B	4005	BCR	C11-C10-C9	10.70	142.29	127.28
21	a	1013	CLA	C4A-NA-C1A	10.70	111.56	106.68
21	1	1112	CLA	C4A-NA-C1A	10.69	111.56	106.68
24	l	4019	BCR	C16-C15-C14	10.68	145.38	123.52
24	A	4008	BCR	C16-C15-C14	10.68	145.37	123.52
21	b	1221	CLA	C4A-NA-C1A	10.67	111.55	106.68
21	B	1217	CLA	C4A-NA-C1A	10.64	111.53	106.68
21	2	1213	CLA	C4A-NA-C1A	10.64	111.53	106.68
21	a	1112	CLA	C4A-NA-C1A	10.63	111.53	106.68
21	B	1207	CLA	C4A-NA-C1A	10.62	111.53	106.68
21	j	1302	CLA	C4A-NA-C1A	10.62	111.52	106.68
21	b	1231	CLA	C4A-NA-C1A	10.60	111.51	106.68
24	1	4008	BCR	C11-C10-C9	10.59	142.13	127.28
21	2	1216	CLA	C4A-NA-C1A	10.59	111.51	106.68
21	1	1119	CLA	C4A-NA-C1A	10.57	111.50	106.68
21	2	1232	CLA	C4A-NA-C1A	10.57	111.50	106.68
24	0	4019	BCR	C11-C10-C9	10.56	142.09	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1123	CLA	C4A-NA-C1A	10.55	111.49	106.68
21	a	1106	CLA	C4A-NA-C1A	10.55	111.49	106.68
21	B	1203	CLA	C4A-NA-C1A	10.54	111.49	106.68
21	1	1126	CLA	C4A-NA-C1A	10.54	111.49	106.68
21	a	1122	CLA	C4A-NA-C1A	10.52	111.48	106.68
21	2	1021	CLA	C4A-NA-C1A	10.52	111.48	106.68
21	A	1139	CLA	C4A-NA-C1A	10.50	111.47	106.68
21	2	1212	CLA	C4A-NA-C1A	10.49	111.46	106.68
21	A	1108	CLA	C4A-NA-C1A	10.48	111.46	106.68
24	b	4017	BCR	C21-C20-C19	10.48	153.57	123.20
21	2	1206	CLA	C4A-NA-C1A	10.48	111.46	106.68
21	2	1205	CLA	C4A-NA-C1A	10.48	111.46	106.68
21	b	1207	CLA	C4A-NA-C1A	10.47	111.46	106.68
21	J	1303	CLA	C4A-NA-C1A	10.46	111.45	106.68
21	k	1402	CLA	C4A-NA-C1A	10.45	111.45	106.68
21	B	1211	CLA	C4A-NA-C1A	10.44	111.44	106.68
24	a	4007	BCR	C11-C10-C9	10.43	141.91	127.28
21	a	1801	CLA	C4A-NA-C1A	10.42	111.43	106.68
21	B	1229	CLA	C4A-NA-C1A	10.42	111.43	106.68
21	1	1139	CLA	C4A-NA-C1A	10.42	111.43	106.68
21	a	1138	CLA	C4A-NA-C1A	10.40	111.43	106.68
28	h	4020	45D	C42-C38-C36	-10.40	112.69	127.28
21	b	1211	CLA	C4A-NA-C1A	10.40	111.42	106.68
21	7	1302	CLA	C4A-NA-C1A	10.40	111.42	106.68
21	A	1126	CLA	C4A-NA-C1A	10.38	111.42	106.68
21	1	1133	CLA	C4A-NA-C1A	10.37	111.41	106.68
24	2	4017	BCR	C21-C20-C19	10.34	153.17	123.20
21	2	1223	CLA	C4A-NA-C1A	10.34	111.39	106.68
21	2	1022	CLA	C4A-NA-C1A	10.32	111.39	106.68
21	b	1224	CLA	C4A-NA-C1A	10.32	111.39	106.68
21	b	1240	CLA	C4A-NA-C1A	10.30	111.38	106.68
24	2	4011	BCR	C11-C10-C9	10.29	141.71	127.28
21	a	1108	CLA	C4A-NA-C1A	10.28	111.37	106.68
21	A	1111	CLA	C4A-NA-C1A	10.27	111.37	106.68
24	0	4022	BCR	C16-C15-C14	10.27	144.52	123.52
21	2	1228	CLA	C4A-NA-C1A	10.26	111.36	106.68
24	2	4011	BCR	C16-C15-C14	10.26	144.51	123.52
24	B	4017	BCR	C21-C20-C19	10.25	152.91	123.20
21	B	1206	CLA	C4A-NA-C1A	10.25	111.36	106.68
21	b	1021	CLA	C4A-NA-C1A	10.25	111.36	106.68
21	B	1215	CLA	C4A-NA-C1A	10.25	111.35	106.68
21	1	1125	CLA	C4A-NA-C1A	10.25	111.35	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	k	1401	CLA	C4A-NA-C1A	10.24	111.35	106.68
21	a	1103	CLA	C4A-NA-C1A	10.24	111.35	106.68
21	b	1206	CLA	C4A-NA-C1A	10.23	111.35	106.68
21	1	1102	CLA	C4A-NA-C1A	10.23	111.35	106.68
21	b	1220	CLA	C4A-NA-C1A	10.22	111.34	106.68
21	1	1109	CLA	C4A-NA-C1A	10.22	111.34	106.68
21	l	1501	CLA	C4A-NA-C1A	10.21	111.34	106.68
21	A	1103	CLA	C4A-NA-C1A	10.19	111.33	106.68
21	A	1102	CLA	C4A-NA-C1A	10.19	111.33	106.68
21	A	1012	CLA	C4A-NA-C1A	10.18	111.33	106.68
21	1	1118	CLA	C4A-NA-C1A	10.17	111.32	106.68
21	2	1235	CLA	C4A-NA-C1A	10.17	111.32	106.68
21	7	1303	CLA	C4A-NA-C1A	10.16	111.32	106.68
24	8	4001	BCR	C11-C10-C9	10.15	141.52	127.28
21	A	1107	CLA	C4A-NA-C1A	10.15	111.31	106.68
21	A	1138	CLA	C4A-NA-C1A	10.14	111.31	106.68
21	2	1224	CLA	C4A-NA-C1A	10.14	111.31	106.68
21	1	1110	CLA	C4A-NA-C1A	10.14	111.30	106.68
21	B	1232	CLA	C4A-NA-C1A	10.13	111.30	106.68
21	B	1205	CLA	C4A-NA-C1A	10.12	111.30	106.68
21	a	1134	CLA	C4A-NA-C1A	10.11	111.29	106.68
21	b	1201	CLA	C4A-NA-C1A	10.11	111.29	106.68
21	2	1209	CLA	C4A-NA-C1A	10.11	111.29	106.68
21	B	1202	CLA	C4A-NA-C1A	10.10	111.29	106.68
21	2	1202	CLA	C4A-NA-C1A	10.10	111.28	106.68
21	B	1222	CLA	C4A-NA-C1A	10.09	111.28	106.68
21	1	1134	CLA	C4A-NA-C1A	10.08	111.28	106.68
30	2	4006	ECH	C16-C17-C18	-10.07	113.15	127.28
21	L	1501	CLA	C4A-NA-C1A	10.07	111.27	106.68
21	1	1104	CLA	C4A-NA-C1A	10.07	111.27	106.68
21	a	1115	CLA	C4A-NA-C1A	10.05	111.27	106.68
21	a	1124	CLA	C4A-NA-C1A	10.05	111.26	106.68
21	b	1228	CLA	C4A-NA-C1A	10.04	111.26	106.68
21	B	1230	CLA	C4A-NA-C1A	10.03	111.26	106.68
21	2	1240	CLA	C4A-NA-C1A	10.03	111.25	106.68
21	a	1136	CLA	C4A-NA-C1A	10.03	111.25	106.68
21	B	1224	CLA	C4A-NA-C1A	10.03	111.25	106.68
21	A	1121	CLA	C4A-NA-C1A	10.02	111.25	106.68
21	2	1222	CLA	C4A-NA-C1A	10.02	111.25	106.68
24	i	4018	BCR	C21-C20-C19	10.02	152.22	123.20
21	b	1213	CLA	C4A-NA-C1A	10.01	111.25	106.68
21	2	1230	CLA	C4A-NA-C1A	10.00	111.24	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	4020	ECH	C15-C14-C13	-9.99	113.26	127.28
21	B	1209	CLA	C4A-NA-C1A	9.99	111.24	106.68
21	B	1221	CLA	C4A-NA-C1A	9.99	111.24	106.68
21	a	1125	CLA	C4A-NA-C1A	9.99	111.23	106.68
21	a	1139	CLA	C4A-NA-C1A	9.99	111.23	106.68
21	1	1113	CLA	C4A-NA-C1A	9.99	111.23	106.68
21	2	1207	CLA	C4A-NA-C1A	9.99	111.23	106.68
21	a	1012	CLA	C4A-NA-C1A	9.98	111.23	106.68
24	B	4014	BCR	C16-C15-C14	9.98	143.93	123.52
21	B	1231	CLA	C4A-NA-C1A	9.97	111.23	106.68
21	1	1116	CLA	C4A-NA-C1A	9.97	111.23	106.68
21	2	1239	CLA	C4A-NA-C1A	9.97	111.23	106.68
21	2	1234	CLA	C4A-NA-C1A	9.97	111.23	106.68
21	A	1134	CLA	C4A-NA-C1A	9.96	111.22	106.68
21	B	1218	CLA	C4A-NA-C1A	9.96	111.22	106.68
21	B	1220	CLA	C4A-NA-C1A	9.95	111.22	106.68
21	8	1402	CLA	C4A-NA-C1A	9.95	111.22	106.68
21	2	1221	CLA	C4A-NA-C1A	9.93	111.21	106.68
21	b	1216	CLA	C4A-NA-C1A	9.92	111.20	106.68
21	A	1115	CLA	C4A-NA-C1A	9.92	111.20	106.68
24	2	4018	BCR	C21-C20-C19	9.91	151.93	123.20
21	2	1217	CLA	C4A-NA-C1A	9.91	111.20	106.68
21	A	1013	CLA	C4A-NA-C1A	9.91	111.20	106.68
21	b	1232	CLA	C4A-NA-C1A	9.91	111.20	106.68
21	a	1128	CLA	C4A-NA-C1A	9.91	111.20	106.68
21	2	1211	CLA	C4A-NA-C1A	9.90	111.20	106.68
21	2	1231	CLA	C4A-NA-C1A	9.90	111.20	106.68
21	a	1104	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	1	1108	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	b	1239	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	a	1111	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	1	1122	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	1	1106	CLA	C4A-NA-C1A	9.89	111.19	106.68
21	2	1226	CLA	C4A-NA-C1A	9.88	111.19	106.68
21	1	1120	CLA	C4A-NA-C1A	9.88	111.19	106.68
24	h	4018	BCR	C21-C20-C19	9.87	151.80	123.20
21	A	1104	CLA	C4A-NA-C1A	9.87	111.18	106.68
21	a	1120	CLA	C4A-NA-C1A	9.87	111.18	106.68
21	b	1236	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	1	1121	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	a	1110	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	b	1218	CLA	C4A-NA-C1A	9.86	111.18	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1209	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	A	1109	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	8	1401	CLA	C4A-NA-C1A	9.86	111.18	106.68
21	a	1130	CLA	C4A-NA-C1A	9.85	111.17	106.68
21	B	1239	CLA	C4A-NA-C1A	9.85	111.17	106.68
21	F	1302	CLA	C4A-NA-C1A	9.85	111.17	106.68
21	2	1210	CLA	C4A-NA-C1A	9.84	111.17	106.68
21	2	1220	CLA	C4A-NA-C1A	9.84	111.17	106.68
21	A	1140	CLA	C4A-NA-C1A	9.82	111.16	106.68
21	F	1301	CLA	C4A-NA-C1A	9.82	111.16	106.68
21	a	1101	CLA	C4A-NA-C1A	9.82	111.16	106.68
21	A	1801	CLA	C4A-NA-C1A	9.82	111.16	106.68
21	b	1022	CLA	C4A-NA-C1A	9.82	111.16	106.68
21	a	1113	CLA	C4A-NA-C1A	9.80	111.15	106.68
21	b	1227	CLA	C4A-NA-C1A	9.80	111.15	106.68
21	1	1131	CLA	C4A-NA-C1A	9.80	111.15	106.68
21	2	1204	CLA	C4A-NA-C1A	9.80	111.15	106.68
21	b	1203	CLA	C4A-NA-C1A	9.78	111.14	106.68
21	L	1502	CLA	C4A-NA-C1A	9.78	111.14	106.68
21	a	1131	CLA	C4A-NA-C1A	9.78	111.14	106.68
21	0	1502	CLA	C4A-NA-C1A	9.77	111.14	106.68
21	B	1216	CLA	C4A-NA-C1A	9.77	111.14	106.68
24	9	4021	BCR	C21-C20-C19	9.77	151.50	123.20
21	B	1223	CLA	C4A-NA-C1A	9.76	111.13	106.68
24	1	4002	BCR	C11-C10-C9	9.76	140.96	127.28
21	b	1222	CLA	C4A-NA-C1A	9.75	111.13	106.68
21	a	1116	CLA	C4A-NA-C1A	9.75	111.13	106.68
21	b	1208	CLA	C4A-NA-C1A	9.75	111.12	106.68
21	2	1227	CLA	C4A-NA-C1A	9.74	111.12	106.68
21	1	1137	CLA	C4A-NA-C1A	9.73	111.12	106.68
21	a	1123	CLA	C4A-NA-C1A	9.73	111.12	106.68
21	B	1022	CLA	C4A-NA-C1A	9.73	111.12	106.68
21	a	1114	CLA	C4A-NA-C1A	9.71	111.11	106.68
21	1	1101	CLA	C4A-NA-C1A	9.71	111.11	106.68
21	2	1229	CLA	C4A-NA-C1A	9.71	111.11	106.68
21	b	1210	CLA	C4A-NA-C1A	9.70	111.11	106.68
34	j	4015	ZEX	C21-C26-C25	-9.70	115.34	122.84
21	B	1201	CLA	C4A-NA-C1A	9.69	111.10	106.68
21	1	1801	CLA	C4A-NA-C1A	9.69	111.10	106.68
21	B	1228	CLA	C4A-NA-C1A	9.69	111.10	106.68
21	1	1132	CLA	C4A-NA-C1A	9.68	111.10	106.68
21	2	1219	CLA	C4A-NA-C1A	9.68	111.10	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1107	CLA	C4A-NA-C1A	9.67	111.09	106.68
21	2	1215	CLA	C4A-NA-C1A	9.67	111.09	106.68
21	a	1117	CLA	C4A-NA-C1A	9.67	111.09	106.68
21	1	1111	CLA	C4A-NA-C1A	9.66	111.09	106.68
21	a	1121	CLA	C4A-NA-C1A	9.66	111.09	106.68
21	a	1140	CLA	C4A-NA-C1A	9.66	111.09	106.68
21	A	1125	CLA	C4A-NA-C1A	9.66	111.09	106.68
21	b	1223	CLA	C4A-NA-C1A	9.64	111.08	106.68
21	b	1235	CLA	C4A-NA-C1A	9.64	111.08	106.68
24	b	4010	BCR	C11-C10-C9	9.64	140.79	127.28
21	A	1116	CLA	C4A-NA-C1A	9.63	111.07	106.68
21	B	1225	CLA	C4A-NA-C1A	9.63	111.07	106.68
21	1	1117	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	L	1503	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	f	1302	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	A	1110	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	B	1213	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	A	1137	CLA	C4A-NA-C1A	9.62	111.07	106.68
21	1	1115	CLA	C4A-NA-C1A	9.60	111.06	106.68
21	B	1234	CLA	C4A-NA-C1A	9.60	111.06	106.68
21	B	1210	CLA	C4A-NA-C1A	9.59	111.05	106.68
21	B	1227	CLA	C4A-NA-C1A	9.59	111.05	106.68
21	B	1237	CLA	C4A-NA-C1A	9.59	111.05	106.68
28	h	4020	45D	C24-C26-C30	-9.58	103.94	119.01
24	A	4001	BCR	C11-C10-C9	9.58	140.71	127.28
21	2	1203	CLA	C4A-NA-C1A	9.58	111.05	106.68
21	a	1132	CLA	C4A-NA-C1A	9.57	111.05	106.68
24	2	4010	BCR	C20-C19-C18	9.57	152.59	126.36
21	1	1136	CLA	C4A-NA-C1A	9.56	111.04	106.68
21	a	1137	CLA	C4A-NA-C1A	9.56	111.04	106.68
24	2	4017	BCR	C20-C19-C18	9.53	152.50	126.36
21	A	1130	CLA	C4A-NA-C1A	9.53	111.03	106.68
24	a	4012	BCR	C11-C10-C9	9.53	140.64	127.28
21	1	1107	CLA	C4A-NA-C1A	9.53	111.03	106.68
21	A	1106	CLA	C4A-NA-C1A	9.52	111.02	106.68
24	b	4018	BCR	C11-C10-C9	9.52	140.63	127.28
21	1	1138	CLA	C4A-NA-C1A	9.52	111.02	106.68
21	B	1240	CLA	C4A-NA-C1A	9.51	111.02	106.68
21	a	1105	CLA	C4A-NA-C1A	9.51	111.02	106.68
21	2	1218	CLA	C4A-NA-C1A	9.51	111.02	106.68
21	0	1501	CLA	C4A-NA-C1A	9.51	111.02	106.68
21	1	1105	CLA	C4A-NA-C1A	9.50	111.02	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1226	CLA	C4A-NA-C1A	9.50	111.01	106.68
21	1	1130	CLA	C4A-NA-C1A	9.50	111.01	106.68
21	2	1208	CLA	C4A-NA-C1A	9.49	111.01	106.68
21	1	1127	CLA	C4A-NA-C1A	9.47	111.00	106.68
21	b	1219	CLA	C4A-NA-C1A	9.46	111.00	106.68
21	1	1123	CLA	C4A-NA-C1A	9.45	110.99	106.68
21	a	1127	CLA	C4A-NA-C1A	9.45	110.99	106.68
21	a	1119	CLA	C4A-NA-C1A	9.43	110.98	106.68
21	2	1236	CLA	C4A-NA-C1A	9.42	110.98	106.68
21	l	1502	CLA	C4A-NA-C1A	9.41	110.97	106.68
21	K	1402	CLA	C4A-NA-C1A	9.41	110.97	106.68
21	b	1217	CLA	C4A-NA-C1A	9.40	110.97	106.68
21	1	1140	CLA	C4A-NA-C1A	9.39	110.97	106.68
24	b	4018	BCR	C20-C19-C18	9.38	152.09	126.36
21	A	1131	CLA	C4A-NA-C1A	9.37	110.95	106.68
21	a	1118	CLA	C4A-NA-C1A	9.36	110.95	106.68
21	B	1208	CLA	C4A-NA-C1A	9.36	110.95	106.68
21	A	1136	CLA	C4A-NA-C1A	9.36	110.95	106.68
21	b	1229	CLA	C4A-NA-C1A	9.35	110.94	106.68
21	B	1236	CLA	C4A-NA-C1A	9.35	110.94	106.68
21	0	1503	CLA	C4A-NA-C1A	9.35	110.94	106.68
21	B	1212	CLA	C4A-NA-C1A	9.35	110.94	106.68
21	1	1128	CLA	C4A-NA-C1A	9.35	110.94	106.68
21	A	1122	CLA	C4A-NA-C1A	9.34	110.94	106.68
21	b	1237	CLA	C4A-NA-C1A	9.34	110.94	106.68
21	j	1303	CLA	C4A-NA-C1A	9.34	110.94	106.68
21	B	1214	CLA	C4A-NA-C1A	9.34	110.94	106.68
21	A	1118	CLA	C4A-NA-C1A	9.33	110.94	106.68
21	1	1114	CLA	C4A-NA-C1A	9.33	110.94	106.68
30	B	4006	ECH	C16-C17-C18	-9.33	114.20	127.28
21	b	1215	CLA	C4A-NA-C1A	9.32	110.93	106.68
21	b	1234	CLA	C4A-NA-C1A	9.32	110.93	106.68
21	b	1238	CLA	C4A-NA-C1A	9.31	110.93	106.68
21	A	1124	CLA	C4A-NA-C1A	9.30	110.92	106.68
21	A	1128	CLA	C4A-NA-C1A	9.29	110.92	106.68
21	K	1401	CLA	C4A-NA-C1A	9.29	110.92	106.68
24	L	4019	BCR	C11-C10-C9	9.29	140.31	127.28
21	2	1237	CLA	C4A-NA-C1A	9.28	110.92	106.68
21	2	1225	CLA	C4A-NA-C1A	9.27	110.91	106.68
21	A	1114	CLA	C4A-NA-C1A	9.27	110.91	106.68
21	A	1129	CLA	C4A-NA-C1A	9.25	110.90	106.68
21	A	1127	CLA	C4A-NA-C1A	9.25	110.90	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1214	CLA	C4A-NA-C1A	9.25	110.90	106.68
21	b	1205	CLA	C4A-NA-C1A	9.25	110.90	106.68
21	A	1117	CLA	C4A-NA-C1A	9.24	110.89	106.68
21	b	1225	CLA	C4A-NA-C1A	9.23	110.89	106.68
21	B	1219	CLA	C4A-NA-C1A	9.22	110.89	106.68
21	A	1113	CLA	C4A-NA-C1A	9.21	110.88	106.68
21	a	1129	CLA	C4A-NA-C1A	9.20	110.88	106.68
24	b	4017	BCR	C20-C19-C18	9.18	151.54	126.36
21	b	1204	CLA	C4A-NA-C1A	9.18	110.87	106.68
21	f	1301	CLA	C4A-NA-C1A	9.16	110.86	106.68
24	a	4008	BCR	C20-C19-C18	9.16	151.49	126.36
21	A	1101	CLA	C4A-NA-C1A	9.16	110.86	106.68
21	6	1301	CLA	C4A-NA-C1A	9.15	110.86	106.68
21	A	1132	CLA	C4A-NA-C1A	9.14	110.85	106.68
21	A	1119	CLA	C4A-NA-C1A	9.13	110.84	106.68
24	2	4011	BCR	C20-C19-C18	9.11	151.35	126.36
24	B	4018	BCR	C20-C19-C18	9.10	151.33	126.36
21	1	1135	CLA	C4A-NA-C1A	9.10	110.83	106.68
21	a	1133	CLA	C4A-NA-C1A	9.10	110.83	106.68
21	l	1503	CLA	C4A-NA-C1A	9.10	110.83	106.68
24	1	4007	BCR	C20-C19-C18	9.10	151.31	126.36
21	2	1238	CLA	C4A-NA-C1A	9.09	110.83	106.68
24	a	4012	BCR	C20-C19-C18	9.06	151.19	126.36
24	B	4005	BCR	C20-C19-C18	9.05	151.17	126.36
21	1	1129	CLA	C4A-NA-C1A	9.04	110.80	106.68
21	A	1120	CLA	C4A-NA-C1A	9.03	110.80	106.68
24	A	4007	BCR	C11-C10-C9	9.02	139.92	127.28
21	1	1124	CLA	C4A-NA-C1A	8.96	110.77	106.68
24	A	4008	BCR	C11-C10-C9	8.95	139.83	127.28
24	a	4002	BCR	C20-C19-C18	8.94	150.88	126.36
30	b	4011	ECH	C15-C14-C13	-8.94	114.74	127.28
21	A	1135	CLA	C4A-NA-C1A	8.93	110.75	106.68
24	A	4007	BCR	C20-C19-C18	8.88	150.71	126.36
24	0	4019	BCR	C20-C19-C18	8.87	150.68	126.36
24	L	4019	BCR	C16-C15-C14	8.87	141.66	123.52
24	B	4017	BCR	C20-C19-C18	8.84	150.60	126.36
21	A	1105	CLA	C4A-NA-C1A	8.82	110.70	106.68
30	b	4006	ECH	C20-C21-C22	-8.80	114.94	127.28
21	a	1135	CLA	C4A-NA-C1A	8.72	110.66	106.68
24	2	4005	BCR	C20-C19-C18	8.69	150.19	126.36
24	A	4019	BCR	C20-C19-C18	8.67	150.13	126.36
24	l	4019	BCR	C11-C10-C9	8.66	139.43	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	4005	BCR	C20-C19-C18	8.66	150.10	126.36
21	B	1204	CLA	C4A-NA-C1A	8.63	110.62	106.68
21	b	1212	CLA	C4A-NA-C1A	8.63	110.62	106.68
21	A	1133	CLA	C4A-NA-C1A	8.61	110.61	106.68
24	a	4001	BCR	C20-C19-C18	8.54	149.78	126.36
21	2	1214	CLA	C4A-NA-C1A	8.54	110.58	106.68
21	B	1238	CLA	C4A-NA-C1A	8.52	110.57	106.68
24	I	4018	BCR	C21-C20-C19	8.50	147.84	123.20
28	h	4020	45D	C32-C34-C36	-8.46	103.16	126.36
24	L	4019	BCR	C20-C19-C18	8.44	149.50	126.36
21	b	1226	CLA	C4A-NA-C1A	8.36	110.50	106.68
24	l	4019	BCR	C20-C19-C18	8.29	149.09	126.36
24	1	4019	BCR	C20-C19-C18	8.25	148.99	126.36
24	K	4001	BCR	C20-C19-C18	8.22	148.91	126.36
24	a	4003	BCR	C20-C19-C18	8.21	148.87	126.36
24	1	4012	BCR	C20-C19-C18	8.21	148.87	126.36
24	J	4013	BCR	C20-C19-C18	8.18	148.79	126.36
24	k	4001	BCR	C20-C19-C18	8.13	148.65	126.36
24	6	4016	BCR	C20-C19-C18	8.06	148.47	126.36
24	A	4008	BCR	C20-C19-C18	8.02	148.37	126.36
24	A	4002	BCR	C20-C19-C18	8.00	148.31	126.36
24	L	4022	BCR	C20-C19-C18	7.94	148.14	126.36
34	J	4015	ZEX	C21-C26-C25	-7.85	116.78	122.84
24	1	4008	BCR	C20-C19-C18	7.84	147.87	126.36
24	A	4001	BCR	C20-C19-C18	7.82	147.82	126.36
24	B	4010	BCR	C20-C19-C18	7.78	147.70	126.36
24	f	4016	BCR	C20-C19-C18	7.78	147.70	126.36
24	a	4007	BCR	C20-C19-C18	7.69	147.45	126.36
24	1	4001	BCR	C20-C19-C18	7.65	147.33	126.36
30	2	4006	ECH	C24-C23-C22	-7.59	115.01	126.23
28	h	4020	45D	C32-C30-C26	7.55	137.86	127.28
24	8	4001	BCR	C20-C19-C18	7.53	147.02	126.36
34	7	4015	ZEX	C21-C26-C25	-7.46	117.07	122.84
24	b	4004	BCR	C20-C19-C18	7.39	146.62	126.36
24	2	4004	BCR	C20-C19-C18	7.37	146.57	126.36
24	A	4012	BCR	C20-C19-C18	7.35	146.50	126.36
24	B	4014	BCR	C20-C19-C18	7.28	146.33	126.36
24	l	4022	BCR	C20-C19-C18	7.22	146.17	126.36
24	1	4003	BCR	C20-C19-C18	7.21	146.14	126.36
24	b	4014	BCR	C20-C19-C18	7.08	145.78	126.36
24	B	4004	BCR	C20-C19-C18	7.03	145.64	126.36
24	b	4010	BCR	C20-C19-C18	6.99	145.53	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	j	4013	BCR	C20-C19-C18	6.99	145.52	126.36
24	7	4013	BCR	C20-C19-C18	6.97	145.47	126.36
24	1	4002	BCR	C20-C19-C18	6.96	145.44	126.36
24	2	4014	BCR	C20-C19-C18	6.87	145.21	126.36
24	A	4003	BCR	C20-C19-C18	6.82	145.07	126.36
30	B	4006	ECH	C24-C23-C22	-6.74	116.26	126.23
28	h	4020	45D	C24-C20-C08	-6.74	109.00	127.00
24	a	4019	BCR	C20-C19-C18	6.54	144.29	126.36
28	B	4011	45D	C20-C24-C26	-6.39	116.79	126.23
21	1	1109	CLA	CMD-C2D-C1D	6.35	135.91	124.73
34	F	4016	ZEX	C28-C27-C26	-6.27	116.86	126.94
30	i	4020	ECH	C7-C8-C9	-6.24	117.01	126.23
24	9	4021	BCR	C20-C19-C18	6.15	143.22	126.36
24	0	4022	BCR	C20-C19-C18	6.14	143.19	126.36
30	b	4011	ECH	C20-C21-C22	-6.12	118.70	127.28
21	A	1121	CLA	CMD-C2D-C1D	6.11	135.48	124.73
21	2	1228	CLA	CMD-C2D-C1D	6.09	135.45	124.73
28	h	4020	45D	C28-C26-C24	6.09	127.38	118.09
21	b	1213	CLA	CMD-C2D-C1D	6.05	135.38	124.73
21	b	1226	CLA	CMD-C2D-C1D	6.02	135.32	124.73
21	2	1221	CLA	CMD-C2D-C1D	5.99	135.28	124.73
21	a	1136	CLA	CMD-C2D-C1D	5.97	135.25	124.73
21	1	1801	CLA	CMD-C2D-C1D	5.97	135.24	124.73
21	a	1107	CLA	CMD-C2D-C1D	5.96	135.22	124.73
28	B	4011	45D	C41-C37-C35	-5.95	118.94	127.28
21	b	1231	CLA	CMD-C2D-C1D	5.91	135.14	124.73
21	1	1122	CLA	CMD-C2D-C1D	5.86	135.05	124.73
21	k	1402	CLA	O2A-C1-C2	5.86	122.93	108.99
21	A	1120	CLA	CMD-C2D-C1D	5.85	135.03	124.73
21	2	1227	CLA	CMD-C2D-C1D	5.85	135.02	124.73
21	a	1103	CLA	CMD-C2D-C1D	5.84	135.01	124.73
21	2	1201	CLA	CMD-C2D-C1D	5.82	134.98	124.73
21	2	1211	CLA	CMD-C2D-C1D	5.82	134.98	124.73
24	2	4018	BCR	C20-C19-C18	5.81	142.28	126.36
21	7	1302	CLA	CMD-C2D-C1D	5.80	134.95	124.73
21	A	1131	CLA	CMD-C2D-C1D	5.79	134.92	124.73
21	B	1217	CLA	CMD-C2D-C1D	5.78	134.90	124.73
21	2	1224	CLA	CMD-C2D-C1D	5.78	134.90	124.73
21	b	1232	CLA	CMD-C2D-C1D	5.76	134.88	124.73
21	A	1011	CLA	O2D-CGD-CBD	5.76	121.31	111.23
21	1	1111	CLA	CMD-C2D-C1D	5.76	134.87	124.73
21	a	1101	CLA	CMD-C2D-C1D	5.76	134.87	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1205	CLA	CMD-C2D-C1D	5.75	134.86	124.73
21	a	1109	CLA	CMD-C2D-C1D	5.75	134.85	124.73
21	A	1124	CLA	CMD-C2D-C1D	5.74	134.84	124.73
21	b	1023	CLA	CMD-C2D-C1D	5.73	134.83	124.73
21	B	1208	CLA	CMD-C2D-C1D	5.73	134.82	124.73
21	A	1113	CLA	CMD-C2D-C1D	5.72	134.80	124.73
21	A	1103	CLA	CMD-C2D-C1D	5.72	134.80	124.73
21	b	1202	CLA	CMD-C2D-C1D	5.72	134.79	124.73
21	b	1211	CLA	CMD-C2D-C1D	5.71	134.79	124.73
21	k	1402	CLA	CMD-C2D-C1D	5.71	134.78	124.73
21	1	1135	CLA	CMD-C2D-C1D	5.71	134.78	124.73
21	B	1232	CLA	CMD-C2D-C1D	5.70	134.77	124.73
21	a	1139	CLA	CMD-C2D-C1D	5.70	134.77	124.73
21	1	1134	CLA	CMD-C2D-C1D	5.70	134.76	124.73
21	B	1231	CLA	CMD-C2D-C1D	5.69	134.75	124.73
21	b	1236	CLA	CMD-C2D-C1D	5.69	134.75	124.73
21	2	1212	CLA	CMD-C2D-C1D	5.69	134.75	124.73
28	h	4020	45D	C20-C24-C26	5.69	134.65	126.23
21	8	1401	CLA	CMD-C2D-C1D	5.69	134.75	124.73
30	B	4006	ECH	C16-C15-C14	-5.68	111.89	123.52
21	2	1240	CLA	CMD-C2D-C1D	5.68	134.72	124.73
21	b	1240	CLA	CMD-C2D-C1D	5.67	134.72	124.73
21	b	1222	CLA	CMD-C2D-C1D	5.67	134.71	124.73
21	2	1230	CLA	CMD-C2D-C1D	5.67	134.71	124.73
21	B	1221	CLA	CMD-C2D-C1D	5.67	134.71	124.73
21	a	1123	CLA	CMD-C2D-C1D	5.66	134.70	124.73
21	7	1303	CLA	CMD-C2D-C1D	5.66	134.70	124.73
21	a	1104	CLA	CMD-C2D-C1D	5.65	134.67	124.73
21	2	1225	CLA	CMD-C2D-C1D	5.65	134.67	124.73
21	a	1106	CLA	CMD-C2D-C1D	5.64	134.66	124.73
21	2	1203	CLA	CMD-C2D-C1D	5.64	134.66	124.73
21	2	1209	CLA	CMD-C2D-C1D	5.64	134.66	124.73
21	1	1112	CLA	CMD-C2D-C1D	5.64	134.65	124.73
21	b	1216	CLA	CMD-C2D-C1D	5.64	134.65	124.73
21	2	1234	CLA	CMD-C2D-C1D	5.63	134.65	124.73
21	2	1232	CLA	CMD-C2D-C1D	5.63	134.65	124.73
21	a	1126	CLA	CMD-C2D-C1D	5.63	134.64	124.73
21	a	1113	CLA	CMD-C2D-C1D	5.63	134.64	124.73
21	b	1217	CLA	CMD-C2D-C1D	5.63	134.64	124.73
21	2	1206	CLA	CMD-C2D-C1D	5.62	134.63	124.73
21	b	1228	CLA	CMD-C2D-C1D	5.62	134.62	124.73
21	1	1104	CLA	CMD-C2D-C1D	5.62	134.62	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1223	CLA	CMD-C2D-C1D	5.61	134.61	124.73
21	2	1213	CLA	CMD-C2D-C1D	5.61	134.60	124.73
21	1	1121	CLA	CMD-C2D-C1D	5.61	134.60	124.73
21	8	1402	CLA	CMD-C2D-C1D	5.60	134.60	124.73
21	6	1302	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	1	1131	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	2	1204	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	2	1226	CLA	CMD-C2D-C1D	5.60	134.59	124.73
21	1	1101	CLA	CMD-C2D-C1D	5.59	134.58	124.73
21	2	1208	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	a	1135	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	1	1113	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	1	1140	CLA	CMD-C2D-C1D	5.59	134.57	124.73
21	K	1402	CLA	CMD-C2D-C1D	5.58	134.56	124.73
21	B	1214	CLA	CMD-C2D-C1D	5.58	134.56	124.73
21	1	1116	CLA	CMD-C2D-C1D	5.58	134.56	124.73
21	j	1302	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	2	1231	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	a	1114	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	2	1219	CLA	CMD-C2D-C1D	5.58	134.55	124.73
21	f	1301	CLA	CMD-C2D-C1D	5.57	134.54	124.73
21	a	1121	CLA	CMD-C2D-C1D	5.57	134.54	124.73
21	2	1021	CLA	CMD-C2D-C1D	5.57	134.53	124.73
21	1	1139	CLA	CMD-C2D-C1D	5.56	134.53	124.73
21	J	1303	CLA	CMD-C2D-C1D	5.56	134.53	124.73
21	a	1105	CLA	CMD-C2D-C1D	5.56	134.53	124.73
21	2	1229	CLA	CMD-C2D-C1D	5.56	134.52	124.73
21	B	1230	CLA	CMD-C2D-C1D	5.56	134.52	124.73
21	1	1103	CLA	CMD-C2D-C1D	5.56	134.52	124.73
21	A	1110	CLA	CMD-C2D-C1D	5.56	134.52	124.73
36	I	4020	EQ3	C11-C10-C9	-5.56	119.48	127.28
21	b	1209	CLA	CMD-C2D-C1D	5.56	134.52	124.73
21	a	1102	CLA	CMD-C2D-C1D	5.56	134.51	124.73
21	a	1137	CLA	CMD-C2D-C1D	5.56	134.51	124.73
21	B	1240	CLA	CMD-C2D-C1D	5.56	134.51	124.73
21	2	1210	CLA	CMD-C2D-C1D	5.55	134.51	124.73
21	1	1119	CLA	CMD-C2D-C1D	5.55	134.50	124.73
30	B	4006	ECH	C11-C10-C9	-5.55	119.50	127.28
21	b	1227	CLA	CMD-C2D-C1D	5.54	134.49	124.73
21	1	1124	CLA	CMD-C2D-C1D	5.54	134.49	124.73
21	2	1222	CLA	CMD-C2D-C1D	5.54	134.49	124.73
21	1	1114	CLA	CMD-C2D-C1D	5.54	134.48	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1213	CLA	CMD-C2D-C1D	5.53	134.46	124.73
21	a	1134	CLA	CMD-C2D-C1D	5.52	134.45	124.73
25	M	5001	LHG	O7-C7-C8	5.52	123.43	111.48
21	a	1801	CLA	CMD-C2D-C1D	5.52	134.45	124.73
21	B	1219	CLA	CMD-C2D-C1D	5.52	134.45	124.73
28	B	4011	45D	C31-C29-C25	-5.52	119.54	127.28
21	a	1108	CLA	CMD-C2D-C1D	5.52	134.44	124.73
21	a	1112	CLA	CMD-C2D-C1D	5.51	134.44	124.73
21	A	1135	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	B	1226	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	1	1105	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	1	1110	CLA	CMD-C2D-C1D	5.51	134.43	124.73
21	B	1220	CLA	CMD-C2D-C1D	5.51	134.42	124.73
21	B	1212	CLA	CMD-C2D-C1D	5.50	134.42	124.73
21	A	1102	CLA	CMD-C2D-C1D	5.50	134.42	124.73
21	a	1119	CLA	CMD-C2D-C1D	5.50	134.42	124.73
21	1	1130	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	a	1127	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	l	1502	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	1	1102	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	a	1117	CLA	CMD-C2D-C1D	5.50	134.41	124.73
21	2	1235	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	b	1219	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	1	1115	CLA	CMD-C2D-C1D	5.49	134.40	124.73
21	b	1229	CLA	CMD-C2D-C1D	5.49	134.39	124.73
21	B	1210	CLA	CMD-C2D-C1D	5.48	134.39	124.73
21	a	1110	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	1	1117	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	2	1220	CLA	CMD-C2D-C1D	5.48	134.38	124.73
21	A	1129	CLA	CMD-C2D-C1D	5.48	134.37	124.73
21	A	1140	CLA	CMD-C2D-C1D	5.48	134.37	124.73
21	A	1138	CLA	CMD-C2D-C1D	5.47	134.37	124.73
21	2	1238	CLA	CMD-C2D-C1D	5.47	134.37	124.73
21	F	1302	CLA	CMD-C2D-C1D	5.47	134.37	124.73
21	2	1218	CLA	CMD-C2D-C1D	5.47	134.36	124.73
21	a	1140	CLA	CMD-C2D-C1D	5.47	134.36	124.73
21	a	1122	CLA	CMD-C2D-C1D	5.47	134.36	124.73
21	a	1120	CLA	CMD-C2D-C1D	5.46	134.35	124.73
21	1	1106	CLA	CMD-C2D-C1D	5.46	134.35	124.73
21	a	1115	CLA	CMD-C2D-C1D	5.46	134.34	124.73
21	1	1108	CLA	CMD-C2D-C1D	5.46	134.34	124.73
21	1	1138	CLA	CMD-C2D-C1D	5.46	134.34	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	l	1501	CLA	CMD-C2D-C1D	5.46	134.34	124.73
21	A	1125	CLA	CMD-C2D-C1D	5.45	134.33	124.73
21	B	1227	CLA	CMD-C2D-C1D	5.45	134.33	124.73
21	B	1202	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	A	1122	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	b	1022	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	2	1214	CLA	CMD-C2D-C1D	5.45	134.32	124.73
21	1	1123	CLA	CMD-C2D-C1D	5.44	134.32	124.73
21	b	1235	CLA	CMD-C2D-C1D	5.44	134.31	124.73
21	B	1216	CLA	CMD-C2D-C1D	5.44	134.31	124.73
21	j	1303	CLA	CMD-C2D-C1D	5.44	134.30	124.73
21	A	1011	CLA	CMD-C2D-C1D	5.44	134.30	124.73
21	2	1215	CLA	CMD-C2D-C1D	5.43	134.29	124.73
21	b	1201	CLA	CMD-C2D-C1D	5.43	134.29	124.73
21	b	1208	CLA	CMD-C2D-C1D	5.43	134.29	124.73
21	2	1237	CLA	CMD-C2D-C1D	5.43	134.28	124.73
21	a	1133	CLA	CMD-C2D-C1D	5.43	134.28	124.73
21	f	1302	CLA	CMD-C2D-C1D	5.42	134.27	124.73
21	b	1215	CLA	CMD-C2D-C1D	5.42	134.27	124.73
21	a	1125	CLA	CMD-C2D-C1D	5.41	134.25	124.73
21	A	1101	CLA	CMD-C2D-C1D	5.41	134.25	124.73
21	2	1022	CLA	CMD-C2D-C1D	5.41	134.25	124.73
21	b	1224	CLA	CMD-C2D-C1D	5.40	134.24	124.73
21	A	1801	CLA	CMD-C2D-C1D	5.40	134.23	124.73
21	A	1111	CLA	CMD-C2D-C1D	5.40	134.23	124.73
36	I	4020	EQ3	C33-C5-C6	-5.39	118.60	124.48
21	a	1131	CLA	CMD-C2D-C1D	5.39	134.22	124.73
21	B	1234	CLA	CMD-C2D-C1D	5.39	134.21	124.73
21	a	1111	CLA	CMD-C2D-C1D	5.38	134.21	124.73
21	1	1120	CLA	CMD-C2D-C1D	5.38	134.21	124.73
21	0	1503	CLA	CMD-C2D-C1D	5.38	134.21	124.73
21	a	1129	CLA	CMD-C2D-C1D	5.38	134.20	124.73
21	B	1224	CLA	CMD-C2D-C1D	5.38	134.20	124.73
21	A	1134	CLA	CMD-C2D-C1D	5.38	134.20	124.73
21	a	1130	CLA	CMD-C2D-C1D	5.38	134.19	124.73
21	B	1218	CLA	CMD-C2D-C1D	5.37	134.19	124.73
21	a	1116	CLA	CMD-C2D-C1D	5.37	134.18	124.73
21	6	1301	CLA	CMD-C2D-C1D	5.37	134.18	124.73
21	A	1105	CLA	CMD-C2D-C1D	5.36	134.18	124.73
21	b	1212	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	1	1011	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	2	1217	CLA	CMD-C2D-C1D	5.36	134.17	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1115	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	B	1235	CLA	CMD-C2D-C1D	5.36	134.16	124.73
21	B	1229	CLA	CMD-C2D-C1D	5.36	134.16	124.73
21	b	1238	CLA	CMD-C2D-C1D	5.35	134.15	124.73
21	1	1118	CLA	CMD-C2D-C1D	5.35	134.15	124.73
21	a	1124	CLA	CMD-C2D-C1D	5.35	134.14	124.73
21	A	1117	CLA	CMD-C2D-C1D	5.34	134.14	124.73
21	B	1204	CLA	CMD-C2D-C1D	5.34	134.13	124.73
21	1	1125	CLA	CMD-C2D-C1D	5.34	134.12	124.73
34	j	4015	ZEX	C7-C8-C9	-5.33	118.34	126.23
21	b	1230	CLA	CMD-C2D-C1D	5.33	134.11	124.73
21	2	1223	CLA	CMD-C2D-C1D	5.32	134.10	124.73
21	B	1215	CLA	CMD-C2D-C1D	5.32	134.10	124.73
21	2	1236	CLA	CMD-C2D-C1D	5.32	134.09	124.73
21	F	1301	CLA	CMD-C2D-C1D	5.32	134.09	124.73
21	a	1136	CLA	O2D-CGD-CBD	5.32	120.53	111.23
21	a	1132	CLA	CMD-C2D-C1D	5.31	134.09	124.73
21	A	1108	CLA	CMD-C2D-C1D	5.31	134.07	124.73
21	B	1021	CLA	CMD-C2D-C1D	5.31	134.07	124.73
21	A	1114	CLA	CMD-C2D-C1D	5.30	134.07	124.73
21	B	1238	CLA	CMD-C2D-C1D	5.30	134.07	124.73
21	J	1302	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	A	1119	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	B	1209	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	1	1136	CLA	CMD-C2D-C1D	5.30	134.06	124.73
21	A	1130	CLA	CMD-C2D-C1D	5.29	134.05	124.73
21	b	1239	CLA	CMD-C2D-C1D	5.29	134.04	124.73
21	b	1210	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	B	1228	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	1	1137	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	2	1207	CLA	CMD-C2D-C1D	5.28	134.02	124.73
21	a	1118	CLA	CMD-C2D-C1D	5.28	134.02	124.73
21	1	1133	CLA	CMD-C2D-C1D	5.27	134.02	124.73
21	b	1221	CLA	CMD-C2D-C1D	5.27	134.02	124.73
21	l	1503	CLA	CMD-C2D-C1D	5.27	134.00	124.73
21	2	1202	CLA	CMD-C2D-C1D	5.27	134.00	124.73
21	2	1216	CLA	CMD-C2D-C1D	5.26	134.00	124.73
21	B	1023	CLA	CMD-C2D-C1D	5.26	133.99	124.73
21	L	1502	CLA	CMD-C2D-C1D	5.25	133.98	124.73
21	0	1501	CLA	CMD-C2D-C1D	5.24	133.96	124.73
21	b	1234	CLA	CMD-C2D-C1D	5.24	133.96	124.73
21	1	1128	CLA	CMD-C2D-C1D	5.23	133.94	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1134	CLA	O2A-C1-C2	5.23	121.44	108.99
21	B	1236	CLA	CMD-C2D-C1D	5.22	133.93	124.73
21	b	1214	CLA	CMD-C2D-C1D	5.22	133.93	124.73
21	1	1126	CLA	CMD-C2D-C1D	5.22	133.92	124.73
21	A	1104	CLA	CMD-C2D-C1D	5.21	133.91	124.73
21	b	1204	CLA	CMD-C2D-C1D	5.21	133.90	124.73
21	B	1211	CLA	CMD-C2D-C1D	5.20	133.89	124.73
21	B	1203	CLA	CMD-C2D-C1D	5.20	133.89	124.73
21	1	1132	CLA	CMD-C2D-C1D	5.20	133.88	124.73
21	A	1013	CLA	CMD-C2D-C1D	5.19	133.88	124.73
21	1	1129	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	b	1223	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	1	1012	CLA	CMD-C2D-C1D	5.18	133.85	124.73
21	B	1209	CLA	O2D-CGD-CBD	5.17	120.27	111.23
21	b	1218	CLA	CMD-C2D-C1D	5.17	133.83	124.73
21	A	1139	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	A	1132	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	b	1220	CLA	CMD-C2D-C1D	5.16	133.82	124.73
21	b	1205	CLA	CMD-C2D-C1D	5.14	133.78	124.73
21	A	1133	CLA	CMD-C2D-C1D	5.13	133.77	124.73
21	A	1106	CLA	CMD-C2D-C1D	5.13	133.76	124.73
21	B	1237	CLA	CMD-C2D-C1D	5.13	133.76	124.73
21	L	1503	CLA	CMD-C2D-C1D	5.13	133.75	124.73
21	A	1012	CLA	CMD-C2D-C1D	5.12	133.75	124.73
21	A	1118	CLA	CMD-C2D-C1D	5.12	133.74	124.73
25	A	5007	LHG	O7-C7-C8	5.12	122.56	111.48
21	2	1239	CLA	CMD-C2D-C1D	5.12	133.74	124.73
21	B	1205	CLA	CMD-C2D-C1D	5.12	133.74	124.73
21	B	1222	CLA	CMD-C2D-C1D	5.10	133.72	124.73
21	A	1116	CLA	CMD-C2D-C1D	5.09	133.70	124.73
21	2	1023	CLA	CMD-C2D-C1D	5.09	133.70	124.73
21	1	1107	CLA	CMD-C2D-C1D	5.08	133.67	124.73
21	A	1107	CLA	CMD-C2D-C1D	5.08	133.67	124.73
21	A	1112	CLA	CMD-C2D-C1D	5.08	133.67	124.73
21	b	1203	CLA	CMD-C2D-C1D	5.07	133.66	124.73
21	0	1502	CLA	CMD-C2D-C1D	5.07	133.66	124.73
21	B	1201	CLA	CMD-C2D-C1D	5.05	133.63	124.73
21	K	1401	CLA	CMD-C2D-C1D	5.05	133.62	124.73
21	k	1401	CLA	CMD-C2D-C1D	5.03	133.58	124.73
21	B	1206	CLA	CMD-C2D-C1D	5.02	133.57	124.73
21	B	1239	CLA	CMD-C2D-C1D	4.99	133.51	124.73
21	A	1137	CLA	CMD-C2D-C1D	4.98	133.50	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1109	CLA	CMD-C2D-C1D	4.97	133.48	124.73
26	a	5004	LMG	O7-C10-C11	4.97	122.23	111.48
21	B	1225	CLA	CMD-C2D-C1D	4.97	133.48	124.73
21	a	1138	CLA	CMD-C2D-C1D	4.96	133.46	124.73
21	A	1123	CLA	CMD-C2D-C1D	4.95	133.45	124.73
21	B	1207	CLA	CMD-C2D-C1D	4.95	133.45	124.73
21	2	1228	CLA	O2D-CGD-CBD	4.95	119.88	111.23
21	b	1237	CLA	CMD-C2D-C1D	4.94	133.42	124.73
21	b	1215	CLA	O2A-C1-C2	4.94	127.10	108.11
30	2	4006	ECH	C16-C15-C14	-4.93	113.44	123.52
21	A	1136	CLA	CMD-C2D-C1D	4.92	133.40	124.73
21	a	1013	CLA	CMD-C2D-C1D	4.91	133.38	124.73
21	6	1302	CLA	O2D-CGD-CBD	4.89	119.78	111.23
25	a	5005	LHG	O7-C7-C8	4.89	122.05	111.48
21	b	1225	CLA	CMD-C2D-C1D	4.88	133.33	124.73
34	7	4015	ZEX	C7-C8-C9	-4.88	119.02	126.23
21	b	1207	CLA	CMD-C2D-C1D	4.85	133.27	124.73
30	b	4011	ECH	C7-C8-C9	-4.84	119.08	126.23
30	b	4006	ECH	C33-C5-C6	-4.82	119.22	124.48
21	2	1221	CLA	O2D-CGD-CBD	4.82	119.66	111.23
26	K	5009	LMG	O7-C10-C11	4.81	121.88	111.48
21	A	1128	CLA	CMD-C2D-C1D	4.80	133.18	124.73
30	b	4006	ECH	C7-C8-C9	-4.79	119.15	126.23
21	A	1126	CLA	CMD-C2D-C1D	4.79	133.16	124.73
21	a	1011	CLA	CMD-C2D-C1D	4.78	133.15	124.73
21	1	1127	CLA	CMD-C2D-C1D	4.78	133.14	124.73
21	A	1128	CLA	O2A-C1-C2	4.76	126.42	108.11
21	a	1012	CLA	CMD-C2D-C1D	4.75	133.10	124.73
21	a	1128	CLA	CMD-C2D-C1D	4.74	133.08	124.73
30	B	4006	ECH	C33-C5-C6	-4.74	119.31	124.48
30	b	4006	ECH	C24-C23-C22	-4.73	119.23	126.23
21	b	1221	CLA	O2D-CGD-CBD	4.70	119.45	111.23
21	A	1127	CLA	CMD-C2D-C1D	4.70	133.00	124.73
34	J	4015	ZEX	C7-C8-C9	-4.68	119.31	126.23
21	1	1013	CLA	CMD-C2D-C1D	4.67	132.95	124.73
21	B	1239	CLA	O2A-C1-C2	4.66	126.05	108.11
21	B	1022	CLA	CMD-C2D-C1D	4.64	132.90	124.73
21	B	1240	CLA	O2D-CGD-CBD	4.54	119.17	111.23
30	i	4020	ECH	C15-C16-C17	-4.53	114.25	123.52
21	b	1021	CLA	CMD-C2D-C1D	4.53	132.70	124.73
36	I	4020	EQ3	C16-C17-C18	-4.53	120.93	127.28
21	b	1206	CLA	CMD-C2D-C1D	4.51	132.67	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	2002	PQN	C11-C12-C13	-4.51	119.06	126.83
30	B	4006	ECH	C20-C21-C22	-4.48	121.00	127.28
30	2	4006	ECH	C33-C5-C6	-4.48	119.60	124.48
30	2	4006	ECH	C7-C8-C9	-4.47	119.63	126.23
21	A	1138	CLA	O2A-C1-C2	4.45	125.23	108.11
21	B	1221	CLA	O2D-CGD-CBD	4.44	119.00	111.23
21	b	1239	CLA	O2A-C1-C2	4.44	125.21	108.11
21	1	1128	CLA	O2A-C1-C2	4.43	125.17	108.11
34	j	4015	ZEX	C28-C27-C26	-4.42	119.83	126.94
21	A	1135	CLA	O2A-C1-C2	4.42	125.11	108.11
26	b	5005	LMG	O7-C10-C11	4.40	120.99	111.48
21	2	1215	CLA	O2A-C1-C2	4.39	125.01	108.11
30	b	4006	ECH	C15-C14-C13	-4.38	121.14	127.28
25	A	5006	LHG	O7-C7-C8	4.37	120.94	111.48
21	a	1125	CLA	O2A-C1-C2	4.37	124.94	108.11
21	1	1129	CLA	O2D-CGD-CBD	4.37	118.87	111.23
21	2	1205	CLA	O2D-CGD-CBD	4.37	118.86	111.23
21	2	1239	CLA	O2A-C1-C2	4.37	124.91	108.11
21	2	1213	CLA	O2D-CGD-CBD	4.36	118.86	111.23
21	B	1205	CLA	O2D-CGD-CBD	4.36	118.86	111.23
21	A	1130	CLA	O2A-C1-C2	4.36	124.88	108.11
30	m	4021	ECH	C20-C21-C22	-4.36	121.17	127.28
28	h	4020	45D	C41-C37-C35	-4.35	121.18	127.28
25	1	5007	LHG	O7-C7-C8	4.34	120.88	111.48
25	1	5005	LHG	O7-C7-C8	4.34	120.87	111.48
21	B	1206	CLA	O2A-C1-C2	4.33	124.78	108.11
21	L	1501	CLA	CMD-C2D-C1D	4.31	132.32	124.73
25	a	5001	LHG	O7-C7-C8	4.31	120.80	111.48
21	2	1202	CLA	O2D-CGD-CBD	4.30	118.75	111.23
21	1	1012	CLA	O2A-C1-C2	4.30	124.66	108.11
24	B	4014	BCR	C15-C14-C13	4.29	133.29	127.28
25	B	5004	LHG	O7-C7-C8	4.29	120.75	111.48
26	A	5002	LMG	O7-C10-C11	4.28	120.75	111.48
25	l	5001	LHG	O7-C7-C8	4.27	120.73	111.48
37	L	5004	DGD	O2G-C1B-C2B	4.27	120.72	111.48
25	A	5005	LHG	O7-C7-C8	4.27	120.72	111.48
30	b	4011	ECH	C12-C13-C14	4.26	125.71	119.01
21	b	1230	CLA	O2D-CGD-CBD	4.25	118.67	111.23
21	K	1402	CLA	O2D-CGD-CBD	4.25	118.65	111.23
26	A	5008	LMG	O7-C10-C11	4.24	120.66	111.48
21	A	1107	CLA	O2A-C1-C2	4.24	124.43	108.11
21	a	1102	CLA	O2D-CGD-CBD	4.24	118.64	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1128	CLA	O2D-CGD-CBD	4.23	118.62	111.23
21	1	1132	CLA	O2A-C1-C2	4.22	124.36	108.11
26	b	5002	LMG	O7-C10-C11	4.21	120.58	111.48
30	i	4020	ECH	C10-C11-C12	-4.21	111.01	123.20
25	1	5003	LHG	O7-C7-C8	4.20	120.58	111.48
21	A	1125	CLA	O2A-C1-C2	4.20	124.29	108.11
21	2	1229	CLA	CHD-C1D-ND	-4.20	118.89	124.80
21	2	1211	CLA	O2D-CGD-CBD	4.20	118.57	111.23
30	b	4011	ECH	C24-C23-C22	-4.18	120.05	126.23
25	2	5004	LHG	O7-C7-C8	4.18	120.52	111.48
21	1	1123	CLA	O2D-CGD-CBD	4.17	118.51	111.23
21	b	1234	CLA	O2D-CGD-CBD	4.15	118.48	111.23
21	b	1212	CLA	O2D-CGD-CBD	4.15	118.48	111.23
21	B	1213	CLA	O2D-CGD-CBD	4.15	118.48	111.23
21	a	1106	CLA	O2D-CGD-CBD	4.14	118.46	111.23
25	l	5004	LHG	O7-C7-C8	4.14	120.43	111.48
30	m	4021	ECH	C7-C8-C9	-4.13	120.12	126.23
21	2	1230	CLA	O2D-CGD-CBD	4.13	118.44	111.23
25	1	5001	LHG	O7-C7-C8	4.12	120.40	111.48
25	B	5006	LHG	O7-C7-C8	4.12	120.39	111.48
21	b	1205	CLA	O2D-CGD-CBD	4.12	118.43	111.23
21	B	1234	CLA	O2A-C1-C2	4.09	123.85	108.11
21	b	1231	CLA	O2A-C1-C2	4.09	123.84	108.11
21	1	1133	CLA	O2D-CGD-CBD	4.08	118.36	111.23
21	1	1128	CLA	O2D-CGD-CBD	4.07	118.35	111.23
21	F	1302	CLA	O2D-CGD-CBD	4.07	118.34	111.23
21	1	1125	CLA	O2A-C1-C2	4.07	123.77	108.11
34	j	4015	ZEX	C31-C32-C33	-4.07	115.21	126.36
30	b	4011	ECH	C28-C27-C26	-4.07	114.99	118.64
21	A	1801	CLA	O2D-CGD-CBD	4.06	118.34	111.23
21	1	1132	CLA	O2D-CGD-CBD	4.06	118.33	111.23
25	l	5002	LHG	O7-C7-C8	4.06	120.27	111.48
21	j	1302	CLA	O2D-CGD-CBD	4.06	118.33	111.23
25	0	5004	LHG	O7-C7-C8	4.05	120.24	111.48
25	b	5004	LHG	O7-C7-C8	4.04	120.23	111.48
26	B	5005	LMG	O7-C10-C11	4.04	120.23	111.48
26	1	5002	LMG	O7-C10-C11	4.04	120.22	111.48
30	M	4021	ECH	C24-C23-C22	-4.04	120.26	126.23
28	h	4020	45D	C30-C32-C34	4.04	134.90	123.20
21	B	1230	CLA	O2D-CGD-CBD	4.04	118.28	111.23
21	A	1102	CLA	O2D-CGD-CBD	4.04	118.28	111.23
21	a	1132	CLA	O2D-CGD-CBD	4.03	118.28	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1111	CLA	O2A-C1-C2	4.03	123.62	108.11
30	M	4021	ECH	C33-C5-C6	-4.03	120.09	124.48
21	a	1013	CLA	O2D-CGD-CBD	4.02	118.27	111.23
25	a	5003	LHG	O7-C7-C8	4.02	120.18	111.48
21	B	1235	CLA	O2A-C1-C2	4.02	123.58	108.11
21	J	1303	CLA	O2D-CGD-CBD	4.02	118.26	111.23
26	a	5002	LMG	O7-C10-C11	4.01	120.16	111.48
21	L	1503	CLA	O2A-C1-C2	4.01	123.55	108.11
30	M	4021	ECH	C7-C8-C9	-4.01	120.31	126.23
21	A	1124	CLA	O2D-CGD-CBD	4.00	118.23	111.23
21	K	1401	CLA	O2D-CGD-CBD	4.00	118.23	111.23
21	b	1227	CLA	O2D-CGD-CBD	4.00	118.23	111.23
21	b	1209	CLA	O2A-C1-C2	4.00	123.50	108.11
21	b	1226	CLA	O2D-CGD-CBD	4.00	118.22	111.23
21	B	1238	CLA	C1D-ND-C4D	-4.00	103.51	106.31
21	1	1102	CLA	O2D-CGD-CBD	3.99	118.21	111.23
21	A	1120	CLA	O2A-C1-C2	3.99	123.47	108.11
28	B	4011	45D	C42-C38-C36	-3.99	121.69	127.28
21	2	1237	CLA	O2D-CGD-CBD	3.98	118.19	111.23
21	1	1113	CLA	O2D-CGD-CBD	3.98	118.19	111.23
21	A	1113	CLA	O2D-CGD-CBD	3.98	118.19	111.23
21	a	1138	CLA	O2A-C1-C2	3.98	123.41	108.11
21	2	1210	CLA	O2D-CGD-CBD	3.97	118.18	111.23
21	A	1123	CLA	O2D-CGD-CBD	3.97	118.17	111.23
21	l	1503	CLA	O2A-C1-C2	3.97	123.38	108.11
35	l	6001	LMT	O5B-C5B-C4B	3.97	116.85	109.70
24	6	4016	BCR	C40-C30-C25	-3.96	104.03	110.24
21	A	1106	CLA	O2D-CGD-CBD	3.96	118.16	111.23
21	A	1128	CLA	O2D-CGD-CBD	3.96	118.16	111.23
21	B	1213	CLA	O2A-C1-C2	3.96	123.34	108.11
21	B	1231	CLA	O2A-C1-C2	3.95	123.32	108.11
21	a	1140	CLA	O2A-C1-C2	3.95	123.31	108.11
21	2	1240	CLA	C1D-ND-C4D	-3.95	103.54	106.31
22	2	2002	PQN	C11-C12-C13	-3.95	120.03	126.83
21	A	1125	CLA	O2D-CGD-CBD	3.95	118.13	111.23
21	B	1216	CLA	O2A-C1-C2	3.95	123.29	108.11
21	A	1129	CLA	O2D-CGD-CBD	3.94	118.12	111.23
26	1	5004	LMG	O7-C10-C11	3.94	120.00	111.48
34	j	4015	ZEX	C31-C30-C29	-3.93	121.76	127.28
21	b	1225	CLA	O2A-C1-C2	3.93	123.24	108.11
30	M	4021	ECH	C20-C21-C22	-3.93	121.76	127.28
21	B	1239	CLA	O2D-CGD-CBD	3.92	118.09	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1013	CLA	O2A-C1-C2	3.92	123.20	108.11
21	a	1137	CLA	O2D-CGD-CBD	3.92	118.08	111.23
21	L	1503	CLA	O2D-CGD-CBD	3.92	118.08	111.23
21	0	1503	CLA	O2A-C1-C2	3.91	123.17	108.11
25	A	5003	LHG	O7-C7-C8	3.91	119.93	111.48
21	a	1127	CLA	O2A-C1-C2	3.90	123.13	108.11
21	1	1112	CLA	O2A-C1-C2	3.90	123.13	108.11
21	1	1106	CLA	O2D-CGD-CBD	3.90	118.05	111.23
25	a	5007	LHG	O7-C7-C8	3.90	119.92	111.48
21	B	1226	CLA	O2D-CGD-CBD	3.90	118.05	111.23
24	9	4021	BCR	C30-C25-C26	-3.90	117.31	122.64
21	j	1303	CLA	O2D-CGD-CBD	3.90	118.05	111.23
21	2	1225	CLA	O2A-C1-C2	3.90	123.11	108.11
21	b	1220	CLA	O2A-C1-C2	3.90	123.11	108.11
26	b	5007	LMG	O7-C10-C11	3.90	119.91	111.48
21	1	1105	CLA	O2D-CGD-CBD	3.90	118.04	111.23
21	1	1135	CLA	O2A-C1-C2	3.90	123.10	108.11
24	a	4003	BCR	C30-C25-C26	-3.89	117.31	122.64
21	1	1134	CLA	O2D-CGD-CBD	3.89	118.04	111.23
26	0	5001	LMG	O7-C10-C11	3.89	119.89	111.48
21	B	1227	CLA	C1D-ND-C4D	-3.89	103.58	106.31
21	1	1138	CLA	O2A-C1-C2	3.88	123.05	108.11
21	a	1121	CLA	O2D-CGD-CBD	3.88	118.01	111.23
21	1	1135	CLA	O2D-CGD-CBD	3.88	118.01	111.23
21	B	1023	CLA	O2A-C1-C2	3.87	123.02	108.11
30	m	4021	ECH	C33-C5-C6	-3.87	120.26	124.48
24	6	4016	BCR	C35-C13-C14	-3.87	116.54	122.82
21	2	1238	CLA	O2D-CGD-CBD	3.87	118.00	111.23
21	a	1129	CLA	O2D-CGD-CBD	3.87	118.00	111.23
21	l	1502	CLA	O2D-CGD-CBD	3.87	118.00	111.23
21	A	1109	CLA	O2A-C1-C2	3.87	123.00	108.11
25	A	5001	LHG	O7-C7-C8	3.87	119.85	111.48
21	a	1105	CLA	O2D-CGD-CBD	3.87	117.99	111.23
21	a	1120	CLA	O2D-CGD-CBD	3.87	117.99	111.23
21	a	1101	CLA	O2A-C1-C2	3.86	122.98	108.11
21	A	1110	CLA	O2D-CGD-CBD	3.86	117.98	111.23
21	b	1219	CLA	O2A-C1-C2	3.86	122.96	108.11
21	b	1234	CLA	O2A-C1-C2	3.86	122.95	108.11
21	a	1123	CLA	O2D-CGD-CBD	3.85	117.97	111.23
21	a	1129	CLA	O2A-C1-C2	3.85	122.94	108.11
21	a	1107	CLA	O2A-C1-C2	3.85	122.94	108.11
21	a	1122	CLA	O2A-C1-C2	3.85	122.94	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1012	CLA	O2A-C1-C2	3.85	122.93	108.11
21	2	1234	CLA	O2A-C1-C2	3.85	122.91	108.11
24	A	4008	BCR	C39-C30-C25	-3.84	104.22	110.24
21	1	1130	CLA	O2D-CGD-CBD	3.84	117.95	111.23
21	A	1116	CLA	O2D-CGD-CBD	3.84	117.95	111.23
21	2	1021	CLA	O2D-CGD-CBD	3.84	117.94	111.23
21	a	1114	CLA	O2A-C1-C2	3.84	122.88	108.11
21	K	1401	CLA	O2A-C1-C2	3.84	122.87	108.11
21	1	1110	CLA	O2D-CGD-CBD	3.83	117.93	111.23
21	l	1501	CLA	O2D-CGD-CBD	3.83	117.93	111.23
21	a	1135	CLA	O2A-C1-C2	3.83	122.85	108.11
21	1	1115	CLA	O2A-C1-C2	3.83	122.84	108.11
21	a	1012	CLA	O2D-CGD-CBD	3.83	117.92	111.23
21	a	1110	CLA	O2D-CGD-CBD	3.83	117.92	111.23
26	2	5005	LMG	O7-C10-C11	3.83	119.76	111.48
21	A	1106	CLA	O2A-C1-C2	3.82	122.82	108.11
21	1	1119	CLA	O2D-CGD-CBD	3.82	117.90	111.23
21	a	1115	CLA	O2A-C1-C2	3.82	122.79	108.11
21	2	1204	CLA	O2D-CGD-CBD	3.81	117.89	111.23
21	2	1235	CLA	O2A-C1-C2	3.81	122.78	108.11
21	a	1110	CLA	O2A-C1-C2	3.81	122.78	108.11
21	k	1401	CLA	O2A-C1-C2	3.81	122.77	108.11
24	b	4004	BCR	C39-C30-C25	-3.81	104.27	110.24
24	0	4022	BCR	C36-C18-C19	-3.81	112.27	118.09
21	A	1111	CLA	O2D-CGD-CBD	3.81	117.89	111.23
21	b	1216	CLA	O2A-C1-C2	3.81	122.76	108.11
30	b	4011	ECH	C10-C11-C12	-3.81	112.17	123.20
21	a	1126	CLA	O2A-C1-C2	3.81	122.76	108.11
21	1	1140	CLA	O2A-C1-C2	3.81	122.75	108.11
21	b	1235	CLA	O2A-C1-C2	3.81	122.75	108.11
21	B	1208	CLA	O2D-CGD-CBD	3.80	117.88	111.23
30	b	4011	ECH	C33-C5-C6	-3.80	120.34	124.48
25	l	5003	LHG	O7-C7-C8	3.80	119.70	111.48
26	A	5004	LMG	O7-C10-C11	3.80	119.70	111.48
21	A	1132	CLA	O2A-C1-C2	3.79	122.71	108.11
21	1	1012	CLA	O2D-CGD-CBD	3.79	117.86	111.23
21	B	1225	CLA	O2A-C1-C2	3.79	122.71	108.11
21	6	1301	CLA	O2D-CGD-CBD	3.79	117.86	111.23
21	A	1101	CLA	O2A-C1-C2	3.79	122.70	108.11
21	B	1222	CLA	O2D-CGD-CBD	3.79	117.85	111.23
21	b	1229	CLA	O2D-CGD-CBD	3.79	117.85	111.23
25	0	5002	LHG	O7-C7-C8	3.78	119.67	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1228	CLA	O2D-CGD-CBD	3.78	117.84	111.23
28	h	4020	45D	C23-C19-C07	-3.78	116.90	127.00
36	I	4020	EQ3	C15-C14-C13	-3.78	121.98	127.28
21	B	1227	CLA	O2D-CGD-CBD	3.78	117.84	111.23
21	a	1101	CLA	O2D-CGD-CBD	3.78	117.83	111.23
21	b	1211	CLA	O2D-CGD-CBD	3.78	117.83	111.23
21	B	1232	CLA	O2A-C1-C2	3.78	122.64	108.11
21	B	1224	CLA	O2D-CGD-CBD	3.77	117.83	111.23
30	m	4021	ECH	C15-C14-C13	-3.77	121.99	127.28
36	I	4020	EQ3	C7-C8-C9	-3.77	120.65	126.23
21	A	1140	CLA	O2D-CGD-CBD	3.77	117.83	111.23
21	B	1209	CLA	O2A-C1-C2	3.77	122.62	108.11
21	a	1105	CLA	O2A-C1-C2	3.77	122.61	108.11
21	1	1120	CLA	O2D-CGD-CBD	3.77	117.82	111.23
21	a	1120	CLA	O2A-C1-C2	3.77	122.61	108.11
21	2	1022	CLA	O2A-C1-C2	3.77	122.61	108.11
21	a	1106	CLA	O2A-C1-C2	3.77	122.61	108.11
21	2	1208	CLA	O2D-CGD-CBD	3.77	117.82	111.23
21	f	1302	CLA	O2A-C1-C2	3.76	122.59	108.11
21	A	1133	CLA	O2D-CGD-CBD	3.76	117.80	111.23
21	2	1218	CLA	O2A-C1-C2	3.76	122.57	108.11
21	l	1503	CLA	O2D-CGD-CBD	3.75	117.79	111.23
36	I	4020	EQ3	C23-C24-C25	-3.75	116.97	127.00
21	1	1116	CLA	O2A-C1-C2	3.75	122.55	108.11
24	7	4013	BCR	C38-C26-C25	-3.75	120.39	124.48
21	1	1103	CLA	O2D-CGD-CBD	3.75	117.78	111.23
21	a	1138	CLA	O2D-CGD-CBD	3.75	117.78	111.23
21	2	1216	CLA	C1D-ND-C4D	-3.74	103.69	106.31
21	J	1302	CLA	O2A-C1-C2	3.74	122.50	108.11
21	6	1301	CLA	O2A-C1-C2	3.74	121.81	108.40
21	8	1401	CLA	O2D-CGD-CBD	3.74	117.76	111.23
21	1	1801	CLA	O2A-C1-C2	3.74	122.49	108.11
21	a	1140	CLA	O2D-CGD-CBD	3.73	117.76	111.23
21	J	1302	CLA	O2D-CGD-CBD	3.73	117.75	111.23
24	0	4022	BCR	C19-C18-C17	3.73	124.88	119.01
21	2	1212	CLA	O2D-CGD-CBD	3.73	117.75	111.23
21	1	1122	CLA	O2A-C1-C2	3.73	122.45	108.11
21	A	1101	CLA	CAA-C2A-C3A	-3.73	102.93	113.00
21	b	1237	CLA	O2D-CGD-CBD	3.72	117.74	111.23
21	a	1128	CLA	O2A-C1-C2	3.72	122.44	108.11
21	1	1111	CLA	O2A-C1-C2	3.72	122.44	108.11
21	A	1120	CLA	O2D-CGD-CBD	3.72	117.74	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1112	CLA	O2A-C1-C2	3.72	122.42	108.11
21	b	1202	CLA	O2D-CGD-CBD	3.72	117.73	111.23
21	b	1206	CLA	O2A-C1-C2	3.72	122.42	108.11
21	A	1104	CLA	O2A-C1-C2	3.72	122.41	108.11
21	1	1101	CLA	O2D-CGD-CBD	3.72	117.73	111.23
26	B	5002	LMG	O7-C10-C11	3.72	119.52	111.48
21	A	1105	CLA	O2D-CGD-CBD	3.71	117.72	111.23
21	a	1119	CLA	O2D-CGD-CBD	3.71	117.72	111.23
21	B	1204	CLA	O2D-CGD-CBD	3.71	117.72	111.23
21	B	1234	CLA	O2D-CGD-CBD	3.71	117.72	111.23
21	B	1236	CLA	O2A-C1-C2	3.71	122.38	108.11
21	B	1021	CLA	O2D-CGD-CBD	3.71	117.71	111.23
21	1	1102	CLA	O2A-C1-C2	3.71	122.38	108.11
21	A	1109	CLA	O2D-CGD-CBD	3.71	117.71	111.23
21	0	1502	CLA	O2A-C1-C2	3.70	122.36	108.11
36	I	4020	EQ3	C8-C7-C6	-3.70	117.11	127.00
21	B	1206	CLA	O2D-CGD-CBD	3.70	117.70	111.23
21	a	1012	CLA	O2A-C1-C2	3.70	122.35	108.11
21	2	1216	CLA	O2D-CGD-CBD	3.70	117.70	111.23
21	A	1115	CLA	O2A-C1-C2	3.70	122.34	108.11
21	A	1101	CLA	O2D-CGD-CBD	3.70	117.69	111.23
21	b	1239	CLA	O2D-CGD-CBD	3.70	117.69	111.23
21	j	1303	CLA	O2A-C1-C2	3.69	122.32	108.11
21	A	1126	CLA	O2D-CGD-CBD	3.69	117.68	111.23
21	a	1108	CLA	O2D-CGD-CBD	3.69	117.68	111.23
21	l	1502	CLA	O2A-C1-C2	3.69	122.31	108.11
21	A	1132	CLA	O2D-CGD-CBD	3.69	117.68	111.23
21	a	1112	CLA	O2A-C1-C2	3.69	122.30	108.11
25	F	5002	LHG	O7-C7-C8	3.69	119.46	111.48
21	A	1013	CLA	O2A-C1-C2	3.69	122.30	108.11
21	2	1206	CLA	O2A-C1-C2	3.69	122.29	108.11
21	a	1116	CLA	O2D-CGD-CBD	3.68	117.67	111.23
21	A	1126	CLA	O2A-C1-C2	3.68	122.28	108.11
21	b	1219	CLA	O2D-CGD-CBD	3.68	117.67	111.23
21	B	1234	CLA	C1D-ND-C4D	-3.68	103.73	106.31
21	a	1114	CLA	O2D-CGD-CBD	3.68	117.66	111.23
21	l	1503	CLA	C1D-ND-C4D	-3.67	103.73	106.31
21	2	1213	CLA	O2A-C1-C2	3.67	122.24	108.11
21	1	1129	CLA	O2A-C1-C2	3.67	122.23	108.11
28	B	4011	45D	C05-C03-C07	3.67	115.77	110.44
35	0	6001	LMT	C3'-C4'-C5'	-3.67	102.80	110.93
21	B	1219	CLA	O2A-C1-C2	3.66	122.21	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1222	CLA	O2A-C1-C2	3.66	122.21	108.11
30	B	4006	ECH	C20-C19-C18	-3.66	116.32	126.36
21	b	1229	CLA	C1D-ND-C4D	-3.66	103.74	106.31
21	1	1139	CLA	O2D-CGD-CBD	3.66	117.63	111.23
21	b	1213	CLA	O2A-C1-C2	3.66	122.20	108.11
21	1	1140	CLA	O2D-CGD-CBD	3.66	117.63	111.23
21	1	1120	CLA	O2A-C1-C2	3.66	122.19	108.11
21	b	1205	CLA	C1D-ND-C4D	-3.66	103.75	106.31
21	a	1101	CLA	CAA-C2A-C3A	-3.66	103.12	113.00
21	B	1240	CLA	O2A-C1-C2	3.65	122.17	108.11
21	b	1203	CLA	O2A-C1-C2	3.65	122.17	108.11
21	F	1302	CLA	O2A-C1-C2	3.65	122.16	108.11
21	2	1205	CLA	O2A-C1-C2	3.65	122.16	108.11
24	2	4018	BCR	C38-C26-C25	-3.65	120.50	124.48
21	b	1209	CLA	O2D-CGD-CBD	3.65	117.61	111.23
21	b	1236	CLA	O2A-C1-C2	3.65	122.14	108.11
21	2	1214	CLA	O2A-C1-C2	3.65	122.14	108.11
21	l	1502	CLA	C1D-ND-C4D	-3.64	103.75	106.31
21	a	1137	CLA	O2A-C1-C2	3.64	122.13	108.11
21	a	1113	CLA	O2A-C1-C2	3.64	122.13	108.11
21	A	1134	CLA	O2A-C1-C2	3.64	122.12	108.11
21	A	1012	CLA	O2D-CGD-CBD	3.64	117.60	111.23
26	2	5002	LMG	O7-C10-C11	3.64	119.36	111.48
24	B	4005	BCR	C38-C26-C25	-3.64	120.51	124.48
21	a	1131	CLA	O2D-CGD-CBD	3.64	117.59	111.23
21	b	1231	CLA	O2D-CGD-CBD	3.64	117.59	111.23
21	1	1107	CLA	O2A-C1-C2	3.64	122.11	108.11
21	b	1240	CLA	O2A-C1-C2	3.64	122.11	108.11
21	B	1219	CLA	O2D-CGD-CBD	3.64	117.59	111.23
21	1	1105	CLA	O2A-C1-C2	3.64	122.10	108.11
21	2	1023	CLA	O2A-C1-C2	3.64	122.10	108.11
21	a	1113	CLA	O2D-CGD-CBD	3.64	117.59	111.23
21	1	1119	CLA	O2A-C1-C2	3.63	122.09	108.11
30	2	4006	ECH	C19-C18-C17	3.63	124.72	119.01
21	b	1023	CLA	O2A-C1-C2	3.63	122.08	108.11
21	1	1139	CLA	O2A-C1-C2	3.63	122.08	108.11
30	i	4020	ECH	C33-C5-C6	-3.63	120.53	124.48
21	1	1101	CLA	O2A-C1-C2	3.63	122.06	108.11
28	B	4011	45D	C21-C15-C17	3.62	120.98	115.49
21	B	1211	CLA	O2D-CGD-CBD	3.62	117.56	111.23
21	1	1116	CLA	O2D-CGD-CBD	3.62	117.56	111.23
24	A	4002	BCR	C15-C14-C13	3.62	132.36	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1133	CLA	O2A-C1-C2	3.62	122.04	108.11
21	a	1133	CLA	O2D-CGD-CBD	3.62	117.56	111.23
21	B	1217	CLA	O2D-CGD-CBD	3.62	117.56	111.23
24	j	4013	BCR	C38-C26-C25	-3.62	120.53	124.48
21	0	1501	CLA	O2A-C1-C2	3.62	122.04	108.11
21	f	1301	CLA	O2A-C1-C2	3.62	122.04	108.11
21	b	1214	CLA	O2D-CGD-CBD	3.62	117.56	111.23
21	1	1112	CLA	O2D-CGD-CBD	3.62	117.56	111.23
28	h	4020	45D	C28-C26-C30	3.62	128.67	122.82
21	2	1237	CLA	O2A-C1-C2	3.61	122.02	108.11
21	1	1133	CLA	O2A-C1-C2	3.61	122.02	108.11
21	a	1127	CLA	O2D-CGD-CBD	3.61	117.55	111.23
21	b	1217	CLA	O2D-CGD-CBD	3.61	117.55	111.23
21	A	1130	CLA	O2D-CGD-CBD	3.61	117.54	111.23
24	f	4016	BCR	C35-C13-C14	-3.61	116.97	122.82
21	B	1229	CLA	O2D-CGD-CBD	3.61	117.54	111.23
21	a	1134	CLA	O2D-CGD-CBD	3.60	117.53	111.23
24	A	4008	BCR	C15-C14-C13	3.60	132.33	127.28
21	b	1222	CLA	O2D-CGD-CBD	3.60	117.53	111.23
21	2	1214	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	a	4019	BCR	C15-C14-C13	-3.60	122.23	127.28
21	1	1801	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	2	4014	BCR	C15-C14-C13	3.60	132.32	127.28
21	A	1013	CLA	O2D-CGD-CBD	3.60	117.52	111.23
21	2	1230	CLA	O2A-C1-C2	3.60	121.30	108.40
21	A	1129	CLA	O2A-C1-C2	3.59	121.94	108.11
21	L	1502	CLA	O2D-CGD-CBD	3.59	117.51	111.23
21	0	1501	CLA	O2D-CGD-CBD	3.59	117.51	111.23
21	L	1501	CLA	O2A-C1-C2	3.59	121.92	108.11
21	B	1212	CLA	O2D-CGD-CBD	3.59	117.50	111.23
21	b	1208	CLA	O2D-CGD-CBD	3.59	117.50	111.23
21	A	1119	CLA	O2A-C1-C2	3.58	121.90	108.11
21	b	1204	CLA	O2D-CGD-CBD	3.58	117.50	111.23
21	A	1131	CLA	O2A-C1-C2	3.58	121.90	108.11
21	1	1108	CLA	O2D-CGD-CBD	3.58	117.49	111.23
21	b	1237	CLA	O2A-C1-C2	3.58	121.88	108.11
21	B	1231	CLA	O2D-CGD-CBD	3.58	117.48	111.23
21	A	1117	CLA	O2D-CGD-CBD	3.58	117.48	111.23
21	2	1219	CLA	O2D-CGD-CBD	3.58	117.48	111.23
21	A	1119	CLA	O2D-CGD-CBD	3.58	117.48	111.23
21	b	1205	CLA	O2A-C1-C2	3.57	121.86	108.11
21	2	1221	CLA	O2A-C1-C2	3.57	121.86	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	4013	BCR	C38-C26-C25	-3.57	120.58	124.48
21	2	1215	CLA	O2D-CGD-CBD	3.57	117.47	111.23
21	b	1240	CLA	O2D-CGD-CBD	3.57	117.47	111.23
21	0	1502	CLA	O2D-CGD-CBD	3.57	117.47	111.23
21	A	1118	CLA	O2A-C1-C2	3.57	121.84	108.11
21	2	1202	CLA	O2A-C1-C2	3.57	121.84	108.11
24	2	4011	BCR	C15-C14-C13	3.57	132.28	127.28
34	F	4016	ZEX	C7-C8-C9	-3.57	120.96	126.23
21	A	1114	CLA	O2A-C1-C2	3.56	121.83	108.11
21	a	1135	CLA	O2D-CGD-CBD	3.56	117.46	111.23
30	b	4011	ECH	C35-C13-C12	-3.56	112.64	118.09
21	B	1223	CLA	O2A-C1-C2	3.56	121.82	108.11
21	1	1138	CLA	O2D-CGD-CBD	3.56	117.46	111.23
21	b	1218	CLA	O2A-C1-C2	3.56	121.81	108.11
21	2	1226	CLA	O2D-CGD-CBD	3.56	117.46	111.23
21	2	1201	CLA	O2D-CGD-CBD	3.56	117.45	111.23
30	B	4006	ECH	C28-C27-C26	-3.56	115.45	118.64
24	A	4003	BCR	C1-C6-C5	-3.56	117.77	122.64
21	L	1502	CLA	O2A-C1-C2	3.56	121.80	108.11
21	b	1232	CLA	O2A-C1-C2	3.56	121.80	108.11
21	1	1107	CLA	O2D-CGD-CBD	3.56	117.45	111.23
21	A	1011	CLA	CHD-C1D-ND	-3.56	119.80	124.80
26	a	5004	LMG	O1-C1-C2	3.56	113.67	108.27
21	B	1208	CLA	O2A-C1-C2	3.55	121.79	108.11
21	F	1301	CLA	O2A-C1-C2	3.55	121.79	108.11
21	B	1212	CLA	O2A-C1-C2	3.55	121.78	108.11
21	2	1203	CLA	O2D-CGD-CBD	3.55	117.44	111.23
21	2	1217	CLA	O2A-C1-C2	3.55	121.77	108.11
21	a	1104	CLA	O2D-CGD-CBD	3.55	117.44	111.23
21	a	1125	CLA	O2D-CGD-CBD	3.55	117.44	111.23
21	a	1111	CLA	O2D-CGD-CBD	3.55	117.43	111.23
21	A	1121	CLA	O2A-C1-C2	3.54	121.75	108.11
21	1	1137	CLA	O2A-C1-C2	3.54	121.74	108.11
21	A	1140	CLA	O2A-C1-C2	3.54	121.74	108.11
21	a	1102	CLA	O2A-C1-C2	3.54	121.73	108.11
21	A	1801	CLA	O2A-C1-C2	3.54	121.73	108.11
21	a	1116	CLA	O2A-C1-C2	3.54	121.72	108.11
21	B	1225	CLA	C1D-ND-C4D	-3.54	103.83	106.31
21	a	1118	CLA	O2D-CGD-CBD	3.54	117.41	111.23
21	B	1218	CLA	O2A-C1-C2	3.54	121.72	108.11
30	i	4020	ECH	C12-C13-C14	3.54	124.57	119.01
21	A	1123	CLA	O2A-C1-C2	3.54	121.71	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	4011	45D	C23-C19-C07	-3.53	117.56	127.00
21	f	1301	CLA	O2D-CGD-CBD	3.53	117.40	111.23
21	7	1302	CLA	O2D-CGD-CBD	3.53	117.40	111.23
21	j	1302	CLA	CMA-C3A-C4A	3.53	121.26	111.77
21	2	1226	CLA	O2A-C1-C2	3.53	121.69	108.11
21	2	1217	CLA	O2D-CGD-CBD	3.53	117.40	111.23
21	A	1107	CLA	O2D-CGD-CBD	3.53	117.40	111.23
21	b	1228	CLA	O2A-C1-C2	3.53	121.68	108.11
21	a	1124	CLA	O2A-C1-C2	3.53	121.68	108.11
21	a	1132	CLA	O2A-C1-C2	3.52	121.67	108.11
21	b	1210	CLA	O2D-CGD-CBD	3.52	117.39	111.23
21	1	1124	CLA	O2D-CGD-CBD	3.52	117.39	111.23
30	b	4011	ECH	C15-C16-C17	-3.52	116.31	123.52
21	1	1126	CLA	O2A-C1-C2	3.52	121.66	108.11
21	b	1213	CLA	O2D-CGD-CBD	3.52	117.38	111.23
24	2	4005	BCR	C40-C30-C25	-3.52	104.72	110.24
21	J	1303	CLA	O2A-C1-C2	3.52	121.65	108.11
21	a	1121	CLA	O2A-C1-C2	3.52	121.64	108.11
21	1	1101	CLA	CAA-C2A-C3A	-3.52	103.50	113.00
21	2	1022	CLA	O2D-CGD-CBD	3.52	117.38	111.23
21	a	1115	CLA	O2D-CGD-CBD	3.51	117.37	111.23
24	8	4001	BCR	C40-C30-C25	-3.51	104.73	110.24
21	A	1137	CLA	O2D-CGD-CBD	3.51	117.37	111.23
21	a	1108	CLA	O2A-C1-C2	3.51	121.62	108.11
21	0	1503	CLA	O2D-CGD-CBD	3.51	117.37	111.23
21	A	1126	CLA	C1D-ND-C4D	-3.51	103.85	106.31
21	1	1126	CLA	O2D-CGD-CBD	3.51	117.36	111.23
24	b	4004	BCR	C30-C25-C24	3.51	125.17	115.65
21	B	1202	CLA	O2D-CGD-CBD	3.51	117.36	111.23
21	B	1229	CLA	CHD-C1D-ND	-3.51	119.87	124.80
21	b	1203	CLA	O2D-CGD-CBD	3.50	117.36	111.23
30	2	4006	ECH	C28-C27-C26	-3.50	115.50	118.64
25	L	5005	LHG	O7-C7-C8	3.50	119.06	111.48
21	2	1203	CLA	O2A-C1-C2	3.50	121.58	108.11
21	B	1229	CLA	C1D-ND-C4D	-3.50	103.86	106.31
21	a	1103	CLA	O2D-CGD-CBD	3.50	117.35	111.23
21	B	1235	CLA	O2D-CGD-CBD	3.50	117.35	111.23
21	1	1117	CLA	O2A-C1-C2	3.50	121.57	108.11
21	A	1131	CLA	O2D-CGD-CBD	3.50	117.35	111.23
21	2	1236	CLA	O2A-C1-C2	3.50	121.57	108.11
21	A	1115	CLA	O2D-CGD-CBD	3.50	117.34	111.23
21	2	1223	CLA	O2A-C1-C2	3.50	121.56	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1219	CLA	C1D-ND-C4D	-3.49	103.86	106.31
21	2	1218	CLA	O2D-CGD-CBD	3.49	117.33	111.23
21	b	1202	CLA	CHD-C1D-ND	-3.49	119.89	124.80
21	1	1130	CLA	O2A-C1-C2	3.49	121.53	108.11
21	B	1216	CLA	O2D-CGD-CBD	3.49	117.33	111.23
21	1	1127	CLA	O2A-C1-C2	3.49	121.53	108.11
21	1	1109	CLA	O2A-C1-C2	3.49	121.53	108.11
21	1	1134	CLA	O2A-C1-C2	3.49	121.53	108.11
21	B	1220	CLA	O2A-C1-C2	3.48	121.52	108.11
21	a	1126	CLA	O2D-CGD-CBD	3.48	117.32	111.23
21	1	1011	CLA	O2A-C1-C2	3.48	121.51	108.11
21	1	1013	CLA	O2D-CGD-CBD	3.48	117.31	111.23
21	a	1112	CLA	O2D-CGD-CBD	3.47	117.30	111.23
21	f	1302	CLA	O2D-CGD-CBD	3.47	117.30	111.23
21	B	1224	CLA	O2A-C1-C2	3.47	121.48	108.11
21	1	1110	CLA	O2A-C1-C2	3.47	121.47	108.11
21	2	1231	CLA	O2D-CGD-CBD	3.47	117.30	111.23
24	L	4019	BCR	C15-C14-C13	3.47	132.14	127.28
21	1	1121	CLA	O2A-C1-C2	3.47	121.45	108.11
21	b	1215	CLA	C1-O2A-CGA	3.47	125.05	116.65
21	F	1301	CLA	O2D-CGD-CBD	3.46	117.28	111.23
21	B	1218	CLA	O2D-CGD-CBD	3.46	117.28	111.23
21	2	1240	CLA	O2D-CGD-CBD	3.46	117.28	111.23
21	a	1139	CLA	O2A-C1-C2	3.46	121.43	108.11
21	a	1115	CLA	C1D-ND-C4D	-3.46	103.89	106.31
21	B	1022	CLA	O2A-C1-C2	3.46	121.42	108.11
21	A	1103	CLA	O2D-CGD-CBD	3.46	117.28	111.23
24	L	4019	BCR	C40-C30-C25	-3.46	104.82	110.24
21	a	1126	CLA	C1D-ND-C4D	-3.45	103.89	106.31
21	1	1125	CLA	O2D-CGD-CBD	3.45	117.27	111.23
21	2	1229	CLA	O2D-CGD-CBD	3.45	117.27	111.23
21	b	1232	CLA	O2D-CGD-CBD	3.45	117.26	111.23
21	7	1303	CLA	O2D-CGD-CBD	3.45	117.26	111.23
21	0	1502	CLA	C1D-ND-C4D	-3.45	103.89	106.31
30	2	4006	ECH	C21-C20-C19	-3.45	113.21	123.20
21	2	1224	CLA	O2A-C1-C2	3.45	121.38	108.11
21	b	1229	CLA	CHD-C1D-ND	-3.45	119.95	124.80
21	2	1209	CLA	O2D-CGD-CBD	3.44	117.25	111.23
21	1	1136	CLA	O2D-CGD-CBD	3.44	117.25	111.23
21	a	1130	CLA	O2A-C1-C2	3.44	121.34	108.11
21	b	1211	CLA	C1D-ND-C4D	-3.43	103.90	106.31
21	1	1104	CLA	O2D-CGD-CBD	3.43	117.23	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	4019	BCR	C40-C30-C25	-3.43	104.86	110.24
21	B	1205	CLA	C1D-ND-C4D	-3.43	103.91	106.31
24	2	4004	BCR	C40-C30-C25	-3.43	104.87	110.24
26	K	5009	LMG	C1-C2-C3	3.43	117.22	110.01
21	b	1222	CLA	O2A-C1-C2	3.43	121.29	108.11
21	1	1131	CLA	O2D-CGD-CBD	3.42	117.21	111.23
21	A	1108	CLA	O2A-C1-C2	3.42	121.28	108.11
21	a	1133	CLA	C1D-ND-C4D	-3.42	103.91	106.31
21	B	1223	CLA	O2D-CGD-CBD	3.42	117.21	111.23
21	2	1210	CLA	O2A-C1-C2	3.42	121.28	108.11
21	B	1215	CLA	O2D-CGD-CBD	3.42	117.21	111.23
21	B	1230	CLA	C1D-ND-C4D	-3.42	103.91	106.31
21	B	1203	CLA	O2D-CGD-CBD	3.42	117.21	111.23
24	a	4002	BCR	C40-C30-C25	-3.42	104.88	110.24
21	B	1210	CLA	O2D-CGD-CBD	3.42	117.20	111.23
21	1	1115	CLA	O2D-CGD-CBD	3.42	117.20	111.23
30	B	4006	ECH	C11-C12-C13	-3.42	117.00	126.36
24	a	4007	BCR	C40-C30-C25	-3.42	104.89	110.24
21	b	1222	CLA	C1D-ND-C4D	-3.41	103.92	106.31
21	a	1109	CLA	O2D-CGD-CBD	3.41	117.20	111.23
21	b	1215	CLA	O2D-CGD-CBD	3.41	117.19	111.23
21	1	1136	CLA	O2A-C1-C2	3.41	121.22	108.11
21	A	1139	CLA	O2D-CGD-CBD	3.41	117.18	111.23
21	2	1227	CLA	O2D-CGD-CBD	3.40	117.18	111.23
30	i	4020	ECH	C20-C21-C22	-3.40	122.50	127.28
21	a	1135	CLA	CHD-C1D-ND	-3.40	120.01	124.80
21	b	1230	CLA	C1D-ND-C4D	-3.40	103.92	106.31
21	B	1205	CLA	O2A-C1-C2	3.40	121.20	108.11
21	B	1217	CLA	O2A-C1-C2	3.40	121.19	108.11
21	b	1223	CLA	O2A-C1-C2	3.40	121.19	108.11
21	B	1226	CLA	O2A-C1-C2	3.40	121.18	108.11
21	2	1220	CLA	O2D-CGD-CBD	3.40	117.17	111.23
21	B	1225	CLA	O2D-CGD-CBD	3.40	117.17	111.23
21	b	1209	CLA	C1D-ND-C4D	-3.40	103.93	106.31
21	a	1104	CLA	O2A-C1-C2	3.40	121.17	108.11
21	A	1113	CLA	O2A-C1-C2	3.39	121.17	108.11
21	1	1114	CLA	O2D-CGD-CBD	3.39	117.16	111.23
21	b	1023	CLA	CHD-C1D-ND	-3.39	120.03	124.80
30	M	4021	ECH	C16-C17-C18	-3.39	122.52	127.28
21	1	1134	CLA	C1D-ND-C4D	-3.39	103.93	106.31
30	B	4006	ECH	C7-C8-C9	-3.39	121.22	126.23
21	1	1115	CLA	C1D-ND-C4D	-3.39	103.94	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1239	CLA	O2D-CGD-CBD	3.38	117.15	111.23
21	1	1118	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	1	1127	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	B	1212	CLA	C1D-ND-C4D	-3.38	103.94	106.31
21	b	1022	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	a	1111	CLA	O2A-C1-C2	3.38	121.11	108.11
21	B	1222	CLA	O2A-C1-C2	3.38	121.11	108.11
21	a	1801	CLA	O2D-CGD-CBD	3.38	117.14	111.23
30	b	4011	ECH	C20-C19-C18	-3.38	117.10	126.36
21	A	1112	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	8	1402	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	1	1103	CLA	O2A-C1-C2	3.38	121.10	108.11
30	M	4021	ECH	C15-C14-C13	-3.37	122.55	127.28
21	A	1103	CLA	O2A-C1-C2	3.37	121.09	108.11
21	2	1234	CLA	C1D-ND-C4D	-3.37	103.95	106.31
21	A	1129	CLA	C1D-ND-C4D	-3.37	103.95	106.31
21	B	1232	CLA	O2D-CGD-CBD	3.37	117.12	111.23
21	L	1501	CLA	O2D-CGD-CBD	3.37	117.12	111.23
21	a	1131	CLA	O2A-C1-C2	3.37	121.06	108.11
21	A	1117	CLA	CMA-C3A-C4A	3.37	120.82	111.77
21	A	1134	CLA	O2D-CGD-CBD	3.37	117.11	111.23
21	1	1121	CLA	O2D-CGD-CBD	3.36	117.11	111.23
21	B	1237	CLA	C1D-ND-C4D	-3.36	103.95	106.31
21	B	1235	CLA	C1D-ND-C4D	-3.36	103.95	106.31
21	2	1236	CLA	C1D-ND-C4D	-3.36	103.95	106.31
21	a	1124	CLA	O2D-CGD-CBD	3.36	117.10	111.23
21	b	1235	CLA	O2D-CGD-CBD	3.36	117.10	111.23
21	a	1124	CLA	C1D-ND-C4D	-3.36	103.96	106.31
21	1	1104	CLA	O2A-C1-C2	3.35	121.02	108.11
21	a	1136	CLA	O2A-C1-C2	3.35	121.01	108.11
21	1	1123	CLA	O2A-C1-C2	3.35	121.01	108.11
21	2	1225	CLA	O2D-CGD-CBD	3.35	117.09	111.23
24	b	4017	BCR	C39-C30-C25	-3.35	104.99	110.24
22	b	2002	PQN	C14-C13-C15	3.35	121.04	115.23
21	2	1211	CLA	O2A-C1-C2	3.35	120.98	108.11
21	1	1137	CLA	O2D-CGD-CBD	3.34	117.08	111.23
24	b	4005	BCR	C40-C30-C25	-3.34	105.00	110.24
21	A	1133	CLA	O2A-C1-C2	3.34	120.97	108.11
21	B	1201	CLA	O2A-C1-C2	3.34	120.97	108.11
21	A	1120	CLA	C1D-ND-C4D	-3.34	103.97	106.31
21	A	1121	CLA	C1D-ND-C4D	-3.34	103.97	106.31
21	2	1219	CLA	C1D-ND-C4D	-3.34	103.97	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1102	CLA	O2A-C1-C2	3.34	120.97	108.11
28	h	4020	45D	C34-C36-C38	3.34	124.26	119.01
21	a	1139	CLA	O2D-CGD-CBD	3.34	117.07	111.23
21	k	1402	CLA	C1D-ND-C4D	-3.34	103.97	106.31
21	l	1501	CLA	O2A-C1-C2	3.34	120.95	108.11
21	a	1130	CLA	O2D-CGD-CBD	3.34	117.06	111.23
21	A	1104	CLA	O2D-CGD-CBD	3.34	117.06	111.23
24	a	4012	BCR	C39-C30-C25	-3.34	105.01	110.24
21	B	1229	CLA	C2D-C1D-ND	3.33	113.42	110.13
21	2	1208	CLA	O2A-C1-C2	3.33	120.92	108.11
24	a	4001	BCR	C30-C25-C26	-3.33	118.09	122.64
21	a	1119	CLA	O2A-C1-C2	3.32	120.90	108.11
21	2	1229	CLA	C1D-ND-C4D	-3.32	103.98	106.31
21	A	1114	CLA	O2D-CGD-CBD	3.32	117.04	111.23
21	a	1107	CLA	O2D-CGD-CBD	3.32	117.04	111.23
21	2	1223	CLA	O2D-CGD-CBD	3.32	117.04	111.23
24	f	4016	BCR	C40-C30-C25	-3.32	105.03	110.24
22	A	2001	PQN	C14-C13-C15	3.32	120.99	115.23
21	B	1204	CLA	O2A-C1-C2	3.32	120.88	108.11
21	A	1130	CLA	O2A-CGA-CBA	3.32	121.95	111.83
24	1	4002	BCR	C38-C26-C25	-3.32	120.86	124.48
21	2	1219	CLA	O2A-C1-C2	3.32	120.87	108.11
21	B	1236	CLA	O2D-CGD-CBD	3.32	117.03	111.23
21	B	1221	CLA	O2A-C1-C2	3.32	120.87	108.11
21	A	1105	CLA	O2A-C1-C2	3.31	120.86	108.11
21	1	1801	CLA	C1D-ND-C4D	-3.31	103.99	106.31
21	B	1220	CLA	O2D-CGD-CBD	3.31	117.02	111.23
24	h	4018	BCR	C40-C30-C25	-3.31	105.05	110.24
21	2	1226	CLA	C3B-C4B-NB	-3.31	107.58	110.53
21	2	1239	CLA	C1D-ND-C4D	-3.31	103.99	106.31
30	b	4006	ECH	C21-C20-C19	3.30	132.78	123.20
21	A	1120	CLA	CHD-C1D-ND	-3.30	120.15	124.80
21	b	1221	CLA	O2A-C1-C2	3.30	120.82	108.11
25	l	5002	LHG	C5-O7-C7	-3.30	109.89	117.80
21	2	1222	CLA	O2D-CGD-CBD	3.30	117.00	111.23
21	1	1131	CLA	C1D-ND-C4D	-3.30	104.00	106.31
21	2	1229	CLA	O2A-C1-C2	3.30	120.81	108.11
26	b	5007	LMG	O1-C1-C2	3.30	113.29	108.27
21	a	1117	CLA	O2D-CGD-CBD	3.30	117.00	111.23
24	A	4002	BCR	C40-C30-C25	-3.30	105.07	110.24
21	K	1402	CLA	C1D-ND-C4D	-3.30	104.00	106.31
21	b	1214	CLA	O2A-C1-C2	3.30	120.79	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1202	CLA	CHD-C1D-ND	-3.30	120.17	124.80
21	2	1210	CLA	C1D-ND-C4D	-3.30	104.00	106.31
21	b	1206	CLA	O2D-CGD-CBD	3.29	116.99	111.23
21	2	1238	CLA	O2A-C1-C2	3.29	120.78	108.11
21	A	1137	CLA	O2A-C1-C2	3.29	120.78	108.11
21	a	1117	CLA	O2A-C1-C2	3.29	120.78	108.11
21	1	1118	CLA	O2A-C1-C2	3.29	120.78	108.11
21	b	1236	CLA	O2D-CGD-CBD	3.29	116.98	111.23
21	b	1021	CLA	O2D-CGD-CBD	3.29	116.98	111.23
21	A	1128	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
21	B	1229	CLA	O2A-C1-C2	3.29	120.75	108.11
21	2	1023	CLA	CHD-C1D-ND	-3.28	120.18	124.80
21	a	1103	CLA	O2A-C1-C2	3.28	120.74	108.11
24	B	4005	BCR	C40-C30-C25	-3.28	105.10	110.24
21	1	1109	CLA	O2D-CGD-CBD	3.28	116.97	111.23
21	A	1127	CLA	O2A-C1-C2	3.28	120.72	108.11
30	i	4020	ECH	C23-C24-C25	-3.28	118.24	127.00
21	b	1212	CLA	O2A-C1-C2	3.28	120.72	108.11
21	K	1402	CLA	CHD-C1D-ND	-3.28	120.19	124.80
21	A	1108	CLA	C1D-ND-C4D	-3.27	104.02	106.31
21	a	1123	CLA	CMA-C3A-C4A	3.27	120.56	111.77
21	A	1801	CLA	C1D-ND-C4D	-3.27	104.02	106.31
26	0	5001	LMG	O6-C5-C4	3.27	115.59	109.70
21	k	1402	CLA	O2D-CGD-CBD	3.26	116.94	111.23
21	1	1105	CLA	C1D-ND-C4D	-3.26	104.02	106.31
21	1	1109	CLA	CMA-C3A-C4A	3.26	120.54	111.77
21	1	1106	CLA	O2A-C1-C2	3.26	120.66	108.11
21	b	1235	CLA	C1D-ND-C4D	-3.26	104.03	106.31
21	1	1136	CLA	C1D-ND-C4D	-3.26	104.03	106.31
21	B	1237	CLA	O2D-CGD-CBD	3.26	116.92	111.23
21	1	1117	CLA	CMA-C3A-C4A	3.26	120.52	111.77
30	m	4021	ECH	C24-C23-C22	-3.26	121.42	126.23
21	2	1207	CLA	CHD-C1D-ND	-3.25	120.22	124.80
21	a	1120	CLA	C1D-ND-C4D	-3.25	104.03	106.31
21	A	1122	CLA	O2A-C1-C2	3.25	120.63	108.11
34	7	4015	ZEX	C31-C32-C33	-3.25	117.44	126.36
21	B	1211	CLA	O2A-C1-C2	3.25	120.62	108.11
25	A	5001	LHG	O8-C23-C24	3.25	121.75	111.83
21	a	1120	CLA	CMA-C3A-C4A	3.25	120.51	111.77
21	L	1503	CLA	C1D-ND-C4D	-3.25	104.03	106.31
21	0	1502	CLA	CMA-C3A-C4A	3.25	120.50	111.77
22	A	2001	PQN	C11-C12-C13	-3.25	121.24	126.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1011	CLA	CHA-C1A-NA	-3.25	119.04	126.39
21	2	1224	CLA	O2D-CGD-CBD	3.24	116.90	111.23
21	a	1116	CLA	CHD-C1D-ND	-3.24	120.24	124.80
21	2	1204	CLA	C1D-ND-C4D	-3.24	104.04	106.31
21	b	1229	CLA	O2A-C1-C2	3.24	120.58	108.11
35	l	6001	LMT	C3'-C4'-C5'	-3.24	103.75	110.93
21	2	1201	CLA	O2A-C1-C2	3.24	120.57	108.11
34	J	4015	ZEX	C31-C32-C33	-3.23	117.50	126.36
24	1	4002	BCR	C40-C30-C25	-3.23	105.17	110.24
21	b	1202	CLA	O2A-C1-C2	3.23	120.55	108.11
21	b	1207	CLA	C1-O2A-CGA	3.23	124.47	116.65
21	1	1136	CLA	C3B-C4B-NB	-3.23	107.65	110.53
21	a	1109	CLA	CMA-C3A-C4A	3.23	120.45	111.77
21	B	1227	CLA	O2A-C1-C2	3.23	120.53	108.11
30	m	4021	ECH	C16-C17-C18	-3.23	122.75	127.28
21	A	1103	CLA	CHD-C1D-ND	-3.23	120.26	124.80
21	2	1240	CLA	CMA-C3A-C4A	3.23	120.44	111.77
21	1	1124	CLA	O2A-C1-C2	3.22	120.51	108.11
24	b	4005	BCR	C38-C26-C25	-3.22	120.97	124.48
21	B	1231	CLA	CHD-C1D-ND	-3.22	120.27	124.80
21	1	1122	CLA	O2D-CGD-CBD	3.22	116.86	111.23
21	B	1210	CLA	O2A-C1-C2	3.22	120.50	108.11
24	f	4016	BCR	C2-C1-C6	3.22	115.11	110.44
22	1	2001	PQN	C14-C13-C15	3.22	120.81	115.23
21	a	1108	CLA	CMA-C3A-C4A	3.22	120.42	111.77
21	a	1136	CLA	CMA-C3A-C4A	3.22	120.42	111.77
24	f	4016	BCR	C15-C14-C13	3.22	131.79	127.28
21	2	1218	CLA	C1D-ND-C4D	-3.21	104.06	106.31
21	B	1021	CLA	O2A-C1-C2	3.21	120.47	108.11
21	L	1502	CLA	C1D-ND-C4D	-3.21	104.06	106.31
21	1	1012	CLA	C1D-ND-C4D	-3.21	104.06	106.31
21	2	1207	CLA	O2D-CGD-CBD	3.21	116.85	111.23
21	a	1109	CLA	O2A-C1-C2	3.21	120.47	108.11
21	a	1801	CLA	O2A-C1-C2	3.21	120.46	108.11
36	I	4020	EQ3	C21-C20-C19	-3.21	113.91	123.20
21	A	1110	CLA	O2A-C1-C2	3.20	120.44	108.11
24	f	4016	BCR	C12-C13-C14	3.20	124.04	119.01
21	a	1134	CLA	CHD-C1D-ND	-3.20	120.30	124.80
21	a	1117	CLA	CMA-C3A-C4A	3.20	120.38	111.77
21	b	1224	CLA	O2D-CGD-CBD	3.20	116.82	111.23
24	h	4018	BCR	C39-C30-C25	-3.20	105.23	110.24
21	2	1207	CLA	O2A-C1-C2	3.20	120.42	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1135	CLA	CHD-C1D-ND	-3.20	120.30	124.80
30	b	4006	ECH	C19-C18-C17	-3.20	113.98	119.01
21	A	1139	CLA	O2A-C1-C2	3.20	120.42	108.11
21	A	1136	CLA	C1D-ND-C4D	-3.20	104.07	106.31
21	a	1011	CLA	O2A-C1-C2	3.19	120.40	108.11
21	B	1237	CLA	O2A-CGA-CBA	3.19	121.57	111.83
21	2	1234	CLA	CMA-C3A-C4A	3.19	120.35	111.77
21	b	1210	CLA	O2A-C1-C2	3.19	120.39	108.11
21	A	1140	CLA	C1D-ND-C4D	-3.19	104.07	106.31
21	1	1126	CLA	C1D-ND-C4D	-3.19	104.07	106.31
21	b	1226	CLA	CHD-C1D-ND	-3.19	120.31	124.80
21	A	1139	CLA	CMA-C3A-C4A	3.19	120.35	111.77
21	A	1131	CLA	CHD-C1D-ND	-3.19	120.32	124.80
24	2	4011	BCR	C39-C30-C25	-3.18	105.25	110.24
21	A	1117	CLA	C1D-ND-C4D	-3.18	104.08	106.31
21	b	1223	CLA	O2D-CGD-CBD	3.18	116.79	111.23
21	B	1207	CLA	O2A-CGA-CBA	3.18	121.52	111.83
21	A	1136	CLA	O2A-C1-C2	3.18	120.33	108.11
21	2	1229	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	1	1132	CLA	C1D-ND-C4D	-3.18	104.08	106.31
21	a	1123	CLA	CHD-C1D-ND	-3.17	120.34	124.80
21	A	1121	CLA	O2D-CGD-CBD	3.17	116.77	111.23
21	A	1127	CLA	O2D-CGD-CBD	3.17	116.77	111.23
21	1	1108	CLA	CMA-C3A-C4A	3.17	120.28	111.77
21	A	1117	CLA	O2A-C1-C2	3.17	120.29	108.11
21	A	1140	CLA	C3B-C4B-NB	-3.16	107.70	110.53
24	0	4022	BCR	C40-C30-C25	-3.16	105.29	110.24
21	2	1232	CLA	O2D-CGD-CBD	3.16	116.75	111.23
21	2	1204	CLA	CHD-C1D-ND	-3.16	120.36	124.80
21	A	1101	CLA	C3B-C4B-NB	-3.16	107.71	110.53
21	a	1101	CLA	CHD-C1D-ND	-3.16	120.36	124.80
21	1	1139	CLA	CMA-C3A-C4A	3.16	120.25	111.77
21	A	1135	CLA	C1D-ND-C4D	-3.16	104.10	106.31
21	B	1209	CLA	C1D-ND-C4D	-3.16	104.10	106.31
26	b	5002	LMG	O8-C28-C29	3.15	121.45	111.83
21	1	1124	CLA	C1D-ND-C4D	-3.15	104.10	106.31
21	2	1202	CLA	CHD-C1D-ND	-3.15	120.36	124.80
21	B	1228	CLA	O2A-C1-C2	3.15	120.24	108.11
21	2	1211	CLA	CMA-C3A-C4A	3.15	120.25	111.77
21	B	1022	CLA	O2D-CGD-CBD	3.15	116.74	111.23
21	b	1232	CLA	C1D-ND-C4D	-3.15	104.10	106.31
21	j	1302	CLA	C1D-ND-C4D	-3.15	104.10	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1216	CLA	O2A-C1-C2	3.15	120.23	108.11
21	8	1401	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	a	1135	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	B	1240	CLA	CMA-C3A-C4A	3.14	120.22	111.77
21	B	1214	CLA	O2D-CGD-CBD	3.14	116.72	111.23
21	B	1229	CLA	C3B-C4B-NB	-3.14	107.73	110.53
21	B	1228	CLA	C1D-ND-C4D	-3.14	104.11	106.31
21	a	1013	CLA	O2A-C1-C2	3.14	120.18	108.11
21	j	1303	CLA	C1D-ND-C4D	-3.13	104.11	106.31
24	1	4008	BCR	C40-C30-C25	-3.13	105.33	110.24
21	2	1021	CLA	O2A-C1-C2	3.13	120.16	108.11
21	B	1239	CLA	C1D-ND-C4D	-3.13	104.11	106.31
21	b	1227	CLA	O2A-C1-C2	3.13	120.16	108.11
21	2	1236	CLA	CMA-C3A-C4A	3.13	120.19	111.77
21	2	1235	CLA	O2D-CGD-CBD	3.13	116.70	111.23
21	A	1114	CLA	C1D-ND-C4D	-3.13	104.11	106.31
21	B	1214	CLA	O2A-C1-C2	3.13	120.15	108.11
21	a	1123	CLA	O2A-C1-C2	3.13	120.15	108.11
21	A	1133	CLA	C1D-ND-C4D	-3.13	104.12	106.31
21	1	1135	CLA	CHD-C1D-ND	-3.13	120.40	124.80
21	b	1230	CLA	O2A-C1-C2	3.13	120.14	108.11
21	b	1209	CLA	CMA-C3A-C4A	3.13	120.18	111.77
21	2	1224	CLA	C1D-ND-C4D	-3.13	104.12	106.31
28	h	4020	45D	C31-C29-C25	-3.12	122.90	127.28
28	h	4020	45D	C40-C36-C38	-3.12	117.75	122.82
21	2	1220	CLA	CMA-C3A-C4A	3.12	120.17	111.77
21	b	1238	CLA	O2A-C1-C2	3.12	120.12	108.11
21	2	1218	CLA	CMA-C3A-C4A	3.12	120.16	111.77
21	a	1122	CLA	O2D-CGD-CBD	3.12	116.69	111.23
21	B	1203	CLA	O2A-C1-C2	3.12	120.12	108.11
30	b	4006	ECH	C28-C27-C26	-3.12	115.84	118.64
26	0	5001	LMG	C1-O6-C5	3.12	119.81	113.72
21	1	1128	CLA	C1D-ND-C4D	-3.12	104.12	106.31
21	1	1108	CLA	CHD-C1D-ND	-3.12	120.41	124.80
21	j	1302	CLA	O2A-C1-C2	3.12	120.11	108.11
21	b	1231	CLA	CHD-C1D-ND	-3.12	120.42	124.80
21	A	1136	CLA	C3B-C4B-NB	-3.11	107.75	110.53
21	b	1212	CLA	C1D-ND-C4D	-3.11	104.13	106.31
21	b	1238	CLA	O2D-CGD-CBD	3.11	116.67	111.23
21	b	1208	CLA	C1D-ND-C4D	-3.11	104.13	106.31
36	I	4020	EQ3	C24-C23-C22	-3.11	121.64	126.23
21	A	1133	CLA	C3B-C4B-NB	-3.11	107.76	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1023	CLA	C3B-C4B-NB	-3.11	107.76	110.53
21	B	1236	CLA	C1D-ND-C4D	-3.11	104.13	106.31
21	1	1126	CLA	CMA-C3A-C4A	3.11	120.12	111.77
24	A	4003	BCR	C40-C30-C25	-3.10	105.37	110.24
21	b	1212	CLA	C3B-C4B-NB	-3.10	107.76	110.53
21	A	1108	CLA	O2D-CGD-CBD	3.10	116.66	111.23
21	b	1022	CLA	O2A-C1-C2	3.10	120.05	108.11
21	b	1219	CLA	CMA-C3A-C4A	3.10	120.11	111.77
21	b	1216	CLA	O2D-CGD-CBD	3.10	116.65	111.23
25	A	5001	LHG	C5-O7-C7	-3.10	110.37	117.80
21	6	1302	CLA	CMA-C3A-C4A	3.10	120.10	111.77
21	A	1132	CLA	C1D-ND-C4D	-3.10	104.14	106.31
21	b	1229	CLA	C2D-C1D-ND	3.10	113.19	110.13
21	2	1231	CLA	CHD-C1D-ND	-3.10	120.44	124.80
21	b	1021	CLA	C3B-C4B-NB	-3.10	107.77	110.53
21	B	1224	CLA	O2A-CGA-CBA	3.10	121.27	111.83
21	2	1204	CLA	O2A-CGA-CBA	3.09	121.27	111.83
21	b	1225	CLA	O2D-CGD-CBD	3.09	116.64	111.23
21	b	1213	CLA	C1D-ND-C4D	-3.09	104.14	106.31
21	B	1224	CLA	C1D-ND-C4D	-3.09	104.15	106.31
21	A	1101	CLA	CHD-C1D-ND	-3.09	120.46	124.80
34	J	4015	ZEX	C37-C21-C26	-3.08	105.42	110.25
21	2	1209	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	7	1303	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	A	1102	CLA	O2A-CGA-CBA	3.08	121.23	111.83
21	1	1131	CLA	CHD-C1D-ND	-3.08	120.47	124.80
21	J	1302	CLA	CMA-C3A-C4A	3.08	120.05	111.77
21	B	1237	CLA	O2A-C1-C2	3.08	119.96	108.11
21	B	1212	CLA	C3B-C4B-NB	-3.08	107.78	110.53
21	7	1302	CLA	C1D-ND-C4D	-3.08	104.15	106.31
21	b	1226	CLA	C3B-C4B-NB	-3.08	107.78	110.53
21	b	1238	CLA	C1D-ND-C4D	-3.08	104.15	106.31
21	8	1402	CLA	C1D-ND-C4D	-3.07	104.16	106.31
21	B	1220	CLA	CMA-C3A-C4A	3.07	120.03	111.77
21	j	1303	CLA	CMA-C3A-C4A	3.07	120.02	111.77
21	A	1124	CLA	CHD-C1D-ND	-3.07	120.48	124.80
21	a	1126	CLA	CMA-C3A-C4A	3.07	120.02	111.77
21	1	1113	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	2	1223	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	2	1222	CLA	C1D-ND-C4D	-3.07	104.16	106.31
21	2	1208	CLA	CMA-C3A-C4A	3.06	120.01	111.77
21	1	1136	CLA	CMA-C3A-C4A	3.06	120.01	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1207	CLA	C1D-ND-C4D	-3.06	104.16	106.31
24	L	4019	BCR	C39-C30-C25	-3.06	105.44	110.24
21	1	1120	CLA	CMA-C3A-C4A	3.06	120.00	111.77
36	I	4020	EQ3	C16-C15-C14	-3.06	117.26	123.52
21	2	1217	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	b	1222	CLA	CHD-C1D-ND	-3.06	120.50	124.80
21	1	1122	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	b	1224	CLA	O2A-C1-C2	3.06	119.88	108.11
21	B	1023	CLA	C3B-C4B-NB	-3.06	107.80	110.53
21	2	1235	CLA	C1D-ND-C4D	-3.06	104.17	106.31
26	A	5002	LMG	O8-C28-C29	3.06	121.15	111.83
21	A	1136	CLA	O2D-CGD-CBD	3.06	116.57	111.23
21	b	1237	CLA	O2A-CGA-CBA	3.06	121.15	111.83
21	A	1103	CLA	C1D-ND-C4D	-3.05	104.17	106.31
21	2	1204	CLA	O2A-C1-C2	3.05	119.84	108.11
21	1	1011	CLA	O2D-CGD-CBD	3.05	116.56	111.23
35	L	6001	LMT	O5B-C1B-C2B	3.05	116.63	110.37
21	A	1115	CLA	C1D-ND-C4D	-3.05	104.17	106.31
21	B	1238	CLA	C2D-C1D-ND	3.05	113.14	110.13
21	b	1215	CLA	CHD-C1D-ND	-3.04	120.52	124.80
21	B	1207	CLA	O2A-C1-C2	3.04	119.82	108.11
21	B	1230	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	1	1104	CLA	CHD-C1D-ND	-3.04	120.52	124.80
21	a	1117	CLA	C1D-ND-C4D	-3.04	104.18	106.31
21	1	1138	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	k	1401	CLA	O2D-CGD-CBD	3.04	116.55	111.23
21	b	1236	CLA	CHD-C1D-ND	-3.04	120.52	124.80
21	K	1401	CLA	C1D-ND-C4D	-3.04	104.18	106.31
21	1	1110	CLA	CMA-C3A-C4A	3.04	119.94	111.77
21	2	1203	CLA	C1D-ND-C4D	-3.04	104.18	106.31
26	a	5004	LMG	O8-C28-C29	3.04	121.09	111.83
22	b	2002	PQN	C17-C16-C15	-3.04	105.17	113.26
21	A	1012	CLA	C1D-ND-C4D	-3.04	104.18	106.31
21	a	1012	CLA	C2D-C1D-ND	3.03	113.13	110.13
21	1	1137	CLA	CHD-C1D-ND	-3.03	120.53	124.80
21	b	1225	CLA	C1D-ND-C4D	-3.03	104.19	106.31
21	1	1114	CLA	CMA-C3A-C4A	3.03	119.92	111.77
21	2	1206	CLA	O2D-CGD-CBD	3.03	116.52	111.23
21	b	1220	CLA	O2D-CGD-CBD	3.03	116.52	111.23
21	B	1219	CLA	CHD-C1D-ND	-3.03	120.54	124.80
22	a	2001	PQN	C12-C11-C3	-3.03	104.63	112.08
21	1	1105	CLA	CMA-C3A-C4A	3.03	119.90	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	4003	BCR	C27-C26-C25	-3.02	118.62	122.70
21	A	1127	CLA	C1D-ND-C4D	-3.02	104.19	106.31
21	f	1301	CLA	C1D-ND-C4D	-3.02	104.19	106.31
21	a	1121	CLA	CMA-C3A-C4A	3.02	119.90	111.77
21	B	1234	CLA	CHD-C1D-ND	-3.02	120.55	124.80
21	1	1135	CLA	C1D-ND-C4D	-3.02	104.19	106.31
21	A	1011	CLA	C3B-C4B-NB	-3.02	107.83	110.53
25	1	5003	LHG	C5-O7-C7	-3.02	110.57	117.80
21	A	1105	CLA	C1D-ND-C4D	-3.02	104.19	106.31
21	a	1127	CLA	C1D-ND-C4D	-3.02	104.19	106.31
21	b	1229	CLA	C3B-C4B-NB	-3.02	107.83	110.53
21	A	1116	CLA	CHD-C1D-ND	-3.02	120.55	124.80
21	2	1212	CLA	C1D-ND-C4D	-3.02	104.19	106.31
36	I	4020	EQ3	C10-C11-C12	-3.02	114.46	123.20
21	A	1122	CLA	CMA-C3A-C4A	3.02	119.88	111.77
21	B	1207	CLA	CMA-C3A-C4A	3.02	119.88	111.77
21	a	1106	CLA	C1D-ND-C4D	-3.02	104.20	106.31
21	1	1801	CLA	CHD-C1D-ND	-3.01	120.56	124.80
21	A	1139	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	a	1139	CLA	CMA-C3A-C4A	3.01	119.87	111.77
24	B	4004	BCR	C38-C26-C25	-3.01	121.20	124.48
21	1	1102	CLA	O2A-CGA-CBA	3.01	121.02	111.83
21	A	1011	CLA	C2A-C1A-CHA	3.01	129.09	123.87
21	A	1107	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	a	1136	CLA	O2A-CGA-CBA	3.01	121.02	111.83
21	A	1114	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	J	1303	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	B	1232	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	a	1114	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	b	1228	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	B	1225	CLA	CMA-C3A-C4A	3.01	119.86	111.77
24	9	4021	BCR	C30-C25-C24	3.01	123.81	115.65
24	9	4021	BCR	C40-C30-C25	-3.01	105.53	110.24
21	a	1138	CLA	CMA-C3A-C4A	3.01	119.85	111.77
21	B	1240	CLA	C3B-C4B-NB	-3.01	107.85	110.53
34	7	4015	ZEX	C17-C1-C6	-3.01	105.53	110.24
21	A	1108	CLA	CHD-C1D-ND	-3.01	120.57	124.80
21	b	1236	CLA	C1D-ND-C4D	-3.00	104.20	106.31
21	A	1131	CLA	C1D-ND-C4D	-3.00	104.20	106.31
21	B	1227	CLA	C3B-C4B-NB	-3.00	107.85	110.53
21	B	1238	CLA	C3B-C4B-NB	-3.00	107.85	110.53
24	l	4022	BCR	C40-C30-C25	-3.00	105.54	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	5006	LHG	O8-C23-C24	3.00	120.99	111.83
21	1	1112	CLA	CMA-C3A-C4A	3.00	119.84	111.77
24	I	4018	BCR	C35-C13-C12	3.00	122.67	118.09
21	b	1240	CLA	C1D-ND-C4D	-3.00	104.21	106.31
35	L	6001	LMT	C1B-C2B-C3B	3.00	116.32	110.01
21	2	1219	CLA	CMA-C3A-C4A	3.00	119.83	111.77
21	1	1123	CLA	CHD-C1D-ND	-3.00	120.58	124.80
21	0	1502	CLA	C3B-C4B-NB	-3.00	107.85	110.53
21	1	1117	CLA	O2D-CGD-CBD	3.00	116.47	111.23
21	2	1207	CLA	O2A-CGA-CBA	3.00	120.97	111.83
21	1	1140	CLA	CMA-C3A-C4A	3.00	119.83	111.77
21	a	1119	CLA	C1D-ND-C4D	-3.00	104.21	106.31
21	2	1225	CLA	C1D-ND-C4D	-3.00	104.21	106.31
21	1	1140	CLA	C3B-C4B-NB	-3.00	107.86	110.53
25	a	5003	LHG	O8-C23-C24	3.00	120.97	111.83
21	b	1232	CLA	CMA-C3A-C4A	3.00	119.82	111.77
21	B	1202	CLA	O2A-CGA-CBA	2.99	120.96	111.83
30	b	4011	ECH	C23-C24-C25	-2.99	119.00	127.00
21	1	1104	CLA	C1D-ND-C4D	-2.99	104.21	106.31
21	a	1127	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	1	1101	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	b	1209	CLA	C1-O2A-CGA	2.99	123.89	116.65
21	b	1210	CLA	CMA-C3A-C4A	2.99	119.80	111.77
21	2	1215	CLA	C1-O2A-CGA	2.99	123.88	116.65
24	a	4008	BCR	C38-C26-C25	-2.99	121.23	124.48
21	A	1130	CLA	C1-O2A-CGA	2.99	123.88	116.65
35	F	6001	LMT	C3'-C4'-C5'	-2.99	104.31	110.93
21	2	1208	CLA	CHD-C1D-ND	-2.98	120.60	124.80
22	B	2002	PQN	C14-C13-C15	2.98	120.41	115.23
21	b	1216	CLA	CHD-C1D-ND	-2.98	120.60	124.80
21	1	1101	CLA	CHD-C1D-ND	-2.98	120.60	124.80
21	A	1106	CLA	C1D-ND-C4D	-2.98	104.22	106.31
21	a	1136	CLA	C1D-ND-C4D	-2.98	104.22	106.31
21	F	1302	CLA	CMA-C3A-C4A	2.98	119.79	111.77
21	B	1238	CLA	CHD-C1D-ND	-2.98	120.61	124.80
21	2	1225	CLA	CMA-C3A-C4A	2.98	119.79	111.77
21	B	1202	CLA	O2A-C1-C2	2.98	119.58	108.11
21	K	1401	CLA	CHD-C1D-ND	-2.98	120.61	124.80
21	2	1235	CLA	CHD-C1D-ND	-2.98	120.61	124.80
21	b	1219	CLA	C1D-ND-C4D	-2.98	104.22	106.31
21	b	1217	CLA	O2A-C1-C2	2.98	119.57	108.11
21	a	1801	CLA	CMA-C3A-C4A	2.98	119.78	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	4003	BCR	C1-C6-C5	-2.98	118.57	122.64
21	b	1203	CLA	C1D-ND-C4D	-2.98	104.22	106.31
21	B	1232	CLA	C1D-ND-C4D	-2.98	104.22	106.31
21	a	1122	CLA	CMA-C3A-C4A	2.98	119.77	111.77
24	2	4010	BCR	C15-C14-C13	2.97	131.45	127.28
31	F	5001	SQD	O7-S-C6	-2.97	102.31	106.76
21	b	1239	CLA	CHD-C1D-ND	-2.97	120.62	124.80
21	B	1222	CLA	C1D-ND-C4D	-2.97	104.23	106.31
21	a	1124	CLA	C2D-C1D-ND	2.97	113.07	110.13
21	2	1023	CLA	O2D-CGD-CBD	2.97	116.43	111.23
21	k	1401	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	1	1125	CLA	CMA-C3A-C4A	2.97	119.75	111.77
21	1	1129	CLA	CHD-C1D-ND	-2.97	120.62	124.80
21	a	1137	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	I	4018	BCR	C15-C14-C13	2.97	131.44	127.28
21	a	1121	CLA	CHD-C1D-ND	-2.97	120.62	124.80
21	1	1801	CLA	C3B-C4B-NB	-2.97	107.88	110.53
21	a	1125	CLA	C1-O2A-CGA	2.97	123.84	116.65
21	1	1116	CLA	C3B-C4B-NB	-2.97	107.88	110.53
25	1	5003	LHG	O8-C23-C24	2.97	120.88	111.83
21	B	1232	CLA	CHD-C1D-ND	-2.97	120.63	124.80
24	K	4001	BCR	C40-C30-C25	-2.97	105.59	110.24
24	A	4019	BCR	C8-C7-C6	2.97	134.92	127.00
21	1	1109	CLA	CMD-C2D-C3D	-2.97	120.89	127.69
21	b	1218	CLA	C1D-ND-C4D	-2.96	104.23	106.31
30	2	4006	ECH	C23-C22-C21	-2.96	114.35	119.01
28	h	4020	45D	C19-C23-C25	-2.96	121.85	126.23
21	2	1232	CLA	CHD-C1D-ND	-2.96	120.64	124.80
21	B	1216	CLA	C1D-ND-C4D	-2.96	104.23	106.31
21	B	1218	CLA	C1D-ND-C4D	-2.96	104.23	106.31
21	a	1129	CLA	C1D-ND-C4D	-2.96	104.23	106.31
21	B	1023	CLA	CHD-C1D-ND	-2.96	120.64	124.80
21	2	1204	CLA	C1-O2A-CGA	2.96	123.81	116.65
21	A	1118	CLA	O2D-CGD-CBD	2.96	116.40	111.23
36	I	4020	EQ3	C35-C13-C12	2.95	122.60	118.09
26	B	5002	LMG	O8-C28-C29	2.95	120.84	111.83
24	B	4014	BCR	C39-C30-C25	-2.95	105.61	110.24
21	2	1238	CLA	CMA-C3A-C4A	2.95	119.71	111.77
21	A	1109	CLA	C1D-ND-C4D	-2.95	104.24	106.31
21	b	1214	CLA	C1D-ND-C4D	-2.95	104.24	106.31
24	7	4013	BCR	C40-C30-C25	-2.95	105.62	110.24
21	b	1217	CLA	CMA-C3A-C4A	2.95	119.70	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1120	CLA	CHD-C1D-ND	-2.95	120.65	124.80
21	b	1021	CLA	O2A-C1-C2	2.95	119.45	108.11
21	a	1114	CLA	CMA-C3A-C4A	2.95	119.69	111.77
21	A	1013	CLA	CHD-C1D-ND	-2.95	120.66	124.80
21	A	1116	CLA	C1D-ND-C4D	-2.95	104.25	106.31
21	a	1122	CLA	C1D-ND-C4D	-2.95	104.25	106.31
21	A	1101	CLA	C1D-ND-C4D	-2.94	104.25	106.31
21	2	1228	CLA	C3B-C4B-NB	-2.94	107.90	110.53
21	A	1109	CLA	O2A-CGA-CBA	2.94	120.81	111.83
21	B	1201	CLA	O2D-CGD-CBD	2.94	116.37	111.23
21	a	1108	CLA	C3B-C4B-NB	-2.94	107.90	110.53
28	B	4011	45D	C31-C33-C35	-2.94	118.30	126.36
21	b	1207	CLA	CMA-C3A-C4A	2.94	119.67	111.77
21	1	1131	CLA	O2A-C1-C2	2.94	119.42	108.11
21	A	1121	CLA	CHD-C1D-ND	-2.94	120.67	124.80
24	0	4019	BCR	C40-C30-C25	-2.94	105.64	110.24
21	1	1123	CLA	CMA-C3A-C4A	2.94	119.67	111.77
21	b	1227	CLA	C1D-ND-C4D	-2.93	104.25	106.31
21	1	1137	CLA	O2A-CGA-CBA	2.93	120.78	111.83
21	a	1113	CLA	CMA-C3A-C4A	2.93	119.66	111.77
21	a	1121	CLA	C1D-ND-C4D	-2.93	104.25	106.31
21	1	1103	CLA	CHD-C1D-ND	-2.93	120.68	124.80
21	1	1139	CLA	C1D-ND-C4D	-2.93	104.25	106.31
21	1	1124	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	b	1224	CLA	O2A-CGA-CBA	2.93	120.77	111.83
21	1	1129	CLA	C1D-ND-C4D	-2.93	104.26	106.31
21	b	1204	CLA	CHD-C1D-ND	-2.93	120.68	124.80
21	2	1227	CLA	C3B-C4B-NB	-2.93	107.92	110.53
21	B	1214	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	2	1213	CLA	C1D-ND-C4D	-2.93	104.26	106.31
21	A	1108	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	b	1211	CLA	O2A-C1-C2	2.93	119.38	108.11
21	b	1238	CLA	CMA-C3A-C4A	2.93	119.64	111.77
22	2	2002	PQN	C2M-C2-C3	-2.93	119.64	124.45
21	B	1204	CLA	C1D-ND-C4D	-2.93	104.26	106.31
21	b	1240	CLA	CHD-C1D-ND	-2.93	120.69	124.80
21	l	1502	CLA	C3B-C4B-NB	-2.92	107.92	110.53
21	K	1402	CLA	O2A-C1-C2	2.92	119.36	108.11
21	B	1223	CLA	CMA-C3A-C4A	2.92	119.63	111.77
36	I	4020	EQ3	C20-C21-C22	-2.92	123.18	127.28
21	a	1132	CLA	C1D-ND-C4D	-2.92	104.26	106.31
21	1	1122	CLA	C1D-ND-C4D	-2.92	104.26	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1209	CLA	CHD-C1D-ND	-2.92	120.69	124.80
21	a	1124	CLA	CMA-C3A-C4A	2.92	119.61	111.77
24	9	4021	BCR	C35-C13-C14	-2.92	118.09	122.82
21	a	1116	CLA	CMA-C3A-C4A	2.92	119.61	111.77
21	1	1108	CLA	C1D-ND-C4D	-2.91	104.27	106.31
21	2	1215	CLA	C3B-C4B-NB	-2.91	107.93	110.53
28	h	4020	45D	C21-C15-C17	2.91	119.90	115.49
25	0	5002	LHG	O8-C23-C24	2.91	120.72	111.83
21	b	1223	CLA	CMA-C3A-C4A	2.91	119.60	111.77
21	b	1234	CLA	C1D-ND-C4D	-2.91	104.27	106.31
22	2	2002	PQN	C14-C13-C15	2.91	120.28	115.23
24	I	4018	BCR	C40-C30-C25	-2.91	105.68	110.24
21	a	1140	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	b	4014	BCR	C39-C30-C25	-2.91	105.68	110.24
21	b	1230	CLA	C2D-C1D-ND	2.91	113.00	110.13
21	b	1214	CLA	CMA-C3A-C4A	2.91	119.59	111.77
21	b	1234	CLA	CHD-C1D-ND	-2.91	120.71	124.80
21	2	1203	CLA	CHD-C1D-ND	-2.91	120.71	124.80
21	l	1502	CLA	C2D-C1D-ND	2.91	113.00	110.13
34	j	4015	ZEX	C39-C29-C30	-2.91	118.11	122.82
24	j	4013	BCR	C39-C30-C25	-2.91	105.69	110.24
21	2	1212	CLA	CMA-C3A-C4A	2.91	119.58	111.77
21	b	1205	CLA	O2A-CGA-CBA	2.91	120.69	111.83
21	b	1210	CLA	C1D-ND-C4D	-2.90	104.27	106.31
21	1	1114	CLA	C1D-ND-C4D	-2.90	104.28	106.31
26	0	5001	LMG	C3-C4-C5	2.90	115.50	110.23
21	a	1013	CLA	CHD-C1D-ND	-2.90	120.72	124.80
21	2	1206	CLA	CHD-C1D-ND	-2.90	120.72	124.80
21	a	1012	CLA	C1D-ND-C4D	-2.90	104.28	106.31
21	A	1122	CLA	C1D-ND-C4D	-2.90	104.28	106.31
21	B	1219	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	A	1105	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	a	1131	CLA	CHD-C1D-ND	-2.90	120.72	124.80
21	b	1224	CLA	CHD-C1D-ND	-2.90	120.72	124.80
21	1	1124	CLA	O2A-CGA-CBA	2.90	120.67	111.83
25	a	5001	LHG	C5-O7-C7	-2.90	110.86	117.80
21	a	1125	CLA	CHD-C1D-ND	-2.90	120.73	124.80
21	0	1503	CLA	C1D-ND-C4D	-2.90	104.28	106.31
21	1	1011	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	B	4018	BCR	C15-C14-C13	-2.90	123.22	127.28
21	B	1211	CLA	CMA-C3A-C4A	2.90	119.56	111.77
24	A	4012	BCR	C38-C26-C25	-2.89	121.33	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	1503	CLA	CHD-C1D-ND	-2.89	120.73	124.80
21	7	1302	CLA	CHD-C1D-ND	-2.89	120.73	124.80
21	a	1125	CLA	CMA-C3A-C4A	2.89	119.55	111.77
24	i	4018	BCR	C40-C30-C25	-2.89	105.71	110.24
21	A	1110	CLA	C1D-ND-C4D	-2.89	104.28	106.31
21	a	1107	CLA	CMA-C3A-C4A	2.89	119.54	111.77
21	a	1113	CLA	C1D-ND-C4D	-2.89	104.29	106.31
24	A	4019	BCR	C8-C9-C10	2.89	123.55	119.01
21	B	1203	CLA	C1D-ND-C4D	-2.89	104.29	106.31
34	j	4015	ZEX	C28-C29-C30	2.89	123.55	119.01
21	f	1302	CLA	CHD-C1D-ND	-2.89	120.74	124.80
24	2	4018	BCR	C36-C18-C19	-2.88	113.68	118.09
21	a	1103	CLA	CHD-C1D-ND	-2.88	120.74	124.80
21	A	1138	CLA	CHD-C1D-ND	-2.88	120.75	124.80
21	1	1116	CLA	CHD-C1D-ND	-2.88	120.75	124.80
21	7	1302	CLA	CMA-C3A-C4A	2.88	119.52	111.77
26	0	5001	LMG	O8-C28-C29	2.88	120.62	111.83
21	F	1302	CLA	CHD-C1D-ND	-2.88	120.75	124.80
21	1	1013	CLA	CHD-C1D-ND	-2.88	120.75	124.80
21	A	1123	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	1	1137	CLA	C1D-ND-C4D	-2.88	104.29	106.31
28	B	4011	45D	C09-C05-C03	2.88	117.42	113.21
25	A	5006	LHG	O8-C23-C24	2.87	120.60	111.83
21	1	1129	CLA	C3B-C4B-NB	-2.87	107.96	110.53
21	1	1138	CLA	CMA-C3A-C4A	2.87	119.50	111.77
21	K	1402	CLA	O2A-CGA-CBA	2.87	120.60	111.83
21	B	1212	CLA	CMA-C3A-C4A	2.87	119.50	111.77
21	b	1211	CLA	CHD-C1D-ND	-2.87	120.76	124.80
21	l	1503	CLA	CHD-C1D-ND	-2.87	120.76	124.80
21	2	1239	CLA	O2A-CGA-CBA	2.87	120.59	111.83
21	2	1229	CLA	CMA-C3A-C4A	2.87	119.49	111.77
21	2	1215	CLA	CHD-C1D-ND	-2.87	120.76	124.80
21	2	1234	CLA	CHD-C1D-ND	-2.87	120.76	124.80
21	1	1127	CLA	CMA-C3A-C4A	2.87	119.49	111.77
21	B	1234	CLA	C2D-C1D-ND	2.87	112.97	110.13
21	A	1106	CLA	O2A-CGA-CBA	2.87	120.59	111.83
21	0	1502	CLA	C2D-C1D-ND	2.87	112.97	110.13
21	A	1125	CLA	C1D-ND-C4D	-2.87	104.30	106.31
21	B	1217	CLA	C1D-ND-C4D	-2.87	104.30	106.31
21	a	1801	CLA	C1D-ND-C4D	-2.87	104.30	106.31
21	b	1202	CLA	O2A-CGA-CBA	2.87	120.58	111.83
21	a	1011	CLA	CHA-C1A-NA	-2.87	119.89	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	4011	45D	O02-C18-C16	-2.87	118.40	120.98
21	1	1110	CLA	C3B-C4B-NB	-2.87	107.97	110.53
24	0	4019	BCR	C38-C26-C25	-2.86	121.36	124.48
24	I	4018	BCR	C2-C1-C6	2.86	114.60	110.44
21	a	1134	CLA	C3B-C4B-NB	-2.86	107.97	110.53
21	2	1022	CLA	CHD-C1D-ND	-2.86	120.77	124.80
21	B	1221	CLA	CHD-C1D-ND	-2.86	120.77	124.80
21	a	1122	CLA	CHD-C1D-ND	-2.86	120.77	124.80
21	1	1111	CLA	O2D-CGD-CBD	2.86	116.23	111.23
24	2	4018	BCR	C19-C18-C17	2.86	123.51	119.01
21	B	1231	CLA	C1D-ND-C4D	-2.86	104.31	106.31
21	0	1501	CLA	C1D-ND-C4D	-2.86	104.31	106.31
21	2	1239	CLA	CMA-C3A-C4A	2.86	119.45	111.77
26	K	5009	LMG	O8-C28-C29	2.86	120.55	111.83
21	1	1115	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	1	1121	CLA	CMA-C3A-C4A	2.85	119.44	111.77
21	a	1129	CLA	C3B-C4B-NB	-2.85	107.98	110.53
21	A	1116	CLA	O2A-C1-C2	2.85	119.07	108.11
21	B	1227	CLA	C2D-C1D-ND	2.85	112.94	110.13
21	2	1212	CLA	CHD-C1D-ND	-2.85	120.79	124.80
21	B	1223	CLA	C1D-ND-C4D	-2.85	104.31	106.31
21	A	1140	CLA	CMA-C3A-C4A	2.85	119.42	111.77
21	b	1228	CLA	O2D-CGD-CBD	2.85	116.21	111.23
21	1	1801	CLA	C2D-C1D-ND	2.85	112.94	110.13
21	B	1215	CLA	O2A-C1-C2	2.85	119.06	108.11
21	b	1022	CLA	C1D-ND-C4D	-2.84	104.32	106.31
21	b	1235	CLA	CHD-C1D-ND	-2.84	120.80	124.80
21	a	1130	CLA	CHD-C1D-ND	-2.84	120.80	124.80
21	0	1503	CLA	CHD-C1D-ND	-2.84	120.80	124.80
34	F	4016	ZEX	C1-C6-C5	-2.84	118.75	122.64
21	A	1129	CLA	CHD-C1D-ND	-2.84	120.80	124.80
21	B	1209	CLA	CMA-C3A-C4A	2.84	119.41	111.77
21	A	1112	CLA	O2A-CGA-CBA	2.84	120.49	111.83
24	J	4013	BCR	C39-C30-C25	-2.84	105.79	110.24
21	2	1205	CLA	O2A-CGA-CBA	2.84	120.49	111.83
21	B	1216	CLA	CHD-C1D-ND	-2.84	120.81	124.80
25	a	5007	LHG	O8-C23-C24	2.84	120.49	111.83
21	l	1501	CLA	C1D-ND-C4D	-2.84	104.32	106.31
21	2	1238	CLA	C1D-ND-C4D	-2.84	104.32	106.31
21	b	1207	CLA	O2D-CGD-CBD	2.84	116.19	111.23
21	A	1113	CLA	CMA-C3A-C4A	2.84	119.39	111.77
21	b	1239	CLA	C1D-ND-C4D	-2.83	104.32	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1219	CLA	CHD-C1D-ND	-2.83	120.81	124.80
21	2	1219	CLA	O2A-CGA-CBA	2.83	120.47	111.83
21	B	1208	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	B	1215	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	2	1225	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	A	1122	CLA	O2D-CGD-CBD	2.83	116.18	111.23
21	1	1113	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	2	1201	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	b	1023	CLA	C3B-C4B-NB	-2.83	108.00	110.53
21	2	1215	CLA	CMA-C3A-C4A	2.83	119.38	111.77
21	1	1105	CLA	C3B-C4B-NB	-2.83	108.00	110.53
28	h	4020	45D	C31-C33-C35	-2.83	118.60	126.36
34	7	4015	ZEX	C37-C21-C26	-2.83	105.82	110.25
25	b	5004	LHG	O8-C23-C24	2.83	120.46	111.83
21	b	1225	CLA	CHD-C1D-ND	-2.83	120.82	124.80
21	1	1137	CLA	CMA-C3A-C4A	2.83	119.37	111.77
21	A	1133	CLA	CHD-C1D-ND	-2.83	120.83	124.80
21	b	1217	CLA	C1D-ND-C4D	-2.83	104.33	106.31
24	b	4005	BCR	C37-C22-C23	2.83	122.41	118.09
24	9	4021	BCR	C12-C13-C14	2.83	123.45	119.01
21	b	1202	CLA	C1D-ND-C4D	-2.82	104.33	106.31
24	B	4004	BCR	C40-C30-C25	-2.82	105.82	110.24
24	2	4018	BCR	C29-C28-C27	2.82	117.48	111.28
35	1	6001	LMT	C1'-O5'-C5'	-2.82	108.21	113.72
21	A	1136	CLA	CMA-C3A-C4A	2.82	119.36	111.77
26	b	5005	LMG	O8-C28-C29	2.82	120.43	111.83
21	b	1202	CLA	C1-O2A-CGA	2.82	123.47	116.65
21	B	1022	CLA	C1D-ND-C4D	-2.82	104.33	106.31
21	b	1237	CLA	C1D-ND-C4D	-2.82	104.33	106.31
24	A	4003	BCR	C36-C18-C19	-2.82	113.78	118.09
24	1	4007	BCR	C40-C30-C25	-2.82	105.83	110.24
26	A	5008	LMG	O8-C28-C29	2.82	120.42	111.83
21	1	1121	CLA	CHD-C1D-ND	-2.82	120.84	124.80
21	2	1221	CLA	CHD-C1D-ND	-2.82	120.84	124.80
21	A	1124	CLA	C1D-ND-C4D	-2.82	104.34	106.31
21	b	1240	CLA	CMA-C3A-C4A	2.82	119.34	111.77
21	2	1222	CLA	C3B-C4B-NB	-2.82	108.02	110.53
21	2	1205	CLA	CHD-C1D-ND	-2.81	120.84	124.80
21	A	1013	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	2	1223	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	a	1107	CLA	CHD-C1D-ND	-2.81	120.84	124.80
21	a	1129	CLA	CHD-C1D-ND	-2.81	120.84	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1226	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	B	1235	CLA	C2D-C1D-ND	2.81	112.91	110.13
21	1	1106	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	B	1231	CLA	C1-O2A-CGA	2.81	123.45	116.65
21	6	1302	CLA	CHD-C1D-ND	-2.81	120.85	124.80
21	2	1208	CLA	C3B-C4B-NB	-2.81	108.02	110.53
21	2	1205	CLA	CMA-C3A-C4A	2.81	119.33	111.77
21	a	1135	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	1	1107	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	1	1119	CLA	CHD-C1D-ND	-2.81	120.85	124.80
26	b	5007	LMG	O8-C28-C29	2.81	120.40	111.83
21	B	1215	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	b	1201	CLA	O2D-CGD-CBD	2.81	116.14	111.23
21	A	1126	CLA	C2D-C1D-ND	2.81	112.90	110.13
21	a	1105	CLA	C1D-ND-C4D	-2.81	104.34	106.31
21	a	1105	CLA	CMA-C3A-C4A	2.81	119.31	111.77
21	1	1132	CLA	C2D-C1D-ND	2.81	112.90	110.13
21	1	1137	CLA	CAA-CBA-CGA	-2.81	105.24	113.21
21	1	1130	CLA	CHD-C1D-ND	-2.80	120.86	124.80
25	a	5001	LHG	O8-C23-C24	2.80	120.39	111.83
21	1	1118	CLA	CHD-C1D-ND	-2.80	120.86	124.80
21	A	1128	CLA	C1D-ND-C4D	-2.80	104.34	106.31
21	1	1117	CLA	C1D-ND-C4D	-2.80	104.34	106.31
21	1	1128	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	a	1114	CLA	O2A-CGA-CBA	2.80	120.38	111.83
21	f	1302	CLA	C1D-ND-C4D	-2.80	104.35	106.31
21	a	1118	CLA	O2A-C1-C2	2.80	118.89	108.11
21	B	1207	CLA	CAC-C3C-C2C	2.80	132.70	127.56
21	A	1134	CLA	C1D-ND-C4D	-2.80	104.35	106.31
21	B	1213	CLA	CMA-C3A-C4A	2.80	119.30	111.77
21	A	1110	CLA	CHD-C1D-ND	-2.80	120.86	124.80
21	B	1021	CLA	CHD-C1D-ND	-2.80	120.86	124.80
24	B	4014	BCR	C36-C18-C19	-2.80	113.81	118.09
21	B	1204	CLA	CHD-C1D-ND	-2.80	120.86	124.80
24	I	4018	BCR	C39-C30-C25	-2.80	105.86	110.24
21	1	1135	CLA	CMA-C3A-C4A	2.80	119.29	111.77
21	B	1214	CLA	CHD-C1D-ND	-2.80	120.87	124.80
24	2	4018	BCR	C23-C24-C25	2.80	134.47	127.00
21	a	1140	CLA	CMA-C3A-C4A	2.80	119.29	111.77
24	a	4008	BCR	C39-C30-C25	-2.79	105.86	110.24
21	B	1210	CLA	CMA-C3A-C4A	2.79	119.28	111.77
24	2	4005	BCR	C38-C26-C25	-2.79	121.44	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1221	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	A	1011	CLA	O2A-C1-C2	2.79	118.86	108.11
21	7	1303	CLA	CHD-C1D-ND	-2.79	120.87	124.80
24	A	4012	BCR	C39-C30-C25	-2.79	105.86	110.24
21	a	1110	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	2	1236	CLA	C2D-C1D-ND	2.79	112.89	110.13
21	a	1108	CLA	C1D-ND-C4D	-2.79	104.35	106.31
21	a	1101	CLA	C1D-ND-C4D	-2.79	104.35	106.31
21	1	1109	CLA	C1D-ND-C4D	-2.79	104.35	106.31
21	1	1801	CLA	O2A-CGA-CBA	2.79	120.34	111.83
21	B	1230	CLA	CHD-C1D-ND	-2.79	120.88	124.80
21	B	1208	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	A	1134	CLA	CHD-C1D-ND	-2.79	120.88	124.80
30	m	4021	ECH	C37-C22-C23	-2.79	113.83	118.09
21	2	1237	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	B	1228	CLA	C2D-C1D-ND	2.79	112.89	110.13
21	a	1101	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	A	1102	CLA	CHD-C1D-ND	-2.79	120.88	124.80
21	B	1238	CLA	O2D-CGD-CBD	2.79	116.10	111.23
21	B	1238	CLA	CMA-C3A-C4A	2.79	119.26	111.77
21	b	1231	CLA	C1D-ND-C4D	-2.79	104.36	106.31
21	b	1217	CLA	CHD-C1D-ND	-2.79	120.88	124.80
30	i	4020	ECH	C28-C29-C30	-2.78	109.14	113.21
24	2	4014	BCR	C40-C30-C25	-2.78	105.88	110.24
21	a	1117	CLA	CHD-C1D-ND	-2.78	120.89	124.80
21	b	1215	CLA	C1D-ND-C4D	-2.78	104.36	106.31
21	A	1108	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	1	1134	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	1	1139	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	1	1011	CLA	CHA-C1A-NA	-2.78	120.09	126.39
26	A	5004	LMG	O1-C1-C2	2.78	112.50	108.27
21	A	1119	CLA	C1D-ND-C4D	-2.78	104.36	106.31
21	a	1107	CLA	C1D-ND-C4D	-2.78	104.36	106.31
21	b	1226	CLA	CMD-C2D-C3D	-2.78	121.31	127.69
21	a	1112	CLA	CHD-C1D-ND	-2.78	120.89	124.80
21	2	1223	CLA	CHD-C1D-ND	-2.78	120.89	124.80
21	A	1110	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	A	1111	CLA	C1D-ND-C4D	-2.78	104.36	106.31
21	b	1212	CLA	CHD-C1D-ND	-2.78	120.89	124.80
21	f	1302	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	2	1240	CLA	C2D-C1D-ND	2.78	112.88	110.13
24	A	4003	BCR	C19-C18-C17	2.78	123.38	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1132	CLA	C2D-C1D-ND	2.78	112.87	110.13
21	b	1218	CLA	C2D-C1D-ND	2.78	112.87	110.13
25	A	5005	LHG	C5-O7-C7	-2.78	111.15	117.80
21	A	1124	CLA	O2A-C1-C2	2.78	118.79	108.11
21	b	1234	CLA	CMA-C3A-C4A	2.78	119.23	111.77
26	2	5005	LMG	O8-C28-C29	2.78	120.30	111.83
21	b	1204	CLA	C1-O2A-CGA	2.77	123.37	116.65
21	B	1218	CLA	CHD-C1D-ND	-2.77	120.90	124.80
21	B	1236	CLA	CHD-C1D-ND	-2.77	120.90	124.80
21	b	1204	CLA	O2A-C1-C2	2.77	118.78	108.11
21	A	1113	CLA	C1D-ND-C4D	-2.77	104.37	106.31
21	6	1301	CLA	C1D-ND-C4D	-2.77	104.37	106.31
21	1	1120	CLA	C1D-ND-C4D	-2.77	104.37	106.31
21	b	1218	CLA	O2D-CGD-CBD	2.77	116.07	111.23
21	K	1402	CLA	CMA-C3A-C4A	2.77	119.22	111.77
24	B	4014	BCR	C19-C18-C17	2.77	123.36	119.01
21	2	1230	CLA	C1D-ND-C4D	-2.77	104.37	106.31
21	B	1217	CLA	CHD-C1D-ND	-2.77	120.91	124.80
24	B	4018	BCR	C38-C26-C25	-2.77	121.46	124.48
21	a	1136	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	A	1111	CLA	CHD-C1D-ND	-2.77	120.91	124.80
21	1	1109	CLA	CHD-C1D-ND	-2.77	120.91	124.80
24	b	4014	BCR	C36-C18-C19	-2.77	113.86	118.09
21	J	1303	CLA	C1D-ND-C4D	-2.77	104.37	106.31
21	a	1110	CLA	CHD-C1D-ND	-2.77	120.91	124.80
21	b	1201	CLA	O2A-C1-C2	2.76	118.75	108.11
21	1	1115	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	A	1128	CLA	O2A-CGA-CBA	2.76	120.26	111.83
31	b	5006	SQD	O7-S-C6	-2.76	102.63	106.76
21	A	1121	CLA	CMA-C3A-C4A	2.76	119.20	111.77
21	b	1240	CLA	C2D-C1D-ND	2.76	112.86	110.13
21	a	1124	CLA	O2A-CGA-CBA	2.76	120.26	111.83
21	b	1231	CLA	C1-O2A-CGA	2.76	123.34	116.65
21	A	1101	CLA	CHA-C1A-NA	-2.76	120.14	126.39
21	J	1302	CLA	C1-O2A-CGA	2.76	123.34	116.65
21	a	1118	CLA	CHD-C1D-ND	-2.76	120.92	124.80
21	A	1013	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	1	1133	CLA	C3B-C4B-NB	-2.76	108.06	110.53
21	2	1231	CLA	C1D-ND-C4D	-2.76	104.38	106.31
21	B	1230	CLA	O2A-C1-C2	2.76	118.73	108.11
21	2	1226	CLA	CHA-C4D-ND	2.76	138.24	132.55
21	a	1011	CLA	C3B-C4B-NB	-2.76	108.07	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	5004	LMG	O8-C28-C29	2.76	120.25	111.83
21	B	1239	CLA	O2A-CGA-CBA	2.76	120.25	111.83
36	I	4020	EQ3	C29-C30-C25	2.76	114.44	110.44
21	B	1234	CLA	CMA-C3A-C4A	2.76	119.18	111.77
25	F	5002	LHG	O8-C23-C24	2.76	120.24	111.83
21	a	1128	CLA	CMB-C2B-C1B	-2.75	121.22	125.42
21	1	1134	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	2	1226	CLA	CMA-C3A-C4A	2.75	119.17	111.77
24	f	4016	BCR	C32-C1-C6	-2.75	105.93	110.24
21	A	1129	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	b	4005	BCR	C39-C30-C25	-2.75	105.93	110.24
21	A	1119	CLA	CHD-C1D-ND	-2.75	120.93	124.80
21	A	1137	CLA	CHD-C1D-ND	-2.75	120.93	124.80
26	A	5004	LMG	O8-C28-C29	2.75	120.22	111.83
31	L	5001	SQD	O7-S-C6	-2.75	102.65	106.76
24	K	4001	BCR	C23-C24-C25	-2.75	119.66	127.00
22	a	2001	PQN	C14-C13-C15	2.75	119.99	115.23
21	A	1120	CLA	CMA-C3A-C4A	2.74	119.15	111.77
21	a	1011	CLA	CHD-C1D-ND	-2.74	120.94	124.80
21	a	1013	CLA	C2D-C1D-ND	2.74	112.84	110.13
24	1	4007	BCR	C38-C26-C25	-2.74	121.49	124.48
21	1	1127	CLA	C3B-C4B-NB	-2.74	108.08	110.53
21	A	1011	CLA	CED-O2D-CGD	-2.74	109.69	115.92
21	b	1210	CLA	CHD-C1D-ND	-2.74	120.94	124.80
21	2	1232	CLA	CMA-C3A-C4A	2.74	119.14	111.77
21	b	1209	CLA	CHD-C1D-ND	-2.74	120.94	124.80
21	b	1239	CLA	O2A-CGA-CBA	2.74	120.19	111.83
21	a	1130	CLA	C1D-ND-C4D	-2.74	104.39	106.31
21	B	1235	CLA	CHD-C1D-ND	-2.74	120.95	124.80
21	B	1201	CLA	O2A-CGA-CBA	2.74	120.19	111.83
21	A	1801	CLA	C2D-C1D-ND	2.74	112.84	110.13
28	B	4011	45D	C19-C23-C25	-2.74	122.18	126.23
21	a	1127	CLA	C3B-C4B-NB	-2.74	108.08	110.53
21	B	1209	CLA	CHD-C1D-ND	-2.74	120.95	124.80
21	a	1011	CLA	C2A-C1A-CHA	2.74	128.62	123.87
21	b	1220	CLA	O2A-CGA-CBA	2.74	120.19	111.83
21	b	1237	CLA	C1-O2A-CGA	2.74	123.28	116.65
26	B	5005	LMG	O8-C28-C29	2.74	120.18	111.83
21	a	1111	CLA	CHD-C1D-ND	-2.74	120.95	124.80
21	b	1201	CLA	CHD-C1D-ND	-2.74	120.95	124.80
21	B	1217	CLA	C1-O2A-CGA	2.74	123.28	116.65
21	2	1214	CLA	C1D-ND-C4D	-2.74	104.39	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	4014	BCR	C19-C18-C17	2.74	123.31	119.01
25	0	5004	LHG	O8-C23-C24	2.74	120.18	111.83
24	l	4019	BCR	C40-C30-C25	-2.74	105.95	110.24
21	a	1108	CLA	CHD-C1D-ND	-2.74	120.95	124.80
21	B	1207	CLA	C3B-C4B-NB	-2.73	108.09	110.53
21	B	1212	CLA	C2D-C1D-ND	2.73	112.83	110.13
21	1	1012	CLA	C2D-C1D-ND	2.73	112.83	110.13
21	A	1137	CLA	C1D-ND-C4D	-2.73	104.39	106.31
21	B	1208	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	1	5001	LHG	O8-C23-C24	2.73	120.17	111.83
21	a	1118	CLA	C1D-ND-C4D	-2.73	104.39	106.31
21	2	1205	CLA	C1D-ND-C4D	-2.73	104.39	106.31
21	a	1139	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	b	4004	BCR	C38-C26-C25	-2.73	121.50	124.48
21	b	1218	CLA	CMA-C3A-C4A	2.73	119.11	111.77
24	j	4013	BCR	C8-C9-C10	2.73	123.30	119.01
21	a	1104	CLA	CHD-C1D-ND	-2.73	120.96	124.80
21	a	1140	CLA	CHD-C1D-ND	-2.73	120.96	124.80
21	B	1229	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
21	1	1117	CLA	CHD-C1D-ND	-2.73	120.96	124.80
21	2	1230	CLA	CHD-C1D-ND	-2.73	120.96	124.80
21	a	1111	CLA	C1D-ND-C4D	-2.73	104.40	106.31
21	1	1127	CLA	C1D-ND-C4D	-2.73	104.40	106.31
21	1	1107	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
21	b	1213	CLA	CHD-C1D-ND	-2.73	120.96	124.80
21	A	1011	CLA	C1D-ND-C4D	-2.73	104.40	106.31
21	B	1202	CLA	C1-O2A-CGA	2.73	123.25	116.65
24	a	4007	BCR	C38-C26-C25	-2.73	121.51	124.48
21	2	1201	CLA	O2A-CGA-CBA	2.73	120.15	111.83
21	a	1114	CLA	C1-O2A-CGA	2.73	123.25	116.65
21	L	1502	CLA	C2D-C1D-ND	2.73	112.83	110.13
21	a	1104	CLA	C2D-C1D-ND	2.73	112.83	110.13
21	l	1503	CLA	C2D-C1D-ND	2.73	112.83	110.13
21	a	1126	CLA	CHD-C1D-ND	-2.73	120.97	124.80
25	a	5005	LHG	O8-C23-C24	2.73	120.15	111.83
21	2	1234	CLA	C2D-C1D-ND	2.73	112.82	110.13
21	A	1139	CLA	C3B-C4B-NB	-2.73	108.10	110.53
21	B	1206	CLA	C1-O2A-CGA	2.72	123.25	116.65
30	b	4006	ECH	C36-C18-C19	2.72	122.25	118.09
21	1	1125	CLA	C1-O2A-CGA	2.72	123.25	116.65
21	B	1240	CLA	C1D-ND-C4D	-2.72	104.40	106.31
21	a	1104	CLA	C1D-ND-C4D	-2.72	104.40	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1107	CLA	CMA-C3A-C4A	2.72	119.09	111.77
24	b	4014	BCR	C15-C14-C13	2.72	131.10	127.28
21	B	1216	CLA	CMA-C3A-C4A	2.72	119.09	111.77
21	a	1113	CLA	CHD-C1D-ND	-2.72	120.97	124.80
21	B	1225	CLA	CHD-C1D-ND	-2.72	120.97	124.80
21	B	1224	CLA	C2D-C1D-ND	2.72	112.82	110.13
21	j	1302	CLA	C2D-C1D-ND	2.72	112.82	110.13
21	A	1129	CLA	C3B-C4B-NB	-2.72	108.10	110.53
21	F	1301	CLA	C1D-ND-C4D	-2.72	104.40	106.31
21	1	1133	CLA	CHD-C1D-ND	-2.72	120.98	124.80
21	l	1502	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	a	1133	CLA	CHD-C1D-ND	-2.72	120.98	124.80
21	1	1116	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	B	1204	CLA	C1-O2A-CGA	2.72	123.23	116.65
21	a	1013	CLA	C1D-ND-C4D	-2.72	104.41	106.31
24	A	4001	BCR	C35-C13-C12	2.72	122.24	118.09
21	2	1234	CLA	O2D-CGD-CBD	2.72	115.98	111.23
24	b	4017	BCR	C38-C26-C25	-2.72	121.52	124.48
21	2	1238	CLA	C3B-C4B-NB	-2.72	108.11	110.53
21	k	1402	CLA	O2A-CGA-CBA	2.72	120.11	111.83
21	1	1133	CLA	C1D-ND-C4D	-2.72	104.41	106.31
21	A	1132	CLA	CHD-C1D-ND	-2.71	120.98	124.80
21	2	1221	CLA	CHA-C4D-ND	2.71	138.15	132.55
21	A	1140	CLA	CHD-C1D-ND	-2.71	120.98	124.80
21	b	1230	CLA	CMA-C3A-C4A	2.71	119.07	111.77
21	1	1131	CLA	C3B-C4B-NB	-2.71	108.11	110.53
35	L	6001	LMT	C3B-C4B-C5B	-2.71	105.31	110.23
21	b	1214	CLA	CHD-C1D-ND	-2.71	120.98	124.80
36	I	4020	EQ3	C15-C16-C17	-2.71	117.97	123.52
21	B	1207	CLA	C1D-ND-C4D	-2.71	104.41	106.31
24	L	4019	BCR	C37-C22-C23	2.71	122.23	118.09
21	a	1101	CLA	CHA-C1A-NA	-2.71	120.25	126.39
24	i	4018	BCR	C39-C30-C25	-2.71	105.99	110.24
21	b	1203	CLA	CHD-C1D-ND	-2.71	120.99	124.80
24	l	4019	BCR	C34-C9-C10	-2.71	118.42	122.82
24	1	4012	BCR	C39-C30-C25	-2.71	105.99	110.24
24	b	4018	BCR	C38-C26-C25	-2.71	121.53	124.48
21	6	1302	CLA	C3B-C4B-NB	-2.71	108.11	110.53
21	1	1110	CLA	CHD-C1D-ND	-2.71	120.99	124.80
21	a	1110	CLA	C1D-ND-C4D	-2.71	104.41	106.31
21	b	1214	CLA	C3B-C4B-NB	-2.71	108.11	110.53
21	b	1230	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})
21	B	1225	CLA	C2D-C1D-ND	2.71	112.81	110.13
21	a	1125	CLA	C1D-ND-C4D	-2.71	104.41	106.31
21	2	1201	CLA	C3B-C4B-NB	-2.71	108.11	110.53
21	B	1204	CLA	O2A-CGA-CBA	2.71	120.08	111.83
25	l	5001	LHG	O8-C23-C24	2.71	120.08	111.83
21	a	1131	CLA	C1D-ND-C4D	-2.71	104.41	106.31
25	l	5001	LHG	C5-O7-C7	-2.71	111.32	117.80
21	2	1237	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	2	1228	CLA	CHD-C1D-ND	-2.70	121.00	124.80
24	A	4007	BCR	C40-C30-C25	-2.70	106.00	110.24
21	A	1801	CLA	O2A-CGA-CBA	2.70	120.08	111.83
24	B	4018	BCR	C39-C30-C25	-2.70	106.00	110.24
24	0	4022	BCR	C29-C28-C27	2.70	117.22	111.28
21	a	1115	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	2	1210	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	a	1127	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	a	1101	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	k	4001	BCR	C40-C30-C25	-2.70	106.01	110.24
21	b	1219	CLA	O2A-CGA-CBA	2.70	120.07	111.83
36	I	4020	EQ3	C7-C6-C5	-2.70	115.33	121.56
21	a	1137	CLA	C1D-ND-C4D	-2.70	104.42	106.31
21	1	1107	CLA	C1D-ND-C4D	-2.70	104.42	106.31
24	1	4003	BCR	C39-C30-C25	-2.70	106.01	110.24
21	B	1207	CLA	CHD-C1D-ND	-2.70	121.00	124.80
21	2	1202	CLA	CMA-C3A-C4A	2.70	119.03	111.77
21	a	1136	CLA	C2D-C1D-ND	2.70	112.80	110.13
21	2	1203	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	2	1224	CLA	O2A-CGA-CBA	2.70	120.06	111.83
24	2	4018	BCR	C30-C25-C24	2.70	122.96	115.65
21	2	1210	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	A	1130	CLA	C1D-ND-C4D	-2.70	104.42	106.31
21	a	1106	CLA	CHD-C1D-ND	-2.69	121.01	124.80
21	a	1102	CLA	C1D-ND-C4D	-2.69	104.42	106.31
24	b	4010	BCR	C40-C30-C25	-2.69	106.02	110.24
21	2	1206	CLA	CMA-C3A-C4A	2.69	119.01	111.77
21	B	1217	CLA	CMA-C3A-C4A	2.69	119.01	111.77
21	a	1115	CLA	CMA-C3A-C4A	2.69	119.01	111.77
24	b	4004	BCR	C30-C25-C26	-2.69	118.96	122.64
24	2	4014	BCR	C39-C30-C25	-2.69	106.02	110.24
21	A	1106	CLA	C2D-C1D-ND	2.69	112.79	110.13
21	1	1140	CLA	CHD-C1D-ND	-2.69	121.02	124.80
31	f	5001	SQD	O7-S-C6	-2.69	102.74	106.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1211	CLA	C3B-C4B-NB	-2.69	108.13	110.53
21	B	1239	CLA	C2D-C1D-ND	2.69	112.79	110.13
21	L	1501	CLA	CMA-C3A-C4A	2.69	119.00	111.77
21	1	1011	CLA	CHA-C4D-ND	2.69	138.09	132.55
25	l	5004	LHG	O8-C23-C24	2.69	120.03	111.83
21	b	1220	CLA	CHD-C1D-ND	-2.68	121.02	124.80
21	a	1119	CLA	CMA-C3A-C4A	2.68	118.99	111.77
34	J	4015	ZEX	C31-C30-C29	-2.68	123.51	127.28
28	B	4011	45D	C30-C32-C34	-2.68	115.42	123.20
21	a	1134	CLA	CMA-C3A-C4A	2.68	118.98	111.77
21	A	1124	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	J	1302	CLA	C1D-ND-C4D	-2.68	104.43	106.31
21	1	1101	CLA	C1D-ND-C4D	-2.68	104.43	106.31
21	B	1212	CLA	CHD-C1D-ND	-2.68	121.03	124.80
24	B	4017	BCR	C36-C18-C19	-2.68	113.99	118.09
21	A	1132	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	1	1109	CLA	CHA-C4D-ND	2.68	138.08	132.55
21	A	1131	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	a	1115	CLA	C2D-C1D-ND	2.68	112.78	110.13
21	1	1126	CLA	C2D-C1D-ND	2.68	112.78	110.13
21	1	1136	CLA	C2D-C1D-ND	2.68	112.78	110.13
21	8	1402	CLA	C2D-C1D-ND	2.68	112.78	110.13
21	b	1219	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	L	5005	LHG	O8-C23-C24	2.68	120.00	111.83
21	2	1223	CLA	O2A-CGA-CBA	2.68	120.00	111.83
21	a	1119	CLA	CHD-C1D-ND	-2.68	121.03	124.80
30	b	4006	ECH	C20-C19-C18	2.68	133.71	126.36
21	K	1401	CLA	CMA-C3A-C4A	2.68	118.97	111.77
21	2	1202	CLA	O2A-CGA-CBA	2.68	120.00	111.83
21	B	1238	CLA	C1-O2A-CGA	2.68	123.13	116.65
21	b	1226	CLA	O2A-C1-C2	2.68	118.41	108.11
21	2	1222	CLA	CHD-C1D-ND	-2.68	121.04	124.80
21	B	1230	CLA	C2D-C1D-ND	2.68	112.77	110.13
21	2	1213	CLA	CMA-C3A-C4A	2.68	118.96	111.77
21	1	1136	CLA	CHD-C1D-ND	-2.67	121.04	124.80
21	2	1221	CLA	CMD-C2D-C3D	-2.67	121.56	127.69
30	B	4006	ECH	C8-C7-C6	-2.67	119.86	127.00
34	J	4015	ZEX	C39-C29-C30	-2.67	118.48	122.82
21	k	1401	CLA	C1D-ND-C4D	-2.67	104.44	106.31
21	a	1112	CLA	O2A-CGA-CBA	2.67	119.98	111.83
25	l	5003	LHG	O8-C23-C24	2.67	119.98	111.83
21	1	1106	CLA	CMA-C3A-C4A	2.67	118.95	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1138	CLA	CHD-C1D-ND	-2.67	121.04	124.80
21	1	1011	CLA	O2A-CGA-CBA	2.67	119.98	111.83
21	B	1023	CLA	O2D-CGD-CBD	2.67	115.90	111.23
21	2	1239	CLA	C2D-C1D-ND	2.67	112.77	110.13
21	2	1021	CLA	CHA-C4D-ND	2.67	138.06	132.55
21	A	1117	CLA	CHD-C1D-ND	-2.67	121.05	124.80
21	2	1218	CLA	C2D-C1D-ND	2.67	112.77	110.13
21	A	1135	CLA	CMA-C3A-C4A	2.67	118.94	111.77
21	1	1137	CLA	C3B-C4B-NB	-2.67	108.15	110.53
24	B	4017	BCR	C38-C26-C25	-2.67	121.57	124.48
21	b	1023	CLA	O2D-CGD-CBD	2.67	115.89	111.23
21	a	1116	CLA	C1D-ND-C4D	-2.67	104.44	106.31
21	A	1124	CLA	CMA-C3A-C4A	2.67	118.94	111.77
24	A	4001	BCR	C40-C30-C25	-2.67	106.06	110.24
21	1	1013	CLA	C3B-C4B-NB	-2.67	108.15	110.53
21	A	1109	CLA	CHD-C1D-ND	-2.67	121.05	124.80
21	A	1129	CLA	C2D-C1D-ND	2.67	112.76	110.13
21	1	1130	CLA	C1D-ND-C4D	-2.67	104.44	106.31
21	A	1117	CLA	C3B-C4B-NB	-2.66	108.15	110.53
21	a	1118	CLA	C3B-C4B-NB	-2.66	108.15	110.53
21	L	1501	CLA	C1D-ND-C4D	-2.66	104.44	106.31
21	B	1226	CLA	CHD-C1D-ND	-2.66	121.05	124.80
21	8	1402	CLA	CMA-C3A-C4A	2.66	118.93	111.77
21	2	1209	CLA	CHA-C4D-ND	2.66	138.04	132.55
21	A	1115	CLA	C2D-C1D-ND	2.66	112.76	110.13
21	b	1236	CLA	O2A-CGA-CBA	2.66	119.94	111.83
21	A	1138	CLA	C1-O2A-CGA	2.66	123.09	116.65
21	B	1214	CLA	O2A-CGA-CBA	2.66	119.94	111.83
21	b	1238	CLA	C1-O2A-CGA	2.66	123.08	116.65
21	1	1128	CLA	C1-O2A-CGA	2.66	123.08	116.65
21	A	1113	CLA	CHD-C1D-ND	-2.66	121.06	124.80
21	1	1122	CLA	CHD-C1D-ND	-2.66	121.06	124.80
24	i	4018	BCR	C38-C26-C25	-2.66	121.58	124.48
21	B	1235	CLA	CMA-C3A-C4A	2.66	118.92	111.77
21	a	1112	CLA	CMA-C3A-C4A	2.66	118.92	111.77
21	1	1115	CLA	CHD-C1D-ND	-2.66	121.06	124.80
21	b	1235	CLA	C3B-C4B-NB	-2.66	108.16	110.53
21	0	1501	CLA	CMA-C3A-C4A	2.66	118.91	111.77
21	2	1212	CLA	C2D-C1D-ND	2.66	112.75	110.13
21	A	1136	CLA	C2D-C1D-ND	2.65	112.75	110.13
21	b	1021	CLA	CHA-C4D-ND	2.65	138.03	132.55
21	a	1109	CLA	C1D-ND-C4D	-2.65	104.45	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	4018	BCR	C12-C13-C14	-2.65	114.83	119.01
21	A	1012	CLA	C2D-C1D-ND	2.65	112.75	110.13
21	J	1302	CLA	C3B-C4B-NB	-2.65	108.16	110.53
21	2	1208	CLA	C1D-ND-C4D	-2.65	104.45	106.31
21	2	1217	CLA	C1D-ND-C4D	-2.65	104.45	106.31
21	a	1136	CLA	C1-O2A-CGA	2.65	123.07	116.65
25	1	5005	LHG	O8-C23-C24	2.65	119.92	111.83
21	2	1218	CLA	CHD-C1D-ND	-2.65	121.07	124.80
21	2	1227	CLA	CHD-C1D-ND	-2.65	121.07	124.80
24	A	4002	BCR	C35-C13-C12	2.65	122.14	118.09
21	A	1109	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	J	4013	BCR	C40-C30-C25	-2.65	106.09	110.24
24	a	4008	BCR	C40-C30-C25	-2.65	106.09	110.24
21	b	1204	CLA	C1D-ND-C4D	-2.65	104.45	106.31
21	k	1402	CLA	CHD-C1D-ND	-2.65	121.07	124.80
21	A	1130	CLA	CHD-C1D-ND	-2.65	121.08	124.80
21	1	1116	CLA	C1D-ND-C4D	-2.65	104.45	106.31
21	b	1206	CLA	C1-O2A-CGA	2.65	123.06	116.65
24	6	4016	BCR	C30-C25-C26	-2.65	119.02	122.64
21	2	1222	CLA	O2A-CGA-CBA	2.65	119.91	111.83
21	a	1130	CLA	CMA-C3A-C4A	2.65	118.89	111.77
21	a	1137	CLA	CHA-C4D-ND	2.65	138.01	132.55
21	B	1218	CLA	CMA-C3A-C4A	2.65	118.88	111.77
21	2	1201	CLA	CMA-C3A-C4A	2.65	118.88	111.77
21	1	1125	CLA	C1D-ND-C4D	-2.65	104.46	106.31
21	a	1126	CLA	C2D-C1D-ND	2.65	112.74	110.13
21	2	1210	CLA	C2D-C1D-ND	2.65	112.74	110.13
30	m	4021	ECH	C28-C27-C26	-2.64	116.27	118.64
21	1	1101	CLA	O2A-CGA-CBA	2.64	119.90	111.83
21	2	1213	CLA	CHD-C1D-ND	-2.64	121.08	124.80
21	b	1212	CLA	C2D-C1D-ND	2.64	112.74	110.13
21	1	1125	CLA	CHD-C1D-ND	-2.64	121.08	124.80
21	a	1137	CLA	O2A-CGA-CBA	2.64	119.89	111.83
21	B	1224	CLA	CHD-C1D-ND	-2.64	121.08	124.80
21	1	1112	CLA	CHD-C1D-ND	-2.64	121.08	124.80
25	A	5007	LHG	O7-C7-O9	-2.64	117.53	123.70
21	1	1101	CLA	CHA-C1A-NA	-2.64	120.41	126.39
30	i	4020	ECH	C29-C30-C25	-2.64	106.60	110.44
21	a	1129	CLA	C1-O2A-CGA	2.64	123.04	116.65
21	A	1120	CLA	C2D-C1D-ND	2.64	112.74	110.13
21	a	1011	CLA	CHA-C4D-ND	2.64	138.00	132.55
21	b	1224	CLA	C1D-ND-C4D	-2.64	104.46	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	1401	CLA	C1D-ND-C4D	-2.64	104.46	106.31
21	j	1303	CLA	CHD-C1D-ND	-2.64	121.09	124.80
24	1	4007	BCR	C39-C30-C25	-2.64	106.11	110.24
21	A	1104	CLA	CHD-C1D-ND	-2.64	121.09	124.80
21	2	1240	CLA	CHD-C1D-ND	-2.64	121.09	124.80
25	A	5007	LHG	O8-C23-C24	2.64	119.88	111.83
21	7	1302	CLA	C2D-C1D-ND	2.64	112.74	110.13
21	1	1011	CLA	C2A-C1A-CHA	2.64	128.44	123.87
21	1	1134	CLA	CHD-C1D-ND	-2.64	121.09	124.80
25	l	5002	LHG	O8-C23-C24	2.63	119.87	111.83
21	F	1302	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	6	4016	BCR	C12-C13-C14	2.63	123.15	119.01
21	1	1134	CLA	C2D-C1D-ND	2.63	112.73	110.13
21	1	1128	CLA	O2A-CGA-CBA	2.63	119.86	111.83
21	A	1013	CLA	C1-O2A-CGA	2.63	123.02	116.65
21	a	1139	CLA	C1-O2A-CGA	2.63	123.02	116.65
21	b	1212	CLA	CHA-C4D-ND	2.63	137.98	132.55
21	2	1216	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	2	1229	CLA	C2D-C1D-ND	2.63	112.73	110.13
24	1	4019	BCR	C40-C30-C25	-2.63	106.12	110.24
24	A	4019	BCR	C30-C25-C26	-2.63	119.04	122.64
21	A	1140	CLA	C2D-C1D-ND	2.63	112.73	110.13
21	a	1105	CLA	O2A-CGA-CBA	2.63	119.85	111.83
21	a	1128	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	B	1220	CLA	CHD-C1D-ND	-2.63	121.10	124.80
21	b	1205	CLA	C2D-C1D-ND	2.63	112.73	110.13
21	b	1223	CLA	CHD-C1D-ND	-2.63	121.11	124.80
21	b	1214	CLA	O2A-CGA-CBA	2.63	119.84	111.83
21	B	1023	CLA	CMA-C3A-C4A	2.63	118.83	111.77
21	2	1219	CLA	CHA-C1A-NA	-2.63	120.44	126.39
21	B	1205	CLA	C2D-C1D-ND	2.63	112.72	110.13
21	K	1401	CLA	CAA-CBA-CGA	-2.63	105.75	113.21
21	A	1125	CLA	CHA-C4D-ND	2.63	137.97	132.55
21	B	1223	CLA	CHD-C1D-ND	-2.63	121.11	124.80
21	1	1107	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	1	1138	CLA	C1D-ND-C4D	-2.62	104.47	106.31
21	b	1213	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
21	2	1216	CLA	C2D-C1D-ND	2.62	112.72	110.13
21	2	1212	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	2	1235	CLA	CMA-C3A-C4A	2.62	118.82	111.77
24	a	4012	BCR	C8-C9-C10	2.62	123.13	119.01
21	1	1801	CLA	CMA-C3A-C4A	2.62	118.81	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1801	CLA	CHD-C1D-ND	-2.62	121.12	124.80
21	A	1105	CLA	C3B-C4B-NB	-2.62	108.19	110.53
21	a	1109	CLA	CHA-C4D-ND	2.62	137.95	132.55
22	b	2002	PQN	C2M-C2-C3	-2.62	120.15	124.45
21	b	1220	CLA	C1D-ND-C4D	-2.62	104.48	106.31
21	2	1214	CLA	CHD-C1D-ND	-2.62	121.12	124.80
21	a	1116	CLA	O2A-CGA-CBA	2.61	119.81	111.83
21	A	1128	CLA	C1-O2A-CGA	2.61	122.98	116.65
21	A	1138	CLA	C1D-ND-C4D	-2.61	104.48	106.31
37	L	5004	DGD	O1G-C1A-C2A	2.61	119.80	111.83
21	b	1220	CLA	CHA-C4D-ND	2.61	137.94	132.55
21	J	1302	CLA	C2D-C1D-ND	2.61	112.71	110.13
30	i	4020	ECH	C28-C27-C26	-2.61	116.30	118.64
21	B	1021	CLA	CHA-C4D-ND	2.61	137.94	132.55
21	A	1108	CLA	C2D-C1D-ND	2.61	112.71	110.13
21	k	1402	CLA	C2D-C1D-ND	2.61	112.71	110.13
21	k	1402	CLA	CMA-C3A-C4A	2.61	118.79	111.77
21	A	1134	CLA	O2A-CGA-CBA	2.61	119.79	111.83
21	B	1217	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	a	1105	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	a	1124	CLA	CHD-C1D-ND	-2.61	121.13	124.80
21	b	1208	CLA	C1-O2A-CGA	2.61	122.97	116.65
21	j	1303	CLA	C3B-C4B-NB	-2.61	108.20	110.53
21	b	1022	CLA	CHD-C1D-ND	-2.61	121.13	124.80
21	A	1112	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	B	4017	BCR	C40-C30-C25	-2.61	106.15	110.24
24	a	4003	BCR	C39-C30-C25	-2.61	106.16	110.24
21	2	1237	CLA	C1D-ND-C4D	-2.61	104.48	106.31
21	2	1211	CLA	C1D-ND-C4D	-2.61	104.48	106.31
21	A	1121	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
21	2	1022	CLA	CMA-C3A-C4A	2.61	118.78	111.77
21	B	1210	CLA	CHA-C4D-ND	2.61	137.93	132.55
21	l	1502	CLA	CHD-C1D-ND	-2.61	121.14	124.80
21	a	1102	CLA	CMA-C3A-C4A	2.60	118.77	111.77
21	A	1122	CLA	CHD-C1D-ND	-2.60	121.14	124.80
21	A	1112	CLA	CHD-C1D-ND	-2.60	121.14	124.80
21	b	1218	CLA	O2A-CGA-CBA	2.60	119.77	111.83
21	1	1129	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
21	A	1138	CLA	CMA-C3A-C4A	2.60	118.77	111.77
30	2	4006	ECH	C8-C7-C6	-2.60	120.05	127.00
21	2	1227	CLA	CHA-C4D-ND	2.60	137.92	132.55
21	2	1228	CLA	CHA-C4D-ND	2.60	137.92	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	7	4015	ZEX	C31-C30-C29	-2.60	123.63	127.28
21	8	1401	CLA	CHD-C1D-ND	-2.60	121.14	124.80
24	a	4008	BCR	C40-C30-C29	2.60	118.94	108.95
21	a	1139	CLA	CHD-C1D-ND	-2.60	121.14	124.80
21	2	1238	CLA	CHD-C1D-ND	-2.60	121.14	124.80
21	B	1225	CLA	O2A-CGA-CBA	2.60	119.76	111.83
21	A	1012	CLA	CHA-C1A-NA	-2.60	120.51	126.39
21	b	1203	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
21	1	1105	CLA	CHD-C1D-ND	-2.60	121.15	124.80
21	b	1223	CLA	C1D-ND-C4D	-2.60	104.49	106.31
21	a	1118	CLA	CMA-C3A-C4A	2.60	118.75	111.77
21	a	1109	CLA	CHD-C1D-ND	-2.60	121.15	124.80
21	a	1104	CLA	CHA-C4D-ND	2.59	137.90	132.55
21	L	1501	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	2	1236	CLA	C3B-C4B-NB	-2.59	108.22	110.53
21	B	1223	CLA	O2A-CGA-CBA	2.59	119.74	111.83
21	B	1022	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	b	1220	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	b	1205	CLA	C3B-C4B-NB	-2.59	108.22	110.53
21	a	1136	CLA	CHD-C1D-ND	-2.59	121.16	124.80
21	B	1209	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	b	1228	CLA	CHD-C1D-ND	-2.59	121.16	124.80
21	2	1236	CLA	CHD-C1D-ND	-2.59	121.16	124.80
21	b	1207	CLA	O2A-CGA-CBA	2.59	119.73	111.83
24	1	4012	BCR	C40-C30-C29	2.59	118.89	108.95
21	1	1011	CLA	CHD-C1D-ND	-2.59	121.16	124.80
25	M	5001	LHG	O8-C23-C24	2.59	119.73	111.83
21	2	1224	CLA	C2D-C1D-ND	2.59	112.69	110.13
24	L	4022	BCR	C39-C30-C25	-2.59	106.18	110.24
24	A	4019	BCR	C15-C14-C13	-2.59	123.65	127.28
21	A	1104	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	B	1207	CLA	C2D-C1D-ND	2.59	112.69	110.13
21	L	1502	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	b	1229	CLA	CMA-C3A-C4A	2.59	118.73	111.77
24	A	4001	BCR	C34-C9-C10	-2.59	118.62	122.82
21	B	1227	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	2	1230	CLA	CMA-C3A-C4A	2.59	118.72	111.77
25	A	5003	LHG	C5-O7-C7	-2.59	111.61	117.80
24	B	4017	BCR	C19-C18-C17	2.59	123.08	119.01
21	a	1106	CLA	C3B-C4B-NB	-2.59	108.22	110.53
21	1	1113	CLA	C1D-ND-C4D	-2.59	104.50	106.31
21	b	1023	CLA	CHA-C4D-ND	2.59	137.88	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	5005	LHG	O8-C23-C24	2.59	119.72	111.83
21	2	1222	CLA	CMA-C3A-C4A	2.58	118.72	111.77
21	A	1101	CLA	C1-O2A-CGA	2.58	122.91	116.65
24	1	4012	BCR	C40-C30-C25	-2.58	106.19	110.24
21	B	1226	CLA	CHA-C4D-ND	2.58	137.88	132.55
21	2	1224	CLA	CHD-C1D-ND	-2.58	121.17	124.80
21	A	1115	CLA	CMA-C3A-C4A	2.58	118.72	111.77
21	k	1402	CLA	C3B-C4B-NB	-2.58	108.22	110.53
24	A	4003	BCR	C39-C30-C25	-2.58	106.19	110.24
24	1	4001	BCR	C40-C30-C25	-2.58	106.19	110.24
26	b	5002	LMG	C7-O1-C1	-2.58	108.26	113.80
21	f	1301	CLA	CMA-C3A-C4A	2.58	118.71	111.77
30	i	4020	ECH	C7-C6-C5	-2.58	115.61	121.56
21	A	1101	CLA	O2A-CGA-CBA	2.58	119.71	111.83
21	1	1126	CLA	O2A-CGA-CBA	2.58	119.71	111.83
21	B	1213	CLA	CHA-C4D-ND	2.58	137.88	132.55
21	1	1140	CLA	C1D-ND-C4D	-2.58	104.50	106.31
21	a	1012	CLA	CHA-C4D-ND	2.58	137.87	132.55
24	B	4014	BCR	C40-C30-C25	-2.58	106.20	110.24
21	a	1131	CLA	C3B-C4B-NB	-2.58	108.23	110.53
21	a	1133	CLA	C3B-C4B-NB	-2.58	108.23	110.53
21	2	1213	CLA	O2A-CGA-CBA	2.58	119.70	111.83
21	J	1303	CLA	CHD-C1D-ND	-2.58	121.17	124.80
21	1	1102	CLA	CHA-C4D-ND	2.58	137.87	132.55
21	A	1013	CLA	C2D-C1D-ND	2.58	112.68	110.13
21	2	1236	CLA	O2D-CGD-CBD	2.58	115.74	111.23
21	1	1126	CLA	CHD-C1D-ND	-2.58	121.18	124.80
24	b	4014	BCR	C40-C30-C25	-2.58	106.20	110.24
21	b	1205	CLA	CHA-C4D-ND	2.58	137.86	132.55
21	8	1402	CLA	CHD-C1D-ND	-2.58	121.18	124.80
24	A	4012	BCR	C40-C30-C29	2.58	118.84	108.95
21	1	1115	CLA	C2D-C1D-ND	2.57	112.67	110.13
21	1	1125	CLA	C2D-C1D-ND	2.57	112.67	110.13
21	b	1215	CLA	C3B-C4B-NB	-2.57	108.23	110.53
25	M	5001	LHG	O7-C7-O9	-2.57	117.69	123.70
24	2	4010	BCR	C39-C30-C25	-2.57	106.21	110.24
21	6	1301	CLA	CMA-C3A-C4A	2.57	118.69	111.77
21	2	1021	CLA	CHD-C1D-ND	-2.57	121.18	124.80
21	B	1238	CLA	O2A-C1-C2	2.57	118.01	108.11
21	1	1121	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	b	1227	CLA	CHD-C1D-ND	-2.57	121.19	124.80
21	1	1105	CLA	C2D-C1D-ND	2.57	112.67	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	h	4018	BCR	C40-C30-C29	2.57	118.82	108.95
21	B	1240	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	A	1013	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	2	1212	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	1	1111	CLA	CHA-C4D-ND	2.57	137.85	132.55
21	1	1126	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	2	1237	CLA	C3B-C4B-NB	-2.57	108.24	110.53
26	b	5005	LMG	O1-C7-C8	-2.57	104.57	110.82
24	a	4001	BCR	C40-C30-C25	-2.57	106.22	110.24
21	B	1232	CLA	C2D-C1D-ND	2.57	112.67	110.13
21	B	1221	CLA	CHA-C4D-ND	2.57	137.84	132.55
26	a	5002	LMG	O8-C28-C29	2.57	119.66	111.83
21	B	1216	CLA	CHA-C4D-ND	2.57	137.84	132.55
24	b	4018	BCR	C40-C30-C29	2.57	118.80	108.95
21	B	1211	CLA	CHD-C1D-ND	-2.56	121.19	124.80
21	b	1021	CLA	CHD-C1D-ND	-2.56	121.19	124.80
21	2	1220	CLA	C3B-C2B-C1B	-2.56	104.15	107.17
21	B	1223	CLA	CHA-C4D-ND	2.56	137.84	132.55
21	b	1240	CLA	O2A-CGA-CBA	2.56	119.65	111.83
21	2	1237	CLA	O2A-CGA-CBA	2.56	119.65	111.83
26	2	5002	LMG	O8-C28-C29	2.56	119.65	111.83
21	B	1221	CLA	CMA-C3A-C4A	2.56	118.67	111.77
21	2	1211	CLA	CHD-C1D-ND	-2.56	121.19	124.80
21	0	1503	CLA	O2A-CGA-CBA	2.56	119.65	111.83
21	a	1106	CLA	C2D-C1D-ND	2.56	112.66	110.13
21	B	1216	CLA	C3B-C4B-NB	-2.56	108.24	110.53
21	1	1127	CLA	O2A-CGA-CBA	2.56	119.65	111.83
24	a	4001	BCR	C40-C30-C29	2.56	118.78	108.95
25	B	5004	LHG	C5-O7-C7	-2.56	111.67	117.80
21	B	1239	CLA	CHD-C1D-ND	-2.56	121.20	124.80
21	1	1107	CLA	CHD-C1D-ND	-2.56	121.20	124.80
24	1	4007	BCR	C40-C30-C29	2.56	118.77	108.95
21	B	1206	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	a	1110	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	b	1216	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	b	1201	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	A	1125	CLA	CHD-C1D-ND	-2.56	121.20	124.80
21	b	1223	CLA	CHA-C4D-ND	2.56	137.83	132.55
21	b	1228	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	2	1230	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	b	1225	CLA	CMA-C3A-C4A	2.56	118.65	111.77
21	0	1501	CLA	CHD-C1D-ND	-2.56	121.20	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	1302	CLA	CHA-C1A-NA	-2.56	120.60	126.39
21	A	1104	CLA	CHA-C4D-ND	2.56	137.82	132.55
21	B	1210	CLA	CAC-C3C-C4C	2.56	128.12	124.79
21	2	1214	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	2	1220	CLA	CHD-C1D-ND	-2.56	121.20	124.80
21	b	1203	CLA	CHA-C4D-ND	2.56	137.82	132.55
24	B	4010	BCR	C39-C30-C25	-2.56	106.23	110.24
24	j	4013	BCR	C40-C30-C29	2.56	118.76	108.95
21	B	1205	CLA	CHA-C4D-ND	2.56	137.82	132.55
21	2	1230	CLA	CHA-C4D-ND	2.56	137.82	132.55
21	B	1214	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	A	1133	CLA	C2D-C1D-ND	2.55	112.65	110.13
21	a	1133	CLA	C2D-C1D-ND	2.55	112.65	110.13
24	A	4003	BCR	C40-C30-C29	2.55	118.75	108.95
24	i	4018	BCR	C40-C30-C29	2.55	118.75	108.95
24	b	4004	BCR	C40-C30-C29	2.55	118.75	108.95
21	2	1215	CLA	C1D-ND-C4D	-2.55	104.52	106.31
24	I	4018	BCR	C40-C30-C29	2.55	118.75	108.95
24	2	4014	BCR	C40-C30-C29	2.55	118.75	108.95
24	2	4017	BCR	C40-C30-C29	2.55	118.75	108.95
21	b	1226	CLA	CMA-C3A-C4A	2.55	118.63	111.77
25	A	5003	LHG	O8-C23-C24	2.55	119.61	111.83
21	a	1136	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	a	1013	CLA	C3B-C4B-NB	-2.55	108.25	110.53
25	a	5003	LHG	C5-O7-C7	-2.55	111.69	117.80
30	i	4020	ECH	C24-C23-C22	-2.55	122.46	126.23
24	a	4019	BCR	C40-C30-C29	2.55	118.74	108.95
24	2	4005	BCR	C40-C30-C29	2.55	118.74	108.95
21	a	1105	CLA	CHD-C1D-ND	-2.55	121.21	124.80
21	b	1207	CLA	CHD-C1D-ND	-2.55	121.21	124.80
21	2	1226	CLA	CHD-C1D-ND	-2.55	121.21	124.80
21	b	1238	CLA	CHD-C1D-ND	-2.55	121.22	124.80
21	B	1203	CLA	CHA-C4D-ND	2.55	137.81	132.55
21	1	1115	CLA	C1-O2A-CGA	2.55	122.82	116.65
21	B	1225	CLA	C3B-C4B-NB	-2.55	108.25	110.53
21	2	1210	CLA	O2A-CGA-CBA	2.55	119.61	111.83
24	9	4021	BCR	C40-C30-C29	2.55	118.73	108.95
24	b	4014	BCR	C40-C30-C29	2.55	118.73	108.95
24	b	4017	BCR	C40-C30-C29	2.55	118.73	108.95
21	b	1022	CLA	O2A-CGA-CBA	2.55	119.60	111.83
21	B	1023	CLA	C2D-C1D-ND	2.55	112.65	110.13
21	7	1302	CLA	C3B-C4B-NB	-2.55	108.26	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	4002	BCR	C40-C30-C29	2.55	118.73	108.95
24	B	4005	BCR	C40-C30-C29	2.55	118.72	108.95
30	2	4006	ECH	C11-C10-C9	-2.55	123.71	127.28
24	6	4016	BCR	C40-C30-C29	2.55	118.72	108.95
21	A	1131	CLA	CHA-C4D-ND	2.55	137.80	132.55
21	a	1138	CLA	O2A-CGA-CBA	2.54	119.59	111.83
24	A	4002	BCR	C38-C26-C25	-2.54	121.71	124.48
21	a	1133	CLA	O2A-CGA-CBA	2.54	119.59	111.83
21	B	1021	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	J	4013	BCR	C40-C30-C29	2.54	118.72	108.95
21	2	1214	CLA	CMA-C3A-C4A	2.54	118.61	111.77
24	l	4019	BCR	C40-C30-C29	2.54	118.72	108.95
24	A	4001	BCR	C40-C30-C29	2.54	118.72	108.95
21	a	1125	CLA	CHA-C4D-ND	2.54	137.80	132.55
21	2	1220	CLA	CHA-C4D-ND	2.54	137.80	132.55
24	7	4013	BCR	C34-C9-C10	-2.54	118.70	122.82
21	a	1120	CLA	CHD-C1D-ND	-2.54	121.22	124.80
24	0	4022	BCR	C40-C30-C29	2.54	118.71	108.95
24	A	4007	BCR	C40-C30-C29	2.54	118.71	108.95
21	a	1135	CLA	C3B-C4B-NB	-2.54	108.26	110.53
21	B	1210	CLA	CHD-C1D-ND	-2.54	121.23	124.80
21	6	1301	CLA	CHD-C1D-ND	-2.54	121.23	124.80
24	b	4005	BCR	C40-C30-C29	2.54	118.71	108.95
21	2	1203	CLA	C2D-C1D-ND	2.54	112.64	110.13
21	A	1134	CLA	CMA-C3A-C4A	2.54	118.60	111.77
21	A	1114	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	a	4007	BCR	C40-C30-C29	2.54	118.70	108.95
21	b	1238	CLA	C2D-C1D-ND	2.54	112.64	110.13
21	B	1239	CLA	CMA-C3A-C4A	2.54	118.60	111.77
24	1	4003	BCR	C40-C30-C29	2.54	118.70	108.95
21	A	1118	CLA	CHA-C4D-ND	2.54	137.79	132.55
24	i	4018	BCR	C37-C22-C23	2.54	121.97	118.09
21	B	1222	CLA	CHD-C1D-ND	-2.54	121.23	124.80
21	2	1236	CLA	O2A-CGA-CBA	2.54	119.58	111.83
21	B	1218	CLA	C2D-C1D-ND	2.54	112.64	110.13
24	L	4022	BCR	C40-C30-C29	2.54	118.69	108.95
24	8	4001	BCR	C40-C30-C29	2.54	118.69	108.95
21	b	1236	CLA	CMA-C3A-C4A	2.54	118.59	111.77
21	A	1125	CLA	C2D-C1D-ND	2.54	112.64	110.13
21	B	1220	CLA	C1D-ND-C4D	-2.54	104.53	106.31
24	2	4018	BCR	C40-C30-C29	2.54	118.69	108.95
24	B	4017	BCR	C40-C30-C29	2.54	118.69	108.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4018	BCR	C40-C30-C29	2.54	118.69	108.95
21	2	1217	CLA	CHD-C1D-ND	-2.54	121.23	124.80
24	K	4001	BCR	C40-C30-C29	2.54	118.69	108.95
24	a	4003	BCR	C40-C30-C29	2.54	118.69	108.95
21	A	1115	CLA	C3B-C4B-NB	-2.54	108.27	110.53
21	B	1209	CLA	CHA-C4D-ND	2.54	137.78	132.55
21	1	1110	CLA	CHA-C4D-ND	2.54	137.78	132.55
24	A	4002	BCR	C40-C30-C29	2.53	118.68	108.95
24	B	4004	BCR	C40-C30-C29	2.53	118.68	108.95
21	L	1502	CLA	CHD-C1D-ND	-2.53	121.23	124.80
21	b	1232	CLA	C2D-C1D-ND	2.53	112.63	110.13
24	2	4011	BCR	C40-C30-C29	2.53	118.68	108.95
21	B	1208	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	B	1231	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	2	1211	CLA	CHA-C4D-ND	2.53	137.78	132.55
21	B	1232	CLA	O2A-CGA-CBA	2.53	119.56	111.83
21	a	1102	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	L	4022	BCR	C35-C13-C12	2.53	121.96	118.09
24	7	4013	BCR	C40-C30-C29	2.53	118.68	108.95
21	2	1207	CLA	CMA-C3A-C4A	2.53	118.58	111.77
21	1	1132	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	f	4016	BCR	C40-C30-C29	2.53	118.67	108.95
21	B	1208	CLA	C1D-ND-C4D	-2.53	104.53	106.31
21	2	1207	CLA	C1D-ND-C4D	-2.53	104.53	106.31
24	2	4010	BCR	C40-C30-C29	2.53	118.67	108.95
21	B	1203	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	1	1139	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	b	1021	CLA	C3B-C2B-C1B	-2.53	104.19	107.17
21	B	1237	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	1	1106	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	1	4002	BCR	C40-C30-C29	2.53	118.67	108.95
21	B	1201	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	a	1139	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	b	1216	CLA	CHA-C4D-ND	2.53	137.77	132.55
24	l	4022	BCR	C40-C30-C29	2.53	118.66	108.95
21	A	1128	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	8	4001	BCR	C29-C28-C27	2.53	116.84	111.28
21	1	1801	CLA	CHA-C4D-ND	2.53	137.77	132.55
21	A	1105	CLA	C2D-C1D-ND	2.53	112.63	110.13
21	1	1801	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
21	A	1105	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	a	1138	CLA	C1D-ND-C4D	-2.53	104.54	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1113	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	B	1239	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	B	1220	CLA	CHA-C4D-ND	2.53	137.76	132.55
24	A	4002	BCR	C8-C9-C10	2.53	122.98	119.01
21	b	1226	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	A	1102	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	b	1232	CLA	CHA-C4D-ND	2.53	137.76	132.55
21	6	1302	CLA	CHA-C4D-ND	2.53	137.76	132.55
24	1	4019	BCR	C40-C30-C29	2.53	118.65	108.95
21	1	1112	CLA	O2A-CGA-CBA	2.53	119.54	111.83
31	0	5005	SQD	O7-S-C6	-2.53	102.98	106.76
21	a	1128	CLA	CHD-C1D-ND	-2.53	121.25	124.80
21	A	1127	CLA	CMA-C3A-C4A	2.52	118.56	111.77
21	1	1133	CLA	CHA-C4D-ND	2.52	137.76	132.55
21	B	1226	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
21	2	1217	CLA	CHA-C4D-ND	2.52	137.76	132.55
21	b	1201	CLA	C1D-ND-C4D	-2.52	104.54	106.31
21	a	1801	CLA	C2D-C1D-ND	2.52	112.62	110.13
21	b	1211	CLA	C2D-C1D-ND	2.52	112.62	110.13
24	2	4010	BCR	C38-C26-C25	-2.52	121.73	124.48
21	6	1302	CLA	C2A-C1A-CHA	2.52	128.25	123.87
24	1	4008	BCR	C40-C30-C29	2.52	118.64	108.95
24	A	4003	BCR	C1-C6-C7	2.52	122.50	115.65
21	A	1105	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	1	5007	LHG	O8-C23-C24	2.52	119.53	111.83
21	a	1138	CLA	C2D-C1D-ND	2.52	112.62	110.13
21	A	1120	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	J	1303	CLA	C3B-C4B-NB	-2.52	108.28	110.53
21	b	1216	CLA	C1D-ND-C4D	-2.52	104.54	106.31
21	1	1125	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	a	1801	CLA	CHD-C1D-ND	-2.52	121.25	124.80
21	1	1114	CLA	CHD-C1D-ND	-2.52	121.25	124.80
21	0	1502	CLA	CHD-C1D-ND	-2.52	121.25	124.80
36	I	4020	EQ3	C38-C26-C27	2.52	119.31	115.49
21	a	1118	CLA	O2A-CGA-CBA	2.52	119.52	111.83
21	b	1232	CLA	O2A-CGA-CBA	2.52	119.52	111.83
21	1	1111	CLA	CMA-C3A-C4A	2.52	118.55	111.77
24	a	4001	BCR	C27-C26-C25	-2.52	119.30	122.70
21	a	1110	CLA	CHA-C4D-ND	2.52	137.75	132.55
21	a	1104	CLA	CMA-C3A-C4A	2.52	118.55	111.77
21	B	1239	CLA	C1-O2A-CGA	2.52	122.75	116.65
21	A	1118	CLA	C1D-ND-C4D	-2.52	104.54	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	4006	ECH	C36-C18-C19	-2.52	114.24	118.09
24	L	4019	BCR	C40-C30-C29	2.52	118.62	108.95
21	1	1127	CLA	CHA-C4D-ND	2.52	137.75	132.55
24	0	4019	BCR	C40-C30-C29	2.52	118.62	108.95
24	A	4001	BCR	C30-C25-C26	-2.52	119.19	122.64
21	b	1230	CLA	CHD-C1D-ND	-2.52	121.26	124.80
21	2	1022	CLA	C1D-ND-C4D	-2.52	104.55	106.31
21	b	1223	CLA	C2D-C1D-ND	2.52	112.62	110.13
21	B	1023	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
21	A	1112	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	l	1503	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	B	1240	CLA	CHD-C1D-ND	-2.52	121.26	124.80
21	2	1218	CLA	O2A-CGA-CBA	2.52	119.51	111.83
24	A	4019	BCR	C40-C30-C29	2.52	118.61	108.95
21	A	1125	CLA	C3D-C2D-C1D	-2.52	102.40	105.83
24	1	4001	BCR	C40-C30-C29	2.52	118.61	108.95
24	a	4012	BCR	C40-C30-C29	2.52	118.61	108.95
21	A	1117	CLA	O2A-CGA-CBA	2.52	119.50	111.83
21	a	1108	CLA	CHA-C4D-ND	2.51	137.74	132.55
21	B	1206	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	2	1210	CLA	CMA-C3A-C4A	2.51	118.53	111.77
21	1	1012	CLA	CHA-C1A-NA	-2.51	120.70	126.39
21	A	1104	CLA	C1D-ND-C4D	-2.51	104.55	106.31
21	B	1232	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	A	1012	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	1	1140	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	1132	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	b	1221	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	1103	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	1101	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	2	1223	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	1127	CLA	CHA-C4D-ND	2.51	137.73	132.55
21	a	1138	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	2	1235	CLA	C2D-C1D-ND	2.51	112.61	110.13
28	h	4020	45D	C03-C07-C19	2.51	122.45	115.65
24	B	4010	BCR	C40-C30-C29	2.51	118.58	108.95
21	B	1210	CLA	C1D-ND-C4D	-2.51	104.55	106.31
21	2	1209	CLA	C1D-ND-C4D	-2.51	104.55	106.31
24	0	4022	BCR	C38-C26-C25	-2.51	121.75	124.48
21	b	1220	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	l	1501	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	a	1801	CLA	CHA-C4D-ND	2.51	137.72	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1116	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	b	4010	BCR	C40-C30-C29	2.51	118.58	108.95
21	1	1136	CLA	O2A-CGA-CBA	2.51	119.48	111.83
21	b	1212	CLA	C1-O2A-CGA	2.51	122.72	116.65
24	B	4014	BCR	C40-C30-C29	2.51	118.58	108.95
21	1	1103	CLA	C1D-ND-C4D	-2.51	104.55	106.31
24	7	4013	BCR	C8-C9-C10	2.51	122.95	119.01
21	b	1218	CLA	CHD-C1D-ND	-2.51	121.28	124.80
21	b	1213	CLA	C1-O2A-CGA	2.51	122.72	116.65
21	B	1231	CLA	C3B-C2B-C1B	-2.51	104.22	107.17
21	a	1104	CLA	C3D-C2D-C1D	-2.51	102.41	105.83
21	b	1217	CLA	C3B-C4B-NB	-2.51	108.29	110.53
21	1	1801	CLA	C1-O2A-CGA	2.51	122.72	116.65
21	A	1801	CLA	C3B-C4B-NB	-2.50	108.29	110.53
24	1	4008	BCR	C37-C22-C23	2.50	121.91	118.09
21	1	1107	CLA	C3B-C2B-C1B	-2.50	104.22	107.17
30	2	4006	ECH	C37-C22-C21	2.50	126.87	122.82
24	a	4002	BCR	C38-C26-C25	-2.50	121.75	124.48
21	A	1117	CLA	C2D-C1D-ND	2.50	112.60	110.13
24	2	4004	BCR	C40-C30-C29	2.50	118.56	108.95
21	a	1124	CLA	C3D-C2D-C1D	-2.50	102.42	105.83
21	b	1217	CLA	O2A-CGA-CBA	2.50	119.47	111.83
21	1	1102	CLA	C1-O2A-CGA	2.50	122.71	116.65
21	B	1211	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	a	1123	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	2	1023	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	A	1119	CLA	CHA-C4D-ND	2.50	137.71	132.55
22	2	2002	PQN	C11-C3-C2	-2.50	120.60	124.89
21	A	1138	CLA	O2D-CGD-CBD	2.50	115.60	111.23
21	b	1206	CLA	CMA-C3A-C4A	2.50	118.49	111.77
21	b	1208	CLA	CHD-C1D-ND	-2.50	121.28	124.80
21	b	1213	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	2	1232	CLA	CHA-C4D-ND	2.50	137.71	132.55
21	b	1209	CLA	C2D-C1D-ND	2.50	112.60	110.13
21	7	1303	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	1	1111	CLA	CAC-C3C-C4C	2.50	128.04	124.79
21	l	1503	CLA	O2A-CGA-CBA	2.50	119.45	111.83
25	B	5004	LHG	O8-C23-C24	2.50	119.45	111.83
21	1	1012	CLA	CHD-C1D-ND	-2.50	121.29	124.80
21	A	1127	CLA	O2A-CGA-CBA	2.50	119.45	111.83
21	2	1206	CLA	O2A-CGA-CBA	2.50	119.45	111.83
21	1	1112	CLA	CHA-C4D-ND	2.50	137.70	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	4016	ZEX	C11-C12-C13	-2.50	119.52	126.36
21	1	1125	CLA	C3B-C4B-NB	-2.50	108.30	110.53
21	1	1104	CLA	C2D-C1D-ND	2.50	112.60	110.13
21	b	1228	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	a	1123	CLA	C1D-ND-C4D	-2.50	104.56	106.31
21	J	1303	CLA	O2A-CGA-CBA	2.50	119.44	111.83
24	A	4002	BCR	C37-C22-C23	2.50	121.90	118.09
21	A	1113	CLA	CHA-C4D-ND	2.50	137.70	132.55
21	l	1503	CLA	C1-O2A-CGA	2.49	122.69	116.65
21	2	1227	CLA	CMA-C3A-C4A	2.49	118.48	111.77
21	A	1106	CLA	C3B-C4B-NB	-2.49	108.30	110.53
24	1	4003	BCR	C40-C30-C25	-2.49	106.33	110.24
21	l	1501	CLA	CMA-C3A-C4A	2.49	118.48	111.77
21	1	1128	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	L	4022	BCR	C15-C14-C13	2.49	130.78	127.28
21	A	1011	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
28	h	4020	45D	C10-C18-C16	2.49	120.88	118.64
21	A	1130	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	2	1227	CLA	C1D-ND-C4D	-2.49	104.56	106.31
21	A	1139	CLA	C2D-C1D-ND	2.49	112.59	110.13
21	1	1137	CLA	C2D-C1D-ND	2.49	112.59	110.13
21	b	1239	CLA	C3B-C4B-NB	-2.49	108.31	110.53
21	A	1121	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	K	1402	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	1	1116	CLA	O2A-CGA-CBA	2.49	119.43	111.83
21	b	1208	CLA	C3B-C4B-NB	-2.49	108.31	110.53
21	b	1217	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	a	1120	CLA	C2D-C1D-ND	2.49	112.59	110.13
21	b	1206	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	b	1221	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	b	1223	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
25	a	5007	LHG	C5-O7-C7	-2.49	111.84	117.80
21	2	1214	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	A	1801	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	J	1302	CLA	CHA-C4D-ND	2.49	137.69	132.55
21	B	1237	CLA	CMA-C3A-C4A	2.49	118.46	111.77
21	1	1120	CLA	C3B-C4B-NB	-2.49	108.31	110.53
21	1	1130	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	B	1023	CLA	O2A-CGA-CBA	2.49	119.42	111.83
21	a	1113	CLA	C2D-C1D-ND	2.49	112.59	110.13
21	B	1202	CLA	C1D-ND-C4D	-2.49	104.57	106.31
21	a	1140	CLA	CHA-C4D-ND	2.49	137.68	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1012	CLA	O2A-CGA-CBA	2.49	119.42	111.83
28	h	4020	45D	C21-C15-C07	-2.49	120.11	124.11
21	b	1215	CLA	C2D-C1D-ND	2.49	112.59	110.13
21	2	1225	CLA	CHA-C4D-ND	2.49	137.68	132.55
24	b	4004	BCR	C24-C25-C26	-2.49	115.83	121.56
21	b	1212	CLA	CHA-C1A-NA	-2.49	120.76	126.39
21	a	1106	CLA	CMA-C3A-C4A	2.49	118.46	111.77
21	A	1109	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	A	1120	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	1	1119	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	a	1013	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	1	1104	CLA	CHA-C4D-ND	2.49	137.68	132.55
21	F	1301	CLA	CMA-C3A-C4A	2.48	118.45	111.77
21	b	1219	CLA	C1-O2A-CGA	2.48	122.66	116.65
21	a	1107	CLA	CMD-C2D-C3D	-2.48	121.99	127.69
21	F	1302	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	a	4019	BCR	C30-C25-C26	-2.48	119.24	122.64
21	A	1127	CLA	CHD-C1D-ND	-2.48	121.31	124.80
24	2	4010	BCR	C8-C9-C10	2.48	122.91	119.01
21	A	1123	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	A	4008	BCR	C40-C30-C29	2.48	118.48	108.95
21	a	1115	CLA	C3B-C4B-NB	-2.48	108.31	110.53
21	A	1127	CLA	CHA-C4D-ND	2.48	137.67	132.55
24	j	4013	BCR	C34-C9-C10	-2.48	118.80	122.82
21	B	1204	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	L	1503	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	2	1208	CLA	CHA-C4D-ND	2.48	137.67	132.55
21	A	1124	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
21	2	1223	CLA	C3B-C4B-NB	-2.48	108.31	110.53
24	k	4001	BCR	C40-C30-C29	2.48	118.47	108.95
21	A	1136	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	b	1240	CLA	CHA-C4D-ND	2.48	137.67	132.55
21	B	1231	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	a	4002	BCR	C8-C9-C10	2.48	122.91	119.01
21	A	1133	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	B	1202	CLA	CHA-C4D-ND	2.48	137.66	132.55
24	a	4012	BCR	C30-C25-C26	-2.48	119.25	122.64
21	B	1213	CLA	C1D-ND-C4D	-2.48	104.57	106.31
24	7	4013	BCR	C29-C28-C27	2.48	116.73	111.28
21	a	1136	CLA	C3D-C2D-C1D	-2.48	102.45	105.83
21	B	1214	CLA	C1D-ND-C4D	-2.48	104.57	106.31
21	b	1210	CLA	O2A-CGA-CBA	2.48	119.39	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1232	CLA	C3B-C4B-NB	-2.48	108.32	110.53
21	b	1231	CLA	CHA-C4D-ND	2.48	137.66	132.55
25	B	5006	LHG	C5-O7-C7	-2.48	111.87	117.80
21	B	1023	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	L	5002	SQD	O7-S-C6	-2.48	103.06	106.76
21	2	1216	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	A	1134	CLA	C3B-C4B-NB	-2.48	108.32	110.53
21	a	1116	CLA	C3B-C4B-NB	-2.48	108.32	110.53
21	a	1128	CLA	O2A-CGA-CBA	2.48	119.38	111.83
21	a	1133	CLA	CMA-C3A-C4A	2.48	118.43	111.77
21	J	1303	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	1	1123	CLA	CHA-C4D-ND	2.48	137.66	132.55
21	2	1219	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
21	1	1124	CLA	CHA-C4D-ND	2.47	137.66	132.55
21	a	1137	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	a	1132	CLA	C2D-C1D-ND	2.47	112.58	110.13
21	8	1402	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	A	1120	CLA	C1-O2A-CGA	2.47	122.64	116.65
21	1	1139	CLA	C1-O2A-CGA	2.47	122.64	116.65
21	2	1240	CLA	C3B-C4B-NB	-2.47	108.32	110.53
21	a	1132	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	1	1131	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	a	1140	CLA	C1D-ND-C4D	-2.47	104.58	106.31
21	b	1237	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	J	1303	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	L	1503	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	A	1110	CLA	C3B-C4B-NB	-2.47	108.32	110.53
24	k	4001	BCR	C38-C26-C25	-2.47	121.79	124.48
24	l	4019	BCR	C38-C26-C25	-2.47	121.79	124.48
21	a	1118	CLA	CHA-C4D-ND	2.47	137.65	132.55
21	b	1231	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
21	k	1402	CLA	C1-O2A-CGA	2.47	122.63	116.65
21	A	1101	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	b	1206	CLA	C3B-C4B-NB	-2.47	108.33	110.53
21	2	1228	CLA	C1D-ND-C4D	-2.47	104.58	106.31
21	B	1205	CLA	O2A-CGA-CBA	2.47	119.36	111.83
21	1	1114	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	l	1501	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	2	1201	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	B	1236	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	1	1110	CLA	C1D-ND-C4D	-2.47	104.58	106.31
21	A	1101	CLA	CHA-C4D-ND	2.47	137.64	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1214	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	B	1206	CLA	O2A-CGA-CBA	2.47	119.36	111.83
21	2	1023	CLA	O2A-CGA-CBA	2.47	119.36	111.83
21	b	1208	CLA	CMA-C3A-C4A	2.47	118.41	111.77
21	2	1205	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	a	1012	CLA	CMA-C3A-C4A	2.47	118.41	111.77
21	b	1219	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	a	1139	CLA	C1D-ND-C4D	-2.47	104.58	106.31
21	B	1211	CLA	C3B-C4B-NB	-2.47	108.33	110.53
21	7	1302	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	a	1125	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	2	1237	CLA	CHA-C4D-ND	2.47	137.64	132.55
21	A	1115	CLA	CHD-C1D-ND	-2.47	121.33	124.80
21	b	1232	CLA	CHD-C1D-ND	-2.47	121.33	124.80
21	1	1139	CLA	CHD-C1D-ND	-2.47	121.33	124.80
21	a	1117	CLA	C2D-C1D-ND	2.47	112.57	110.13
21	1	1013	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	a	1102	CLA	O2A-CGA-CBA	2.46	119.35	111.83
21	B	1240	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	b	1208	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	a	1132	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	2	1217	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	A	1113	CLA	O2A-CGA-CBA	2.46	119.34	111.83
24	a	4003	BCR	C40-C30-C25	-2.46	106.38	110.24
21	b	1208	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	a	1012	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
21	1	1127	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	A	1012	CLA	O2A-CGA-CBA	2.46	119.34	111.83
21	B	1022	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	1	1101	CLA	CHA-C4D-ND	2.46	137.63	132.55
21	2	1228	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
21	1	1135	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	K	1401	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
24	2	4004	BCR	C38-C26-C25	-2.46	121.80	124.48
21	A	1110	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	2	1224	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	B	1237	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	A	1128	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	B	1234	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	2	1213	CLA	C3B-C4B-NB	-2.46	108.34	110.53
21	0	1501	CLA	C3B-C4B-NB	-2.46	108.34	110.53
21	1	1111	CLA	CHD-C1D-ND	-2.46	121.34	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1102	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	A	1109	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	1	1118	CLA	C1D-ND-C4D	-2.46	104.59	106.31
21	a	1134	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	2	1213	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	B	1219	CLA	C3B-C4B-NB	-2.46	108.34	110.53
25	2	5004	LHG	O8-C23-C24	2.46	119.33	111.83
24	b	4018	BCR	C29-C28-C27	2.46	116.68	111.28
21	b	1216	CLA	O2A-CGA-CBA	2.46	119.32	111.83
21	A	1137	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	B	1220	CLA	O2A-CGA-CBA	2.46	119.32	111.83
21	2	1215	CLA	C2D-C1D-ND	2.46	112.56	110.13
21	b	1223	CLA	O2A-CGA-CBA	2.46	119.32	111.83
21	B	1212	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	2	1206	CLA	CHA-C4D-ND	2.45	137.61	132.55
30	M	4021	ECH	C23-C24-C25	-2.45	120.44	127.00
21	b	1022	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	1	1111	CLA	C1D-ND-C4D	-2.45	104.59	106.31
21	A	1129	CLA	O2A-CGA-CBA	2.45	119.32	111.83
21	k	1401	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	B	1221	CLA	C1D-ND-C4D	-2.45	104.59	106.31
21	j	1303	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	1	1129	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	B	1227	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	2	1212	CLA	CAA-C2A-C3A	-2.45	110.61	116.23
21	b	1227	CLA	C2D-C1D-ND	2.45	112.55	110.13
21	1	1118	CLA	CMA-C3A-C4A	2.45	118.36	111.77
21	1	1124	CLA	C1-O2A-CGA	2.45	122.58	116.65
21	a	1121	CLA	CHA-C4D-ND	2.45	137.61	132.55
21	b	1209	CLA	O2A-CGA-CBA	2.45	119.31	111.83
21	a	1108	CLA	C2D-C1D-ND	2.45	112.55	110.13
21	1	1139	CLA	C2D-C1D-ND	2.45	112.55	110.13
21	f	1301	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	2	1022	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	a	1116	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	j	1302	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	8	1401	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	A	1139	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	b	1220	CLA	CMA-C3A-C4A	2.45	118.35	111.77
24	1	4008	BCR	C29-C28-C27	2.45	116.66	111.28
25	b	5004	LHG	C5-O7-C7	-2.45	111.94	117.80
22	A	2001	PQN	C11-C3-C2	-2.45	120.69	124.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1222	CLA	C2D-C1D-ND	2.45	112.55	110.13
24	1	4008	BCR	C38-C26-C25	-2.45	121.81	124.48
21	A	1012	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	a	1113	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	B	1236	CLA	C3B-C4B-NB	-2.45	108.35	110.53
21	f	1302	CLA	C3B-C4B-NB	-2.45	108.35	110.53
21	b	1225	CLA	O2A-CGA-CBA	2.45	119.29	111.83
21	2	1227	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
21	2	1228	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
21	B	1239	CLA	CHA-C4D-ND	2.45	137.60	132.55
21	a	1110	CLA	C2D-C1D-ND	2.45	112.55	110.13
21	b	1235	CLA	C2D-C1D-ND	2.45	112.55	110.13
21	B	1207	CLA	C1-O2A-CGA	2.45	122.57	116.65
21	A	1107	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	B	1203	CLA	C2D-C1D-ND	2.45	112.55	110.13
24	2	4017	BCR	C40-C30-C25	-2.44	106.41	110.24
21	A	1102	CLA	C1D-ND-C4D	-2.44	104.60	106.31
21	2	1214	CLA	C2D-C1D-ND	2.44	112.55	110.13
21	A	1111	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	B	1215	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	b	1230	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	1	1116	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	A	1011	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
21	1	1118	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	1	1119	CLA	C3B-C4B-NB	-2.44	108.35	110.53
21	B	1206	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	b	1228	CLA	CMA-C3A-C4A	2.44	118.34	111.77
21	a	1011	CLA	O2A-CGA-CBA	2.44	119.28	111.83
21	J	1302	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	B	1201	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	B	1232	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	B	1217	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	2	1222	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	1	1135	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
24	a	4002	BCR	C29-C28-C27	2.44	116.64	111.28
21	1	1106	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	2	1234	CLA	O2A-CGA-CBA	2.44	119.28	111.83
36	I	4020	EQ3	C37-C22-C23	2.44	121.82	118.09
21	B	1210	CLA	O2A-CGA-CBA	2.44	119.28	111.83
24	9	4021	BCR	C8-C9-C10	2.44	122.85	119.01
21	a	1138	CLA	CHA-C4D-ND	2.44	137.58	132.55
24	9	4021	BCR	C27-C26-C25	-2.44	119.41	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	1503	CLA	O2A-CGA-CBA	2.44	119.27	111.83
36	I	4020	EQ3	C38-C26-C25	-2.44	120.19	124.11
25	2	5004	LHG	C5-O7-C7	-2.44	111.96	117.80
21	a	1130	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	1	1131	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	2	1219	CLA	CHA-C4D-ND	2.44	137.58	132.55
21	b	1209	CLA	C3B-C4B-NB	-2.44	108.35	110.53
21	2	1206	CLA	C1D-ND-C4D	-2.44	104.60	106.31
21	B	1229	CLA	O2A-CGA-CBA	2.44	119.27	111.83
21	a	1115	CLA	CHA-C4D-ND	2.44	137.58	132.55
21	2	1207	CLA	CHA-C4D-ND	2.44	137.58	132.55
24	2	4014	BCR	C36-C18-C19	-2.44	114.36	118.09
21	a	1114	CLA	CHA-C4D-ND	2.44	137.58	132.55
21	1	1124	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	1	1112	CLA	C3B-C4B-NB	-2.44	108.36	110.53
21	b	1235	CLA	CMA-C3A-C4A	2.44	118.32	111.77
21	2	1204	CLA	CMA-C3A-C4A	2.44	118.32	111.77
21	B	1211	CLA	C1D-ND-C4D	-2.44	104.60	106.31
21	b	1231	CLA	C3B-C4B-NB	-2.44	108.36	110.53
21	2	1202	CLA	CHA-C4D-ND	2.44	137.57	132.55
21	2	1213	CLA	C2D-C1D-ND	2.44	112.54	110.13
21	2	1211	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
21	1	1128	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	A	1115	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	2	1215	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	A	1115	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
21	1	1125	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
21	2	1219	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	2	1238	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	A	1131	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	2	1239	CLA	CAA-CBA-CGA	-2.43	106.30	113.21
21	K	1401	CLA	CAA-C2A-C1A	-2.43	104.00	111.97
21	b	1215	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	a	1012	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
21	a	1128	CLA	CHA-C4D-ND	2.43	137.57	132.55
21	a	1112	CLA	C1D-ND-C4D	-2.43	104.61	106.31
21	a	1112	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	1	1119	CLA	CMA-C3A-C4A	2.43	118.31	111.77
21	A	1121	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	1	1128	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	A	1114	CLA	CHD-C1D-ND	-2.43	121.38	124.80
24	a	4012	BCR	C27-C26-C25	-2.43	119.42	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1138	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	2	1023	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	2	1226	CLA	O2A-CGA-CBA	2.43	119.24	111.83
21	A	1123	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	b	1228	CLA	C2D-C1D-ND	2.43	112.53	110.13
21	a	1103	CLA	C1D-ND-C4D	-2.43	104.61	106.31
21	a	1138	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	1	1105	CLA	O2A-CGA-CBA	2.43	119.24	111.83
21	B	1208	CLA	O2A-CGA-CBA	2.43	119.24	111.83
31	B	5008	SQD	O7-S-C6	-2.43	103.13	106.76
21	a	1136	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
21	b	1206	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	a	1122	CLA	C1-O2A-CGA	2.43	122.53	116.65
21	f	1302	CLA	CHA-C4D-ND	2.43	137.56	132.55
21	A	1103	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
21	A	1118	CLA	C3B-C4B-NB	-2.43	108.36	110.53
21	a	1105	CLA	CHA-C4D-ND	2.43	137.55	132.55
21	b	1240	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
21	a	1126	CLA	CHA-C4D-ND	2.43	137.55	132.55
21	B	1208	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
21	a	1106	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	B	1217	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	b	1227	CLA	CHA-C4D-ND	2.42	137.55	132.55
30	i	4020	ECH	C8-C9-C10	-2.42	115.20	119.01
21	a	1107	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	a	1103	CLA	CMA-C3A-C4A	2.42	118.28	111.77
21	k	1401	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	b	5005	LMG	O6-C1-O1	-2.42	104.32	110.04
21	1	1111	CLA	C1-O2A-CGA	2.42	122.51	116.65
21	B	1224	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	k	1402	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	2	1203	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	A	1120	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
21	A	1106	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
21	a	1135	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	A	1011	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	a	1113	CLA	O2A-CGA-CBA	2.42	119.21	111.83
21	b	1236	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
21	1	1113	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	2	1216	CLA	CHD-C1D-ND	-2.42	121.40	124.80
21	A	1134	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	A	1138	CLA	C3B-C4B-NB	-2.42	108.37	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1134	CLA	C1D-ND-C4D	-2.42	104.62	106.31
21	F	1301	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	b	1210	CLA	CHA-C4D-ND	2.42	137.54	132.55
21	B	1211	CLA	C2D-C1D-ND	2.42	112.52	110.13
21	a	1127	CLA	C2D-C1D-ND	2.42	112.52	110.13
21	a	1119	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	a	1133	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	b	1218	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	A	1137	CLA	C2D-C1D-ND	2.42	112.52	110.13
21	B	1228	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	b	1219	CLA	CHA-C4D-ND	2.42	137.53	132.55
21	1	1013	CLA	C2D-C1D-ND	2.41	112.52	110.13
21	0	1501	CLA	CHA-C4D-ND	2.41	137.53	132.55
21	1	1122	CLA	CHA-C4D-ND	2.41	137.53	132.55
21	b	1222	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
21	b	1215	CLA	O2A-CGA-CBA	2.41	119.19	111.83
21	b	1229	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
21	B	1219	CLA	C2D-C1D-ND	2.41	112.51	110.13
21	a	1129	CLA	CHA-C4D-ND	2.41	137.53	132.55
21	1	1107	CLA	O2A-CGA-CBA	2.41	119.19	111.83
21	1	1133	CLA	O2A-CGA-CBA	2.41	119.19	111.83
24	2	4010	BCR	C36-C18-C19	-2.41	114.40	118.09
21	l	1501	CLA	O2A-CGA-CBA	2.41	119.19	111.83
30	i	4020	ECH	C35-C13-C12	-2.41	114.41	118.09
21	a	1119	CLA	C2D-C1D-ND	2.41	112.51	110.13
26	1	5002	LMG	O8-C28-C29	2.41	119.18	111.83
21	b	1212	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
21	b	1021	CLA	O2A-CGA-CBA	2.41	119.18	111.83
21	b	1201	CLA	O2A-CGA-CBA	2.41	119.18	111.83
21	b	1234	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	1	1109	CLA	C3B-C4B-NB	-2.41	108.38	110.53
21	2	1207	CLA	C3B-C4B-NB	-2.41	108.38	110.53
21	b	1236	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	B	1223	CLA	C3B-C4B-NB	-2.41	108.38	110.53
21	A	1113	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
21	2	1216	CLA	CHA-C1A-NA	-2.41	120.94	126.39
21	1	1103	CLA	CHA-C4D-ND	2.41	137.51	132.55
21	f	1302	CLA	C2D-C1D-ND	2.41	112.51	110.13
21	1	1134	CLA	CHA-C4D-ND	2.41	137.51	132.55
30	M	4021	ECH	C28-C27-C26	-2.41	116.48	118.64
21	A	1137	CLA	O2A-CGA-CBA	2.41	119.17	111.83
21	a	1125	CLA	O2A-CGA-CBA	2.41	119.17	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1126	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	A	1114	CLA	CHA-C4D-ND	2.40	137.51	132.55
28	B	4011	45D	C06-C04-C08	2.40	113.93	110.44
21	L	1502	CLA	C3B-C4B-NB	-2.40	108.38	110.53
21	1	1114	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	2	1219	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	B	1206	CLA	CHA-C4D-ND	2.40	137.51	132.55
21	8	1402	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
24	I	4018	BCR	C32-C1-C6	-2.40	106.47	110.24
21	b	1023	CLA	C1D-ND-C4D	-2.40	104.63	106.31
21	1	1121	CLA	C1D-ND-C4D	-2.40	104.63	106.31
21	K	1401	CLA	C1-O2A-CGA	2.40	122.47	116.65
21	1	1129	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	A	1129	CLA	CHA-C4D-ND	2.40	137.50	132.55
21	B	1227	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	2	1228	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	b	1201	CLA	CMA-C3A-C4A	2.40	118.23	111.77
24	0	4019	BCR	C32-C1-C6	-2.40	106.48	110.24
21	7	1302	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
21	2	1021	CLA	O2A-CGA-CBA	2.40	119.16	111.83
21	A	1135	CLA	O2D-CGD-CBD	2.40	115.43	111.23
21	a	1111	CLA	CHA-C4D-ND	2.40	137.50	132.55
21	2	1225	CLA	C3B-C4B-NB	-2.40	108.39	110.53
21	B	1206	CLA	CMA-C3A-C4A	2.40	118.22	111.77
22	B	2002	PQN	O4-C4-C5	-2.40	117.73	121.57
21	B	1219	CLA	O2A-CGA-CBA	2.40	119.15	111.83
24	a	4007	BCR	C35-C13-C12	2.40	121.75	118.09
24	0	4019	BCR	C34-C9-C10	-2.40	118.93	122.82
21	a	1114	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	b	1214	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	b	1234	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	2	1212	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
21	a	1131	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	a	5005	LHG	O7-C7-O9	-2.40	118.10	123.70
21	A	1114	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	b	1239	CLA	C2D-C1D-ND	2.40	112.50	110.13
24	b	4017	BCR	C40-C30-C25	-2.40	106.48	110.24
21	1	1101	CLA	C3B-C4B-NB	-2.40	108.39	110.53
21	1	1105	CLA	CHA-C4D-ND	2.40	137.49	132.55
24	2	4018	BCR	C40-C30-C25	-2.40	106.49	110.24
21	b	1222	CLA	C2D-C1D-ND	2.40	112.50	110.13
21	7	1302	CLA	CAA-C2A-C3A	-2.40	110.74	116.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1120	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	1	1012	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	A	1116	CLA	C2D-C1D-ND	2.39	112.50	110.13
21	a	1120	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	2	1210	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	A	1104	CLA	C3D-C2D-C1D	-2.39	102.56	105.83
22	b	2002	PQN	O1-C1-C10	-2.39	117.74	121.57
24	A	4001	BCR	C8-C9-C10	2.39	122.77	119.01
21	1	1121	CLA	CHA-C1A-NA	-2.39	120.97	126.39
21	b	1218	CLA	C3D-C2D-C1D	-2.39	102.56	105.83
21	2	1023	CLA	C3D-C2D-C1D	-2.39	102.56	105.83
21	B	1022	CLA	CHA-C4D-ND	2.39	137.49	132.55
21	A	1133	CLA	C1-C2-C3	-2.39	122.28	126.20
21	2	1234	CLA	CHA-C4D-ND	2.39	137.48	132.55
21	0	1503	CLA	CHA-C4D-ND	2.39	137.48	132.55
21	2	1205	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
21	K	1402	CLA	C2D-C1D-ND	2.39	112.49	110.13
21	B	1209	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
22	1	2001	PQN	C12-C11-C3	-2.39	106.19	112.08
21	1	1132	CLA	CHA-C4D-ND	2.39	137.48	132.55
21	A	1119	CLA	C2D-C1D-ND	2.39	112.49	110.13
21	2	1230	CLA	C2D-C1D-ND	2.39	112.49	110.13
21	2	1209	CLA	C3B-C4B-NB	-2.39	108.40	110.53
21	a	1134	CLA	O2A-CGA-CBA	2.39	119.12	111.83
21	1	1134	CLA	O2A-CGA-CBA	2.39	119.12	111.83
21	a	1122	CLA	C2D-C1D-ND	2.39	112.49	110.13
21	a	1103	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
21	A	1112	CLA	CHA-C4D-ND	2.39	137.48	132.55
21	a	1121	CLA	C2D-C1D-ND	2.39	112.49	110.13
21	B	1228	CLA	O2A-CGA-CBA	2.39	119.12	111.83
21	1	1120	CLA	C2D-C1D-ND	2.39	112.49	110.13
24	a	4008	BCR	C32-C1-C6	-2.39	106.50	110.24
21	1	1122	CLA	C2D-C1D-ND	2.39	112.49	110.13
28	B	4011	45D	C21-C15-C07	-2.39	120.27	124.11
21	A	1137	CLA	C3B-C4B-NB	-2.39	108.40	110.53
21	b	1208	CLA	O2A-C1-C2	2.39	117.29	108.11
21	A	1107	CLA	O2A-CGA-CBA	2.39	119.11	111.83
21	A	1105	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	A	1140	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	2	1218	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	a	1115	CLA	C1-O2A-CGA	2.39	122.42	116.65
24	2	4018	BCR	C37-C22-C23	2.39	121.73	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1231	CLA	CHA-C4D-ND	2.39	137.47	132.55
21	A	1012	CLA	C2A-C1A-CHA	2.38	128.01	123.87
21	b	1023	CLA	O2A-CGA-CBA	2.38	119.11	111.83
21	2	1204	CLA	C2D-C1D-ND	2.38	112.49	110.13
21	a	1013	CLA	C3D-C2D-C1D	-2.38	102.58	105.83
21	1	1012	CLA	O2A-CGA-CBA	2.38	119.10	111.83
35	L	6001	LMT	C3'-C4'-C5'	-2.38	105.65	110.93
25	0	5004	LHG	C5-O7-C7	-2.38	112.09	117.80
21	a	1130	CLA	CHA-C4D-ND	2.38	137.47	132.55
21	k	1401	CLA	O2A-CGA-CBA	2.38	119.10	111.83
21	A	1116	CLA	C3B-C4B-NB	-2.38	108.40	110.53
21	b	1229	CLA	C1-O2A-CGA	2.38	122.42	116.65
21	F	1301	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	b	1022	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	A	1134	CLA	CHA-C1A-NA	-2.38	121.00	126.39
21	B	1210	CLA	CHA-C1A-NA	-2.38	121.00	126.39
21	2	1214	CLA	CHA-C1A-NA	-2.38	121.00	126.39
21	1	1111	CLA	CHA-C1A-NA	-2.38	121.00	126.39
21	a	1114	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	k	1401	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	A	1012	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
21	2	1223	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	B	1228	CLA	C3B-C4B-NB	-2.38	108.41	110.53
21	b	1227	CLA	CMA-C3A-C4A	2.38	118.17	111.77
21	B	1220	CLA	C2D-C1D-ND	2.38	112.48	110.13
30	M	4021	ECH	C8-C7-C6	-2.38	120.64	127.00
24	A	4008	BCR	C32-C1-C6	-2.38	106.51	110.24
21	6	1301	CLA	CHA-C4D-ND	2.38	137.46	132.55
21	A	1136	CLA	CHA-C4D-ND	2.38	137.46	132.55
21	B	1213	CLA	CHA-C1A-NA	-2.38	121.01	126.39
21	b	1224	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	2	1240	CLA	CHA-C4D-ND	2.38	137.45	132.55
30	m	4021	ECH	C23-C24-C25	-2.38	120.65	127.00
21	2	1231	CLA	C2D-C1D-ND	2.38	112.48	110.13
24	1	4012	BCR	C37-C22-C23	2.38	121.72	118.09
21	b	1023	CLA	C3D-C2D-C1D	-2.38	102.59	105.83
21	2	1225	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
21	1	1102	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
21	b	1209	CLA	CHA-C4D-ND	2.38	137.45	132.55
21	b	1217	CLA	C2D-C1D-ND	2.38	112.48	110.13
21	F	1301	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	a	1107	CLA	C1-O2A-CGA	2.37	122.40	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	4002	BCR	C34-C9-C10	-2.37	118.97	122.82
24	B	4005	BCR	C39-C30-C25	-2.37	106.52	110.24
21	j	1302	CLA	CHD-C1D-ND	-2.37	121.46	124.80
21	A	1104	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
21	B	1207	CLA	CHA-C4D-ND	2.37	137.45	132.55
21	b	1211	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
21	a	1137	CLA	C2D-C1D-ND	2.37	112.47	110.13
21	A	1124	CLA	C1-O2A-CGA	2.37	122.39	116.65
21	1	1136	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
24	a	4001	BCR	C2-C1-C6	2.37	113.88	110.44
21	A	1122	CLA	CHA-C4D-ND	2.37	137.44	132.55
21	a	1102	CLA	C2D-C1D-ND	2.37	112.47	110.13
21	j	1303	CLA	C2D-C1D-ND	2.37	112.47	110.13
24	6	4016	BCR	C37-C22-C23	2.37	121.71	118.09
21	1	1117	CLA	CHA-C4D-ND	2.37	137.44	132.55
24	a	4001	BCR	C39-C30-C25	-2.37	106.53	110.24
21	A	1135	CLA	CHA-C4D-ND	2.37	137.44	132.55
21	2	1222	CLA	CHA-C4D-ND	2.37	137.44	132.55
21	j	1302	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
21	2	1203	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
24	f	4016	BCR	C29-C28-C27	2.37	116.48	111.28
21	2	1235	CLA	C3B-C4B-NB	-2.37	108.42	110.53
21	B	1230	CLA	CHA-C4D-ND	2.37	137.43	132.55
21	1	1138	CLA	C4B-CHC-C1C	2.37	131.81	126.25
24	j	4013	BCR	C37-C22-C23	2.37	121.70	118.09
21	B	1204	CLA	CHA-C4D-ND	2.37	137.43	132.55
21	1	1132	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
21	a	1128	CLA	C1D-ND-C4D	-2.37	104.65	106.31
21	b	1214	CLA	CHA-C4D-ND	2.37	137.43	132.55
26	b	5002	LMG	O7-C10-O9	-2.37	118.17	123.70
21	1	1134	CLA	C4B-CHC-C1C	2.37	131.81	126.25
21	2	1221	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
21	f	1301	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	a	1109	CLA	CMD-C2D-C3D	-2.37	122.27	127.69
24	a	4001	BCR	C23-C24-C25	2.37	133.32	127.00
21	a	1140	CLA	C1-O2A-CGA	2.36	122.38	116.65
21	a	1101	CLA	C1-O2A-CGA	2.36	122.38	116.65
21	b	1212	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
21	2	1203	CLA	CMA-C3A-C4A	2.36	118.13	111.77
21	B	1023	CLA	C1D-ND-C4D	-2.36	104.65	106.31
21	B	1206	CLA	C1D-ND-C4D	-2.36	104.65	106.31
21	A	1139	CLA	CHA-C4D-ND	2.36	137.43	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	1303	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
21	A	1106	CLA	CHA-C4D-ND	2.36	137.43	132.55
24	2	4010	BCR	C34-C9-C10	-2.36	118.99	122.82
21	A	1118	CLA	O2A-CGA-CBA	2.36	119.04	111.83
21	1	1106	CLA	C3B-C4B-NB	-2.36	108.42	110.53
21	a	1125	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
21	2	1211	CLA	C3B-C4B-NB	-2.36	108.42	110.53
21	B	1223	CLA	C2D-C1D-ND	2.36	112.46	110.13
21	0	1502	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
21	B	1236	CLA	O2A-CGA-CBA	2.36	119.03	111.83
22	A	2001	PQN	C2M-C2-C3	-2.36	120.57	124.45
21	a	1111	CLA	CMA-C3A-C4A	2.36	118.11	111.77
24	i	4018	BCR	C2-C1-C6	2.36	113.87	110.44
21	2	1230	CLA	O2A-CGA-CBA	2.36	119.03	111.83
21	b	1213	CLA	C2D-C1D-ND	2.36	112.46	110.13
21	A	1125	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	B	1205	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	1	1115	CLA	CHA-C4D-ND	2.36	137.41	132.55
25	l	5004	LHG	C5-O7-C7	-2.36	112.15	117.80
21	b	1022	CLA	CMA-C3A-C4A	2.36	118.11	111.77
24	a	4008	BCR	C35-C13-C12	2.36	121.69	118.09
21	1	1110	CLA	C2D-C1D-ND	2.36	112.46	110.13
21	1	1113	CLA	C2D-C1D-ND	2.36	112.46	110.13
30	b	4006	ECH	C15-C16-C17	-2.36	118.70	123.52
24	2	4017	BCR	C39-C30-C25	-2.36	106.55	110.24
21	2	1215	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
21	1	1126	CLA	CHA-C4D-ND	2.36	137.41	132.55
34	j	4015	ZEX	C11-C12-C13	-2.36	119.90	126.36
21	a	1124	CLA	C3B-C4B-NB	-2.36	108.43	110.53
31	f	5001	SQD	O3-C3-C2	-2.36	104.82	110.38
34	7	4015	ZEX	C39-C29-C30	-2.36	119.00	122.82
21	a	1112	CLA	C2D-C1D-ND	2.36	112.46	110.13
21	1	1124	CLA	C2D-C1D-ND	2.36	112.46	110.13
21	1	1122	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
21	2	1234	CLA	C3D-C2D-C1D	-2.36	102.62	105.83
21	2	1235	CLA	CHA-C4D-ND	2.36	137.41	132.55
21	A	1121	CLA	O2A-CGA-CBA	2.35	119.01	111.83
21	B	1237	CLA	C1-O2A-CGA	2.35	122.35	116.65
21	B	1216	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	1	1107	CLA	CHA-C4D-ND	2.35	137.40	132.55
21	F	1302	CLA	C1D-ND-C4D	-2.35	104.66	106.31
21	1	1132	CLA	C3B-C4B-NB	-2.35	108.43	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1118	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	1	1119	CLA	O2A-CGA-CBA	2.35	119.01	111.83
24	2	4018	BCR	C10-C11-C12	-2.35	116.39	123.20
21	2	1239	CLA	CHA-C4D-ND	2.35	137.40	132.55
21	L	1501	CLA	CHD-C1D-ND	-2.35	121.49	124.80
36	I	4020	EQ3	C12-C13-C14	-2.35	115.31	119.01
21	k	1401	CLA	C1-O2A-CGA	2.35	122.34	116.65
21	b	1239	CLA	CMA-C3A-C4A	2.35	118.09	111.77
21	a	1112	CLA	C3B-C4B-NB	-2.35	108.43	110.53
21	A	1117	CLA	CHA-C4D-ND	2.35	137.40	132.55
21	b	1226	CLA	C1-O2A-CGA	2.35	122.34	116.65
21	0	1503	CLA	CMA-C3A-C4A	2.35	118.09	111.77
21	B	1231	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
21	a	1012	CLA	CHA-C1A-NA	-2.35	121.07	126.39
21	b	1225	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	h	4020	45D	C27-C25-C23	2.35	121.68	118.09
21	B	1240	CLA	O2A-CGA-CBA	2.35	119.00	111.83
21	a	1136	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
21	1	1130	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	a	1121	CLA	CHA-C1A-NA	-2.35	121.07	126.39
21	B	1224	CLA	C3B-C4B-NB	-2.35	108.43	110.53
21	b	1220	CLA	C3D-C2D-C1D	-2.35	102.63	105.83
21	a	1118	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	L	1502	CLA	O2A-CGA-CBA	2.35	118.99	111.83
21	b	1204	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	b	1023	CLA	C2D-C1D-ND	2.35	112.45	110.13
21	1	1116	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
21	B	1234	CLA	C3D-C2D-C1D	-2.35	102.63	105.83
21	B	1228	CLA	CHD-C1D-ND	-2.35	121.50	124.80
30	m	4021	ECH	C8-C7-C6	-2.35	120.73	127.00
24	B	4017	BCR	C39-C30-C25	-2.34	106.57	110.24
21	1	1102	CLA	C1D-ND-C4D	-2.34	104.67	106.31
21	a	1104	CLA	O2A-CGA-CBA	2.34	118.98	111.83
21	A	1115	CLA	C1-O2A-CGA	2.34	122.33	116.65
24	B	4004	BCR	C29-C28-C27	2.34	116.43	111.28
21	B	1207	CLA	O2D-CGD-CBD	2.34	115.33	111.23
21	b	1207	CLA	C2D-C1D-ND	2.34	112.45	110.13
21	f	1301	CLA	C2D-C1D-ND	2.34	112.45	110.13
21	1	1133	CLA	CMA-C3A-C4A	2.34	118.07	111.77
21	a	1117	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	B	1222	CLA	CBC-CAC-C3C	-2.34	106.07	112.42
21	b	1224	CLA	CHA-C4D-ND	2.34	137.38	132.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	4013	BCR	C37-C22-C23	2.34	121.67	118.09
24	A	4019	BCR	C40-C30-C25	-2.34	106.57	110.24
24	A	4007	BCR	C37-C22-C23	2.34	121.67	118.09
21	1	1108	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	B	1232	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	A	1130	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
21	A	1106	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
24	A	4002	BCR	C34-C9-C10	-2.34	119.02	122.82
21	b	1210	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	l	1502	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	l	1501	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	a	1101	CLA	O2A-CGA-CBA	2.34	118.97	111.83
21	a	1124	CLA	CAA-CBA-CGA	-2.34	106.56	113.21
21	B	1222	CLA	CHA-C4D-ND	2.34	137.38	132.55
21	B	1210	CLA	C2D-C1D-ND	2.34	112.44	110.13
21	1	1121	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
21	J	1302	CLA	O2A-CGA-CBA	2.34	118.97	111.83
21	B	1235	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	k	1401	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	A	1127	CLA	C3B-C4B-NB	-2.34	108.44	110.53
21	A	1108	CLA	CHA-C4D-ND	2.34	137.37	132.55
21	b	1213	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
21	l	1502	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	A	1106	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	A	1104	CLA	CHA-C1A-NA	-2.34	121.10	126.39
21	2	1201	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
21	b	1230	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	B	1213	CLA	CHD-C1D-ND	-2.34	121.52	124.80
21	2	1210	CLA	C3B-C2B-C1B	-2.34	104.42	107.17
21	A	1109	CLA	CMA-C3A-C4A	2.34	118.05	111.77
21	b	1237	CLA	CHA-C4D-ND	2.34	137.37	132.55
21	a	1121	CLA	O2A-CGA-CBA	2.33	118.95	111.83
21	B	1213	CLA	C2D-C1D-ND	2.33	112.44	110.13
21	2	1022	CLA	C2D-C1D-ND	2.33	112.44	110.13
21	A	1132	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	b	1238	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	B	1226	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
24	K	4001	BCR	C37-C22-C23	2.33	121.65	118.09
21	1	1013	CLA	CMA-C3A-C4A	2.33	118.04	111.77
21	A	1106	CLA	CMA-C3A-C4A	2.33	118.04	111.77
21	1	1111	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
21	2	1229	CLA	C3D-C2D-C1D	-2.33	102.65	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1210	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	a	1119	CLA	O2A-CGA-CBA	2.33	118.94	111.83
21	1	1102	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	a	1101	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
21	K	1401	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	1	1104	CLA	CMA-C3A-C4A	2.33	118.04	111.77
21	A	1126	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	2	1224	CLA	CHA-C1A-NA	-2.33	121.11	126.39
21	b	1235	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	b	1239	CLA	CHA-C4D-ND	2.33	137.36	132.55
21	A	1131	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
21	2	1216	CLA	CMA-C3A-C4A	2.33	118.03	111.77
21	A	1127	CLA	C2D-C1D-ND	2.33	112.43	110.13
21	1	1133	CLA	C2D-C1D-ND	2.33	112.43	110.13
21	b	1225	CLA	CHA-C4D-ND	2.33	137.35	132.55
21	b	1235	CLA	O2A-CGA-CBA	2.33	118.94	111.83
21	j	1302	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	2	1204	CLA	CHA-C4D-ND	2.33	137.35	132.55
21	A	1130	CLA	C2D-C1D-ND	2.33	112.43	110.13
21	2	1239	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	B	1224	CLA	C3D-C2D-C1D	-2.33	102.66	105.83
21	2	1224	CLA	CMA-C3A-C4A	2.33	118.03	111.77
24	2	4014	BCR	C19-C18-C17	2.33	122.67	119.01
21	A	1119	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	b	1223	CLA	C3B-C4B-NB	-2.33	108.45	110.53
21	2	1021	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
21	2	1222	CLA	C3B-C2B-C1B	-2.33	104.43	107.17
21	1	1107	CLA	C2D-C1D-ND	2.32	112.43	110.13
21	A	1116	CLA	CHA-C4D-ND	2.32	137.34	132.55
21	L	1501	CLA	CHA-C4D-ND	2.32	137.34	132.55
21	A	1107	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
30	b	4006	ECH	C37-C22-C23	-2.32	114.54	118.09
21	1	1131	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
21	J	1302	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
21	B	1235	CLA	O2A-CGA-CBA	2.32	118.92	111.83
21	a	1122	CLA	CHA-C4D-ND	2.32	137.34	132.55
21	1	1122	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
21	1	1129	CLA	O2A-CGA-CBA	2.32	118.92	111.83
24	b	4018	BCR	C37-C22-C23	2.32	121.64	118.09
21	2	1207	CLA	CHA-C1A-NA	-2.32	121.13	126.39
30	b	4011	ECH	C7-C6-C5	-2.32	116.21	121.56
21	A	1125	CLA	O2D-CGD-O1D	-2.32	119.33	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	l	4019	BCR	C39-C30-C25	-2.32	106.61	110.24
21	A	1118	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	2	4005	BCR	C39-C30-C25	-2.32	106.61	110.24
21	A	1013	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
21	a	1011	CLA	C3B-C2B-C1B	-2.32	104.44	107.17
21	2	1221	CLA	CMA-C3A-C4A	2.32	118.00	111.77
21	a	1124	CLA	CHA-C4D-ND	2.32	137.33	132.55
21	a	1013	CLA	O2A-CGA-CBA	2.32	118.90	111.83
21	a	1123	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
21	1	1801	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
21	b	1021	CLA	CHA-C1A-NA	-2.32	121.14	126.39
21	b	1227	CLA	C3B-C4B-NB	-2.32	108.46	110.53
21	B	1022	CLA	O2A-CGA-CBA	2.32	118.90	111.83
21	2	1238	CLA	C2D-C1D-ND	2.32	112.42	110.13
21	A	1111	CLA	CMA-C3A-C4A	2.32	118.00	111.77
21	2	1218	CLA	C3D-C2D-C1D	-2.31	102.67	105.83
30	B	4006	ECH	C12-C13-C14	2.31	122.65	119.01
21	2	1229	CLA	C4B-CHC-C1C	2.31	131.69	126.25
21	B	1201	CLA	C1D-ND-C4D	-2.31	104.69	106.31
21	B	1218	CLA	CHA-C4D-ND	2.31	137.32	132.55
21	2	1023	CLA	CHA-C1A-NA	-2.31	121.15	126.39
21	6	1302	CLA	C3D-C2D-C1D	-2.31	102.67	105.83
21	b	1202	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
21	B	1235	CLA	CHA-C4D-ND	2.31	137.32	132.55
21	b	1222	CLA	CHA-C4D-ND	2.31	137.32	132.55
24	2	4010	BCR	C19-C18-C17	2.31	122.65	119.01
24	1	4002	BCR	C34-C9-C10	-2.31	119.07	122.82
24	L	4019	BCR	C23-C24-C25	2.31	133.18	127.00
21	b	1221	CLA	O2A-CGA-CBA	2.31	118.89	111.83
21	2	1218	CLA	C3B-C4B-NB	-2.31	108.47	110.53
21	a	1106	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	B	1217	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
21	A	1104	CLA	O2A-CGA-CBA	2.31	118.88	111.83
21	B	1237	CLA	CHA-C4D-ND	2.31	137.32	132.55
21	1	1123	CLA	CHA-C1A-NA	-2.31	121.16	126.39
28	B	4011	45D	C28-C26-C30	-2.31	119.07	122.82
21	1	1136	CLA	CHA-C4D-ND	2.31	137.31	132.55
24	A	4012	BCR	C37-C22-C23	2.31	121.62	118.09
21	B	1213	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	2	1224	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	0	1502	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	b	1202	CLA	C2D-C1D-ND	2.31	112.41	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1221	CLA	C3B-C4B-NB	-2.31	108.47	110.53
21	B	1228	CLA	CMA-C3A-C4A	2.31	117.97	111.77
21	b	1216	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
24	j	4013	BCR	C24-C25-C26	-2.31	116.24	121.56
21	1	1112	CLA	C1-O2A-CGA	2.31	122.23	116.65
21	f	1302	CLA	O2A-CGA-CBA	2.31	118.87	111.83
21	0	1503	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	a	4001	BCR	C37-C22-C23	2.31	121.61	118.09
21	k	1401	CLA	CHA-C1A-NA	-2.31	121.17	126.39
21	2	1226	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
21	B	1228	CLA	C3D-C2D-C1D	-2.31	102.69	105.83
21	a	1011	CLA	O2D-CGD-CBD	2.31	115.26	111.23
24	b	4005	BCR	C24-C25-C26	-2.30	116.25	121.56
24	2	4018	BCR	C35-C13-C12	2.30	121.61	118.09
26	A	5002	LMG	O1-C1-C2	2.30	111.77	108.27
21	A	1140	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
24	a	4012	BCR	C40-C30-C25	-2.30	106.63	110.24
21	b	1023	CLA	CHA-C1A-NA	-2.30	121.17	126.39
21	1	1124	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
21	B	1210	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	B	1223	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	1	1130	CLA	C2D-C1D-ND	2.30	112.41	110.13
21	2	1208	CLA	C2D-C1D-ND	2.30	112.41	110.13
21	a	1139	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
21	L	1502	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
24	k	4001	BCR	C37-C22-C23	2.30	121.61	118.09
21	B	1226	CLA	O2A-CGA-CBA	2.30	118.86	111.83
21	A	1105	CLA	C4B-CHC-C1C	2.30	131.66	126.25
26	K	5009	LMG	O7-C10-O9	-2.30	118.32	123.70
21	B	1221	CLA	C3B-C4B-NB	-2.30	108.47	110.53
21	a	1114	CLA	C3B-C4B-NB	-2.30	108.47	110.53
21	1	1119	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	1	1118	CLA	O2A-CGA-CBA	2.30	118.85	111.83
21	B	1206	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	2	1210	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	b	1232	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
21	b	1202	CLA	CHA-C4D-ND	2.30	137.30	132.55
21	B	1222	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
24	1	4007	BCR	C37-C22-C23	2.30	121.60	118.09
21	2	1201	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	b	1213	CLA	CBA-CAA-C2A	2.30	120.64	113.79
21	a	1126	CLA	O2A-CGA-CBA	2.30	118.85	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1112	CLA	C2D-C1D-ND	2.30	112.40	110.13
24	K	4001	BCR	C10-C11-C12	-2.30	116.53	123.20
24	1	4001	BCR	C30-C25-C26	-2.30	119.49	122.64
24	L	4022	BCR	C12-C13-C14	-2.30	115.39	119.01
21	1	1106	CLA	C2D-C1D-ND	2.30	112.40	110.13
21	A	1132	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
31	B	5008	SQD	O3-C3-C2	-2.30	104.96	110.38
21	B	1207	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	2	1223	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	8	1401	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
21	8	1401	CLA	C2D-C1D-ND	2.30	112.40	110.13
21	1	1135	CLA	O2A-CGA-CBA	2.30	118.84	111.83
21	1	1138	CLA	O2A-CGA-CBA	2.30	118.84	111.83
21	1	1137	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
21	B	1219	CLA	CHA-C1A-NA	-2.30	121.19	126.39
24	7	4013	BCR	C30-C25-C24	2.30	121.88	115.65
21	2	1224	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
24	B	4010	BCR	C37-C22-C23	2.30	121.60	118.09
21	B	1201	CLA	CHD-C1D-ND	-2.30	121.57	124.80
22	1	2001	PQN	C2M-C2-C3	-2.30	120.67	124.45
21	B	1212	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
21	2	1211	CLA	O2A-CGA-CBA	2.30	118.84	111.83
28	B	4011	45D	C24-C26-C30	2.30	122.62	119.01
21	2	1208	CLA	O2A-CGA-CBA	2.30	118.84	111.83
21	1	1123	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	2	1021	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	2	1202	CLA	C1D-ND-C4D	-2.30	104.70	106.31
21	B	1225	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	b	1201	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	b	1231	CLA	O2A-CGA-CBA	2.29	118.83	111.83
21	b	1222	CLA	C3B-C4B-NB	-2.29	108.48	110.53
21	1	1129	CLA	CHA-C1A-NA	-2.29	121.20	126.39
21	2	1023	CLA	C2A-C1A-CHA	2.29	127.85	123.87
21	2	1236	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
21	2	1238	CLA	CHA-C1A-NA	-2.29	121.20	126.39
21	A	1107	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	2	1219	CLA	C3B-C4B-NB	-2.29	108.48	110.53
21	7	1303	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
21	b	1209	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
30	B	4006	ECH	C23-C24-C25	-2.29	120.88	127.00
21	b	1229	CLA	CHA-C4D-ND	2.29	137.28	132.55
24	2	4017	BCR	C30-C25-C26	-2.29	119.50	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1124	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	a	1108	CLA	CHA-C1A-NA	-2.29	121.20	126.39
24	B	4004	BCR	C36-C18-C19	-2.29	114.59	118.09
21	1	1104	CLA	O2A-CGA-CBA	2.29	118.82	111.83
21	B	1219	CLA	CHA-C4D-ND	2.29	137.27	132.55
24	1	4002	BCR	C31-C1-C6	-2.29	106.65	110.24
21	2	1217	CLA	C2D-C1D-ND	2.29	112.39	110.13
21	2	1209	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
24	b	4017	BCR	C15-C14-C13	2.29	130.49	127.28
21	a	1110	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
21	b	1232	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
21	B	1210	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
21	B	1215	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
21	A	1120	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
21	b	1204	CLA	CHA-C4D-ND	2.29	137.27	132.55
21	k	1402	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
21	B	1236	CLA	C2D-C1D-ND	2.29	112.39	110.13
21	L	1502	CLA	CHA-C4D-ND	2.29	137.27	132.55
21	2	1022	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
21	A	1116	CLA	O2A-CGA-CBA	2.29	118.81	111.83
21	B	1219	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
21	A	1128	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
21	a	1112	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
21	a	1111	CLA	C2D-C1D-ND	2.29	112.39	110.13
28	B	4011	45D	C10-C18-C16	2.28	120.70	118.64
21	B	1217	CLA	C3D-C2D-C1D	-2.28	102.71	105.83
24	a	4008	BCR	C37-C22-C23	2.28	121.58	118.09
21	B	1221	CLA	C2D-C1D-ND	2.28	112.39	110.13
21	B	1213	CLA	C1-O2A-CGA	2.28	122.18	116.65
21	a	1131	CLA	CMA-C3A-C4A	2.28	117.91	111.77
21	A	1104	CLA	C3B-C4B-NB	-2.28	108.49	110.53
21	K	1401	CLA	CHA-C4D-ND	2.28	137.26	132.55
21	b	1217	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
21	B	1213	CLA	CBA-CAA-C2A	2.28	120.58	113.79
21	b	1203	CLA	C2D-C1D-ND	2.28	112.38	110.13
21	2	1238	CLA	C1-O2A-CGA	2.28	122.17	116.65
21	1	1106	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
24	b	4005	BCR	C35-C13-C12	2.28	121.57	118.09
21	B	1240	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
21	a	1801	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
24	A	4012	BCR	C40-C30-C25	-2.28	106.67	110.24
21	2	1226	CLA	CHA-C1A-NA	-2.28	121.23	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1120	CLA	C1-O2A-CGA	2.28	122.17	116.65
24	1	4002	BCR	C29-C28-C27	2.28	116.29	111.28
26	K	5009	LMG	O6-C1-C2	2.28	115.06	110.37
21	L	1503	CLA	CHA-C4D-ND	2.28	137.25	132.55
21	a	1120	CLA	CHA-C1A-NA	-2.28	121.23	126.39
21	B	1215	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	1	1101	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
21	A	1102	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	a	1125	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	A	1103	CLA	C2D-C1D-ND	2.28	112.38	110.13
21	1	1132	CLA	O2A-CGA-CBA	2.28	118.78	111.83
21	A	1122	CLA	C2D-C1D-ND	2.28	112.38	110.13
21	B	1216	CLA	O2A-CGA-CBA	2.28	118.78	111.83
21	2	1206	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	a	1114	CLA	CHA-C1A-NA	-2.28	121.23	126.39
21	B	1217	CLA	C1-C2-C3	2.28	129.93	126.20
21	a	1118	CLA	CHA-C1A-NA	-2.28	121.23	126.39
30	b	4006	ECH	C23-C24-C25	-2.28	120.92	127.00
21	B	1218	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
21	1	1116	CLA	C2D-C1D-ND	2.28	112.38	110.13
21	0	1501	CLA	C2D-C1D-ND	2.28	112.38	110.13
24	9	4021	BCR	C8-C7-C6	2.28	133.08	127.00
21	A	1110	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
21	2	1240	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
21	2	1236	CLA	CHA-C4D-ND	2.28	137.24	132.55
21	2	1219	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
24	B	4017	BCR	C32-C1-C6	-2.28	106.67	110.24
21	1	1131	CLA	O2A-CGA-CBA	2.27	118.77	111.83
24	a	4019	BCR	C37-C22-C23	2.27	121.56	118.09
21	7	1303	CLA	C1D-ND-C4D	-2.27	104.72	106.31
24	1	4001	BCR	C29-C28-C27	2.27	116.28	111.28
21	A	1135	CLA	C2D-C1D-ND	2.27	112.38	110.13
21	a	1101	CLA	C2D-C1D-ND	2.27	112.38	110.13
24	0	4019	BCR	C39-C30-C25	-2.27	106.68	110.24
21	1	1013	CLA	CHA-C1A-NA	-2.27	121.24	126.39
21	A	1138	CLA	CHA-C4D-ND	2.27	137.24	132.55
21	1	1103	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
21	b	1215	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
21	a	1108	CLA	C1-O2A-CGA	2.27	122.15	116.65
21	b	1211	CLA	CHA-C4D-ND	2.27	137.24	132.55
21	a	1121	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
21	2	1022	CLA	C3D-C2D-C1D	-2.27	102.73	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4010	BCR	C35-C13-C12	2.27	121.56	118.09
24	b	4005	BCR	C30-C25-C24	2.27	121.81	115.65
21	A	1103	CLA	CAA-CBA-CGA	-2.27	106.76	113.21
21	1	1129	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
21	2	1230	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
21	a	1134	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
21	b	1221	CLA	C6-C7-C8	-2.27	108.42	115.97
21	A	1101	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
21	1	1108	CLA	C2D-C1D-ND	2.27	112.37	110.13
21	1	1127	CLA	CHD-C1D-ND	-2.27	121.61	124.80
21	A	1125	CLA	C1-O2A-CGA	2.27	122.14	116.65
21	A	1112	CLA	C1D-ND-C4D	-2.27	104.72	106.31
21	1	1012	CLA	C2A-C1A-CHA	2.27	127.80	123.87
21	B	1206	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
24	B	4014	BCR	C8-C9-C10	2.27	122.58	119.01
21	a	1130	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
21	B	1229	CLA	CHA-C4D-ND	2.27	137.23	132.55
21	2	1227	CLA	CHA-C1A-NA	-2.27	121.26	126.39
21	2	1206	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
21	a	1123	CLA	O2A-CGA-CBA	2.27	118.75	111.83
21	2	1022	CLA	CHA-C1A-NA	-2.27	121.26	126.39
21	A	1131	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
21	2	1214	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
21	A	1111	CLA	C2D-C1D-ND	2.27	112.37	110.13
21	1	1140	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
21	B	1207	CLA	CHA-C1A-NA	-2.27	121.26	126.39
21	A	1109	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
21	B	1218	CLA	O2A-CGA-CBA	2.27	118.74	111.83
24	2	4018	BCR	C15-C14-C13	2.27	130.46	127.28
21	b	1221	CLA	C1D-ND-C4D	-2.26	104.72	106.31
24	6	4016	BCR	C27-C26-C25	-2.26	119.64	122.70
21	B	1021	CLA	O2A-CGA-CBA	2.26	118.74	111.83
21	B	1211	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
21	1	1134	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
21	b	1227	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
21	b	1207	CLA	CHA-C4D-ND	2.26	137.22	132.55
21	B	1021	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
21	1	1129	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
21	a	1105	CLA	C2D-C1D-ND	2.26	112.37	110.13
21	a	1120	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
21	a	1137	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
21	7	1302	CLA	CMD-C2D-C3D	-2.26	122.50	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1023	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
21	l	1503	CLA	CHA-C4D-ND	2.26	137.22	132.55
24	8	4001	BCR	C34-C9-C10	-2.26	119.15	122.82
21	2	1210	CLA	CHA-C1A-NA	-2.26	121.27	126.39
24	A	4001	BCR	C29-C28-C27	2.26	116.25	111.28
21	a	1128	CLA	C3B-C4B-NB	-2.26	108.51	110.53
21	B	1230	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	1	1134	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	a	1109	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	2	1207	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	1	1129	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	l	1502	CLA	O2A-CGA-CBA	2.26	118.73	111.83
21	A	1112	CLA	CHA-C1A-NA	-2.26	121.27	126.39
21	1	1102	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	A	1137	CLA	C4B-CHC-C1C	2.26	131.56	126.25
21	1	1113	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	B	1202	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	a	1129	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	1	1110	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	b	1228	CLA	O2A-CGA-CBA	2.26	118.72	111.83
24	0	4022	BCR	C8-C9-C10	2.26	122.56	119.01
21	1	1124	CLA	C3B-C4B-NB	-2.26	108.51	110.53
21	k	1402	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
24	6	4016	BCR	C15-C14-C13	2.26	130.45	127.28
25	l	5003	LHG	C5-O7-C7	-2.26	112.39	117.80
24	A	4019	BCR	C34-C9-C10	-2.26	119.16	122.82
21	1	1108	CLA	C3B-C4B-NB	-2.26	108.51	110.53
21	B	1227	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	b	1229	CLA	O2A-CGA-CBA	2.26	118.72	111.83
21	A	1134	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	B	1221	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
21	2	1220	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
21	2	1206	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	F	1302	CLA	C2D-C1D-ND	2.26	112.36	110.13
21	1	1119	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
21	a	1101	CLA	CBA-CAA-C2A	2.25	120.50	113.79
21	A	1112	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
21	1	1104	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
21	2	1214	CLA	O2A-CGA-CBA	2.25	118.71	111.83
21	a	1132	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
21	a	1107	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
24	1	4001	BCR	C15-C14-C13	-2.25	124.12	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1135	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
21	b	1228	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
21	B	1214	CLA	CHA-C1A-NA	-2.25	121.29	126.39
21	B	1215	CLA	C1D-ND-C4D	-2.25	104.73	106.31
21	2	1229	CLA	C1-O2A-CGA	2.25	122.11	116.65
21	a	1113	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
21	A	1107	CLA	C2D-C1D-ND	2.25	112.36	110.13
21	1	1112	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
21	f	1301	CLA	C3B-C4B-NB	-2.25	108.52	110.53
21	A	1136	CLA	O2A-CGA-CBA	2.25	118.70	111.83
21	1	1137	CLA	CHA-C4D-ND	2.25	137.19	132.55
21	1	1102	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
21	2	1232	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
21	A	1102	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	1	1126	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
30	b	4006	ECH	C8-C7-C6	-2.25	120.99	127.00
21	b	1231	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	2	1228	CLA	C4B-CHC-C1C	2.25	131.54	126.25
21	a	1131	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	B	1226	CLA	C1D-ND-C4D	-2.25	104.73	106.31
21	1	1112	CLA	CHA-C1A-NA	-2.25	121.30	126.39
21	1	1013	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
35	0	6001	LMT	O1B-C4'-C3'	2.25	112.94	107.23
24	2	4018	BCR	C8-C9-C10	2.25	122.54	119.01
21	K	1402	CLA	C3B-C4B-NB	-2.25	108.52	110.53
21	a	1116	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	b	1225	CLA	C2D-C1D-ND	2.25	112.35	110.13
21	B	1227	CLA	C4B-CHC-C1C	2.25	131.53	126.25
21	2	1236	CLA	CHA-C1A-NA	-2.25	121.30	126.39
28	h	4020	45D	C42-C41-C37	-2.25	118.92	123.52
21	2	1227	CLA	C4B-CHC-C1C	2.25	131.53	126.25
24	h	4018	BCR	C30-C25-C26	-2.25	119.57	122.64
21	A	1108	CLA	C3B-C2B-C1B	-2.25	104.52	107.17
21	A	1011	CLA	C4D-C3D-CAD	-2.25	105.67	108.11
21	a	1125	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
21	2	1209	CLA	CHA-C1A-NA	-2.24	121.31	126.39
24	1	4002	BCR	C37-C22-C23	2.24	121.52	118.09
24	b	4010	BCR	C39-C30-C25	-2.24	106.72	110.24
21	2	1217	CLA	O2A-CGA-CBA	2.24	118.68	111.83
21	2	1204	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
21	2	1213	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
21	b	1237	CLA	CMA-C3A-C4A	2.24	117.80	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1240	CLA	CHA-C1A-NA	-2.24	121.31	126.39
34	7	4015	ZEX	C11-C12-C13	-2.24	120.21	126.36
21	1	1122	CLA	C3B-C4B-NB	-2.24	108.53	110.53
21	2	1225	CLA	O2A-CGA-CBA	2.24	118.67	111.83
21	a	1139	CLA	CHA-C1A-NA	-2.24	121.31	126.39
21	1	1114	CLA	CHA-C1A-NA	-2.24	121.31	126.39
21	1	1112	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	2	1220	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	A	1105	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
21	A	1122	CLA	C3B-C4B-NB	-2.24	108.53	110.53
21	L	1503	CLA	C3B-C4B-NB	-2.24	108.53	110.53
21	b	1205	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
21	B	1229	CLA	CMA-C3A-C4A	2.24	117.80	111.77
21	2	1240	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
21	B	1209	CLA	C3B-C4B-NB	-2.24	108.53	110.53
21	1	1120	CLA	CHA-C1A-NA	-2.24	121.32	126.39
21	b	1226	CLA	O2A-CGA-CBA	2.24	118.67	111.83
21	b	1234	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
21	2	1228	CLA	CHA-C1A-NA	-2.24	121.32	126.39
24	2	4010	BCR	C40-C30-C25	-2.24	106.73	110.24
21	2	1231	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
21	1	1102	CLA	C2D-C1D-ND	2.24	112.34	110.13
21	A	1103	CLA	CHA-C4D-ND	2.24	137.17	132.55
21	a	1135	CLA	O2A-CGA-CBA	2.24	118.66	111.83
21	F	1302	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
21	2	1222	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
21	a	1107	CLA	C2D-C1D-ND	2.24	112.34	110.13
21	a	1126	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
21	1	1116	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
21	A	1011	CLA	O2A-CGA-CBA	2.24	118.66	111.83
21	B	1023	CLA	CHA-C1A-NA	-2.24	121.33	126.39
21	b	1226	CLA	CHA-C1A-NA	-2.24	121.33	126.39
21	2	1208	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
21	8	1401	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
21	B	1221	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
31	0	5005	SQD	O3-C3-C2	-2.24	105.11	110.38
21	B	1222	CLA	CMA-C3A-C4A	2.24	117.78	111.77
24	b	4017	BCR	C34-C9-C10	-2.24	119.19	122.82
21	2	1232	CLA	C1D-ND-C4D	-2.23	104.74	106.31
21	a	1107	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
21	2	1220	CLA	CHA-C1A-NA	-2.23	121.33	126.39
21	F	1301	CLA	O2A-CGA-CBA	2.23	118.64	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1103	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
21	a	1101	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
21	1	1012	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
21	b	1237	CLA	C2D-C1D-ND	2.23	112.33	110.13
21	b	1203	CLA	C3B-C4B-NB	-2.23	108.54	110.53
21	1	1111	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	6	1301	CLA	O2A-CGA-CBA	2.23	118.64	111.83
24	A	4019	BCR	C37-C22-C23	2.23	121.50	118.09
25	1	5005	LHG	O7-C7-O9	-2.23	118.49	123.70
30	2	4006	ECH	C12-C13-C14	-2.23	115.50	119.01
21	A	1139	CLA	C4B-CHC-C1C	2.23	131.49	126.25
21	K	1401	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
21	1	1119	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
21	1	1123	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
21	a	1105	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
21	a	1138	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	A	1114	CLA	CHA-C1A-NA	-2.23	121.35	126.39
21	1	1139	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
24	a	4002	BCR	C31-C1-C6	-2.23	106.75	110.24
21	2	1021	CLA	CHA-C1A-NA	-2.23	121.35	126.39
24	a	4012	BCR	C37-C22-C23	2.23	121.49	118.09
21	8	1402	CLA	CHA-C1A-NA	-2.23	121.35	126.39
21	B	1215	CLA	O2A-CGA-CBA	2.23	118.62	111.83
21	2	1232	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	2	4014	BCR	C8-C9-C10	2.23	122.51	119.01
21	0	1502	CLA	CHA-C4D-ND	2.23	137.14	132.55
21	a	1801	CLA	CHA-C1A-NA	-2.23	121.35	126.39
21	A	1138	CLA	C3B-C2B-C1B	-2.23	104.55	107.17
21	b	1023	CLA	CMD-C2D-C3D	-2.23	122.59	127.69
21	b	1201	CLA	C2D-C1D-ND	2.22	112.33	110.13
21	A	1115	CLA	O2A-CGA-CBA	2.22	118.62	111.83
21	2	1221	CLA	O2A-CGA-CBA	2.22	118.62	111.83
21	a	1140	CLA	C2D-C1D-ND	2.22	112.33	110.13
21	b	1203	CLA	CMA-C3A-C4A	2.22	117.75	111.77
21	a	1131	CLA	O2A-CGA-CBA	2.22	118.61	111.83
21	b	1230	CLA	O2A-CGA-CBA	2.22	118.61	111.83
21	2	1219	CLA	CBA-CAA-C2A	2.22	120.41	113.79
21	B	1209	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	1	1120	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
28	B	4011	45D	C41-C42-C38	-2.22	118.97	123.52
24	B	4018	BCR	C40-C30-C25	-2.22	106.76	110.24
21	8	1401	CLA	CHA-C1A-NA	-2.22	121.36	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1232	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
21	0	1502	CLA	O2A-CGA-CBA	2.22	118.61	111.83
21	b	1021	CLA	C1D-ND-C4D	-2.22	104.75	106.31
21	0	1503	CLA	C2D-C1D-ND	2.22	112.33	110.13
21	B	1220	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	B	1238	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	a	1126	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
24	B	4010	BCR	C40-C30-C25	-2.22	106.76	110.24
21	B	1218	CLA	CHA-C1A-NA	-2.22	121.36	126.39
21	A	1126	CLA	CMA-C3A-C4A	2.22	117.74	111.77
24	A	4007	BCR	C35-C13-C12	2.22	121.48	118.09
21	a	1117	CLA	C3B-C4B-NB	-2.22	108.55	110.53
24	2	4018	BCR	C34-C9-C10	-2.22	119.22	122.82
24	A	4002	BCR	C12-C13-C14	-2.22	115.52	119.01
21	B	1021	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	a	1104	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	a	1133	CLA	CHA-C1A-NA	-2.22	121.37	126.39
24	9	4021	BCR	C23-C24-C25	2.22	132.92	127.00
24	A	4019	BCR	C35-C13-C14	-2.22	119.22	122.82
21	a	1114	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
21	b	1215	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
21	A	1110	CLA	C2D-C1D-ND	2.22	112.32	110.13
21	1	1121	CLA	O2A-CGA-CBA	2.22	118.59	111.83
21	A	1121	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
21	a	1113	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
21	J	1303	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	a	1134	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	f	1301	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	B	1232	CLA	C4B-CHC-C1C	2.22	131.46	126.25
24	A	4007	BCR	C15-C14-C13	2.22	130.38	127.28
21	1	1140	CLA	C1-O2A-CGA	2.22	122.01	116.65
24	b	4004	BCR	C36-C18-C19	-2.22	114.70	118.09
21	A	1113	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
21	a	1137	CLA	CHA-C1A-NA	-2.21	121.38	126.39
24	l	4019	BCR	C35-C13-C12	2.21	121.47	118.09
21	A	1012	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
24	b	4004	BCR	C19-C18-C17	2.21	122.49	119.01
21	F	1302	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	A	1135	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	K	1402	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
21	a	1102	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	A	1114	CLA	O2A-CGA-CBA	2.21	118.58	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1230	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
24	2	4014	BCR	C37-C22-C23	2.21	121.47	118.09
21	B	1214	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
24	2	4017	BCR	C35-C13-C12	2.21	121.47	118.09
21	1	1118	CLA	CHA-C1A-NA	-2.21	121.38	126.39
21	a	1127	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
21	A	1118	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	2	1205	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	B	1218	CLA	C1-O2A-CGA	2.21	122.00	116.65
21	b	1234	CLA	O2A-CGA-CBA	2.21	118.57	111.83
21	1	1128	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	0	4022	BCR	C34-C9-C10	-2.21	119.24	122.82
21	1	1104	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
21	2	1237	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
21	f	1302	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	b	1222	CLA	O2A-CGA-CBA	2.21	118.57	111.83
21	A	1123	CLA	C1D-ND-C4D	-2.21	104.76	106.31
21	A	1011	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
21	1	1012	CLA	CMA-C3A-C4A	2.21	117.71	111.77
21	1	1117	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
21	f	1301	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	1	1114	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	1	1013	CLA	O2A-CGA-CBA	2.21	118.57	111.83
21	A	1118	CLA	CHA-C1A-NA	-2.21	121.39	126.39
21	1	1140	CLA	CHA-C1A-NA	-2.21	121.39	126.39
21	B	1220	CLA	C3B-C4B-NB	-2.21	108.56	110.53
21	a	1108	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	1	1118	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	B	1231	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	2	1225	CLA	C2D-C1D-ND	2.21	112.31	110.13
24	a	4007	BCR	C30-C25-C26	-2.21	119.62	122.64
24	i	4018	BCR	C15-C14-C13	2.21	130.37	127.28
21	1	1117	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	B	1214	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
21	K	1402	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
21	6	1302	CLA	C3B-C2B-C1B	-2.21	104.57	107.17
21	K	1401	CLA	C2D-C1D-ND	2.21	112.31	110.13
21	a	1139	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	J	1302	CLA	CHA-C1A-NA	-2.21	121.40	126.39
21	A	1124	CLA	O2A-CGA-CBA	2.21	118.56	111.83
21	A	1126	CLA	O2A-CGA-CBA	2.21	118.56	111.83
21	b	1209	CLA	CMD-C2D-C3D	-2.21	122.63	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1136	CLA	C1-O2A-CGA	2.20	121.99	116.65
21	a	1102	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
21	a	1115	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
21	b	1202	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
21	A	1122	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
21	1	1138	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
21	2	1209	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
21	a	1111	CLA	CAC-C3C-C4C	2.20	127.66	124.79
21	b	1213	CLA	CMA-C3A-C4A	2.20	117.70	111.77
21	2	1203	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
21	k	1402	CLA	CHA-C1A-NA	-2.20	121.40	126.39
21	1	1112	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
21	1	1801	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
26	a	5004	LMG	O7-C10-O9	-2.20	118.56	123.70
21	a	1129	CLA	CHA-C1A-NA	-2.20	121.40	126.39
21	B	1231	CLA	O2A-CGA-CBA	2.20	118.55	111.83
21	A	1131	CLA	O2A-CGA-CBA	2.20	118.55	111.83
21	A	1129	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	B	1202	CLA	C3B-C4B-NB	-2.20	108.56	110.53
21	a	1132	CLA	CMA-C3A-C4A	2.20	117.69	111.77
25	1	5001	LHG	C6-C5-C4	-2.20	106.65	111.78
24	B	4004	BCR	C19-C18-C17	2.20	122.47	119.01
21	B	1240	CLA	CHA-C1A-NA	-2.20	121.41	126.39
21	f	1301	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
21	b	1201	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	2	1235	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	A	1122	CLA	CHA-C1A-NA	-2.20	121.41	126.39
21	2	1232	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	2	1238	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	A	1135	CLA	O2A-CGA-CBA	2.20	118.54	111.83
21	1	1138	CLA	C2D-C1D-ND	2.20	112.30	110.13
21	A	1120	CLA	O2A-CGA-CBA	2.20	118.54	111.83
24	A	4003	BCR	C35-C13-C12	2.20	121.45	118.09
24	h	4018	BCR	C32-C1-C6	-2.20	106.80	110.24
21	2	1208	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
21	b	1217	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
24	A	4007	BCR	C2-C1-C6	2.20	113.63	110.44
21	a	1125	CLA	CHA-C1A-NA	-2.20	121.41	126.39
21	a	1126	CLA	C3B-C4B-NB	-2.20	108.57	110.53
21	a	1130	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
21	B	1023	CLA	CAC-C3C-C4C	2.20	127.65	124.79
21	b	1229	CLA	C6-C7-C8	-2.20	108.66	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	4021	BCR	C34-C9-C10	-2.20	119.26	122.82
21	2	1202	CLA	C2D-C1D-ND	2.20	112.30	110.13
21	6	1301	CLA	C2D-C1D-ND	2.20	112.30	110.13
21	B	1223	CLA	CHA-C1A-NA	-2.20	121.42	126.39
30	2	4006	ECH	C29-C30-C25	-2.20	107.25	110.44
21	A	1138	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
21	2	1021	CLA	C3B-C4B-NB	-2.20	108.57	110.53
21	A	1111	CLA	C1-O2A-CGA	2.20	121.97	116.65
21	b	1238	CLA	CHA-C1A-NA	-2.20	121.42	126.39
21	1	1120	CLA	C3B-C2B-C1B	-2.19	104.58	107.17
21	A	1113	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
21	2	1220	CLA	C2D-C1D-ND	2.19	112.30	110.13
21	A	1108	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	2	1239	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	A	1128	CLA	C2D-C1D-ND	2.19	112.30	110.13
21	2	1217	CLA	CHA-C1A-NA	-2.19	121.42	126.39
21	A	1102	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	B	1207	CLA	CAC-C3C-C4C	-2.19	121.94	124.79
21	a	1106	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
21	b	1231	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
24	K	4001	BCR	C39-C30-C25	-2.19	106.81	110.24
34	F	4016	ZEX	C39-C29-C28	2.19	121.44	118.09
21	b	1237	CLA	CAC-C3C-C4C	2.19	127.64	124.79
36	I	4020	EQ3	C36-C18-C19	2.19	121.44	118.09
21	a	1102	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
21	1	1114	CLA	C3B-C4B-NB	-2.19	108.57	110.53
34	F	4016	ZEX	C31-C32-C33	-2.19	120.36	126.36
21	2	1209	CLA	C2D-C1D-ND	2.19	112.29	110.13
21	2	1235	CLA	O2A-CGA-CBA	2.19	118.51	111.83
24	1	4008	BCR	C39-C30-C25	-2.19	106.81	110.24
21	2	1205	CLA	C3B-C4B-NB	-2.19	108.58	110.53
21	2	1228	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
21	1	1123	CLA	O2A-CGA-CBA	2.19	118.51	111.83
21	B	1215	CLA	C2D-C1D-ND	2.19	112.29	110.13
24	L	4022	BCR	C37-C22-C23	2.19	121.43	118.09
21	2	1223	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	A	1137	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	a	1114	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	b	1224	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	A	1112	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
21	a	1112	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	A	1135	CLA	CMD-C2D-C3D	-2.19	122.67	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	l	1501	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
21	2	1231	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
21	2	1231	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	B	1022	CLA	C3B-C4B-NB	-2.19	108.58	110.53
21	A	1130	CLA	CMA-C3A-C4A	2.19	117.65	111.77
21	A	1801	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
21	a	1117	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
21	B	1221	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
21	a	1106	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
21	A	1132	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	b	1022	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	1	1102	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	2	1201	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	B	1215	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
21	B	1206	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	B	1214	CLA	C2D-C1D-ND	2.19	112.29	110.13
21	1	1106	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
21	2	1206	CLA	CHA-C1A-NA	-2.19	121.44	126.39
21	b	1209	CLA	CHA-C1A-NA	-2.18	121.44	126.39
21	a	1112	CLA	C3B-C2B-C1B	-2.18	104.59	107.17
21	a	1139	CLA	C2D-C1D-ND	2.18	112.29	110.13
21	b	1239	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
21	1	1011	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
34	F	4016	ZEX	C27-C28-C29	2.18	129.47	126.23
21	1	1139	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
21	B	1204	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
21	A	1113	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	a	1132	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	j	1303	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	B	1226	CLA	CAC-C3C-C4C	2.18	127.63	124.79
21	b	1209	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
21	1	1113	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
21	A	1011	CLA	C2A-C3A-C4A	2.18	105.39	101.87
21	A	1137	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
21	1	1105	CLA	C4B-CHC-C1C	2.18	131.38	126.25
21	A	1111	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
21	2	1240	CLA	CAA-C2A-C3A	-2.18	111.23	116.23
30	M	4021	ECH	C7-C6-C5	-2.18	116.53	121.56
21	A	1105	CLA	CHA-C1A-NA	-2.18	121.45	126.39
21	b	1228	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
21	2	1202	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
21	1	1130	CLA	C3D-C2D-C1D	-2.18	102.86	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1213	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
21	1	1012	CLA	C3B-C4B-NB	-2.18	108.58	110.53
21	A	1135	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
21	a	1129	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
21	1	1124	CLA	CHA-C1A-NA	-2.18	121.46	126.39
21	A	1116	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
21	B	1227	CLA	O2A-CGA-CBA	2.18	118.48	111.83
21	b	1235	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	b	1219	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	2	1212	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
21	b	1206	CLA	C2D-C1D-ND	2.18	112.28	110.13
24	2	4004	BCR	C39-C30-C25	-2.18	106.83	110.24
21	a	1128	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
21	B	1231	CLA	CMA-C3A-C4A	2.18	117.63	111.77
21	a	1013	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
21	f	1301	CLA	O2A-CGA-CBA	2.18	118.47	111.83
24	L	4019	BCR	C32-C1-C6	-2.18	106.83	110.24
21	a	1111	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	8	4001	BCR	C38-C26-C25	-2.18	122.11	124.48
21	a	1135	CLA	C2D-C1D-ND	2.18	112.28	110.13
21	b	1236	CLA	C2D-C1D-ND	2.18	112.28	110.13
21	a	1127	CLA	C1-O2A-CGA	2.18	121.92	116.65
21	a	1113	CLA	CHA-C1A-NA	-2.18	121.46	126.39
21	1	1105	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
31	F	5001	SQD	O3-C3-C2	-2.18	105.25	110.38
21	A	1107	CLA	C1-O2A-CGA	2.18	121.92	116.65
21	b	1215	CLA	CMA-C3A-C4A	2.18	117.62	111.77
21	A	1140	CLA	C1-O2A-CGA	2.18	121.92	116.65
21	2	1215	CLA	O2A-CGA-CBA	2.18	118.47	111.83
21	B	1223	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
21	1	1138	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	a	1103	CLA	O2A-CGA-CBA	2.17	118.47	111.83
21	j	1303	CLA	O2A-CGA-CBA	2.17	118.47	111.83
21	1	1114	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
21	b	1238	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
21	b	1205	CLA	CHD-C1D-ND	-2.17	121.74	124.80
24	a	4002	BCR	C37-C22-C23	2.17	121.41	118.09
21	2	1206	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
21	K	1401	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	7	1303	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
24	7	4013	BCR	C37-C22-C23	2.17	121.41	118.09
31	L	5001	SQD	O3-C3-C2	-2.17	105.25	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1119	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
21	A	1013	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	b	1223	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	a	1122	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	l	1503	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
24	A	4002	BCR	C39-C30-C25	-2.17	106.84	110.24
21	a	1137	CLA	CMA-C3A-C4A	2.17	117.61	111.77
21	7	1303	CLA	CAA-C2A-C3A	-2.17	111.25	116.23
21	1	1105	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
21	K	1401	CLA	O2A-CGA-CBA	2.17	118.45	111.83
21	1	1104	CLA	C3B-C4B-NB	-2.17	108.59	110.53
21	B	1212	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	2	1221	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	2	1204	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	2	1211	CLA	C2D-C1D-ND	2.17	112.27	110.13
26	B	5005	LMG	O7-C10-O9	-2.17	118.63	123.70
21	2	1215	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
21	B	1021	CLA	C1D-ND-C4D	-2.17	104.79	106.31
21	b	1234	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	b	1218	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	2	1220	CLA	C3B-C4B-NB	-2.17	108.59	110.53
21	1	1101	CLA	C2D-C1D-ND	2.17	112.27	110.13
24	1	4003	BCR	C1-C6-C7	2.17	121.53	115.65
24	k	4001	BCR	C29-C28-C27	2.17	116.04	111.28
21	a	1111	CLA	C3B-C4B-NB	-2.17	108.59	110.53
21	1	1115	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	2	1218	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	a	1123	CLA	C2D-C1D-ND	2.17	112.27	110.13
21	A	1135	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
21	B	1202	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	a	1119	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	2	1215	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	A	1130	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
21	a	1133	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
24	K	4001	BCR	C27-C26-C25	-2.17	119.78	122.70
21	1	1140	CLA	C2D-C1D-ND	2.17	112.27	110.13
21	1	1109	CLA	CHA-C1A-NA	-2.17	121.49	126.39
21	a	1011	CLA	C1D-ND-C4D	-2.16	104.79	106.31
24	a	4001	BCR	C32-C1-C6	-2.16	106.85	110.24
26	A	5002	LMG	O7-C10-O9	-2.16	118.64	123.70
21	2	1022	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
21	B	1222	CLA	O2A-CGA-CBA	2.16	118.44	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	4004	BCR	C34-C9-C10	-2.16	119.31	122.82
21	a	1111	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	a	1140	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	2	1238	CLA	O2A-CGA-CBA	2.16	118.43	111.83
24	8	4001	BCR	C37-C22-C23	2.16	121.39	118.09
21	b	1228	CLA	CHA-C1A-NA	-2.16	121.49	126.39
21	b	1022	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	2	1206	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	a	1107	CLA	O2A-CGA-CBA	2.16	118.43	111.83
24	A	4001	BCR	C37-C22-C23	2.16	121.39	118.09
24	l	4019	BCR	C37-C22-C23	2.16	121.39	118.09
24	L	4019	BCR	C38-C26-C25	-2.16	122.12	124.48
21	1	1115	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	b	1023	CLA	CMA-C3A-C4A	2.16	117.59	111.77
24	1	4019	BCR	C39-C30-C25	-2.16	106.85	110.24
21	B	1238	CLA	CHA-C4D-ND	2.16	137.01	132.55
24	A	4007	BCR	C34-C9-C10	-2.16	119.31	122.82
24	l	4022	BCR	C37-C22-C23	2.16	121.39	118.09
21	2	1232	CLA	CHA-C1A-NA	-2.16	121.50	126.39
21	a	1121	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	2	1234	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
24	l	4022	BCR	C35-C13-C12	2.16	121.39	118.09
21	A	1113	CLA	C2D-C1D-ND	2.16	112.27	110.13
24	I	4018	BCR	C10-C11-C12	-2.16	116.94	123.20
21	B	1230	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	a	1104	CLA	C3B-C4B-NB	-2.16	108.60	110.53
21	2	1227	CLA	C2D-C1D-ND	2.16	112.26	110.13
21	6	1302	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
21	A	1125	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
21	B	1240	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
21	1	1130	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
21	a	1109	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	2	1201	CLA	C1D-ND-C4D	-2.16	104.80	106.31
21	2	1203	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
21	A	1119	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
24	L	4019	BCR	C35-C13-C12	2.16	121.39	118.09
21	a	1108	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
21	A	1114	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
21	1	1116	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
25	A	5005	LHG	O7-C7-O9	-2.16	118.66	123.70
21	2	1217	CLA	CAC-C3C-C4C	2.16	127.60	124.79
21	A	1102	CLA	CMD-C2D-C3D	-2.16	122.74	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1102	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
21	A	1136	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
21	0	1503	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
21	a	1135	CLA	CHA-C1A-NA	-2.16	121.51	126.39
24	1	4003	BCR	C37-C22-C23	2.16	121.38	118.09
21	a	1137	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
21	b	1223	CLA	C3B-C2B-C1B	-2.16	104.63	107.17
21	a	1105	CLA	CHA-C1A-NA	-2.16	121.51	126.39
24	l	4019	BCR	C32-C1-C6	-2.15	106.86	110.24
21	j	1303	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
21	1	1108	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
21	a	1128	CLA	C2D-C1D-ND	2.15	112.26	110.13
21	b	1237	CLA	CHA-C1A-NA	-2.15	121.51	126.39
21	b	1206	CLA	CHA-C1A-NA	-2.15	121.51	126.39
24	7	4013	BCR	C36-C18-C19	-2.15	114.80	118.09
21	B	1224	CLA	CMA-C3A-C4A	2.15	117.56	111.77
30	b	4011	ECH	C28-C29-C30	-2.15	110.06	113.21
21	A	1111	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
21	L	1501	CLA	C3B-C4B-NB	-2.15	108.61	110.53
21	F	1301	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
21	1	1012	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
21	a	1129	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
21	L	1503	CLA	C6-C7-C8	-2.15	108.81	115.97
21	B	1229	CLA	C4B-CHC-C1C	2.15	131.31	126.25
24	l	4022	BCR	C36-C18-C19	-2.15	114.80	118.09
21	a	1105	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
24	A	4001	BCR	C8-C7-C6	2.15	132.75	127.00
22	A	2001	PQN	C17-C16-C15	-2.15	107.53	113.26
21	7	1302	CLA	CHA-C1A-NA	-2.15	121.52	126.39
21	2	1230	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
21	2	1208	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	0	4022	BCR	C15-C14-C13	2.15	130.29	127.28
21	A	1135	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
21	B	1234	CLA	CHA-C1A-NA	-2.15	121.52	126.39
21	a	1116	CLA	C1-C2-C3	-2.15	122.68	126.20
21	2	1227	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
21	2	1218	CLA	C1-O2A-CGA	2.15	121.85	116.65
21	2	1221	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
21	b	1240	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
28	h	4020	45D	C29-C31-C33	-2.15	116.98	123.20
21	a	1109	CLA	C3B-C4B-NB	-2.15	108.61	110.53
21	a	1140	CLA	CHA-C1A-NA	-2.15	121.53	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1127	CLA	CHA-C1A-NA	-2.15	121.53	126.39
24	a	4012	BCR	C34-C9-C10	-2.15	119.34	122.82
21	b	1227	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
21	1	1135	CLA	CHA-C1A-NA	-2.15	121.53	126.39
21	A	1140	CLA	O2A-CGA-CBA	2.15	118.38	111.83
30	b	4006	ECH	C11-C10-C9	-2.15	124.27	127.28
21	b	1212	CLA	C4B-CHC-C1C	2.15	131.29	126.25
34	J	4015	ZEX	C40-C33-C34	-2.15	119.34	122.82
21	6	1302	CLA	C2D-C1D-ND	2.15	112.25	110.13
21	2	1235	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
21	b	1219	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
24	B	4018	BCR	C11-C12-C13	-2.15	120.48	126.36
21	A	1013	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
21	a	1136	CLA	CHA-C1A-NA	-2.14	121.53	126.39
21	1	1104	CLA	CHA-C1A-NA	-2.14	121.53	126.39
21	B	1240	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
21	b	1213	CLA	C3B-C4B-NB	-2.14	108.62	110.53
21	a	1103	CLA	C2D-C1D-ND	2.14	112.25	110.13
26	B	5002	LMG	O7-C10-O9	-2.14	118.69	123.70
21	B	1220	CLA	CHA-C1A-NA	-2.14	121.54	126.39
21	a	1122	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	b	1204	CLA	O2A-CGA-CBA	2.14	118.37	111.83
21	a	1135	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	B	1220	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	B	1239	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	B	1216	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	b	1208	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	a	4002	BCR	C10-C11-C12	-2.14	117.00	123.20
21	B	1216	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	a	1127	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	1	1113	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
21	b	1222	CLA	CMA-C3A-C4A	2.14	117.53	111.77
21	F	1301	CLA	CHA-C1A-NA	-2.14	121.54	126.39
21	a	1140	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	2	1207	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	B	1221	CLA	O2A-CGA-CBA	2.14	118.36	111.83
21	A	1134	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	a	1119	CLA	CHA-C1A-NA	-2.14	121.55	126.39
21	1	1108	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	a	1110	CLA	O2A-CGA-CBA	2.14	118.36	111.83
21	b	1203	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
21	a	1127	CLA	CHA-C1A-NA	-2.14	121.55	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1240	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	B	4018	BCR	C12-C13-C14	2.14	122.37	119.01
21	1	1103	CLA	C2D-C1D-ND	2.14	112.24	110.13
21	2	1237	CLA	CHA-C1A-NA	-2.14	121.55	126.39
21	A	1133	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
21	2	1202	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
21	b	1217	CLA	C1-O2A-CGA	2.14	121.82	116.65
21	6	1301	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
21	l	1501	CLA	CAC-C3C-C4C	2.14	127.57	124.79
21	b	1229	CLA	C4B-CHC-C1C	2.14	131.27	126.25
21	B	1022	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
21	B	1239	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
21	1	1115	CLA	C4B-CHC-C1C	2.14	131.27	126.25
21	2	1212	CLA	CHA-C1A-NA	-2.14	121.56	126.39
24	l	4022	BCR	C32-C1-C6	-2.14	106.89	110.24
21	b	1023	CLA	C2A-C1A-CHA	2.14	127.57	123.87
21	a	1105	CLA	CAC-C3C-C4C	2.14	127.57	124.79
21	A	1136	CLA	C4B-CHC-C1C	2.14	131.27	126.25
21	b	1227	CLA	O2A-CGA-CBA	2.13	118.34	111.83
21	A	1139	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	1	1133	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	a	1123	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	2	1211	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	B	1238	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	2	1222	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	B	1203	CLA	O2A-CGA-CBA	2.13	118.34	111.83
21	6	1301	CLA	CHA-C1A-NA	-2.13	121.56	126.39
26	B	5002	LMG	C7-O1-C1	-2.13	109.22	113.80
21	a	1117	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	B	1217	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	A	1121	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	B	1211	CLA	O2A-CGA-CBA	2.13	118.34	111.83
21	b	1216	CLA	CHA-C1A-NA	-2.13	121.56	126.39
21	A	1129	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	1	1106	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	B	1213	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	l	4022	BCR	C19-C18-C17	2.13	122.36	119.01
21	B	1202	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	b	1022	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	2	1210	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	A	1122	CLA	C1-O2A-CGA	2.13	121.81	116.65
21	a	1106	CLA	O2A-CGA-CBA	2.13	118.33	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	4018	BCR	C38-C26-C25	-2.13	122.16	124.48
21	2	1229	CLA	CHA-C4D-ND	2.13	136.94	132.55
21	b	1208	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	2	1238	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	b	1221	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
21	B	1236	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
21	B	1204	CLA	C2D-C1D-ND	2.13	112.23	110.13
24	2	4005	BCR	C37-C22-C23	2.13	121.34	118.09
21	B	1021	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
21	A	1125	CLA	O2A-CGA-CBA	2.13	118.32	111.83
21	1	1128	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
21	B	1217	CLA	O2A-CGA-CBA	2.13	118.32	111.83
24	b	4004	BCR	C35-C13-C12	2.13	121.34	118.09
21	b	1021	CLA	C2D-C1D-ND	2.13	112.23	110.13
21	a	1136	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
21	A	1130	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
24	A	4007	BCR	C38-C26-C25	-2.13	122.17	124.48
21	b	1219	CLA	CHA-C1A-NA	-2.13	121.58	126.39
21	1	1112	CLA	C2D-C1D-ND	2.12	112.23	110.13
21	b	1222	CLA	CBC-CAC-C3C	-2.12	106.66	112.42
21	a	1128	CLA	CHA-C1A-NA	-2.12	121.58	126.39
21	l	1502	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
21	A	1106	CLA	CAA-C2A-C1A	-2.12	105.01	111.97
21	a	1132	CLA	O2A-CGA-CBA	2.12	118.31	111.83
25	A	5006	LHG	O7-C7-O9	-2.12	118.74	123.70
24	1	4019	BCR	C37-C22-C23	2.12	121.33	118.09
24	A	4002	BCR	C31-C1-C6	-2.12	106.91	110.24
21	a	1116	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
21	a	1131	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
21	2	1205	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
21	a	1011	CLA	C2D-C1D-ND	2.12	112.23	110.13
21	a	1130	CLA	C3B-C4B-NB	-2.12	108.64	110.53
21	b	1215	CLA	CHA-C1A-NA	-2.12	121.58	126.39
21	1	1139	CLA	CHA-C1A-NA	-2.12	121.58	126.39
21	2	1207	CLA	C1-O2A-CGA	2.12	121.79	116.65
21	b	1206	CLA	O2A-CGA-CBA	2.12	118.31	111.83
24	2	4011	BCR	C37-C22-C23	2.12	121.33	118.09
21	1	1110	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
21	a	1139	CLA	C4B-CHC-C1C	2.12	131.24	126.25
31	b	5006	SQD	O3-C3-C2	-2.12	105.38	110.38
21	A	1125	CLA	CHA-C1A-NA	-2.12	121.59	126.39
21	2	1229	CLA	CMD-C2D-C3D	-2.12	122.83	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1138	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	b	1221	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	1	1140	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	a	1122	CLA	CHA-C1A-NA	-2.12	121.59	126.39
21	A	1110	CLA	C4B-CHC-C1C	2.12	131.23	126.25
21	2	1022	CLA	C1-O2A-CGA	2.12	121.78	116.65
21	F	1302	CLA	O2A-CGA-CBA	2.12	118.30	111.83
21	1	1111	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	A	1128	CLA	C3B-C4B-NB	-2.12	108.64	110.53
21	1	1801	CLA	CHA-C1A-NA	-2.12	121.59	126.39
30	b	4006	ECH	C4-C5-C6	-2.12	119.84	122.70
21	A	1119	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	b	1207	CLA	CHA-C1A-NA	-2.12	121.59	126.39
21	a	1137	CLA	C4B-CHC-C1C	2.12	131.23	126.25
21	2	1239	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
24	A	4007	BCR	C39-C30-C25	-2.12	106.92	110.24
21	A	1013	CLA	O2A-CGA-CBA	2.12	118.29	111.83
21	a	1801	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
24	2	4018	BCR	C30-C25-C26	-2.12	119.74	122.64
21	B	1211	CLA	CHA-C1A-NA	-2.12	121.60	126.39
21	A	1117	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	a	1115	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
21	1	1126	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
21	1	1102	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
24	7	4013	BCR	C19-C18-C17	2.12	122.34	119.01
21	b	1022	CLA	C3B-C2B-C1B	-2.12	104.68	107.17
21	2	1217	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
21	A	1126	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
21	a	1133	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
21	a	1108	CLA	O2A-CGA-CBA	2.11	118.28	111.83
21	B	1228	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
21	a	1105	CLA	C4B-CHC-C1C	2.11	131.22	126.25
21	B	1231	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
21	b	1213	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
21	2	1203	CLA	O2A-CGA-CBA	2.11	118.28	111.83
24	2	4010	BCR	C1-C6-C5	-2.11	119.75	122.64
21	b	1204	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
21	2	1239	CLA	C1-O2A-CGA	2.11	121.76	116.65
21	j	1302	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
21	0	1502	CLA	C4B-CHC-C1C	2.11	131.21	126.25
21	A	1120	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	b	1216	CLA	C3D-C2D-C1D	-2.11	102.95	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1011	CLA	C2D-C1D-ND	2.11	112.22	110.13
21	2	1201	CLA	C2D-C1D-ND	2.11	112.22	110.13
24	h	4018	BCR	C2-C1-C6	2.11	113.50	110.44
21	B	1209	CLA	O2A-CGA-CBA	2.11	118.27	111.83
24	2	4004	BCR	C37-C22-C23	2.11	121.31	118.09
21	a	1121	CLA	C3B-C4B-NB	-2.11	108.65	110.53
21	2	1202	CLA	C3B-C4B-NB	-2.11	108.65	110.53
21	a	1123	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	j	1303	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
24	A	4002	BCR	C30-C25-C26	-2.11	119.75	122.64
21	2	1232	CLA	C2D-C1D-ND	2.11	112.21	110.13
21	a	1131	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
21	a	1012	CLA	C2A-C1A-CHA	2.11	127.53	123.87
21	a	1107	CLA	CHA-C1A-NA	-2.11	121.61	126.39
21	b	1210	CLA	C3B-C4B-NB	-2.11	108.65	110.53
21	2	1207	CLA	CMA-C3A-C2A	2.11	122.14	113.98
21	a	1112	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
24	K	4001	BCR	C35-C13-C12	2.11	121.31	118.09
21	a	1109	CLA	CHA-C1A-NA	-2.11	121.62	126.39
21	8	1402	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
21	b	1238	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
21	L	1501	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
35	1	6001	LMT	C3'-C4'-C5'	-2.11	106.26	110.93
21	B	1217	CLA	C4B-CHC-C1C	2.11	131.20	126.25
21	1	1013	CLA	C2A-C1A-CHA	2.11	127.53	123.87
21	b	1217	CLA	CHA-C1A-NA	-2.11	121.62	126.39
21	B	1209	CLA	C4B-CHC-C1C	2.11	131.20	126.25
21	F	1302	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
21	1	1113	CLA	C3B-C4B-NB	-2.11	108.65	110.53
21	A	1801	CLA	C1-O2A-CGA	2.11	121.75	116.65
21	B	1022	CLA	CMA-C3A-C4A	2.11	117.44	111.77
21	1	1129	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
21	2	1222	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
21	B	1213	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
21	B	1234	CLA	O2A-CGA-CBA	2.11	118.26	111.83
21	B	1217	CLA	CAC-C3C-C4C	2.11	127.53	124.79
24	1	4002	BCR	C30-C25-C24	2.11	121.36	115.65
21	b	1231	CLA	C3B-C2B-C1B	-2.11	104.69	107.17
21	j	1302	CLA	CHA-C1A-NA	-2.11	121.62	126.39
21	A	1123	CLA	C1-O2A-CGA	2.11	121.75	116.65
21	1	1011	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
21	1	1101	CLA	C3D-C2D-C1D	-2.10	102.96	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	1302	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
30	m	4021	ECH	C7-C6-C5	-2.10	116.71	121.56
21	L	1503	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
24	1	4012	BCR	C8-C9-C10	2.10	122.32	119.01
21	B	1209	CLA	C1-O2A-CGA	2.10	121.74	116.65
21	2	1230	CLA	CHA-C1A-NA	-2.10	121.63	126.39
21	a	1110	CLA	CHA-C1A-NA	-2.10	121.63	126.39
21	J	1303	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
21	2	1234	CLA	C3B-C4B-NB	-2.10	108.65	110.53
21	A	1801	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
24	B	4004	BCR	C37-C22-C23	2.10	121.30	118.09
21	a	1129	CLA	O2A-CGA-CBA	2.10	118.24	111.83
21	6	1302	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
21	b	1206	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
21	A	1132	CLA	O2A-CGA-CBA	2.10	118.24	111.83
21	2	1237	CLA	C2D-C1D-ND	2.10	112.20	110.13
21	2	1220	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
21	A	1114	CLA	C4B-CHC-C1C	2.10	131.19	126.25
21	1	1113	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	a	1124	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	b	1213	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	b	1207	CLA	C3B-C4B-NB	-2.10	108.66	110.53
21	b	1211	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
21	a	1136	CLA	C4B-CHC-C1C	2.10	131.18	126.25
21	1	1011	CLA	C2D-C1D-ND	2.10	112.20	110.13
24	A	4019	BCR	C1-C6-C5	-2.10	119.77	122.64
21	7	1303	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	1	1136	CLA	C3B-C2B-C1B	-2.10	104.70	107.17
21	b	1227	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	1	1125	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	b	1222	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
21	B	1212	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
21	1	1109	CLA	CAC-C3C-C4C	2.10	127.52	124.79
21	1	1122	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	2	1205	CLA	CBC-CAC-C3C	-2.10	106.74	112.42
21	b	1201	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
21	b	1224	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	1	1132	CLA	CMA-C3A-C4A	2.10	117.41	111.77
21	B	1022	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	B	1228	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	B	1203	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
21	B	1230	CLA	C4B-CHC-C1C	2.10	131.17	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4010	BCR	C38-C26-C25	-2.10	122.20	124.48
24	j	4013	BCR	C40-C30-C25	-2.09	106.96	110.24
21	B	1201	CLA	C2D-C1D-ND	2.09	112.20	110.13
21	2	1206	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
22	b	2002	PQN	C11-C12-C13	-2.09	123.22	126.83
21	L	1503	CLA	C1-O2A-CGA	2.09	121.72	116.65
24	B	4018	BCR	C37-C22-C23	2.09	121.29	118.09
21	2	1216	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
21	2	1234	CLA	CHA-C1A-NA	-2.09	121.65	126.39
21	a	1116	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
21	l	1502	CLA	CHA-C1A-NA	-2.09	121.65	126.39
26	b	5002	LMG	C30-C29-C28	-2.09	106.03	113.69
21	b	1220	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
24	b	4017	BCR	C10-C11-C12	-2.09	117.14	123.20
21	a	1102	CLA	C3B-C4B-NB	-2.09	108.66	110.53
21	1	1119	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	2	1021	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
21	A	1138	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	a	1111	CLA	C4B-CHC-C1C	2.09	131.16	126.25
21	j	1302	CLA	C4B-CHC-C1C	2.09	131.16	126.25
21	a	1109	CLA	O2A-CGA-CBA	2.09	118.21	111.83
21	A	1129	CLA	CMA-C3A-C4A	2.09	117.39	111.77
21	2	1219	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
30	2	4006	ECH	C15-C16-C17	2.09	127.80	123.52
24	9	4021	BCR	C39-C30-C25	-2.09	106.97	110.24
21	1	1136	CLA	C1-O2A-CGA	2.09	121.71	116.65
26	B	5002	LMG	C30-C29-C28	-2.09	106.04	113.69
21	A	1127	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	2	1211	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	A	5003	LHG	O8-C23-O10	-2.09	118.40	123.63
21	1	1137	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	B	1226	CLA	C3B-C4B-NB	-2.09	108.67	110.53
21	b	1220	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	A	1108	CLA	O2A-CGA-CBA	2.09	118.20	111.83
24	b	4014	BCR	C8-C9-C10	2.09	122.29	119.01
21	A	1132	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
21	A	1138	CLA	CHA-C1A-NA	-2.09	121.67	126.39
21	A	1137	CLA	CMA-C3A-C4A	2.09	117.38	111.77
21	2	1229	CLA	O2A-CGA-CBA	2.09	118.20	111.83
21	b	1205	CLA	C4B-CHC-C1C	2.09	131.15	126.25
34	F	4016	ZEX	C31-C30-C29	2.09	130.20	127.28
21	B	1219	CLA	C4B-CHC-C1C	2.09	131.15	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	4001	BCR	C37-C22-C23	2.09	121.28	118.09
21	B	1230	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
24	K	4001	BCR	C12-C13-C14	-2.09	115.73	119.01
21	2	1231	CLA	C3B-C4B-NB	-2.09	108.67	110.53
21	a	1120	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
21	f	1301	CLA	C4B-CHC-C1C	2.08	131.15	126.25
21	a	1110	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
21	2	1222	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
21	1	1107	CLA	CHA-C1A-NA	-2.08	121.67	126.39
21	a	1111	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
31	L	5001	SQD	O5-C1-O6	-2.08	105.12	110.04
21	2	1217	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	b	1206	CLA	CAC-C3C-C4C	2.08	127.50	124.79
21	B	1236	CLA	CHA-C1A-NA	-2.08	121.67	126.39
21	b	1224	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
21	f	1302	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
24	A	4008	BCR	C37-C22-C23	2.08	121.27	118.09
24	a	4007	BCR	C37-C22-C23	2.08	121.27	118.09
21	b	1210	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
34	j	4015	ZEX	C17-C1-C6	-2.08	106.98	110.24
24	0	4022	BCR	C1-C6-C5	-2.08	119.79	122.64
21	b	1222	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
21	2	1234	CLA	C1-O2A-CGA	2.08	121.69	116.65
21	A	1121	CLA	C3B-C4B-NB	-2.08	108.67	110.53
21	B	1212	CLA	C4B-CHC-C1C	2.08	131.14	126.25
21	1	1140	CLA	O2A-CGA-CBA	2.08	118.18	111.83
21	K	1402	CLA	CHA-C1A-NA	-2.08	121.68	126.39
21	1	1130	CLA	CHA-C1A-NA	-2.08	121.68	126.39
21	B	1202	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
21	l	1501	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	A	1132	CLA	C1-O2A-CGA	2.08	121.69	116.65
26	b	5002	LMG	O1-C1-C2	2.08	111.43	108.27
21	A	1117	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
21	A	1801	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
21	a	1104	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
35	0	6001	LMT	C1'-C2'-C3'	2.08	114.39	110.01
21	1	1117	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	1	1110	CLA	O2A-CGA-CBA	2.08	118.17	111.83
21	B	1215	CLA	CAC-C3C-C4C	2.08	127.50	124.79
21	1	1136	CLA	CHA-C1A-NA	-2.08	121.68	126.39
21	L	1503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	b	1235	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1202	CLA	CMA-C3A-C4A	2.08	117.36	111.77
21	a	1801	CLA	O2A-CGA-CBA	2.08	118.17	111.83
21	A	1135	CLA	C1-C2-C3	-2.08	122.79	126.20
21	B	1227	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
21	1	1127	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
21	a	1127	CLA	C4B-CHC-C1C	2.08	131.13	126.25
21	b	1216	CLA	C2D-C1D-ND	2.08	112.18	110.13
24	2	4004	BCR	C30-C25-C26	-2.08	119.80	122.64
21	A	1130	CLA	C4B-CHC-C1C	2.08	131.13	126.25
21	1	1137	CLA	C4B-CHC-C1C	2.08	131.13	126.25
21	a	1118	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
21	a	1130	CLA	C4B-CHC-C1C	2.08	131.13	126.25
21	B	1210	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
21	b	1221	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	b	1227	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
21	2	1212	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
21	B	1215	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	L	1503	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	B	1201	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
21	b	1214	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
34	j	4015	ZEX	C19-C9-C10	-2.08	119.45	122.82
21	A	1111	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	B	1216	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	1	1013	CLA	C1D-ND-C4D	-2.08	104.86	106.31
24	L	4022	BCR	C10-C11-C12	-2.07	117.19	123.20
24	h	4018	BCR	C38-C26-C25	-2.07	122.22	124.48
21	1	1101	CLA	C4B-CHC-C1C	2.07	131.12	126.25
21	B	1222	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	B	1202	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
21	B	1022	CLA	C3B-C2B-C1B	-2.07	104.72	107.17
21	b	1239	CLA	CHA-C1A-NA	-2.07	121.70	126.39
21	A	1111	CLA	CAC-C3C-C4C	2.07	127.49	124.79
21	a	1136	CLA	CAA-CBA-CGA	-2.07	107.32	113.21
21	l	1501	CLA	CHA-C1A-NA	-2.07	121.70	126.39
21	b	1218	CLA	C3B-C4B-NB	-2.07	108.68	110.53
21	1	1103	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	A	1124	CLA	CHA-C1A-NA	-2.07	121.70	126.39
21	A	1123	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
24	a	4012	BCR	C32-C1-C6	-2.07	107.00	110.24
21	L	1502	CLA	CHA-C1A-NA	-2.07	121.70	126.39
21	B	1201	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
30	M	4021	ECH	C11-C10-C9	-2.07	124.37	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	1116	CLA	CHA-C1A-NA	-2.07	121.70	126.39
24	L	4019	BCR	C34-C9-C10	-2.07	119.46	122.82
21	B	1208	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
21	2	1214	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
21	a	1013	CLA	C1-O2A-CGA	2.07	121.66	116.65
24	a	4003	BCR	C1-C6-C5	-2.07	119.81	122.64
21	A	1140	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
21	B	1204	CLA	C4B-CHC-C1C	2.07	131.11	126.25
21	7	1303	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
21	1	1132	CLA	C1-O2A-CGA	2.07	121.66	116.65
21	a	1107	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
21	a	1111	CLA	O2A-CGA-CBA	2.07	118.14	111.83
21	1	1108	CLA	CHA-C1A-NA	-2.07	121.71	126.39
21	a	1011	CLA	C1-O2A-CGA	2.07	121.65	116.65
25	l	5002	LHG	O7-C7-O9	-2.07	118.87	123.70
21	B	1205	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
21	A	1131	CLA	CHA-C1A-NA	-2.07	121.71	126.39
21	1	1103	CLA	O2A-CGA-CBA	2.07	118.13	111.83
21	l	1502	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
21	a	1125	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
24	7	4013	BCR	C39-C30-C25	-2.07	107.00	110.24
24	l	4022	BCR	C29-C28-C27	2.07	115.82	111.28
21	a	1133	CLA	C1-O2A-CGA	2.07	121.65	116.65
24	B	4005	BCR	C37-C22-C23	2.07	121.24	118.09
21	A	1124	CLA	C2D-C1D-ND	2.07	112.17	110.13
21	A	1102	CLA	C3B-C2B-C1B	-2.06	104.73	107.17
21	A	1110	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
21	2	1226	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
21	A	1101	CLA	C2A-C1A-CHA	2.06	127.45	123.87
21	A	1012	CLA	CMA-C3A-C4A	2.06	117.32	111.77
21	B	1208	CLA	CHA-C1A-NA	-2.06	121.72	126.39
21	b	1210	CLA	CHA-C1A-NA	-2.06	121.72	126.39
21	2	1231	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
21	1	1110	CLA	C4B-CHC-C1C	2.06	131.10	126.25
25	1	5007	LHG	O7-C7-O9	-2.06	118.88	123.70
21	A	1111	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	k	1401	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	b	1221	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
31	L	5002	SQD	O3-C3-C2	-2.06	105.52	110.38
21	B	1236	CLA	CMA-C3A-C4A	2.06	117.31	111.77
24	B	4014	BCR	C34-C9-C10	-2.06	119.48	122.82
35	1	6001	LMT	O5B-C5B-C6B	2.06	111.55	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	1132	CLA	CHA-C1A-NA	-2.06	121.72	126.39
21	B	1203	CLA	CMA-C3A-C4A	2.06	117.31	111.77
21	1	1117	CLA	C3B-C4B-NB	-2.06	108.69	110.53
21	2	1218	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
30	B	4006	ECH	C19-C18-C17	2.06	122.25	119.01
21	b	1203	CLA	O2A-CGA-CBA	2.06	118.11	111.83
21	A	1134	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	2	1239	CLA	C3B-C4B-NB	-2.06	108.69	110.53
21	A	1801	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	B	1201	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
21	2	1226	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
21	1	1132	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
21	a	1140	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
24	j	4013	BCR	C30-C25-C24	2.06	121.23	115.65
24	a	4007	BCR	C15-C14-C13	2.06	130.16	127.28
21	A	1116	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	a	1128	CLA	C1-O2A-CGA	2.06	121.63	116.65
21	1	1106	CLA	O2A-CGA-CBA	2.06	118.10	111.83
24	2	4017	BCR	C15-C14-C13	2.06	130.16	127.28
21	A	1128	CLA	CMA-C3A-C4A	2.06	117.30	111.77
24	B	4017	BCR	C2-C1-C6	2.06	113.42	110.44
21	1	1011	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
21	b	1205	CLA	CMD-C2D-C3D	-2.06	122.98	127.69
21	j	1302	CLA	O2A-CGA-CBA	2.05	118.10	111.83
21	1	1138	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	b	1204	CLA	CAC-C3C-C4C	2.05	127.46	124.79
21	A	1113	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	1	1128	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	a	1134	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
21	A	1123	CLA	CMA-C3A-C2A	2.05	121.92	113.98
21	6	1302	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
21	a	1118	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
24	A	4019	BCR	C29-C28-C27	2.05	115.79	111.28
35	l	6001	LMT	C1B-O5B-C5B	2.05	117.73	113.72
24	1	4007	BCR	C31-C1-C6	-2.05	107.03	110.24
21	1	1133	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	0	1501	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
24	K	4001	BCR	C38-C26-C27	2.05	117.97	113.60
21	a	1126	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
21	f	1302	CLA	CHA-C1A-NA	-2.05	121.75	126.39
24	K	4001	BCR	C38-C26-C25	-2.05	122.25	124.48
21	b	1238	CLA	CMD-C2D-C3D	-2.05	122.99	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1232	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	6	1301	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	B	1221	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	1	1116	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	1	1117	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	0	1501	CLA	O2A-CGA-CBA	2.05	118.08	111.83
21	1	1119	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	2	1201	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
21	1	1126	CLA	CHA-C1A-NA	-2.05	121.75	126.39
21	B	1216	CLA	C1-O2A-CGA	2.05	121.61	116.65
21	1	1120	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
24	a	4002	BCR	C2-C1-C6	2.05	113.41	110.44
21	F	1301	CLA	C4B-CHC-C1C	2.05	131.06	126.25
24	l	4022	BCR	C30-C25-C26	-2.05	119.84	122.64
21	A	1133	CLA	O2A-CGA-CBA	2.05	118.08	111.83
21	b	1202	CLA	C3B-C2B-C1B	-2.05	104.76	107.17
21	b	1204	CLA	C4B-CHC-C1C	2.05	131.06	126.25
21	A	1119	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
21	b	1236	CLA	CHA-C1A-NA	-2.04	121.76	126.39
21	B	1226	CLA	CMA-C3A-C4A	2.04	117.27	111.77
21	B	1213	CLA	C2A-C1A-CHA	2.04	127.42	123.87
21	7	1303	CLA	C2D-C1D-ND	2.04	112.15	110.13
21	6	1301	CLA	C4B-CHC-C1C	2.04	131.05	126.25
21	B	1205	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
21	b	1215	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
21	1	1105	CLA	CHA-C1A-NA	-2.04	121.76	126.39
26	a	5002	LMG	O7-C10-O9	-2.04	118.93	123.70
21	0	1501	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
21	b	1208	CLA	C3B-C2B-C1B	-2.04	104.76	107.17
24	a	4003	BCR	C37-C22-C23	2.04	121.21	118.09
21	6	1302	CLA	C1D-ND-C4D	-2.04	104.88	106.31
21	a	1129	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	f	1302	CLA	C3B-C2B-C1B	-2.04	104.76	107.17
21	2	1231	CLA	CMA-C3A-C4A	2.04	117.26	111.77
21	1	1110	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	1	1135	CLA	C2D-C1D-ND	2.04	112.15	110.13
21	1	1107	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	1	1134	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	A	1101	CLA	C3B-C2B-C1B	-2.04	104.76	107.17
21	A	1122	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	A	1111	CLA	C3B-C4B-NB	-2.04	108.71	110.53
21	F	1302	CLA	C1-O2A-CGA	2.04	121.59	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1234	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
22	1	2001	PQN	C11-C3-C2	-2.04	121.39	124.89
21	B	1208	CLA	C2D-C1D-ND	2.04	112.14	110.13
21	A	1103	CLA	O2A-CGA-CBA	2.04	118.05	111.83
24	a	4012	BCR	C8-C7-C6	2.04	132.44	127.00
21	F	1301	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	B	1231	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	0	1503	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	2	1226	CLA	C4B-CHC-C1C	2.04	131.04	126.25
21	1	1131	CLA	CMA-C3A-C4A	2.04	117.25	111.77
21	A	1101	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	B	1237	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	B	1240	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
21	1	1131	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	a	4007	BCR	C29-C28-C27	2.04	115.75	111.28
21	B	1226	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	A	1012	CLA	C3B-C4B-NB	-2.04	108.71	110.53
21	2	1022	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	B	1208	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	b	1201	CLA	CHA-C1A-NA	-2.04	121.78	126.39
21	B	1220	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
21	b	1219	CLA	C4B-CHC-C1C	2.04	131.03	126.25
21	2	1221	CLA	C1D-ND-C4D	-2.04	104.88	106.31
21	A	1130	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
21	B	1224	CLA	CHA-C1A-NA	-2.03	121.78	126.39
21	b	1201	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
21	A	1109	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
24	f	4016	BCR	C37-C22-C23	2.03	121.19	118.09
24	j	4013	BCR	C36-C18-C19	-2.03	114.98	118.09
24	J	4013	BCR	C34-C9-C10	-2.03	119.52	122.82
21	b	1234	CLA	C3B-C4B-NB	-2.03	108.72	110.53
21	a	1115	CLA	O2A-CGA-CBA	2.03	118.03	111.83
21	A	1127	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
21	b	1210	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	A	1119	CLA	CHA-C1A-NA	-2.03	121.79	126.39
21	2	1238	CLA	C4B-CHC-C1C	2.03	131.03	126.25
21	2	1225	CLA	CHA-C1A-NA	-2.03	121.79	126.39
21	A	1104	CLA	CMA-C3A-C4A	2.03	117.23	111.77
21	2	1022	CLA	C3B-C4B-NB	-2.03	108.72	110.53
34	j	4015	ZEX	C21-C26-C27	-2.03	110.14	115.65
21	0	1501	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	1	1128	CLA	CMD-C2D-C3D	-2.03	123.03	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	1203	CLA	CHA-C1A-NA	-2.03	121.79	126.39
21	1	1136	CLA	C4B-CHC-C1C	2.03	131.02	126.25
21	B	1201	CLA	CHA-C1A-NA	-2.03	121.79	126.39
21	b	1207	CLA	O2A-C1-C2	2.03	115.92	108.11
21	2	1221	CLA	CMA-C3A-C2A	2.03	121.83	113.98
25	1	5007	LHG	C5-O7-C7	-2.03	112.94	117.80
21	1	1118	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
30	b	4011	ECH	C19-C18-C17	2.03	122.20	119.01
24	a	4019	BCR	C35-C13-C14	-2.03	119.53	122.82
21	A	1125	CLA	OBD-CAD-C3D	-2.03	123.67	128.42
24	2	4010	BCR	C37-C22-C23	2.03	121.19	118.09
21	a	1128	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
21	a	1127	CLA	O2A-CGA-CBA	2.03	118.02	111.83
21	a	1129	CLA	CMA-C3A-C4A	2.03	117.22	111.77
21	b	1234	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	2	1230	CLA	C4B-CHC-C1C	2.03	131.01	126.25
21	b	1234	CLA	C4B-CHC-C1C	2.03	131.01	126.25
21	A	1115	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	a	1134	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
21	B	1229	CLA	C1-O2A-CGA	2.03	121.56	116.65
21	l	1501	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
21	A	1140	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	A	1114	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
24	2	4011	BCR	C38-C26-C25	-2.03	122.27	124.48
21	B	1235	CLA	C3B-C4B-NB	-2.03	108.72	110.53
21	b	1235	CLA	C1-O2A-CGA	2.03	121.55	116.65
21	2	1214	CLA	C1-O2A-CGA	2.02	121.55	116.65
21	A	1129	CLA	CHA-C1A-NA	-2.02	121.81	126.39
21	B	1232	CLA	CHA-C1A-NA	-2.02	121.81	126.39
21	2	1239	CLA	CHA-C1A-NA	-2.02	121.81	126.39
34	7	4015	ZEX	C15-C35-C34	-2.02	119.38	123.52
21	b	1230	CLA	C4B-CHC-C1C	2.02	131.01	126.25
21	1	1129	CLA	C1-O2A-CGA	2.02	121.55	116.65
24	2	4017	BCR	C38-C26-C25	-2.02	122.28	124.48
21	2	1222	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
26	b	5005	LMG	O8-C28-O10	-2.02	118.57	123.63
24	B	4010	BCR	C34-C9-C10	-2.02	119.54	122.82
24	9	4021	BCR	C11-C12-C13	-2.02	120.82	126.36
30	i	4020	ECH	C16-C15-C14	2.02	127.66	123.52
24	j	4013	BCR	C19-C18-C17	2.02	122.19	119.01
24	9	4021	BCR	C37-C22-C23	2.02	121.18	118.09
21	B	1204	CLA	C3B-C4B-NB	-2.02	108.72	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	5006	LHG	C5-O7-C7	-2.02	112.96	117.80
35	F	6001	LMT	C1'-O5'-C5'	-2.02	109.77	113.72
21	A	1105	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
21	B	1215	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
21	B	1226	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
21	1	1111	CLA	C4B-CHC-C1C	2.02	131.00	126.25
24	0	4019	BCR	C15-C14-C13	2.02	130.11	127.28
21	A	1102	CLA	CMA-C3A-C4A	2.02	117.20	111.77
21	b	1214	CLA	CHA-C1A-NA	-2.02	121.82	126.39
21	2	1228	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	A	1103	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	B	1225	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	1	1117	CLA	O2A-CGA-CBA	2.02	117.99	111.83
21	a	1117	CLA	C4B-CHC-C1C	2.02	131.00	126.25
21	1	1121	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	A	1102	CLA	CHA-C1A-NA	-2.02	121.82	126.39
21	b	1221	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
21	a	1111	CLA	C3B-C2B-C1B	-2.02	104.79	107.17
34	J	4015	ZEX	C17-C1-C6	-2.02	107.08	110.24
21	A	1118	CLA	C4B-CHC-C1C	2.02	130.99	126.25
21	b	1216	CLA	C4B-CHC-C1C	2.02	130.99	126.25
24	B	4017	BCR	C35-C13-C12	2.02	121.17	118.09
21	A	1011	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	A	1123	CLA	CHA-C1A-NA	-2.02	121.82	126.39
24	0	4022	BCR	C37-C22-C23	2.02	121.17	118.09
21	A	1108	CLA	C4B-CHC-C1C	2.02	130.99	126.25
21	a	1013	CLA	CHA-C1A-NA	-2.02	121.82	126.39
21	b	1239	CLA	C1-O2A-CGA	2.02	121.53	116.65
30	M	4021	ECH	C37-C22-C23	-2.02	115.01	118.09
21	1	1133	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
21	a	1122	CLA	C3B-C2B-C1B	-2.02	104.79	107.17
24	7	4013	BCR	C23-C24-C25	2.02	132.38	127.00
21	B	1209	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
24	b	4017	BCR	C35-C13-C12	2.02	121.17	118.09
30	2	4006	ECH	C10-C11-C12	-2.02	117.36	123.20
21	A	1123	CLA	C2D-C1D-ND	2.02	112.12	110.13
21	2	1234	CLA	C4B-CHC-C1C	2.02	130.99	126.25
21	A	1012	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
21	a	1120	CLA	CAC-C3C-C4C	2.02	127.41	124.79
21	2	1207	CLA	CMD-C2D-C3D	-2.02	123.07	127.69
21	b	1230	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
21	2	1208	CLA	C4B-CHC-C1C	2.02	130.99	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	0	1503	CLA	CHA-C1A-NA	-2.02	121.83	126.39
21	a	1130	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
30	b	4011	ECH	O27-C27-C26	2.01	122.79	120.98
21	B	1204	CLA	CHA-C1A-NA	-2.01	121.83	126.39
21	b	1229	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
21	A	1109	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
21	A	1112	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
21	B	1234	CLA	C3B-C4B-NB	-2.01	108.73	110.53
21	2	1204	CLA	C3B-C4B-NB	-2.01	108.73	110.53
24	1	4002	BCR	C35-C13-C12	2.01	121.16	118.09
21	A	1132	CLA	CMA-C3A-C4A	2.01	117.18	111.77
21	b	1214	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
21	A	1128	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
21	a	1140	CLA	O2A-CGA-CBA	2.01	117.97	111.83
21	b	1202	CLA	C3B-C4B-NB	-2.01	108.73	110.53
21	b	1209	CLA	CAC-C3C-C4C	2.01	127.41	124.79
21	2	1023	CLA	C1D-ND-C4D	-2.01	104.90	106.31
21	b	1224	CLA	CMA-C3A-C4A	2.01	117.17	111.77
34	J	4015	ZEX	C11-C12-C13	-2.01	120.85	126.36
21	2	1202	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
21	2	1225	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	b	1225	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
21	l	1503	CLA	C3B-C4B-NB	-2.01	108.74	110.53
21	A	1133	CLA	CHA-C1A-NA	-2.01	121.84	126.39
21	2	1226	CLA	C1D-ND-C4D	-2.01	104.90	106.31
21	B	1212	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
21	1	1125	CLA	C4B-CHC-C1C	2.01	130.97	126.25
24	j	4013	BCR	C23-C24-C25	2.01	132.36	127.00
21	b	1224	CLA	CAC-C3C-C4C	2.01	127.40	124.79
21	A	1126	CLA	C3B-C4B-NB	-2.01	108.74	110.53
21	B	1218	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
30	b	4011	ECH	C8-C7-C6	-2.01	121.64	127.00
21	2	1237	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	2	4004	BCR	C35-C13-C12	2.01	121.15	118.09
21	b	1206	CLA	C3B-C2B-C1B	-2.01	104.81	107.17
21	A	1108	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
26	0	5001	LMG	O6-C5-C6	2.01	111.41	106.44
21	B	1216	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
21	2	1236	CLA	C4B-CHC-C1C	2.01	130.96	126.25
21	B	1219	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
21	a	1129	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
21	2	1215	CLA	CMD-C2D-C3D	-2.00	123.09	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	5003	LHG	O7-C7-O9	-2.00	119.02	123.70
21	a	1132	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
24	2	4011	BCR	C40-C30-C25	-2.00	107.10	110.24
21	B	1237	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
21	A	1106	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	2	1202	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	1	1119	CLA	C2D-C1D-ND	2.00	112.11	110.13
21	1	1121	CLA	C2D-C1D-ND	2.00	112.11	110.13
21	a	1135	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
21	1	1116	CLA	C4B-CHC-C1C	2.00	130.96	126.25
21	B	1230	CLA	O2A-CGA-CBA	2.00	117.94	111.83
21	J	1303	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
21	1	1120	CLA	C1-O2A-CGA	2.00	121.50	116.65
24	f	4016	BCR	C30-C25-C26	-2.00	119.90	122.64
21	a	1133	CLA	C4B-CHC-C1C	2.00	130.95	126.25
21	a	1103	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	b	1205	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	A	1109	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	B	1229	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	a	1118	CLA	C4B-CHC-C1C	2.00	130.95	126.25
21	A	1118	CLA	CMD-C2D-C3D	-2.00	123.10	127.69

All (256) chirality outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	A	1117	CLA	ND
21	A	1118	CLA	ND
21	A	1119	CLA	ND
21	A	1120	CLA	ND
21	A	1121	CLA	ND
21	A	1122	CLA	ND
21	A	1123	CLA	ND
21	A	1124	CLA	ND
21	A	1126	CLA	ND
21	A	1127	CLA	ND
21	A	1128	CLA	ND
21	A	1131	CLA	ND
21	A	1132	CLA	ND
21	A	1133	CLA	ND
21	A	1134	CLA	ND
21	A	1136	CLA	ND
21	A	1137	CLA	ND
21	A	1138	CLA	ND
21	A	1139	CLA	ND
21	A	1140	CLA	ND
21	A	1130	CLA	ND
21	A	1801	CLA	ND
21	A	1012	CLA	ND
21	B	1022	CLA	ND
21	B	1237	CLA	ND
21	B	1021	CLA	ND
21	B	1023	CLA	ND
21	B	1201	CLA	ND
21	B	1202	CLA	ND
21	B	1203	CLA	ND
21	B	1204	CLA	ND
21	B	1205	CLA	ND
21	B	1206	CLA	ND
21	B	1208	CLA	ND
21	B	1211	CLA	ND
21	B	1212	CLA	ND
21	B	1213	CLA	ND
21	B	1214	CLA	ND
21	B	1215	CLA	ND
21	B	1216	CLA	ND
21	B	1217	CLA	ND
21	B	1218	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	B	1220	CLA	ND
21	B	1221	CLA	ND
21	B	1222	CLA	ND
21	B	1223	CLA	ND
21	B	1224	CLA	ND
21	B	1225	CLA	ND
21	B	1226	CLA	ND
21	B	1228	CLA	ND
21	B	1229	CLA	ND
21	B	1232	CLA	ND
21	B	1235	CLA	ND
21	B	1236	CLA	ND
21	B	1238	CLA	ND
21	B	1239	CLA	ND
21	B	1240	CLA	ND
21	B	1230	CLA	ND
21	F	1301	CLA	ND
21	F	1302	CLA	ND
21	J	1302	CLA	ND
21	J	1303	CLA	ND
21	K	1401	CLA	ND
21	L	1501	CLA	ND
21	L	1502	CLA	ND
21	a	1011	CLA	ND
21	a	1013	CLA	ND
21	a	1102	CLA	ND
21	a	1103	CLA	ND
21	a	1104	CLA	ND
21	a	1105	CLA	ND
21	a	1106	CLA	ND
21	a	1107	CLA	ND
21	a	1108	CLA	ND
21	a	1109	CLA	ND
21	a	1110	CLA	ND
21	a	1111	CLA	ND
21	a	1112	CLA	ND
21	a	1113	CLA	ND
21	a	1114	CLA	ND
21	a	1116	CLA	ND
21	a	1117	CLA	ND
21	a	1118	CLA	ND
21	a	1119	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	a	1121	CLA	ND
21	a	1122	CLA	ND
21	a	1123	CLA	ND
21	a	1124	CLA	ND
21	a	1125	CLA	ND
21	a	1126	CLA	ND
21	a	1127	CLA	ND
21	a	1128	CLA	ND
21	a	1129	CLA	ND
21	a	1131	CLA	ND
21	a	1134	CLA	ND
21	a	1135	CLA	ND
21	a	1136	CLA	ND
21	a	1137	CLA	ND
21	a	1139	CLA	ND
21	a	1140	CLA	ND
21	a	1801	CLA	ND
21	a	1130	CLA	ND
21	a	1138	CLA	ND
21	a	1132	CLA	ND
21	a	1012	CLA	ND
21	b	1022	CLA	ND
21	b	1237	CLA	ND
21	b	1021	CLA	ND
21	b	1023	CLA	ND
21	b	1202	CLA	ND
21	b	1203	CLA	ND
21	b	1204	CLA	ND
21	b	1205	CLA	ND
21	b	1206	CLA	ND
21	b	1208	CLA	ND
21	b	1211	CLA	ND
21	b	1213	CLA	ND
21	b	1214	CLA	ND
21	b	1215	CLA	ND
21	b	1216	CLA	ND
21	b	1217	CLA	ND
21	b	1218	CLA	ND
21	b	1219	CLA	ND
21	b	1220	CLA	ND
21	b	1221	CLA	ND
21	b	1222	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	b	1223	CLA	ND
21	b	1224	CLA	ND
21	b	1225	CLA	ND
21	b	1226	CLA	ND
21	b	1227	CLA	ND
21	b	1228	CLA	ND
21	b	1229	CLA	ND
21	b	1231	CLA	ND
21	b	1232	CLA	ND
21	b	1234	CLA	ND
21	b	1235	CLA	ND
21	b	1236	CLA	ND
21	b	1238	CLA	ND
21	b	1239	CLA	ND
21	b	1240	CLA	ND
21	b	1230	CLA	ND
21	b	1201	CLA	ND
21	f	1301	CLA	ND
21	f	1302	CLA	ND
21	j	1302	CLA	ND
21	j	1303	CLA	ND
21	k	1401	CLA	ND
21	k	1402	CLA	ND
21	l	1501	CLA	ND
21	l	1502	CLA	ND
21	l	1503	CLA	ND
21	1	1011	CLA	ND
21	1	1013	CLA	ND
21	1	1102	CLA	ND
21	1	1103	CLA	ND
21	1	1104	CLA	ND
21	1	1105	CLA	ND
21	1	1106	CLA	ND
21	1	1107	CLA	ND
21	1	1108	CLA	ND
21	1	1109	CLA	ND
21	1	1110	CLA	ND
21	1	1111	CLA	ND
21	1	1112	CLA	ND
21	1	1113	CLA	ND
21	1	1114	CLA	ND
21	1	1115	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	1	1116	CLA	ND
21	1	1117	CLA	ND
21	1	1118	CLA	ND
21	1	1119	CLA	ND
21	1	1120	CLA	ND
21	1	1121	CLA	ND
21	1	1122	CLA	ND
21	1	1124	CLA	ND
21	1	1125	CLA	ND
21	1	1126	CLA	ND
21	1	1127	CLA	ND
21	1	1128	CLA	ND
21	1	1129	CLA	ND
21	1	1131	CLA	ND
21	1	1132	CLA	ND
21	1	1133	CLA	ND
21	1	1134	CLA	ND
21	1	1136	CLA	ND
21	1	1137	CLA	ND
21	1	1138	CLA	ND
21	1	1140	CLA	ND
21	1	1801	CLA	ND
21	1	1130	CLA	ND
21	1	1139	CLA	ND
21	1	1012	CLA	ND
21	2	1022	CLA	ND
21	2	1237	CLA	ND
21	2	1021	CLA	ND
21	2	1023	CLA	ND
21	2	1201	CLA	ND
21	2	1202	CLA	ND
21	2	1203	CLA	ND
21	2	1204	CLA	ND
21	2	1205	CLA	ND
21	2	1206	CLA	ND
21	2	1208	CLA	ND
21	2	1211	CLA	ND
21	2	1212	CLA	ND
21	2	1213	CLA	ND
21	2	1214	CLA	ND
21	2	1215	CLA	ND
21	2	1216	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	2	1217	CLA	ND
21	2	1218	CLA	ND
21	2	1220	CLA	ND
21	2	1221	CLA	ND
21	2	1222	CLA	ND
21	2	1224	CLA	ND
21	2	1225	CLA	ND
21	2	1226	CLA	ND
21	2	1227	CLA	ND
21	2	1228	CLA	ND
21	2	1229	CLA	ND
21	2	1231	CLA	ND
21	2	1232	CLA	ND
21	2	1234	CLA	ND
21	2	1235	CLA	ND
21	2	1236	CLA	ND
21	2	1238	CLA	ND
21	2	1239	CLA	ND
21	2	1230	CLA	ND
21	6	1301	CLA	ND
21	6	1302	CLA	ND
21	7	1302	CLA	ND
21	7	1303	CLA	ND
21	8	1401	CLA	ND
21	8	1402	CLA	ND
21	0	1501	CLA	ND
21	0	1502	CLA	ND
21	0	1503	CLA	ND
34	F	4016	ZEX	C24

All (5927) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	1102	CLA	C11-C10-C8-C9
21	A	1103	CLA	C1A-C2A-CAA-CBA
21	A	1103	CLA	C3A-C2A-CAA-CBA
21	A	1103	CLA	CAD-CBD-CGD-O1D
21	A	1103	CLA	CAD-CBD-CGD-O2D
21	A	1106	CLA	C1A-C2A-CAA-CBA
21	A	1106	CLA	CHA-CBD-CGD-O1D
21	A	1106	CLA	CHA-CBD-CGD-O2D
21	A	1107	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1107	CLA	C2-C1-O2A-CGA
21	A	1107	CLA	CBD-CGD-O2D-CED
21	A	1108	CLA	C1A-C2A-CAA-CBA
21	A	1110	CLA	C1A-C2A-CAA-CBA
21	A	1110	CLA	C3A-C2A-CAA-CBA
21	A	1111	CLA	C3A-C2A-CAA-CBA
21	A	1112	CLA	C1A-C2A-CAA-CBA
21	A	1112	CLA	C3A-C2A-CAA-CBA
21	A	1113	CLA	CAD-CBD-CGD-O2D
21	A	1114	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	C4B-C3B-CAB-CBB
21	A	1118	CLA	CBD-CGD-O2D-CED
21	A	1119	CLA	C1A-C2A-CAA-CBA
21	A	1119	CLA	C3A-C2A-CAA-CBA
21	A	1119	CLA	C11-C10-C8-C9
21	A	1121	CLA	C1A-C2A-CAA-CBA
21	A	1121	CLA	C6-C7-C8-C9
21	A	1122	CLA	C1A-C2A-CAA-CBA
21	A	1123	CLA	CHA-CBD-CGD-O1D
21	A	1123	CLA	CHA-CBD-CGD-O2D
21	A	1124	CLA	C11-C12-C13-C14
21	A	1126	CLA	C2-C1-O2A-CGA
21	A	1126	CLA	CBD-CGD-O2D-CED
21	A	1128	CLA	C2-C1-O2A-CGA
21	A	1128	CLA	CHA-CBD-CGD-O1D
21	A	1128	CLA	CHA-CBD-CGD-O2D
21	A	1129	CLA	C6-C7-C8-C9
21	A	1131	CLA	C6-C7-C8-C9
21	A	1132	CLA	CHA-CBD-CGD-O1D
21	A	1132	CLA	CHA-CBD-CGD-O2D
21	A	1134	CLA	C1A-C2A-CAA-CBA
21	A	1135	CLA	CBD-CGD-O2D-CED
21	A	1139	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	C2-C1-O2A-CGA
21	A	1140	CLA	C11-C12-C13-C14
21	A	1801	CLA	CAD-CBD-CGD-O1D
21	A	1801	CLA	CAD-CBD-CGD-O2D
21	A	1012	CLA	CAD-CBD-CGD-O1D
21	A	1012	CLA	CAD-CBD-CGD-O2D
21	B	1237	CLA	CBA-CGA-O2A-C1
21	B	1237	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1021	CLA	CBD-CGD-O2D-CED
21	B	1201	CLA	CBD-CGD-O2D-CED
21	B	1202	CLA	C3A-C2A-CAA-CBA
21	B	1202	CLA	CAD-CBD-CGD-O1D
21	B	1202	CLA	CAD-CBD-CGD-O2D
21	B	1203	CLA	CBD-CGD-O2D-CED
21	B	1205	CLA	CHA-CBD-CGD-O1D
21	B	1205	CLA	CHA-CBD-CGD-O2D
21	B	1206	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	CBD-CGD-O2D-CED
21	B	1209	CLA	C1A-C2A-CAA-CBA
21	B	1209	CLA	C3A-C2A-CAA-CBA
21	B	1209	CLA	CHA-CBD-CGD-O1D
21	B	1209	CLA	CHA-CBD-CGD-O2D
21	B	1209	CLA	C11-C10-C8-C9
21	B	1210	CLA	C1A-C2A-CAA-CBA
21	B	1212	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	C1A-C2A-CAA-CBA
21	B	1213	CLA	CHA-CBD-CGD-O1D
21	B	1213	CLA	CHA-CBD-CGD-O2D
21	B	1214	CLA	C6-C7-C8-C9
21	B	1215	CLA	C1A-C2A-CAA-CBA
21	B	1215	CLA	C3A-C2A-CAA-CBA
21	B	1215	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	C1A-C2A-CAA-CBA
21	B	1216	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	C1A-C2A-CAA-CBA
21	B	1217	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	C14-C13-C15-C16
21	B	1218	CLA	C1A-C2A-CAA-CBA
21	B	1219	CLA	C1A-C2A-CAA-CBA
21	B	1219	CLA	CBA-CGA-O2A-C1
21	B	1219	CLA	O1A-CGA-O2A-C1
21	B	1220	CLA	C6-C7-C8-C9
21	B	1221	CLA	CHA-CBD-CGD-O1D
21	B	1221	CLA	CHA-CBD-CGD-O2D
21	B	1223	CLA	C2B-C3B-CAB-CBB
21	B	1223	CLA	C4B-C3B-CAB-CBB
21	B	1224	CLA	C1A-C2A-CAA-CBA
21	B	1224	CLA	C3A-C2A-CAA-CBA
21	B	1224	CLA	CBD-CGD-O2D-CED
21	B	1225	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1225	CLA	C3A-C2A-CAA-CBA
21	B	1226	CLA	CAD-CBD-CGD-O2D
21	B	1226	CLA	C14-C13-C15-C16
21	B	1227	CLA	C1A-C2A-CAA-CBA
21	B	1227	CLA	C3A-C2A-CAA-CBA
21	B	1227	CLA	C2-C1-O2A-CGA
21	B	1229	CLA	C1A-C2A-CAA-CBA
21	B	1229	CLA	C3A-C2A-CAA-CBA
21	B	1231	CLA	C2-C1-O2A-CGA
21	B	1234	CLA	C1A-C2A-CAA-CBA
21	B	1236	CLA	C2-C1-O2A-CGA
21	B	1239	CLA	C1A-C2A-CAA-CBA
21	B	1239	CLA	C3A-C2A-CAA-CBA
21	B	1239	CLA	C2-C1-O2A-CGA
21	B	1240	CLA	C1A-C2A-CAA-CBA
21	B	1240	CLA	C3A-C2A-CAA-CBA
21	B	1240	CLA	CHA-CBD-CGD-O1D
21	B	1240	CLA	CHA-CBD-CGD-O2D
21	B	1207	CLA	C11-C12-C13-C14
21	B	1230	CLA	C1A-C2A-CAA-CBA
21	B	1230	CLA	C3A-C2A-CAA-CBA
21	F	1301	CLA	C11-C10-C8-C7
21	F	1302	CLA	C1A-C2A-CAA-CBA
21	F	1302	CLA	C3A-C2A-CAA-CBA
21	F	1302	CLA	C4B-C3B-CAB-CBB
21	F	1302	CLA	CHA-CBD-CGD-O1D
21	F	1302	CLA	CHA-CBD-CGD-O2D
21	J	1303	CLA	CHA-CBD-CGD-O1D
21	J	1303	CLA	CHA-CBD-CGD-O2D
21	J	1303	CLA	C12-C13-C15-C16
21	L	1501	CLA	C1A-C2A-CAA-CBA
21	L	1501	CLA	C3A-C2A-CAA-CBA
21	L	1502	CLA	C1A-C2A-CAA-CBA
21	L	1502	CLA	C3A-C2A-CAA-CBA
21	L	1503	CLA	C1A-C2A-CAA-CBA
21	a	1013	CLA	C2-C1-O2A-CGA
21	a	1102	CLA	CHA-CBD-CGD-O1D
21	a	1102	CLA	CHA-CBD-CGD-O2D
21	a	1103	CLA	C1A-C2A-CAA-CBA
21	a	1103	CLA	C3A-C2A-CAA-CBA
21	a	1103	CLA	CAD-CBD-CGD-O1D
21	a	1103	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1106	CLA	C3A-C2A-CAA-CBA
21	a	1106	CLA	CHA-CBD-CGD-O1D
21	a	1106	CLA	CHA-CBD-CGD-O2D
21	a	1107	CLA	CBD-CGD-O2D-CED
21	a	1108	CLA	C1A-C2A-CAA-CBA
21	a	1109	CLA	C1A-C2A-CAA-CBA
21	a	1109	CLA	C3A-C2A-CAA-CBA
21	a	1109	CLA	CBD-CGD-O2D-CED
21	a	1110	CLA	C1A-C2A-CAA-CBA
21	a	1110	CLA	C3A-C2A-CAA-CBA
21	a	1111	CLA	C3A-C2A-CAA-CBA
21	a	1111	CLA	C2-C3-C5-C6
21	a	1111	CLA	C4-C3-C5-C6
21	a	1112	CLA	C1A-C2A-CAA-CBA
21	a	1112	CLA	C3A-C2A-CAA-CBA
21	a	1112	CLA	C2-C1-O2A-CGA
21	a	1112	CLA	CBD-CGD-O2D-CED
21	a	1113	CLA	CHA-CBD-CGD-O1D
21	a	1113	CLA	CHA-CBD-CGD-O2D
21	a	1114	CLA	C1A-C2A-CAA-CBA
21	a	1114	CLA	CBA-CGA-O2A-C1
21	a	1114	CLA	O1A-CGA-O2A-C1
21	a	1114	CLA	C3-C5-C6-C7
21	a	1116	CLA	C3A-C2A-CAA-CBA
21	a	1116	CLA	CBD-CGD-O2D-CED
21	a	1117	CLA	C1A-C2A-CAA-CBA
21	a	1117	CLA	C3A-C2A-CAA-CBA
21	a	1118	CLA	CBD-CGD-O2D-CED
21	a	1119	CLA	CBD-CGD-O2D-CED
21	a	1120	CLA	C1A-C2A-CAA-CBA
21	a	1120	CLA	CHA-CBD-CGD-O2D
21	a	1121	CLA	C1A-C2A-CAA-CBA
21	a	1121	CLA	C2-C3-C5-C6
21	a	1121	CLA	C4-C3-C5-C6
21	a	1122	CLA	C1A-C2A-CAA-CBA
21	a	1123	CLA	C2-C1-O2A-CGA
21	a	1123	CLA	CHA-CBD-CGD-O1D
21	a	1123	CLA	CHA-CBD-CGD-O2D
21	a	1125	CLA	C2-C1-O2A-CGA
21	a	1126	CLA	CBD-CGD-O2D-CED
21	a	1128	CLA	C2-C1-O2A-CGA
21	a	1128	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1128	CLA	CHA-CBD-CGD-O2D
21	a	1129	CLA	C3A-C2A-CAA-CBA
21	a	1131	CLA	C2B-C3B-CAB-CBB
21	a	1131	CLA	C4B-C3B-CAB-CBB
21	a	1133	CLA	C2-C1-O2A-CGA
21	a	1134	CLA	C1A-C2A-CAA-CBA
21	a	1136	CLA	CHA-CBD-CGD-O1D
21	a	1136	CLA	CHA-CBD-CGD-O2D
21	a	1140	CLA	CBD-CGD-O2D-CED
21	a	1801	CLA	C1A-C2A-CAA-CBA
21	a	1801	CLA	C3A-C2A-CAA-CBA
21	a	1801	CLA	CBD-CGD-O2D-CED
21	a	1130	CLA	C4-C3-C5-C6
21	a	1138	CLA	C2-C1-O2A-CGA
21	a	1132	CLA	CHA-CBD-CGD-O1D
21	a	1132	CLA	CHA-CBD-CGD-O2D
21	a	1012	CLA	CAD-CBD-CGD-O1D
21	a	1012	CLA	CAD-CBD-CGD-O2D
21	b	1237	CLA	CBA-CGA-O2A-C1
21	b	1237	CLA	O1A-CGA-O2A-C1
21	b	1237	CLA	CBD-CGD-O2D-CED
21	b	1202	CLA	C3A-C2A-CAA-CBA
21	b	1205	CLA	CHA-CBD-CGD-O1D
21	b	1205	CLA	CHA-CBD-CGD-O2D
21	b	1206	CLA	C2-C1-O2A-CGA
21	b	1208	CLA	C1A-C2A-CAA-CBA
21	b	1208	CLA	C3A-C2A-CAA-CBA
21	b	1209	CLA	C1A-C2A-CAA-CBA
21	b	1209	CLA	C3A-C2A-CAA-CBA
21	b	1209	CLA	C6-C7-C8-C9
21	b	1210	CLA	C1A-C2A-CAA-CBA
21	b	1213	CLA	C1A-C2A-CAA-CBA
21	b	1213	CLA	CHA-CBD-CGD-O1D
21	b	1213	CLA	CHA-CBD-CGD-O2D
21	b	1213	CLA	CBD-CGD-O2D-CED
21	b	1214	CLA	C2B-C3B-CAB-CBB
21	b	1214	CLA	C4B-C3B-CAB-CBB
21	b	1214	CLA	C6-C7-C8-C9
21	b	1215	CLA	C1A-C2A-CAA-CBA
21	b	1215	CLA	C3A-C2A-CAA-CBA
21	b	1215	CLA	C2-C1-O2A-CGA
21	b	1216	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1216	CLA	C3A-C2A-CAA-CBA
21	b	1216	CLA	C2-C1-O2A-CGA
21	b	1217	CLA	C3A-C2A-CAA-CBA
21	b	1217	CLA	C2-C3-C5-C6
21	b	1217	CLA	C4-C3-C5-C6
21	b	1219	CLA	C3A-C2A-CAA-CBA
21	b	1220	CLA	C4B-C3B-CAB-CBB
21	b	1220	CLA	CBD-CGD-O2D-CED
21	b	1221	CLA	CHA-CBD-CGD-O1D
21	b	1221	CLA	CHA-CBD-CGD-O2D
21	b	1224	CLA	C3A-C2A-CAA-CBA
21	b	1224	CLA	CBD-CGD-O2D-CED
21	b	1225	CLA	C1A-C2A-CAA-CBA
21	b	1225	CLA	C3A-C2A-CAA-CBA
21	b	1228	CLA	C1A-C2A-CAA-CBA
21	b	1229	CLA	C1A-C2A-CAA-CBA
21	b	1229	CLA	C3A-C2A-CAA-CBA
21	b	1229	CLA	CBD-CGD-O2D-CED
21	b	1231	CLA	C2-C1-O2A-CGA
21	b	1231	CLA	CBD-CGD-O2D-CED
21	b	1232	CLA	C1A-C2A-CAA-CBA
21	b	1232	CLA	C3A-C2A-CAA-CBA
21	b	1239	CLA	C1A-C2A-CAA-CBA
21	b	1239	CLA	C3A-C2A-CAA-CBA
21	b	1239	CLA	C2-C1-O2A-CGA
21	b	1240	CLA	C3A-C2A-CAA-CBA
21	b	1240	CLA	CAD-CBD-CGD-O1D
21	b	1240	CLA	CAD-CBD-CGD-O2D
21	b	1230	CLA	C3A-C2A-CAA-CBA
21	b	1230	CLA	C2-C1-O2A-CGA
21	b	1230	CLA	CHA-CBD-CGD-O1D
21	b	1230	CLA	CHA-CBD-CGD-O2D
21	f	1301	CLA	CBD-CGD-O2D-CED
21	f	1302	CLA	CAD-CBD-CGD-O1D
21	f	1302	CLA	CAD-CBD-CGD-O2D
21	f	1302	CLA	C6-C7-C8-C9
21	j	1302	CLA	C2-C1-O2A-CGA
21	j	1303	CLA	C2-C1-O2A-CGA
21	k	1402	CLA	C2-C1-O2A-CGA
21	k	1402	CLA	C4B-C3B-CAB-CBB
21	l	1501	CLA	C3A-C2A-CAA-CBA
21	l	1501	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	l	1503	CLA	CBD-CGD-O2D-CED
21	1	1011	CLA	C1A-C2A-CAA-CBA
21	1	1102	CLA	C3A-C2A-CAA-CBA
21	1	1102	CLA	CBA-CGA-O2A-C1
21	1	1102	CLA	O1A-CGA-O2A-C1
21	1	1102	CLA	CAD-CBD-CGD-O1D
21	1	1102	CLA	CAD-CBD-CGD-O2D
21	1	1103	CLA	C1A-C2A-CAA-CBA
21	1	1103	CLA	C3A-C2A-CAA-CBA
21	1	1103	CLA	CAD-CBD-CGD-O2D
21	1	1104	CLA	CBD-CGD-O2D-CED
21	1	1106	CLA	C1A-C2A-CAA-CBA
21	1	1106	CLA	C3A-C2A-CAA-CBA
21	1	1106	CLA	CHA-CBD-CGD-O1D
21	1	1106	CLA	CHA-CBD-CGD-O2D
21	1	1106	CLA	C14-C13-C15-C16
21	1	1107	CLA	C1A-C2A-CAA-CBA
21	1	1108	CLA	C1A-C2A-CAA-CBA
21	1	1108	CLA	CBD-CGD-O2D-CED
21	1	1109	CLA	CBD-CGD-O2D-CED
21	1	1110	CLA	C1A-C2A-CAA-CBA
21	1	1110	CLA	C3A-C2A-CAA-CBA
21	1	1111	CLA	C3A-C2A-CAA-CBA
21	1	1112	CLA	C1A-C2A-CAA-CBA
21	1	1112	CLA	C3A-C2A-CAA-CBA
21	1	1112	CLA	C2-C1-O2A-CGA
21	1	1112	CLA	CBD-CGD-O2D-CED
21	1	1113	CLA	C2A-CAA-CBA-CGA
21	1	1113	CLA	CAA-CBA-CGA-O1A
21	1	1116	CLA	C1A-C2A-CAA-CBA
21	1	1116	CLA	C3A-C2A-CAA-CBA
21	1	1116	CLA	CBD-CGD-O2D-CED
21	1	1116	CLA	C6-C7-C8-C9
21	1	1117	CLA	C1A-C2A-CAA-CBA
21	1	1117	CLA	C3A-C2A-CAA-CBA
21	1	1121	CLA	C1A-C2A-CAA-CBA
21	1	1121	CLA	C3A-C2A-CAA-CBA
21	1	1121	CLA	CBD-CGD-O2D-CED
21	1	1123	CLA	C2-C1-O2A-CGA
21	1	1124	CLA	C6-C7-C8-C9
21	1	1125	CLA	C1A-C2A-CAA-CBA
21	1	1125	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1126	CLA	C1A-C2A-CAA-CBA
21	1	1126	CLA	C3A-C2A-CAA-CBA
21	1	1126	CLA	CBD-CGD-O2D-CED
21	1	1127	CLA	C4-C3-C5-C6
21	1	1128	CLA	C2-C1-O2A-CGA
21	1	1128	CLA	CHA-CBD-CGD-O1D
21	1	1128	CLA	CHA-CBD-CGD-O2D
21	1	1129	CLA	C1A-C2A-CAA-CBA
21	1	1129	CLA	C3A-C2A-CAA-CBA
21	1	1132	CLA	CHA-CBD-CGD-O1D
21	1	1132	CLA	CHA-CBD-CGD-O2D
21	1	1133	CLA	C2-C1-O2A-CGA
21	1	1134	CLA	C2-C1-O2A-CGA
21	1	1134	CLA	CHA-CBD-CGD-O1D
21	1	1134	CLA	CHA-CBD-CGD-O2D
21	1	1134	CLA	CBD-CGD-O2D-CED
21	1	1134	CLA	C4-C3-C5-C6
21	1	1135	CLA	C3-C5-C6-C7
21	1	1138	CLA	C2-C1-O2A-CGA
21	1	1138	CLA	CBD-CGD-O2D-CED
21	1	1140	CLA	C2-C1-O2A-CGA
21	1	1140	CLA	CBD-CGD-O2D-CED
21	1	1801	CLA	CBA-CGA-O2A-C1
21	1	1801	CLA	O1A-CGA-O2A-C1
21	1	1801	CLA	CAD-CBD-CGD-O1D
21	1	1801	CLA	CAD-CBD-CGD-O2D
21	1	1130	CLA	C2-C3-C5-C6
21	1	1130	CLA	C4-C3-C5-C6
21	1	1139	CLA	CBD-CGD-O2D-CED
21	1	1012	CLA	CAD-CBD-CGD-O1D
21	1	1012	CLA	CAD-CBD-CGD-O2D
21	2	1023	CLA	CBD-CGD-O2D-CED
21	2	1202	CLA	C3A-C2A-CAA-CBA
21	2	1203	CLA	C2-C3-C5-C6
21	2	1203	CLA	C4-C3-C5-C6
21	2	1205	CLA	C4B-C3B-CAB-CBB
21	2	1205	CLA	CHA-CBD-CGD-O1D
21	2	1205	CLA	CHA-CBD-CGD-O2D
21	2	1206	CLA	C2-C1-O2A-CGA
21	2	1206	CLA	C14-C13-C15-C16
21	2	1207	CLA	CBD-CGD-O2D-CED
21	2	1208	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1209	CLA	C1A-C2A-CAA-CBA
21	2	1209	CLA	C3A-C2A-CAA-CBA
21	2	1210	CLA	C1A-C2A-CAA-CBA
21	2	1210	CLA	C3A-C2A-CAA-CBA
21	2	1211	CLA	C1A-C2A-CAA-CBA
21	2	1211	CLA	C3A-C2A-CAA-CBA
21	2	1211	CLA	CHA-CBD-CGD-O1D
21	2	1211	CLA	CHA-CBD-CGD-O2D
21	2	1212	CLA	CBD-CGD-O2D-CED
21	2	1213	CLA	CHA-CBD-CGD-O1D
21	2	1213	CLA	CHA-CBD-CGD-O2D
21	2	1215	CLA	C1A-C2A-CAA-CBA
21	2	1215	CLA	C3A-C2A-CAA-CBA
21	2	1215	CLA	C2-C1-O2A-CGA
21	2	1217	CLA	C1A-C2A-CAA-CBA
21	2	1217	CLA	C3A-C2A-CAA-CBA
21	2	1217	CLA	CBD-CGD-O2D-CED
21	2	1218	CLA	C3A-C2A-CAA-CBA
21	2	1218	CLA	CBA-CGA-O2A-C1
21	2	1218	CLA	O1A-CGA-O2A-C1
21	2	1218	CLA	CBD-CGD-O2D-CED
21	2	1218	CLA	C14-C13-C15-C16
21	2	1219	CLA	C1A-C2A-CAA-CBA
21	2	1219	CLA	C2-C1-O2A-CGA
21	2	1221	CLA	CHA-CBD-CGD-O1D
21	2	1221	CLA	CHA-CBD-CGD-O2D
21	2	1222	CLA	C3A-C2A-CAA-CBA
21	2	1224	CLA	C1A-C2A-CAA-CBA
21	2	1224	CLA	C3A-C2A-CAA-CBA
21	2	1225	CLA	C1A-C2A-CAA-CBA
21	2	1225	CLA	C3A-C2A-CAA-CBA
21	2	1226	CLA	CAD-CBD-CGD-O1D
21	2	1226	CLA	CAD-CBD-CGD-O2D
21	2	1228	CLA	C1A-C2A-CAA-CBA
21	2	1228	CLA	C3A-C2A-CAA-CBA
21	2	1228	CLA	CHA-CBD-CGD-O1D
21	2	1228	CLA	CHA-CBD-CGD-O2D
21	2	1229	CLA	C1A-C2A-CAA-CBA
21	2	1229	CLA	C3A-C2A-CAA-CBA
21	2	1229	CLA	CBD-CGD-O2D-CED
21	2	1229	CLA	C11-C12-C13-C15
21	2	1231	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1232	CLA	CBD-CGD-O2D-CED
21	2	1234	CLA	C1A-C2A-CAA-CBA
21	2	1234	CLA	C3A-C2A-CAA-CBA
21	2	1236	CLA	CBD-CGD-O2D-CED
21	2	1239	CLA	C1A-C2A-CAA-CBA
21	2	1239	CLA	C3A-C2A-CAA-CBA
21	2	1239	CLA	C2-C1-O2A-CGA
21	2	1230	CLA	C3A-C2A-CAA-CBA
21	2	1230	CLA	CHA-CBD-CGD-O1D
21	2	1230	CLA	CHA-CBD-CGD-O2D
21	7	1302	CLA	CBD-CGD-O2D-CED
21	7	1303	CLA	CBD-CGD-O2D-CED
21	8	1401	CLA	C1A-C2A-CAA-CBA
21	8	1401	CLA	C3A-C2A-CAA-CBA
21	8	1402	CLA	CBA-CGA-O2A-C1
21	0	1501	CLA	C1A-C2A-CAA-CBA
21	0	1501	CLA	C3A-C2A-CAA-CBA
24	A	4001	BCR	C11-C10-C9-C8
24	A	4001	BCR	C11-C10-C9-C34
24	A	4001	BCR	C11-C12-C13-C14
24	A	4001	BCR	C11-C12-C13-C35
24	A	4002	BCR	C11-C10-C9-C8
24	A	4002	BCR	C11-C10-C9-C34
24	A	4002	BCR	C11-C12-C13-C14
24	A	4003	BCR	C11-C10-C9-C8
24	A	4003	BCR	C11-C10-C9-C34
24	A	4003	BCR	C13-C14-C15-C16
24	A	4003	BCR	C21-C22-C23-C24
24	A	4003	BCR	C37-C22-C23-C24
24	A	4007	BCR	C11-C12-C13-C14
24	A	4008	BCR	C23-C24-C25-C26
24	A	4019	BCR	C7-C8-C9-C10
24	A	4012	BCR	C5-C6-C7-C8
24	A	4012	BCR	C11-C10-C9-C8
24	A	4012	BCR	C11-C10-C9-C34
24	A	4012	BCR	C11-C12-C13-C14
24	A	4012	BCR	C11-C12-C13-C35
24	B	4004	BCR	C1-C6-C7-C8
24	B	4004	BCR	C5-C6-C7-C8
24	B	4004	BCR	C11-C10-C9-C8
24	B	4004	BCR	C11-C10-C9-C34
24	B	4004	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	4004	BCR	C11-C12-C13-C35
24	B	4004	BCR	C21-C22-C23-C24
24	B	4004	BCR	C37-C22-C23-C24
24	B	4004	BCR	C23-C24-C25-C26
24	B	4004	BCR	C23-C24-C25-C30
24	B	4005	BCR	C11-C10-C9-C8
24	B	4005	BCR	C11-C10-C9-C34
24	B	4005	BCR	C13-C14-C15-C16
24	B	4005	BCR	C17-C18-C19-C20
24	B	4005	BCR	C36-C18-C19-C20
24	B	4005	BCR	C37-C22-C23-C24
24	B	4010	BCR	C11-C10-C9-C8
24	B	4010	BCR	C11-C10-C9-C34
24	B	4010	BCR	C10-C11-C12-C13
24	B	4010	BCR	C17-C18-C19-C20
24	B	4017	BCR	C11-C10-C9-C8
24	B	4017	BCR	C11-C10-C9-C34
24	B	4017	BCR	C10-C11-C12-C13
24	B	4017	BCR	C11-C12-C13-C14
24	B	4017	BCR	C11-C12-C13-C35
24	B	4017	BCR	C17-C18-C19-C20
24	B	4017	BCR	C36-C18-C19-C20
24	B	4018	BCR	C17-C18-C19-C20
24	B	4018	BCR	C36-C18-C19-C20
24	B	4018	BCR	C18-C19-C20-C21
24	B	4014	BCR	C11-C10-C9-C8
24	B	4014	BCR	C11-C10-C9-C34
24	B	4014	BCR	C21-C22-C23-C24
24	B	4014	BCR	C37-C22-C23-C24
24	I	4018	BCR	C11-C10-C9-C34
24	I	4018	BCR	C19-C20-C21-C22
24	J	4013	BCR	C11-C10-C9-C8
24	J	4013	BCR	C11-C10-C9-C34
24	J	4013	BCR	C10-C11-C12-C13
24	J	4013	BCR	C15-C16-C17-C18
24	J	4013	BCR	C17-C18-C19-C20
24	K	4001	BCR	C11-C10-C9-C8
24	K	4001	BCR	C11-C10-C9-C34
24	K	4001	BCR	C15-C16-C17-C18
24	K	4001	BCR	C17-C18-C19-C20
24	L	4022	BCR	C11-C10-C9-C8
24	L	4022	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	L	4022	BCR	C10-C11-C12-C13
24	L	4022	BCR	C17-C18-C19-C20
24	a	4001	BCR	C11-C10-C9-C8
24	a	4001	BCR	C11-C10-C9-C34
24	a	4001	BCR	C10-C11-C12-C13
24	a	4001	BCR	C11-C12-C13-C14
24	a	4001	BCR	C11-C12-C13-C35
24	a	4001	BCR	C17-C18-C19-C20
24	a	4001	BCR	C36-C18-C19-C20
24	a	4002	BCR	C11-C10-C9-C8
24	a	4002	BCR	C11-C10-C9-C34
24	a	4002	BCR	C11-C12-C13-C14
24	a	4002	BCR	C21-C22-C23-C24
24	a	4003	BCR	C11-C10-C9-C8
24	a	4003	BCR	C11-C10-C9-C34
24	a	4007	BCR	C11-C10-C9-C8
24	a	4007	BCR	C11-C10-C9-C34
24	a	4007	BCR	C17-C18-C19-C20
24	a	4007	BCR	C36-C18-C19-C20
24	a	4008	BCR	C11-C10-C9-C8
24	a	4008	BCR	C11-C10-C9-C34
24	a	4008	BCR	C13-C14-C15-C16
24	a	4008	BCR	C17-C18-C19-C20
24	a	4019	BCR	C11-C10-C9-C8
24	a	4019	BCR	C11-C10-C9-C34
24	a	4019	BCR	C10-C11-C12-C13
24	a	4019	BCR	C17-C18-C19-C20
24	a	4019	BCR	C21-C22-C23-C24
24	a	4019	BCR	C37-C22-C23-C24
24	a	4012	BCR	C11-C10-C9-C8
24	a	4012	BCR	C11-C10-C9-C34
24	b	4004	BCR	C1-C6-C7-C8
24	b	4004	BCR	C5-C6-C7-C8
24	b	4004	BCR	C11-C10-C9-C8
24	b	4004	BCR	C11-C10-C9-C34
24	b	4004	BCR	C10-C11-C12-C13
24	b	4004	BCR	C23-C24-C25-C26
24	b	4004	BCR	C23-C24-C25-C30
24	b	4005	BCR	C11-C10-C9-C8
24	b	4005	BCR	C11-C10-C9-C34
24	b	4005	BCR	C10-C11-C12-C13
24	b	4010	BCR	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	4010	BCR	C36-C18-C19-C20
24	b	4017	BCR	C11-C10-C9-C8
24	b	4017	BCR	C11-C10-C9-C34
24	b	4017	BCR	C11-C12-C13-C14
24	b	4017	BCR	C17-C18-C19-C20
24	b	4018	BCR	C23-C24-C25-C26
24	b	4018	BCR	C23-C24-C25-C30
24	b	4014	BCR	C11-C10-C9-C8
24	b	4014	BCR	C11-C10-C9-C34
24	b	4014	BCR	C21-C22-C23-C24
24	b	4014	BCR	C37-C22-C23-C24
24	f	4016	BCR	C10-C11-C12-C13
24	f	4016	BCR	C11-C12-C13-C14
24	f	4016	BCR	C11-C12-C13-C35
24	f	4016	BCR	C21-C22-C23-C24
24	f	4016	BCR	C37-C22-C23-C24
24	i	4018	BCR	C11-C10-C9-C8
24	i	4018	BCR	C11-C10-C9-C34
24	i	4018	BCR	C10-C11-C12-C13
24	i	4018	BCR	C11-C12-C13-C35
24	i	4018	BCR	C17-C18-C19-C20
24	i	4018	BCR	C36-C18-C19-C20
24	j	4013	BCR	C11-C10-C9-C8
24	j	4013	BCR	C11-C10-C9-C34
24	j	4013	BCR	C23-C24-C25-C26
24	j	4013	BCR	C23-C24-C25-C30
24	k	4001	BCR	C11-C10-C9-C8
24	k	4001	BCR	C11-C10-C9-C34
24	k	4001	BCR	C10-C11-C12-C13
24	k	4001	BCR	C17-C18-C19-C20
24	k	4001	BCR	C36-C18-C19-C20
24	l	4019	BCR	C7-C8-C9-C10
24	l	4019	BCR	C7-C8-C9-C34
24	l	4019	BCR	C23-C24-C25-C26
24	l	4022	BCR	C7-C8-C9-C10
24	l	4022	BCR	C7-C8-C9-C34
24	l	4022	BCR	C10-C11-C12-C13
24	l	4022	BCR	C11-C12-C13-C14
24	l	4022	BCR	C11-C12-C13-C35
24	l	4022	BCR	C21-C22-C23-C24
24	l	4022	BCR	C37-C22-C23-C24
24	1	4001	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	4001	BCR	C11-C10-C9-C34
24	1	4001	BCR	C10-C11-C12-C13
24	1	4002	BCR	C11-C10-C9-C8
24	1	4002	BCR	C11-C10-C9-C34
24	1	4002	BCR	C13-C14-C15-C16
24	1	4002	BCR	C17-C18-C19-C20
24	1	4002	BCR	C21-C22-C23-C24
24	1	4003	BCR	C11-C10-C9-C8
24	1	4003	BCR	C11-C10-C9-C34
24	1	4007	BCR	C11-C10-C9-C8
24	1	4007	BCR	C11-C10-C9-C34
24	1	4007	BCR	C21-C22-C23-C24
24	1	4019	BCR	C7-C8-C9-C10
24	1	4019	BCR	C7-C8-C9-C34
24	1	4019	BCR	C10-C11-C12-C13
24	1	4019	BCR	C17-C18-C19-C20
24	1	4019	BCR	C36-C18-C19-C20
24	1	4012	BCR	C11-C10-C9-C8
24	1	4012	BCR	C11-C10-C9-C34
24	1	4012	BCR	C11-C12-C13-C14
24	1	4012	BCR	C11-C12-C13-C35
24	1	4012	BCR	C21-C22-C23-C24
24	2	4011	BCR	C7-C8-C9-C10
24	2	4011	BCR	C17-C18-C19-C20
24	2	4011	BCR	C21-C22-C23-C24
24	2	4011	BCR	C37-C22-C23-C24
24	2	4004	BCR	C1-C6-C7-C8
24	2	4004	BCR	C5-C6-C7-C8
24	2	4004	BCR	C7-C8-C9-C10
24	2	4004	BCR	C7-C8-C9-C34
24	2	4004	BCR	C11-C10-C9-C8
24	2	4004	BCR	C11-C10-C9-C34
24	2	4004	BCR	C11-C12-C13-C14
24	2	4004	BCR	C11-C12-C13-C35
24	2	4004	BCR	C17-C18-C19-C20
24	2	4005	BCR	C11-C10-C9-C8
24	2	4005	BCR	C11-C10-C9-C34
24	2	4005	BCR	C10-C11-C12-C13
24	2	4005	BCR	C17-C18-C19-C20
24	2	4005	BCR	C21-C22-C23-C24
24	2	4005	BCR	C37-C22-C23-C24
24	2	4010	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	4010	BCR	C11-C10-C9-C34
24	2	4010	BCR	C11-C12-C13-C14
24	2	4010	BCR	C11-C12-C13-C35
24	2	4010	BCR	C17-C18-C19-C20
24	2	4010	BCR	C36-C18-C19-C20
24	2	4010	BCR	C18-C19-C20-C21
24	2	4017	BCR	C11-C10-C9-C8
24	2	4017	BCR	C11-C10-C9-C34
24	2	4017	BCR	C17-C18-C19-C20
24	2	4017	BCR	C36-C18-C19-C20
24	2	4018	BCR	C11-C10-C9-C8
24	2	4018	BCR	C17-C18-C19-C20
24	2	4018	BCR	C23-C24-C25-C26
24	2	4018	BCR	C23-C24-C25-C30
24	2	4014	BCR	C11-C10-C9-C8
24	2	4014	BCR	C11-C10-C9-C34
24	2	4014	BCR	C21-C22-C23-C24
24	2	4014	BCR	C37-C22-C23-C24
24	6	4016	BCR	C10-C11-C12-C13
24	6	4016	BCR	C11-C12-C13-C14
24	6	4016	BCR	C21-C22-C23-C24
24	6	4016	BCR	C37-C22-C23-C24
24	h	4018	BCR	C11-C10-C9-C8
24	h	4018	BCR	C11-C10-C9-C34
24	h	4018	BCR	C10-C11-C12-C13
24	h	4018	BCR	C11-C12-C13-C14
24	h	4018	BCR	C11-C12-C13-C35
24	h	4018	BCR	C17-C18-C19-C20
24	7	4013	BCR	C11-C10-C9-C8
24	7	4013	BCR	C11-C10-C9-C34
24	7	4013	BCR	C11-C12-C13-C35
24	7	4013	BCR	C23-C24-C25-C26
24	7	4013	BCR	C23-C24-C25-C30
24	8	4001	BCR	C11-C10-C9-C8
24	8	4001	BCR	C11-C10-C9-C34
24	8	4001	BCR	C11-C12-C13-C14
24	8	4001	BCR	C11-C12-C13-C35
24	8	4001	BCR	C21-C22-C23-C24
24	8	4001	BCR	C37-C22-C23-C24
24	0	4019	BCR	C11-C10-C9-C8
24	0	4019	BCR	C11-C10-C9-C34
24	0	4019	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	0	4022	BCR	C11-C10-C9-C8
24	0	4022	BCR	C11-C10-C9-C34
24	0	4022	BCR	C10-C11-C12-C13
24	9	4021	BCR	C1-C6-C7-C8
24	9	4021	BCR	C5-C6-C7-C8
24	9	4021	BCR	C11-C10-C9-C8
24	9	4021	BCR	C11-C10-C9-C34
24	9	4021	BCR	C10-C11-C12-C13
24	9	4021	BCR	C11-C12-C13-C14
24	9	4021	BCR	C21-C22-C23-C24
25	A	5001	LHG	C3-O3-P-O5
25	A	5001	LHG	C4-O6-P-O3
25	A	5001	LHG	C4-O6-P-O4
25	A	5003	LHG	C3-O3-P-O6
25	A	5003	LHG	C4-O6-P-O3
25	A	5003	LHG	C4-O6-P-O4
25	A	5005	LHG	C1-C2-C3-O3
25	A	5005	LHG	C4-O6-P-O3
25	A	5005	LHG	C4-O6-P-O4
25	A	5005	LHG	C4-O6-P-O5
25	A	5005	LHG	O9-C7-O7-C5
25	A	5005	LHG	C8-C7-O7-C5
25	A	5007	LHG	O1-C1-C2-C3
25	A	5007	LHG	O2-C2-C3-O3
25	A	5007	LHG	C3-O3-P-O5
25	A	5007	LHG	C3-O3-P-O6
25	A	5007	LHG	C4-O6-P-O3
25	A	5007	LHG	C4-O6-P-O4
25	A	5007	LHG	O9-C7-O7-C5
25	A	5007	LHG	C8-C7-O7-C5
25	A	5006	LHG	O1-C1-C2-C3
25	A	5006	LHG	C3-O3-P-O5
25	A	5006	LHG	O9-C7-O7-C5
25	A	5006	LHG	C8-C7-O7-C5
25	B	5004	LHG	C3-O3-P-O6
25	B	5004	LHG	C4-O6-P-O3
25	B	5004	LHG	C4-O6-P-O4
25	B	5004	LHG	C4-O6-P-O5
25	B	5006	LHG	O1-C1-C2-C3
25	B	5006	LHG	C3-O3-P-O4
25	B	5006	LHG	C3-O3-P-O5
25	B	5006	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	5006	LHG	C4-O6-P-O3
25	B	5006	LHG	O9-C7-O7-C5
25	F	5002	LHG	O1-C1-C2-C3
25	F	5002	LHG	O2-C2-C3-O3
25	F	5002	LHG	C3-O3-P-O4
25	F	5002	LHG	C3-O3-P-O6
25	F	5002	LHG	C4-O6-P-O3
25	F	5002	LHG	C4-O6-P-O4
25	F	5002	LHG	C4-O6-P-O5
25	L	5005	LHG	C3-O3-P-O6
25	M	5001	LHG	C4-O6-P-O3
25	M	5001	LHG	C4-O6-P-O4
25	M	5001	LHG	C4-O6-P-O5
25	M	5001	LHG	O9-C7-O7-C5
25	M	5001	LHG	C8-C7-O7-C5
25	a	5001	LHG	O1-C1-C2-C3
25	a	5001	LHG	C1-C2-C3-O3
25	a	5001	LHG	C4-O6-P-O3
25	a	5001	LHG	C4-O6-P-O4
25	a	5003	LHG	O1-C1-C2-C3
25	a	5003	LHG	C3-O3-P-O6
25	a	5003	LHG	C4-O6-P-O3
25	a	5003	LHG	C4-O6-P-O4
25	a	5003	LHG	C4-O6-P-O5
25	a	5003	LHG	O7-C5-C6-O8
25	a	5005	LHG	C1-C2-C3-O3
25	a	5005	LHG	C2-C3-O3-P
25	a	5005	LHG	C3-O3-P-O6
25	a	5005	LHG	C4-O6-P-O5
25	a	5005	LHG	O9-C7-O7-C5
25	a	5005	LHG	C8-C7-O7-C5
25	a	5007	LHG	O1-C1-C2-C3
25	a	5007	LHG	C4-O6-P-O3
25	a	5007	LHG	C4-O6-P-O4
25	a	5007	LHG	C4-O6-P-O5
25	l	5001	LHG	O1-C1-C2-C3
25	l	5001	LHG	O2-C2-C3-O3
25	l	5001	LHG	C3-O3-P-O6
25	l	5001	LHG	C4-O6-P-O3
25	l	5001	LHG	C4-O6-P-O4
25	l	5001	LHG	C4-O6-P-O5
25	l	5003	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	l	5003	LHG	C3-O3-P-O5
25	l	5003	LHG	C3-O3-P-O6
25	l	5003	LHG	C4-O6-P-O3
25	l	5003	LHG	C4-O6-P-O4
25	l	5004	LHG	C3-O3-P-O4
25	l	5004	LHG	C3-O3-P-O6
25	l	5002	LHG	C1-C2-C3-O3
25	l	5002	LHG	C3-O3-P-O6
25	l	5002	LHG	C4-O6-P-O3
25	l	5002	LHG	C4-O6-P-O4
25	l	5002	LHG	C4-O6-P-O5
25	l	5002	LHG	O6-C4-C5-O7
25	1	5005	LHG	O1-C1-C2-C3
25	1	5005	LHG	C3-O3-P-O4
25	1	5005	LHG	C3-O3-P-O6
25	1	5005	LHG	O9-C7-O7-C5
25	1	5005	LHG	C8-C7-O7-C5
25	1	5007	LHG	C3-O3-P-O4
25	1	5007	LHG	C3-O3-P-O5
25	1	5007	LHG	C3-O3-P-O6
25	1	5007	LHG	C4-O6-P-O3
25	1	5007	LHG	C4-O6-P-O4
25	1	5007	LHG	C8-C7-O7-C5
25	1	5001	LHG	O1-C1-C2-C3
25	1	5001	LHG	C1-C2-C3-O3
25	1	5001	LHG	O7-C5-C6-O8
25	1	5003	LHG	O1-C1-C2-C3
25	1	5003	LHG	C1-C2-C3-O3
25	1	5003	LHG	C3-O3-P-O6
25	1	5003	LHG	C4-O6-P-O3
25	1	5003	LHG	C4-O6-P-O4
25	1	5003	LHG	C4-O6-P-O5
25	2	5004	LHG	C3-O3-P-O6
25	0	5002	LHG	O1-C1-C2-C3
25	0	5002	LHG	C3-O3-P-O4
25	0	5002	LHG	C3-O3-P-O6
25	0	5004	LHG	C3-O3-P-O6
26	A	5002	LMG	O6-C1-O1-C7
26	A	5002	LMG	O1-C7-C8-O7
26	A	5002	LMG	O9-C10-O7-C8
26	A	5002	LMG	C11-C10-O7-C8
26	A	5008	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	5008	LMG	O9-C10-O7-C8
26	A	5008	LMG	C11-C10-O7-C8
26	K	5009	LMG	O6-C1-O1-C7
26	K	5009	LMG	O9-C10-O7-C8
26	K	5009	LMG	C11-C10-O7-C8
26	a	5002	LMG	O9-C10-O7-C8
26	a	5002	LMG	C11-C10-O7-C8
26	a	5004	LMG	C2-C1-O1-C7
26	a	5004	LMG	C11-C10-O7-C8
26	b	5005	LMG	O6-C1-O1-C7
26	b	5005	LMG	C11-C10-O7-C8
26	b	5007	LMG	O6-C1-O1-C7
26	b	5007	LMG	C11-C10-O7-C8
26	1	5002	LMG	C2-C1-O1-C7
26	1	5002	LMG	O6-C1-O1-C7
26	1	5002	LMG	C11-C10-O7-C8
26	2	5005	LMG	C2-C1-O1-C7
26	2	5005	LMG	O6-C1-O1-C7
26	0	5001	LMG	C2-C1-O1-C7
26	0	5001	LMG	O6-C1-O1-C7
28	B	4011	45D	C19-C23-C25-C27
28	B	4011	45D	C19-C23-C25-C29
28	B	4011	45D	C31-C33-C35-C37
28	B	4011	45D	C31-C33-C35-C39
28	h	4020	45D	C19-C23-C25-C27
28	h	4020	45D	C19-C23-C25-C29
28	h	4020	45D	C31-C33-C35-C37
28	h	4020	45D	C31-C33-C35-C39
28	h	4020	45D	C35-C37-C41-C42
30	M	4021	ECH	C21-C22-C23-C24
30	M	4021	ECH	C37-C22-C23-C24
30	M	4021	ECH	C23-C24-C25-C26
30	b	4011	ECH	C21-C22-C23-C24
30	i	4020	ECH	C5-C6-C7-C8
30	i	4020	ECH	C7-C8-C9-C10
30	m	4021	ECH	C21-C22-C23-C24
30	m	4021	ECH	C37-C22-C23-C24
30	m	4021	ECH	C23-C24-C25-C26
30	2	4006	ECH	C23-C24-C25-C26
31	B	5008	SQD	C2-C1-O6-C44
31	F	5001	SQD	O5-C5-C6-S
31	L	5001	SQD	O5-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	L	5001	SQD	O5-C5-C6-S
31	L	5001	SQD	C5-C6-S-O7
31	L	5001	SQD	C5-C6-S-O8
31	L	5001	SQD	C5-C6-S-O9
31	L	5002	SQD	O5-C5-C6-S
31	b	5006	SQD	C8-C7-O47-C45
31	b	5006	SQD	O5-C5-C6-S
31	0	5005	SQD	O5-C5-C6-S
34	F	4016	ZEX	C1-C6-C7-C8
34	F	4016	ZEX	C5-C6-C7-C8
34	F	4016	ZEX	C25-C26-C27-C28
34	F	4016	ZEX	C7-C8-C9-C19
34	F	4016	ZEX	C7-C8-C9-C10
34	j	4015	ZEX	C25-C26-C27-C28
34	j	4015	ZEX	C31-C32-C33-C34
34	7	4015	ZEX	C7-C8-C9-C10
35	F	6001	LMT	C2-C1-O1'-C1'
35	L	6001	LMT	O5'-C1'-O1'-C1
36	I	4020	EQ3	C21-C22-C23-C24
37	L	5004	DGD	C2B-C1B-O2G-C2G
37	L	5004	DGD	C2D-C1D-O3G-C3G
37	L	5004	DGD	O6D-C1D-O3G-C3G
37	L	5004	DGD	C4D-C5D-C6D-O5D
37	L	5004	DGD	O6E-C1E-O5D-C6D
21	B	1227	CLA	O1D-CGD-O2D-CED
21	a	1138	CLA	O1D-CGD-O2D-CED
21	B	1207	CLA	C4C-C3C-CAC-CBC
21	A	1104	CLA	O1D-CGD-O2D-CED
21	B	1220	CLA	O1D-CGD-O2D-CED
21	a	1104	CLA	O1D-CGD-O2D-CED
21	b	1218	CLA	O1D-CGD-O2D-CED
21	1	1138	CLA	O1D-CGD-O2D-CED
21	2	1021	CLA	O1D-CGD-O2D-CED
21	2	1220	CLA	O1D-CGD-O2D-CED
21	8	1402	CLA	O1D-CGD-O2D-CED
21	A	1104	CLA	CBD-CGD-O2D-CED
21	A	1105	CLA	CBD-CGD-O2D-CED
21	A	1109	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	CBD-CGD-O2D-CED
21	A	1119	CLA	CBD-CGD-O2D-CED
21	A	1120	CLA	CBD-CGD-O2D-CED
21	A	1121	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1138	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	CBD-CGD-O2D-CED
21	B	1022	CLA	CBD-CGD-O2D-CED
21	B	1204	CLA	CBD-CGD-O2D-CED
21	B	1206	CLA	CBD-CGD-O2D-CED
21	B	1217	CLA	CBD-CGD-O2D-CED
21	B	1218	CLA	CBD-CGD-O2D-CED
21	B	1219	CLA	CBD-CGD-O2D-CED
21	B	1220	CLA	CBD-CGD-O2D-CED
21	B	1227	CLA	CBD-CGD-O2D-CED
21	B	1229	CLA	CBD-CGD-O2D-CED
21	B	1231	CLA	CBD-CGD-O2D-CED
21	B	1232	CLA	CBD-CGD-O2D-CED
21	B	1235	CLA	CBD-CGD-O2D-CED
21	B	1240	CLA	CBD-CGD-O2D-CED
21	F	1301	CLA	CBD-CGD-O2D-CED
21	F	1302	CLA	CBD-CGD-O2D-CED
21	J	1302	CLA	CBD-CGD-O2D-CED
21	a	1103	CLA	CBD-CGD-O2D-CED
21	a	1104	CLA	CBD-CGD-O2D-CED
21	a	1106	CLA	CBD-CGD-O2D-CED
21	a	1113	CLA	CBD-CGD-O2D-CED
21	a	1114	CLA	CBD-CGD-O2D-CED
21	a	1117	CLA	CBD-CGD-O2D-CED
21	a	1121	CLA	CBD-CGD-O2D-CED
21	a	1122	CLA	CBD-CGD-O2D-CED
21	a	1133	CLA	CBD-CGD-O2D-CED
21	a	1136	CLA	CBD-CGD-O2D-CED
21	a	1137	CLA	CBD-CGD-O2D-CED
21	a	1139	CLA	CBD-CGD-O2D-CED
21	a	1138	CLA	CBD-CGD-O2D-CED
21	b	1022	CLA	CBD-CGD-O2D-CED
21	b	1203	CLA	CBD-CGD-O2D-CED
21	b	1215	CLA	CBD-CGD-O2D-CED
21	b	1217	CLA	CBD-CGD-O2D-CED
21	b	1218	CLA	CBD-CGD-O2D-CED
21	b	1219	CLA	CBD-CGD-O2D-CED
21	b	1223	CLA	CBD-CGD-O2D-CED
21	b	1227	CLA	CBD-CGD-O2D-CED
21	b	1232	CLA	CBD-CGD-O2D-CED
21	b	1235	CLA	CBD-CGD-O2D-CED
21	b	1239	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1201	CLA	CBD-CGD-O2D-CED
21	f	1302	CLA	CBD-CGD-O2D-CED
21	j	1302	CLA	CBD-CGD-O2D-CED
21	j	1303	CLA	CBD-CGD-O2D-CED
21	l	1501	CLA	CBD-CGD-O2D-CED
21	1	1011	CLA	CBD-CGD-O2D-CED
21	1	1106	CLA	CBD-CGD-O2D-CED
21	1	1107	CLA	CBD-CGD-O2D-CED
21	1	1110	CLA	CBD-CGD-O2D-CED
21	1	1113	CLA	CBD-CGD-O2D-CED
21	1	1114	CLA	CBD-CGD-O2D-CED
21	1	1118	CLA	CBD-CGD-O2D-CED
21	1	1125	CLA	CBD-CGD-O2D-CED
21	1	1131	CLA	CBD-CGD-O2D-CED
21	1	1137	CLA	CBD-CGD-O2D-CED
21	1	1130	CLA	CBD-CGD-O2D-CED
21	2	1021	CLA	CBD-CGD-O2D-CED
21	2	1201	CLA	CBD-CGD-O2D-CED
21	2	1203	CLA	CBD-CGD-O2D-CED
21	2	1210	CLA	CBD-CGD-O2D-CED
21	2	1213	CLA	CBD-CGD-O2D-CED
21	2	1214	CLA	CBD-CGD-O2D-CED
21	2	1215	CLA	CBD-CGD-O2D-CED
21	2	1219	CLA	CBD-CGD-O2D-CED
21	2	1220	CLA	CBD-CGD-O2D-CED
21	2	1224	CLA	CBD-CGD-O2D-CED
21	2	1228	CLA	CBD-CGD-O2D-CED
21	2	1240	CLA	CBD-CGD-O2D-CED
21	6	1301	CLA	CBD-CGD-O2D-CED
21	8	1401	CLA	CBD-CGD-O2D-CED
21	8	1402	CLA	CBD-CGD-O2D-CED
21	A	1114	CLA	O1A-CGA-O2A-C1
21	A	1801	CLA	O1A-CGA-O2A-C1
21	a	1110	CLA	O1A-CGA-O2A-C1
21	b	1219	CLA	O1A-CGA-O2A-C1
21	1	1109	CLA	O1A-CGA-O2A-C1
21	2	1204	CLA	O1A-CGA-O2A-C1
21	2	1219	CLA	O1A-CGA-O2A-C1
25	1	5005	LHG	O10-C23-O8-C6
26	A	5002	LMG	O10-C28-O8-C9
26	B	5005	LMG	O10-C28-O8-C9
26	a	5002	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	2	5005	LMG	O10-C28-O8-C9
31	f	5001	SQD	O10-C23-O48-C46
21	8	1402	CLA	O1A-CGA-O2A-C1
21	K	1402	CLA	C15-C16-C17-C18
21	B	1218	CLA	O1D-CGD-O2D-CED
21	B	1219	CLA	O1D-CGD-O2D-CED
21	F	1301	CLA	O1D-CGD-O2D-CED
21	a	1139	CLA	O1D-CGD-O2D-CED
21	b	1219	CLA	O1D-CGD-O2D-CED
21	f	1302	CLA	O1D-CGD-O2D-CED
21	1	1114	CLA	O1D-CGD-O2D-CED
21	2	1214	CLA	O1D-CGD-O2D-CED
21	2	1219	CLA	O1D-CGD-O2D-CED
21	A	1801	CLA	CBA-CGA-O2A-C1
21	a	1110	CLA	CBA-CGA-O2A-C1
21	b	1219	CLA	CBA-CGA-O2A-C1
21	1	1109	CLA	CBA-CGA-O2A-C1
21	2	1219	CLA	CBA-CGA-O2A-C1
25	1	5005	LHG	C24-C23-O8-C6
26	A	5002	LMG	C29-C28-O8-C9
26	B	5005	LMG	C29-C28-O8-C9
26	a	5002	LMG	C29-C28-O8-C9
26	2	5005	LMG	C29-C28-O8-C9
31	f	5001	SQD	C24-C23-O48-C46
21	B	1214	CLA	CBD-CGD-O2D-CED
21	B	1238	CLA	CBD-CGD-O2D-CED
21	L	1503	CLA	CBD-CGD-O2D-CED
21	a	1120	CLA	CBD-CGD-O2D-CED
21	a	1132	CLA	CBD-CGD-O2D-CED
21	b	1206	CLA	CBD-CGD-O2D-CED
21	b	1230	CLA	CBD-CGD-O2D-CED
21	2	1211	CLA	CBD-CGD-O2D-CED
21	A	1109	CLA	O1A-CGA-O2A-C1
21	A	1110	CLA	O1A-CGA-O2A-C1
21	A	1129	CLA	O1A-CGA-O2A-C1
21	A	1130	CLA	O1A-CGA-O2A-C1
21	B	1204	CLA	O1A-CGA-O2A-C1
21	B	1206	CLA	O1A-CGA-O2A-C1
21	B	1227	CLA	O1A-CGA-O2A-C1
21	B	1235	CLA	O1A-CGA-O2A-C1
21	a	1104	CLA	O1A-CGA-O2A-C1
21	a	1136	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1214	CLA	O1A-CGA-O2A-C1
21	b	1218	CLA	O1A-CGA-O2A-C1
21	b	1227	CLA	O1A-CGA-O2A-C1
21	b	1235	CLA	O1A-CGA-O2A-C1
21	f	1302	CLA	O1A-CGA-O2A-C1
21	k	1402	CLA	O1A-CGA-O2A-C1
21	l	1501	CLA	O1A-CGA-O2A-C1
21	1	1013	CLA	O1A-CGA-O2A-C1
21	1	1104	CLA	O1A-CGA-O2A-C1
21	1	1110	CLA	O1A-CGA-O2A-C1
21	2	1237	CLA	O1A-CGA-O2A-C1
21	2	1221	CLA	O1A-CGA-O2A-C1
21	2	1235	CLA	O1A-CGA-O2A-C1
26	A	5004	LMG	O10-C28-O8-C9
26	1	5002	LMG	O10-C28-O8-C9
26	1	5004	LMG	O10-C28-O8-C9
31	0	5005	SQD	O10-C23-O48-C46
35	0	6001	LMT	C3'-C4'-O1B-C1B
21	B	1207	CLA	C2C-C3C-CAC-CBC
21	A	1118	CLA	O1D-CGD-O2D-CED
21	A	1139	CLA	O1D-CGD-O2D-CED
21	B	1203	CLA	O1D-CGD-O2D-CED
21	B	1232	CLA	O1D-CGD-O2D-CED
21	a	1107	CLA	O1D-CGD-O2D-CED
21	a	1801	CLA	O1D-CGD-O2D-CED
21	2	1207	CLA	O1D-CGD-O2D-CED
21	2	1208	CLA	O1D-CGD-O2D-CED
21	2	1217	CLA	O1D-CGD-O2D-CED
21	2	1218	CLA	O1D-CGD-O2D-CED
21	2	1224	CLA	O1D-CGD-O2D-CED
21	2	1231	CLA	O1D-CGD-O2D-CED
21	2	1240	CLA	O1D-CGD-O2D-CED
21	7	1303	CLA	O1D-CGD-O2D-CED
21	A	1107	CLA	O1D-CGD-O2D-CED
21	A	1135	CLA	O1D-CGD-O2D-CED
21	B	1021	CLA	O1D-CGD-O2D-CED
21	B	1201	CLA	O1D-CGD-O2D-CED
21	B	1212	CLA	O1D-CGD-O2D-CED
21	a	1112	CLA	O1D-CGD-O2D-CED
21	a	1118	CLA	O1D-CGD-O2D-CED
21	b	1224	CLA	O1D-CGD-O2D-CED
21	b	1229	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1231	CLA	O1D-CGD-O2D-CED
21	f	1301	CLA	O1D-CGD-O2D-CED
21	l	1503	CLA	O1D-CGD-O2D-CED
21	1	1104	CLA	O1D-CGD-O2D-CED
21	1	1108	CLA	O1D-CGD-O2D-CED
21	1	1109	CLA	O1D-CGD-O2D-CED
21	1	1116	CLA	O1D-CGD-O2D-CED
21	1	1121	CLA	O1D-CGD-O2D-CED
21	1	1126	CLA	O1D-CGD-O2D-CED
21	1	1140	CLA	O1D-CGD-O2D-CED
21	1	1139	CLA	O1D-CGD-O2D-CED
21	2	1212	CLA	O1D-CGD-O2D-CED
21	2	1229	CLA	O1D-CGD-O2D-CED
21	2	1236	CLA	O1D-CGD-O2D-CED
26	0	5001	LMG	O6-C5-C6-O5
21	A	1115	CLA	CBD-CGD-O2D-CED
21	1	1103	CLA	CBD-CGD-O2D-CED
21	2	1239	CLA	CBD-CGD-O2D-CED
21	B	1212	CLA	O1A-CGA-O2A-C1
21	L	1501	CLA	O1A-CGA-O2A-C1
25	1	5007	LHG	O9-C7-O7-C5
26	a	5004	LMG	O9-C10-O7-C8
26	1	5002	LMG	O9-C10-O7-C8
31	b	5006	SQD	O49-C7-O47-C45
21	A	1114	CLA	O1D-CGD-O2D-CED
21	b	1220	CLA	O1D-CGD-O2D-CED
21	7	1302	CLA	O1D-CGD-O2D-CED
21	2	1231	CLA	CBA-CGA-O2A-C1
21	A	1108	CLA	C3-C5-C6-C7
21	A	1109	CLA	C3-C5-C6-C7
21	A	1114	CLA	C3-C5-C6-C7
21	A	1115	CLA	C3-C5-C6-C7
21	A	1116	CLA	C3-C5-C6-C7
21	A	1120	CLA	C3-C5-C6-C7
21	A	1137	CLA	C3-C5-C6-C7
21	B	1209	CLA	C3-C5-C6-C7
21	B	1218	CLA	C3-C5-C6-C7
21	B	1228	CLA	C3-C5-C6-C7
21	a	1011	CLA	C3-C5-C6-C7
21	a	1108	CLA	C3-C5-C6-C7
21	a	1115	CLA	C3-C5-C6-C7
21	a	1120	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1124	CLA	C3-C5-C6-C7
21	a	1127	CLA	C3-C5-C6-C7
21	a	1801	CLA	C3-C5-C6-C7
21	b	1206	CLA	C3-C5-C6-C7
21	b	1207	CLA	C3-C5-C6-C7
21	b	1221	CLA	C3-C5-C6-C7
21	b	1224	CLA	C3-C5-C6-C7
21	b	1231	CLA	C3-C5-C6-C7
21	b	1240	CLA	C3-C5-C6-C7
21	l	1503	CLA	C3-C5-C6-C7
21	1	1103	CLA	C3-C5-C6-C7
21	1	1104	CLA	C3-C5-C6-C7
21	1	1111	CLA	C3-C5-C6-C7
21	1	1116	CLA	C3-C5-C6-C7
21	1	1120	CLA	C3-C5-C6-C7
21	1	1122	CLA	C3-C5-C6-C7
21	1	1124	CLA	C3-C5-C6-C7
21	1	1133	CLA	C3-C5-C6-C7
21	2	1237	CLA	C3-C5-C6-C7
21	2	1021	CLA	C3-C5-C6-C7
21	2	1203	CLA	C3-C5-C6-C7
21	2	1205	CLA	C3-C5-C6-C7
21	2	1206	CLA	C3-C5-C6-C7
21	2	1218	CLA	C3-C5-C6-C7
21	2	1238	CLA	C3-C5-C6-C7
21	B	1206	CLA	O1D-CGD-O2D-CED
21	a	1126	CLA	O1D-CGD-O2D-CED
21	b	1237	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	CBA-CGA-O2A-C1
21	A	1114	CLA	CBA-CGA-O2A-C1
21	A	1129	CLA	CBA-CGA-O2A-C1
21	A	1130	CLA	CBA-CGA-O2A-C1
21	B	1227	CLA	CBA-CGA-O2A-C1
21	B	1228	CLA	CBA-CGA-O2A-C1
21	B	1230	CLA	CBA-CGA-O2A-C1
21	J	1303	CLA	CBA-CGA-O2A-C1
21	a	1124	CLA	CBA-CGA-O2A-C1
21	b	1214	CLA	CBA-CGA-O2A-C1
21	b	1235	CLA	CBA-CGA-O2A-C1
21	f	1302	CLA	CBA-CGA-O2A-C1
21	l	1501	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1110	CLA	CBA-CGA-O2A-C1
21	1	1126	CLA	CBA-CGA-O2A-C1
21	1	1134	CLA	CBA-CGA-O2A-C1
21	1	1130	CLA	CBA-CGA-O2A-C1
21	2	1237	CLA	CBA-CGA-O2A-C1
21	2	1204	CLA	CBA-CGA-O2A-C1
21	2	1207	CLA	CBA-CGA-O2A-C1
21	2	1221	CLA	CBA-CGA-O2A-C1
21	2	1235	CLA	CBA-CGA-O2A-C1
21	0	1501	CLA	CBA-CGA-O2A-C1
26	A	5004	LMG	C29-C28-O8-C9
26	1	5002	LMG	C29-C28-O8-C9
26	1	5004	LMG	C29-C28-O8-C9
21	A	1102	CLA	CBD-CGD-O2D-CED
21	A	1103	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	CBD-CGD-O2D-CED
21	A	1012	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	CBD-CGD-O2D-CED
21	J	1303	CLA	CBD-CGD-O2D-CED
21	K	1402	CLA	CBD-CGD-O2D-CED
21	a	1013	CLA	CBD-CGD-O2D-CED
21	a	1105	CLA	CBD-CGD-O2D-CED
21	a	1110	CLA	CBD-CGD-O2D-CED
21	a	1115	CLA	CBD-CGD-O2D-CED
21	a	1124	CLA	CBD-CGD-O2D-CED
21	a	1127	CLA	CBD-CGD-O2D-CED
21	a	1135	CLA	CBD-CGD-O2D-CED
21	b	1204	CLA	CBD-CGD-O2D-CED
21	b	1208	CLA	CBD-CGD-O2D-CED
21	b	1214	CLA	CBD-CGD-O2D-CED
21	b	1226	CLA	CBD-CGD-O2D-CED
21	b	1228	CLA	CBD-CGD-O2D-CED
21	b	1240	CLA	CBD-CGD-O2D-CED
21	1	1102	CLA	CBD-CGD-O2D-CED
21	1	1119	CLA	CBD-CGD-O2D-CED
21	1	1120	CLA	CBD-CGD-O2D-CED
21	1	1123	CLA	CBD-CGD-O2D-CED
21	1	1128	CLA	CBD-CGD-O2D-CED
21	1	1132	CLA	CBD-CGD-O2D-CED
21	1	1135	CLA	CBD-CGD-O2D-CED
21	1	1801	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1012	CLA	CBD-CGD-O2D-CED
21	2	1022	CLA	CBD-CGD-O2D-CED
21	2	1204	CLA	CBD-CGD-O2D-CED
21	2	1205	CLA	CBD-CGD-O2D-CED
21	2	1222	CLA	CBD-CGD-O2D-CED
21	2	1235	CLA	CBD-CGD-O2D-CED
21	2	1230	CLA	CBD-CGD-O2D-CED
21	0	1503	CLA	CBD-CGD-O2D-CED
25	B	5006	LHG	C8-C7-O7-C5
21	2	1230	CLA	C2-C1-O2A-CGA
21	A	1120	CLA	O1D-CGD-O2D-CED
21	A	1138	CLA	O1D-CGD-O2D-CED
21	B	1208	CLA	O1D-CGD-O2D-CED
21	B	1215	CLA	O1D-CGD-O2D-CED
21	B	1224	CLA	O1D-CGD-O2D-CED
21	J	1302	CLA	O1D-CGD-O2D-CED
21	a	1103	CLA	O1D-CGD-O2D-CED
21	a	1109	CLA	O1D-CGD-O2D-CED
21	a	1116	CLA	O1D-CGD-O2D-CED
21	a	1119	CLA	O1D-CGD-O2D-CED
21	a	1140	CLA	O1D-CGD-O2D-CED
21	b	1213	CLA	O1D-CGD-O2D-CED
21	b	1215	CLA	O1D-CGD-O2D-CED
21	b	1223	CLA	O1D-CGD-O2D-CED
21	b	1201	CLA	O1D-CGD-O2D-CED
21	1	1107	CLA	O1D-CGD-O2D-CED
21	1	1112	CLA	O1D-CGD-O2D-CED
21	1	1134	CLA	O1D-CGD-O2D-CED
21	2	1023	CLA	O1D-CGD-O2D-CED
21	2	1232	CLA	O1D-CGD-O2D-CED
21	8	1401	CLA	O1D-CGD-O2D-CED
21	b	1202	CLA	O1A-CGA-O2A-C1
21	j	1303	CLA	O1A-CGA-O2A-C1
21	2	1231	CLA	O1A-CGA-O2A-C1
21	6	1301	CLA	C2-C1-O2A-CGA
35	l	6001	LMT	O5B-C5B-C6B-O6B
21	A	1126	CLA	O1D-CGD-O2D-CED
21	b	1203	CLA	O1D-CGD-O2D-CED
21	A	1113	CLA	C4-C3-C5-C6
21	A	1116	CLA	C4-C3-C5-C6
21	A	1128	CLA	C4-C3-C5-C6
21	A	1012	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1237	CLA	C4-C3-C5-C6
21	B	1021	CLA	C4-C3-C5-C6
21	B	1215	CLA	C4-C3-C5-C6
21	B	1226	CLA	C4-C3-C5-C6
21	B	1235	CLA	C4-C3-C5-C6
21	L	1503	CLA	C4-C3-C5-C6
21	a	1103	CLA	C4-C3-C5-C6
21	a	1104	CLA	C4-C3-C5-C6
21	a	1116	CLA	C4-C3-C5-C6
21	a	1128	CLA	C4-C3-C5-C6
21	a	1133	CLA	C4-C3-C5-C6
21	a	1012	CLA	C4-C3-C5-C6
21	b	1021	CLA	C4-C3-C5-C6
21	b	1208	CLA	C4-C3-C5-C6
21	b	1209	CLA	C4-C3-C5-C6
21	b	1216	CLA	C4-C3-C5-C6
21	b	1219	CLA	C4-C3-C5-C6
21	b	1222	CLA	C4-C3-C5-C6
21	b	1230	CLA	C4-C3-C5-C6
21	1	1109	CLA	C4-C3-C5-C6
21	1	1126	CLA	C4-C3-C5-C6
21	1	1135	CLA	C4-C3-C5-C6
21	1	1012	CLA	C4-C3-C5-C6
21	2	1226	CLA	C4-C3-C5-C6
21	A	1113	CLA	C2-C3-C5-C6
21	A	1116	CLA	C2-C3-C5-C6
21	A	1128	CLA	C2-C3-C5-C6
21	A	1012	CLA	C2-C3-C5-C6
21	B	1237	CLA	C2-C3-C5-C6
21	B	1021	CLA	C2-C3-C5-C6
21	B	1215	CLA	C2-C3-C5-C6
21	L	1503	CLA	C2-C3-C5-C6
21	a	1103	CLA	C2-C3-C5-C6
21	a	1104	CLA	C2-C3-C5-C6
21	a	1116	CLA	C2-C3-C5-C6
21	a	1128	CLA	C2-C3-C5-C6
21	a	1130	CLA	C2-C3-C5-C6
21	a	1012	CLA	C2-C3-C5-C6
21	b	1208	CLA	C2-C3-C5-C6
21	b	1219	CLA	C2-C3-C5-C6
21	b	1222	CLA	C2-C3-C5-C6
21	b	1230	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1126	CLA	C2-C3-C5-C6
21	1	1127	CLA	C2-C3-C5-C6
21	1	1134	CLA	C2-C3-C5-C6
21	1	1108	CLA	CBA-CGA-O2A-C1
21	A	1112	CLA	CBD-CGD-O2D-CED
21	B	1210	CLA	CBD-CGD-O2D-CED
21	B	1234	CLA	CBD-CGD-O2D-CED
21	a	1128	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	O1D-CGD-O2D-CED
21	b	1239	CLA	O1D-CGD-O2D-CED
21	1	1011	CLA	O1D-CGD-O2D-CED
21	A	1122	CLA	C2A-CAA-CBA-CGA
21	a	1129	CLA	C3-C5-C6-C7
21	2	1217	CLA	C3-C5-C6-C7
21	A	1113	CLA	C3-C5-C6-C7
21	A	1128	CLA	C3-C5-C6-C7
21	L	1503	CLA	C3-C5-C6-C7
21	a	1126	CLA	C3-C5-C6-C7
21	a	1128	CLA	C3-C5-C6-C7
21	b	1237	CLA	C3-C5-C6-C7
21	b	1232	CLA	C3-C5-C6-C7
21	f	1302	CLA	C3-C5-C6-C7
21	j	1303	CLA	C3-C5-C6-C7
21	1	1125	CLA	C3-C5-C6-C7
21	1	1139	CLA	C3-C5-C6-C7
21	2	1207	CLA	C3-C5-C6-C7
21	2	1215	CLA	C3-C5-C6-C7
21	A	1104	CLA	CBA-CGA-O2A-C1
21	B	1202	CLA	CBA-CGA-O2A-C1
21	B	1204	CLA	CBA-CGA-O2A-C1
21	B	1206	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	CBA-CGA-O2A-C1
21	B	1218	CLA	CBA-CGA-O2A-C1
21	B	1235	CLA	CBA-CGA-O2A-C1
21	L	1501	CLA	CBA-CGA-O2A-C1
21	a	1013	CLA	CBA-CGA-O2A-C1
21	a	1104	CLA	CBA-CGA-O2A-C1
21	a	1136	CLA	CBA-CGA-O2A-C1
21	b	1218	CLA	CBA-CGA-O2A-C1
21	b	1227	CLA	CBA-CGA-O2A-C1
21	k	1402	CLA	CBA-CGA-O2A-C1
21	1	1013	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1104	CLA	CBA-CGA-O2A-C1
21	1	1121	CLA	CBA-CGA-O2A-C1
21	1	1124	CLA	CBA-CGA-O2A-C1
25	a	5007	LHG	C24-C23-O8-C6
31	b	5006	SQD	C24-C23-O48-C46
31	0	5005	SQD	C24-C23-O48-C46
26	A	5002	LMG	C38-C39-C40-C41
26	A	5002	LMG	C41-C42-C43-C44
26	B	5002	LMG	C20-C21-C22-C23
26	2	5002	LMG	C20-C21-C22-C23
26	2	5005	LMG	C41-C42-C43-C44
26	0	5001	LMG	C23-C24-C25-C26
26	b	5002	LMG	C20-C21-C22-C23
26	2	5005	LMG	C38-C39-C40-C41
26	A	5004	LMG	C23-C24-C25-C26
37	L	5004	DGD	C8A-C9A-CAA-CBA
24	A	4002	BCR	C13-C14-C15-C16
24	B	4017	BCR	C13-C14-C15-C16
24	B	4018	BCR	C19-C20-C21-C22
24	I	4018	BCR	C13-C14-C15-C16
24	b	4017	BCR	C13-C14-C15-C16
24	b	4018	BCR	C13-C14-C15-C16
24	i	4018	BCR	C13-C14-C15-C16
24	i	4018	BCR	C15-C16-C17-C18
24	2	4017	BCR	C13-C14-C15-C16
24	h	4018	BCR	C13-C14-C15-C16
24	0	4019	BCR	C13-C14-C15-C16
28	h	4020	45D	C26-C30-C32-C34
21	A	1102	CLA	O1A-CGA-O2A-C1
21	B	1202	CLA	O1A-CGA-O2A-C1
21	B	1209	CLA	O1A-CGA-O2A-C1
21	B	1214	CLA	O1A-CGA-O2A-C1
21	B	1218	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	O1A-CGA-O2A-C1
21	J	1303	CLA	O1A-CGA-O2A-C1
21	a	1013	CLA	O1A-CGA-O2A-C1
21	a	1121	CLA	O1A-CGA-O2A-C1
21	1	1121	CLA	O1A-CGA-O2A-C1
21	1	1126	CLA	O1A-CGA-O2A-C1
21	1	1138	CLA	O1A-CGA-O2A-C1
21	2	1207	CLA	O1A-CGA-O2A-C1
25	0	5002	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	5005	LMG	O9-C10-O7-C8
26	b	5007	LMG	O9-C10-O7-C8
37	L	5004	DGD	O1B-C1B-O2G-C2G
21	j	1303	CLA	O1D-CGD-O2D-CED
21	2	1215	CLA	O1D-CGD-O2D-CED
26	B	5005	LMG	C38-C39-C40-C41
26	b	5007	LMG	C23-C24-C25-C26
26	1	5002	LMG	C41-C42-C43-C44
26	0	5001	LMG	C38-C39-C40-C41
21	1	1108	CLA	O1A-CGA-O2A-C1
26	A	5002	LMG	C17-C18-C19-C20
26	A	5004	LMG	C17-C18-C19-C20
26	A	5008	LMG	C20-C21-C22-C23
26	A	5008	LMG	C35-C36-C37-C38
26	B	5002	LMG	C23-C24-C25-C26
26	B	5002	LMG	C35-C36-C37-C38
26	B	5005	LMG	C41-C42-C43-C44
26	a	5002	LMG	C17-C18-C19-C20
26	a	5002	LMG	C38-C39-C40-C41
26	a	5002	LMG	C41-C42-C43-C44
26	a	5004	LMG	C17-C18-C19-C20
26	a	5004	LMG	C20-C21-C22-C23
26	b	5002	LMG	C23-C24-C25-C26
26	b	5002	LMG	C35-C36-C37-C38
26	b	5005	LMG	C38-C39-C40-C41
26	b	5007	LMG	C20-C21-C22-C23
26	b	5007	LMG	C35-C36-C37-C38
26	b	5007	LMG	C41-C42-C43-C44
26	1	5002	LMG	C17-C18-C19-C20
26	1	5002	LMG	C38-C39-C40-C41
26	1	5004	LMG	C23-C24-C25-C26
26	1	5004	LMG	C35-C36-C37-C38
26	2	5002	LMG	C23-C24-C25-C26
26	2	5002	LMG	C35-C36-C37-C38
26	0	5001	LMG	C20-C21-C22-C23
37	L	5004	DGD	CEA-CFA-CGA-CHA
37	L	5004	DGD	CEB-CFB-CGB-CHB
21	A	1116	CLA	O1D-CGD-O2D-CED
21	B	1022	CLA	O1D-CGD-O2D-CED
21	B	1204	CLA	O1D-CGD-O2D-CED
21	B	1240	CLA	O1D-CGD-O2D-CED
21	a	1114	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1136	CLA	O1D-CGD-O2D-CED
21	a	1137	CLA	O1D-CGD-O2D-CED
21	b	1217	CLA	O1D-CGD-O2D-CED
21	b	1232	CLA	O1D-CGD-O2D-CED
21	1	1113	CLA	O1D-CGD-O2D-CED
21	1	1137	CLA	O1D-CGD-O2D-CED
21	2	1210	CLA	O1D-CGD-O2D-CED
21	A	1111	CLA	C3-C5-C6-C7
21	B	1205	CLA	C3-C5-C6-C7
21	F	1301	CLA	C3-C5-C6-C7
21	K	1401	CLA	C3-C5-C6-C7
21	a	1105	CLA	C3-C5-C6-C7
21	b	1205	CLA	C3-C5-C6-C7
21	b	1218	CLA	C3-C5-C6-C7
21	b	1227	CLA	C3-C5-C6-C7
21	b	1236	CLA	C3-C5-C6-C7
21	2	1221	CLA	C3-C5-C6-C7
21	2	1226	CLA	C3-C5-C6-C7
21	0	1503	CLA	C3-C5-C6-C7
21	A	1131	CLA	CBD-CGD-O2D-CED
21	B	1226	CLA	CBD-CGD-O2D-CED
21	B	1239	CLA	CBD-CGD-O2D-CED
21	a	1101	CLA	CBD-CGD-O2D-CED
21	1	1105	CLA	CBD-CGD-O2D-CED
21	1	1101	CLA	CBD-CGD-O2D-CED
21	2	1216	CLA	CBD-CGD-O2D-CED
25	l	5001	LHG	C31-C32-C33-C34
26	b	5005	LMG	C41-C42-C43-C44
25	A	5005	LHG	O2-C2-C3-O3
25	A	5006	LHG	O2-C2-C3-O3
25	L	5005	LHG	O2-C2-C3-O3
25	l	5004	LHG	O2-C2-C3-O3
25	1	5005	LHG	O2-C2-C3-O3
25	1	5001	LHG	O2-C2-C3-O3
25	6	5001	LHG	O2-C2-C3-O3
25	0	5004	LHG	O2-C2-C3-O3
21	A	1119	CLA	O1D-CGD-O2D-CED
21	B	1217	CLA	O1D-CGD-O2D-CED
21	a	1113	CLA	O1D-CGD-O2D-CED
21	a	1117	CLA	O1D-CGD-O2D-CED
21	a	1122	CLA	O1D-CGD-O2D-CED
21	2	1201	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1203	CLA	O1D-CGD-O2D-CED
21	A	1102	CLA	CBA-CGA-O2A-C1
21	B	1207	CLA	CBA-CGA-O2A-C1
21	L	1503	CLA	CBA-CGA-O2A-C1
21	a	1117	CLA	CBA-CGA-O2A-C1
21	a	1121	CLA	CBA-CGA-O2A-C1
21	a	1134	CLA	CBA-CGA-O2A-C1
21	a	1138	CLA	CBA-CGA-O2A-C1
21	j	1303	CLA	CBA-CGA-O2A-C1
21	1	1117	CLA	CBA-CGA-O2A-C1
21	1	1135	CLA	CBA-CGA-O2A-C1
21	A	1104	CLA	O1A-CGA-O2A-C1
21	B	1207	CLA	O1A-CGA-O2A-C1
21	B	1230	CLA	O1A-CGA-O2A-C1
21	a	1124	CLA	O1A-CGA-O2A-C1
21	1	1124	CLA	O1A-CGA-O2A-C1
21	1	1134	CLA	O1A-CGA-O2A-C1
21	1	1130	CLA	O1A-CGA-O2A-C1
21	0	1501	CLA	O1A-CGA-O2A-C1
31	b	5006	SQD	O10-C23-O48-C46
21	A	1105	CLA	O1D-CGD-O2D-CED
21	A	1121	CLA	O1D-CGD-O2D-CED
21	j	1302	CLA	O1D-CGD-O2D-CED
21	l	1501	CLA	O1D-CGD-O2D-CED
21	1	1118	CLA	O1D-CGD-O2D-CED
35	0	6001	LMT	O5B-C5B-C6B-O6B
26	0	5001	LMG	C4-C5-C6-O5
21	A	1124	CLA	CBD-CGD-O2D-CED
21	A	1127	CLA	CBD-CGD-O2D-CED
21	A	1128	CLA	CBD-CGD-O2D-CED
21	B	1209	CLA	CBD-CGD-O2D-CED
21	B	1211	CLA	CBD-CGD-O2D-CED
21	b	1207	CLA	CBD-CGD-O2D-CED
21	1	1125	CLA	O1D-CGD-O2D-CED
21	1	1130	CLA	O1D-CGD-O2D-CED
21	a	1138	CLA	O1A-CGA-O2A-C1
21	B	1229	CLA	O1D-CGD-O2D-CED
21	1	1131	CLA	O1D-CGD-O2D-CED
21	A	1140	CLA	C3-C5-C6-C7
21	B	1203	CLA	C3-C5-C6-C7
21	B	1215	CLA	C3-C5-C6-C7
21	B	1216	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	F	1302	CLA	C3-C5-C6-C7
21	b	1230	CLA	C3-C5-C6-C7
21	1	1012	CLA	C3-C5-C6-C7
21	a	1011	CLA	CBD-CGD-O2D-CED
21	a	1129	CLA	CBD-CGD-O2D-CED
21	a	1012	CLA	CBD-CGD-O2D-CED
21	k	1402	CLA	CBD-CGD-O2D-CED
21	1	1115	CLA	CBD-CGD-O2D-CED
21	1	1122	CLA	CBD-CGD-O2D-CED
21	1	1136	CLA	CBD-CGD-O2D-CED
21	2	1206	CLA	CBD-CGD-O2D-CED
21	B	1231	CLA	O1D-CGD-O2D-CED
21	F	1302	CLA	O1D-CGD-O2D-CED
21	a	1133	CLA	O1D-CGD-O2D-CED
21	b	1022	CLA	O1D-CGD-O2D-CED
21	b	1206	CLA	O1D-CGD-O2D-CED
21	b	1227	CLA	O1D-CGD-O2D-CED
21	b	1235	CLA	O1D-CGD-O2D-CED
21	1	1106	CLA	O1D-CGD-O2D-CED
21	2	1213	CLA	O1D-CGD-O2D-CED
21	6	1301	CLA	O1D-CGD-O2D-CED
21	A	1126	CLA	CBA-CGA-O2A-C1
21	B	1209	CLA	CBA-CGA-O2A-C1
21	B	1214	CLA	CBA-CGA-O2A-C1
21	a	1126	CLA	CBA-CGA-O2A-C1
21	b	1202	CLA	CBA-CGA-O2A-C1
21	1	1138	CLA	CBA-CGA-O2A-C1
25	0	5002	LHG	C24-C23-O8-C6
21	A	1107	CLA	C4-C3-C5-C6
21	A	1133	CLA	C4-C3-C5-C6
21	B	1225	CLA	C4-C3-C5-C6
21	a	1122	CLA	C4-C3-C5-C6
21	a	1127	CLA	C4-C3-C5-C6
21	a	1135	CLA	C4-C3-C5-C6
21	b	1237	CLA	C4-C3-C5-C6
21	b	1225	CLA	C4-C3-C5-C6
21	b	1235	CLA	C4-C3-C5-C6
21	1	1121	CLA	C4-C3-C5-C6
21	1	1140	CLA	C4-C3-C5-C6
21	2	1217	CLA	C4-C3-C5-C6
21	A	1107	CLA	C2-C3-C5-C6
21	A	1133	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1226	CLA	C2-C3-C5-C6
21	B	1235	CLA	C2-C3-C5-C6
21	a	1122	CLA	C2-C3-C5-C6
21	a	1133	CLA	C2-C3-C5-C6
21	a	1135	CLA	C2-C3-C5-C6
21	a	1140	CLA	C2-C3-C5-C6
21	b	1237	CLA	C2-C3-C5-C6
21	b	1021	CLA	C2-C3-C5-C6
21	b	1215	CLA	C2-C3-C5-C6
21	b	1216	CLA	C2-C3-C5-C6
21	b	1225	CLA	C2-C3-C5-C6
21	1	1121	CLA	C2-C3-C5-C6
21	1	1135	CLA	C2-C3-C5-C6
21	1	1140	CLA	C2-C3-C5-C6
21	1	1012	CLA	C2-C3-C5-C6
21	2	1217	CLA	C2-C3-C5-C6
21	2	1218	CLA	C2-C3-C5-C6
21	0	1503	CLA	C2-C3-C5-C6
21	L	1503	CLA	O1A-CGA-O2A-C1
21	a	1134	CLA	O1A-CGA-O2A-C1
25	a	5007	LHG	O10-C23-O8-C6
21	B	1202	CLA	CBD-CGD-O2D-CED
21	a	1125	CLA	CBD-CGD-O2D-CED
21	2	1237	CLA	CBD-CGD-O2D-CED
21	2	1202	CLA	CBD-CGD-O2D-CED
21	B	1214	CLA	O1D-CGD-O2D-CED
25	l	5004	LHG	C2-C3-O3-P
35	1	6001	LMT	O5B-C5B-C6B-O6B
35	l	6001	LMT	C4B-C5B-C6B-O6B
21	B	1240	CLA	C2A-CAA-CBA-CGA
21	J	1303	CLA	C2A-CAA-CBA-CGA
21	A	1109	CLA	O1D-CGD-O2D-CED
21	B	1238	CLA	O1D-CGD-O2D-CED
21	a	1106	CLA	O1D-CGD-O2D-CED
21	a	1120	CLA	O1D-CGD-O2D-CED
21	1	1110	CLA	O1D-CGD-O2D-CED
21	2	1228	CLA	O1D-CGD-O2D-CED
21	A	1126	CLA	O1A-CGA-O2A-C1
21	a	1126	CLA	O1A-CGA-O2A-C1
21	b	1206	CLA	O1A-CGA-O2A-C1
21	a	1103	CLA	C3-C5-C6-C7
26	a	5002	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	5004	LMG	O6-C1-O1-C7
31	B	5008	SQD	O5-C1-O6-C44
31	b	5006	SQD	O5-C1-O6-C44
21	B	1235	CLA	O1D-CGD-O2D-CED
21	a	1121	CLA	O1D-CGD-O2D-CED
21	2	1206	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	CBD-CGD-O2D-CED
21	A	1111	CLA	CBD-CGD-O2D-CED
21	A	1117	CLA	CBD-CGD-O2D-CED
21	A	1133	CLA	CBD-CGD-O2D-CED
21	A	1136	CLA	CBD-CGD-O2D-CED
21	B	1237	CLA	CBD-CGD-O2D-CED
21	B	1207	CLA	CBD-CGD-O2D-CED
21	B	1230	CLA	CBD-CGD-O2D-CED
21	L	1501	CLA	CBD-CGD-O2D-CED
21	a	1130	CLA	CBD-CGD-O2D-CED
21	b	1209	CLA	CBD-CGD-O2D-CED
21	b	1212	CLA	CBD-CGD-O2D-CED
21	b	1234	CLA	CBD-CGD-O2D-CED
21	l	1502	CLA	CBD-CGD-O2D-CED
21	1	1129	CLA	CBD-CGD-O2D-CED
21	2	1209	CLA	CBD-CGD-O2D-CED
21	2	1238	CLA	CBD-CGD-O2D-CED
21	6	1302	CLA	CBD-CGD-O2D-CED
21	a	1117	CLA	O1A-CGA-O2A-C1
21	1	1117	CLA	O1A-CGA-O2A-C1
21	1	1135	CLA	O1A-CGA-O2A-C1
25	l	5004	LHG	C28-C29-C30-C31
26	a	5004	LMG	C36-C37-C38-C39
21	A	1115	CLA	O1D-CGD-O2D-CED
21	L	1503	CLA	O1D-CGD-O2D-CED
21	a	1132	CLA	O1D-CGD-O2D-CED
21	b	1230	CLA	O1D-CGD-O2D-CED
21	2	1211	CLA	O1D-CGD-O2D-CED
21	2	1239	CLA	O1D-CGD-O2D-CED
26	2	5005	LMG	C32-C33-C34-C35
21	A	1129	CLA	CBD-CGD-O2D-CED
21	a	1102	CLA	CBD-CGD-O2D-CED
21	a	1108	CLA	CBD-CGD-O2D-CED
21	b	1210	CLA	CBD-CGD-O2D-CED
25	2	5004	LHG	C7-C8-C9-C10
21	a	1106	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1231	CLA	C3-C5-C6-C7
21	b	1208	CLA	C3-C5-C6-C7
25	a	5007	LHG	C13-C14-C15-C16
25	a	5007	LHG	C30-C31-C32-C33
24	h	4018	BCR	C15-C16-C17-C18
21	b	1239	CLA	O1A-CGA-O2A-C1
21	2	1210	CLA	O1A-CGA-O2A-C1
25	A	5006	LHG	C1-C2-C3-O3
25	B	5004	LHG	C1-C2-C3-O3
25	F	5002	LHG	C1-C2-C3-O3
25	a	5003	LHG	C1-C2-C3-O3
25	a	5007	LHG	C1-C2-C3-O3
25	l	5003	LHG	C1-C2-C3-O3
25	1	5005	LHG	C1-C2-C3-O3
25	1	5007	LHG	C1-C2-C3-O3
25	2	5004	LHG	C1-C2-C3-O3
21	A	1121	CLA	CBA-CGA-O2A-C1
21	A	1135	CLA	CBA-CGA-O2A-C1
21	B	1208	CLA	CBA-CGA-O2A-C1
21	B	1239	CLA	CBA-CGA-O2A-C1
21	a	1112	CLA	CBA-CGA-O2A-C1
21	a	1123	CLA	CBA-CGA-O2A-C1
21	a	1128	CLA	CBA-CGA-O2A-C1
21	a	1137	CLA	CBA-CGA-O2A-C1
21	a	1130	CLA	CBA-CGA-O2A-C1
21	b	1023	CLA	CBA-CGA-O2A-C1
21	b	1206	CLA	CBA-CGA-O2A-C1
21	b	1212	CLA	CBA-CGA-O2A-C1
21	b	1216	CLA	CBA-CGA-O2A-C1
21	b	1221	CLA	CBA-CGA-O2A-C1
21	b	1239	CLA	CBA-CGA-O2A-C1
21	b	1240	CLA	CBA-CGA-O2A-C1
21	l	1502	CLA	CBA-CGA-O2A-C1
21	l	1503	CLA	CBA-CGA-O2A-C1
21	1	1123	CLA	CBA-CGA-O2A-C1
21	1	1128	CLA	CBA-CGA-O2A-C1
21	2	1023	CLA	CBA-CGA-O2A-C1
21	2	1201	CLA	CBA-CGA-O2A-C1
21	2	1202	CLA	CBA-CGA-O2A-C1
21	2	1210	CLA	CBA-CGA-O2A-C1
21	2	1236	CLA	CBA-CGA-O2A-C1
21	2	1239	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	K	5009	LMG	C29-C28-O8-C9
26	0	5001	LMG	C29-C28-O8-C9
21	b	1236	CLA	CBD-CGD-O2D-CED
21	1	1117	CLA	CBD-CGD-O2D-CED
25	l	5003	LHG	C33-C34-C35-C36
21	A	1102	CLA	O1D-CGD-O2D-CED
21	J	1303	CLA	O1D-CGD-O2D-CED
21	a	1013	CLA	O1D-CGD-O2D-CED
21	a	1105	CLA	O1D-CGD-O2D-CED
21	a	1124	CLA	O1D-CGD-O2D-CED
21	1	1103	CLA	O1D-CGD-O2D-CED
21	1	1120	CLA	O1D-CGD-O2D-CED
21	1	1128	CLA	O1D-CGD-O2D-CED
21	1	1123	CLA	O1A-CGA-O2A-C1
25	b	5004	LHG	C13-C14-C15-C16
21	A	1121	CLA	C4-C3-C5-C6
21	A	1126	CLA	C4-C3-C5-C6
21	A	1134	CLA	C4-C3-C5-C6
21	B	1203	CLA	C4-C3-C5-C6
21	B	1212	CLA	C4-C3-C5-C6
21	a	1140	CLA	C4-C3-C5-C6
21	b	1215	CLA	C4-C3-C5-C6
21	1	1116	CLA	C4-C3-C5-C6
21	2	1237	CLA	C4-C3-C5-C6
21	2	1218	CLA	C4-C3-C5-C6
21	0	1503	CLA	C4-C3-C5-C6
21	A	1121	CLA	C2-C3-C5-C6
21	A	1126	CLA	C2-C3-C5-C6
21	A	1134	CLA	C2-C3-C5-C6
21	B	1203	CLA	C2-C3-C5-C6
21	a	1127	CLA	C2-C3-C5-C6
21	b	1209	CLA	C2-C3-C5-C6
21	b	1235	CLA	C2-C3-C5-C6
21	1	1109	CLA	C2-C3-C5-C6
21	1	1116	CLA	C2-C3-C5-C6
21	2	1237	CLA	C2-C3-C5-C6
21	2	1226	CLA	C2-C3-C5-C6
21	A	1801	CLA	C3-C5-C6-C7
21	B	1226	CLA	C3-C5-C6-C7
21	b	1238	CLA	C3-C5-C6-C7
21	B	1205	CLA	CBD-CGD-O2D-CED
21	b	1021	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1127	CLA	CBD-CGD-O2D-CED
21	A	1106	CLA	C14-C13-C15-C16
21	A	1107	CLA	C6-C7-C8-C9
21	A	1107	CLA	C14-C13-C15-C16
21	A	1110	CLA	C6-C7-C8-C9
21	A	1116	CLA	C6-C7-C8-C9
21	A	1116	CLA	C11-C10-C8-C9
21	A	1118	CLA	C11-C10-C8-C9
21	A	1125	CLA	C14-C13-C15-C16
21	A	1126	CLA	C14-C13-C15-C16
21	A	1129	CLA	C11-C10-C8-C9
21	A	1131	CLA	C11-C10-C8-C9
21	A	1134	CLA	C14-C13-C15-C16
21	A	1137	CLA	C11-C12-C13-C14
21	A	1012	CLA	C11-C10-C8-C9
21	A	1012	CLA	C11-C12-C13-C14
21	B	1023	CLA	C11-C12-C13-C14
21	B	1201	CLA	C11-C10-C8-C9
21	B	1206	CLA	C14-C13-C15-C16
21	B	1215	CLA	C6-C7-C8-C9
21	B	1221	CLA	C11-C12-C13-C14
21	B	1228	CLA	C6-C7-C8-C9
21	F	1301	CLA	C14-C13-C15-C16
21	F	1302	CLA	C11-C12-C13-C14
21	L	1502	CLA	C6-C7-C8-C9
21	a	1013	CLA	C14-C13-C15-C16
21	a	1106	CLA	C14-C13-C15-C16
21	a	1110	CLA	C6-C7-C8-C9
21	a	1111	CLA	C11-C12-C13-C14
21	a	1115	CLA	C11-C12-C13-C14
21	a	1117	CLA	C14-C13-C15-C16
21	a	1118	CLA	C11-C12-C13-C14
21	a	1119	CLA	C11-C10-C8-C9
21	a	1122	CLA	C14-C13-C15-C16
21	a	1123	CLA	C6-C7-C8-C9
21	a	1126	CLA	C11-C12-C13-C14
21	a	1126	CLA	C14-C13-C15-C16
21	a	1128	CLA	C11-C12-C13-C14
21	a	1131	CLA	C6-C7-C8-C9
21	a	1140	CLA	C11-C12-C13-C14
21	a	1130	CLA	C6-C7-C8-C9
21	a	1130	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1012	CLA	C11-C10-C8-C9
21	a	1012	CLA	C11-C12-C13-C14
21	b	1202	CLA	C14-C13-C15-C16
21	b	1206	CLA	C14-C13-C15-C16
21	b	1208	CLA	C6-C7-C8-C9
21	b	1211	CLA	C11-C12-C13-C14
21	b	1219	CLA	C11-C10-C8-C9
21	b	1222	CLA	C11-C12-C13-C14
21	b	1232	CLA	C6-C7-C8-C9
21	l	1503	CLA	C14-C13-C15-C16
21	1	1115	CLA	C6-C7-C8-C9
21	1	1120	CLA	C11-C12-C13-C14
21	1	1122	CLA	C6-C7-C8-C9
21	1	1126	CLA	C6-C7-C8-C9
21	1	1128	CLA	C11-C10-C8-C9
21	1	1133	CLA	C11-C10-C8-C9
21	1	1133	CLA	C14-C13-C15-C16
21	2	1022	CLA	C11-C12-C13-C14
21	2	1210	CLA	C6-C7-C8-C9
21	0	1502	CLA	C6-C7-C8-C9
22	b	2002	PQN	C21-C22-C23-C24
35	0	6001	LMT	C4B-C5B-C6B-O6B
21	A	1012	CLA	O1D-CGD-O2D-CED
21	b	1204	CLA	O1D-CGD-O2D-CED
21	b	1240	CLA	O1D-CGD-O2D-CED
21	1	1123	CLA	O1D-CGD-O2D-CED
21	1	1135	CLA	O1D-CGD-O2D-CED
21	2	1235	CLA	O1D-CGD-O2D-CED
21	2	1230	CLA	O1D-CGD-O2D-CED
21	0	1503	CLA	O1D-CGD-O2D-CED
26	A	5002	LMG	C2-C1-O1-C7
26	A	5008	LMG	C2-C1-O1-C7
26	a	5002	LMG	C2-C1-O1-C7
26	b	5007	LMG	C2-C1-O1-C7
31	L	5001	SQD	C2-C1-O6-C44
35	L	6001	LMT	C2'-C1'-O1'-C1
25	b	5004	LHG	C23-C24-C25-C26
25	B	5004	LHG	O2-C2-C3-O3
25	a	5001	LHG	O2-C2-C3-O3
25	a	5003	LHG	O2-C2-C3-O3
25	a	5005	LHG	O2-C2-C3-O3
25	l	5003	LHG	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	1	5007	LHG	O2-C2-C3-O3
25	2	5004	LHG	O2-C2-C3-O3
21	b	1214	CLA	O1D-CGD-O2D-CED
21	a	1123	CLA	O1A-CGA-O2A-C1
21	b	1023	CLA	O1A-CGA-O2A-C1
21	b	1216	CLA	O1A-CGA-O2A-C1
21	b	1221	CLA	O1A-CGA-O2A-C1
21	b	1240	CLA	O1A-CGA-O2A-C1
21	2	1236	CLA	O1A-CGA-O2A-C1
21	K	1402	CLA	O1D-CGD-O2D-CED
21	a	1127	CLA	O1D-CGD-O2D-CED
21	b	1208	CLA	O1D-CGD-O2D-CED
21	b	1228	CLA	O1D-CGD-O2D-CED
21	1	1102	CLA	O1D-CGD-O2D-CED
21	1	1012	CLA	O1D-CGD-O2D-CED
24	A	4002	BCR	C11-C12-C13-C35
24	A	4003	BCR	C36-C18-C19-C20
24	A	4007	BCR	C11-C12-C13-C35
24	A	4019	BCR	C7-C8-C9-C34
24	B	4004	BCR	C7-C8-C9-C34
24	B	4010	BCR	C36-C18-C19-C20
24	B	4014	BCR	C11-C12-C13-C35
24	I	4018	BCR	C36-C18-C19-C20
24	J	4013	BCR	C7-C8-C9-C34
24	J	4013	BCR	C11-C12-C13-C35
24	J	4013	BCR	C36-C18-C19-C20
24	K	4001	BCR	C36-C18-C19-C20
24	L	4019	BCR	C7-C8-C9-C34
24	L	4022	BCR	C36-C18-C19-C20
24	a	4001	BCR	C37-C22-C23-C24
24	a	4002	BCR	C11-C12-C13-C35
24	a	4002	BCR	C37-C22-C23-C24
24	a	4008	BCR	C36-C18-C19-C20
24	a	4019	BCR	C36-C18-C19-C20
24	b	4004	BCR	C11-C12-C13-C35
24	b	4004	BCR	C37-C22-C23-C24
24	b	4005	BCR	C36-C18-C19-C20
24	b	4017	BCR	C11-C12-C13-C35
24	b	4017	BCR	C36-C18-C19-C20
24	b	4018	BCR	C37-C22-C23-C24
24	b	4014	BCR	C11-C12-C13-C35
24	j	4013	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	4001	BCR	C11-C12-C13-C35
24	1	4002	BCR	C36-C18-C19-C20
24	1	4002	BCR	C37-C22-C23-C24
24	1	4003	BCR	C11-C12-C13-C35
24	1	4003	BCR	C37-C22-C23-C24
24	1	4007	BCR	C37-C22-C23-C24
24	1	4012	BCR	C37-C22-C23-C24
24	2	4011	BCR	C7-C8-C9-C34
24	2	4011	BCR	C36-C18-C19-C20
24	2	4004	BCR	C36-C18-C19-C20
24	2	4004	BCR	C37-C22-C23-C24
24	2	4005	BCR	C36-C18-C19-C20
24	2	4017	BCR	C11-C12-C13-C35
24	2	4018	BCR	C36-C18-C19-C20
24	2	4014	BCR	C11-C12-C13-C35
24	6	4016	BCR	C11-C12-C13-C35
24	6	4016	BCR	C36-C18-C19-C20
24	h	4018	BCR	C36-C18-C19-C20
24	7	4013	BCR	C37-C22-C23-C24
24	0	4019	BCR	C11-C12-C13-C35
24	0	4019	BCR	C37-C22-C23-C24
24	0	4022	BCR	C37-C22-C23-C24
24	9	4021	BCR	C11-C12-C13-C35
24	9	4021	BCR	C37-C22-C23-C24
30	b	4011	ECH	C7-C8-C9-C34
30	b	4011	ECH	C37-C22-C23-C24
30	b	4006	ECH	C37-C22-C23-C24
30	i	4020	ECH	C11-C12-C13-C35
30	i	4020	ECH	C37-C22-C23-C24
30	2	4006	ECH	C37-C22-C23-C24
34	j	4015	ZEX	C31-C32-C33-C40
34	7	4015	ZEX	C7-C8-C9-C19
36	I	4020	EQ3	C37-C22-C23-C24
24	B	4005	BCR	C21-C22-C23-C24
24	B	4014	BCR	C11-C12-C13-C14
24	I	4018	BCR	C17-C18-C19-C20
24	J	4013	BCR	C11-C12-C13-C14
24	b	4004	BCR	C11-C12-C13-C14
24	b	4004	BCR	C21-C22-C23-C24
24	b	4014	BCR	C11-C12-C13-C14
24	i	4018	BCR	C11-C12-C13-C14
24	j	4013	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	4001	BCR	C11-C12-C13-C14
24	2	4017	BCR	C11-C12-C13-C14
24	2	4014	BCR	C11-C12-C13-C14
24	7	4013	BCR	C11-C12-C13-C14
24	7	4013	BCR	C21-C22-C23-C24
24	0	4019	BCR	C11-C12-C13-C14
24	0	4019	BCR	C21-C22-C23-C24
30	b	4011	ECH	C7-C8-C9-C10
30	i	4020	ECH	C11-C12-C13-C14
30	2	4006	ECH	C21-C22-C23-C24
21	A	1127	CLA	C2A-CAA-CBA-CGA
21	B	1225	CLA	C2A-CAA-CBA-CGA
21	B	1239	CLA	C2A-CAA-CBA-CGA
21	k	1402	CLA	C2A-CAA-CBA-CGA
21	2	1214	CLA	C2A-CAA-CBA-CGA
25	a	5007	LHG	C7-C8-C9-C10
21	A	1121	CLA	O1A-CGA-O2A-C1
21	a	1112	CLA	O1A-CGA-O2A-C1
21	a	1130	CLA	O1A-CGA-O2A-C1
21	b	1212	CLA	O1A-CGA-O2A-C1
21	l	1503	CLA	O1A-CGA-O2A-C1
21	1	1128	CLA	O1A-CGA-O2A-C1
21	2	1023	CLA	O1A-CGA-O2A-C1
21	2	1201	CLA	O1A-CGA-O2A-C1
21	B	1210	CLA	C3-C5-C6-C7
21	L	1502	CLA	C3-C5-C6-C7
21	b	1210	CLA	C3-C5-C6-C7
21	b	1215	CLA	C3-C5-C6-C7
21	a	1133	CLA	C8-C10-C11-C12
37	L	5004	DGD	O6D-C5D-C6D-O5D
25	F	5002	LHG	C8-C7-O7-C5
21	b	1232	CLA	CBA-CGA-O2A-C1
21	A	1133	CLA	C15-C16-C17-C18
21	A	1136	CLA	C15-C16-C17-C18
21	B	1203	CLA	C13-C15-C16-C17
21	B	1223	CLA	C8-C10-C11-C12
21	F	1302	CLA	C8-C10-C11-C12
21	K	1401	CLA	C13-C15-C16-C17
21	a	1136	CLA	C13-C15-C16-C17
21	b	1237	CLA	C5-C6-C7-C8
21	b	1213	CLA	C5-C6-C7-C8
21	b	1214	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1118	CLA	C15-C16-C17-C18
25	1	5007	LHG	C7-C8-C9-C10
21	A	1104	CLA	C2-C1-O2A-CGA
21	A	1108	CLA	C2-C1-O2A-CGA
21	A	1111	CLA	C2-C1-O2A-CGA
21	A	1112	CLA	C2-C1-O2A-CGA
21	A	1119	CLA	C2-C1-O2A-CGA
21	A	1123	CLA	C2-C1-O2A-CGA
21	A	1137	CLA	C2-C1-O2A-CGA
21	A	1138	CLA	C2-C1-O2A-CGA
21	A	1139	CLA	C2-C1-O2A-CGA
21	A	1101	CLA	C2-C1-O2A-CGA
21	B	1203	CLA	C2-C1-O2A-CGA
21	B	1228	CLA	C2-C1-O2A-CGA
21	B	1229	CLA	C2-C1-O2A-CGA
21	J	1302	CLA	C2-C1-O2A-CGA
21	a	1104	CLA	C2-C1-O2A-CGA
21	a	1107	CLA	C2-C1-O2A-CGA
21	a	1108	CLA	C2-C1-O2A-CGA
21	a	1111	CLA	C2-C1-O2A-CGA
21	a	1118	CLA	C2-C1-O2A-CGA
21	a	1119	CLA	C2-C1-O2A-CGA
21	a	1126	CLA	C2-C1-O2A-CGA
21	a	1129	CLA	C2-C1-O2A-CGA
21	a	1139	CLA	C2-C1-O2A-CGA
21	a	1140	CLA	C2-C1-O2A-CGA
21	b	1023	CLA	C2-C1-O2A-CGA
21	b	1209	CLA	C2-C1-O2A-CGA
21	b	1227	CLA	C2-C1-O2A-CGA
21	b	1229	CLA	C2-C1-O2A-CGA
21	f	1301	CLA	C2-C1-O2A-CGA
21	1	1013	CLA	C2-C1-O2A-CGA
21	1	1104	CLA	C2-C1-O2A-CGA
21	1	1111	CLA	C2-C1-O2A-CGA
21	1	1118	CLA	C2-C1-O2A-CGA
21	1	1122	CLA	C2-C1-O2A-CGA
21	1	1125	CLA	C2-C1-O2A-CGA
21	1	1126	CLA	C2-C1-O2A-CGA
21	1	1137	CLA	C2-C1-O2A-CGA
21	1	1139	CLA	C2-C1-O2A-CGA
21	1	1101	CLA	C2-C1-O2A-CGA
21	2	1022	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1023	CLA	C2-C1-O2A-CGA
21	2	1203	CLA	C2-C1-O2A-CGA
21	2	1214	CLA	C2-C1-O2A-CGA
21	2	1217	CLA	C2-C1-O2A-CGA
21	2	1229	CLA	C2-C1-O2A-CGA
21	A	1132	CLA	O1D-CGD-O2D-CED
21	a	1110	CLA	O1D-CGD-O2D-CED
21	a	1115	CLA	O1D-CGD-O2D-CED
21	2	1022	CLA	O1D-CGD-O2D-CED
21	2	1204	CLA	O1D-CGD-O2D-CED
21	B	1222	CLA	CBD-CGD-O2D-CED
25	A	5001	LHG	C11-C12-C13-C14
35	L	6001	LMT	C5'-C4'-O1B-C1B
21	A	1132	CLA	C13-C15-C16-C17
21	A	1133	CLA	C8-C10-C11-C12
21	B	1205	CLA	C8-C10-C11-C12
21	B	1208	CLA	C5-C6-C7-C8
21	B	1213	CLA	C15-C16-C17-C18
21	B	1240	CLA	C15-C16-C17-C18
21	F	1302	CLA	C15-C16-C17-C18
21	J	1303	CLA	C8-C10-C11-C12
21	a	1111	CLA	C10-C11-C12-C13
21	b	1021	CLA	C5-C6-C7-C8
21	b	1207	CLA	C10-C11-C12-C13
21	b	1213	CLA	C15-C16-C17-C18
21	b	1225	CLA	C5-C6-C7-C8
21	b	1231	CLA	C5-C6-C7-C8
21	b	1232	CLA	C15-C16-C17-C18
21	1	1125	CLA	C10-C11-C12-C13
21	1	1126	CLA	C13-C15-C16-C17
21	1	1134	CLA	C8-C10-C11-C12
21	1	1801	CLA	C5-C6-C7-C8
21	2	1210	CLA	C13-C15-C16-C17
21	0	1503	CLA	C10-C11-C12-C13
25	0	5002	LHG	O1-C1-C2-O2
21	b	1203	CLA	C3-C5-C6-C7
21	B	1213	CLA	O1D-CGD-O2D-CED
21	2	1205	CLA	O1D-CGD-O2D-CED
21	A	1135	CLA	O1A-CGA-O2A-C1
21	2	1239	CLA	O1A-CGA-O2A-C1
21	a	1106	CLA	C10-C11-C12-C13
21	1	1101	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1013	CLA	CBD-CGD-O2D-CED
21	K	1401	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	C6-C7-C8-C10
21	A	1117	CLA	C11-C10-C8-C7
21	B	1211	CLA	C11-C10-C8-C7
21	B	1216	CLA	C11-C12-C13-C15
21	a	1121	CLA	C11-C12-C13-C15
21	a	1125	CLA	C11-C12-C13-C15
21	a	1136	CLA	C11-C10-C8-C7
21	b	1021	CLA	C11-C12-C13-C15
21	b	1208	CLA	C11-C10-C8-C7
21	b	1210	CLA	C11-C10-C8-C7
21	b	1211	CLA	C11-C10-C8-C7
21	l	1503	CLA	C11-C12-C13-C15
21	1	1131	CLA	C6-C7-C8-C10
21	1	1101	CLA	C11-C12-C13-C15
21	2	1210	CLA	C11-C12-C13-C15
21	A	1113	CLA	CBA-CGA-O2A-C1
21	A	1134	CLA	CBA-CGA-O2A-C1
21	A	1139	CLA	CBA-CGA-O2A-C1
21	a	1113	CLA	CBA-CGA-O2A-C1
21	b	1209	CLA	CBA-CGA-O2A-C1
21	b	1217	CLA	CBA-CGA-O2A-C1
21	b	1201	CLA	CBA-CGA-O2A-C1
21	j	1302	CLA	CBA-CGA-O2A-C1
21	2	1234	CLA	CBA-CGA-O2A-C1
25	F	5002	LHG	C24-C23-O8-C6
25	a	5005	LHG	C24-C23-O8-C6
21	f	1302	CLA	C4-C3-C5-C6
21	A	1131	CLA	C5-C6-C7-C8
21	A	1101	CLA	C10-C11-C12-C13
21	B	1203	CLA	C10-C11-C12-C13
21	L	1503	CLA	C8-C10-C11-C12
21	a	1013	CLA	C13-C15-C16-C17
21	1	1128	CLA	C8-C10-C11-C12
25	a	5003	LHG	C23-C24-C25-C26
24	A	4001	BCR	C19-C20-C21-C22
24	B	4018	BCR	C13-C14-C15-C16
24	I	4018	BCR	C15-C16-C17-C18
24	a	4003	BCR	C13-C14-C15-C16
24	1	4007	BCR	C13-C14-C15-C16
24	1	4008	BCR	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	4019	BCR	C9-C10-C11-C12
24	2	4011	BCR	C19-C20-C21-C22
24	2	4010	BCR	C19-C20-C21-C22
35	F	6001	LMT	O1'-C1-C2-C3
21	A	1103	CLA	O1D-CGD-O2D-CED
21	2	1222	CLA	O1D-CGD-O2D-CED
21	A	1130	CLA	C3-C5-C6-C7
21	B	1237	CLA	C3-C5-C6-C7
21	B	1204	CLA	C3-C5-C6-C7
21	B	1227	CLA	C3-C5-C6-C7
21	a	1122	CLA	C3-C5-C6-C7
21	2	1204	CLA	C3-C5-C6-C7
21	A	1110	CLA	C8-C10-C11-C12
21	B	1225	CLA	C13-C15-C16-C17
21	B	1240	CLA	C13-C15-C16-C17
21	L	1501	CLA	C13-C15-C16-C17
21	a	1118	CLA	C5-C6-C7-C8
21	a	1125	CLA	C13-C15-C16-C17
21	a	1135	CLA	C13-C15-C16-C17
21	j	1302	CLA	C5-C6-C7-C8
21	1	1118	CLA	C10-C11-C12-C13
21	1	1012	CLA	C5-C6-C7-C8
25	A	5001	LHG	C23-C24-C25-C26
25	A	5006	LHG	C7-C8-C9-C10
25	F	5002	LHG	C23-C24-C25-C26
25	a	5001	LHG	C7-C8-C9-C10
25	a	5005	LHG	C7-C8-C9-C10
25	l	5001	LHG	C7-C8-C9-C10
25	l	5001	LHG	C23-C24-C25-C26
25	l	5003	LHG	C23-C24-C25-C26
25	1	5005	LHG	C7-C8-C9-C10
25	1	5007	LHG	C23-C24-C25-C26
26	1	5002	LMG	C28-C29-C30-C31
21	a	1137	CLA	O1A-CGA-O2A-C1
21	2	1206	CLA	O1A-CGA-O2A-C1
21	A	1106	CLA	CBD-CGD-O2D-CED
21	a	1135	CLA	O1D-CGD-O2D-CED
21	B	1216	CLA	CBA-CGA-O2A-C1
21	A	1102	CLA	C10-C11-C12-C13
21	A	1106	CLA	C8-C10-C11-C12
21	A	1110	CLA	C10-C11-C12-C13
21	A	1111	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1116	CLA	C5-C6-C7-C8
21	A	1125	CLA	C5-C6-C7-C8
21	A	1140	CLA	C8-C10-C11-C12
21	A	1130	CLA	C5-C6-C7-C8
21	A	1012	CLA	C5-C6-C7-C8
21	B	1209	CLA	C15-C16-C17-C18
21	B	1214	CLA	C13-C15-C16-C17
21	B	1214	CLA	C15-C16-C17-C18
21	B	1217	CLA	C10-C11-C12-C13
21	B	1218	CLA	C5-C6-C7-C8
21	B	1218	CLA	C10-C11-C12-C13
21	B	1225	CLA	C5-C6-C7-C8
21	B	1228	CLA	C15-C16-C17-C18
21	B	1207	CLA	C13-C15-C16-C17
21	a	1013	CLA	C10-C11-C12-C13
21	a	1117	CLA	C13-C15-C16-C17
21	a	1127	CLA	C15-C16-C17-C18
21	a	1135	CLA	C10-C11-C12-C13
21	a	1130	CLA	C15-C16-C17-C18
21	b	1214	CLA	C8-C10-C11-C12
21	b	1215	CLA	C5-C6-C7-C8
21	b	1223	CLA	C15-C16-C17-C18
21	b	1228	CLA	C5-C6-C7-C8
21	b	1228	CLA	C13-C15-C16-C17
21	b	1239	CLA	C8-C10-C11-C12
21	l	1503	CLA	C10-C11-C12-C13
21	2	1205	CLA	C8-C10-C11-C12
21	2	1215	CLA	C8-C10-C11-C12
21	2	1225	CLA	C5-C6-C7-C8
22	2	2002	PQN	C23-C25-C26-C27
21	A	1113	CLA	C2A-CAA-CBA-CGA
21	A	1135	CLA	C2A-CAA-CBA-CGA
21	A	1801	CLA	C2A-CAA-CBA-CGA
21	B	1238	CLA	C2A-CAA-CBA-CGA
21	F	1302	CLA	C2A-CAA-CBA-CGA
21	a	1109	CLA	C2A-CAA-CBA-CGA
21	a	1114	CLA	C2A-CAA-CBA-CGA
21	b	1214	CLA	C2A-CAA-CBA-CGA
21	b	1216	CLA	C2A-CAA-CBA-CGA
21	b	1238	CLA	C2A-CAA-CBA-CGA
21	l	1501	CLA	C2A-CAA-CBA-CGA
21	1	1135	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1237	CLA	C2A-CAA-CBA-CGA
21	2	1211	CLA	C2A-CAA-CBA-CGA
21	2	1238	CLA	C2A-CAA-CBA-CGA
21	8	1402	CLA	C2A-CAA-CBA-CGA
21	0	1503	CLA	C2A-CAA-CBA-CGA
21	1	1132	CLA	O1D-CGD-O2D-CED
24	A	4003	BCR	C10-C11-C12-C13
24	B	4018	BCR	C10-C11-C12-C13
24	2	4010	BCR	C10-C11-C12-C13
21	A	1103	CLA	C13-C15-C16-C17
21	A	1104	CLA	C15-C16-C17-C18
21	A	1106	CLA	C15-C16-C17-C18
21	A	1110	CLA	C13-C15-C16-C17
21	A	1113	CLA	C13-C15-C16-C17
21	A	1134	CLA	C15-C16-C17-C18
21	A	1136	CLA	C5-C6-C7-C8
21	A	1137	CLA	C8-C10-C11-C12
21	B	1201	CLA	C10-C11-C12-C13
21	B	1206	CLA	C10-C11-C12-C13
21	B	1215	CLA	C10-C11-C12-C13
21	B	1215	CLA	C13-C15-C16-C17
21	B	1223	CLA	C5-C6-C7-C8
21	a	1121	CLA	C10-C11-C12-C13
21	a	1131	CLA	C10-C11-C12-C13
21	b	1208	CLA	C8-C10-C11-C12
21	b	1218	CLA	C10-C11-C12-C13
21	b	1218	CLA	C13-C15-C16-C17
21	b	1222	CLA	C10-C11-C12-C13
21	j	1302	CLA	C10-C11-C12-C13
21	1	1103	CLA	C5-C6-C7-C8
21	1	1106	CLA	C13-C15-C16-C17
21	1	1109	CLA	C10-C11-C12-C13
21	1	1122	CLA	C10-C11-C12-C13
21	1	1125	CLA	C15-C16-C17-C18
21	1	1126	CLA	C10-C11-C12-C13
21	1	1128	CLA	C10-C11-C12-C13
21	1	1131	CLA	C13-C15-C16-C17
21	1	1133	CLA	C15-C16-C17-C18
21	1	1134	CLA	C5-C6-C7-C8
21	1	1136	CLA	C8-C10-C11-C12
21	2	1202	CLA	C13-C15-C16-C17
21	2	1210	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	A	5003	LHG	C23-C24-C25-C26
25	B	5006	LHG	C7-C8-C9-C10
25	l	5004	LHG	C23-C24-C25-C26
25	1	5005	LHG	C23-C24-C25-C26
25	0	5004	LHG	C23-C24-C25-C26
21	1	1801	CLA	O1D-CGD-O2D-CED
21	B	1208	CLA	O1A-CGA-O2A-C1
26	K	5009	LMG	O10-C28-O8-C9
21	A	1013	CLA	C10-C11-C12-C13
21	A	1103	CLA	C15-C16-C17-C18
21	A	1105	CLA	C15-C16-C17-C18
21	A	1106	CLA	C13-C15-C16-C17
21	A	1107	CLA	C5-C6-C7-C8
21	A	1110	CLA	C5-C6-C7-C8
21	A	1114	CLA	C10-C11-C12-C13
21	A	1118	CLA	C5-C6-C7-C8
21	A	1120	CLA	C13-C15-C16-C17
21	A	1134	CLA	C5-C6-C7-C8
21	A	1134	CLA	C8-C10-C11-C12
21	B	1023	CLA	C8-C10-C11-C12
21	B	1208	CLA	C15-C16-C17-C18
21	B	1211	CLA	C8-C10-C11-C12
21	B	1215	CLA	C5-C6-C7-C8
21	B	1216	CLA	C8-C10-C11-C12
21	B	1216	CLA	C15-C16-C17-C18
21	B	1218	CLA	C13-C15-C16-C17
21	B	1221	CLA	C15-C16-C17-C18
21	B	1229	CLA	C5-C6-C7-C8
21	B	1229	CLA	C8-C10-C11-C12
21	B	1234	CLA	C5-C6-C7-C8
21	B	1234	CLA	C10-C11-C12-C13
21	B	1238	CLA	C5-C6-C7-C8
21	J	1302	CLA	C8-C10-C11-C12
21	K	1401	CLA	C5-C6-C7-C8
21	K	1401	CLA	C15-C16-C17-C18
21	K	1402	CLA	C13-C15-C16-C17
21	L	1503	CLA	C15-C16-C17-C18
21	a	1111	CLA	C5-C6-C7-C8
21	a	1112	CLA	C5-C6-C7-C8
21	a	1122	CLA	C13-C15-C16-C17
21	a	1123	CLA	C15-C16-C17-C18
21	a	1124	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1133	CLA	C15-C16-C17-C18
21	a	1139	CLA	C13-C15-C16-C17
21	b	1209	CLA	C15-C16-C17-C18
21	b	1216	CLA	C5-C6-C7-C8
21	b	1218	CLA	C5-C6-C7-C8
21	b	1219	CLA	C8-C10-C11-C12
21	b	1220	CLA	C15-C16-C17-C18
21	b	1224	CLA	C5-C6-C7-C8
21	b	1231	CLA	C15-C16-C17-C18
21	b	1240	CLA	C8-C10-C11-C12
21	b	1201	CLA	C13-C15-C16-C17
21	j	1303	CLA	C5-C6-C7-C8
21	1	1117	CLA	C15-C16-C17-C18
21	1	1131	CLA	C5-C6-C7-C8
21	1	1101	CLA	C15-C16-C17-C18
21	2	1208	CLA	C8-C10-C11-C12
22	1	2001	PQN	C18-C20-C21-C22
25	A	5003	LHG	O2-C2-C3-O3
25	B	5006	LHG	O2-C2-C3-O3
25	a	5007	LHG	O2-C2-C3-O3
25	l	5002	LHG	O2-C2-C3-O3
25	1	5003	LHG	O2-C2-C3-O3
21	A	1112	CLA	O1D-CGD-O2D-CED
21	a	1109	CLA	CBA-CGA-O2A-C1
21	2	1208	CLA	CBA-CGA-O2A-C1
21	B	1228	CLA	CBD-CGD-O2D-CED
21	1	1133	CLA	CBD-CGD-O2D-CED
21	B	1239	CLA	O1A-CGA-O2A-C1
21	a	1128	CLA	O1A-CGA-O2A-C1
21	2	1202	CLA	O1A-CGA-O2A-C1
26	0	5001	LMG	O10-C28-O8-C9
25	A	5003	LHG	C7-C8-C9-C10
25	a	5007	LHG	C23-C24-C25-C26
31	L	5002	SQD	C7-C8-C9-C10
31	0	5005	SQD	C23-C24-C25-C26
21	B	1205	CLA	C5-C6-C7-C8
21	B	1213	CLA	C13-C15-C16-C17
21	b	1206	CLA	C15-C16-C17-C18
21	b	1231	CLA	C13-C15-C16-C17
21	b	1236	CLA	C13-C15-C16-C17
21	b	1201	CLA	C8-C10-C11-C12
21	l	1502	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	l	1502	CLA	C10-C11-C12-C13
21	1	1103	CLA	C15-C16-C17-C18
21	2	1210	CLA	C5-C6-C7-C8
25	F	5002	LHG	O9-C7-O7-C5
21	a	1106	CLA	C3-C5-C6-C7
21	A	1113	CLA	O1D-CGD-O2D-CED
21	B	1210	CLA	O1D-CGD-O2D-CED
21	B	1226	CLA	O1D-CGD-O2D-CED
21	B	1234	CLA	O1D-CGD-O2D-CED
21	a	1128	CLA	O1D-CGD-O2D-CED
21	a	1101	CLA	O1D-CGD-O2D-CED
21	b	1226	CLA	O1D-CGD-O2D-CED
21	1	1119	CLA	O1D-CGD-O2D-CED
21	1	1101	CLA	O1D-CGD-O2D-CED
21	2	1216	CLA	O1D-CGD-O2D-CED
21	A	1126	CLA	C10-C11-C12-C13
21	A	1131	CLA	C13-C15-C16-C17
21	A	1138	CLA	C8-C10-C11-C12
21	B	1202	CLA	C15-C16-C17-C18
21	B	1214	CLA	C8-C10-C11-C12
21	B	1224	CLA	C10-C11-C12-C13
21	B	1231	CLA	C5-C6-C7-C8
21	B	1234	CLA	C8-C10-C11-C12
21	F	1301	CLA	C15-C16-C17-C18
21	a	1103	CLA	C13-C15-C16-C17
21	a	1106	CLA	C13-C15-C16-C17
21	a	1120	CLA	C5-C6-C7-C8
21	a	1121	CLA	C8-C10-C11-C12
21	a	1130	CLA	C13-C15-C16-C17
21	a	1138	CLA	C15-C16-C17-C18
21	b	1205	CLA	C10-C11-C12-C13
21	b	1214	CLA	C5-C6-C7-C8
21	b	1225	CLA	C13-C15-C16-C17
21	b	1228	CLA	C10-C11-C12-C13
21	1	1106	CLA	C15-C16-C17-C18
21	2	1201	CLA	C13-C15-C16-C17
21	2	1205	CLA	C13-C15-C16-C17
22	a	2001	PQN	C18-C20-C21-C22
21	b	1202	CLA	CBD-CGD-O2D-CED
21	b	1214	CLA	C4-C3-C5-C6
21	a	1113	CLA	O1A-CGA-O2A-C1
21	l	1502	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1234	CLA	O1A-CGA-O2A-C1
25	A	5007	LHG	C23-C24-C25-C26
26	A	5008	LMG	C28-C29-C30-C31
26	b	5007	LMG	C28-C29-C30-C31
25	l	5003	LHG	C9-C10-C11-C12
21	A	1131	CLA	O1D-CGD-O2D-CED
21	B	1239	CLA	O1D-CGD-O2D-CED
35	L	6001	LMT	O5B-C5B-C6B-O6B
21	A	1137	CLA	C13-C15-C16-C17
21	A	1140	CLA	C10-C11-C12-C13
21	B	1214	CLA	C5-C6-C7-C8
21	B	1229	CLA	C10-C11-C12-C13
21	F	1301	CLA	C13-C15-C16-C17
21	a	1102	CLA	C5-C6-C7-C8
21	a	1131	CLA	C8-C10-C11-C12
21	b	1021	CLA	C13-C15-C16-C17
21	b	1207	CLA	C8-C10-C11-C12
21	f	1302	CLA	C5-C6-C7-C8
21	1	1127	CLA	C15-C16-C17-C18
21	0	1501	CLA	C13-C15-C16-C17
21	A	1123	CLA	CBA-CGA-O2A-C1
21	B	1201	CLA	CBA-CGA-O2A-C1
21	B	1210	CLA	CBA-CGA-O2A-C1
21	a	1118	CLA	CBA-CGA-O2A-C1
21	a	1135	CLA	CBA-CGA-O2A-C1
21	b	1226	CLA	CBA-CGA-O2A-C1
21	1	1133	CLA	CBA-CGA-O2A-C1
21	1	1136	CLA	CBA-CGA-O2A-C1
21	2	1216	CLA	CBA-CGA-O2A-C1
21	2	1222	CLA	CBA-CGA-O2A-C1
21	A	1108	CLA	CBD-CGD-O2D-CED
21	2	1223	CLA	CBD-CGD-O2D-CED
21	2	1234	CLA	CBD-CGD-O2D-CED
26	2	5005	LMG	C11-C10-O7-C8
21	A	1139	CLA	O1A-CGA-O2A-C1
21	b	1217	CLA	O1A-CGA-O2A-C1
21	B	1211	CLA	O1D-CGD-O2D-CED
21	b	1207	CLA	O1D-CGD-O2D-CED
21	b	1209	CLA	C3-C5-C6-C7
21	1	1127	CLA	C3-C5-C6-C7
25	0	5002	LHG	C5-C6-O8-C23
21	1	1013	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	4019	BCR	C19-C20-C21-C22
24	2	4010	BCR	C13-C14-C15-C16
24	8	4001	BCR	C19-C20-C21-C22
21	A	1139	CLA	C8-C10-C11-C12
21	b	1201	CLA	C10-C11-C12-C13
34	7	4015	ZEX	C25-C26-C27-C28
25	1	5003	LHG	C23-C24-C25-C26
26	2	5005	LMG	O9-C10-O7-C8
35	L	6001	LMT	C3'-C4'-O1B-C1B
25	A	5003	LHG	C1-C2-C3-O3
25	A	5007	LHG	C1-C2-C3-O3
25	B	5006	LHG	C1-C2-C3-O3
25	L	5005	LHG	C1-C2-C3-O3
25	l	5001	LHG	C1-C2-C3-O3
21	A	1108	CLA	C2A-CAA-CBA-CGA
21	B	1214	CLA	C2A-CAA-CBA-CGA
21	B	1216	CLA	C2A-CAA-CBA-CGA
21	B	1218	CLA	C2A-CAA-CBA-CGA
21	B	1229	CLA	C2A-CAA-CBA-CGA
21	a	1127	CLA	C2A-CAA-CBA-CGA
21	b	1237	CLA	C2A-CAA-CBA-CGA
21	b	1240	CLA	C2A-CAA-CBA-CGA
21	1	1106	CLA	C2A-CAA-CBA-CGA
21	1	1127	CLA	C2A-CAA-CBA-CGA
21	2	1213	CLA	C2A-CAA-CBA-CGA
21	2	1225	CLA	C2A-CAA-CBA-CGA
21	A	1136	CLA	CBA-CGA-O2A-C1
21	A	1137	CLA	CBA-CGA-O2A-C1
21	B	1221	CLA	CBA-CGA-O2A-C1
21	B	1232	CLA	CBA-CGA-O2A-C1
21	a	1102	CLA	CBA-CGA-O2A-C1
21	b	1231	CLA	CBA-CGA-O2A-C1
21	1	1120	CLA	CBA-CGA-O2A-C1
21	A	1013	CLA	C13-C15-C16-C17
21	A	1111	CLA	C10-C11-C12-C13
21	A	1113	CLA	C5-C6-C7-C8
21	A	1116	CLA	C8-C10-C11-C12
21	A	1125	CLA	C15-C16-C17-C18
21	B	1206	CLA	C15-C16-C17-C18
21	B	1216	CLA	C10-C11-C12-C13
21	L	1501	CLA	C10-C11-C12-C13
21	a	1102	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1104	CLA	C5-C6-C7-C8
21	a	1105	CLA	C5-C6-C7-C8
21	a	1108	CLA	C5-C6-C7-C8
21	a	1117	CLA	C5-C6-C7-C8
21	a	1126	CLA	C8-C10-C11-C12
21	a	1133	CLA	C5-C6-C7-C8
21	b	1213	CLA	C13-C15-C16-C17
21	b	1220	CLA	C5-C6-C7-C8
21	b	1221	CLA	C15-C16-C17-C18
21	b	1232	CLA	C10-C11-C12-C13
21	b	1235	CLA	C15-C16-C17-C18
21	1	1106	CLA	C10-C11-C12-C13
21	1	1118	CLA	C8-C10-C11-C12
21	1	1120	CLA	C5-C6-C7-C8
21	1	1125	CLA	C8-C10-C11-C12
21	1	1134	CLA	C15-C16-C17-C18
21	1	1136	CLA	C13-C15-C16-C17
21	2	1203	CLA	C13-C15-C16-C17
21	2	1221	CLA	C13-C15-C16-C17
21	0	1502	CLA	C13-C15-C16-C17
21	0	1503	CLA	C5-C6-C7-C8
21	b	1216	CLA	CBD-CGD-O2D-CED
21	A	1012	CLA	C3-C5-C6-C7
21	1	1121	CLA	C3-C5-C6-C7
21	A	1127	CLA	O1D-CGD-O2D-CED
21	B	1209	CLA	O1D-CGD-O2D-CED
21	a	1011	CLA	O1D-CGD-O2D-CED
21	a	1012	CLA	O1D-CGD-O2D-CED
21	1	1105	CLA	O1D-CGD-O2D-CED
21	1	1122	CLA	O1D-CGD-O2D-CED
25	B	5004	LHG	C23-C24-C25-C26
21	A	1119	CLA	C5-C6-C7-C8
21	A	1121	CLA	C8-C10-C11-C12
21	A	1121	CLA	C15-C16-C17-C18
21	A	1135	CLA	C15-C16-C17-C18
21	B	1210	CLA	C10-C11-C12-C13
21	B	1215	CLA	C8-C10-C11-C12
21	B	1228	CLA	C5-C6-C7-C8
21	b	1203	CLA	C13-C15-C16-C17
21	b	1204	CLA	C13-C15-C16-C17
21	b	1236	CLA	C10-C11-C12-C13
21	b	1240	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	f	1302	CLA	C15-C16-C17-C18
21	1	1106	CLA	C5-C6-C7-C8
21	2	1201	CLA	C10-C11-C12-C13
21	2	1202	CLA	C10-C11-C12-C13
21	0	1503	CLA	C13-C15-C16-C17
21	A	1125	CLA	CBD-CGD-O2D-CED
26	K	5009	LMG	O6-C5-C6-O5
26	a	5004	LMG	O6-C5-C6-O5
21	A	1109	CLA	C13-C15-C16-C17
21	A	1110	CLA	C15-C16-C17-C18
21	A	1124	CLA	C8-C10-C11-C12
21	A	1101	CLA	C8-C10-C11-C12
21	B	1205	CLA	C10-C11-C12-C13
21	F	1302	CLA	C10-C11-C12-C13
21	J	1303	CLA	C13-C15-C16-C17
21	a	1110	CLA	C5-C6-C7-C8
21	a	1111	CLA	C13-C15-C16-C17
21	a	1138	CLA	C13-C15-C16-C17
21	b	1230	CLA	C8-C10-C11-C12
21	1	1122	CLA	C5-C6-C7-C8
21	1	1139	CLA	C13-C15-C16-C17
21	2	1206	CLA	C13-C15-C16-C17
21	2	1208	CLA	C10-C11-C12-C13
21	2	1221	CLA	C10-C11-C12-C13
21	2	1229	CLA	C15-C16-C17-C18
21	0	1501	CLA	C15-C16-C17-C18
22	A	2001	PQN	C18-C20-C21-C22
22	b	2002	PQN	C18-C20-C21-C22
21	b	1232	CLA	O1A-CGA-O2A-C1
21	A	1124	CLA	O1D-CGD-O2D-CED
21	k	1402	CLA	O1D-CGD-O2D-CED
21	1	1112	CLA	CBA-CGA-O2A-C1
21	1	1137	CLA	CBA-CGA-O2A-C1
21	6	1302	CLA	C2A-CAA-CBA-CGA
21	B	1216	CLA	C4-C3-C5-C6
21	a	1101	CLA	C4-C3-C5-C6
21	l	1503	CLA	C4-C3-C5-C6
21	1	1139	CLA	C4-C3-C5-C6
21	2	1208	CLA	C4-C3-C5-C6
21	B	1225	CLA	C2-C3-C5-C6
25	1	5003	LHG	C17-C18-C19-C20
21	A	1128	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1115	CLA	O1D-CGD-O2D-CED
21	A	1120	CLA	C15-C16-C17-C18
21	A	1122	CLA	C10-C11-C12-C13
21	B	1219	CLA	C13-C15-C16-C17
21	b	1210	CLA	C8-C10-C11-C12
21	1	1104	CLA	C10-C11-C12-C13
21	2	1202	CLA	C15-C16-C17-C18
21	2	1215	CLA	C10-C11-C12-C13
21	B	1229	CLA	C3-C5-C6-C7
21	1	1124	CLA	CBD-CGD-O2D-CED
25	1	5001	LHG	C8-C7-O7-C5
31	f	5001	SQD	C8-C7-O47-C45
21	b	1231	CLA	C14-C13-C15-C16
21	A	1113	CLA	O1A-CGA-O2A-C1
21	b	1209	CLA	O1A-CGA-O2A-C1
21	b	1201	CLA	O1A-CGA-O2A-C1
25	a	5005	LHG	O10-C23-O8-C6
25	1	5001	LHG	O9-C7-O7-C5
31	f	5001	SQD	O49-C7-O47-C45
21	b	1211	CLA	C15-C16-C17-C18
21	1	1124	CLA	C5-C6-C7-C8
21	a	1129	CLA	O1D-CGD-O2D-CED
21	1	1136	CLA	O1D-CGD-O2D-CED
21	A	1120	CLA	CBA-CGA-O2A-C1
21	A	1107	CLA	C16-C17-C18-C19
21	A	1117	CLA	C16-C17-C18-C20
21	A	1125	CLA	C16-C17-C18-C20
21	A	1801	CLA	C16-C17-C18-C19
21	2	1224	CLA	C6-C7-C8-C9
21	b	1211	CLA	C5-C6-C7-C8
24	A	4007	BCR	C11-C10-C9-C34
24	A	4019	BCR	C11-C10-C9-C34
24	b	4010	BCR	C11-C10-C9-C34
24	f	4016	BCR	C11-C10-C9-C34
24	1	4019	BCR	C11-C10-C9-C34
24	2	4011	BCR	C11-C10-C9-C34
24	2	4018	BCR	C11-C10-C9-C34
24	6	4016	BCR	C11-C10-C9-C34
25	l	5003	LHG	C7-C8-C9-C10
21	L	1502	CLA	C13-C15-C16-C17
24	A	4003	BCR	C7-C8-C9-C34
24	A	4003	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	4008	BCR	C37-C22-C23-C24
24	A	4019	BCR	C36-C18-C19-C20
24	A	4012	BCR	C37-C22-C23-C24
24	B	4010	BCR	C37-C22-C23-C24
24	B	4014	BCR	C7-C8-C9-C34
24	K	4001	BCR	C11-C12-C13-C35
24	L	4019	BCR	C37-C22-C23-C24
24	a	4003	BCR	C11-C12-C13-C35
24	a	4003	BCR	C37-C22-C23-C24
24	a	4008	BCR	C37-C22-C23-C24
24	a	4012	BCR	C11-C12-C13-C35
24	b	4005	BCR	C37-C22-C23-C24
24	b	4010	BCR	C37-C22-C23-C24
24	j	4013	BCR	C37-C22-C23-C24
24	l	4019	BCR	C37-C22-C23-C24
24	1	4007	BCR	C7-C8-C9-C34
24	1	4008	BCR	C36-C18-C19-C20
24	1	4019	BCR	C37-C22-C23-C24
24	0	4022	BCR	C11-C12-C13-C35
30	b	4011	ECH	C11-C12-C13-C35
30	i	4020	ECH	C7-C8-C9-C34
30	2	4006	ECH	C7-C8-C9-C34
30	2	4006	ECH	C36-C18-C19-C20
36	I	4020	EQ3	C7-C8-C9-C34
26	A	5002	LMG	C32-C33-C34-C35
21	B	1220	CLA	C8-C10-C11-C12
24	A	4003	BCR	C11-C12-C13-C14
24	A	4008	BCR	C21-C22-C23-C24
24	A	4019	BCR	C17-C18-C19-C20
24	B	4010	BCR	C21-C22-C23-C24
24	J	4013	BCR	C7-C8-C9-C10
24	K	4001	BCR	C11-C12-C13-C14
24	L	4019	BCR	C21-C22-C23-C24
24	a	4001	BCR	C21-C22-C23-C24
24	a	4003	BCR	C11-C12-C13-C14
24	a	4003	BCR	C21-C22-C23-C24
24	a	4012	BCR	C11-C12-C13-C14
24	b	4005	BCR	C21-C22-C23-C24
24	b	4010	BCR	C21-C22-C23-C24
24	b	4018	BCR	C21-C22-C23-C24
24	j	4013	BCR	C21-C22-C23-C24
24	l	4019	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1	4003	BCR	C11-C12-C13-C14
24	1	4003	BCR	C21-C22-C23-C24
24	1	4019	BCR	C21-C22-C23-C24
24	2	4004	BCR	C21-C22-C23-C24
24	0	4022	BCR	C11-C12-C13-C14
24	0	4022	BCR	C21-C22-C23-C24
30	b	4011	ECH	C11-C12-C13-C14
30	b	4006	ECH	C21-C22-C23-C24
30	i	4020	ECH	C21-C22-C23-C24
30	2	4006	ECH	C17-C18-C19-C20
21	A	1134	CLA	O1A-CGA-O2A-C1
21	B	1232	CLA	O1A-CGA-O2A-C1
21	j	1302	CLA	O1A-CGA-O2A-C1
25	F	5002	LHG	O10-C23-O8-C6
25	2	5004	LHG	C34-C35-C36-C37
31	f	5001	SQD	C28-C29-C30-C31
21	A	1119	CLA	C2A-CAA-CBA-CGA
21	A	1125	CLA	C2A-CAA-CBA-CGA
21	A	1012	CLA	C2A-CAA-CBA-CGA
21	B	1204	CLA	C2A-CAA-CBA-CGA
21	a	1108	CLA	C2A-CAA-CBA-CGA
21	a	1128	CLA	C2A-CAA-CBA-CGA
21	b	1225	CLA	C2A-CAA-CBA-CGA
21	b	1239	CLA	C2A-CAA-CBA-CGA
21	2	1236	CLA	C2A-CAA-CBA-CGA
21	A	1109	CLA	C15-C16-C17-C18
21	A	1114	CLA	C5-C6-C7-C8
21	J	1302	CLA	C5-C6-C7-C8
25	A	5001	LHG	O1-C1-C2-C3
25	A	5005	LHG	O1-C1-C2-C3
25	B	5004	LHG	O1-C1-C2-C3
25	M	5001	LHG	O1-C1-C2-C3
25	b	5004	LHG	O1-C1-C2-C3
25	l	5004	LHG	O1-C1-C2-C3
25	2	5004	LHG	O1-C1-C2-C3
25	0	5004	LHG	O1-C1-C2-C3
24	a	4002	BCR	C13-C14-C15-C16
24	1	4001	BCR	C13-C14-C15-C16
24	1	4003	BCR	C13-C14-C15-C16
21	A	1102	CLA	C16-C17-C18-C19
21	A	1110	CLA	C16-C17-C18-C20
21	A	1114	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1116	CLA	C16-C17-C18-C19
21	A	1135	CLA	C16-C17-C18-C20
21	A	1139	CLA	C16-C17-C18-C19
21	A	1139	CLA	C16-C17-C18-C20
21	A	1140	CLA	C16-C17-C18-C20
21	B	1203	CLA	C16-C17-C18-C20
21	B	1228	CLA	C16-C17-C18-C20
21	J	1302	CLA	C16-C17-C18-C19
21	J	1303	CLA	C16-C17-C18-C19
21	a	1801	CLA	C6-C7-C8-C10
21	a	1012	CLA	C16-C17-C18-C20
21	b	1216	CLA	C16-C17-C18-C20
21	b	1218	CLA	C16-C17-C18-C20
21	1	1013	CLA	C16-C17-C18-C20
21	1	1122	CLA	C11-C12-C13-C14
21	1	1127	CLA	C16-C17-C18-C20
21	1	1133	CLA	C16-C17-C18-C19
21	1	1140	CLA	C16-C17-C18-C19
21	2	1203	CLA	C16-C17-C18-C20
21	2	1223	CLA	C6-C7-C8-C10
21	2	1226	CLA	C6-C7-C8-C10
21	2	1206	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	O1A-CGA-O2A-C1
21	B	1201	CLA	O1A-CGA-O2A-C1
21	B	1216	CLA	O1A-CGA-O2A-C1
21	a	1109	CLA	O1A-CGA-O2A-C1
21	b	1231	CLA	O1A-CGA-O2A-C1
21	1	1120	CLA	O1A-CGA-O2A-C1
21	1	1136	CLA	O1A-CGA-O2A-C1
21	2	1208	CLA	O1A-CGA-O2A-C1
21	2	1222	CLA	O1A-CGA-O2A-C1
21	A	1133	CLA	C3-C5-C6-C7
21	B	1201	CLA	C3-C5-C6-C7
21	1	1115	CLA	C3-C5-C6-C7
21	2	1229	CLA	C3-C5-C6-C7
26	A	5008	LMG	O6-C5-C6-O5
21	A	1112	CLA	C15-C16-C17-C18
21	B	1238	CLA	C8-C10-C11-C12
21	1	1109	CLA	C5-C6-C7-C8
24	A	4007	BCR	C11-C10-C9-C8
24	A	4019	BCR	C11-C10-C9-C8
24	I	4018	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	4010	BCR	C11-C10-C9-C8
24	f	4016	BCR	C11-C10-C9-C8
24	1	4019	BCR	C11-C10-C9-C8
24	2	4011	BCR	C11-C10-C9-C8
24	6	4016	BCR	C11-C10-C9-C8
31	0	5005	SQD	O5-C1-O6-C44
21	b	1222	CLA	C8-C10-C11-C12
21	B	1212	CLA	C2-C3-C5-C6
35	L	6001	LMT	C1-C2-C3-C4
21	A	1136	CLA	O1D-CGD-O2D-CED
21	B	1237	CLA	O1D-CGD-O2D-CED
21	B	1202	CLA	O1D-CGD-O2D-CED
21	2	1209	CLA	O1D-CGD-O2D-CED
21	A	1123	CLA	O1A-CGA-O2A-C1
21	a	1125	CLA	O1D-CGD-O2D-CED
21	2	1237	CLA	O1D-CGD-O2D-CED
21	b	1210	CLA	CBA-CGA-O2A-C1
21	B	1202	CLA	C13-C15-C16-C17
21	a	1132	CLA	C5-C6-C7-C8
21	2	1226	CLA	CBD-CGD-O2D-CED
25	M	5001	LHG	C23-C24-C25-C26
25	1	5001	LHG	C7-C8-C9-C10
21	A	1013	CLA	C2-C1-O2A-CGA
21	A	1118	CLA	C2-C1-O2A-CGA
21	A	1125	CLA	C2-C1-O2A-CGA
21	B	1023	CLA	C2-C1-O2A-CGA
21	B	1216	CLA	C2-C1-O2A-CGA
21	B	1218	CLA	C2-C1-O2A-CGA
21	B	1220	CLA	C2-C1-O2A-CGA
21	B	1230	CLA	C2-C1-O2A-CGA
21	a	1109	CLA	C2-C1-O2A-CGA
21	a	1122	CLA	C2-C1-O2A-CGA
21	a	1127	CLA	C2-C1-O2A-CGA
21	a	1137	CLA	C2-C1-O2A-CGA
21	a	1101	CLA	C2-C1-O2A-CGA
21	b	1235	CLA	C2-C1-O2A-CGA
21	b	1236	CLA	C2-C1-O2A-CGA
21	k	1401	CLA	C2-C1-O2A-CGA
21	1	1105	CLA	C2-C1-O2A-CGA
21	1	1107	CLA	C2-C1-O2A-CGA
21	2	1236	CLA	C2-C1-O2A-CGA
21	A	1110	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1125	CLA	C16-C17-C18-C19
21	A	1127	CLA	C16-C17-C18-C19
21	B	1203	CLA	C16-C17-C18-C19
21	B	1215	CLA	C16-C17-C18-C19
21	a	1117	CLA	C16-C17-C18-C20
21	a	1140	CLA	C16-C17-C18-C20
21	a	1012	CLA	C16-C17-C18-C19
21	b	1211	CLA	C16-C17-C18-C20
21	b	1212	CLA	C16-C17-C18-C19
21	b	1231	CLA	C16-C17-C18-C20
21	1	1122	CLA	C11-C12-C13-C15
21	2	1237	CLA	C16-C17-C18-C20
21	2	1223	CLA	C6-C7-C8-C9
21	B	1210	CLA	O1A-CGA-O2A-C1
21	b	1212	CLA	C8-C10-C11-C12
21	b	1215	CLA	C8-C10-C11-C12
21	2	1202	CLA	O1D-CGD-O2D-CED
21	2	1238	CLA	O1D-CGD-O2D-CED
21	6	1302	CLA	O1D-CGD-O2D-CED
25	A	5006	LHG	C25-C26-C27-C28
25	B	5006	LHG	C26-C27-C28-C29
25	l	5003	LHG	C32-C33-C34-C35
26	A	5008	LMG	C36-C37-C38-C39
31	0	5005	SQD	C31-C32-C33-C34
21	a	1110	CLA	C10-C11-C12-C13
25	A	5006	LHG	C13-C14-C15-C16
25	F	5002	LHG	C17-C18-C19-C20
25	F	5002	LHG	C29-C30-C31-C32
25	a	5001	LHG	C11-C12-C13-C14
25	a	5003	LHG	C29-C30-C31-C32
25	l	5004	LHG	C25-C26-C27-C28
25	1	5003	LHG	C9-C10-C11-C12
26	A	5008	LMG	C21-C22-C23-C24
26	B	5002	LMG	C22-C23-C24-C25
31	B	5008	SQD	C13-C14-C15-C16
21	A	1117	CLA	O1D-CGD-O2D-CED
31	b	5006	SQD	C7-C8-C9-C10
21	A	1114	CLA	C15-C16-C17-C18
21	1	1115	CLA	C8-C10-C11-C12
25	B	5004	LHG	C34-C35-C36-C37
25	F	5002	LHG	C31-C32-C33-C34
25	L	5005	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	L	5005	LHG	C32-C33-C34-C35
25	l	5003	LHG	C29-C30-C31-C32
25	1	5005	LHG	C28-C29-C30-C31
31	B	5008	SQD	C31-C32-C33-C34
31	f	5001	SQD	C24-C25-C26-C27
21	B	1221	CLA	O1A-CGA-O2A-C1
21	b	1226	CLA	O1A-CGA-O2A-C1
21	1	1133	CLA	O1A-CGA-O2A-C1
21	1	1119	CLA	CBA-CGA-O2A-C1
21	1	1122	CLA	CBA-CGA-O2A-C1
21	2	1230	CLA	CBA-CGA-O2A-C1
25	A	5007	LHG	C30-C31-C32-C33
25	A	5006	LHG	C28-C29-C30-C31
25	B	5004	LHG	C11-C12-C13-C14
25	a	5005	LHG	C24-C25-C26-C27
25	l	5004	LHG	C11-C12-C13-C14
25	l	5002	LHG	C13-C14-C15-C16
25	1	5003	LHG	C13-C14-C15-C16
25	2	5004	LHG	C13-C14-C15-C16
26	A	5002	LMG	C15-C16-C17-C18
26	B	5005	LMG	C21-C22-C23-C24
26	1	5004	LMG	C29-C30-C31-C32
26	0	5001	LMG	C39-C40-C41-C42
25	A	5005	LHG	O1-C1-C2-O2
25	A	5007	LHG	O1-C1-C2-O2
25	A	5006	LHG	O1-C1-C2-O2
25	B	5004	LHG	O1-C1-C2-O2
25	F	5002	LHG	O1-C1-C2-O2
25	M	5001	LHG	O1-C1-C2-O2
25	a	5001	LHG	O1-C1-C2-O2
25	b	5004	LHG	O1-C1-C2-O2
25	l	5003	LHG	O1-C1-C2-O2
25	1	5005	LHG	O1-C1-C2-O2
25	1	5001	LHG	O1-C1-C2-O2
25	1	5003	LHG	O1-C1-C2-O2
25	2	5004	LHG	O1-C1-C2-O2
25	0	5004	LHG	O1-C1-C2-O2
35	0	6001	LMT	C2-C1-O1'-C1'
25	A	5006	LHG	C11-C10-C9-C8
25	B	5006	LHG	C31-C32-C33-C34
25	F	5002	LHG	C34-C35-C36-C37
25	a	5007	LHG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	L	1501	CLA	O1D-CGD-O2D-CED
21	b	1235	CLA	C13-C15-C16-C17
21	a	1115	CLA	C4B-C3B-CAB-CBB
21	1	1116	CLA	C4B-C3B-CAB-CBB
25	a	5001	LHG	C23-C24-C25-C26
25	l	5002	LHG	C23-C24-C25-C26
25	0	5002	LHG	C23-C24-C25-C26
25	B	5006	LHG	C11-C12-C13-C14
25	M	5001	LHG	C24-C25-C26-C27
25	0	5004	LHG	C24-C25-C26-C27
26	A	5002	LMG	C30-C31-C32-C33
31	F	5001	SQD	C11-C12-C13-C14
31	F	5001	SQD	C12-C13-C14-C15
37	L	5004	DGD	C6A-C7A-C8A-C9A
21	A	1102	CLA	C16-C17-C18-C20
21	A	1103	CLA	C16-C17-C18-C19
21	A	1107	CLA	C16-C17-C18-C20
21	A	1114	CLA	C16-C17-C18-C19
21	A	1116	CLA	C16-C17-C18-C20
21	A	1120	CLA	C16-C17-C18-C19
21	A	1127	CLA	C16-C17-C18-C20
21	A	1135	CLA	C16-C17-C18-C19
21	A	1140	CLA	C16-C17-C18-C19
21	B	1208	CLA	C16-C17-C18-C19
21	B	1209	CLA	C16-C17-C18-C19
21	B	1228	CLA	C16-C17-C18-C19
21	J	1303	CLA	C16-C17-C18-C20
21	a	1117	CLA	C16-C17-C18-C19
21	a	1140	CLA	C16-C17-C18-C19
21	a	1801	CLA	C6-C7-C8-C9
21	b	1212	CLA	C16-C17-C18-C20
21	b	1216	CLA	C16-C17-C18-C19
21	b	1218	CLA	C16-C17-C18-C19
21	1	1011	CLA	C16-C17-C18-C19
21	1	1011	CLA	C16-C17-C18-C20
21	1	1013	CLA	C16-C17-C18-C19
21	1	1121	CLA	C6-C7-C8-C10
21	1	1127	CLA	C16-C17-C18-C19
21	1	1140	CLA	C16-C17-C18-C20
21	2	1202	CLA	C16-C17-C18-C19
21	2	1226	CLA	C6-C7-C8-C9
21	a	1130	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	l	1502	CLA	O1D-CGD-O2D-CED
21	a	1118	CLA	O1A-CGA-O2A-C1
21	a	1135	CLA	O1A-CGA-O2A-C1
21	a	1138	CLA	C2A-CAA-CBA-CGA
21	b	1235	CLA	C2A-CAA-CBA-CGA
21	2	1224	CLA	C2A-CAA-CBA-CGA
25	A	5007	LHG	C13-C14-C15-C16
25	1	5003	LHG	C30-C31-C32-C33
21	B	1204	CLA	C5-C6-C7-C8
21	B	1217	CLA	C8-C10-C11-C12
21	a	1104	CLA	C15-C16-C17-C18
21	a	1106	CLA	C8-C10-C11-C12
21	a	1801	CLA	C5-C6-C7-C8
21	b	1206	CLA	C10-C11-C12-C13
21	b	1211	CLA	C8-C10-C11-C12
21	b	1224	CLA	C10-C11-C12-C13
21	2	1214	CLA	C5-C6-C7-C8
25	A	5001	LHG	C8-C7-O7-C5
26	1	5004	LMG	C11-C10-O7-C8
31	0	5005	SQD	C8-C7-O47-C45
35	F	6001	LMT	O5'-C5'-C6'-O6'
21	A	1102	CLA	C6-C7-C8-C10
21	A	1119	CLA	C12-C13-C15-C16
21	A	1120	CLA	C12-C13-C15-C16
21	B	1206	CLA	C12-C13-C15-C16
21	B	1210	CLA	C12-C13-C15-C16
21	B	1218	CLA	C6-C7-C8-C10
21	F	1301	CLA	C11-C12-C13-C15
21	a	1118	CLA	C12-C13-C15-C16
21	a	1132	CLA	C12-C13-C15-C16
21	b	1023	CLA	C11-C10-C8-C7
21	2	1203	CLA	C11-C10-C8-C7
21	2	1205	CLA	C6-C7-C8-C10
26	0	5001	LMG	C29-C30-C31-C32
25	M	5001	LHG	O2-C2-C3-O3
25	A	5006	LHG	C23-C24-C25-C26
25	2	5004	LHG	C23-C24-C25-C26
21	B	1217	CLA	C5-C6-C7-C8
21	1	1140	CLA	C13-C15-C16-C17
21	2	1205	CLA	C10-C11-C12-C13
25	L	5005	LHG	C11-C12-C13-C14
25	a	5005	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	5005	LHG	C13-C14-C15-C16
25	a	5005	LHG	C17-C18-C19-C20
25	b	5004	LHG	C29-C30-C31-C32
25	l	5001	LHG	C13-C14-C15-C16
31	b	5006	SQD	C28-C29-C30-C31
35	1	6001	LMT	C4-C5-C6-C7
21	a	1102	CLA	O1A-CGA-O2A-C1
21	a	1013	CLA	C3-C5-C6-C7
21	a	1135	CLA	C3-C5-C6-C7
21	a	1101	CLA	C3-C5-C6-C7
21	b	1204	CLA	C3-C5-C6-C7
21	l	1501	CLA	C3-C5-C6-C7
21	A	1104	CLA	C3A-C2A-CAA-CBA
21	A	1107	CLA	C3A-C2A-CAA-CBA
21	A	1121	CLA	C3A-C2A-CAA-CBA
21	A	1125	CLA	C3A-C2A-CAA-CBA
21	A	1134	CLA	C3A-C2A-CAA-CBA
21	A	1135	CLA	C3A-C2A-CAA-CBA
21	B	1210	CLA	C3A-C2A-CAA-CBA
21	B	1213	CLA	C3A-C2A-CAA-CBA
21	B	1234	CLA	C3A-C2A-CAA-CBA
21	L	1503	CLA	C3A-C2A-CAA-CBA
21	a	1104	CLA	C3A-C2A-CAA-CBA
21	a	1107	CLA	C3A-C2A-CAA-CBA
21	a	1108	CLA	C3A-C2A-CAA-CBA
21	a	1113	CLA	C3A-C2A-CAA-CBA
21	a	1121	CLA	C3A-C2A-CAA-CBA
21	a	1122	CLA	C3A-C2A-CAA-CBA
21	a	1134	CLA	C3A-C2A-CAA-CBA
21	a	1135	CLA	C3A-C2A-CAA-CBA
21	b	1022	CLA	C3A-C2A-CAA-CBA
21	b	1210	CLA	C3A-C2A-CAA-CBA
21	b	1213	CLA	C3A-C2A-CAA-CBA
21	b	1228	CLA	C3A-C2A-CAA-CBA
21	b	1234	CLA	C3A-C2A-CAA-CBA
21	1	1011	CLA	C3A-C2A-CAA-CBA
21	1	1104	CLA	C3A-C2A-CAA-CBA
21	1	1107	CLA	C3A-C2A-CAA-CBA
21	1	1108	CLA	C3A-C2A-CAA-CBA
21	1	1135	CLA	C3A-C2A-CAA-CBA
21	2	1219	CLA	C3A-C2A-CAA-CBA
21	B	1207	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1230	CLA	O1D-CGD-O2D-CED
21	b	1209	CLA	O1D-CGD-O2D-CED
25	1	5001	LHG	C28-C29-C30-C31
25	1	5003	LHG	C27-C28-C29-C30
26	b	5007	LMG	C22-C23-C24-C25
26	1	5002	LMG	C14-C15-C16-C17
31	L	5002	SQD	C10-C11-C12-C13
21	B	1021	CLA	C5-C6-C7-C8
21	B	1206	CLA	C13-C15-C16-C17
21	a	1136	CLA	C5-C6-C7-C8
21	b	1222	CLA	C13-C15-C16-C17
21	1	1116	CLA	C13-C15-C16-C17
21	1	1120	CLA	C15-C16-C17-C18
21	1	1012	CLA	C8-C10-C11-C12
21	2	1237	CLA	C13-C15-C16-C17
21	0	1503	CLA	C8-C10-C11-C12
21	A	1133	CLA	O1D-CGD-O2D-CED
21	b	1212	CLA	O1D-CGD-O2D-CED
24	B	4017	BCR	C15-C16-C17-C18
24	a	4012	BCR	C19-C20-C21-C22
24	1	4002	BCR	C19-C20-C21-C22
24	1	4019	BCR	C13-C14-C15-C16
28	h	4020	45D	C25-C29-C31-C33
21	B	1209	CLA	C16-C17-C18-C20
21	a	1132	CLA	C16-C17-C18-C19
21	a	1132	CLA	C16-C17-C18-C20
21	1	1134	CLA	C16-C17-C18-C20
21	2	1237	CLA	C16-C17-C18-C19
21	2	1021	CLA	C16-C17-C18-C19
21	A	1120	CLA	O1A-CGA-O2A-C1
21	A	1137	CLA	O1A-CGA-O2A-C1
21	1	1112	CLA	O1A-CGA-O2A-C1
21	1	1137	CLA	O1A-CGA-O2A-C1
21	2	1216	CLA	O1A-CGA-O2A-C1
25	l	5002	LHG	C11-C12-C13-C14
25	A	5001	LHG	C26-C27-C28-C29
25	A	5007	LHG	C12-C13-C14-C15
25	a	5003	LHG	C13-C14-C15-C16
25	a	5007	LHG	C25-C26-C27-C28
25	l	5001	LHG	C34-C35-C36-C37
25	0	5004	LHG	C11-C12-C13-C14
25	M	5001	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	K	1401	CLA	CBA-CGA-O2A-C1
21	K	1402	CLA	CBA-CGA-O2A-C1
21	b	1222	CLA	CBA-CGA-O2A-C1
25	A	5005	LHG	C16-C17-C18-C19
25	A	5007	LHG	C34-C35-C36-C37
25	A	5006	LHG	C16-C17-C18-C19
25	a	5001	LHG	C13-C14-C15-C16
25	1	5005	LHG	C13-C14-C15-C16
25	1	5007	LHG	C32-C33-C34-C35
25	0	5004	LHG	C26-C27-C28-C29
21	A	1122	CLA	C3-C5-C6-C7
21	b	1228	CLA	C3-C5-C6-C7
25	1	5003	LHG	C7-C8-C9-C10
21	b	1236	CLA	C5-C6-C7-C8
25	M	5001	LHG	C29-C30-C31-C32
25	M	5001	LHG	C30-C31-C32-C33
25	a	5003	LHG	C17-C18-C19-C20
25	a	5005	LHG	C11-C12-C13-C14
25	a	5005	LHG	C18-C19-C20-C21
25	b	5004	LHG	C30-C31-C32-C33
25	l	5001	LHG	C11-C10-C9-C8
26	A	5008	LMG	C14-C15-C16-C17
31	L	5001	SQD	C16-C17-C18-C19
35	L	6001	LMT	C6-C7-C8-C9
37	L	5004	DGD	C3A-C4A-C5A-C6A
21	b	1210	CLA	O1A-CGA-O2A-C1
34	j	4015	ZEX	C21-C26-C27-C28
25	A	5003	LHG	C28-C29-C30-C31
25	0	5002	LHG	C34-C35-C36-C37
31	F	5001	SQD	C14-C15-C16-C17
21	A	1111	CLA	O1D-CGD-O2D-CED
25	l	5001	LHG	C30-C31-C32-C33
21	b	1210	CLA	O1D-CGD-O2D-CED
21	b	1234	CLA	O1D-CGD-O2D-CED
25	A	5003	LHG	C34-C35-C36-C37
25	l	5003	LHG	C28-C29-C30-C31
25	1	5003	LHG	C10-C11-C12-C13
21	B	1215	CLA	C16-C17-C18-C20
21	2	1202	CLA	C16-C17-C18-C20
26	K	5009	LMG	C28-C29-C30-C31
21	A	1116	CLA	C2B-C3B-CAB-CBB
21	F	1302	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1220	CLA	C2B-C3B-CAB-CBB
21	k	1402	CLA	C2B-C3B-CAB-CBB
21	1	1116	CLA	C2B-C3B-CAB-CBB
21	2	1205	CLA	C2B-C3B-CAB-CBB
24	A	4008	BCR	C23-C24-C25-C30
24	A	4012	BCR	C1-C6-C7-C8
24	A	4012	BCR	C23-C24-C25-C26
24	A	4012	BCR	C23-C24-C25-C30
24	B	4010	BCR	C23-C24-C25-C26
24	B	4010	BCR	C23-C24-C25-C30
24	L	4019	BCR	C23-C24-C25-C26
24	L	4019	BCR	C23-C24-C25-C30
24	a	4007	BCR	C23-C24-C25-C26
24	a	4007	BCR	C23-C24-C25-C30
24	k	4001	BCR	C23-C24-C25-C30
24	l	4019	BCR	C23-C24-C25-C30
24	1	4012	BCR	C1-C6-C7-C8
24	1	4012	BCR	C5-C6-C7-C8
24	2	4011	BCR	C23-C24-C25-C26
24	2	4011	BCR	C23-C24-C25-C30
24	0	4019	BCR	C23-C24-C25-C30
24	0	4022	BCR	C1-C6-C7-C8
24	0	4022	BCR	C5-C6-C7-C8
28	B	4011	45D	C03-C07-C19-C23
30	B	4006	ECH	C23-C24-C25-C26
30	M	4021	ECH	C5-C6-C7-C8
30	b	4011	ECH	C23-C24-C25-C26
25	a	5001	LHG	C8-C7-O7-C5
25	0	5002	LHG	C8-C7-O7-C5
21	B	1231	CLA	CBA-CGA-O2A-C1
21	B	1236	CLA	CBA-CGA-O2A-C1
21	b	1228	CLA	CBA-CGA-O2A-C1
21	2	1226	CLA	CBA-CGA-O2A-C1
21	a	1122	CLA	C5-C6-C7-C8
25	0	5004	LHG	C25-C26-C27-C28
26	b	5002	LMG	C21-C22-C23-C24
26	2	5005	LMG	C31-C32-C33-C34
21	a	1110	CLA	C11-C12-C13-C14
21	A	1110	CLA	O1D-CGD-O2D-CED
21	a	1108	CLA	O1D-CGD-O2D-CED
21	1	1129	CLA	O1D-CGD-O2D-CED
25	a	5007	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	l	5001	LHG	C26-C27-C28-C29
25	l	5002	LHG	C26-C27-C28-C29
25	0	5004	LHG	C29-C30-C31-C32
21	B	1237	CLA	C2A-CAA-CBA-CGA
21	L	1503	CLA	C2A-CAA-CBA-CGA
21	a	1106	CLA	C2A-CAA-CBA-CGA
21	a	1135	CLA	C2A-CAA-CBA-CGA
21	a	1136	CLA	C2A-CAA-CBA-CGA
21	1	1013	CLA	C2A-CAA-CBA-CGA
21	1	1136	CLA	C2A-CAA-CBA-CGA
21	1	1138	CLA	C2A-CAA-CBA-CGA
25	0	5004	LHG	C7-C8-C9-C10
21	B	1237	CLA	C5-C6-C7-C8
21	a	1103	CLA	C10-C11-C12-C13
25	A	5003	LHG	C11-C12-C13-C14
25	1	5005	LHG	C12-C13-C14-C15
31	L	5002	SQD	C30-C31-C32-C33
21	B	1231	CLA	O1A-CGA-O2A-C1
21	1	1119	CLA	O1A-CGA-O2A-C1
21	1	1122	CLA	O1A-CGA-O2A-C1
21	2	1230	CLA	O1A-CGA-O2A-C1
26	A	5004	LMG	O6-C5-C6-O5
26	B	5005	LMG	C15-C16-C17-C18
26	1	5004	LMG	O9-C10-O7-C8
31	0	5005	SQD	O49-C7-O47-C45
21	A	1139	CLA	C4-C3-C5-C6
21	1	1117	CLA	O1D-CGD-O2D-CED
25	a	5001	LHG	C12-C13-C14-C15
25	l	5003	LHG	C13-C14-C15-C16
26	A	5008	LMG	C13-C14-C15-C16
26	1	5004	LMG	C21-C22-C23-C24
24	B	4005	BCR	C10-C11-C12-C13
24	K	4001	BCR	C10-C11-C12-C13
24	a	4003	BCR	C10-C11-C12-C13
24	b	4017	BCR	C10-C11-C12-C13
24	b	4018	BCR	C10-C11-C12-C13
24	1	4003	BCR	C10-C11-C12-C13
24	1	4008	BCR	C10-C11-C12-C13
24	2	4017	BCR	C10-C11-C12-C13
24	7	4013	BCR	C10-C11-C12-C13
21	A	1119	CLA	C13-C15-C16-C17
21	a	1118	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1135	CLA	C5-C6-C7-C8
21	b	1209	CLA	C13-C15-C16-C17
21	1	1134	CLA	C10-C11-C12-C13
21	2	1204	CLA	C5-C6-C7-C8
21	A	1139	CLA	C2-C3-C5-C6
21	a	1101	CLA	C2-C3-C5-C6
21	f	1302	CLA	C2-C3-C5-C6
21	l	1503	CLA	C2-C3-C5-C6
21	1	1139	CLA	C2-C3-C5-C6
21	2	1208	CLA	C2-C3-C5-C6
21	B	1204	CLA	C16-C17-C18-C20
21	J	1302	CLA	C16-C17-C18-C20
21	1	1121	CLA	C6-C7-C8-C9
25	M	5001	LHG	C25-C26-C27-C28
25	l	5003	LHG	C11-C10-C9-C8
25	1	5005	LHG	C11-C12-C13-C14
25	1	5003	LHG	C16-C17-C18-C19
26	a	5004	LMG	C21-C22-C23-C24
26	2	5005	LMG	C13-C14-C15-C16
26	0	5001	LMG	C22-C23-C24-C25
31	F	5001	SQD	C10-C11-C12-C13
35	F	6001	LMT	C2-C3-C4-C5
21	A	1011	CLA	CBA-CGA-O2A-C1
21	A	1106	CLA	CBA-CGA-O2A-C1
21	A	1116	CLA	CBA-CGA-O2A-C1
21	F	1301	CLA	CBA-CGA-O2A-C1
21	F	1302	CLA	CBA-CGA-O2A-C1
21	a	1119	CLA	CBA-CGA-O2A-C1
21	a	1133	CLA	CBA-CGA-O2A-C1
21	b	1236	CLA	CBA-CGA-O2A-C1
21	b	1230	CLA	CBA-CGA-O2A-C1
21	2	1021	CLA	CBA-CGA-O2A-C1
21	A	1126	CLA	C6-C7-C8-C9
21	B	1230	CLA	C11-C10-C8-C9
21	K	1402	CLA	C11-C10-C8-C9
21	L	1503	CLA	C11-C10-C8-C9
21	1	1118	CLA	C11-C10-C8-C9
21	1	1134	CLA	C14-C13-C15-C16
25	A	5006	LHG	C9-C10-C11-C12
25	M	5001	LHG	C11-C10-C9-C8
25	1	5007	LHG	C16-C17-C18-C19
31	L	5001	SQD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1122	CLA	C8-C10-C11-C12
21	A	1136	CLA	C8-C10-C11-C12
21	B	1231	CLA	C10-C11-C12-C13
21	a	1103	CLA	C15-C16-C17-C18
25	A	5003	LHG	C13-C14-C15-C16
25	b	5004	LHG	C11-C12-C13-C14
25	l	5001	LHG	C11-C12-C13-C14
31	b	5006	SQD	C12-C13-C14-C15
25	0	5002	LHG	C13-C14-C15-C16
25	0	5002	LHG	C28-C29-C30-C31
26	B	5005	LMG	C39-C40-C41-C42
31	L	5002	SQD	C34-C35-C36-C37
26	b	5005	LMG	C2-C1-O1-C7
21	B	1205	CLA	C13-C15-C16-C17
21	b	1212	CLA	C15-C16-C17-C18
21	1	1128	CLA	C5-C6-C7-C8
21	2	1238	CLA	C13-C15-C16-C17
25	L	5005	LHG	C34-C35-C36-C37
25	l	5004	LHG	C13-C14-C15-C16
25	M	5001	LHG	C31-C32-C33-C34
25	a	5001	LHG	C28-C29-C30-C31
31	b	5006	SQD	C16-C17-C18-C19
21	A	1102	CLA	C3-C5-C6-C7
21	A	1135	CLA	C3-C5-C6-C7
21	B	1203	CLA	CBA-CGA-O2A-C1
24	B	4005	BCR	C15-C16-C17-C18
24	K	4001	BCR	C13-C14-C15-C16
24	b	4017	BCR	C15-C16-C17-C18
24	b	4018	BCR	C19-C20-C21-C22
24	7	4013	BCR	C19-C20-C21-C22
25	B	5006	LHG	C35-C36-C37-C38
21	B	1229	CLA	C16-C17-C18-C19
21	2	1224	CLA	C6-C7-C8-C10
25	L	5005	LHG	C8-C7-O7-C5
25	a	5003	LHG	C8-C7-O7-C5
25	0	5004	LHG	C8-C7-O7-C5
26	A	5004	LMG	C11-C10-O7-C8
31	B	5008	SQD	C8-C7-O47-C45
31	F	5001	SQD	C8-C7-O47-C45
25	l	5003	LHG	C34-C35-C36-C37
21	a	1104	CLA	C8-C10-C11-C12
21	a	1106	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1205	CLA	C5-C6-C7-C8
25	0	5004	LHG	O9-C7-O7-C5
25	A	5001	LHG	C24-C25-C26-C27
25	a	5003	LHG	C34-C35-C36-C37
25	l	5003	LHG	C10-C11-C12-C13
26	1	5002	LMG	C36-C37-C38-C39
31	B	5008	SQD	C30-C31-C32-C33
25	A	5006	LHG	C35-C36-C37-C38
21	A	1127	CLA	C15-C16-C17-C18
21	B	1209	CLA	C5-C6-C7-C8
21	b	1236	CLA	C15-C16-C17-C18
21	2	1201	CLA	C8-C10-C11-C12
21	2	1225	CLA	C15-C16-C17-C18
21	0	1501	CLA	C10-C11-C12-C13
24	A	4007	BCR	C37-C22-C23-C24
24	B	4004	BCR	C36-C18-C19-C20
34	j	4015	ZEX	C27-C28-C29-C39
25	1	5003	LHG	C25-C26-C27-C28
25	2	5004	LHG	C11-C10-C9-C8
26	K	5009	LMG	C40-C41-C42-C43
25	1	5001	LHG	C23-C24-C25-C26
25	A	5005	LHG	C34-C35-C36-C37
25	0	5004	LHG	C33-C34-C35-C36
24	A	4003	BCR	C17-C18-C19-C20
24	A	4012	BCR	C21-C22-C23-C24
24	b	4005	BCR	C17-C18-C19-C20
34	j	4015	ZEX	C27-C28-C29-C30
31	0	5005	SQD	C45-C44-O6-C1
25	A	5001	LHG	C13-C14-C15-C16
25	A	5003	LHG	C9-C10-C11-C12
25	F	5002	LHG	C13-C14-C15-C16
26	A	5002	LMG	C37-C38-C39-C40
21	B	1236	CLA	C2A-CAA-CBA-CGA
21	B	1204	CLA	C16-C17-C18-C19
21	B	1208	CLA	C16-C17-C18-C20
21	B	1221	CLA	C16-C17-C18-C19
21	b	1211	CLA	C16-C17-C18-C19
21	b	1231	CLA	C16-C17-C18-C19
21	1	1132	CLA	C16-C17-C18-C19
21	1	1132	CLA	C16-C17-C18-C20
21	1	1133	CLA	C16-C17-C18-C20
21	0	1502	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	F	5002	LHG	C11-C12-C13-C14
25	0	5004	LHG	C11-C10-C9-C8
21	B	1229	CLA	C4-C3-C5-C6
25	l	5003	LHG	C11-C12-C13-C14
25	1	5001	LHG	C11-C12-C13-C14
31	L	5001	SQD	C13-C14-C15-C16
31	b	5006	SQD	C26-C27-C28-C29
25	1	5005	LHG	C35-C36-C37-C38
21	A	1139	CLA	C13-C15-C16-C17
21	a	1118	CLA	C10-C11-C12-C13
21	K	1401	CLA	O1A-CGA-O2A-C1
21	b	1222	CLA	O1A-CGA-O2A-C1
21	A	1011	CLA	C3-C5-C6-C7
21	a	1139	CLA	C3-C5-C6-C7
21	b	1216	CLA	C3-C5-C6-C7
21	B	1213	CLA	C5-C6-C7-C8
21	B	1239	CLA	C8-C10-C11-C12
21	J	1303	CLA	C10-C11-C12-C13
21	a	1109	CLA	C15-C16-C17-C18
21	b	1211	CLA	C13-C15-C16-C17
21	1	1103	CLA	C8-C10-C11-C12
21	1	1104	CLA	C5-C6-C7-C8
21	1	1119	CLA	C10-C11-C12-C13
21	1	1119	CLA	C13-C15-C16-C17
25	L	5005	LHG	C27-C28-C29-C30
35	F	6001	LMT	C1-C2-C3-C4
21	b	1021	CLA	O1D-CGD-O2D-CED
25	L	5005	LHG	C7-C8-C9-C10
26	b	5005	LMG	C28-C29-C30-C31
35	l	6001	LMT	O1'-C1-C2-C3
25	A	5001	LHG	O9-C7-O7-C5
25	F	5002	LHG	O6-C4-C5-O7
25	1	5005	LHG	O6-C4-C5-O7
21	1	1127	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	C35-C36-C37-C38
21	A	1137	CLA	C10-C11-C12-C13
21	B	1203	CLA	C5-C6-C7-C8
21	a	1135	CLA	C15-C16-C17-C18
21	a	1101	CLA	C15-C16-C17-C18
21	a	1012	CLA	C5-C6-C7-C8
21	A	1132	CLA	C16-C17-C18-C20
21	B	1214	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1134	CLA	C16-C17-C18-C19
25	A	5005	LHG	C31-C32-C33-C34
21	B	1236	CLA	O1A-CGA-O2A-C1
21	F	1301	CLA	O1A-CGA-O2A-C1
21	K	1402	CLA	O1A-CGA-O2A-C1
21	2	1226	CLA	O1A-CGA-O2A-C1
25	A	5003	LHG	C10-C11-C12-C13
25	0	5002	LHG	C26-C27-C28-C29
26	0	5001	LMG	C21-C22-C23-C24
21	A	1105	CLA	C13-C15-C16-C17
21	a	1103	CLA	C8-C10-C11-C12
21	a	1126	CLA	C5-C6-C7-C8
21	l	1502	CLA	C13-C15-C16-C17
21	1	1119	CLA	C15-C16-C17-C18
21	2	1225	CLA	C8-C10-C11-C12
25	A	5001	LHG	C25-C26-C27-C28
25	L	5005	LHG	C33-C34-C35-C36
25	a	5007	LHG	C11-C12-C13-C14
26	b	5007	LMG	O6-C5-C6-O5
21	b	1221	CLA	CBD-CGD-O2D-CED
25	l	5001	LHG	O7-C5-C6-O8
31	L	5001	SQD	O6-C44-C45-O47
21	A	1129	CLA	O1D-CGD-O2D-CED
21	a	1102	CLA	O1D-CGD-O2D-CED
21	a	1111	CLA	CBA-CGA-O2A-C1
21	A	1011	CLA	O1A-CGA-O2A-C1
21	a	1133	CLA	O1A-CGA-O2A-C1
25	A	5001	LHG	C28-C29-C30-C31
25	0	5002	LHG	C11-C12-C13-C14
31	L	5001	SQD	C14-C15-C16-C17
35	0	6001	LMT	C4-C5-C6-C7
21	B	1231	CLA	C13-C15-C16-C17
21	B	1239	CLA	C10-C11-C12-C13
21	b	1224	CLA	C13-C15-C16-C17
21	1	1133	CLA	C13-C15-C16-C17
26	b	5002	LMG	C10-C11-C12-C13
25	A	5003	LHG	C33-C34-C35-C36
25	a	5003	LHG	C11-C12-C13-C14
25	b	5004	LHG	C9-C10-C11-C12
26	a	5002	LMG	C39-C40-C41-C42
26	b	5007	LMG	C40-C41-C42-C43
25	M	5001	LHG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	l	5002	LHG	C25-C26-C27-C28
25	0	5004	LHG	C28-C29-C30-C31
21	b	1203	CLA	C2-C1-O2A-CGA
21	b	1225	CLA	C2-C1-O2A-CGA
21	1	1110	CLA	C2-C1-O2A-CGA
21	1	1119	CLA	C2-C1-O2A-CGA
21	0	1503	CLA	C2-C1-O2A-CGA
26	B	5002	LMG	O6-C5-C6-O5
26	b	5002	LMG	O6-C5-C6-O5
21	A	1117	CLA	C16-C17-C18-C19
21	b	1021	CLA	C16-C17-C18-C19
21	2	1203	CLA	C16-C17-C18-C19
21	B	1211	CLA	C15-C16-C17-C18
21	l	1501	CLA	C13-C15-C16-C17
25	a	5003	LHG	C10-C11-C12-C13
34	J	4015	ZEX	C25-C26-C27-C28
21	B	1240	CLA	C4-C3-C5-C6
21	a	1132	CLA	C4-C3-C5-C6
21	B	1240	CLA	C2-C3-C5-C6
26	A	5004	LMG	O9-C10-O7-C8
31	F	5001	SQD	O49-C7-O47-C45
21	B	1225	CLA	C15-C16-C17-C18
25	b	5004	LHG	C10-C11-C12-C13
26	B	5005	LMG	C11-C12-C13-C14
37	L	5004	DGD	CCA-CDA-CEA-CFA
21	A	1106	CLA	C2A-CAA-CBA-CGA
21	b	1217	CLA	C2A-CAA-CBA-CGA
21	1	1110	CLA	C2A-CAA-CBA-CGA
21	1	1012	CLA	C2A-CAA-CBA-CGA
21	2	1204	CLA	C2A-CAA-CBA-CGA
21	a	1123	CLA	CBD-CGD-O2D-CED
21	A	1128	CLA	CBA-CGA-O2A-C1
25	A	5007	LHG	C11-C12-C13-C14
25	M	5001	LHG	C13-C14-C15-C16
25	1	5007	LHG	C12-C13-C14-C15
26	2	5002	LMG	C13-C14-C15-C16
25	a	5001	LHG	C9-C10-C11-C12
21	a	1126	CLA	C10-C11-C12-C13
21	b	1214	CLA	C15-C16-C17-C18
21	1	1117	CLA	C5-C6-C7-C8
25	a	5007	LHG	C28-C29-C30-C31
25	A	5005	LHG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	5002	LMG	C32-C33-C34-C35
21	A	1013	CLA	C16-C17-C18-C20
21	2	1206	CLA	C10-C11-C12-C13
25	B	5006	LHG	O1-C1-C2-O2
25	a	5003	LHG	O1-C1-C2-O2
25	a	5007	LHG	O1-C1-C2-O2
25	l	5004	LHG	O1-C1-C2-O2
21	b	1228	CLA	O1A-CGA-O2A-C1
21	b	1230	CLA	O1A-CGA-O2A-C1
21	a	1140	CLA	C3-C5-C6-C7
21	2	1224	CLA	C3-C5-C6-C7
25	A	5003	LHG	C25-C26-C27-C28
25	1	5003	LHG	C11-C12-C13-C14
31	L	5002	SQD	C11-C12-C13-C14
21	A	1104	CLA	C1A-C2A-CAA-CBA
21	A	1105	CLA	C1A-C2A-CAA-CBA
21	A	1111	CLA	C1A-C2A-CAA-CBA
21	A	1116	CLA	C1A-C2A-CAA-CBA
21	A	1120	CLA	C1A-C2A-CAA-CBA
21	A	1125	CLA	C1A-C2A-CAA-CBA
21	A	1135	CLA	C1A-C2A-CAA-CBA
21	A	1137	CLA	C1A-C2A-CAA-CBA
21	A	1801	CLA	C1A-C2A-CAA-CBA
21	B	1202	CLA	C1A-C2A-CAA-CBA
21	B	1220	CLA	C1A-C2A-CAA-CBA
21	B	1236	CLA	C1A-C2A-CAA-CBA
21	a	1104	CLA	C1A-C2A-CAA-CBA
21	a	1106	CLA	C1A-C2A-CAA-CBA
21	a	1107	CLA	C1A-C2A-CAA-CBA
21	a	1111	CLA	C1A-C2A-CAA-CBA
21	a	1113	CLA	C1A-C2A-CAA-CBA
21	a	1116	CLA	C1A-C2A-CAA-CBA
21	a	1129	CLA	C1A-C2A-CAA-CBA
21	a	1135	CLA	C1A-C2A-CAA-CBA
21	a	1130	CLA	C1A-C2A-CAA-CBA
21	b	1202	CLA	C1A-C2A-CAA-CBA
21	b	1212	CLA	C1A-C2A-CAA-CBA
21	b	1217	CLA	C1A-C2A-CAA-CBA
21	b	1219	CLA	C1A-C2A-CAA-CBA
21	b	1220	CLA	C1A-C2A-CAA-CBA
21	b	1224	CLA	C1A-C2A-CAA-CBA
21	b	1234	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1236	CLA	C1A-C2A-CAA-CBA
21	b	1240	CLA	C1A-C2A-CAA-CBA
21	b	1230	CLA	C1A-C2A-CAA-CBA
21	k	1401	CLA	C1A-C2A-CAA-CBA
21	l	1501	CLA	C1A-C2A-CAA-CBA
21	1	1102	CLA	C1A-C2A-CAA-CBA
21	1	1104	CLA	C1A-C2A-CAA-CBA
21	1	1109	CLA	C1A-C2A-CAA-CBA
21	1	1111	CLA	C1A-C2A-CAA-CBA
21	1	1113	CLA	C1A-C2A-CAA-CBA
21	1	1114	CLA	C1A-C2A-CAA-CBA
21	1	1120	CLA	C1A-C2A-CAA-CBA
21	1	1127	CLA	C1A-C2A-CAA-CBA
21	1	1134	CLA	C1A-C2A-CAA-CBA
21	1	1135	CLA	C1A-C2A-CAA-CBA
21	1	1130	CLA	C1A-C2A-CAA-CBA
21	2	1202	CLA	C1A-C2A-CAA-CBA
21	2	1208	CLA	C1A-C2A-CAA-CBA
21	2	1216	CLA	C1A-C2A-CAA-CBA
21	2	1218	CLA	C1A-C2A-CAA-CBA
21	2	1222	CLA	C1A-C2A-CAA-CBA
21	2	1236	CLA	C1A-C2A-CAA-CBA
21	2	1230	CLA	C1A-C2A-CAA-CBA
21	6	1302	CLA	C1A-C2A-CAA-CBA
26	K	5009	LMG	C10-C11-C12-C13
21	A	1140	CLA	C13-C15-C16-C17
21	B	1201	CLA	C15-C16-C17-C18
21	a	1110	CLA	C8-C10-C11-C12
21	b	1204	CLA	C5-C6-C7-C8
21	b	1236	CLA	O1D-CGD-O2D-CED
25	l	5003	LHG	C30-C31-C32-C33
26	K	5009	LMG	C33-C34-C35-C36
21	A	1116	CLA	O1A-CGA-O2A-C1
21	2	1021	CLA	O1A-CGA-O2A-C1
21	j	1302	CLA	C13-C15-C16-C17
21	1	1126	CLA	C15-C16-C17-C18
25	A	5007	LHG	O6-C4-C5-C6
25	F	5002	LHG	O6-C4-C5-C6
25	b	5004	LHG	O6-C4-C5-C6
25	l	5002	LHG	O6-C4-C5-C6
25	1	5001	LHG	O6-C4-C5-C6
25	L	5005	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	0	5002	LHG	O9-C7-O7-C5
31	B	5008	SQD	O49-C7-O47-C45
25	B	5004	LHG	C28-C29-C30-C31
25	L	5005	LHG	C17-C18-C19-C20
31	B	5008	SQD	C12-C13-C14-C15
25	A	5005	LHG	C23-C24-C25-C26
21	A	1107	CLA	C11-C12-C13-C15
21	A	1119	CLA	C11-C12-C13-C15
21	A	1121	CLA	C6-C7-C8-C10
21	A	1122	CLA	C6-C7-C8-C10
21	A	1124	CLA	C11-C10-C8-C7
21	A	1128	CLA	C6-C7-C8-C10
21	A	1129	CLA	C11-C10-C8-C7
21	A	1131	CLA	C6-C7-C8-C10
21	A	1131	CLA	C11-C10-C8-C7
21	A	1131	CLA	C12-C13-C15-C16
21	A	1135	CLA	C11-C10-C8-C7
21	A	1139	CLA	C6-C7-C8-C10
21	A	1139	CLA	C12-C13-C15-C16
21	B	1023	CLA	C11-C12-C13-C15
21	B	1203	CLA	C11-C10-C8-C7
21	B	1215	CLA	C6-C7-C8-C10
21	B	1217	CLA	C12-C13-C15-C16
21	B	1235	CLA	C12-C13-C15-C16
21	B	1239	CLA	C11-C12-C13-C15
21	F	1302	CLA	C11-C12-C13-C15
21	J	1303	CLA	C6-C7-C8-C10
21	J	1303	CLA	C11-C12-C13-C15
21	a	1011	CLA	C12-C13-C15-C16
21	a	1103	CLA	C6-C7-C8-C10
21	a	1103	CLA	C11-C10-C8-C7
21	a	1104	CLA	C11-C12-C13-C15
21	a	1110	CLA	C6-C7-C8-C10
21	a	1112	CLA	C12-C13-C15-C16
21	a	1119	CLA	C12-C13-C15-C16
21	a	1121	CLA	C12-C13-C15-C16
21	a	1122	CLA	C12-C13-C15-C16
21	a	1127	CLA	C6-C7-C8-C10
21	a	1127	CLA	C12-C13-C15-C16
21	a	1131	CLA	C11-C12-C13-C15
21	a	1130	CLA	C11-C12-C13-C15
21	a	1012	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1237	CLA	C6-C7-C8-C10
21	b	1021	CLA	C11-C10-C8-C7
21	b	1207	CLA	C6-C7-C8-C10
21	b	1211	CLA	C6-C7-C8-C10
21	b	1211	CLA	C11-C12-C13-C15
21	b	1212	CLA	C11-C10-C8-C7
21	b	1218	CLA	C12-C13-C15-C16
21	b	1219	CLA	C6-C7-C8-C10
21	b	1224	CLA	C11-C12-C13-C15
21	b	1226	CLA	C11-C10-C8-C7
21	b	1235	CLA	C6-C7-C8-C10
21	b	1240	CLA	C12-C13-C15-C16
21	b	1201	CLA	C11-C10-C8-C7
21	f	1302	CLA	C6-C7-C8-C10
21	j	1302	CLA	C6-C7-C8-C10
21	l	1502	CLA	C12-C13-C15-C16
21	l	1503	CLA	C6-C7-C8-C10
21	1	1013	CLA	C6-C7-C8-C10
21	1	1104	CLA	C12-C13-C15-C16
21	1	1109	CLA	C11-C12-C13-C15
21	1	1111	CLA	C6-C7-C8-C10
21	1	1111	CLA	C11-C10-C8-C7
21	1	1117	CLA	C12-C13-C15-C16
21	1	1123	CLA	C11-C10-C8-C7
21	1	1126	CLA	C6-C7-C8-C10
21	1	1127	CLA	C12-C13-C15-C16
21	1	1133	CLA	C11-C12-C13-C15
21	1	1136	CLA	C11-C12-C13-C15
21	2	1023	CLA	C11-C10-C8-C7
21	2	1210	CLA	C6-C7-C8-C10
21	2	1218	CLA	C11-C10-C8-C7
21	2	1218	CLA	C11-C12-C13-C15
21	2	1229	CLA	C12-C13-C15-C16
21	0	1501	CLA	C12-C13-C15-C16
21	0	1502	CLA	C12-C13-C15-C16
21	0	1503	CLA	C11-C12-C13-C15
22	A	2001	PQN	C21-C22-C23-C25
22	B	2002	PQN	C21-C22-C23-C25
22	a	2001	PQN	C21-C22-C23-C25
22	2	2002	PQN	C17-C18-C20-C21
31	L	5002	SQD	C29-C30-C31-C32
21	A	1135	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1128	CLA	O1A-CGA-O2A-C1
21	B	1203	CLA	O1A-CGA-O2A-C1
21	F	1302	CLA	O1A-CGA-O2A-C1
21	a	1104	CLA	C13-C15-C16-C17
21	1	1134	CLA	C13-C15-C16-C17
21	2	1239	CLA	C10-C11-C12-C13
21	A	1117	CLA	C4-C3-C5-C6
35	1	6001	LMT	C4B-C5B-C6B-O6B
21	A	1117	CLA	C2-C3-C5-C6
21	B	1216	CLA	C2-C3-C5-C6
21	a	1132	CLA	C2-C3-C5-C6
21	1	1123	CLA	C2-C3-C5-C6
26	a	5002	LMG	C11-C12-C13-C14
26	a	5004	LMG	C15-C16-C17-C18
35	F	6001	LMT	C6-C7-C8-C9
21	a	1111	CLA	O1A-CGA-O2A-C1
21	a	1119	CLA	O1A-CGA-O2A-C1
21	b	1236	CLA	O1A-CGA-O2A-C1
25	1	5003	LHG	C24-C25-C26-C27
21	a	1125	CLA	C15-C16-C17-C18
21	1	1101	CLA	C8-C10-C11-C12
25	l	5004	LHG	C8-C7-O7-C5
21	A	1013	CLA	O1D-CGD-O2D-CED
21	A	1110	CLA	C2A-CAA-CBA-CGA
21	A	1116	CLA	C2A-CAA-CBA-CGA
21	A	1138	CLA	C2A-CAA-CBA-CGA
21	B	1022	CLA	C2A-CAA-CBA-CGA
21	2	1228	CLA	C2A-CAA-CBA-CGA
21	A	1119	CLA	C11-C12-C13-C14
21	A	1119	CLA	C14-C13-C15-C16
21	A	1123	CLA	C11-C10-C8-C9
21	A	1124	CLA	C14-C13-C15-C16
21	A	1127	CLA	C14-C13-C15-C16
21	A	1128	CLA	C6-C7-C8-C9
21	A	1131	CLA	C14-C13-C15-C16
21	A	1132	CLA	C14-C13-C15-C16
21	A	1138	CLA	C11-C10-C8-C9
21	A	1139	CLA	C6-C7-C8-C9
21	B	1209	CLA	C11-C12-C13-C14
21	B	1210	CLA	C14-C13-C15-C16
21	B	1216	CLA	C14-C13-C15-C16
21	B	1218	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1231	CLA	C6-C7-C8-C9
21	B	1234	CLA	C11-C12-C13-C14
21	B	1235	CLA	C14-C13-C15-C16
21	B	1240	CLA	C11-C10-C8-C9
21	K	1401	CLA	C6-C7-C8-C9
21	a	1011	CLA	C11-C10-C8-C9
21	a	1119	CLA	C14-C13-C15-C16
21	a	1121	CLA	C11-C12-C13-C14
21	a	1128	CLA	C6-C7-C8-C9
21	a	1135	CLA	C11-C10-C8-C9
21	a	1132	CLA	C14-C13-C15-C16
21	b	1237	CLA	C6-C7-C8-C9
21	b	1023	CLA	C11-C10-C8-C9
21	b	1202	CLA	C11-C12-C13-C14
21	b	1207	CLA	C11-C12-C13-C14
21	b	1221	CLA	C6-C7-C8-C9
21	b	1224	CLA	C11-C12-C13-C14
21	b	1226	CLA	C11-C10-C8-C9
21	b	1235	CLA	C6-C7-C8-C9
21	b	1230	CLA	C11-C10-C8-C9
21	f	1302	CLA	C11-C10-C8-C9
21	j	1302	CLA	C6-C7-C8-C9
21	1	1104	CLA	C14-C13-C15-C16
21	1	1111	CLA	C6-C7-C8-C9
21	1	1126	CLA	C14-C13-C15-C16
21	1	1131	CLA	C6-C7-C8-C9
21	1	1136	CLA	C11-C12-C13-C14
21	1	1012	CLA	C11-C10-C8-C9
21	2	1023	CLA	C11-C10-C8-C9
21	2	1204	CLA	C6-C7-C8-C9
21	2	1218	CLA	C11-C10-C8-C9
21	2	1218	CLA	C11-C12-C13-C14
21	2	1225	CLA	C6-C7-C8-C9
21	2	1225	CLA	C14-C13-C15-C16
21	2	1229	CLA	C14-C13-C15-C16
22	a	2001	PQN	C21-C22-C23-C24
25	l	5003	LHG	C26-C27-C28-C29
25	0	5004	LHG	C13-C14-C15-C16
24	a	4001	BCR	C13-C14-C15-C16
25	a	5001	LHG	C25-C26-C27-C28
25	0	5002	LHG	C31-C32-C33-C34
31	F	5001	SQD	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1108	CLA	O1D-CGD-O2D-CED
21	B	1211	CLA	CBA-CGA-O2A-C1
21	a	1125	CLA	CBA-CGA-O2A-C1
21	0	1503	CLA	CBA-CGA-O2A-C1
21	a	1128	CLA	C15-C16-C17-C18
21	b	1210	CLA	C15-C16-C17-C18
31	f	5001	SQD	C10-C11-C12-C13
25	a	5001	LHG	O9-C7-O7-C5
26	B	5005	LMG	C2-C1-O1-C7
26	K	5009	LMG	C2-C1-O1-C7
25	A	5007	LHG	C4-C5-C6-O8
25	L	5005	LHG	C4-C5-C6-O8
25	b	5004	LHG	C4-C5-C6-O8
25	1	5005	LHG	C4-C5-C6-O8
25	1	5001	LHG	C4-C5-C6-O8
26	1	5002	LMG	C7-C8-C9-O8
31	L	5001	SQD	C44-C45-C46-O48
31	b	5006	SQD	O6-C44-C45-C46
31	0	5005	SQD	O6-C44-C45-C46
25	2	5004	LHG	C11-C12-C13-C14
31	b	5006	SQD	C13-C14-C15-C16
26	a	5002	LMG	O6-C5-C6-O5
21	B	1208	CLA	C8-C10-C11-C12
21	a	1115	CLA	C15-C16-C17-C18
21	b	1232	CLA	C13-C15-C16-C17
25	F	5002	LHG	C26-C27-C28-C29
25	a	5003	LHG	C26-C27-C28-C29
31	B	5008	SQD	C33-C34-C35-C36
31	L	5002	SQD	C31-C32-C33-C34
37	L	5004	DGD	C7B-C8B-C9B-CAB
21	B	1205	CLA	O1D-CGD-O2D-CED
21	K	1401	CLA	O1D-CGD-O2D-CED
21	B	1222	CLA	CBA-CGA-O2A-C1
21	1	1116	CLA	CBA-CGA-O2A-C1
21	1	1129	CLA	CBA-CGA-O2A-C1
21	2	1203	CLA	CBA-CGA-O2A-C1
21	0	1502	CLA	CBA-CGA-O2A-C1
21	A	1120	CLA	C16-C17-C18-C20
21	B	1221	CLA	C16-C17-C18-C20
21	B	1224	CLA	C16-C17-C18-C20
21	b	1221	CLA	C16-C17-C18-C19
25	A	5006	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	5004	LHG	C29-C30-C31-C32
25	F	5002	LHG	C30-C31-C32-C33
31	L	5001	SQD	C15-C16-C17-C18
21	B	1222	CLA	O1D-CGD-O2D-CED
21	a	1109	CLA	C8-C10-C11-C12
21	b	1216	CLA	C8-C10-C11-C12
25	a	5007	LHG	C29-C30-C31-C32
25	1	5007	LHG	C34-C35-C36-C37
21	b	1216	CLA	O1D-CGD-O2D-CED
21	1	1123	CLA	C4-C3-C5-C6
21	B	1210	CLA	C2-C3-C5-C6
21	B	1227	CLA	C2-C3-C5-C6
21	B	1229	CLA	C2-C3-C5-C6
21	b	1214	CLA	C2-C3-C5-C6
21	b	1231	CLA	C2-C3-C5-C6
21	1	1136	CLA	C2-C3-C5-C6
35	1	6001	LMT	C5-C6-C7-C8
21	A	1118	CLA	C13-C15-C16-C17
21	a	1121	CLA	C15-C16-C17-C18
21	a	1133	CLA	C10-C11-C12-C13
21	a	1012	CLA	C13-C15-C16-C17
21	j	1302	CLA	C15-C16-C17-C18
21	1	1103	CLA	C10-C11-C12-C13
22	b	2002	PQN	C20-C21-C22-C23
24	a	4002	BCR	C36-C18-C19-C20
24	1	4007	BCR	C36-C18-C19-C20
25	F	5002	LHG	C19-C20-C21-C22
26	A	5004	LMG	C16-C17-C18-C19
26	2	5002	LMG	C36-C37-C38-C39
21	B	1214	CLA	C16-C17-C18-C19
25	b	5004	LHG	C28-C29-C30-C31
31	L	5001	SQD	C29-C30-C31-C32
31	0	5005	SQD	C24-C25-C26-C27
24	B	4018	BCR	C21-C22-C23-C24
24	L	4019	BCR	C7-C8-C9-C10
30	B	4006	ECH	C21-C22-C23-C24
21	a	1125	CLA	O1A-CGA-O2A-C1
21	A	1127	CLA	C5-C6-C7-C8
21	a	1111	CLA	C8-C10-C11-C12
21	a	1121	CLA	C13-C15-C16-C17
21	a	1130	CLA	C8-C10-C11-C12
21	2	1203	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1221	CLA	C5-C6-C7-C8
25	L	5005	LHG	C28-C29-C30-C31
25	l	5002	LHG	C34-C35-C36-C37
26	b	5002	LMG	C32-C33-C34-C35
21	B	1215	CLA	C15-C16-C17-C18
21	B	1230	CLA	C8-C10-C11-C12
31	B	5008	SQD	C14-C15-C16-C17
25	1	5005	LHG	C31-C32-C33-C34
21	B	1240	CLA	CBA-CGA-O2A-C1
21	1	1118	CLA	CBA-CGA-O2A-C1
25	a	5007	LHG	C19-C20-C21-C22
25	F	5002	LHG	C6-C5-O7-C7
26	a	5004	LMG	C7-C8-O7-C10
25	B	5006	LHG	C17-C18-C19-C20
25	l	5002	LHG	C28-C29-C30-C31
24	1	4002	BCR	C10-C11-C12-C13
24	0	4019	BCR	C10-C11-C12-C13
21	A	1109	CLA	C8-C10-C11-C12
21	l	1501	CLA	C10-C11-C12-C13
25	B	5006	LHG	C13-C14-C15-C16
25	M	5001	LHG	C27-C28-C29-C30
25	a	5003	LHG	C33-C34-C35-C36
25	1	5003	LHG	C28-C29-C30-C31
25	2	5004	LHG	C30-C31-C32-C33
25	0	5002	LHG	C33-C34-C35-C36
35	0	6001	LMT	C7-C8-C9-C10
24	A	4003	BCR	C15-C16-C17-C18
24	b	4005	BCR	C13-C14-C15-C16
24	j	4013	BCR	C19-C20-C21-C22
24	1	4002	BCR	C15-C16-C17-C18
24	1	4012	BCR	C13-C14-C15-C16
24	h	4018	BCR	C19-C20-C21-C22
28	B	4011	45D	C25-C29-C31-C33
34	j	4015	ZEX	C29-C30-C31-C32
21	A	1013	CLA	C16-C17-C18-C19
21	b	1203	CLA	C16-C17-C18-C20
21	1	1111	CLA	C16-C17-C18-C20
25	A	5005	LHG	C28-C29-C30-C31
25	a	5003	LHG	C31-C32-C33-C34
31	f	5001	SQD	C32-C33-C34-C35
25	M	5001	LHG	C34-C35-C36-C37
31	0	5005	SQD	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	5001	LHG	O6-C4-C5-O7
21	B	1209	CLA	C10-C11-C12-C13
21	B	1226	CLA	C5-C6-C7-C8
21	b	1218	CLA	C8-C10-C11-C12
25	a	5003	LHG	C9-C10-C11-C12
21	a	1127	CLA	CBA-CGA-O2A-C1
26	B	5005	LMG	C14-C15-C16-C17
25	A	5005	LHG	C17-C18-C19-C20
21	b	1223	CLA	C4-C3-C5-C6
25	L	5005	LHG	C12-C13-C14-C15
25	l	5001	LHG	C28-C29-C30-C31
21	B	1224	CLA	C16-C17-C18-C19
21	a	1115	CLA	C16-C17-C18-C19
21	a	1127	CLA	C16-C17-C18-C20
25	B	5006	LHG	C9-C10-C11-C12
25	B	5006	LHG	C27-C28-C29-C30
25	M	5001	LHG	C12-C13-C14-C15
25	b	5004	LHG	C25-C26-C27-C28
31	L	5002	SQD	C32-C33-C34-C35
21	2	1214	CLA	C11-C12-C13-C14
21	a	1122	CLA	C8-C10-C11-C12
25	1	5005	LHG	C33-C34-C35-C36
25	a	5001	LHG	O7-C5-C6-O8
25	a	5001	LHG	C35-C36-C37-C38
25	a	5003	LHG	C11-C10-C9-C8
31	L	5002	SQD	C24-C25-C26-C27
21	A	1013	CLA	CBA-CGA-O2A-C1
21	1	1140	CLA	CBA-CGA-O2A-C1
25	1	5007	LHG	C33-C34-C35-C36
25	2	5004	LHG	C26-C27-C28-C29
21	1	1131	CLA	C8-C10-C11-C12
21	A	1106	CLA	O1D-CGD-O2D-CED
21	1	1133	CLA	O1D-CGD-O2D-CED
21	2	1223	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	C33-C34-C35-C36
31	L	5002	SQD	C25-C26-C27-C28
21	2	1023	CLA	C2A-CAA-CBA-CGA
21	a	1111	CLA	C3-C5-C6-C7
21	b	1220	CLA	C3-C5-C6-C7
21	2	1208	CLA	C3-C5-C6-C7
21	1	1116	CLA	C5-C6-C7-C8
25	1	5005	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1103	CLA	C16-C17-C18-C19
21	A	1106	CLA	O1A-CGA-O2A-C1
21	0	1503	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	O1D-CGD-O2D-CED
21	A	1117	CLA	CBA-CGA-O2A-C1
21	B	1226	CLA	CBA-CGA-O2A-C1
21	2	1217	CLA	CBA-CGA-O2A-C1
25	1	5007	LHG	C24-C23-O8-C6
21	a	1131	CLA	CBD-CGD-O2D-CED
25	a	5003	LHG	C19-C20-C21-C22
21	A	1013	CLA	C8-C10-C11-C12
21	2	1203	CLA	C8-C10-C11-C12
25	A	5007	LHG	C28-C29-C30-C31
21	1	1013	CLA	O1D-CGD-O2D-CED
21	A	1113	CLA	C10-C11-C12-C13
21	A	1125	CLA	C10-C11-C12-C13
21	B	1231	CLA	C15-C16-C17-C18
21	B	1230	CLA	C5-C6-C7-C8
21	F	1301	CLA	C10-C11-C12-C13
21	a	1121	CLA	C5-C6-C7-C8
21	A	1112	CLA	C16-C17-C18-C20
21	j	1303	CLA	C6-C7-C8-C10
21	0	1503	CLA	C16-C17-C18-C20
21	A	1108	CLA	C4-C3-C5-C6
21	B	1210	CLA	C4-C3-C5-C6
21	B	1227	CLA	C4-C3-C5-C6
21	B	1231	CLA	C4-C3-C5-C6
21	b	1202	CLA	C4-C3-C5-C6
21	b	1204	CLA	C4-C3-C5-C6
21	b	1231	CLA	C4-C3-C5-C6
21	1	1119	CLA	C4-C3-C5-C6
21	1	1136	CLA	C4-C3-C5-C6
21	2	1023	CLA	C4-C3-C5-C6
21	B	1222	CLA	O1A-CGA-O2A-C1
25	l	5001	LHG	C9-C10-C11-C12
25	1	5007	LHG	C29-C30-C31-C32
21	A	1140	CLA	CBA-CGA-O2A-C1
21	a	1801	CLA	CBA-CGA-O2A-C1
21	1	1011	CLA	CBA-CGA-O2A-C1
21	B	1216	CLA	C13-C15-C16-C17
25	M	5001	LHG	C14-C15-C16-C17
25	2	5004	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	5008	LMG	C12-C13-C14-C15
31	L	5002	SQD	C16-C17-C18-C19
25	a	5003	LHG	O9-C7-O7-C5
25	l	5001	LHG	O1-C1-C2-O2
25	l	5002	LHG	O1-C1-C2-O2
35	L	6001	LMT	C2-C1-O1'-C1'
21	A	1013	CLA	C14-C13-C15-C16
21	A	1109	CLA	C11-C12-C13-C14
21	A	1124	CLA	C11-C10-C8-C9
21	A	1128	CLA	C11-C12-C13-C14
21	A	1135	CLA	C11-C10-C8-C9
21	A	1139	CLA	C14-C13-C15-C16
21	B	1208	CLA	C11-C10-C8-C9
21	B	1224	CLA	C11-C12-C13-C14
21	B	1226	CLA	C11-C10-C8-C9
21	B	1229	CLA	C6-C7-C8-C9
21	B	1231	CLA	C11-C10-C8-C9
21	B	1235	CLA	C11-C10-C8-C9
21	B	1238	CLA	C11-C10-C8-C9
21	B	1239	CLA	C11-C10-C8-C9
21	B	1230	CLA	C11-C12-C13-C14
21	F	1302	CLA	C14-C13-C15-C16
21	J	1302	CLA	C11-C12-C13-C14
21	J	1303	CLA	C6-C7-C8-C9
21	J	1303	CLA	C11-C12-C13-C14
21	L	1502	CLA	C14-C13-C15-C16
21	a	1103	CLA	C6-C7-C8-C9
21	a	1103	CLA	C11-C10-C8-C9
21	a	1103	CLA	C11-C12-C13-C14
21	a	1104	CLA	C11-C12-C13-C14
21	a	1108	CLA	C6-C7-C8-C9
21	a	1112	CLA	C14-C13-C15-C16
21	a	1121	CLA	C14-C13-C15-C16
21	a	1126	CLA	C11-C10-C8-C9
21	a	1131	CLA	C11-C12-C13-C14
21	b	1021	CLA	C11-C10-C8-C9
21	b	1021	CLA	C11-C12-C13-C14
21	b	1021	CLA	C14-C13-C15-C16
21	b	1210	CLA	C11-C10-C8-C9
21	b	1211	CLA	C6-C7-C8-C9
21	b	1211	CLA	C11-C10-C8-C9
21	b	1218	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1219	CLA	C6-C7-C8-C9
21	b	1223	CLA	C14-C13-C15-C16
21	b	1235	CLA	C11-C10-C8-C9
21	b	1235	CLA	C11-C12-C13-C14
21	b	1240	CLA	C14-C13-C15-C16
21	b	1201	CLA	C11-C10-C8-C9
21	l	1502	CLA	C14-C13-C15-C16
21	l	1503	CLA	C6-C7-C8-C9
21	1	1013	CLA	C6-C7-C8-C9
21	1	1109	CLA	C11-C12-C13-C14
21	1	1111	CLA	C11-C10-C8-C9
21	1	1117	CLA	C14-C13-C15-C16
21	1	1123	CLA	C11-C10-C8-C9
21	1	1127	CLA	C14-C13-C15-C16
21	1	1131	CLA	C14-C13-C15-C16
21	1	1133	CLA	C11-C12-C13-C14
21	2	1203	CLA	C14-C13-C15-C16
21	2	1229	CLA	C6-C7-C8-C9
21	0	1501	CLA	C14-C13-C15-C16
21	0	1502	CLA	C11-C10-C8-C9
21	0	1503	CLA	C14-C13-C15-C16
22	A	2001	PQN	C21-C22-C23-C24
22	1	2001	PQN	C21-C22-C23-C24
21	A	1129	CLA	C5-C6-C7-C8
21	B	1201	CLA	C13-C15-C16-C17
21	b	1023	CLA	C10-C11-C12-C13
21	b	1209	CLA	C8-C10-C11-C12
21	1	1101	CLA	C13-C15-C16-C17
25	l	5003	LHG	C35-C36-C37-C38
21	A	1115	CLA	C4B-C3B-CAB-CBB
21	B	1224	CLA	C4B-C3B-CAB-CBB
21	a	1125	CLA	C4B-C3B-CAB-CBB
21	b	1204	CLA	C4B-C3B-CAB-CBB
21	1	1108	CLA	C4B-C3B-CAB-CBB
21	1	1112	CLA	C4B-C3B-CAB-CBB
21	1	1122	CLA	C4B-C3B-CAB-CBB
21	1	1133	CLA	C4B-C3B-CAB-CBB
21	2	1237	CLA	C4B-C3B-CAB-CBB
21	2	1212	CLA	C4B-C3B-CAB-CBB
21	2	1217	CLA	C4B-C3B-CAB-CBB
25	l	5004	LHG	C31-C32-C33-C34
25	1	5007	LHG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	1	5003	LHG	C29-C30-C31-C32
31	f	5001	SQD	C34-C35-C36-C37
25	A	5003	LHG	C19-C20-C21-C22
26	a	5002	LMG	C10-C11-C12-C13
21	A	1011	CLA	CAA-CBA-CGA-O2A
25	a	5003	LHG	O8-C23-C24-C25
21	F	1301	CLA	C8-C10-C11-C12
21	1	1111	CLA	C10-C11-C12-C13
21	2	1239	CLA	C13-C15-C16-C17
21	b	1240	CLA	C16-C17-C18-C19
31	f	5001	SQD	C26-C27-C28-C29
25	A	5001	LHG	C34-C35-C36-C37
31	b	5006	SQD	C31-C32-C33-C34
31	f	5001	SQD	C2-C1-O6-C44
31	0	5005	SQD	C2-C1-O6-C44
25	2	5004	LHG	C29-C30-C31-C32
25	0	5004	LHG	C30-C31-C32-C33
21	1	1140	CLA	C3-C5-C6-C7
25	A	5005	LHG	C35-C36-C37-C38
25	1	5001	LHG	C35-C36-C37-C38
25	a	5001	LHG	O6-C4-C5-C6
25	1	5005	LHG	O6-C4-C5-C6
25	2	5004	LHG	O6-C4-C5-C6
25	0	5004	LHG	O6-C4-C5-C6
25	0	5004	LHG	C9-C10-C11-C12
26	A	5008	LMG	C34-C35-C36-C37
25	A	5001	LHG	C19-C20-C21-C22
25	1	5003	LHG	C35-C36-C37-C38
25	0	5004	LHG	C35-C36-C37-C38
21	A	1102	CLA	C11-C10-C8-C7
21	A	1107	CLA	C12-C13-C15-C16
21	A	1109	CLA	C11-C12-C13-C15
21	A	1112	CLA	C11-C10-C8-C7
21	A	1113	CLA	C12-C13-C15-C16
21	A	1114	CLA	C12-C13-C15-C16
21	A	1123	CLA	C11-C10-C8-C7
21	A	1124	CLA	C11-C12-C13-C15
21	A	1126	CLA	C12-C13-C15-C16
21	A	1127	CLA	C12-C13-C15-C16
21	A	1132	CLA	C12-C13-C15-C16
21	A	1136	CLA	C11-C12-C13-C15
21	A	1138	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1140	CLA	C11-C12-C13-C15
21	A	1101	CLA	C11-C12-C13-C15
21	A	1012	CLA	C11-C10-C8-C7
21	A	1012	CLA	C11-C12-C13-C15
21	B	1208	CLA	C11-C10-C8-C7
21	B	1209	CLA	C11-C10-C8-C7
21	B	1209	CLA	C11-C12-C13-C15
21	B	1213	CLA	C11-C12-C13-C15
21	B	1214	CLA	C6-C7-C8-C10
21	B	1216	CLA	C6-C7-C8-C10
21	B	1216	CLA	C12-C13-C15-C16
21	B	1218	CLA	C11-C10-C8-C7
21	B	1224	CLA	C11-C12-C13-C15
21	B	1226	CLA	C6-C7-C8-C10
21	B	1226	CLA	C11-C10-C8-C7
21	B	1226	CLA	C12-C13-C15-C16
21	B	1229	CLA	C6-C7-C8-C10
21	B	1231	CLA	C6-C7-C8-C10
21	B	1231	CLA	C11-C10-C8-C7
21	B	1235	CLA	C11-C10-C8-C7
21	B	1238	CLA	C11-C10-C8-C7
21	B	1240	CLA	C11-C10-C8-C7
21	B	1207	CLA	C11-C12-C13-C15
21	F	1302	CLA	C12-C13-C15-C16
21	J	1302	CLA	C11-C12-C13-C15
21	K	1401	CLA	C6-C7-C8-C10
21	L	1502	CLA	C12-C13-C15-C16
21	a	1011	CLA	C11-C10-C8-C7
21	a	1103	CLA	C11-C12-C13-C15
21	a	1112	CLA	C11-C10-C8-C7
21	a	1117	CLA	C12-C13-C15-C16
21	a	1119	CLA	C11-C10-C8-C7
21	a	1126	CLA	C11-C10-C8-C7
21	a	1128	CLA	C6-C7-C8-C10
21	a	1135	CLA	C11-C10-C8-C7
21	b	1021	CLA	C12-C13-C15-C16
21	b	1023	CLA	C6-C7-C8-C10
21	b	1202	CLA	C11-C12-C13-C15
21	b	1206	CLA	C6-C7-C8-C10
21	b	1206	CLA	C12-C13-C15-C16
21	b	1207	CLA	C11-C12-C13-C15
21	b	1209	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1214	CLA	C6-C7-C8-C10
21	b	1221	CLA	C6-C7-C8-C10
21	b	1235	CLA	C11-C10-C8-C7
21	b	1235	CLA	C11-C12-C13-C15
21	b	1230	CLA	C11-C10-C8-C7
21	f	1302	CLA	C11-C10-C8-C7
21	l	1501	CLA	C12-C13-C15-C16
21	l	1503	CLA	C12-C13-C15-C16
21	1	1103	CLA	C12-C13-C15-C16
21	1	1109	CLA	C11-C10-C8-C7
21	1	1116	CLA	C6-C7-C8-C10
21	1	1120	CLA	C12-C13-C15-C16
21	1	1126	CLA	C12-C13-C15-C16
21	1	1131	CLA	C12-C13-C15-C16
21	1	1133	CLA	C11-C10-C8-C7
21	1	1012	CLA	C11-C12-C13-C15
21	2	1206	CLA	C12-C13-C15-C16
21	2	1225	CLA	C6-C7-C8-C10
21	2	1225	CLA	C12-C13-C15-C16
21	2	1229	CLA	C6-C7-C8-C10
21	2	1239	CLA	C6-C7-C8-C10
21	0	1502	CLA	C11-C10-C8-C7
22	1	2001	PQN	C21-C22-C23-C25
21	B	1214	CLA	C10-C11-C12-C13
21	B	1219	CLA	C10-C11-C12-C13
21	b	1237	CLA	C13-C15-C16-C17
21	2	1204	CLA	C15-C16-C17-C18
21	2	1225	CLA	C13-C15-C16-C17
21	2	1229	CLA	C8-C10-C11-C12
21	2	1238	CLA	C8-C10-C11-C12
21	0	1502	CLA	O1A-CGA-O2A-C1
31	L	5002	SQD	C15-C16-C17-C18
26	A	5002	LMG	C28-C29-C30-C31
26	1	5002	LMG	C10-C11-C12-C13
25	a	5003	LHG	C28-C29-C30-C31
31	b	5006	SQD	C10-C11-C12-C13
21	A	1118	CLA	CBA-CGA-O2A-C1
21	A	1801	CLA	C16-C17-C18-C20
21	b	1203	CLA	C16-C17-C18-C19
21	b	1228	CLA	C16-C17-C18-C19
26	2	5005	LMG	C42-C43-C44-C45
31	F	5001	SQD	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1105	CLA	C3A-C2A-CAA-CBA
21	A	1106	CLA	C3A-C2A-CAA-CBA
21	A	1140	CLA	C3A-C2A-CAA-CBA
21	A	1801	CLA	C3A-C2A-CAA-CBA
21	B	1202	CLA	C4-C3-C5-C6
21	B	1218	CLA	C3A-C2A-CAA-CBA
21	b	1210	CLA	C4-C3-C5-C6
21	1	1119	CLA	C3A-C2A-CAA-CBA
21	1	1127	CLA	C3A-C2A-CAA-CBA
21	1	1128	CLA	C3A-C2A-CAA-CBA
21	1	1131	CLA	C4-C3-C5-C6
25	B	5006	LHG	C14-C15-C16-C17
21	l	1502	CLA	C2-C3-C5-C6
21	1	1124	CLA	O1D-CGD-O2D-CED
25	F	5002	LHG	C35-C36-C37-C38
25	l	5001	LHG	C33-C34-C35-C36
21	B	1211	CLA	O1A-CGA-O2A-C1
21	B	1240	CLA	O1A-CGA-O2A-C1
21	1	1116	CLA	O1A-CGA-O2A-C1
21	1	1129	CLA	O1A-CGA-O2A-C1
21	2	1203	CLA	O1A-CGA-O2A-C1
21	B	1220	CLA	C5-C6-C7-C8
21	1	1130	CLA	C5-C6-C7-C8
21	2	1237	CLA	C5-C6-C7-C8
25	B	5006	LHG	C29-C30-C31-C32
26	K	5009	LMG	C32-C33-C34-C35
26	a	5002	LMG	C37-C38-C39-C40
24	B	4010	BCR	C19-C20-C21-C22
24	2	4005	BCR	C13-C14-C15-C16
24	2	4017	BCR	C19-C20-C21-C22
24	h	4018	BCR	C9-C10-C11-C12
21	0	1502	CLA	C3-C5-C6-C7
21	2	1210	CLA	C2C-C3C-CAC-CBC
25	a	5007	LHG	C26-C27-C28-C29
21	1	1118	CLA	O1A-CGA-O2A-C1
21	2	1226	CLA	O1D-CGD-O2D-CED
21	2	1234	CLA	O1D-CGD-O2D-CED
26	1	5002	LMG	C15-C16-C17-C18
21	A	1140	CLA	C15-C16-C17-C18
24	B	4004	BCR	C7-C8-C9-C10
25	B	5004	LHG	C9-C10-C11-C12
25	1	5007	LHG	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	5006	SQD	C14-C15-C16-C17
25	0	5004	LHG	C1-C2-C3-O3
21	B	1228	CLA	C2A-CAA-CBA-CGA
21	a	1113	CLA	C2A-CAA-CBA-CGA
21	1	1119	CLA	C2A-CAA-CBA-CGA
26	0	5001	LMG	C24-C25-C26-C27
21	A	1131	CLA	CBA-CGA-O2A-C1
21	1	1127	CLA	CBA-CGA-O2A-C1
21	6	1301	CLA	CBA-CGA-O2A-C1
21	B	1227	CLA	C5-C6-C7-C8
25	A	5005	LHG	C4-C5-C6-O8
25	a	5007	LHG	C4-C5-C6-O8
25	l	5001	LHG	C4-C5-C6-O8
26	0	5001	LMG	C7-C8-C9-O8
31	b	5006	SQD	C44-C45-C46-O48
31	L	5002	SQD	C35-C36-C37-C38
21	A	1104	CLA	C3-C5-C6-C7
21	b	1211	CLA	C3-C5-C6-C7
21	j	1302	CLA	C3-C5-C6-C7
31	F	5001	SQD	C17-C18-C19-C20
31	b	5006	SQD	C9-C10-C11-C12
21	A	1112	CLA	C16-C17-C18-C19
21	B	1229	CLA	C16-C17-C18-C20
21	a	1121	CLA	C16-C17-C18-C20
21	B	1230	CLA	C13-C15-C16-C17
25	F	5002	LHG	C25-C26-C27-C28
34	J	4015	ZEX	C21-C26-C27-C28
34	7	4015	ZEX	C21-C26-C27-C28
21	A	1103	CLA	C10-C11-C12-C13
21	1	1127	CLA	C13-C15-C16-C17
26	b	5002	LMG	C11-C12-C13-C14
21	A	1122	CLA	C4-C3-C5-C6
21	B	1214	CLA	C4-C3-C5-C6
21	J	1303	CLA	C4-C3-C5-C6
21	K	1402	CLA	C4-C3-C5-C6
21	L	1501	CLA	C4-C3-C5-C6
21	l	1502	CLA	C4-C3-C5-C6
26	b	5007	LMG	C21-C22-C23-C24
26	1	5004	LMG	C16-C17-C18-C19
26	0	5001	LMG	C18-C19-C20-C21
21	A	1108	CLA	C2-C3-C5-C6
21	b	1204	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1119	CLA	C2-C3-C5-C6
31	F	5001	SQD	C13-C14-C15-C16
21	A	1125	CLA	O1D-CGD-O2D-CED
21	b	1202	CLA	O1D-CGD-O2D-CED
26	a	5002	LMG	C34-C35-C36-C37
25	1	5007	LHG	C13-C14-C15-C16
25	1	5001	LHG	C25-C26-C27-C28
21	K	1402	CLA	C16-C17-C18-C19
21	a	1115	CLA	C16-C17-C18-C20
21	a	1128	CLA	C16-C17-C18-C20
21	j	1303	CLA	C6-C7-C8-C9
25	A	5007	LHG	O6-C4-C5-O7
25	B	5004	LHG	O6-C4-C5-O7
25	b	5004	LHG	O6-C4-C5-O7
25	l	5001	LHG	O6-C4-C5-O7
21	A	1013	CLA	O1A-CGA-O2A-C1
26	a	5002	LMG	C42-C43-C44-C45
24	A	4002	BCR	C1-C6-C7-C8
24	A	4003	BCR	C1-C6-C7-C8
24	J	4013	BCR	C1-C6-C7-C8
24	K	4001	BCR	C1-C6-C7-C8
24	L	4022	BCR	C1-C6-C7-C8
24	a	4001	BCR	C23-C24-C25-C26
24	a	4008	BCR	C23-C24-C25-C30
24	a	4012	BCR	C1-C6-C7-C8
24	b	4005	BCR	C1-C6-C7-C8
24	1	4002	BCR	C1-C6-C7-C8
24	1	4002	BCR	C23-C24-C25-C30
24	1	4003	BCR	C1-C6-C7-C8
24	1	4007	BCR	C23-C24-C25-C30
24	2	4005	BCR	C1-C6-C7-C8
24	2	4018	BCR	C1-C6-C7-C8
24	h	4018	BCR	C1-C6-C7-C8
30	b	4011	ECH	C23-C24-C25-C30
30	i	4020	ECH	C1-C6-C7-C8
30	m	4021	ECH	C23-C24-C25-C30
25	B	5004	LHG	C30-C31-C32-C33
25	l	5003	LHG	C27-C28-C29-C30
21	A	1107	CLA	CBA-CGA-O2A-C1
21	2	1224	CLA	CBA-CGA-O2A-C1
21	A	1137	CLA	C15-C16-C17-C18
25	1	5005	LHG	C2-C3-O3-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	5003	LHG	C30-C31-C32-C33
25	1	5003	LHG	C33-C34-C35-C36
25	2	5004	LHG	C35-C36-C37-C38
21	B	1221	CLA	C8-C10-C11-C12
21	B	1223	CLA	C13-C15-C16-C17
21	a	1116	CLA	C5-C6-C7-C8
21	a	1126	CLA	C15-C16-C17-C18
26	A	5004	LMG	C14-C15-C16-C17
26	B	5002	LMG	C15-C16-C17-C18
26	1	5002	LMG	C30-C31-C32-C33
31	f	5001	SQD	C25-C26-C27-C28
31	0	5005	SQD	C29-C30-C31-C32
35	0	6001	LMT	C5-C6-C7-C8
37	L	5004	DGD	CFB-CGB-CHB-CIB
31	F	5001	SQD	C9-C10-C11-C12
21	a	1127	CLA	C16-C17-C18-C19
21	b	1232	CLA	C16-C17-C18-C20
21	2	1021	CLA	C16-C17-C18-C20
25	B	5006	LHG	C23-C24-C25-C26
21	A	1107	CLA	C8-C10-C11-C12
21	B	1239	CLA	C15-C16-C17-C18
22	a	2001	PQN	C25-C26-C27-C28
25	A	5001	LHG	O7-C5-C6-O8
25	A	5005	LHG	O7-C5-C6-O8
25	A	5007	LHG	O7-C5-C6-O8
25	l	5003	LHG	O7-C5-C6-O8
26	b	5005	LMG	O7-C8-C9-O8
26	0	5001	LMG	O7-C8-C9-O8
31	b	5006	SQD	O6-C44-C45-O47
21	1	1011	CLA	O1A-CGA-O2A-C1
25	l	5002	LHG	C31-C32-C33-C34
21	a	1012	CLA	C3-C5-C6-C7
21	1	1130	CLA	C3-C5-C6-C7
35	1	6001	LMT	C2-C3-C4-C5
26	b	5007	LMG	C24-C25-C26-C27
21	a	1126	CLA	C4-C3-C5-C6
21	2	1214	CLA	C4-C3-C5-C6
25	A	5005	LHG	C33-C34-C35-C36
24	a	4007	BCR	C10-C11-C12-C13
21	a	1119	CLA	C5-C6-C7-C8
21	a	1132	CLA	C13-C15-C16-C17
21	B	1202	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	K	1402	CLA	C2-C3-C5-C6
21	b	1202	CLA	C2-C3-C5-C6
21	1	1131	CLA	C2-C3-C5-C6
31	L	5002	SQD	C11-C10-C9-C8
21	A	1103	CLA	C16-C17-C18-C20
21	b	1021	CLA	C16-C17-C18-C20
25	F	5002	LHG	C10-C11-C12-C13
25	a	5007	LHG	C11-C10-C9-C8
26	2	5002	LMG	C32-C33-C34-C35
26	0	5001	LMG	C28-C29-C30-C31
25	A	5005	LHG	C24-C23-O8-C6
21	1	1011	CLA	C3-C5-C6-C7
25	a	5005	LHG	C35-C36-C37-C38
21	A	1113	CLA	C14-C13-C15-C16
21	A	1114	CLA	C14-C13-C15-C16
21	A	1115	CLA	C11-C12-C13-C14
21	A	1122	CLA	C6-C7-C8-C9
21	A	1123	CLA	C11-C12-C13-C14
21	B	1206	CLA	C11-C10-C8-C9
21	B	1211	CLA	C11-C10-C8-C9
21	B	1216	CLA	C6-C7-C8-C9
21	B	1228	CLA	C11-C10-C8-C9
21	F	1301	CLA	C11-C10-C8-C9
21	J	1303	CLA	C14-C13-C15-C16
21	a	1127	CLA	C14-C13-C15-C16
21	b	1206	CLA	C6-C7-C8-C9
21	b	1226	CLA	C11-C12-C13-C14
21	b	1236	CLA	C6-C7-C8-C9
21	f	1302	CLA	C11-C12-C13-C14
21	1	1012	CLA	C11-C12-C13-C14
21	2	1225	CLA	C11-C12-C13-C14
21	2	1229	CLA	C11-C10-C8-C9
21	2	1229	CLA	C11-C12-C13-C14
21	0	1502	CLA	C14-C13-C15-C16
25	1	5007	LHG	C10-C11-C12-C13
21	A	1135	CLA	C10-C11-C12-C13
21	a	1127	CLA	O1A-CGA-O2A-C1
31	L	5002	SQD	C27-C28-C29-C30
31	F	5001	SQD	C11-C10-C9-C8
31	F	5001	SQD	C16-C17-C18-C19
21	A	1104	CLA	C16-C17-C18-C19
21	B	1231	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	0	1502	CLA	C16-C17-C18-C20
21	b	1221	CLA	O1D-CGD-O2D-CED
21	b	1212	CLA	C3-C5-C6-C7
37	L	5004	DGD	C2E-C1E-O5D-C6D
21	B	1218	CLA	C15-C16-C17-C18
21	b	1210	CLA	C13-C15-C16-C17
21	b	1229	CLA	C5-C6-C7-C8
25	1	5001	LHG	C26-C27-C28-C29
25	A	5006	LHG	C32-C33-C34-C35
25	b	5004	LHG	C7-C8-C9-C10
25	M	5001	LHG	C19-C20-C21-C22
25	A	5001	LHG	O1-C1-C2-O2
25	L	5005	LHG	O1-C1-C2-O2
21	a	1123	CLA	O1D-CGD-O2D-CED
21	2	1205	CLA	C4-C3-C5-C6
25	2	5004	LHG	C15-C16-C17-C18
24	b	4010	BCR	C19-C20-C21-C22
24	l	4022	BCR	C9-C10-C11-C12
25	0	5004	LHG	O8-C23-C24-C25
31	B	5008	SQD	O47-C7-C8-C9
21	B	1231	CLA	C2-C3-C5-C6
21	A	1012	CLA	C16-C17-C18-C20
21	a	1135	CLA	C16-C17-C18-C19
21	0	1503	CLA	C16-C17-C18-C19
21	A	1102	CLA	C5-C6-C7-C8
21	A	1123	CLA	C13-C15-C16-C17
31	0	5005	SQD	C30-C31-C32-C33
35	0	6001	LMT	C3-C4-C5-C6
21	a	1140	CLA	C5-C6-C7-C8
21	b	1022	CLA	C15-C16-C17-C18
25	l	5004	LHG	C1-C2-C3-O3
25	6	5001	LHG	C1-C2-C3-O3
21	b	1207	CLA	CBA-CGA-O2A-C1
21	B	1216	CLA	C5-C6-C7-C8
21	b	1210	CLA	C5-C6-C7-C8
21	2	1201	CLA	C15-C16-C17-C18
21	b	1229	CLA	C2C-C3C-CAC-CBC
25	A	5001	LHG	O6-C4-C5-C6
25	B	5006	LHG	O6-C4-C5-C6
25	l	5003	LHG	O6-C4-C5-C6
21	A	1132	CLA	C16-C17-C18-C19
21	a	1011	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1127	CLA	O1A-CGA-O2A-C1
21	A	1105	CLA	C5-C6-C7-C8
21	B	1226	CLA	C15-C16-C17-C18
21	b	1230	CLA	C10-C11-C12-C13
21	1	1103	CLA	C13-C15-C16-C17
22	b	2002	PQN	C23-C25-C26-C27
24	B	4018	BCR	C37-C22-C23-C24
30	B	4006	ECH	C37-C22-C23-C24
25	b	5004	LHG	C11-C10-C9-C8
21	A	1103	CLA	C11-C12-C13-C15
21	A	1103	CLA	C12-C13-C15-C16
21	A	1106	CLA	C6-C7-C8-C10
21	A	1106	CLA	C12-C13-C15-C16
21	A	1121	CLA	C12-C13-C15-C16
21	A	1125	CLA	C12-C13-C15-C16
21	A	1126	CLA	C11-C12-C13-C15
21	A	1129	CLA	C6-C7-C8-C10
21	A	1138	CLA	C11-C12-C13-C15
21	B	1206	CLA	C11-C10-C8-C7
21	B	1239	CLA	C6-C7-C8-C10
21	B	1230	CLA	C6-C7-C8-C10
21	B	1230	CLA	C11-C12-C13-C15
21	L	1501	CLA	C11-C12-C13-C15
21	L	1501	CLA	C12-C13-C15-C16
21	a	1104	CLA	C11-C10-C8-C7
21	a	1106	CLA	C12-C13-C15-C16
21	a	1109	CLA	C12-C13-C15-C16
21	a	1110	CLA	C11-C10-C8-C7
21	a	1111	CLA	C11-C12-C13-C15
21	a	1118	CLA	C11-C10-C8-C7
21	a	1122	CLA	C11-C10-C8-C7
21	a	1128	CLA	C11-C12-C13-C15
21	a	1131	CLA	C6-C7-C8-C10
21	b	1206	CLA	C11-C10-C8-C7
21	b	1236	CLA	C6-C7-C8-C10
21	1	1118	CLA	C11-C12-C13-C15
21	1	1120	CLA	C6-C7-C8-C10
21	2	1021	CLA	C6-C7-C8-C10
21	2	1229	CLA	C11-C10-C8-C7
31	b	5006	SQD	C25-C26-C27-C28
25	A	5003	LHG	C35-C36-C37-C38
26	2	5002	LMG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	5004	LHG	C31-C32-C33-C34
21	A	1012	CLA	C10-C11-C12-C13
21	B	1208	CLA	C10-C11-C12-C13
21	1	1109	CLA	C8-C10-C11-C12
21	1	1109	CLA	C15-C16-C17-C18
21	1	1115	CLA	C15-C16-C17-C18
21	1	1121	CLA	C5-C6-C7-C8
25	a	5005	LHG	C19-C20-C21-C22
24	A	4003	BCR	C7-C8-C9-C10
24	B	4004	BCR	C17-C18-C19-C20
24	B	4014	BCR	C7-C8-C9-C10
24	1	4008	BCR	C17-C18-C19-C20
24	6	4016	BCR	C17-C18-C19-C20
28	h	4020	45D	C32-C34-C36-C38
30	2	4006	ECH	C7-C8-C9-C10
25	a	5005	LHG	C16-C17-C18-C19
21	1	1140	CLA	O1A-CGA-O2A-C1
26	A	5008	LMG	C8-C7-O1-C1
26	b	5007	LMG	C8-C7-O1-C1
21	b	1203	CLA	C15-C16-C17-C18
21	1	1120	CLA	C13-C15-C16-C17
21	2	1023	CLA	C10-C11-C12-C13
21	A	1131	CLA	C2A-CAA-CBA-CGA
21	a	1110	CLA	C2A-CAA-CBA-CGA
21	a	1129	CLA	C2A-CAA-CBA-CGA
21	b	1201	CLA	C2A-CAA-CBA-CGA
31	0	5005	SQD	C27-C28-C29-C30
21	B	1230	CLA	C16-C17-C18-C19
21	b	1227	CLA	C16-C17-C18-C20
21	b	1240	CLA	C16-C17-C18-C20
21	1	1111	CLA	C16-C17-C18-C19
26	0	5001	LMG	C11-C10-O7-C8
21	A	1136	CLA	C4-C3-C5-C6
25	a	5001	LHG	O8-C23-C24-C25
21	A	1107	CLA	O1A-CGA-O2A-C1
21	A	1118	CLA	O1A-CGA-O2A-C1
21	A	1140	CLA	O1A-CGA-O2A-C1
21	2	1217	CLA	O1A-CGA-O2A-C1
25	1	5007	LHG	O10-C23-O8-C6
21	L	1501	CLA	C2-C3-C5-C6
21	b	1210	CLA	C2-C3-C5-C6
21	a	1130	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	A	5005	LHG	C10-C11-C12-C13
25	A	5007	LHG	C9-C10-C11-C12
21	A	1111	CLA	C13-C15-C16-C17
21	l	1501	CLA	C8-C10-C11-C12
21	1	1013	CLA	C5-C6-C7-C8
21	A	1117	CLA	O1A-CGA-O2A-C1
21	A	1131	CLA	O1A-CGA-O2A-C1
21	a	1801	CLA	O1A-CGA-O2A-C1
21	6	1301	CLA	O1A-CGA-O2A-C1
21	B	1224	CLA	C15-C16-C17-C18
21	B	1230	CLA	C10-C11-C12-C13
21	b	1219	CLA	C5-C6-C7-C8
25	a	5005	LHG	C10-C11-C12-C13
25	a	5005	LHG	C26-C27-C28-C29
21	a	1121	CLA	C16-C17-C18-C19
21	b	1221	CLA	C16-C17-C18-C20
21	2	1221	CLA	C16-C17-C18-C20
35	0	6001	LMT	C5'-C4'-O1B-C1B
21	B	1226	CLA	O1A-CGA-O2A-C1
21	A	1125	CLA	C13-C15-C16-C17
21	1	1123	CLA	C13-C15-C16-C17
31	b	5006	SQD	C19-C20-C21-C22
21	L	1503	CLA	C13-C15-C16-C17
26	0	5001	LMG	O9-C10-O7-C8
25	A	5006	LHG	O6-C4-C5-O7
25	a	5003	LHG	O6-C4-C5-O7
25	1	5001	LHG	O6-C4-C5-O7
35	L	6001	LMT	C4B-C5B-C6B-O6B
21	a	1134	CLA	O2A-C1-C2-C3
26	B	5002	LMG	C16-C17-C18-C19
31	F	5001	SQD	O5-C1-O6-C44
25	A	5006	LHG	C4-C5-C6-O8
25	a	5001	LHG	C4-C5-C6-O8
25	l	5002	LHG	C4-C5-C6-O8
26	A	5002	LMG	O1-C7-C8-C9
31	B	5008	SQD	O6-C44-C45-C46
21	A	1129	CLA	C10-C11-C12-C13
21	1	1127	CLA	C5-C6-C7-C8
21	A	1133	CLA	C16-C17-C18-C19
21	1	1103	CLA	C16-C17-C18-C20
25	1	5001	LHG	C17-C18-C19-C20
21	2	1224	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1128	CLA	C10-C11-C12-C13
21	b	1240	CLA	C5-C6-C7-C8
21	1	1140	CLA	C15-C16-C17-C18
31	b	5006	SQD	C27-C28-C29-C30
21	b	1229	CLA	C2A-CAA-CBA-CGA
21	1	1125	CLA	C2A-CAA-CBA-CGA
21	1	1801	CLA	C2A-CAA-CBA-CGA
21	A	1136	CLA	C2-C3-C5-C6
21	b	1223	CLA	C2-C3-C5-C6
21	2	1205	CLA	C2-C3-C5-C6
26	K	5009	LMG	C30-C31-C32-C33
25	A	5001	LHG	C17-C18-C19-C20
25	a	5007	LHG	C24-C25-C26-C27
37	L	5004	DGD	C2A-C3A-C4A-C5A
21	A	1132	CLA	C3-C5-C6-C7
21	a	1104	CLA	C3-C5-C6-C7
25	L	5005	LHG	O7-C5-C6-O8
25	1	5005	LHG	O7-C5-C6-O8
26	A	5008	LMG	O7-C8-C9-O8
31	B	5008	SQD	O6-C44-C45-O47
31	b	5006	SQD	O47-C45-C46-O48
31	f	5001	SQD	O47-C45-C46-O48
21	B	1210	CLA	C5-C6-C7-C8
21	A	1103	CLA	C11-C12-C13-C14
21	A	1104	CLA	C11-C12-C13-C14
21	A	1136	CLA	C11-C12-C13-C14
21	A	1138	CLA	C11-C12-C13-C14
21	A	1801	CLA	C6-C7-C8-C9
21	B	1205	CLA	C11-C12-C13-C14
21	B	1211	CLA	C6-C7-C8-C9
21	B	1219	CLA	C11-C12-C13-C14
21	B	1239	CLA	C6-C7-C8-C9
21	L	1501	CLA	C14-C13-C15-C16
21	a	1118	CLA	C11-C10-C8-C9
21	a	1138	CLA	C14-C13-C15-C16
21	b	1208	CLA	C11-C10-C8-C9
21	b	1218	CLA	C6-C7-C8-C9
21	b	1222	CLA	C6-C7-C8-C9
21	1	1120	CLA	C6-C7-C8-C9
21	1	1128	CLA	C11-C12-C13-C14
21	2	1201	CLA	C14-C13-C15-C16
21	a	1138	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	5006	SQD	C18-C19-C20-C21
21	A	1116	CLA	CAA-CBA-CGA-O2A
25	l	5004	LHG	O9-C7-O7-C5
25	1	5007	LHG	C35-C36-C37-C38
25	A	5003	LHG	C31-C32-C33-C34
25	A	5006	LHG	C11-C12-C13-C14
25	L	5005	LHG	C35-C36-C37-C38
25	A	5006	LHG	C24-C25-C26-C27
21	A	1113	CLA	C8-C10-C11-C12
21	A	1115	CLA	C10-C11-C12-C13
21	A	1118	CLA	C8-C10-C11-C12
21	a	1136	CLA	C8-C10-C11-C12
21	2	1221	CLA	C15-C16-C17-C18
25	0	5004	LHG	C16-C17-C18-C19
31	0	5005	SQD	C12-C13-C14-C15
21	A	1116	CLA	C13-C15-C16-C17
21	2	1226	CLA	C5-C6-C7-C8
25	B	5006	LHG	C28-C29-C30-C31
21	2	1224	CLA	CAA-CBA-CGA-O2A
26	a	5004	LMG	O7-C10-C11-C12
21	A	1129	CLA	C2-C1-O2A-CGA
21	a	1102	CLA	C2-C1-O2A-CGA
21	a	1121	CLA	C2-C1-O2A-CGA
21	b	1022	CLA	C2-C1-O2A-CGA
21	2	1225	CLA	C2-C1-O2A-CGA
24	a	4007	BCR	C19-C20-C21-C22
21	A	1104	CLA	C16-C17-C18-C20
21	B	1021	CLA	C16-C17-C18-C20
21	a	1135	CLA	C16-C17-C18-C20
21	b	1205	CLA	C16-C17-C18-C20
21	b	1214	CLA	C16-C17-C18-C20
21	b	1232	CLA	C16-C17-C18-C19
21	1	1125	CLA	C16-C17-C18-C19
22	A	2001	PQN	C26-C27-C28-C30
25	0	5004	LHG	C2-C3-O3-P
25	A	5006	LHG	C17-C18-C19-C20
31	0	5005	SQD	C18-C19-C20-C21
25	l	5004	LHG	C35-C36-C37-C38
21	a	1136	CLA	C4-C3-C5-C6
21	b	1203	CLA	C4-C3-C5-C6
26	K	5009	LMG	C4-C5-C6-O5
21	b	1225	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	2002	PQN	C15-C16-C17-C18
21	1	1116	CLA	C2A-CAA-CBA-CGA
25	B	5006	LHG	C34-C35-C36-C37
21	A	1122	CLA	C11-C12-C13-C14
21	B	1212	CLA	C6-C7-C8-C10
21	a	1122	CLA	C16-C17-C18-C20
21	2	1205	CLA	C16-C17-C18-C20
21	2	1210	CLA	C16-C17-C18-C19
21	b	1206	CLA	C13-C15-C16-C17
35	F	6001	LMT	C11-C10-C9-C8
21	a	1131	CLA	O1D-CGD-O2D-CED
21	b	1225	CLA	O1D-CGD-O2D-CED
21	B	1023	CLA	C2C-C3C-CAC-CBC
31	b	5006	SQD	C4-C5-C6-S
37	L	5004	DGD	C6B-C7B-C8B-C9B
24	2	4018	BCR	C10-C11-C12-C13
21	K	1402	CLA	C16-C17-C18-C20
21	b	1228	CLA	C16-C17-C18-C20
21	A	1013	CLA	C3-C5-C6-C7
21	1	1134	CLA	C3-C5-C6-C7
21	a	1127	CLA	C5-C6-C7-C8
28	h	4020	45D	C20-C24-C26-C28
21	A	1011	CLA	C1A-C2A-CAA-CBA
21	A	1131	CLA	C4B-C3B-CAB-CBB
21	A	1133	CLA	C4B-C3B-CAB-CBB
21	A	1140	CLA	C4B-C3B-CAB-CBB
21	B	1204	CLA	C1A-C2A-CAA-CBA
21	B	1212	CLA	C1A-C2A-CAA-CBA
21	B	1214	CLA	C4B-C3B-CAB-CBB
21	B	1216	CLA	C4B-C3B-CAB-CBB
21	B	1225	CLA	C4B-C3B-CAB-CBB
21	B	1240	CLA	C4B-C3B-CAB-CBB
21	a	1108	CLA	C4B-C3B-CAB-CBB
21	a	1110	CLA	C4B-C3B-CAB-CBB
21	a	1134	CLA	C4B-C3B-CAB-CBB
21	b	1216	CLA	C4B-C3B-CAB-CBB
21	b	1217	CLA	C4B-C3B-CAB-CBB
21	b	1239	CLA	C4B-C3B-CAB-CBB
21	f	1302	CLA	C4B-C3B-CAB-CBB
21	1	1119	CLA	C1A-C2A-CAA-CBA
21	1	1139	CLA	C4B-C3B-CAB-CBB
21	2	1204	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1219	CLA	C4B-C3B-CAB-CBB
21	2	1225	CLA	C4B-C3B-CAB-CBB
21	2	1230	CLA	C4B-C3B-CAB-CBB
21	2	1213	CLA	CBA-CGA-O2A-C1
21	B	1205	CLA	C4-C3-C5-C6
21	B	1219	CLA	C4-C3-C5-C6
21	F	1302	CLA	C13-C15-C16-C17
21	a	1101	CLA	CAA-CBA-CGA-O2A
21	b	1215	CLA	CAA-CBA-CGA-O2A
31	0	5005	SQD	C13-C14-C15-C16
24	A	4007	BCR	C21-C22-C23-C24
24	a	4008	BCR	C21-C22-C23-C24
24	1	4007	BCR	C7-C8-C9-C10
24	a	4001	BCR	C15-C16-C17-C18
24	b	4005	BCR	C15-C16-C17-C18
21	b	1219	CLA	C3-C5-C6-C7
21	a	1140	CLA	C10-C11-C12-C13
25	1	5007	LHG	C26-C27-C28-C29
26	a	5004	LMG	C32-C33-C34-C35
21	b	1226	CLA	C8-C10-C11-C12
25	A	5006	LHG	O6-C4-C5-C6
25	a	5003	LHG	O6-C4-C5-C6
25	l	5001	LHG	O6-C4-C5-C6
31	F	5001	SQD	C33-C34-C35-C36
21	1	1137	CLA	C2-C3-C5-C6
35	1	6001	LMT	C3-C4-C5-C6
21	A	1104	CLA	C11-C12-C13-C15
21	A	1104	CLA	C12-C13-C15-C16
21	A	1107	CLA	C6-C7-C8-C10
21	A	1112	CLA	C11-C12-C13-C15
21	A	1114	CLA	C6-C7-C8-C10
21	A	1116	CLA	C11-C10-C8-C7
21	A	1118	CLA	C11-C12-C13-C15
21	A	1120	CLA	C11-C10-C8-C7
21	A	1134	CLA	C12-C13-C15-C16
21	A	1130	CLA	C11-C10-C8-C7
21	B	1201	CLA	C11-C10-C8-C7
21	B	1208	CLA	C12-C13-C15-C16
21	B	1221	CLA	C11-C12-C13-C15
21	F	1301	CLA	C12-C13-C15-C16
21	K	1401	CLA	C12-C13-C15-C16
21	K	1402	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	L	1502	CLA	C6-C7-C8-C10
21	a	1112	CLA	C11-C12-C13-C15
21	a	1117	CLA	C6-C7-C8-C10
21	a	1135	CLA	C12-C13-C15-C16
21	a	1139	CLA	C12-C13-C15-C16
21	a	1012	CLA	C11-C12-C13-C15
21	b	1213	CLA	C11-C12-C13-C15
21	b	1216	CLA	C6-C7-C8-C10
21	b	1220	CLA	C11-C12-C13-C15
21	b	1231	CLA	C6-C7-C8-C10
21	b	1232	CLA	C11-C12-C13-C15
21	b	1230	CLA	C6-C7-C8-C10
21	l	1501	CLA	C11-C10-C8-C7
21	1	1103	CLA	C6-C7-C8-C10
21	1	1117	CLA	C6-C7-C8-C10
21	1	1128	CLA	C11-C10-C8-C7
21	1	1136	CLA	C6-C7-C8-C10
21	1	1138	CLA	C11-C10-C8-C7
21	1	1139	CLA	C12-C13-C15-C16
21	2	1023	CLA	C6-C7-C8-C10
21	2	1205	CLA	C11-C10-C8-C7
21	2	1214	CLA	C6-C7-C8-C10
21	0	1501	CLA	C11-C12-C13-C15
21	A	1106	CLA	C16-C17-C18-C19
21	1	1120	CLA	C16-C17-C18-C20
22	2	2002	PQN	C26-C27-C28-C30
25	B	5006	LHG	C19-C20-C21-C22
21	b	1207	CLA	O1A-CGA-O2A-C1
21	A	1112	CLA	CBA-CGA-O2A-C1
21	A	1119	CLA	CBA-CGA-O2A-C1
21	1	1139	CLA	CBA-CGA-O2A-C1
31	F	5001	SQD	C26-C27-C28-C29
21	B	1224	CLA	C13-C15-C16-C17
25	1	5005	LHG	C9-C10-C11-C12
21	A	1112	CLA	O1A-CGA-O2A-C1
25	A	5005	LHG	O10-C23-O8-C6
25	1	5007	LHG	C2-C3-O3-P
25	A	5005	LHG	C15-C16-C17-C18
25	a	5001	LHG	C31-C32-C33-C34
26	1	5002	LMG	C32-C33-C34-C35
26	1	5004	LMG	C22-C23-C24-C25
21	B	1219	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1118	CLA	C4-C3-C5-C6
21	f	1302	CLA	C16-C17-C18-C19
21	f	1302	CLA	C16-C17-C18-C20
21	B	1202	CLA	CAA-CBA-CGA-O2A
21	a	1012	CLA	C10-C11-C12-C13
21	1	1013	CLA	C8-C10-C11-C12
25	B	5006	LHG	O6-C4-C5-O7
25	2	5004	LHG	O6-C4-C5-O7
25	0	5004	LHG	O6-C4-C5-O7
21	A	1120	CLA	C2A-CAA-CBA-CGA
21	A	1134	CLA	C2A-CAA-CBA-CGA
21	2	1235	CLA	C2A-CAA-CBA-CGA
21	A	1121	CLA	C14-C13-C15-C16
21	A	1126	CLA	C11-C12-C13-C14
21	B	1213	CLA	C11-C12-C13-C14
21	B	1239	CLA	C11-C12-C13-C14
21	B	1230	CLA	C6-C7-C8-C9
21	L	1501	CLA	C11-C12-C13-C14
21	a	1104	CLA	C11-C10-C8-C9
21	a	1109	CLA	C14-C13-C15-C16
21	a	1122	CLA	C11-C10-C8-C9
21	b	1023	CLA	C6-C7-C8-C9
21	b	1206	CLA	C11-C10-C8-C9
21	l	1503	CLA	C11-C10-C8-C9
21	1	1111	CLA	C11-C12-C13-C14
21	1	1118	CLA	C11-C12-C13-C14
21	1	1120	CLA	C14-C13-C15-C16
21	2	1021	CLA	C6-C7-C8-C9
21	2	1205	CLA	C11-C10-C8-C9
21	2	1239	CLA	C6-C7-C8-C9
21	a	1127	CLA	C13-C15-C16-C17
21	l	1503	CLA	C13-C15-C16-C17
31	B	5008	SQD	C18-C19-C20-C21
24	i	4018	BCR	C19-C20-C21-C22
24	1	4012	BCR	C19-C20-C21-C22
21	A	1137	CLA	C16-C17-C18-C19
21	L	1503	CLA	C5-C6-C7-C8
21	b	1222	CLA	C5-C6-C7-C8
21	2	1207	CLA	C5-C6-C7-C8
26	B	5005	LMG	C30-C31-C32-C33
21	a	1134	CLA	C1-C2-C3-C4
21	k	1402	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1217	CLA	C3-C5-C6-C7
21	A	1138	CLA	O1A-CGA-O2A-C1
21	1	1139	CLA	O1A-CGA-O2A-C1
25	A	5006	LHG	O7-C5-C6-O8
25	a	5007	LHG	O7-C5-C6-O8
25	b	5004	LHG	O7-C5-C6-O8
25	1	5007	LHG	O7-C5-C6-O8
31	L	5001	SQD	O47-C45-C46-O48
31	0	5005	SQD	O6-C44-C45-O47
26	b	5005	LMG	C14-C15-C16-C17
21	A	1112	CLA	C5-C6-C7-C8
21	B	1221	CLA	C10-C11-C12-C13
21	B	1238	CLA	C10-C11-C12-C13
21	a	1112	CLA	C15-C16-C17-C18
21	b	1202	CLA	C8-C10-C11-C12
26	A	5008	LMG	C33-C34-C35-C36
31	B	5008	SQD	C34-C35-C36-C37
31	0	5005	SQD	C19-C20-C21-C22
21	b	1222	CLA	CBD-CGD-O2D-CED
25	a	5003	LHG	C4-C5-C6-O8
26	A	5008	LMG	C7-C8-C9-O8
31	L	5001	SQD	O6-C44-C45-C46
21	2	1207	CLA	C4-C3-C5-C6
25	1	5001	LHG	C9-C10-C11-C12
21	2	1206	CLA	C15-C16-C17-C18
31	F	5001	SQD	O47-C7-C8-C9
21	b	1235	CLA	C3-C5-C6-C7
25	1	5001	LHG	C19-C20-C21-C22
21	A	1111	CLA	CAD-CBD-CGD-O2D
21	A	1125	CLA	CAD-CBD-CGD-O2D
21	B	1211	CLA	CAD-CBD-CGD-O2D
21	B	1220	CLA	CAD-CBD-CGD-O2D
21	a	1801	CLA	CAD-CBD-CGD-O2D
21	b	1202	CLA	CAD-CBD-CGD-O2D
21	b	1210	CLA	CAD-CBD-CGD-O2D
21	b	1211	CLA	CAD-CBD-CGD-O2D
21	b	1220	CLA	CAD-CBD-CGD-O2D
21	b	1226	CLA	CAD-CBD-CGD-O2D
21	l	1501	CLA	CAD-CBD-CGD-O2D
21	1	1113	CLA	CAD-CBD-CGD-O2D
21	1	1123	CLA	CAD-CBD-CGD-O2D
21	1	1125	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1202	CLA	CAD-CBD-CGD-O2D
21	2	1210	CLA	CAD-CBD-CGD-O2D
21	2	1212	CLA	CAD-CBD-CGD-O2D
21	2	1220	CLA	CAD-CBD-CGD-O2D
21	7	1302	CLA	CAD-CBD-CGD-O2D
21	7	1303	CLA	CAD-CBD-CGD-O2D
21	A	1140	CLA	C5-C6-C7-C8
21	a	1011	CLA	C5-C6-C7-C8
25	F	5002	LHG	C11-C10-C9-C8
21	2	1210	CLA	C4C-C3C-CAC-CBC
26	a	5002	LMG	C33-C34-C35-C36
21	A	1137	CLA	C16-C17-C18-C20
21	B	1231	CLA	C16-C17-C18-C20
21	a	1119	CLA	C16-C17-C18-C19
21	a	1128	CLA	C16-C17-C18-C19
25	1	5003	LHG	C31-C32-C33-C34
21	1	1132	CLA	C3-C5-C6-C7
21	a	1119	CLA	C2A-CAA-CBA-CGA
21	a	1126	CLA	C2A-CAA-CBA-CGA
21	b	1023	CLA	C2A-CAA-CBA-CGA
21	2	1239	CLA	C2A-CAA-CBA-CGA
25	1	5005	LHG	C27-C28-C29-C30
21	a	1140	CLA	C15-C16-C17-C18
26	1	5002	LMG	C34-C35-C36-C37
26	1	5004	LMG	C14-C15-C16-C17
21	A	1111	CLA	CAD-CBD-CGD-O1D
21	A	1113	CLA	CAD-CBD-CGD-O1D
21	A	1125	CLA	CAD-CBD-CGD-O1D
21	B	1210	CLA	CAD-CBD-CGD-O1D
21	B	1211	CLA	CAD-CBD-CGD-O1D
21	B	1220	CLA	CAD-CBD-CGD-O1D
21	B	1226	CLA	CAD-CBD-CGD-O1D
21	B	1234	CLA	CAD-CBD-CGD-O1D
21	B	1230	CLA	CHA-CBD-CGD-O1D
21	B	1230	CLA	CHA-CBD-CGD-O2D
21	a	1120	CLA	CHA-CBD-CGD-O1D
21	a	1801	CLA	CAD-CBD-CGD-O1D
21	b	1202	CLA	CAD-CBD-CGD-O1D
21	b	1210	CLA	CAD-CBD-CGD-O1D
21	b	1211	CLA	CAD-CBD-CGD-O1D
21	b	1217	CLA	CAD-CBD-CGD-O1D
21	b	1220	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1226	CLA	CAD-CBD-CGD-O1D
21	l	1501	CLA	CAD-CBD-CGD-O1D
21	1	1103	CLA	CAD-CBD-CGD-O1D
21	1	1113	CLA	CAD-CBD-CGD-O1D
21	1	1123	CLA	CAD-CBD-CGD-O1D
21	1	1125	CLA	CAD-CBD-CGD-O1D
21	2	1202	CLA	CAD-CBD-CGD-O1D
21	2	1210	CLA	CAD-CBD-CGD-O1D
21	2	1212	CLA	CAD-CBD-CGD-O1D
21	2	1216	CLA	CHA-CBD-CGD-O2D
21	2	1220	CLA	CAD-CBD-CGD-O1D
21	7	1302	CLA	CAD-CBD-CGD-O1D
21	7	1303	CLA	CAD-CBD-CGD-O1D
24	A	4007	BCR	C9-C10-C11-C12
24	A	4008	BCR	C19-C20-C21-C22
24	B	4004	BCR	C19-C20-C21-C22
24	J	4013	BCR	C13-C14-C15-C16
24	a	4007	BCR	C15-C16-C17-C18
24	2	4005	BCR	C15-C16-C17-C18
25	A	5001	LHG	C4-O6-P-O5
25	A	5003	LHG	C3-O3-P-O5
25	A	5003	LHG	C4-O6-P-O5
25	A	5007	LHG	C3-O3-P-O4
25	A	5006	LHG	C3-O3-P-O6
25	B	5004	LHG	C3-O3-P-O4
25	B	5006	LHG	C4-O6-P-O5
25	L	5005	LHG	C3-O3-P-O5
25	M	5001	LHG	C3-O3-P-O5
25	a	5003	LHG	C3-O3-P-O5
25	a	5005	LHG	C3-O3-P-O5
25	a	5005	LHG	C4-O6-P-O3
25	a	5007	LHG	C3-O3-P-O5
25	l	5001	LHG	C3-O3-P-O5
25	l	5003	LHG	C3-O3-P-O4
25	l	5002	LHG	C3-O3-P-O5
25	1	5003	LHG	C3-O3-P-O5
25	2	5004	LHG	C3-O3-P-O5
25	2	5004	LHG	C4-O6-P-O3
25	2	5004	LHG	C4-O6-P-O4
25	6	5001	LHG	C3-O3-P-O5
25	0	5004	LHG	C3-O3-P-O5
28	h	4020	45D	C36-C38-C42-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	l	5004	LHG	C11-C10-C9-C8
26	A	5002	LMG	C10-C11-C12-C13
25	2	5004	LHG	C25-C26-C27-C28
26	A	5008	LMG	C15-C16-C17-C18
21	B	1202	CLA	C8-C10-C11-C12
21	a	1109	CLA	C4-C3-C5-C6
21	A	1133	CLA	C2B-C3B-CAB-CBB
21	B	1216	CLA	C2B-C3B-CAB-CBB
21	B	1240	CLA	C2B-C3B-CAB-CBB
21	a	1115	CLA	C2B-C3B-CAB-CBB
21	b	1216	CLA	C2B-C3B-CAB-CBB
21	b	1239	CLA	C2B-C3B-CAB-CBB
21	f	1302	CLA	C2B-C3B-CAB-CBB
21	1	1112	CLA	C2B-C3B-CAB-CBB
21	1	1133	CLA	C2B-C3B-CAB-CBB
21	2	1217	CLA	C2B-C3B-CAB-CBB
21	2	1219	CLA	C2B-C3B-CAB-CBB
24	B	4005	BCR	C1-C6-C7-C8
24	a	4001	BCR	C23-C24-C25-C30
24	a	4003	BCR	C23-C24-C25-C26
24	k	4001	BCR	C23-C24-C25-C26
24	l	4022	BCR	C1-C6-C7-C8
24	1	4019	BCR	C1-C6-C7-C8
36	I	4020	EQ3	C1-C6-C7-C8
21	a	1139	CLA	C10-C11-C12-C13
24	b	4004	BCR	C7-C8-C9-C34
24	1	4007	BCR	C11-C12-C13-C35
25	B	5004	LHG	C5-C4-O6-P
25	F	5002	LHG	C2-C3-O3-P
25	l	5001	LHG	C5-C4-O6-P
30	i	4020	ECH	C36-C18-C19-C20
21	B	1207	CLA	C3-C5-C6-C7
21	1	1102	CLA	C3-C5-C6-C7
31	L	5001	SQD	O49-C7-O47-C45
21	j	1302	CLA	C8-C10-C11-C12
22	A	2001	PQN	C23-C25-C26-C27
26	0	5001	LMG	C34-C35-C36-C37
21	A	1012	CLA	C16-C17-C18-C19
21	b	1227	CLA	C16-C17-C18-C19
21	0	1501	CLA	C16-C17-C18-C20
21	A	1101	CLA	CAA-CBA-CGA-O2A
21	A	1124	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1011	CLA	O1A-CGA-O2A-C1
21	2	1213	CLA	O1A-CGA-O2A-C1
25	b	5004	LHG	C35-C36-C37-C38
25	l	5002	LHG	C24-C25-C26-C27
21	B	1206	CLA	C3-C5-C6-C7
21	B	1212	CLA	C3-C5-C6-C7
21	b	1229	CLA	C3-C5-C6-C7
21	A	1119	CLA	O1A-CGA-O2A-C1
21	1	1117	CLA	C16-C17-C18-C20
21	1	1126	CLA	C16-C17-C18-C20
25	a	5005	LHG	O1-C1-C2-C3
25	A	5001	LHG	C31-C32-C33-C34
21	A	1127	CLA	C13-C15-C16-C17
21	B	1217	CLA	C15-C16-C17-C18
31	L	5001	SQD	C8-C7-O47-C45
26	1	5002	LMG	C9-C8-O7-C10
25	l	5002	LHG	C35-C36-C37-C38
24	A	4019	BCR	C18-C19-C20-C21
24	a	4001	BCR	C18-C19-C20-C21
24	a	4019	BCR	C18-C19-C20-C21
24	k	4001	BCR	C18-C19-C20-C21
24	1	4001	BCR	C18-C19-C20-C21
24	2	4018	BCR	C18-C19-C20-C21
24	9	4021	BCR	C18-C19-C20-C21
30	b	4006	ECH	C18-C19-C20-C21
21	a	1011	CLA	CAA-CBA-CGA-O2A
21	b	1202	CLA	CAA-CBA-CGA-O2A
25	B	5006	LHG	O8-C23-C24-C25
21	b	1208	CLA	C5-C6-C7-C8
21	1	1011	CLA	C5-C6-C7-C8
21	2	1023	CLA	C2-C3-C5-C6
25	A	5001	LHG	C12-C13-C14-C15
25	a	5005	LHG	C25-C26-C27-C28
25	l	5003	LHG	C24-C25-C26-C27
25	l	5004	LHG	C26-C27-C28-C29
24	A	4012	BCR	C19-C20-C21-C22
24	1	4007	BCR	C15-C16-C17-C18
24	9	4021	BCR	C19-C20-C21-C22
34	7	4015	ZEX	C33-C34-C35-C15
21	B	1212	CLA	C6-C7-C8-C9
21	B	1230	CLA	C16-C17-C18-C20
21	a	1138	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1215	CLA	C16-C17-C18-C20
21	2	1210	CLA	C16-C17-C18-C20
25	B	5004	LHG	O6-C4-C5-C6
21	A	1127	CLA	CAA-CBA-CGA-O2A
21	A	1104	CLA	C14-C13-C15-C16
21	A	1105	CLA	C11-C10-C8-C9
21	A	1109	CLA	C6-C7-C8-C9
21	A	1112	CLA	C6-C7-C8-C9
21	A	1112	CLA	C11-C10-C8-C9
21	A	1123	CLA	C14-C13-C15-C16
21	B	1201	CLA	C6-C7-C8-C9
21	B	1205	CLA	C14-C13-C15-C16
21	B	1226	CLA	C6-C7-C8-C9
21	a	1112	CLA	C11-C10-C8-C9
21	a	1126	CLA	C6-C7-C8-C9
21	a	1133	CLA	C11-C12-C13-C14
21	a	1136	CLA	C11-C10-C8-C9
21	b	1209	CLA	C11-C12-C13-C14
21	b	1216	CLA	C6-C7-C8-C9
21	b	1231	CLA	C11-C10-C8-C9
21	b	1231	CLA	C11-C12-C13-C14
21	l	1501	CLA	C14-C13-C15-C16
21	1	1103	CLA	C6-C7-C8-C9
21	1	1103	CLA	C14-C13-C15-C16
21	1	1109	CLA	C11-C10-C8-C9
21	1	1117	CLA	C6-C7-C8-C9
21	1	1123	CLA	C11-C12-C13-C14
21	2	1208	CLA	C6-C7-C8-C9
21	2	1210	CLA	C11-C12-C13-C14
22	B	2002	PQN	C21-C22-C23-C24
31	f	5001	SQD	C11-C10-C9-C8
21	A	1112	CLA	C6-C7-C8-C10
21	A	1127	CLA	C11-C12-C13-C15
21	B	1201	CLA	C6-C7-C8-C10
21	B	1206	CLA	C11-C12-C13-C15
21	B	1211	CLA	C6-C7-C8-C10
21	a	1112	CLA	C6-C7-C8-C10
21	a	1133	CLA	C11-C12-C13-C15
21	b	1203	CLA	C11-C10-C8-C7
21	b	1231	CLA	C11-C10-C8-C7
21	b	1232	CLA	C6-C7-C8-C10
21	1	1122	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1127	CLA	C6-C7-C8-C10
21	2	1206	CLA	C11-C12-C13-C15
25	A	5005	LHG	C7-C8-C9-C10
25	A	5001	LHG	O6-C4-C5-O7
25	l	5003	LHG	O6-C4-C5-O7
25	A	5007	LHG	C33-C34-C35-C36
21	A	1122	CLA	C11-C12-C13-C15
21	a	1011	CLA	C16-C17-C18-C20
25	a	5007	LHG	C34-C35-C36-C37
25	1	5003	LHG	C11-C10-C9-C8
25	1	5007	LHG	C15-C16-C17-C18
21	1	1123	CLA	C15-C16-C17-C18
21	A	1109	CLA	C4-C3-C5-C6
21	a	1105	CLA	C4-C3-C5-C6
21	1	1132	CLA	C4-C3-C5-C6
21	2	1215	CLA	CAA-CBA-CGA-O2A
21	a	1118	CLA	C16-C17-C18-C19
21	b	1214	CLA	C16-C17-C18-C19
21	2	1205	CLA	C16-C17-C18-C19
25	1	5001	LHG	C13-C14-C15-C16
25	0	5004	LHG	C12-C13-C14-C15
21	b	1230	CLA	C13-C15-C16-C17
25	A	5005	LHG	C26-C27-C28-C29
35	1	6001	LMT	C11-C10-C9-C8
25	l	5002	LHG	O7-C5-C6-O8
26	A	5004	LMG	O1-C7-C8-O7
26	1	5002	LMG	O7-C8-C9-O8
21	j	1302	CLA	CAA-CBA-CGA-O2A
21	1	1127	CLA	CAA-CBA-CGA-O2A
21	1	1123	CLA	C5-C6-C7-C8
24	7	4013	BCR	C15-C16-C17-C18
21	b	1205	CLA	C16-C17-C18-C19
21	2	1215	CLA	C11-C12-C13-C15
21	2	1238	CLA	C16-C17-C18-C19
25	B	5004	LHG	C26-C27-C28-C29
21	L	1502	CLA	C2A-CAA-CBA-CGA
21	2	1021	CLA	C13-C15-C16-C17
25	l	5001	LHG	C35-C36-C37-C38
31	L	5001	SQD	C9-C10-C11-C12
21	A	1109	CLA	C2-C1-O2A-CGA
21	B	1219	CLA	C2-C1-O2A-CGA
21	1	1135	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	1021	CLA	C2-C1-O2A-CGA
21	B	1211	CLA	C4-C3-C5-C6
21	B	1224	CLA	C4-C3-C5-C6
21	a	1131	CLA	C4-C3-C5-C6
21	1	1138	CLA	C11-C12-C13-C15
21	a	1126	CLA	C2-C3-C5-C6
26	A	5008	LMG	C4-C5-C6-O5
21	B	1230	CLA	C3-C5-C6-C7
21	1	1118	CLA	CAA-CBA-CGA-O2A
21	2	1021	CLA	C15-C16-C17-C18
25	B	5004	LHG	C35-C36-C37-C38
21	a	1122	CLA	C16-C17-C18-C19
24	a	4002	BCR	C17-C18-C19-C20
36	I	4020	EQ3	C7-C8-C9-C10
21	A	1138	CLA	CBA-CGA-O2A-C1
21	A	1117	CLA	C15-C16-C17-C18
21	1	1132	CLA	C13-C15-C16-C17
21	A	1118	CLA	CAA-CBA-CGA-O2A
26	2	5005	LMG	C29-C30-C31-C32
26	b	5007	LMG	C12-C13-C14-C15
21	2	1217	CLA	C2A-CAA-CBA-CGA
24	B	4018	BCR	C15-C16-C17-C18
24	a	4008	BCR	C19-C20-C21-C22
24	1	4008	BCR	C15-C16-C17-C18
24	2	4017	BCR	C15-C16-C17-C18
21	2	1221	CLA	C16-C17-C18-C19
21	B	1220	CLA	C4-C3-C5-C6
21	1	1103	CLA	C4-C3-C5-C6
21	2	1022	CLA	C4-C3-C5-C6
21	1	1132	CLA	C2-C3-C5-C6
25	0	5004	LHG	C34-C35-C36-C37
26	1	5004	LMG	C30-C31-C32-C33
21	b	1225	CLA	CBD-CGD-O2D-CED
21	b	1021	CLA	C15-C16-C17-C18
26	b	5005	LMG	C30-C31-C32-C33
21	1	1102	CLA	C6-C7-C8-C9
21	a	1127	CLA	CAA-CBA-CGA-O2A
25	a	5003	LHG	C7-C8-C9-C10
21	A	1114	CLA	C6-C7-C8-C9
21	A	1120	CLA	C11-C10-C8-C9
21	A	1127	CLA	C11-C12-C13-C14
21	A	1134	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1211	CLA	C14-C13-C15-C16
21	K	1402	CLA	C14-C13-C15-C16
21	a	1133	CLA	C11-C10-C8-C9
21	b	1204	CLA	C11-C10-C8-C9
21	b	1232	CLA	C11-C12-C13-C14
26	a	5002	LMG	C14-C15-C16-C17
21	A	1124	CLA	CBA-CGA-O2A-C1
21	a	1011	CLA	CBA-CGA-O2A-C1
21	a	1120	CLA	CBA-CGA-O2A-C1
21	2	1223	CLA	CBA-CGA-O2A-C1
31	F	5001	SQD	C24-C23-O48-C46
21	f	1301	CLA	O1A-CGA-O2A-C1
21	B	1239	CLA	C4B-C3B-CAB-CBB
21	a	1139	CLA	C4B-C3B-CAB-CBB
21	1	1140	CLA	C4B-C3B-CAB-CBB
21	2	1238	CLA	C4B-C3B-CAB-CBB
25	A	5003	LHG	C15-C16-C17-C18
21	a	1122	CLA	O1A-CGA-O2A-C1
25	F	5002	LHG	C28-C29-C30-C31
21	A	1136	CLA	C16-C17-C18-C19
31	B	5008	SQD	C11-C10-C9-C8
21	a	1122	CLA	CBA-CGA-O2A-C1
21	f	1301	CLA	CBA-CGA-O2A-C1
26	b	5005	LMG	C29-C28-O8-C9
25	B	5006	LHG	C11-C10-C9-C8
21	a	1119	CLA	C8-C10-C11-C12
21	b	1022	CLA	C13-C15-C16-C17
21	a	1120	CLA	O1A-CGA-O2A-C1
21	b	1022	CLA	C2A-CAA-CBA-CGA
21	b	1228	CLA	C2A-CAA-CBA-CGA
21	j	1302	CLA	C2A-CAA-CBA-CGA
21	2	1201	CLA	C2A-CAA-CBA-CGA
21	b	1205	CLA	C4-C3-C5-C6
21	1	1013	CLA	C4-C3-C5-C6
25	A	5007	LHG	C16-C17-C18-C19
21	B	1211	CLA	C2-C3-C5-C6
21	B	1224	CLA	C2-C3-C5-C6
21	2	1022	CLA	C2-C3-C5-C6
25	0	5002	LHG	O6-C4-C5-O7
21	2	1223	CLA	O1A-CGA-O2A-C1
26	b	5005	LMG	O10-C28-O8-C9
24	8	4001	BCR	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	7	4015	ZEX	C29-C30-C31-C32
21	a	1120	CLA	C6-C7-C8-C9
22	A	2001	PQN	C26-C27-C28-C29
31	f	5001	SQD	C7-C8-C9-C10
21	1	1101	CLA	CAA-CBA-CGA-O2A
21	A	1110	CLA	C6-C7-C8-C10
21	A	1120	CLA	C6-C7-C8-C10
21	A	1136	CLA	C12-C13-C15-C16
21	A	1012	CLA	C6-C7-C8-C10
21	B	1205	CLA	C6-C7-C8-C10
21	B	1224	CLA	C6-C7-C8-C10
21	B	1240	CLA	C6-C7-C8-C10
21	a	1104	CLA	C6-C7-C8-C10
21	a	1109	CLA	C11-C10-C8-C7
21	a	1111	CLA	C12-C13-C15-C16
21	b	1209	CLA	C11-C12-C13-C15
21	b	1231	CLA	C11-C12-C13-C15
21	l	1501	CLA	C11-C12-C13-C15
21	1	1104	CLA	C11-C12-C13-C15
21	1	1106	CLA	C11-C10-C8-C7
21	1	1120	CLA	C11-C12-C13-C15
22	B	2002	PQN	C17-C18-C20-C21
22	b	2002	PQN	C21-C22-C23-C25
21	a	1117	CLA	C10-C11-C12-C13
21	2	1225	CLA	C3-C5-C6-C7
25	M	5001	LHG	C33-C34-C35-C36
25	A	5005	LHG	C9-C10-C11-C12
25	1	5005	LHG	C30-C31-C32-C33
21	b	1222	CLA	C16-C17-C18-C19
22	B	2002	PQN	C26-C27-C28-C30
26	b	5002	LMG	C40-C41-C42-C43
21	A	1011	CLA	CAA-CBA-CGA-O1A
31	F	5001	SQD	O10-C23-O48-C46
37	L	5004	DGD	O1G-C1G-C2G-O2G
35	l	6001	LMT	C2B-C1B-O1B-C4'
25	l	5002	LHG	C15-C16-C17-C18
21	A	1102	CLA	C3A-C2A-CAA-CBA
21	A	1108	CLA	C3A-C2A-CAA-CBA
21	A	1118	CLA	C4-C3-C5-C6
21	A	1123	CLA	C4-C3-C5-C6
21	B	1228	CLA	C3A-C2A-CAA-CBA
21	b	1211	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1214	CLA	C3A-C2A-CAA-CBA
21	k	1402	CLA	C3A-C2A-CAA-CBA
21	1	1013	CLA	C3A-C2A-CAA-CBA
21	8	1402	CLA	C3A-C2A-CAA-CBA
21	b	1222	CLA	O1D-CGD-O2D-CED
25	1	5001	LHG	O8-C23-C24-C25
21	B	1205	CLA	C2-C3-C5-C6
21	a	1105	CLA	C2-C3-C5-C6
21	a	1131	CLA	C2-C3-C5-C6
25	A	5003	LHG	C27-C28-C29-C30
21	A	1132	CLA	C5-C6-C7-C8
21	2	1239	CLA	C15-C16-C17-C18
21	b	1215	CLA	C16-C17-C18-C19
21	2	1215	CLA	C11-C12-C13-C14
24	f	4016	BCR	C35-C13-C14-C15
24	l	4022	BCR	C11-C10-C9-C34
24	2	4011	BCR	C16-C17-C18-C36
24	2	4018	BCR	C20-C21-C22-C37
24	6	4016	BCR	C35-C13-C14-C15
24	9	4021	BCR	C35-C13-C14-C15
28	B	4011	45D	C28-C26-C30-C32
28	B	4011	45D	C39-C35-C37-C41
30	B	4006	ECH	C11-C10-C9-C34
30	B	4006	ECH	C35-C13-C14-C15
30	M	4021	ECH	C11-C10-C9-C34
30	b	4011	ECH	C16-C17-C18-C36
30	b	4006	ECH	C11-C10-C9-C34
30	m	4021	ECH	C11-C10-C9-C34
30	2	4006	ECH	C11-C10-C9-C34
34	F	4016	ZEX	C20-C13-C14-C15
36	I	4020	EQ3	C11-C10-C9-C34
25	F	5002	LHG	C9-C10-C11-C12
31	F	5001	SQD	C7-C8-C9-C10
21	A	1104	CLA	C10-C11-C12-C13
25	a	5007	LHG	C35-C36-C37-C38
26	1	5004	LMG	C33-C34-C35-C36
31	f	5001	SQD	C33-C34-C35-C36
21	A	1131	CLA	C2-C1-O2A-CGA
21	B	1225	CLA	C2-C1-O2A-CGA
21	2	1207	CLA	C2-C1-O2A-CGA
21	2	1208	CLA	C2-C1-O2A-CGA
24	K	4001	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	4002	BCR	C9-C10-C11-C12
24	a	4002	BCR	C19-C20-C21-C22
24	1	4001	BCR	C9-C10-C11-C12
25	0	5002	LHG	C15-C16-C17-C18
21	a	1136	CLA	C10-C11-C12-C13
21	1	1106	CLA	C8-C10-C11-C12
25	L	5005	LHG	C2-C3-O3-P
25	M	5001	LHG	C5-C4-O6-P
25	a	5003	LHG	C2-C3-O3-P
25	A	5005	LHG	C19-C20-C21-C22
21	1	1137	CLA	C4-C3-C5-C6
21	B	1223	CLA	O1A-CGA-O2A-C1
21	b	1229	CLA	C10-C11-C12-C13
26	b	5005	LMG	C39-C40-C41-C42
35	F	6001	LMT	O5B-C1B-O1B-C4'
26	a	5004	LMG	C33-C34-C35-C36
21	B	1218	CLA	C8-C10-C11-C12
21	B	1224	CLA	C5-C6-C7-C8
21	a	1011	CLA	C10-C11-C12-C13
21	f	1302	CLA	C10-C11-C12-C13
28	h	4020	45D	C20-C24-C26-C30
35	0	6001	LMT	O1'-C1-C2-C3
21	a	1123	CLA	C4-C3-C5-C6
21	0	1501	CLA	C4-C3-C5-C6
21	B	1219	CLA	C2-C3-C5-C6
21	a	1118	CLA	C2-C3-C5-C6
21	2	1207	CLA	C2-C3-C5-C6
22	B	2002	PQN	C26-C27-C28-C29
21	1	1128	CLA	C13-C15-C16-C17
25	l	5002	LHG	C14-C15-C16-C17
21	A	1136	CLA	C2A-CAA-CBA-CGA
21	a	1013	CLA	C2A-CAA-CBA-CGA
25	0	5002	LHG	C4-C5-C6-O8
26	b	5005	LMG	C7-C8-C9-O8
21	J	1303	CLA	C3-C5-C6-C7
21	A	1801	CLA	C5-C6-C7-C8
21	A	1105	CLA	C14-C13-C15-C16
21	A	1113	CLA	C6-C7-C8-C9
21	A	1120	CLA	C6-C7-C8-C9
21	A	1121	CLA	C11-C10-C8-C9
21	A	1125	CLA	C6-C7-C8-C9
21	A	1126	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1133	CLA	C6-C7-C8-C9
21	A	1136	CLA	C14-C13-C15-C16
21	A	1137	CLA	C14-C13-C15-C16
21	A	1012	CLA	C6-C7-C8-C9
21	B	1201	CLA	C14-C13-C15-C16
21	B	1204	CLA	C6-C7-C8-C9
21	B	1206	CLA	C6-C7-C8-C9
21	B	1216	CLA	C11-C12-C13-C14
21	B	1218	CLA	C6-C7-C8-C9
21	B	1219	CLA	C11-C10-C8-C9
21	B	1224	CLA	C6-C7-C8-C9
21	B	1234	CLA	C11-C10-C8-C9
21	K	1402	CLA	C11-C12-C13-C14
21	a	1104	CLA	C6-C7-C8-C9
21	a	1117	CLA	C11-C10-C8-C9
21	a	1131	CLA	C11-C10-C8-C9
21	a	1133	CLA	C14-C13-C15-C16
21	a	1135	CLA	C11-C12-C13-C14
21	b	1238	CLA	C14-C13-C15-C16
21	l	1501	CLA	C11-C12-C13-C14
21	1	1104	CLA	C11-C12-C13-C14
21	1	1133	CLA	C6-C7-C8-C9
21	1	1140	CLA	C11-C12-C13-C14
21	2	1206	CLA	C11-C10-C8-C9
21	2	1221	CLA	C14-C13-C15-C16
22	b	2002	PQN	C24-C23-C25-C26
25	1	5005	LHG	C26-C27-C28-C29
21	A	1101	CLA	C16-C17-C18-C20
21	b	1022	CLA	C16-C17-C18-C20
21	l	1503	CLA	C16-C17-C18-C20
21	2	1237	CLA	C8-C10-C11-C12
22	a	2001	PQN	C23-C25-C26-C27
25	A	5006	LHG	C27-C28-C29-C30
26	b	5002	LMG	C22-C23-C24-C25
25	F	5002	LHG	C15-C16-C17-C18
21	B	1224	CLA	C8-C10-C11-C12
21	b	1205	CLA	C5-C6-C7-C8
35	l	6001	LMT	C5-C6-C7-C8
24	A	4007	BCR	C19-C20-C21-C22
25	a	5005	LHG	C31-C32-C33-C34
25	0	5004	LHG	C10-C11-C12-C13
21	1	1126	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1205	CLA	C2-C3-C5-C6
21	0	1501	CLA	C2-C3-C5-C6
25	L	5005	LHG	C16-C17-C18-C19
25	0	5002	LHG	C11-C10-C9-C8
26	2	5005	LMG	C40-C41-C42-C43
21	a	1118	CLA	C15-C16-C17-C18
21	L	1501	CLA	C2A-CAA-CBA-CGA
21	a	1111	CLA	C2A-CAA-CBA-CGA
21	l	1503	CLA	C2A-CAA-CBA-CGA
21	2	1022	CLA	C2A-CAA-CBA-CGA
25	a	5003	LHG	O10-C23-C24-C25
21	b	1223	CLA	O1A-CGA-O2A-C1
21	A	1140	CLA	C1A-C2A-CAA-CBA
21	B	1237	CLA	C1A-C2A-CAA-CBA
21	B	1021	CLA	C1A-C2A-CAA-CBA
21	B	1222	CLA	C1A-C2A-CAA-CBA
21	B	1223	CLA	C1A-C2A-CAA-CBA
21	a	1011	CLA	C1A-C2A-CAA-CBA
21	b	1022	CLA	C1A-C2A-CAA-CBA
21	b	1021	CLA	C1A-C2A-CAA-CBA
21	k	1402	CLA	C1A-C2A-CAA-CBA
21	1	1013	CLA	C1A-C2A-CAA-CBA
21	8	1402	CLA	C1A-C2A-CAA-CBA
24	f	4016	BCR	C12-C13-C14-C15
24	l	4022	BCR	C11-C10-C9-C8
24	2	4011	BCR	C16-C17-C18-C19
24	2	4018	BCR	C20-C21-C22-C23
24	6	4016	BCR	C12-C13-C14-C15
24	9	4021	BCR	C12-C13-C14-C15
28	B	4011	45D	C24-C26-C30-C32
28	B	4011	45D	C33-C35-C37-C41
30	B	4006	ECH	C11-C10-C9-C8
30	B	4006	ECH	C12-C13-C14-C15
30	M	4021	ECH	C11-C10-C9-C8
30	b	4011	ECH	C16-C17-C18-C19
30	b	4006	ECH	C11-C10-C9-C8
30	m	4021	ECH	C11-C10-C9-C8
30	2	4006	ECH	C11-C10-C9-C8
34	F	4016	ZEX	C12-C13-C14-C15
36	I	4020	EQ3	C11-C10-C9-C8
25	1	5001	LHG	C31-C32-C33-C34
21	A	1011	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	1225	CLA	C16-C17-C18-C20
37	L	5004	DGD	C5B-C6B-C7B-C8B
21	A	1131	CLA	C2B-C3B-CAB-CBB
21	A	1140	CLA	C2B-C3B-CAB-CBB
21	B	1214	CLA	C2B-C3B-CAB-CBB
21	B	1225	CLA	C2B-C3B-CAB-CBB
21	a	1108	CLA	C2B-C3B-CAB-CBB
21	a	1110	CLA	C2B-C3B-CAB-CBB
21	a	1134	CLA	C2B-C3B-CAB-CBB
21	a	1139	CLA	C2B-C3B-CAB-CBB
21	b	1217	CLA	C2B-C3B-CAB-CBB
21	1	1139	CLA	C2B-C3B-CAB-CBB
21	2	1225	CLA	C2B-C3B-CAB-CBB
21	2	1230	CLA	C2B-C3B-CAB-CBB
24	A	4002	BCR	C5-C6-C7-C8
24	A	4003	BCR	C5-C6-C7-C8
24	B	4005	BCR	C5-C6-C7-C8
24	B	4005	BCR	C23-C24-C25-C30
24	J	4013	BCR	C5-C6-C7-C8
24	K	4001	BCR	C5-C6-C7-C8
24	L	4022	BCR	C5-C6-C7-C8
24	a	4008	BCR	C1-C6-C7-C8
24	a	4012	BCR	C5-C6-C7-C8
24	b	4005	BCR	C5-C6-C7-C8
24	b	4010	BCR	C23-C24-C25-C30
24	b	4014	BCR	C23-C24-C25-C30
24	f	4016	BCR	C1-C6-C7-C8
24	k	4001	BCR	C1-C6-C7-C8
24	1	4002	BCR	C5-C6-C7-C8
24	1	4002	BCR	C23-C24-C25-C26
24	1	4003	BCR	C5-C6-C7-C8
24	1	4003	BCR	C23-C24-C25-C30
24	1	4007	BCR	C23-C24-C25-C26
24	1	4012	BCR	C23-C24-C25-C30
24	2	4011	BCR	C1-C6-C7-C8
24	2	4005	BCR	C5-C6-C7-C8
24	2	4010	BCR	C23-C24-C25-C30
24	2	4018	BCR	C5-C6-C7-C8
24	6	4016	BCR	C1-C6-C7-C8
28	B	4011	45D	C15-C07-C19-C23
28	h	4020	45D	C03-C07-C19-C23
28	h	4020	45D	C04-C08-C20-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	M	4021	ECH	C23-C24-C25-C30
30	b	4011	ECH	C5-C6-C7-C8
30	b	4006	ECH	C5-C6-C7-C8
30	m	4021	ECH	C5-C6-C7-C8
30	2	4006	ECH	C23-C24-C25-C30
31	f	5001	SQD	C15-C16-C17-C18
21	B	1223	CLA	CBA-CGA-O2A-C1
21	2	1238	CLA	O1A-CGA-O2A-C1
25	M	5001	LHG	C2-C3-O3-P
25	a	5007	LHG	C5-C4-O6-P
25	l	5003	LHG	C2-C3-O3-P
25	6	5001	LHG	C2-C3-O3-P
21	A	1801	CLA	C4-C3-C5-C6
21	a	1110	CLA	C4-C3-C5-C6
21	2	1224	CLA	C4-C3-C5-C6
21	2	1235	CLA	C4-C3-C5-C6
25	a	5007	LHG	C14-C15-C16-C17
21	1	1013	CLA	C2-C3-C5-C6
25	A	5007	LHG	C27-C28-C29-C30
25	2	5004	LHG	C16-C17-C18-C19
26	2	5005	LMG	C10-C11-C12-C13
21	2	1232	CLA	CAA-CBA-CGA-O2A
21	a	1105	CLA	C10-C11-C12-C13
25	l	5004	LHG	C9-C10-C11-C12
21	A	1105	CLA	C11-C12-C13-C15
21	A	1106	CLA	C11-C10-C8-C7
21	A	1116	CLA	C6-C7-C8-C10
21	A	1134	CLA	C11-C10-C8-C7
21	B	1206	CLA	C6-C7-C8-C10
21	B	1211	CLA	C12-C13-C15-C16
21	B	1217	CLA	C11-C10-C8-C7
21	a	1104	CLA	C12-C13-C15-C16
21	a	1106	CLA	C6-C7-C8-C10
21	a	1119	CLA	C6-C7-C8-C10
21	b	1204	CLA	C11-C10-C8-C7
21	b	1208	CLA	C6-C7-C8-C10
21	b	1210	CLA	C11-C12-C13-C15
21	b	1216	CLA	C12-C13-C15-C16
21	b	1218	CLA	C11-C12-C13-C15
21	b	1219	CLA	C11-C10-C8-C7
21	1	1103	CLA	C11-C12-C13-C15
21	1	1116	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1128	CLA	C12-C13-C15-C16
21	1	1133	CLA	C12-C13-C15-C16
21	2	1206	CLA	C11-C10-C8-C7
21	2	1221	CLA	C6-C7-C8-C10
22	A	2001	PQN	C22-C23-C25-C26
22	2	2002	PQN	C16-C17-C18-C20
25	A	5005	LHG	C30-C31-C32-C33
21	a	1124	CLA	C6-C7-C8-C9
26	1	5004	LMG	O7-C8-C9-O8
26	2	5005	LMG	C30-C31-C32-C33
25	A	5005	LHG	C13-C14-C15-C16
25	2	5004	LHG	C33-C34-C35-C36
25	A	5005	LHG	C14-C15-C16-C17
24	b	4014	BCR	C7-C8-C9-C34
24	1	4008	BCR	C37-C22-C23-C24
24	2	4018	BCR	C37-C22-C23-C24
28	h	4020	45D	C32-C34-C36-C40
21	F	1302	CLA	C4-C3-C5-C6
21	a	1108	CLA	C4-C3-C5-C6
21	b	1206	CLA	C4-C3-C5-C6
21	1	1120	CLA	C4-C3-C5-C6
22	B	2002	PQN	C14-C13-C15-C16
21	a	1116	CLA	CAA-CBA-CGA-O2A
21	a	1123	CLA	C10-C11-C12-C13
21	A	1118	CLA	C2-C3-C5-C6
21	A	1122	CLA	C2-C3-C5-C6
21	B	1220	CLA	C2-C3-C5-C6
21	J	1303	CLA	C2-C3-C5-C6
21	a	1123	CLA	C2-C3-C5-C6
21	2	1224	CLA	C2-C3-C5-C6
25	a	5001	LHG	C15-C16-C17-C18
21	B	1207	CLA	C2-C1-O2A-CGA
25	a	5005	LHG	C12-C13-C14-C15
21	B	1219	CLA	C15-C16-C17-C18
21	a	1131	CLA	C15-C16-C17-C18
21	b	1223	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	C14-C13-C15-C16
21	A	1112	CLA	C11-C12-C13-C14
22	2	2002	PQN	C21-C22-C23-C24
24	L	4022	BCR	C13-C14-C15-C16
24	2	4004	BCR	C13-C14-C15-C16
21	a	1127	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1231	CLA	C10-C11-C12-C13
21	1	1116	CLA	C15-C16-C17-C18
26	A	5002	LMG	C13-C14-C15-C16
25	1	5005	LHG	C19-C20-C21-C22
21	b	1021	CLA	C3-C5-C6-C7
21	B	1219	CLA	C5-C6-C7-C8
21	b	1227	CLA	C10-C11-C12-C13
21	b	1240	CLA	C13-C15-C16-C17
21	2	1235	CLA	C5-C6-C7-C8
21	A	1013	CLA	C4-C3-C5-C6
21	b	1207	CLA	C4-C3-C5-C6
21	b	1226	CLA	C4-C3-C5-C6
21	1	1124	CLA	C4-C3-C5-C6
21	2	1232	CLA	CAA-CBA-CGA-O1A
25	l	5004	LHG	C5-C4-O6-P
21	A	1109	CLA	C2-C3-C5-C6
21	a	1109	CLA	C2-C3-C5-C6
21	a	1136	CLA	C2-C3-C5-C6
21	1	1124	CLA	C2-C3-C5-C6
25	B	5006	LHG	C33-C34-C35-C36
21	b	1205	CLA	CBD-CGD-O2D-CED
21	b	1021	CLA	O1A-CGA-O2A-C1
21	b	1202	CLA	C15-C16-C17-C18
21	A	1105	CLA	C3-C5-C6-C7
21	a	1133	CLA	C3-C5-C6-C7
21	A	1133	CLA	C10-C11-C12-C13
21	a	1104	CLA	C10-C11-C12-C13
25	A	5007	LHG	C31-C32-C33-C34
21	1	1103	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	C4-C5-C6-O8
26	A	5004	LMG	O1-C7-C8-C9
26	A	5008	LMG	C18-C19-C20-C21
21	1	1107	CLA	O1A-CGA-O2A-C1
21	2	1211	CLA	O1A-CGA-O2A-C1
21	a	1012	CLA	C2A-CAA-CBA-CGA
21	b	1204	CLA	C2A-CAA-CBA-CGA
21	b	1224	CLA	C2A-CAA-CBA-CGA
21	2	1215	CLA	C2A-CAA-CBA-CGA
21	2	1232	CLA	C2A-CAA-CBA-CGA
21	0	1501	CLA	C2A-CAA-CBA-CGA
21	1	1117	CLA	C16-C17-C18-C19
21	1	1138	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	0	6001	LMT	C1-C2-C3-C4
25	l	5003	LHG	O9-C7-O7-C5
21	b	1023	CLA	C15-C16-C17-C18
25	F	5002	LHG	C16-C17-C18-C19
25	A	5003	LHG	O6-C4-C5-O7
21	K	1401	CLA	C4-C3-C5-C6
21	a	1801	CLA	CAA-CBA-CGA-O2A
25	l	5004	LHG	O8-C23-C24-C25
21	B	1217	CLA	C16-C17-C18-C20
21	B	1203	CLA	C15-C16-C17-C18
21	L	1501	CLA	C5-C6-C7-C8
31	B	5008	SQD	C17-C18-C19-C20
25	B	5006	LHG	C10-C11-C12-C13
21	J	1302	CLA	C4B-C3B-CAB-CBB
21	a	1105	CLA	C4B-C3B-CAB-CBB
21	j	1303	CLA	C4B-C3B-CAB-CBB
21	2	1240	CLA	C4B-C3B-CAB-CBB
25	A	5005	LHG	C32-C33-C34-C35
21	1	1011	CLA	CAA-CBA-CGA-O2A
21	2	1202	CLA	CAA-CBA-CGA-O2A
25	a	5005	LHG	O8-C23-C24-C25
21	B	1213	CLA	C16-C17-C18-C20
21	B	1225	CLA	C16-C17-C18-C19
21	b	1209	CLA	C16-C17-C18-C19
21	1	1136	CLA	C16-C17-C18-C19
21	2	1204	CLA	C16-C17-C18-C20
25	b	5004	LHG	C1-C2-C3-O3
24	B	4018	BCR	C11-C10-C9-C34
24	b	4018	BCR	C11-C10-C9-C34
21	b	1210	CLA	C10-C11-C12-C13
21	2	1228	CLA	CAA-CBA-CGA-O2A
21	a	1109	CLA	C13-C15-C16-C17
25	a	5003	LHG	C25-C26-C27-C28
21	A	1113	CLA	C16-C17-C18-C19
21	B	1223	CLA	C16-C17-C18-C20
21	B	1235	CLA	C16-C17-C18-C20
21	a	1116	CLA	C11-C12-C13-C14
21	a	1112	CLA	C4-C3-C5-C6
25	F	5002	LHG	O7-C5-C6-O8
25	M	5001	LHG	O7-C5-C6-O8
21	b	1222	CLA	C15-C16-C17-C18
25	l	5004	LHG	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	5006	SQD	C15-C16-C17-C18
21	a	1108	CLA	C2-C3-C5-C6
21	b	1226	CLA	C2-C3-C5-C6
26	1	5004	LMG	O6-C1-O1-C7
24	I	4018	BCR	C7-C8-C9-C34
21	A	1125	CLA	C6-C7-C8-C10
21	B	1228	CLA	C6-C7-C8-C10
21	a	1117	CLA	C11-C10-C8-C7
21	1	1103	CLA	C11-C10-C8-C7
21	1	1133	CLA	C6-C7-C8-C10
25	l	5002	LHG	C33-C34-C35-C36
25	1	5001	LHG	C33-C34-C35-C36
26	A	5004	LMG	C11-C12-C13-C14
21	1	1013	CLA	C13-C15-C16-C17
26	K	5009	LMG	C24-C25-C26-C27
24	A	4019	BCR	C19-C20-C21-C22
25	A	5001	LHG	C9-C10-C11-C12
25	B	5004	LHG	C32-C33-C34-C35
21	A	1114	CLA	C11-C10-C8-C9
21	B	1208	CLA	C14-C13-C15-C16
21	K	1402	CLA	C6-C7-C8-C9
21	a	1118	CLA	C14-C13-C15-C16
21	a	1123	CLA	C11-C10-C8-C9
21	a	1012	CLA	C6-C7-C8-C9
21	b	1212	CLA	C14-C13-C15-C16
21	b	1215	CLA	C11-C10-C8-C9
21	b	1218	CLA	C11-C10-C8-C9
21	b	1220	CLA	C11-C12-C13-C14
21	b	1228	CLA	C11-C12-C13-C14
21	1	1139	CLA	C14-C13-C15-C16
21	2	1023	CLA	C6-C7-C8-C9
21	2	1203	CLA	C6-C7-C8-C9
21	b	1238	CLA	CBD-CGD-O2D-CED
26	A	5002	LMG	C8-C7-O1-C1
21	B	1224	CLA	C2A-CAA-CBA-CGA
21	J	1302	CLA	C2A-CAA-CBA-CGA
21	1	1128	CLA	C2A-CAA-CBA-CGA
21	2	1218	CLA	C2A-CAA-CBA-CGA
21	K	1401	CLA	C2-C1-O2A-CGA
21	a	1801	CLA	C2-C1-O2A-CGA
21	f	1302	CLA	C2-C1-O2A-CGA
21	1	1801	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	1	5003	LHG	C24-C23-O8-C6
21	A	1011	CLA	C3A-C2A-CAA-CBA
21	A	1126	CLA	C3A-C2A-CAA-CBA
21	A	1138	CLA	C3A-C2A-CAA-CBA
21	B	1022	CLA	C3A-C2A-CAA-CBA
21	B	1222	CLA	C4-C3-C5-C6
21	B	1223	CLA	C3A-C2A-CAA-CBA
21	J	1302	CLA	C4-C3-C5-C6
21	a	1011	CLA	C3A-C2A-CAA-CBA
21	a	1120	CLA	C3A-C2A-CAA-CBA
21	a	1128	CLA	C3A-C2A-CAA-CBA
21	b	1021	CLA	C3A-C2A-CAA-CBA
21	2	1232	CLA	C3A-C2A-CAA-CBA
21	2	1209	CLA	CAA-CBA-CGA-O2A
25	1	5005	LHG	C34-C35-C36-C37
21	a	1103	CLA	CAA-CBA-CGA-O2A
26	A	5008	LMG	O10-C28-O8-C9
21	B	1214	CLA	C2-C3-C5-C6
21	2	1214	CLA	C2-C3-C5-C6
26	A	5008	LMG	C19-C20-C21-C22
31	B	5008	SQD	C15-C16-C17-C18
21	a	1123	CLA	C13-C15-C16-C17
25	B	5004	LHG	C24-C25-C26-C27
26	1	5004	LMG	C2-C1-O1-C7
21	a	1117	CLA	C15-C16-C17-C18
21	A	1012	CLA	O2A-C1-C2-C3
24	I	4018	BCR	C10-C11-C12-C13
24	a	4008	BCR	C10-C11-C12-C13
24	1	4012	BCR	C10-C11-C12-C13
25	B	5004	LHG	C33-C34-C35-C36
21	A	1011	CLA	C16-C17-C18-C20
21	A	1133	CLA	C16-C17-C18-C20
25	a	5003	LHG	C27-C28-C29-C30
31	L	5002	SQD	C28-C29-C30-C31
25	B	5006	LHG	C25-C26-C27-C28
21	B	1211	CLA	C3-C5-C6-C7
21	2	1202	CLA	C3-C5-C6-C7
25	b	5004	LHG	O2-C2-C3-O3
21	1	1107	CLA	CBA-CGA-O2A-C1
25	a	5003	LHG	C14-C15-C16-C17
21	K	1401	CLA	C8-C10-C11-C12
21	b	1224	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1213	CLA	O1A-CGA-O2A-C1
24	B	4018	BCR	C11-C10-C9-C8
24	b	4018	BCR	C11-C10-C9-C8
21	2	1209	CLA	CAA-CBA-CGA-O1A
25	l	5004	LHG	C19-C20-C21-C22
21	a	1105	CLA	C8-C10-C11-C12
25	1	5001	LHG	C12-C13-C14-C15
25	1	5007	LHG	C4-C5-C6-O8
26	1	5004	LMG	C7-C8-C9-O8
37	L	5004	DGD	O1G-C1G-C2G-C3G
21	2	1214	CLA	O1A-CGA-O2A-C1
21	B	1022	CLA	C8-C10-C11-C12
26	a	5004	LMG	C29-C30-C31-C32
26	2	5002	LMG	C22-C23-C24-C25
21	b	1213	CLA	C10-C11-C12-C13
21	2	1228	CLA	CAA-CBA-CGA-O1A
25	A	5001	LHG	C30-C31-C32-C33
31	0	5005	SQD	C14-C15-C16-C17
21	a	1102	CLA	C2A-CAA-CBA-CGA
21	2	1229	CLA	C2A-CAA-CBA-CGA
26	0	5001	LMG	O7-C10-C11-C12
21	A	1123	CLA	C2-C3-C5-C6
24	b	4018	BCR	C15-C16-C17-C18
24	l	4022	BCR	C19-C20-C21-C22
21	B	1213	CLA	C16-C17-C18-C19
21	2	1238	CLA	C16-C17-C18-C20
25	A	5005	LHG	C29-C30-C31-C32
21	b	1212	CLA	C10-C11-C12-C13
21	2	1227	CLA	CAA-CBA-CGA-O2A
25	a	5003	LHG	O7-C7-C8-C9
21	l	1502	CLA	C15-C16-C17-C18
25	B	5006	LHG	C30-C31-C32-C33
25	l	5004	LHG	C24-C25-C26-C27
31	0	5005	SQD	C28-C29-C30-C31
21	A	1103	CLA	C14-C13-C15-C16
21	A	1118	CLA	C11-C12-C13-C14
21	A	1130	CLA	C11-C10-C8-C9
21	B	1237	CLA	C11-C10-C8-C9
21	K	1401	CLA	C14-C13-C15-C16
21	a	1102	CLA	C11-C12-C13-C14
21	a	1112	CLA	C11-C12-C13-C14
21	a	1117	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1125	CLA	C11-C12-C13-C14
21	a	1135	CLA	C14-C13-C15-C16
21	a	1139	CLA	C14-C13-C15-C16
21	b	1213	CLA	C11-C12-C13-C14
21	b	1230	CLA	C6-C7-C8-C9
21	j	1302	CLA	C11-C10-C8-C9
21	l	1501	CLA	C11-C10-C8-C9
21	l	1502	CLA	C6-C7-C8-C9
21	1	1138	CLA	C11-C10-C8-C9
21	1	1012	CLA	C6-C7-C8-C9
21	2	1205	CLA	C6-C7-C8-C9
21	2	1214	CLA	C6-C7-C8-C9
21	0	1501	CLA	C11-C12-C13-C14
22	b	2002	PQN	C19-C18-C20-C21
21	B	1210	CLA	C16-C17-C18-C19
26	0	5001	LMG	C19-C20-C21-C22
21	a	1129	CLA	CAA-CBA-CGA-O2A
25	F	5002	LHG	O8-C23-C24-C25
26	B	5002	LMG	O7-C10-C11-C12
21	b	1239	CLA	C15-C16-C17-C18
25	1	5003	LHG	O10-C23-O8-C6
25	0	5002	LHG	O6-C4-C5-C6
31	0	5005	SQD	C11-C10-C9-C8
21	b	1219	CLA	CAA-CBA-CGA-O2A
21	l	1503	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	O7-C7-C8-C9
21	b	1201	CLA	C16-C17-C18-C19
21	b	1238	CLA	O1D-CGD-O2D-CED
21	A	1112	CLA	C2A-CAA-CBA-CGA
21	B	1201	CLA	C2A-CAA-CBA-CGA
21	b	1215	CLA	C2A-CAA-CBA-CGA
21	A	1110	CLA	C12-C13-C15-C16
21	A	1115	CLA	C12-C13-C15-C16
21	A	1117	CLA	C6-C7-C8-C10
21	A	1117	CLA	C12-C13-C15-C16
21	A	1127	CLA	C6-C7-C8-C10
21	A	1137	CLA	C11-C12-C13-C15
21	A	1801	CLA	C11-C12-C13-C15
21	B	1220	CLA	C11-C10-C8-C7
21	J	1302	CLA	C6-C7-C8-C10
21	a	1115	CLA	C11-C12-C13-C15
21	a	1118	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	a	1123	CLA	C6-C7-C8-C10
21	a	1123	CLA	C11-C10-C8-C7
21	a	1126	CLA	C11-C12-C13-C15
21	a	1130	CLA	C6-C7-C8-C10
21	b	1203	CLA	C11-C12-C13-C15
21	b	1212	CLA	C12-C13-C15-C16
21	b	1213	CLA	C12-C13-C15-C16
21	b	1222	CLA	C11-C12-C13-C15
21	1	1124	CLA	C6-C7-C8-C10
21	2	1202	CLA	C12-C13-C15-C16
21	2	1203	CLA	C6-C7-C8-C10
21	2	1205	CLA	C11-C12-C13-C15
21	2	1207	CLA	C6-C7-C8-C10
21	2	1221	CLA	C11-C10-C8-C7
22	b	2002	PQN	C17-C18-C20-C21
22	2	2002	PQN	C21-C22-C23-C25
37	L	5004	DGD	CAB-CBB-CCB-CDB
21	A	1109	CLA	C2B-C3B-CAB-CBB
21	A	1115	CLA	C2B-C3B-CAB-CBB
21	B	1224	CLA	C2B-C3B-CAB-CBB
21	a	1106	CLA	C2B-C3B-CAB-CBB
21	a	1125	CLA	C2B-C3B-CAB-CBB
21	b	1204	CLA	C2B-C3B-CAB-CBB
21	j	1303	CLA	C2B-C3B-CAB-CBB
21	1	1108	CLA	C2B-C3B-CAB-CBB
21	1	1109	CLA	C2B-C3B-CAB-CBB
21	1	1122	CLA	C2B-C3B-CAB-CBB
21	1	1135	CLA	C2B-C3B-CAB-CBB
21	1	1140	CLA	C2B-C3B-CAB-CBB
21	2	1237	CLA	C2B-C3B-CAB-CBB
21	2	1212	CLA	C2B-C3B-CAB-CBB
21	2	1235	CLA	C2B-C3B-CAB-CBB
21	2	1240	CLA	C2B-C3B-CAB-CBB
24	B	4005	BCR	C23-C24-C25-C26
24	a	4002	BCR	C1-C6-C7-C8
24	a	4002	BCR	C23-C24-C25-C30
24	a	4003	BCR	C23-C24-C25-C30
24	a	4008	BCR	C5-C6-C7-C8
24	b	4010	BCR	C23-C24-C25-C26
24	f	4016	BCR	C5-C6-C7-C8
24	i	4018	BCR	C1-C6-C7-C8
24	k	4001	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	l	4022	BCR	C5-C6-C7-C8
24	1	4012	BCR	C23-C24-C25-C26
24	2	4011	BCR	C5-C6-C7-C8
24	2	4010	BCR	C23-C24-C25-C26
24	2	4017	BCR	C1-C6-C7-C8
24	2	4017	BCR	C5-C6-C7-C8
24	6	4016	BCR	C5-C6-C7-C8
24	h	4018	BCR	C5-C6-C7-C8
28	h	4020	45D	C15-C07-C19-C23
30	b	4006	ECH	C23-C24-C25-C26
30	2	4006	ECH	C5-C6-C7-C8
21	b	1227	CLA	C5-C6-C7-C8
25	l	5003	LHG	C8-C7-O7-C5
25	l	5001	LHG	O7-C7-C8-C9
25	B	5004	LHG	C10-C11-C12-C13
21	A	1105	CLA	C2-C1-O2A-CGA
21	F	1301	CLA	C2-C1-O2A-CGA
21	L	1502	CLA	C2-C1-O2A-CGA
21	a	1011	CLA	C2-C1-O2A-CGA
21	b	1232	CLA	C2-C1-O2A-CGA
21	1	1131	CLA	C2-C1-O2A-CGA
21	2	1210	CLA	C2-C1-O2A-CGA
21	2	1218	CLA	C2-C1-O2A-CGA
21	B	1237	CLA	C16-C17-C18-C19
21	a	1128	CLA	C5-C6-C7-C8
21	A	1121	CLA	C3-C5-C6-C7
25	B	5004	LHG	C16-C17-C18-C19
21	1	1125	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	O8-C23-C24-C25
21	A	1115	CLA	C15-C16-C17-C18
21	2	1211	CLA	CBA-CGA-O2A-C1
21	2	1238	CLA	CBA-CGA-O2A-C1
31	b	5006	SQD	C24-C25-C26-C27
21	b	1022	CLA	C16-C17-C18-C19
21	1	1139	CLA	C10-C11-C12-C13
21	b	1229	CLA	C4-C3-C5-C6
21	1	1106	CLA	C3-C5-C6-C7
31	B	5008	SQD	C7-C8-C9-C10
21	a	1128	CLA	CAA-CBA-CGA-O2A
21	2	1230	CLA	CAA-CBA-CGA-O2A
25	M	5001	LHG	O7-C7-C8-C9
21	A	1132	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1801	CLA	C2-C3-C5-C6
21	a	1110	CLA	C2-C3-C5-C6
21	b	1229	CLA	C2-C3-C5-C6
21	a	1128	CLA	C13-C15-C16-C17
21	a	1116	CLA	C2A-CAA-CBA-CGA
21	2	1202	CLA	C2A-CAA-CBA-CGA
25	l	5002	LHG	C8-C7-O7-C5
31	B	5008	SQD	O49-C7-C8-C9
25	1	5007	LHG	C5-C6-O8-C23
21	b	1216	CLA	CAA-CBA-CGA-O2A
21	k	1402	CLA	CAA-CBA-CGA-O2A
21	1	1136	CLA	CAA-CBA-CGA-O2A
21	2	1214	CLA	CAA-CBA-CGA-O2A
25	l	5002	LHG	O7-C7-C8-C9
21	B	1226	CLA	C8-C10-C11-C12
26	A	5008	LMG	C29-C28-O8-C9
21	1	1108	CLA	CAA-CBA-CGA-O2A
24	A	4019	BCR	C13-C14-C15-C16
21	a	1139	CLA	O1A-CGA-O2A-C1
31	f	5001	SQD	C4-C5-C6-S
31	0	5005	SQD	C4-C5-C6-S
21	B	1206	CLA	C4-C3-C5-C6
26	A	5002	LMG	O8-C28-C29-C30
26	A	5004	LMG	O8-C28-C29-C30
26	2	5002	LMG	O7-C10-C11-C12
21	b	1203	CLA	C2-C3-C5-C6
21	2	1227	CLA	CAA-CBA-CGA-O1A
25	0	5004	LHG	O10-C23-C24-C25
21	A	1112	CLA	C10-C11-C12-C13
25	A	5006	LHG	C15-C16-C17-C18
21	2	1220	CLA	CAA-CBA-CGA-O2A
21	8	1401	CLA	CAA-CBA-CGA-O2A
21	A	1106	CLA	C11-C10-C8-C9
21	B	1217	CLA	C11-C10-C8-C9
21	a	1011	CLA	C14-C13-C15-C16
21	a	1104	CLA	C14-C13-C15-C16
21	a	1106	CLA	C6-C7-C8-C9
21	b	1203	CLA	C14-C13-C15-C16
21	b	1216	CLA	C14-C13-C15-C16
21	b	1231	CLA	C6-C7-C8-C9
21	1	1103	CLA	C11-C12-C13-C14
21	1	1106	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	1136	CLA	C6-C7-C8-C9
21	2	1203	CLA	C11-C10-C8-C9
22	A	2001	PQN	C19-C18-C20-C21
22	B	2002	PQN	C16-C17-C18-C19
21	1	1132	CLA	C5-C6-C7-C8
25	B	5004	LHG	O8-C23-C24-C25
25	a	5007	LHG	O7-C7-C8-C9
25	l	5004	LHG	O7-C7-C8-C9
25	F	5002	LHG	C4-C5-C6-O8
31	L	5002	SQD	O6-C44-C45-C46
21	A	1102	CLA	C1A-C2A-CAA-CBA
21	A	1109	CLA	C4B-C3B-CAB-CBB
21	A	1114	CLA	C1A-C2A-CAA-CBA
21	A	1121	CLA	C4B-C3B-CAB-CBB
21	B	1022	CLA	C1A-C2A-CAA-CBA
21	a	1106	CLA	C4B-C3B-CAB-CBB
21	a	1124	CLA	C1A-C2A-CAA-CBA
21	a	1133	CLA	C4B-C3B-CAB-CBB
21	b	1209	CLA	C4B-C3B-CAB-CBB
21	b	1236	CLA	C4B-C3B-CAB-CBB
21	l	1503	CLA	C1A-C2A-CAA-CBA
21	1	1105	CLA	C1A-C2A-CAA-CBA
21	1	1105	CLA	C4B-C3B-CAB-CBB
21	1	1109	CLA	C4B-C3B-CAB-CBB
21	1	1127	CLA	C4B-C3B-CAB-CBB
21	1	1128	CLA	C1A-C2A-CAA-CBA
21	1	1131	CLA	C4B-C3B-CAB-CBB
21	1	1136	CLA	C4B-C3B-CAB-CBB
21	1	1137	CLA	C4B-C3B-CAB-CBB
21	1	1012	CLA	C1A-C2A-CAA-CBA
21	2	1223	CLA	C4B-C3B-CAB-CBB
21	2	1235	CLA	C4B-C3B-CAB-CBB
21	2	1236	CLA	C4B-C3B-CAB-CBB
21	0	1503	CLA	C1A-C2A-CAA-CBA
26	b	5005	LMG	C11-C12-C13-C14
31	0	5005	SQD	C16-C17-C18-C19
21	B	1221	CLA	C4-C3-C5-C6
21	1	1101	CLA	C5-C6-C7-C8
26	2	5002	LMG	C40-C41-C42-C43
35	1	6001	LMT	C9-C10-C11-C12
21	a	1122	CLA	CAA-CBA-CGA-O2A
21	2	1219	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	5004	LMG	O7-C10-C11-C12
26	K	5009	LMG	O7-C10-C11-C12
31	F	5001	SQD	O48-C23-C24-C25
21	2	1229	CLA	C2-C3-C5-C6
24	b	4004	BCR	C7-C8-C9-C10
24	b	4014	BCR	C7-C8-C9-C10
24	1	4007	BCR	C11-C12-C13-C14
24	1	4007	BCR	C17-C18-C19-C20
24	1	4008	BCR	C21-C22-C23-C24
30	i	4020	ECH	C17-C18-C19-C20
24	l	4022	BCR	C13-C14-C15-C16
34	J	4015	ZEX	C33-C34-C35-C15
21	A	1131	CLA	C10-C11-C12-C13
21	1	1115	CLA	C10-C11-C12-C13
25	l	5002	LHG	O9-C7-O7-C5
21	B	1021	CLA	O1A-CGA-O2A-C1
25	1	5005	LHG	C5-C6-O8-C23
21	L	1503	CLA	C16-C17-C18-C20
25	A	5001	LHG	C24-C23-O8-C6
21	A	1801	CLA	CAA-CBA-CGA-O2A
21	L	1502	CLA	CAA-CBA-CGA-O2A
21	b	1210	CLA	CAA-CBA-CGA-O2A
21	1	1107	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	O10-C23-O8-C6
21	a	1132	CLA	C2A-CAA-CBA-CGA
25	A	5003	LHG	C24-C25-C26-C27
25	1	5003	LHG	C19-C20-C21-C22
25	0	5002	LHG	C19-C20-C21-C22
21	A	1114	CLA	C13-C15-C16-C17
21	b	1221	CLA	C10-C11-C12-C13
21	b	1203	CLA	O1A-CGA-O2A-C1
31	B	5008	SQD	C9-C10-C11-C12
21	B	1222	CLA	C6-C7-C8-C9
21	A	1136	CLA	CAA-CBA-CGA-O2A
21	B	1210	CLA	CAA-CBA-CGA-O2A
21	b	1230	CLA	CAA-CBA-CGA-O2A
21	2	1210	CLA	CAA-CBA-CGA-O2A
25	a	5005	LHG	O7-C7-C8-C9
26	b	5002	LMG	O7-C10-C11-C12
31	L	5001	SQD	O47-C7-C8-C9
21	A	1134	CLA	O1D-CGD-O2D-CED
25	1	5005	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	1011	CLA	C2-C1-O2A-CGA
21	A	1121	CLA	C2-C1-O2A-CGA
21	A	1012	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	C2-C1-O2A-CGA
21	2	1224	CLA	C2-C1-O2A-CGA
21	A	1113	CLA	CAA-CBA-CGA-O2A
21	A	1105	CLA	C6-C7-C8-C10
21	A	1110	CLA	C11-C12-C13-C15
21	A	1118	CLA	C11-C10-C8-C7
21	A	1119	CLA	C11-C10-C8-C7
21	B	1202	CLA	C11-C12-C13-C15
21	B	1220	CLA	C6-C7-C8-C10
21	B	1231	CLA	C11-C12-C13-C15
21	L	1502	CLA	C11-C12-C13-C15
21	a	1125	CLA	C12-C13-C15-C16
21	a	1136	CLA	C11-C12-C13-C15
21	b	1213	CLA	C6-C7-C8-C10
21	b	1218	CLA	C11-C10-C8-C7
21	b	1228	CLA	C6-C7-C8-C10
21	b	1240	CLA	C11-C12-C13-C15
21	b	1201	CLA	C11-C12-C13-C15
21	1	1106	CLA	C12-C13-C15-C16
21	1	1115	CLA	C6-C7-C8-C10
21	1	1134	CLA	C11-C10-C8-C7
21	2	1218	CLA	C12-C13-C15-C16
21	0	1502	CLA	C6-C7-C8-C10
22	A	2001	PQN	C17-C18-C20-C21
22	B	2002	PQN	C16-C17-C18-C20
21	a	1139	CLA	CBA-CGA-O2A-C1
21	b	1021	CLA	CBA-CGA-O2A-C1
21	b	1203	CLA	CBA-CGA-O2A-C1
21	b	1213	CLA	CBA-CGA-O2A-C1
25	A	5003	LHG	C14-C15-C16-C17
25	1	5001	LHG	C18-C19-C20-C21
26	1	5004	LMG	C34-C35-C36-C37
31	B	5008	SQD	C28-C29-C30-C31
21	2	1229	CLA	C2C-C3C-CAC-CBC
25	l	5004	LHG	C29-C30-C31-C32
26	b	5007	LMG	C18-C19-C20-C21
21	a	1107	CLA	CAA-CBA-CGA-O2A
25	F	5002	LHG	O7-C7-C8-C9
26	b	5005	LMG	O8-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	L	5005	LHG	C29-C30-C31-C32
25	A	5005	LHG	C25-C26-C27-C28
21	b	1215	CLA	CAA-CBA-CGA-O1A
21	1	1111	CLA	C15-C16-C17-C18
21	A	1114	CLA	CAA-CBA-CGA-O2A
21	b	1021	CLA	CAA-CBA-CGA-O2A
26	1	5004	LMG	O7-C10-C11-C12
25	A	5001	LHG	O10-C23-C24-C25
31	0	5005	SQD	C35-C36-C37-C38
21	A	1101	CLA	C3A-C2A-CAA-CBA
21	a	1114	CLA	C3A-C2A-CAA-CBA
21	1	1101	CLA	C3A-C2A-CAA-CBA
21	1	1012	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	CAA-CBA-CGA-O1A
25	a	5001	LHG	C26-C27-C28-C29
21	a	1111	CLA	C15-C16-C17-C18
21	b	1021	CLA	C8-C10-C11-C12
26	A	5004	LMG	C4-C5-C6-O5
21	1	1109	CLA	C16-C17-C18-C20
25	a	5001	LHG	O10-C23-C24-C25
26	2	5005	LMG	C16-C17-C18-C19
21	2	1214	CLA	CBA-CGA-O2A-C1
26	A	5004	LMG	C13-C14-C15-C16
21	B	1219	CLA	C8-C10-C11-C12
21	a	1131	CLA	C13-C15-C16-C17
21	1	1104	CLA	C15-C16-C17-C18
21	1	1129	CLA	CAA-CBA-CGA-O2A
21	2	1211	CLA	CAA-CBA-CGA-O2A
25	A	5007	LHG	O7-C7-C8-C9
25	F	5002	LHG	O10-C23-C24-C25
25	M	5001	LHG	O9-C7-C8-C9
25	a	5003	LHG	O9-C7-C8-C9
26	A	5004	LMG	O10-C28-C29-C30
21	B	1209	CLA	C2A-CAA-CBA-CGA
21	A	1107	CLA	C11-C12-C13-C14
21	A	1117	CLA	C14-C13-C15-C16
21	A	1120	CLA	C14-C13-C15-C16
21	A	1801	CLA	C11-C12-C13-C14
21	B	1204	CLA	C11-C10-C8-C9
21	J	1302	CLA	C6-C7-C8-C9
21	a	1110	CLA	C11-C10-C8-C9
21	b	1212	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	1227	CLA	C11-C12-C13-C14
21	b	1240	CLA	C11-C12-C13-C14
21	1	1116	CLA	C11-C12-C13-C14
21	1	1134	CLA	C11-C10-C8-C9
21	2	1221	CLA	C6-C7-C8-C9
22	A	2001	PQN	C24-C23-C25-C26
22	2	2002	PQN	C16-C17-C18-C19
21	j	1303	CLA	CAA-CBA-CGA-O2A
21	1	1136	CLA	CAA-CBA-CGA-O1A
21	2	1214	CLA	CAA-CBA-CGA-O1A
21	2	1219	CLA	CAA-CBA-CGA-O1A
21	2	1224	CLA	CAA-CBA-CGA-O1A
25	B	5004	LHG	O10-C23-C24-C25
25	a	5005	LHG	O9-C7-C8-C9
25	l	5002	LHG	O9-C7-C8-C9
25	l	5001	LHG	C24-C25-C26-C27
21	A	1109	CLA	C5-C6-C7-C8
24	B	4017	BCR	C19-C20-C21-C22
21	8	1401	CLA	CAA-CBA-CGA-O1A
21	2	1023	CLA	C8-C10-C11-C12
21	A	1132	CLA	C4-C3-C5-C6
21	k	1402	CLA	CAA-CBA-CGA-O1A
21	1	1125	CLA	CAA-CBA-CGA-O1A
25	A	5001	LHG	O9-C7-C8-C9
26	A	5002	LMG	O10-C28-C29-C30
26	0	5001	LMG	O9-C10-C11-C12
25	A	5005	LHG	C24-C25-C26-C27
31	f	5001	SQD	O5-C5-C6-S
21	A	1105	CLA	C10-C11-C12-C13
21	A	1127	CLA	C3-C5-C6-C7
21	l	1503	CLA	C16-C17-C18-C19
21	2	1220	CLA	CAA-CBA-CGA-O1A
21	1	1120	CLA	C8-C10-C11-C12
24	2	4018	BCR	C21-C22-C23-C24
34	7	4015	ZEX	C31-C32-C33-C34
21	a	1101	CLA	CAA-CBA-CGA-O1A
21	b	1219	CLA	CAA-CBA-CGA-O1A
21	l	1503	CLA	CAA-CBA-CGA-O1A
21	1	1107	CLA	CAA-CBA-CGA-O1A
26	b	5002	LMG	O9-C10-C11-C12
21	1	1140	CLA	C5-C6-C7-C8
25	l	5001	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	l	5002	LHG	C29-C30-C31-C32
21	A	1113	CLA	CAA-CBA-CGA-O1A
21	A	1136	CLA	CAA-CBA-CGA-O1A
21	a	1128	CLA	CAA-CBA-CGA-O1A
21	a	1129	CLA	CAA-CBA-CGA-O1A
21	b	1216	CLA	CAA-CBA-CGA-O1A
21	b	1230	CLA	CAA-CBA-CGA-O1A
21	2	1230	CLA	CAA-CBA-CGA-O1A
25	l	5001	LHG	O9-C7-C8-C9
21	A	1106	CLA	CAA-CBA-CGA-O2A
25	1	5005	LHG	O8-C23-C24-C25
26	A	5002	LMG	C14-C15-C16-C17
26	0	5001	LMG	O1-C7-C8-C9
21	L	1502	CLA	CAA-CBA-CGA-O1A
21	2	1210	CLA	CAA-CBA-CGA-O1A
25	A	5007	LHG	O9-C7-C8-C9
26	A	5004	LMG	O9-C10-C11-C12
26	B	5002	LMG	O9-C10-C11-C12
21	B	1211	CLA	C5-C6-C7-C8
21	b	1219	CLA	C10-C11-C12-C13
21	b	1223	CLA	C10-C11-C12-C13
21	2	1218	CLA	C8-C10-C11-C12
21	B	1216	CLA	CAA-CBA-CGA-O2A
21	L	1503	CLA	CAA-CBA-CGA-O2A
21	a	1118	CLA	CAA-CBA-CGA-O2A
21	a	1134	CLA	CAA-CBA-CGA-O2A
25	b	5004	LHG	O8-C23-C24-C25
21	1	1103	CLA	C2-C3-C5-C6
21	2	1202	CLA	C2-C3-C5-C6
24	6	4016	BCR	C13-C14-C15-C16
25	l	5004	LHG	O9-C7-C8-C9
21	B	1022	CLA	CAD-CBD-CGD-O2D
21	B	1210	CLA	CAD-CBD-CGD-O2D
21	B	1234	CLA	CAD-CBD-CGD-O2D
21	b	1217	CLA	CAD-CBD-CGD-O2D
21	2	1216	CLA	CAD-CBD-CGD-O2D
35	0	6001	LMT	C6-C7-C8-C9
37	L	5004	DGD	CDA-CEA-CFA-CGA
21	b	1226	CLA	CAA-CBA-CGA-O2A
21	B	1213	CLA	C3-C5-C6-C7
25	a	5007	LHG	C5-C6-O8-C23
26	2	5002	LMG	O9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	F	5001	SQD	O10-C23-C24-C25
21	A	1102	CLA	C13-C15-C16-C17
25	A	5003	LHG	O6-C4-C5-C6
26	b	5007	LMG	C30-C31-C32-C33
21	B	1226	CLA	C2-C1-O2A-CGA
21	b	1202	CLA	C2-C1-O2A-CGA
21	1	1103	CLA	C2-C1-O2A-CGA
21	1	1108	CLA	CAA-CBA-CGA-O1A
25	1	5005	LHG	O10-C23-C24-C25
31	B	5008	SQD	C27-C28-C29-C30
21	a	1128	CLA	C10-C11-C12-C13
21	1	1127	CLA	C10-C11-C12-C13
21	2	1202	CLA	C4-C3-C5-C6
21	2	1229	CLA	C4-C3-C5-C6
26	2	5005	LMG	C21-C22-C23-C24
21	A	1126	CLA	CAA-CBA-CGA-O2A
21	B	1204	CLA	CAA-CBA-CGA-O2A
21	B	1214	CLA	CAA-CBA-CGA-O2A
21	B	1217	CLA	CAA-CBA-CGA-O2A
21	a	1136	CLA	CAA-CBA-CGA-O2A
21	b	1211	CLA	CAA-CBA-CGA-O2A
21	2	1234	CLA	CAA-CBA-CGA-O2A
25	a	5007	LHG	O8-C23-C24-C25
26	b	5005	LMG	O7-C10-C11-C12
21	J	1303	CLA	C15-C16-C17-C18
21	1	1115	CLA	C16-C17-C18-C20
21	A	1801	CLA	CAA-CBA-CGA-O1A
21	b	1210	CLA	CAA-CBA-CGA-O1A
26	K	5009	LMG	O9-C10-C11-C12
31	L	5001	SQD	O49-C7-C8-C9
21	A	1103	CLA	CAA-CBA-CGA-O2A
21	A	1128	CLA	CAA-CBA-CGA-O2A
21	B	1226	CLA	CAA-CBA-CGA-O2A
21	1	1115	CLA	CAA-CBA-CGA-O2A
25	l	5003	LHG	O8-C23-C24-C25
21	B	1210	CLA	CAA-CBA-CGA-O1A
21	a	1122	CLA	CAA-CBA-CGA-O1A
26	b	5005	LMG	O10-C28-C29-C30

There are no ring outliers.

415 monomers are involved in 1664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	1221	CLA	10	0
21	J	1303	CLA	2	0
21	a	1112	CLA	5	0
21	2	1215	CLA	4	0
26	K	5009	LMG	11	0
21	K	1401	CLA	8	0
21	7	1303	CLA	1	0
24	1	4007	BCR	7	0
24	7	4013	BCR	6	0
30	B	4006	ECH	4	0
25	F	5002	LHG	2	0
24	I	4018	BCR	6	0
24	1	4019	BCR	2	0
21	F	1302	CLA	3	0
21	2	1214	CLA	8	0
21	2	1206	CLA	6	0
21	B	1238	CLA	3	0
24	B	4018	BCR	8	0
21	a	1124	CLA	5	0
21	2	1023	CLA	9	0
21	1	1104	CLA	5	0
21	a	1012	CLA	7	0
21	A	1137	CLA	10	0
21	a	1120	CLA	5	0
30	M	4021	ECH	2	0
21	a	1122	CLA	6	0
24	f	4016	BCR	4	0
21	A	1135	CLA	12	0
26	A	5004	LMG	3	0
21	b	1209	CLA	5	0
21	2	1239	CLA	4	0
25	L	5005	LHG	7	0
21	1	1139	CLA	10	0
21	1	1136	CLA	6	0
21	A	1121	CLA	3	0
21	1	1129	CLA	3	0
21	A	1125	CLA	4	0
26	A	5002	LMG	3	0
21	B	1226	CLA	4	0
21	A	1127	CLA	3	0
21	A	1105	CLA	7	0
30	b	4006	ECH	5	0
21	A	1132	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	a	1126	CLA	9	0
21	1	1105	CLA	5	0
21	B	1232	CLA	2	0
25	l	5001	LHG	5	0
21	B	1230	CLA	6	0
21	b	1202	CLA	4	0
28	h	4020	45D	7	0
21	A	1131	CLA	3	0
21	1	1137	CLA	4	0
21	A	1101	CLA	11	0
24	L	4019	BCR	2	0
21	1	1135	CLA	6	0
25	a	5005	LHG	5	0
21	1	1109	CLA	8	0
21	b	1227	CLA	9	0
21	A	1120	CLA	2	0
24	B	4014	BCR	7	0
21	B	1208	CLA	1	0
21	a	1140	CLA	6	0
21	b	1235	CLA	10	0
21	1	1122	CLA	3	0
21	A	1106	CLA	5	0
35	0	6001	LMT	4	0
24	A	4002	BCR	6	0
21	B	1218	CLA	2	0
25	0	5004	LHG	2	0
21	b	1022	CLA	5	0
26	1	5002	LMG	1	0
24	K	4001	BCR	4	0
21	a	1106	CLA	4	0
21	2	1230	CLA	1	0
25	1	5007	LHG	4	0
21	b	1218	CLA	3	0
24	B	4017	BCR	9	0
21	2	1207	CLA	1	0
24	a	4019	BCR	3	0
24	b	4005	BCR	1	0
21	b	1213	CLA	9	0
21	K	1402	CLA	5	0
25	1	5003	LHG	3	0
21	2	1235	CLA	2	0
21	A	1108	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1138	CLA	5	0
21	f	1302	CLA	4	0
25	1	5001	LHG	3	0
21	A	1107	CLA	12	0
24	2	4014	BCR	7	0
21	1	1103	CLA	9	0
24	0	4022	BCR	6	0
21	B	1206	CLA	7	0
21	7	1302	CLA	2	0
26	b	5002	LMG	10	0
21	k	1401	CLA	1	0
21	A	1122	CLA	5	0
21	A	1114	CLA	1	0
21	2	1218	CLA	4	0
21	B	1209	CLA	4	0
21	a	1135	CLA	8	0
21	b	1206	CLA	5	0
21	1	1107	CLA	3	0
21	B	1225	CLA	7	0
21	B	1212	CLA	7	0
21	B	1227	CLA	9	0
21	1	1101	CLA	10	0
23	C	3003	SF4	4	0
21	b	1230	CLA	8	0
21	2	1213	CLA	2	0
26	a	5002	LMG	7	0
21	A	1115	CLA	3	0
21	1	1115	CLA	4	0
21	B	1221	CLA	8	0
21	B	1240	CLA	7	0
24	b	4018	BCR	6	0
21	a	1132	CLA	6	0
24	b	4010	BCR	7	0
21	B	1215	CLA	4	0
21	B	1201	CLA	5	0
21	2	1202	CLA	6	0
24	A	4001	BCR	6	0
21	B	1202	CLA	3	0
24	h	4018	BCR	6	0
30	m	4021	ECH	1	0
21	B	1022	CLA	1	0
21	A	1103	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	5004	LMG	3	0
21	A	1013	CLA	10	0
25	A	5005	LHG	7	0
21	2	1229	CLA	7	0
21	2	1209	CLA	1	0
25	1	5005	LHG	1	0
21	l	1501	CLA	7	0
24	L	4022	BCR	5	0
21	A	1123	CLA	5	0
21	a	1128	CLA	11	0
34	J	4015	ZEX	5	0
24	A	4008	BCR	3	0
24	a	4001	BCR	5	0
21	8	1401	CLA	3	0
21	F	1301	CLA	3	0
21	2	1227	CLA	5	0
21	B	1023	CLA	7	0
21	b	1220	CLA	5	0
35	l	6001	LMT	1	0
24	j	4013	BCR	8	0
24	a	4008	BCR	6	0
21	A	1104	CLA	4	0
25	A	5001	LHG	5	0
24	2	4010	BCR	7	0
21	2	1201	CLA	7	0
24	2	4011	BCR	7	0
21	b	1204	CLA	5	0
24	9	4021	BCR	5	0
21	B	1204	CLA	5	0
21	b	1207	CLA	6	0
24	b	4014	BCR	4	0
21	A	1118	CLA	11	0
21	2	1022	CLA	3	0
25	l	5004	LHG	1	0
21	l	1503	CLA	3	0
21	A	1139	CLA	5	0
21	L	1502	CLA	7	0
24	l	4022	BCR	3	0
21	2	1228	CLA	7	0
21	a	1127	CLA	8	0
21	1	1124	CLA	3	0
21	1	1123	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	5004	LHG	7	0
24	6	4016	BCR	1	0
24	0	4019	BCR	4	0
24	a	4002	BCR	7	0
21	B	1228	CLA	3	0
24	k	4001	BCR	5	0
21	f	1301	CLA	6	0
21	A	1130	CLA	5	0
21	2	1204	CLA	6	0
21	A	1117	CLA	3	0
21	L	1503	CLA	5	0
24	b	4017	BCR	9	0
27	A	7001	ACT	1	0
21	1	1013	CLA	7	0
21	A	1129	CLA	8	0
21	1	1117	CLA	4	0
21	a	1101	CLA	10	0
21	a	1105	CLA	5	0
31	L	5001	SQD	8	0
21	0	1501	CLA	6	0
21	A	1801	CLA	13	0
21	2	1232	CLA	1	0
24	2	4018	BCR	4	0
21	a	1011	CLA	7	0
24	1	4003	BCR	7	0
21	B	1216	CLA	10	0
31	0	5005	SQD	2	0
26	2	5002	LMG	6	0
21	2	1224	CLA	4	0
21	1	1012	CLA	13	0
21	A	1136	CLA	6	0
22	A	2001	PQN	3	0
21	B	1222	CLA	10	0
21	B	1214	CLA	9	0
21	A	1128	CLA	8	0
22	1	2001	PQN	5	0
24	A	4007	BCR	8	0
21	1	1128	CLA	8	0
24	8	4001	BCR	3	0
25	A	5003	LHG	7	0
21	2	1219	CLA	1	0
21	1	1801	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1102	CLA	3	0
21	2	1220	CLA	3	0
21	a	1138	CLA	3	0
21	b	1221	CLA	7	0
31	L	5002	SQD	7	0
21	b	1215	CLA	7	0
21	b	1238	CLA	7	0
21	1	1110	CLA	2	0
21	a	1013	CLA	9	0
21	A	1119	CLA	9	0
24	a	4012	BCR	10	0
21	B	1213	CLA	9	0
30	b	4011	ECH	11	0
21	a	1103	CLA	9	0
21	2	1222	CLA	6	0
21	B	1231	CLA	2	0
21	b	1240	CLA	6	0
21	a	1119	CLA	7	0
21	b	1023	CLA	12	0
21	a	1139	CLA	5	0
24	i	4018	BCR	7	0
21	b	1226	CLA	13	0
21	b	1239	CLA	6	0
21	b	1237	CLA	4	0
21	A	1116	CLA	4	0
21	b	1232	CLA	6	0
21	a	1118	CLA	6	0
28	B	4011	45D	5	0
21	2	1238	CLA	5	0
25	A	5007	LHG	8	0
21	a	1117	CLA	7	0
21	2	1205	CLA	8	0
21	A	1109	CLA	6	0
21	b	1216	CLA	7	0
21	j	1302	CLA	6	0
24	l	4019	BCR	5	0
26	0	5001	LMG	4	0
21	0	1502	CLA	6	0
21	2	1231	CLA	1	0
21	a	1137	CLA	6	0
25	B	5006	LHG	3	0
37	L	5004	DGD	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	b	1234	CLA	7	0
21	1	1102	CLA	4	0
24	b	4004	BCR	6	0
24	B	4010	BCR	9	0
21	B	1210	CLA	4	0
21	b	1214	CLA	10	0
24	B	4005	BCR	5	0
25	2	5004	LHG	5	0
21	B	1203	CLA	6	0
31	B	5008	SQD	5	0
22	a	2001	PQN	4	0
26	1	5004	LMG	4	0
21	1	1131	CLA	4	0
31	F	5001	SQD	4	0
24	a	4007	BCR	1	0
21	b	1203	CLA	10	0
21	a	1801	CLA	2	0
21	2	1216	CLA	4	0
21	b	1225	CLA	9	0
21	1	1125	CLA	8	0
24	1	4001	BCR	7	0
21	1	1140	CLA	4	0
21	b	1210	CLA	4	0
21	A	1113	CLA	3	0
21	b	1205	CLA	7	0
21	1	1113	CLA	1	0
21	B	1236	CLA	7	0
21	B	1239	CLA	4	0
21	B	1021	CLA	8	0
25	M	5001	LHG	2	0
21	A	1011	CLA	4	0
21	2	1225	CLA	7	0
21	b	1201	CLA	5	0
21	a	1115	CLA	5	0
21	a	1104	CLA	5	0
25	a	5001	LHG	4	0
21	a	1110	CLA	6	0
21	b	1211	CLA	5	0
24	1	4008	BCR	3	0
21	A	1126	CLA	8	0
24	A	4012	BCR	6	0
21	2	1210	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1134	CLA	7	0
21	b	1231	CLA	6	0
21	2	1203	CLA	10	0
22	B	2002	PQN	2	0
21	a	1136	CLA	7	0
24	A	4003	BCR	4	0
21	A	1111	CLA	1	0
26	B	5005	LMG	2	0
24	B	4004	BCR	5	0
30	2	4006	ECH	3	0
21	1	1130	CLA	4	0
24	2	4017	BCR	8	0
21	a	1133	CLA	8	0
21	2	1208	CLA	3	0
21	A	1124	CLA	6	0
21	B	1211	CLA	6	0
25	A	5006	LHG	4	0
21	2	1236	CLA	4	0
24	a	4003	BCR	2	0
31	f	5001	SQD	8	0
21	a	1111	CLA	9	0
21	1	1127	CLA	7	0
21	1	1116	CLA	8	0
21	a	1108	CLA	6	0
21	b	1228	CLA	5	0
21	1	1132	CLA	5	0
21	B	1219	CLA	7	0
24	1	4002	BCR	6	0
21	1	1111	CLA	14	0
21	1	1126	CLA	9	0
24	1	4012	BCR	7	0
21	1	1121	CLA	5	0
22	2	2002	PQN	3	0
21	1	1134	CLA	5	0
21	b	1219	CLA	4	0
26	2	5005	LMG	4	0
24	2	4004	BCR	1	0
21	l	1502	CLA	6	0
21	B	1234	CLA	10	0
24	J	4013	BCR	8	0
21	a	1102	CLA	7	0
21	b	1223	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	1207	CLA	9	0
21	B	1224	CLA	11	0
21	k	1402	CLA	1	0
21	2	1211	CLA	1	0
21	1	1011	CLA	4	0
21	2	1226	CLA	3	0
21	0	1503	CLA	6	0
21	a	1107	CLA	4	0
21	6	1301	CLA	6	0
26	b	5007	LMG	2	0
25	a	5007	LHG	3	0
21	b	1021	CLA	8	0
21	8	1402	CLA	1	0
21	b	1222	CLA	13	0
25	a	5003	LHG	8	0
25	l	5003	LHG	6	0
21	a	1109	CLA	3	0
21	B	1220	CLA	7	0
21	a	1113	CLA	1	0
24	2	4005	BCR	5	0
23	c	3002	SF4	1	0
22	b	2002	PQN	2	0
21	1	1138	CLA	5	0
21	2	1234	CLA	3	0
21	A	1110	CLA	6	0
21	6	1302	CLA	1	0
21	2	1240	CLA	1	0
25	l	5002	LHG	5	0
34	7	4015	ZEX	6	0
21	a	1123	CLA	6	0
21	A	1012	CLA	6	0
21	B	1205	CLA	9	0
21	1	1120	CLA	1	0
21	a	1134	CLA	5	0
21	1	1112	CLA	1	0
24	A	4019	BCR	4	0
21	1	1106	CLA	4	0
21	2	1021	CLA	6	0
21	b	1236	CLA	6	0
21	L	1501	CLA	5	0
21	B	1237	CLA	2	0
31	b	5006	SQD	6	0

Continued on next page...

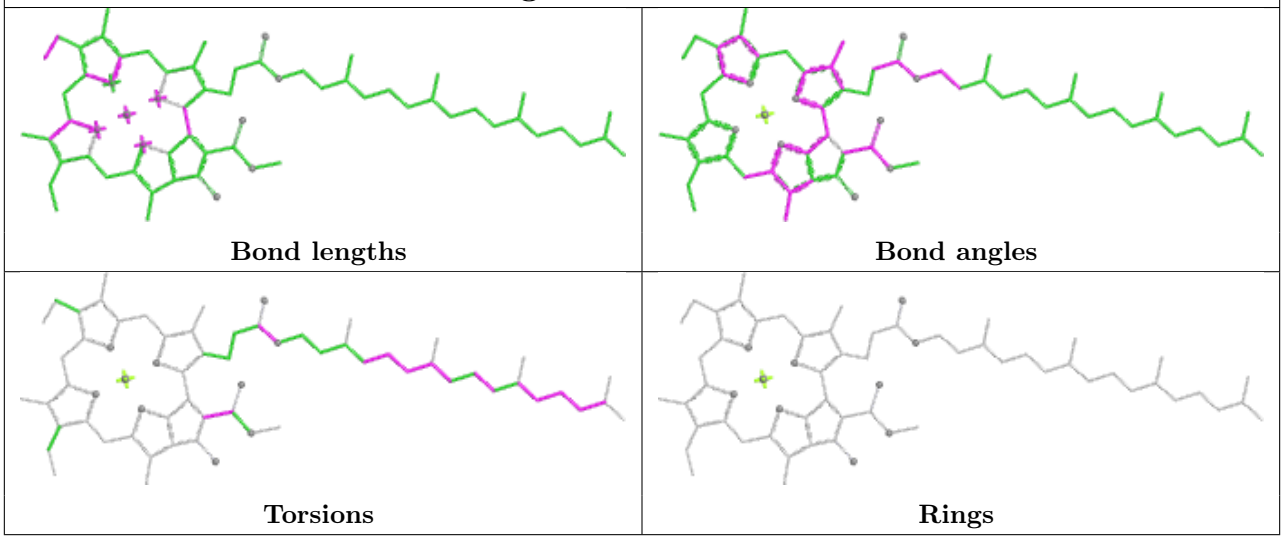
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	b	1212	CLA	14	0
21	a	1125	CLA	6	0
21	1	1119	CLA	9	0
30	i	4020	ECH	3	0
21	b	1217	CLA	5	0
21	B	1223	CLA	4	0
21	B	1217	CLA	7	0
21	a	1129	CLA	10	0
25	B	5004	LHG	9	0
26	A	5008	LMG	6	0
35	L	6001	LMT	1	0
21	A	1133	CLA	9	0
34	F	4016	ZEX	1	0
21	a	1116	CLA	5	0
21	1	1133	CLA	6	0
21	J	1302	CLA	3	0
26	b	5005	LMG	5	0
21	b	1208	CLA	4	0
21	1	1118	CLA	6	0
21	a	1131	CLA	3	0
21	2	1237	CLA	6	0
21	B	1229	CLA	5	0
21	2	1212	CLA	3	0
21	A	1140	CLA	7	0
21	A	1112	CLA	8	0
21	b	1224	CLA	5	0
21	a	1121	CLA	7	0
34	j	4015	ZEX	6	0
21	a	1130	CLA	3	0
21	B	1235	CLA	5	0
25	6	5001	LHG	1	0
21	b	1229	CLA	3	0
26	B	5002	LMG	7	0
21	2	1223	CLA	6	0
21	2	1217	CLA	1	0
25	0	5002	LHG	6	0

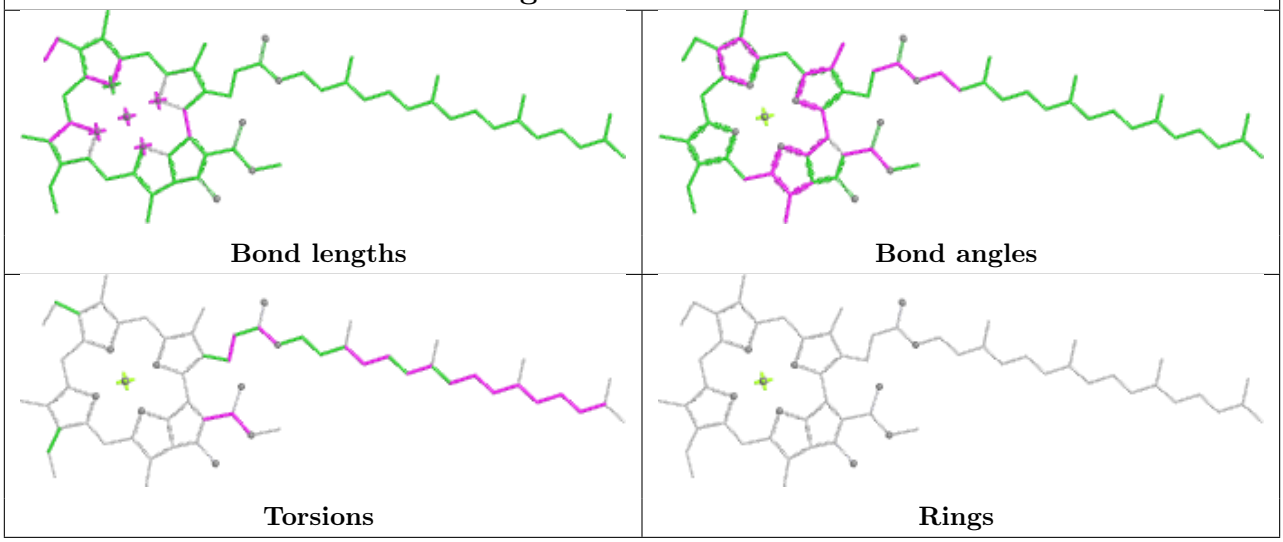
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

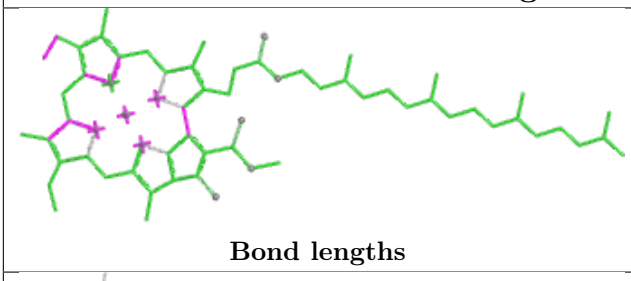
Ligand CLA 2 1221



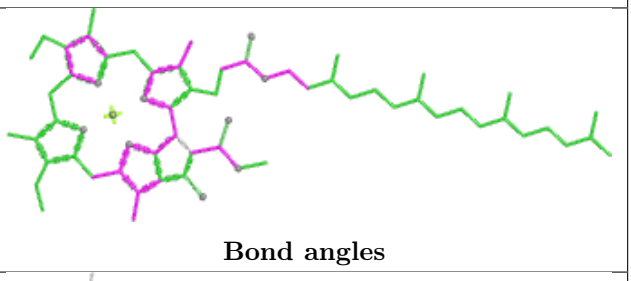
Ligand CLA J 1303



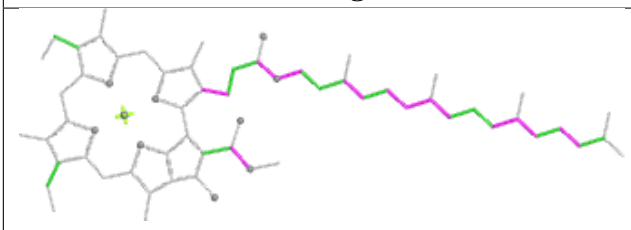
Ligand CLA a 1112



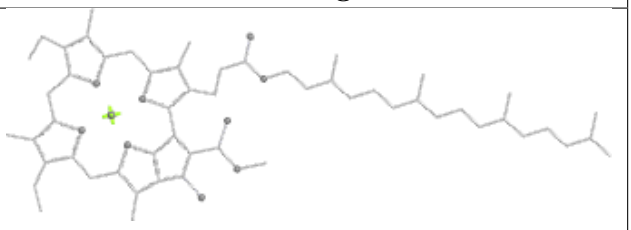
Bond lengths



Bond angles

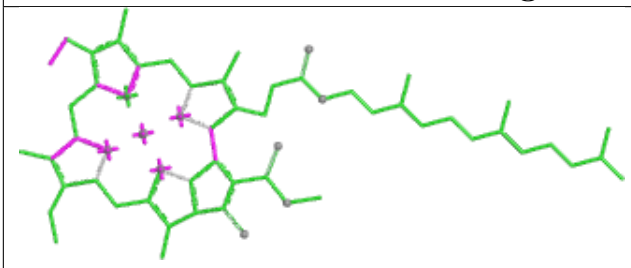


Torsions

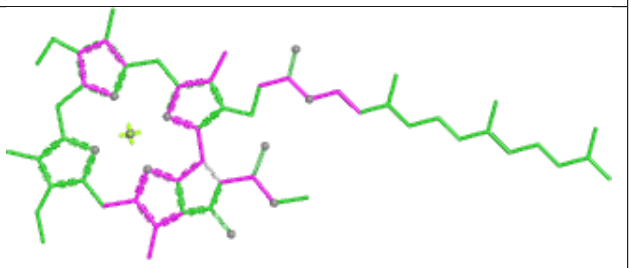


Rings

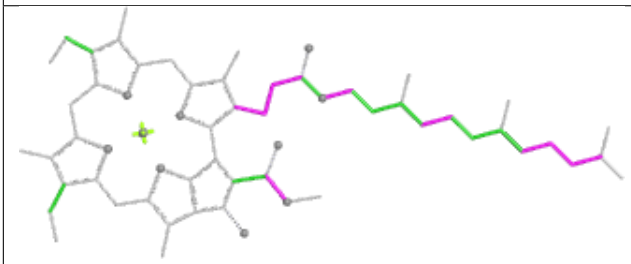
Ligand CLA 2 1215



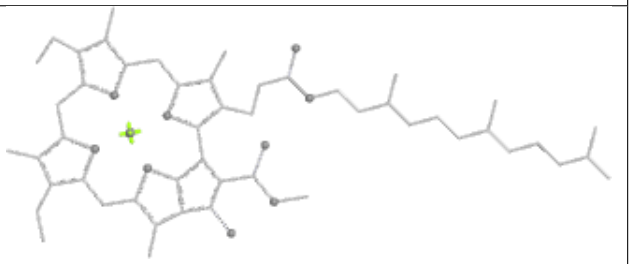
Bond lengths



Bond angles

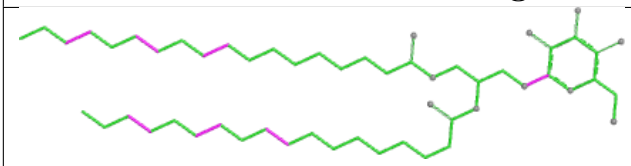


Torsions



Rings

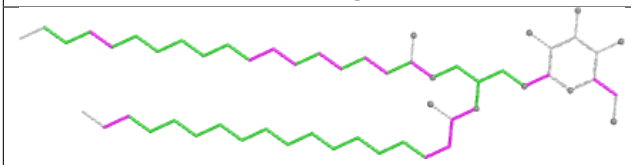
Ligand LMG K 5009



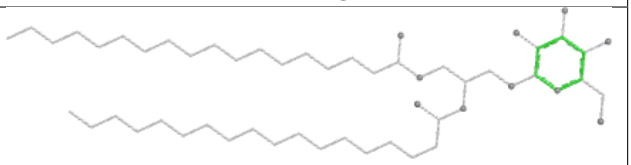
Bond lengths



Bond angles

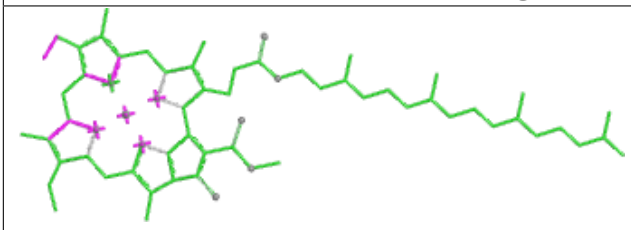


Torsions

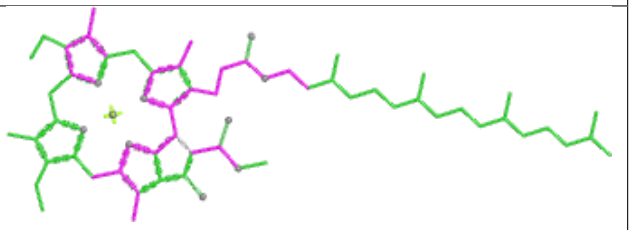


Rings

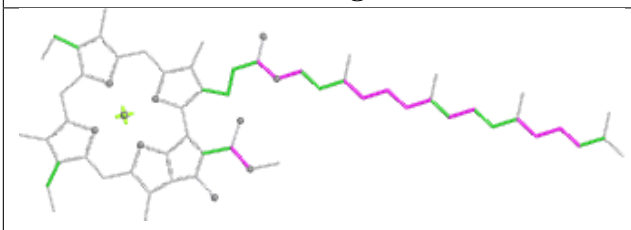
Ligand CLA K 1401



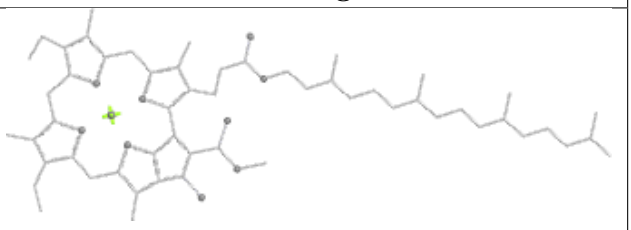
Bond lengths



Bond angles

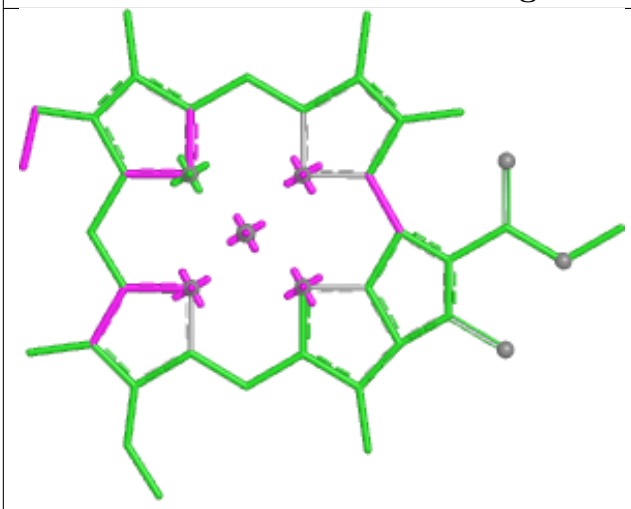


Torsions

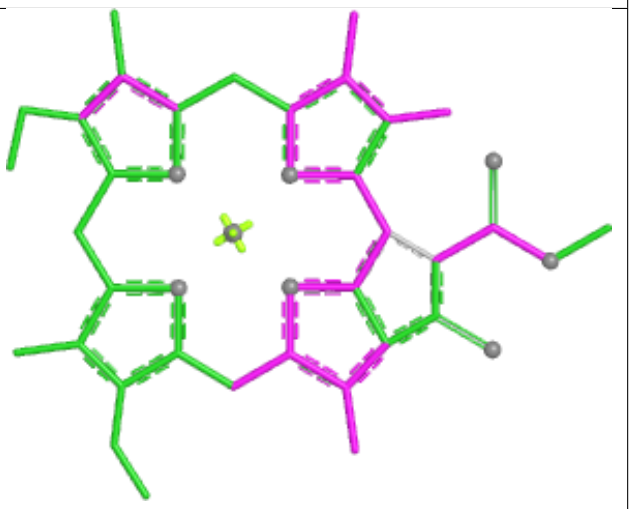


Rings

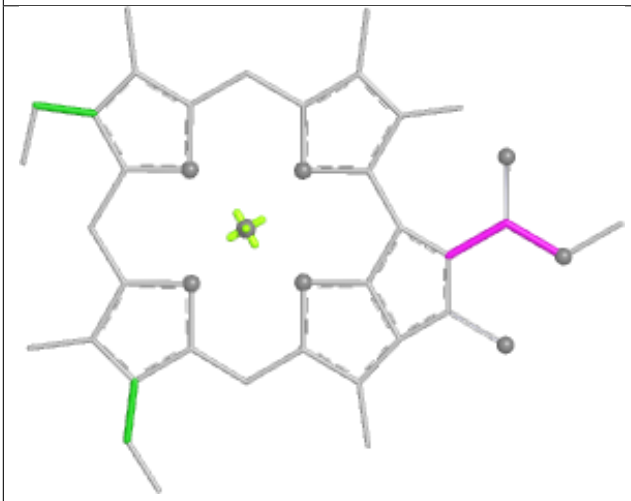
Ligand CLA 7 1303



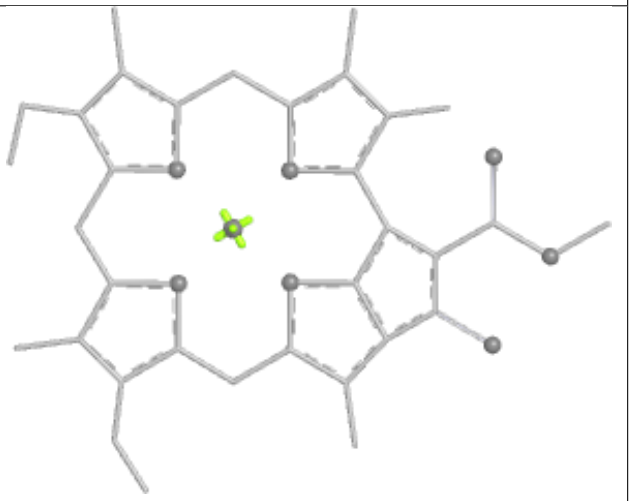
Bond lengths



Bond angles

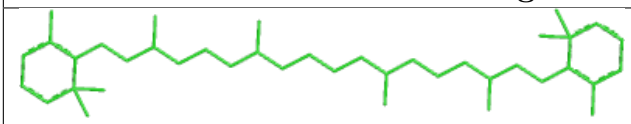


Torsions

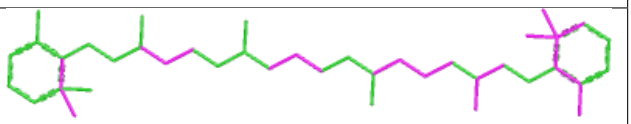


Rings

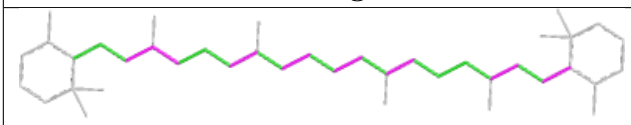
Ligand BCR 1 4007



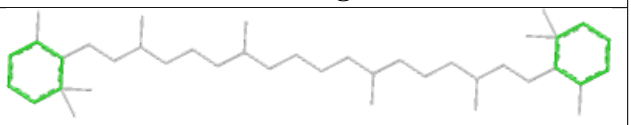
Bond lengths



Bond angles



Torsions

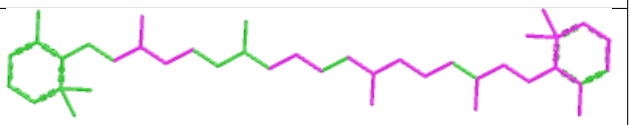


Rings

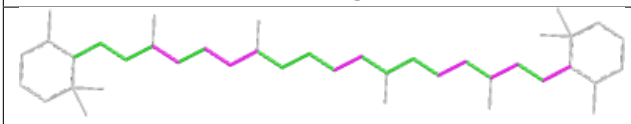
Ligand BCR 7 4013



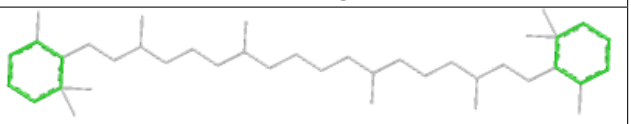
Bond lengths



Bond angles

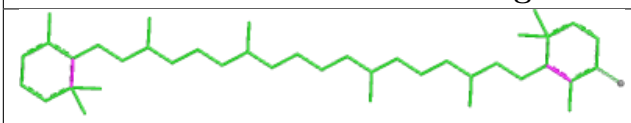


Torsions

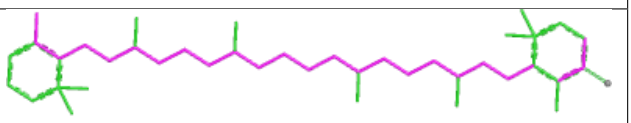


Rings

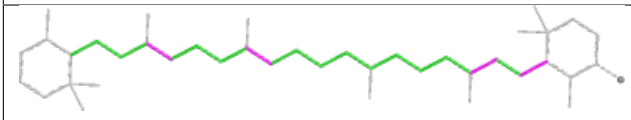
Ligand ECH B 4006



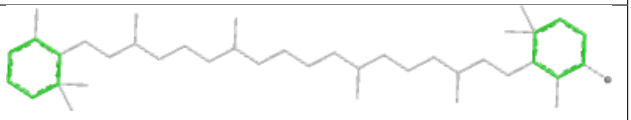
Bond lengths



Bond angles

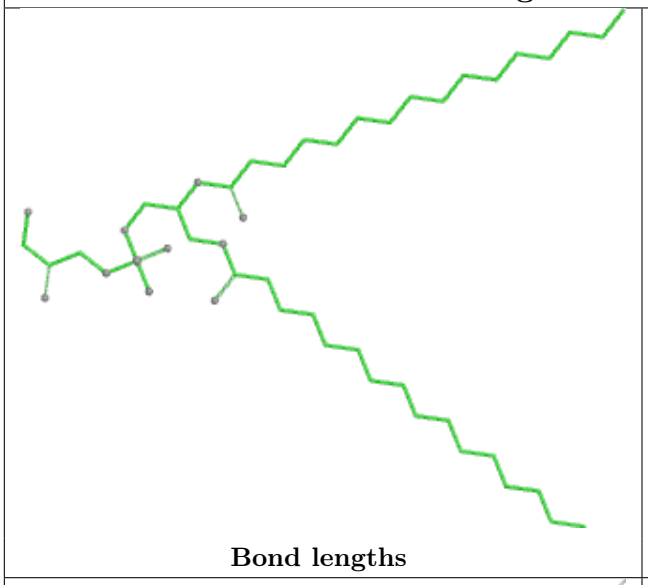


Torsions

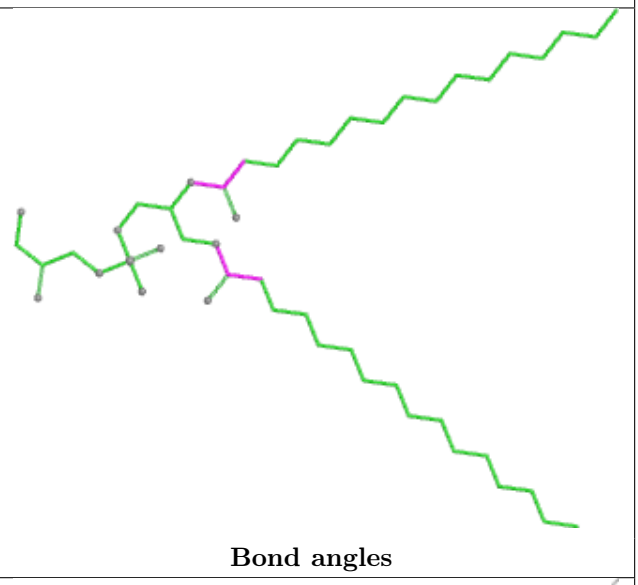


Rings

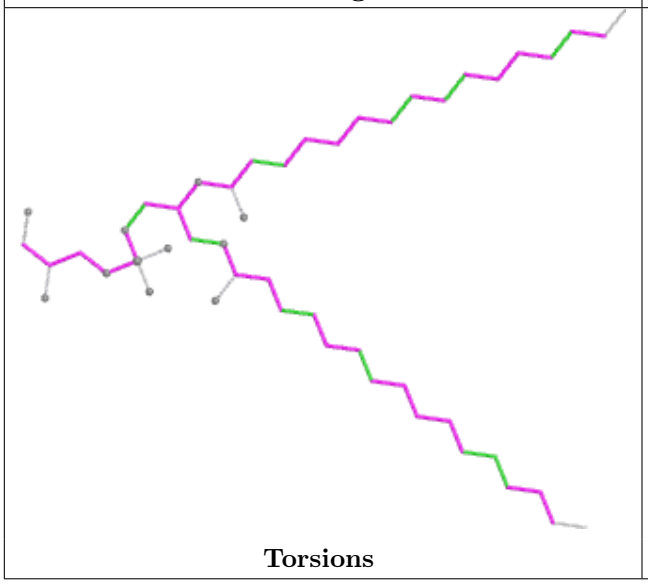
Ligand LHG F 5002



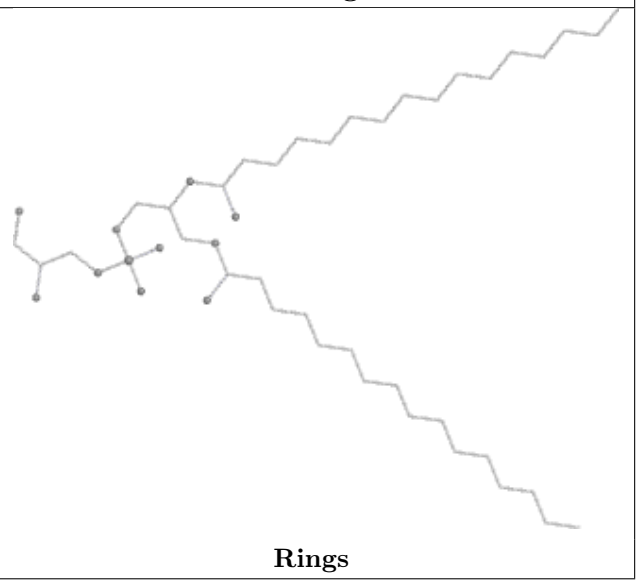
Bond lengths



Bond angles



Torsions

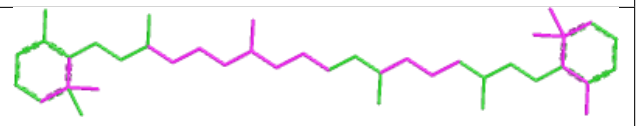


Rings

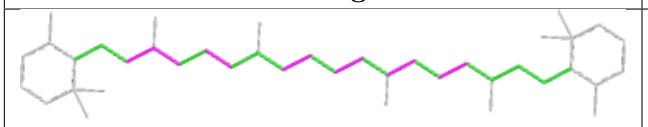
Ligand BCR I 4018



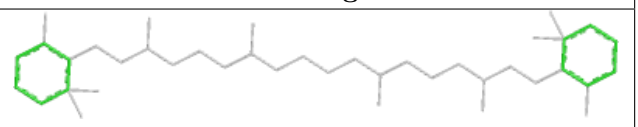
Bond lengths



Bond angles

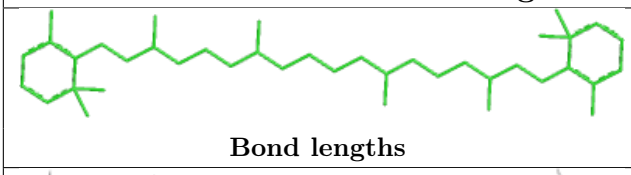


Torsions

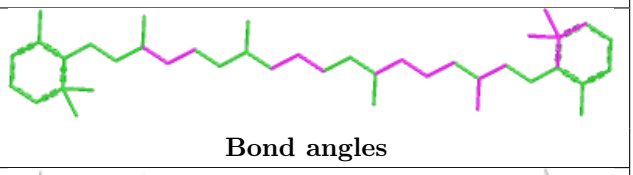


Rings

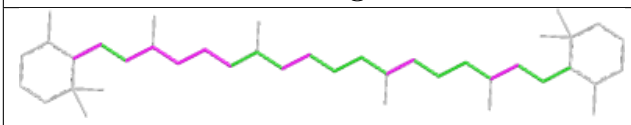
Ligand BCR 1 4019



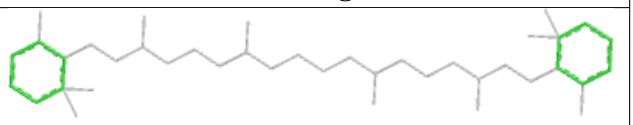
Bond lengths



Bond angles

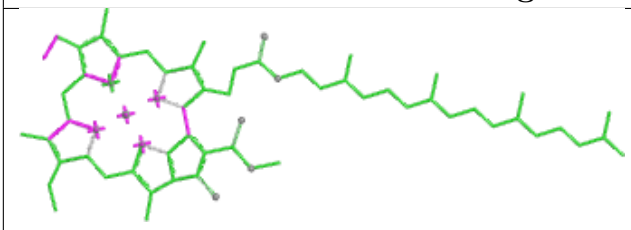


Torsions

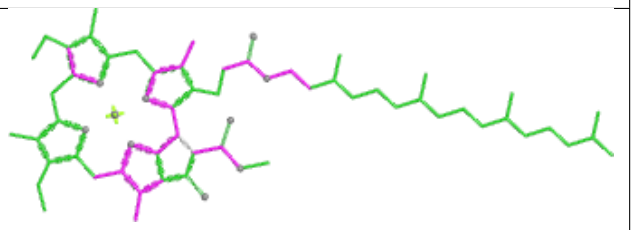


Rings

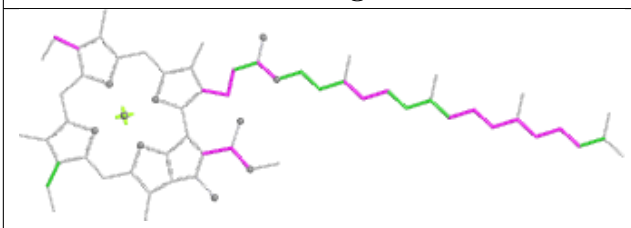
Ligand CLA F 1302



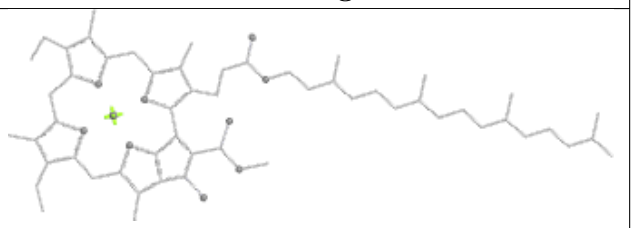
Bond lengths



Bond angles

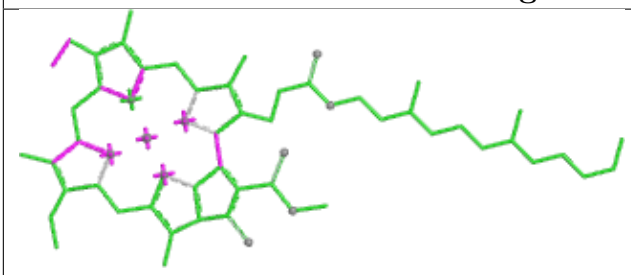


Torsions

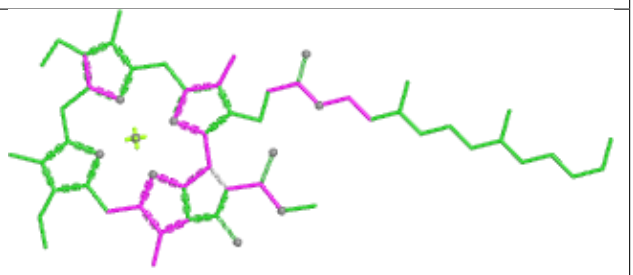


Rings

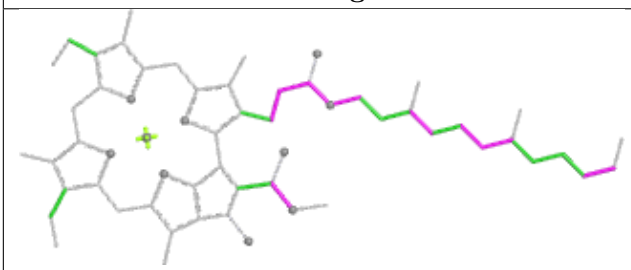
Ligand CLA 2 1214



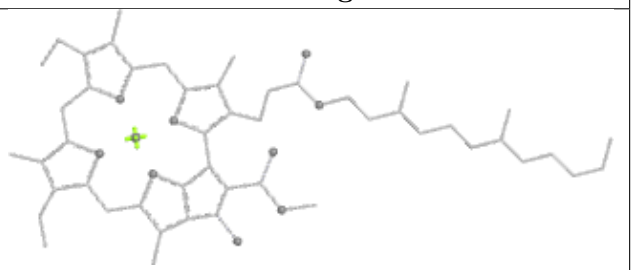
Bond lengths



Bond angles

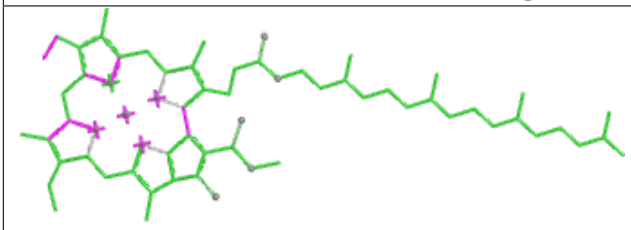


Torsions

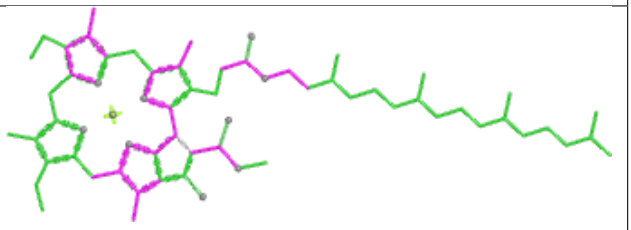


Rings

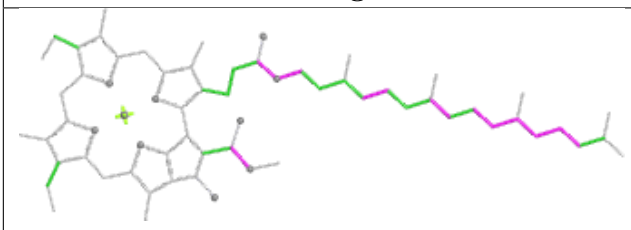
Ligand CLA 2 1206



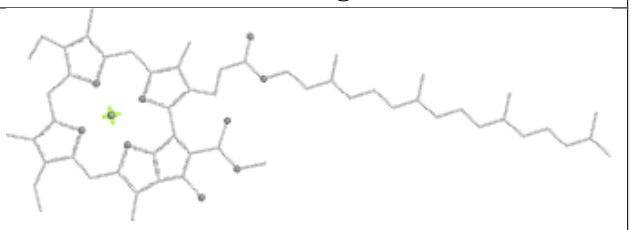
Bond lengths



Bond angles

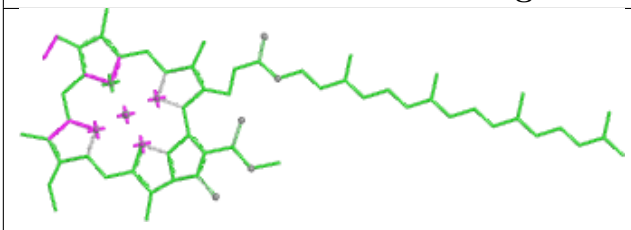


Torsions

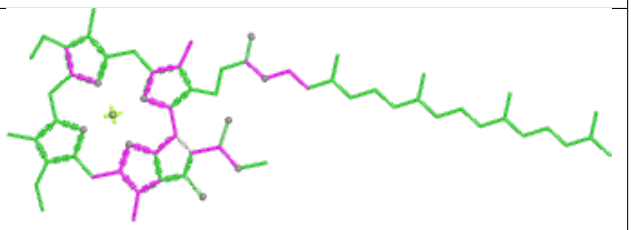


Rings

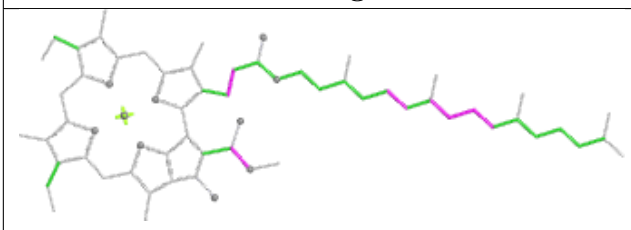
Ligand CLA B 1238



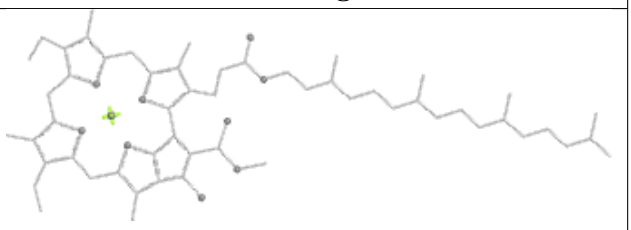
Bond lengths



Bond angles

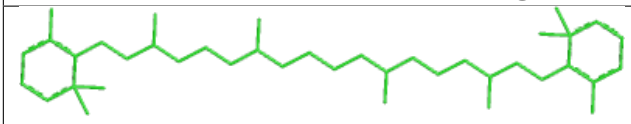


Torsions

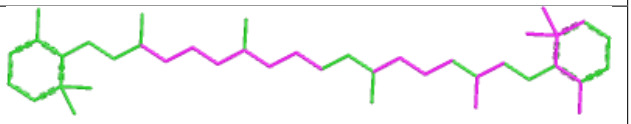


Rings

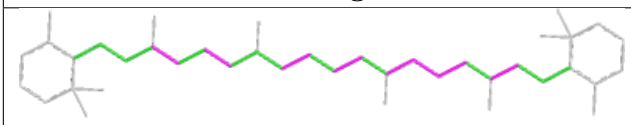
Ligand BCR B 4018



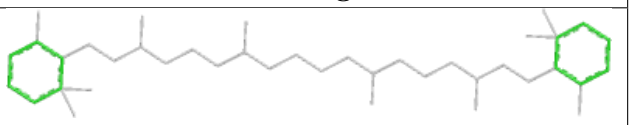
Bond lengths



Bond angles

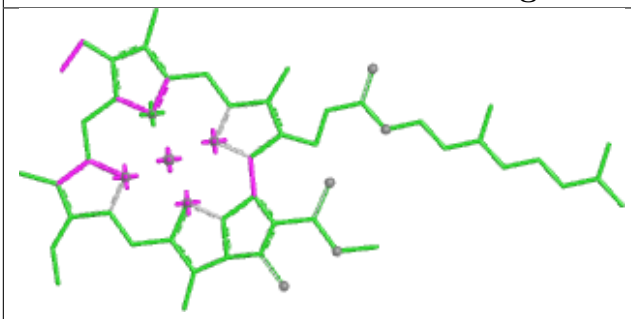


Torsions

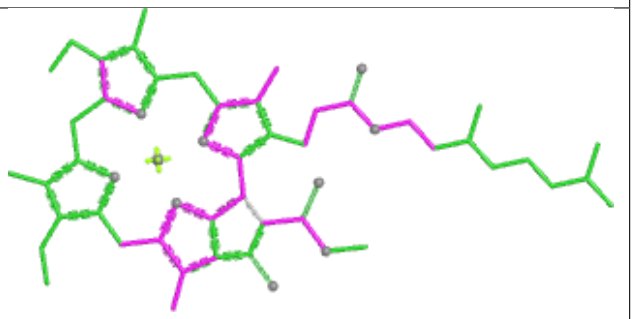


Rings

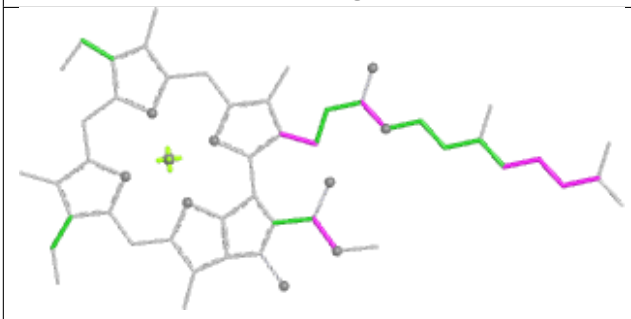
Ligand CLA a 1124



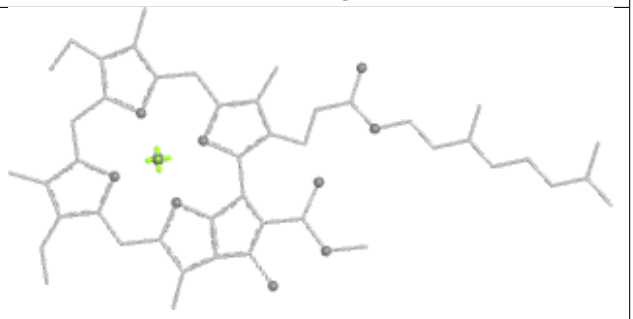
Bond lengths



Bond angles

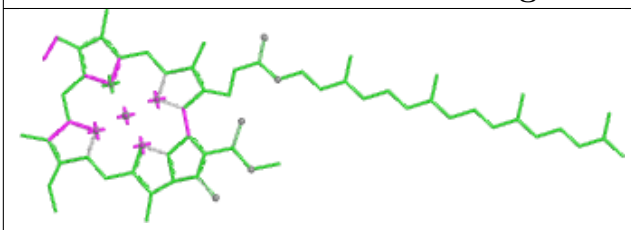


Torsions

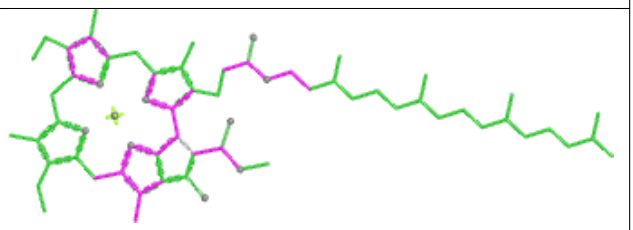


Rings

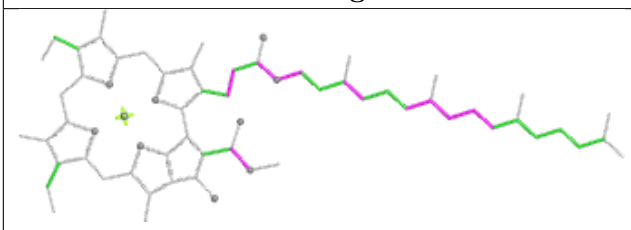
Ligand CLA 2 1023



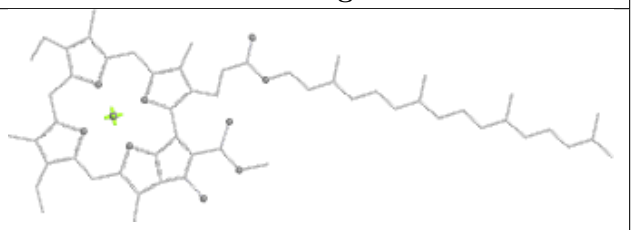
Bond lengths



Bond angles

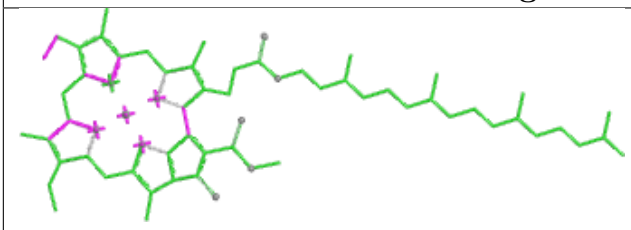


Torsions

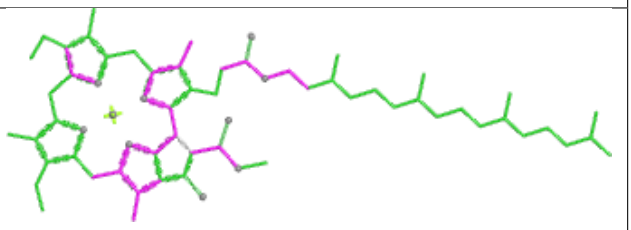


Rings

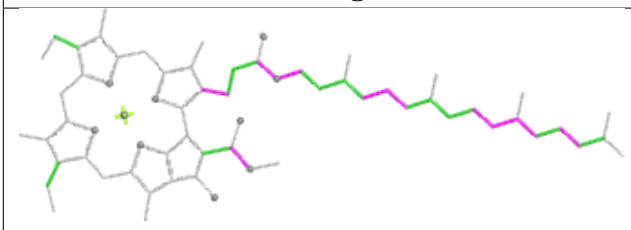
Ligand CLA 1 1104



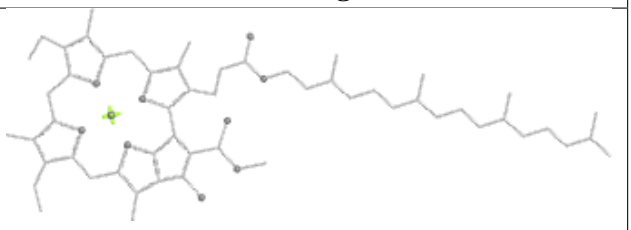
Bond lengths



Bond angles

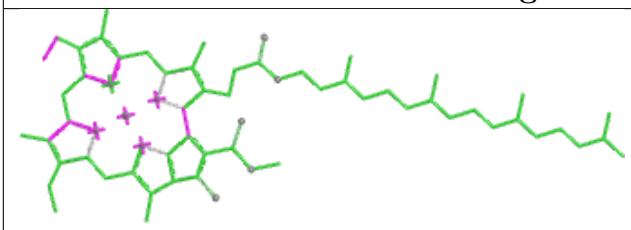


Torsions

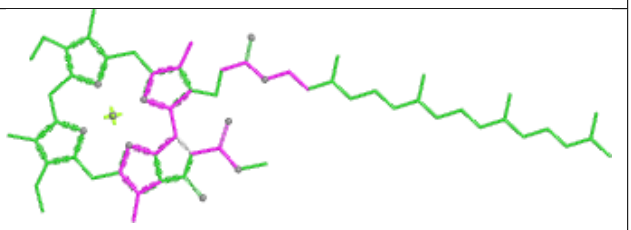


Rings

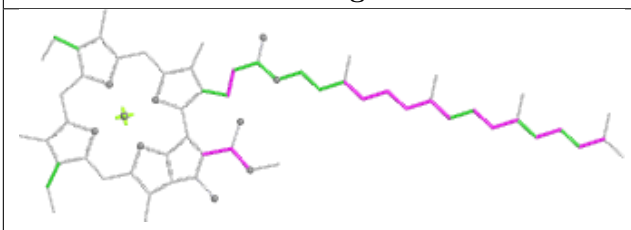
Ligand CLA a 1012



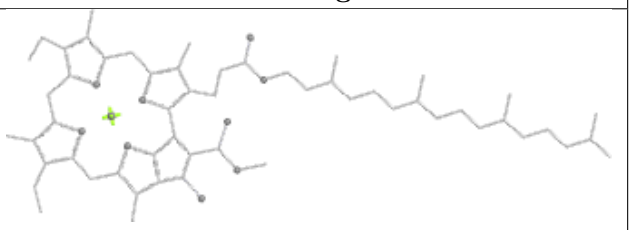
Bond lengths



Bond angles

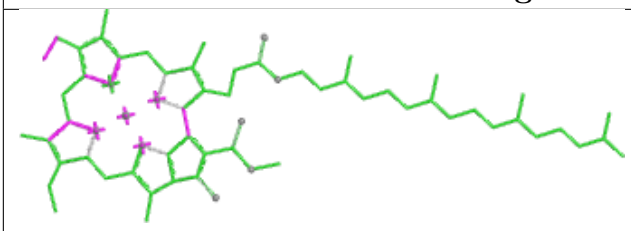


Torsions

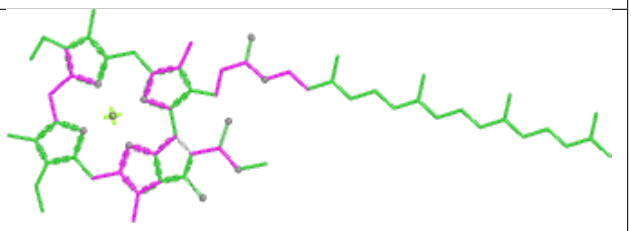


Rings

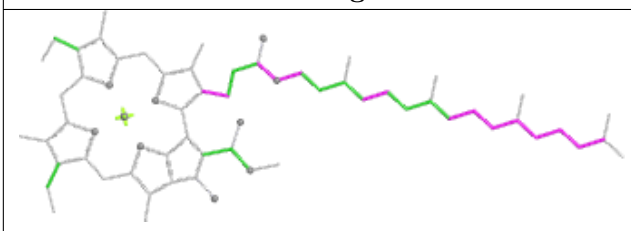
Ligand CLA A 1137



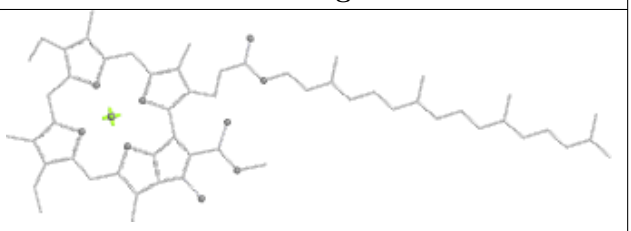
Bond lengths



Bond angles

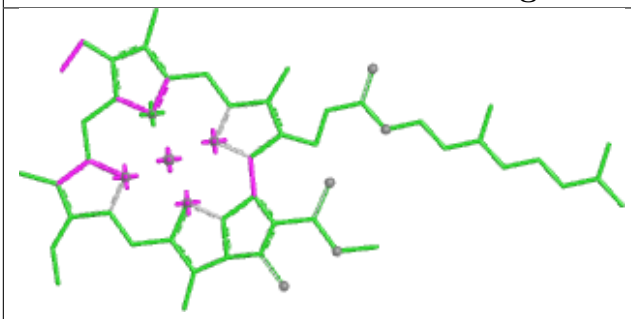


Torsions

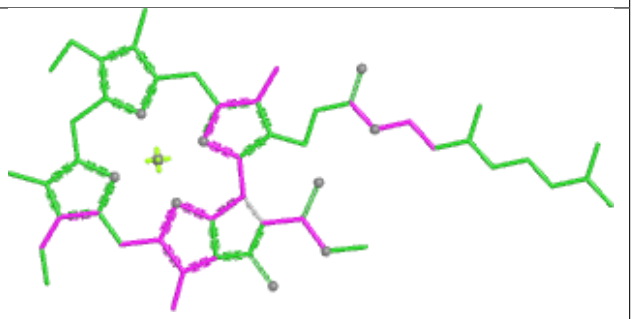


Rings

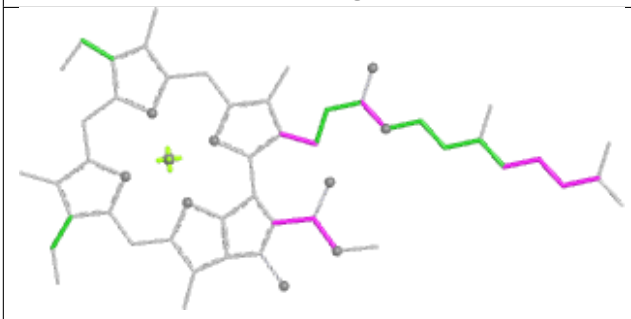
Ligand CLA a 1120



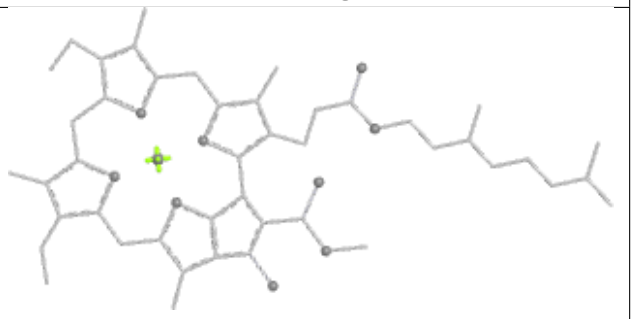
Bond lengths



Bond angles

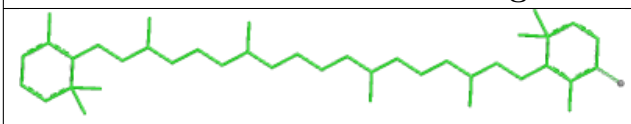


Torsions

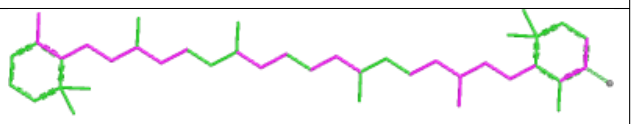


Rings

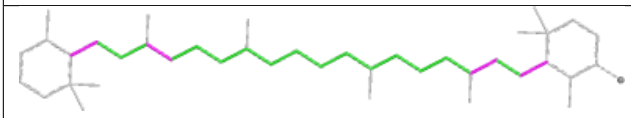
Ligand ECH M 4021



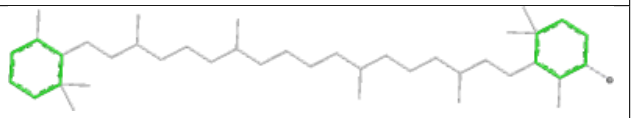
Bond lengths



Bond angles

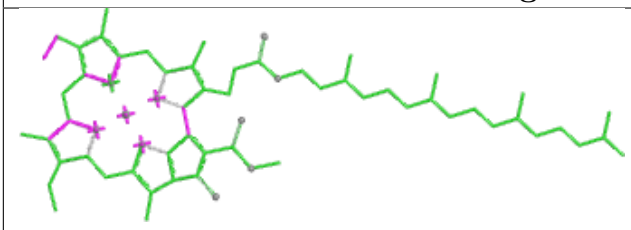


Torsions

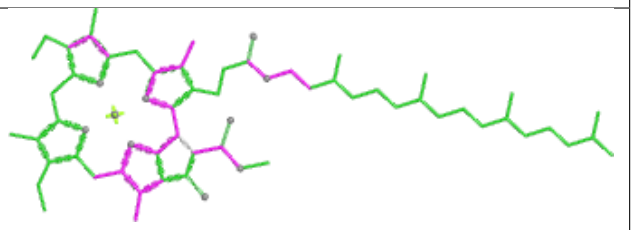


Rings

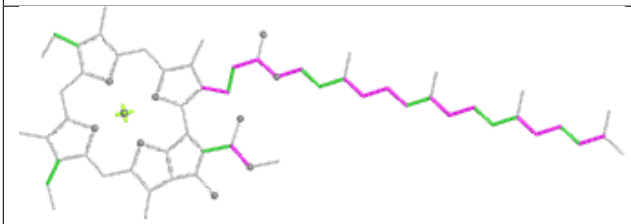
Ligand CLA a 1122



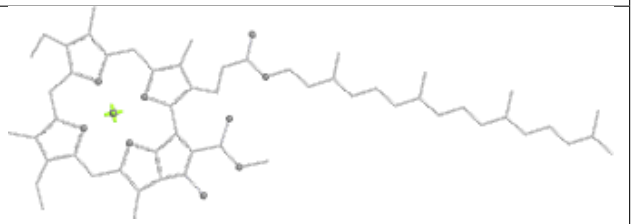
Bond lengths



Bond angles

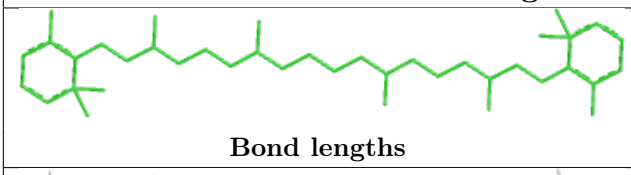


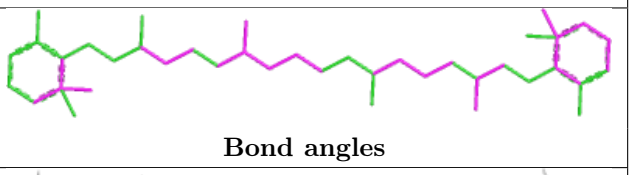
Torsions

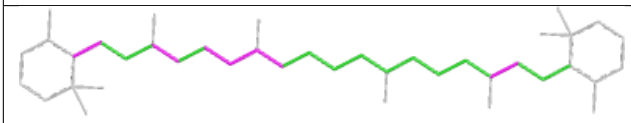


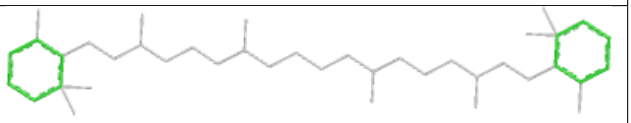
Rings

Ligand BCR f 4016

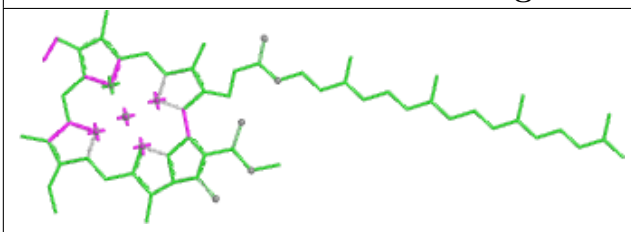

Bond lengths

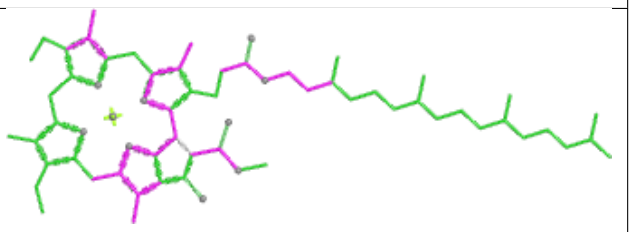

Bond angles

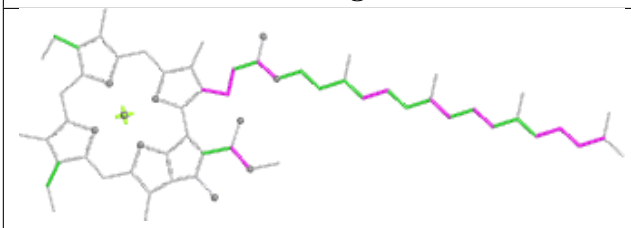

Torsions

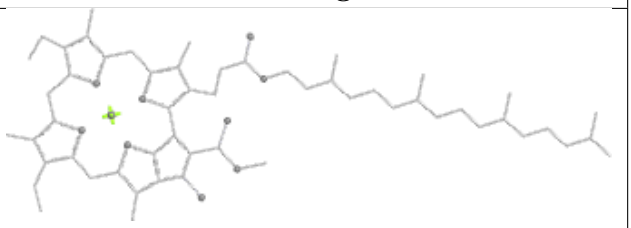

Rings

Ligand CLA A 1135

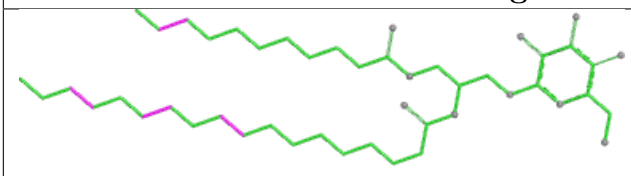

Bond lengths

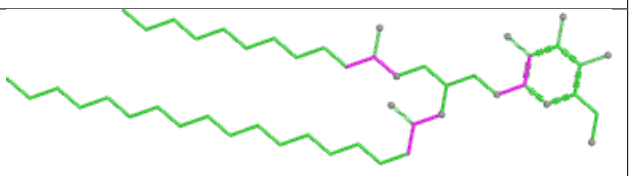

Bond angles

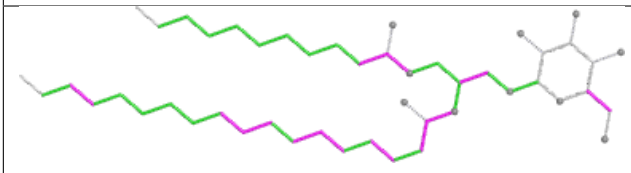

Torsions

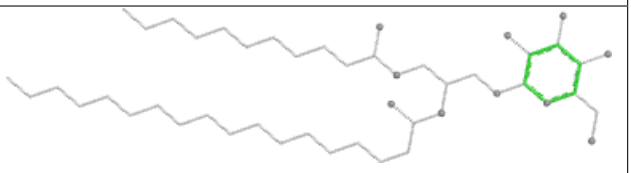

Rings

Ligand LMG A 5004

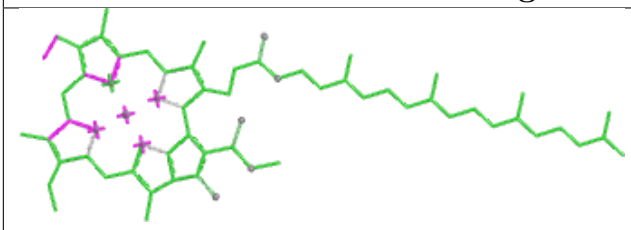

Bond lengths


Bond angles

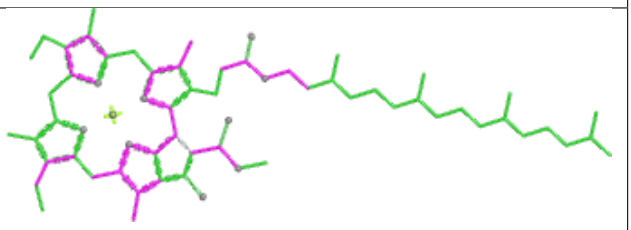

Torsions


Rings

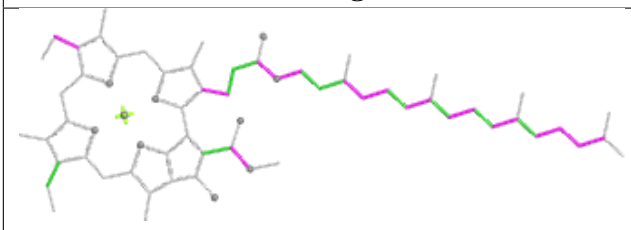
Ligand CLA b 1209



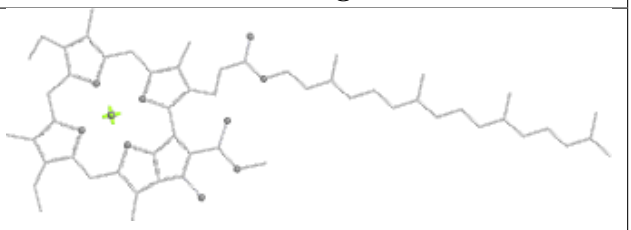
Bond lengths



Bond angles

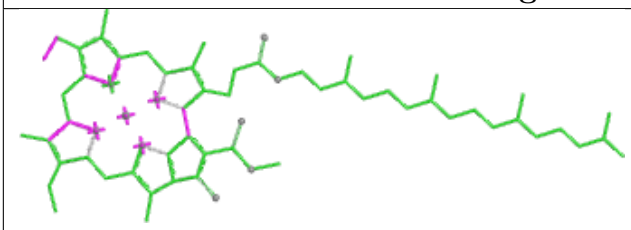


Torsions

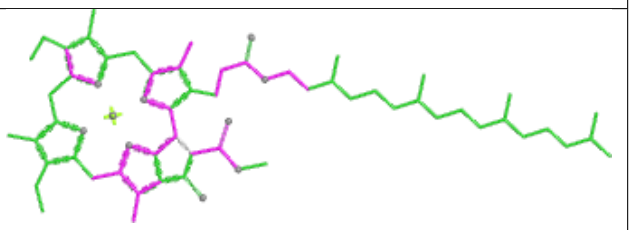


Rings

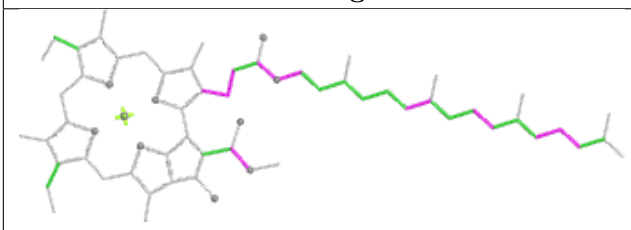
Ligand CLA 2 1239



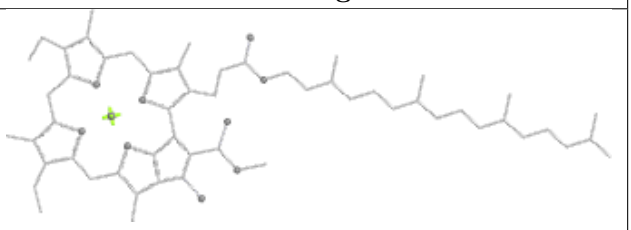
Bond lengths



Bond angles

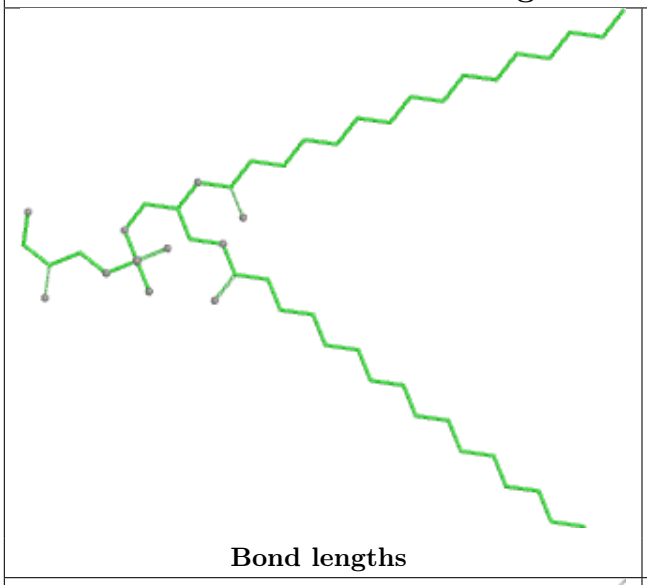


Torsions

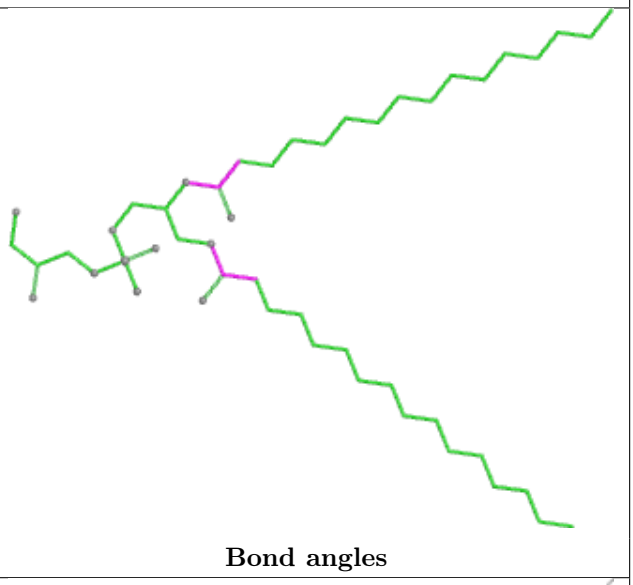


Rings

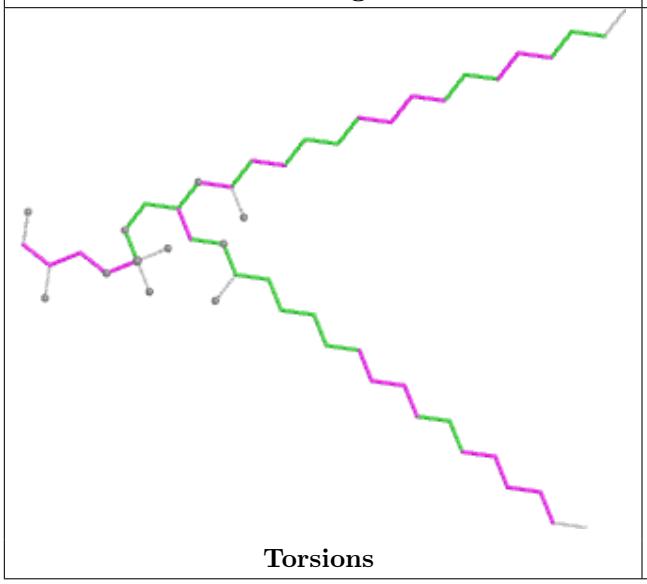
Ligand LHG L 5005



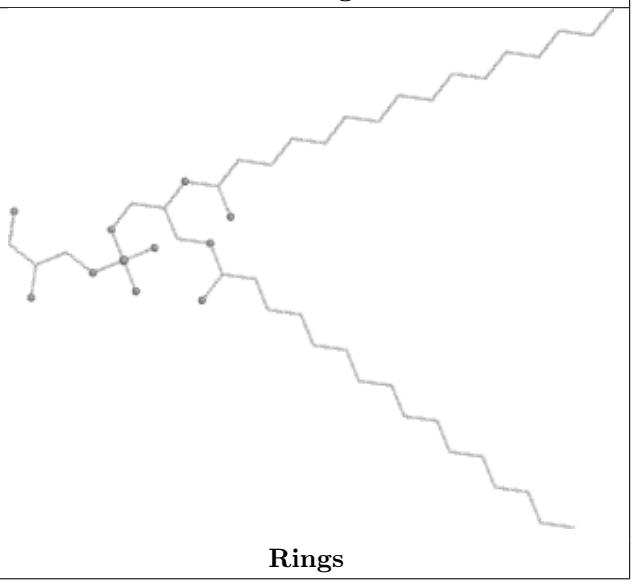
Bond lengths



Bond angles

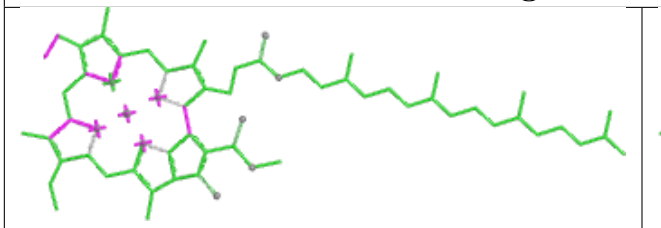


Torsions

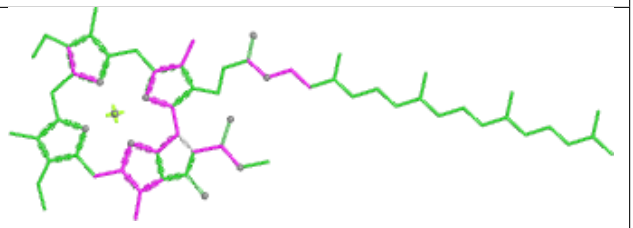


Rings

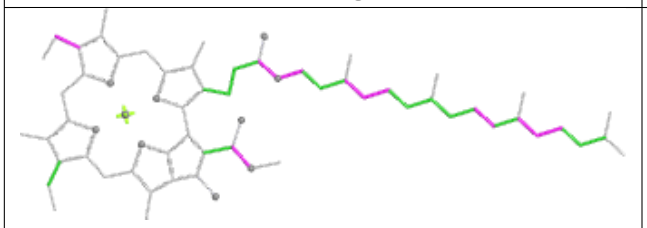
Ligand CLA 1 1139



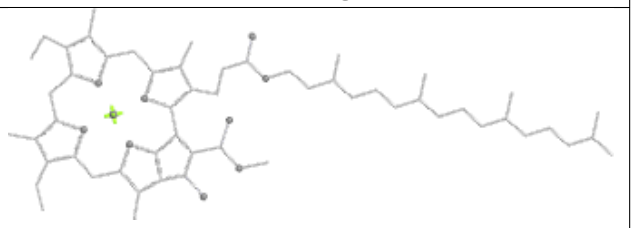
Bond lengths



Bond angles

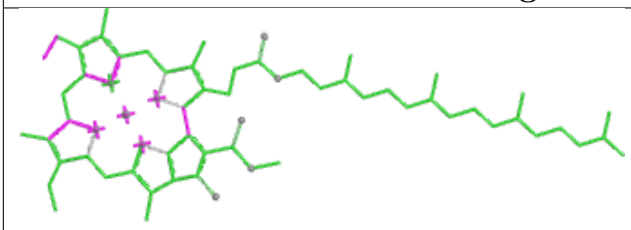


Torsions

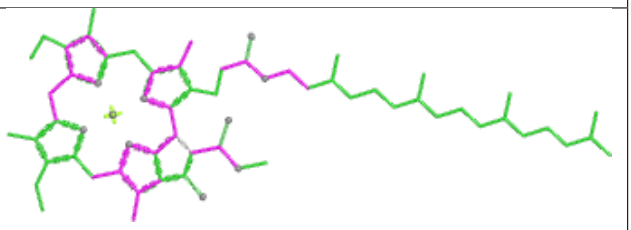


Rings

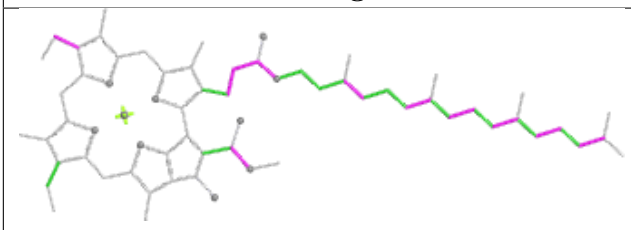
Ligand CLA 1 1136



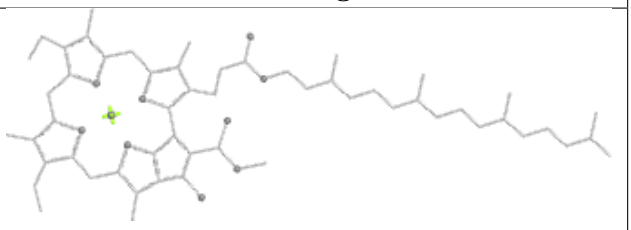
Bond lengths



Bond angles

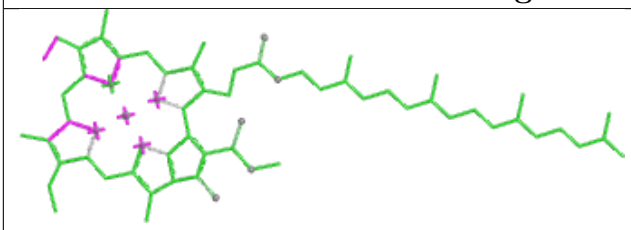


Torsions

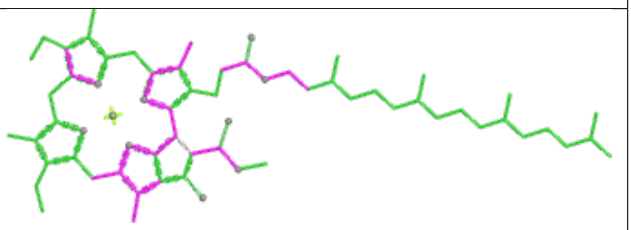


Rings

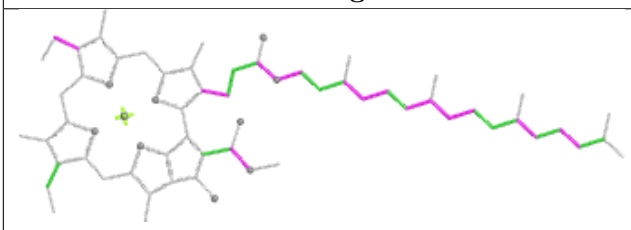
Ligand CLA A 1121



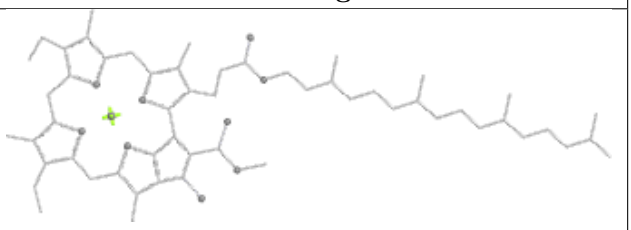
Bond lengths



Bond angles

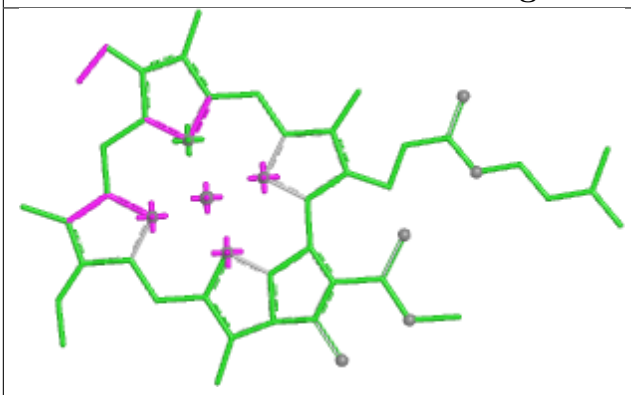


Torsions

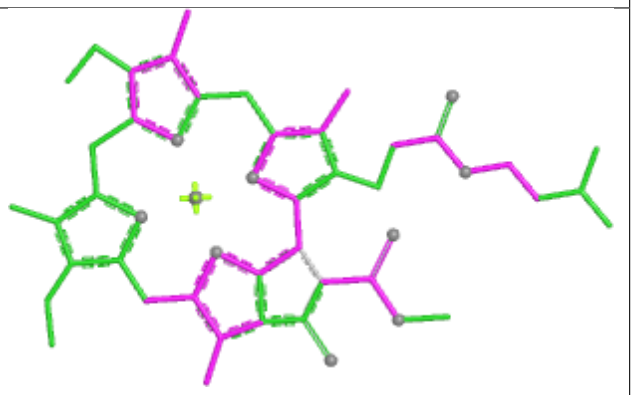


Rings

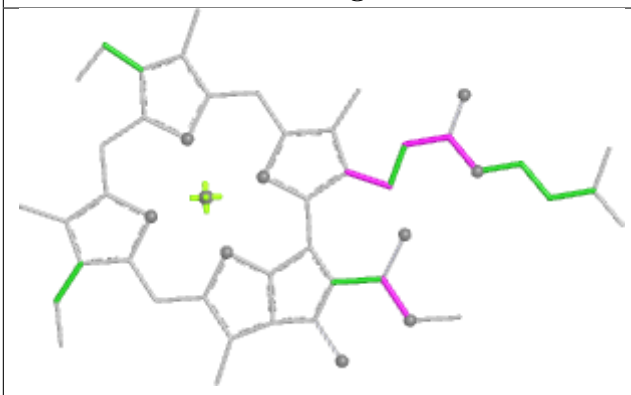
Ligand CLA 1 1129



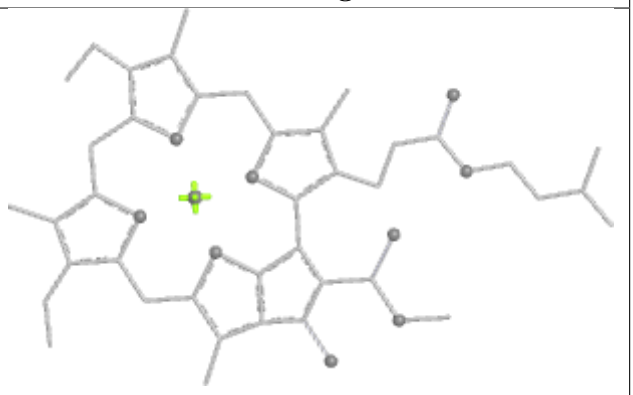
Bond lengths



Bond angles

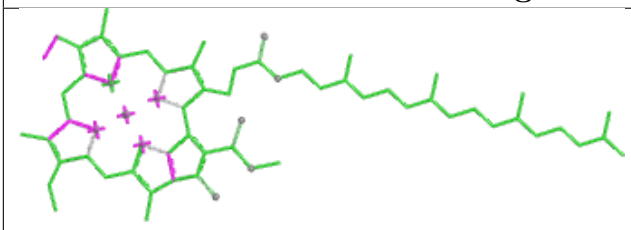


Torsions

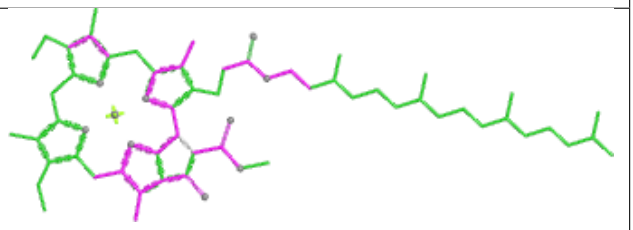


Rings

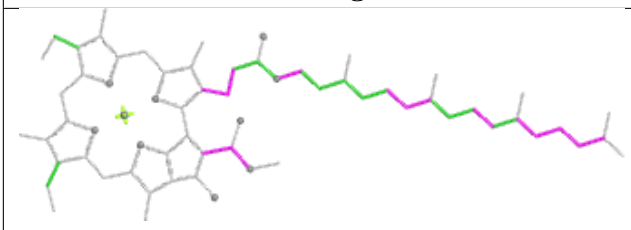
Ligand CLA A 1125



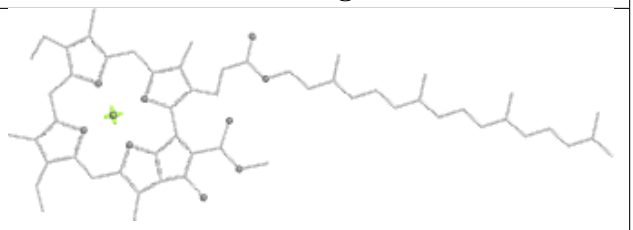
Bond lengths



Bond angles

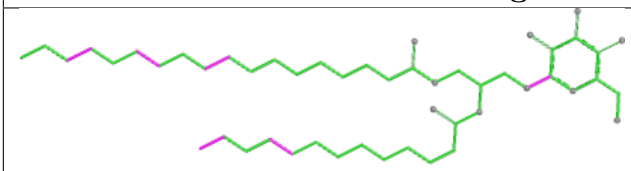


Torsions

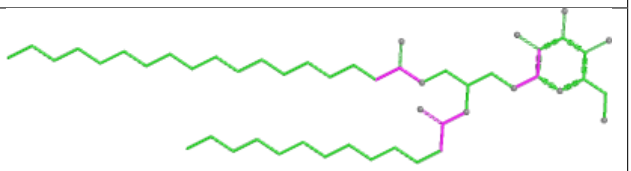


Rings

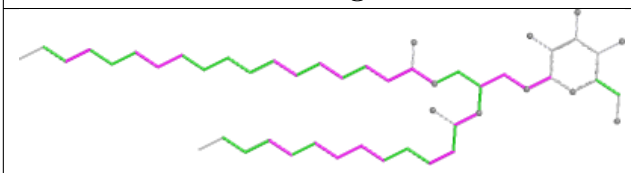
Ligand LMG A 5002



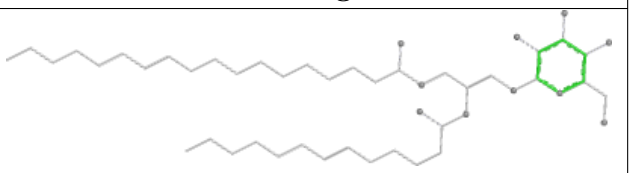
Bond lengths



Bond angles

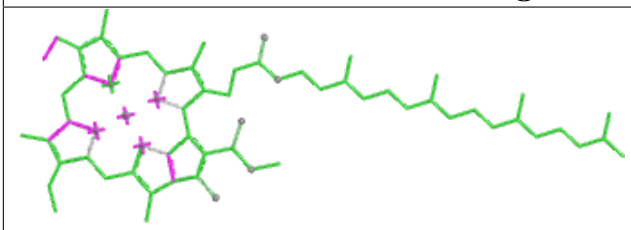


Torsions

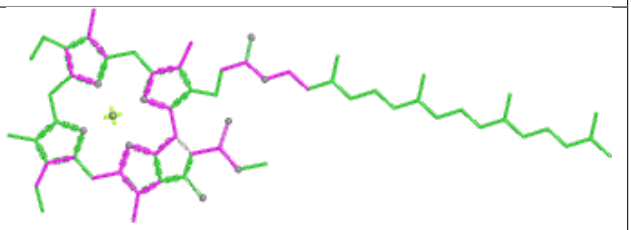


Rings

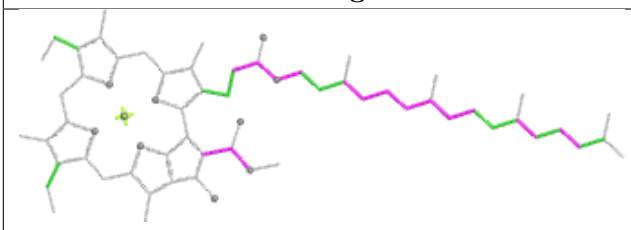
Ligand CLA B 1226



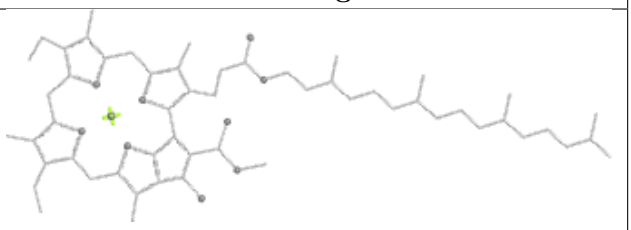
Bond lengths



Bond angles

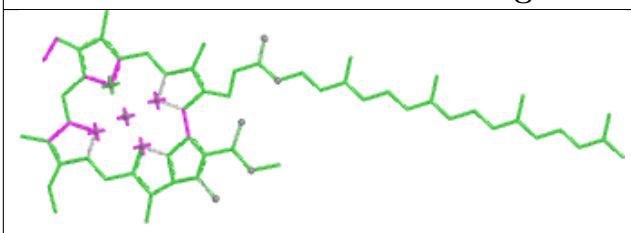


Torsions

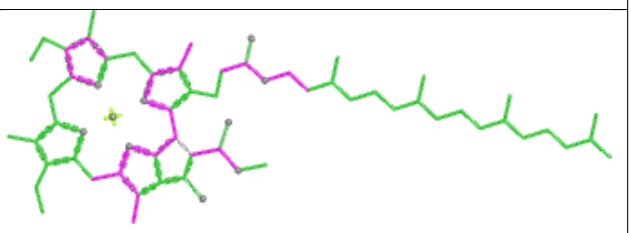


Rings

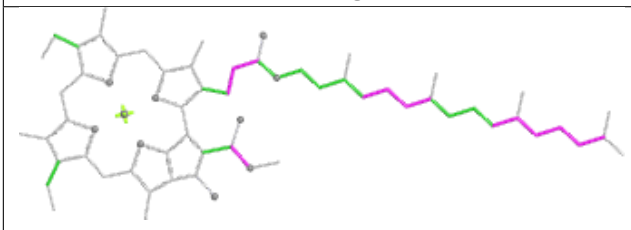
Ligand CLA A 1127



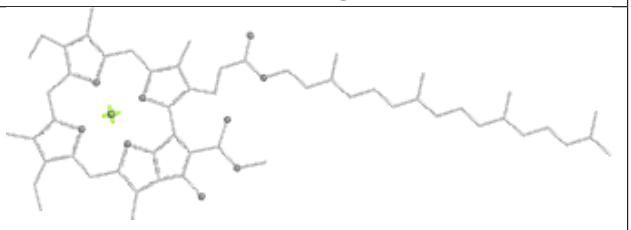
Bond lengths



Bond angles

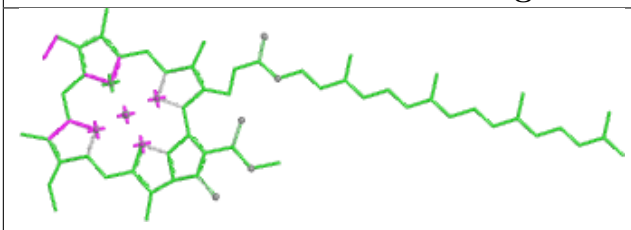


Torsions

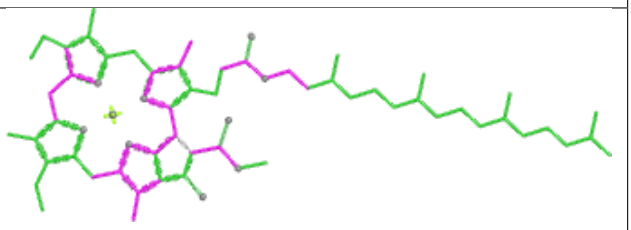


Rings

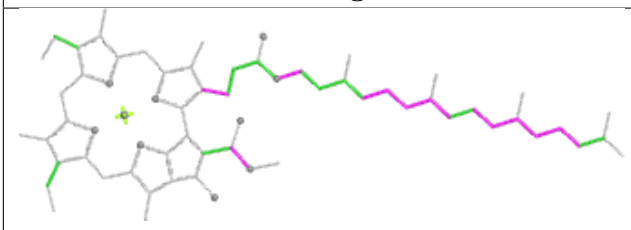
Ligand CLA A 1105



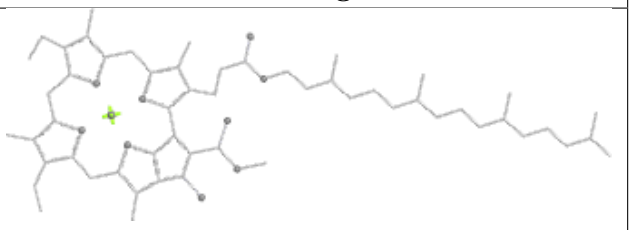
Bond lengths



Bond angles

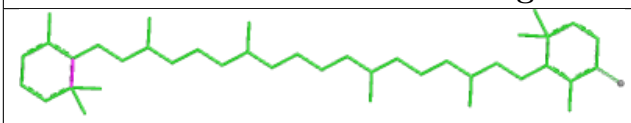


Torsions

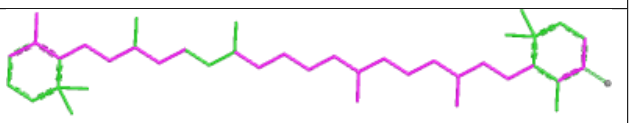


Rings

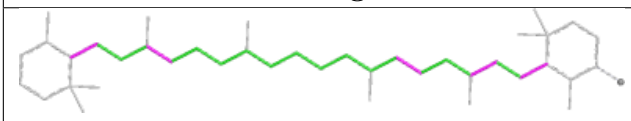
Ligand ECH b 4006



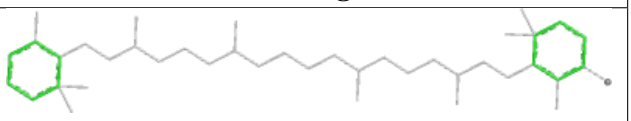
Bond lengths



Bond angles

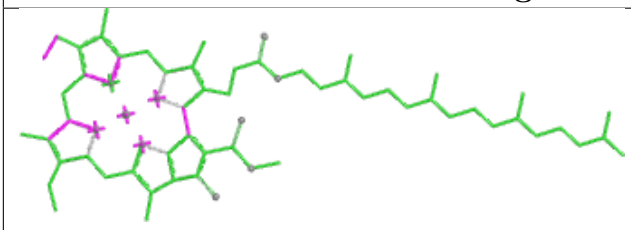


Torsions

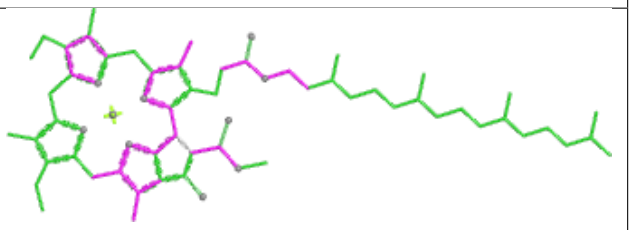


Rings

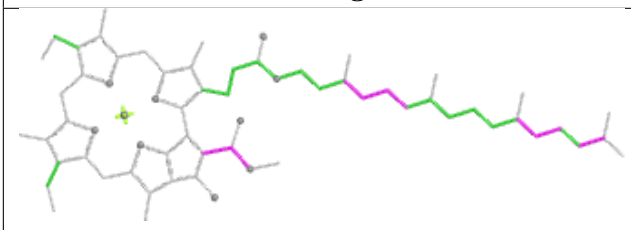
Ligand CLA A 1132



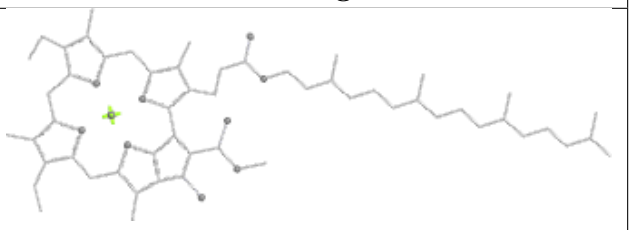
Bond lengths



Bond angles

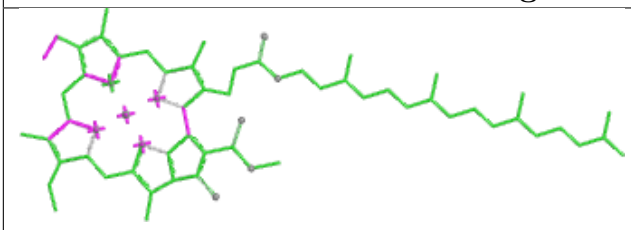


Torsions

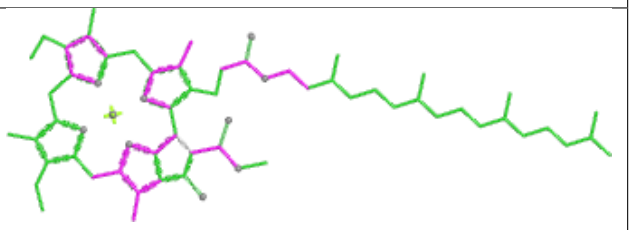


Rings

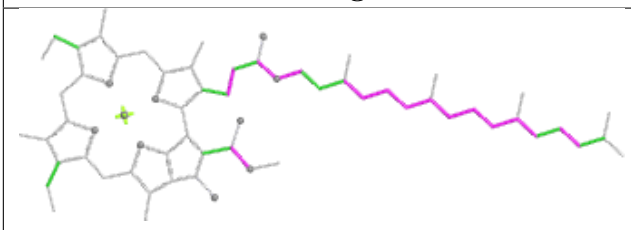
Ligand CLA a 1126



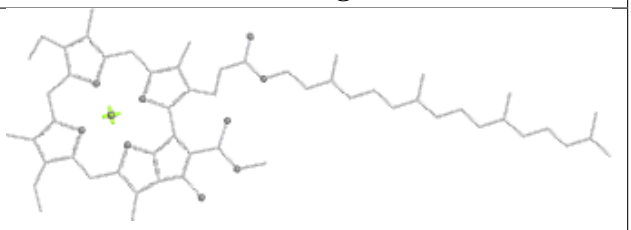
Bond lengths



Bond angles

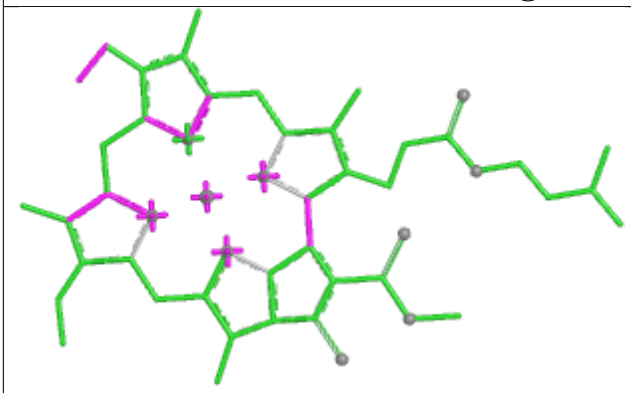


Torsions

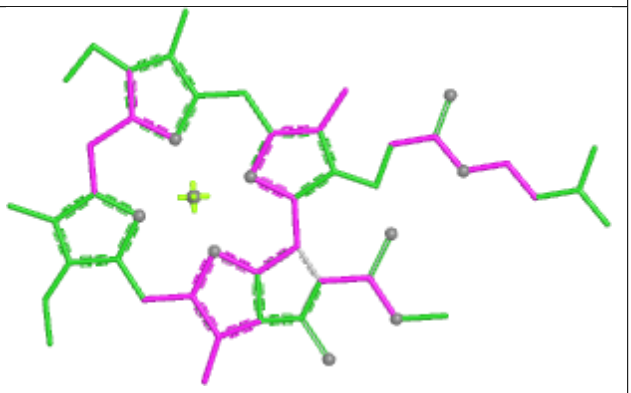


Rings

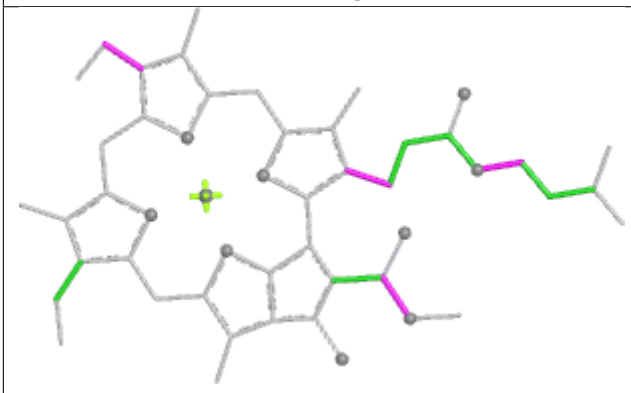
Ligand CLA 1 1105



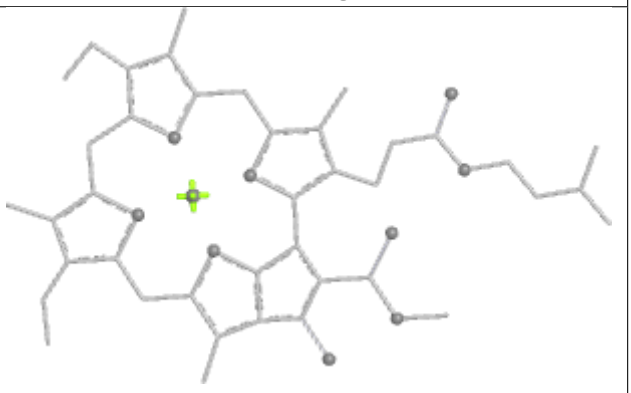
Bond lengths



Bond angles

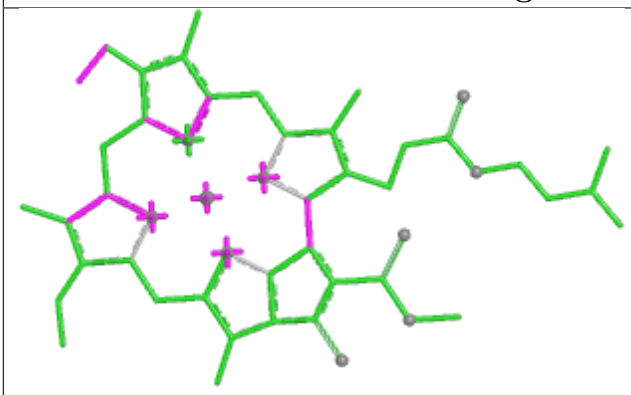


Torsions

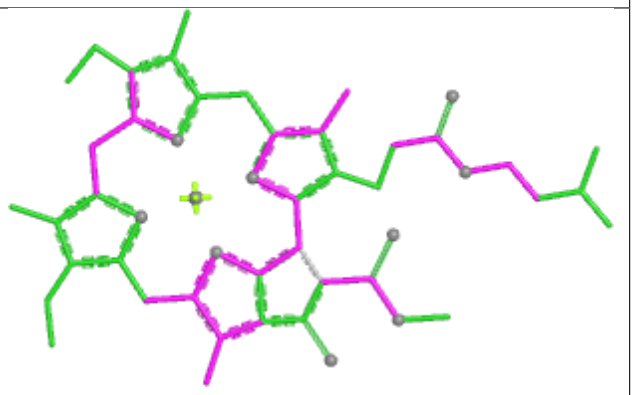


Rings

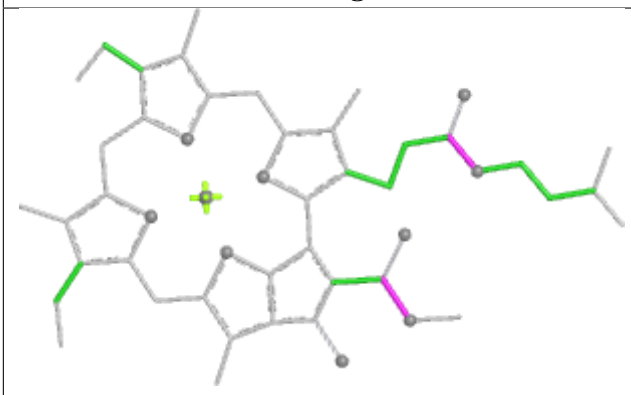
Ligand CLA B 1232



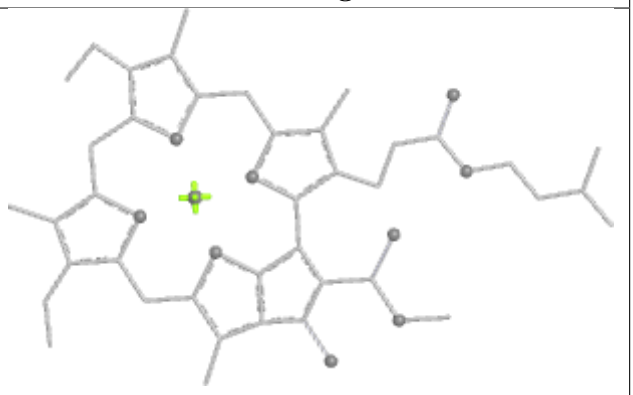
Bond lengths



Bond angles

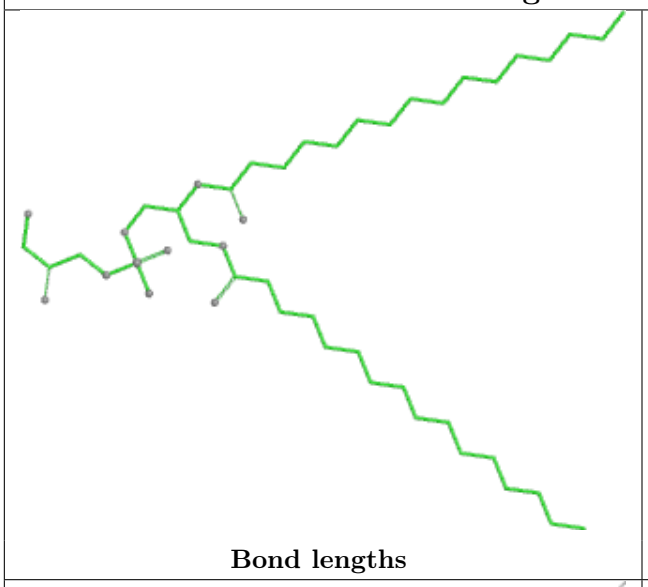


Torsions

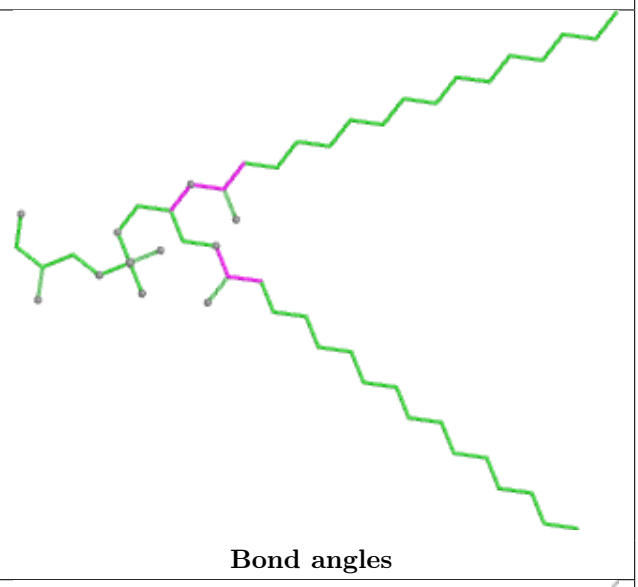


Rings

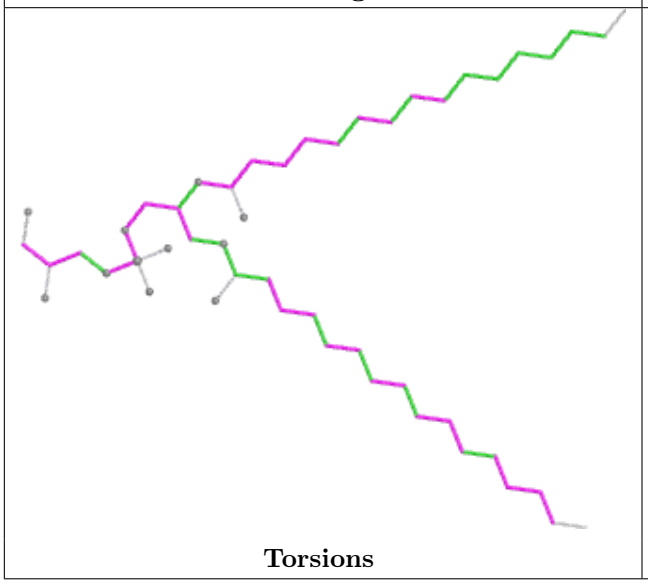
Ligand LHG l 5001



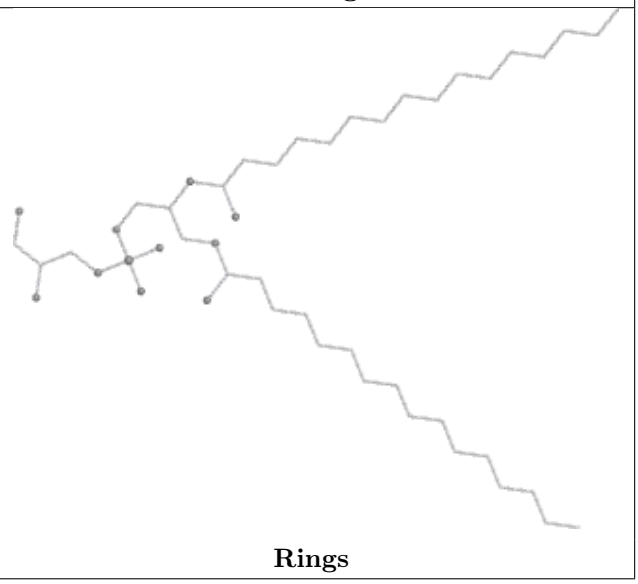
Bond lengths



Bond angles

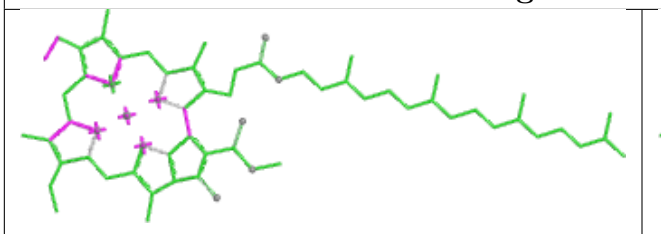


Torsions

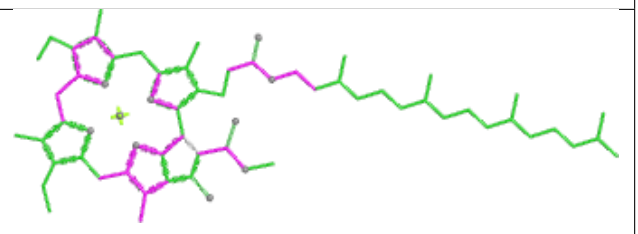


Rings

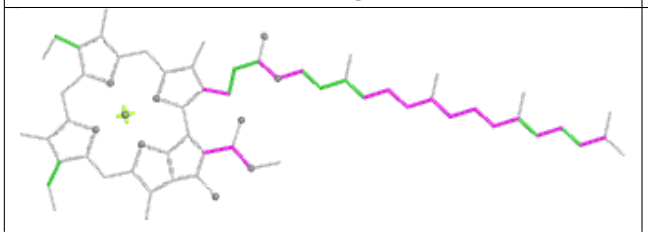
Ligand CLA B 1230



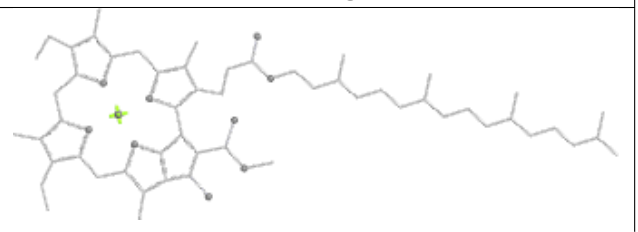
Bond lengths



Bond angles

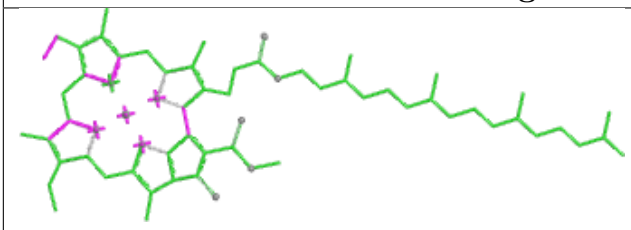


Torsions

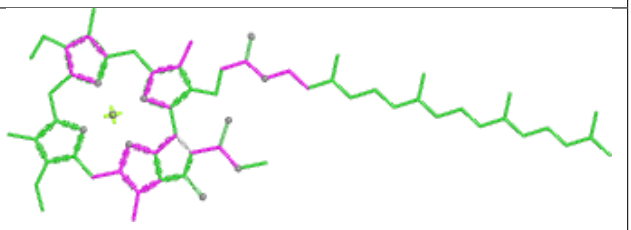


Rings

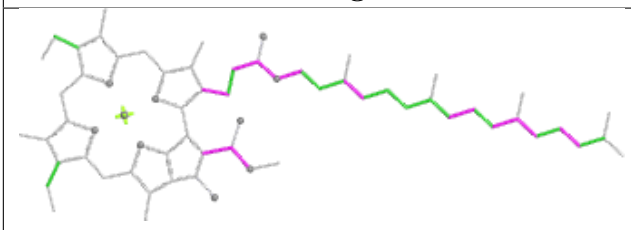
Ligand CLA b 1202



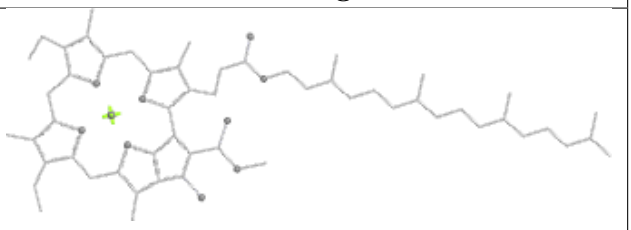
Bond lengths



Bond angles

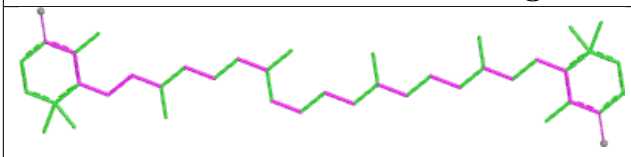


Torsions

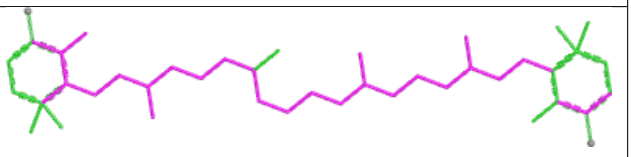


Rings

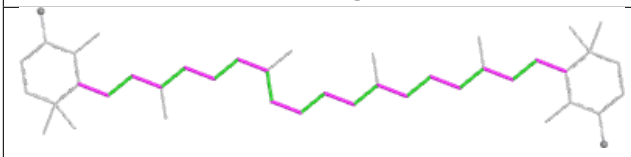
Ligand 45D h 4020



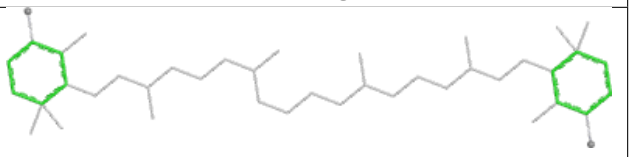
Bond lengths



Bond angles

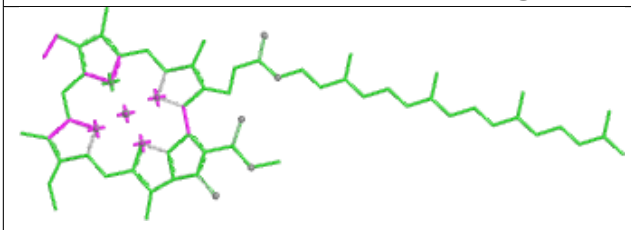


Torsions

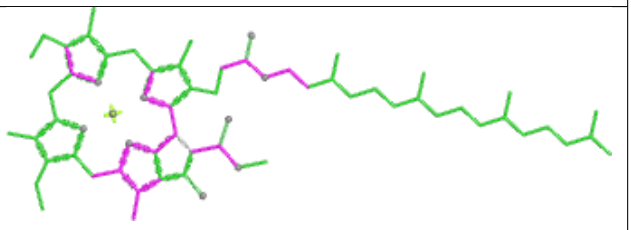


Rings

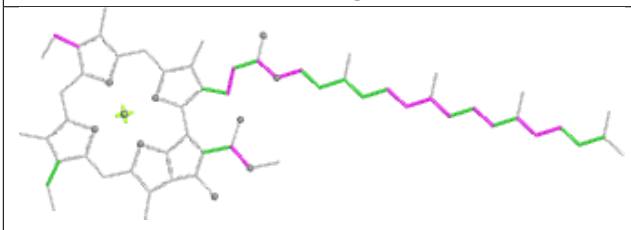
Ligand CLA A 1131



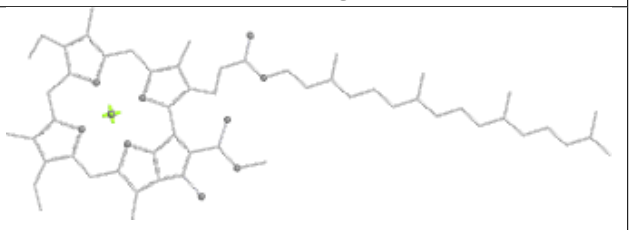
Bond lengths



Bond angles

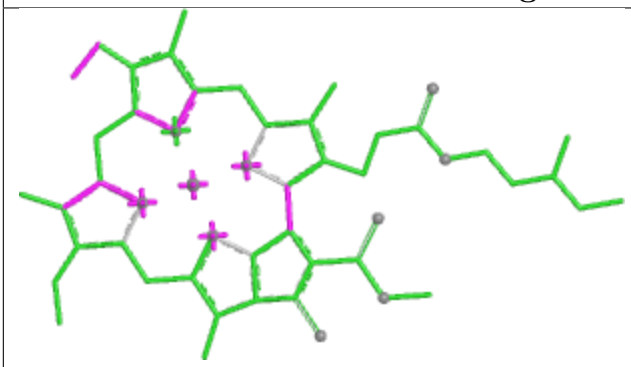


Torsions

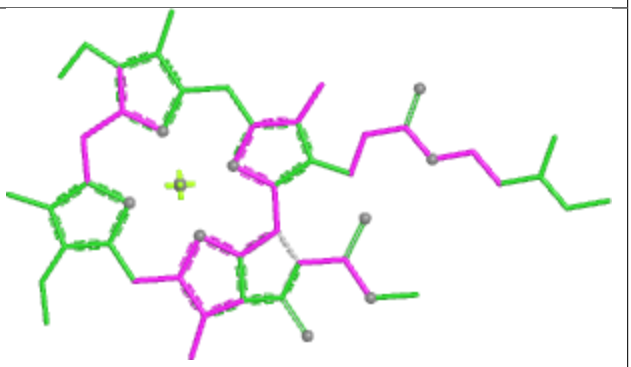


Rings

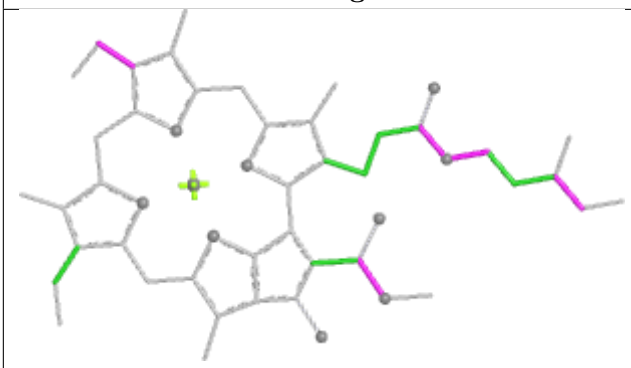
Ligand CLA 1 1137



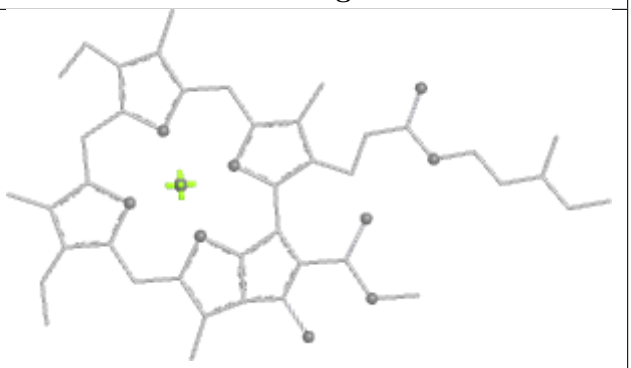
Bond lengths



Bond angles

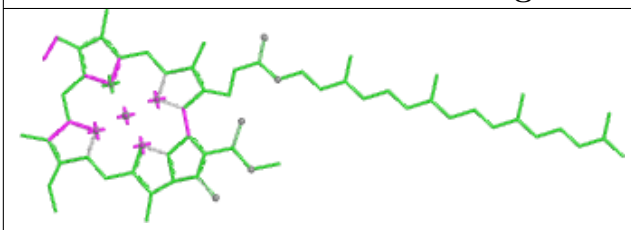


Torsions

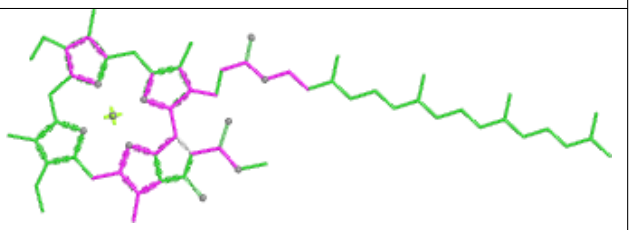


Rings

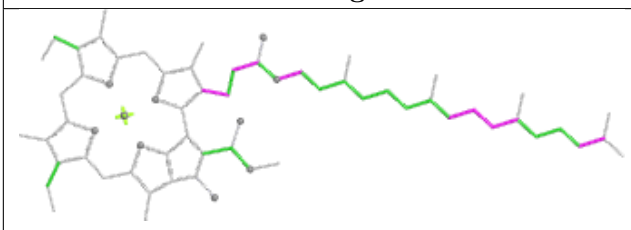
Ligand CLA A 1101



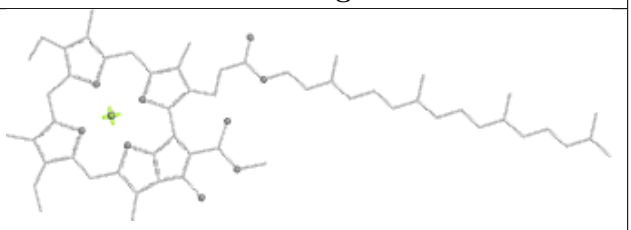
Bond lengths



Bond angles

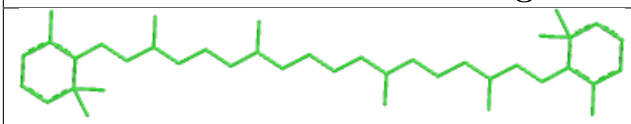


Torsions

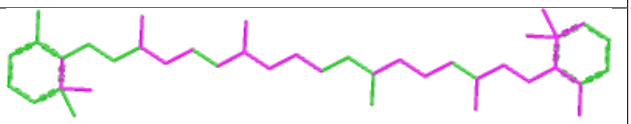


Rings

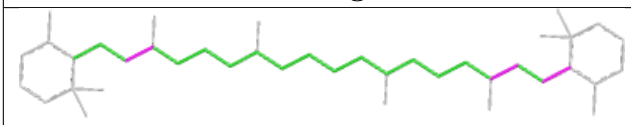
Ligand BCR L 4019



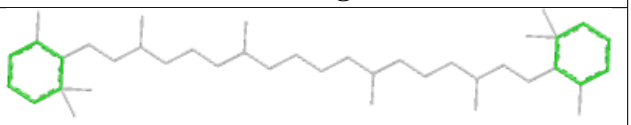
Bond lengths



Bond angles

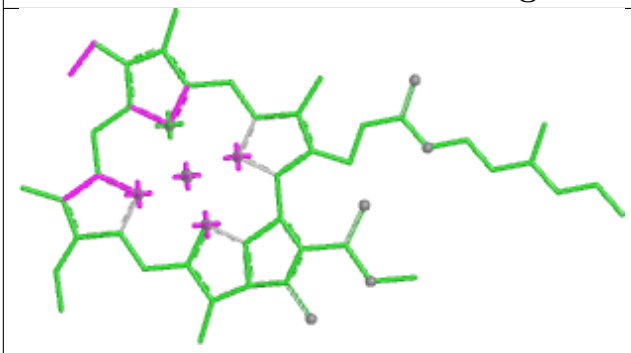


Torsions

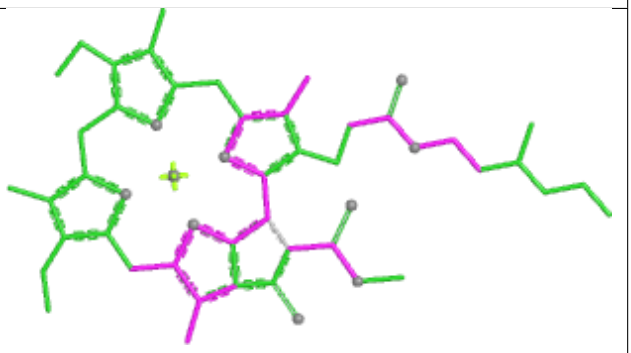


Rings

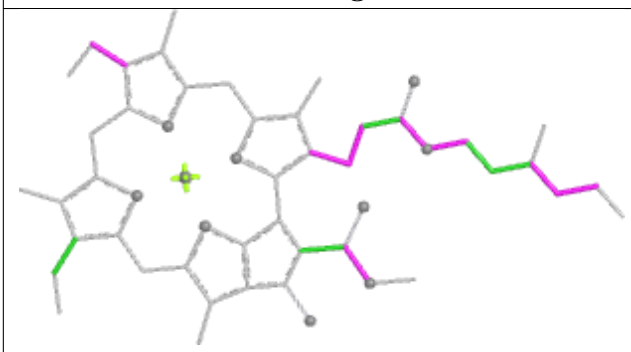
Ligand CLA 1 1135



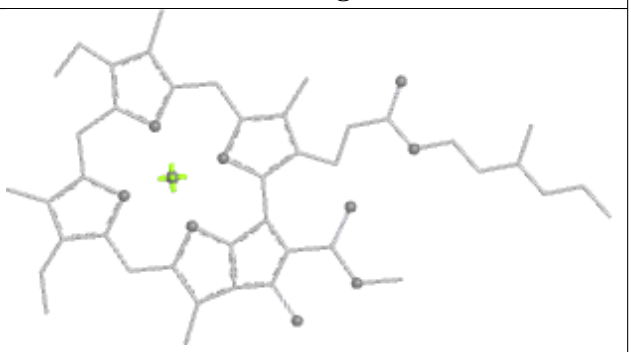
Bond lengths



Bond angles

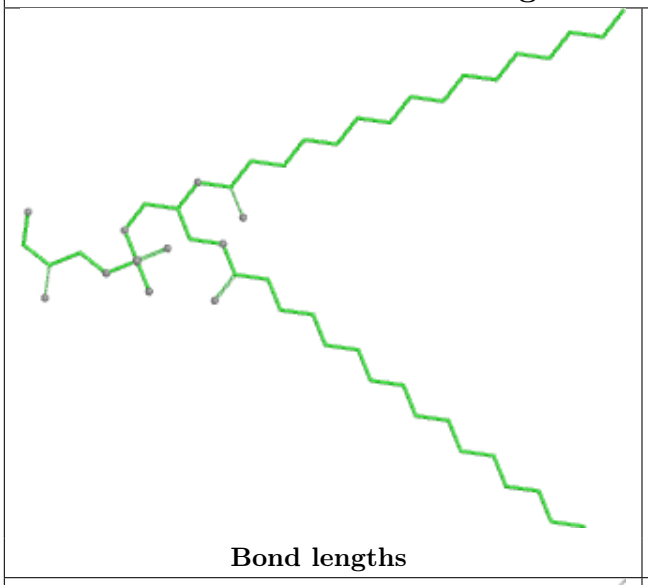


Torsions

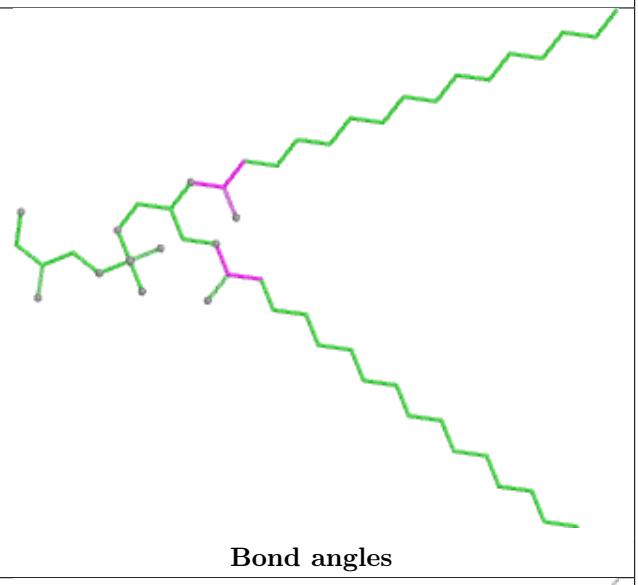


Rings

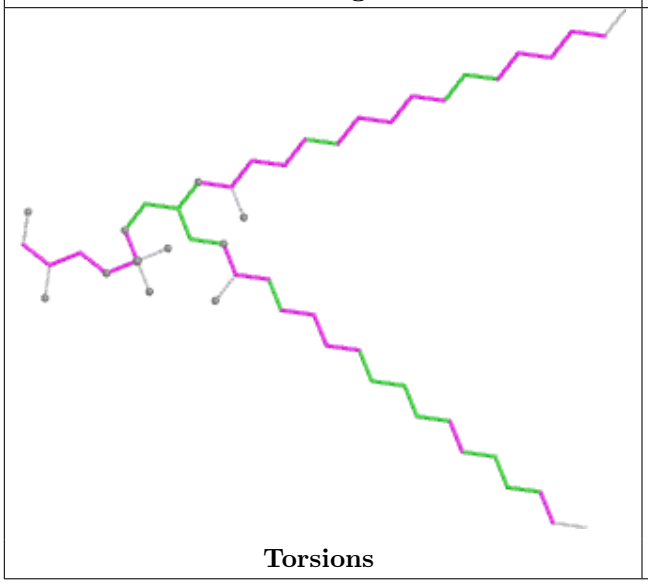
Ligand LHG a 5005



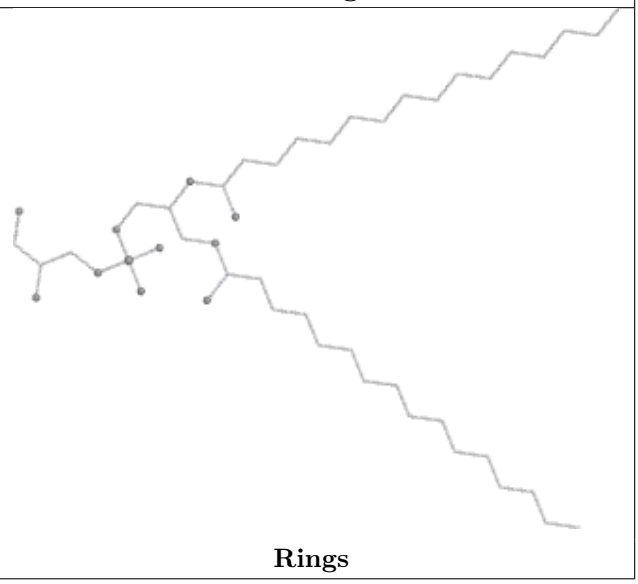
Bond lengths



Bond angles

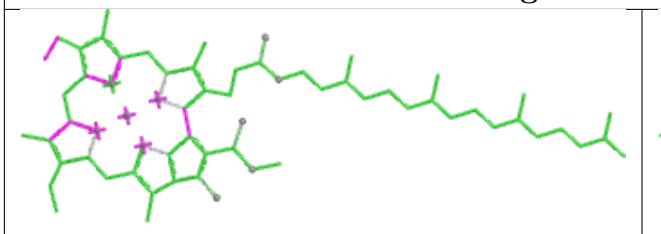


Torsions

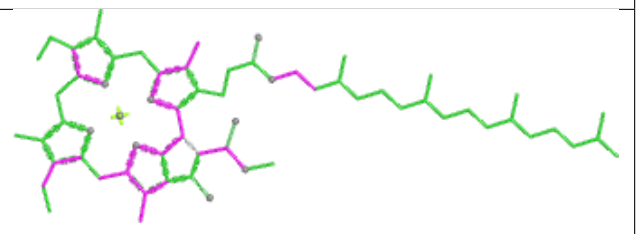


Rings

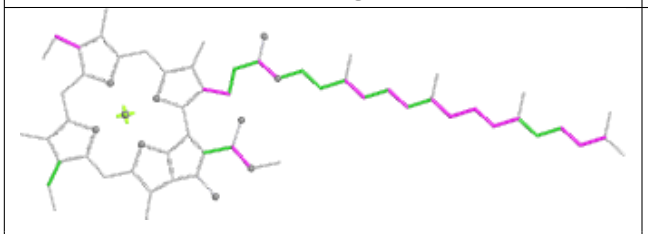
Ligand CLA 1 1109



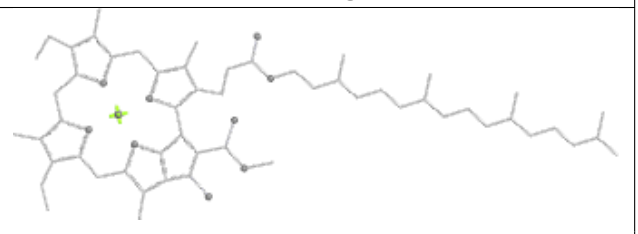
Bond lengths



Bond angles

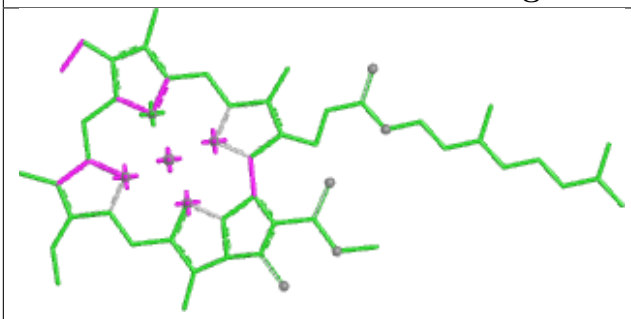


Torsions

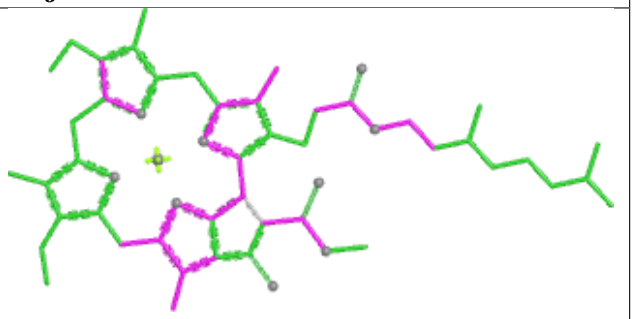


Rings

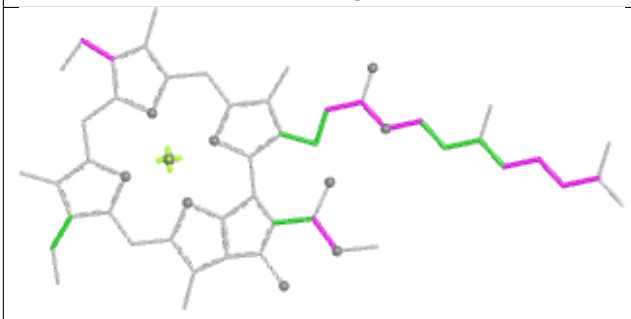
Ligand CLA j 1303



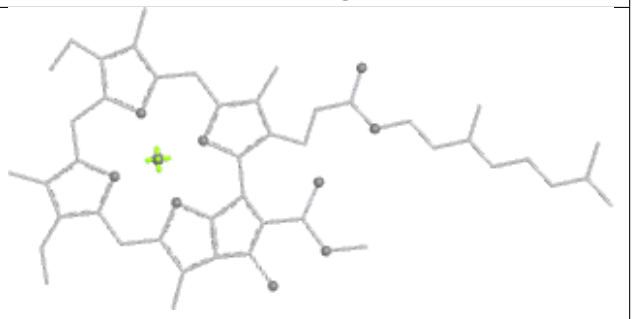
Bond lengths



Bond angles

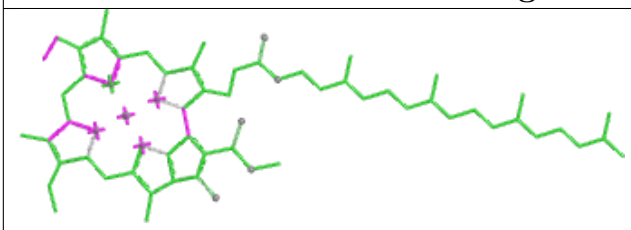


Torsions

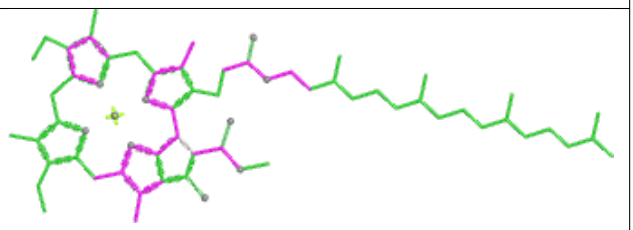


Rings

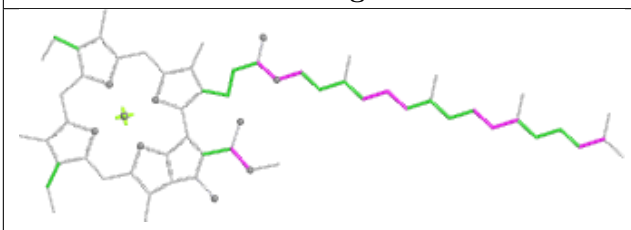
Ligand CLA b 1227



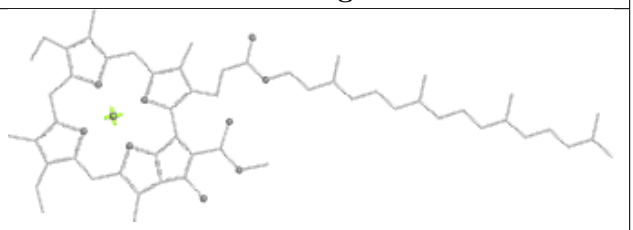
Bond lengths



Bond angles

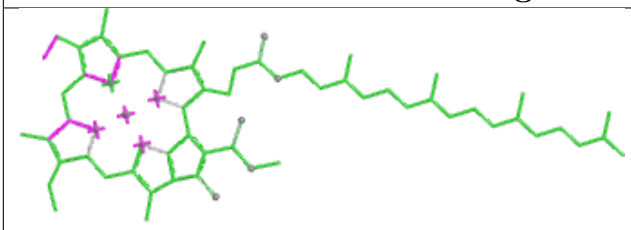


Torsions

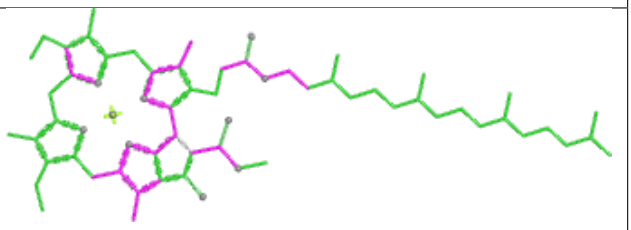


Rings

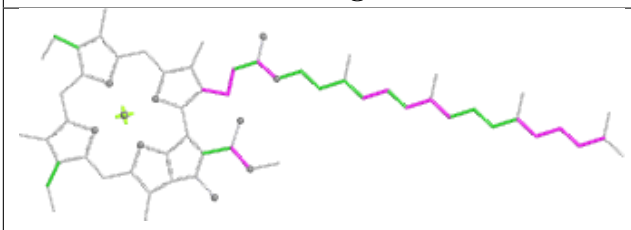
Ligand CLA A 1120



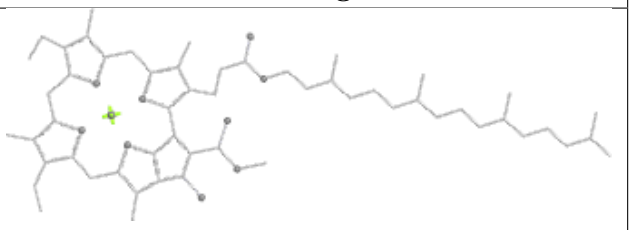
Bond lengths



Bond angles

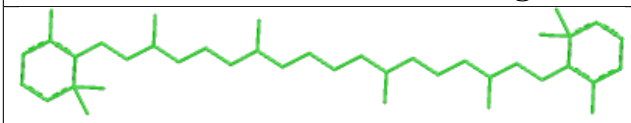


Torsions

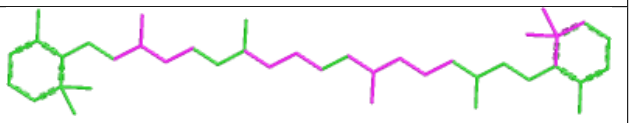


Rings

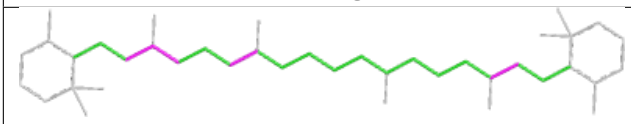
Ligand BCR B 4014



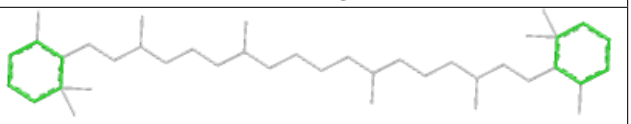
Bond lengths



Bond angles

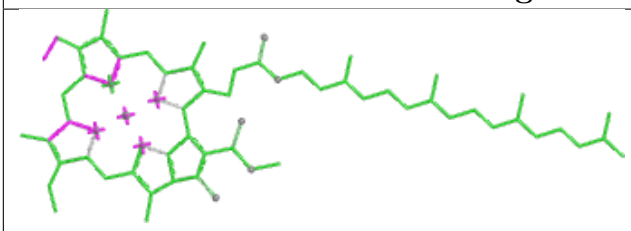


Torsions

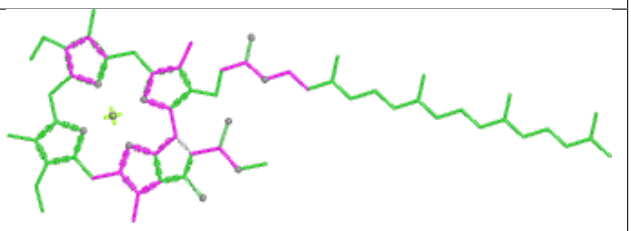


Rings

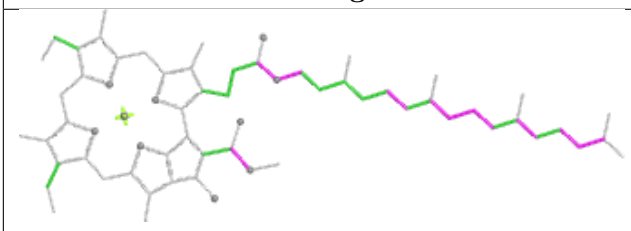
Ligand CLA B 1208



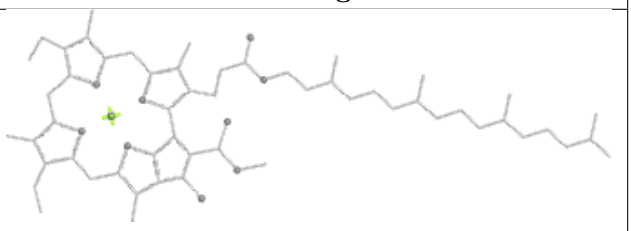
Bond lengths



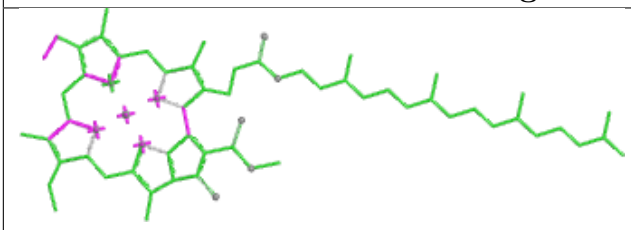
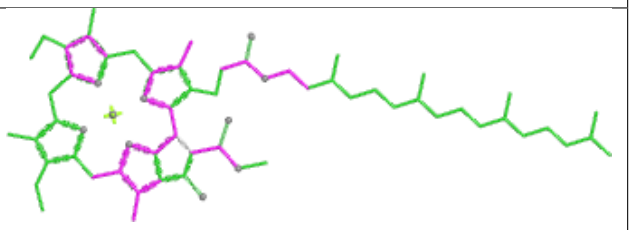
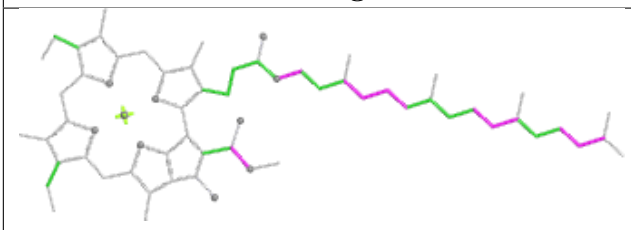
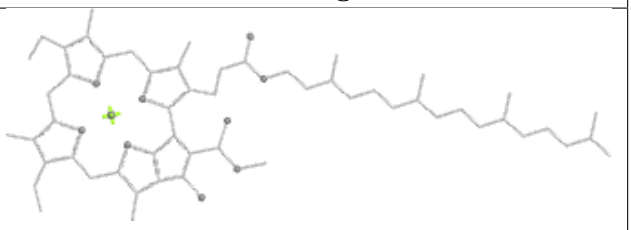
Bond angles

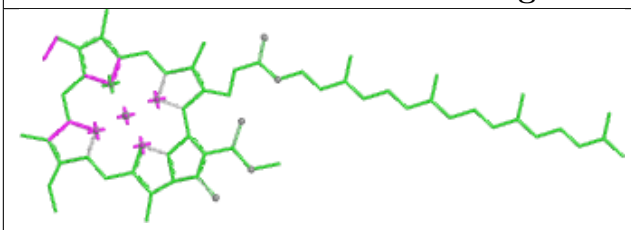
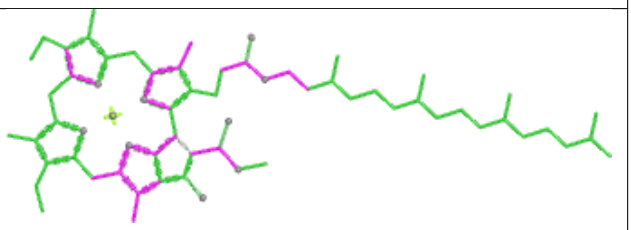
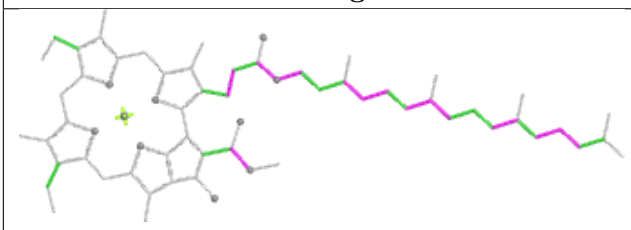
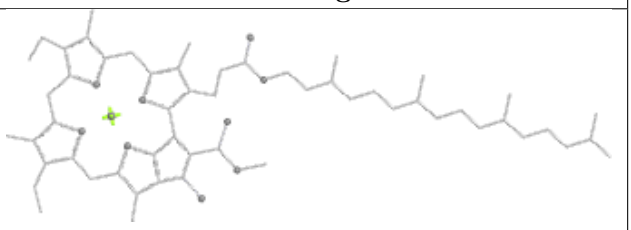


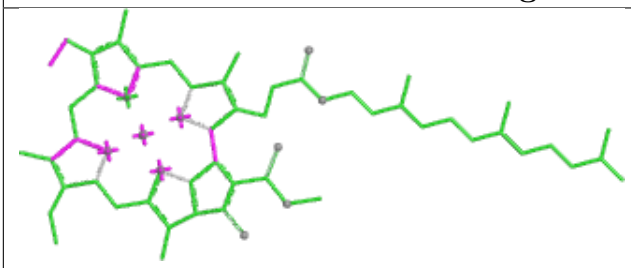
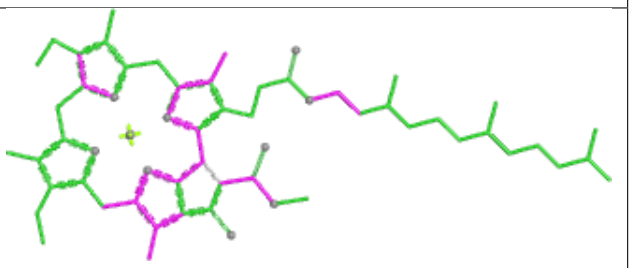
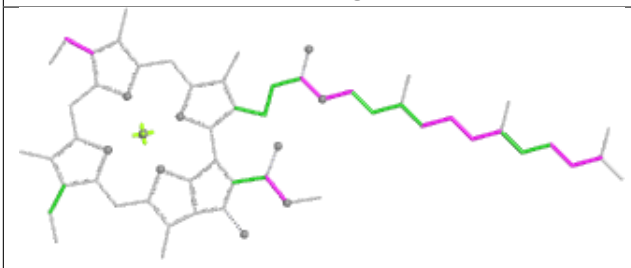
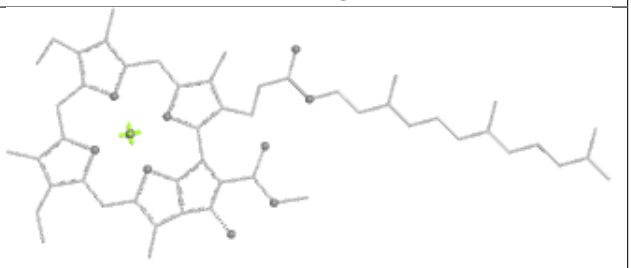
Torsions

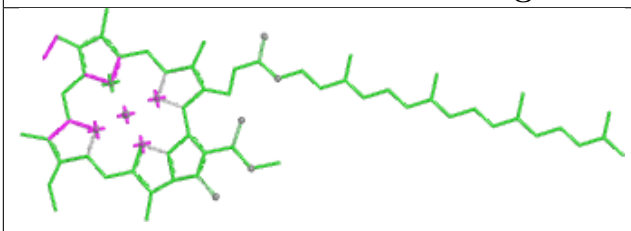
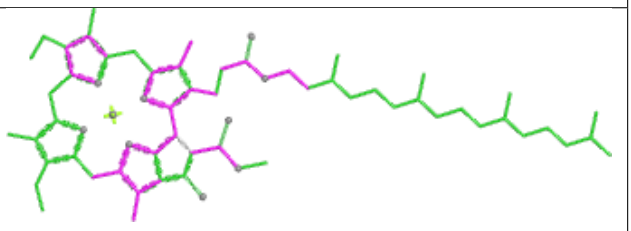
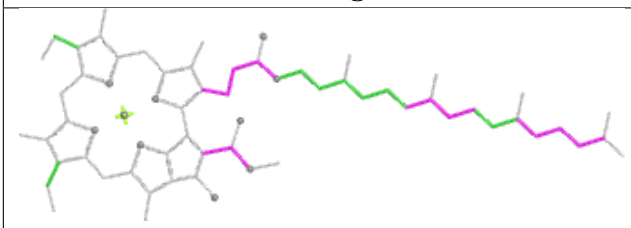
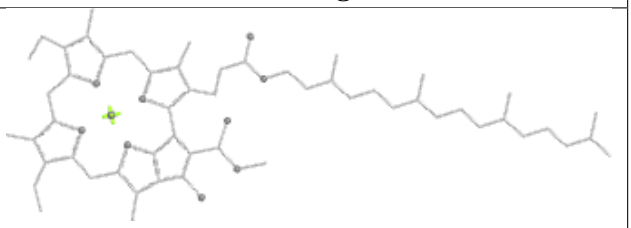


Rings

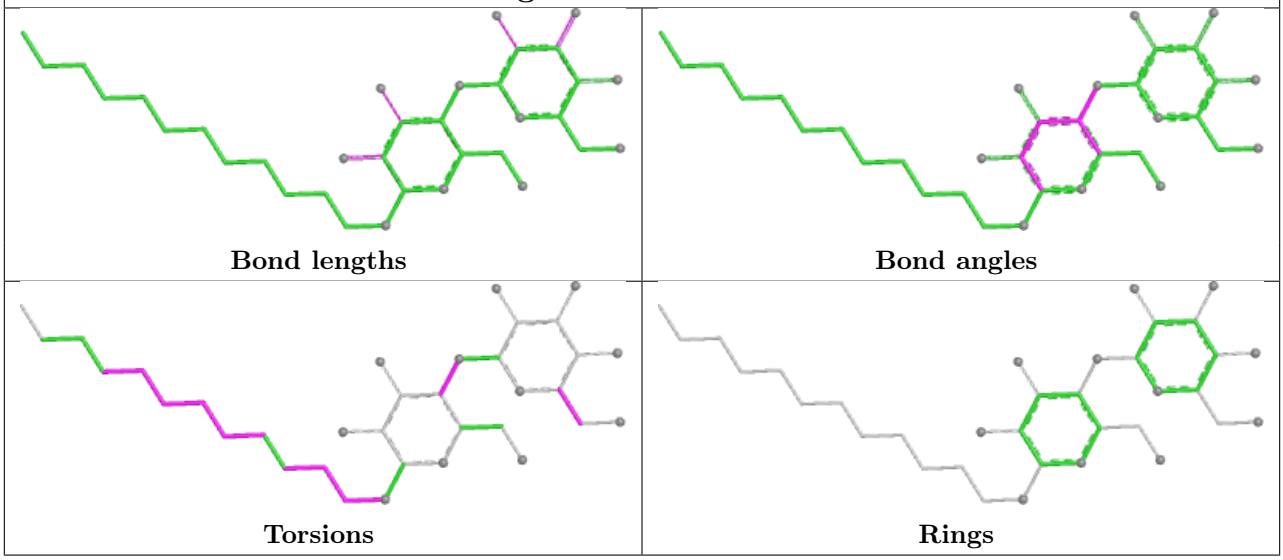
Ligand CLA a 1140	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1235	
	
Bond lengths	Bond angles
	
Torsions	Rings

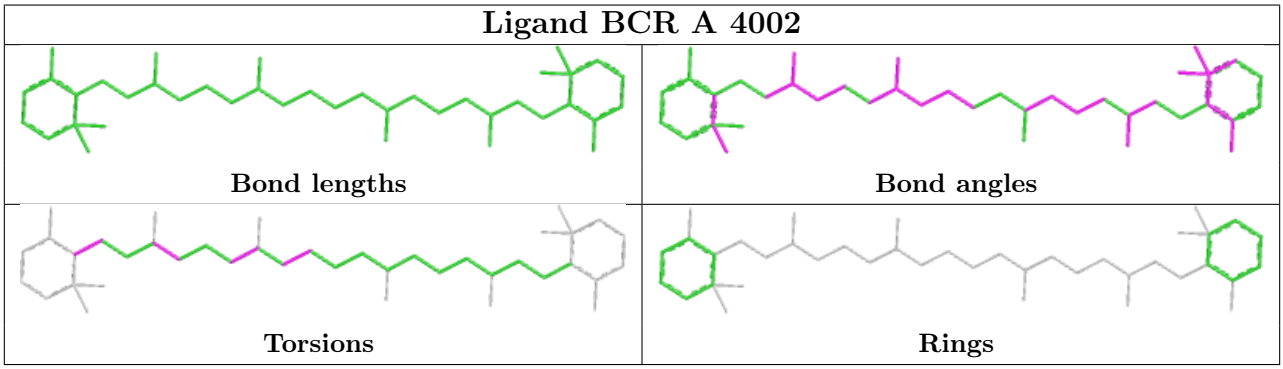
Ligand CLA 1 1122	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1106	
 Bond lengths	 Bond angles
 Torsions	 Rings

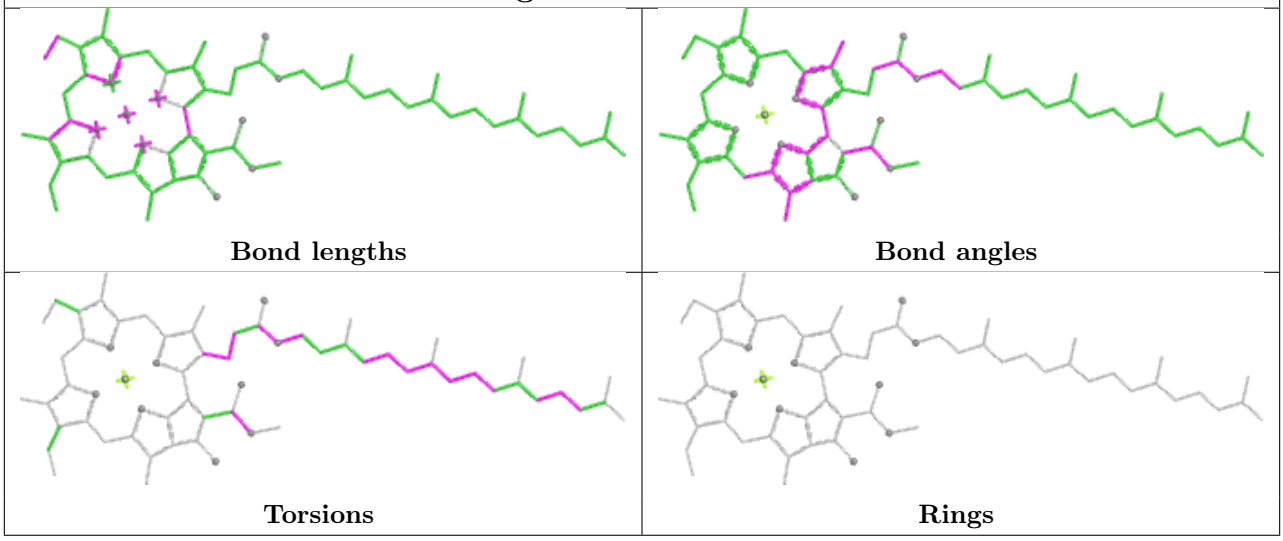
Ligand LMT 0 6001



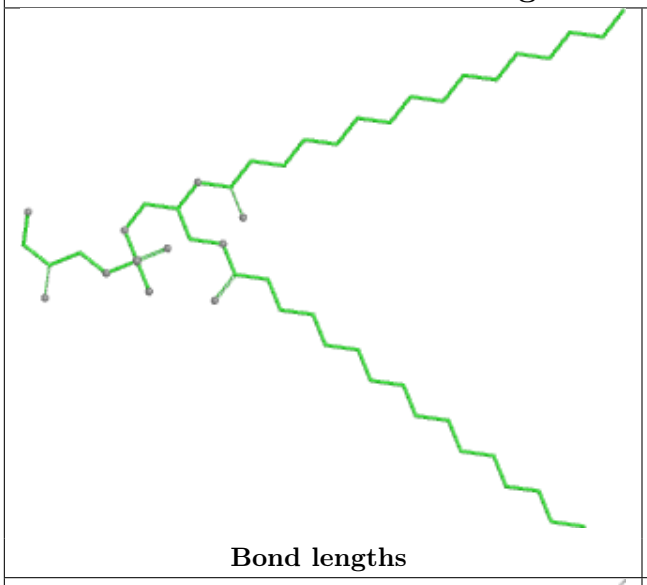
Ligand BCR A 4002



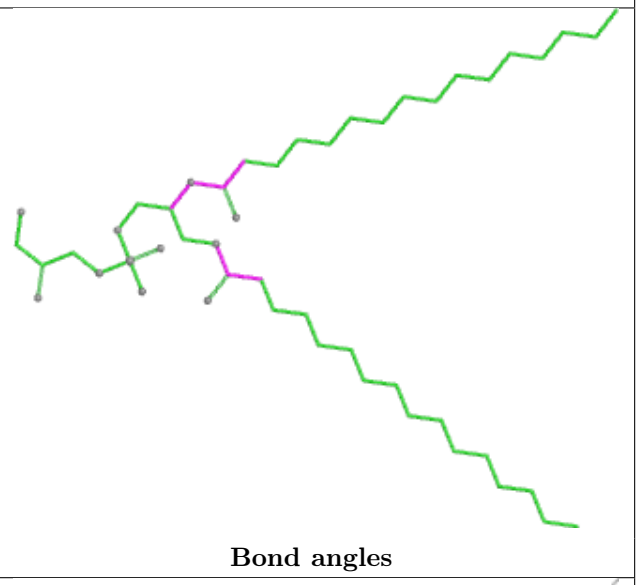
Ligand CLA B 1218



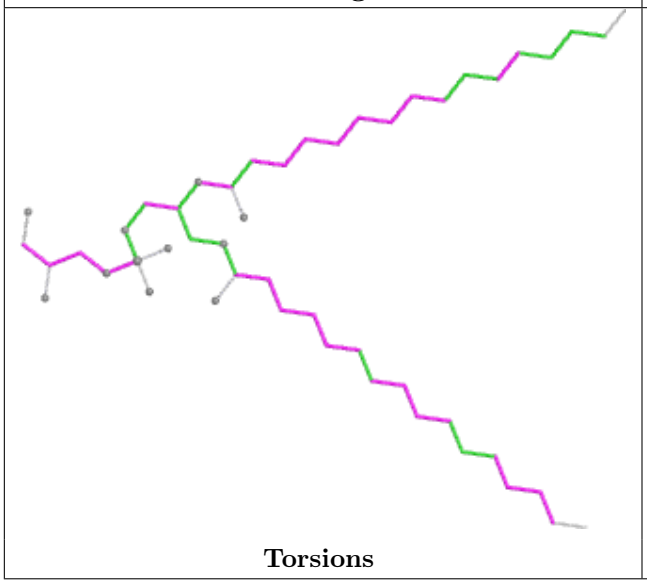
Ligand LHG 0 5004



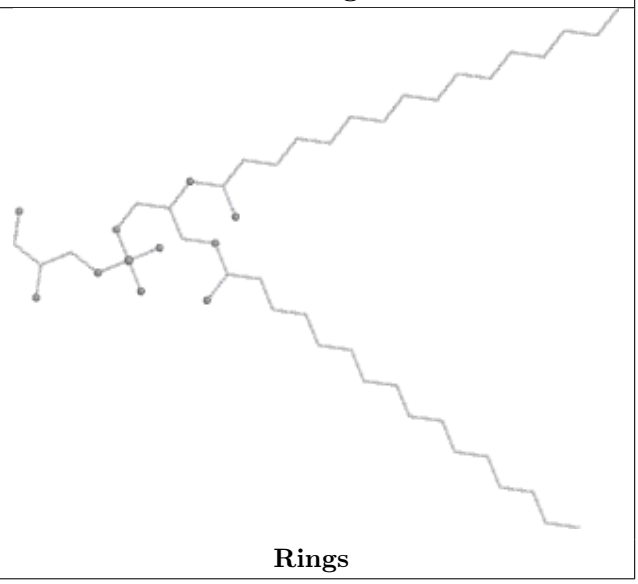
Bond lengths



Bond angles

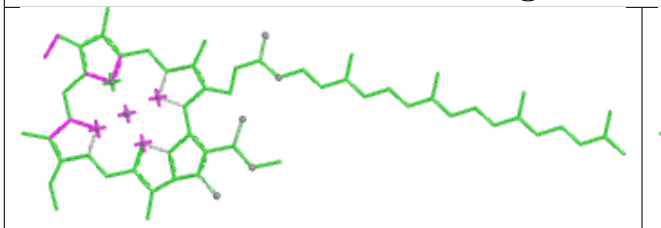


Torsions

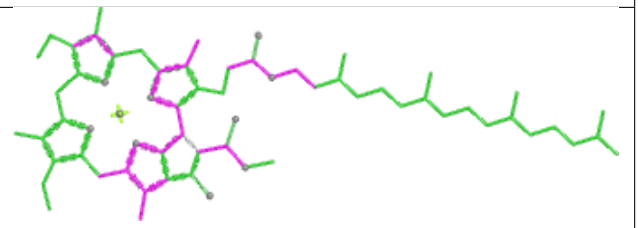


Rings

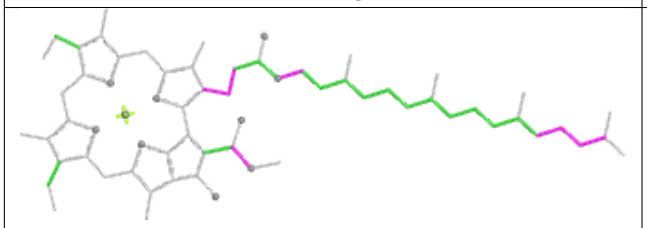
Ligand CLA b 1022



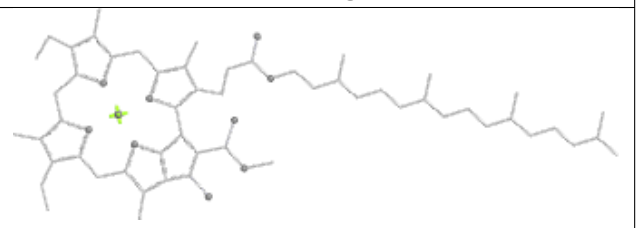
Bond lengths



Bond angles

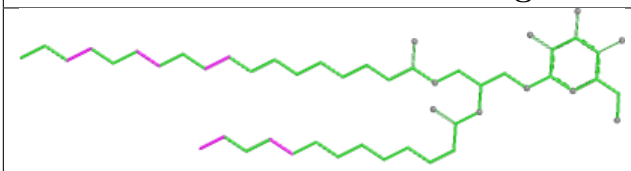


Torsions

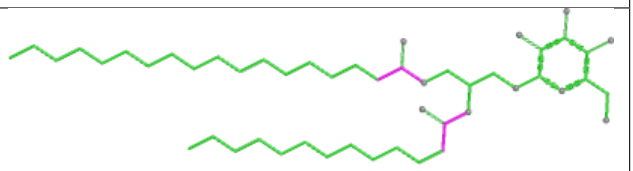


Rings

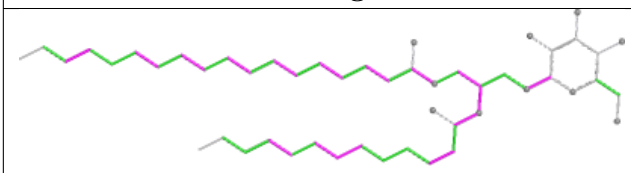
Ligand LMG 1 5002



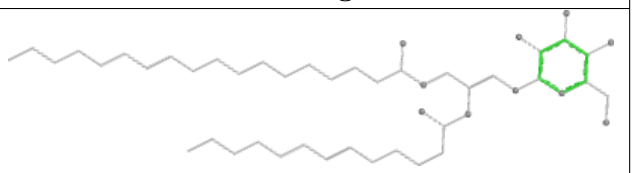
Bond lengths



Bond angles



Torsions

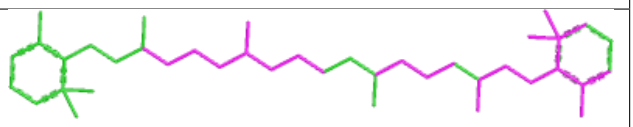


Rings

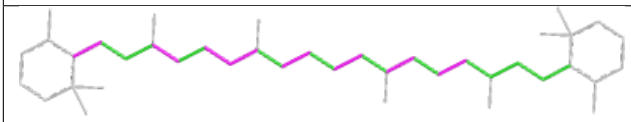
Ligand BCR K 4001



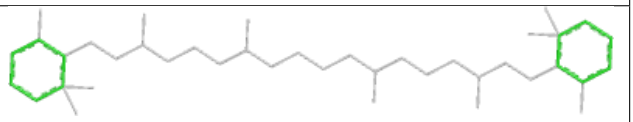
Bond lengths



Bond angles

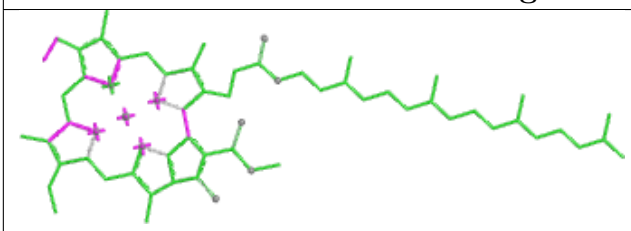


Torsions

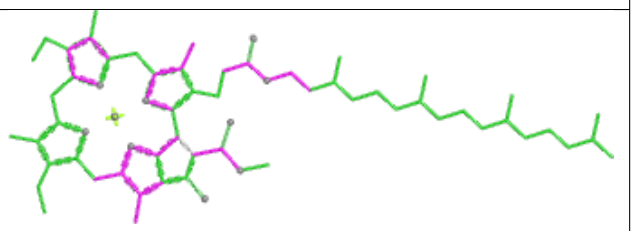


Rings

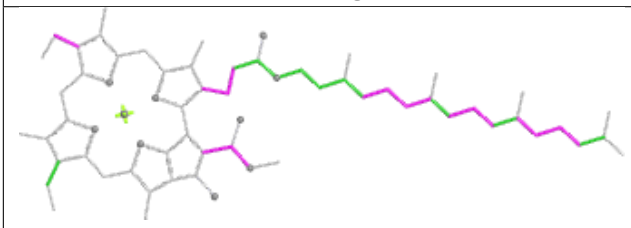
Ligand CLA a 1106



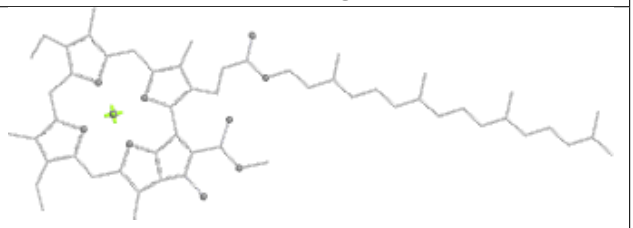
Bond lengths



Bond angles

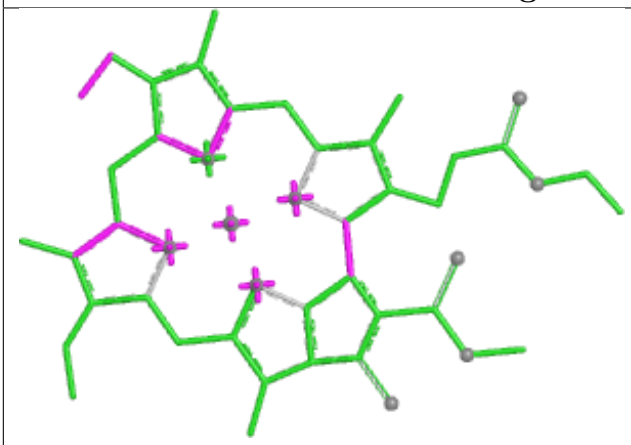


Torsions

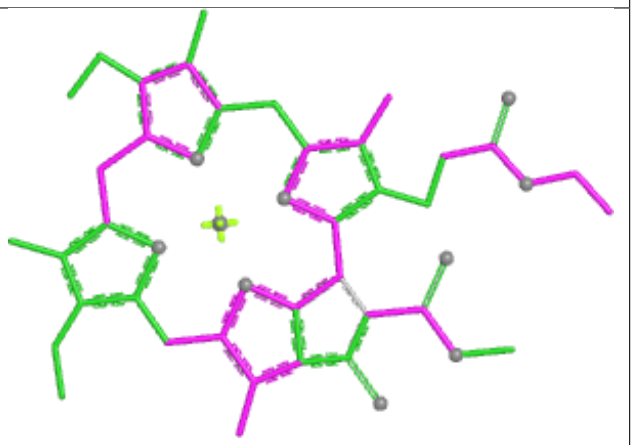


Rings

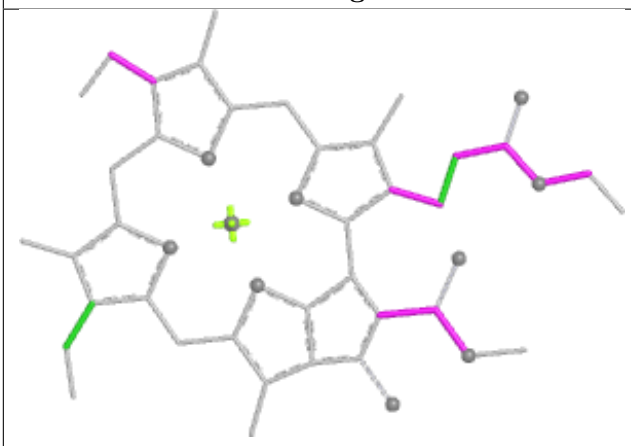
Ligand CLA 2 1230



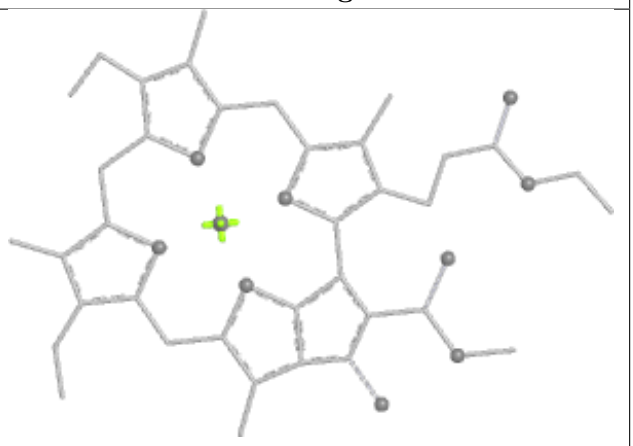
Bond lengths



Bond angles

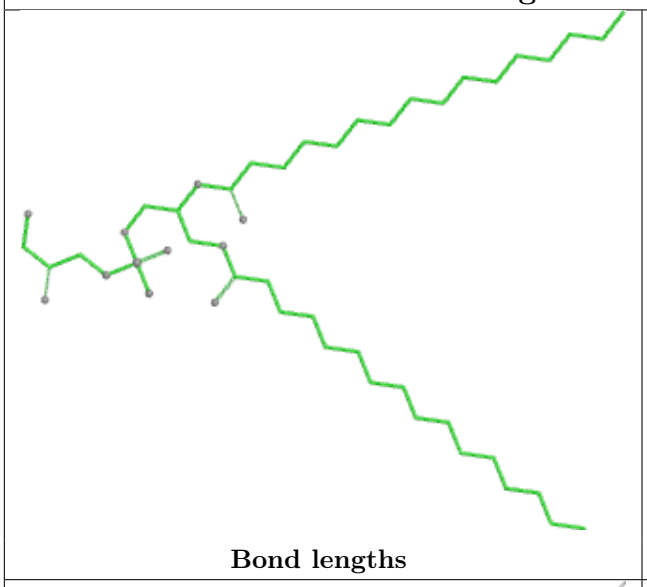


Torsions

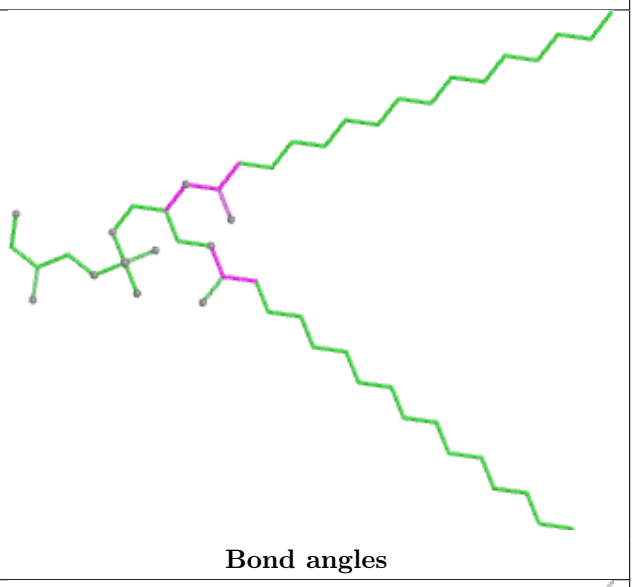


Rings

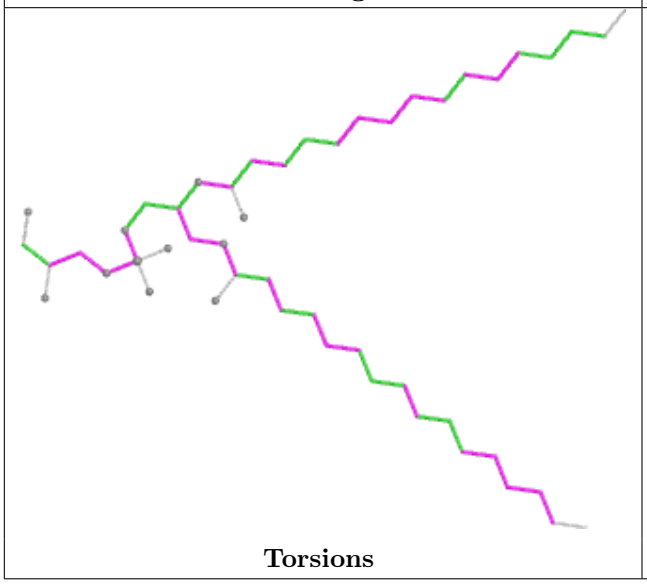
Ligand LHG 1 5007



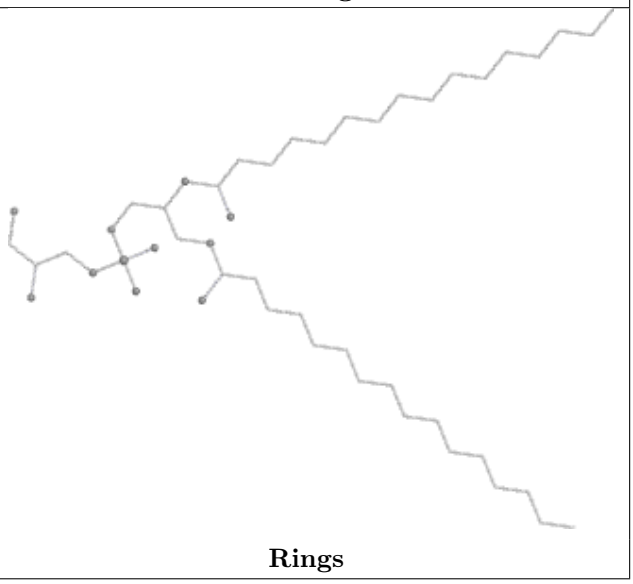
Bond lengths



Bond angles

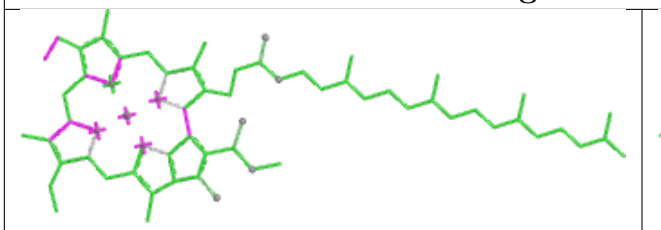


Torsions

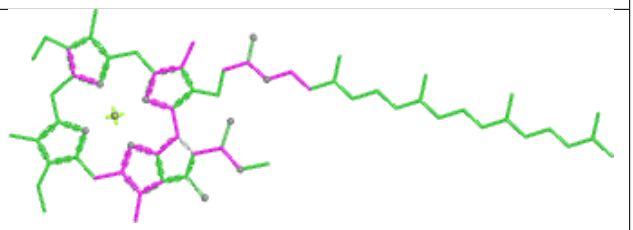


Rings

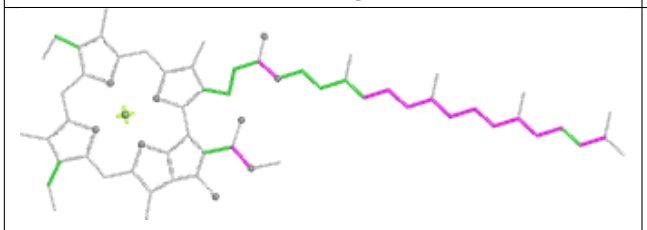
Ligand CLA b 1218



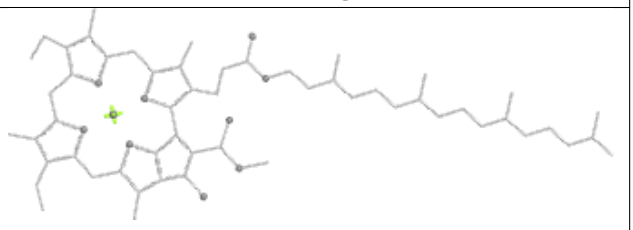
Bond lengths



Bond angles

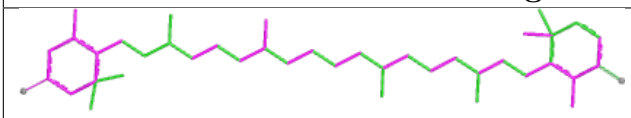


Torsions

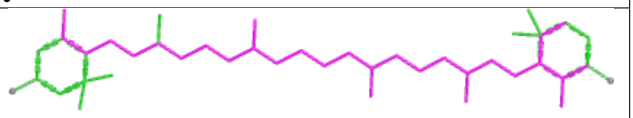


Rings

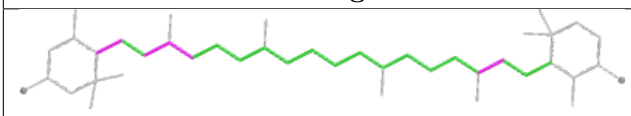
Ligand EQ3 I 4020



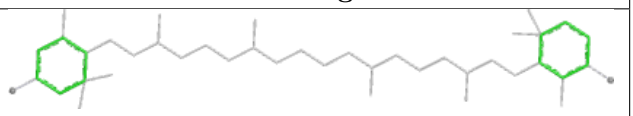
Bond lengths



Bond angles



Torsions



Rings

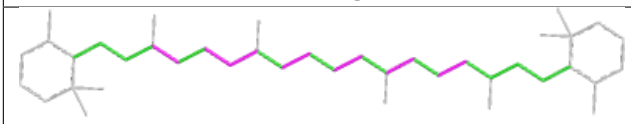
Ligand BCR B 4017



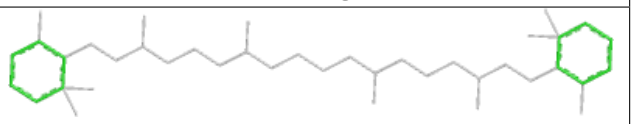
Bond lengths



Bond angles

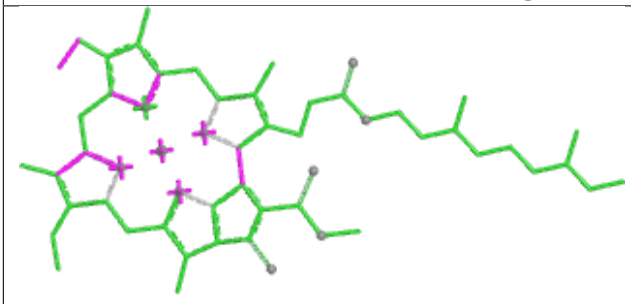


Torsions

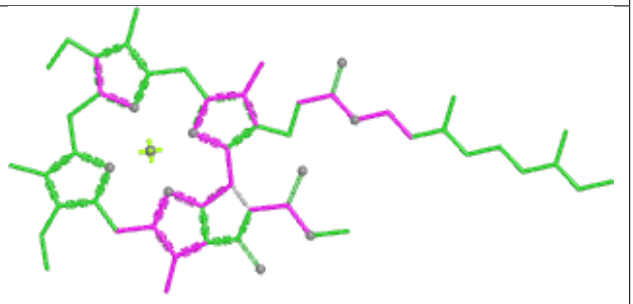


Rings

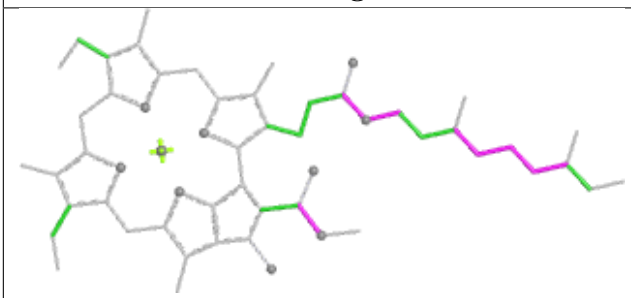
Ligand CLA 2 1207



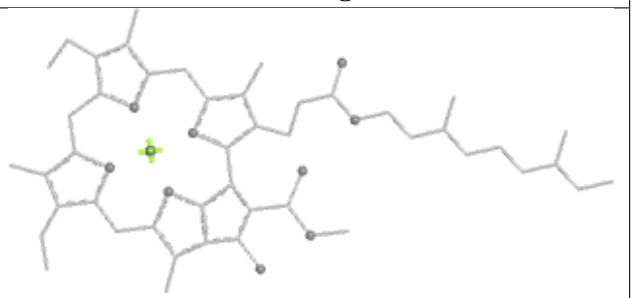
Bond lengths



Bond angles

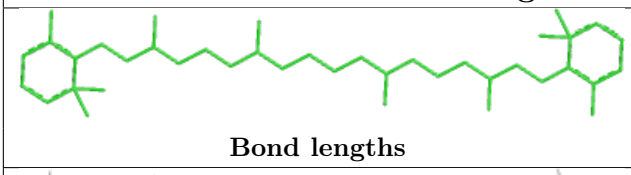


Torsions

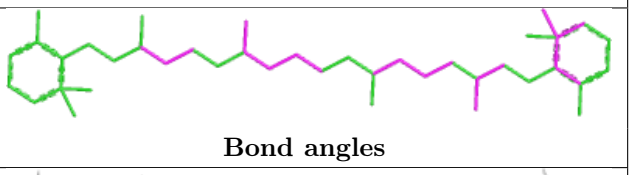


Rings

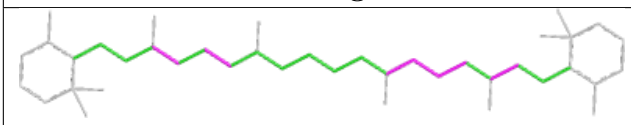
Ligand BCR a 4019



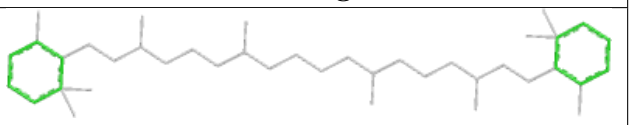
Bond lengths



Bond angles



Torsions

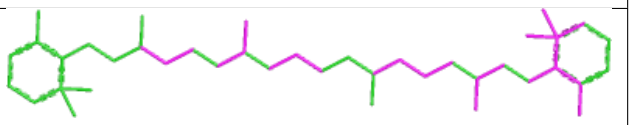


Rings

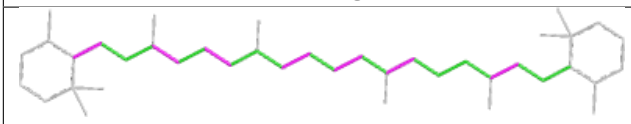
Ligand BCR b 4005



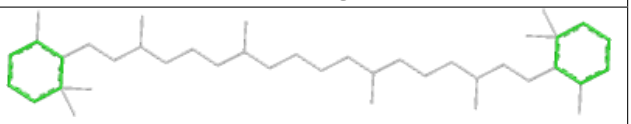
Bond lengths



Bond angles

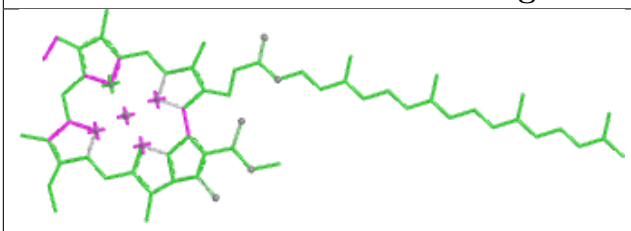


Torsions

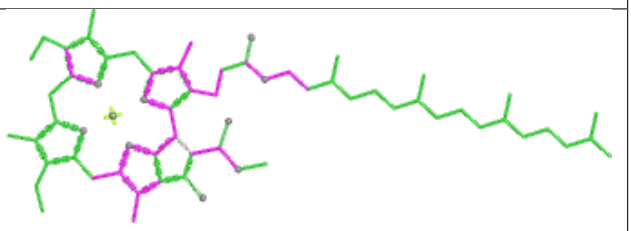


Rings

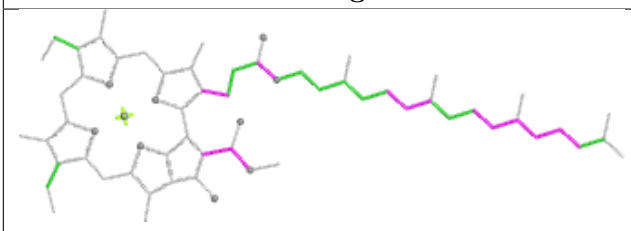
Ligand CLA b 1213



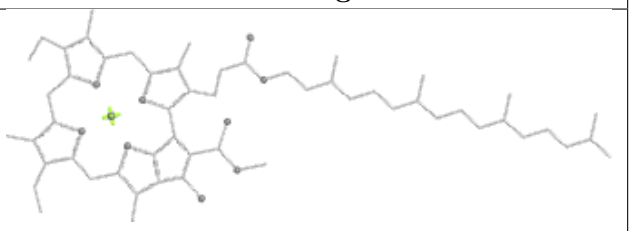
Bond lengths



Bond angles

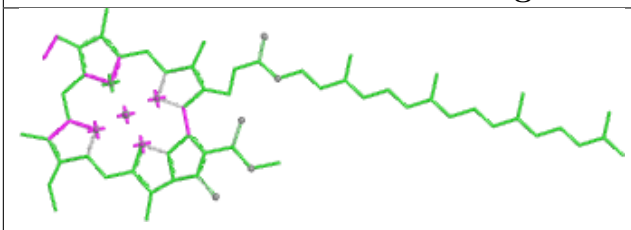


Torsions

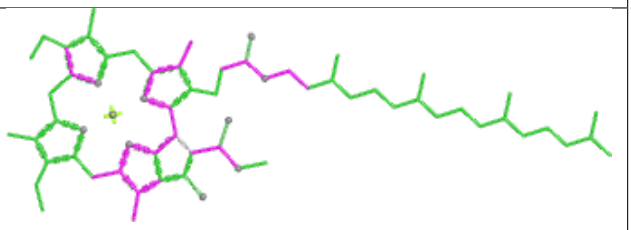


Rings

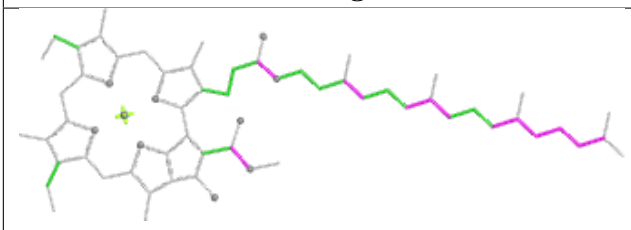
Ligand CLA K 1402



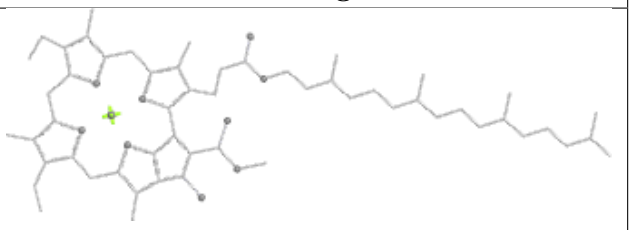
Bond lengths



Bond angles

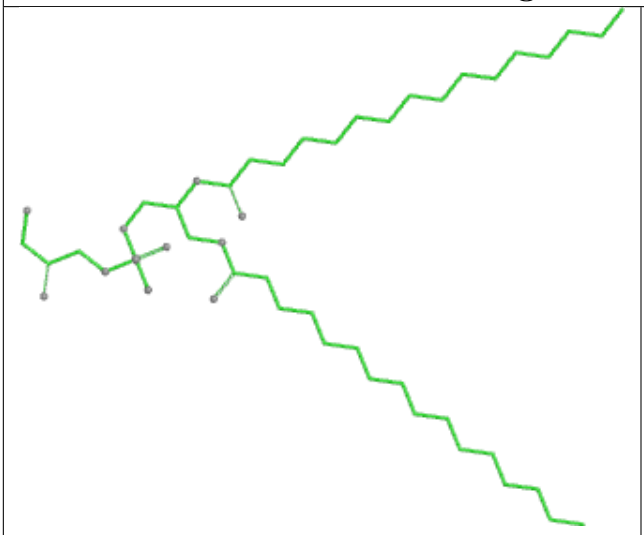


Torsions

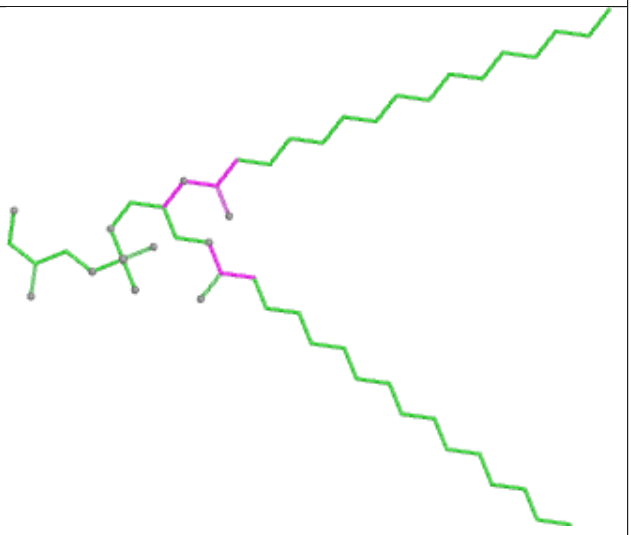


Rings

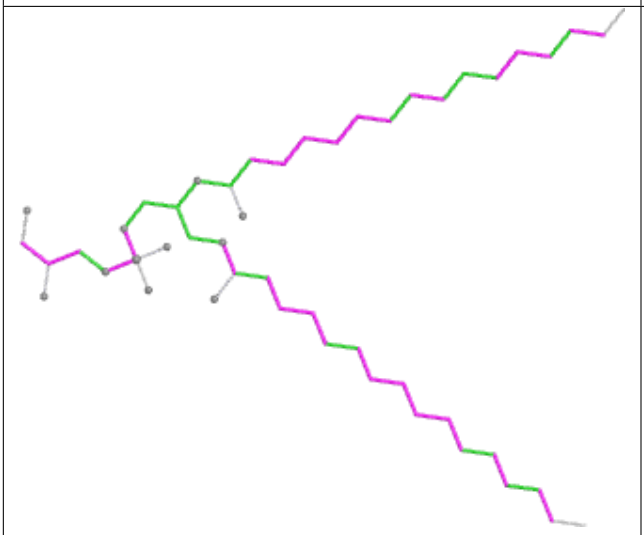
Ligand LHG 1 5003



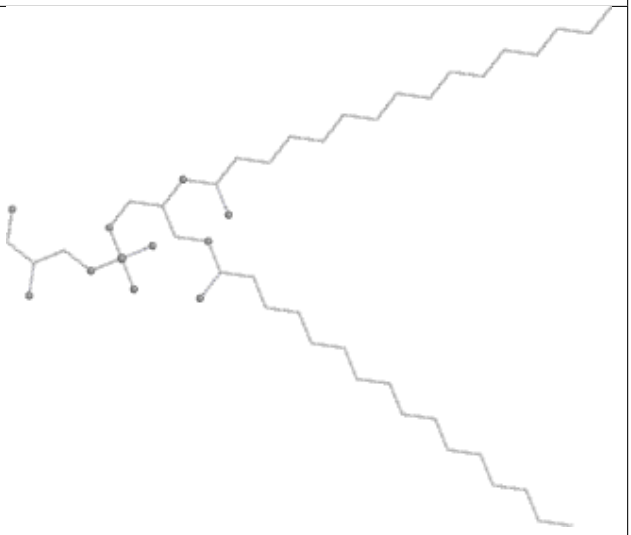
Bond lengths



Bond angles

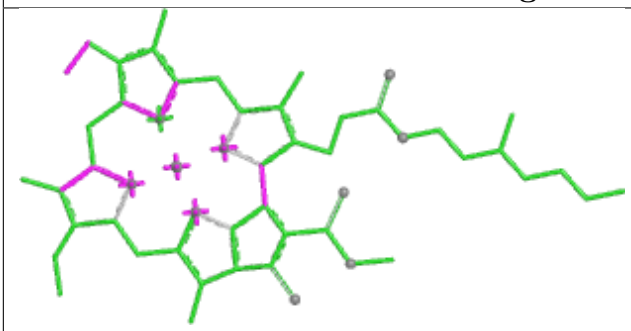


Torsions

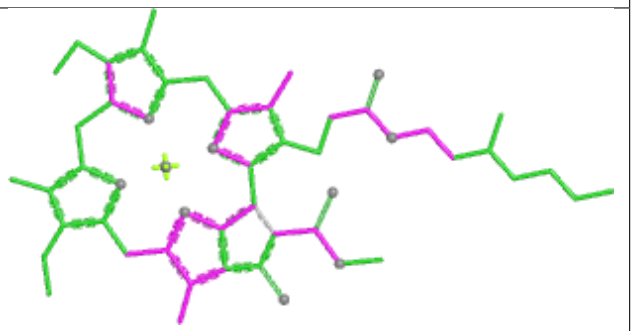


Rings

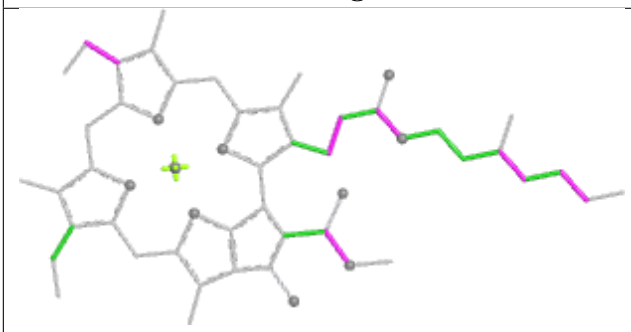
Ligand CLA 2 1235



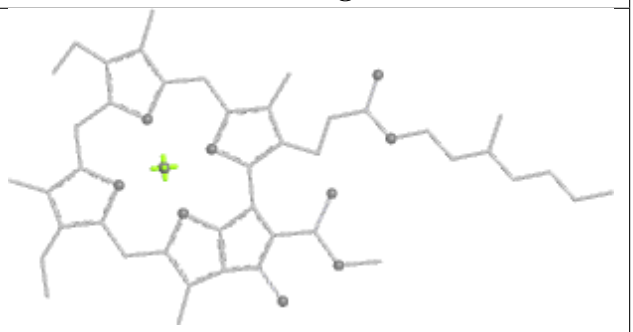
Bond lengths



Bond angles

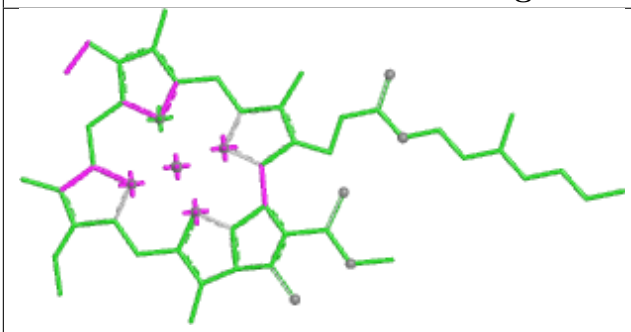


Torsions

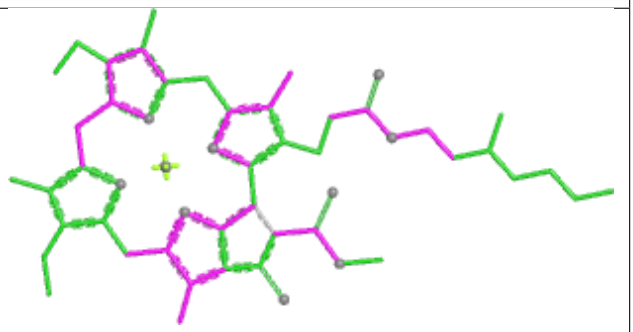


Rings

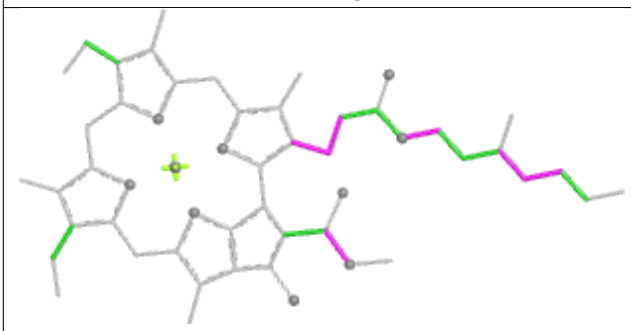
Ligand CLA A 1108



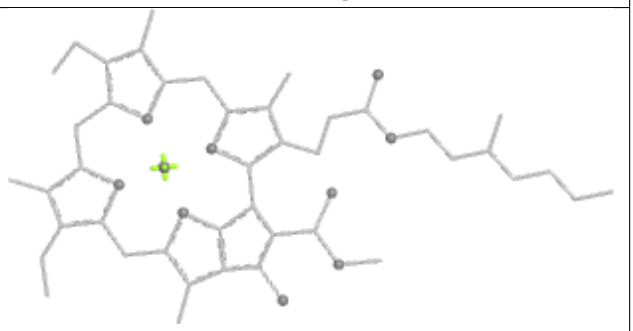
Bond lengths



Bond angles

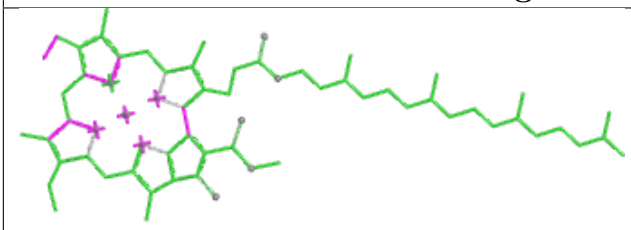


Torsions

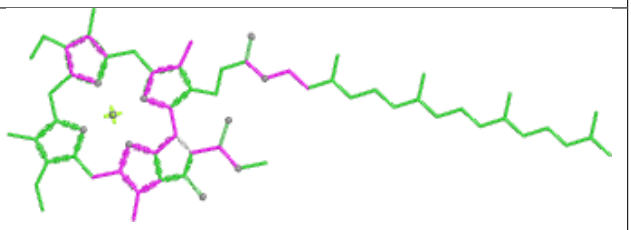


Rings

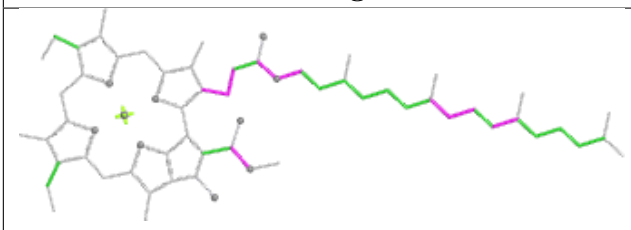
Ligand CLA A 1138



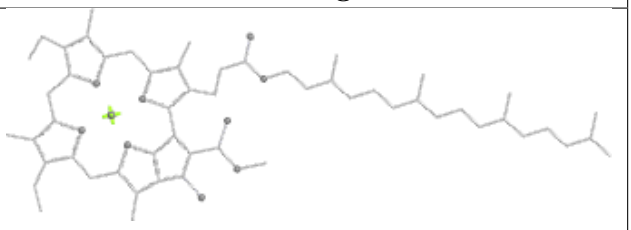
Bond lengths



Bond angles

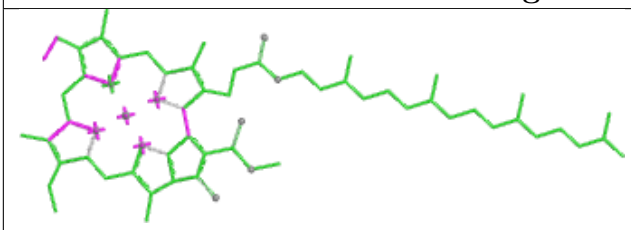


Torsions

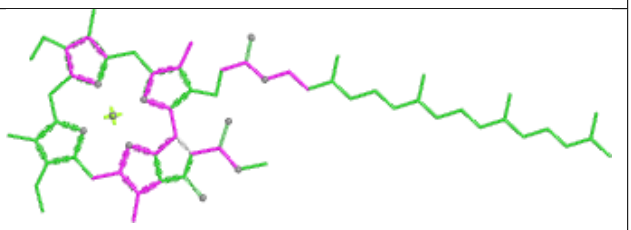


Rings

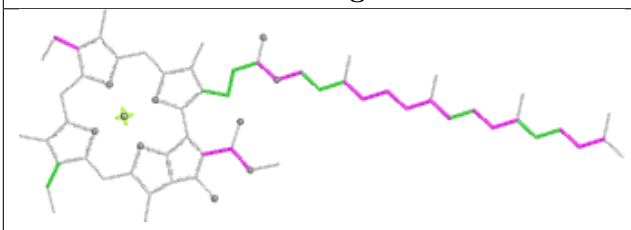
Ligand CLA f 1302



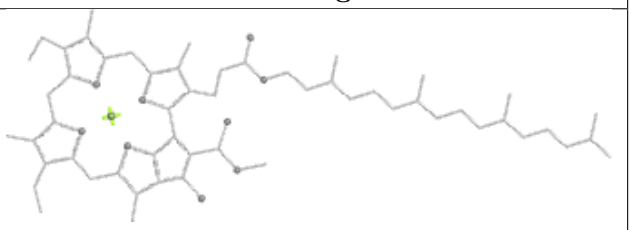
Bond lengths



Bond angles

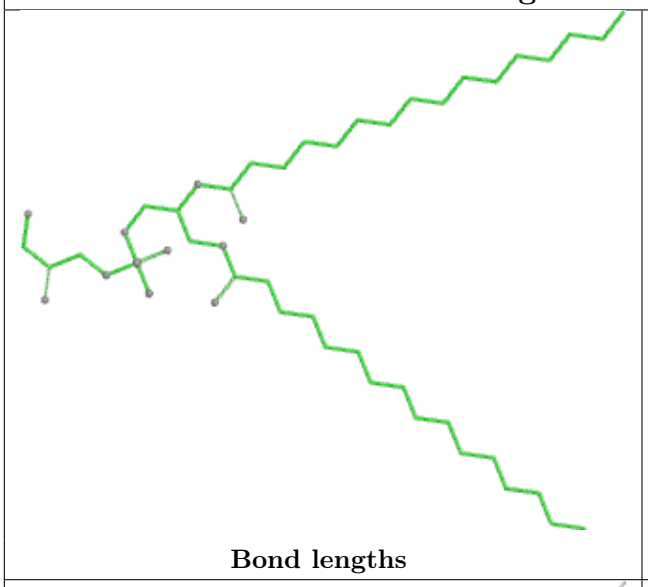


Torsions

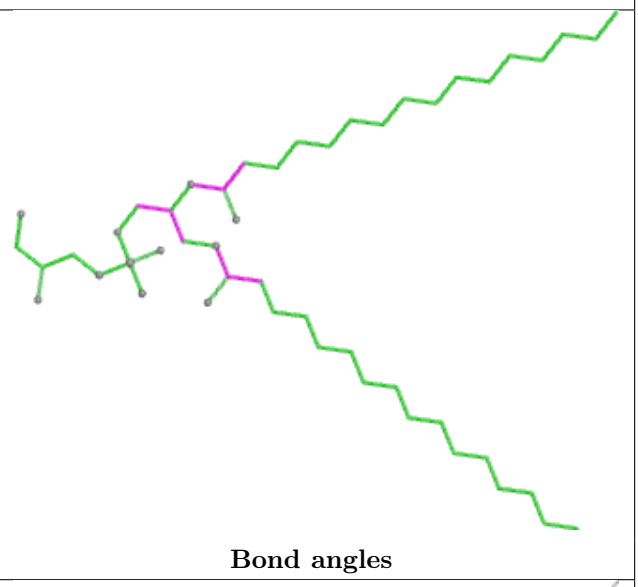


Rings

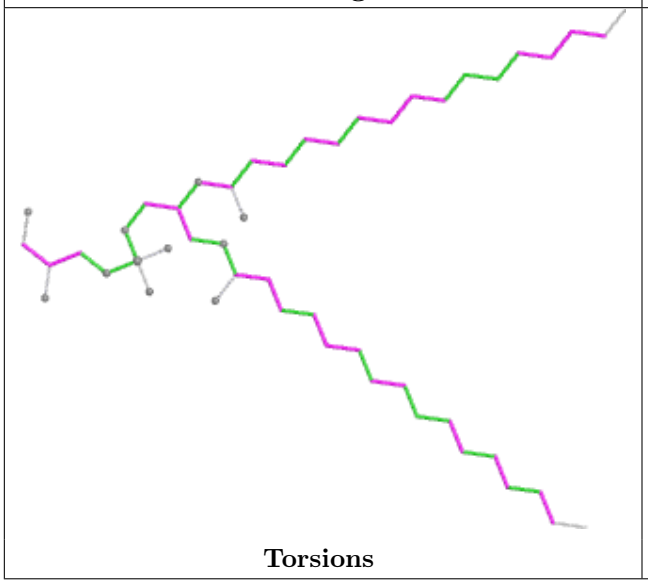
Ligand LHG 1 5001



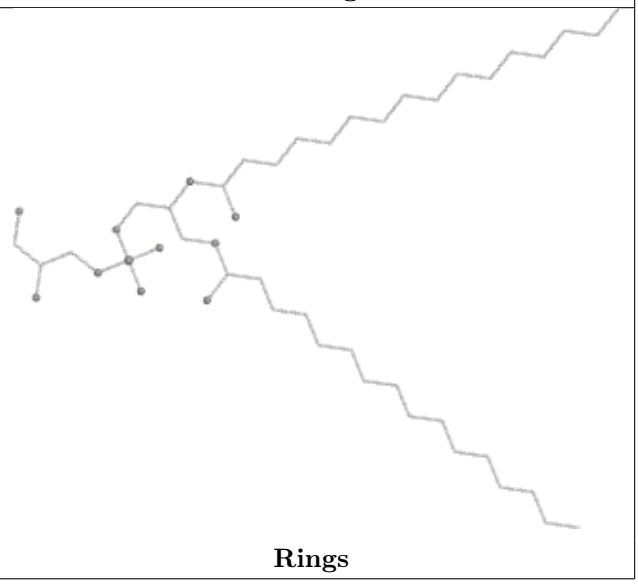
Bond lengths



Bond angles

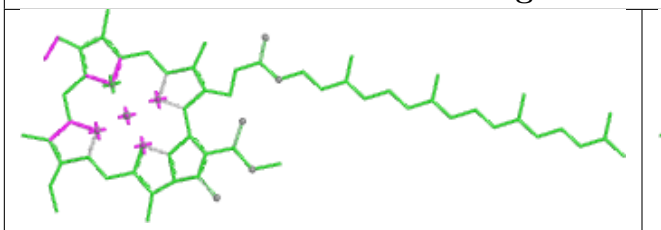


Torsions

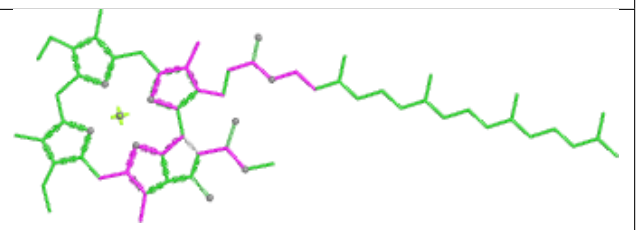


Rings

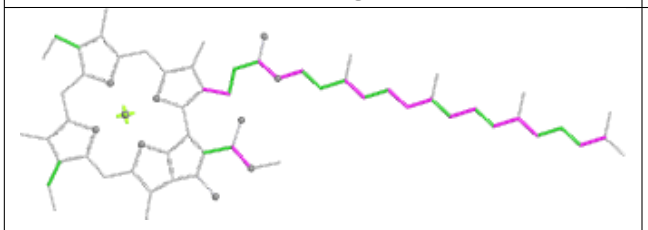
Ligand CLA A 1107



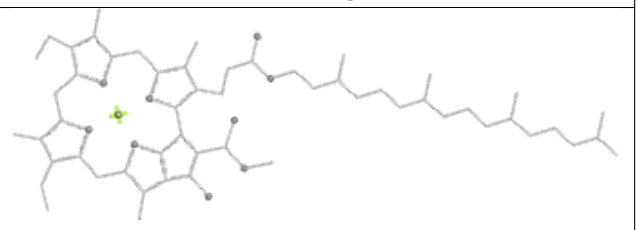
Bond lengths



Bond angles

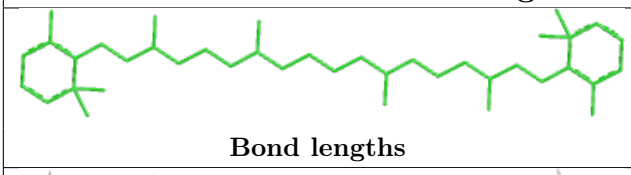


Torsions

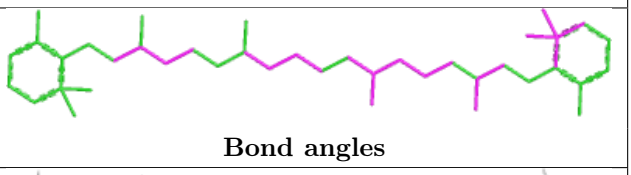


Rings

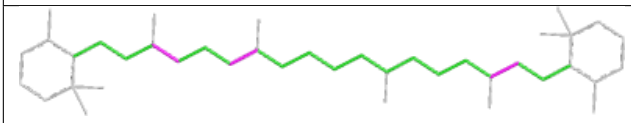
Ligand BCR 2 4014



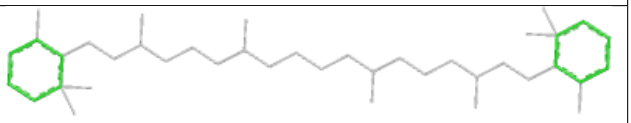
Bond lengths



Bond angles

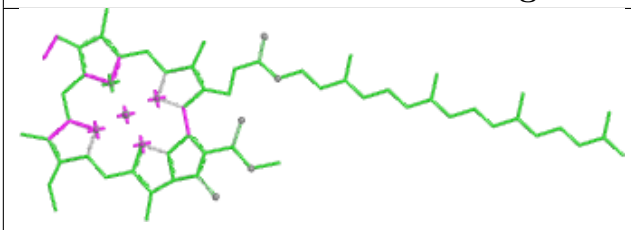


Torsions

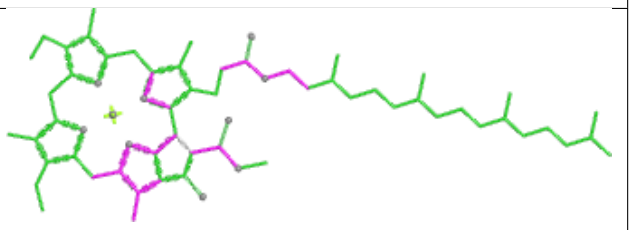


Rings

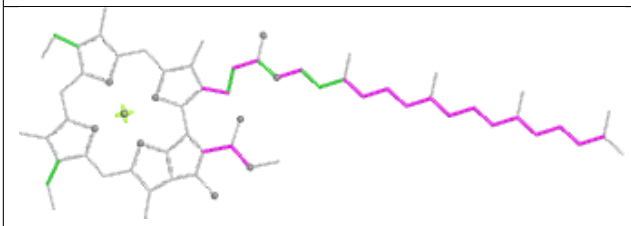
Ligand CLA 1 1103



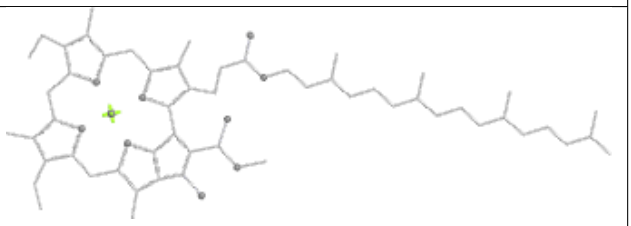
Bond lengths



Bond angles

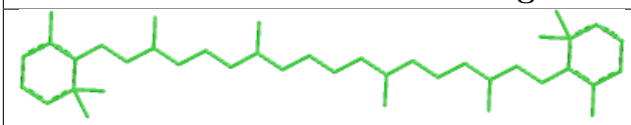


Torsions

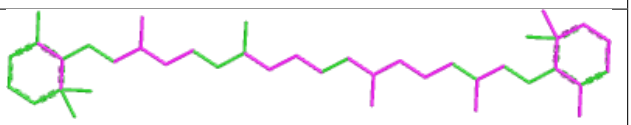


Rings

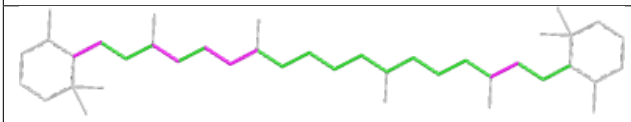
Ligand BCR 0 4022



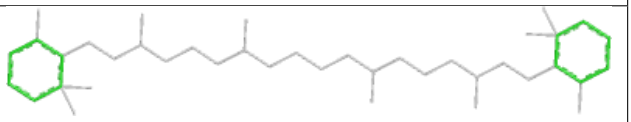
Bond lengths



Bond angles

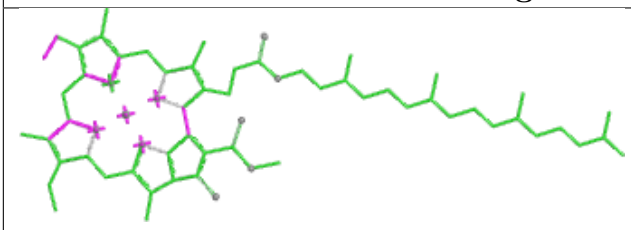


Torsions

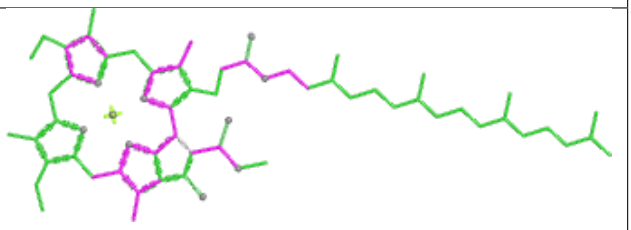


Rings

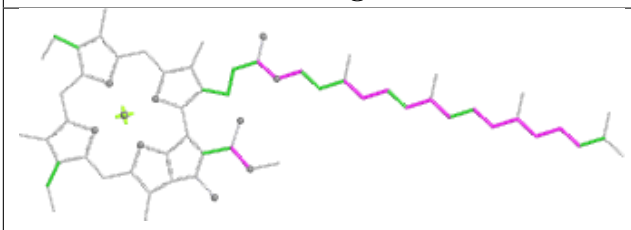
Ligand CLA B 1206



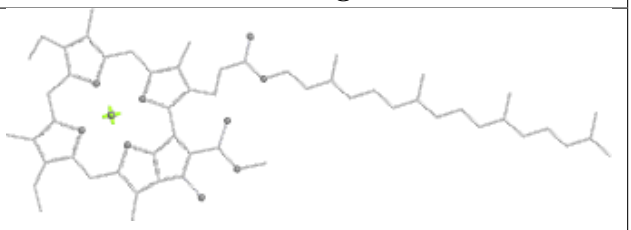
Bond lengths



Bond angles

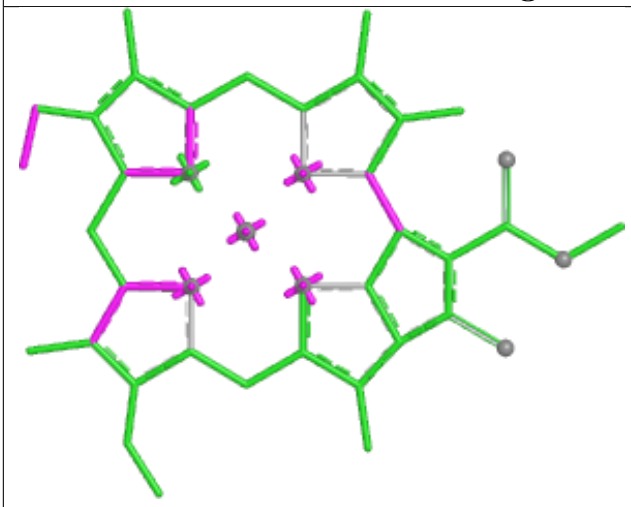


Torsions

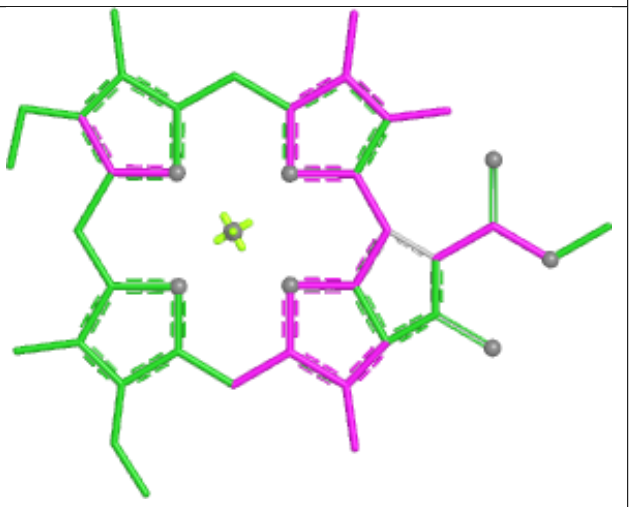


Rings

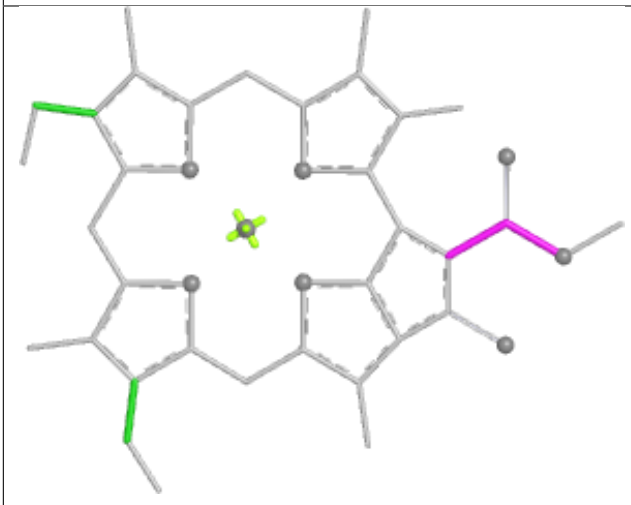
Ligand CLA 7 1302



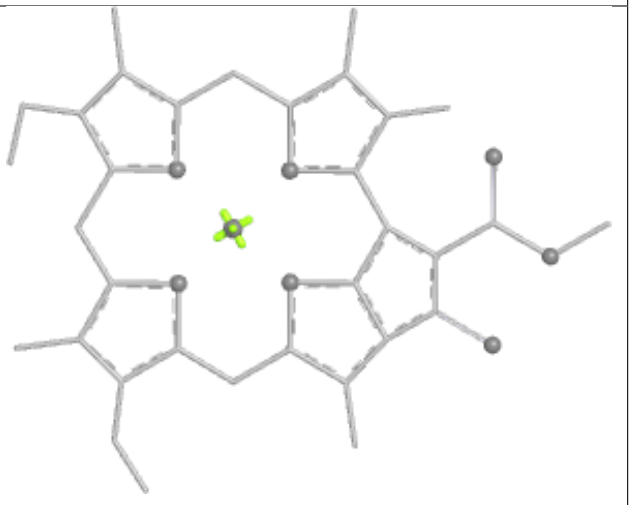
Bond lengths



Bond angles

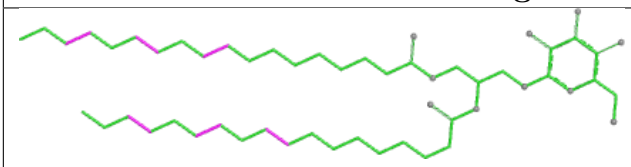


Torsions

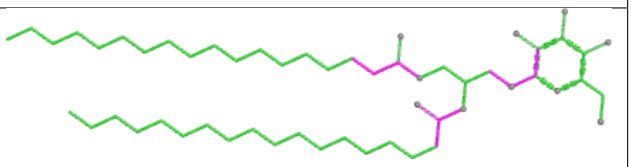


Rings

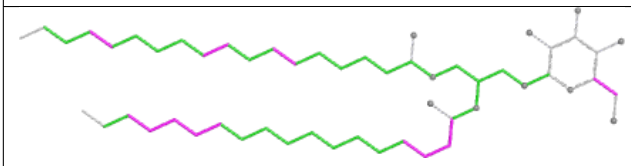
Ligand LMG b 5002



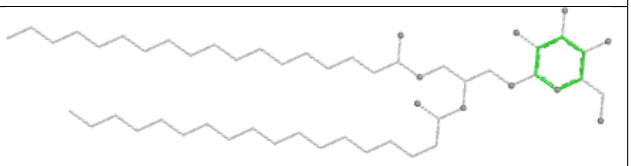
Bond lengths



Bond angles

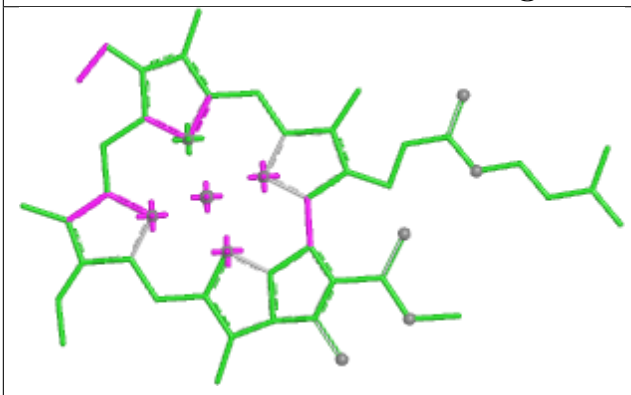


Torsions

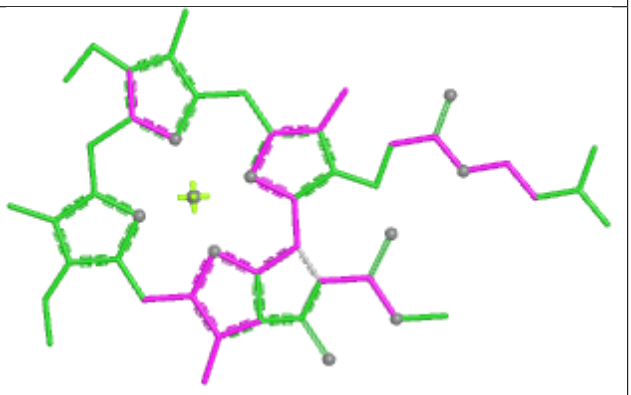


Rings

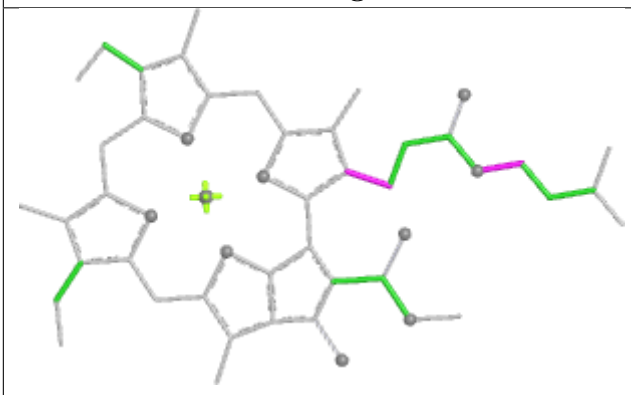
Ligand CLA k 1401



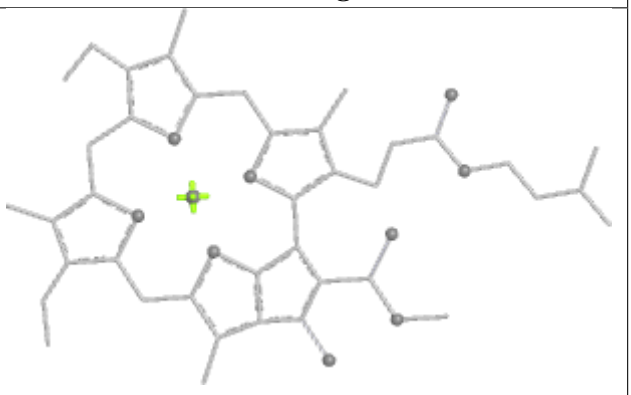
Bond lengths



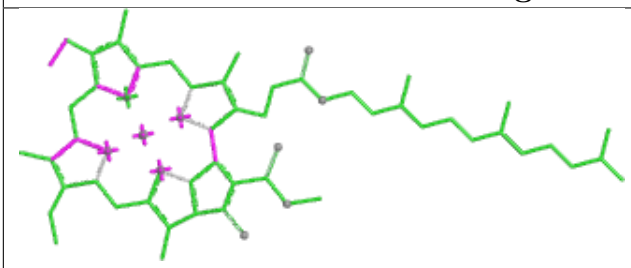
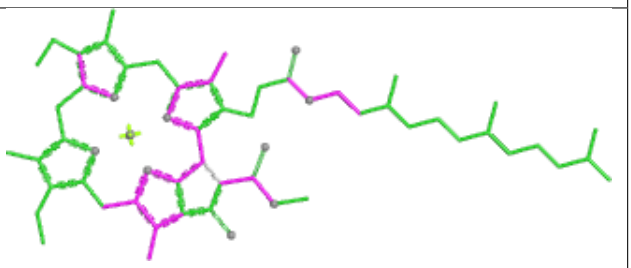
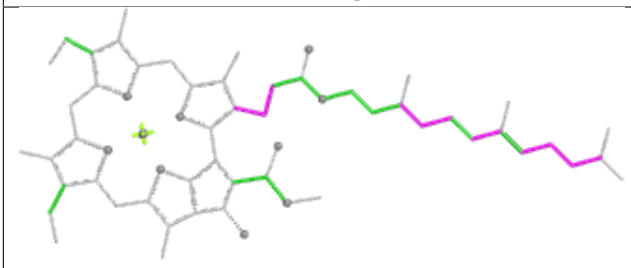
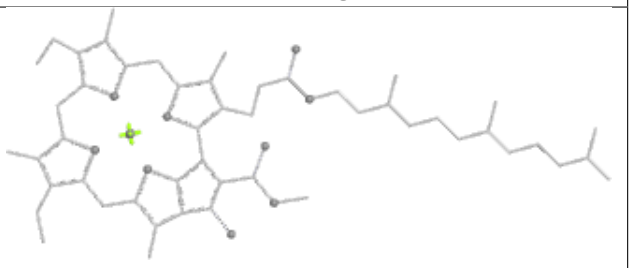
Bond angles

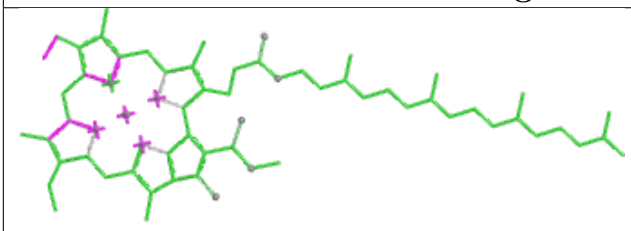
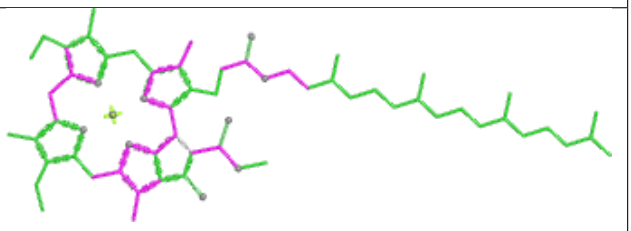
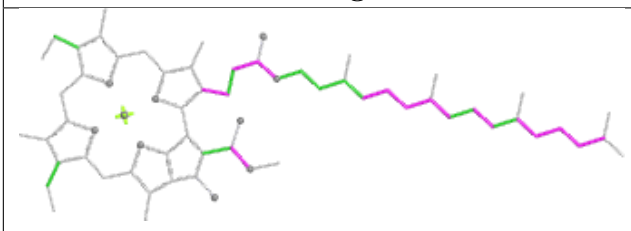
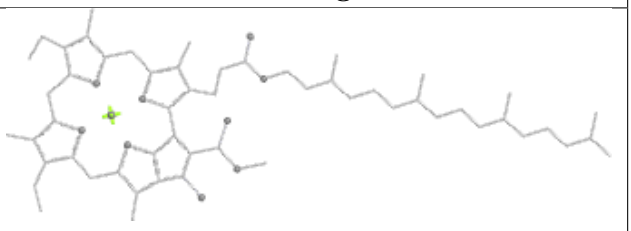


Torsions

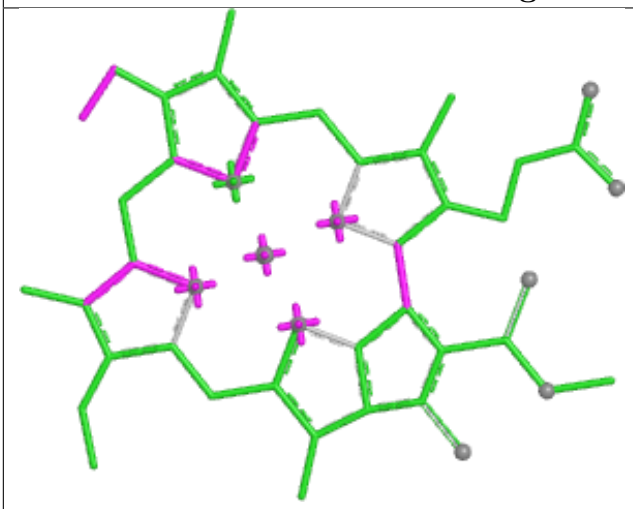


Rings

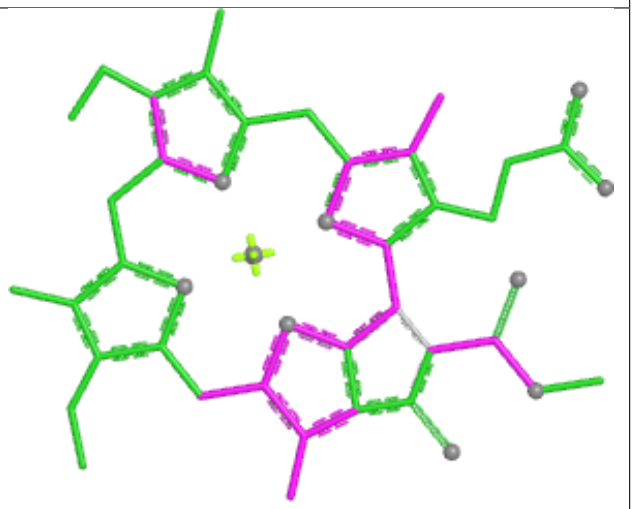
Ligand CLA A 1122	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1114	
	
Bond lengths	Bond angles
	
Torsions	Rings

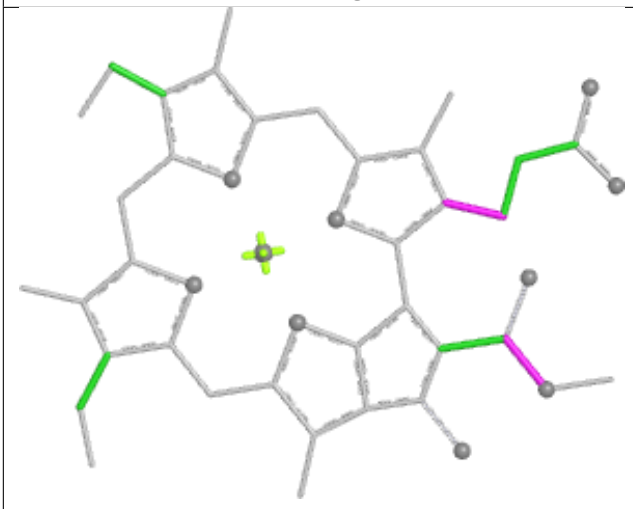
Ligand CLA 1 1114



Bond lengths



Bond angles

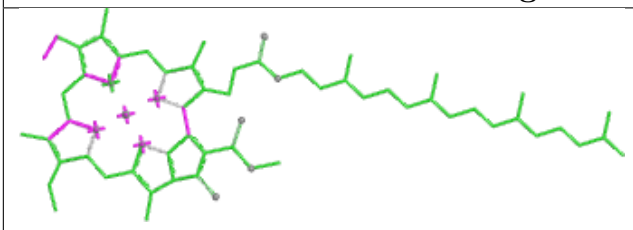


Torsions

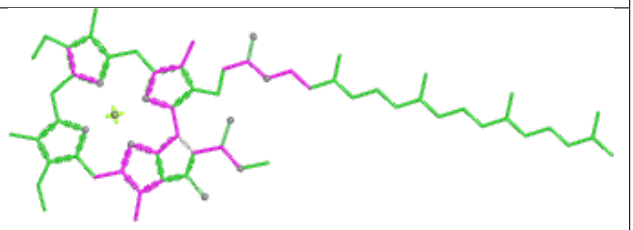


Rings

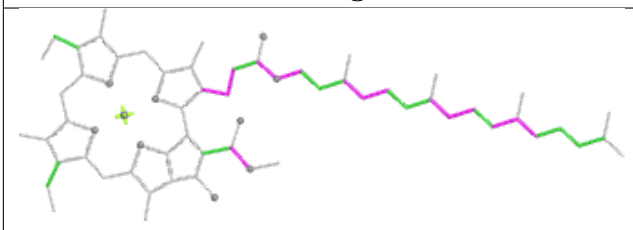
Ligand CLA 2 1218



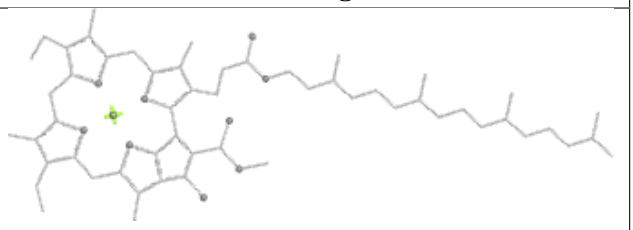
Bond lengths



Bond angles

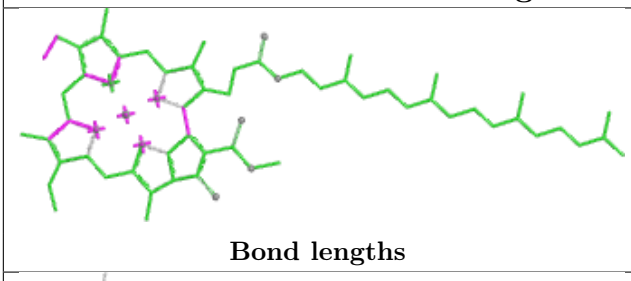


Torsions

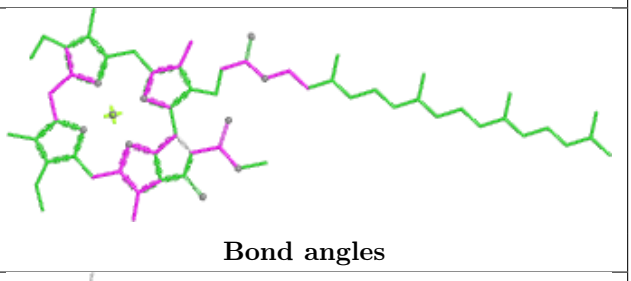


Rings

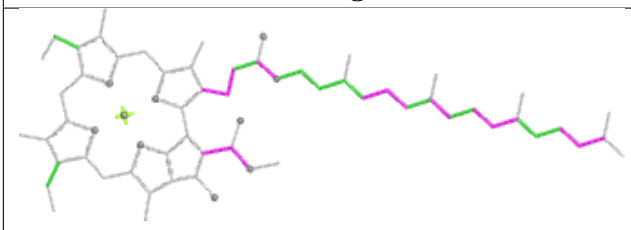
Ligand CLA B 1209



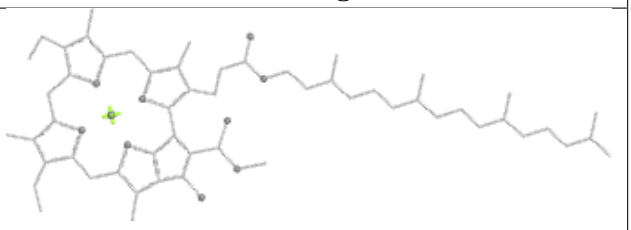
Bond lengths



Bond angles

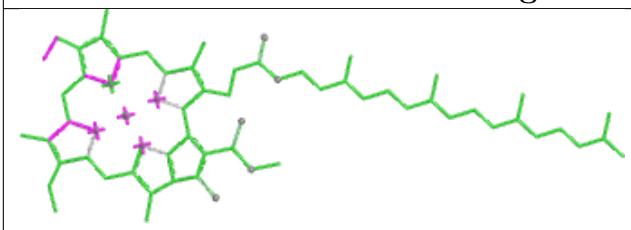


Torsions

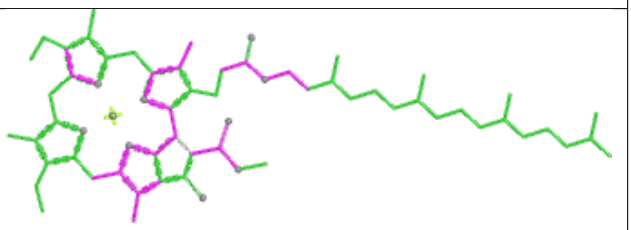


Rings

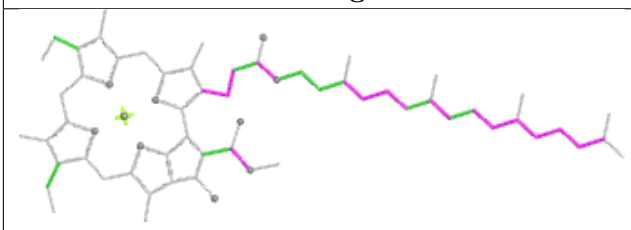
Ligand CLA a 1135



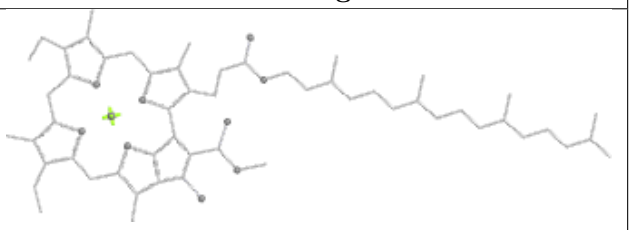
Bond lengths



Bond angles

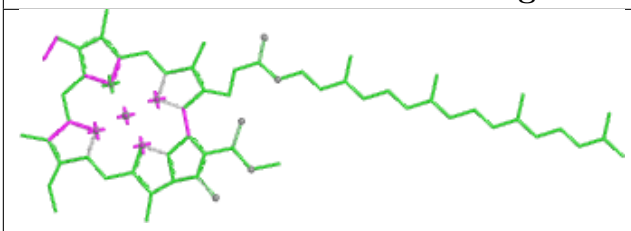


Torsions

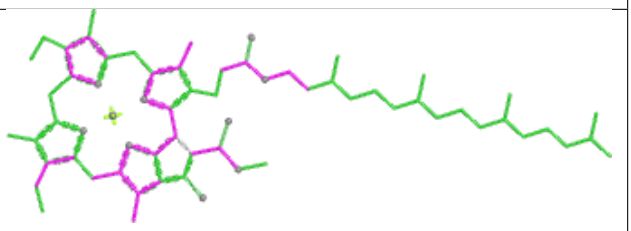


Rings

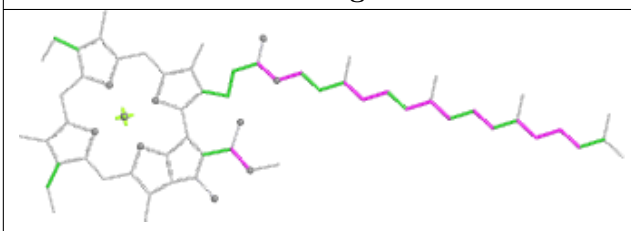
Ligand CLA b 1206



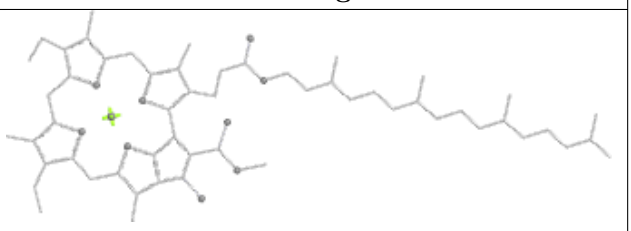
Bond lengths



Bond angles

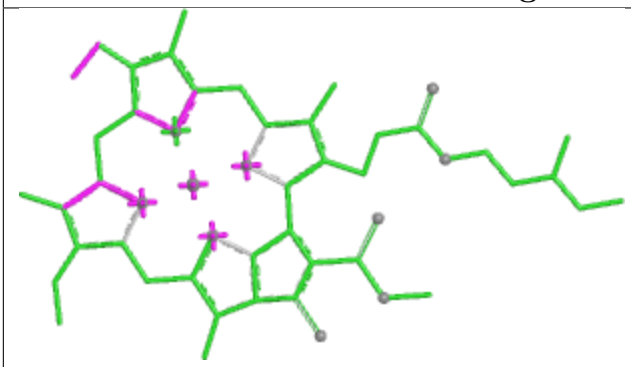


Torsions

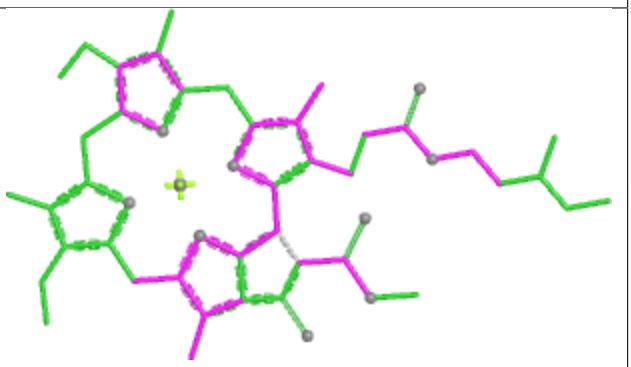


Rings

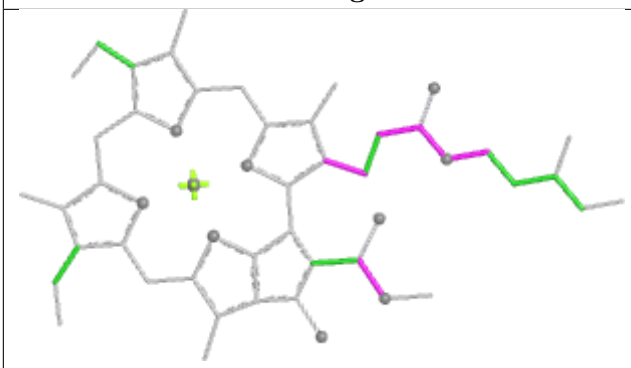
Ligand CLA 1 1107



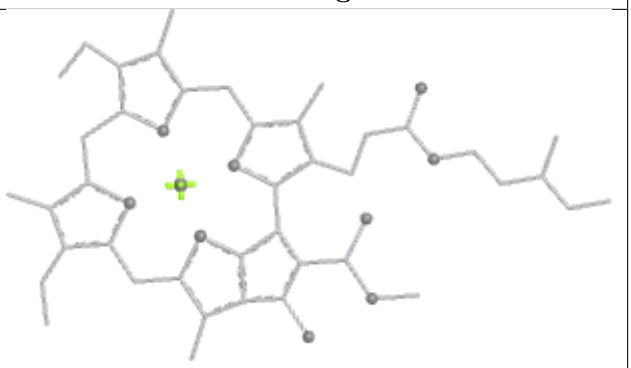
Bond lengths



Bond angles

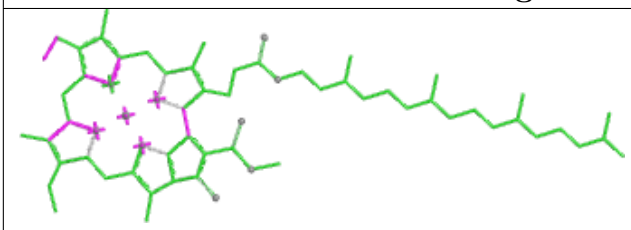


Torsions

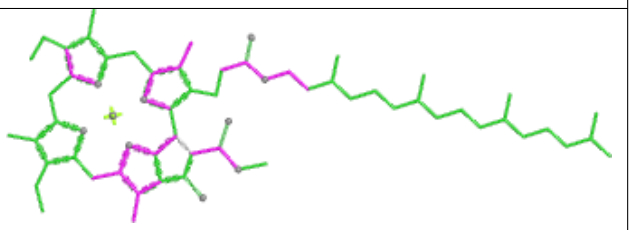


Rings

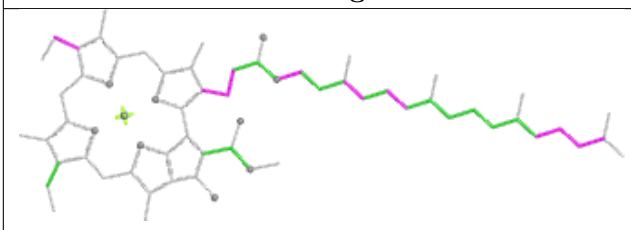
Ligand CLA B 1225



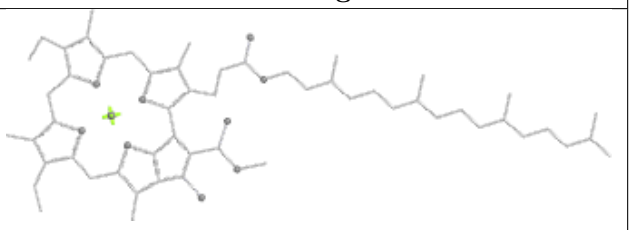
Bond lengths



Bond angles

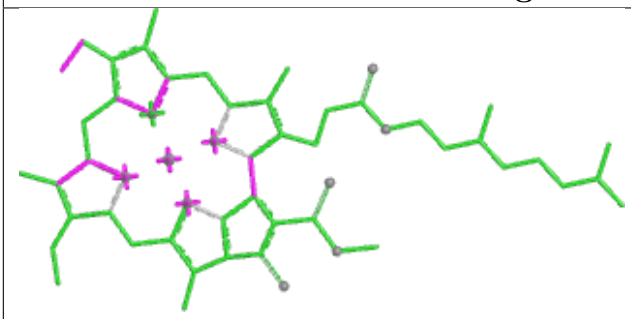


Torsions

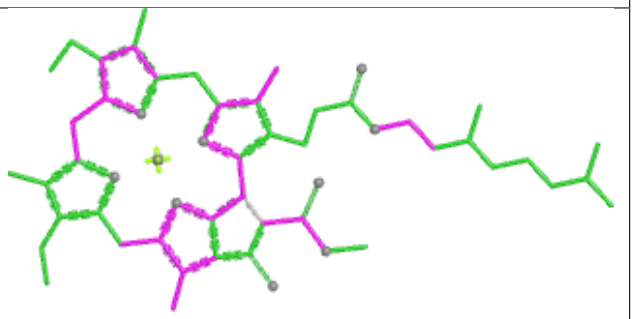


Rings

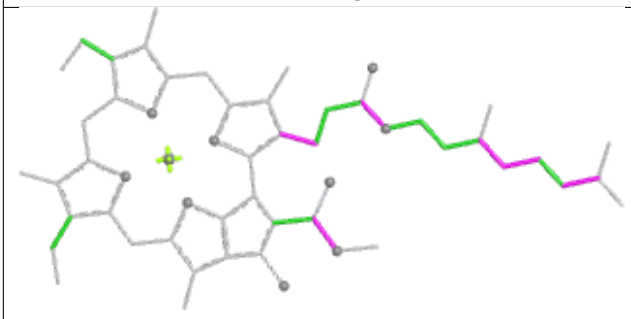
Ligand CLA B 1212



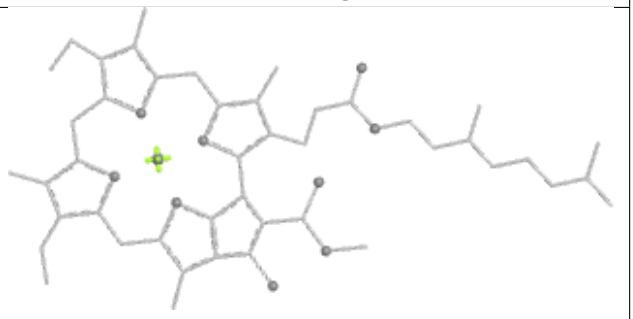
Bond lengths



Bond angles

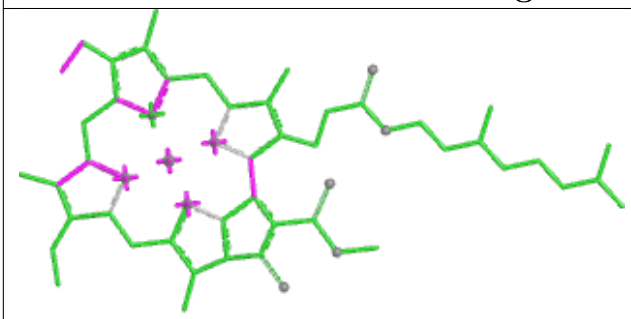


Torsions

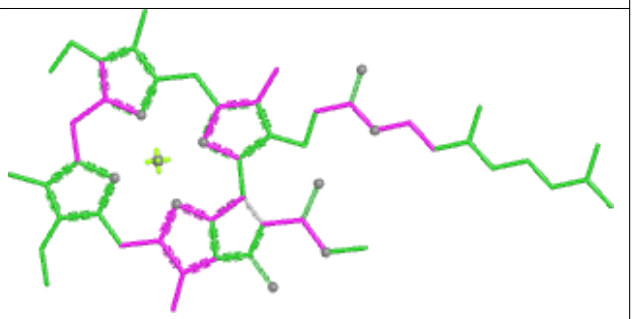


Rings

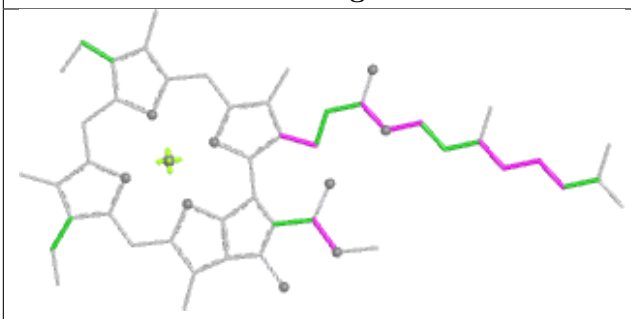
Ligand CLA B 1227



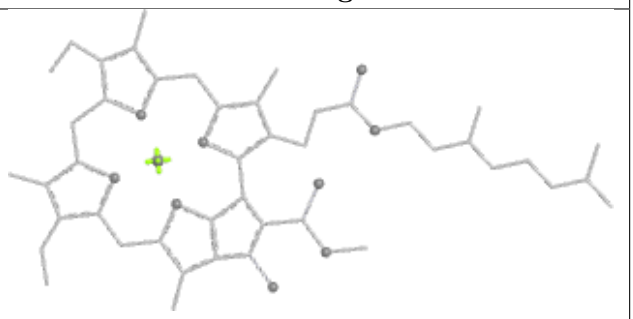
Bond lengths



Bond angles

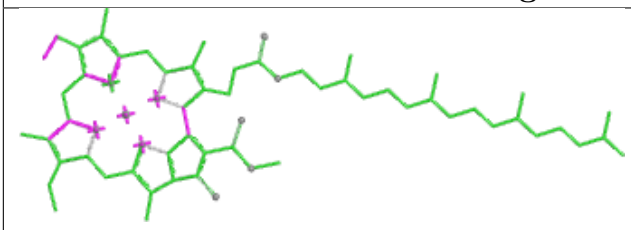


Torsions

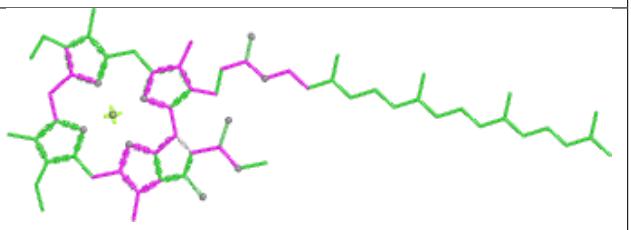


Rings

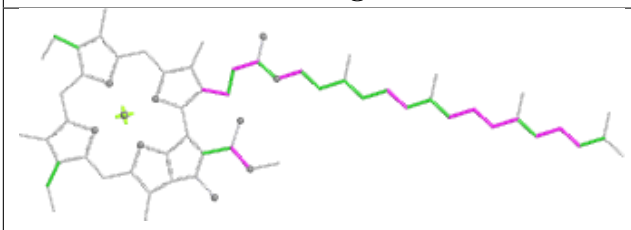
Ligand CLA 1 1101



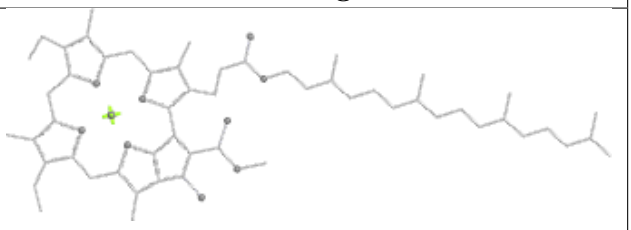
Bond lengths



Bond angles

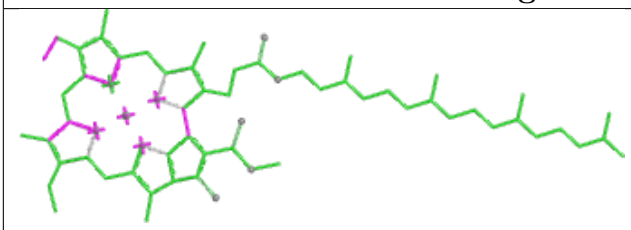


Torsions

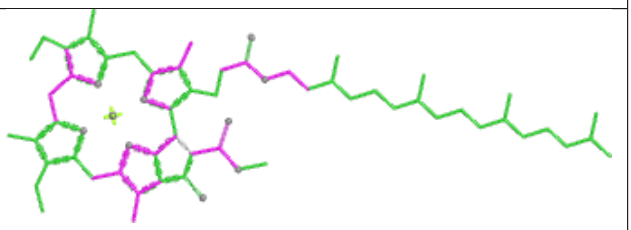


Rings

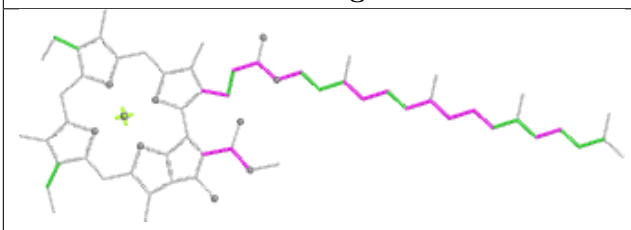
Ligand CLA b 1230



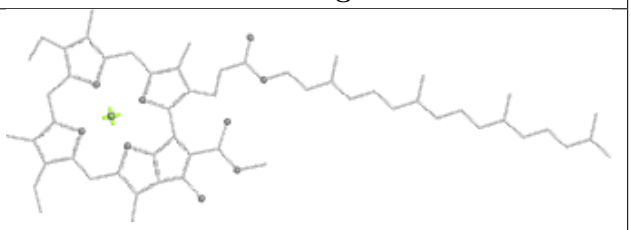
Bond lengths



Bond angles

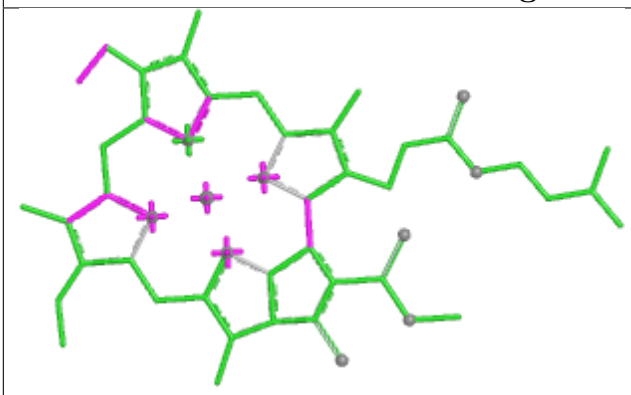


Torsions

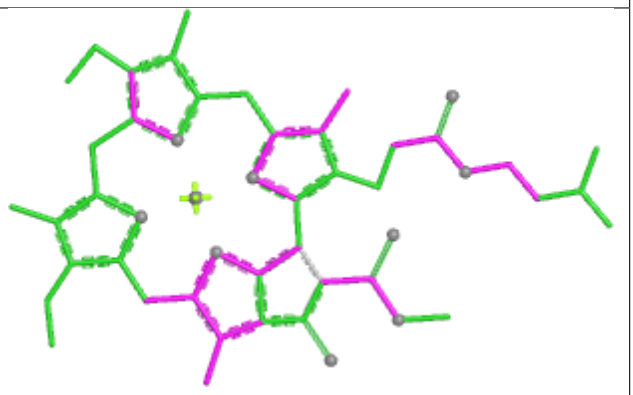


Rings

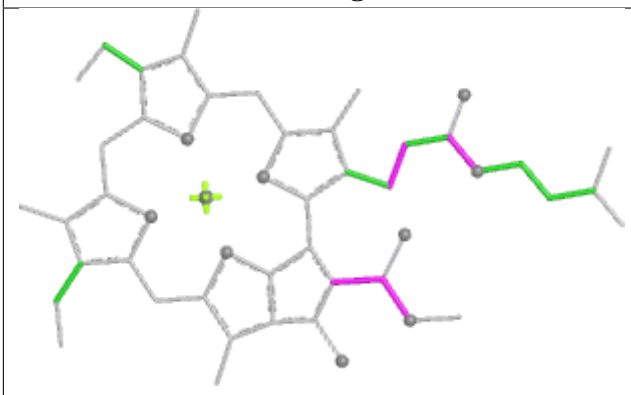
Ligand CLA 2 1213



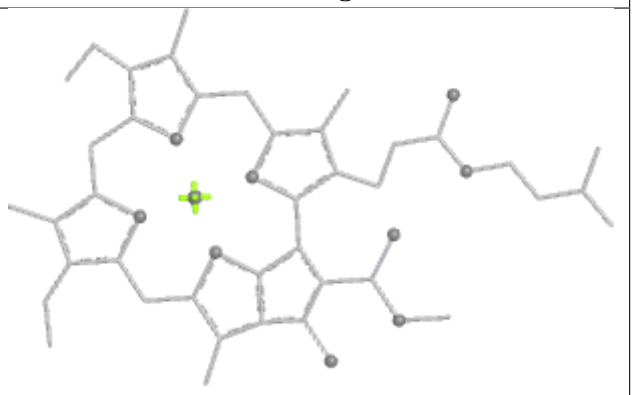
Bond lengths



Bond angles

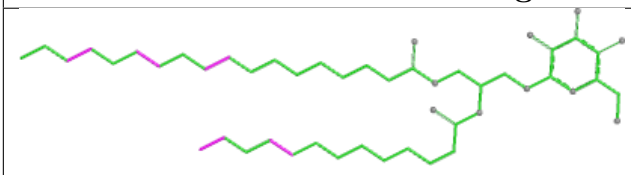


Torsions

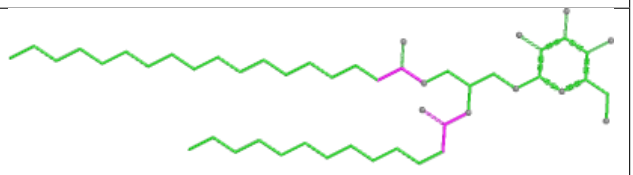


Rings

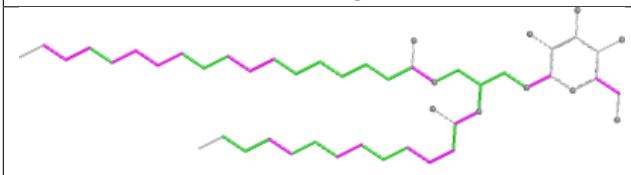
Ligand LMG a 5002



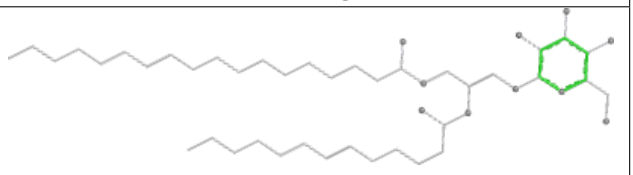
Bond lengths



Bond angles

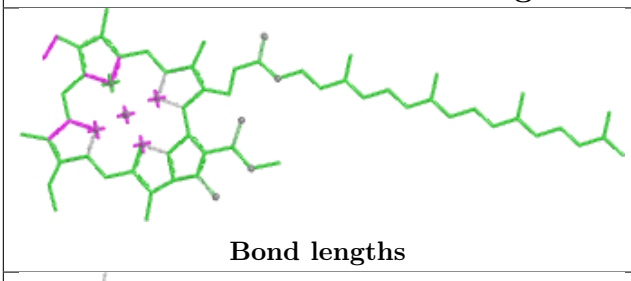


Torsions

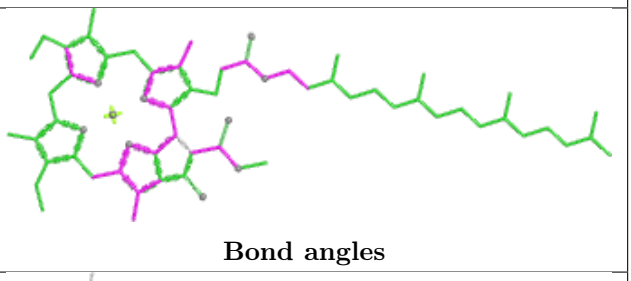


Rings

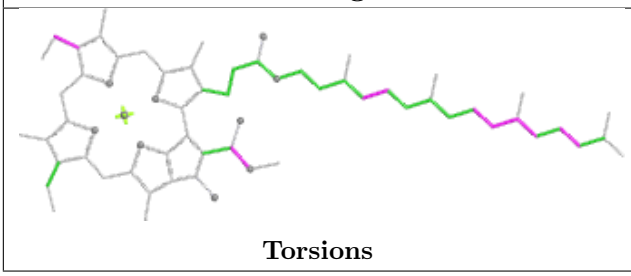
Ligand CLA A 1115



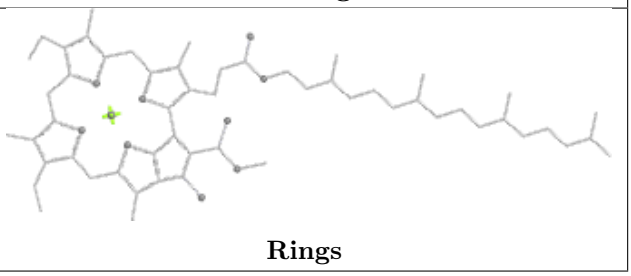
Bond lengths



Bond angles

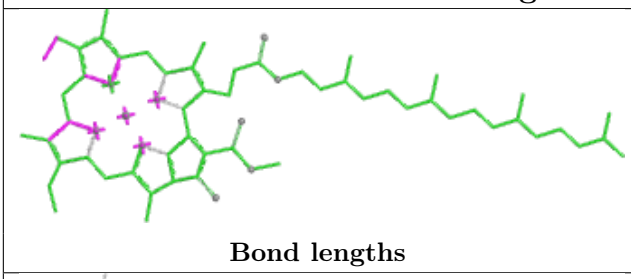


Torsions

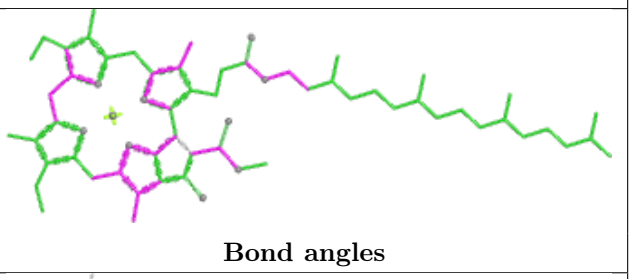


Rings

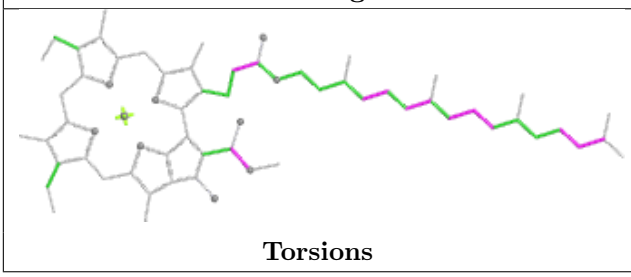
Ligand CLA 1 1115



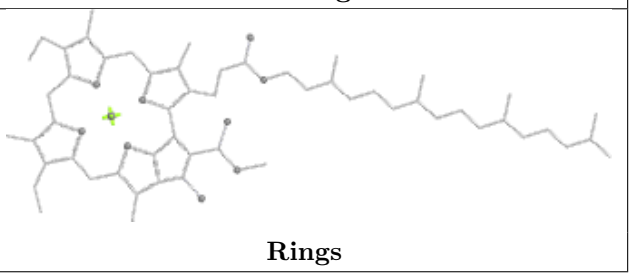
Bond lengths



Bond angles

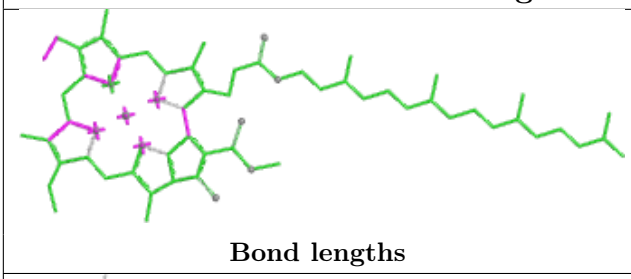


Torsions

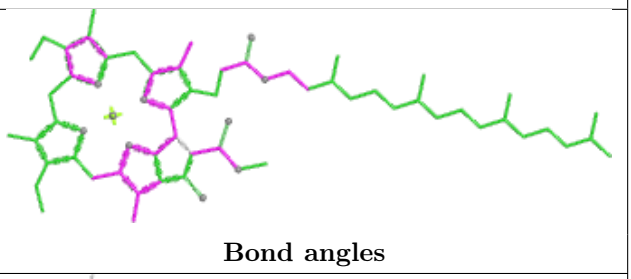


Rings

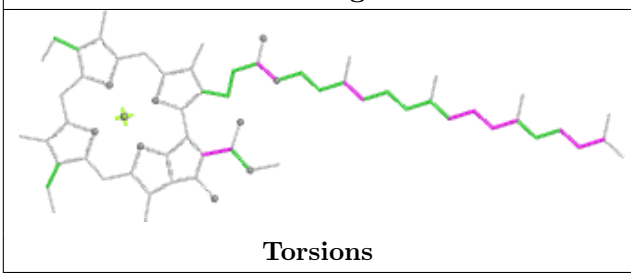
Ligand CLA B 1221



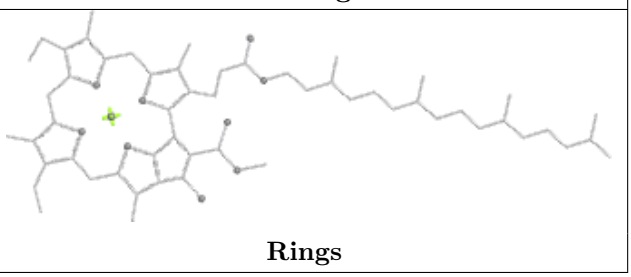
Bond lengths



Bond angles

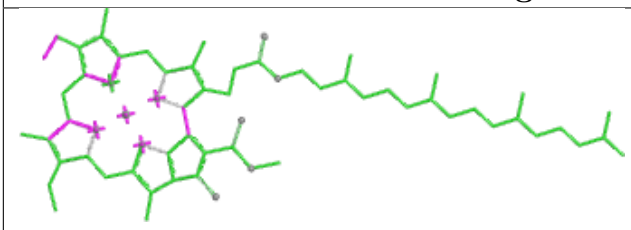


Torsions

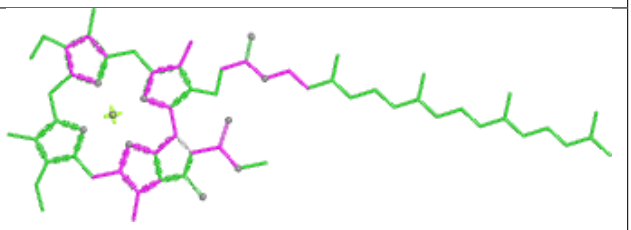


Rings

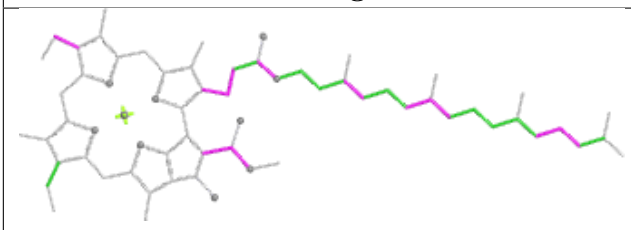
Ligand CLA B 1240



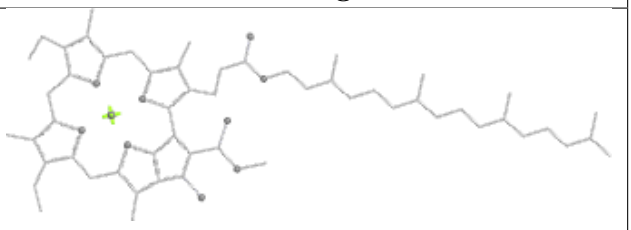
Bond lengths



Bond angles

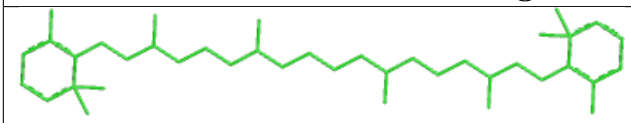


Torsions

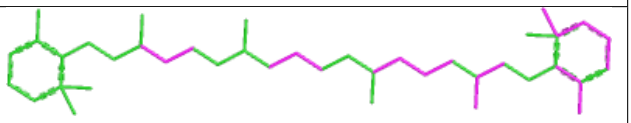


Rings

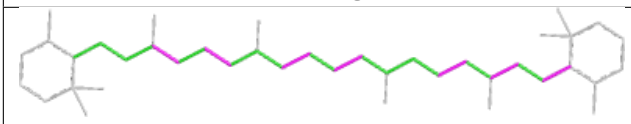
Ligand BCR b 4018



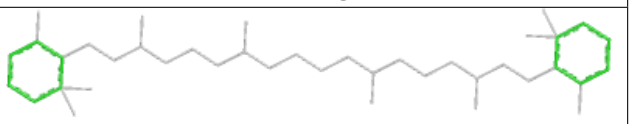
Bond lengths



Bond angles

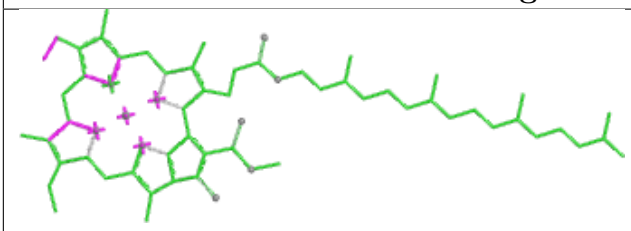


Torsions

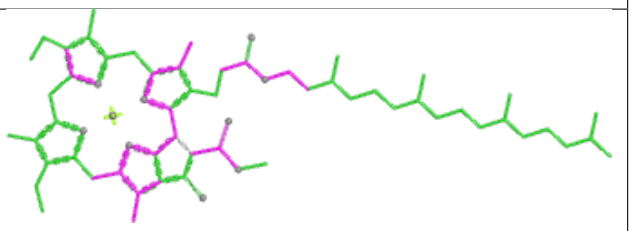


Rings

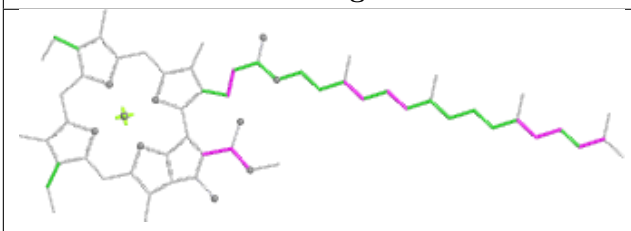
Ligand CLA a 1132



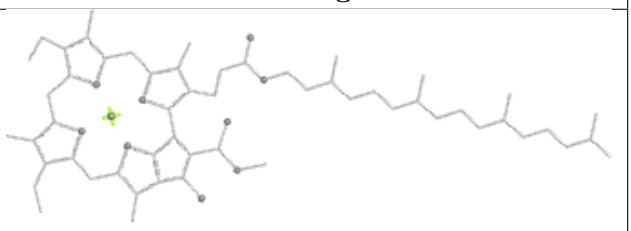
Bond lengths



Bond angles

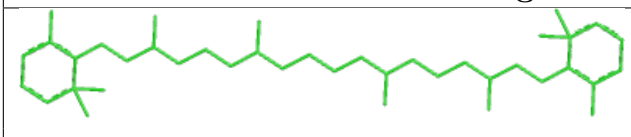


Torsions

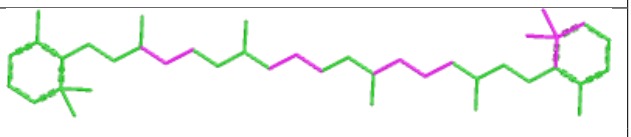


Rings

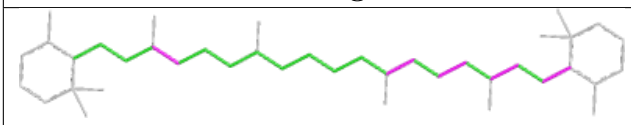
Ligand BCR b 4010



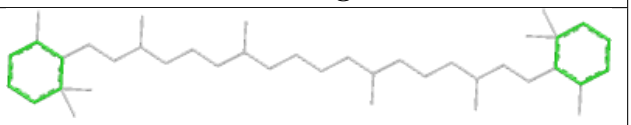
Bond lengths



Bond angles

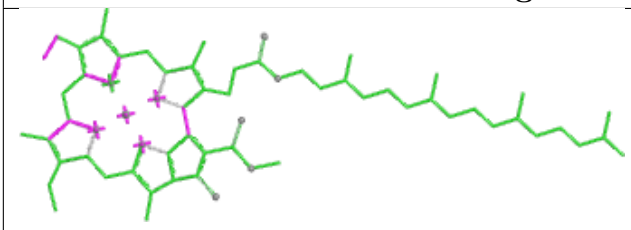


Torsions

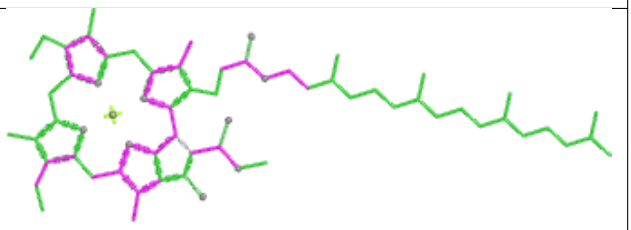


Rings

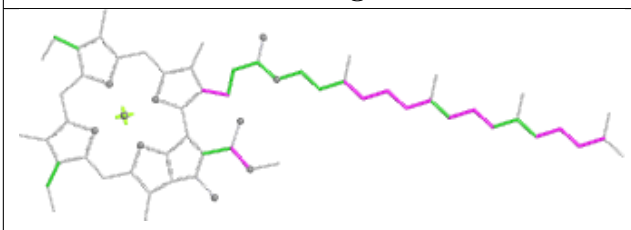
Ligand CLA B 1215



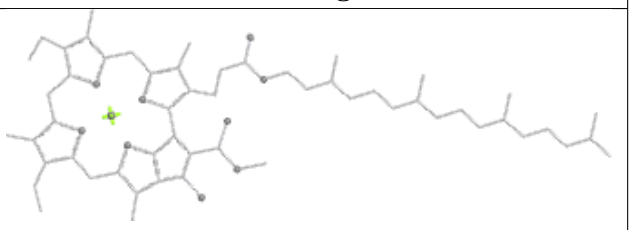
Bond lengths



Bond angles

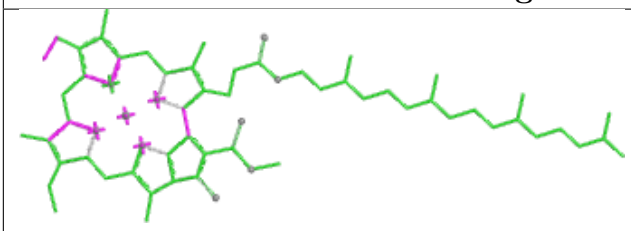


Torsions

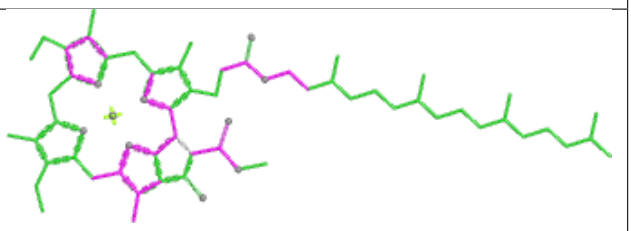


Rings

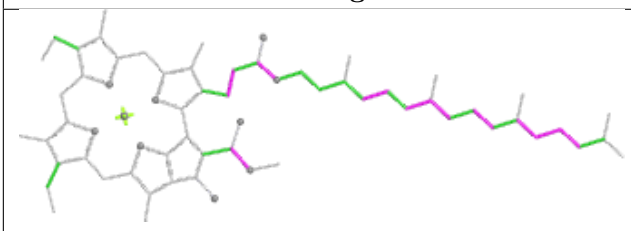
Ligand CLA B 1201



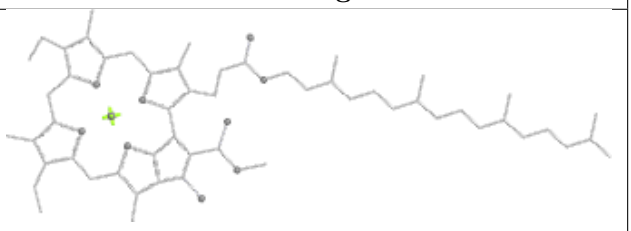
Bond lengths



Bond angles

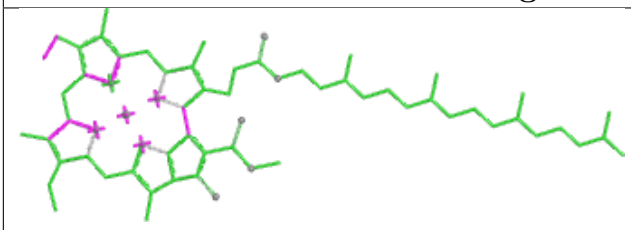


Torsions

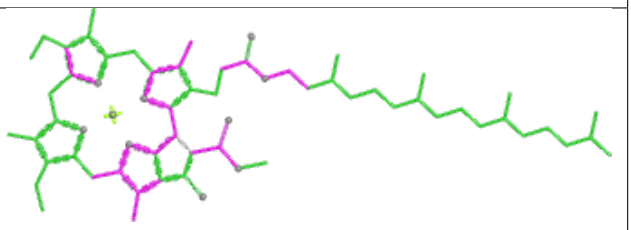


Rings

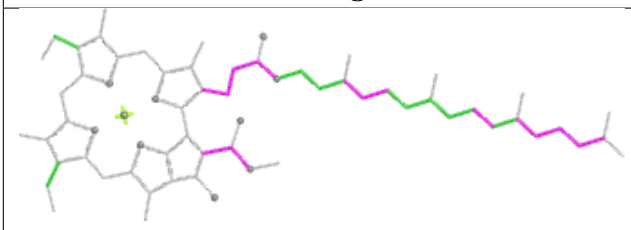
Ligand CLA 2 1202



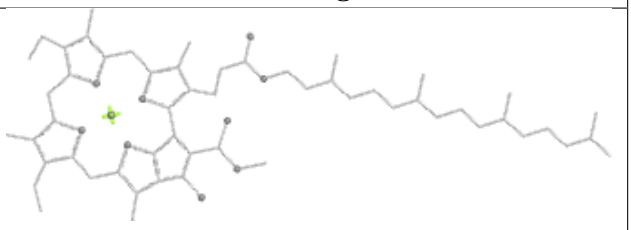
Bond lengths



Bond angles

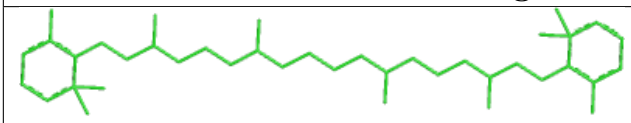


Torsions

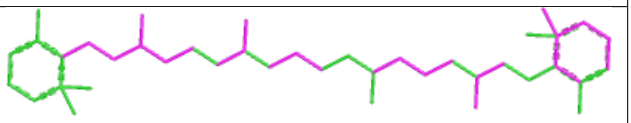


Rings

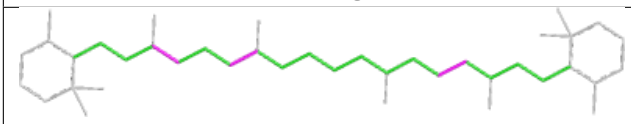
Ligand BCR A 4001



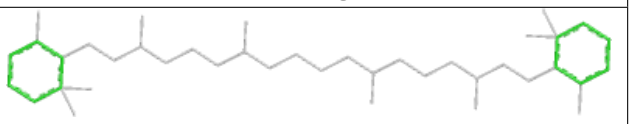
Bond lengths



Bond angles

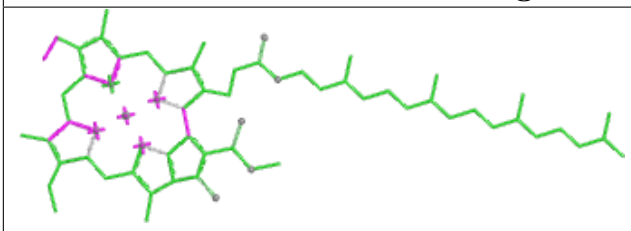


Torsions

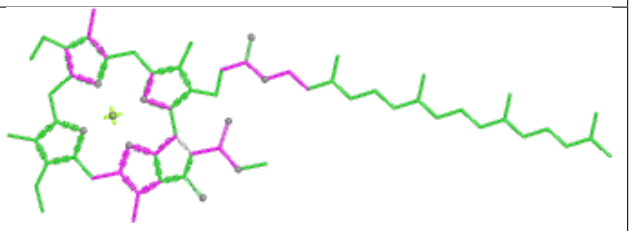


Rings

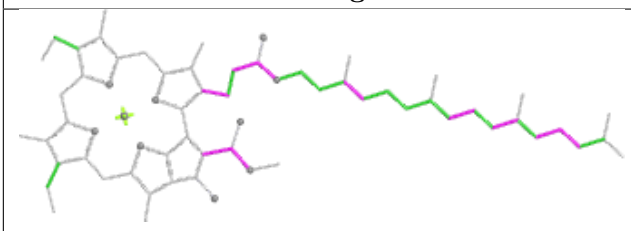
Ligand CLA B 1202



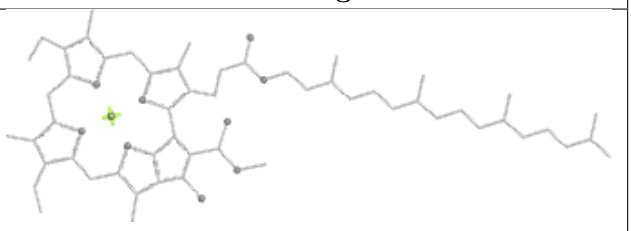
Bond lengths



Bond angles

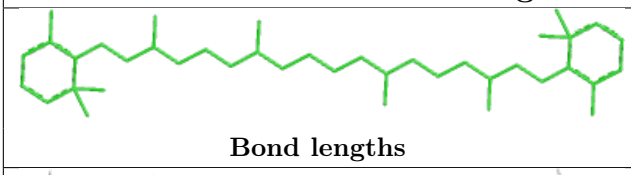


Torsions

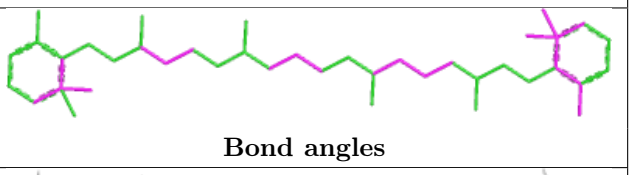


Rings

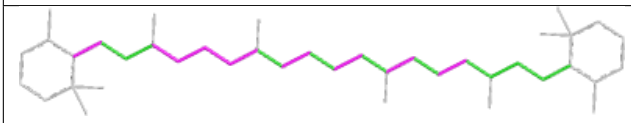
Ligand BCR h 4018



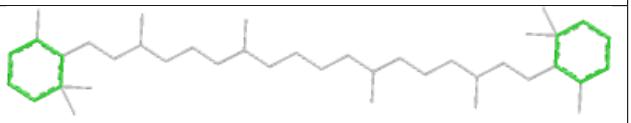
Bond lengths



Bond angles



Torsions



Rings

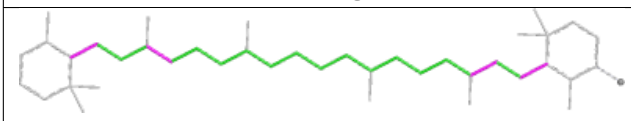
Ligand ECH m 4021



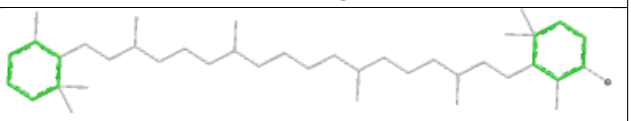
Bond lengths



Bond angles

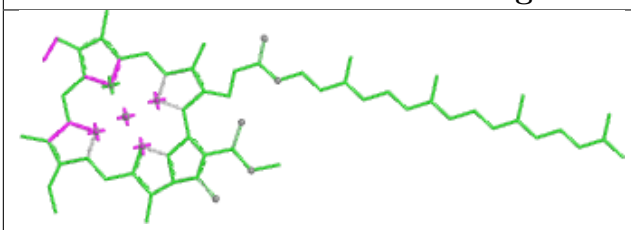


Torsions

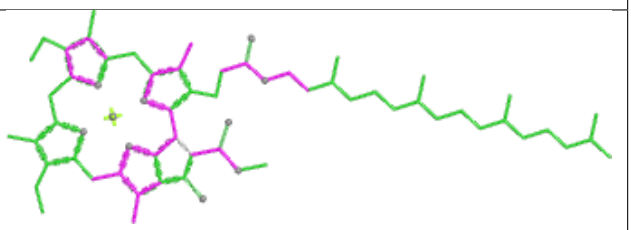


Rings

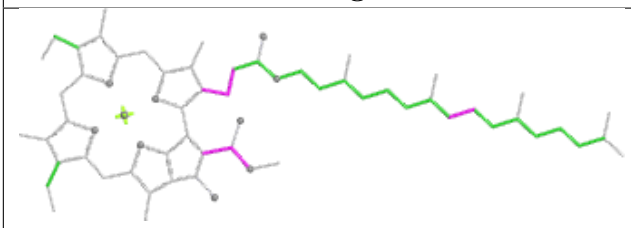
Ligand CLA B 1022



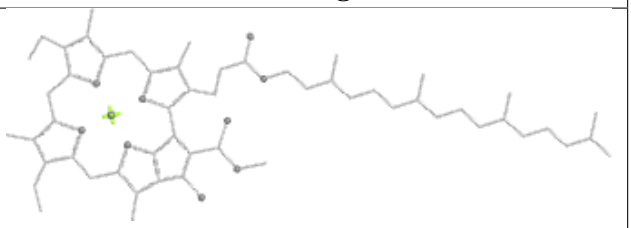
Bond lengths



Bond angles

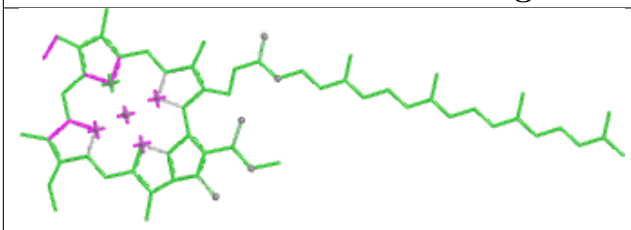


Torsions

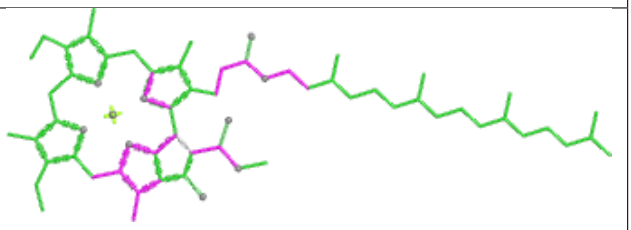


Rings

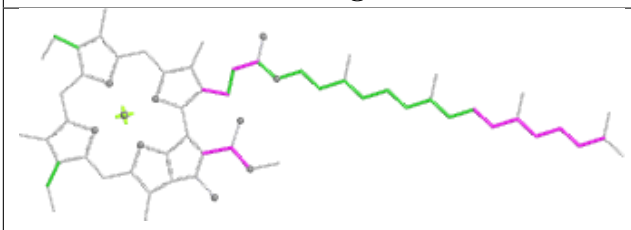
Ligand CLA A 1103



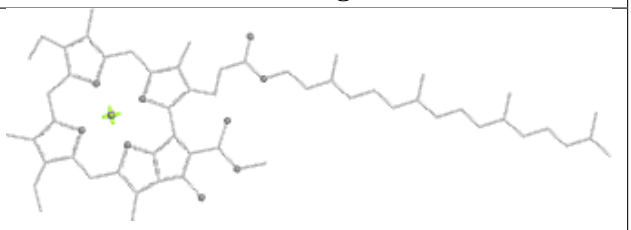
Bond lengths



Bond angles

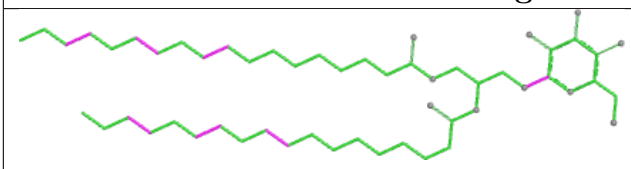


Torsions

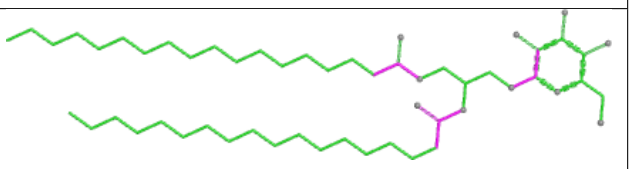


Rings

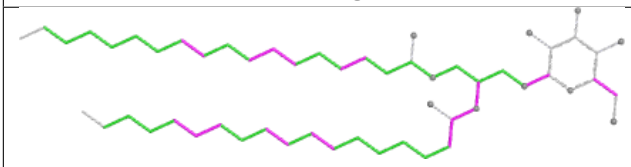
Ligand LMG a 5004



Bond lengths



Bond angles

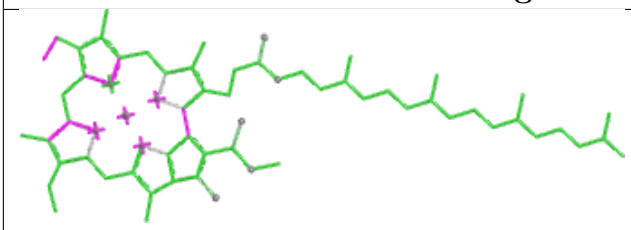


Torsions

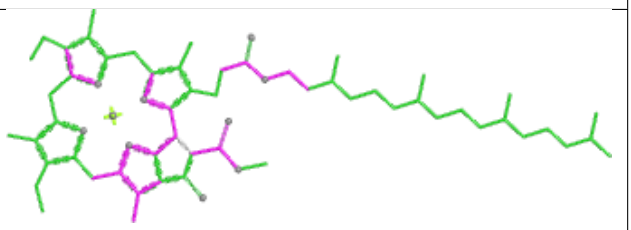


Rings

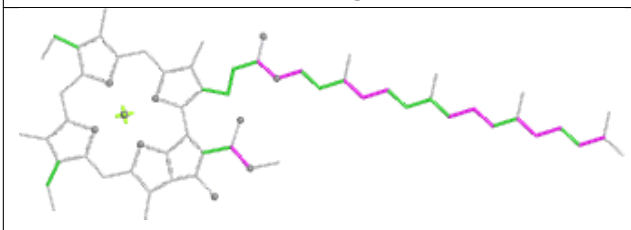
Ligand CLA A 1013



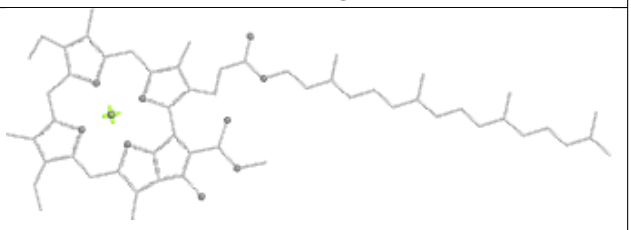
Bond lengths



Bond angles

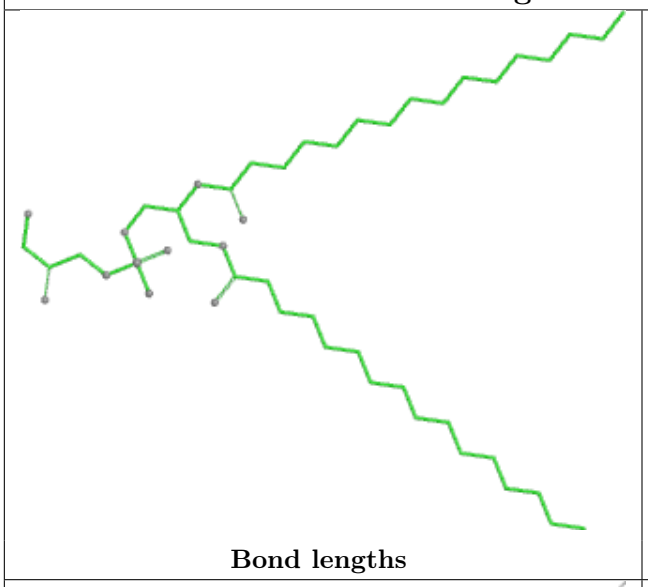


Torsions

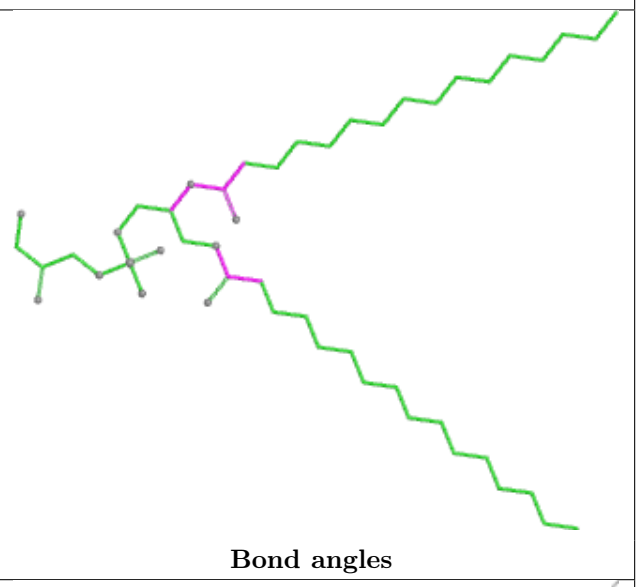


Rings

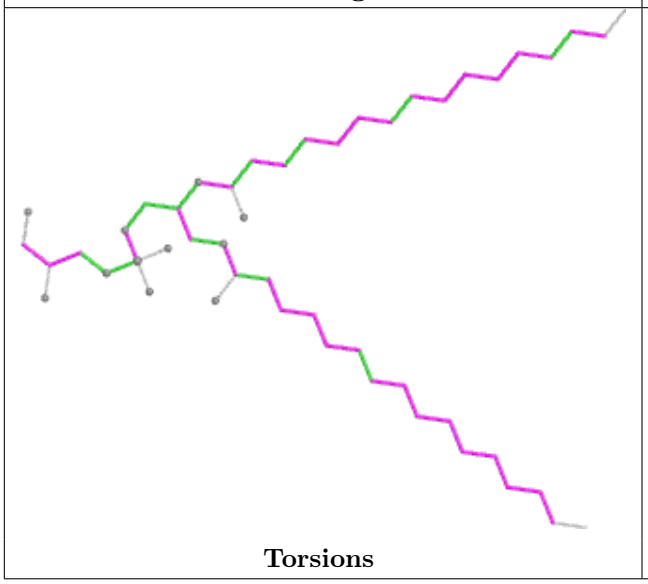
Ligand LHG A 5005



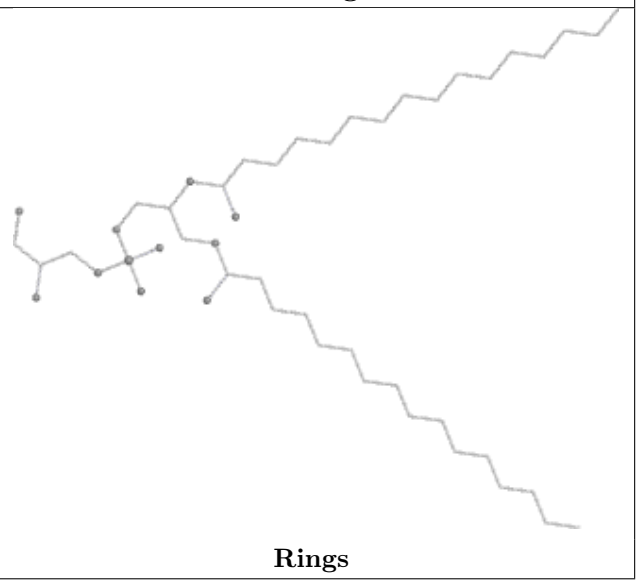
Bond lengths



Bond angles

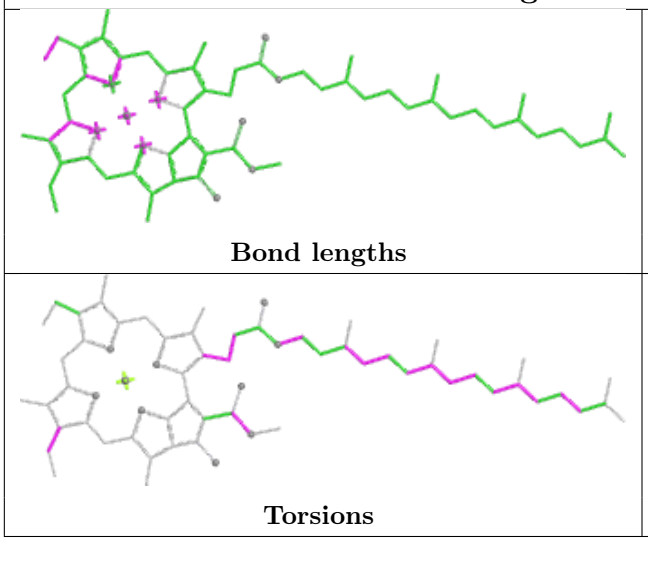


Torsions

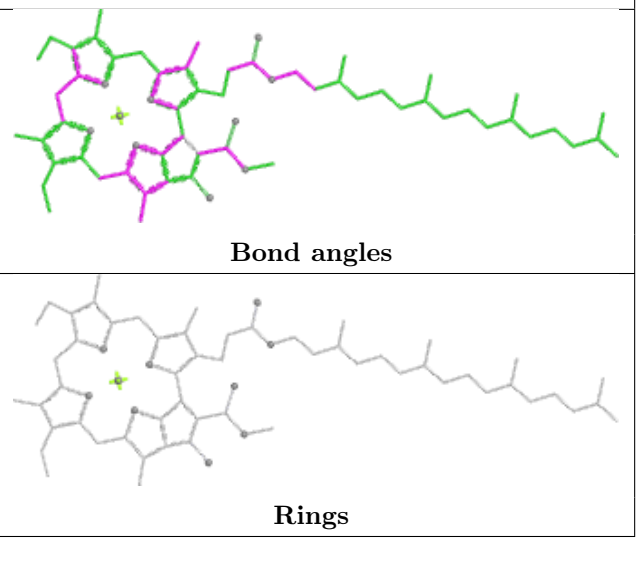


Rings

Ligand CLA 2 1229



Bond lengths

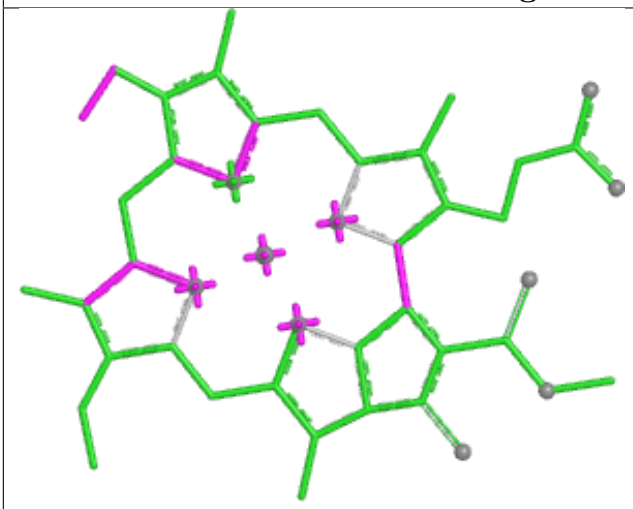


Bond angles

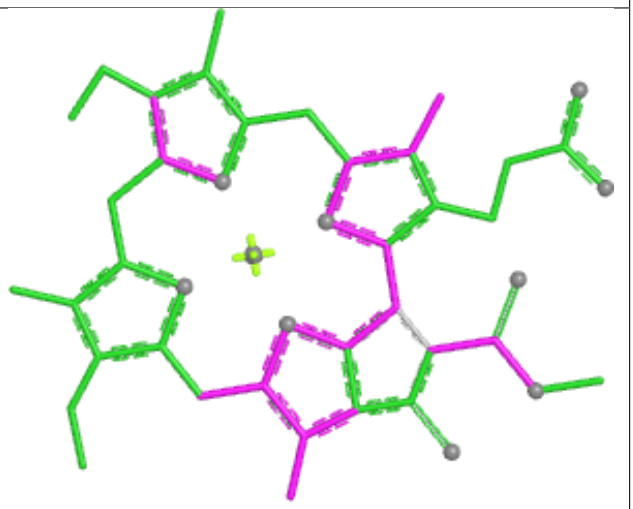
Torsions

Rings

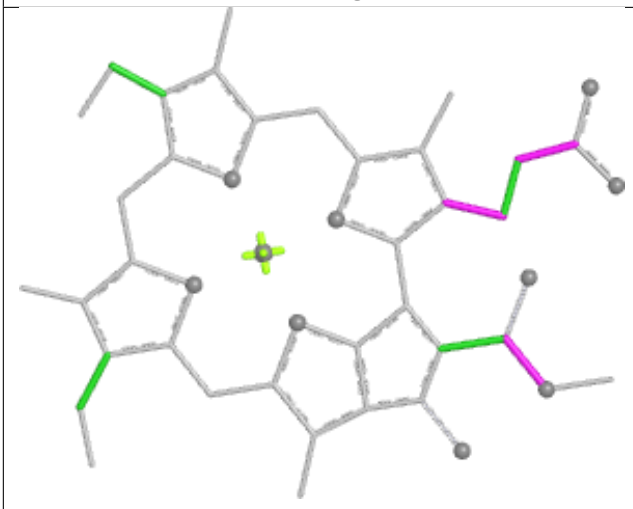
Ligand CLA 2 1209



Bond lengths



Bond angles

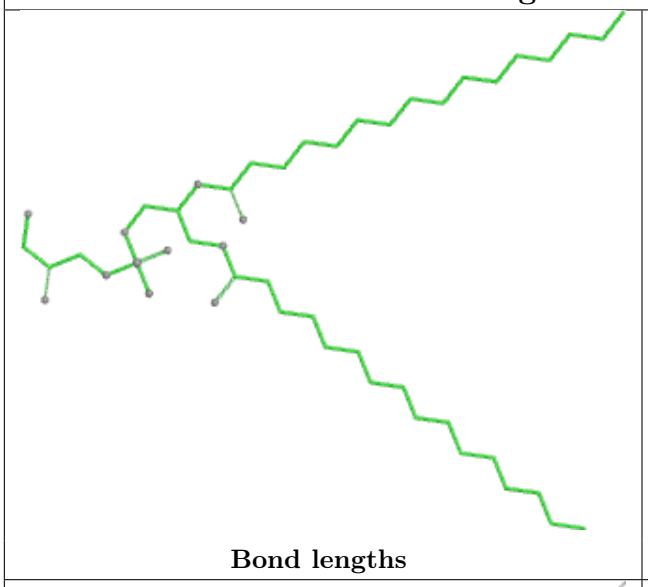


Torsions

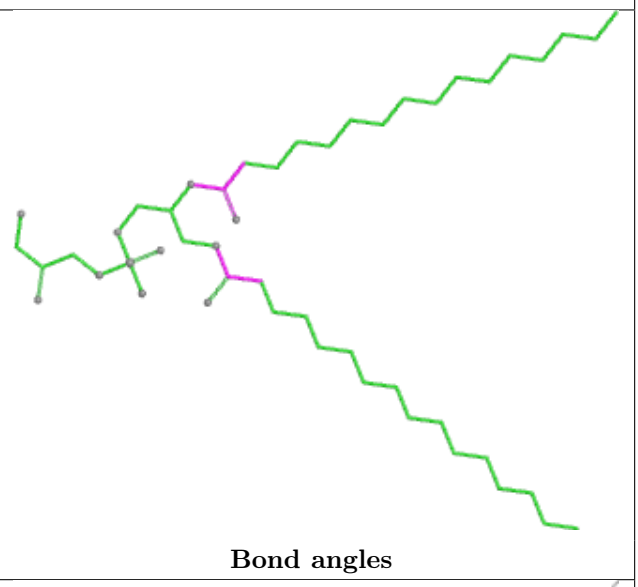


Rings

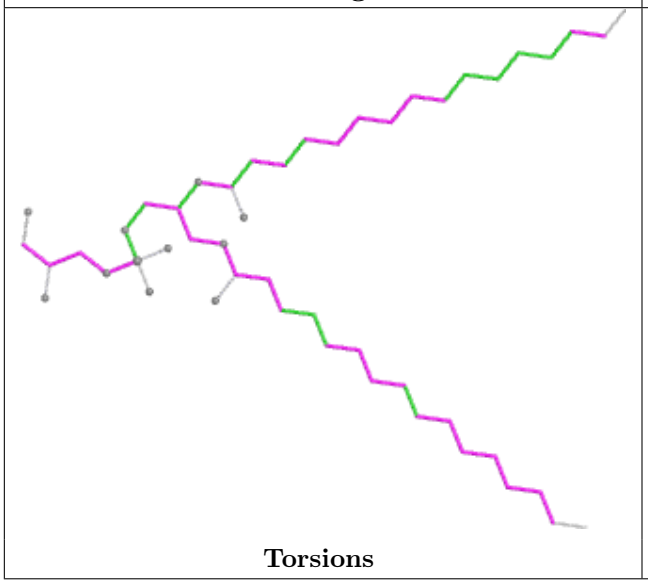
Ligand LHG 1 5005



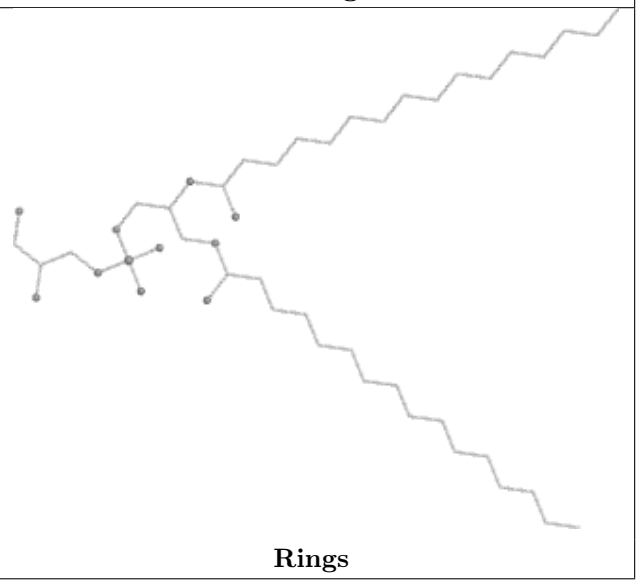
Bond lengths



Bond angles

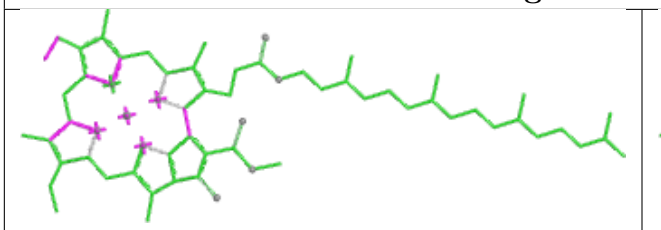


Torsions

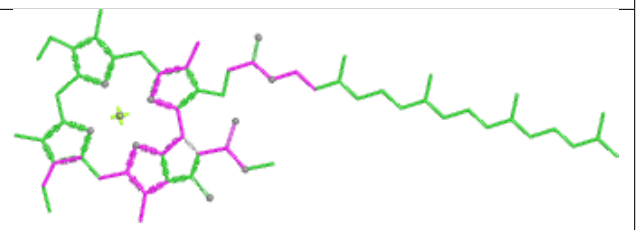


Rings

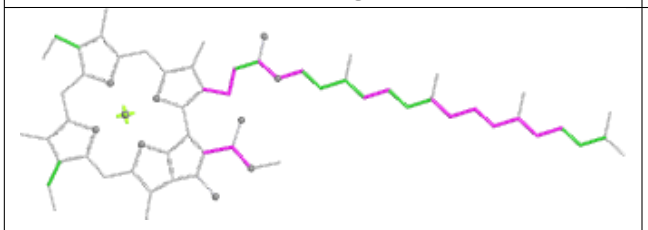
Ligand CLA l 1501



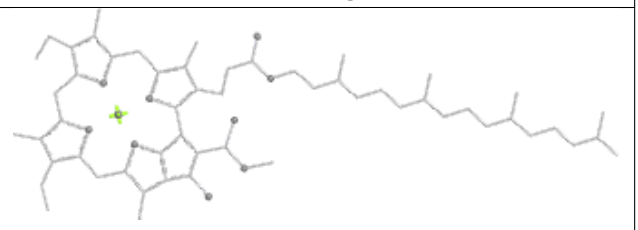
Bond lengths



Bond angles

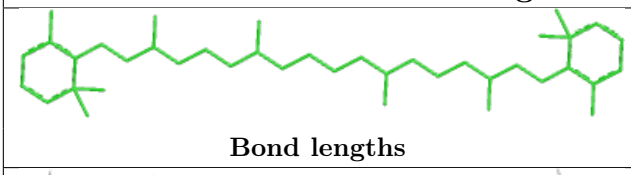


Torsions

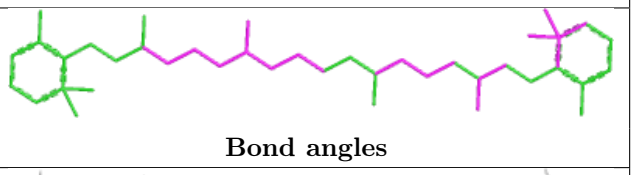


Rings

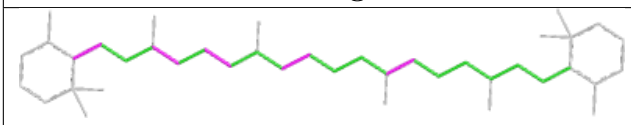
Ligand BCR L 4022



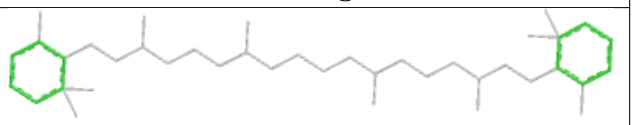
Bond lengths



Bond angles

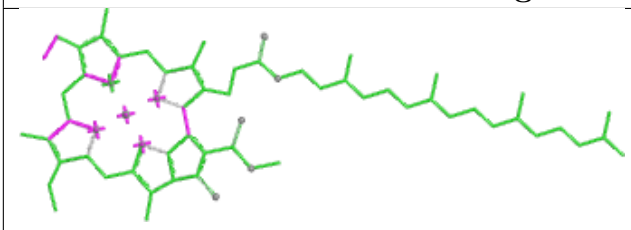


Torsions

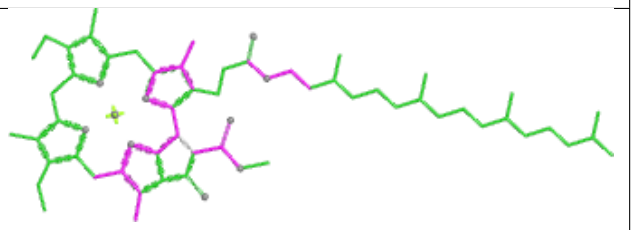


Rings

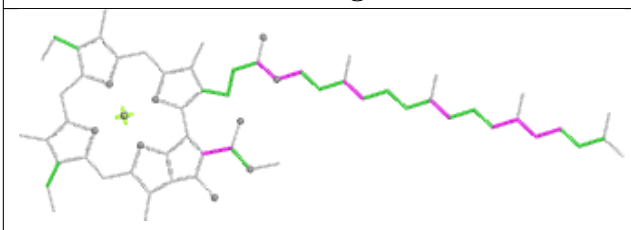
Ligand CLA A 1123



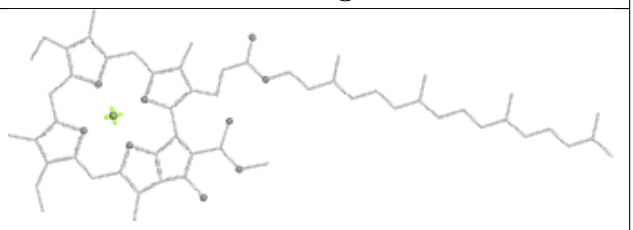
Bond lengths



Bond angles

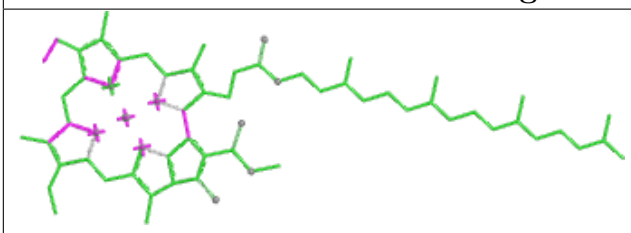


Torsions

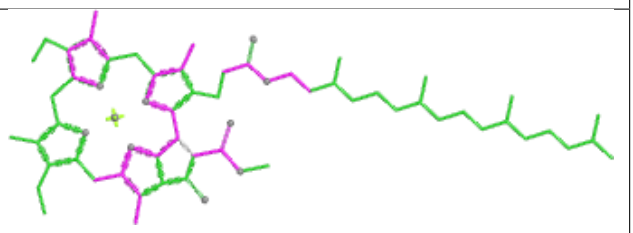


Rings

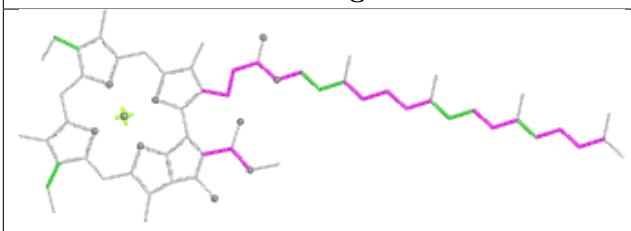
Ligand CLA a 1128



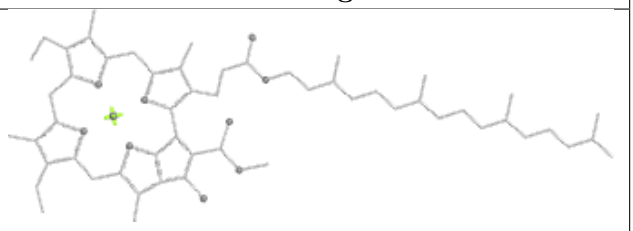
Bond lengths



Bond angles

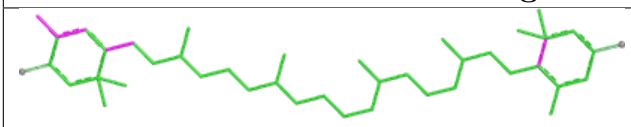


Torsions

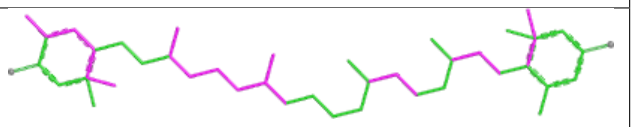


Rings

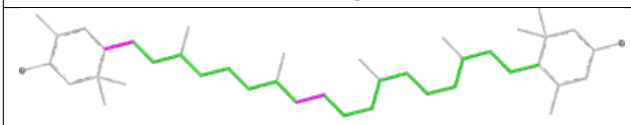
Ligand ZEX J 4015



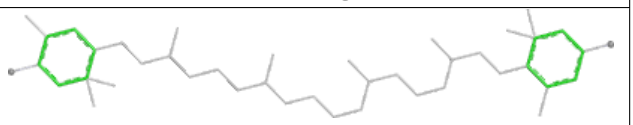
Bond lengths



Bond angles



Torsions

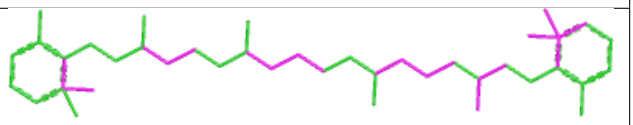


Rings

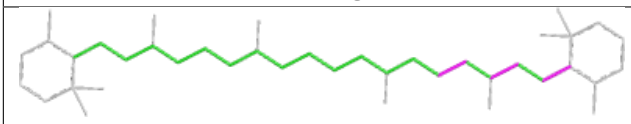
Ligand BCR A 4008



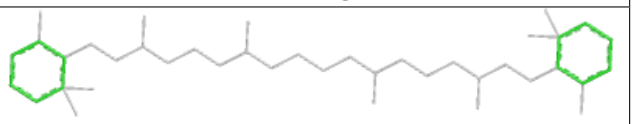
Bond lengths



Bond angles

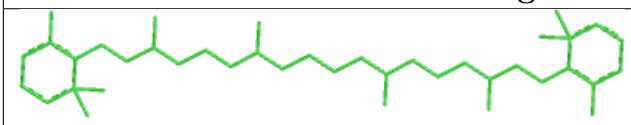


Torsions

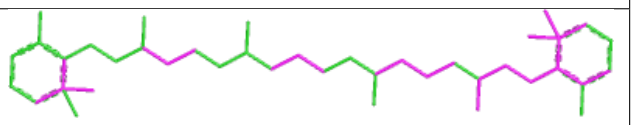


Rings

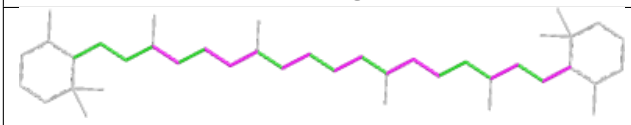
Ligand BCR a 4001



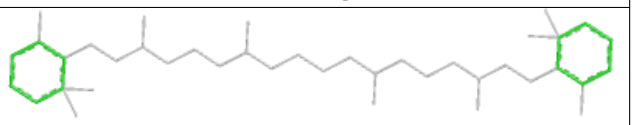
Bond lengths



Bond angles

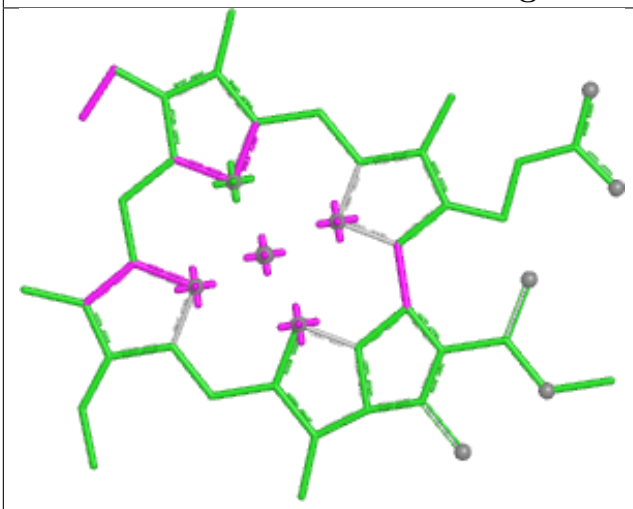


Torsions

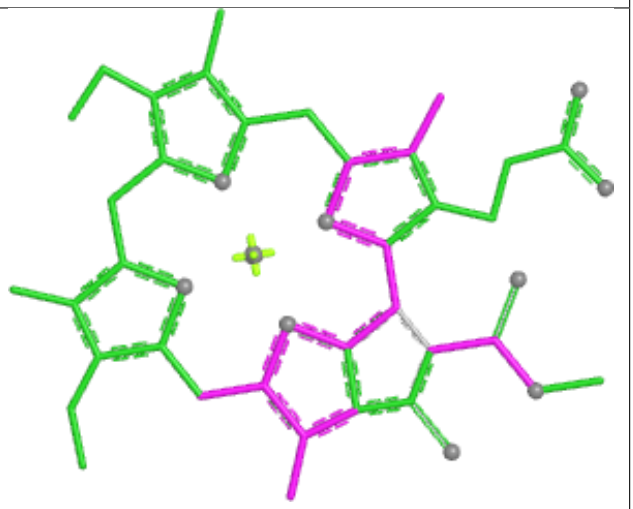


Rings

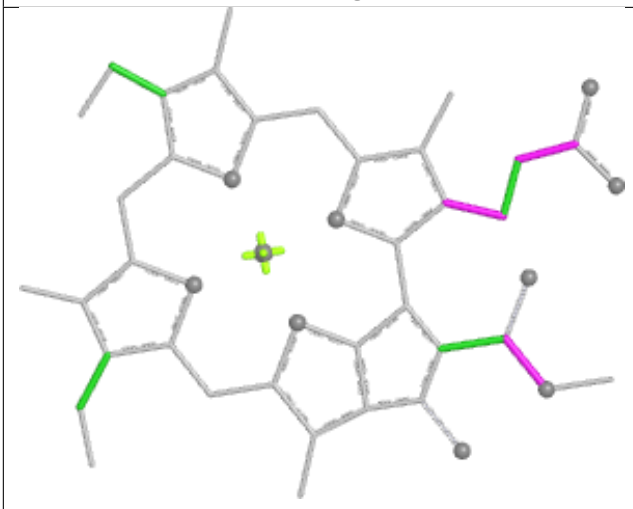
Ligand CLA 8 1401



Bond lengths



Bond angles

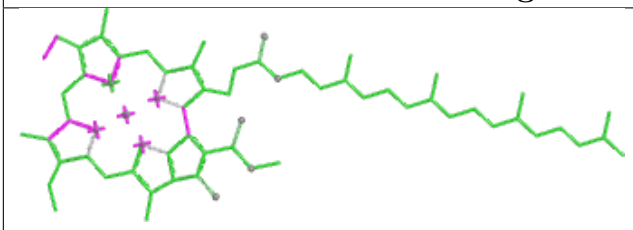


Torsions

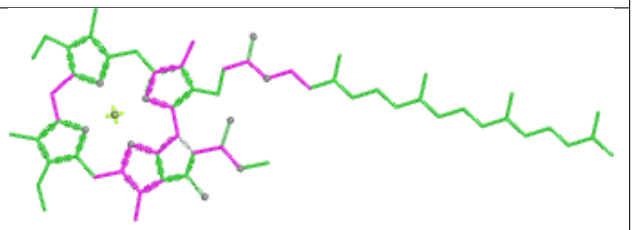


Rings

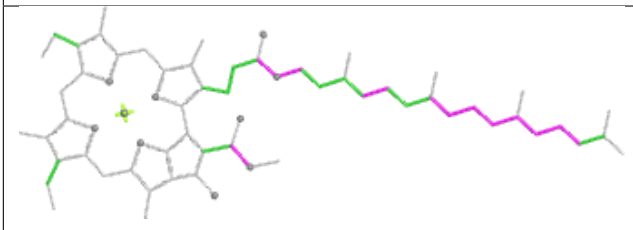
Ligand CLA F 1301



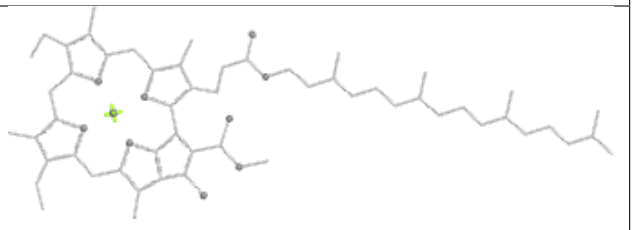
Bond lengths



Bond angles

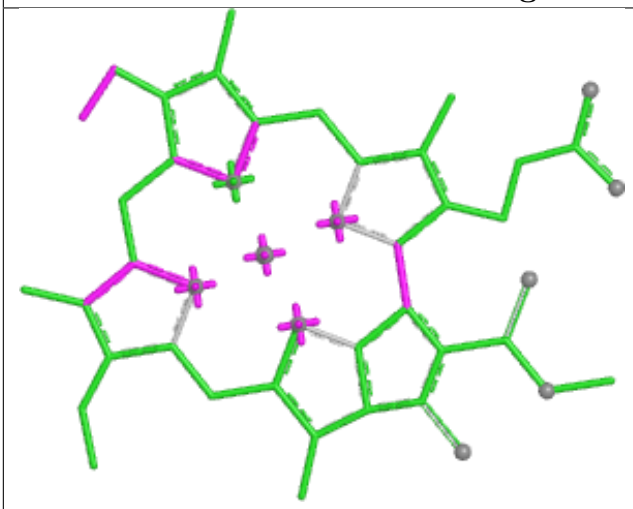


Torsions

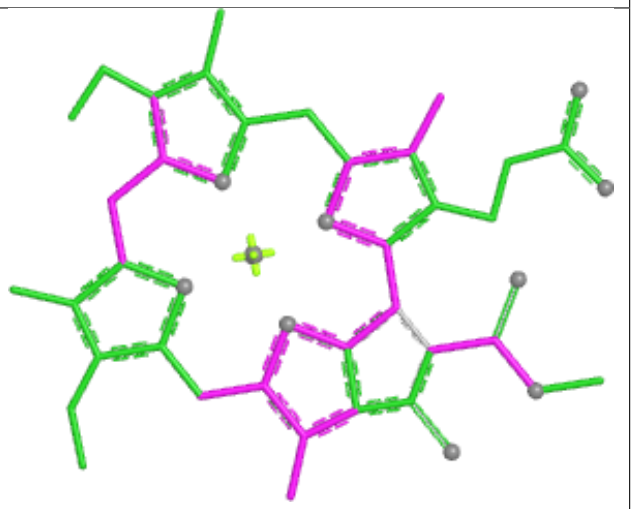


Rings

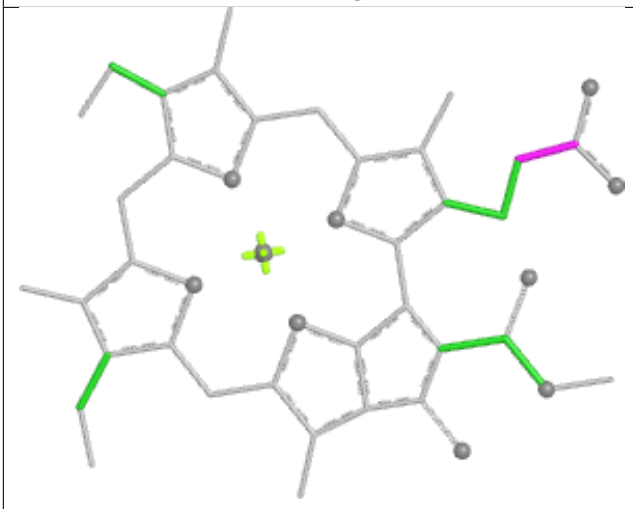
Ligand CLA 2 1227



Bond lengths



Bond angles

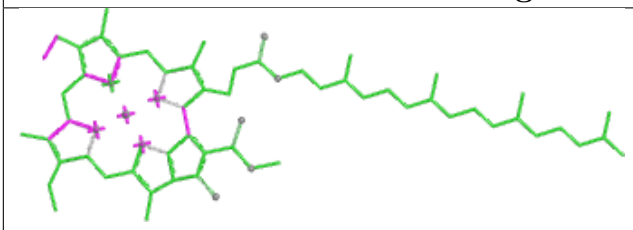


Torsions

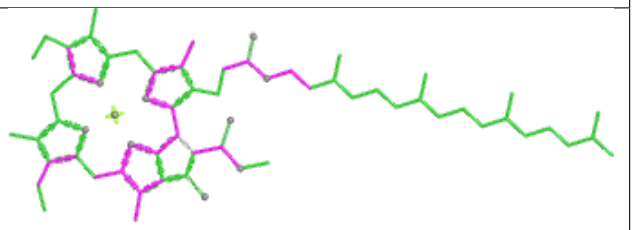


Rings

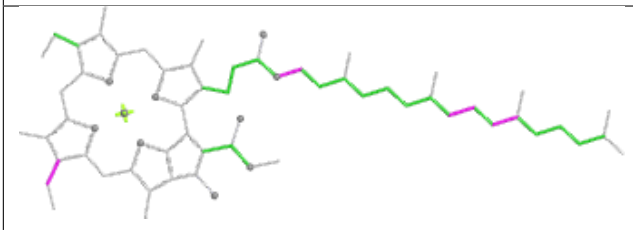
Ligand CLA B 1023



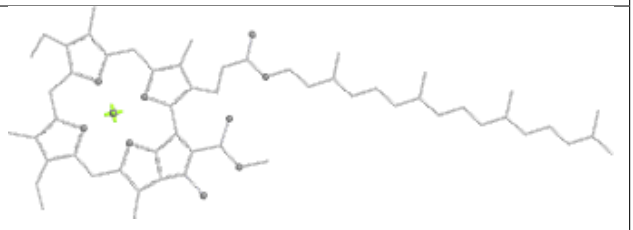
Bond lengths



Bond angles

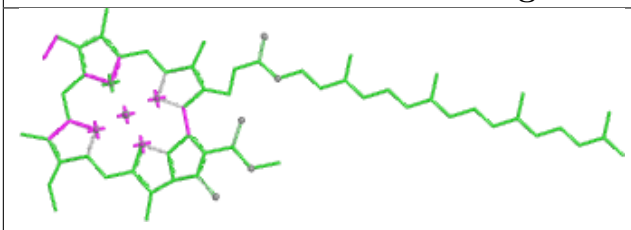


Torsions

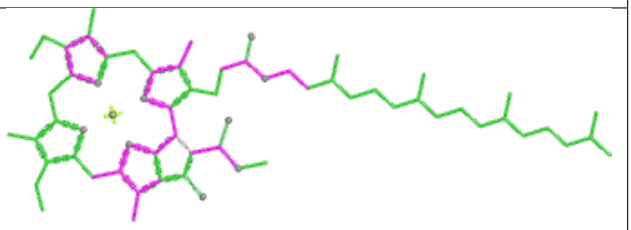


Rings

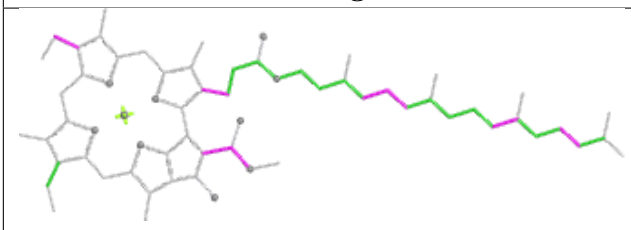
Ligand CLA b 1220



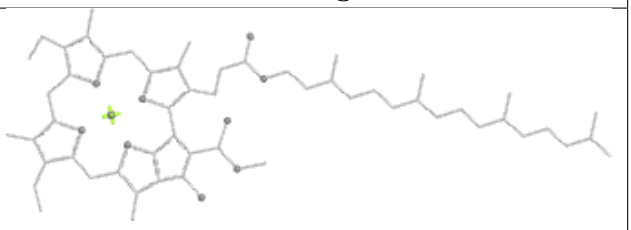
Bond lengths



Bond angles

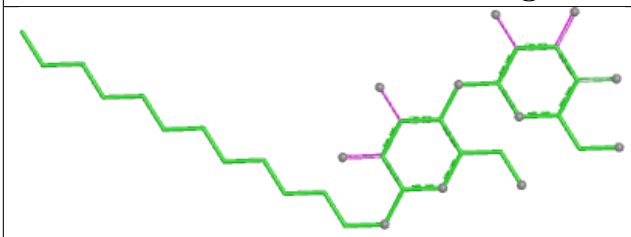


Torsions

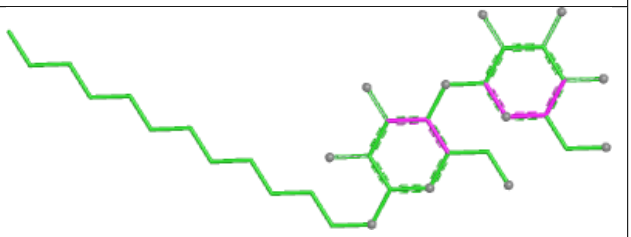


Rings

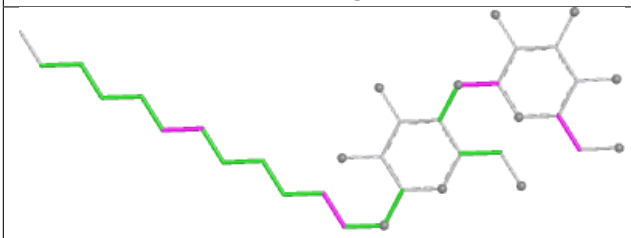
Ligand LMT l 6001



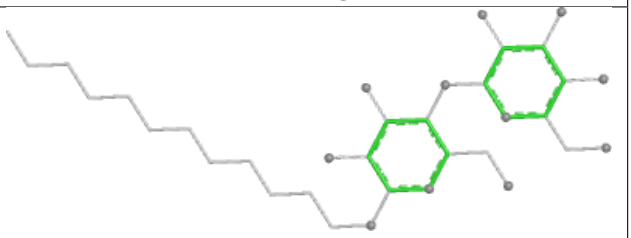
Bond lengths



Bond angles



Torsions

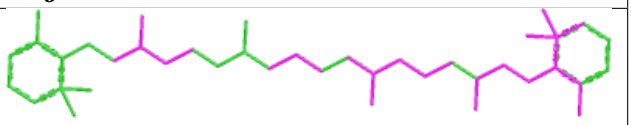


Rings

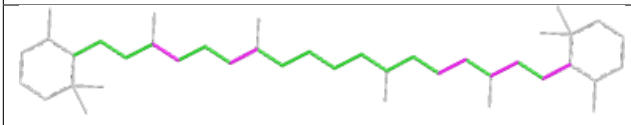
Ligand BCR j 4013



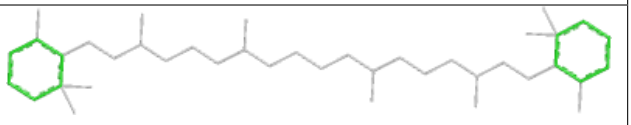
Bond lengths



Bond angles

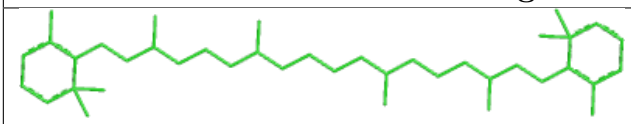


Torsions

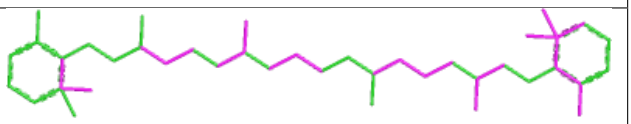


Rings

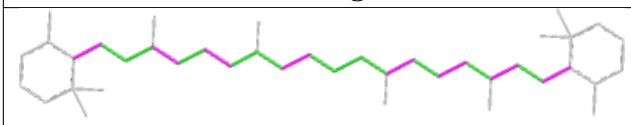
Ligand BCR a 4008



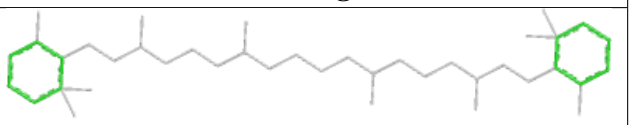
Bond lengths



Bond angles

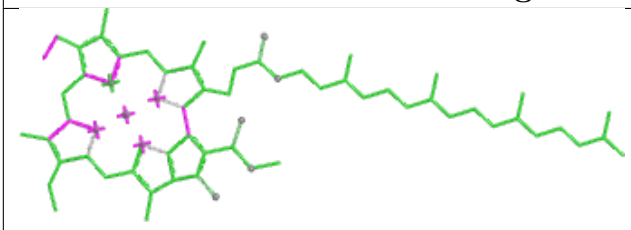


Torsions

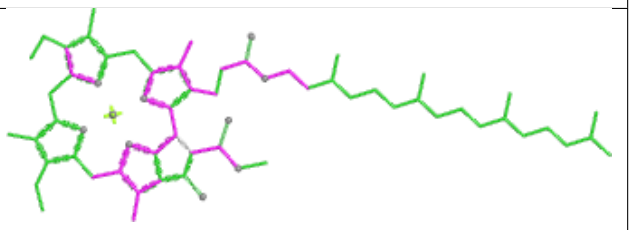


Rings

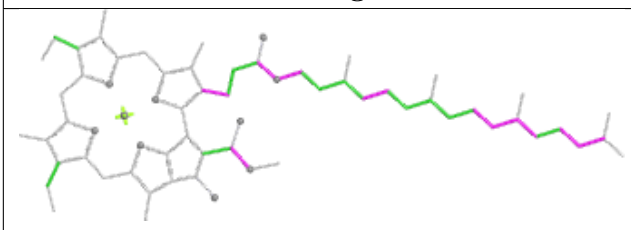
Ligand CLA A 1104



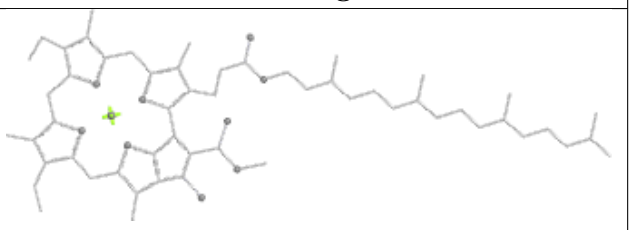
Bond lengths



Bond angles

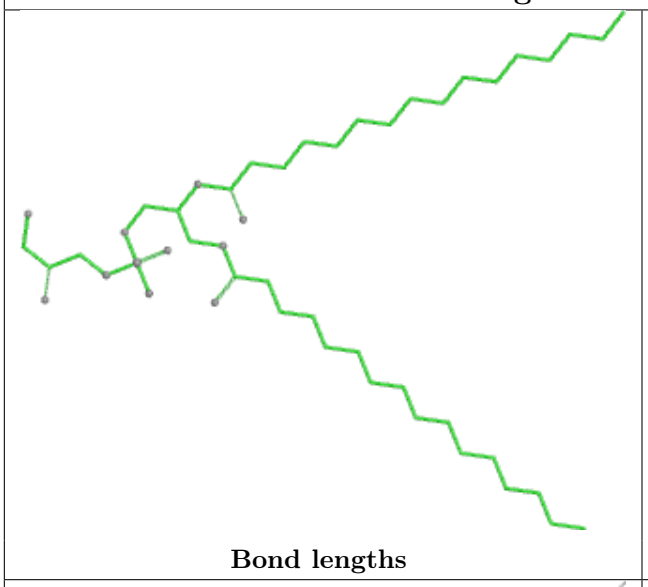


Torsions

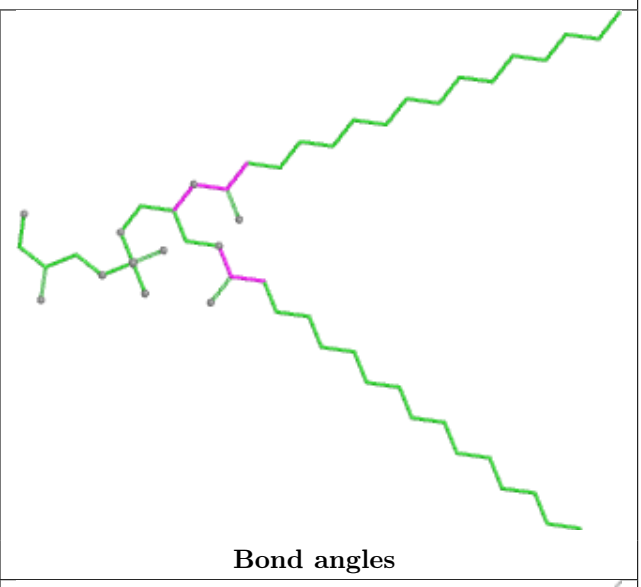


Rings

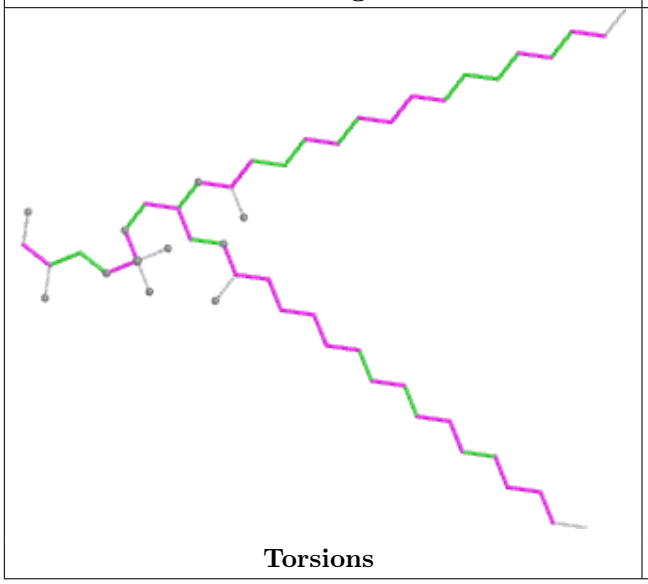
Ligand LHG A 5001



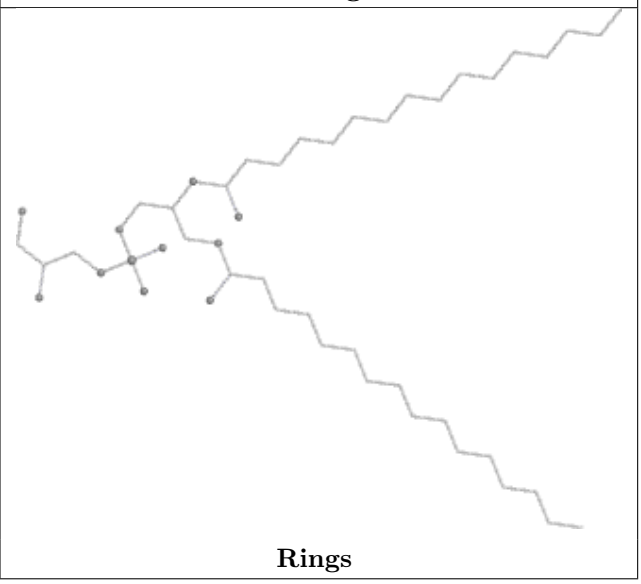
Bond lengths



Bond angles



Torsions

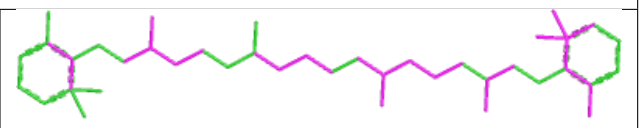


Rings

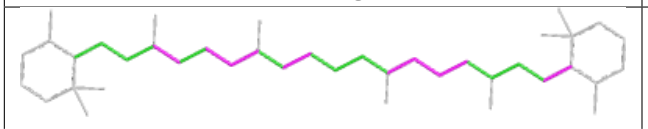
Ligand BCR 2 4010



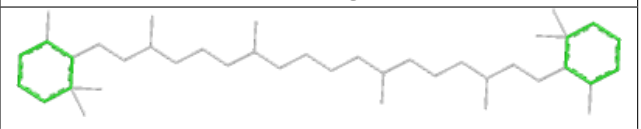
Bond lengths



Bond angles

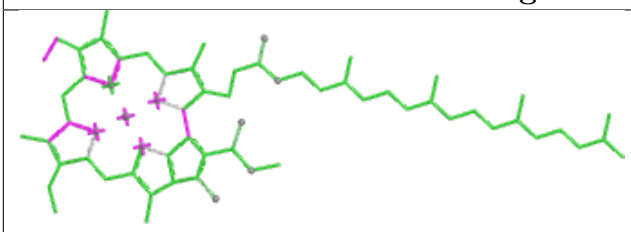


Torsions

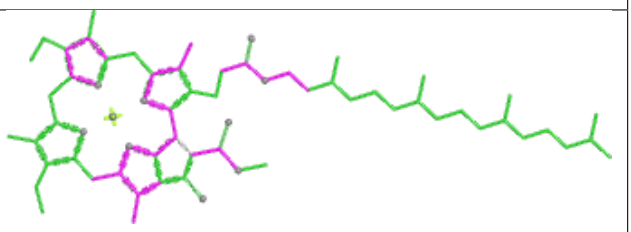


Rings

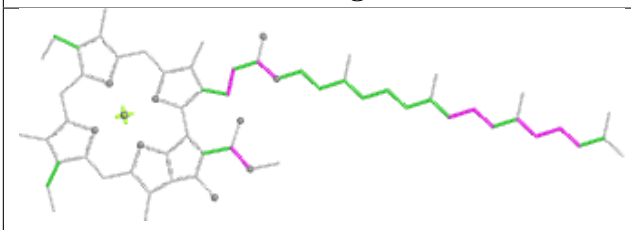
Ligand CLA 2 1201



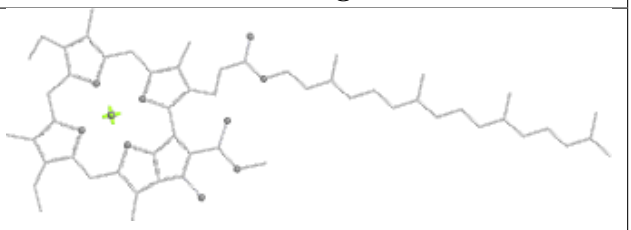
Bond lengths



Bond angles

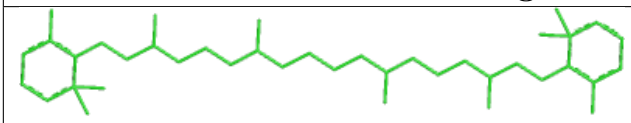


Torsions

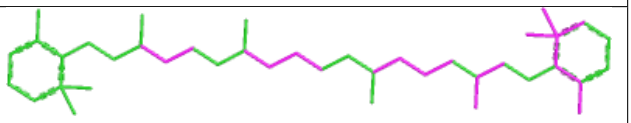


Rings

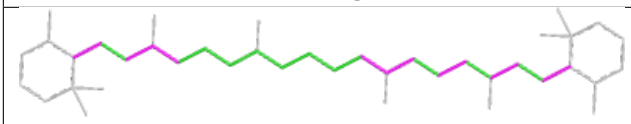
Ligand BCR 2 4011



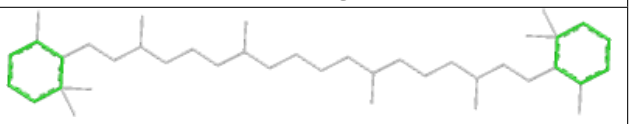
Bond lengths



Bond angles

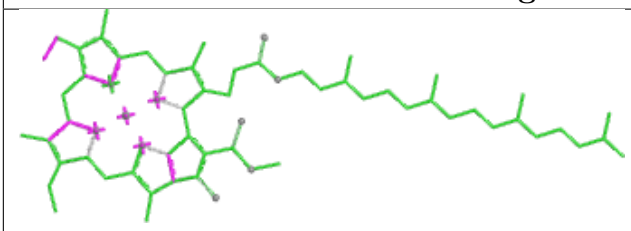


Torsions

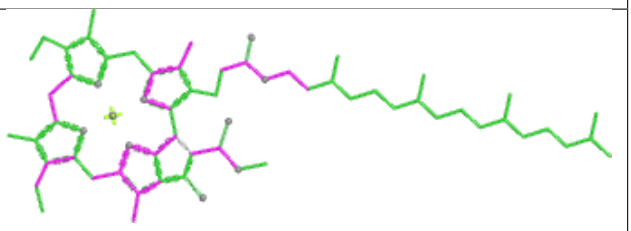


Rings

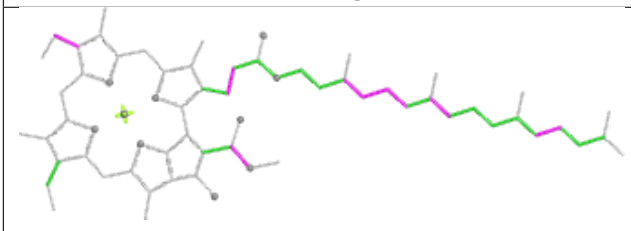
Ligand CLA b 1204



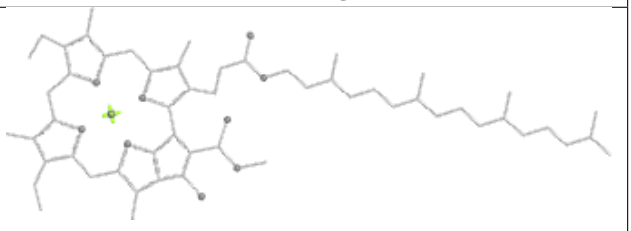
Bond lengths



Bond angles

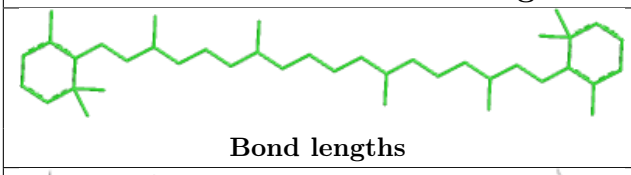


Torsions

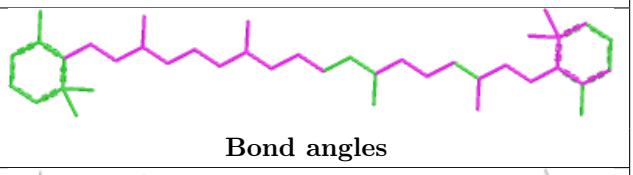


Rings

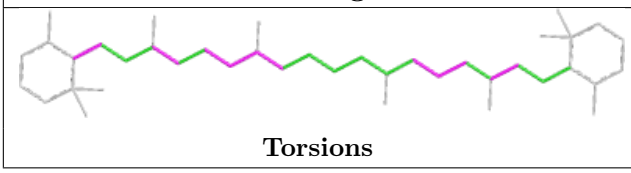
Ligand BCR 9 4021



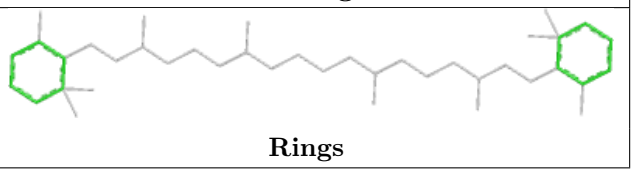
Bond lengths



Bond angles

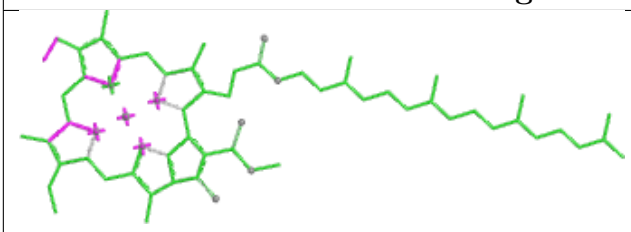


Torsions

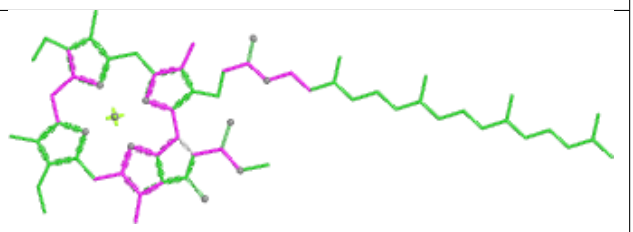


Rings

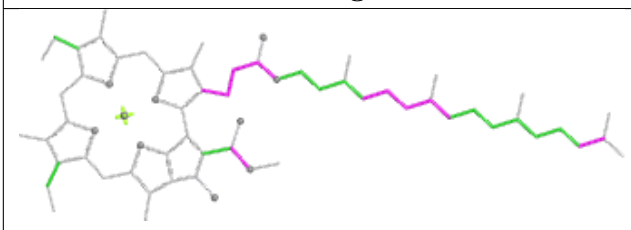
Ligand CLA B 1204



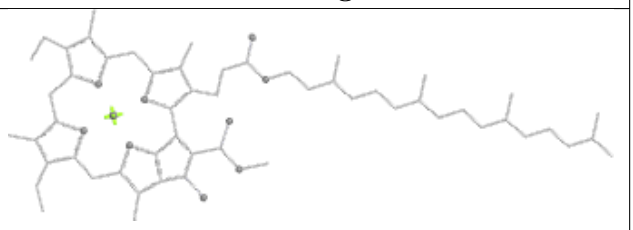
Bond lengths



Bond angles

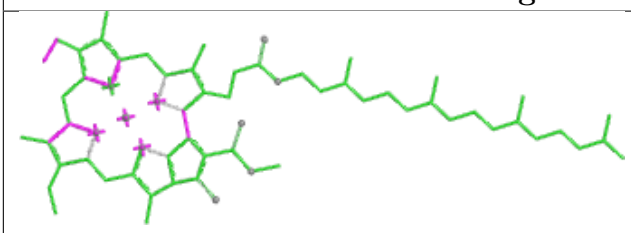


Torsions

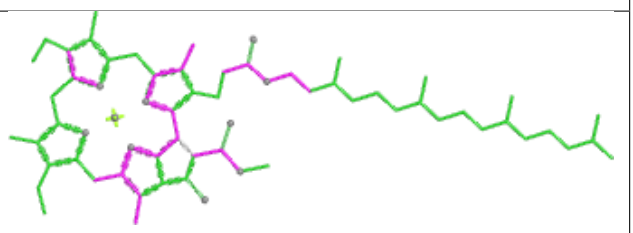


Rings

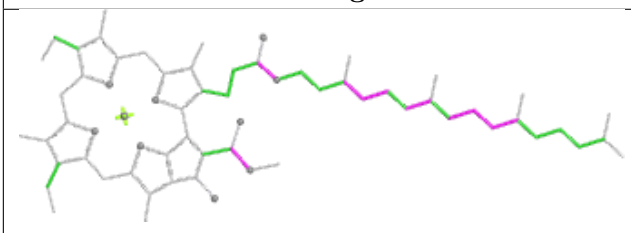
Ligand CLA b 1207



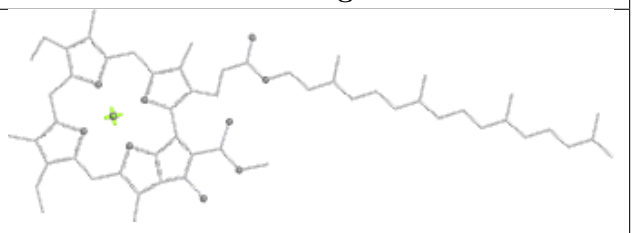
Bond lengths



Bond angles

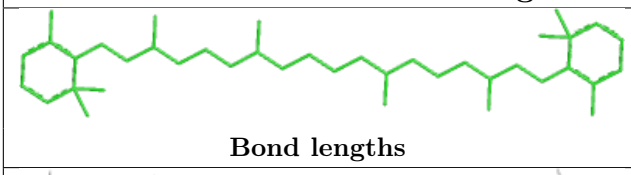


Torsions

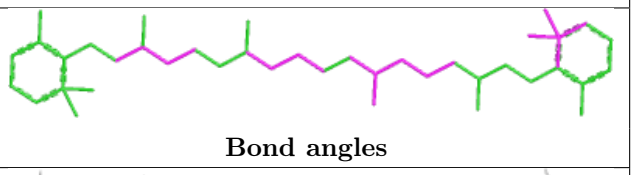


Rings

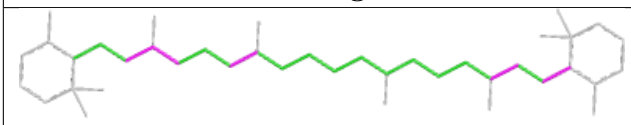
Ligand BCR b 4014



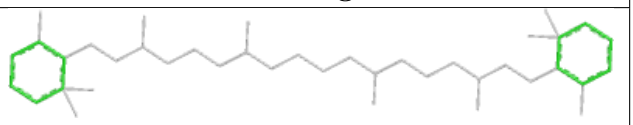
Bond lengths



Bond angles

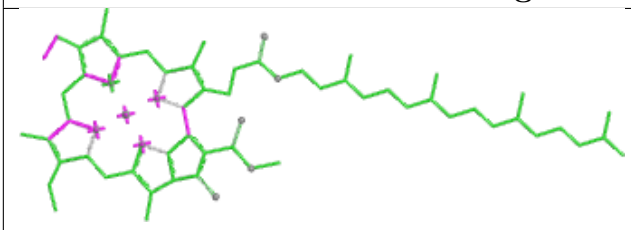


Torsions

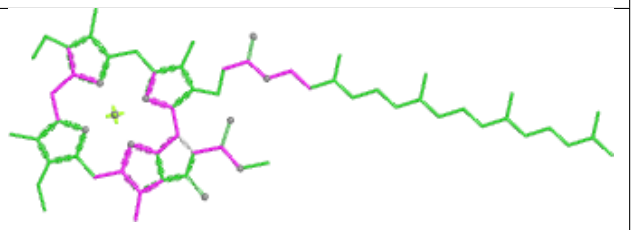


Rings

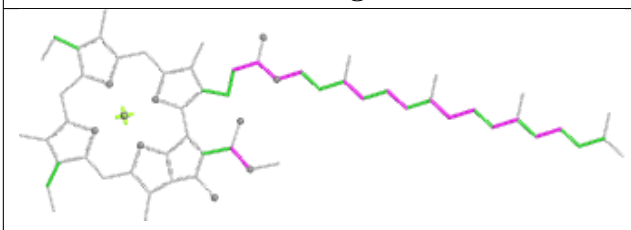
Ligand CLA A 1118



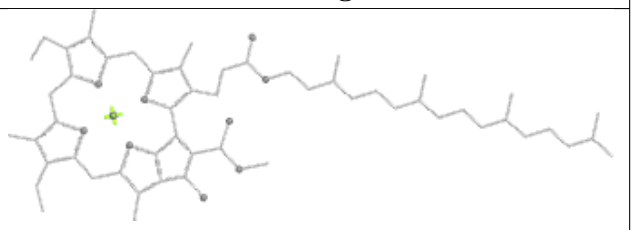
Bond lengths



Bond angles

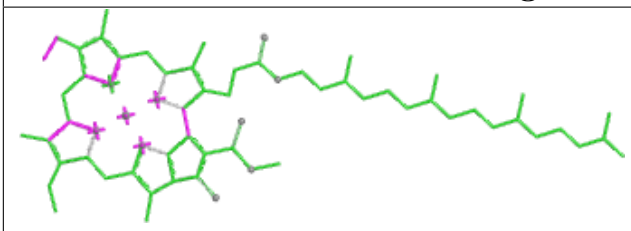


Torsions

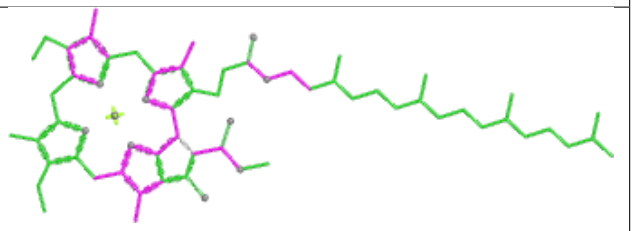


Rings

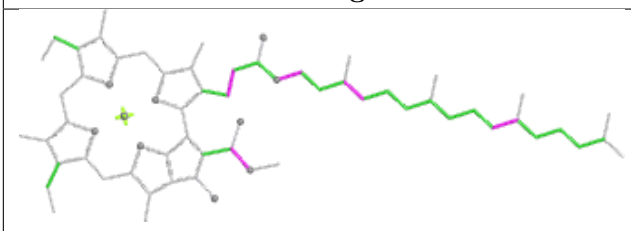
Ligand CLA 2 1022



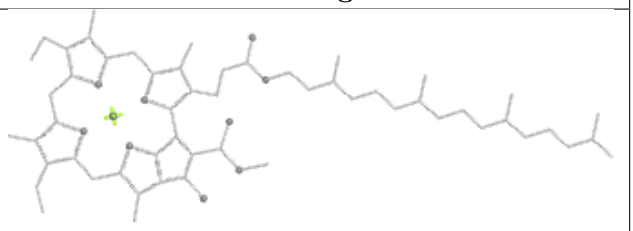
Bond lengths



Bond angles

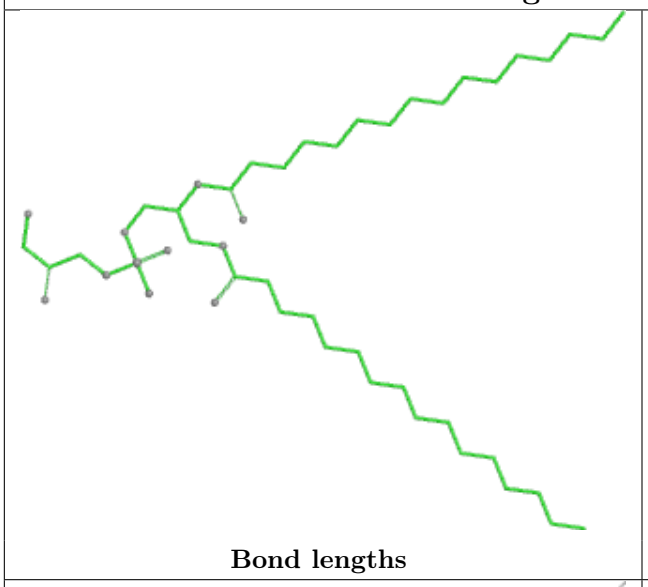


Torsions

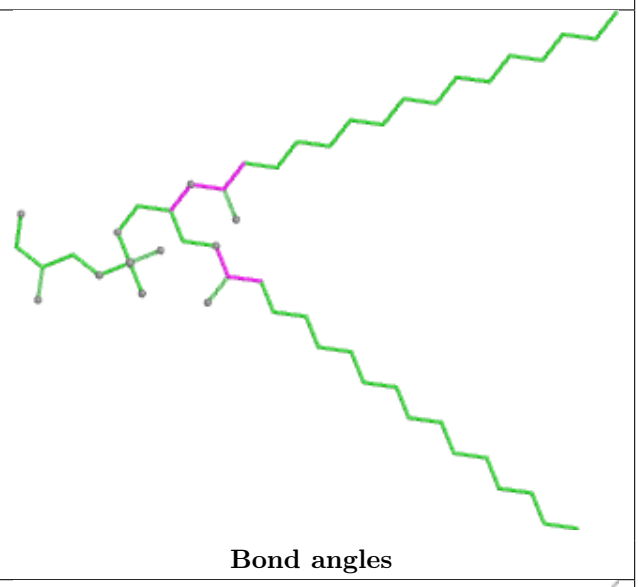


Rings

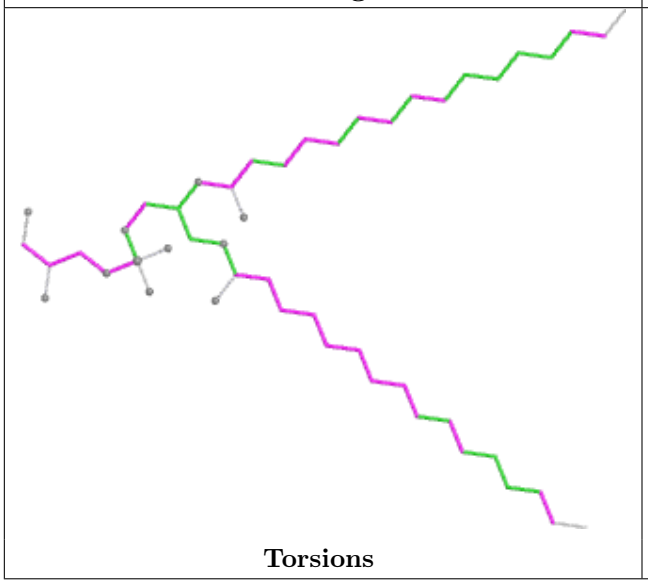
Ligand LHG l 5004



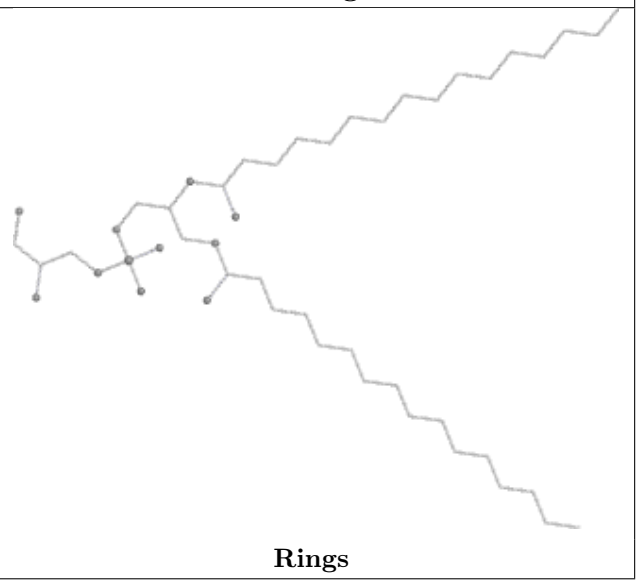
Bond lengths



Bond angles

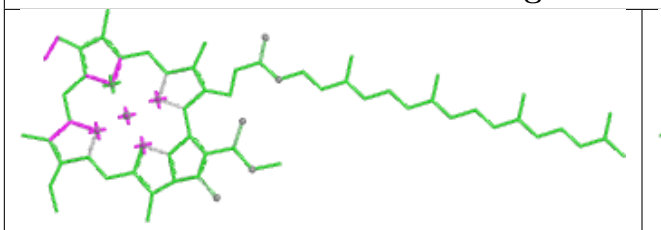


Torsions

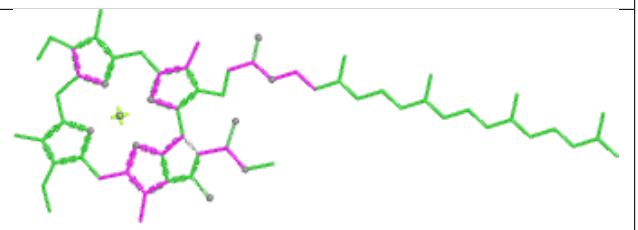


Rings

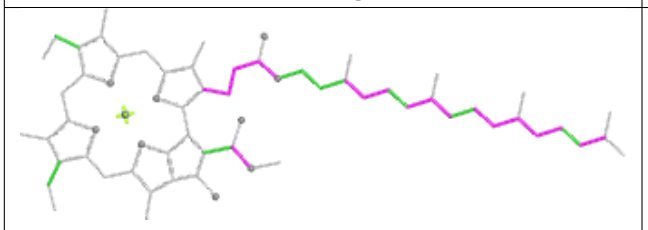
Ligand CLA l 1503



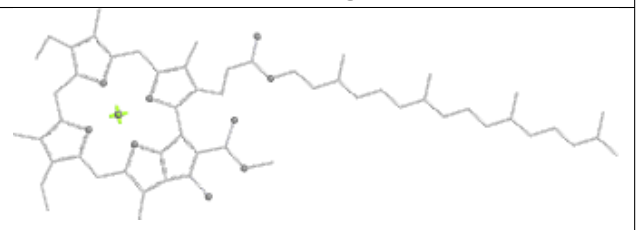
Bond lengths



Bond angles

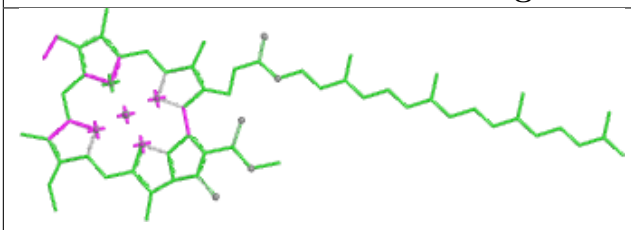


Torsions

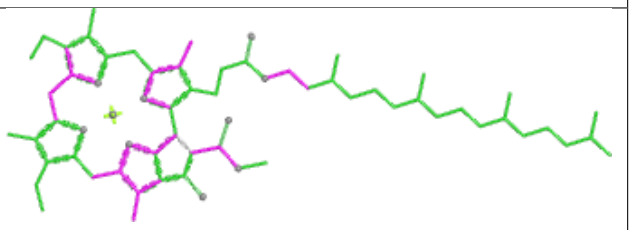


Rings

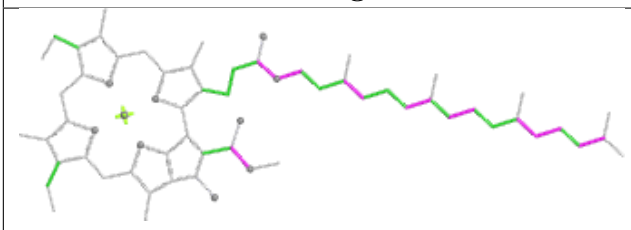
Ligand CLA A 1139



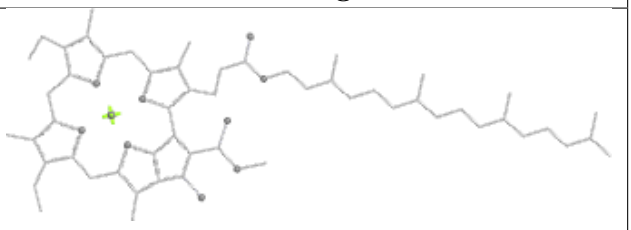
Bond lengths



Bond angles

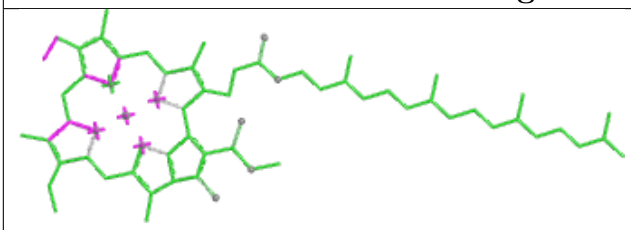


Torsions

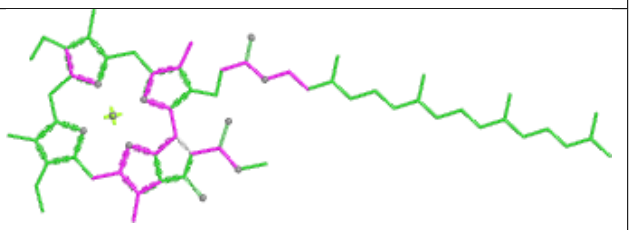


Rings

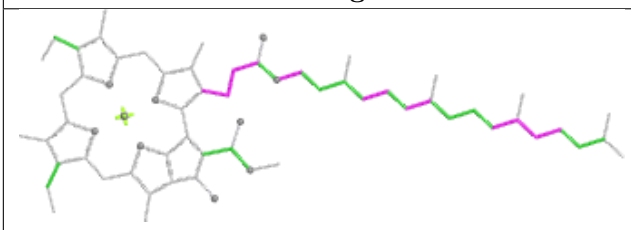
Ligand CLA L 1502



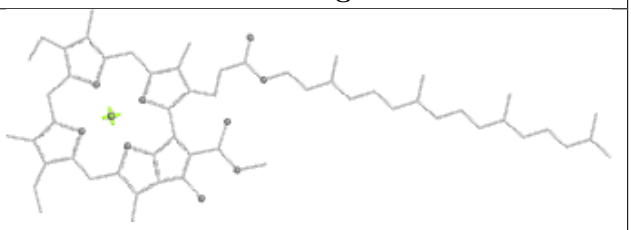
Bond lengths



Bond angles



Torsions

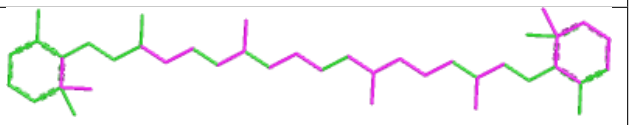


Rings

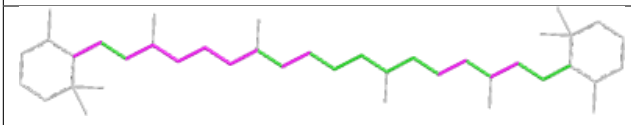
Ligand BCR l 4022



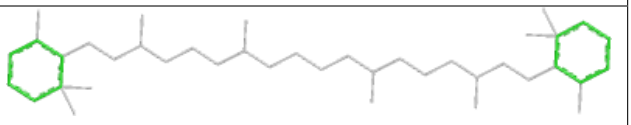
Bond lengths



Bond angles

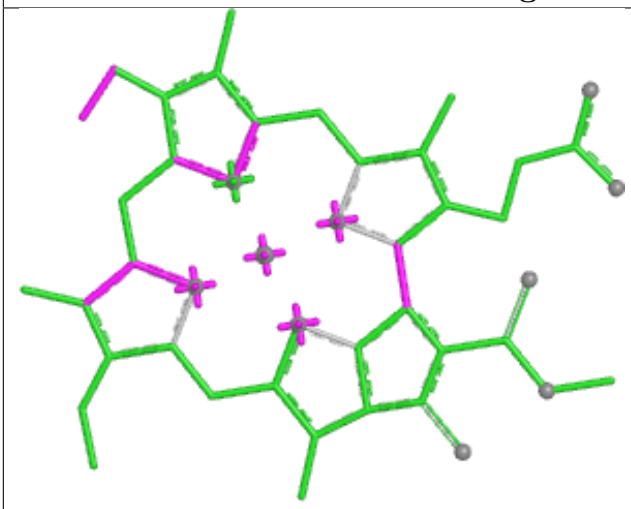


Torsions

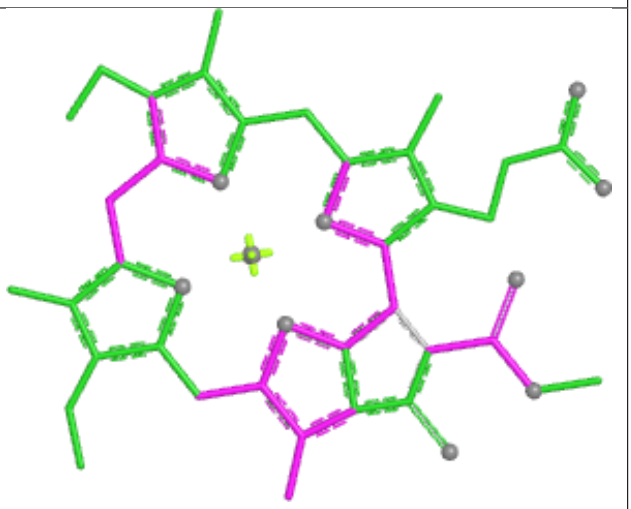


Rings

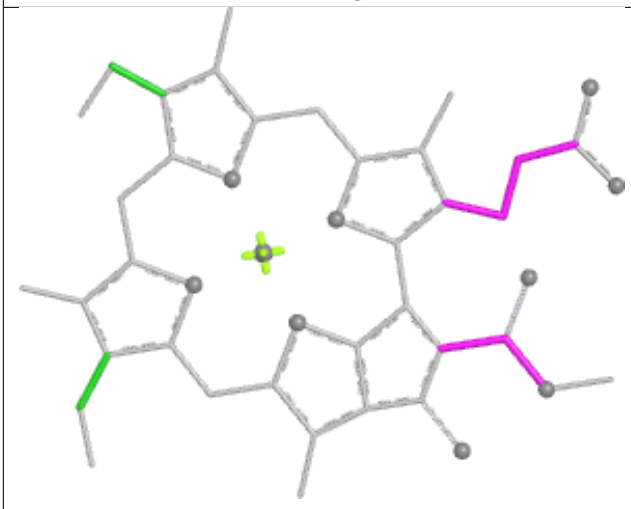
Ligand CLA 2 1228



Bond lengths



Bond angles

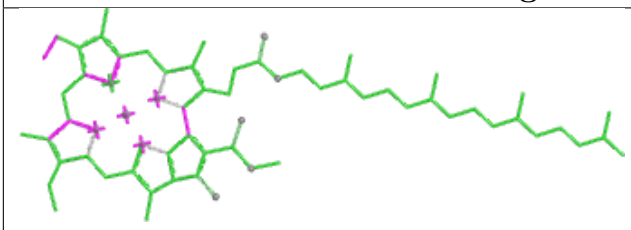


Torsions

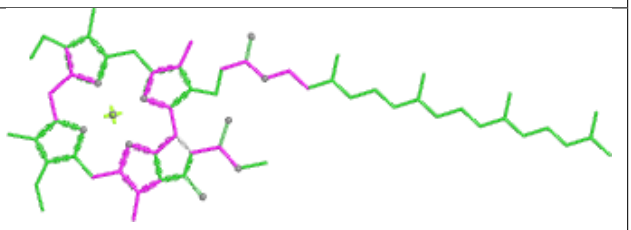


Rings

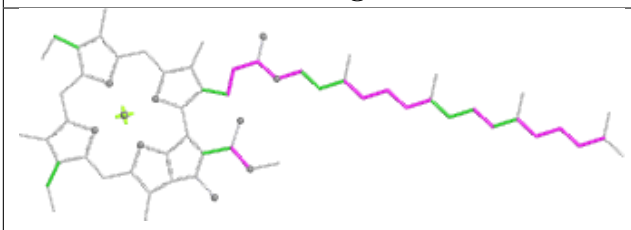
Ligand CLA a 1127



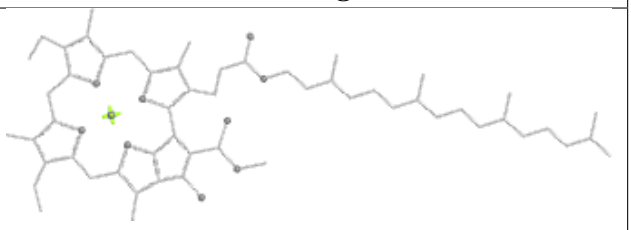
Bond lengths



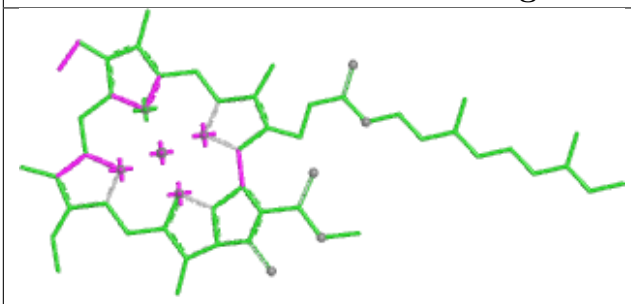
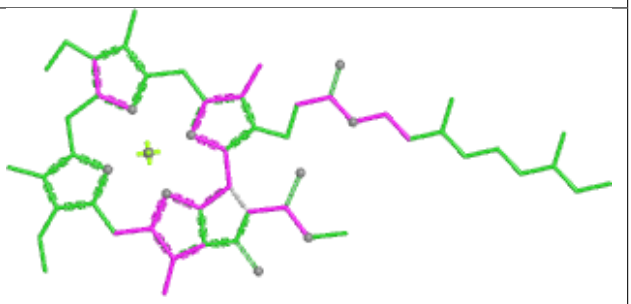
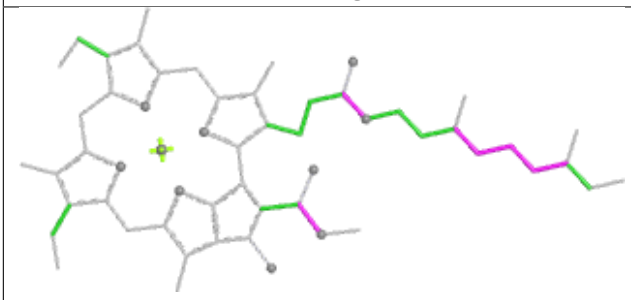
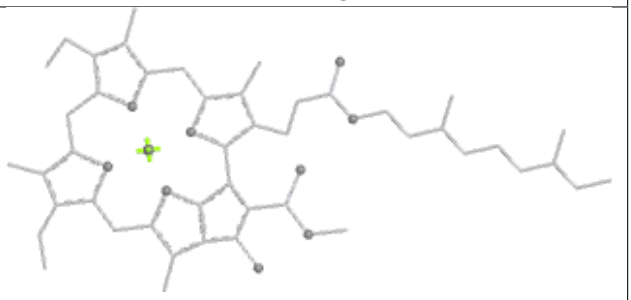
Bond angles

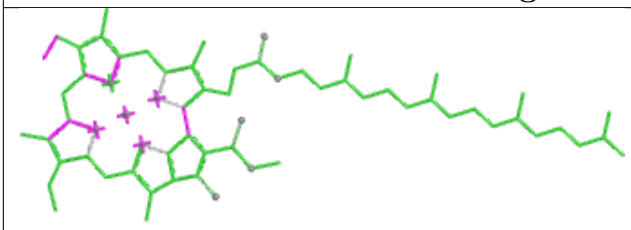
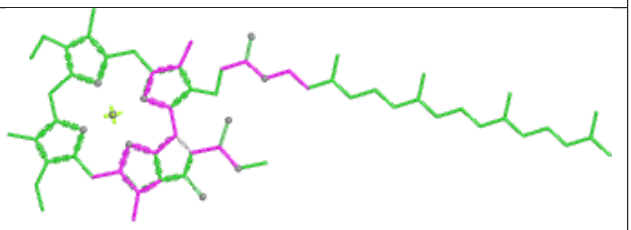
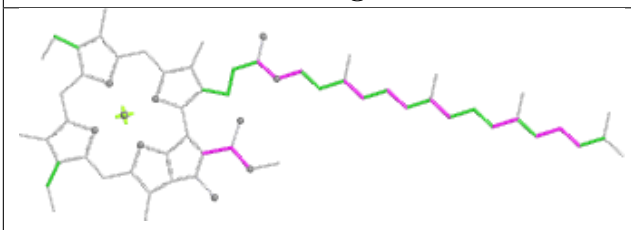
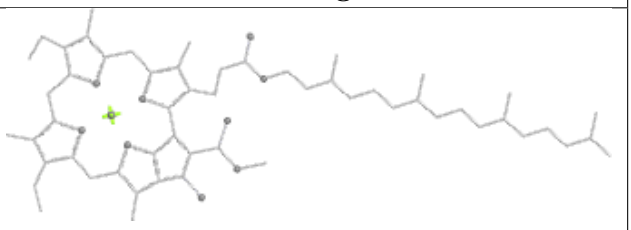


Torsions

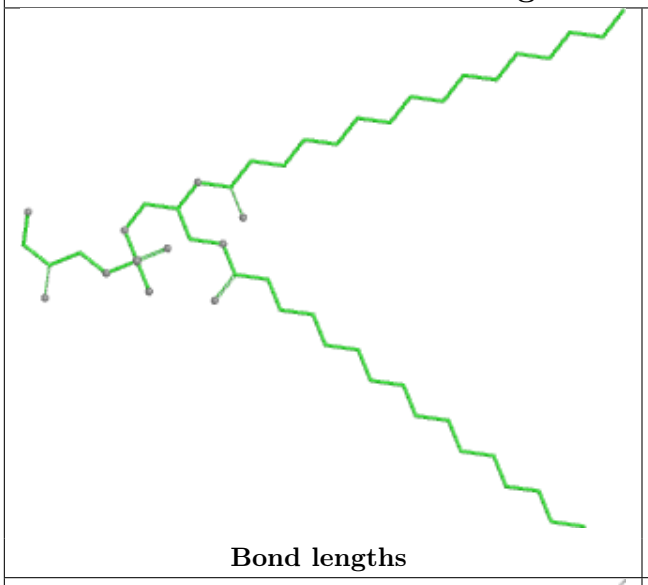


Rings

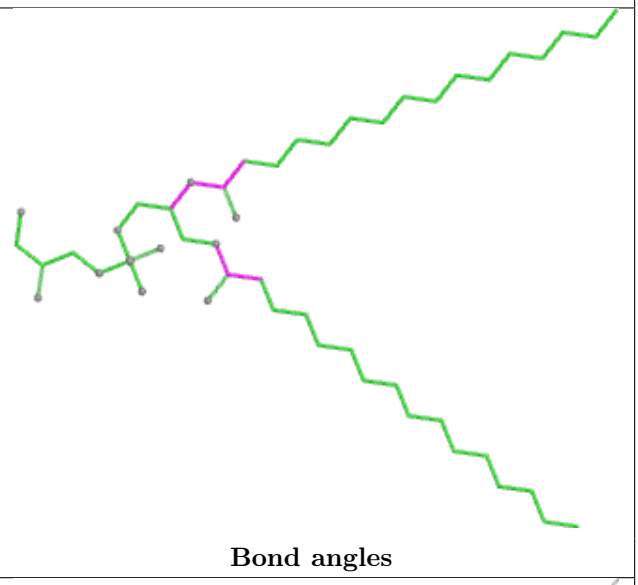
Ligand CLA 1 1124	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

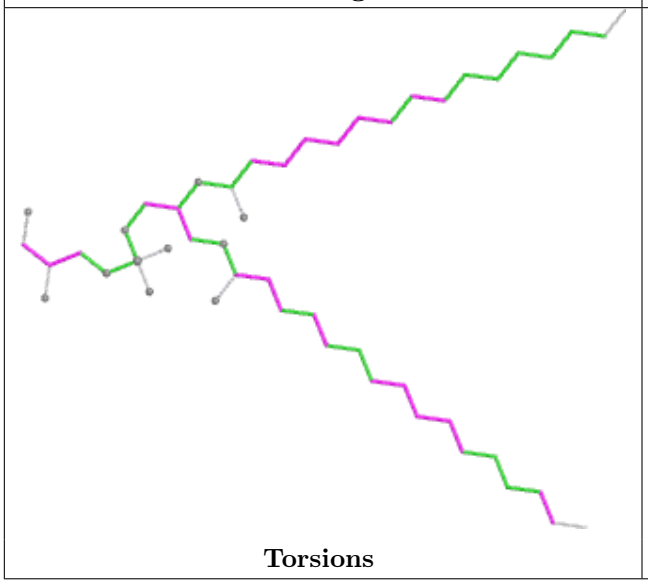
Ligand LHG b 5004



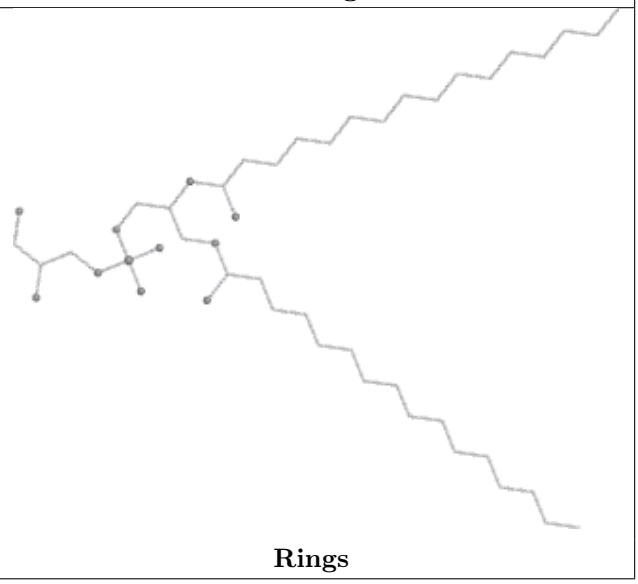
Bond lengths



Bond angles

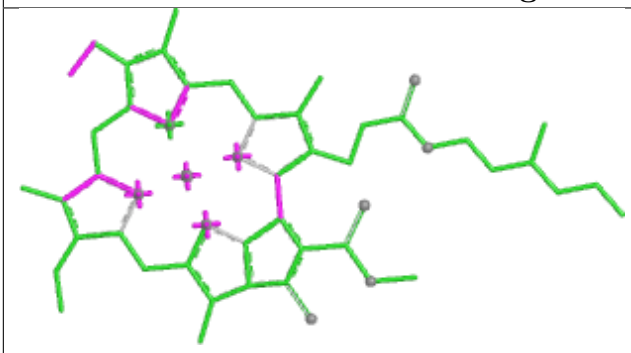


Torsions

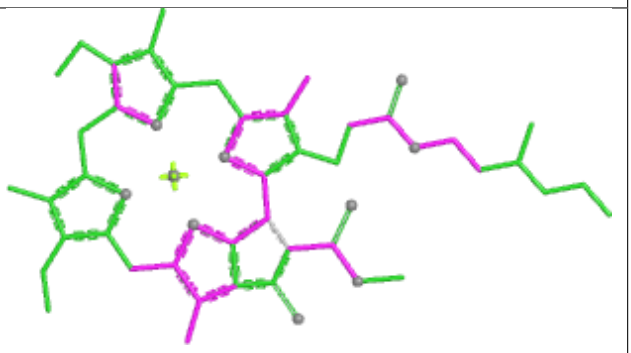


Rings

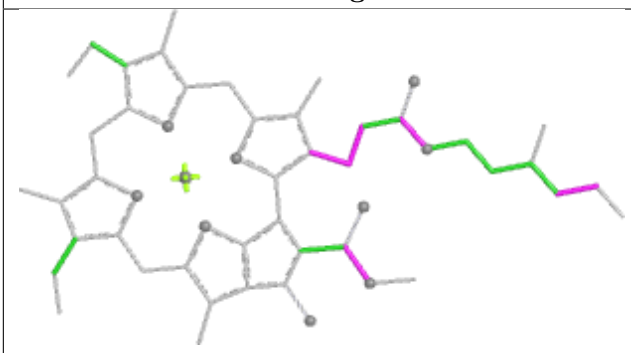
Ligand CLA a 1114



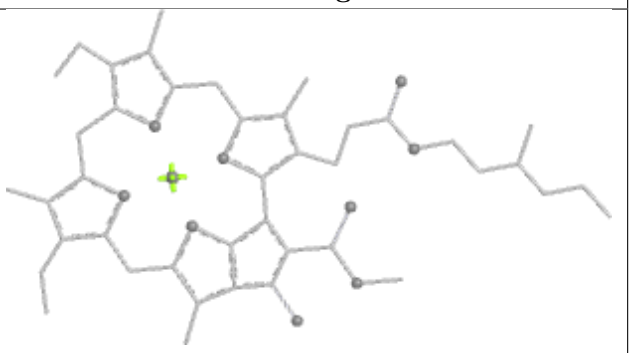
Bond lengths



Bond angles

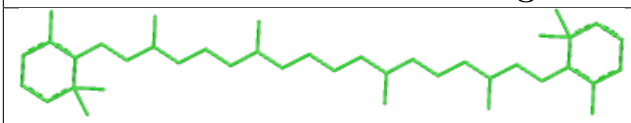


Torsions

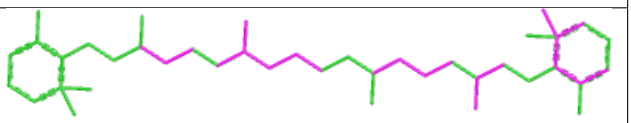


Rings

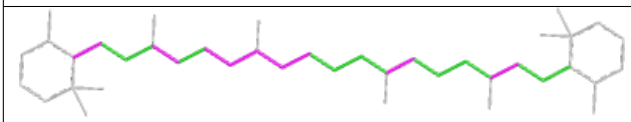
Ligand BCR 6 4016



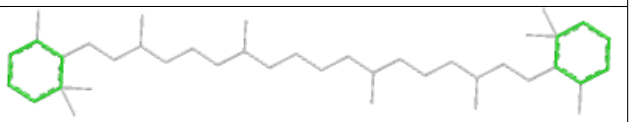
Bond lengths



Bond angles



Torsions

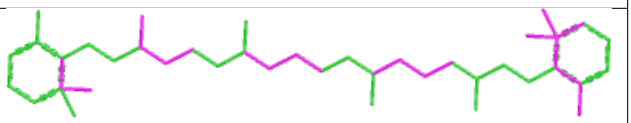


Rings

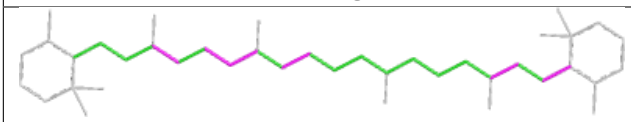
Ligand BCR 0 4019



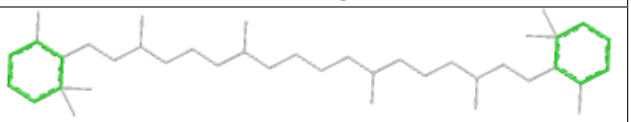
Bond lengths



Bond angles

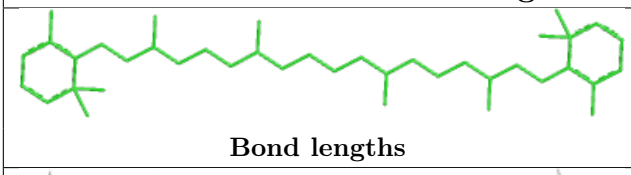


Torsions

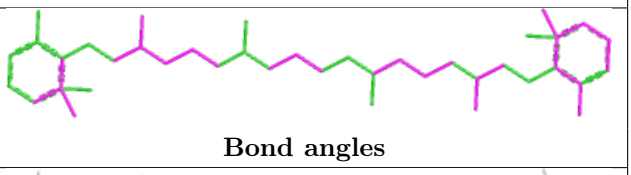


Rings

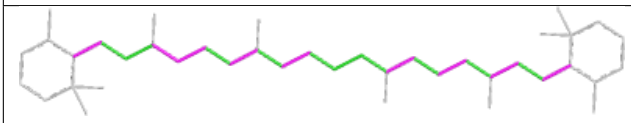
Ligand BCR a 4002



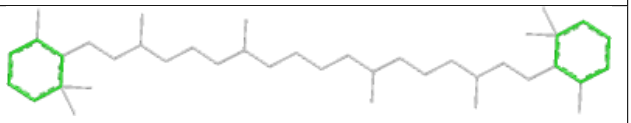
Bond lengths



Bond angles

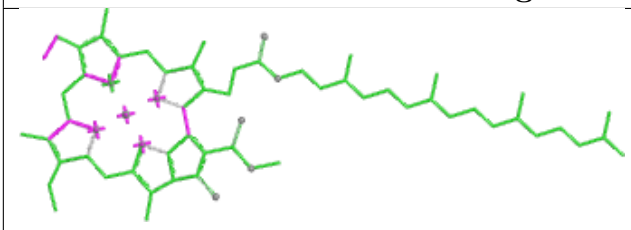


Torsions

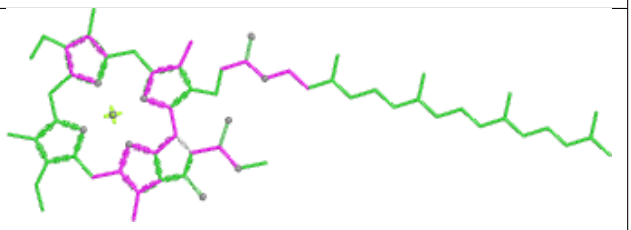


Rings

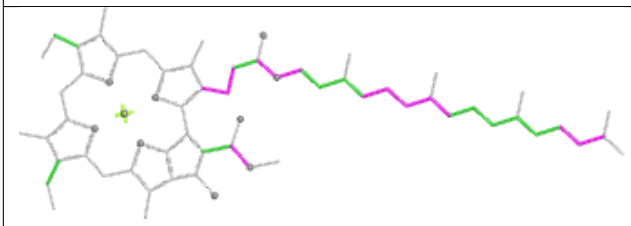
Ligand CLA B 1228



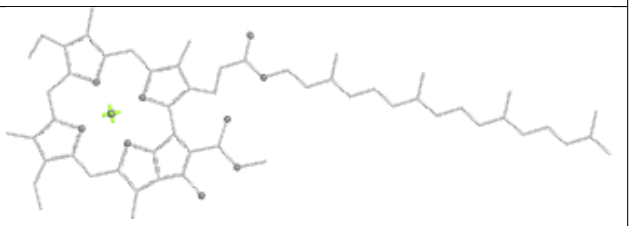
Bond lengths



Bond angles

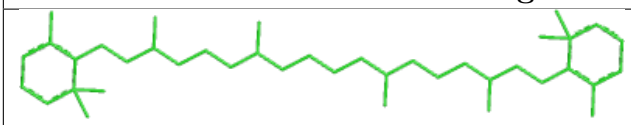


Torsions

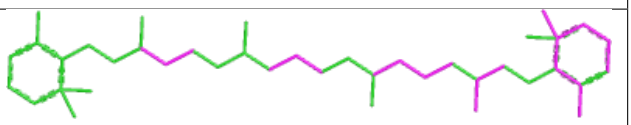


Rings

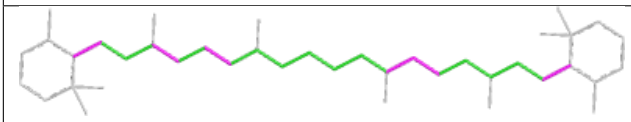
Ligand BCR k 4001



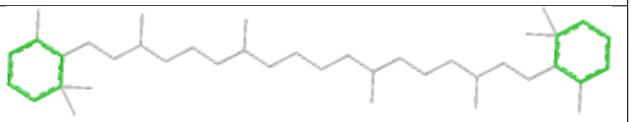
Bond lengths



Bond angles

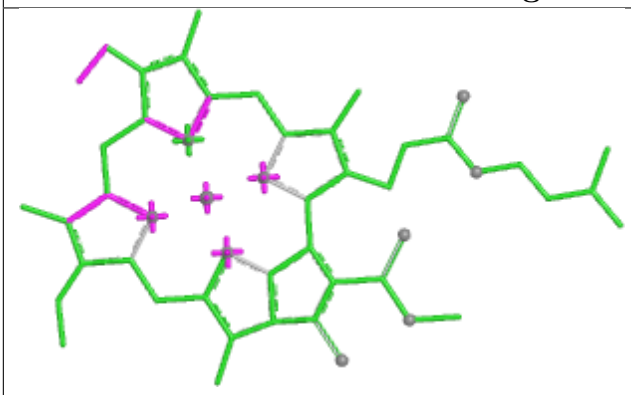


Torsions

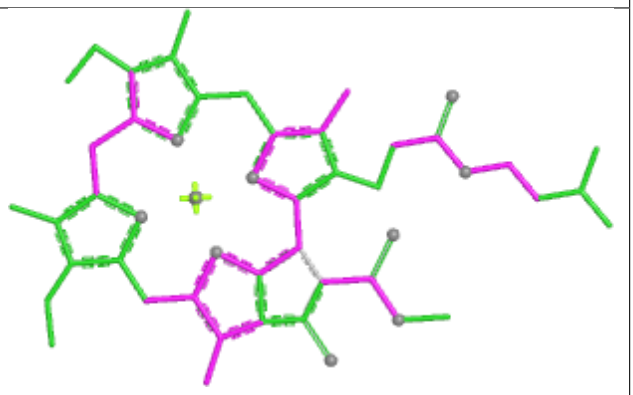


Rings

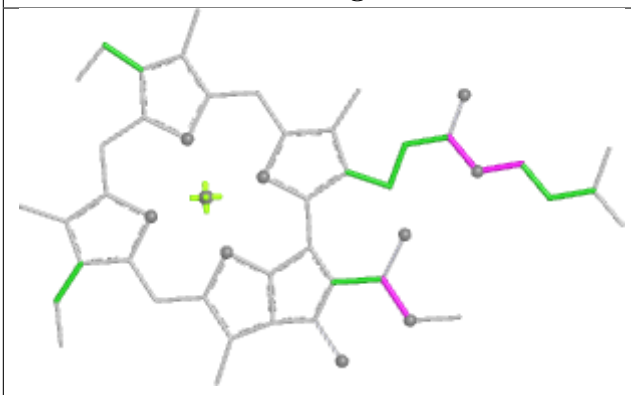
Ligand CLA f 1301



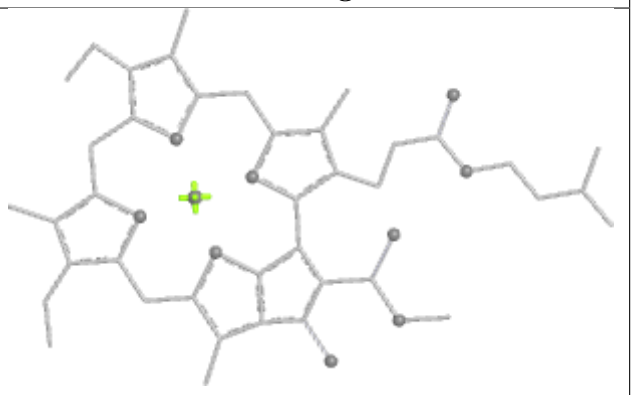
Bond lengths



Bond angles

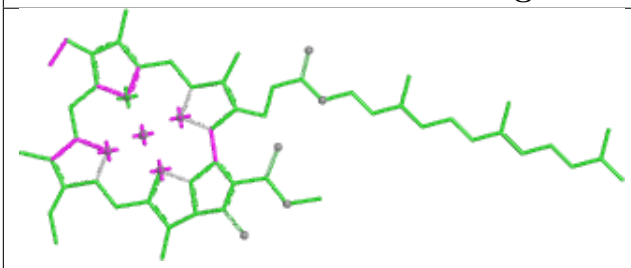


Torsions

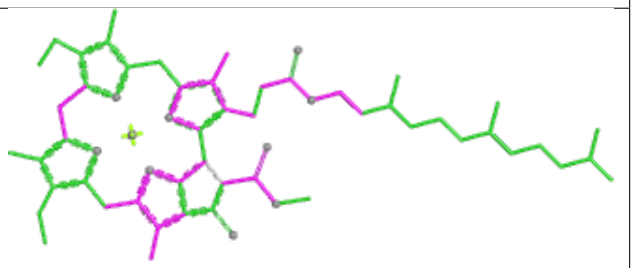


Rings

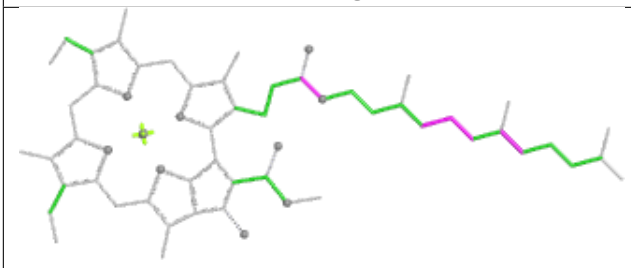
Ligand CLA A 1130



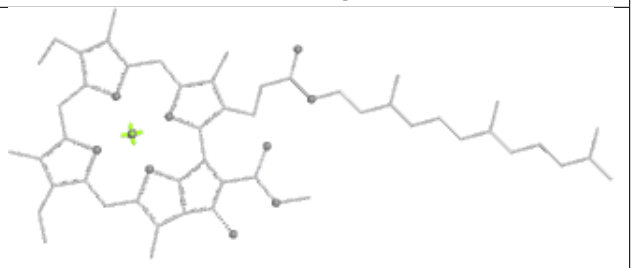
Bond lengths



Bond angles

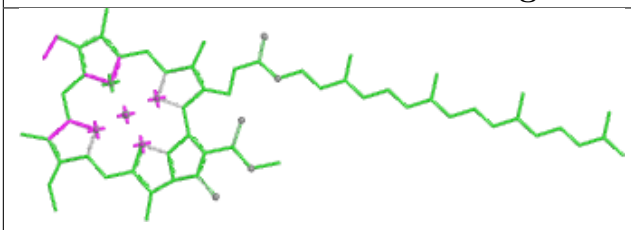


Torsions

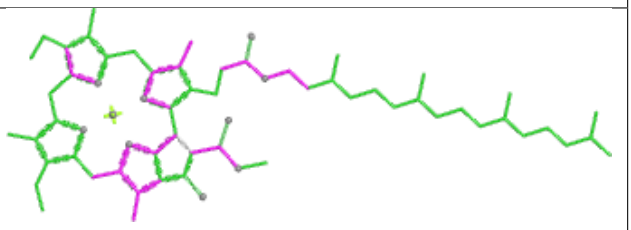


Rings

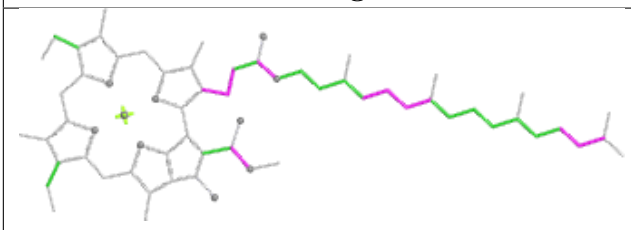
Ligand CLA 2 1204



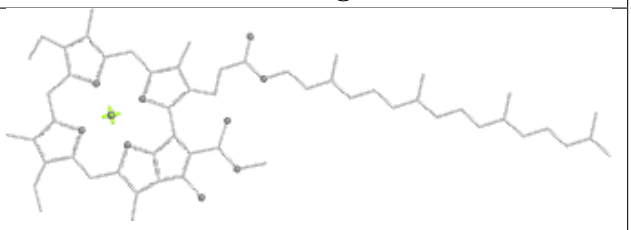
Bond lengths



Bond angles

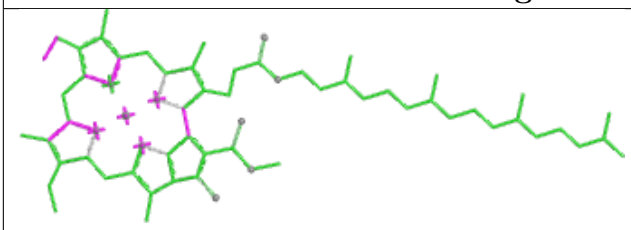


Torsions

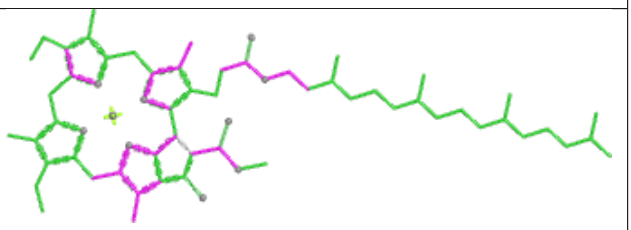


Rings

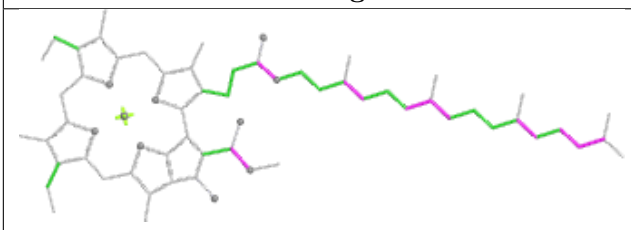
Ligand CLA A 1117



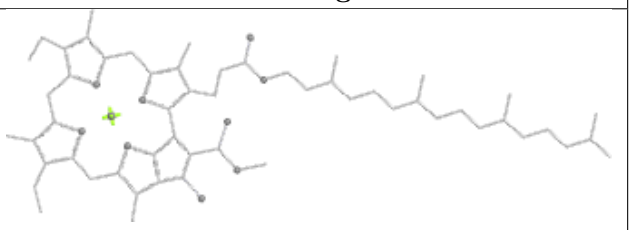
Bond lengths



Bond angles

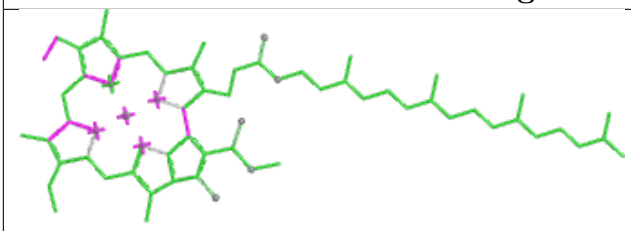


Torsions

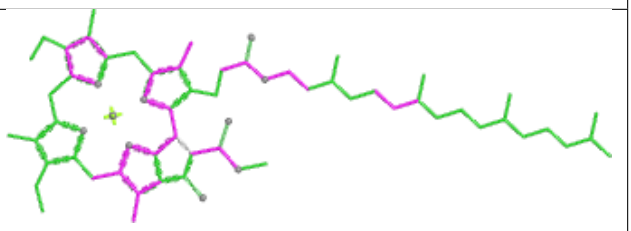


Rings

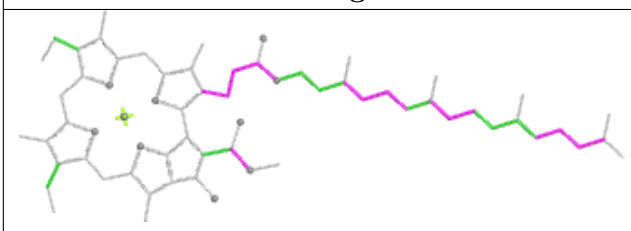
Ligand CLA L 1503



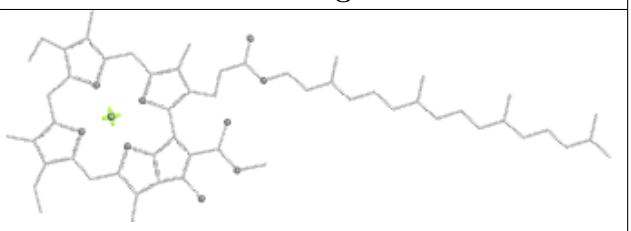
Bond lengths



Bond angles

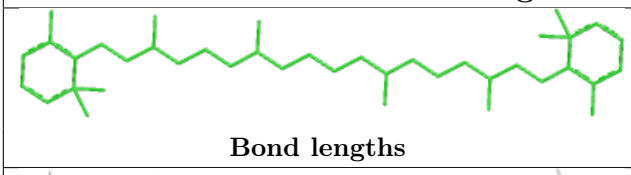


Torsions

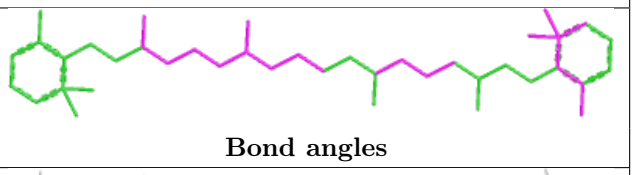


Rings

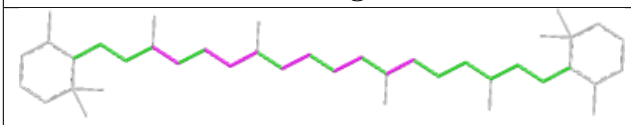
Ligand BCR b 4017



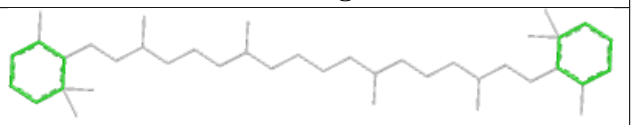
Bond lengths



Bond angles

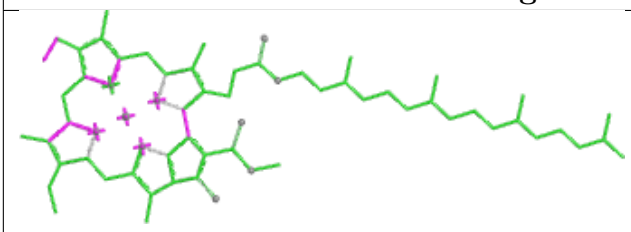


Torsions

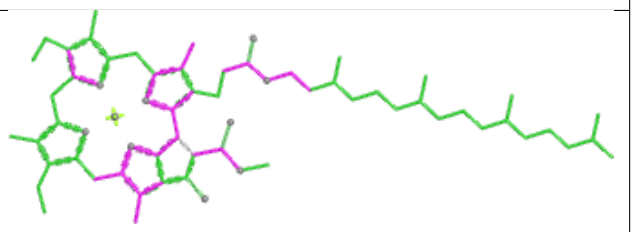


Rings

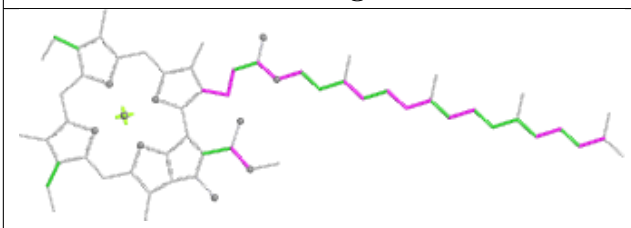
Ligand CLA 1 1013



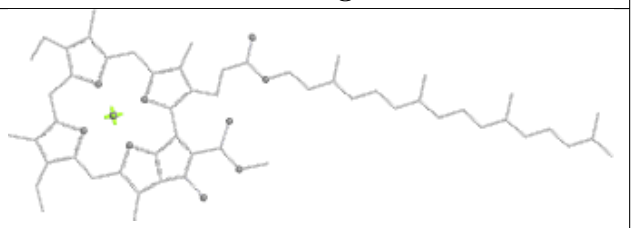
Bond lengths



Bond angles

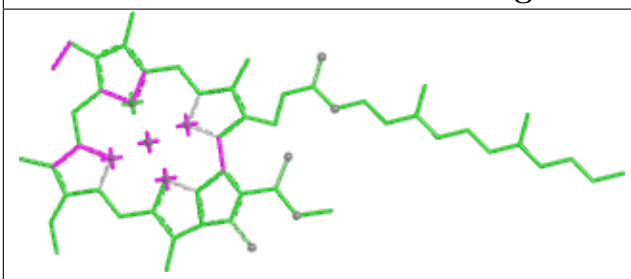


Torsions

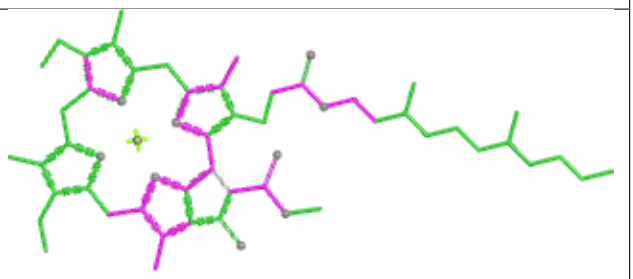


Rings

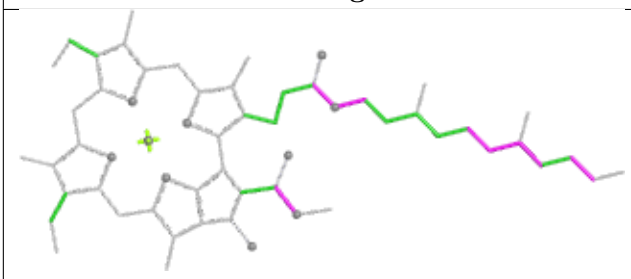
Ligand CLA A 1129



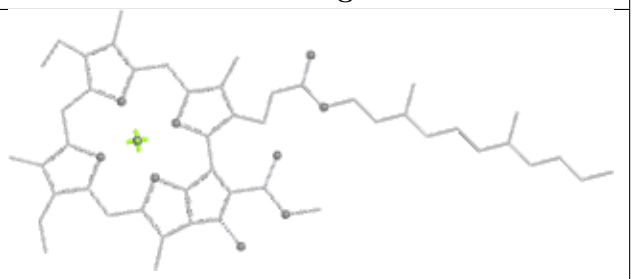
Bond lengths



Bond angles

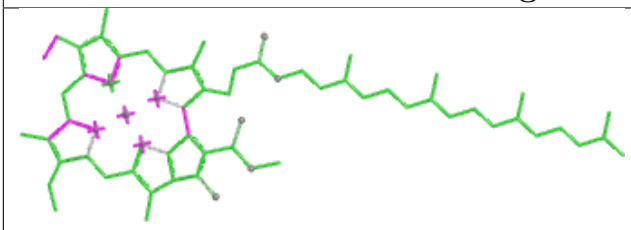


Torsions

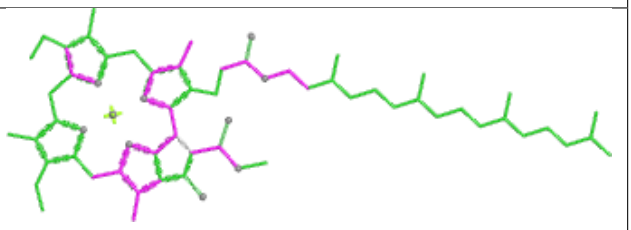


Rings

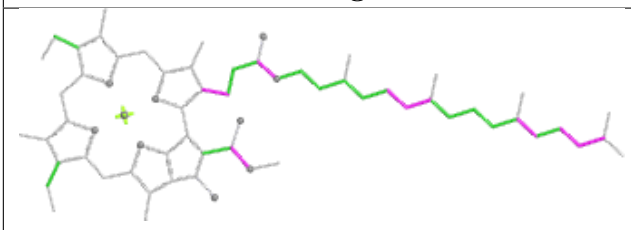
Ligand CLA 1 1117



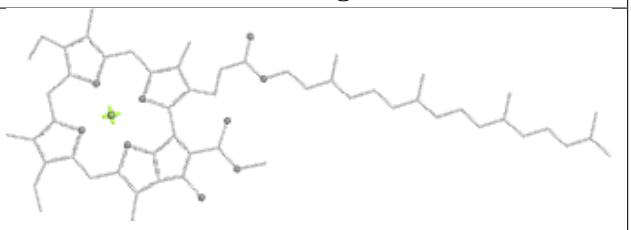
Bond lengths



Bond angles

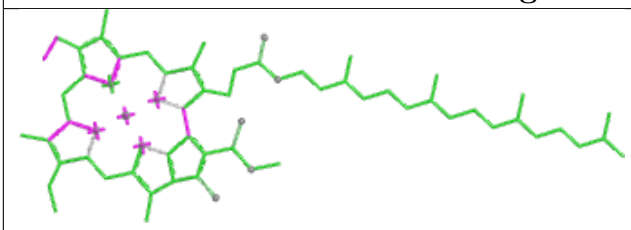


Torsions

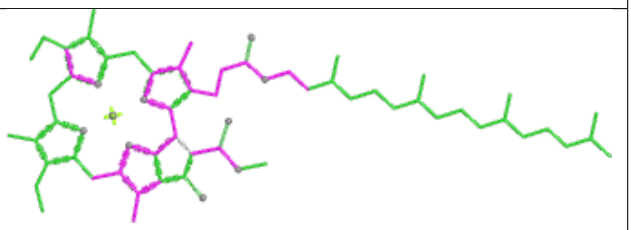


Rings

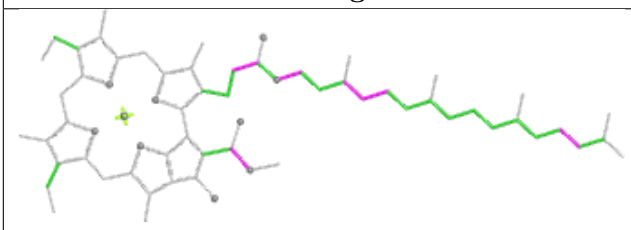
Ligand CLA a 1101



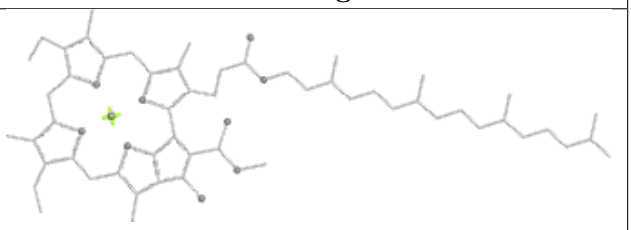
Bond lengths



Bond angles

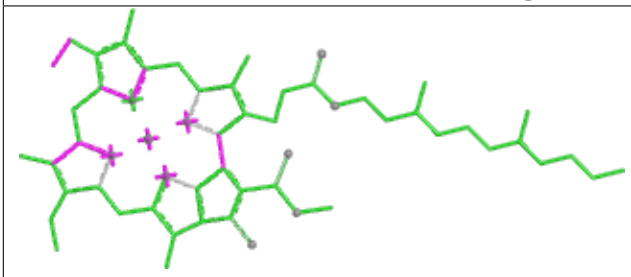


Torsions

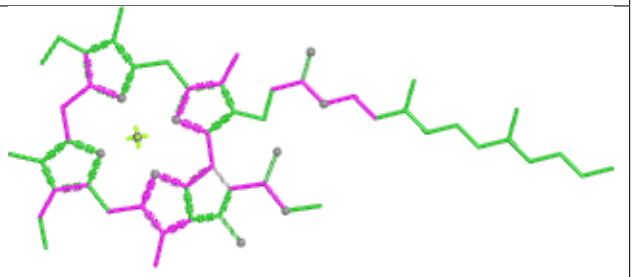


Rings

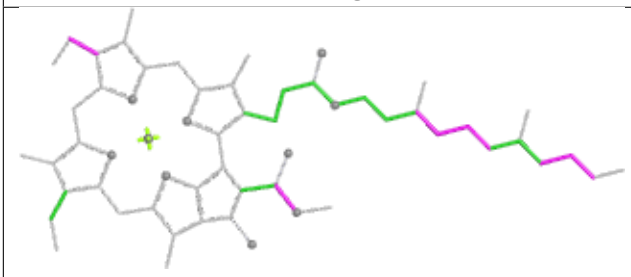
Ligand CLA a 1105



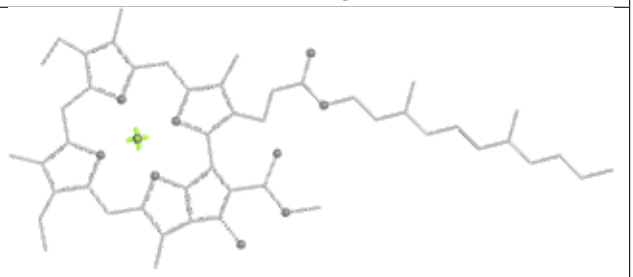
Bond lengths



Bond angles

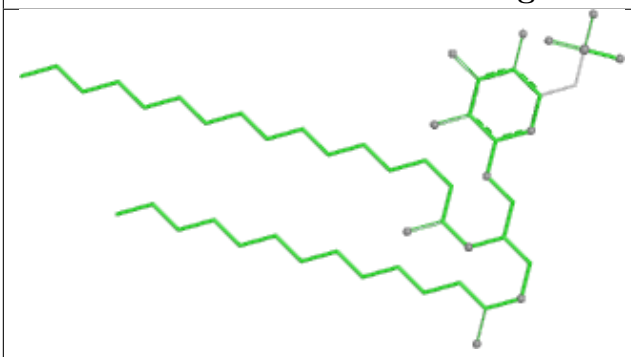


Torsions

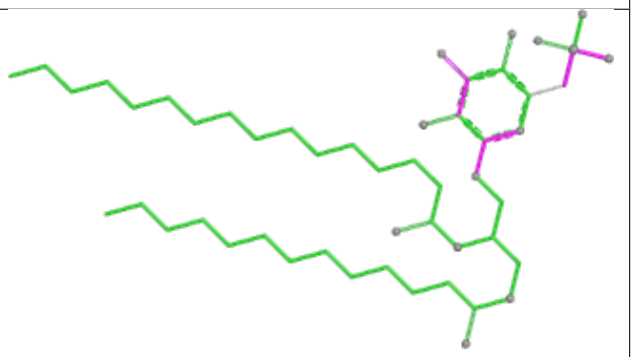


Rings

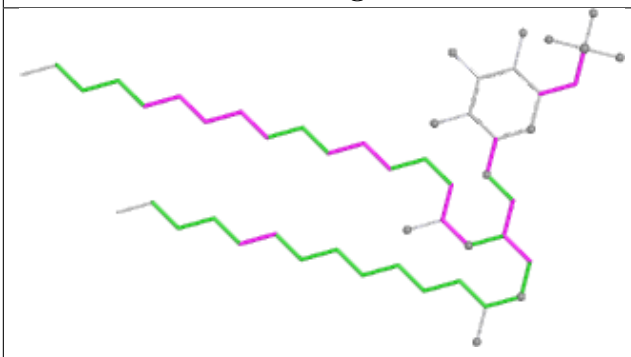
Ligand SQD L 5001



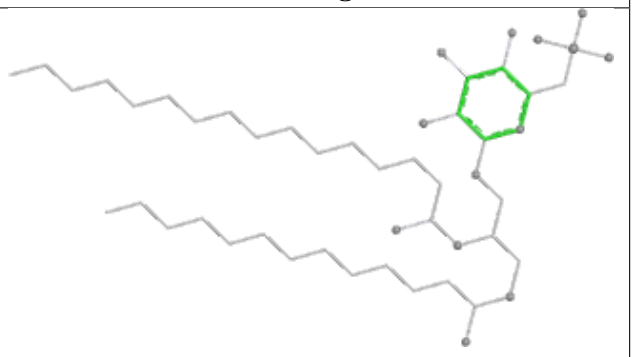
Bond lengths



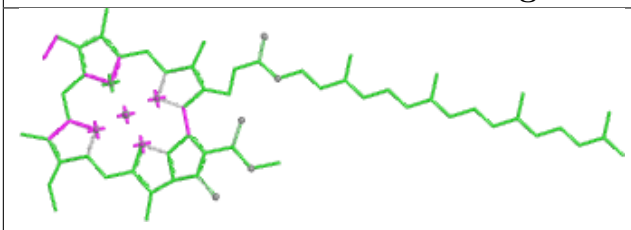
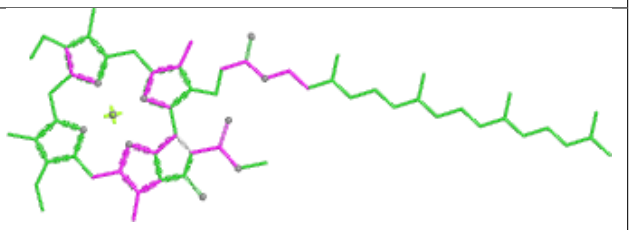
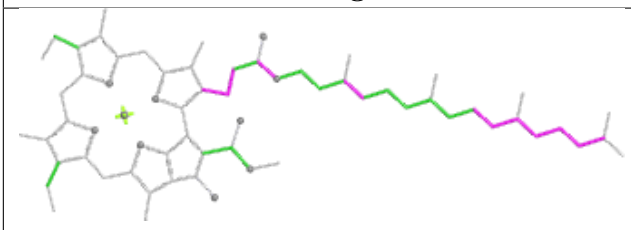
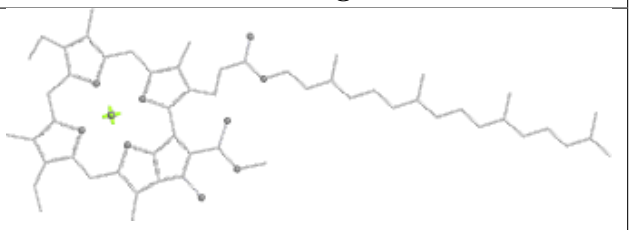
Bond angles

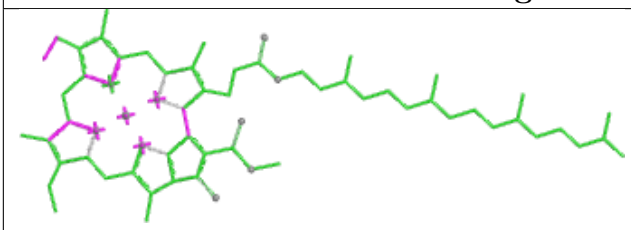
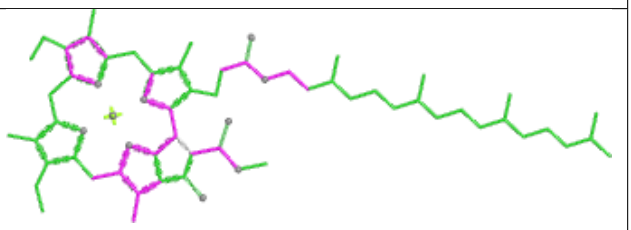
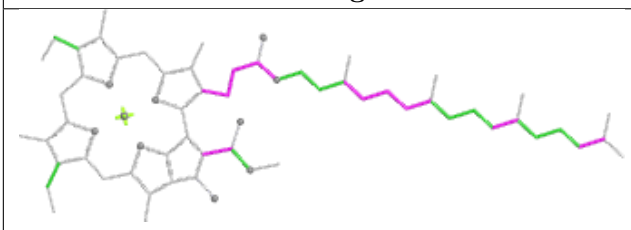
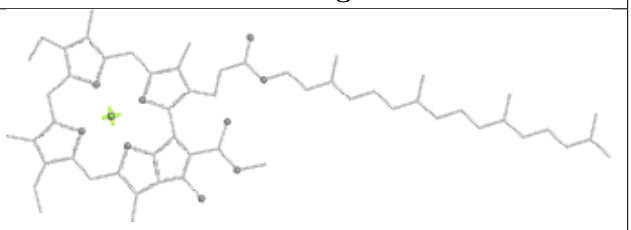


Torsions

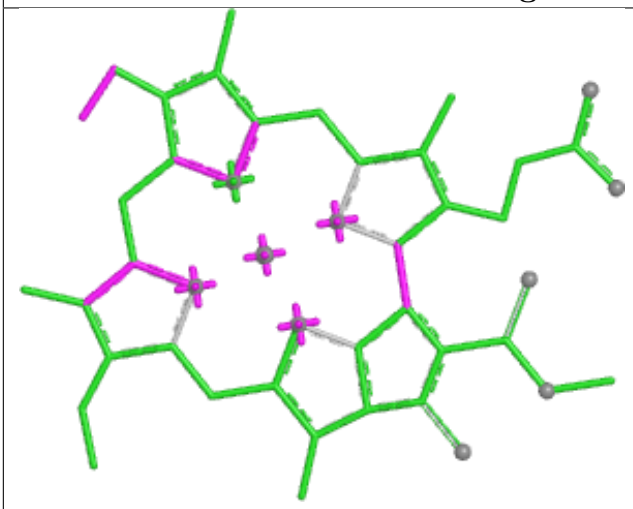


Rings

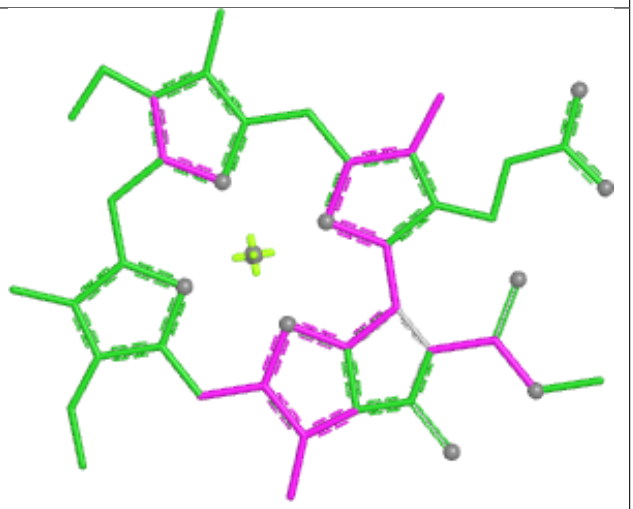
Ligand CLA 0 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

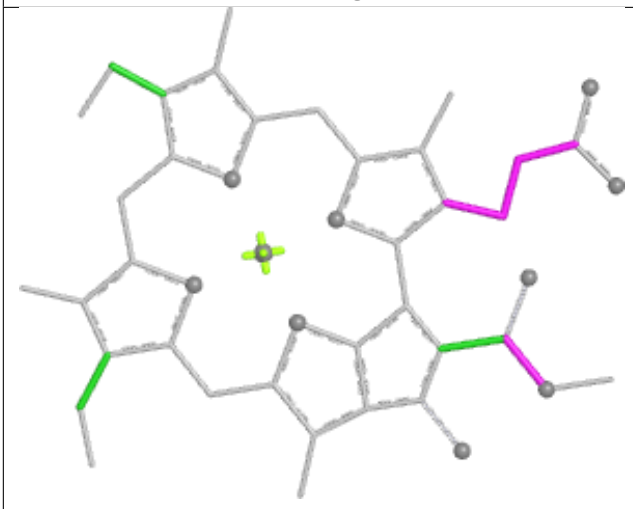
Ligand CLA 2 1232



Bond lengths



Bond angles

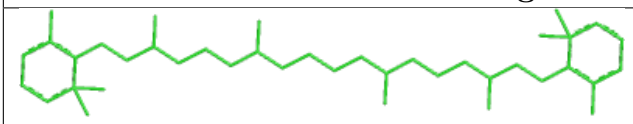


Torsions

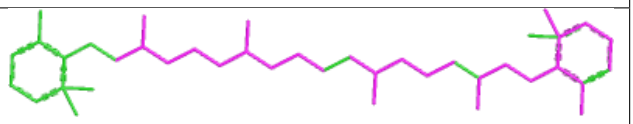


Rings

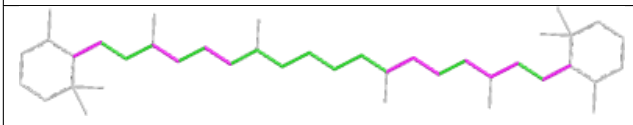
Ligand BCR 2 4018



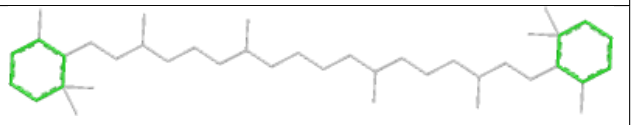
Bond lengths



Bond angles

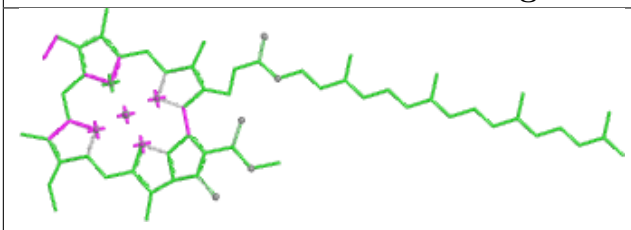


Torsions

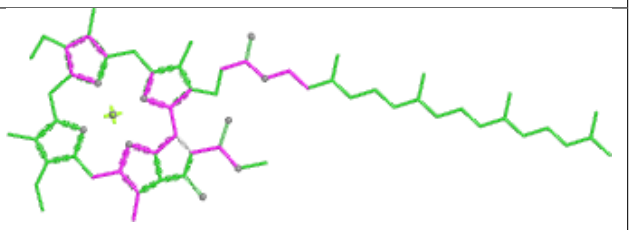


Rings

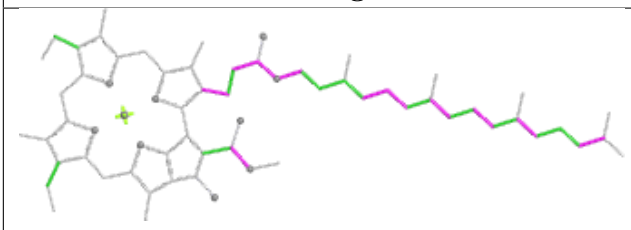
Ligand CLA a 1011



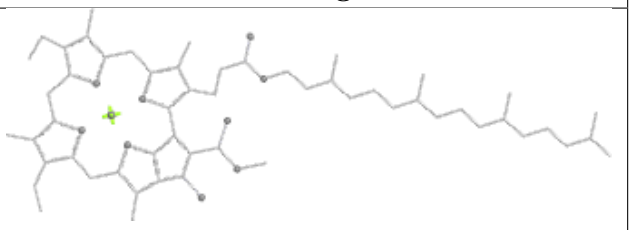
Bond lengths



Bond angles

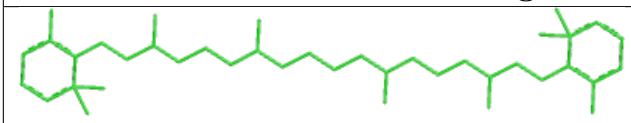


Torsions

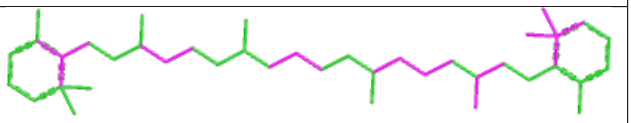


Rings

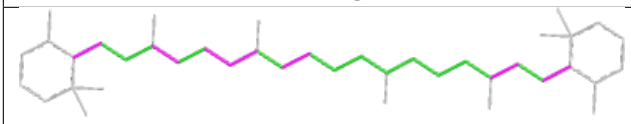
Ligand BCR 1 4003



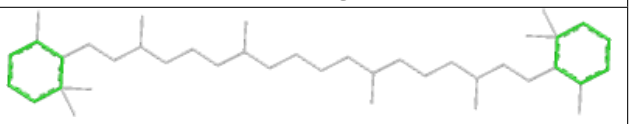
Bond lengths



Bond angles

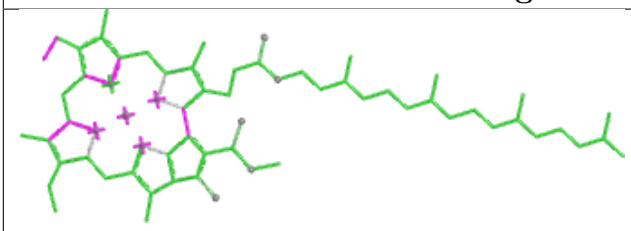


Torsions

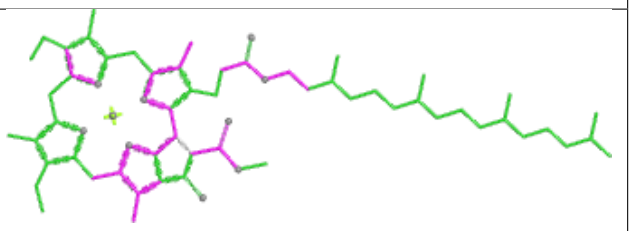


Rings

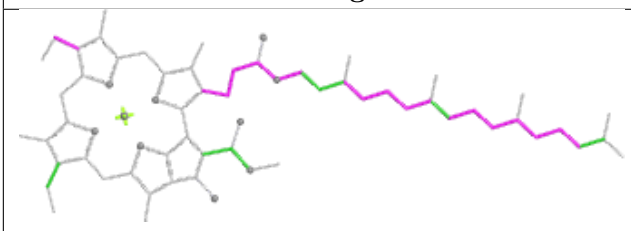
Ligand CLA B 1216



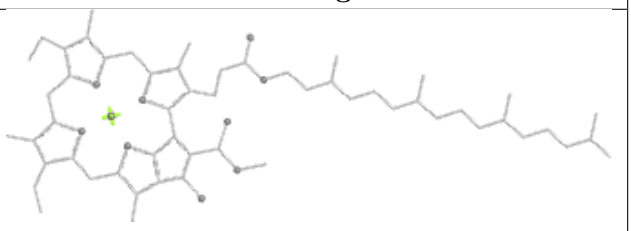
Bond lengths



Bond angles

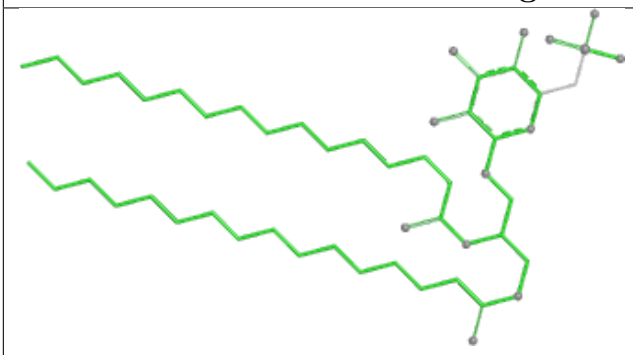


Torsions

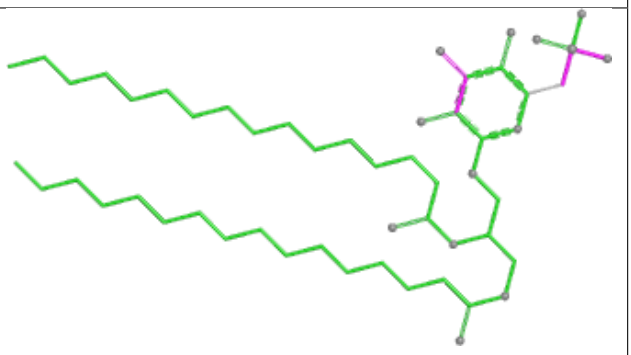


Rings

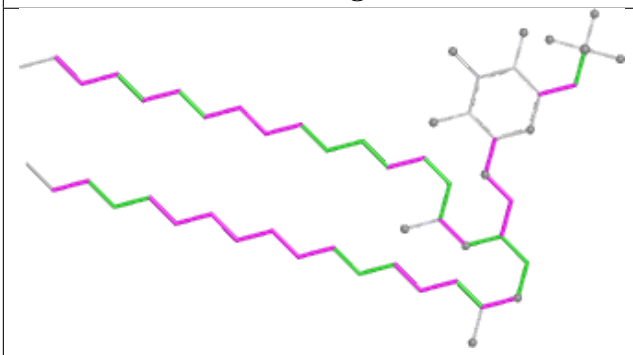
Ligand SQD 0 5005



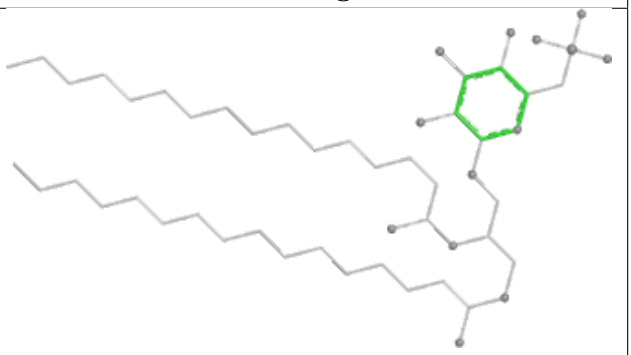
Bond lengths



Bond angles

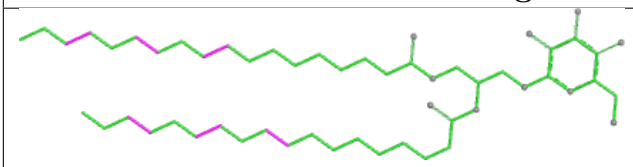


Torsions

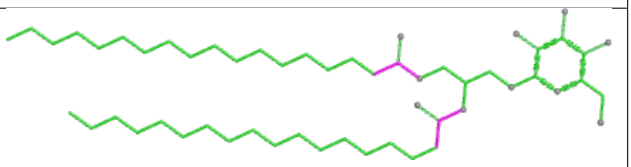


Rings

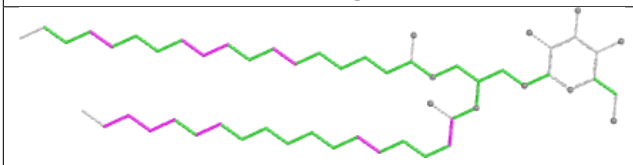
Ligand LMG 2 5002



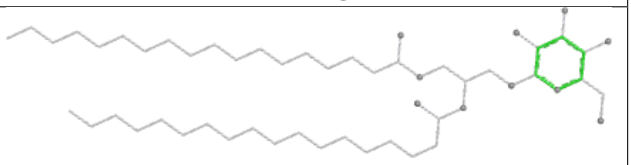
Bond lengths



Bond angles

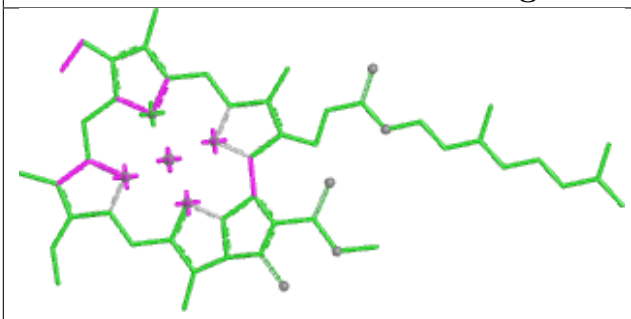


Torsions

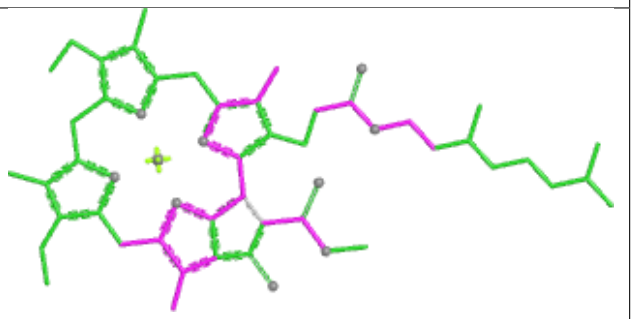


Rings

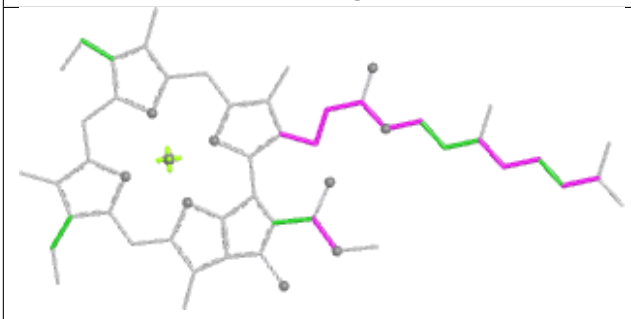
Ligand CLA 2 1224



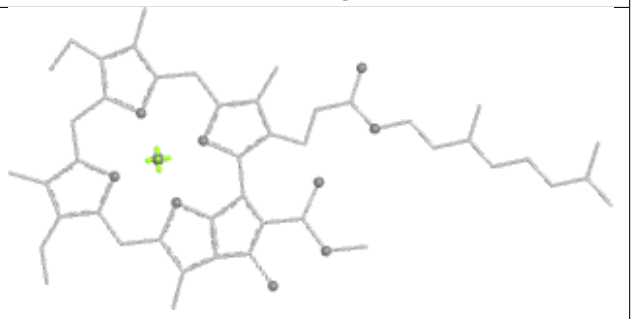
Bond lengths



Bond angles

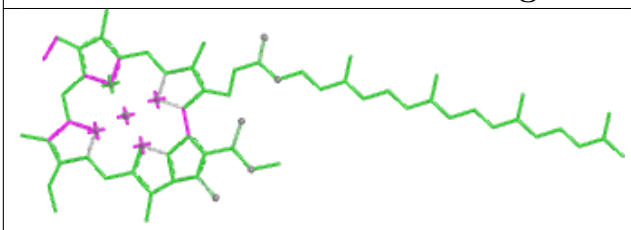


Torsions

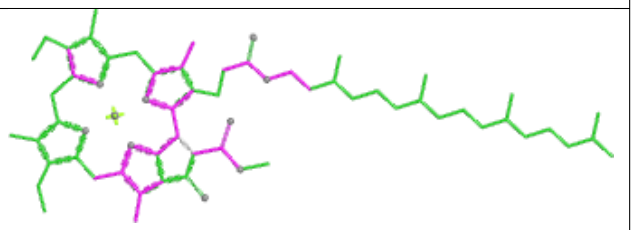


Rings

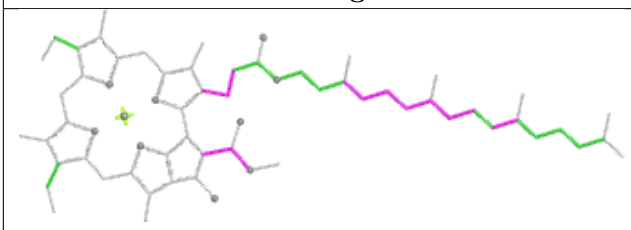
Ligand CLA 1 1012



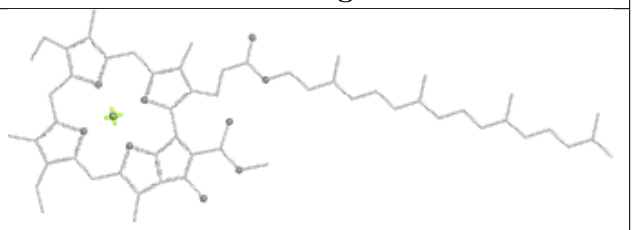
Bond lengths



Bond angles

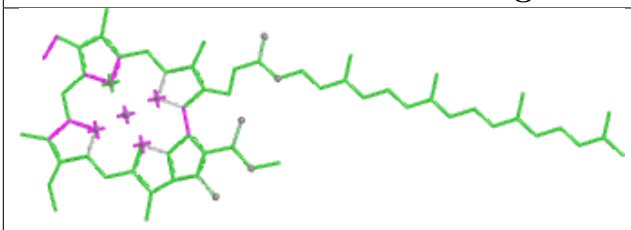


Torsions

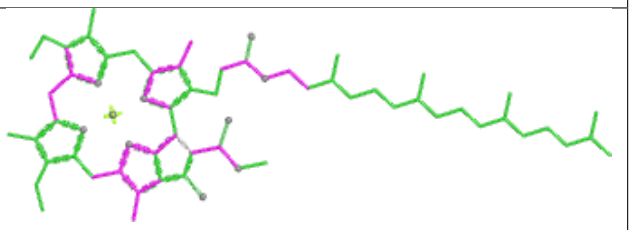


Rings

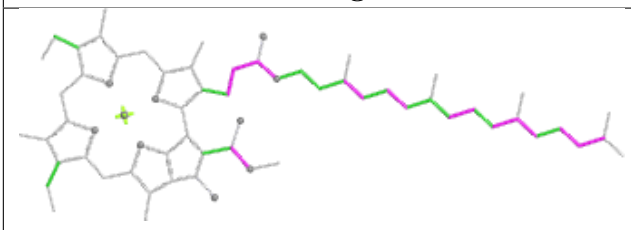
Ligand CLA A 1136



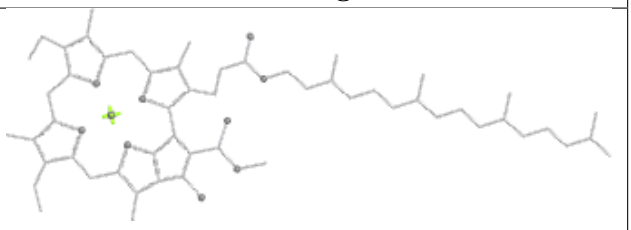
Bond lengths



Bond angles

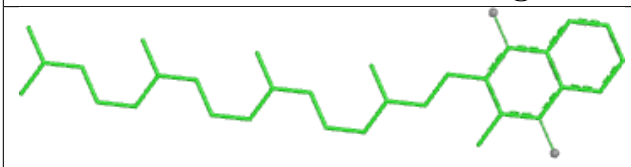


Torsions

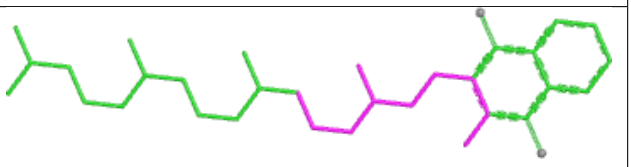


Rings

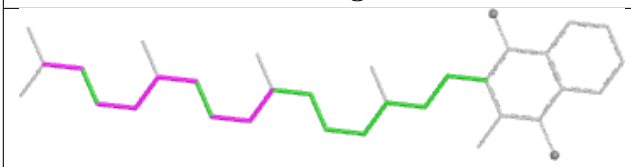
Ligand PQN A 2001



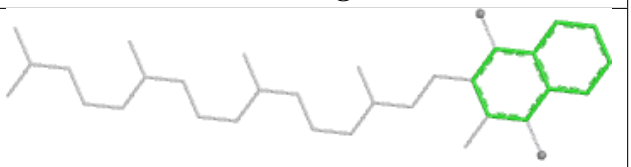
Bond lengths



Bond angles

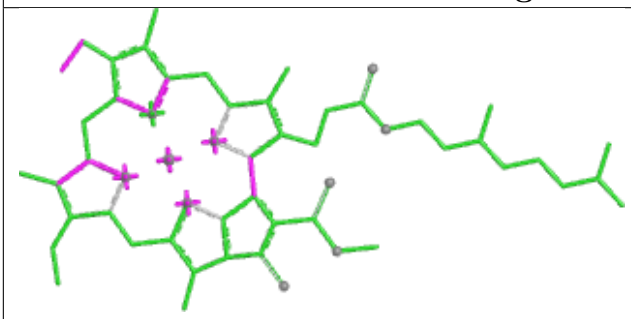


Torsions

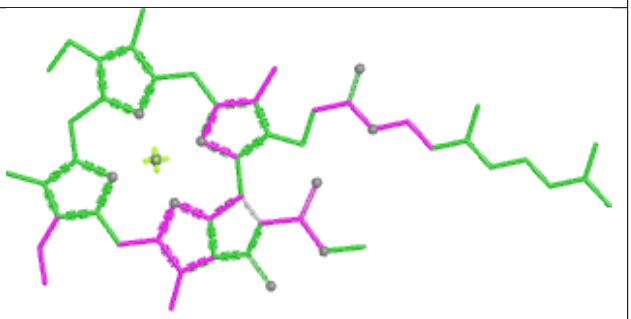


Rings

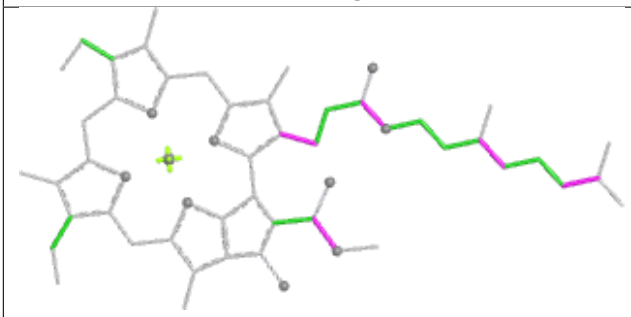
Ligand CLA B 1222



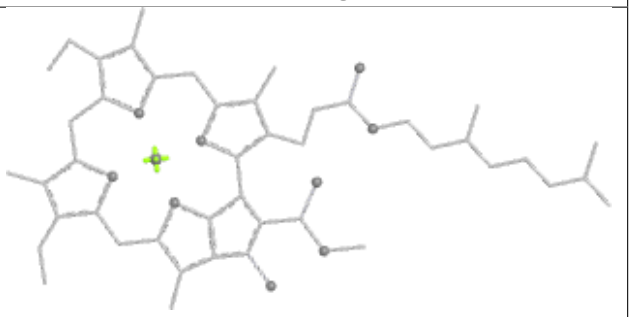
Bond lengths



Bond angles

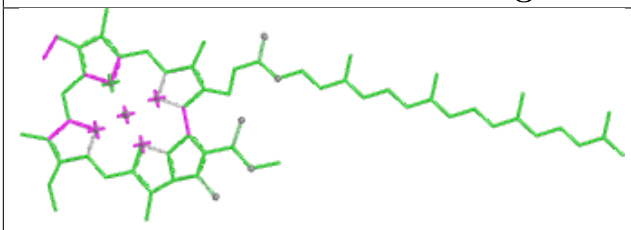


Torsions

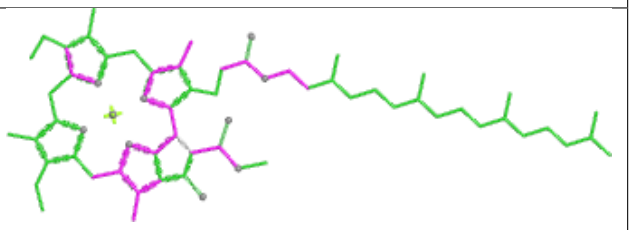


Rings

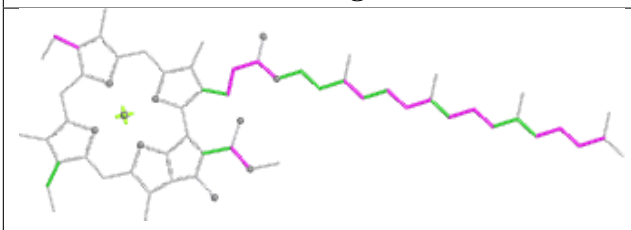
Ligand CLA B 1214



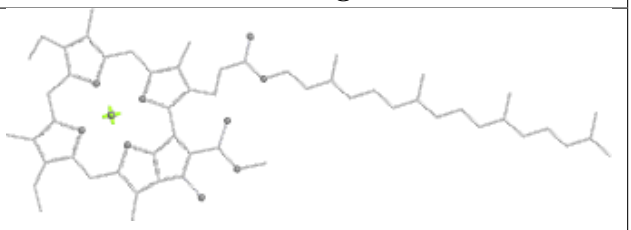
Bond lengths



Bond angles

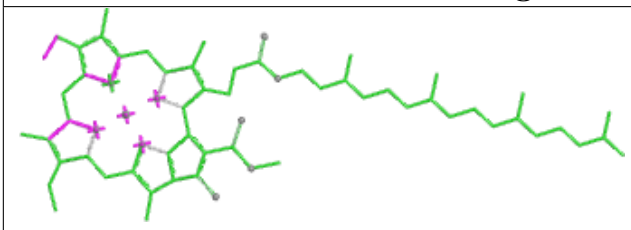


Torsions

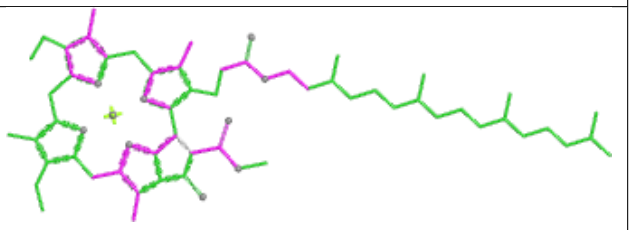


Rings

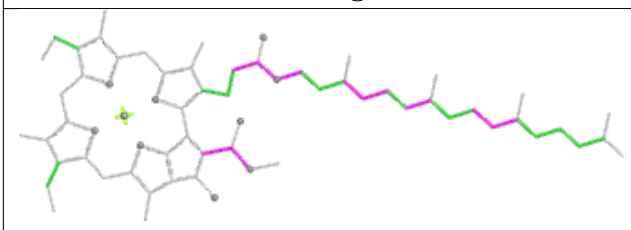
Ligand CLA A 1128



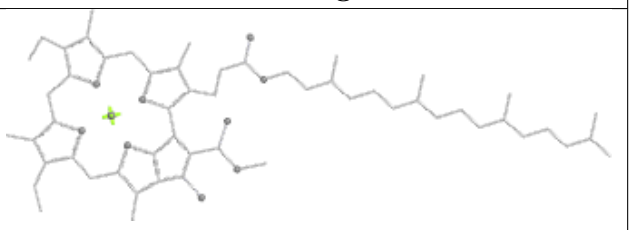
Bond lengths



Bond angles

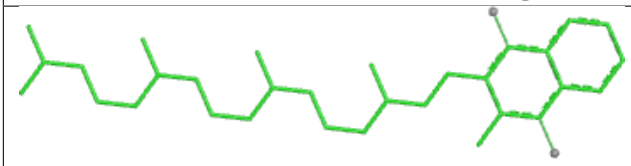


Torsions

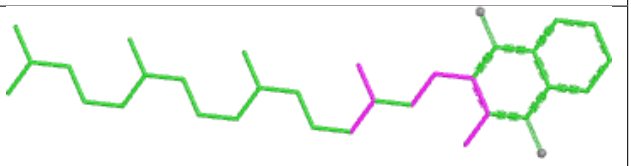


Rings

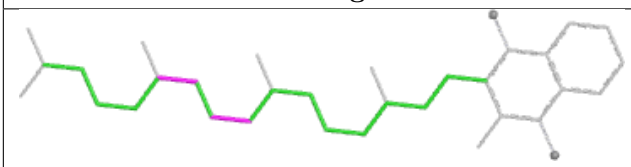
Ligand PQN 1 2001



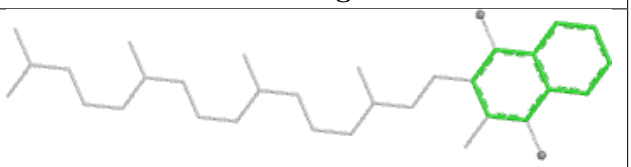
Bond lengths



Bond angles

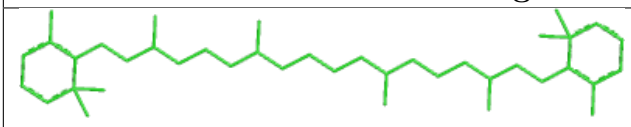


Torsions

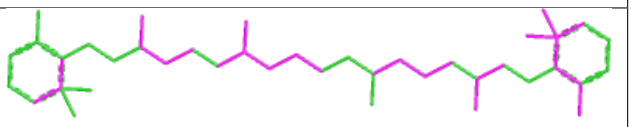


Rings

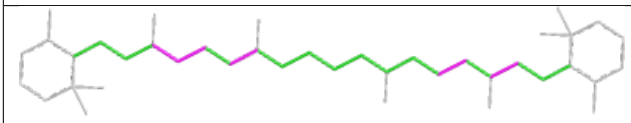
Ligand BCR A 4007



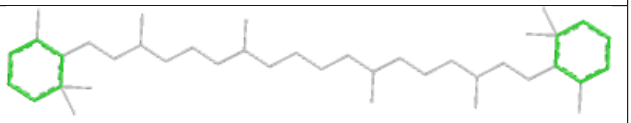
Bond lengths



Bond angles

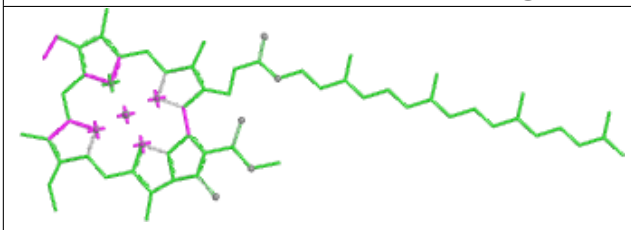


Torsions

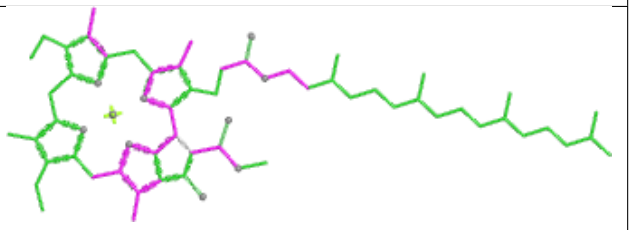


Rings

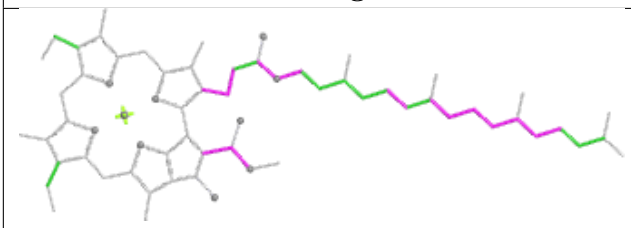
Ligand CLA 1 1128



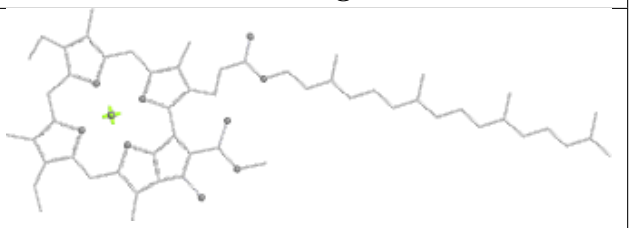
Bond lengths



Bond angles

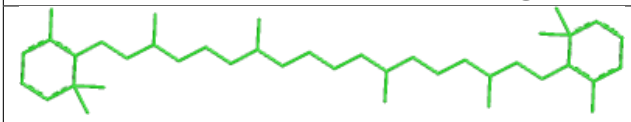


Torsions

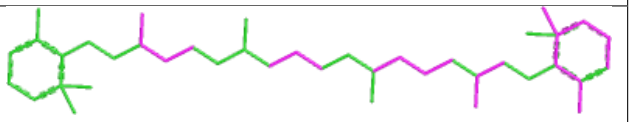


Rings

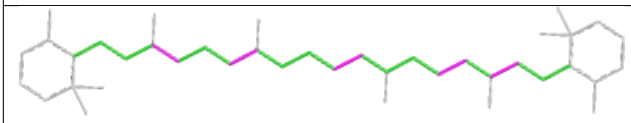
Ligand BCR 8 4001



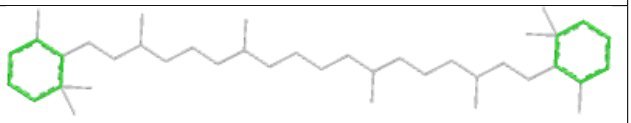
Bond lengths



Bond angles

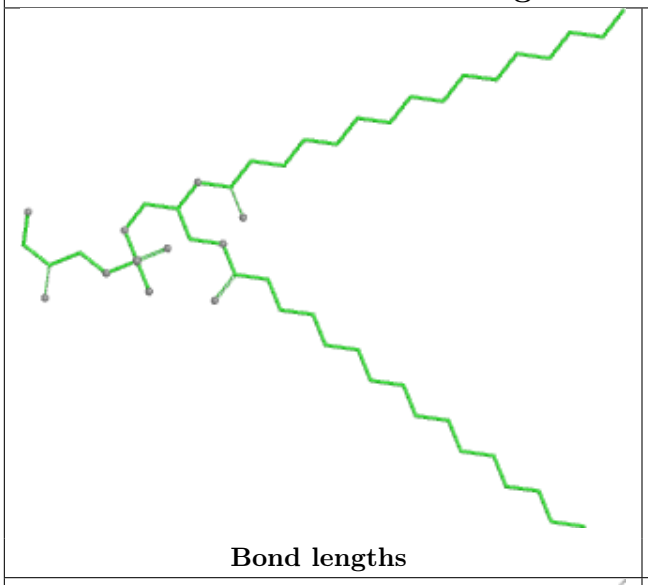


Torsions

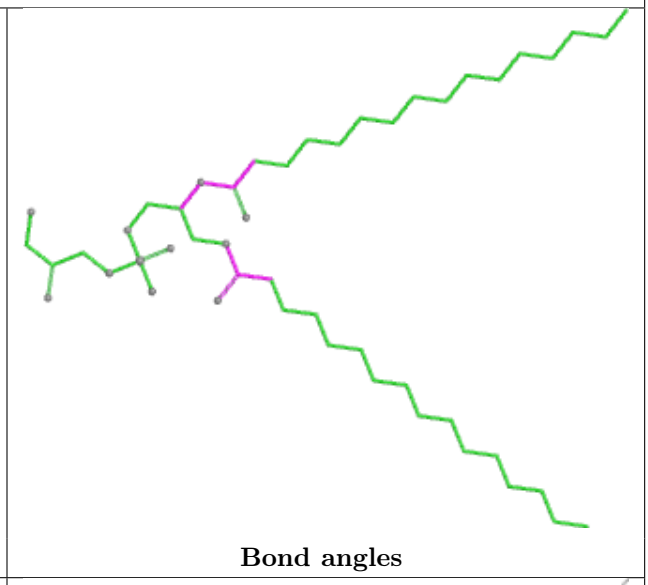


Rings

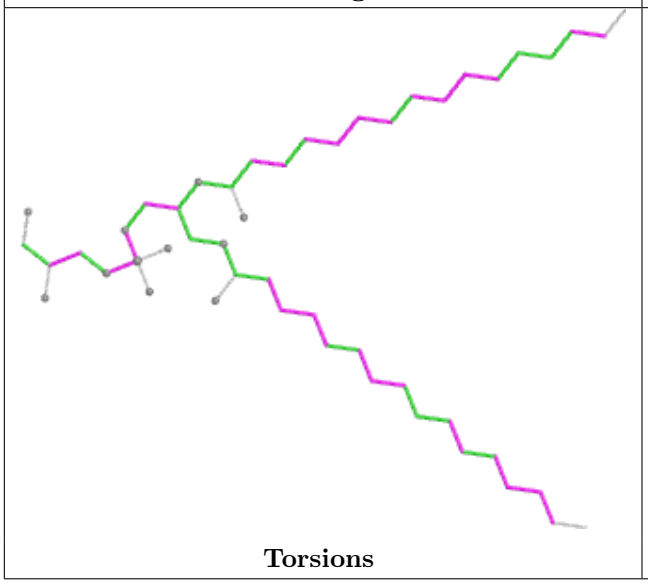
Ligand LHG A 5003



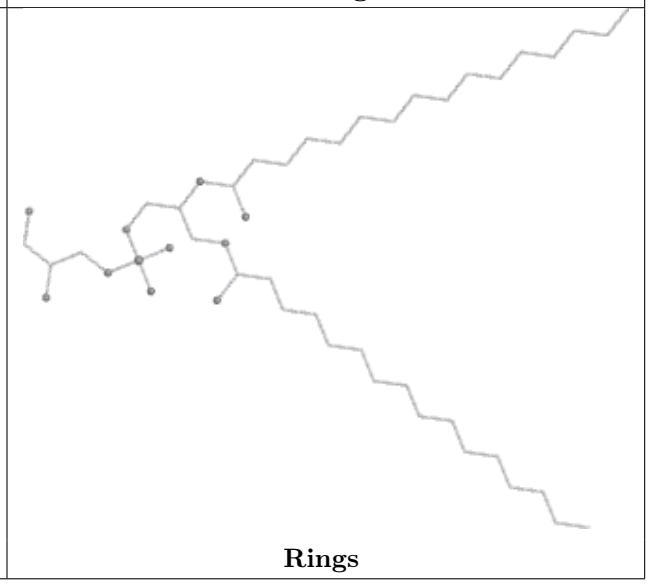
Bond lengths



Bond angles

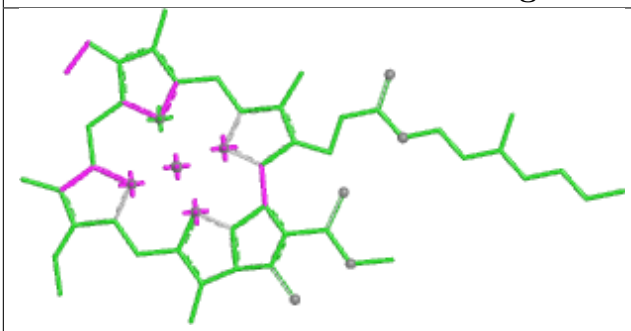


Torsions

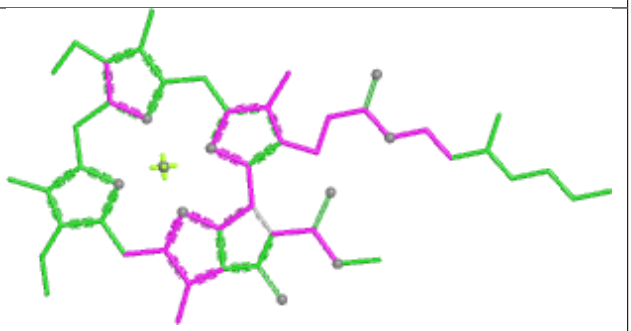


Rings

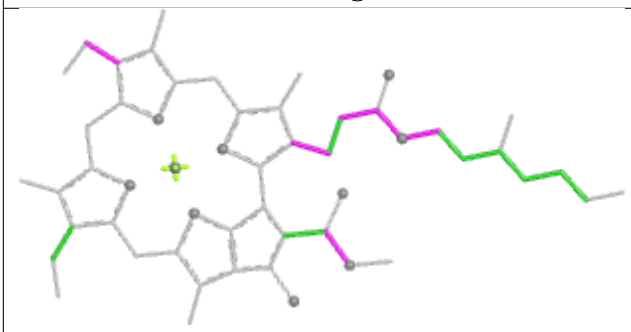
Ligand CLA 2 1219



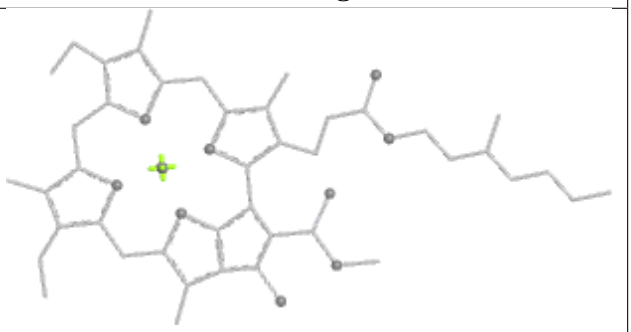
Bond lengths



Bond angles

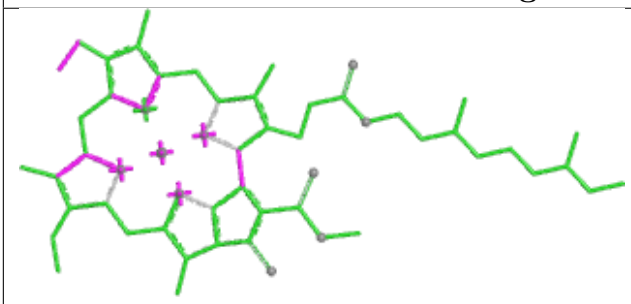


Torsions

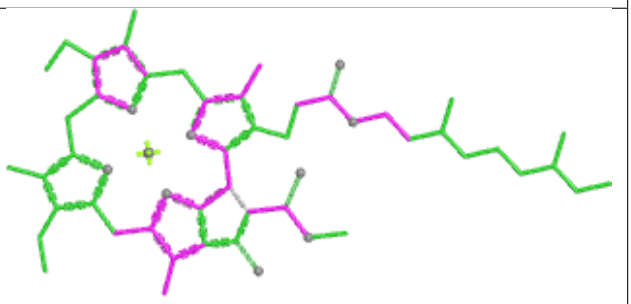


Rings

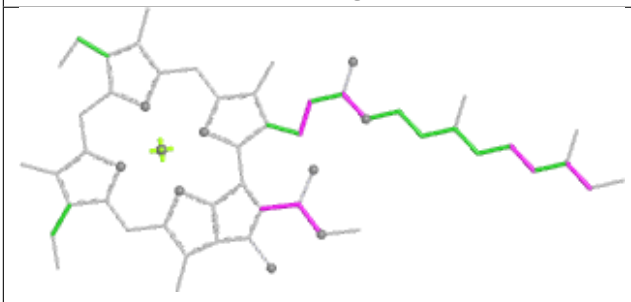
Ligand CLA 1 1801



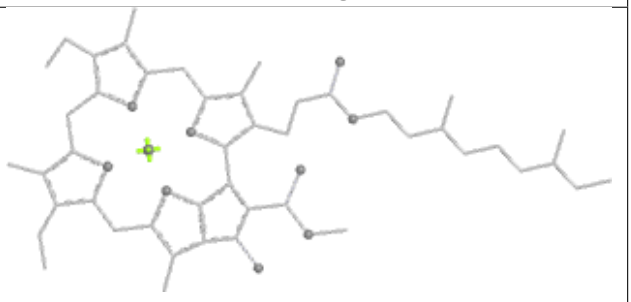
Bond lengths



Bond angles

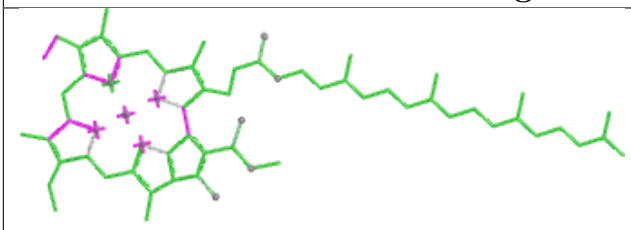


Torsions

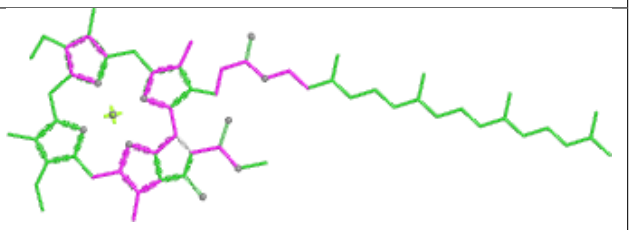


Rings

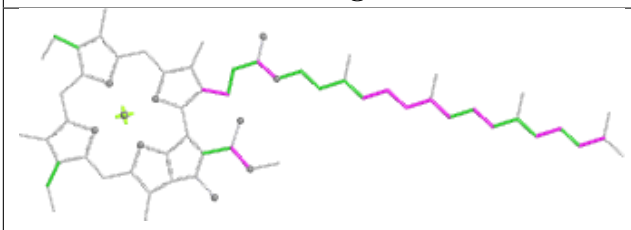
Ligand CLA A 1102



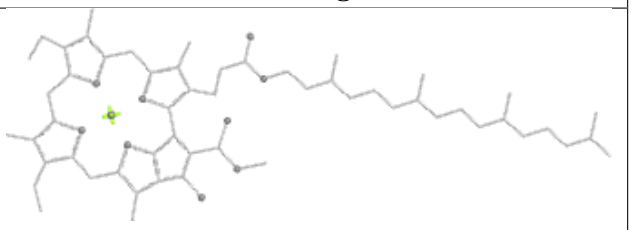
Bond lengths



Bond angles

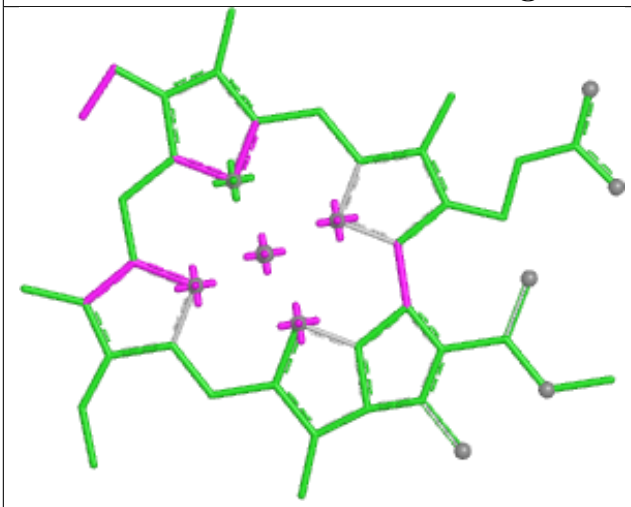


Torsions

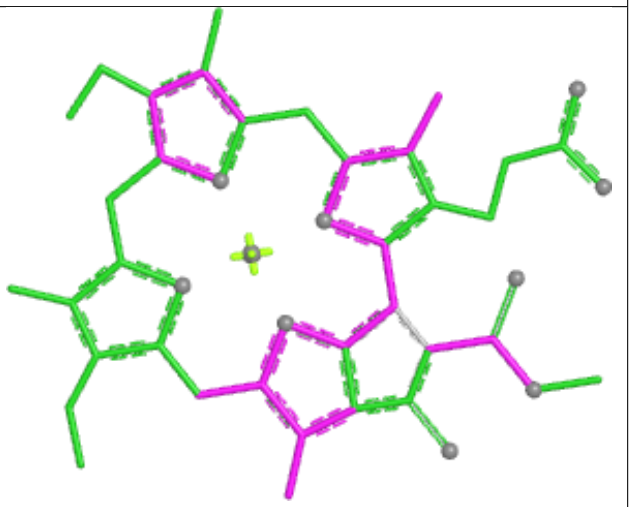


Rings

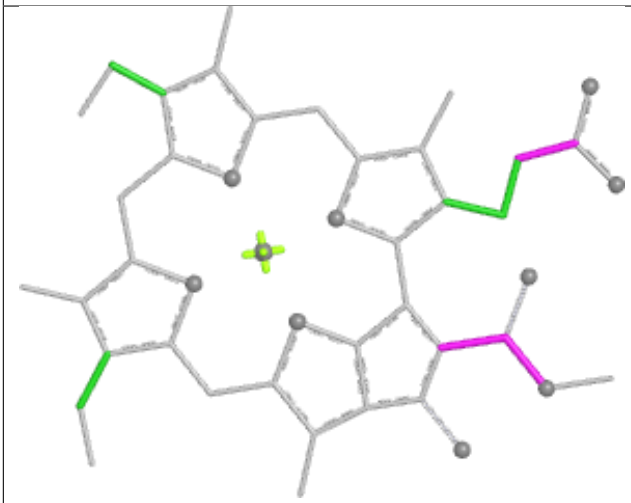
Ligand CLA 2 1220



Bond lengths



Bond angles

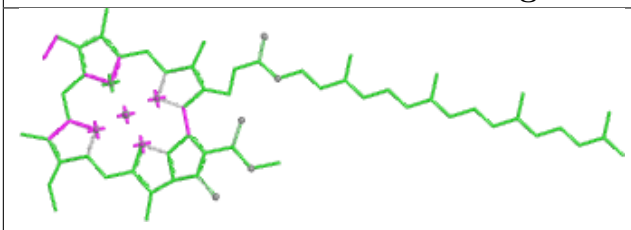


Torsions

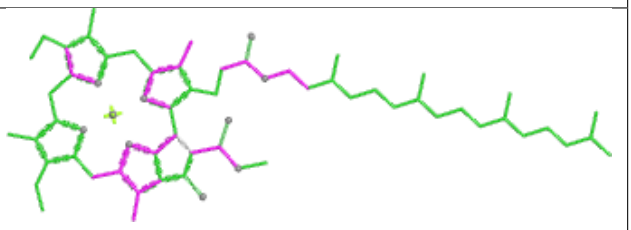


Rings

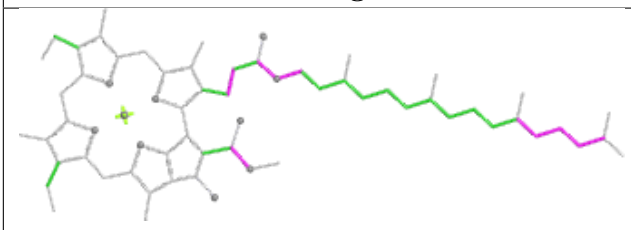
Ligand CLA a 1138



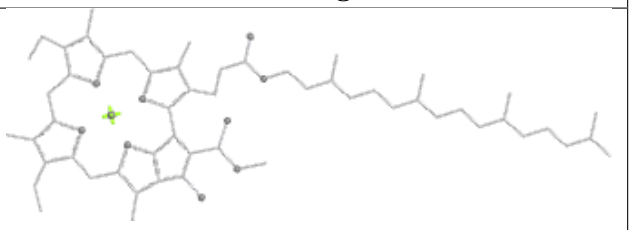
Bond lengths



Bond angles

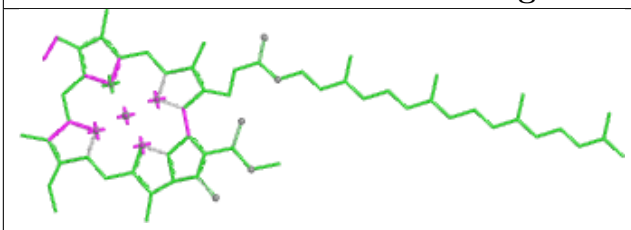


Torsions

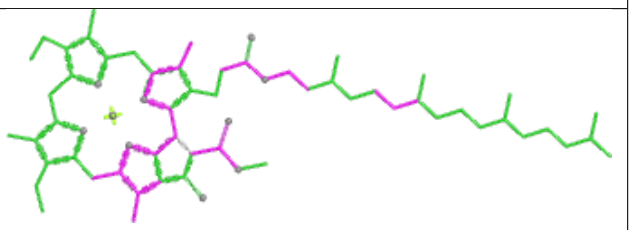


Rings

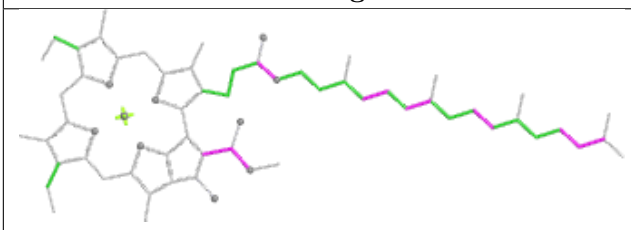
Ligand CLA b 1221



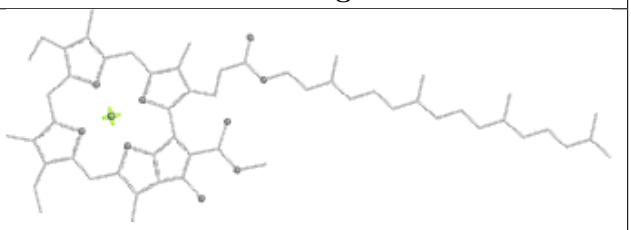
Bond lengths



Bond angles

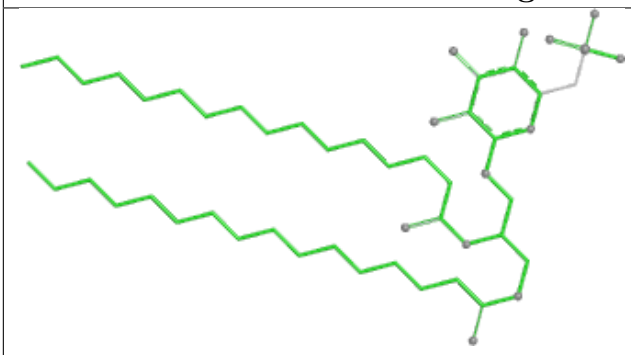


Torsions

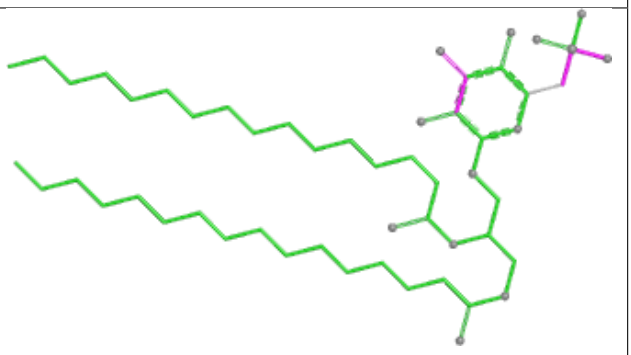


Rings

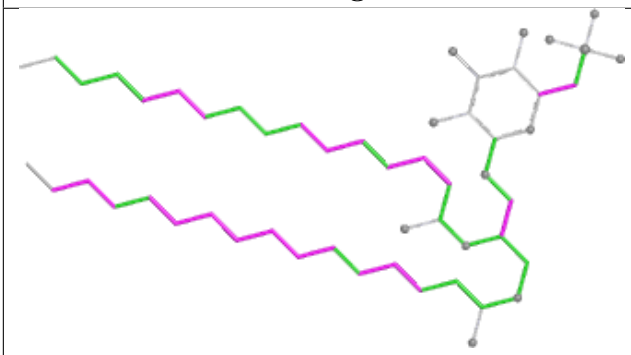
Ligand SQD L 5002



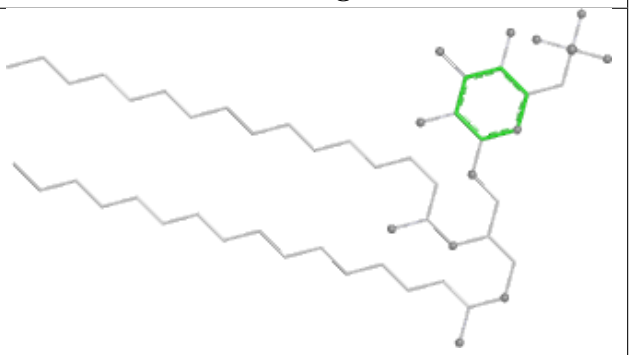
Bond lengths



Bond angles

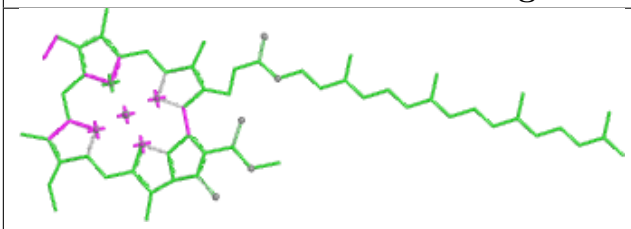


Torsions

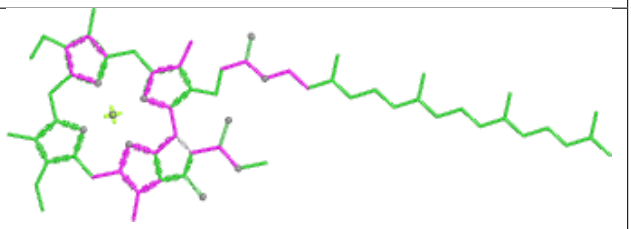


Rings

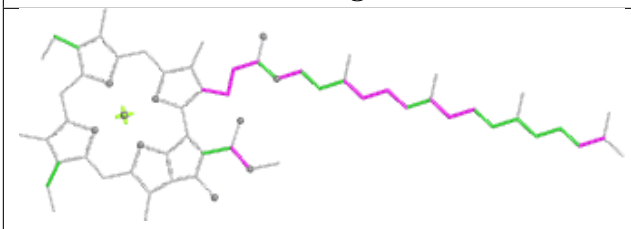
Ligand CLA b 1215



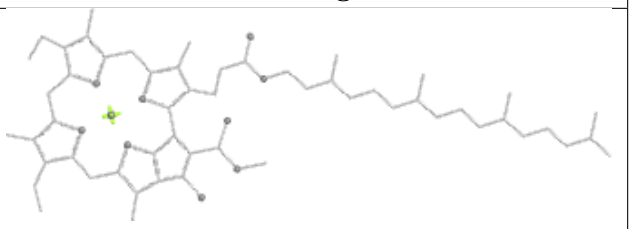
Bond lengths



Bond angles

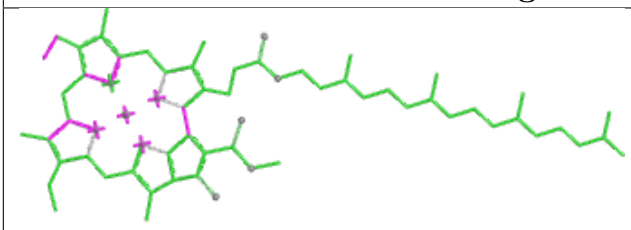


Torsions

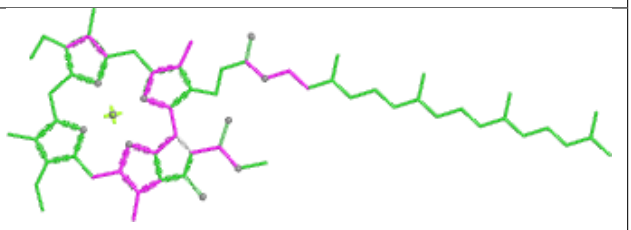


Rings

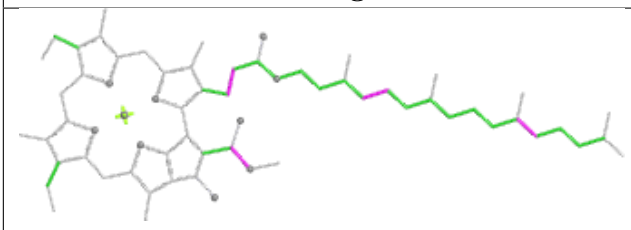
Ligand CLA b 1238



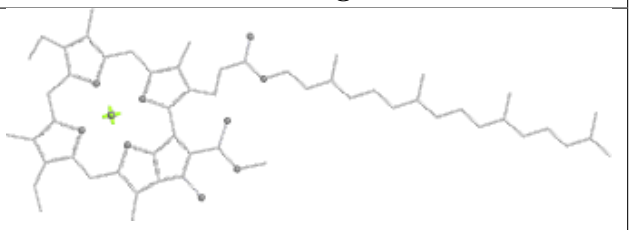
Bond lengths



Bond angles

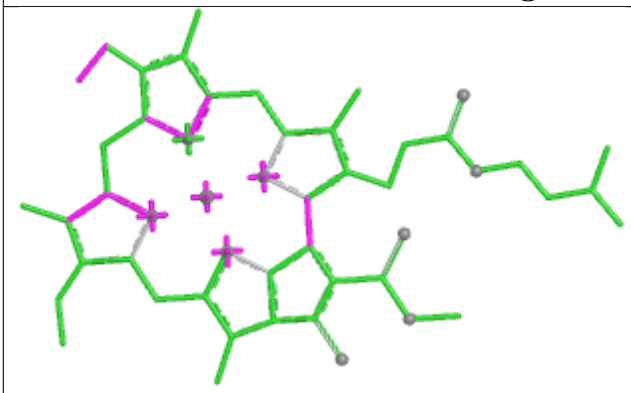


Torsions

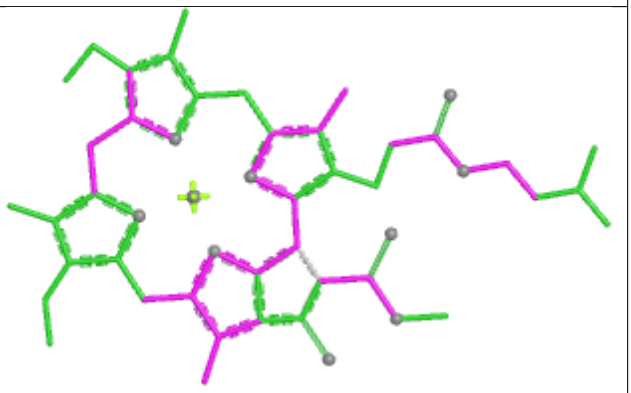


Rings

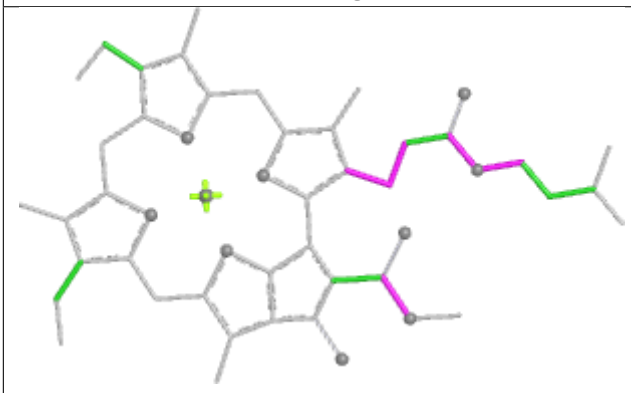
Ligand CLA 1 1110



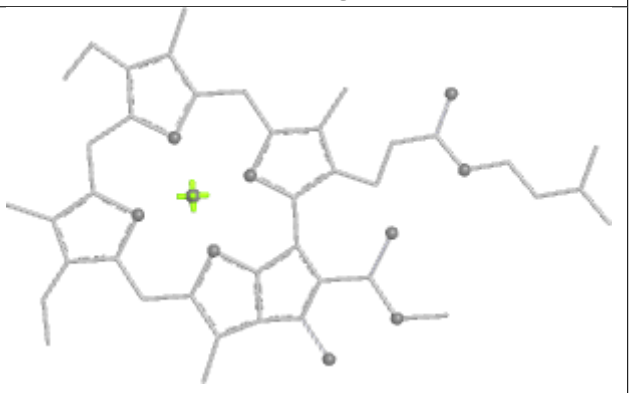
Bond lengths



Bond angles

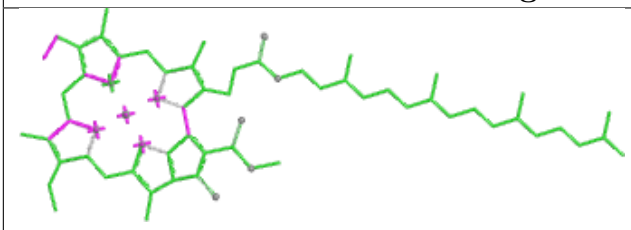


Torsions

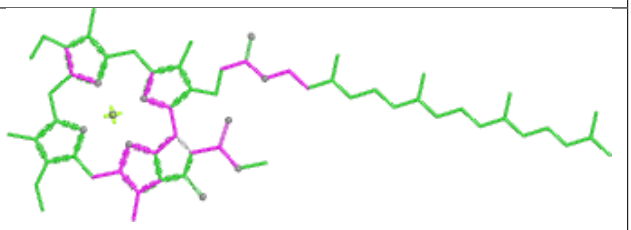


Rings

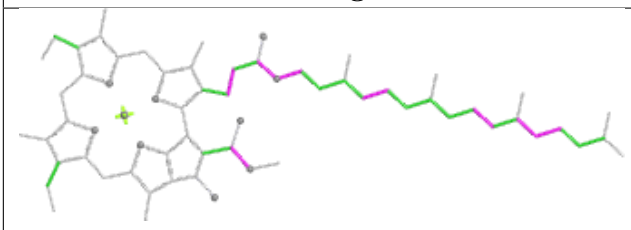
Ligand CLA a 1013



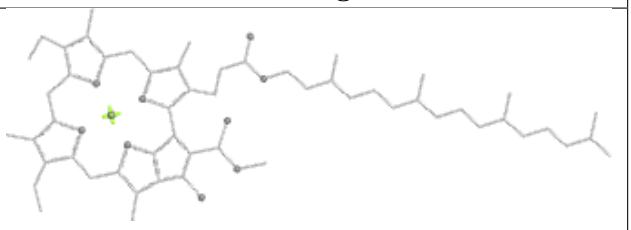
Bond lengths



Bond angles

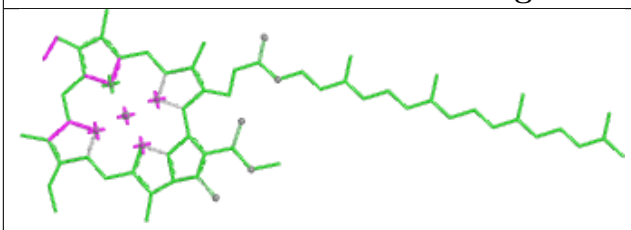


Torsions

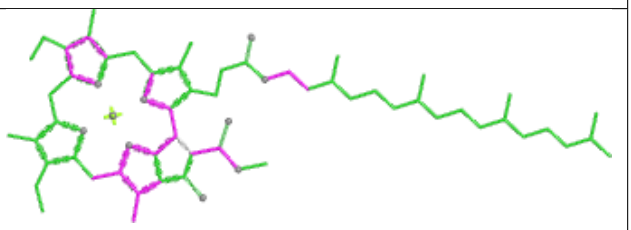


Rings

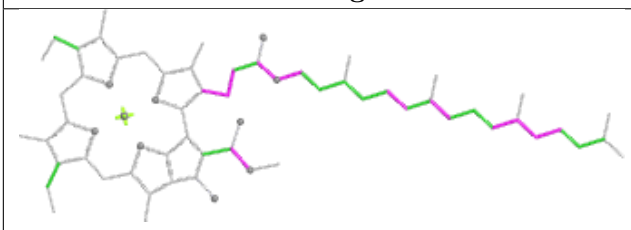
Ligand CLA A 1119



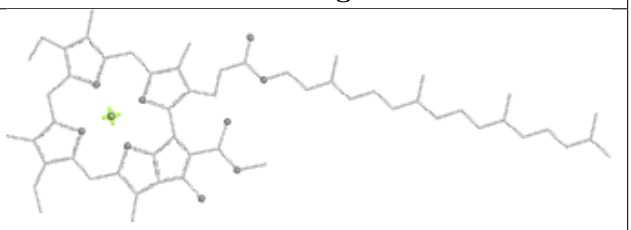
Bond lengths



Bond angles



Torsions

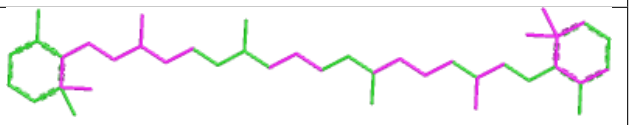


Rings

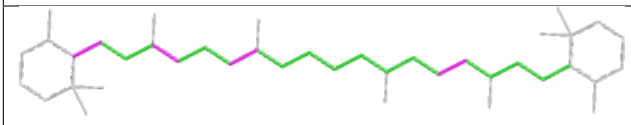
Ligand BCR a 4012



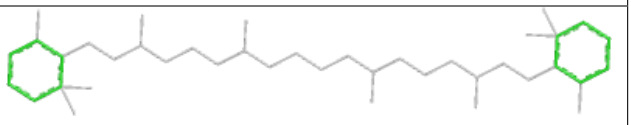
Bond lengths



Bond angles

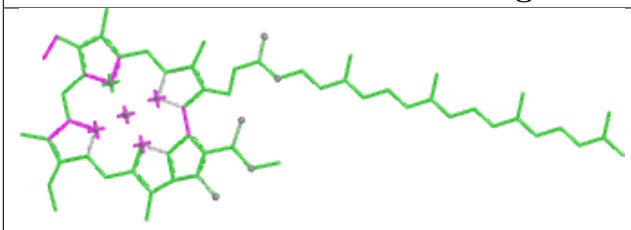


Torsions

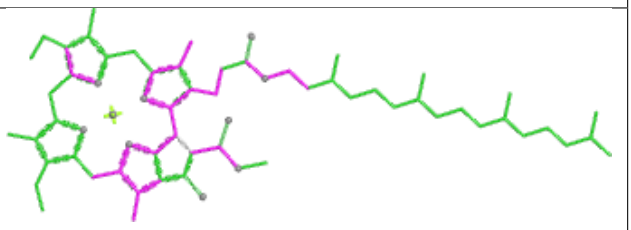


Rings

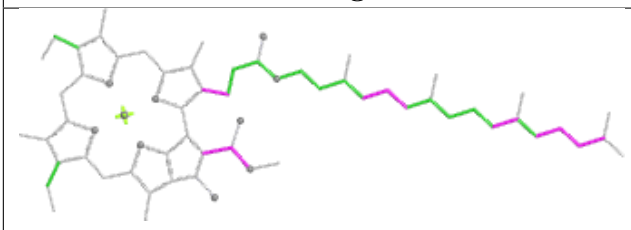
Ligand CLA B 1213



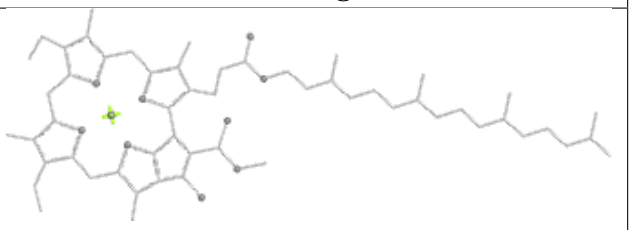
Bond lengths



Bond angles

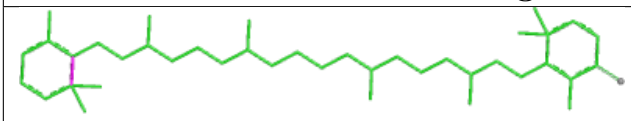


Torsions

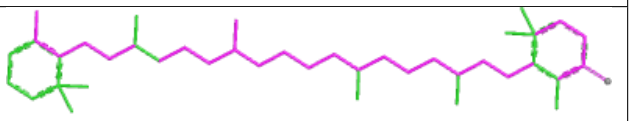


Rings

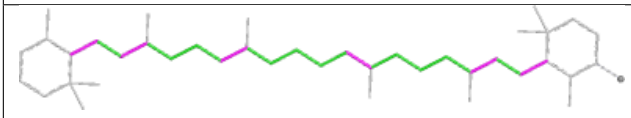
Ligand ECH b 4011



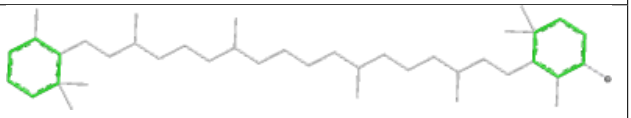
Bond lengths



Bond angles

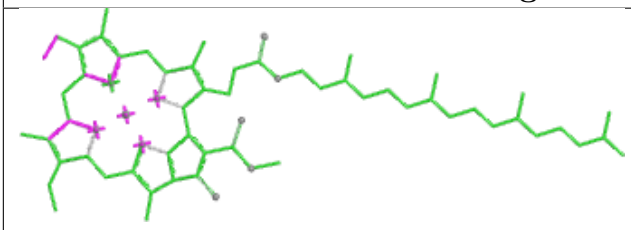


Torsions

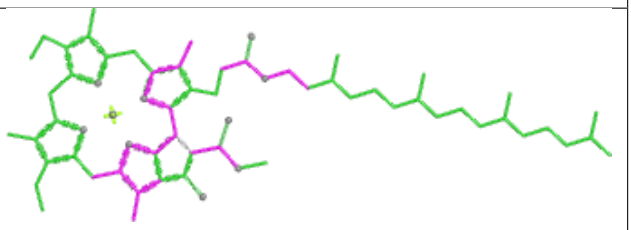


Rings

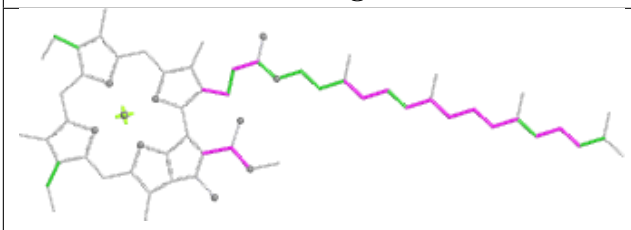
Ligand CLA a 1103



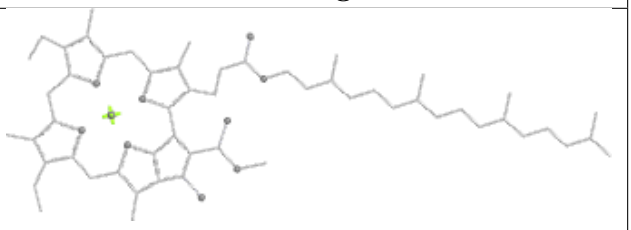
Bond lengths



Bond angles

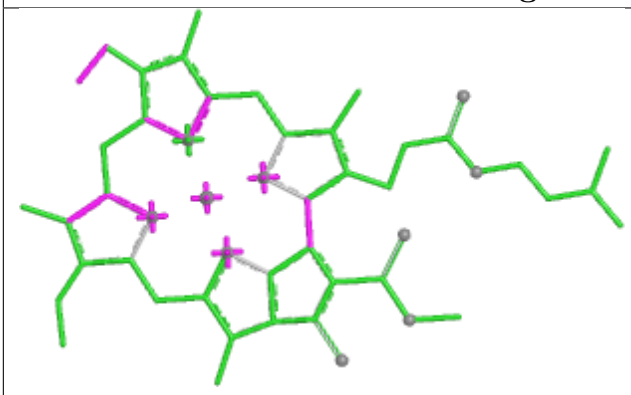


Torsions

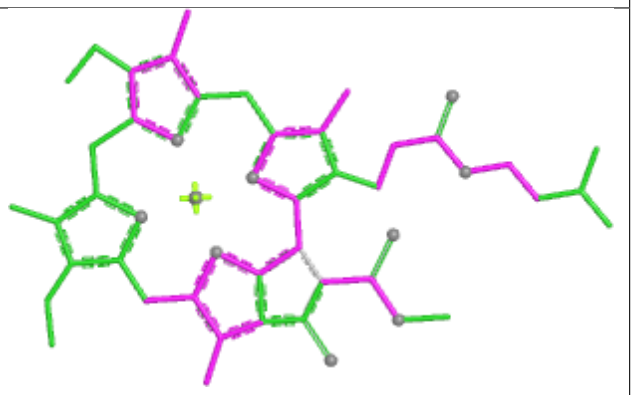


Rings

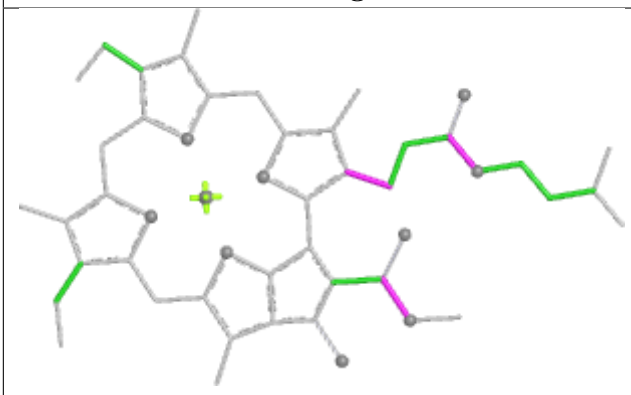
Ligand CLA 2 1222



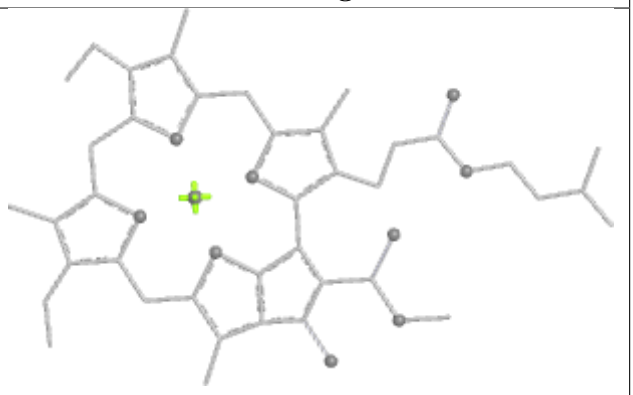
Bond lengths



Bond angles

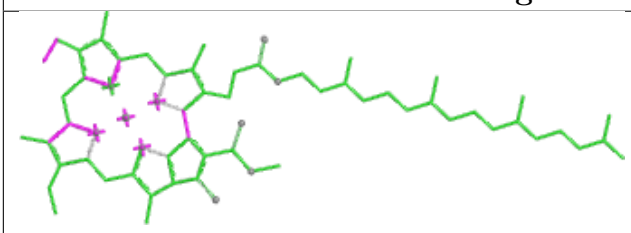


Torsions

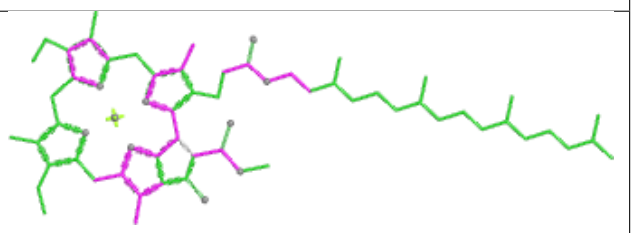


Rings

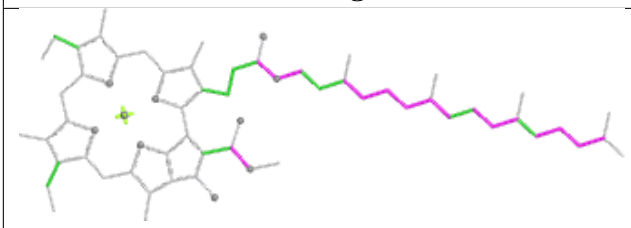
Ligand CLA B 1231



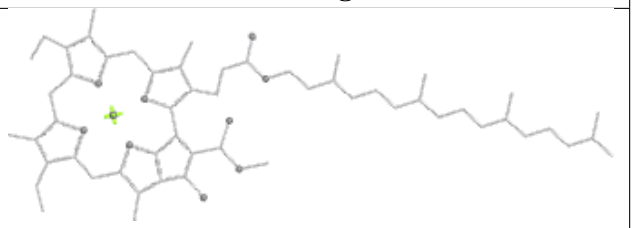
Bond lengths



Bond angles

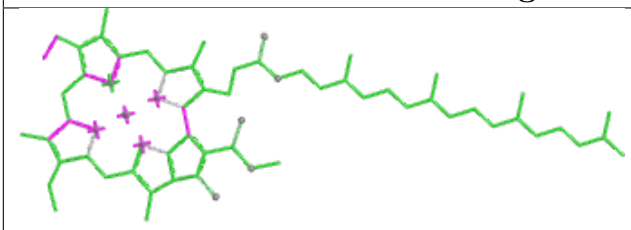


Torsions

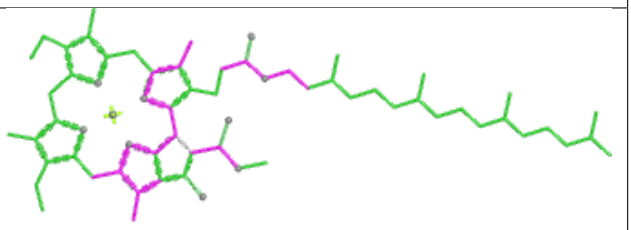


Rings

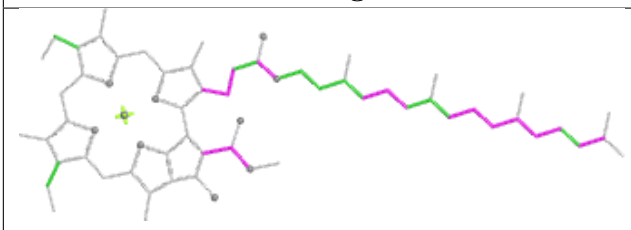
Ligand CLA b 1240



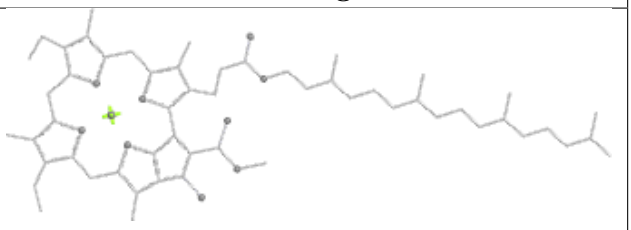
Bond lengths



Bond angles

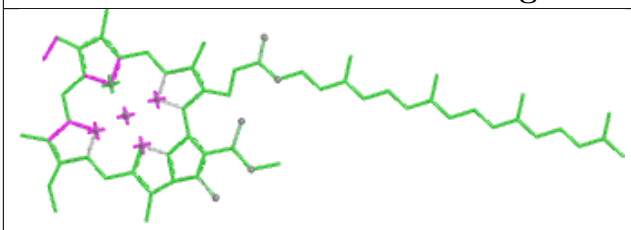


Torsions

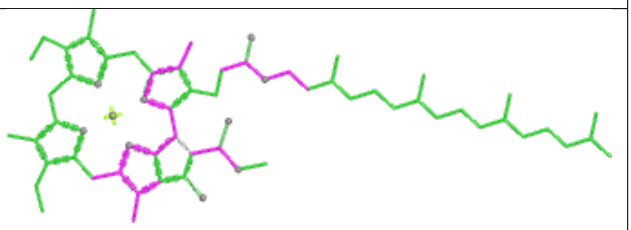


Rings

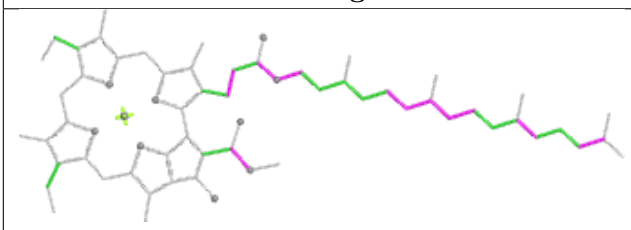
Ligand CLA a 1119



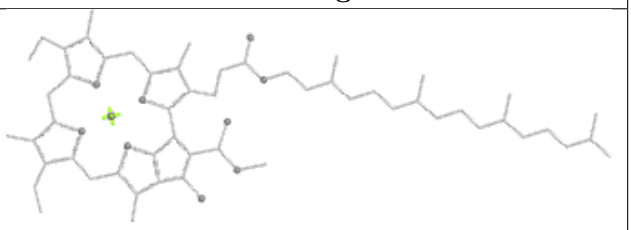
Bond lengths



Bond angles

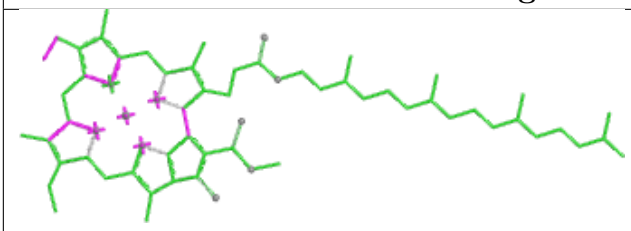


Torsions

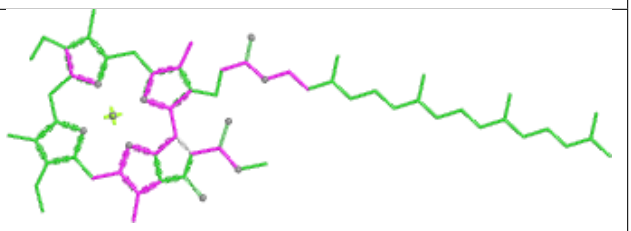


Rings

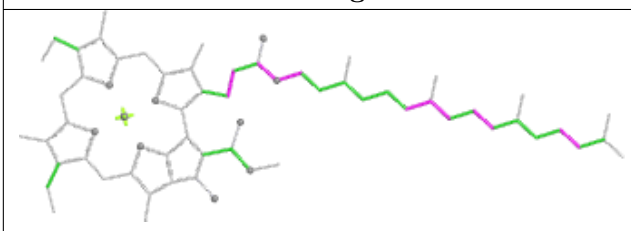
Ligand CLA b 1023



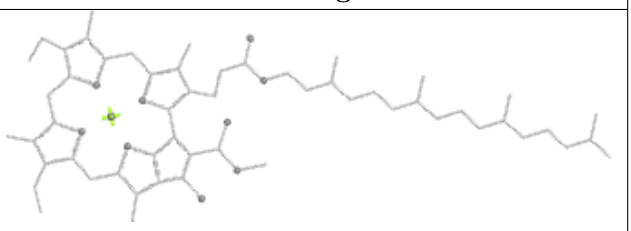
Bond lengths



Bond angles

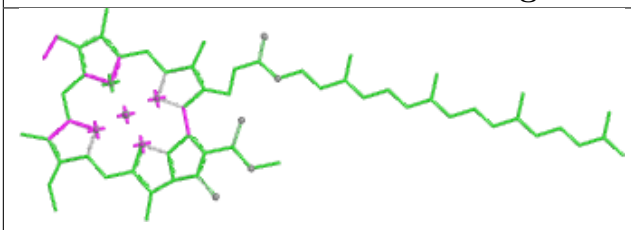


Torsions

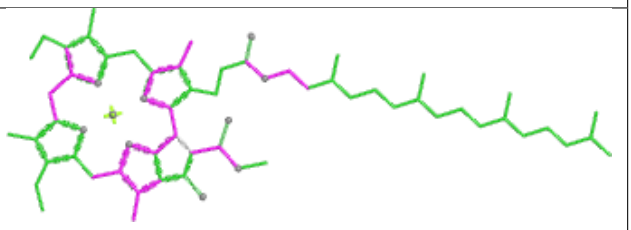


Rings

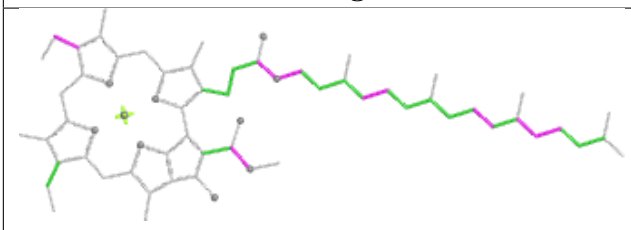
Ligand CLA a 1139



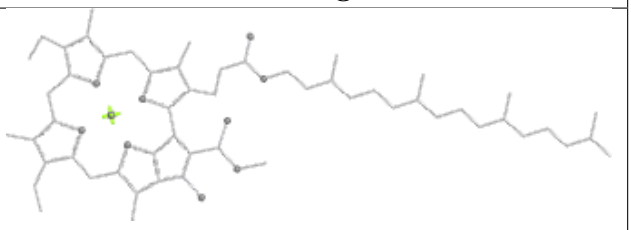
Bond lengths



Bond angles

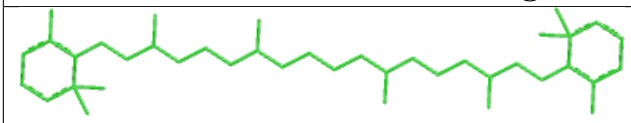


Torsions

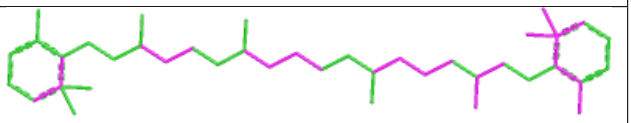


Rings

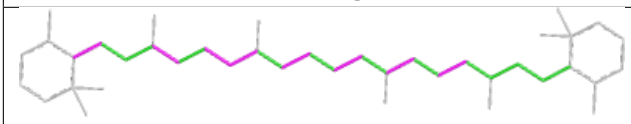
Ligand BCR i 4018



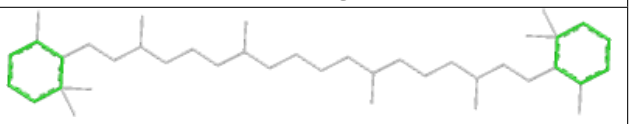
Bond lengths



Bond angles

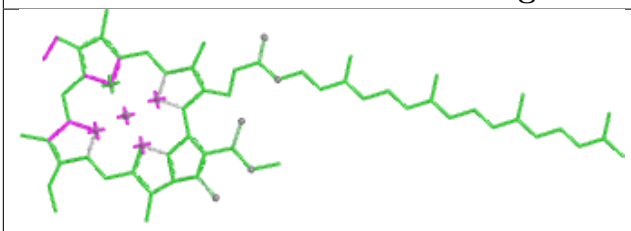


Torsions

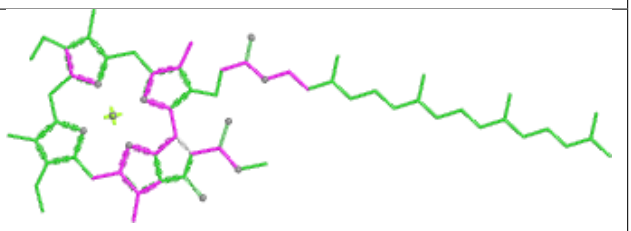


Rings

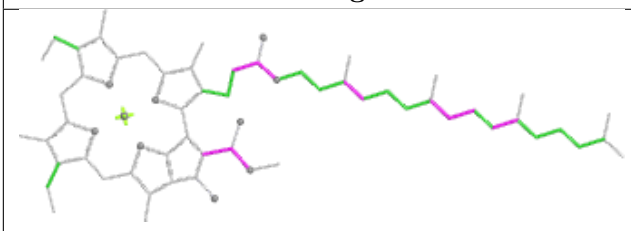
Ligand CLA b 1226



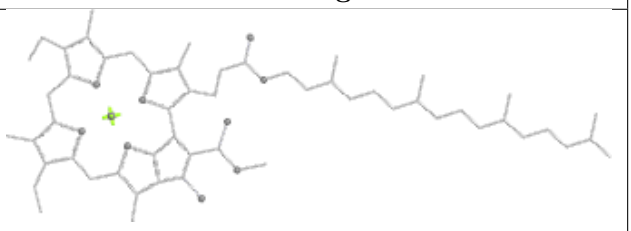
Bond lengths



Bond angles

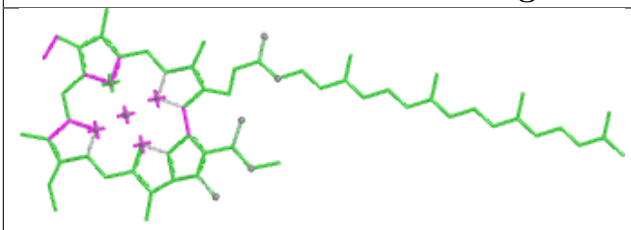


Torsions

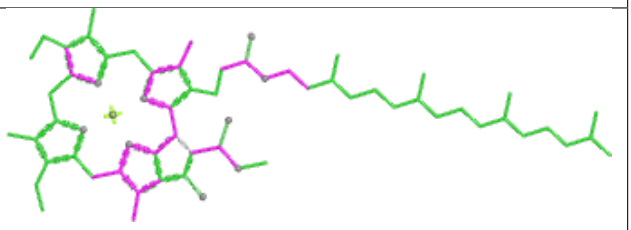


Rings

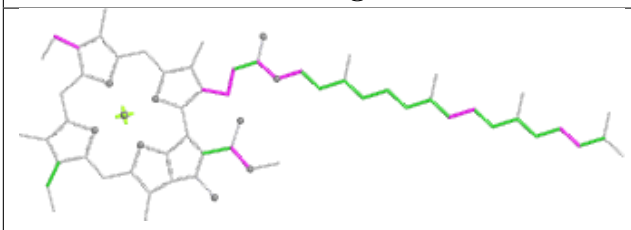
Ligand CLA b 1239



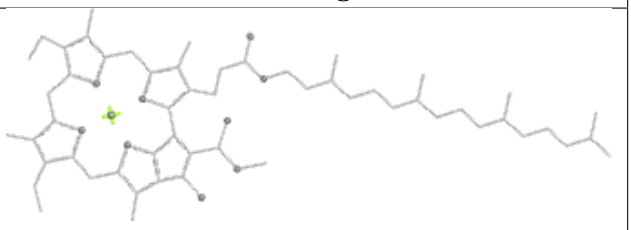
Bond lengths



Bond angles

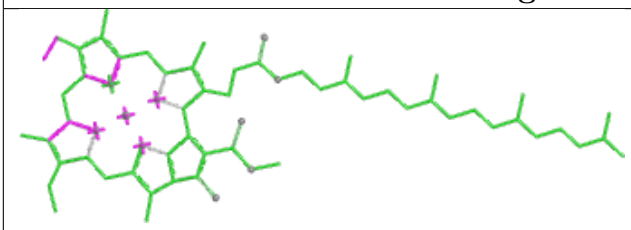


Torsions

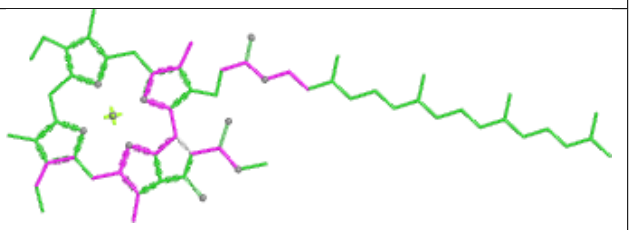


Rings

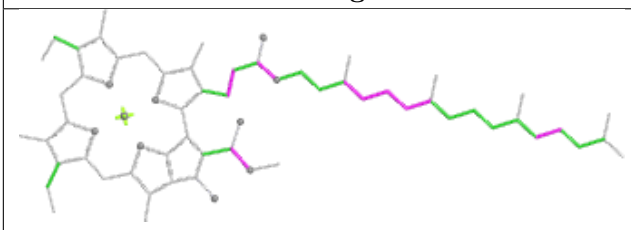
Ligand CLA b 1237



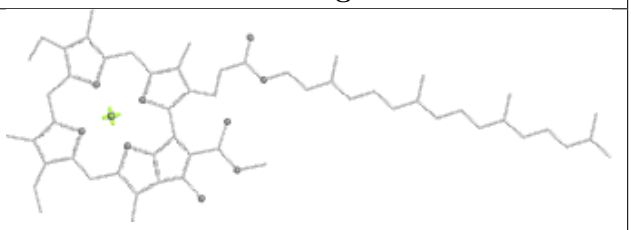
Bond lengths



Bond angles

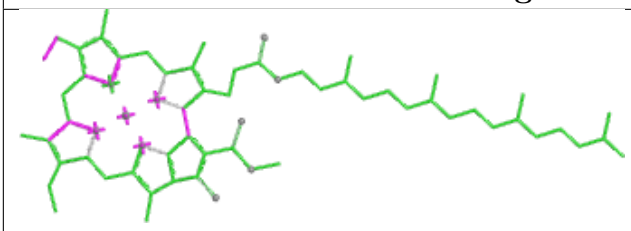


Torsions

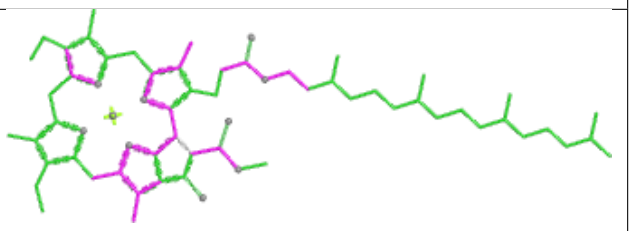


Rings

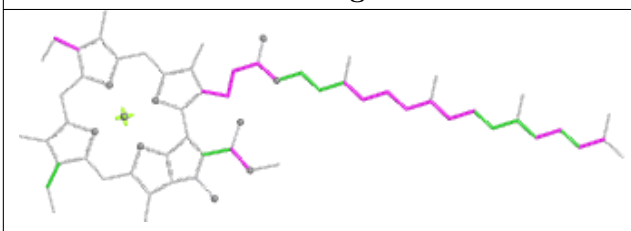
Ligand CLA A 1116



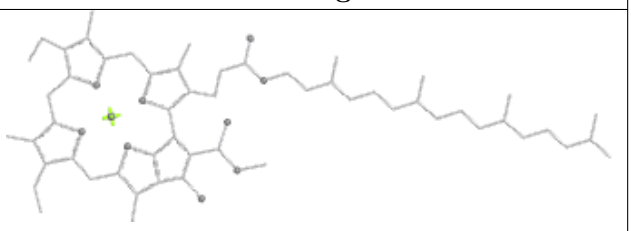
Bond lengths



Bond angles

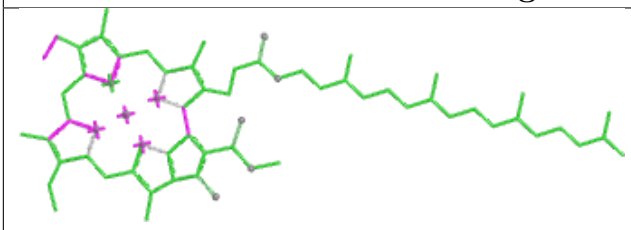


Torsions

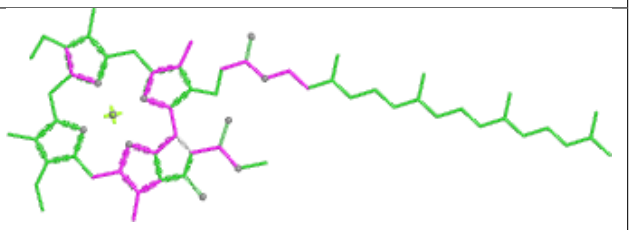


Rings

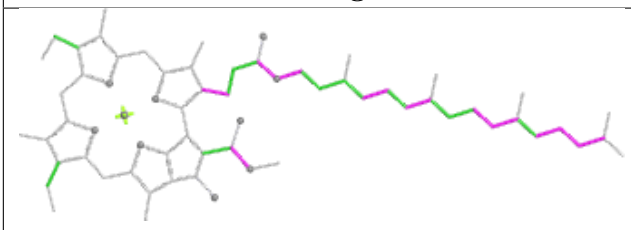
Ligand CLA b 1232



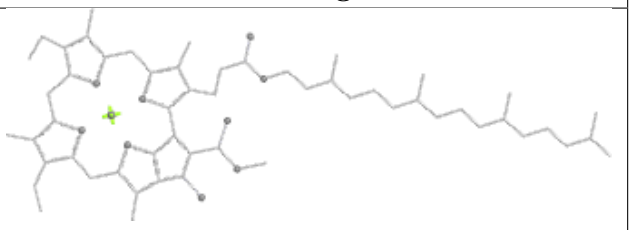
Bond lengths



Bond angles

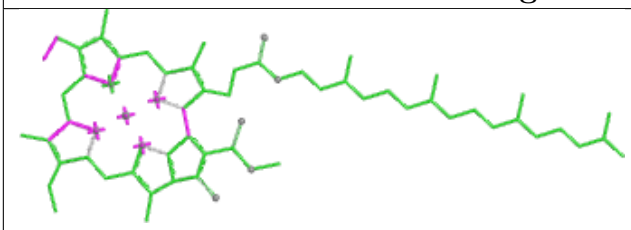


Torsions

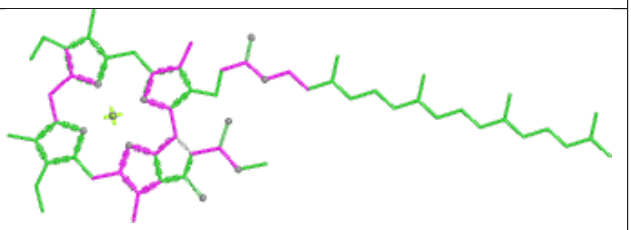


Rings

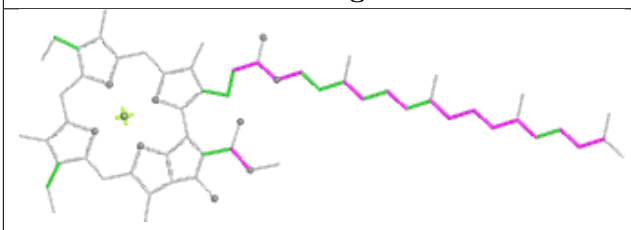
Ligand CLA a 1118



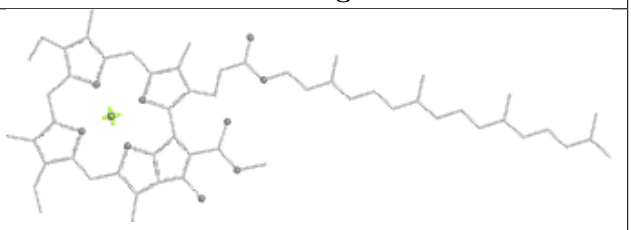
Bond lengths



Bond angles

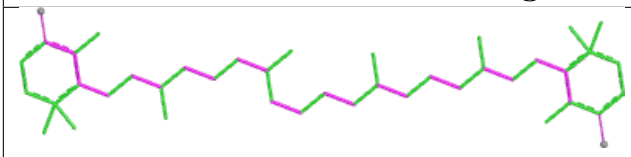


Torsions

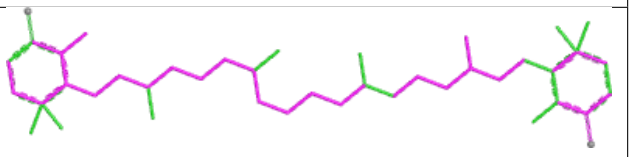


Rings

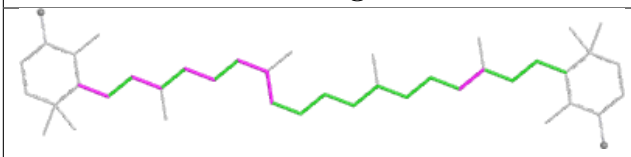
Ligand 45D B 4011



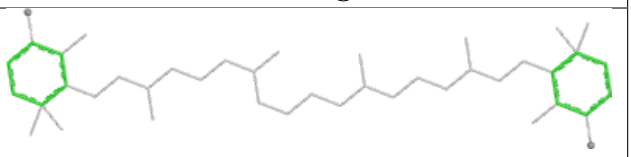
Bond lengths



Bond angles

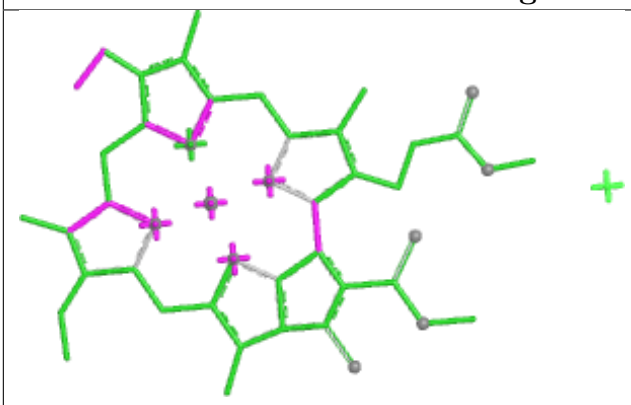


Torsions

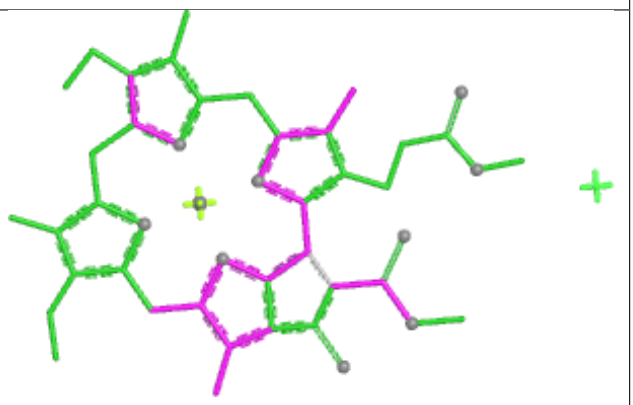


Rings

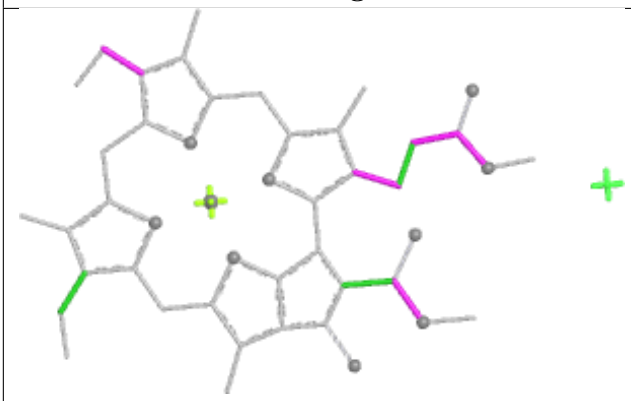
Ligand CLA 1 1108



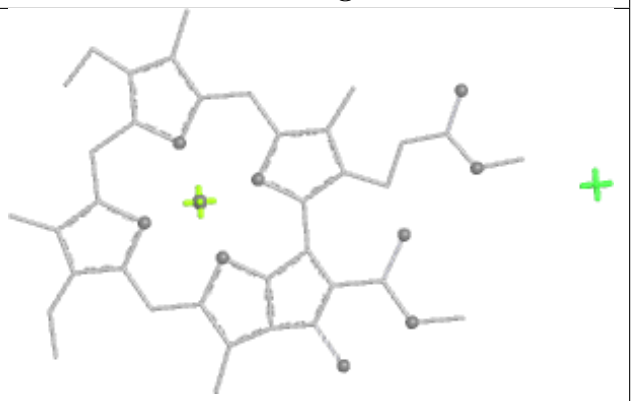
Bond lengths



Bond angles

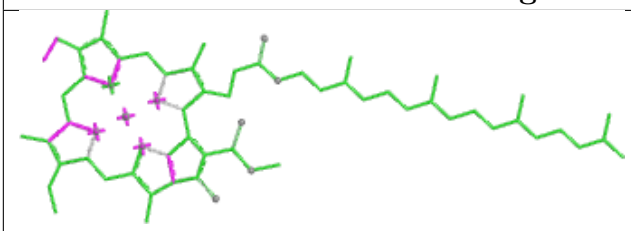


Torsions

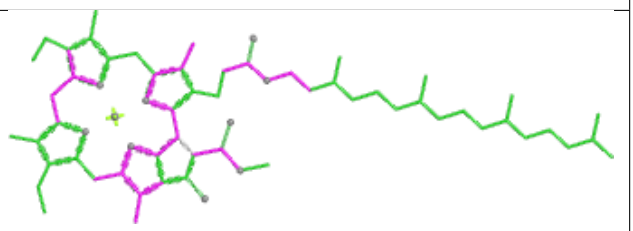


Rings

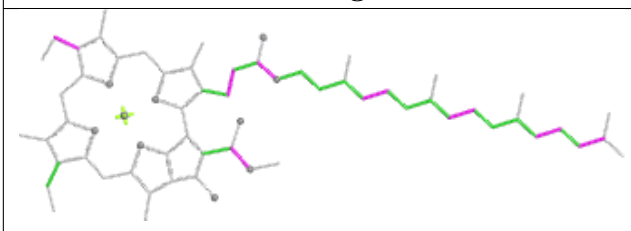
Ligand CLA 2 1238



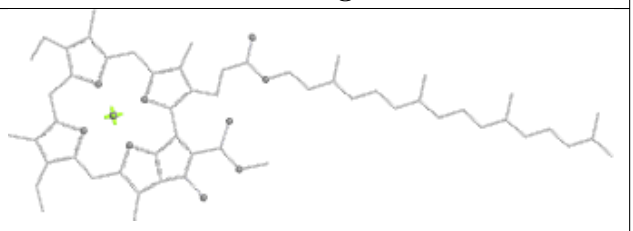
Bond lengths



Bond angles

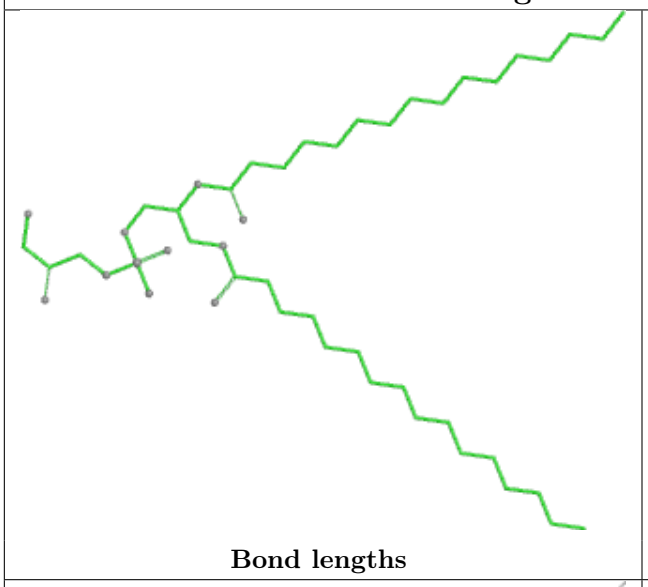


Torsions

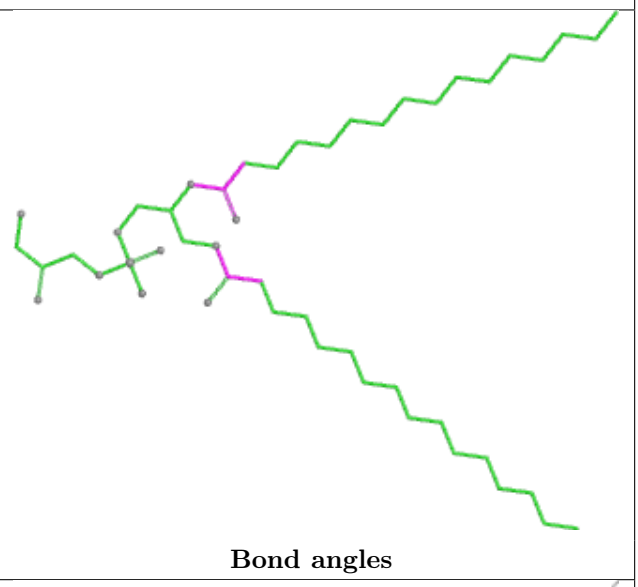


Rings

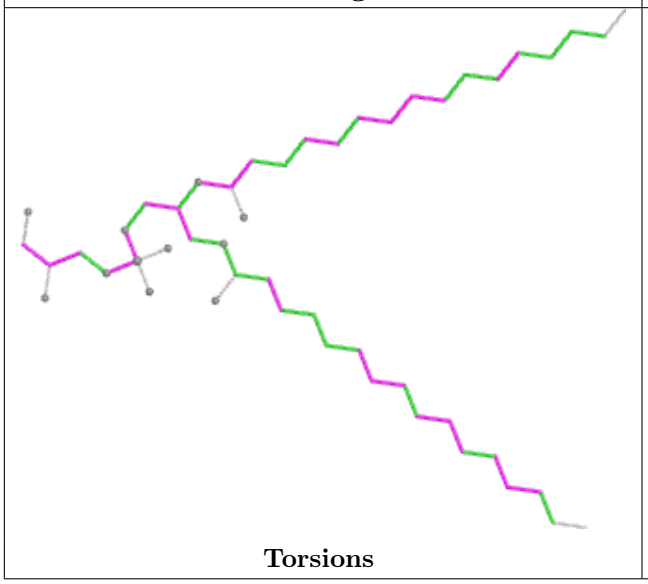
Ligand LHG A 5007



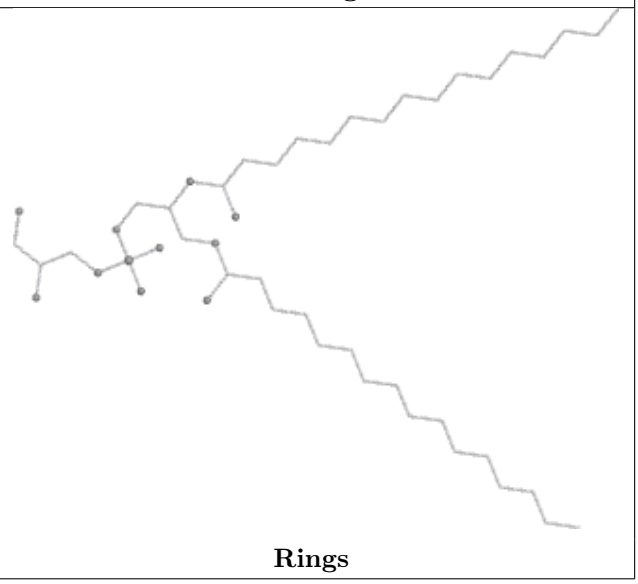
Bond lengths



Bond angles

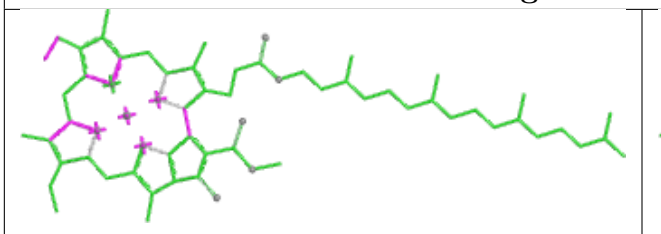


Torsions

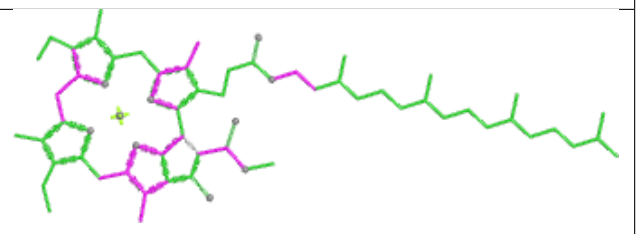


Rings

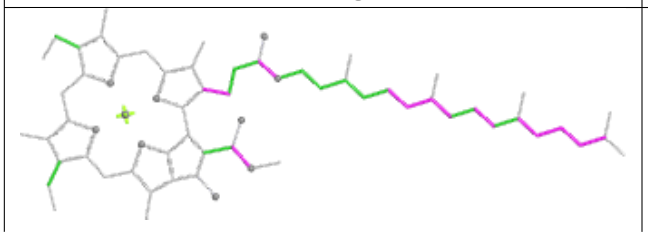
Ligand CLA a 1117



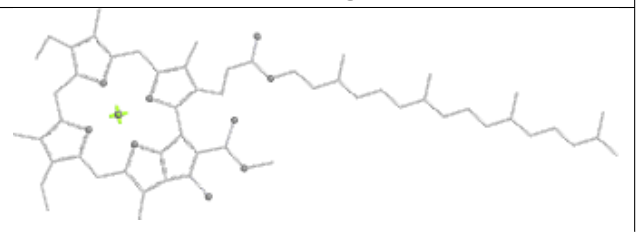
Bond lengths



Bond angles

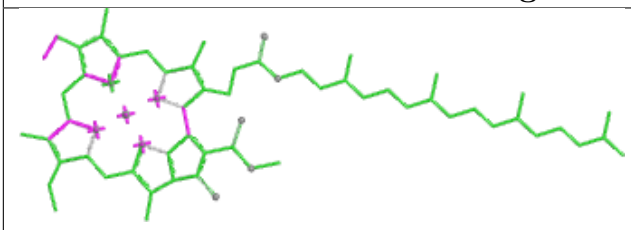


Torsions

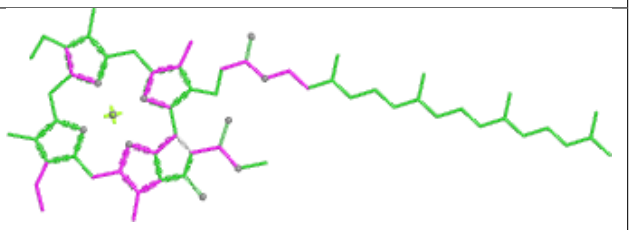


Rings

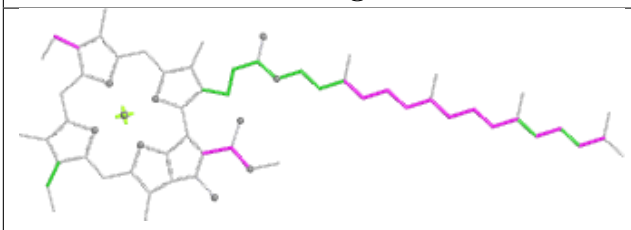
Ligand CLA 2 1205



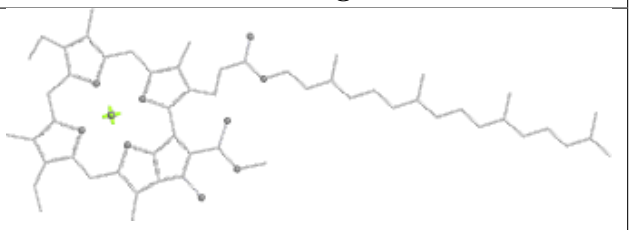
Bond lengths



Bond angles

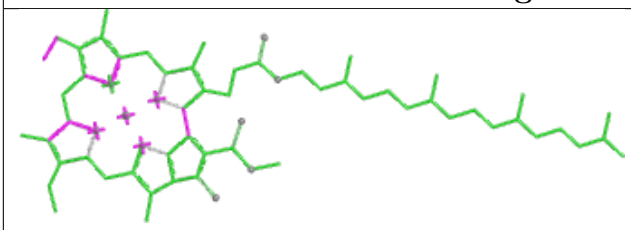


Torsions

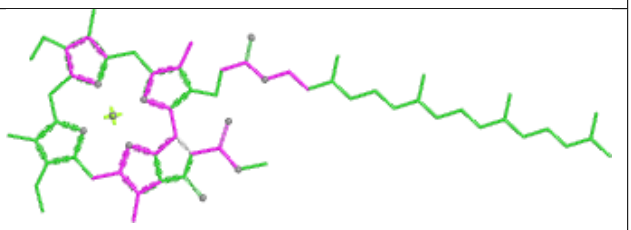


Rings

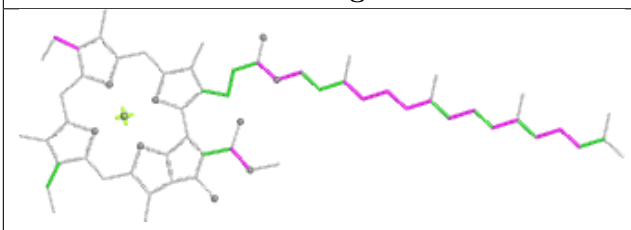
Ligand CLA A 1109



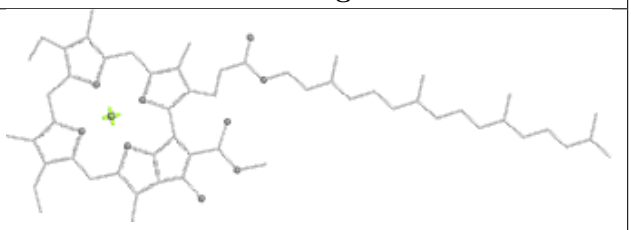
Bond lengths



Bond angles

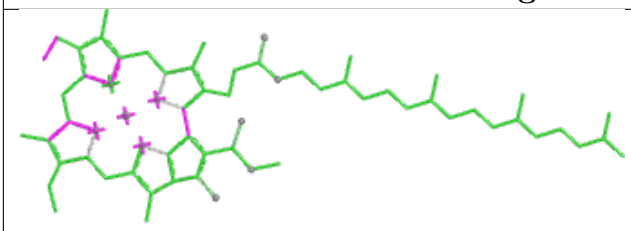


Torsions

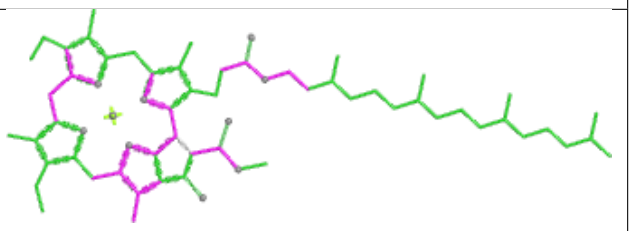


Rings

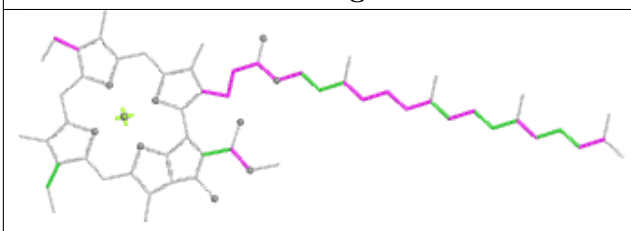
Ligand CLA b 1216



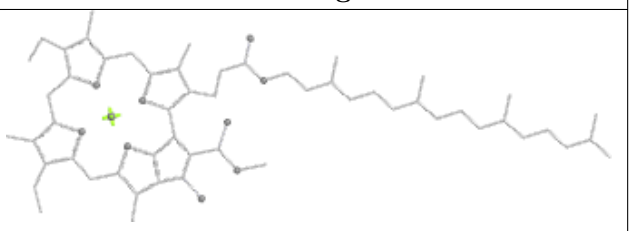
Bond lengths



Bond angles

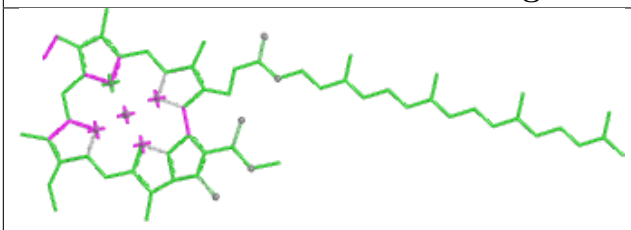


Torsions

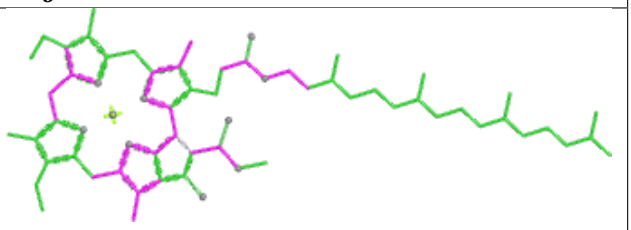


Rings

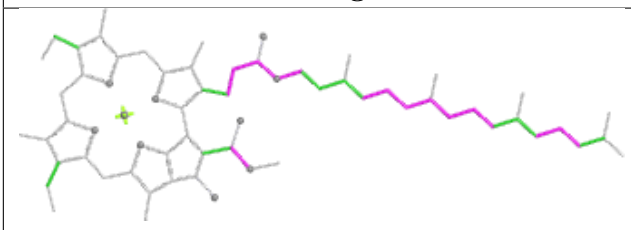
Ligand CLA j 1302



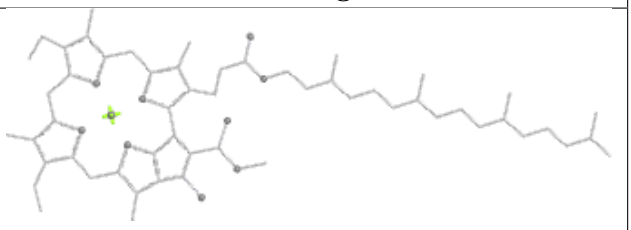
Bond lengths



Bond angles

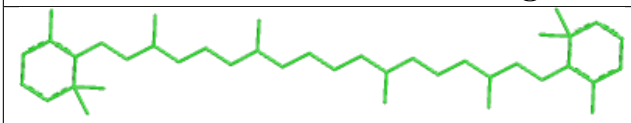


Torsions

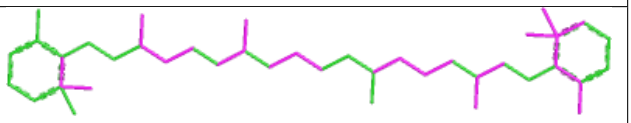


Rings

Ligand BCR l 4019



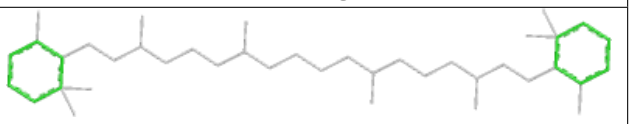
Bond lengths



Bond angles

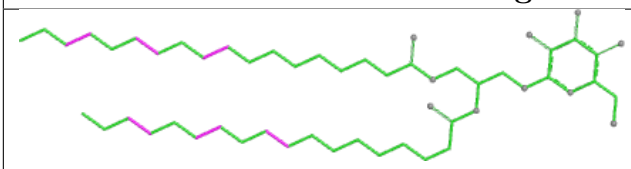


Torsions

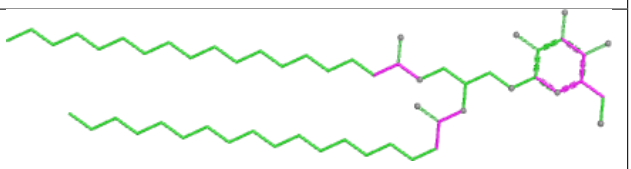


Rings

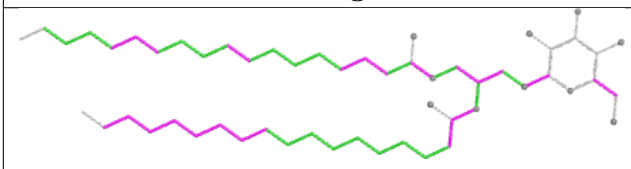
Ligand LMG 0 5001



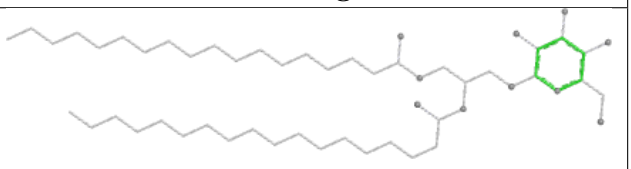
Bond lengths



Bond angles

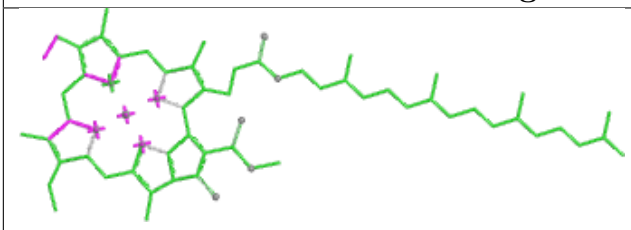


Torsions

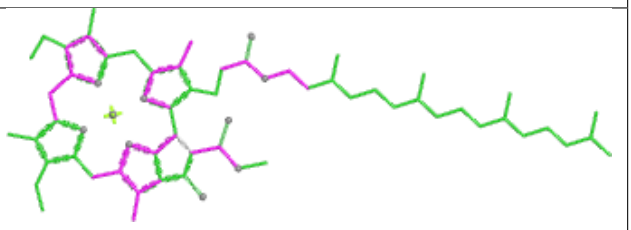


Rings

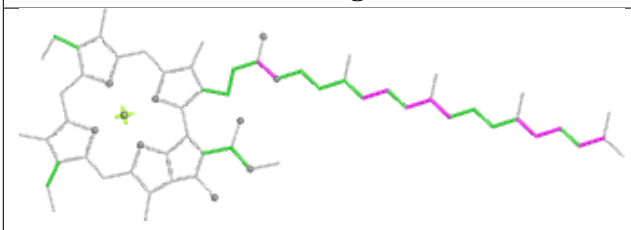
Ligand CLA 0 1502



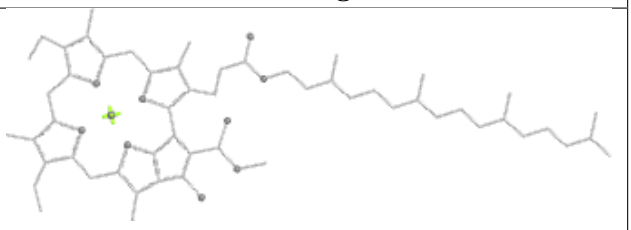
Bond lengths



Bond angles

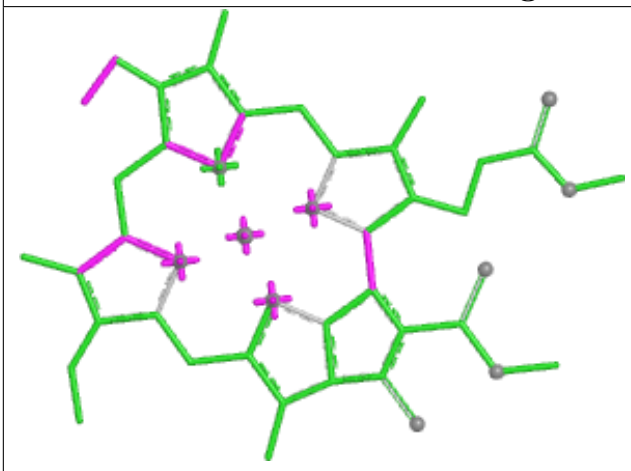


Torsions

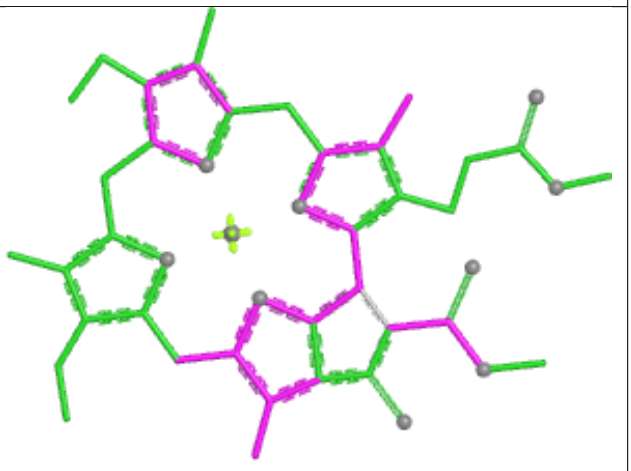


Rings

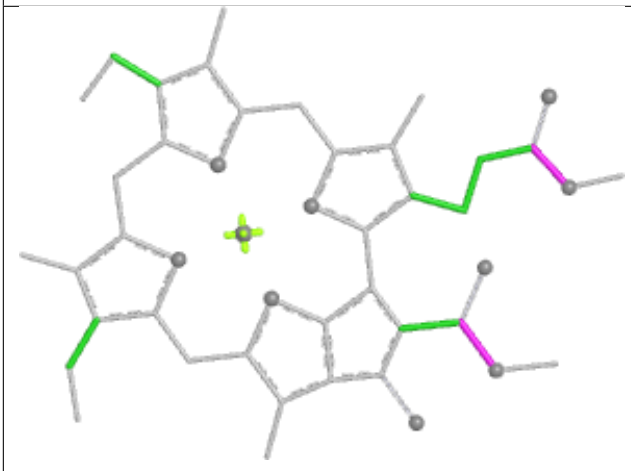
Ligand CLA 2 1231



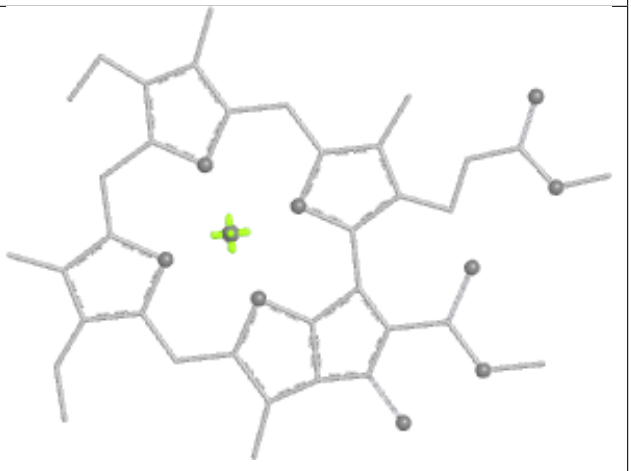
Bond lengths



Bond angles

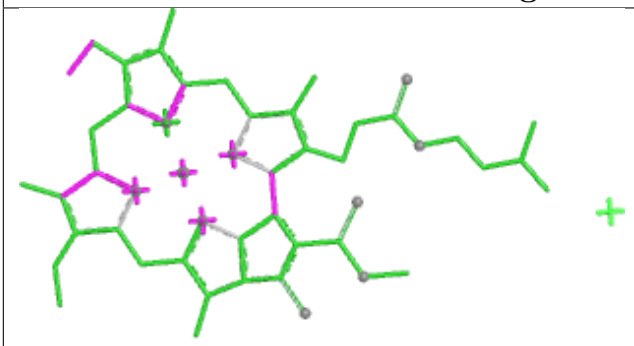


Torsions

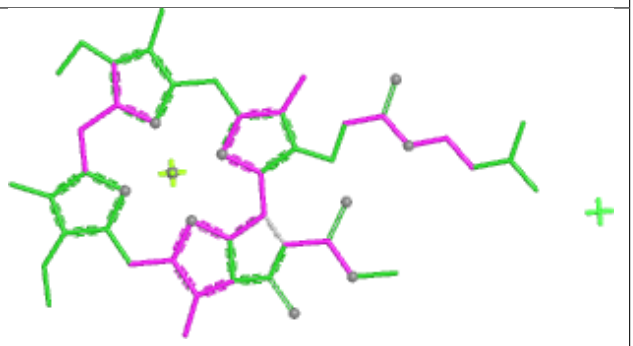


Rings

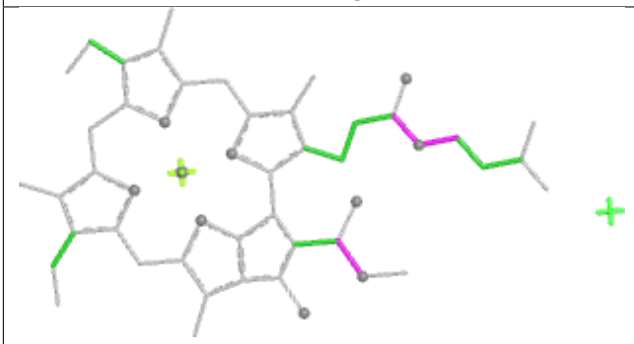
Ligand CLA a 1137



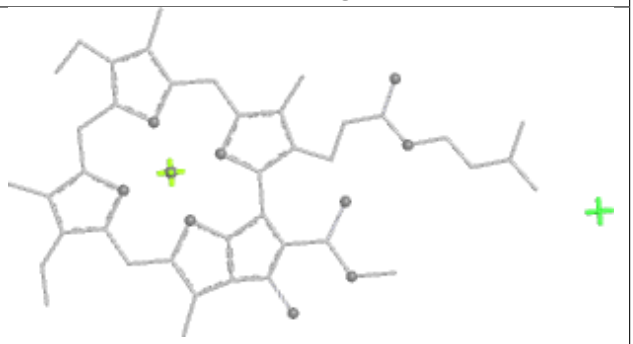
Bond lengths



Bond angles

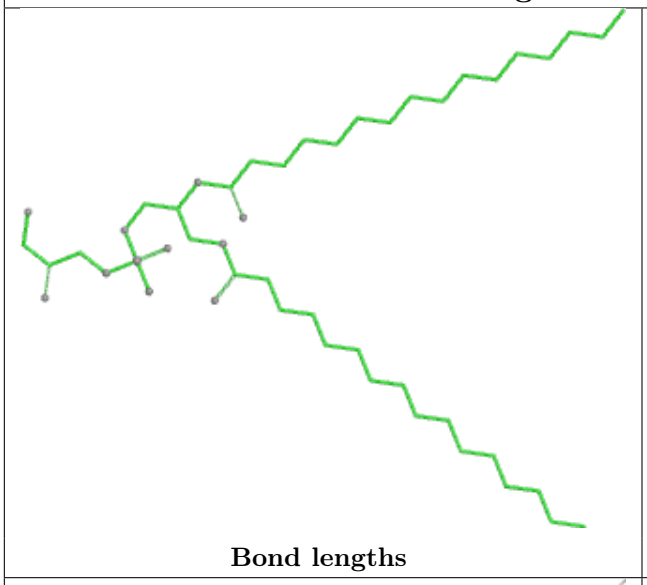


Torsions

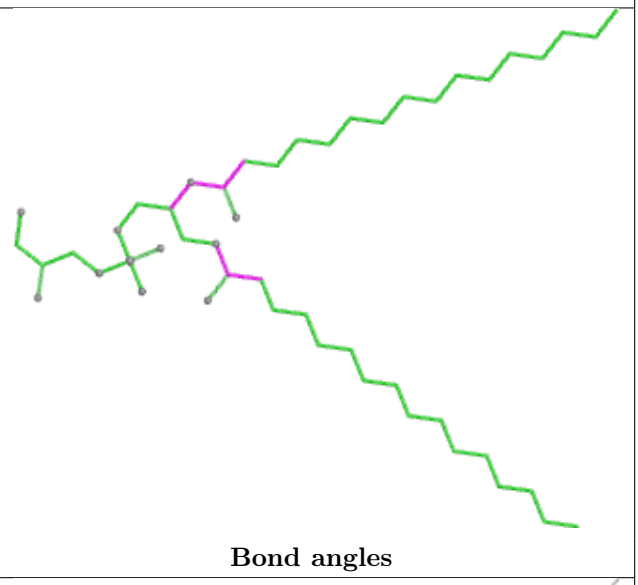


Rings

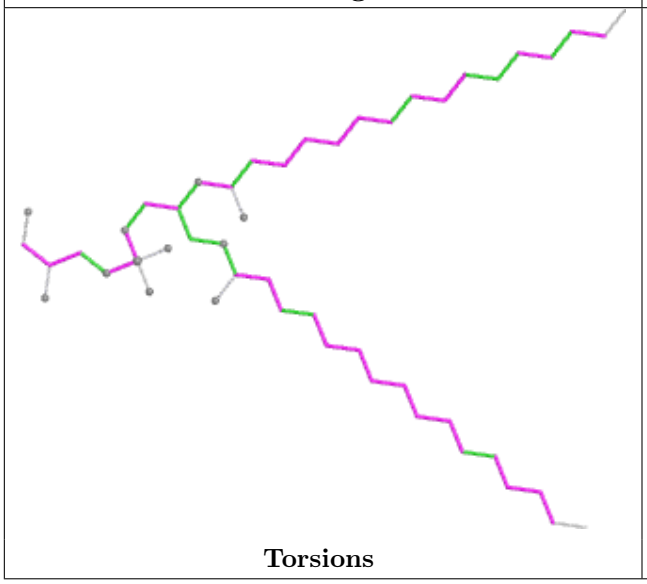
Ligand LHG B 5006



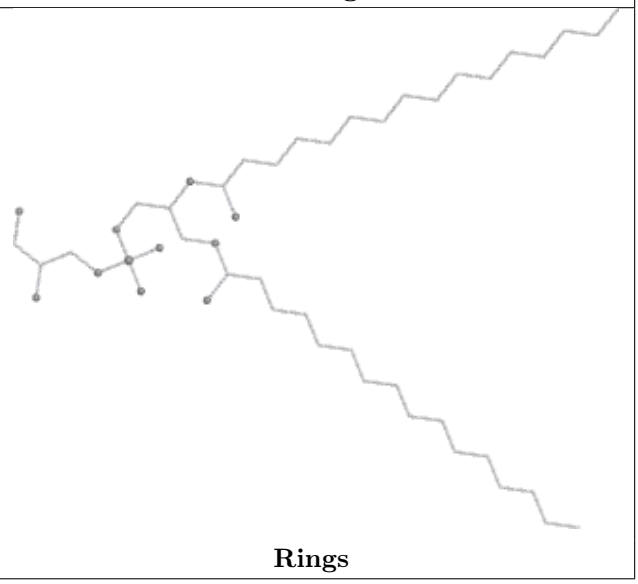
Bond lengths



Bond angles

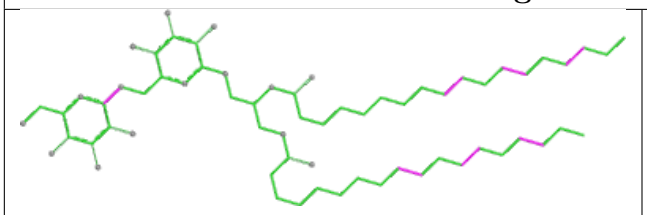


Torsions

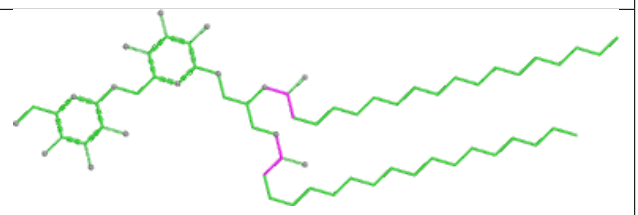


Rings

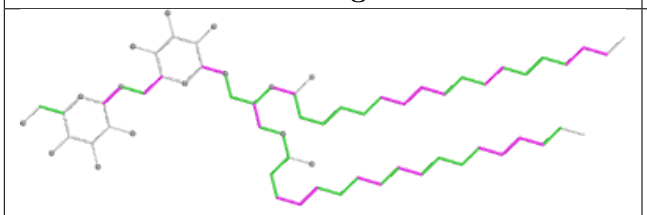
Ligand DGD L 5004



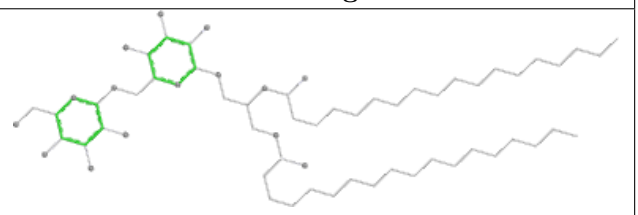
Bond lengths



Bond angles

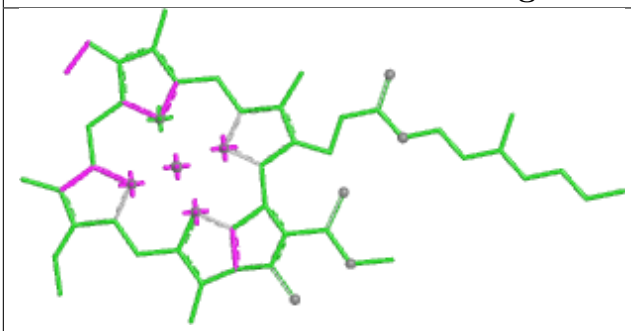


Torsions

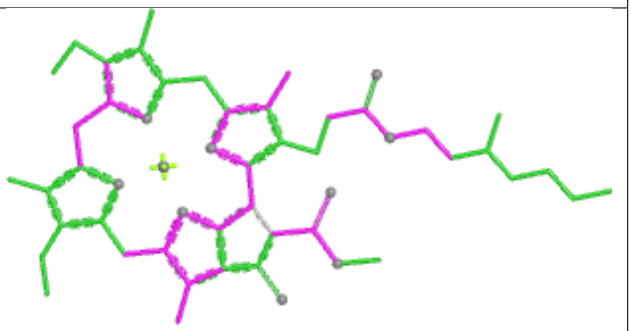


Rings

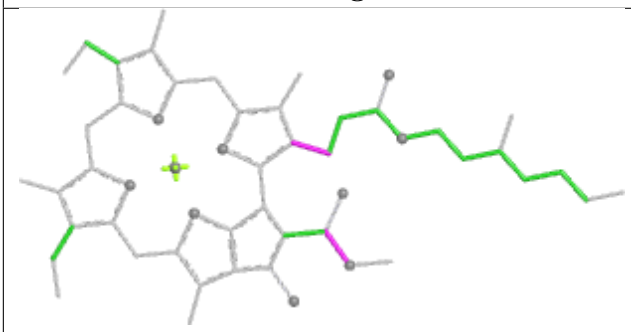
Ligand CLA b 1234



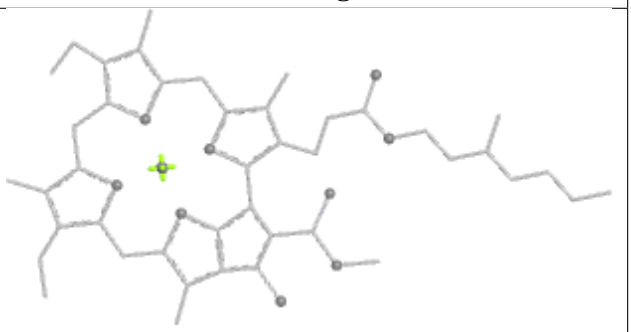
Bond lengths



Bond angles

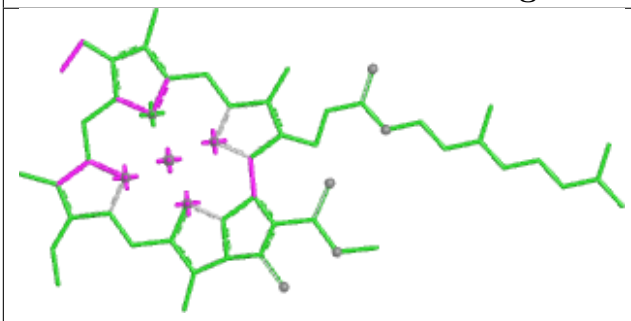


Torsions

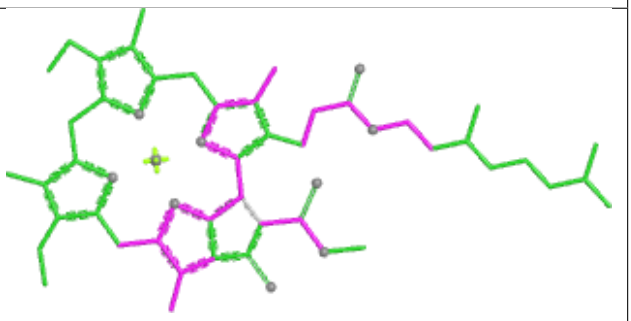


Rings

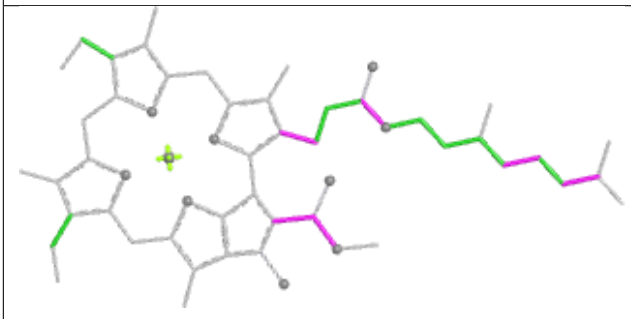
Ligand CLA 1 1102



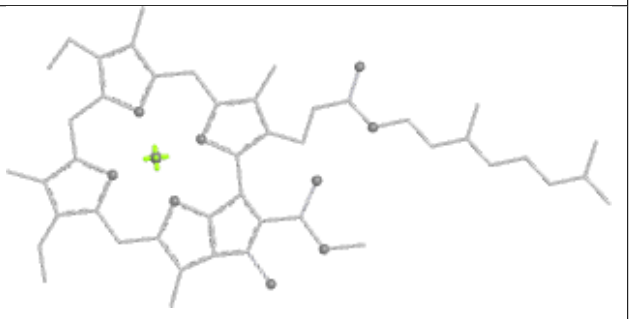
Bond lengths



Bond angles

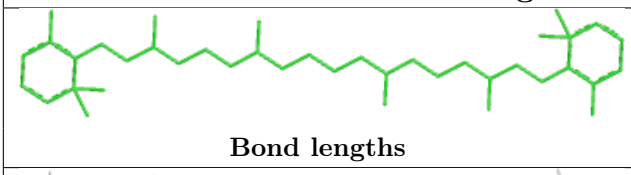


Torsions

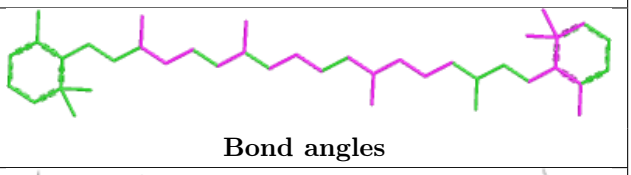


Rings

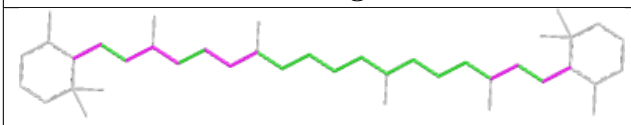
Ligand BCR b 4004



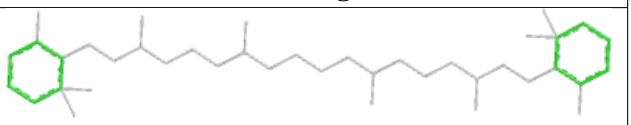
Bond lengths



Bond angles



Torsions

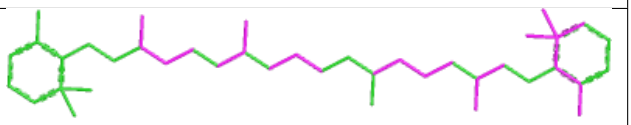


Rings

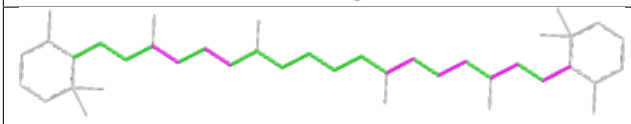
Ligand BCR B 4010



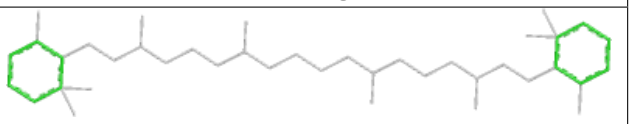
Bond lengths



Bond angles

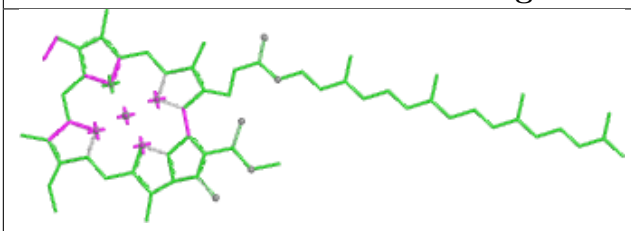


Torsions

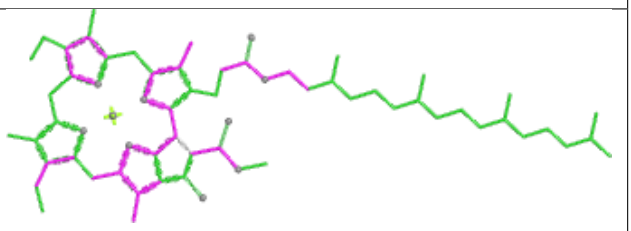


Rings

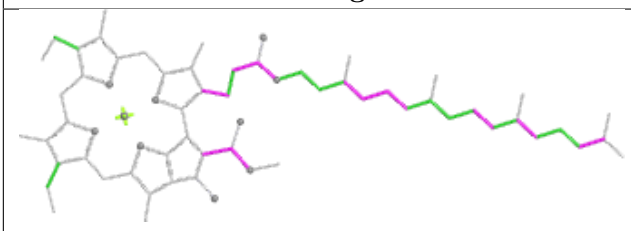
Ligand CLA B 1210



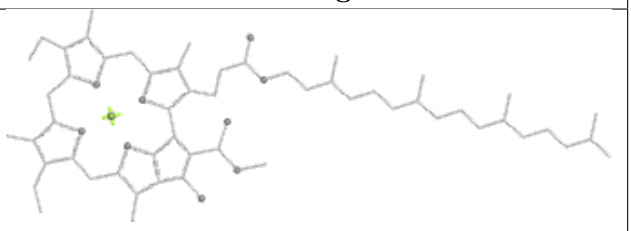
Bond lengths



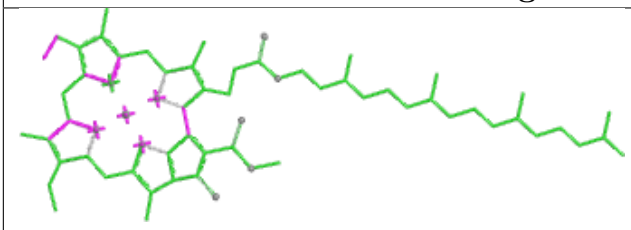
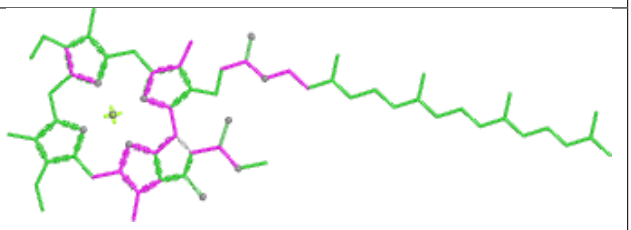
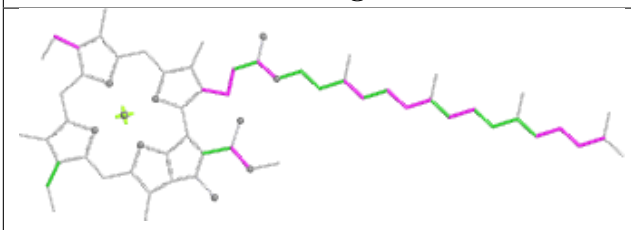
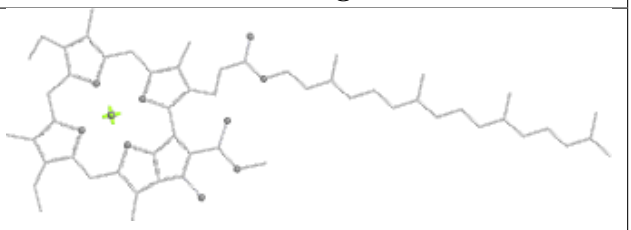
Bond angles

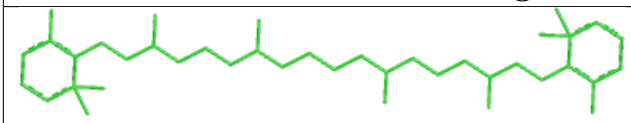
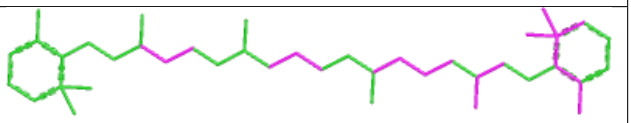
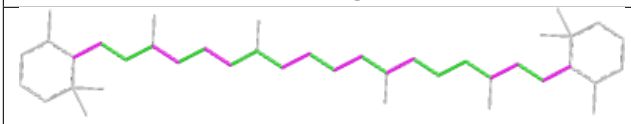
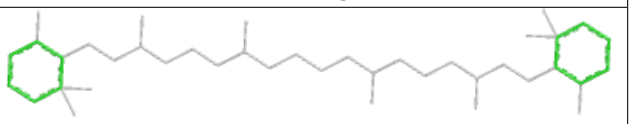


Torsions

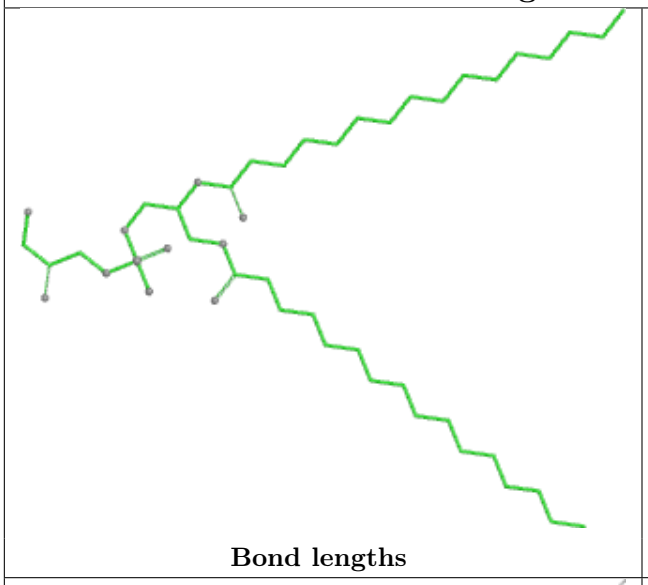


Rings

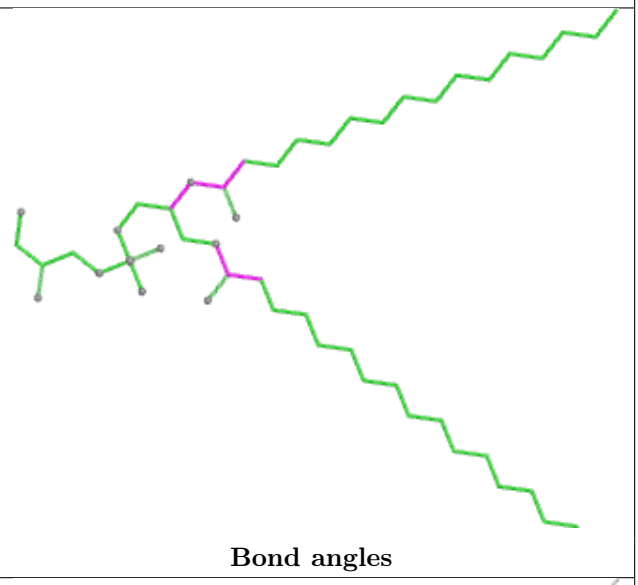
Ligand CLA b 1214	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 4005	
 Bond lengths	 Bond angles
 Torsions	 Rings

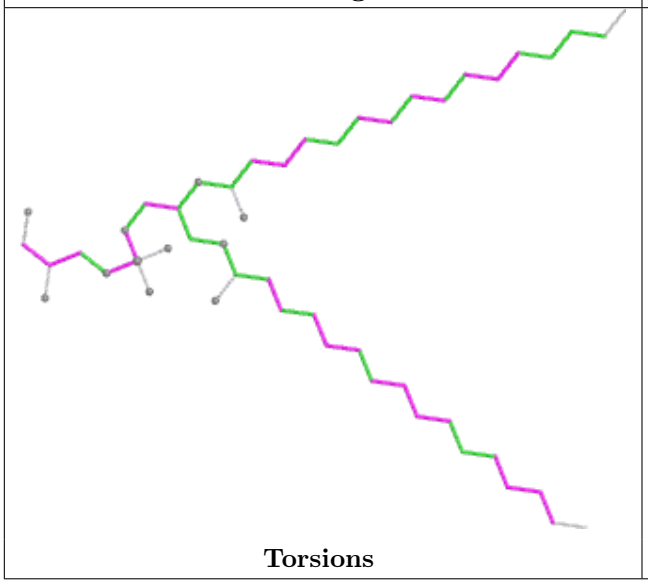
Ligand LHG 2 5004



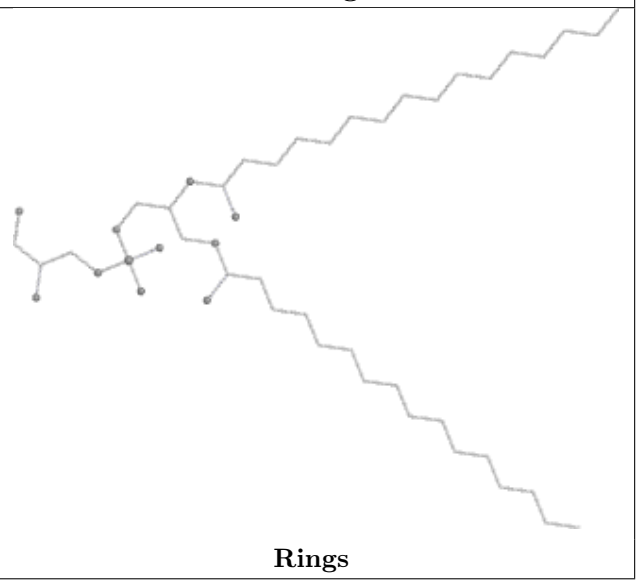
Bond lengths



Bond angles

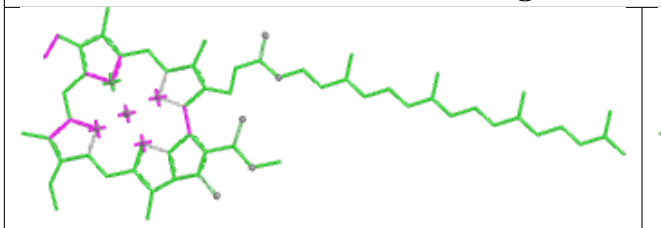


Torsions

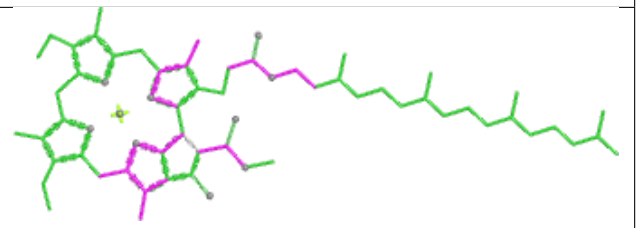


Rings

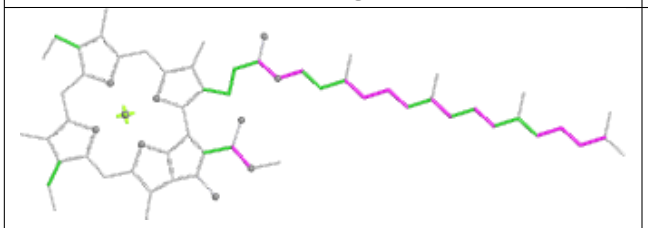
Ligand CLA B 1203



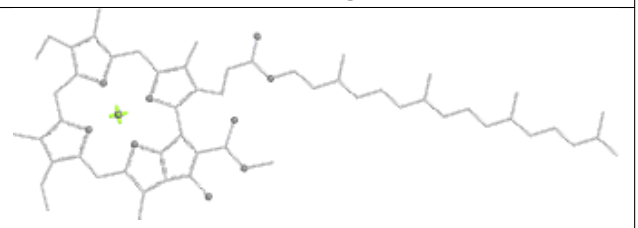
Bond lengths



Bond angles

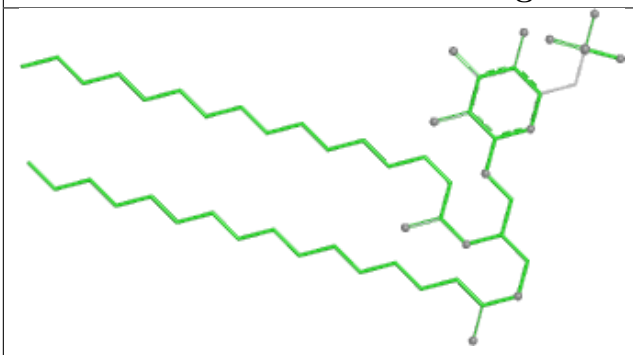


Torsions

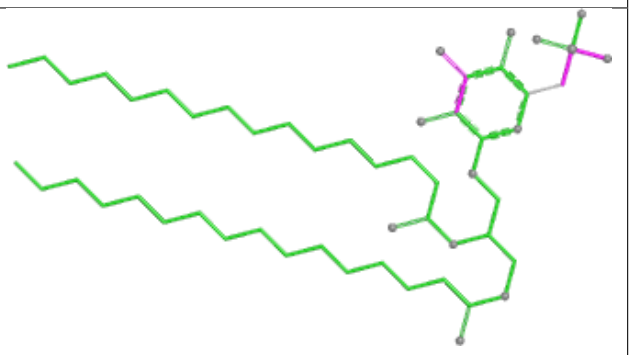


Rings

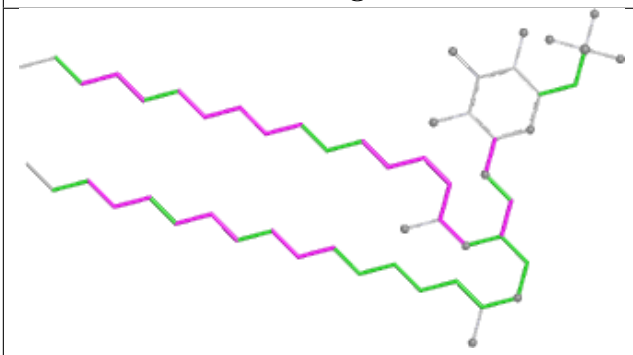
Ligand SQD B 5008



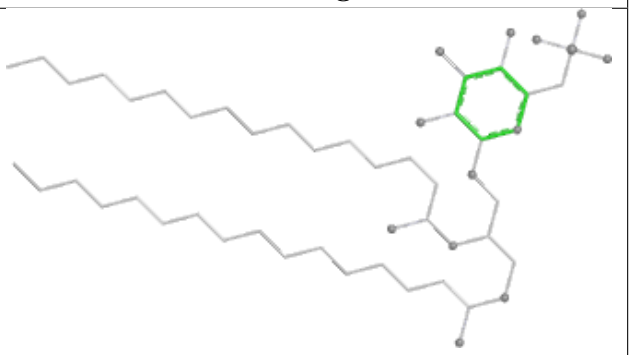
Bond lengths



Bond angles

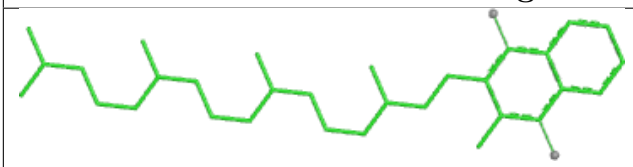


Torsions

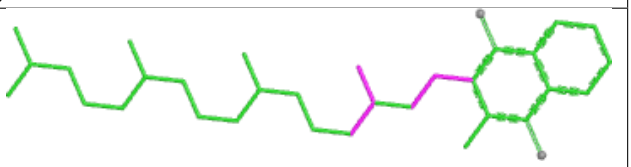


Rings

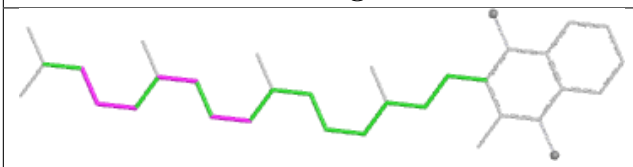
Ligand PQN a 2001



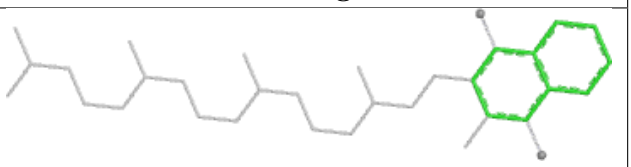
Bond lengths



Bond angles

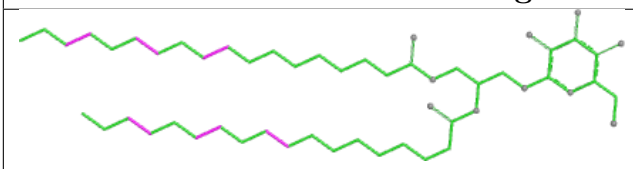


Torsions

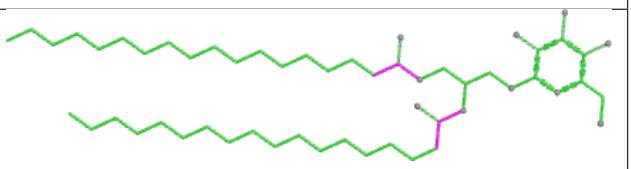


Rings

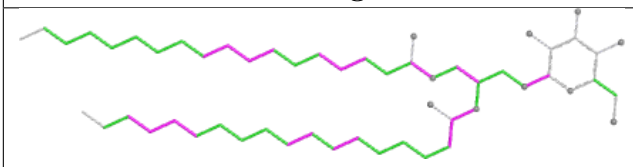
Ligand LMG 1 5004



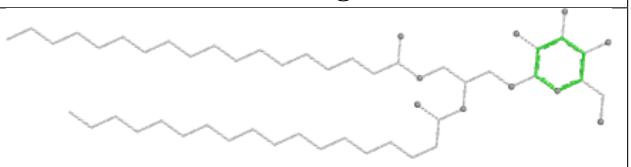
Bond lengths



Bond angles

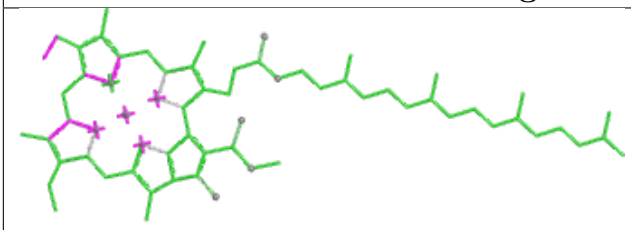


Torsions

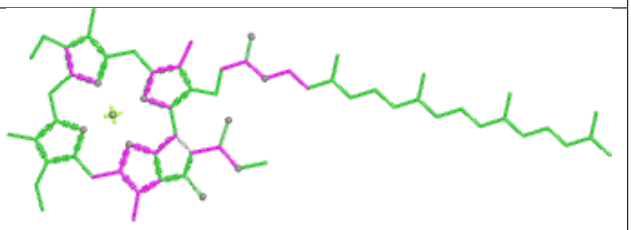


Rings

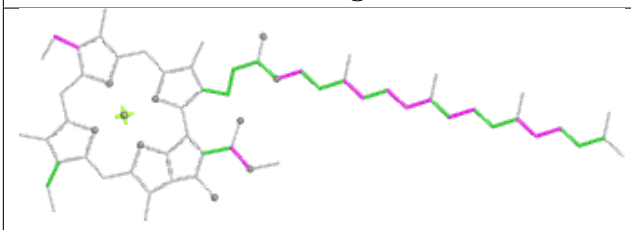
Ligand CLA 1 1131



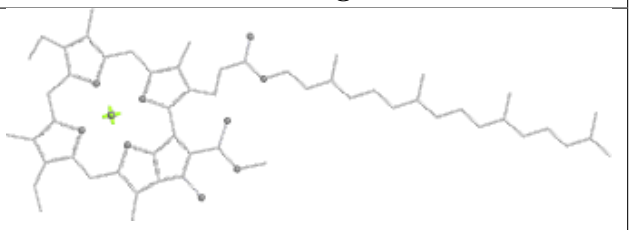
Bond lengths



Bond angles

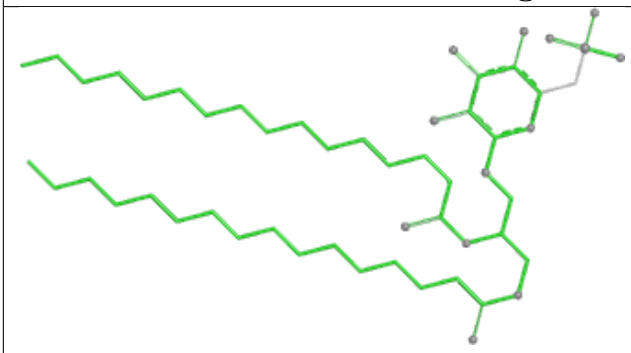


Torsions

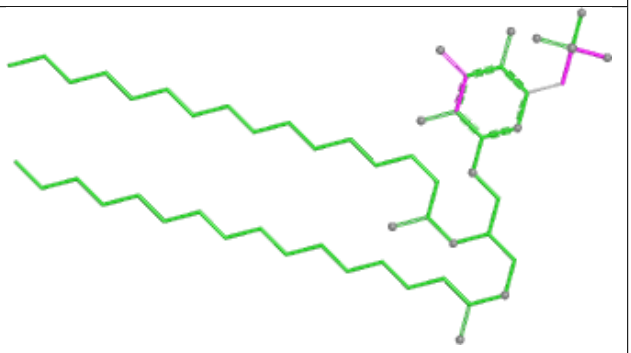


Rings

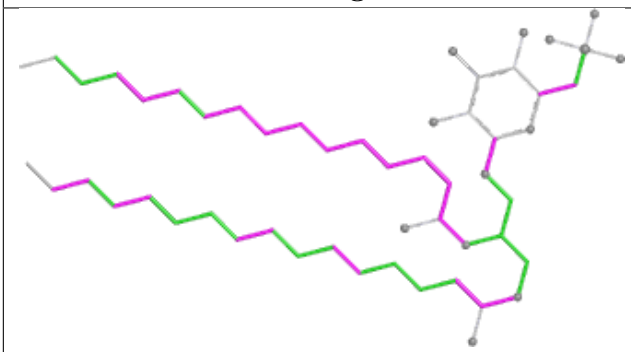
Ligand SQD F 5001



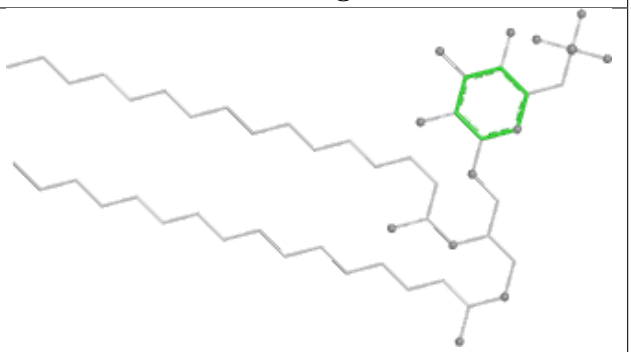
Bond lengths



Bond angles

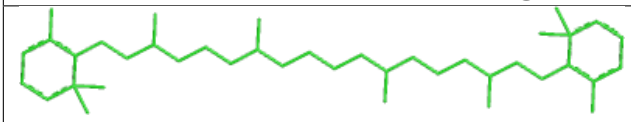


Torsions

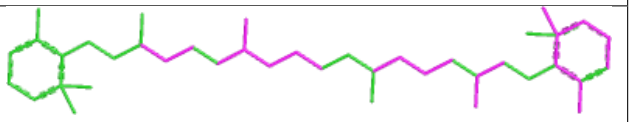


Rings

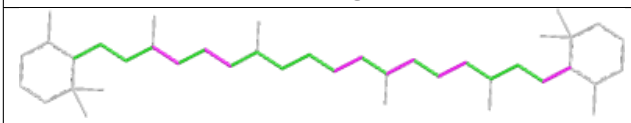
Ligand BCR a 4007



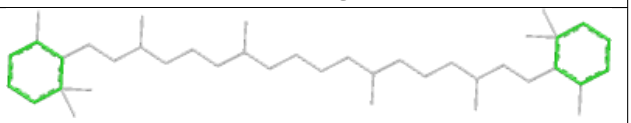
Bond lengths



Bond angles

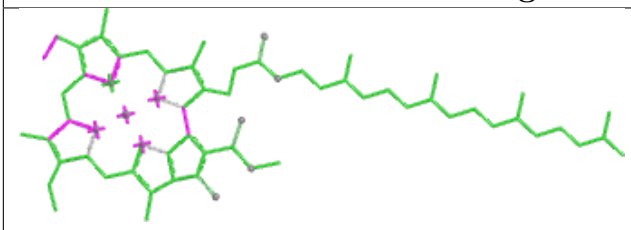


Torsions

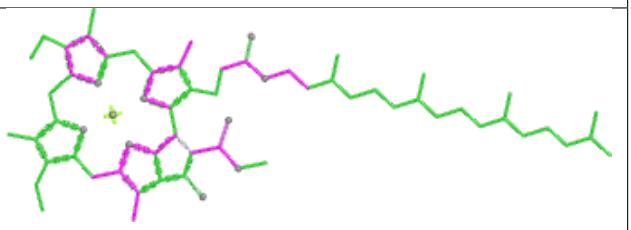


Rings

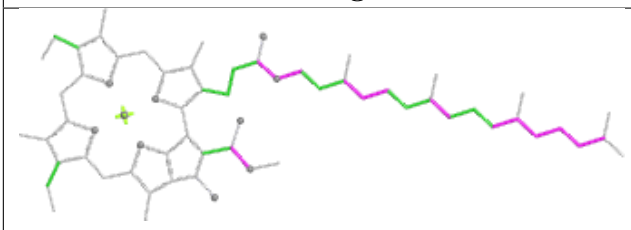
Ligand CLA b 1203



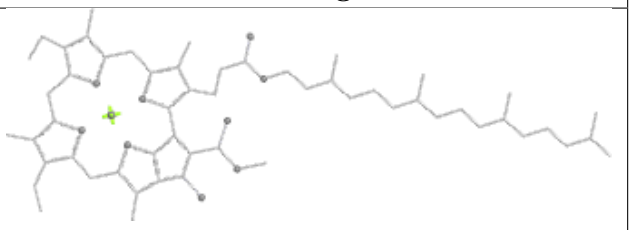
Bond lengths



Bond angles

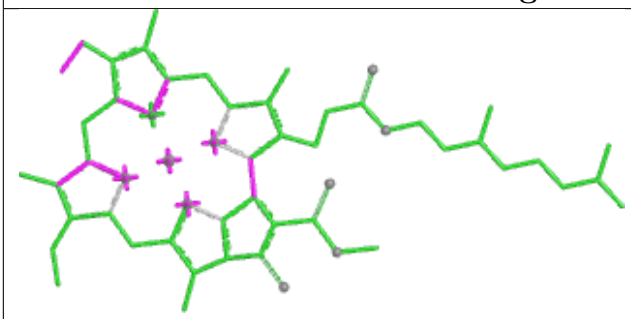


Torsions

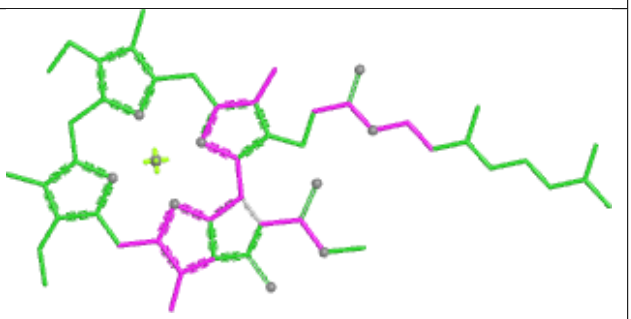


Rings

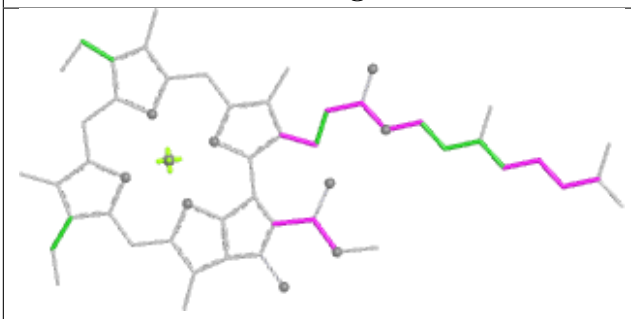
Ligand CLA a 1801



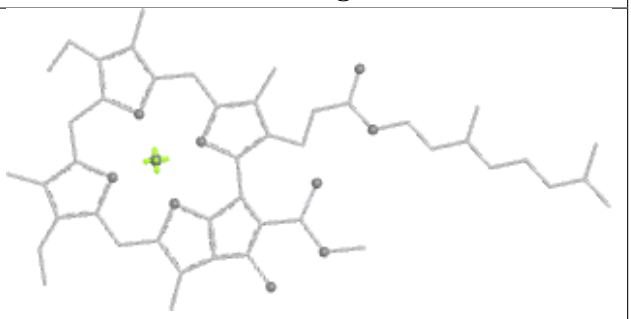
Bond lengths



Bond angles

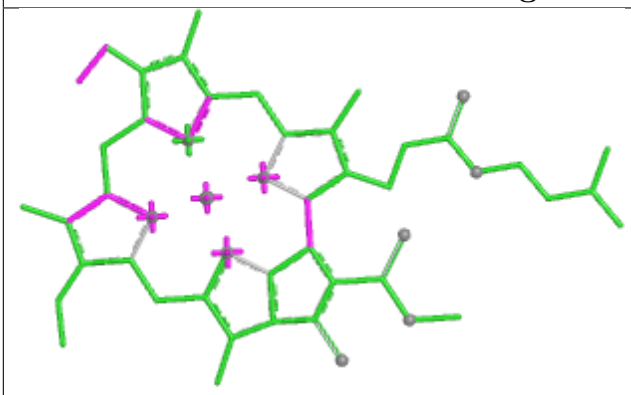


Torsions

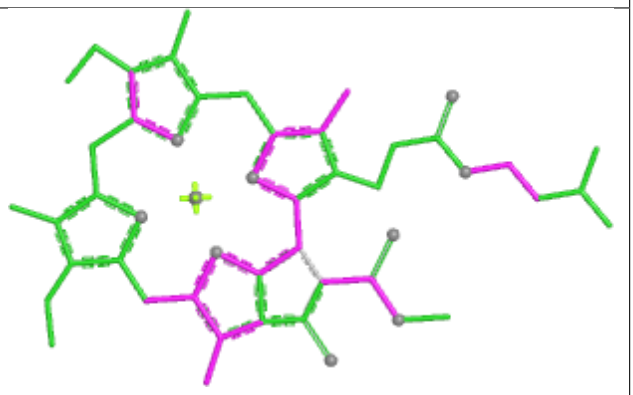


Rings

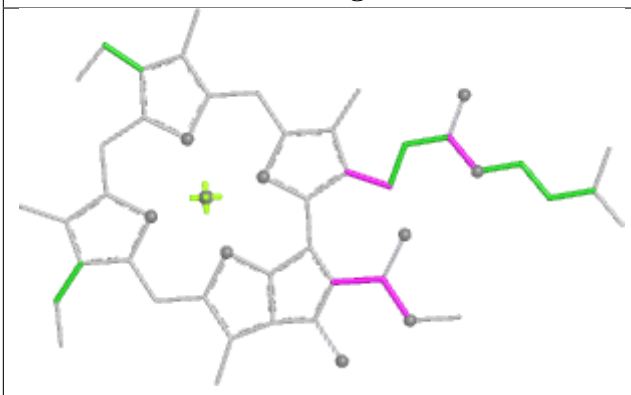
Ligand CLA 2 1216



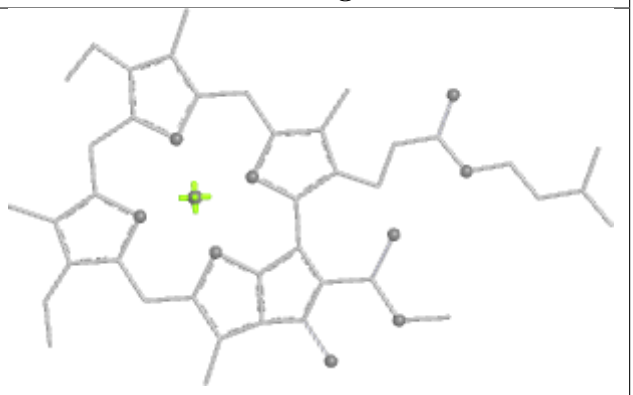
Bond lengths



Bond angles

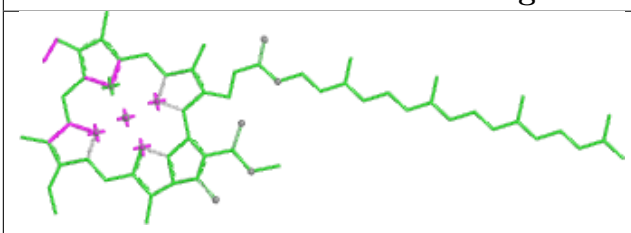


Torsions

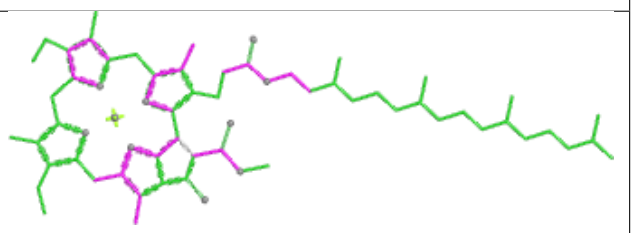


Rings

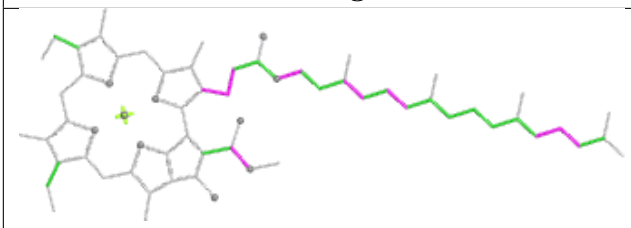
Ligand CLA b 1225



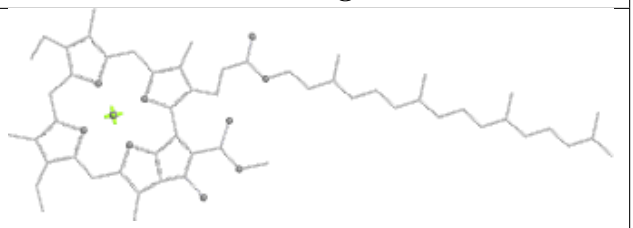
Bond lengths



Bond angles

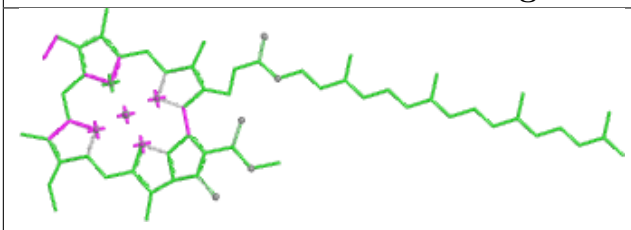


Torsions

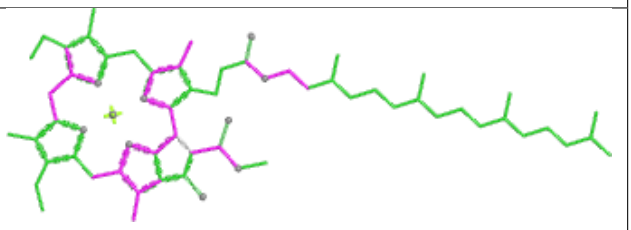


Rings

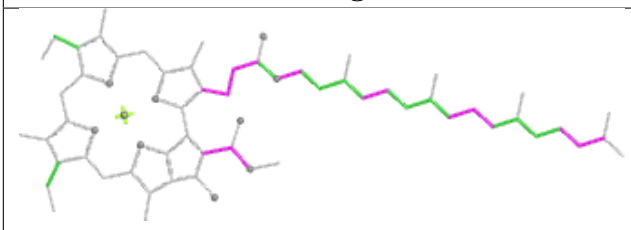
Ligand CLA 1 1125



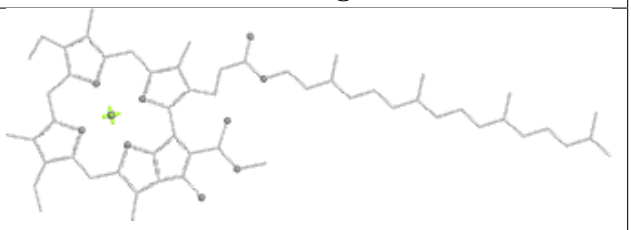
Bond lengths



Bond angles

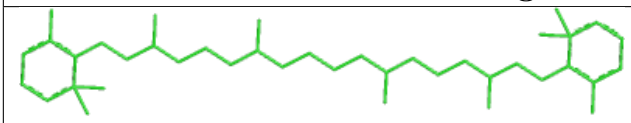


Torsions

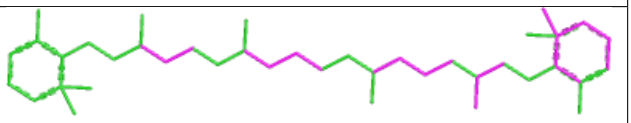


Rings

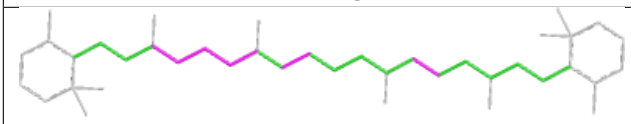
Ligand BCR 1 4001



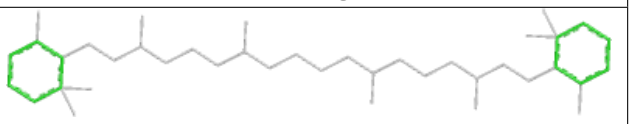
Bond lengths



Bond angles

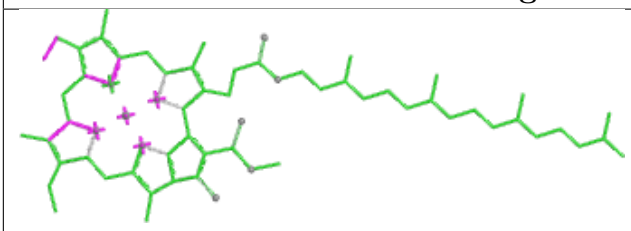


Torsions

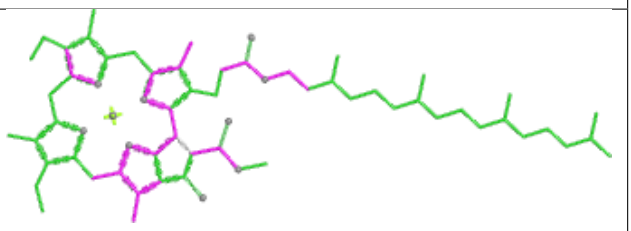


Rings

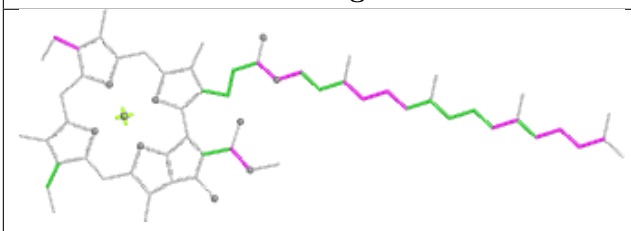
Ligand CLA 1 1140



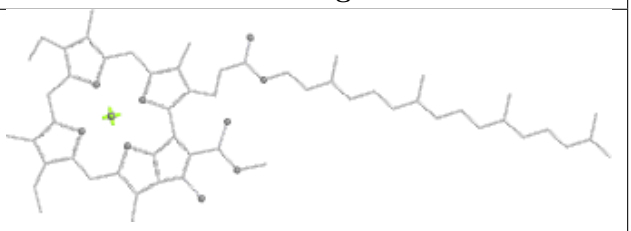
Bond lengths



Bond angles

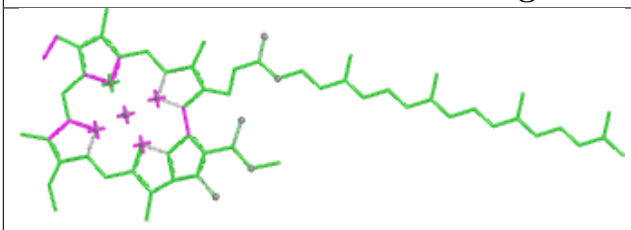


Torsions

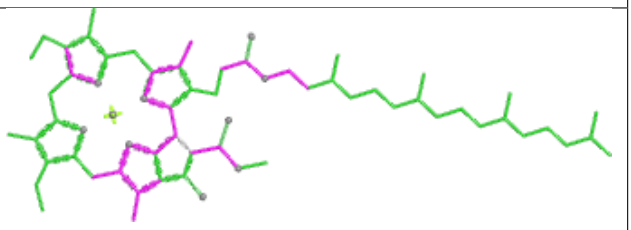


Rings

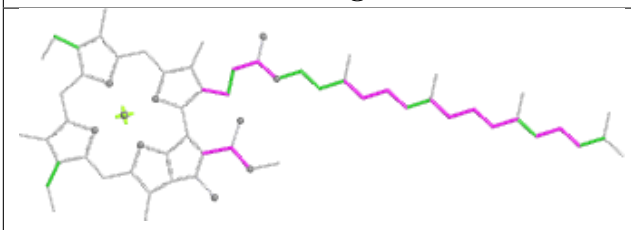
Ligand CLA b 1210



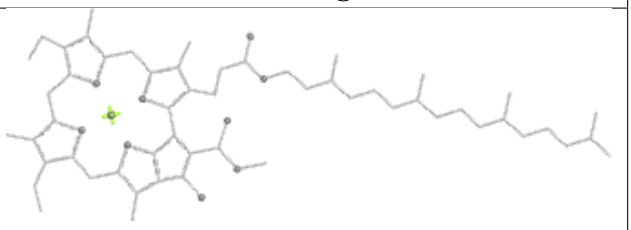
Bond lengths



Bond angles

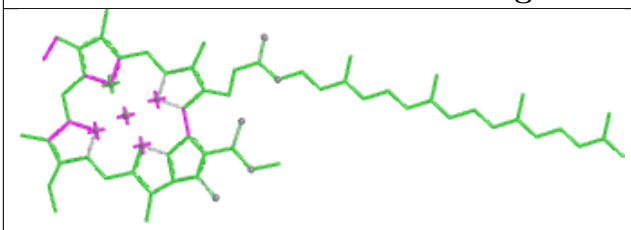


Torsions

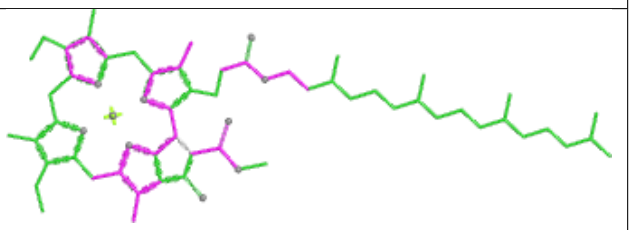


Rings

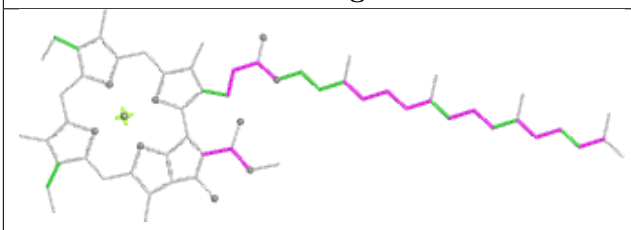
Ligand CLA A 1113



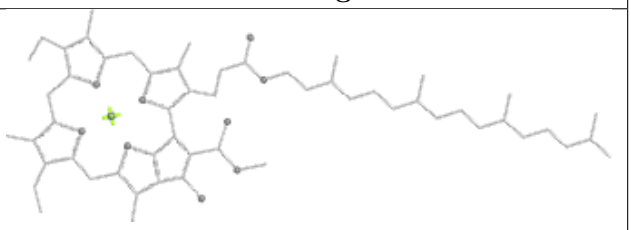
Bond lengths



Bond angles

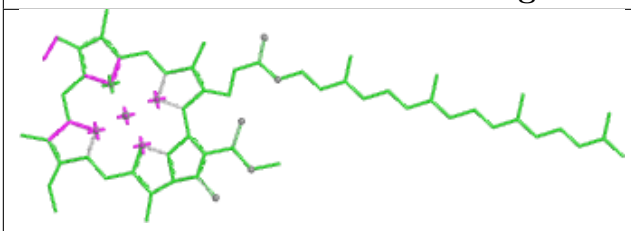


Torsions

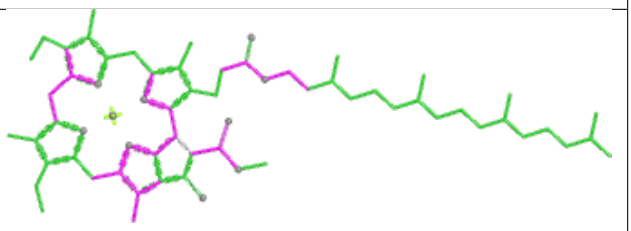


Rings

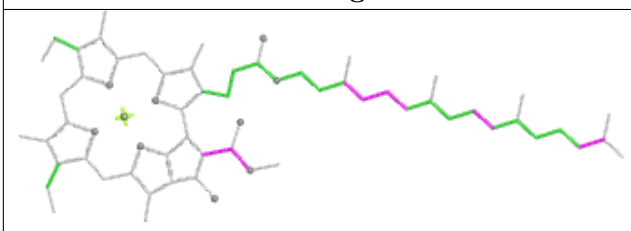
Ligand CLA b 1205



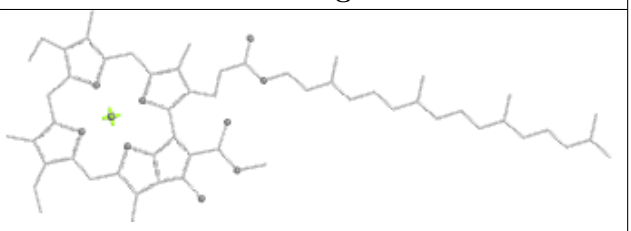
Bond lengths



Bond angles

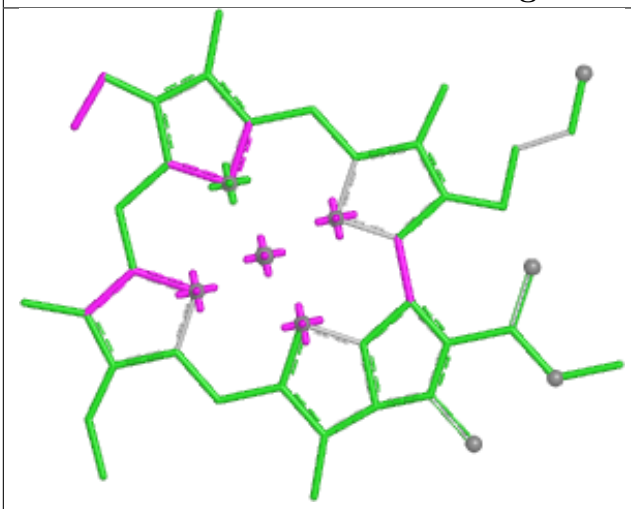


Torsions

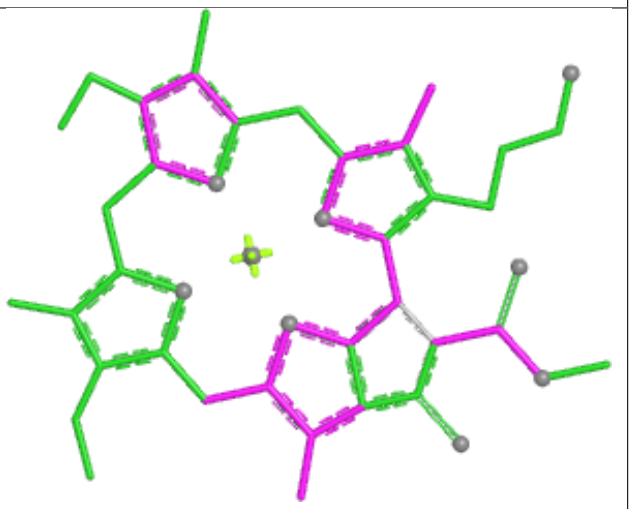


Rings

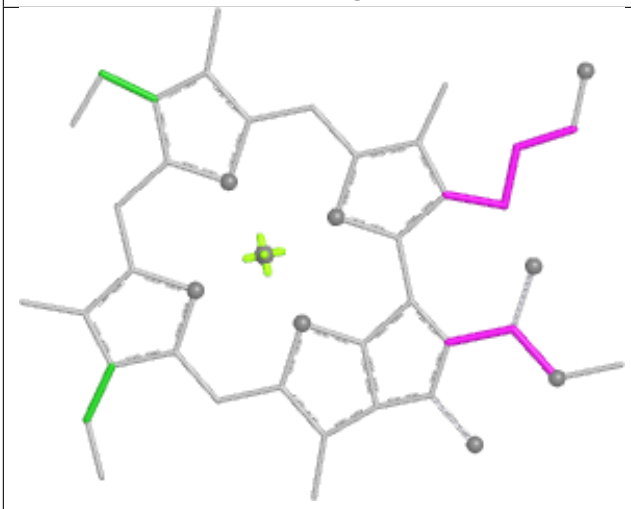
Ligand CLA 1 1113



Bond lengths



Bond angles

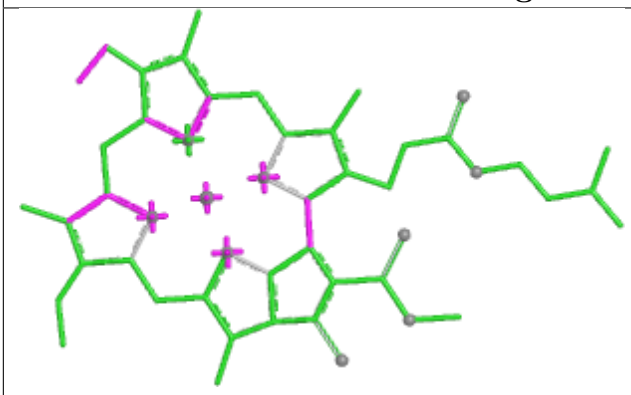


Torsions

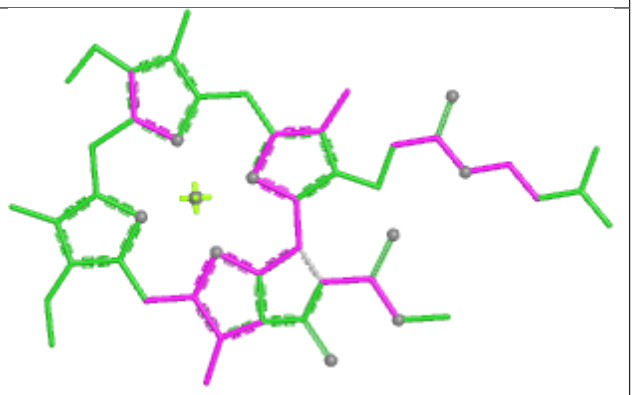


Rings

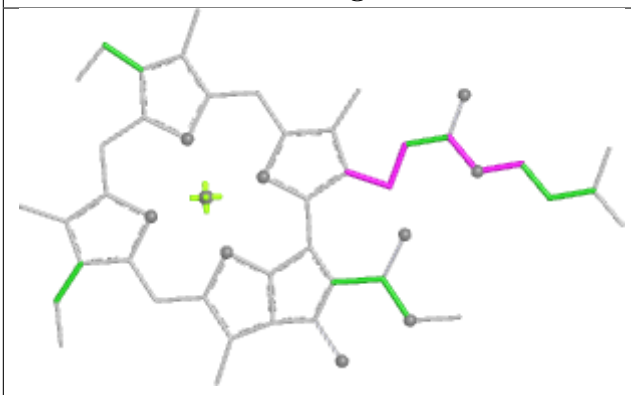
Ligand CLA B 1236



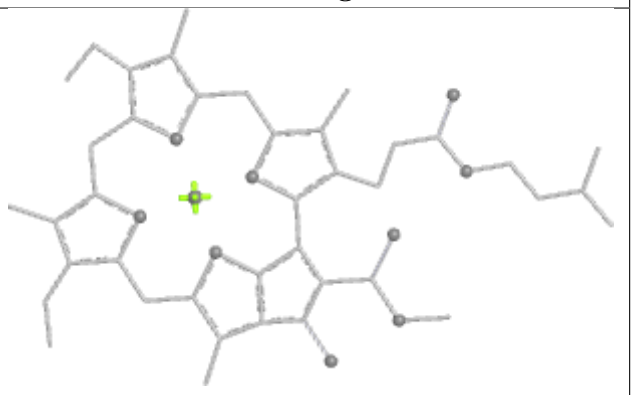
Bond lengths



Bond angles

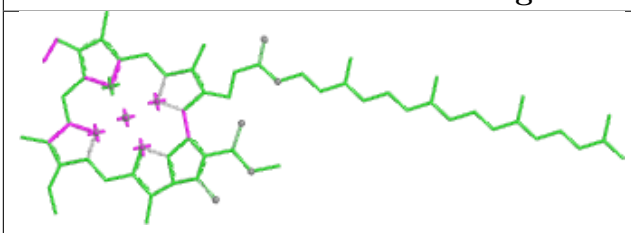


Torsions

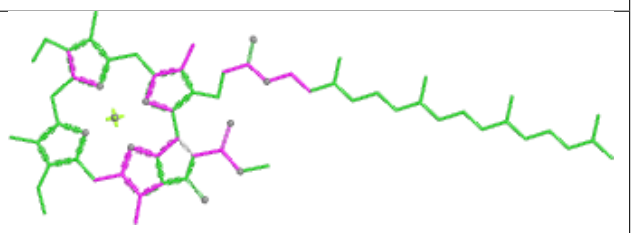


Rings

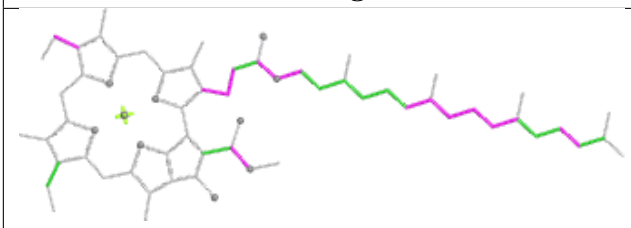
Ligand CLA B 1239



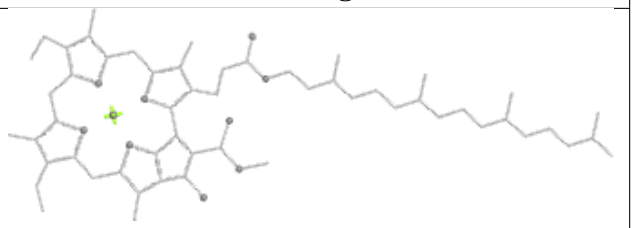
Bond lengths



Bond angles

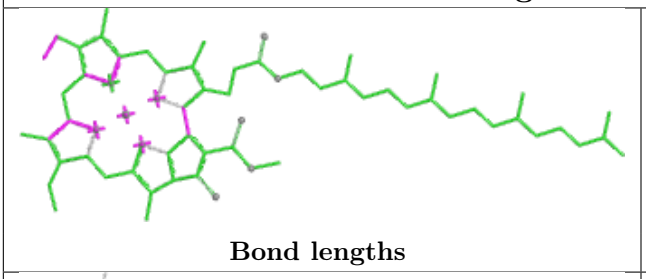


Torsions

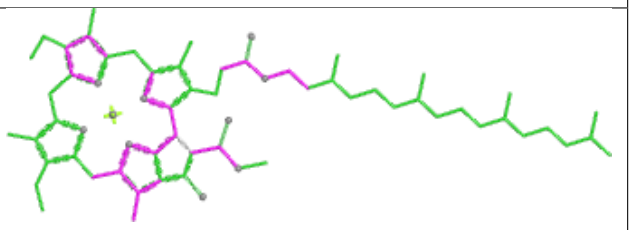


Rings

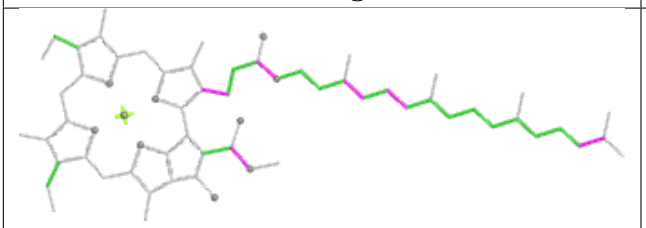
Ligand CLA B 1021



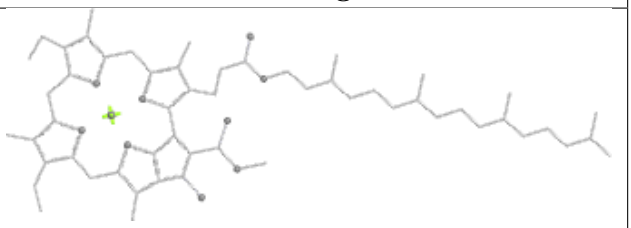
Bond lengths



Bond angles

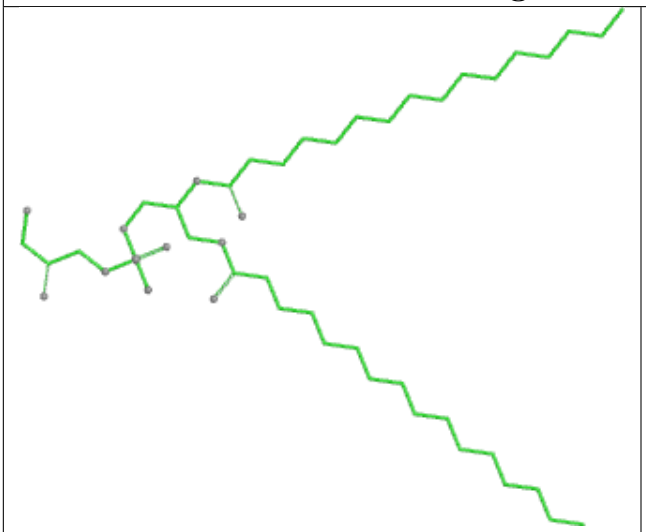


Torsions

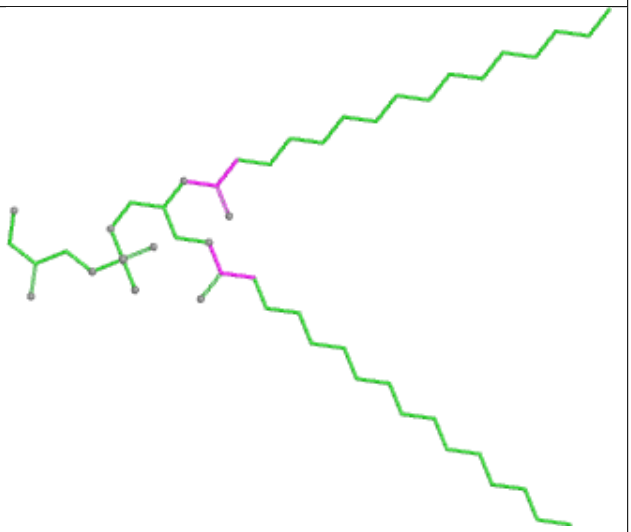


Rings

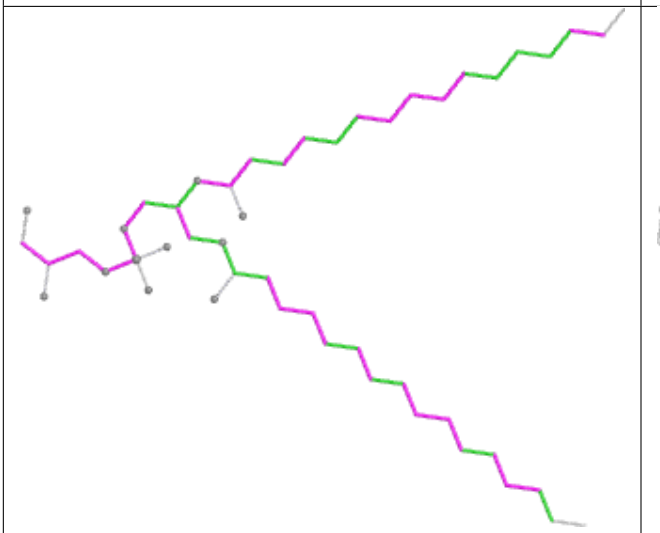
Ligand LHG M 5001



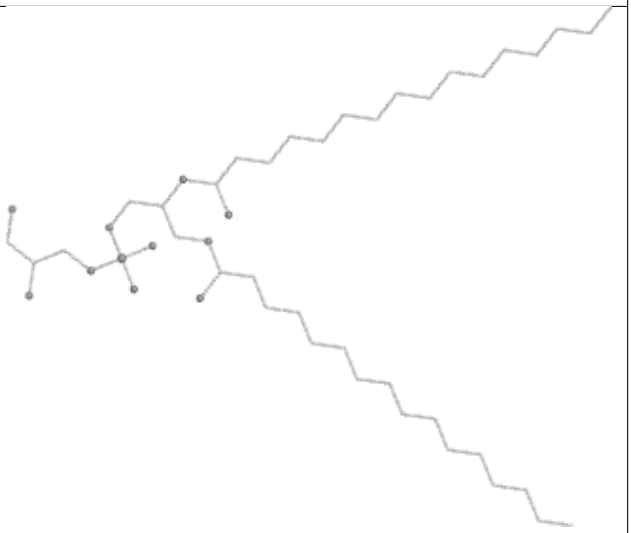
Bond lengths



Bond angles

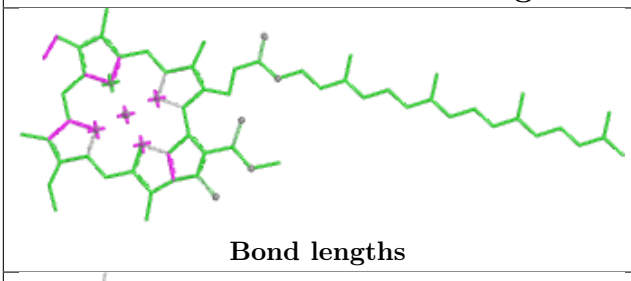


Torsions

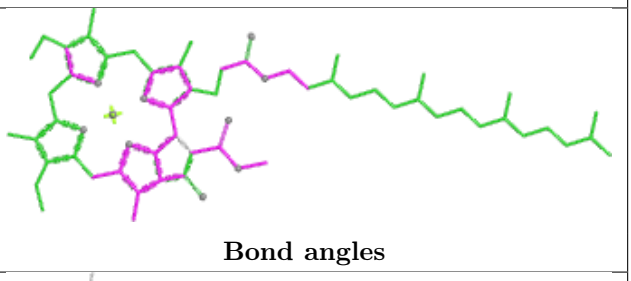


Rings

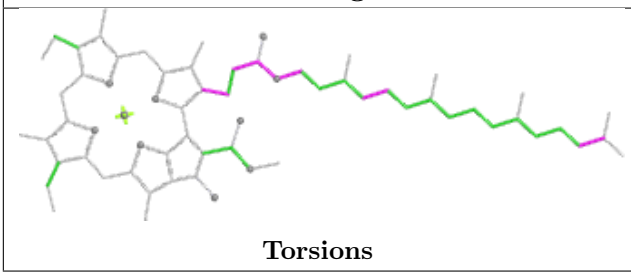
Ligand CLA A 1011



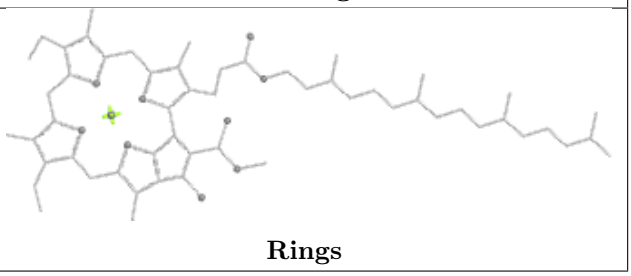
Bond lengths



Bond angles

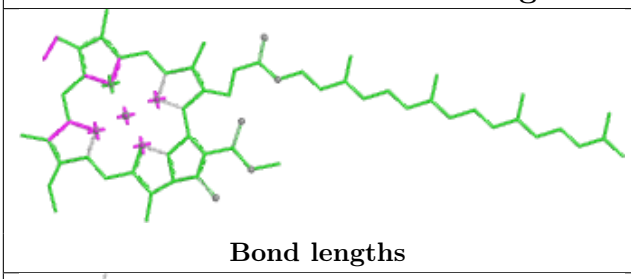


Torsions

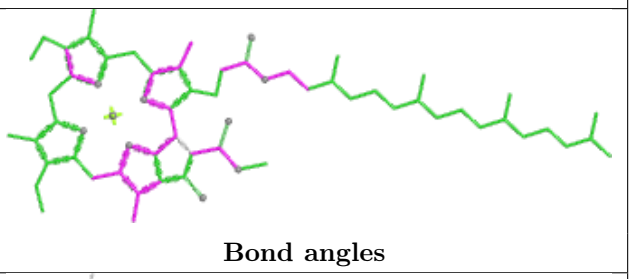


Rings

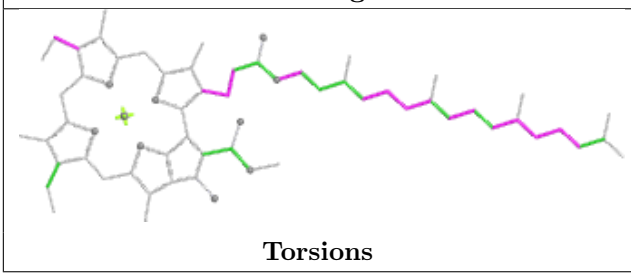
Ligand CLA 2 1225



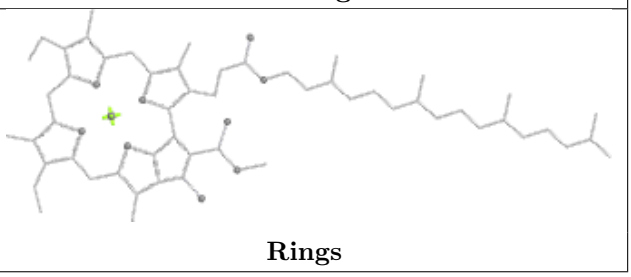
Bond lengths



Bond angles

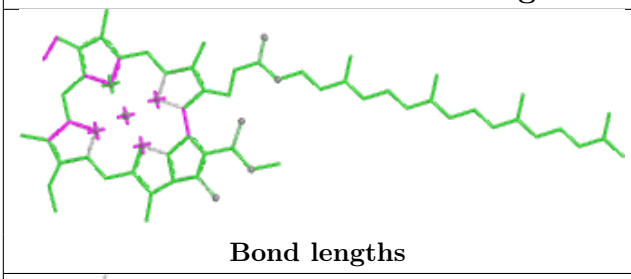


Torsions

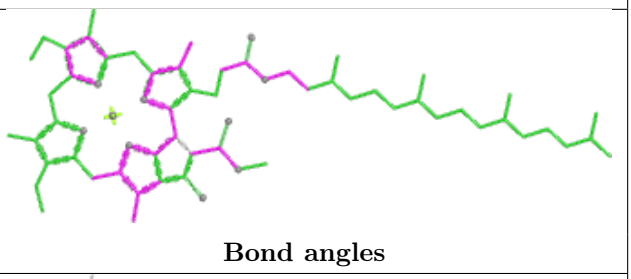


Rings

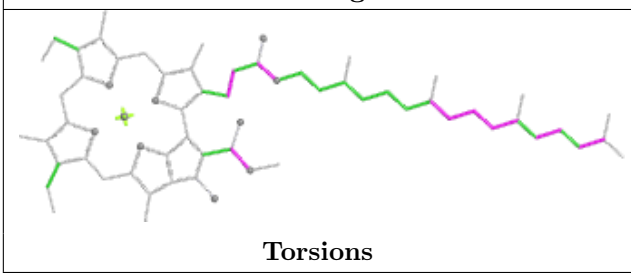
Ligand CLA b 1201



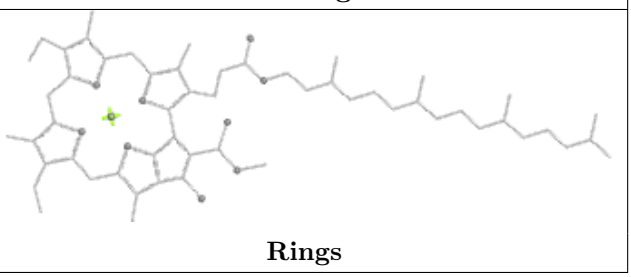
Bond lengths



Bond angles

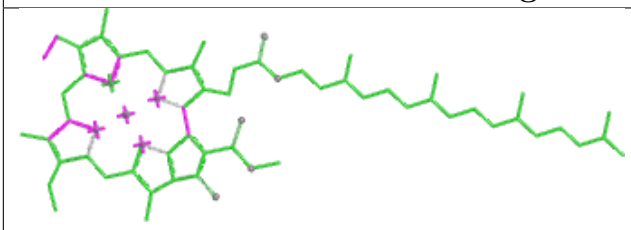


Torsions

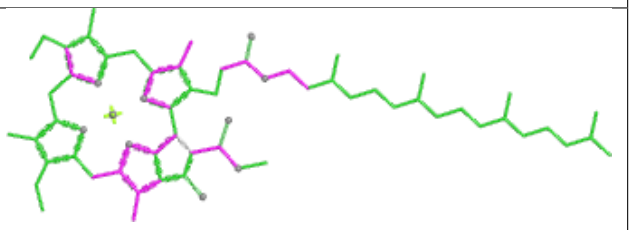


Rings

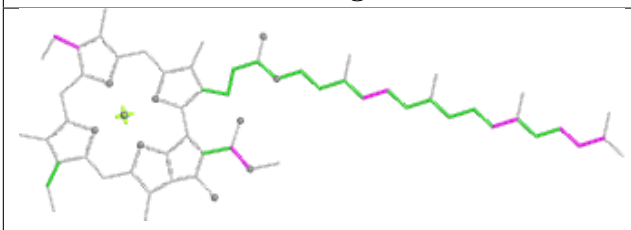
Ligand CLA a 1115



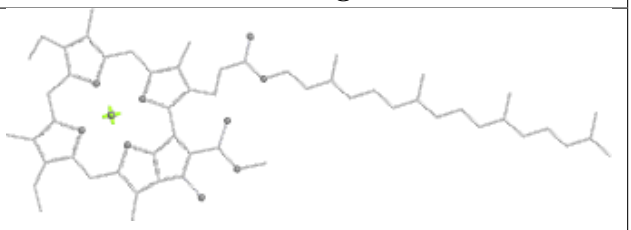
Bond lengths



Bond angles

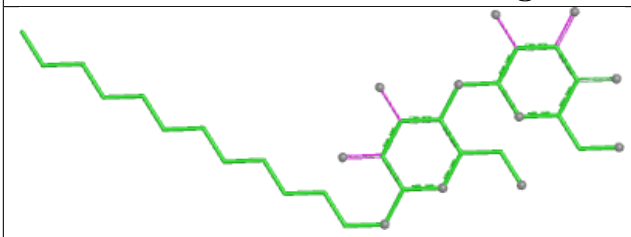


Torsions

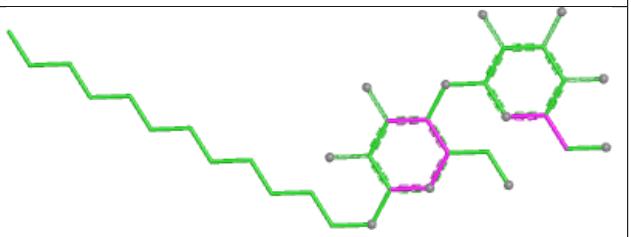


Rings

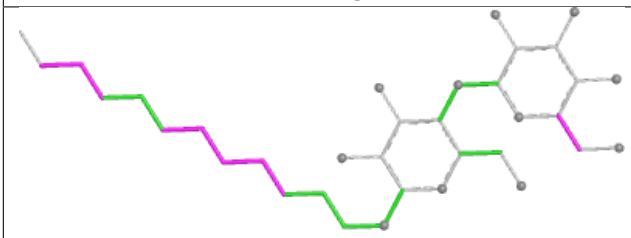
Ligand LMT 1 6001



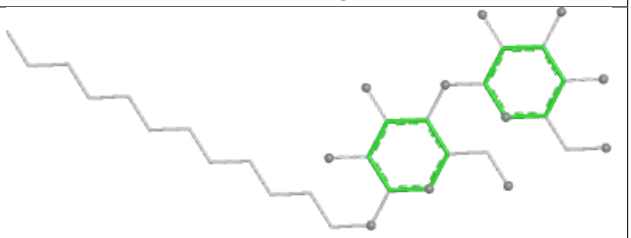
Bond lengths



Bond angles

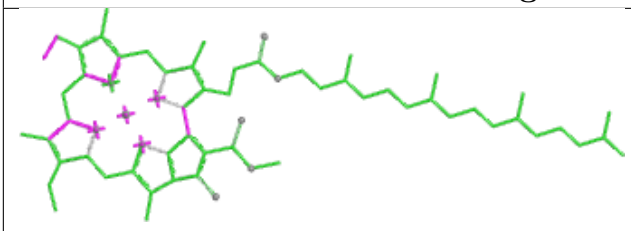


Torsions

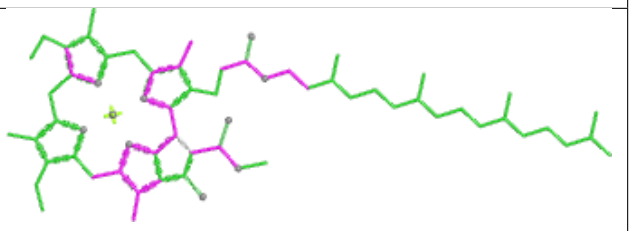


Rings

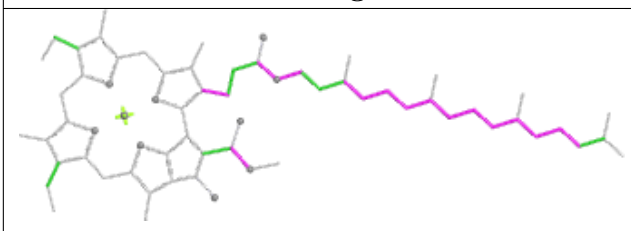
Ligand CLA a 1104



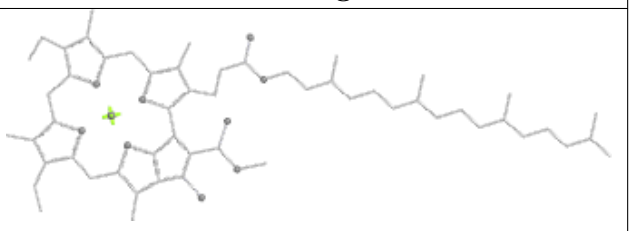
Bond lengths



Bond angles

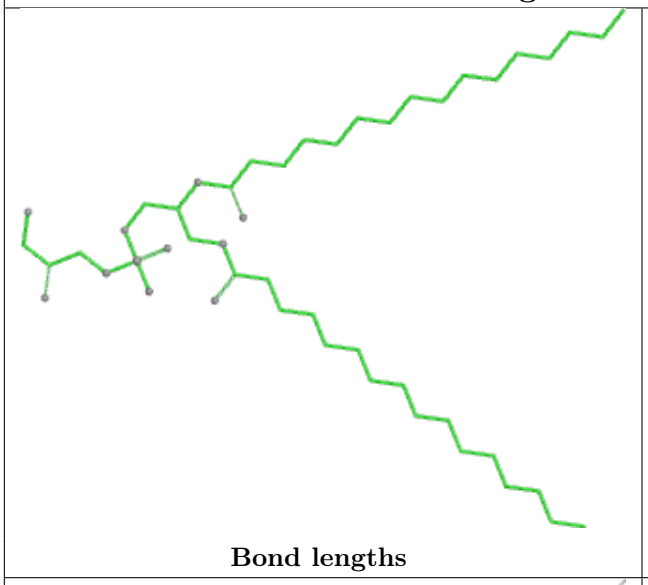


Torsions

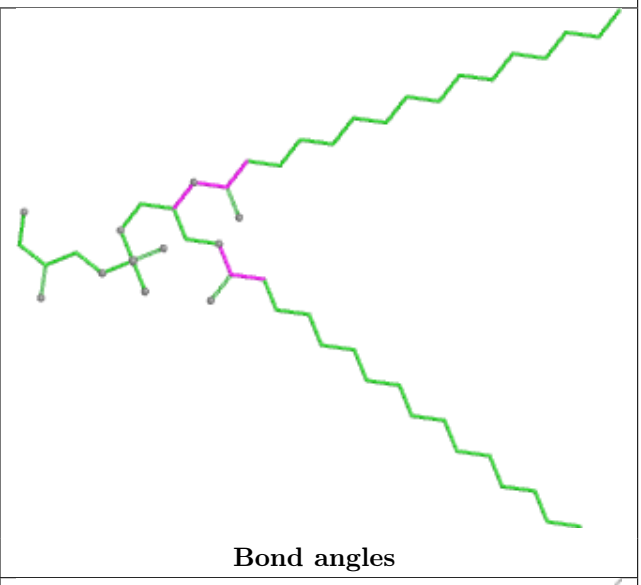


Rings

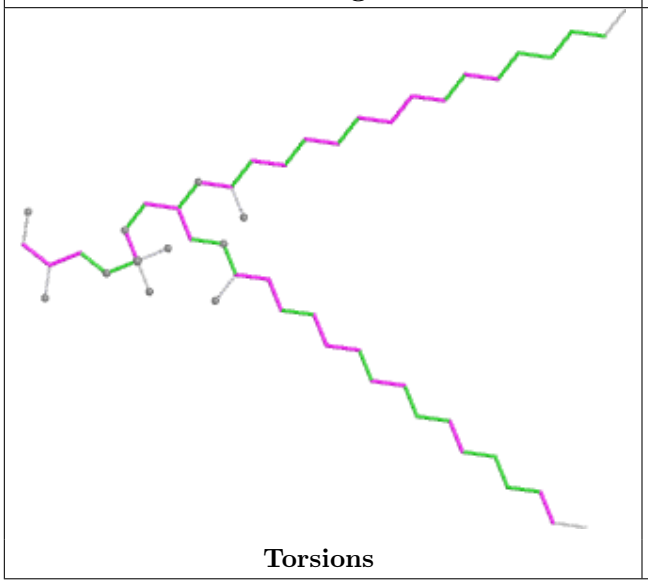
Ligand LHG a 5001



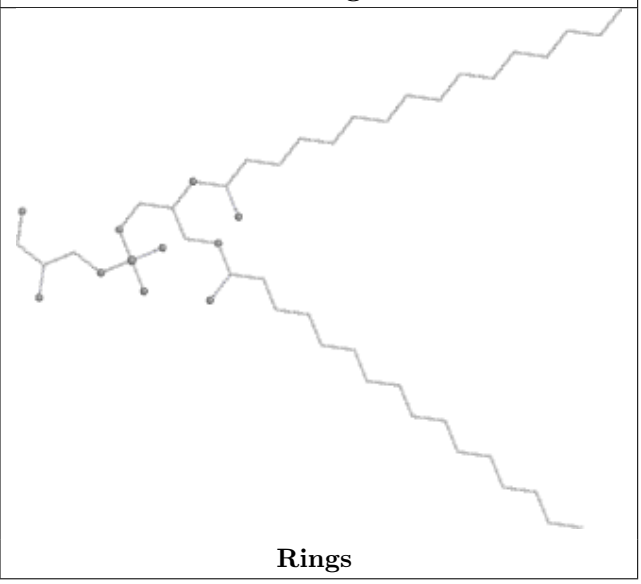
Bond lengths



Bond angles

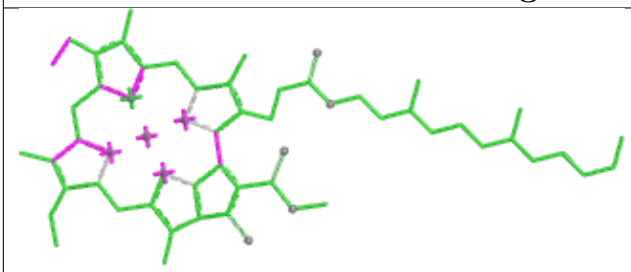


Torsions

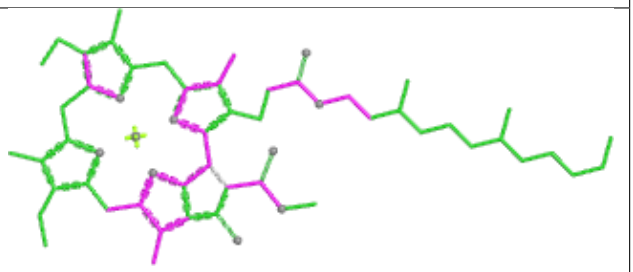


Rings

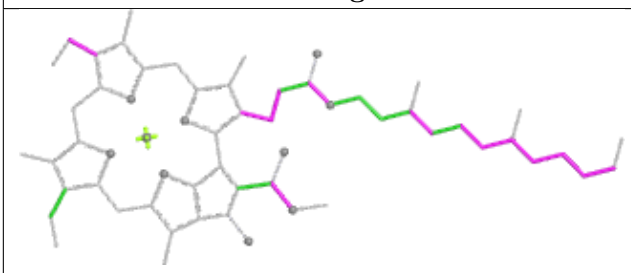
Ligand CLA a 1110



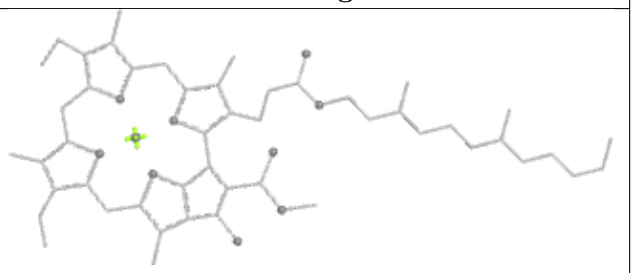
Bond lengths



Bond angles

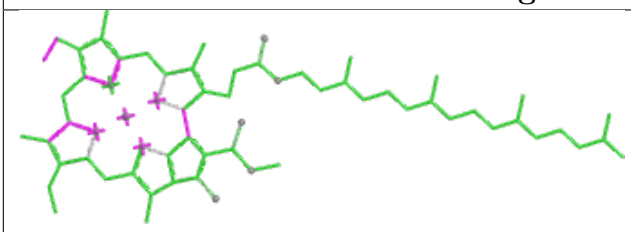


Torsions

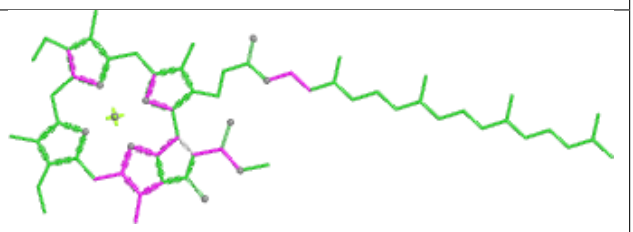


Rings

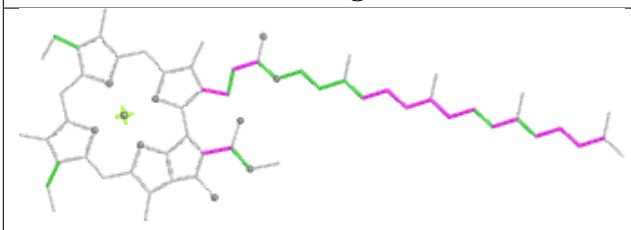
Ligand CLA b 1211



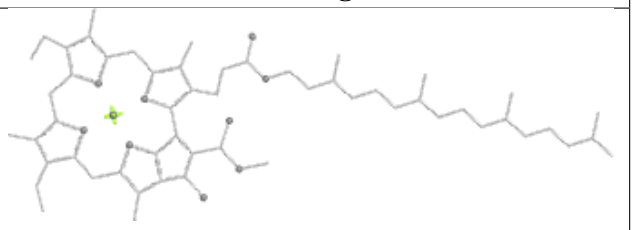
Bond lengths



Bond angles

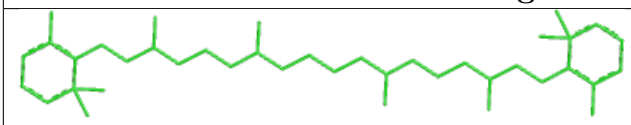


Torsions

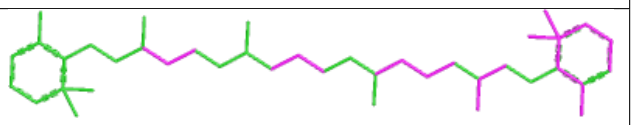


Rings

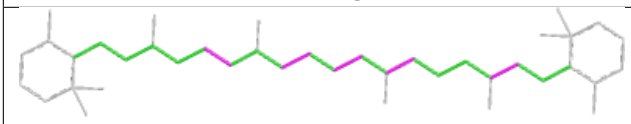
Ligand BCR 1 4008



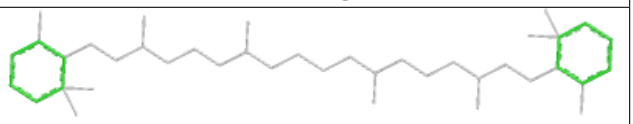
Bond lengths



Bond angles

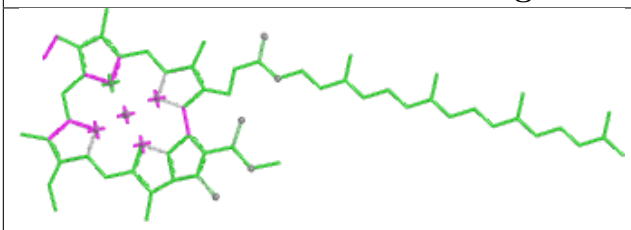


Torsions

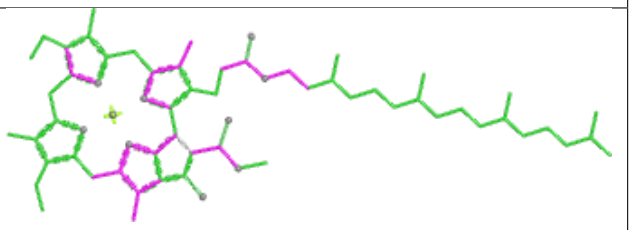


Rings

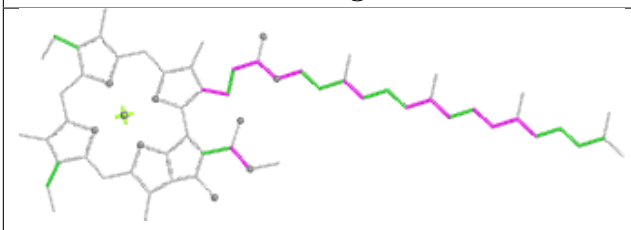
Ligand CLA A 1126



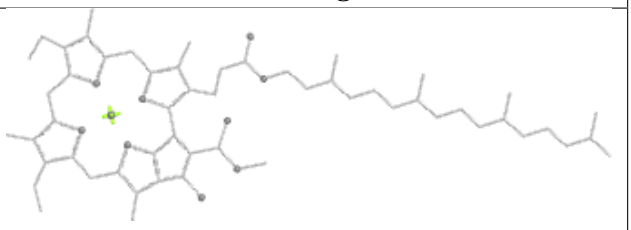
Bond lengths



Bond angles

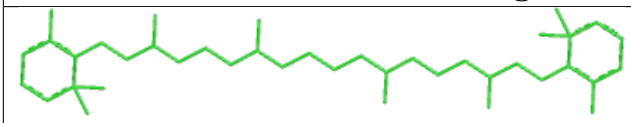


Torsions

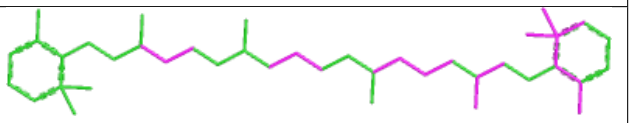


Rings

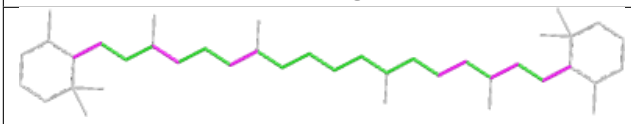
Ligand BCR A 4012



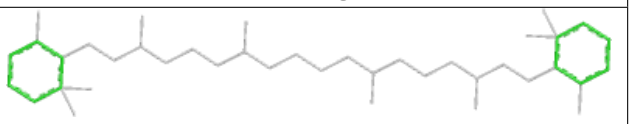
Bond lengths



Bond angles

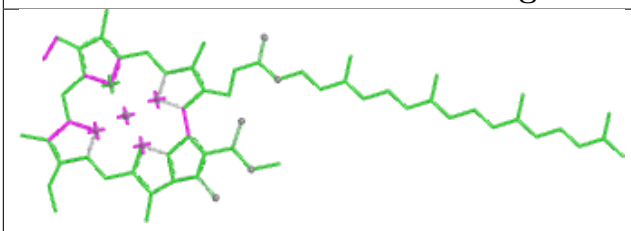


Torsions

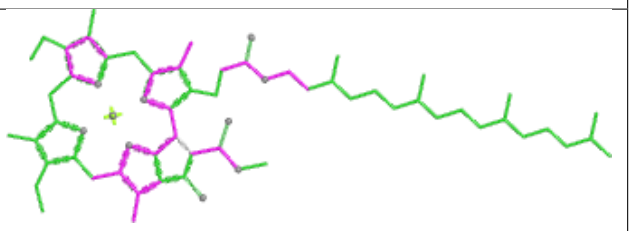


Rings

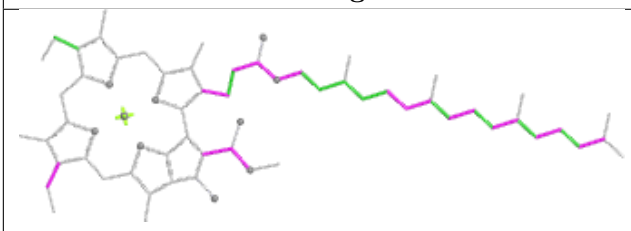
Ligand CLA 2 1210



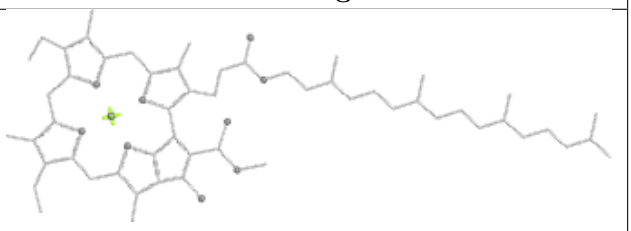
Bond lengths



Bond angles

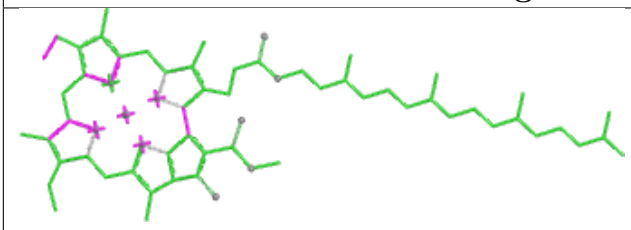


Torsions

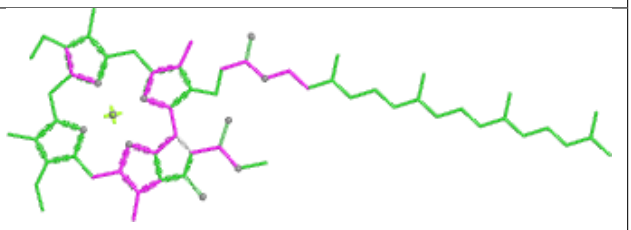


Rings

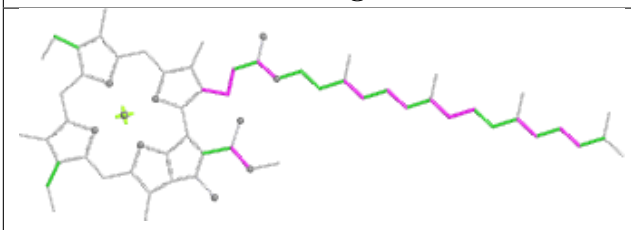
Ligand CLA A 1134



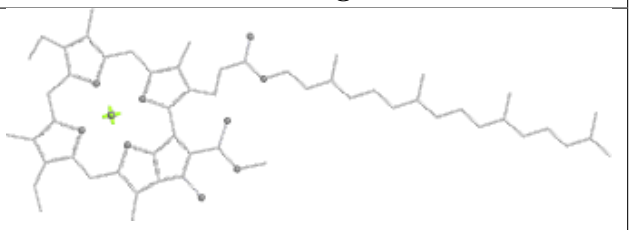
Bond lengths



Bond angles

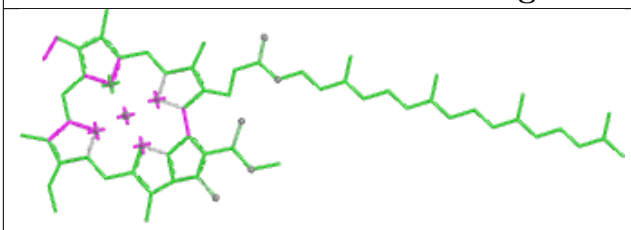


Torsions

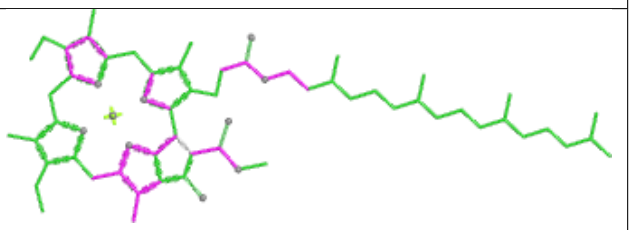


Rings

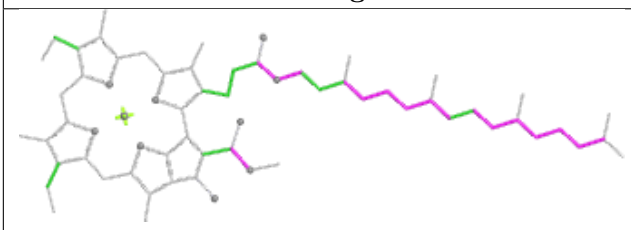
Ligand CLA b 1231



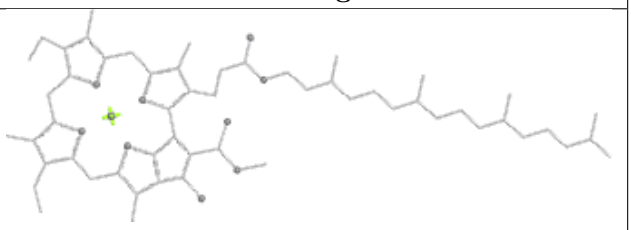
Bond lengths



Bond angles

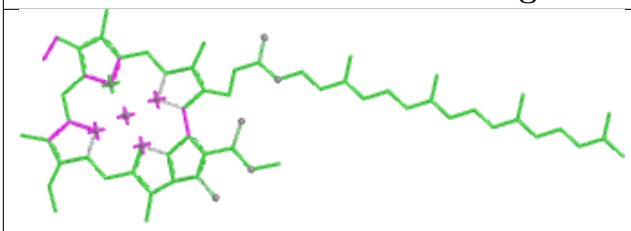


Torsions

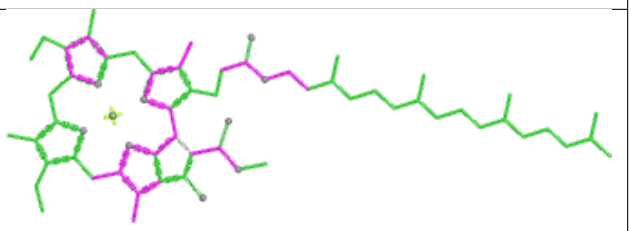


Rings

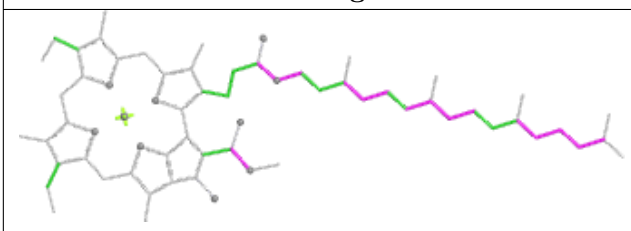
Ligand CLA 2 1203



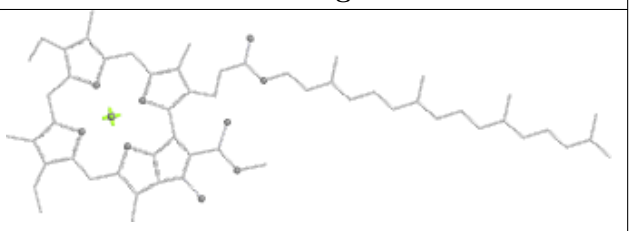
Bond lengths



Bond angles

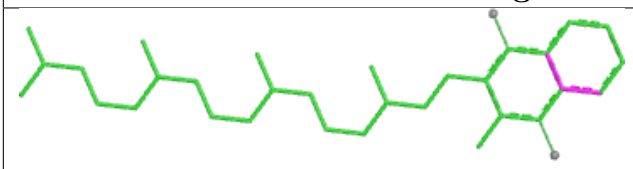


Torsions

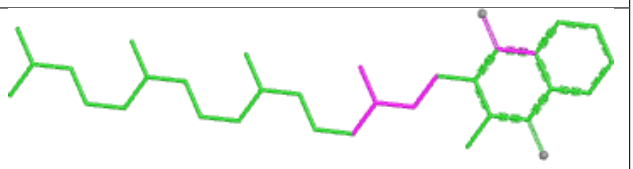


Rings

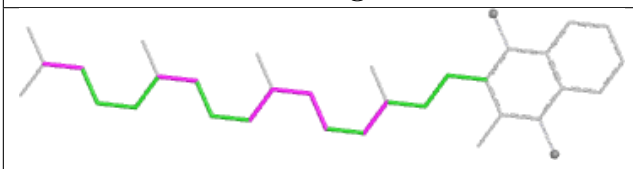
Ligand PQN B 2002



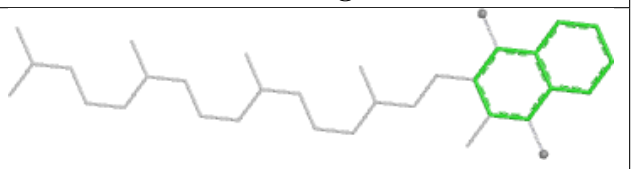
Bond lengths



Bond angles

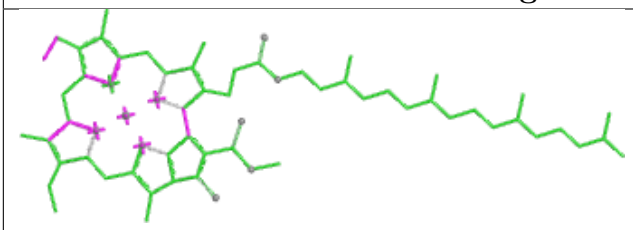


Torsions

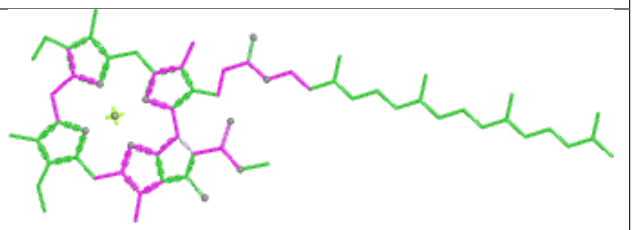


Rings

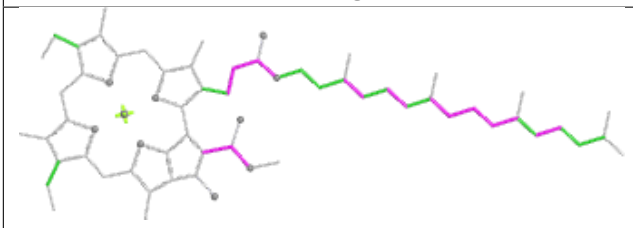
Ligand CLA a 1136



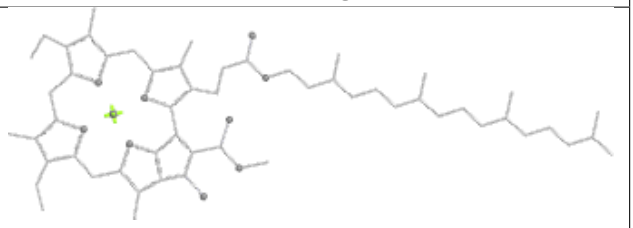
Bond lengths



Bond angles

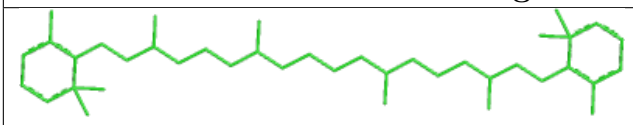


Torsions

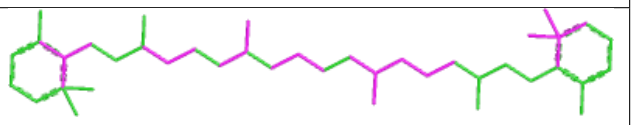


Rings

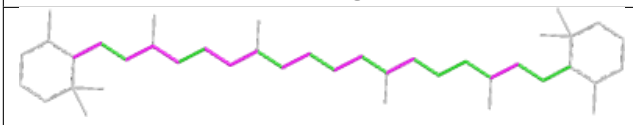
Ligand BCR A 4003



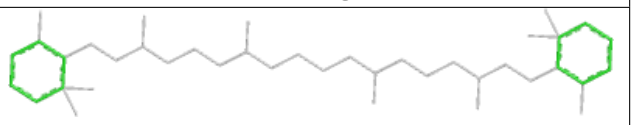
Bond lengths



Bond angles

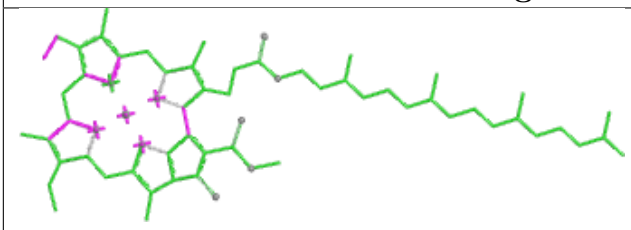


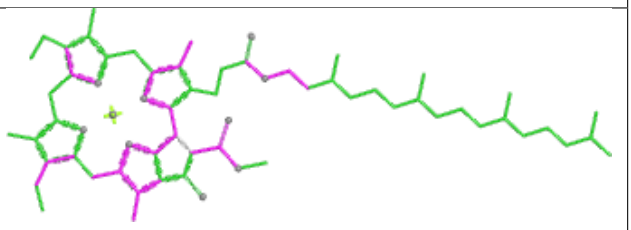
Torsions

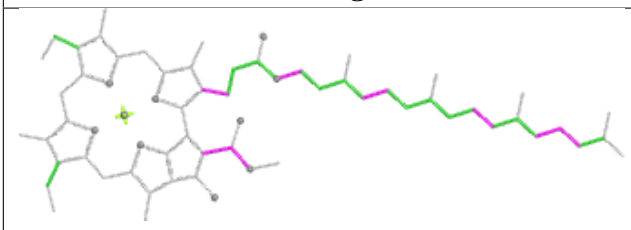


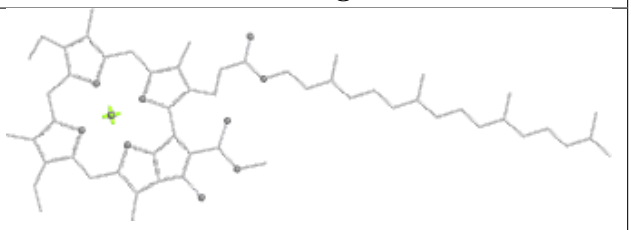
Rings

Ligand CLA A 1111

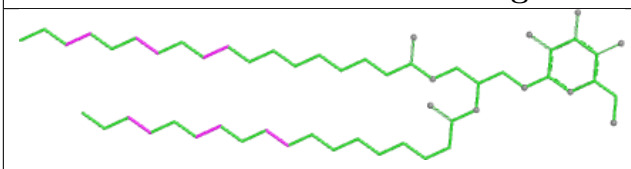

Bond lengths

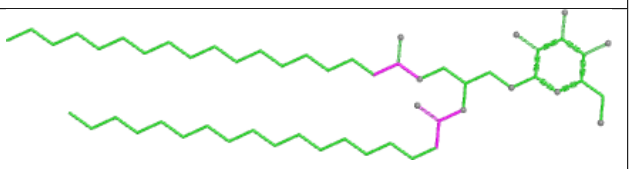

Bond angles

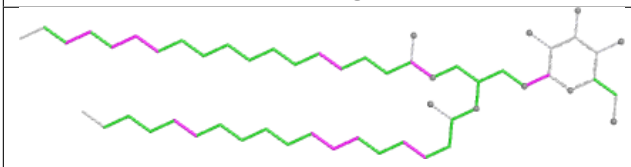

Torsions


Rings

Ligand LMG B 5005


Bond lengths

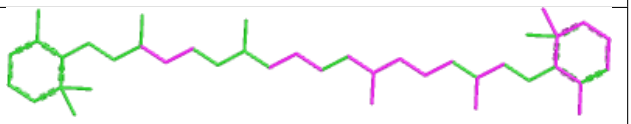

Bond angles

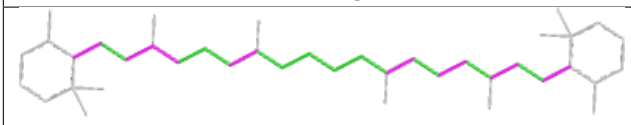

Torsions

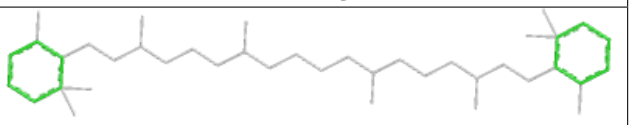

Rings

Ligand BCR B 4004

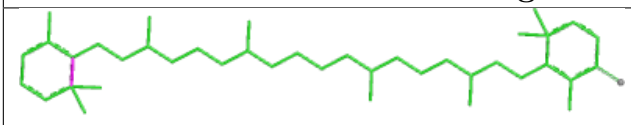

Bond lengths

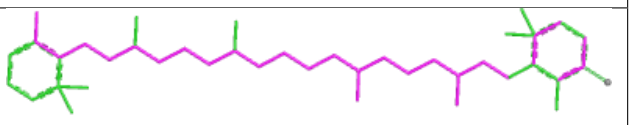

Bond angles

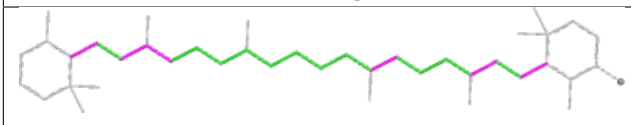

Torsions

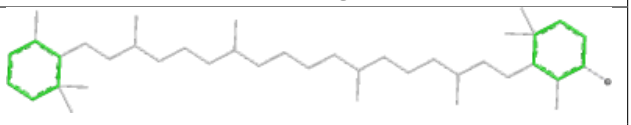

Rings

Ligand ECH 2 4006

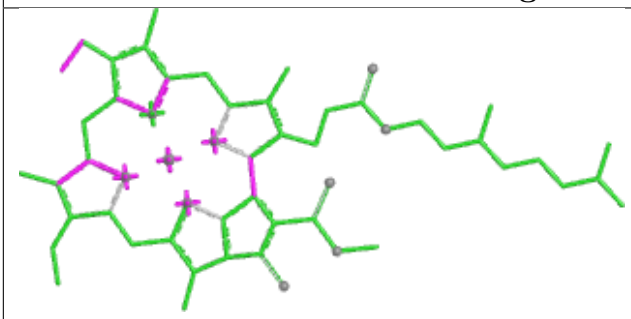

Bond lengths


Bond angles

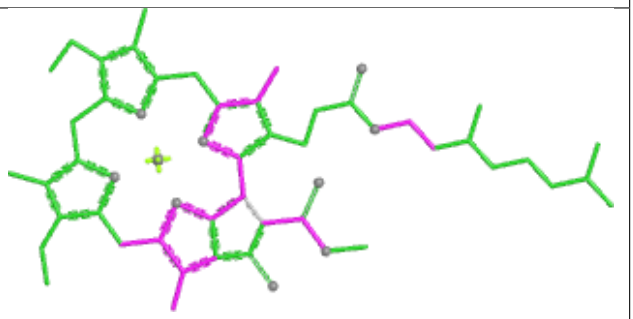

Torsions


Rings

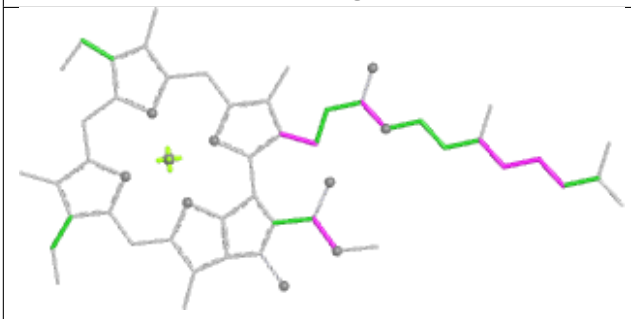
Ligand CLA 1 1130



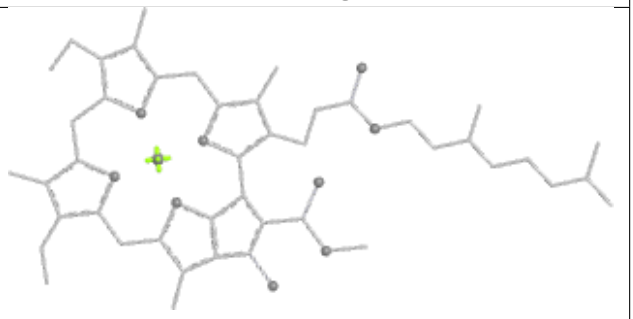
Bond lengths



Bond angles

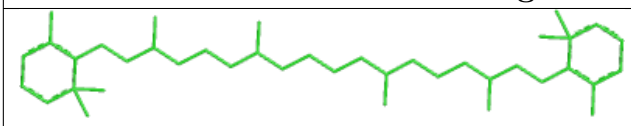


Torsions

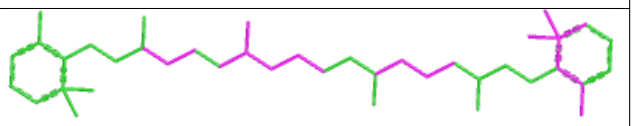


Rings

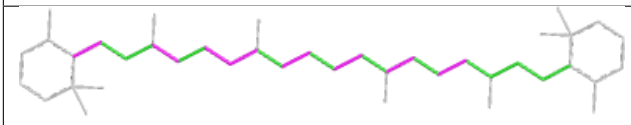
Ligand BCR 2 4017



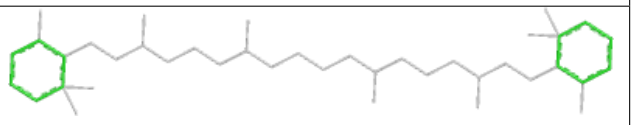
Bond lengths



Bond angles

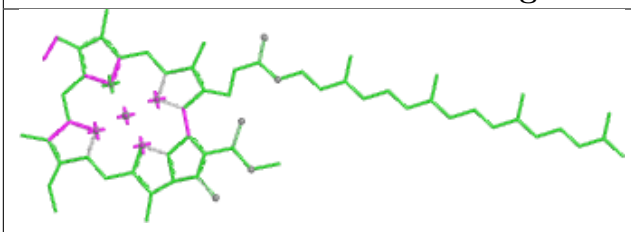


Torsions

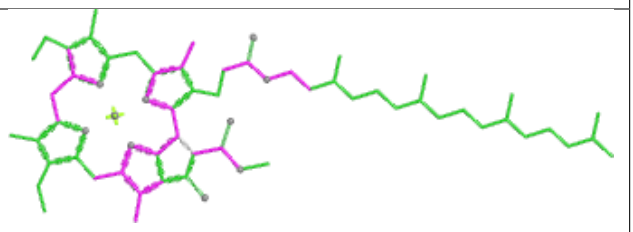


Rings

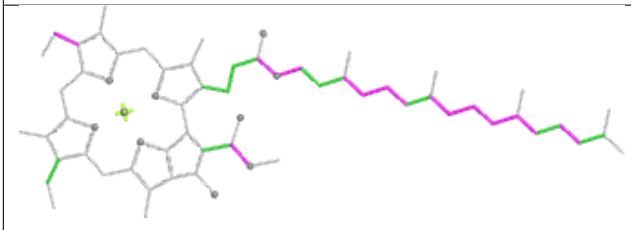
Ligand CLA a 1133



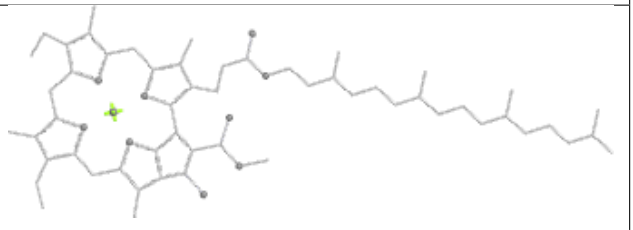
Bond lengths



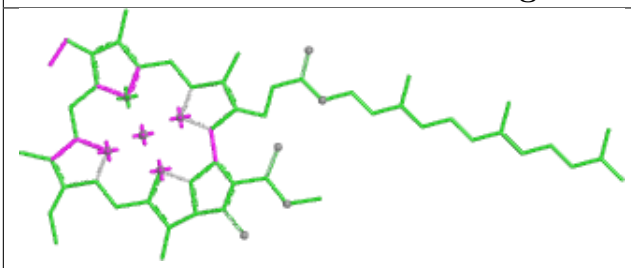
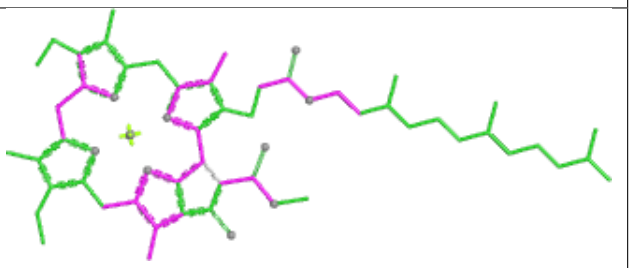
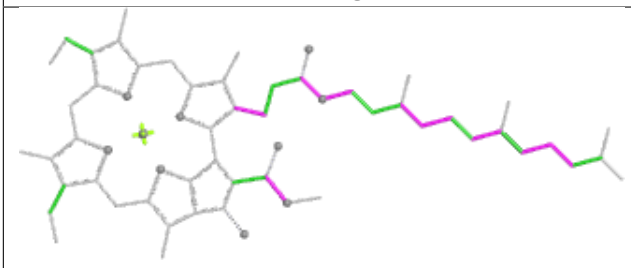
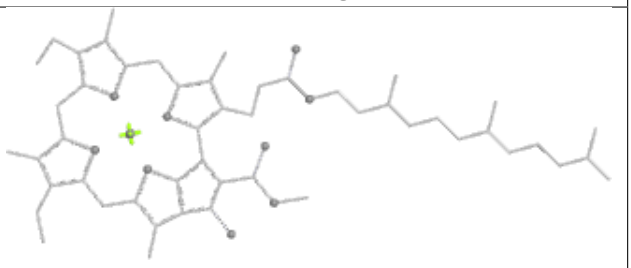
Bond angles

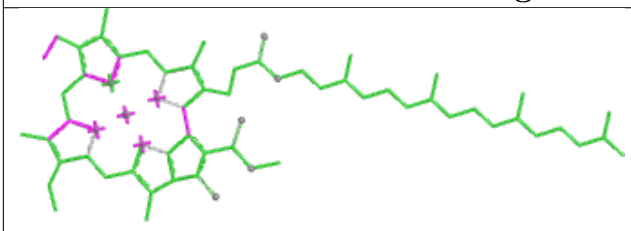
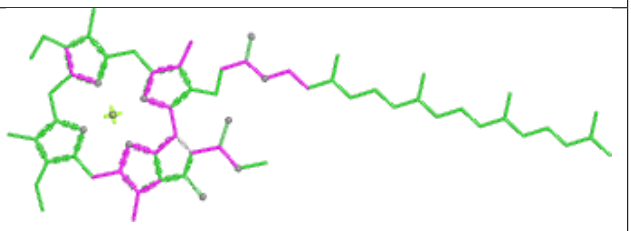
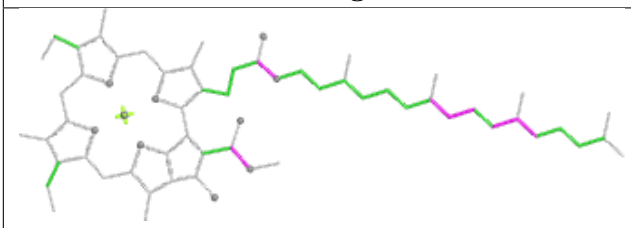
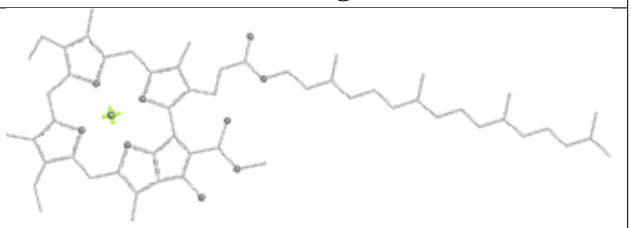


Torsions

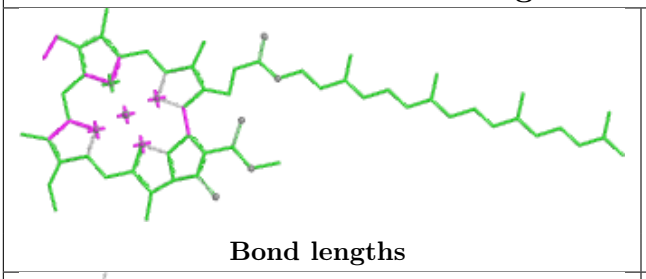


Rings

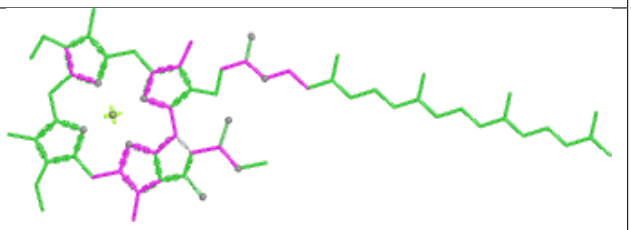
Ligand CLA 2 1208	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

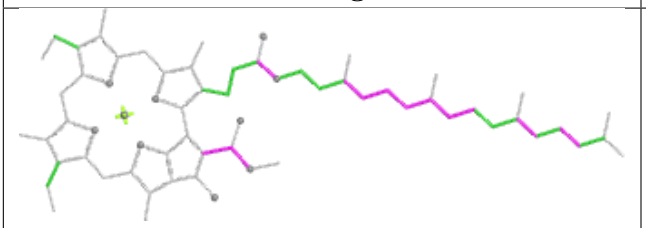
Ligand CLA B 1211



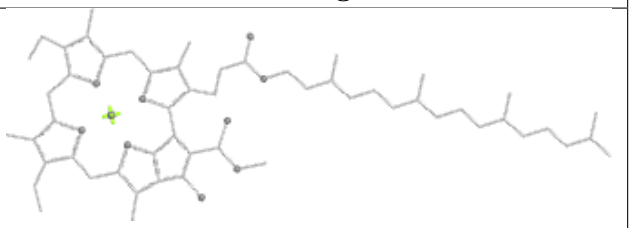
Bond lengths



Bond angles

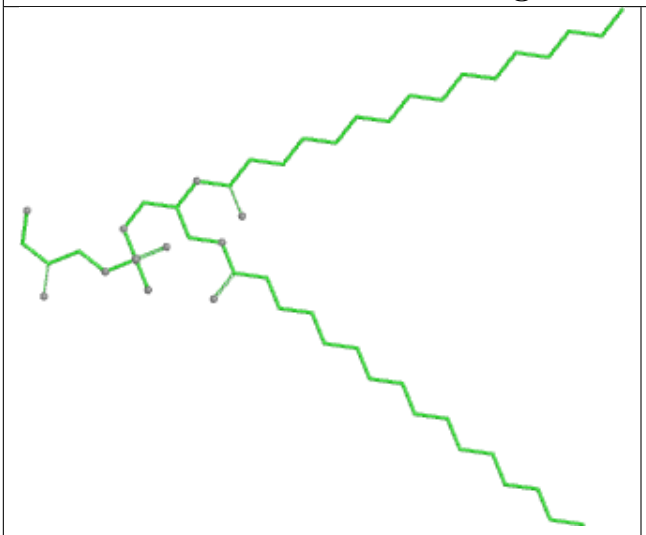


Torsions

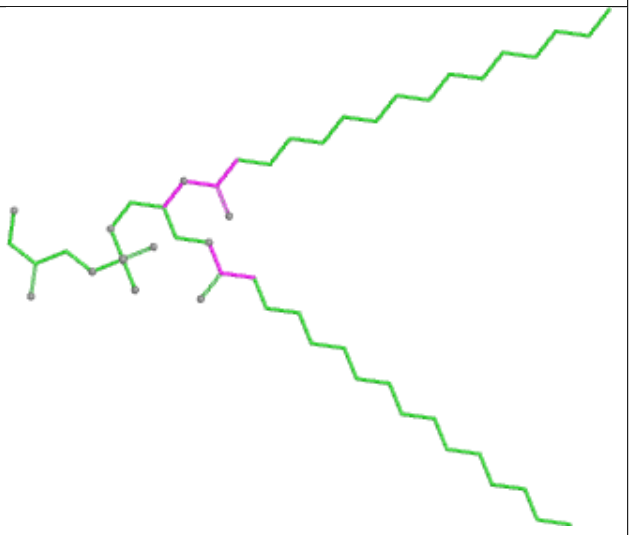


Rings

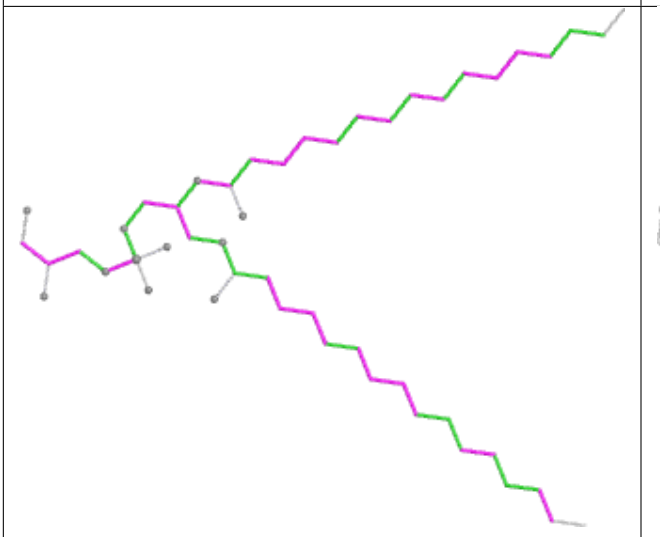
Ligand LHG A 5006



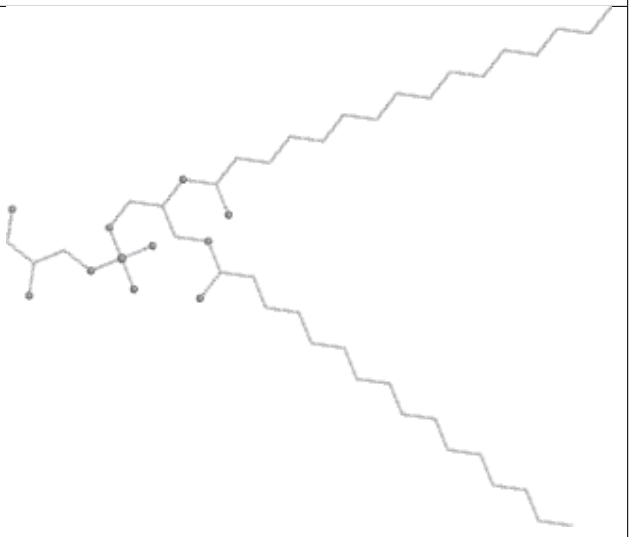
Bond lengths



Bond angles

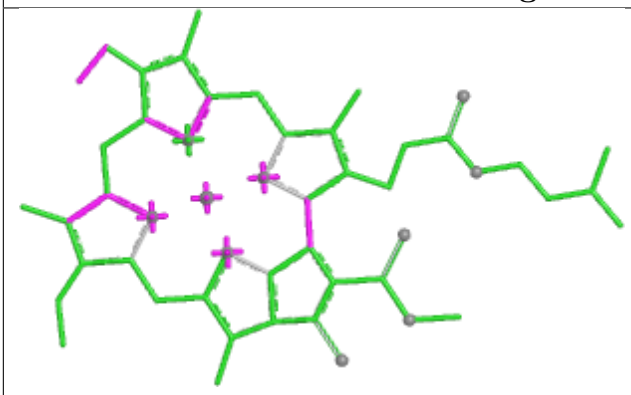


Torsions

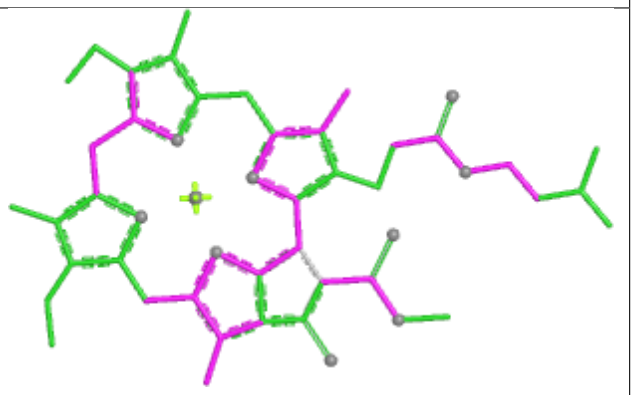


Rings

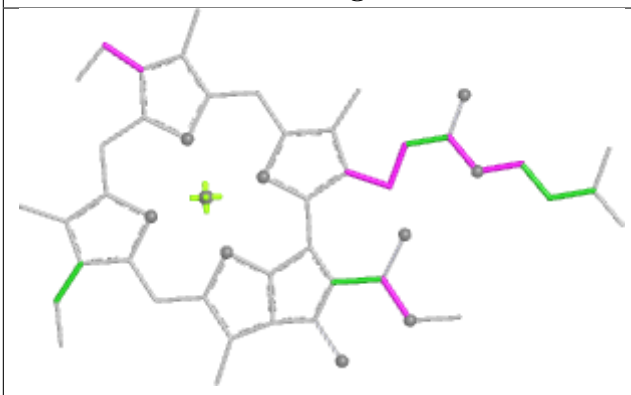
Ligand CLA 2 1236



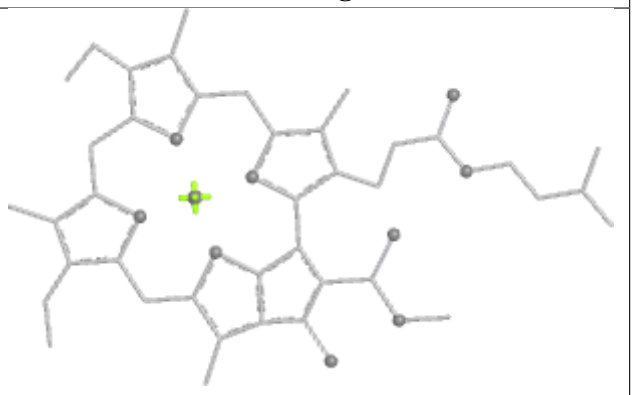
Bond lengths



Bond angles



Torsions

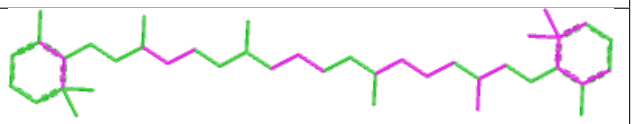


Rings

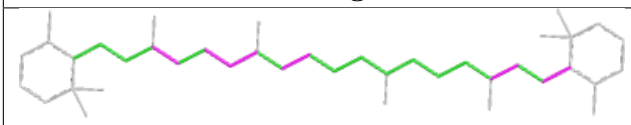
Ligand BCR a 4003



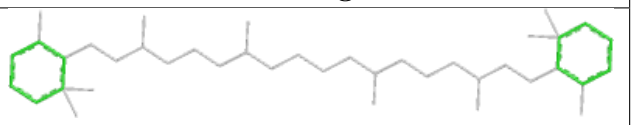
Bond lengths



Bond angles

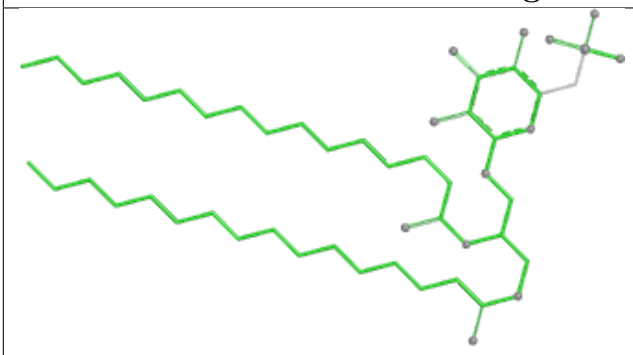


Torsions

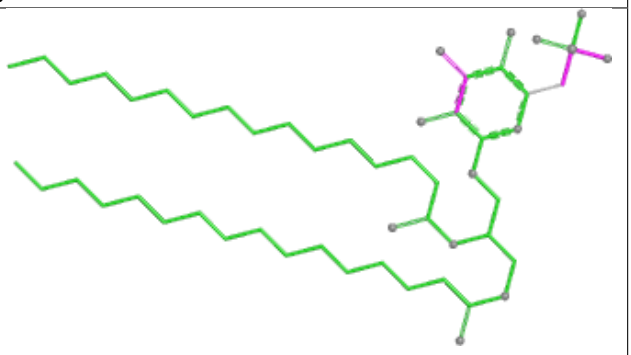


Rings

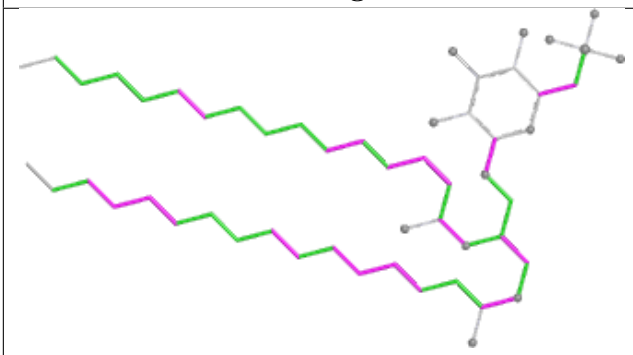
Ligand SQD f 5001



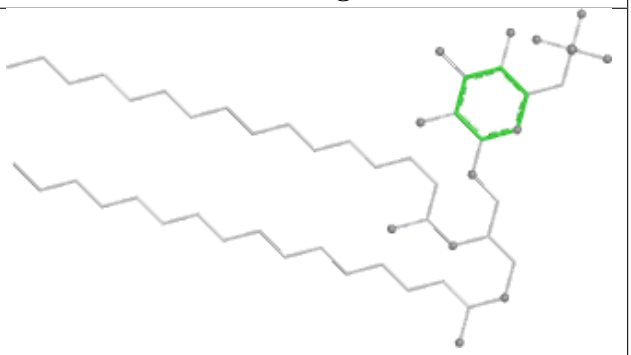
Bond lengths



Bond angles

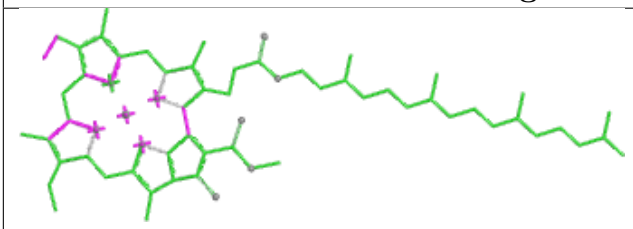


Torsions

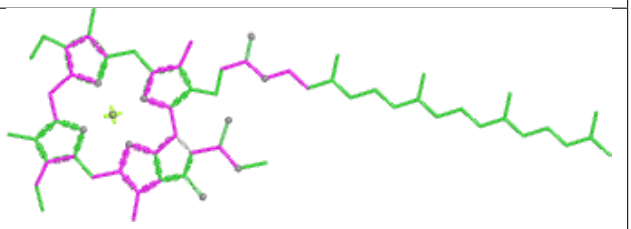


Rings

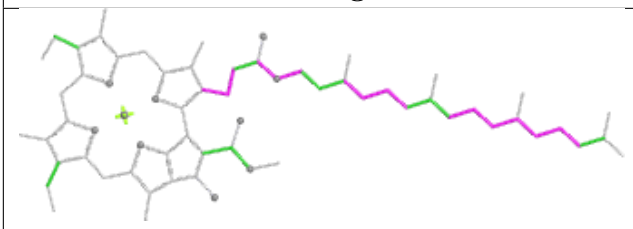
Ligand CLA a 1111



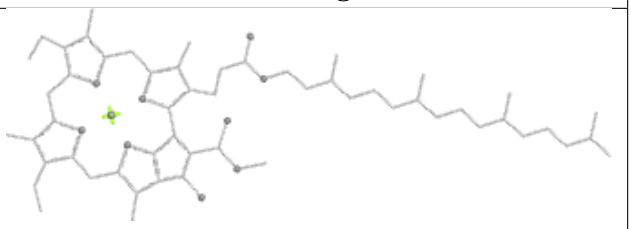
Bond lengths



Bond angles

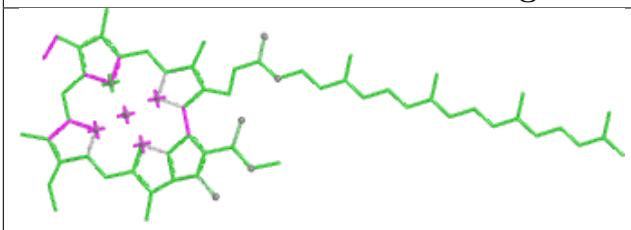


Torsions

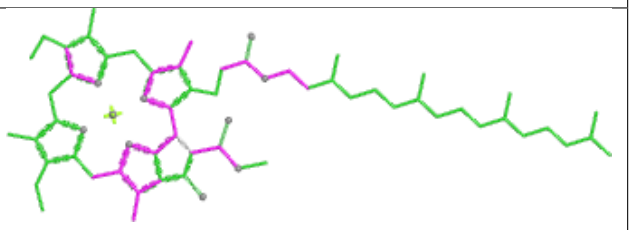


Rings

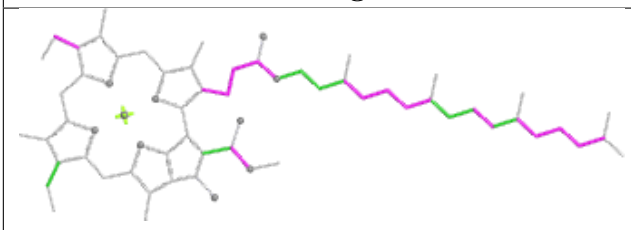
Ligand CLA 1 1127



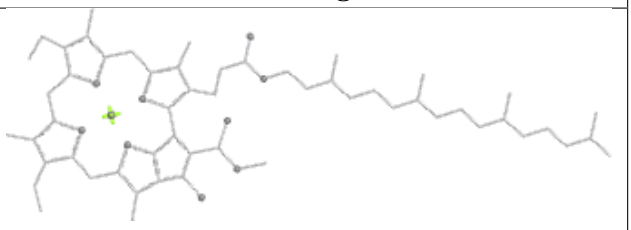
Bond lengths



Bond angles

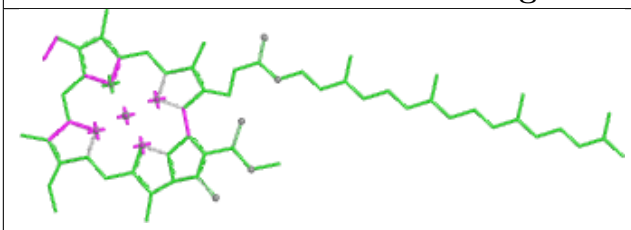


Torsions

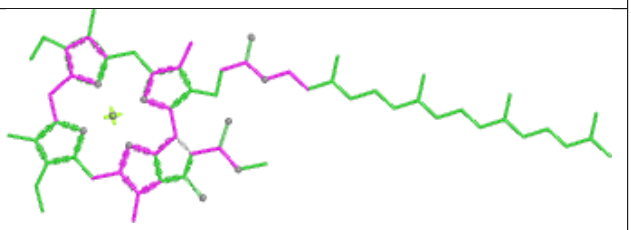


Rings

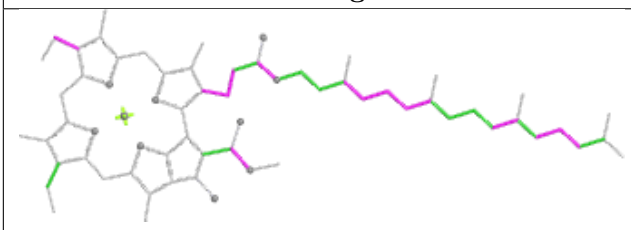
Ligand CLA 1 1116



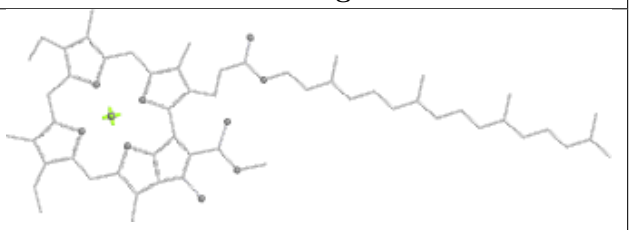
Bond lengths



Bond angles

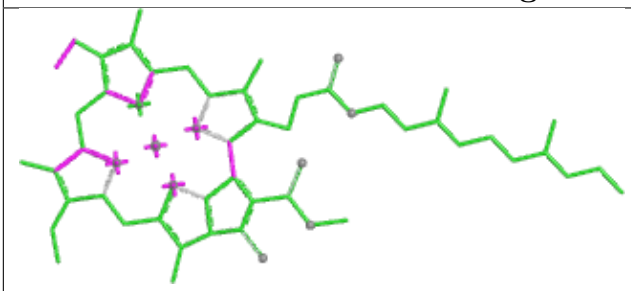


Torsions

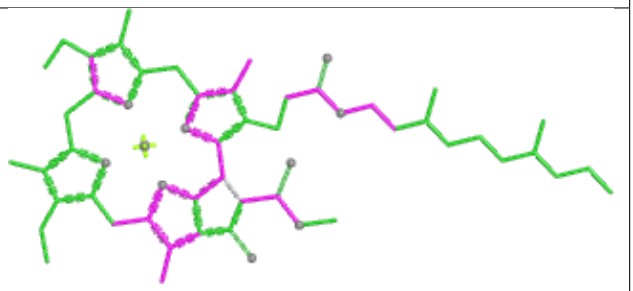


Rings

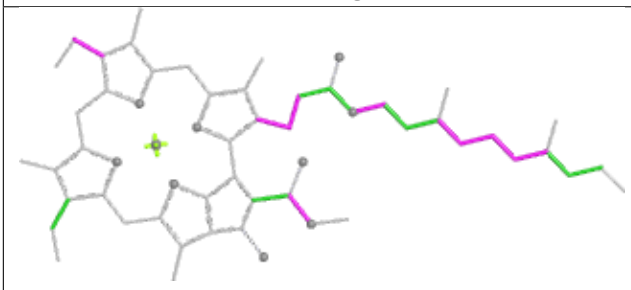
Ligand CLA a 1108



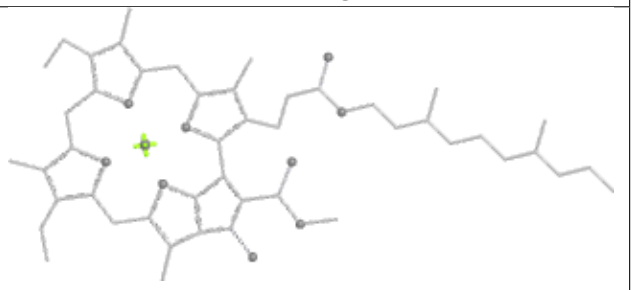
Bond lengths



Bond angles

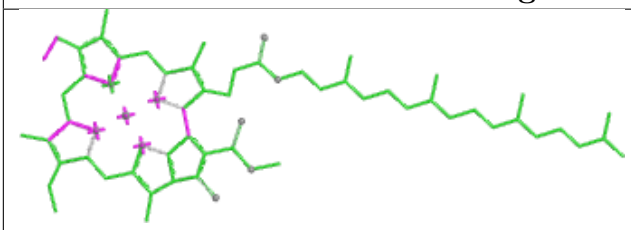


Torsions

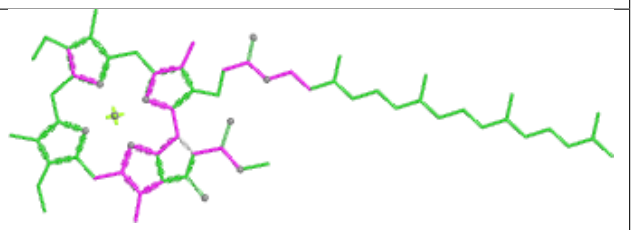


Rings

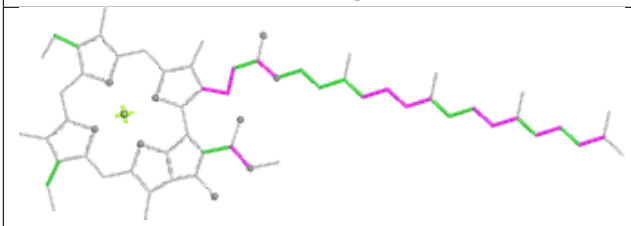
Ligand CLA b 1228



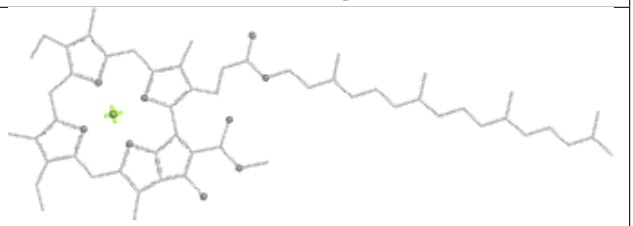
Bond lengths



Bond angles

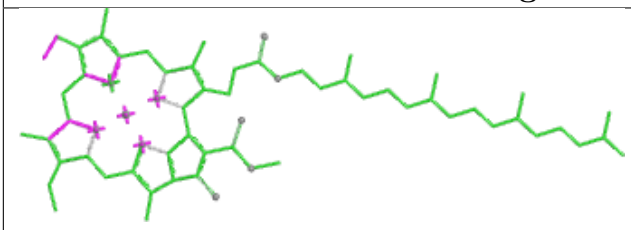


Torsions

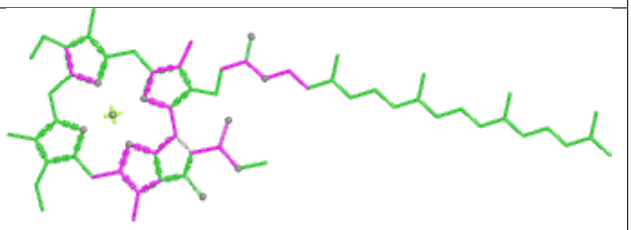


Rings

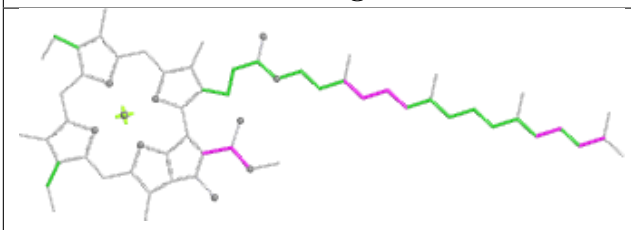
Ligand CLA 1 1132



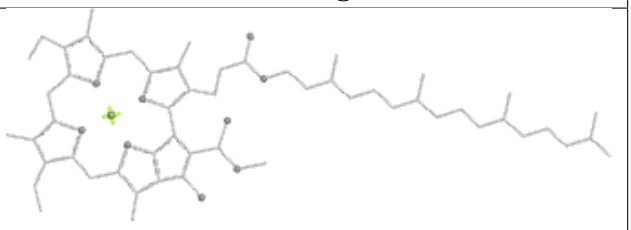
Bond lengths



Bond angles

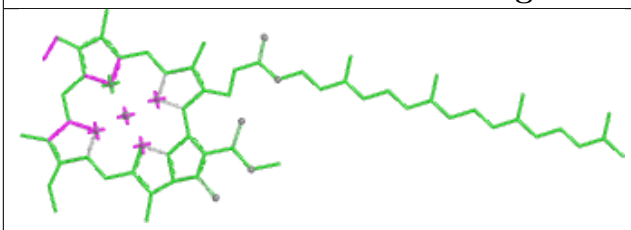


Torsions

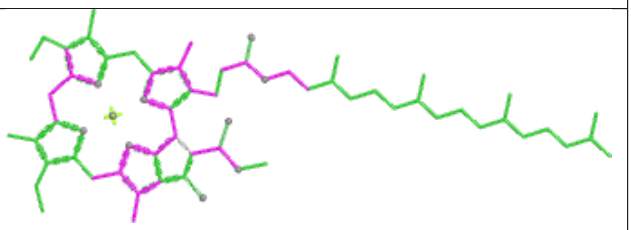


Rings

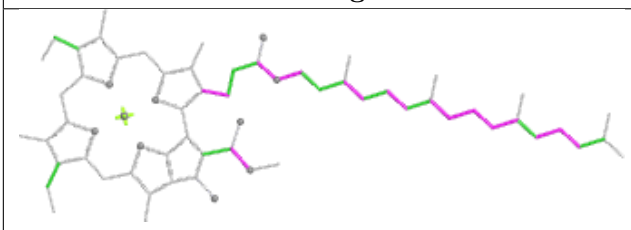
Ligand CLA B 1219



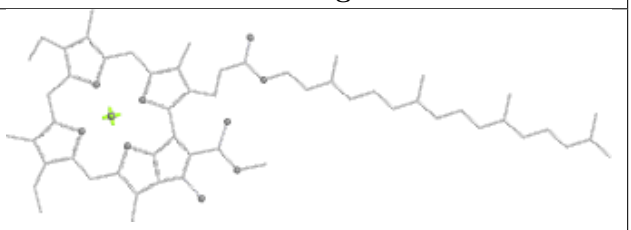
Bond lengths



Bond angles



Torsions

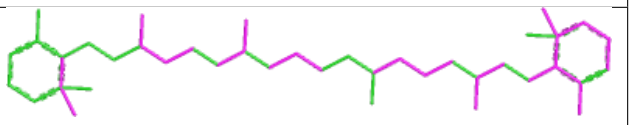


Rings

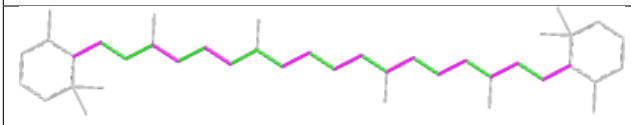
Ligand BCR 1 4002



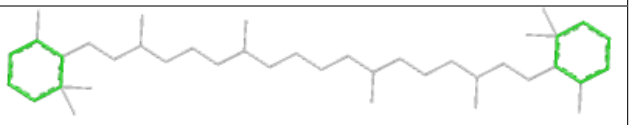
Bond lengths



Bond angles

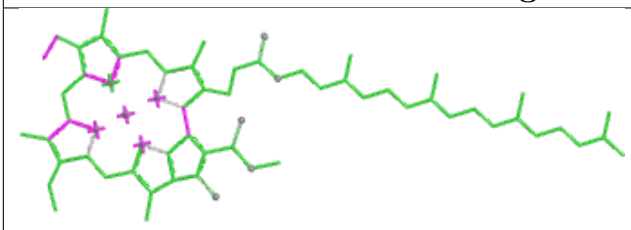


Torsions

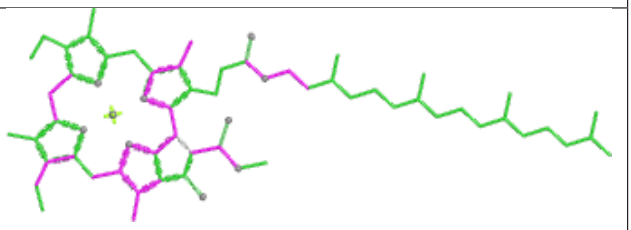


Rings

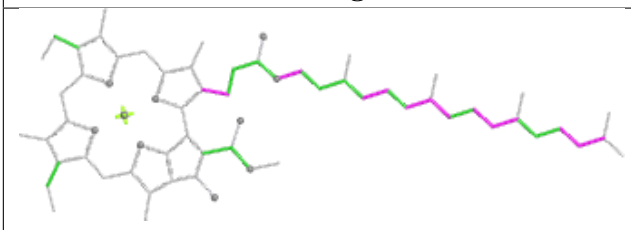
Ligand CLA 1 1111



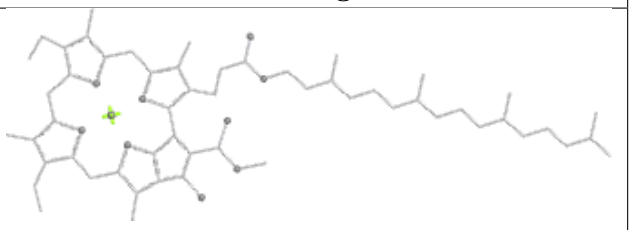
Bond lengths



Bond angles

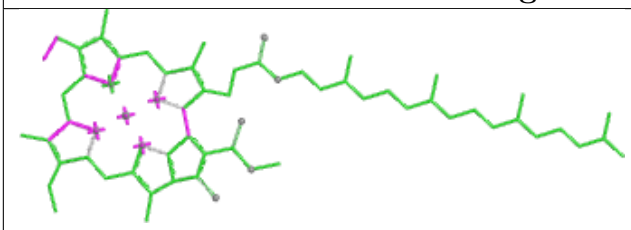


Torsions

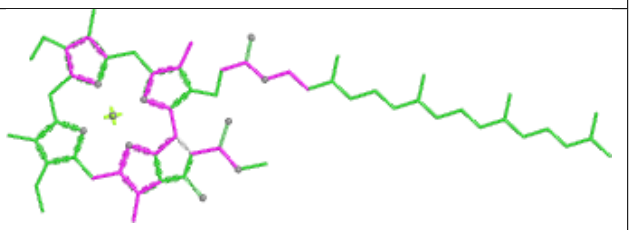


Rings

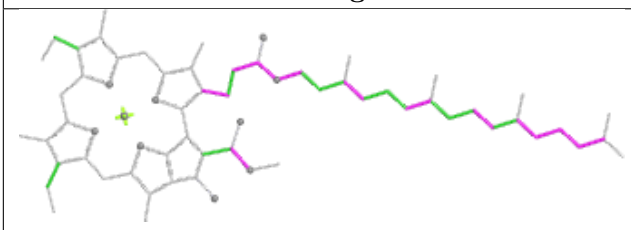
Ligand CLA 1 1126



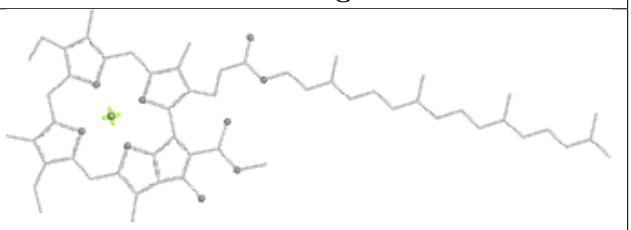
Bond lengths



Bond angles



Torsions

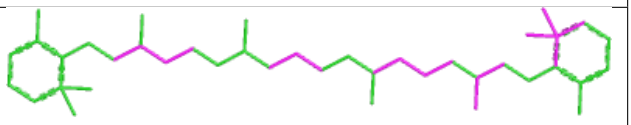


Rings

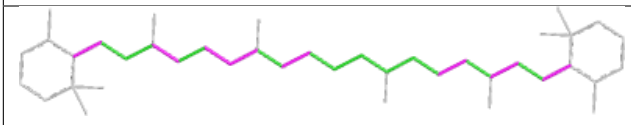
Ligand BCR 1 4012



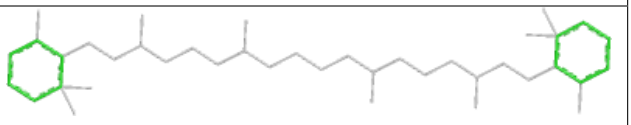
Bond lengths



Bond angles

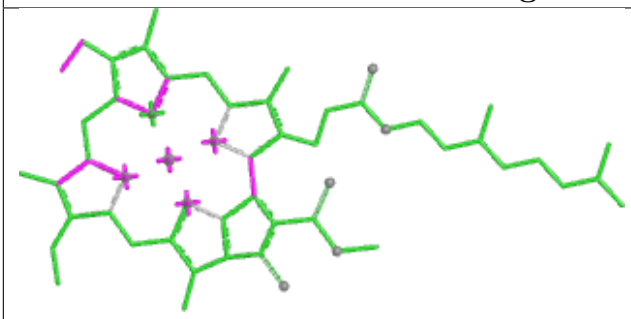


Torsions

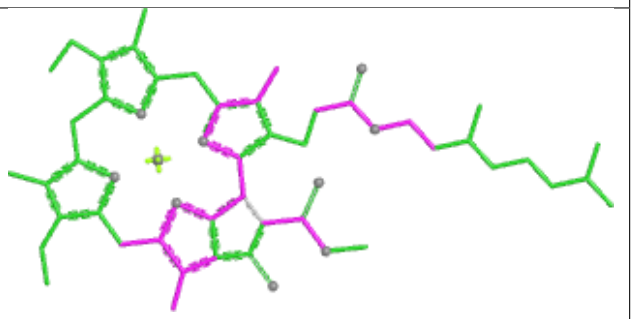


Rings

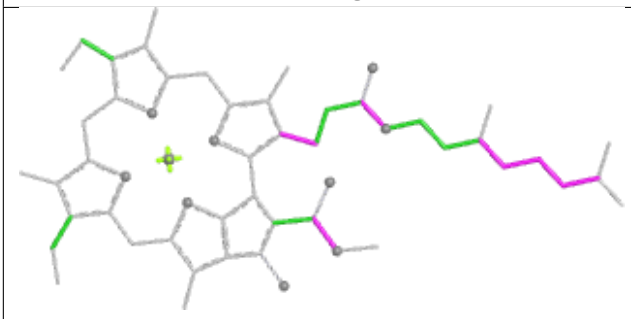
Ligand CLA 1 1121



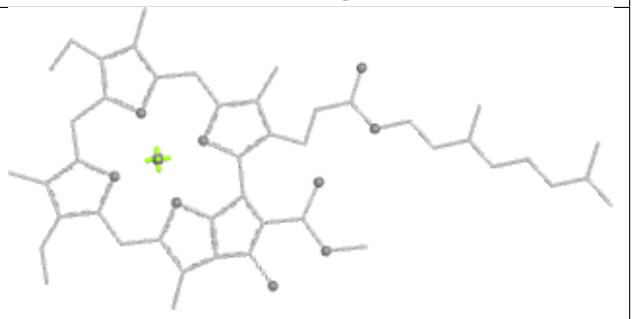
Bond lengths



Bond angles

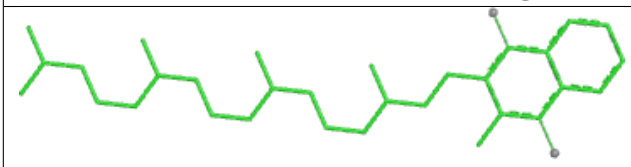


Torsions

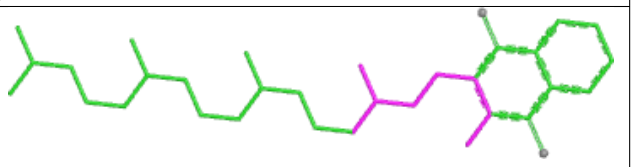


Rings

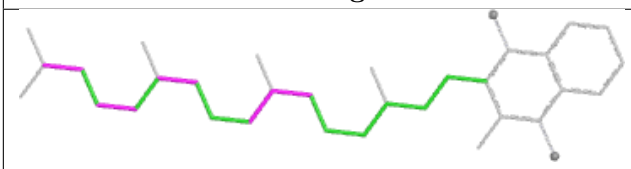
Ligand PQN 2 2002



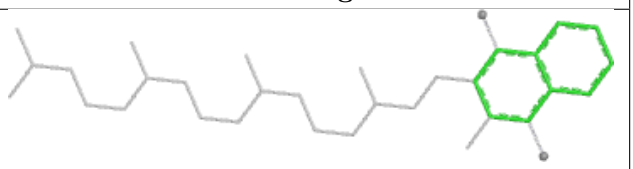
Bond lengths



Bond angles

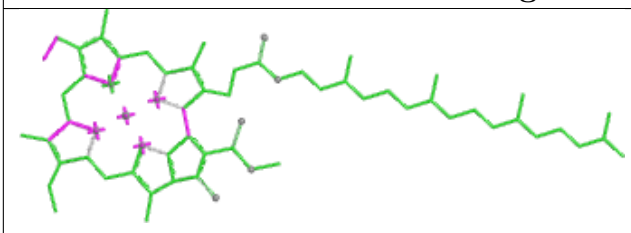


Torsions

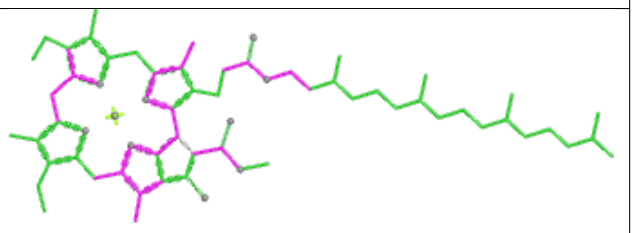


Rings

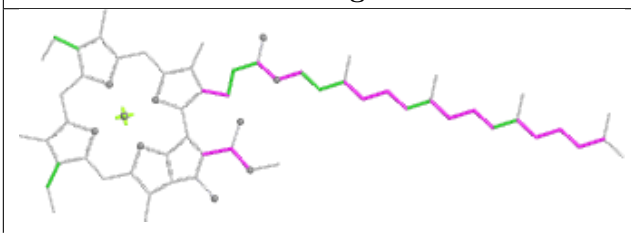
Ligand CLA 1 1134



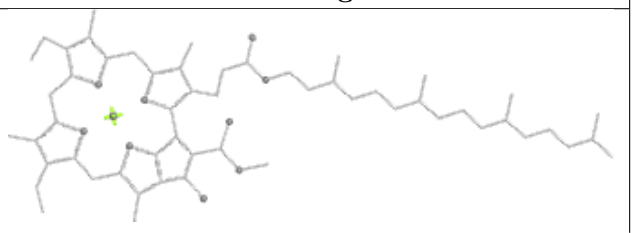
Bond lengths



Bond angles

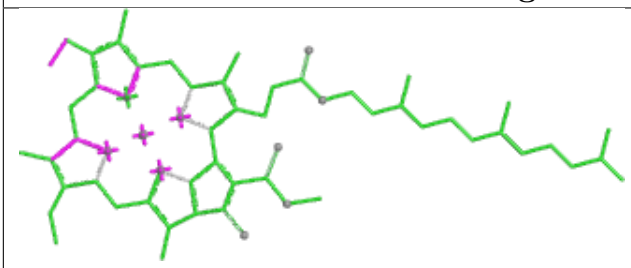


Torsions

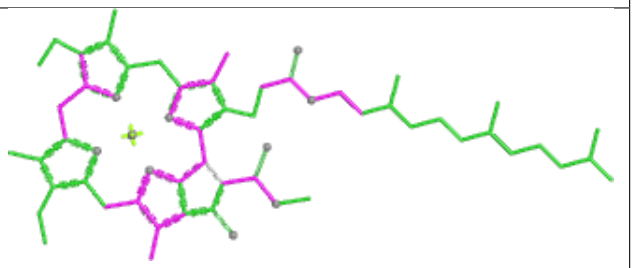


Rings

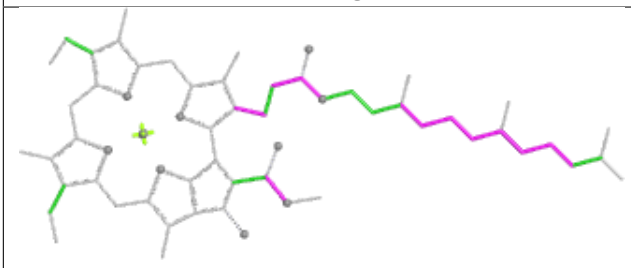
Ligand CLA b 1219



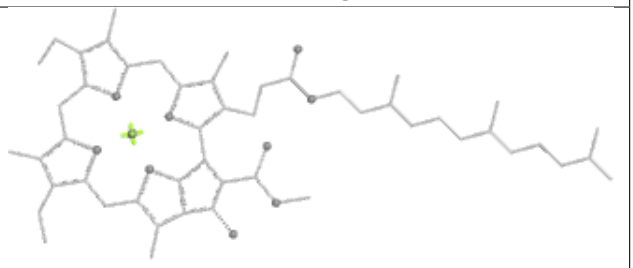
Bond lengths



Bond angles

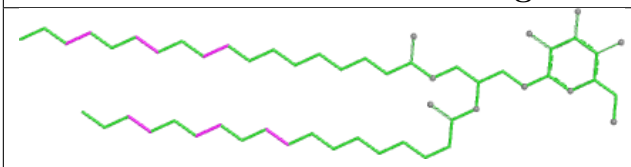


Torsions

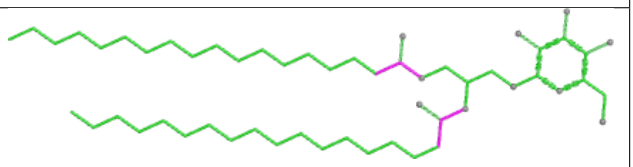


Rings

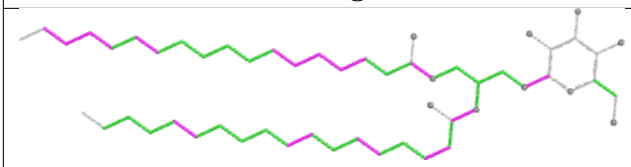
Ligand LMG 2 5005



Bond lengths



Bond angles

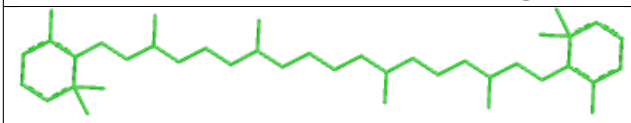


Torsions

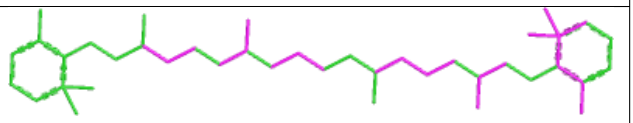


Rings

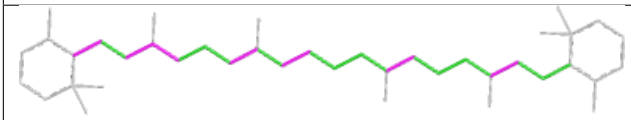
Ligand BCR 2 4004



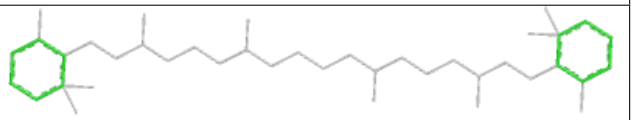
Bond lengths



Bond angles

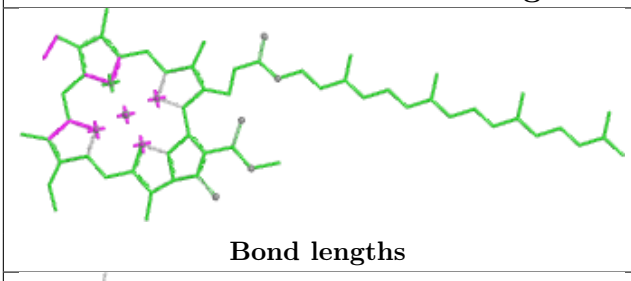


Torsions

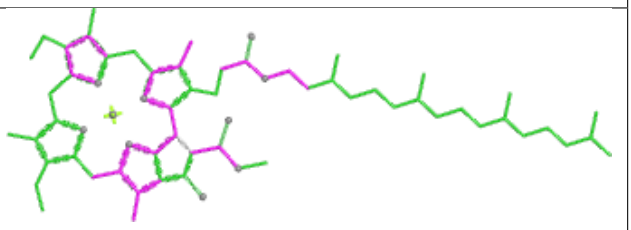


Rings

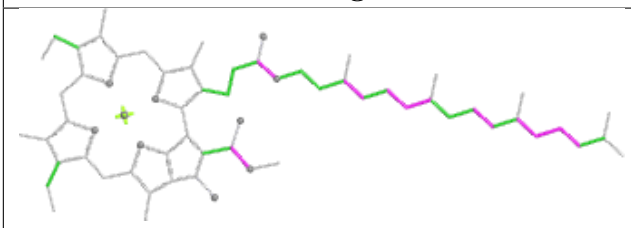
Ligand CLA l 1502



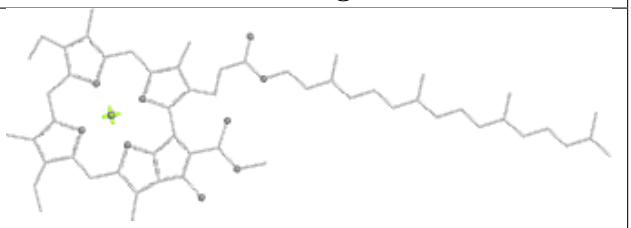
Bond lengths



Bond angles

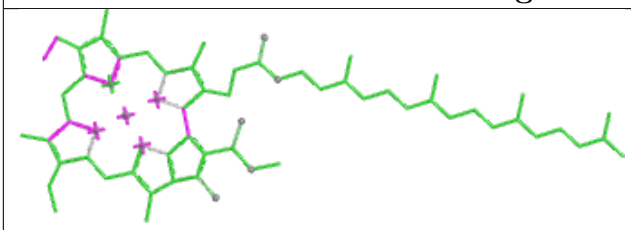


Torsions

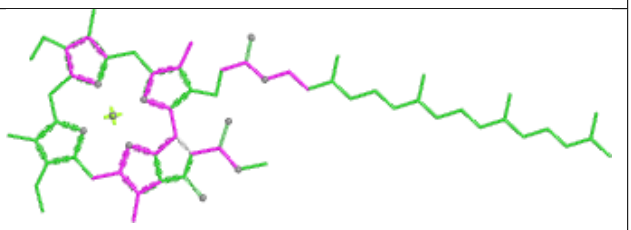


Rings

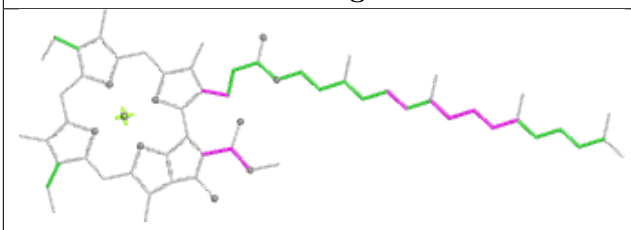
Ligand CLA B 1234



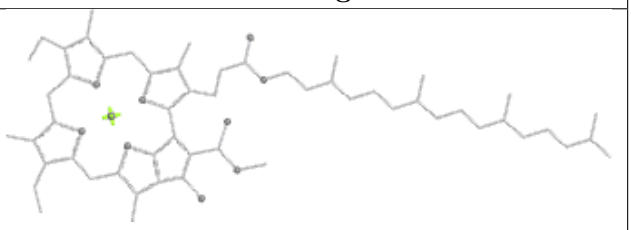
Bond lengths



Bond angles



Torsions

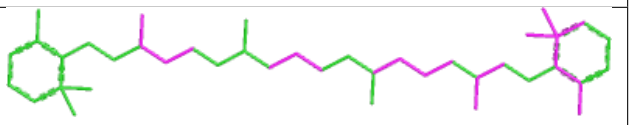


Rings

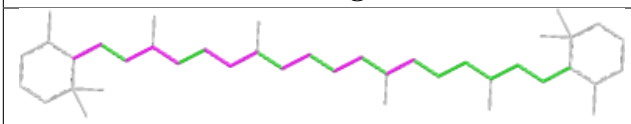
Ligand BCR J 4013



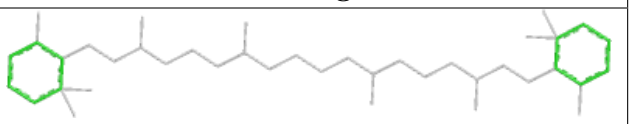
Bond lengths



Bond angles

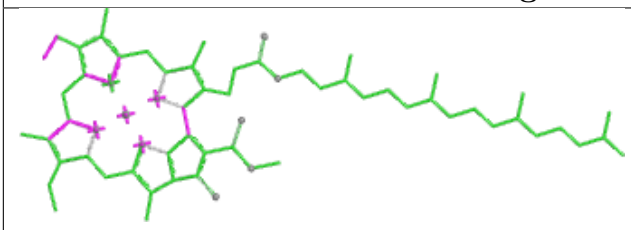


Torsions

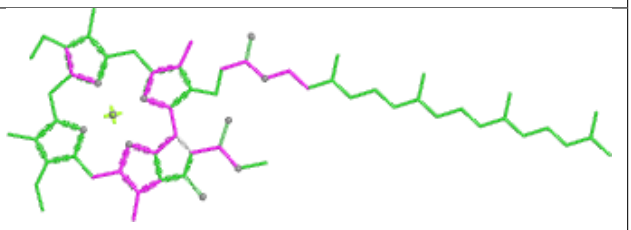


Rings

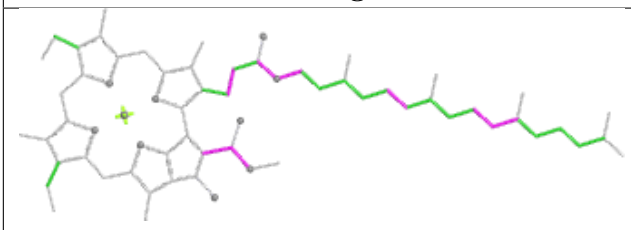
Ligand CLA a 1102



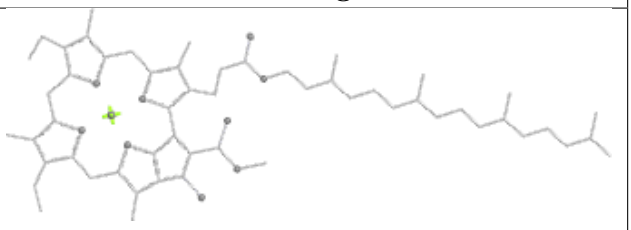
Bond lengths



Bond angles

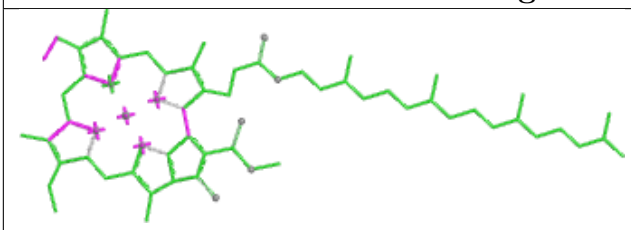


Torsions

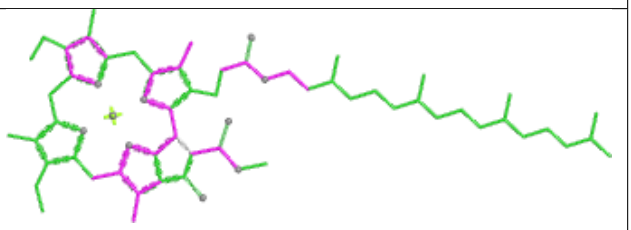


Rings

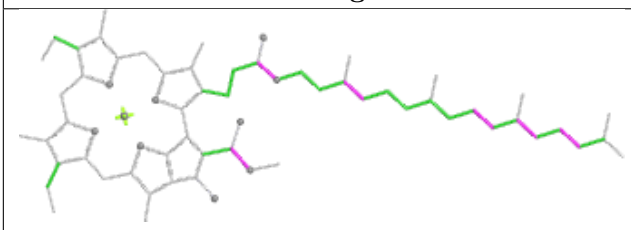
Ligand CLA b 1223



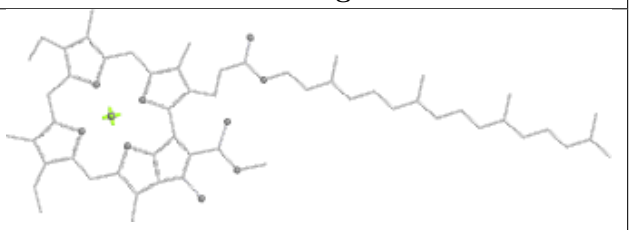
Bond lengths



Bond angles

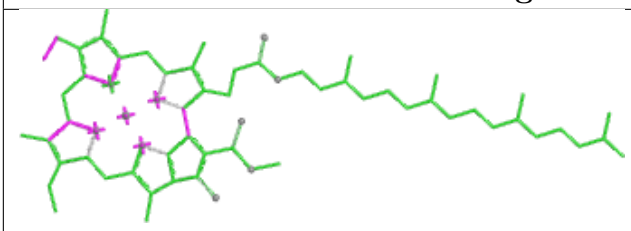


Torsions

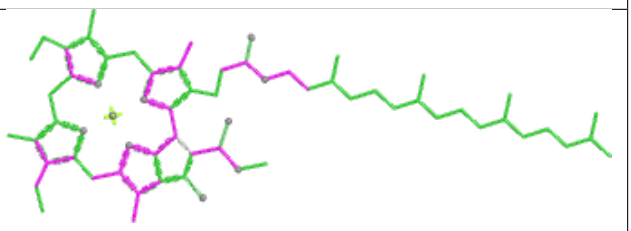


Rings

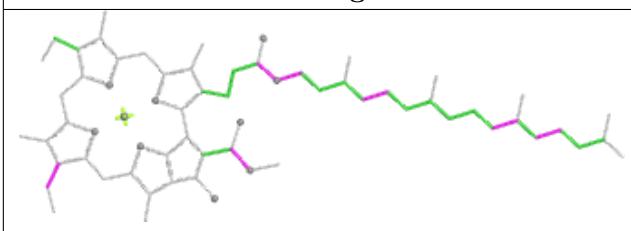
Ligand CLA B 1207



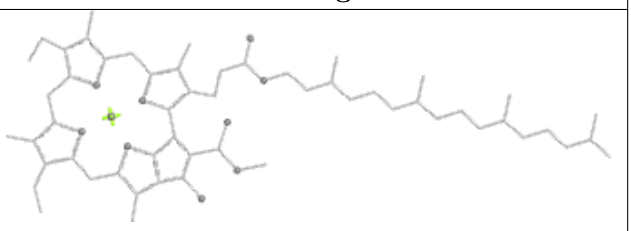
Bond lengths



Bond angles

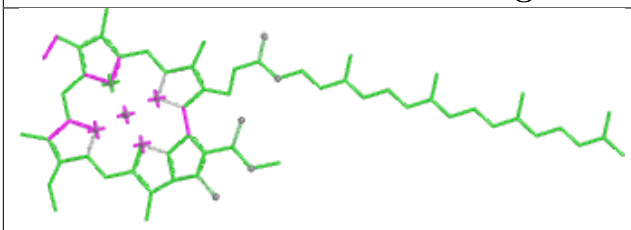


Torsions

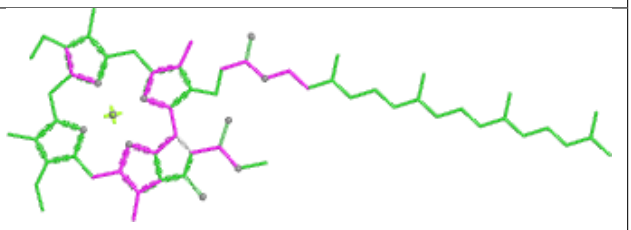


Rings

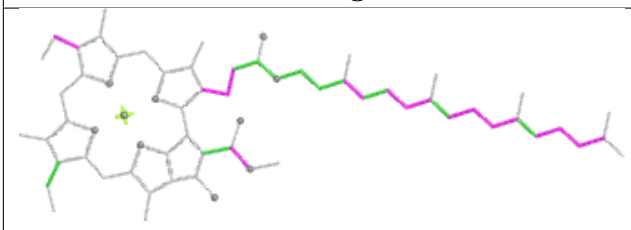
Ligand CLA B 1224



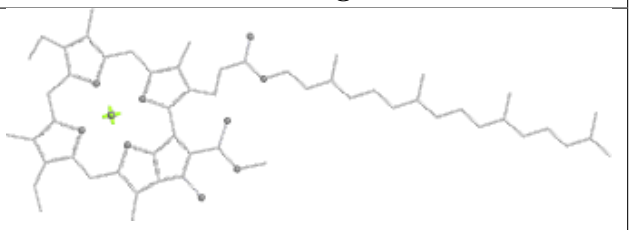
Bond lengths



Bond angles

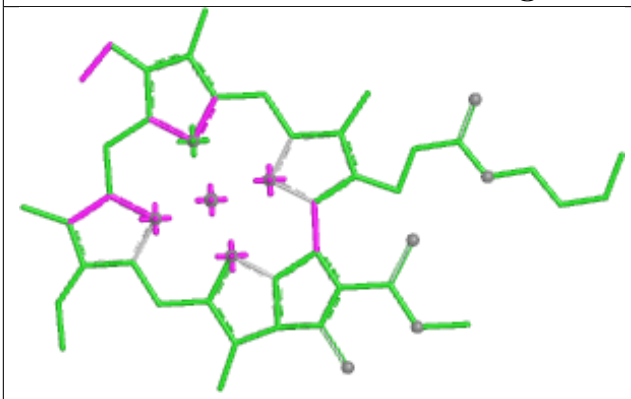


Torsions

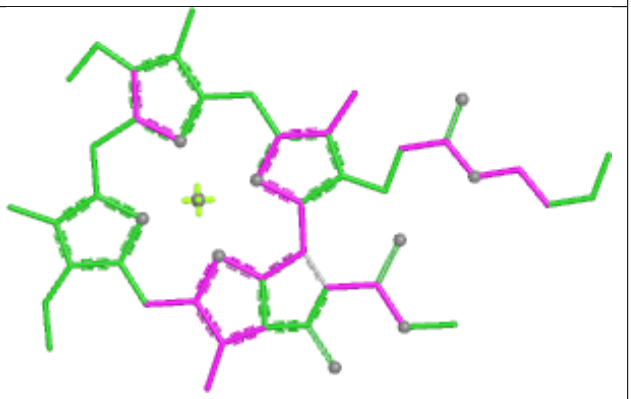


Rings

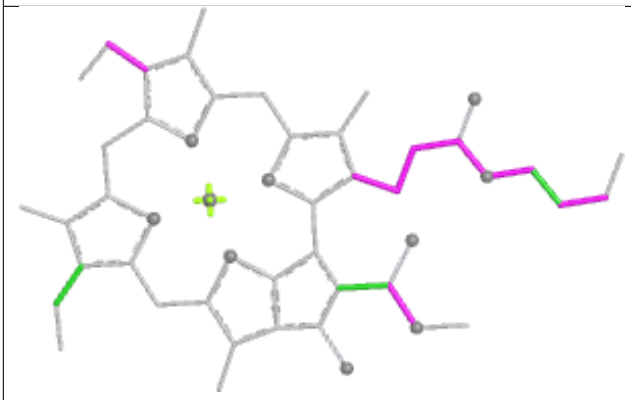
Ligand CLA k 1402



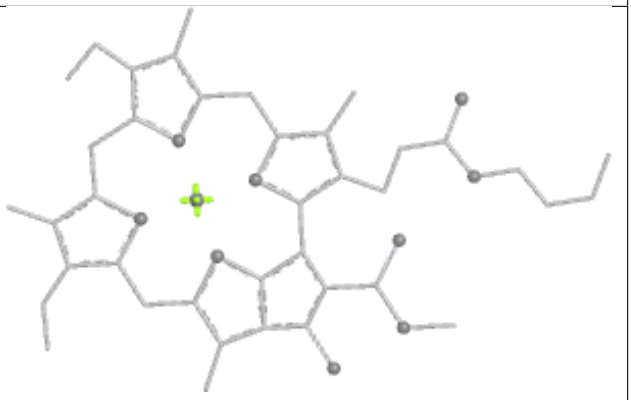
Bond lengths



Bond angles

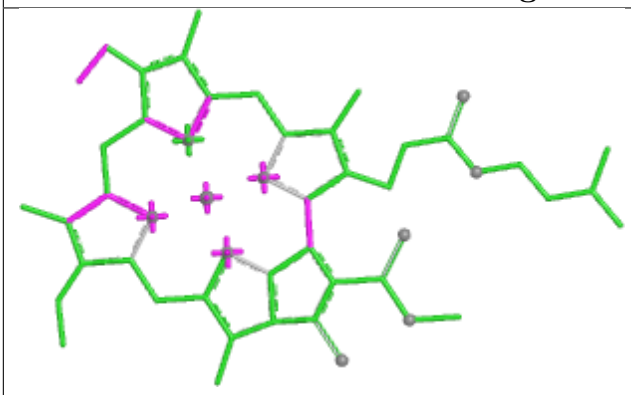


Torsions

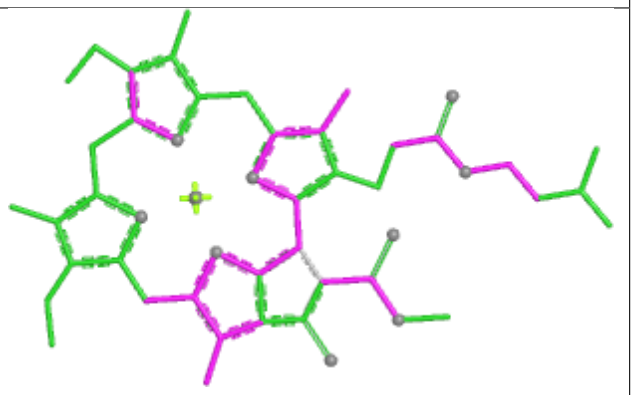


Rings

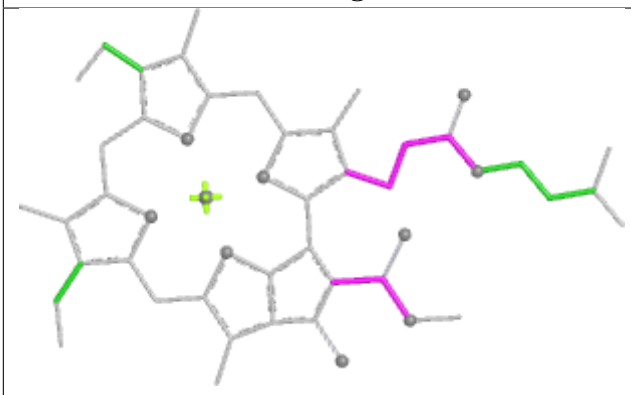
Ligand CLA 2 1211



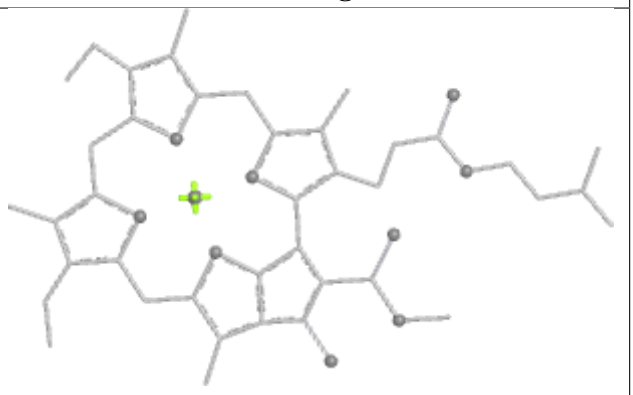
Bond lengths



Bond angles

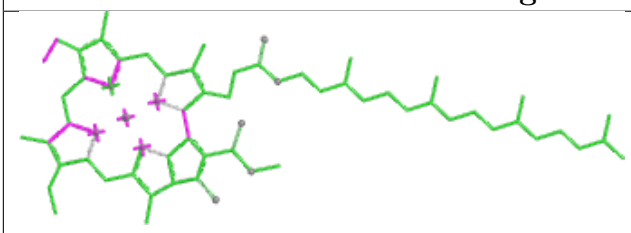


Torsions

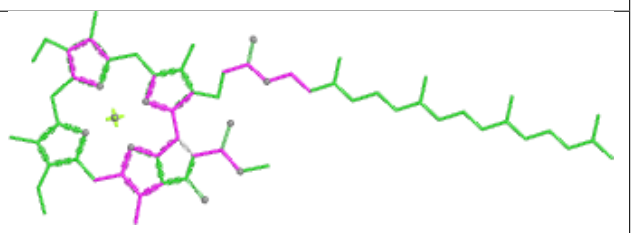


Rings

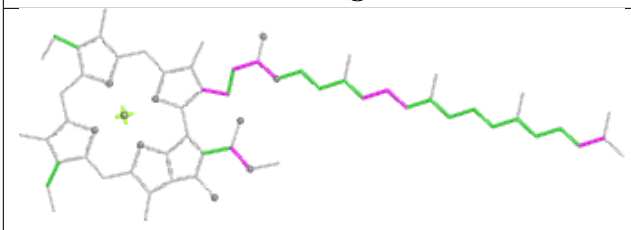
Ligand CLA 1 1011



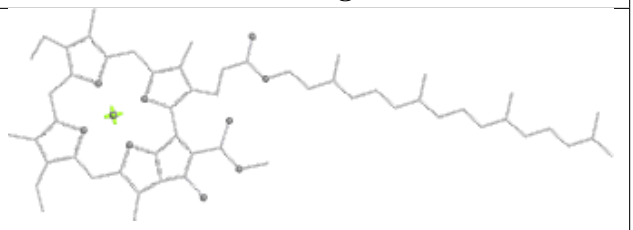
Bond lengths



Bond angles

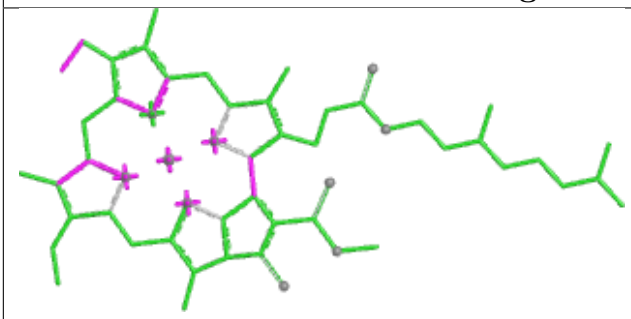


Torsions

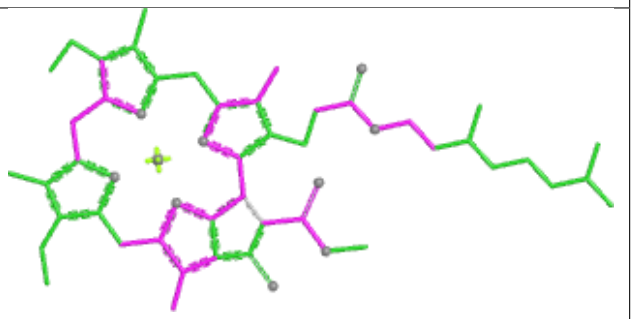


Rings

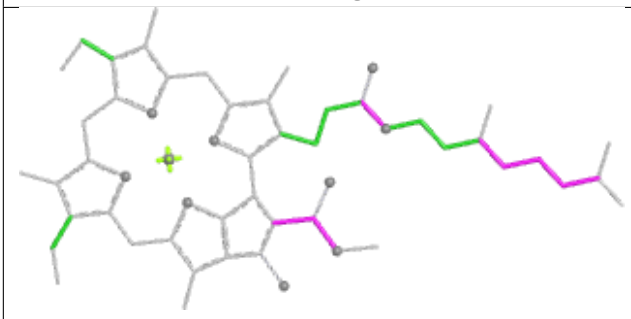
Ligand CLA 2 1226



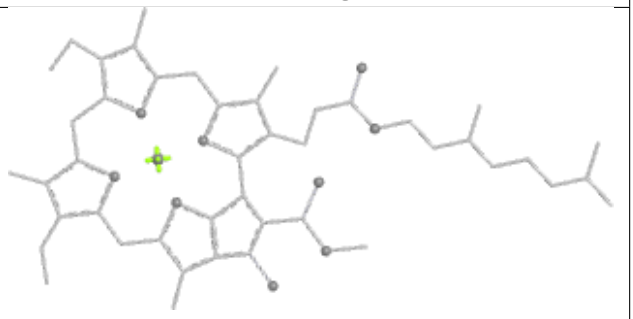
Bond lengths



Bond angles

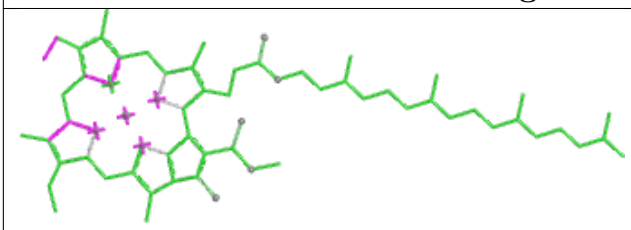


Torsions

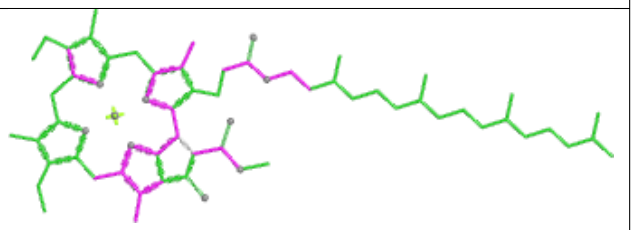


Rings

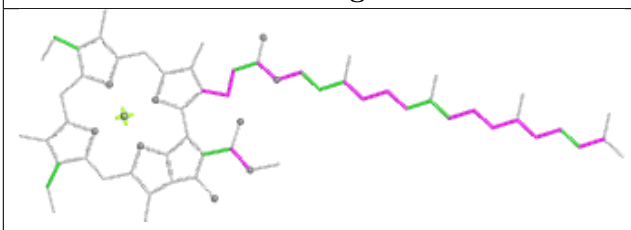
Ligand CLA 0 1503



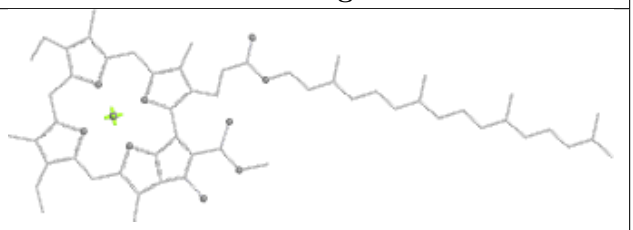
Bond lengths



Bond angles

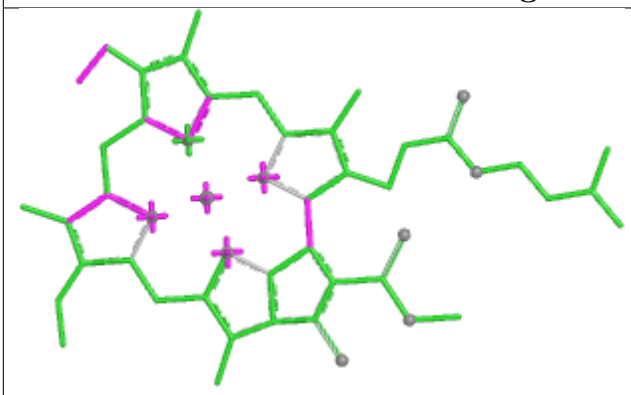


Torsions

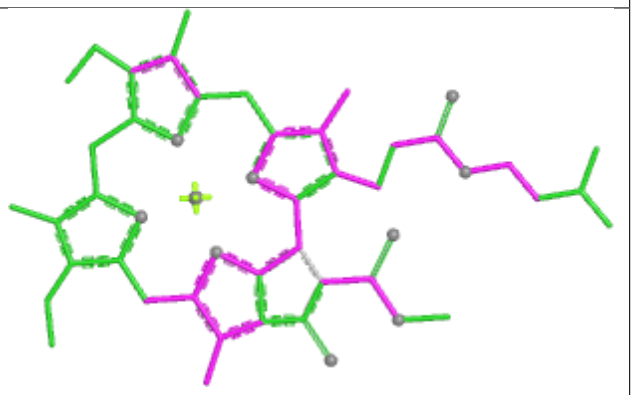


Rings

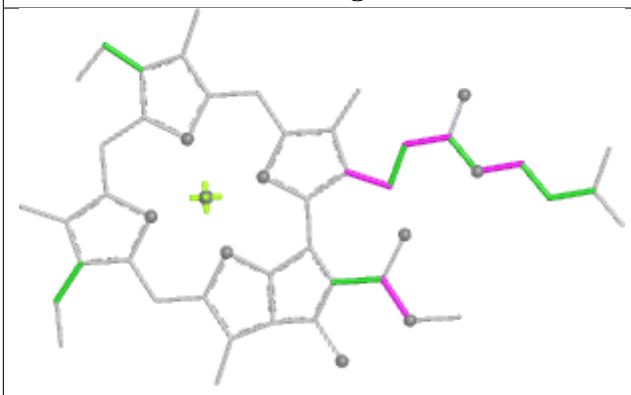
Ligand CLA a 1107



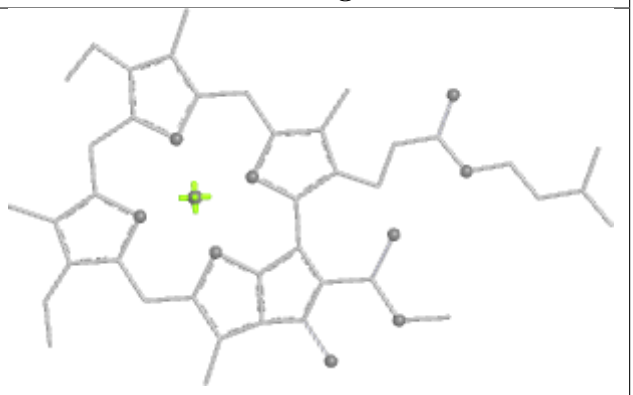
Bond lengths



Bond angles

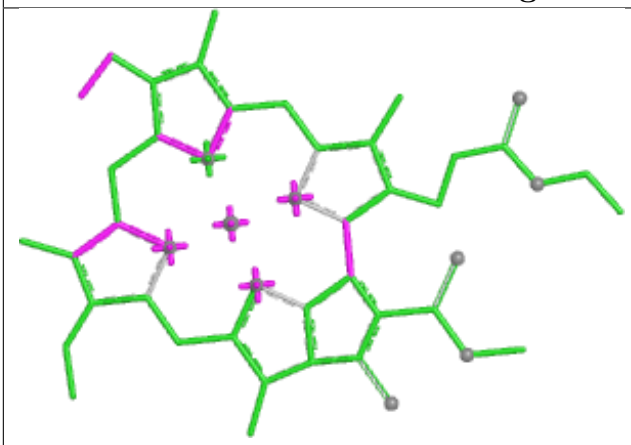


Torsions

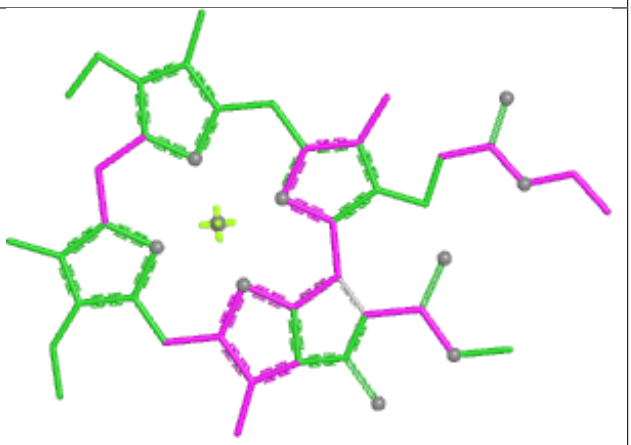


Rings

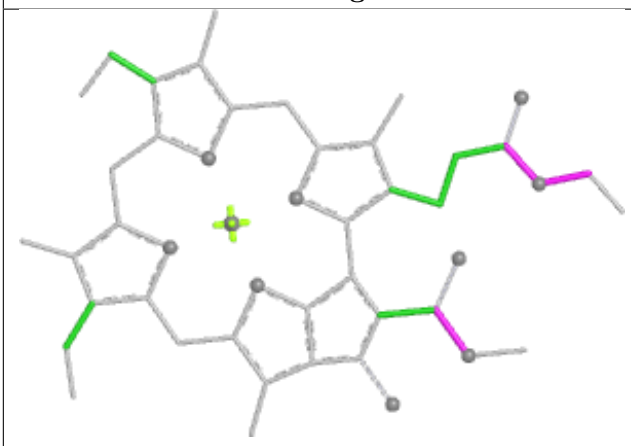
Ligand CLA 6 1301



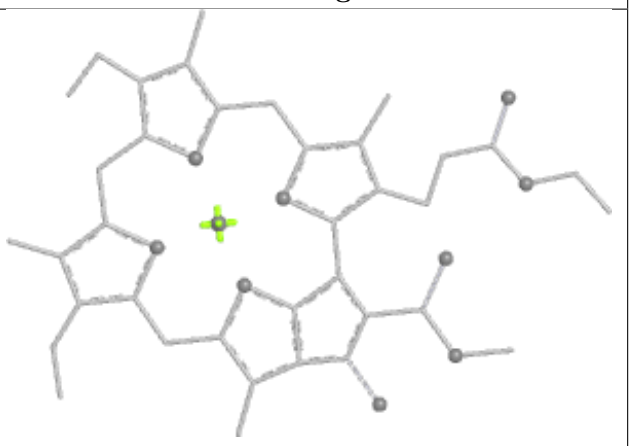
Bond lengths



Bond angles

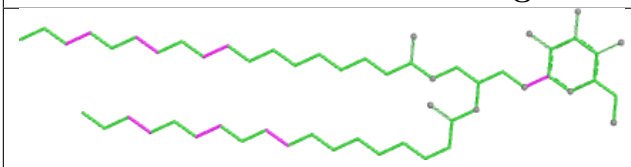


Torsions

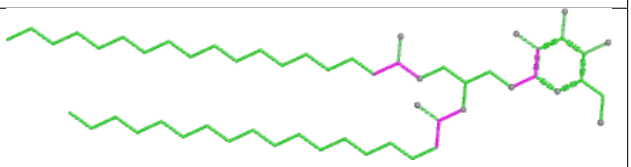


Rings

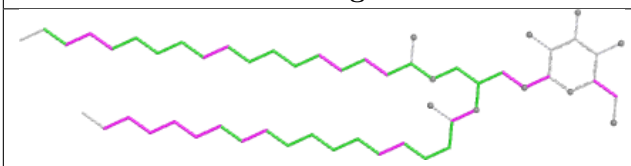
Ligand LMG b 5007



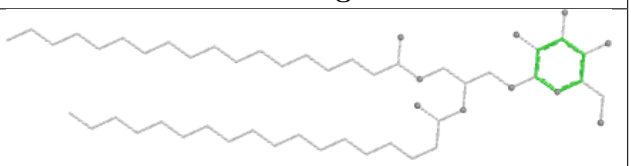
Bond lengths



Bond angles

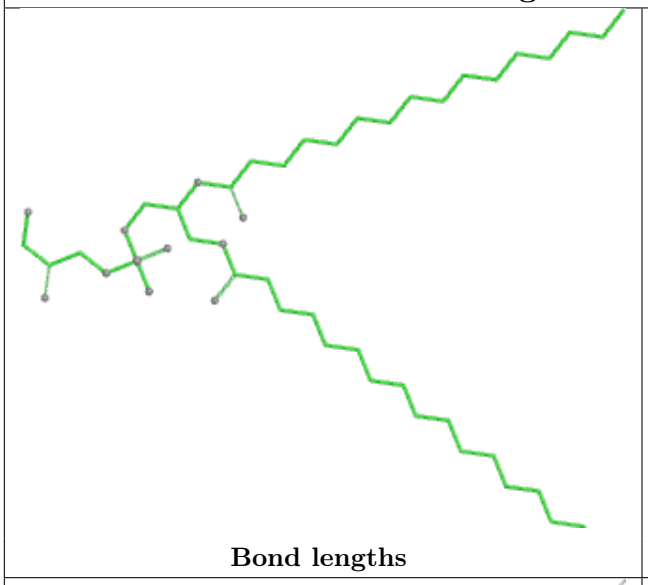


Torsions

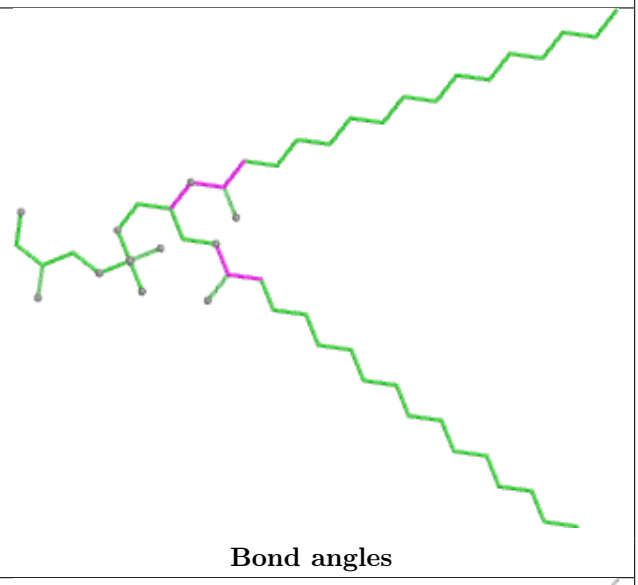


Rings

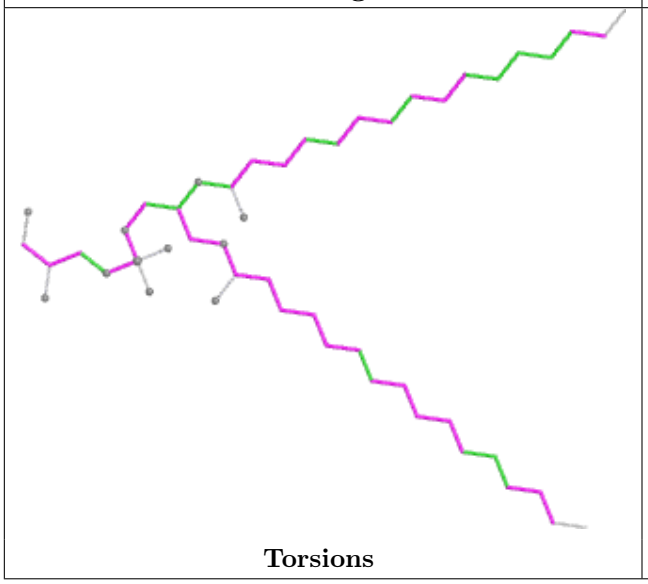
Ligand LHG a 5007



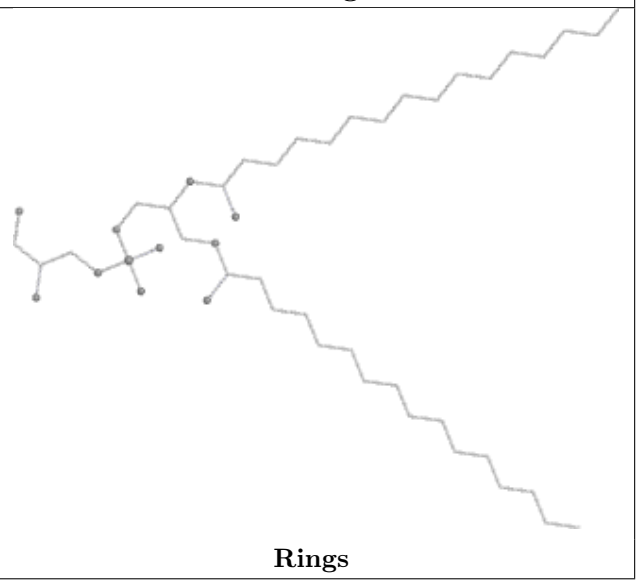
Bond lengths



Bond angles

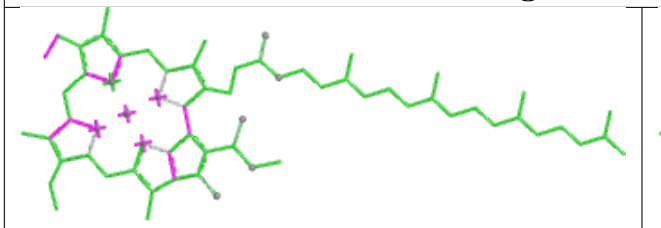


Torsions

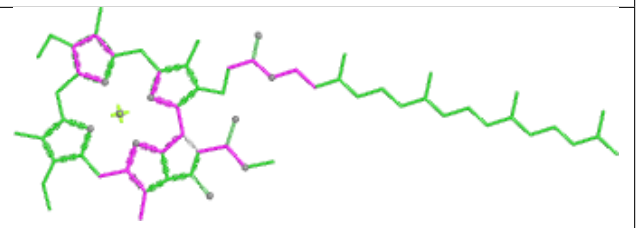


Rings

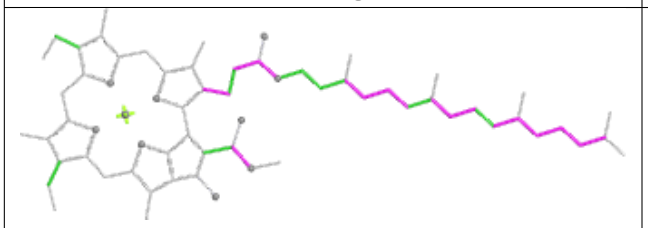
Ligand CLA b 1021



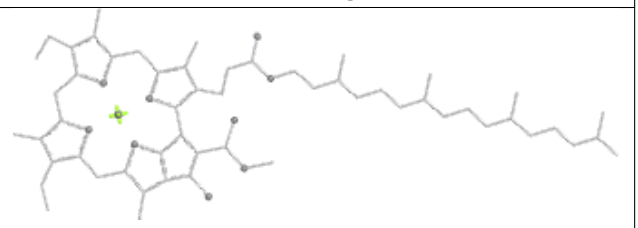
Bond lengths



Bond angles

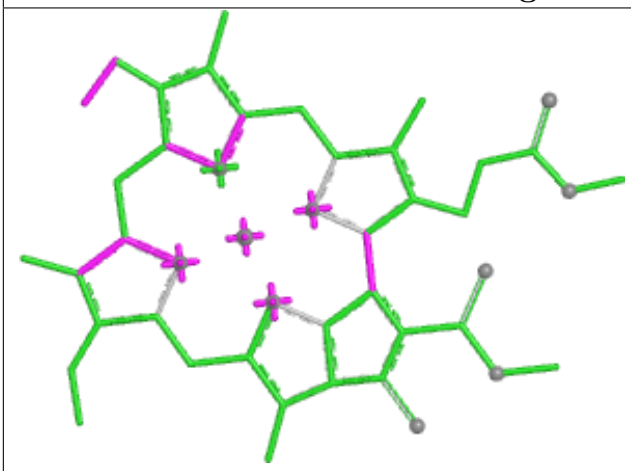


Torsions

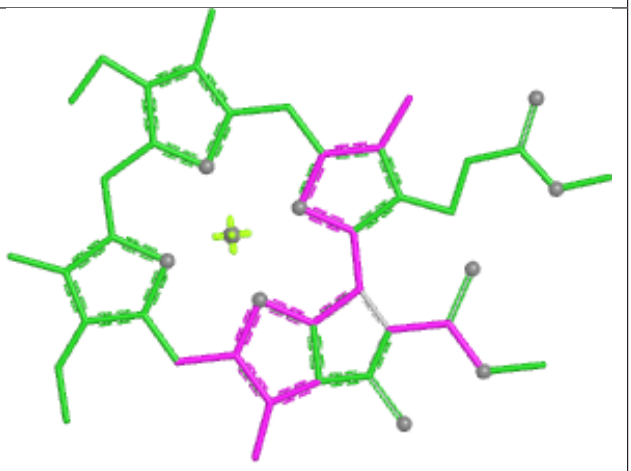


Rings

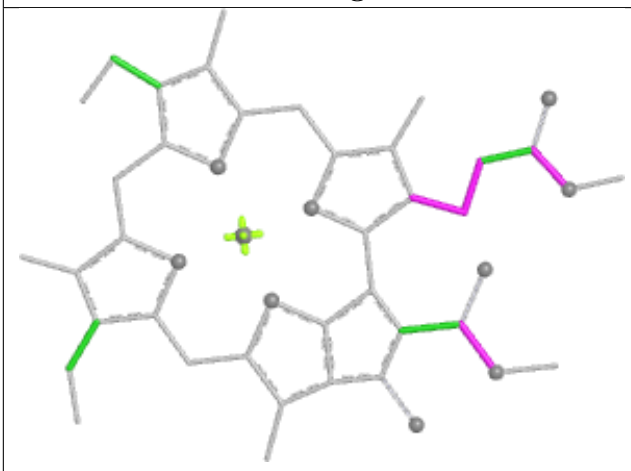
Ligand CLA 8 1402



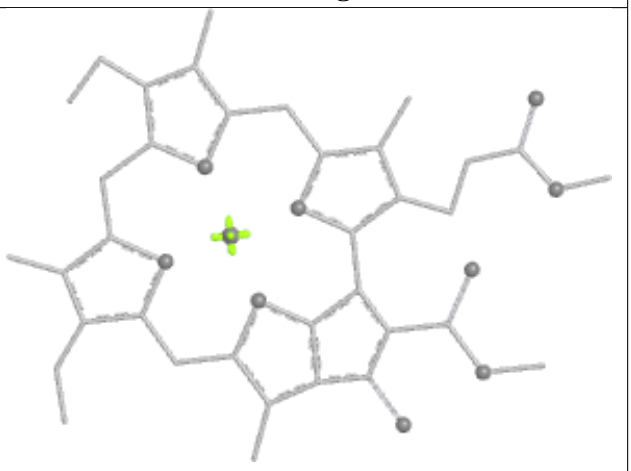
Bond lengths



Bond angles

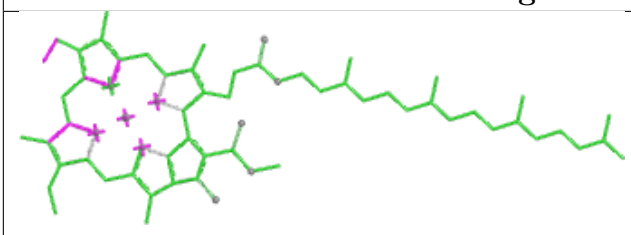


Torsions

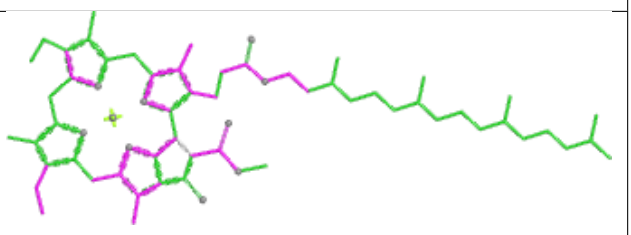


Rings

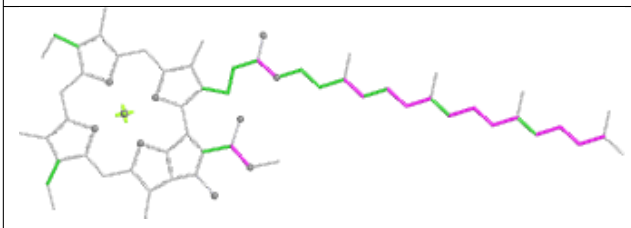
Ligand CLA b 1222



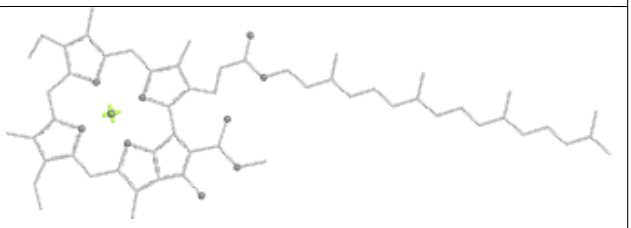
Bond lengths



Bond angles

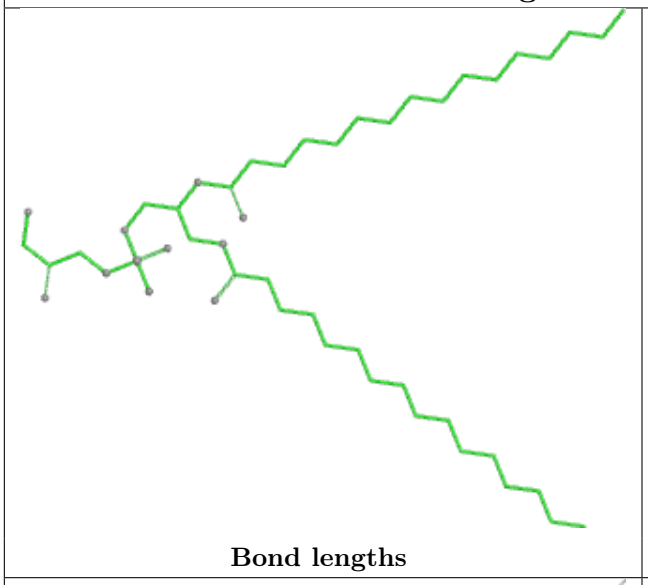


Torsions

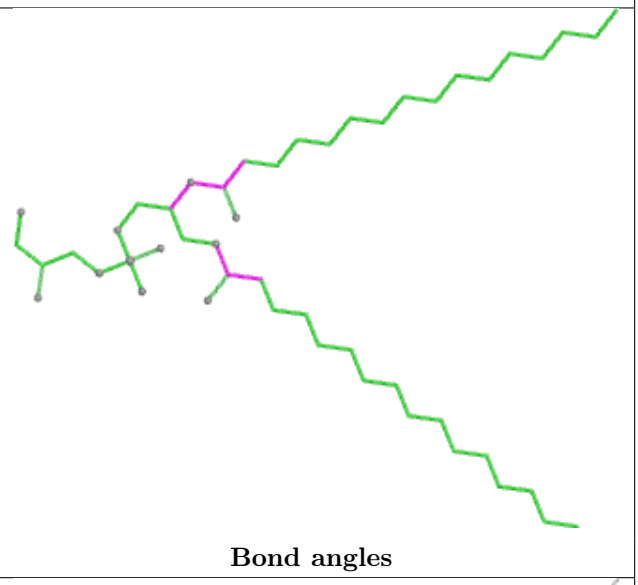


Rings

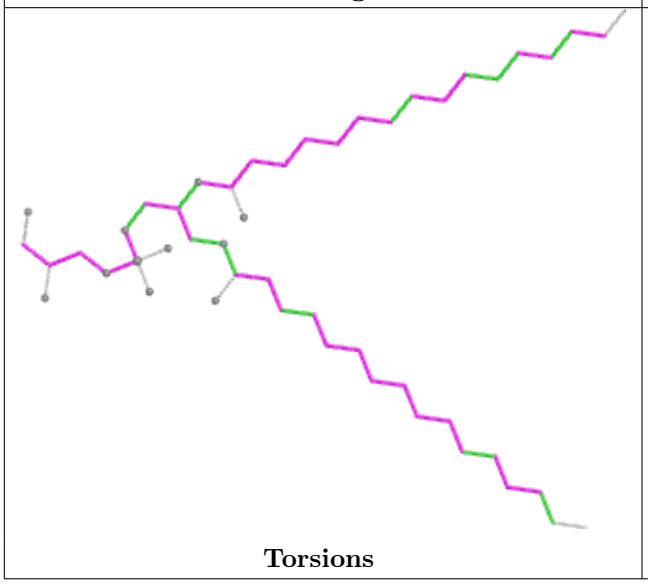
Ligand LHG a 5003



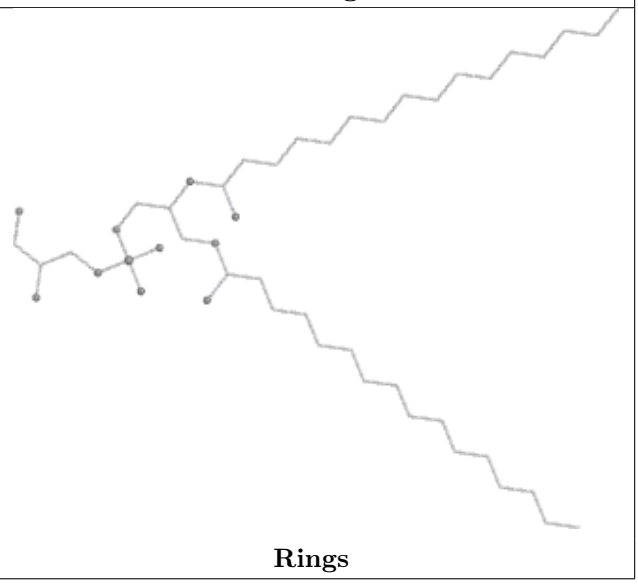
Bond lengths



Bond angles

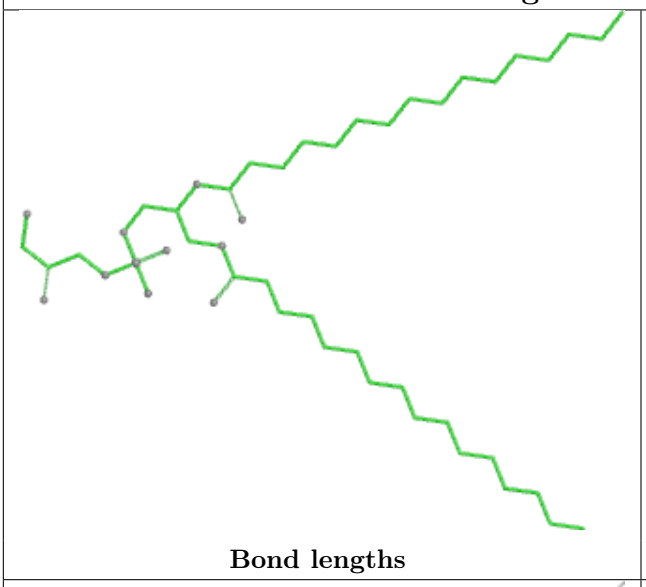


Torsions

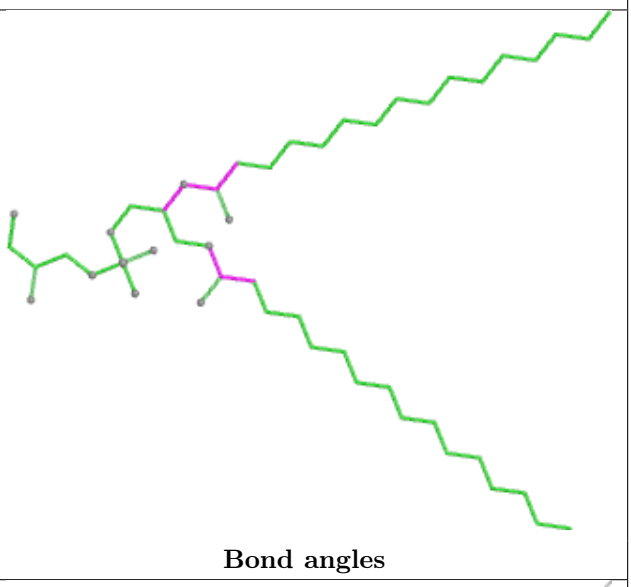


Rings

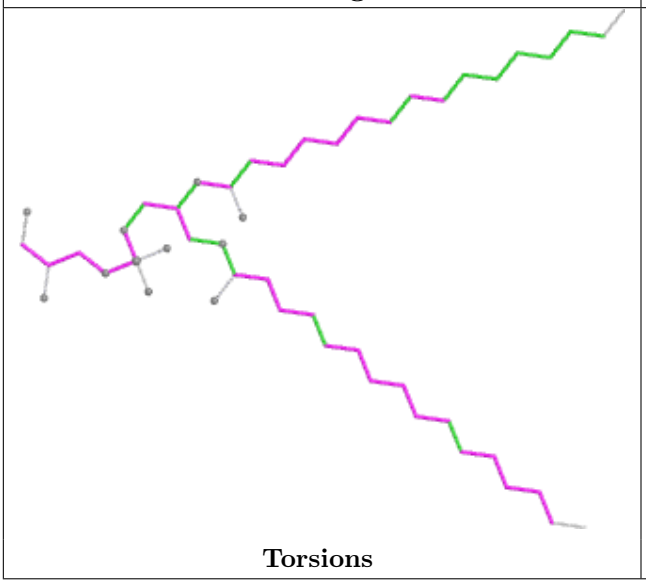
Ligand LHG l 5003



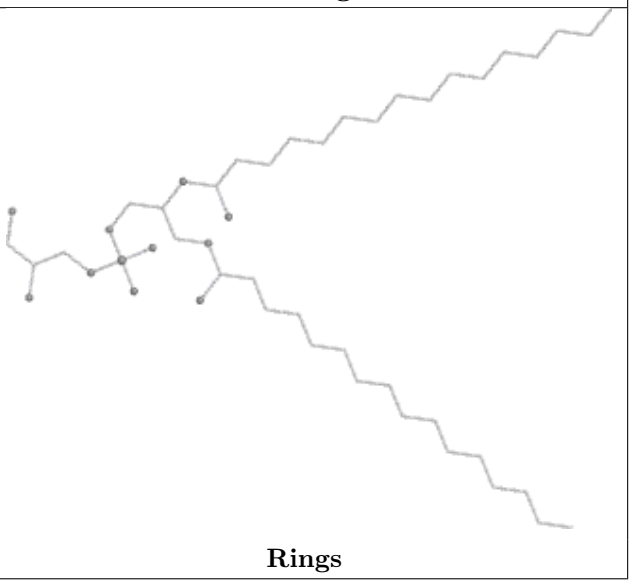
Bond lengths



Bond angles

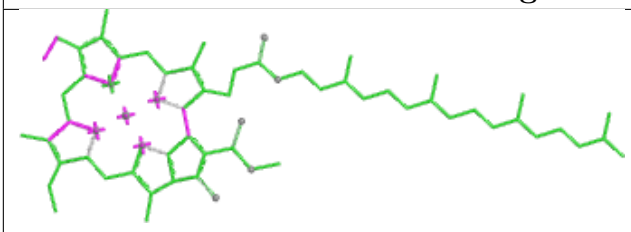


Torsions

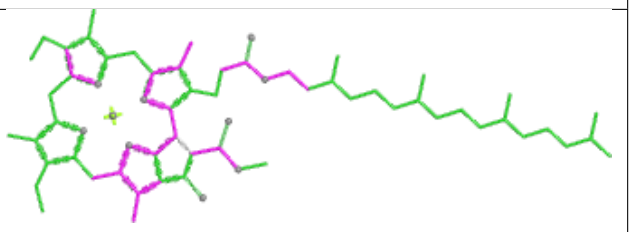


Rings

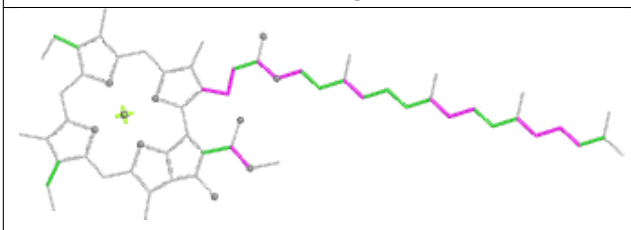
Ligand CLA a 1109



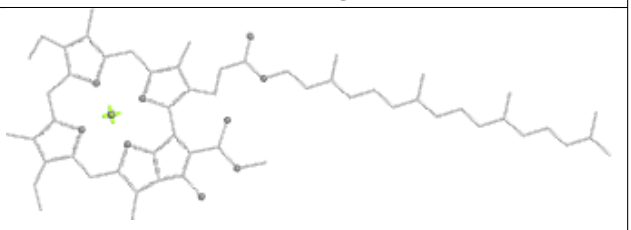
Bond lengths



Bond angles

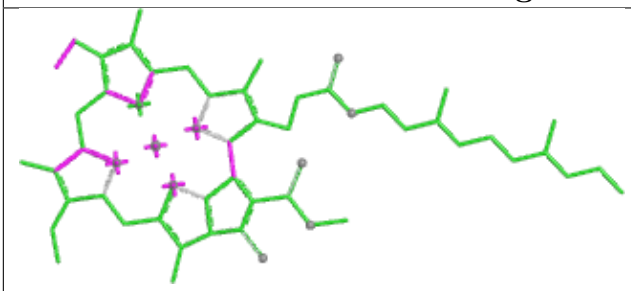


Torsions

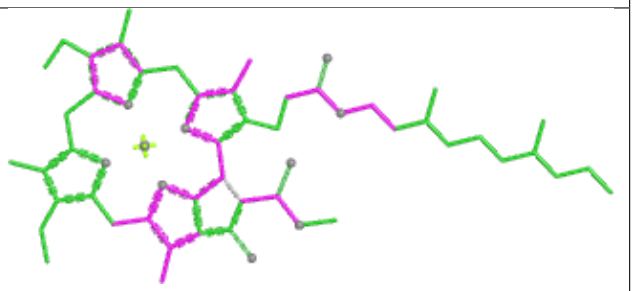


Rings

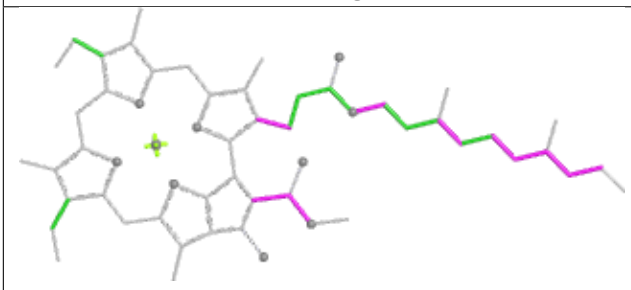
Ligand CLA B 1220



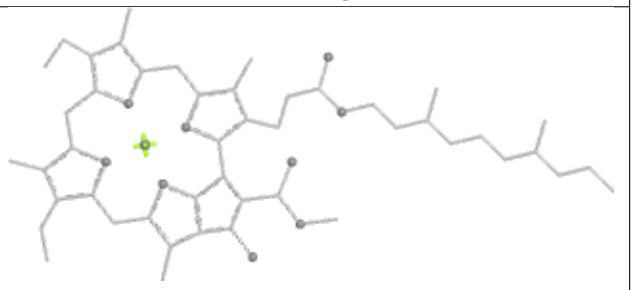
Bond lengths



Bond angles

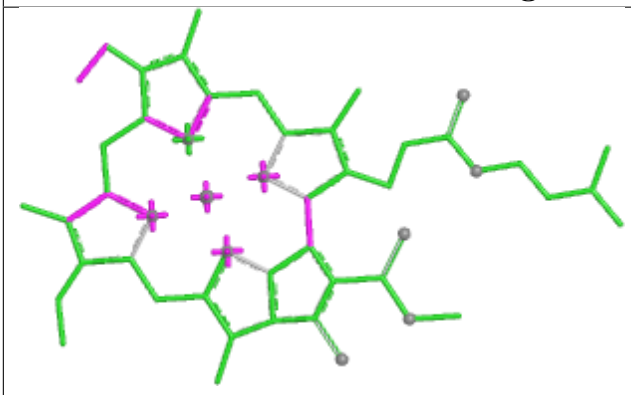


Torsions

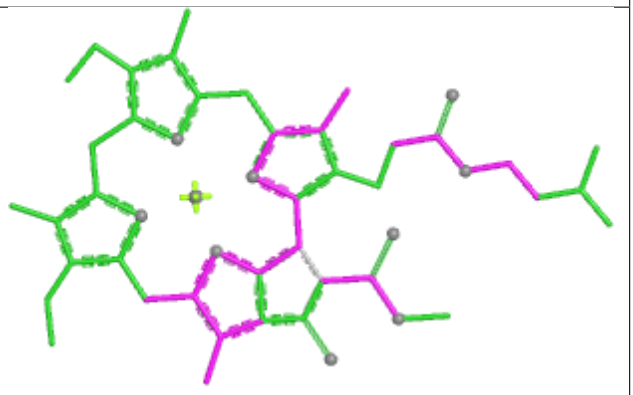


Rings

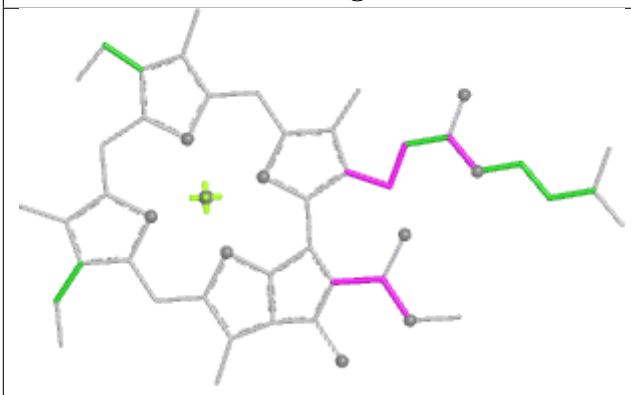
Ligand CLA a 1113



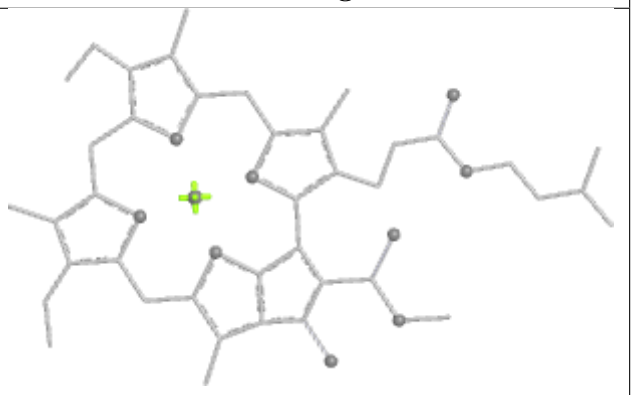
Bond lengths



Bond angles

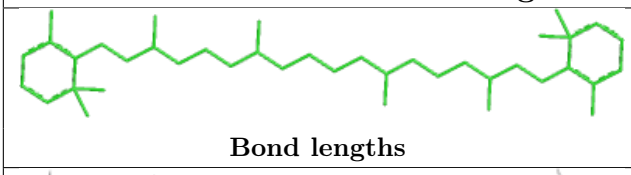


Torsions

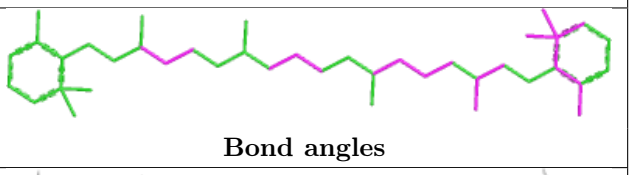


Rings

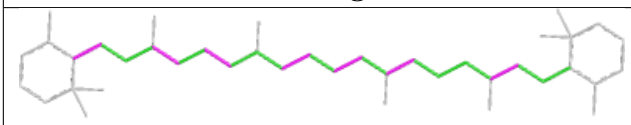
Ligand BCR 2 4005



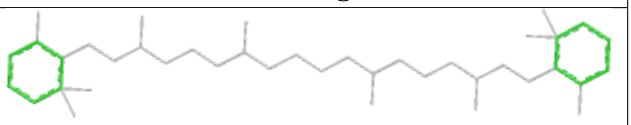
Bond lengths



Bond angles

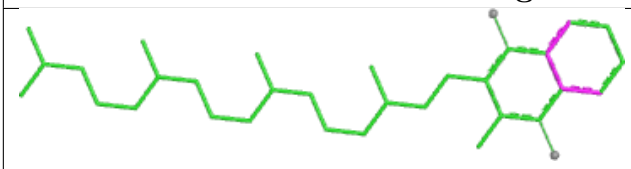


Torsions

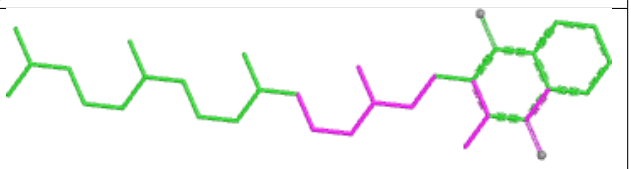


Rings

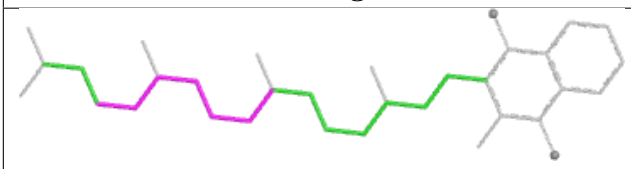
Ligand PQN b 2002



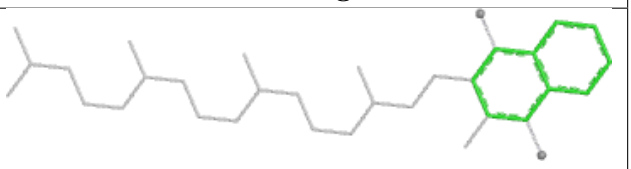
Bond lengths



Bond angles

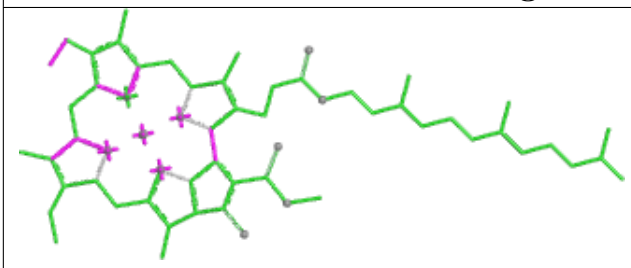


Torsions

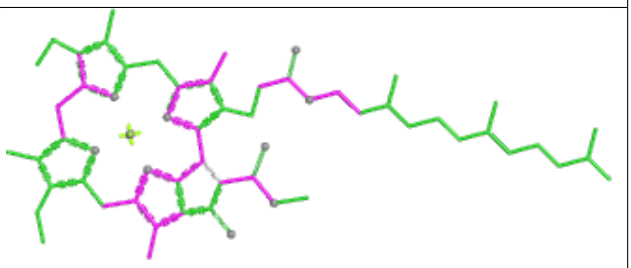


Rings

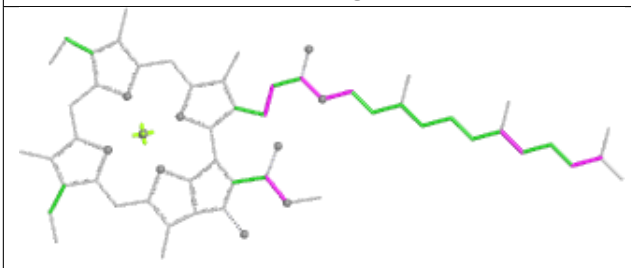
Ligand CLA 1 1138



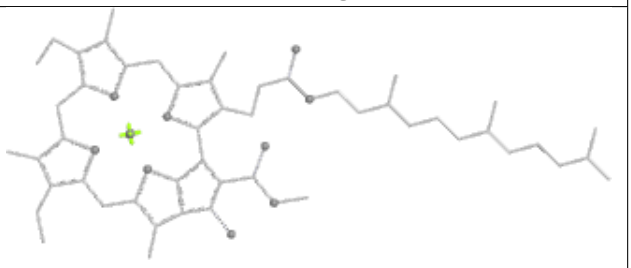
Bond lengths



Bond angles

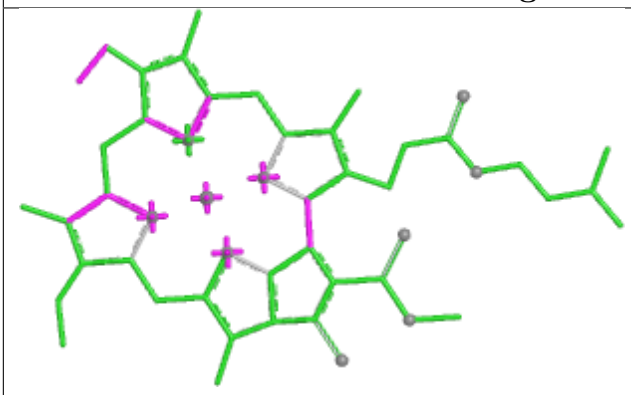


Torsions

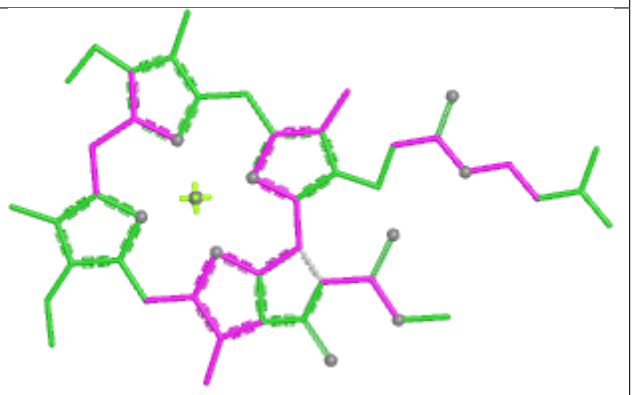


Rings

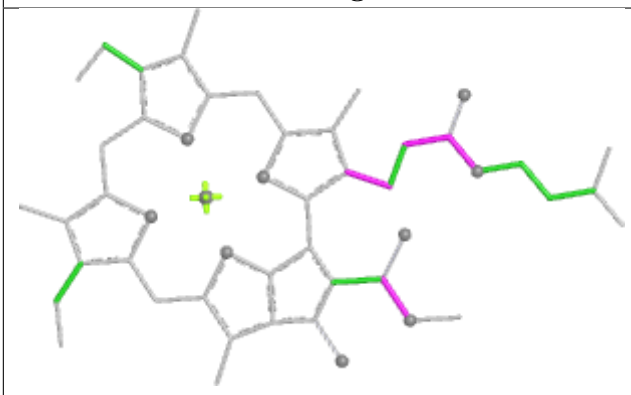
Ligand CLA 2 1234



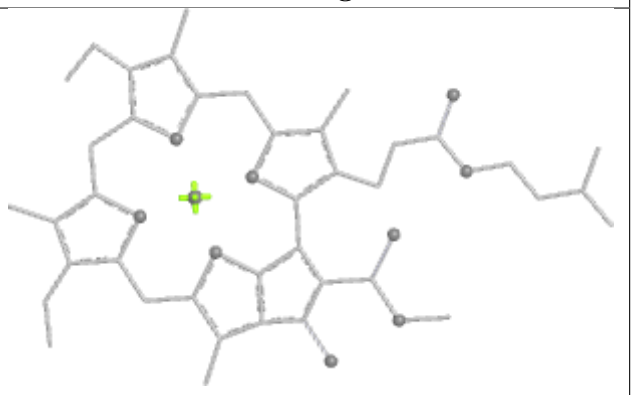
Bond lengths



Bond angles

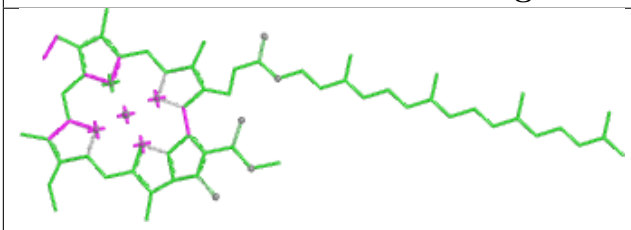


Torsions

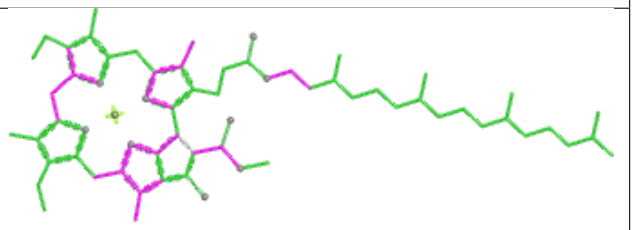


Rings

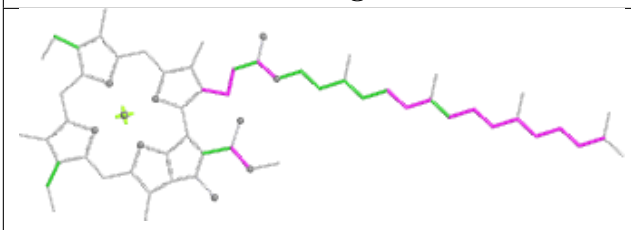
Ligand CLA A 1110



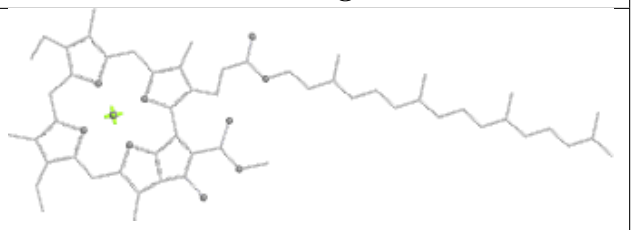
Bond lengths



Bond angles

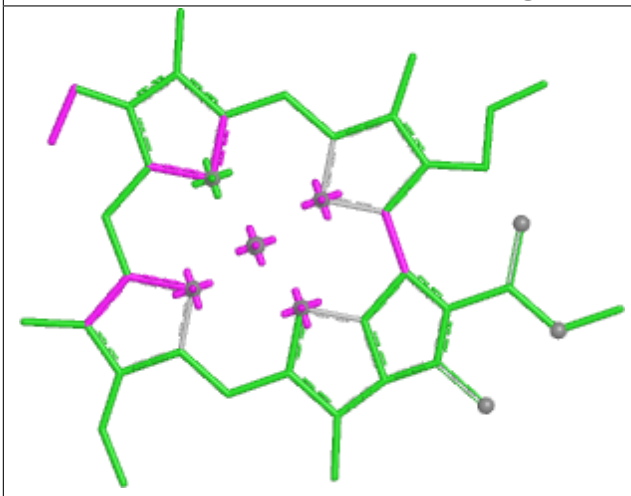


Torsions

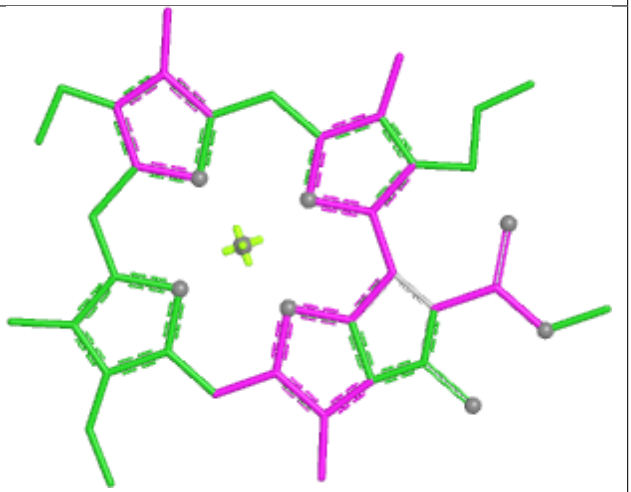


Rings

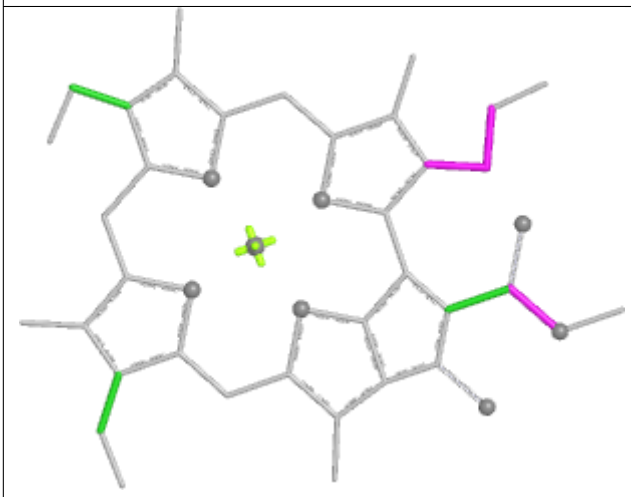
Ligand CLA 6 1302



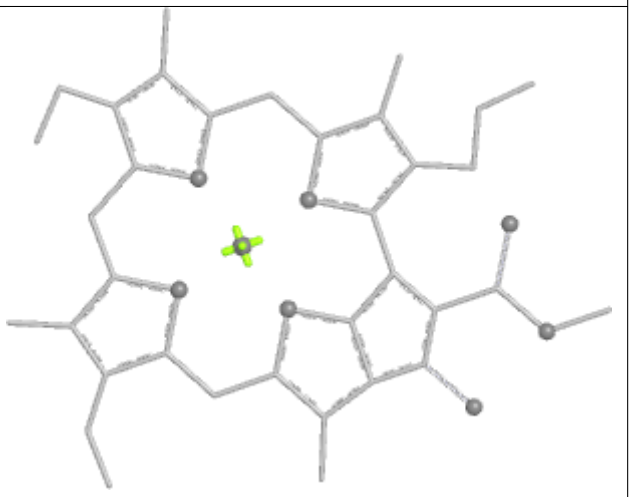
Bond lengths



Bond angles

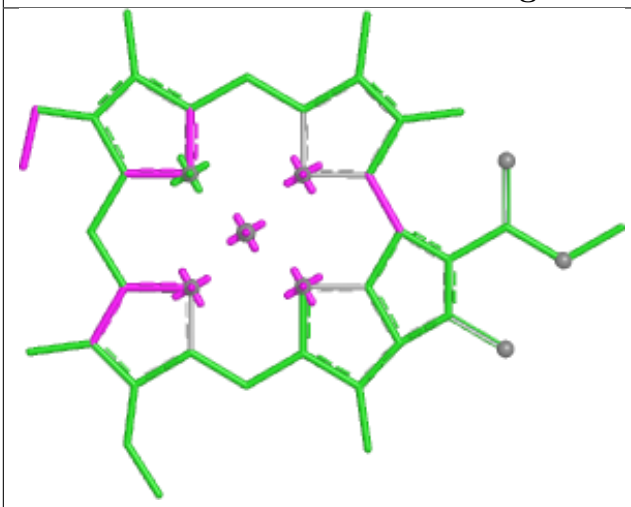


Torsions

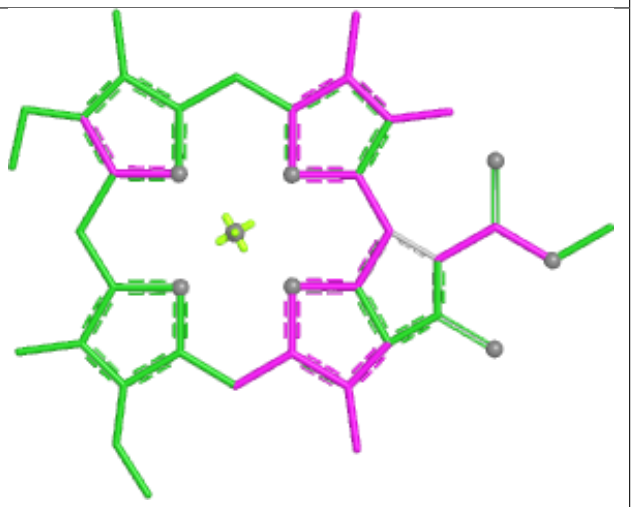


Rings

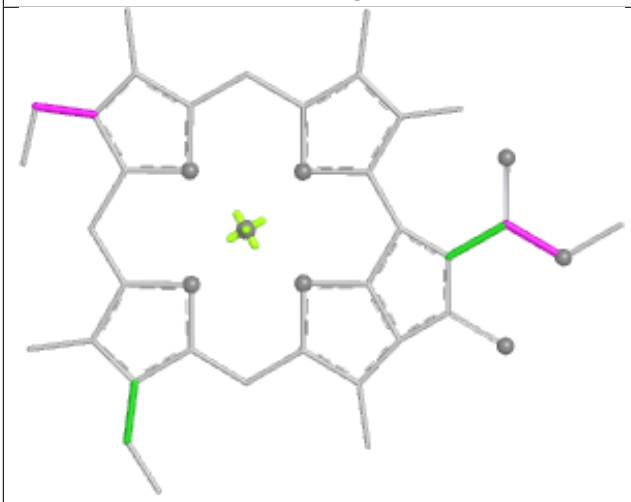
Ligand CLA 2 1240



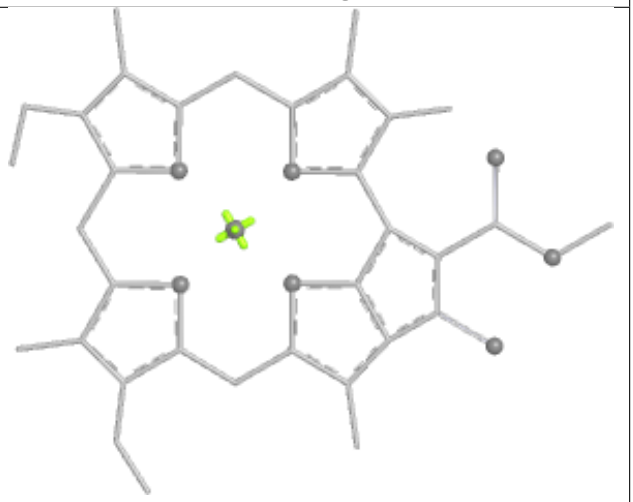
Bond lengths



Bond angles

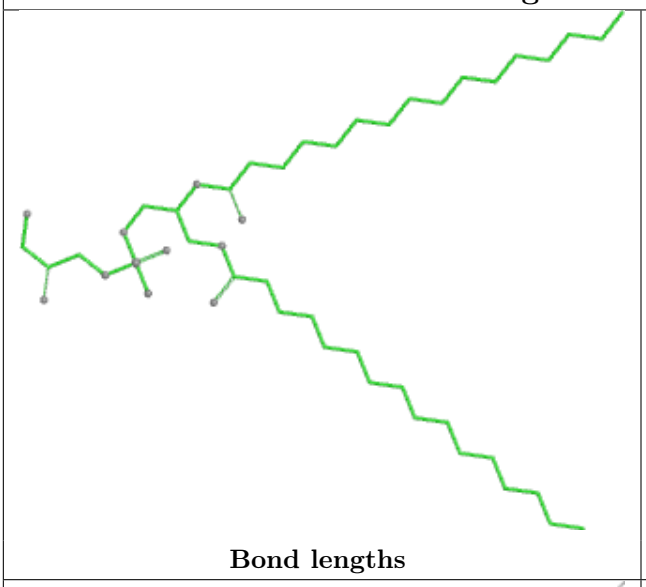


Torsions

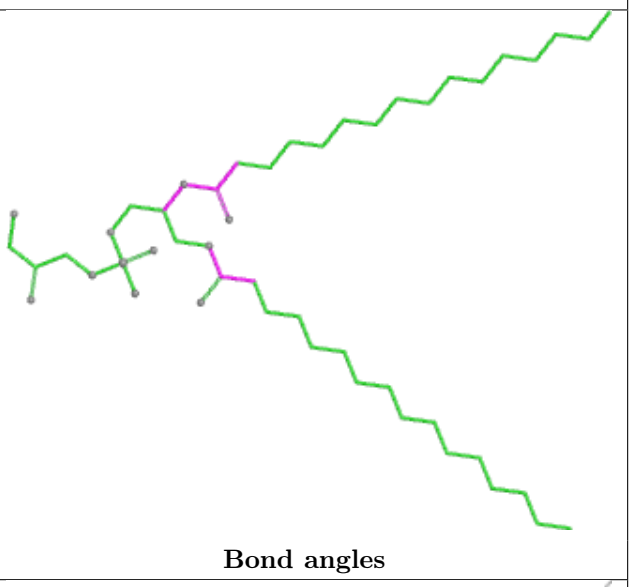


Rings

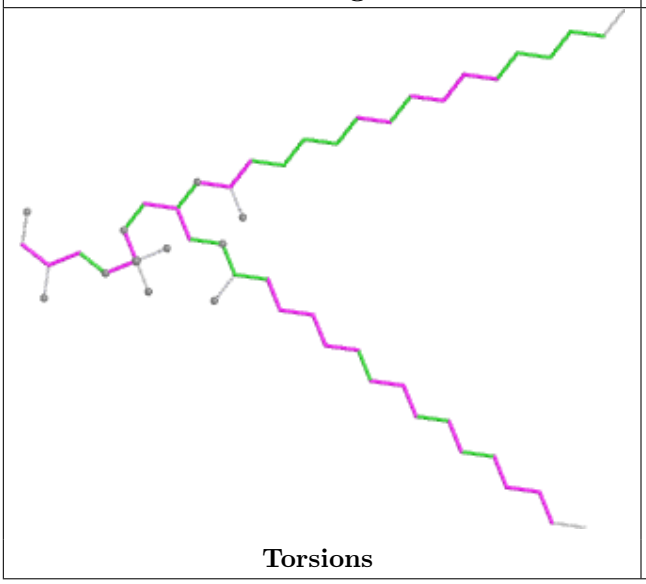
Ligand LHG l 5002



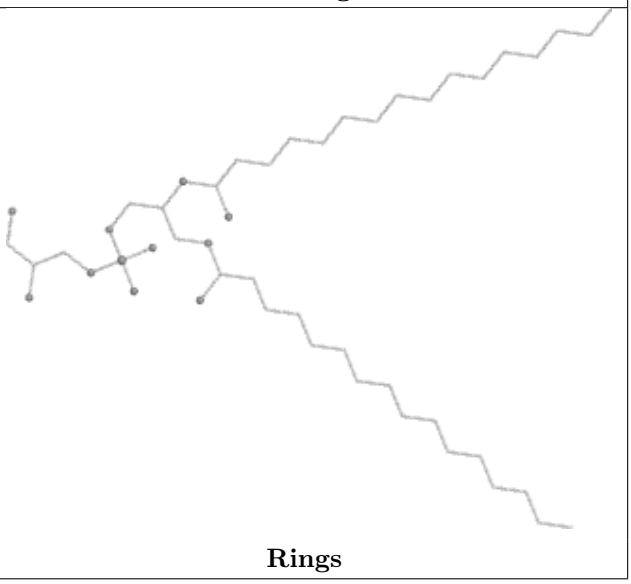
Bond lengths



Bond angles

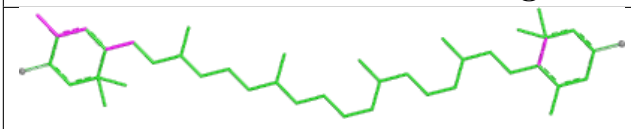


Torsions

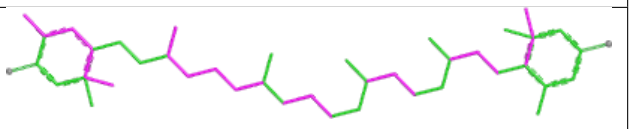


Rings

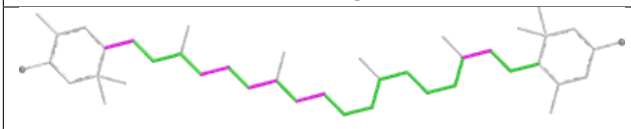
Ligand ZEX 7 4015



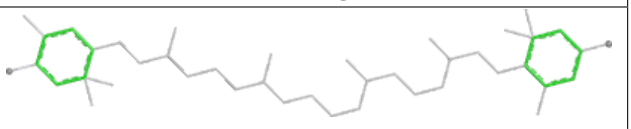
Bond lengths



Bond angles

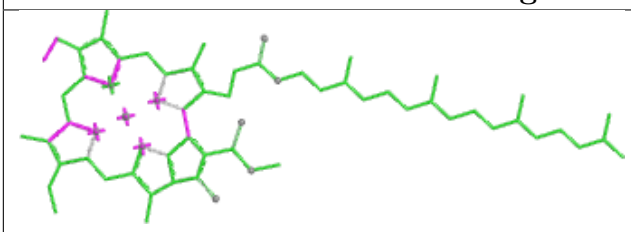


Torsions

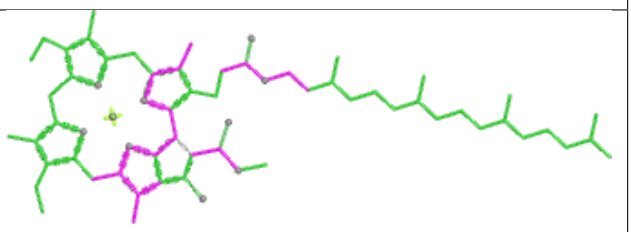


Rings

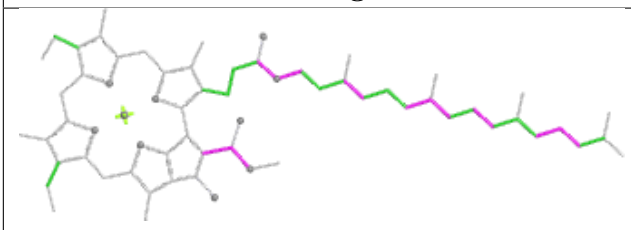
Ligand CLA a 1123



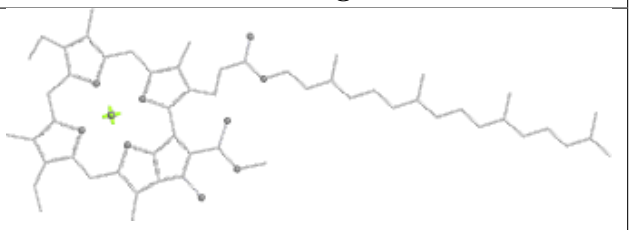
Bond lengths



Bond angles

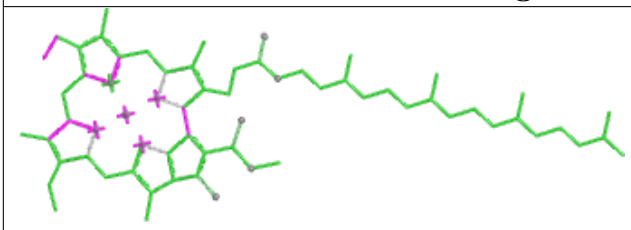


Torsions

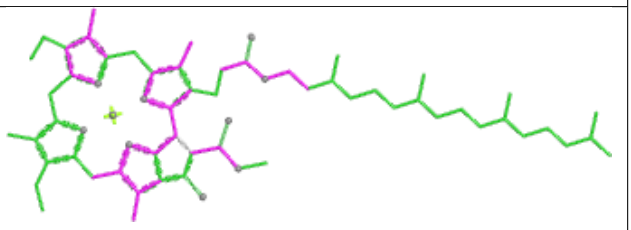


Rings

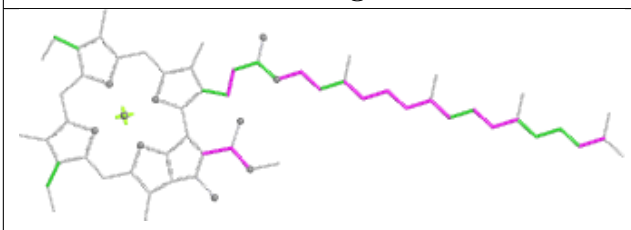
Ligand CLA A 1012



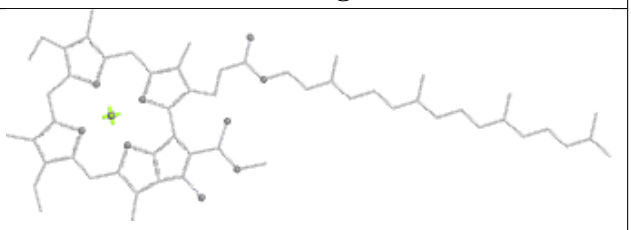
Bond lengths



Bond angles

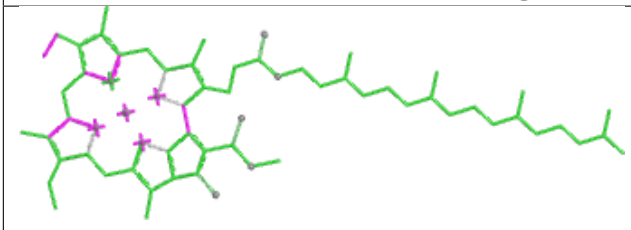


Torsions

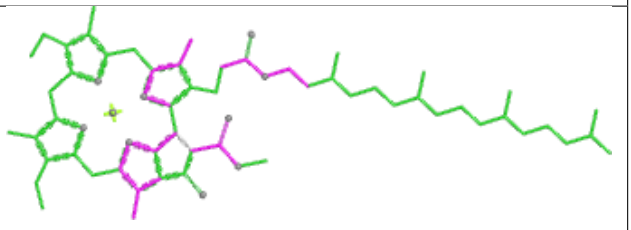


Rings

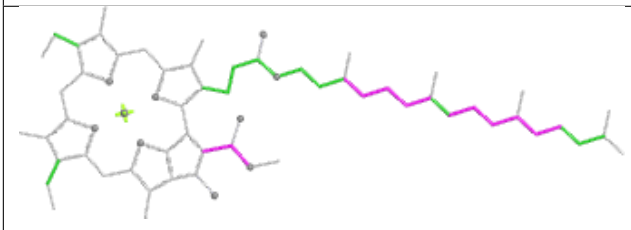
Ligand CLA B 1205



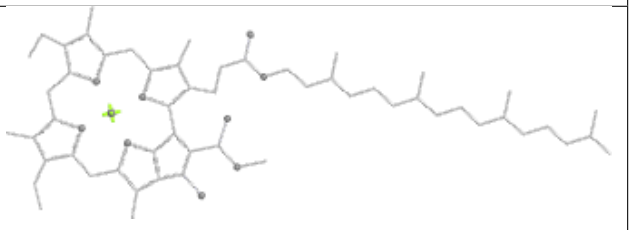
Bond lengths



Bond angles

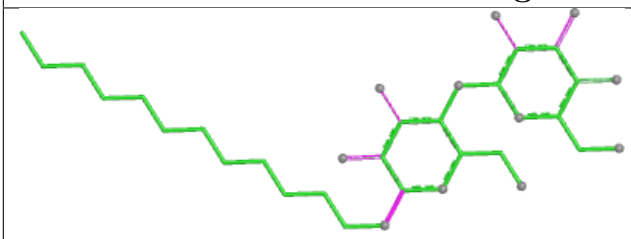


Torsions

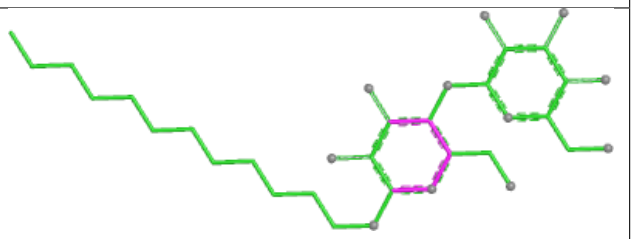


Rings

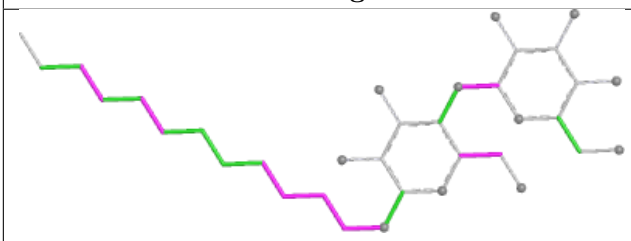
Ligand LMT F 6001



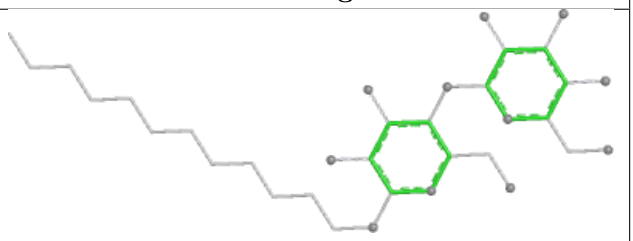
Bond lengths



Bond angles

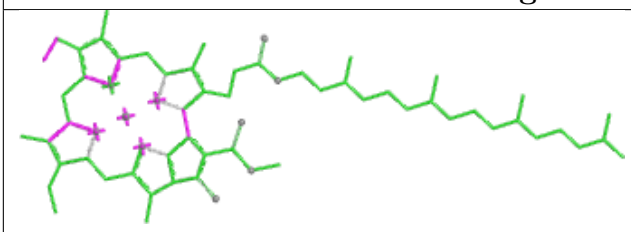


Torsions

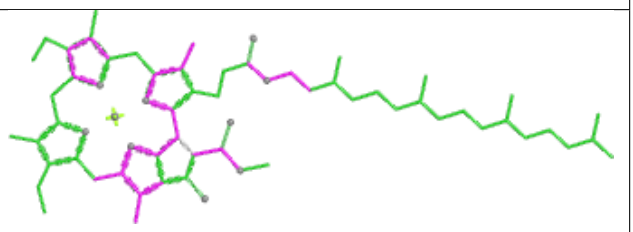


Rings

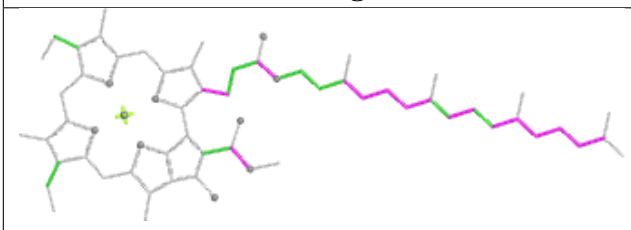
Ligand CLA 1 1120



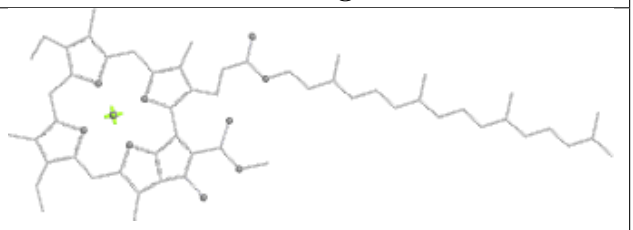
Bond lengths



Bond angles

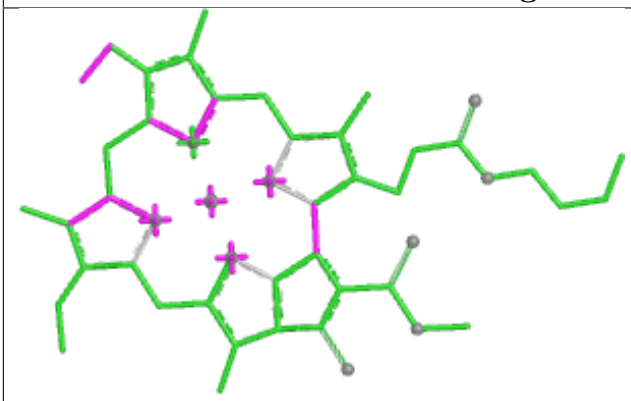


Torsions

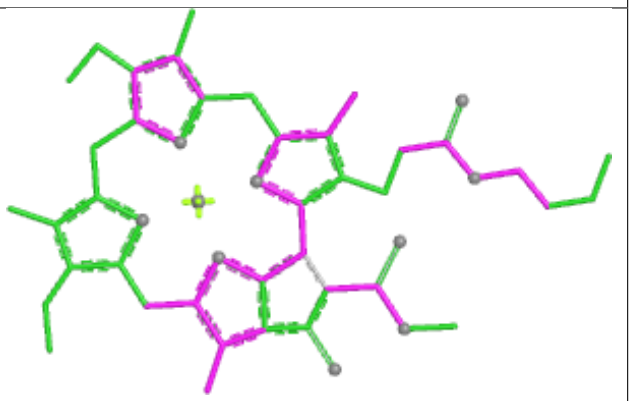


Rings

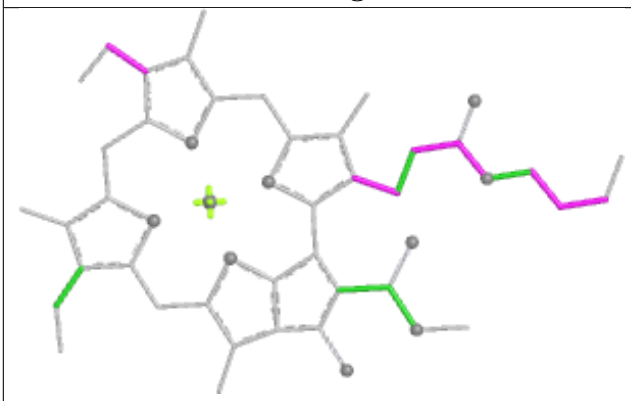
Ligand CLA a 1134



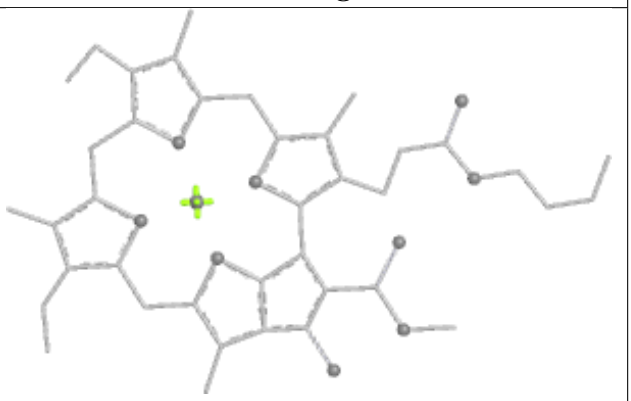
Bond lengths



Bond angles

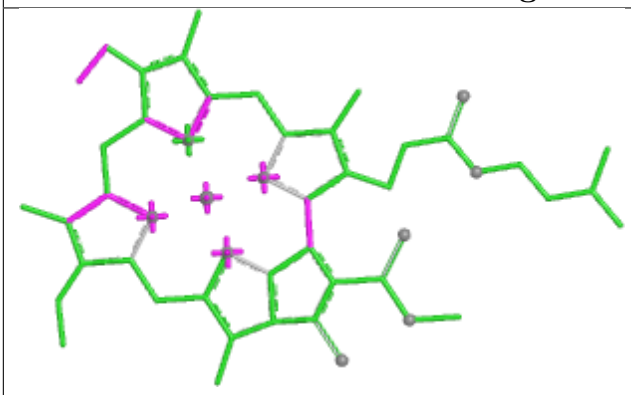


Torsions

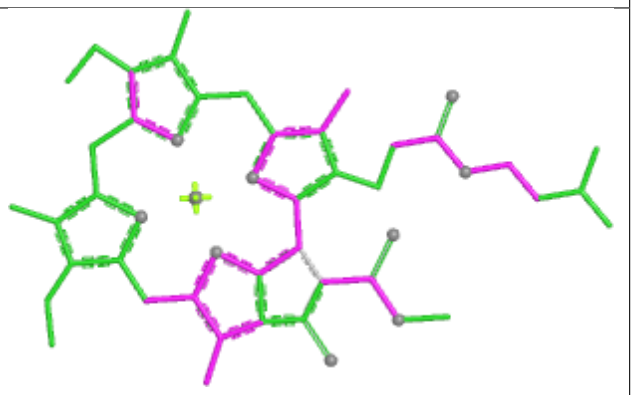


Rings

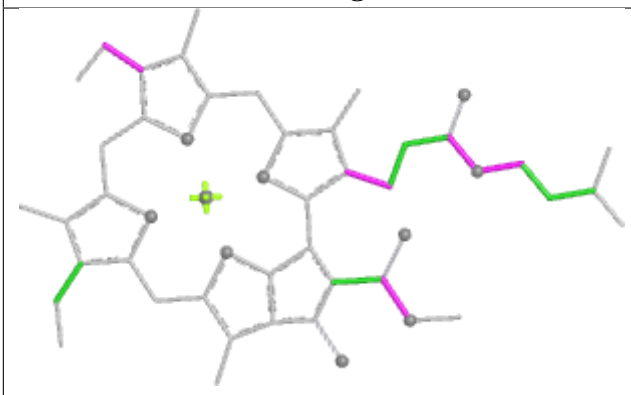
Ligand CLA 1 1112



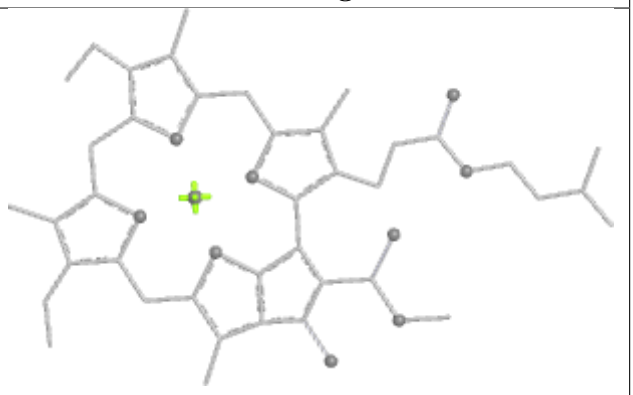
Bond lengths



Bond angles



Torsions

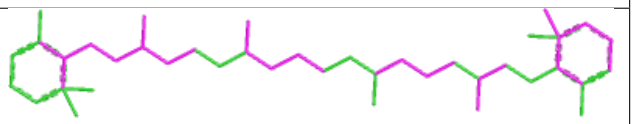


Rings

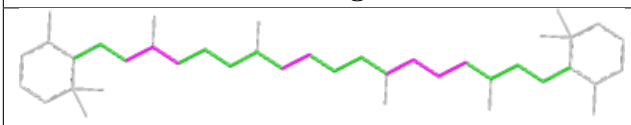
Ligand BCR A 4019



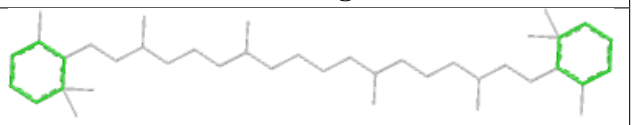
Bond lengths



Bond angles

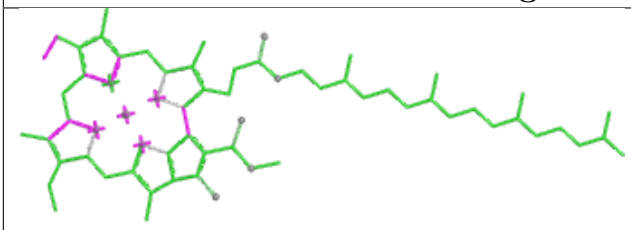


Torsions

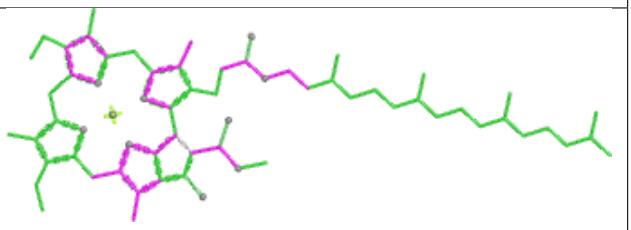


Rings

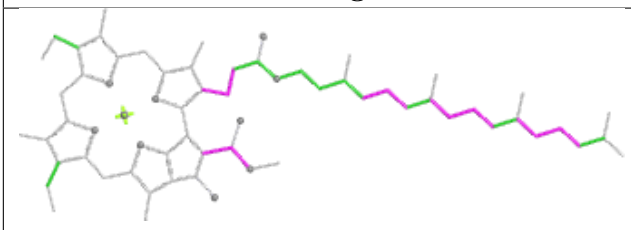
Ligand CLA 1 1106



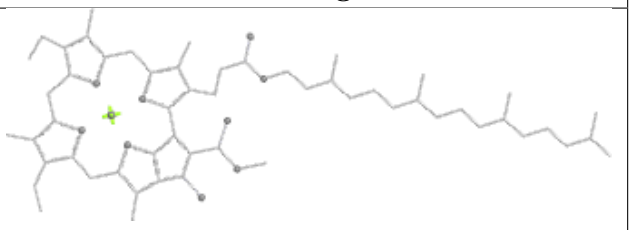
Bond lengths



Bond angles

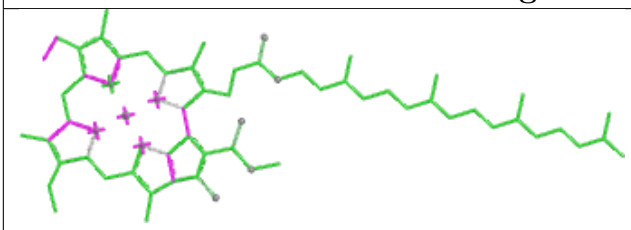


Torsions

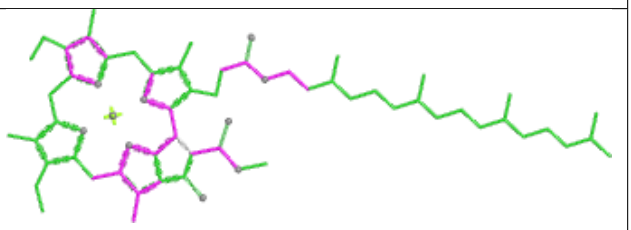


Rings

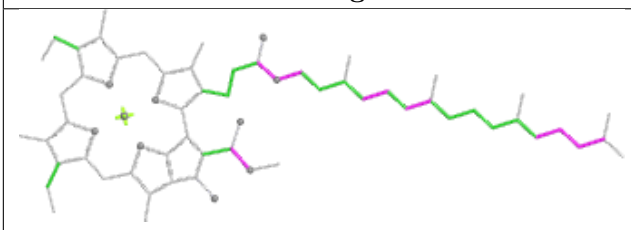
Ligand CLA 2 1021



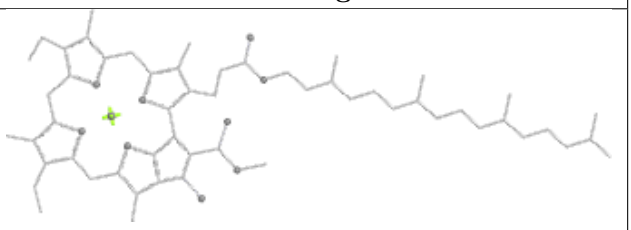
Bond lengths



Bond angles

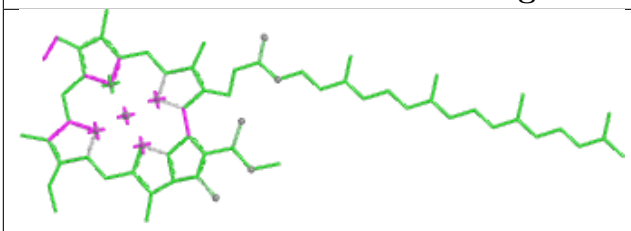


Torsions

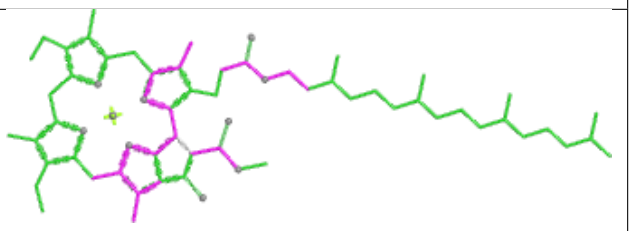


Rings

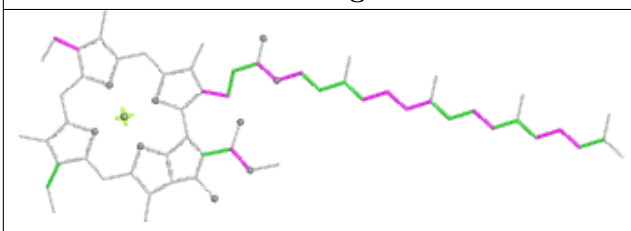
Ligand CLA b 1236



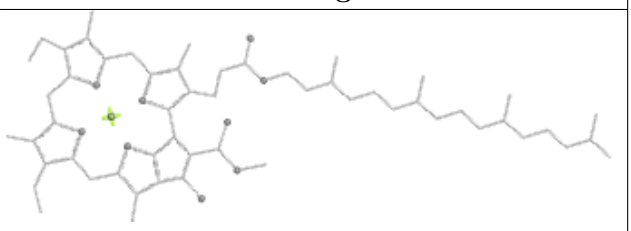
Bond lengths



Bond angles

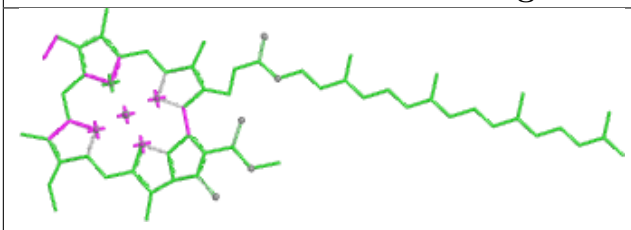


Torsions

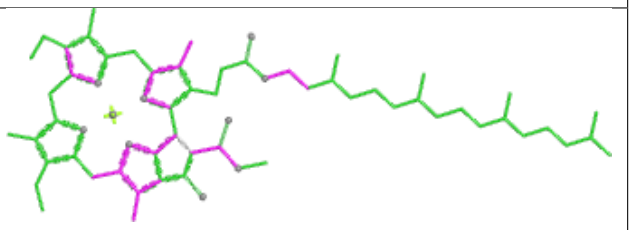


Rings

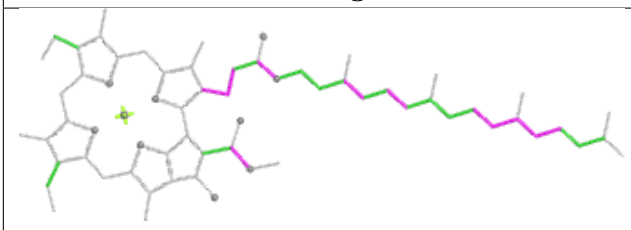
Ligand CLA L 1501



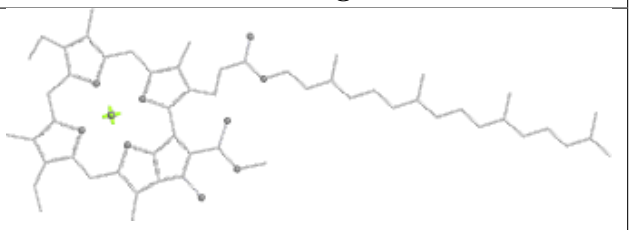
Bond lengths



Bond angles

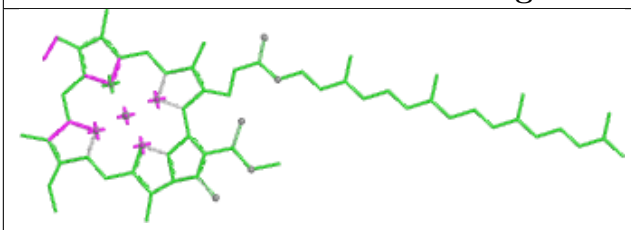


Torsions

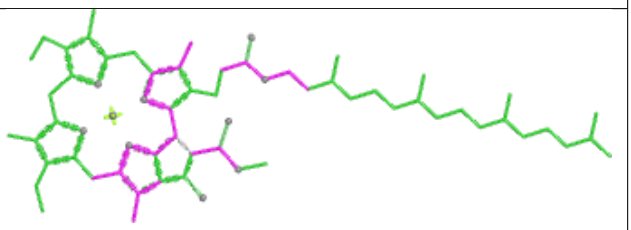


Rings

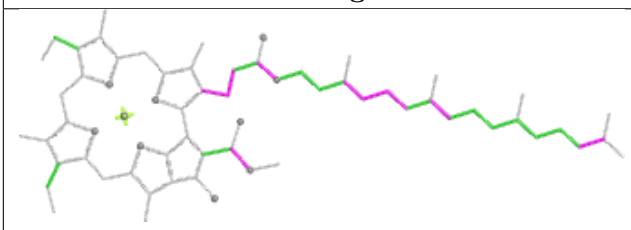
Ligand CLA B 1237



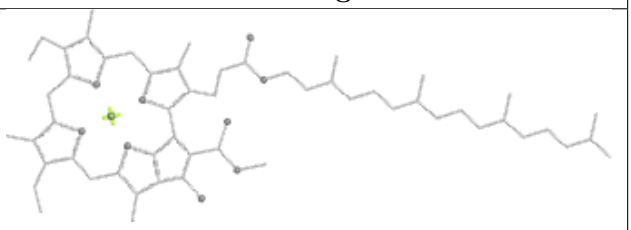
Bond lengths



Bond angles

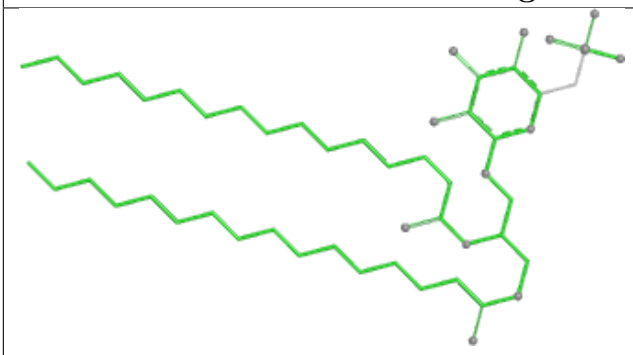


Torsions

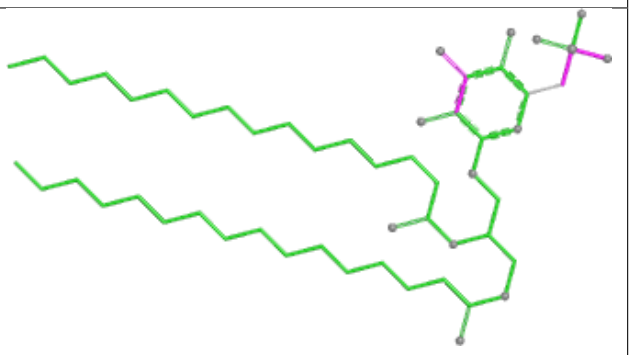


Rings

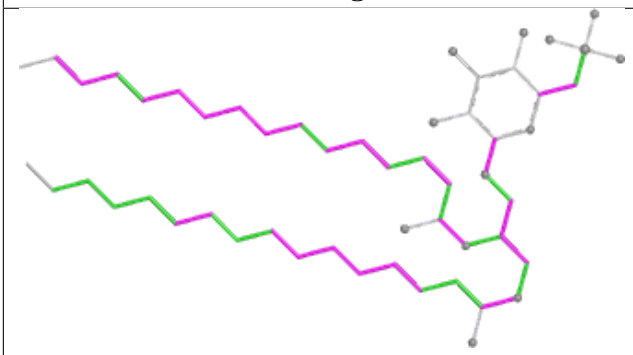
Ligand SQD b 5006



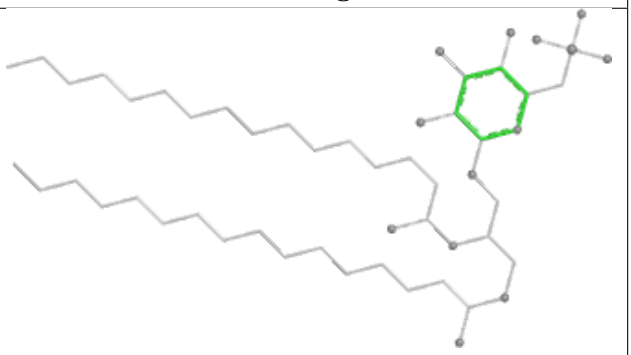
Bond lengths



Bond angles

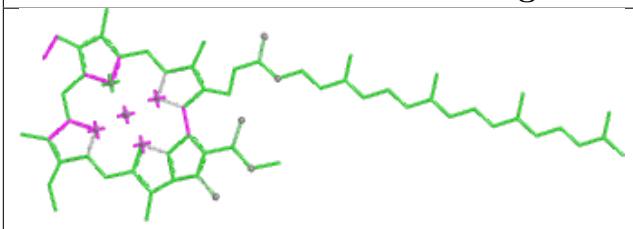


Torsions

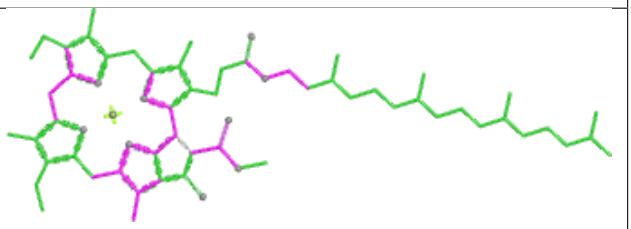


Rings

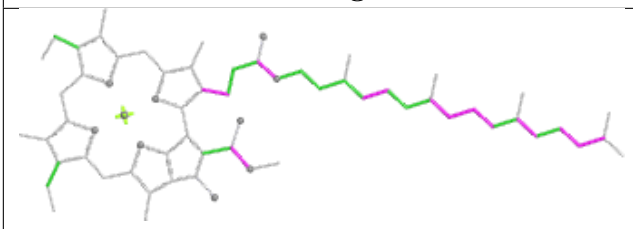
Ligand CLA b 1212



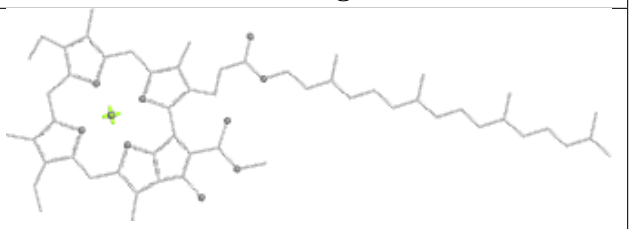
Bond lengths



Bond angles

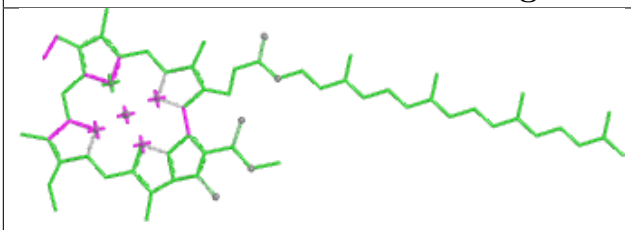


Torsions

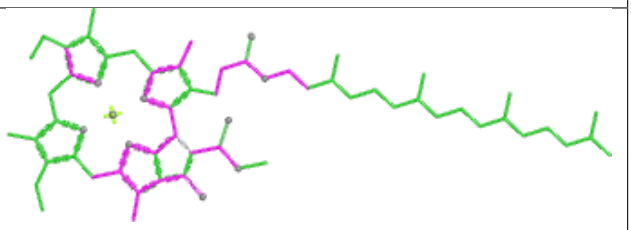


Rings

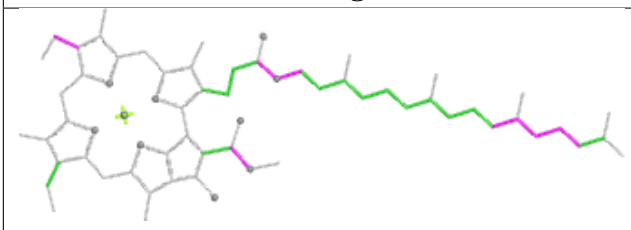
Ligand CLA a 1125



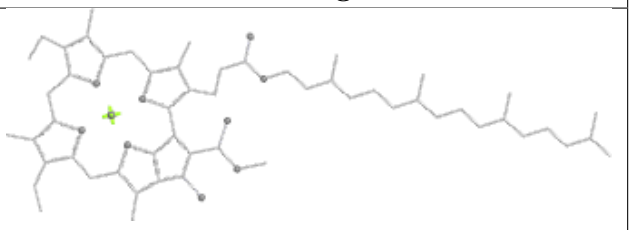
Bond lengths



Bond angles

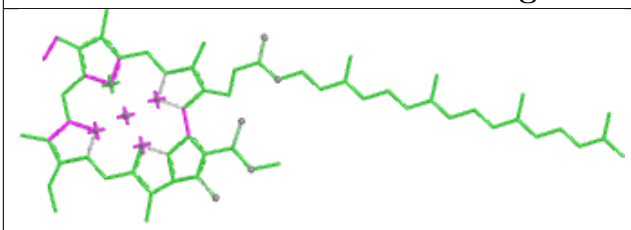


Torsions

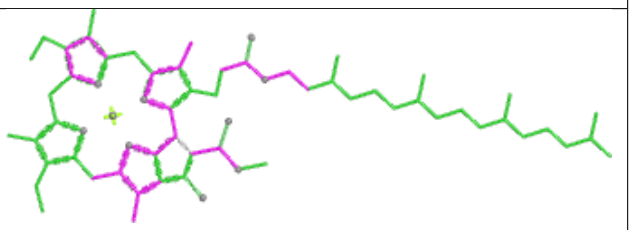


Rings

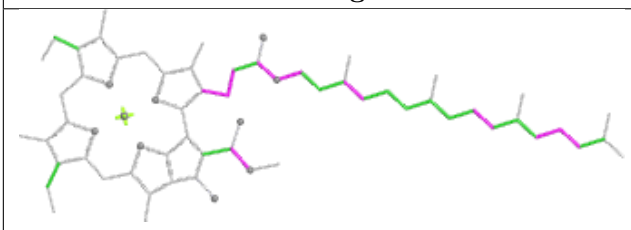
Ligand CLA 1 1119



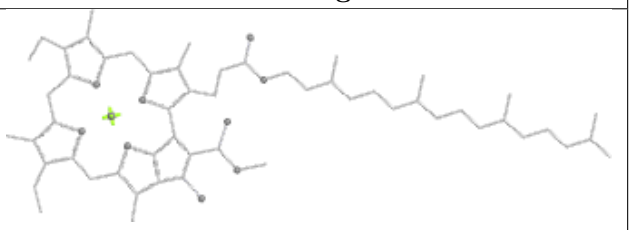
Bond lengths



Bond angles



Torsions

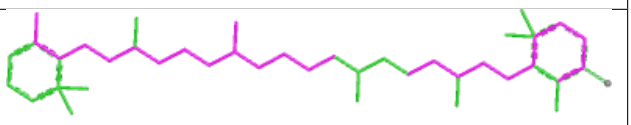


Rings

Ligand ECH i 4020



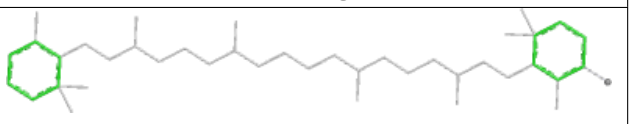
Bond lengths



Bond angles

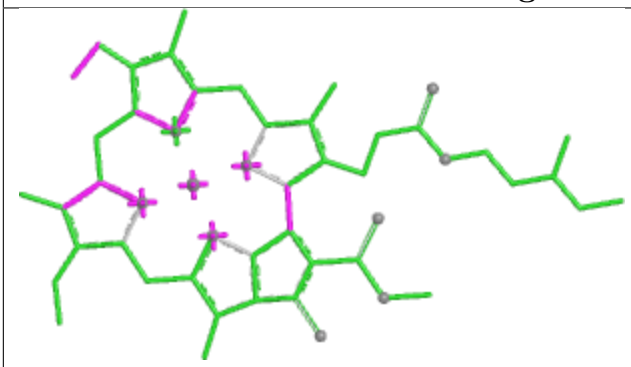


Torsions

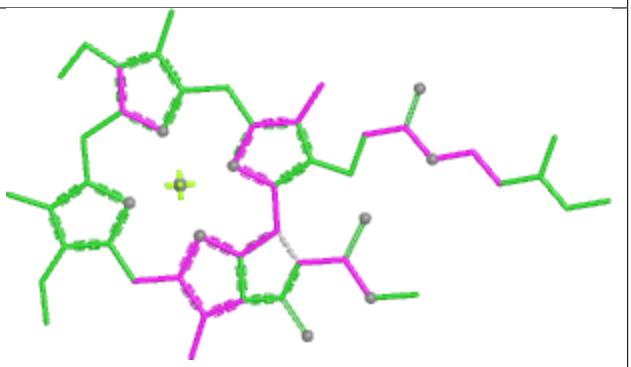


Rings

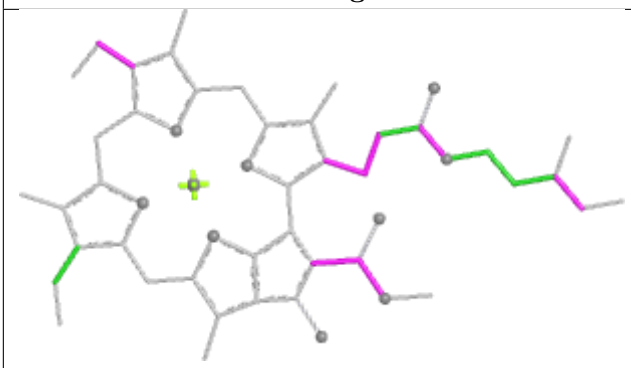
Ligand CLA b 1217



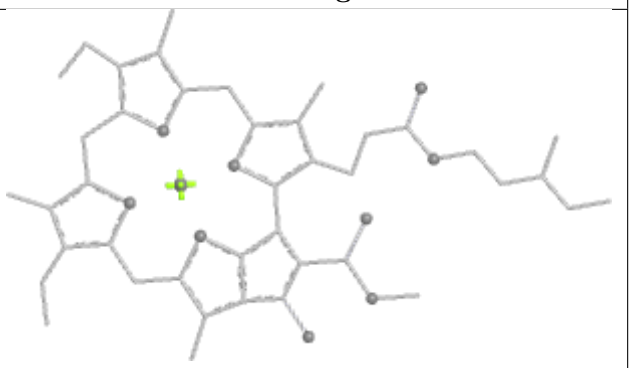
Bond lengths



Bond angles

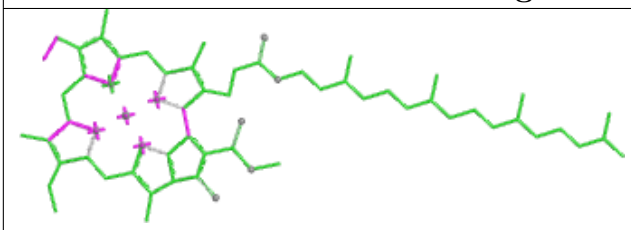


Torsions

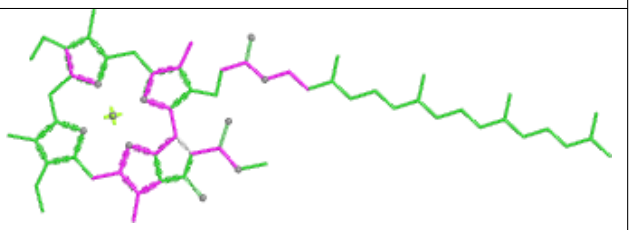


Rings

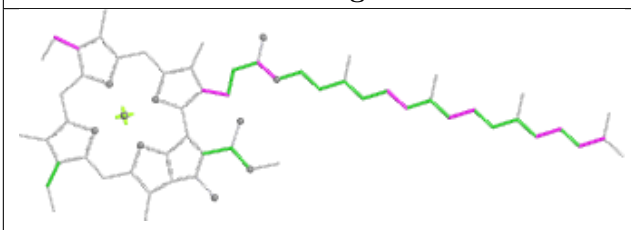
Ligand CLA B 1223



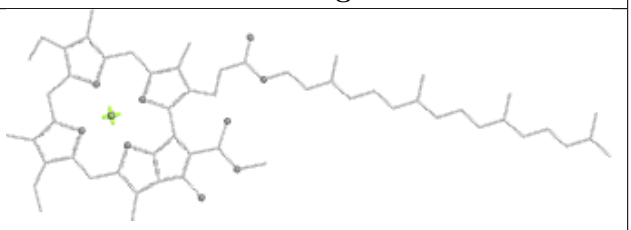
Bond lengths



Bond angles

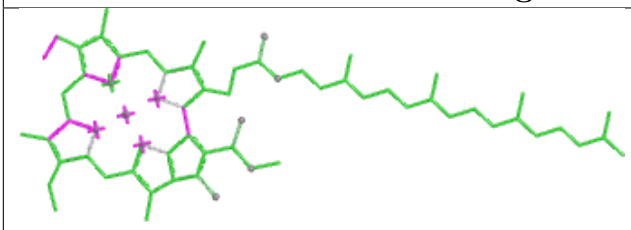


Torsions

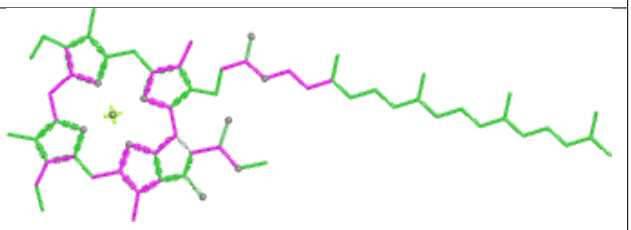


Rings

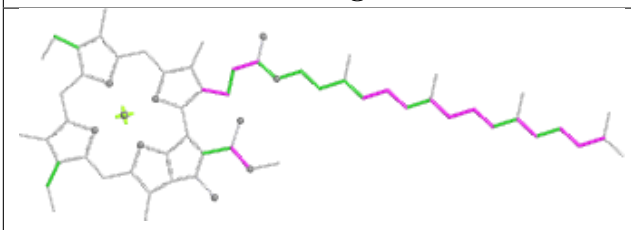
Ligand CLA B 1217



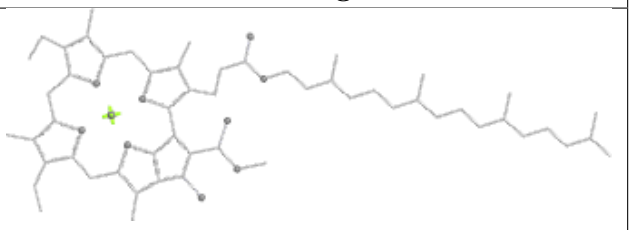
Bond lengths



Bond angles

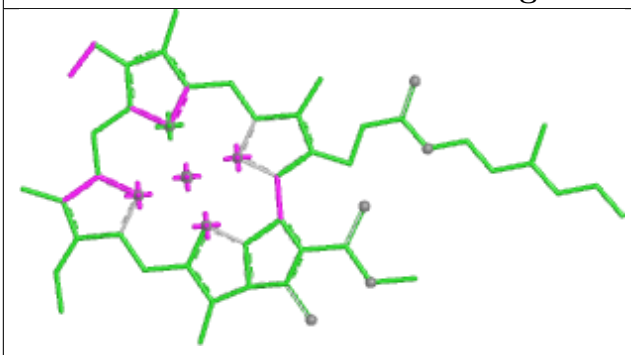


Torsions

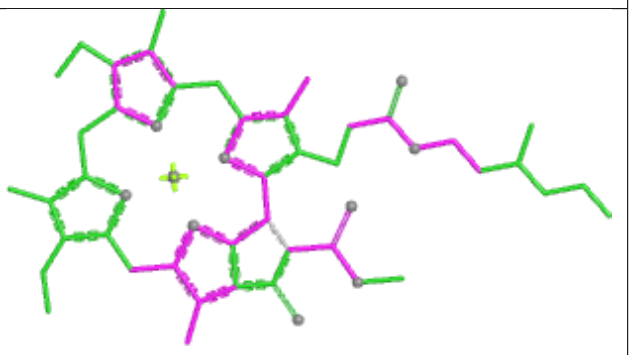


Rings

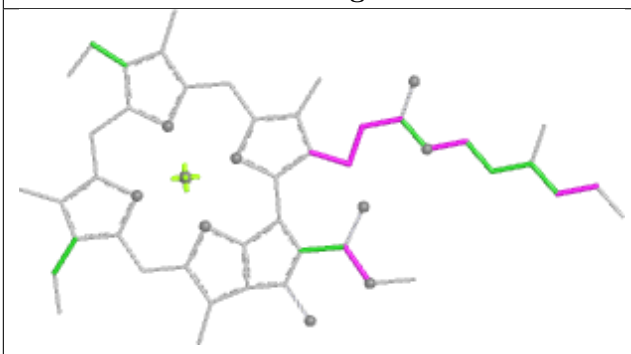
Ligand CLA a 1129



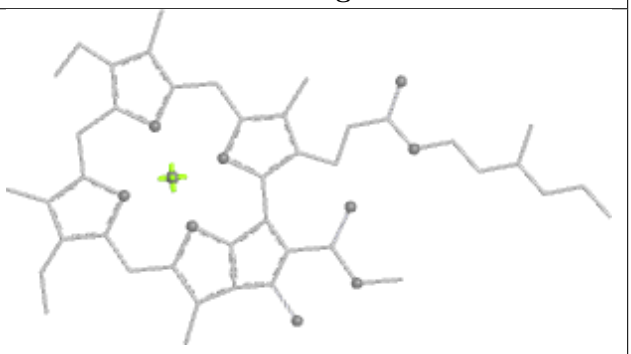
Bond lengths



Bond angles

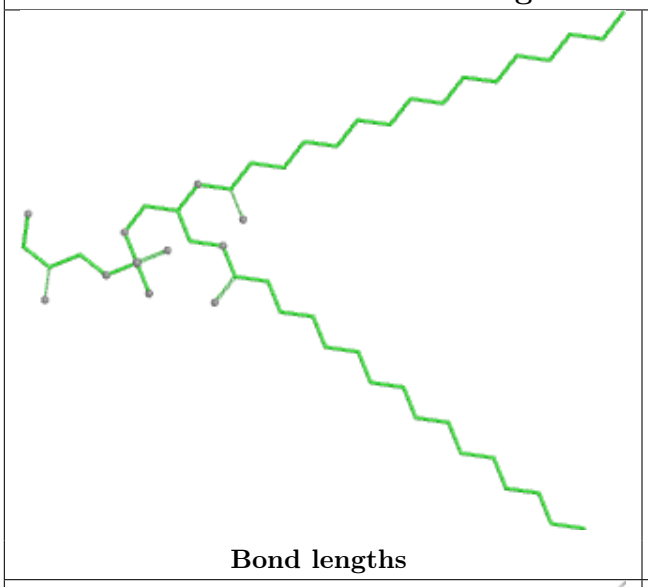


Torsions

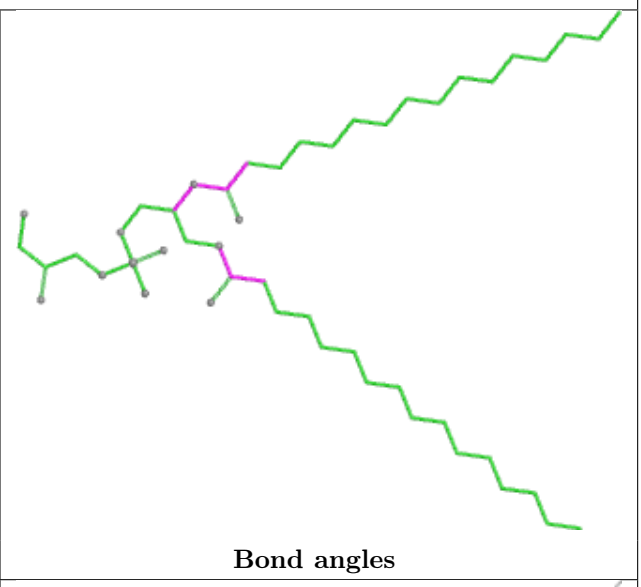


Rings

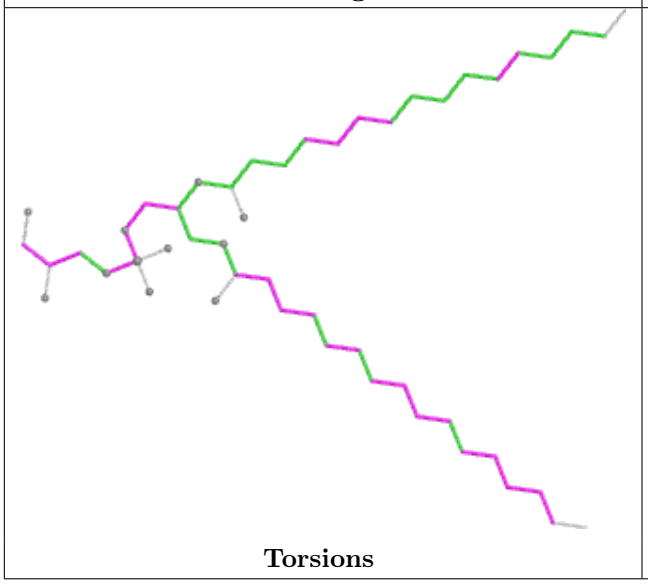
Ligand LHG B 5004



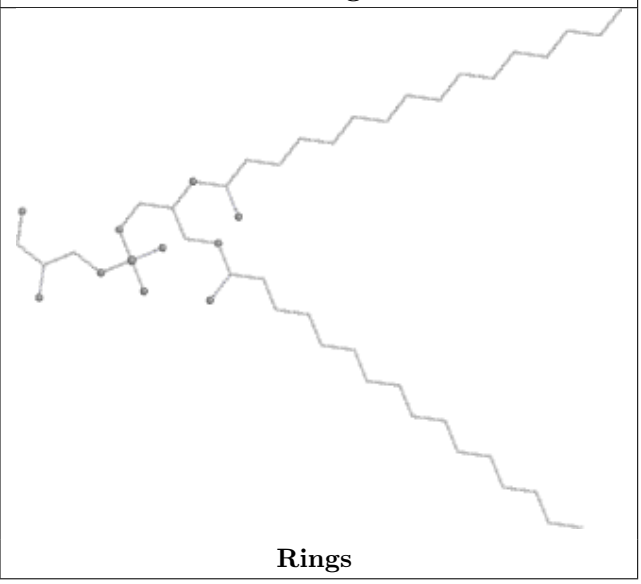
Bond lengths



Bond angles



Torsions

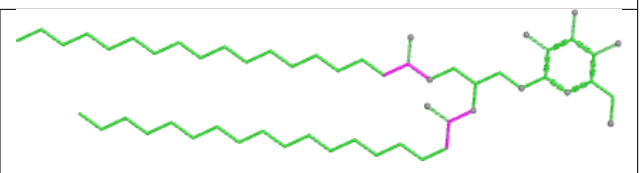


Rings

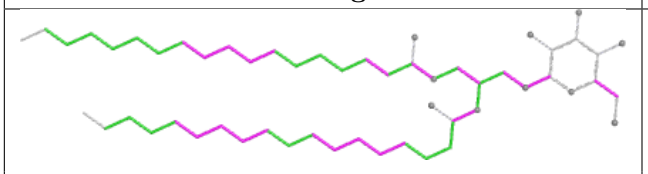
Ligand LMG A 5008



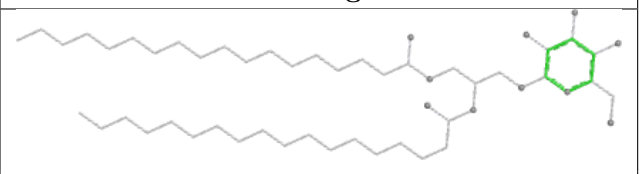
Bond lengths



Bond angles

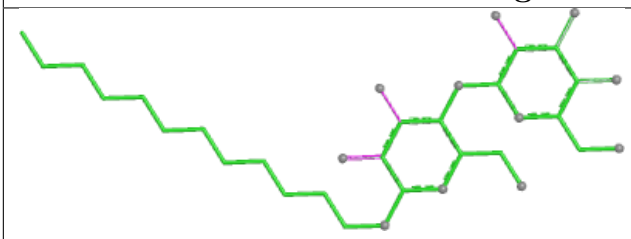


Torsions

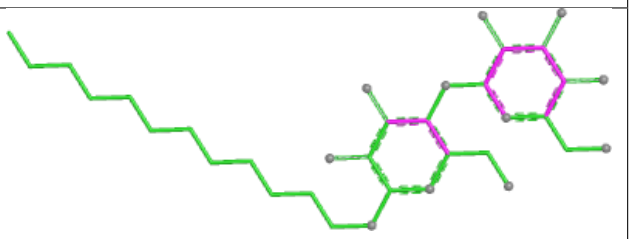


Rings

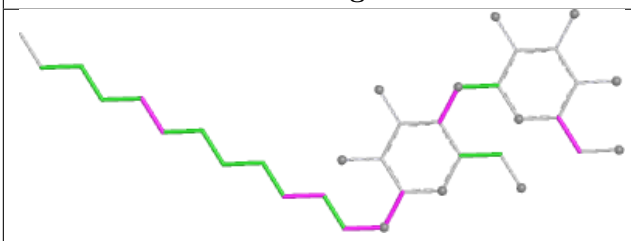
Ligand LMT L 6001



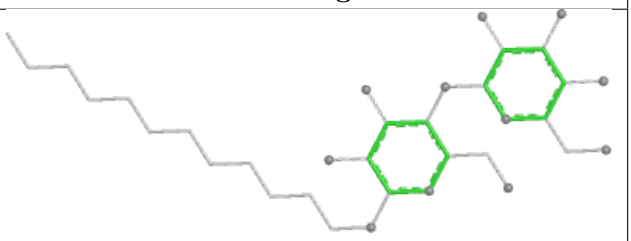
Bond lengths



Bond angles

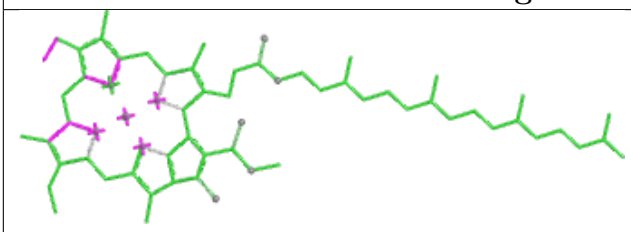


Torsions

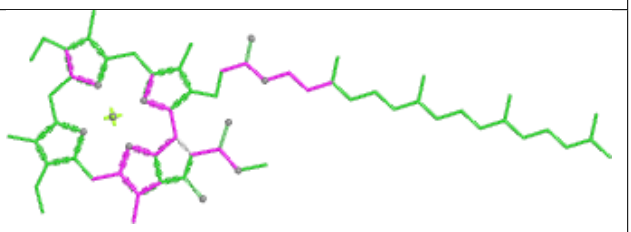


Rings

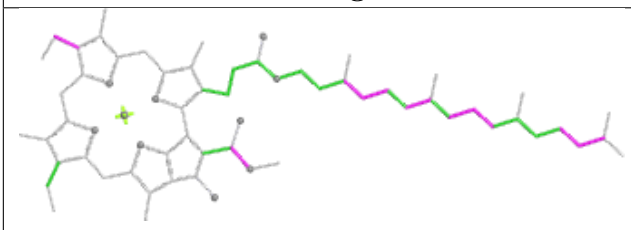
Ligand CLA A 1133



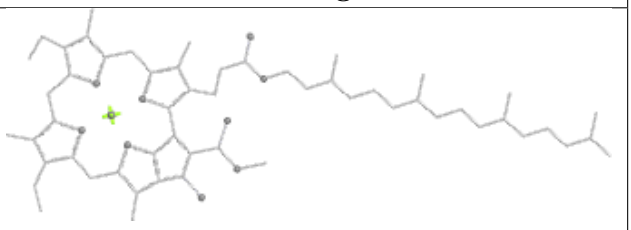
Bond lengths



Bond angles

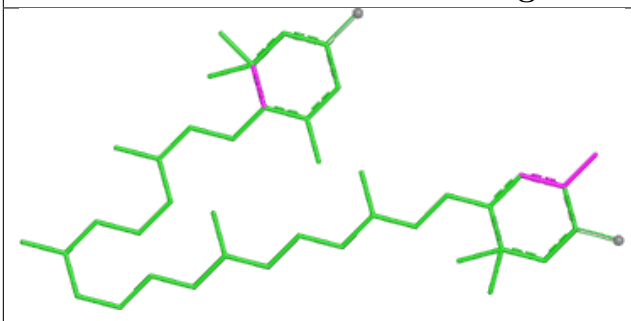


Torsions

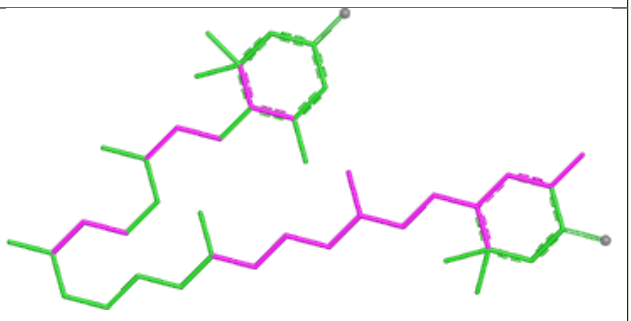


Rings

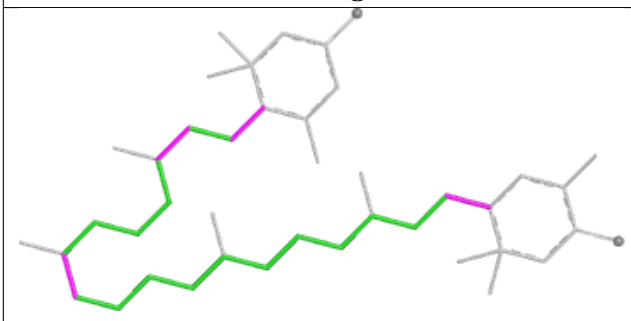
Ligand ZEX F 4016



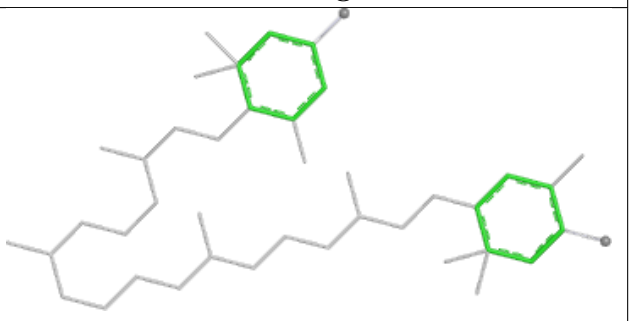
Bond lengths



Bond angles

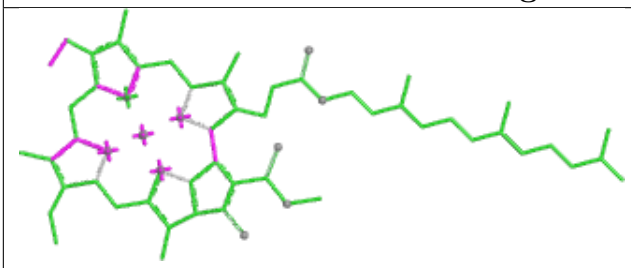


Torsions

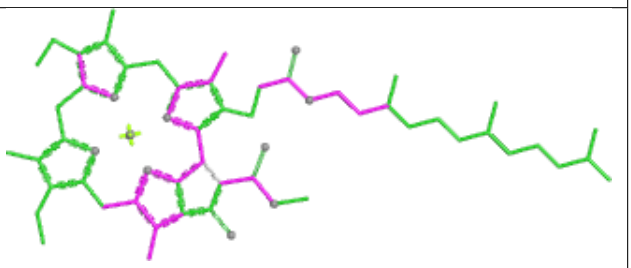


Rings

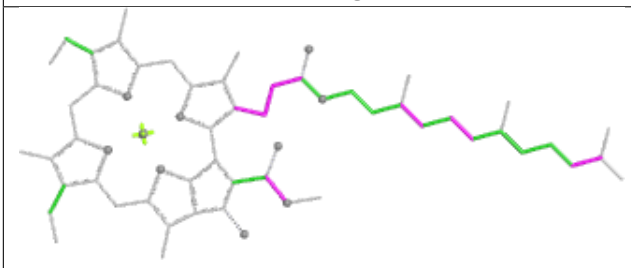
Ligand CLA a 1116



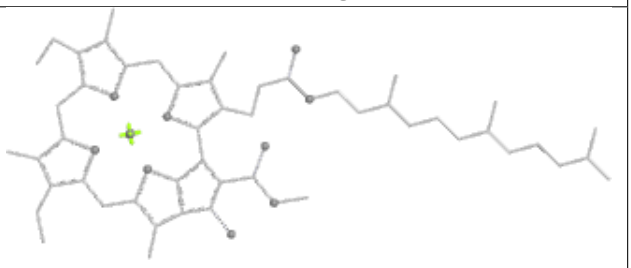
Bond lengths



Bond angles

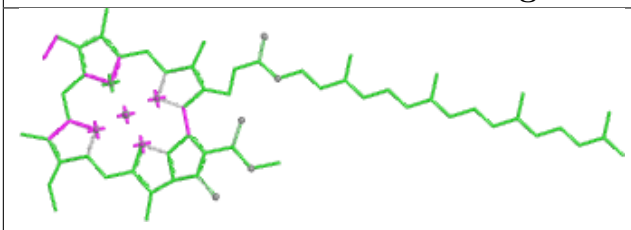


Torsions

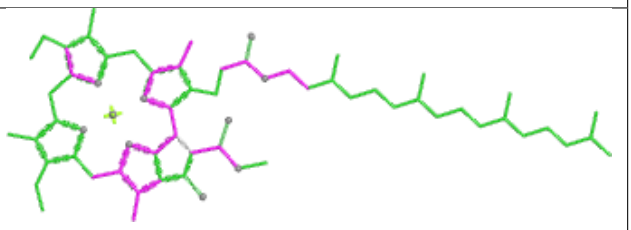


Rings

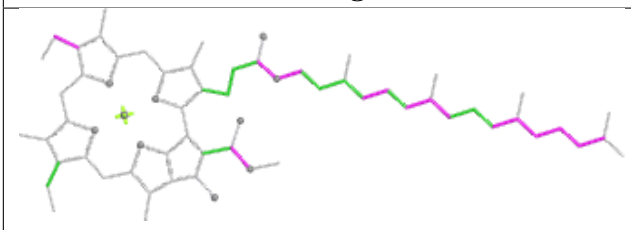
Ligand CLA 1 1133



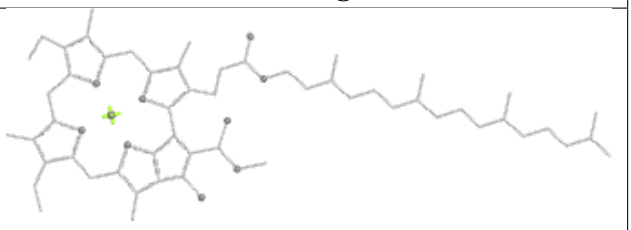
Bond lengths



Bond angles

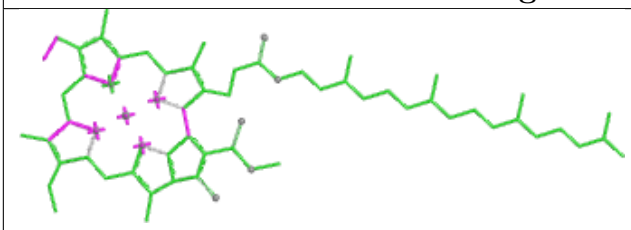


Torsions

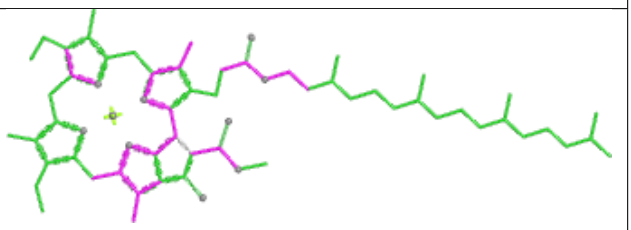


Rings

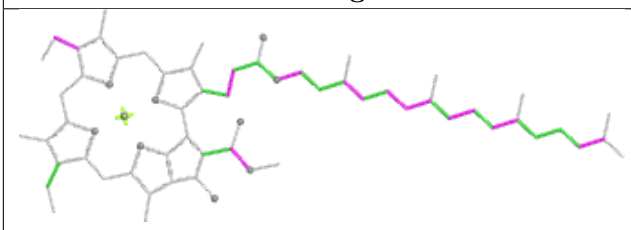
Ligand CLA J 1302



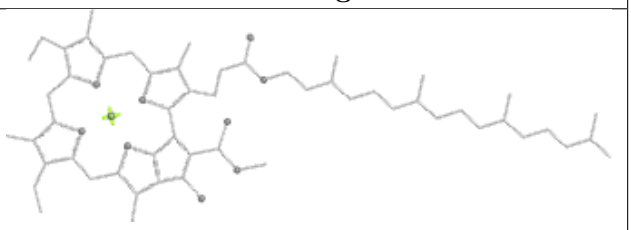
Bond lengths



Bond angles

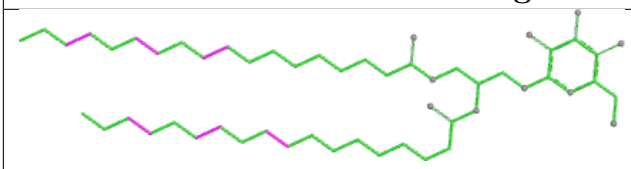


Torsions

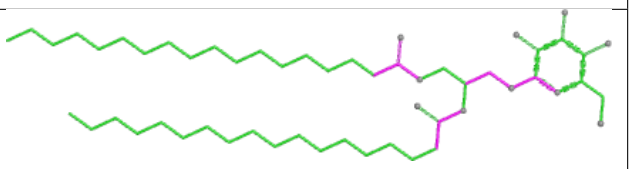


Rings

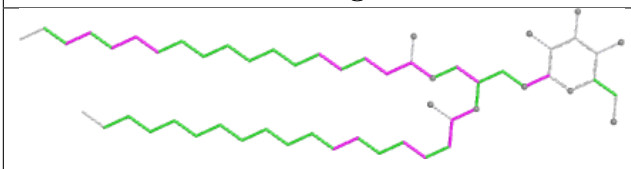
Ligand LMG b 5005



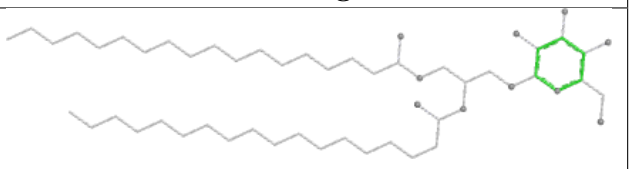
Bond lengths



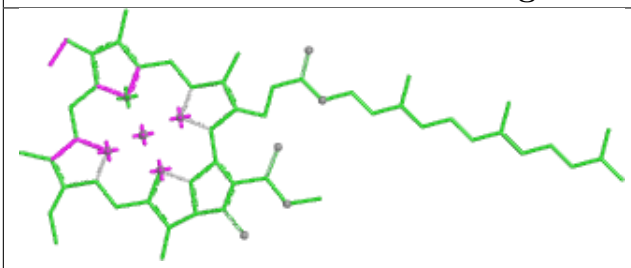
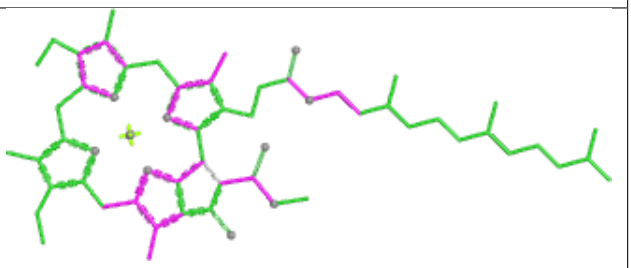
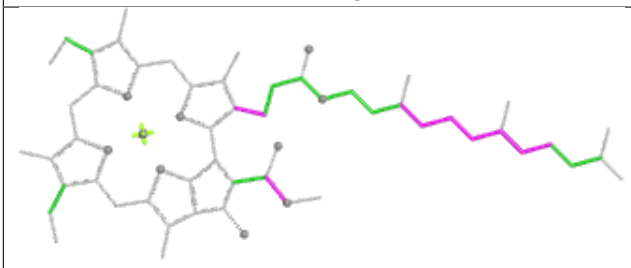
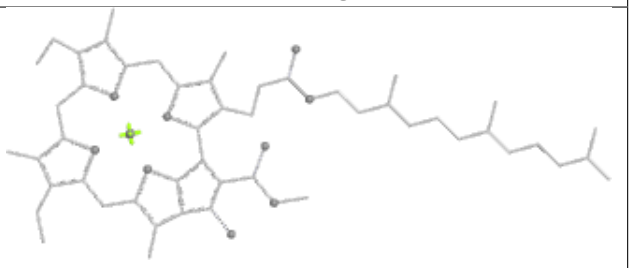
Bond angles

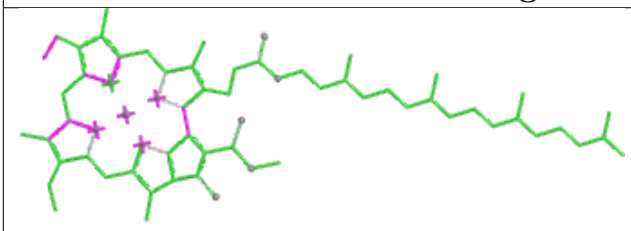
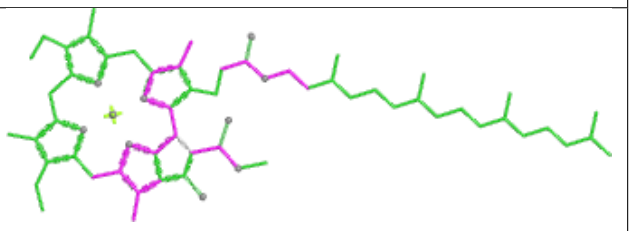
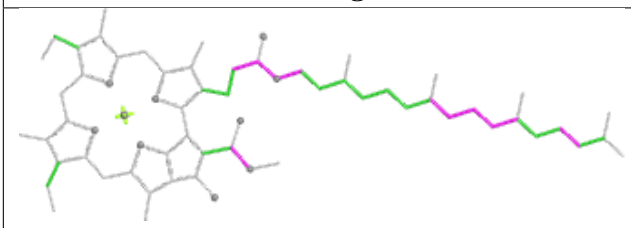
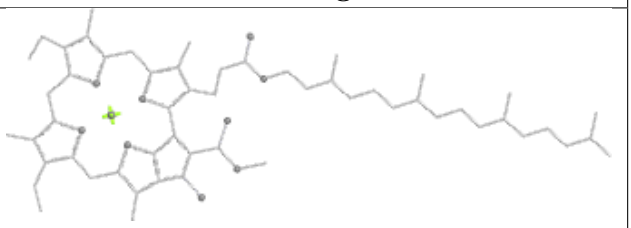


Torsions

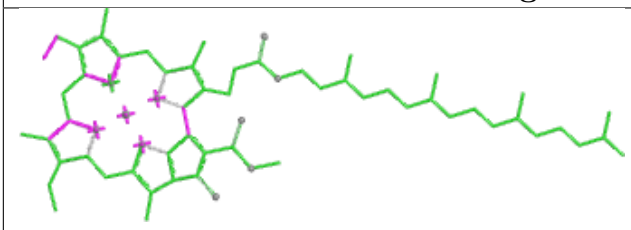


Rings

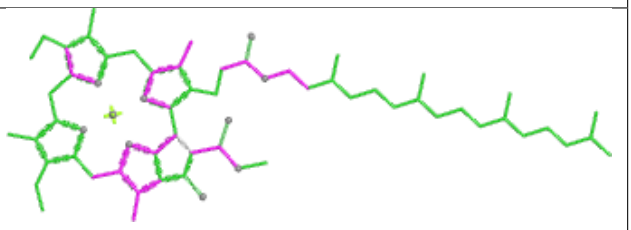
Ligand CLA b 1208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1118	
 Bond lengths	 Bond angles
 Torsions	 Rings

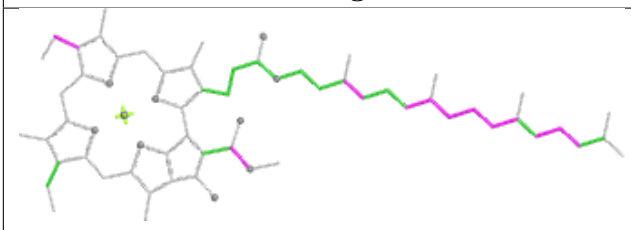
Ligand CLA a 1131



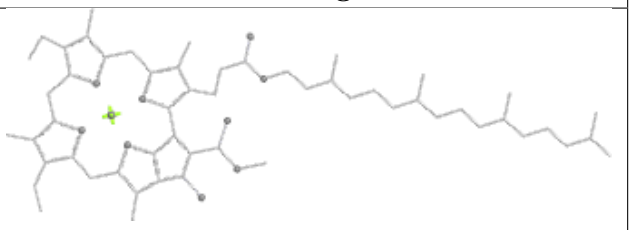
Bond lengths



Bond angles

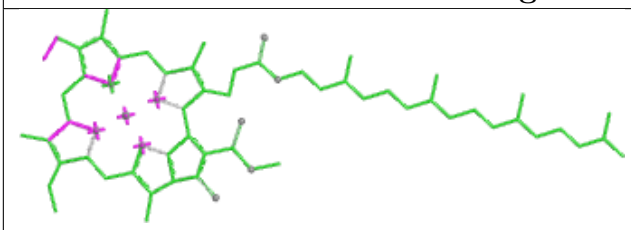


Torsions

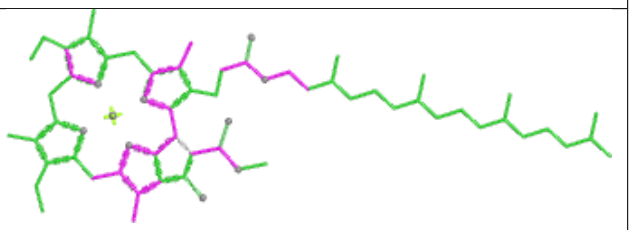


Rings

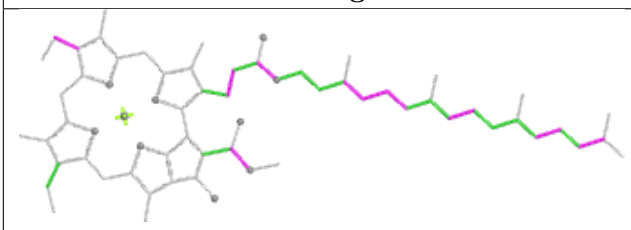
Ligand CLA 2 1237



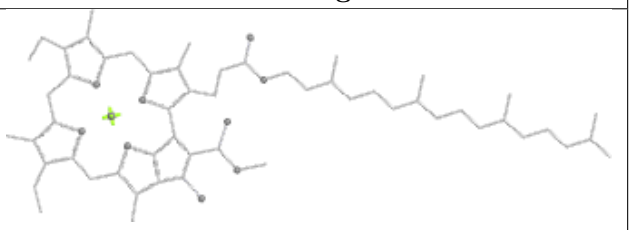
Bond lengths



Bond angles

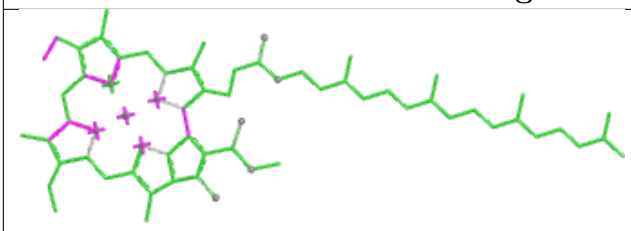


Torsions

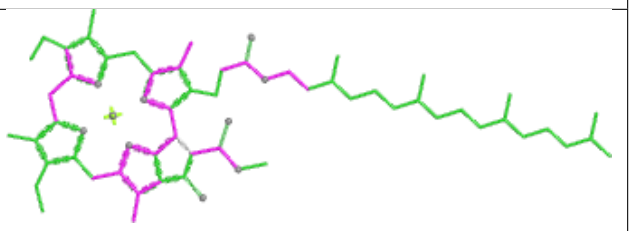


Rings

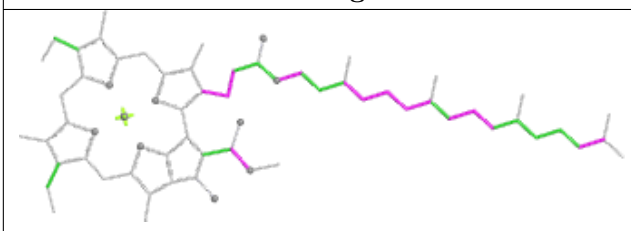
Ligand CLA B 1229



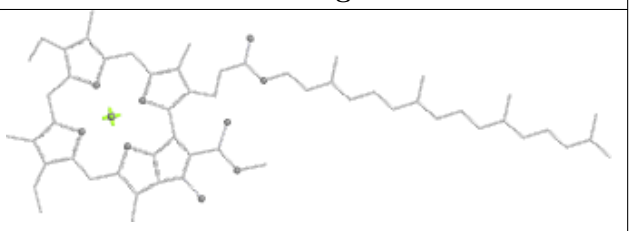
Bond lengths



Bond angles

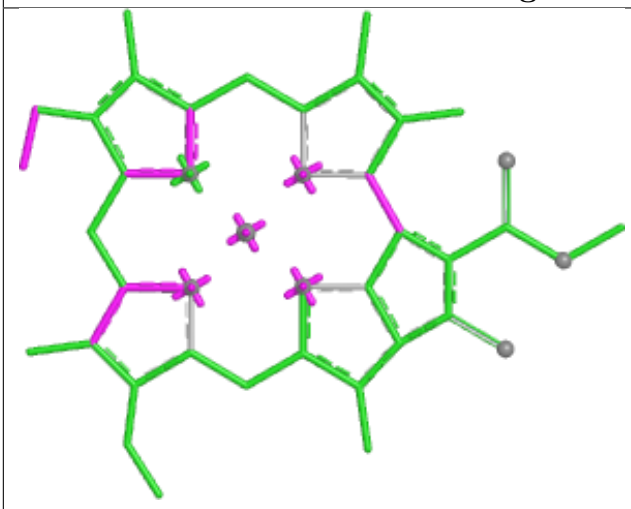


Torsions

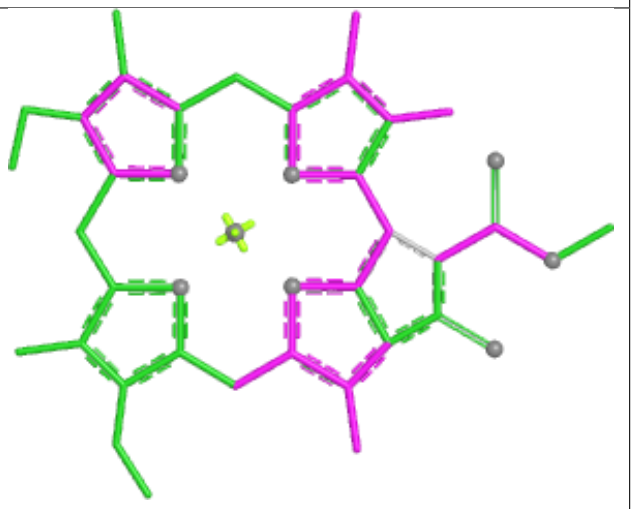


Rings

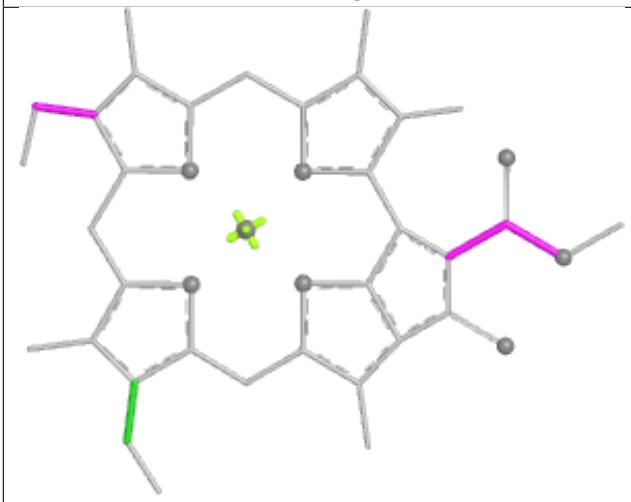
Ligand CLA 2 1212



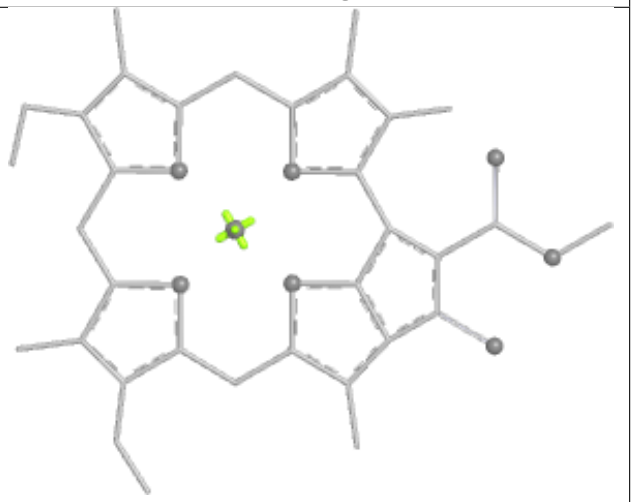
Bond lengths



Bond angles

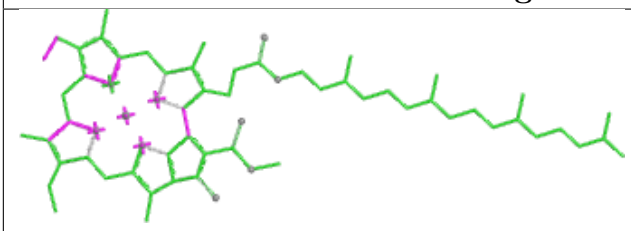


Torsions

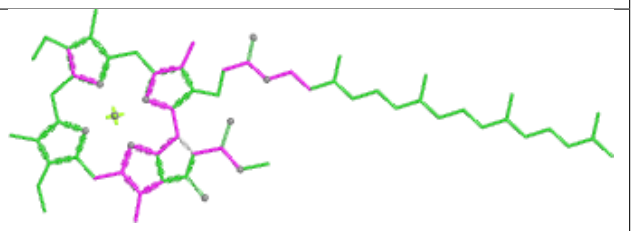


Rings

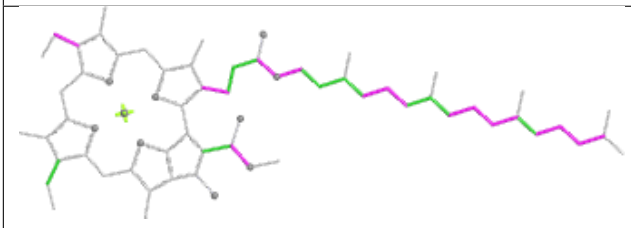
Ligand CLA A 1140



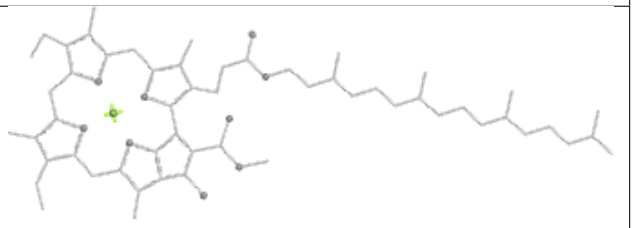
Bond lengths



Bond angles

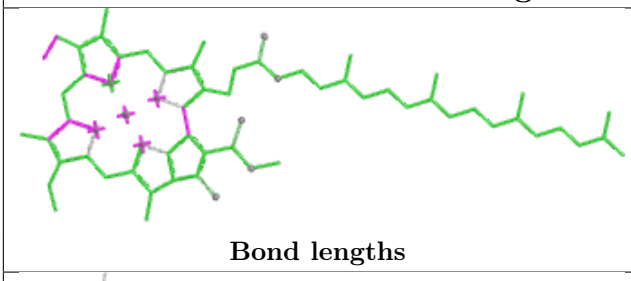


Torsions

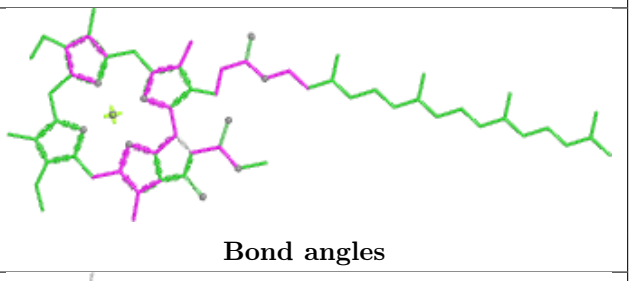


Rings

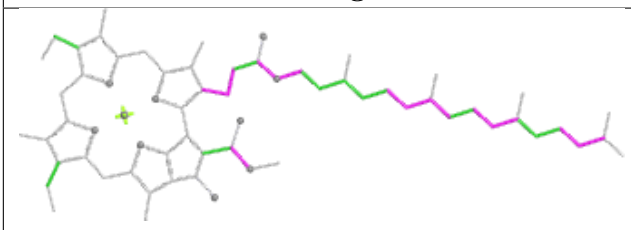
Ligand CLA A 1112



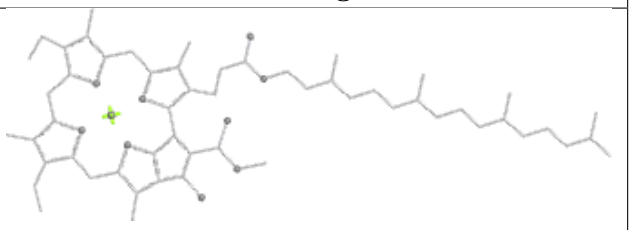
Bond lengths



Bond angles

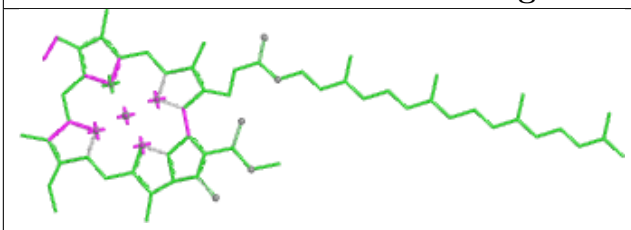


Torsions

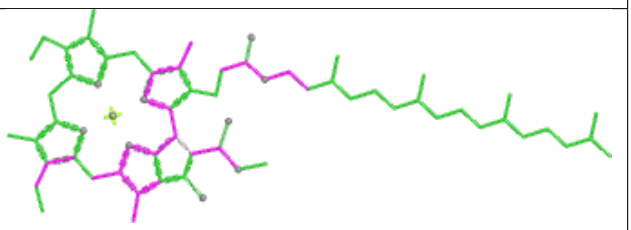


Rings

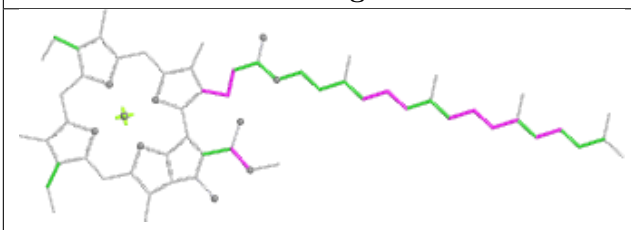
Ligand CLA b 1224



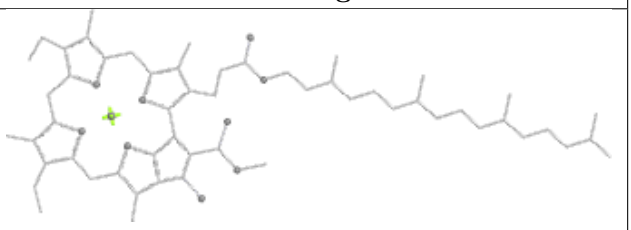
Bond lengths



Bond angles

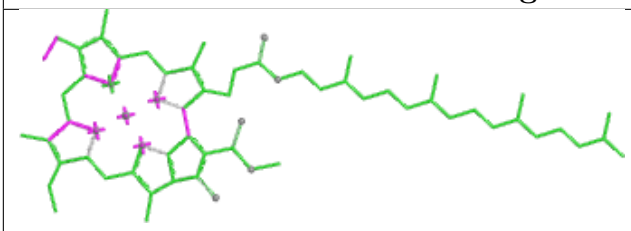


Torsions

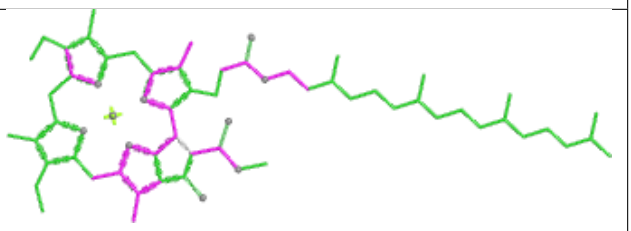


Rings

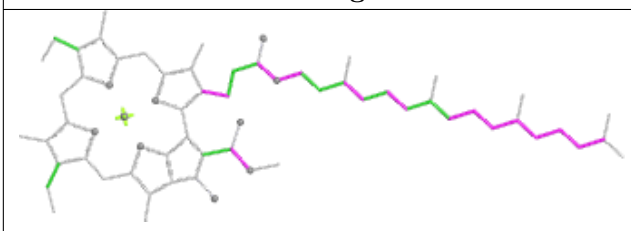
Ligand CLA a 1121



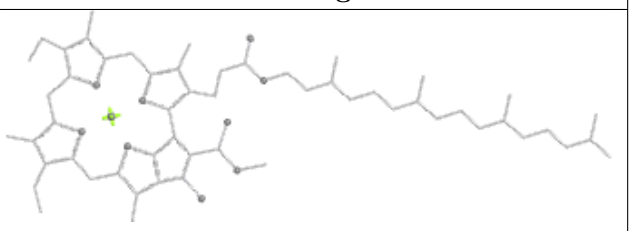
Bond lengths



Bond angles

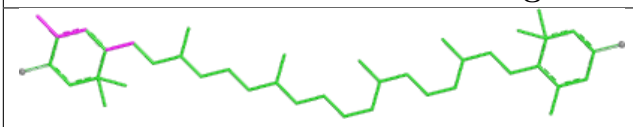


Torsions

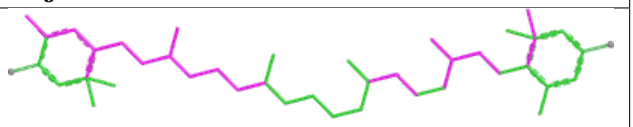


Rings

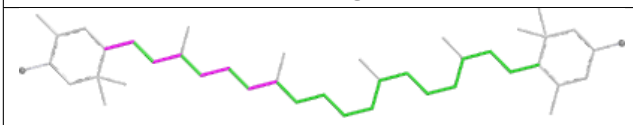
Ligand ZEX j 4015



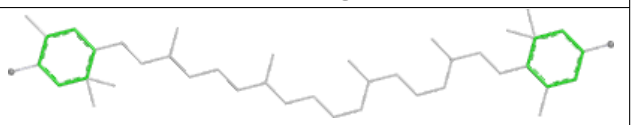
Bond lengths



Bond angles

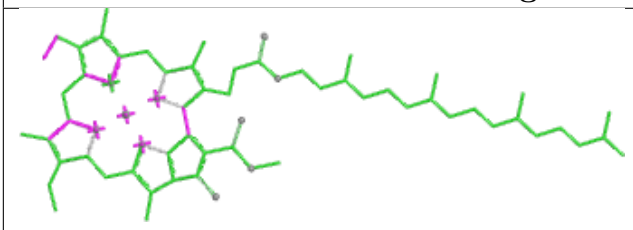


Torsions

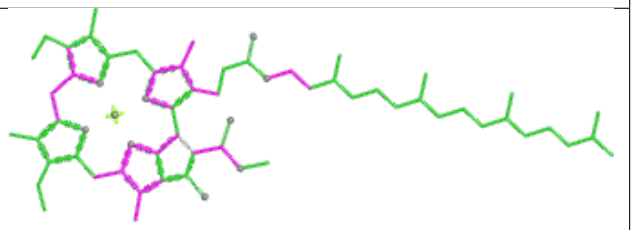


Rings

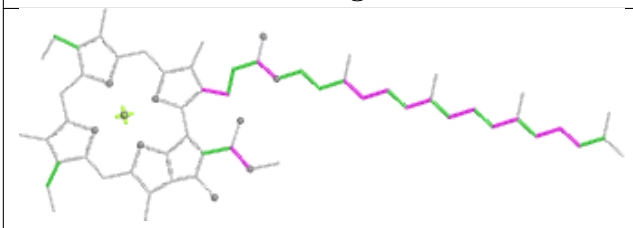
Ligand CLA a 1130



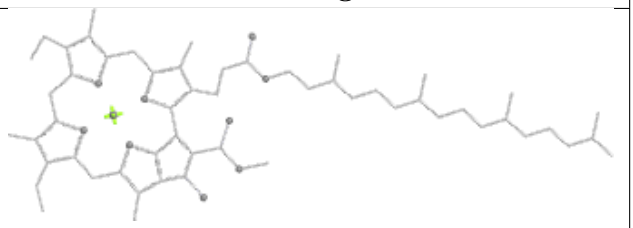
Bond lengths



Bond angles

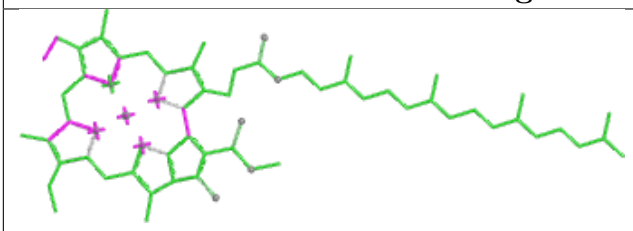


Torsions

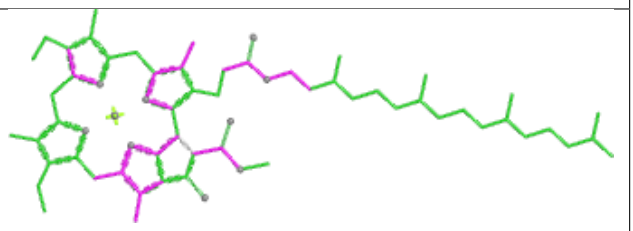


Rings

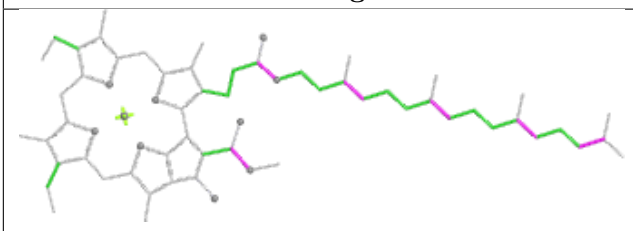
Ligand CLA B 1235



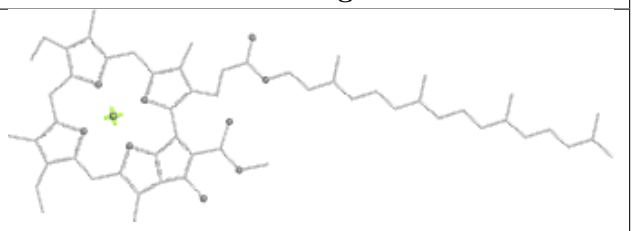
Bond lengths



Bond angles

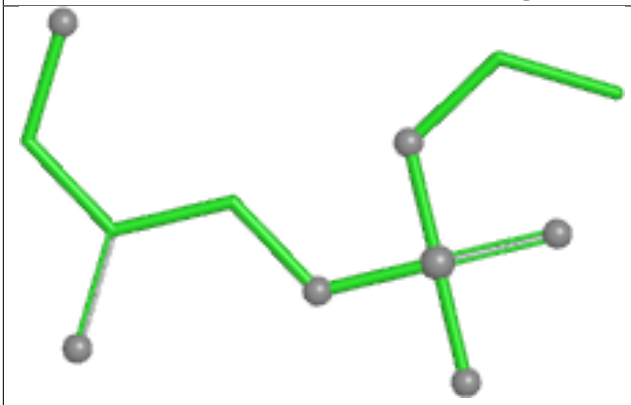


Torsions

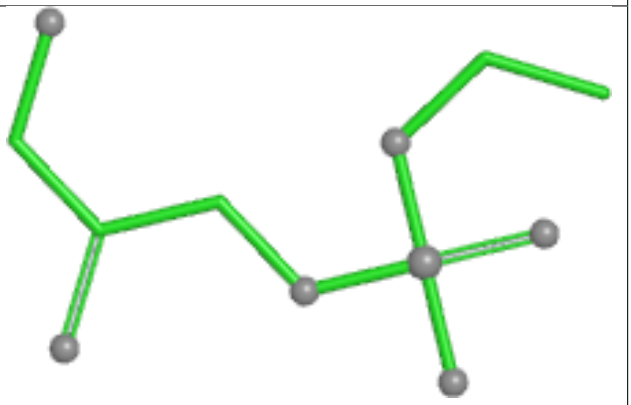


Rings

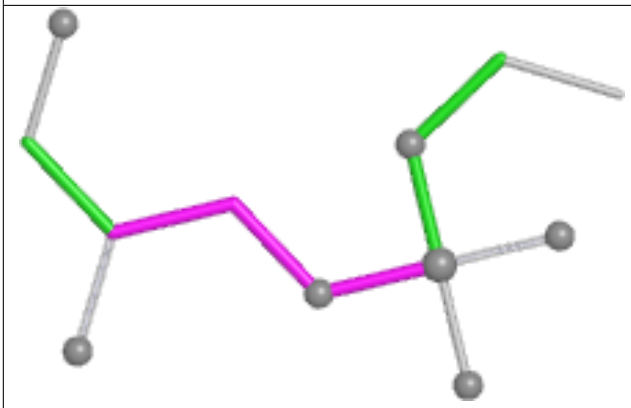
Ligand LHG 6 5001



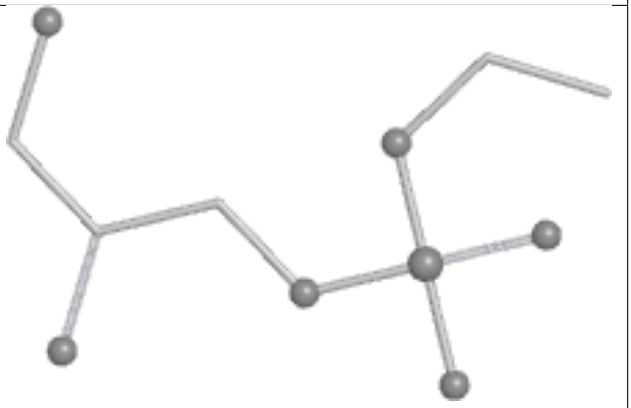
Bond lengths



Bond angles

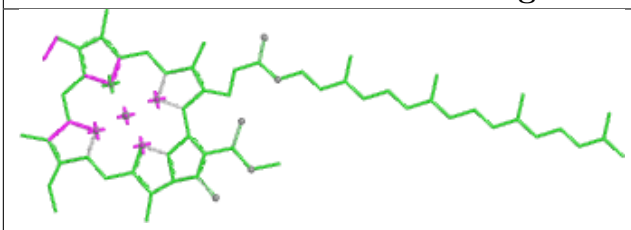


Torsions

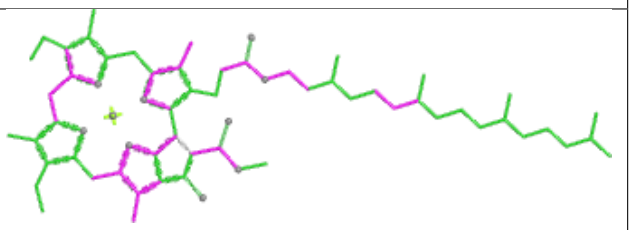


Rings

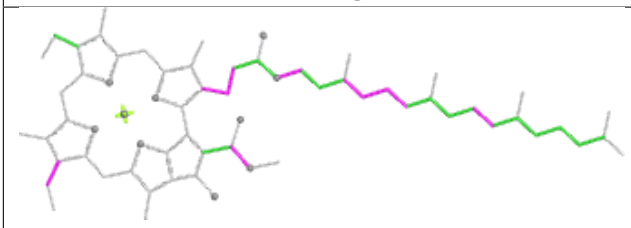
Ligand CLA b 1229



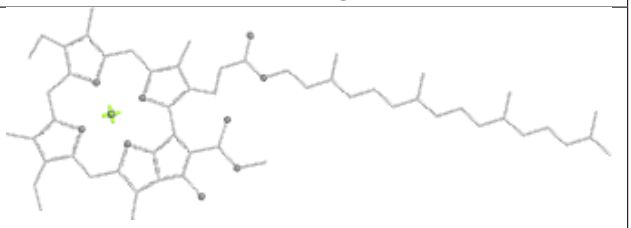
Bond lengths



Bond angles

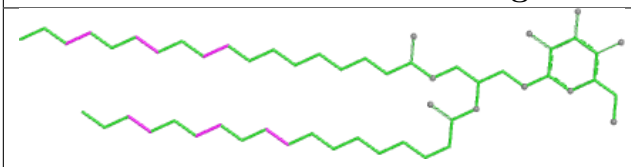


Torsions

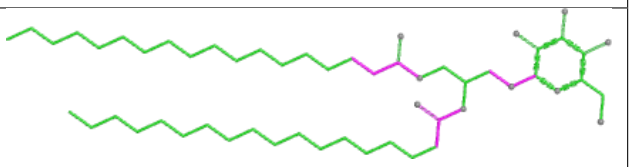


Rings

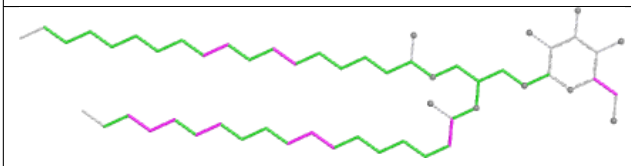
Ligand LMG B 5002



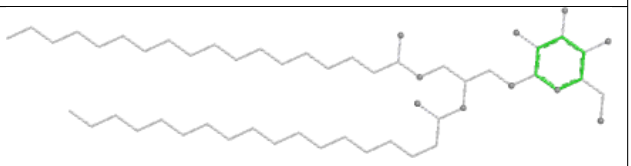
Bond lengths



Bond angles

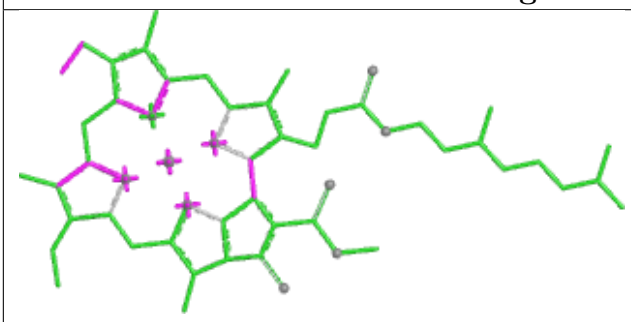


Torsions

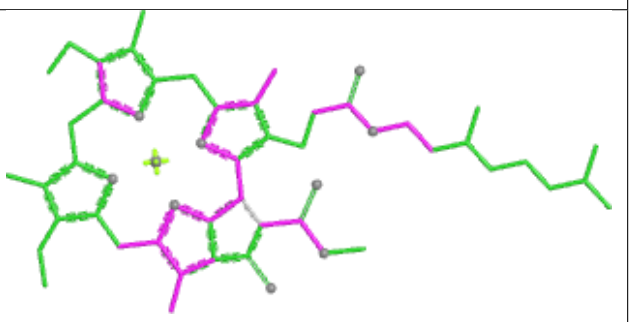


Rings

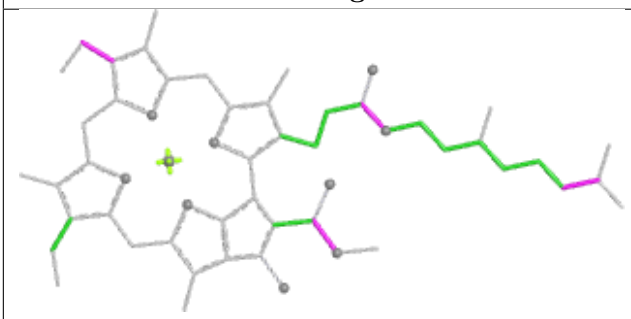
Ligand CLA 2 1223



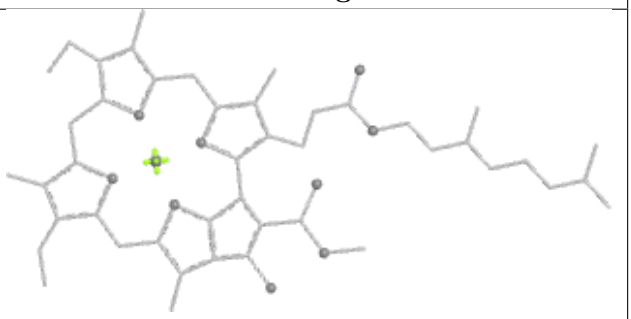
Bond lengths



Bond angles

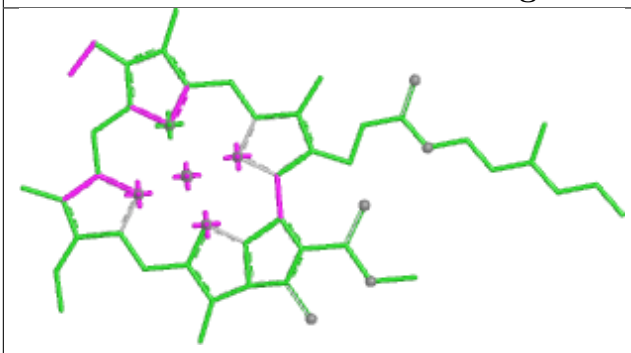


Torsions

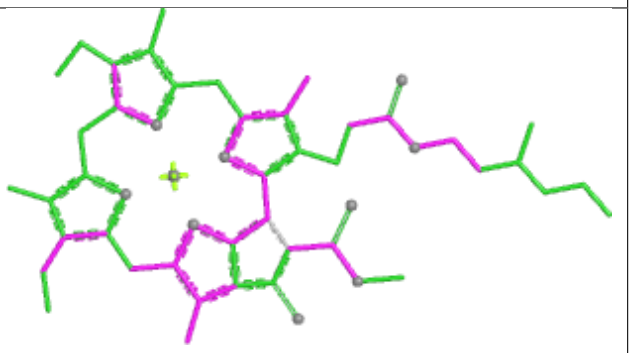


Rings

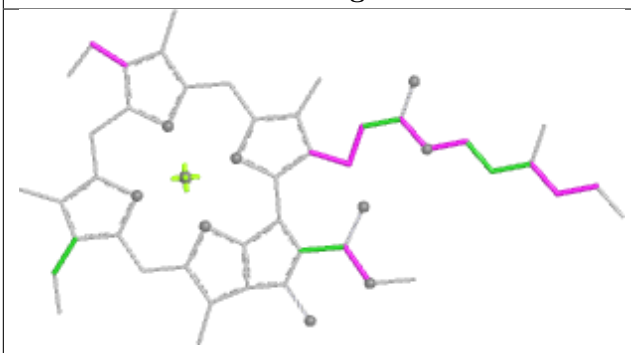
Ligand CLA 2 1217



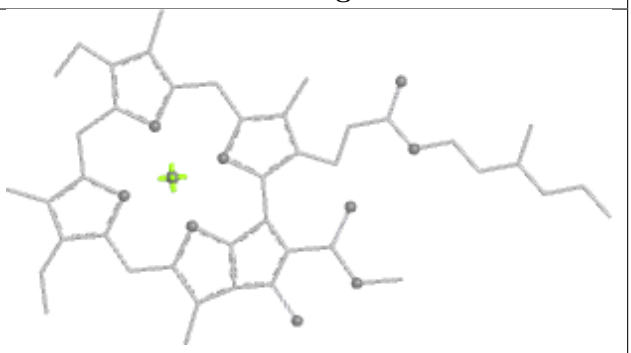
Bond lengths



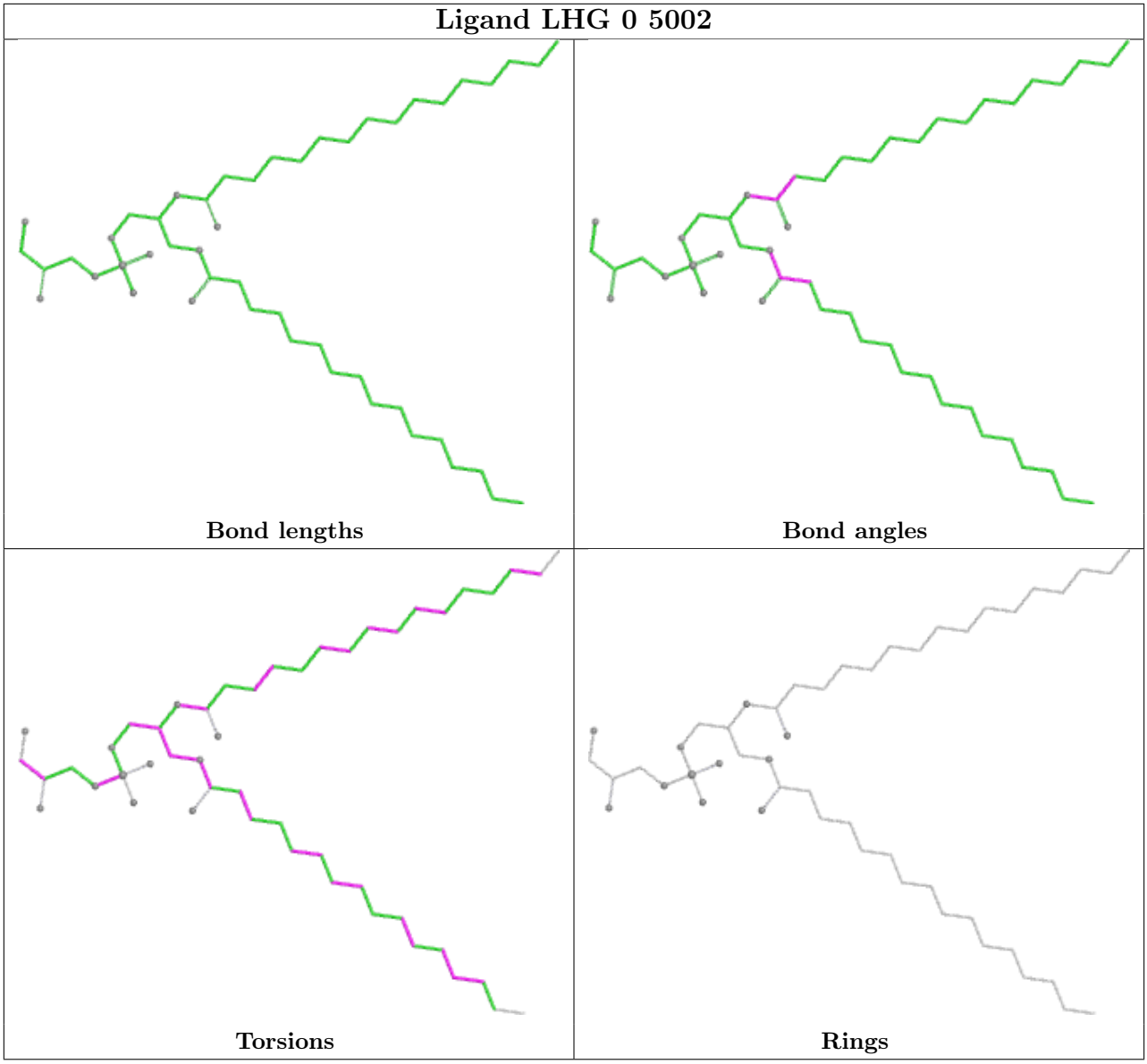
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	751/751 (100%)	0.09	20 (2%) 56 51	29, 47, 72, 134	0
1	a	751/751 (100%)	1.09	114 (15%) 5 4	48, 95, 149, 209	0
2	2	731/731 (100%)	1.07	109 (14%) 5 4	43, 101, 146, 169	0
2	B	731/731 (100%)	0.24	22 (3%) 52 48	29, 56, 90, 152	0
3	3	80/80 (100%)	0.56	4 (5%) 34 30	54, 84, 110, 119	0
3	C	80/80 (100%)	-0.10	1 (1%) 75 71	33, 45, 59, 81	0
4	D	141/141 (100%)	0.05	5 (3%) 47 42	30, 44, 70, 120	0
4	d	141/141 (100%)	0.63	7 (4%) 34 30	56, 82, 106, 136	0
5	5	69/69 (100%)	1.36	14 (20%) 3 2	75, 109, 122, 128	0
5	E	69/69 (100%)	0.50	2 (2%) 53 49	45, 62, 91, 97	0
6	6	143/143 (100%)	1.25	19 (13%) 7 6	114, 141, 158, 189	0
6	F	143/143 (100%)	0.46	5 (3%) 47 42	56, 78, 94, 130	0
6	f	143/143 (100%)	0.68	8 (5%) 30 26	60, 97, 112, 132	0
7	I	40/40 (100%)	-0.04	0 100 100	36, 49, 87, 107	0
7	i	40/40 (100%)	0.23	1 (2%) 58 54	41, 49, 103, 132	0
8	7	40/40 (100%)	0.82	3 (7%) 20 18	109, 128, 152, 165	0
8	J	40/40 (100%)	0.48	3 (7%) 20 18	54, 69, 95, 101	0
8	j	40/40 (100%)	0.61	2 (5%) 34 30	87, 98, 117, 132	0
9	K	80/80 (100%)	1.87	33 (41%) 0 0	39, 64, 113, 128	37 (46%)
10	L	157/157 (100%)	0.03	5 (3%) 50 46	36, 43, 64, 131	0
10	l	157/157 (100%)	0.54	10 (6%) 25 22	45, 60, 107, 184	0
11	9	31/31 (100%)	0.76	5 (16%) 4 4	78, 86, 98, 111	0
11	M	31/31 (100%)	0.33	1 (3%) 50 46	49, 58, 66, 96	0
11	m	31/31 (100%)	-0.03	0 100 100	38, 43, 55, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
12	b	729/729 (100%)	0.32	18 (2%) 58 54	39, 54, 75, 93	0
13	c	81/81 (100%)	0.76	5 (6%) 26 23	54, 69, 83, 96	0
14	e	68/68 (100%)	0.99	5 (7%) 20 18	63, 79, 100, 108	0
15	k	78/78 (100%)	2.46	47 (60%) 0 0	92, 147, 174, 199	36 (46%)
16	1	744/744 (100%)	1.19	111 (14%) 5 4	42, 90, 121, 151	0
17	4	140/140 (100%)	0.55	7 (5%) 34 30	51, 76, 105, 120	0
18	h	38/38 (100%)	0.64	2 (5%) 32 28	54, 68, 95, 96	0
19	8	79/79 (100%)	2.31	46 (58%) 0 0	75, 116, 151, 166	37 (46%)
20	0	154/154 (100%)	0.11	1 (0%) 85 83	38, 51, 73, 108	0
All	All	6771/6771 (100%)	0.67	635 (9%) 14 12	29, 70, 136, 209	110 (1%)

All (635) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	k	81	VAL	11.0
19	8	39	PHE	8.8
1	a	268	TRP	7.8
15	k	14	THR	7.7
1	a	271	TYR	7.1
15	k	11	ALA	6.4
16	1	239	PRO	6.0
16	1	279	GLY	5.9
16	1	51	LEU	5.6
2	B	1	MET	5.5
19	8	87	SER	5.4
10	l	43	GLY	5.4
9	K	52	LEU	5.3
9	K	8	LEU	5.0
19	8	38	TYR	5.0
19	8	18	TRP	4.9
1	a	92	PHE	4.9
6	6	90	ILE	4.9
9	K	12	SER	4.9
2	2	504	SER	4.9
15	k	15	THR	4.8
9	K	42	GLN	4.7
15	k	52	LEU	4.7
9	K	24	ILE	4.6
1	a	47	TRP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	K	86	SER	4.6
9	K	23	GLY	4.5
9	K	44	THR	4.4
2	2	225	PHE	4.4
19	8	19	SER	4.4
19	8	20	LEU	4.4
19	8	16	ALA	4.4
2	2	377	ALA	4.3
12	b	214	SER	4.3
1	a	105	ALA	4.3
1	A	497	THR	4.3
16	1	92	PHE	4.3
19	8	56	ALA	4.3
1	a	272	SER	4.3
13	c	1	MET	4.2
6	6	1	ALA	4.2
15	k	12	SER	4.2
16	1	701	VAL	4.2
2	2	268	LEU	4.2
15	k	84	LEU	4.2
16	1	161	THR	4.1
2	2	379	PHE	4.1
1	a	618	TRP	4.1
9	K	57	SER	4.1
1	a	266	LEU	4.1
1	a	269	GLY	4.1
15	k	19	SER	4.1
1	a	265	THR	4.1
19	8	86	SER	4.0
1	a	12	ALA	4.0
2	2	399	VAL	4.0
1	a	500	ASN	4.0
2	2	618	ARG	4.0
15	k	85	ALA	4.0
2	B	227	THR	4.0
16	1	710	ALA	3.9
9	K	87	SER	3.9
4	D	110	GLU	3.9
19	8	35	VAL	3.9
13	c	62	PHE	3.9
2	2	731	GLY	3.9
16	1	288	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	485	TRP	3.9
1	a	162	ALA	3.9
12	b	731	GLY	3.9
2	2	456	VAL	3.9
19	8	36	ILE	3.8
16	1	244	LEU	3.8
16	1	286	GLY	3.8
6	6	93	SER	3.8
19	8	11	ALA	3.8
1	A	495	GLY	3.8
19	8	24	ILE	3.8
1	a	566	ALA	3.8
2	2	469	LEU	3.8
19	8	55	LEU	3.8
16	1	114	ALA	3.7
2	2	483	ALA	3.7
19	8	9	ALA	3.7
15	k	50	LEU	3.7
1	a	88	SER	3.7
9	K	56	ALA	3.7
2	2	396	TYR	3.6
8	J	33	TYR	3.6
15	k	86	SER	3.6
6	6	107	LEU	3.6
16	1	743	PHE	3.6
15	k	53	PRO	3.6
16	1	246	PRO	3.6
1	a	747	SER	3.6
10	l	154	GLY	3.6
15	k	63	LEU	3.6
1	a	378	TYR	3.6
4	d	77	LYS	3.6
15	k	18	TRP	3.6
1	A	502	LEU	3.6
16	1	505	ALA	3.6
15	k	36	ILE	3.6
15	k	46	LYS	3.5
9	K	10	GLN	3.5
15	k	21	SER	3.5
1	a	38	LEU	3.5
8	J	32	PHE	3.5
9	K	34	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	k	13	PRO	3.5
1	A	2	THR	3.5
16	1	504	THR	3.5
5	5	20	GLY	3.5
9	K	51	ALA	3.5
1	a	264	PHE	3.5
16	1	116	VAL	3.5
15	k	47	GLY	3.5
2	2	286	ILE	3.5
2	2	382	VAL	3.4
1	A	327	ALA	3.4
1	a	243	ILE	3.4
2	2	352	SER	3.4
2	2	532	ILE	3.4
16	1	91	TYR	3.4
16	1	705	ASN	3.4
6	f	55	VAL	3.4
1	A	496	ALA	3.4
2	2	417	ILE	3.4
19	8	57	SER	3.4
3	3	63	LEU	3.4
2	B	731	GLY	3.4
2	2	520	ILE	3.4
10	L	2	ALA	3.4
15	k	16	ALA	3.4
1	a	274	PHE	3.4
1	a	613	MET	3.4
1	a	3	ILE	3.4
1	a	345	THR	3.3
15	k	83	GLY	3.3
2	2	567	ILE	3.3
1	a	2	THR	3.3
15	k	23	GLY	3.3
2	B	730	PHE	3.3
13	c	81	TYR	3.3
1	a	267	ASN	3.3
2	2	505	LEU	3.3
6	f	98	MET	3.3
1	A	500	ASN	3.3
10	L	102	VAL	3.3
16	1	121	VAL	3.3
11	9	5	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2	353	LEU	3.2
16	1	709	VAL	3.2
19	8	15	THR	3.2
1	a	411	PHE	3.2
1	a	37	THR	3.2
16	1	243	ILE	3.2
1	a	275	LEU	3.2
4	D	77	LYS	3.2
2	2	119	GLY	3.2
9	K	22	VAL	3.2
6	6	87	LEU	3.2
1	a	520	VAL	3.2
15	k	24	ILE	3.2
19	8	14	THR	3.2
1	a	257	ALA	3.1
9	K	61	PHE	3.1
19	8	60	THR	3.1
2	B	2	ALA	3.1
1	a	303	LEU	3.1
2	2	506	PHE	3.1
2	2	476	LEU	3.1
11	M	3	LEU	3.1
9	K	45	GLY	3.1
15	k	45	GLY	3.1
1	a	617	VAL	3.1
10	l	156	PHE	3.1
16	1	97	PHE	3.1
19	8	52	LEU	3.1
2	B	83	ASN	3.1
16	1	103	TRP	3.1
9	K	17	GLY	3.1
15	k	79	GLY	3.1
19	8	22	VAL	3.1
1	a	96	LYS	3.0
1	a	748	LEU	3.0
2	2	410	LEU	3.0
1	a	317	ILE	3.0
19	8	10	GLN	3.0
16	1	350	ALA	3.0
1	a	383	TYR	3.0
5	5	19	TYR	3.0
12	b	620	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	263	PHE	3.0
16	1	34	PHE	3.0
9	K	19	SER	3.0
19	8	59	LYS	3.0
16	1	386	GLN	3.0
19	8	41	ILE	3.0
1	a	307	ALA	3.0
9	K	9	ALA	3.0
2	2	160	LYS	3.0
16	1	142	GLY	3.0
1	a	621	VAL	2.9
17	4	103	VAL	2.9
17	4	2	THR	2.9
15	k	55	LEU	2.9
1	a	34	PHE	2.9
16	1	94	GLY	2.9
18	h	38	GLY	2.9
15	k	9	ALA	2.9
16	1	53	ALA	2.9
6	f	24	LEU	2.9
3	C	62	PHE	2.9
15	k	61	PHE	2.9
5	5	47	ASN	2.9
2	2	441	VAL	2.9
2	2	365	THR	2.9
5	5	43	ARG	2.9
1	A	10	ALA	2.9
6	f	43	ALA	2.9
9	K	48	LYS	2.9
5	E	3	LEU	2.9
5	5	18	TRP	2.9
2	2	457	PHE	2.9
2	B	223	MET	2.9
5	5	22	VAL	2.9
1	a	10	ALA	2.9
2	2	92	TRP	2.9
16	1	118	TRP	2.9
19	8	17	GLY	2.9
16	1	481	ILE	2.8
4	d	70	THR	2.8
9	K	53	PRO	2.8
16	1	384	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	1	712	ALA	2.8
16	1	554	LEU	2.8
19	8	50	LEU	2.8
2	2	570	TRP	2.8
2	2	330	PHE	2.8
17	4	107	LYS	2.8
1	a	750	ILE	2.8
11	9	4	SER	2.8
16	1	656	ASN	2.8
1	a	116	VAL	2.8
1	a	6	PRO	2.8
1	A	493	ALA	2.8
9	K	11	ALA	2.8
15	k	39	PHE	2.8
2	2	310	GLY	2.8
2	2	375	TYR	2.8
6	6	106	PRO	2.8
16	1	193	VAL	2.8
2	2	334	LEU	2.8
2	2	727	ALA	2.8
16	1	391	THR	2.8
2	2	302	LYS	2.8
15	k	48	LYS	2.8
1	a	256	PHE	2.8
1	a	609	PHE	2.8
10	l	136	PHE	2.8
2	2	324	ILE	2.8
3	3	65	ILE	2.8
1	a	5	PRO	2.8
1	a	244	LEU	2.8
15	k	56	ALA	2.8
15	k	82	LEU	2.8
12	b	496	ASP	2.8
16	1	52	HIS	2.8
2	2	297	ILE	2.7
2	2	424	SER	2.7
16	1	666	SER	2.7
16	1	657	VAL	2.7
1	a	108	THR	2.7
11	9	3	LEU	2.7
2	2	166	ALA	2.7
15	k	64	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	d	67	ALA	2.7
16	1	12	ALA	2.7
19	8	48	LYS	2.7
2	2	127	ILE	2.7
16	1	720	ILE	2.7
8	7	40	PRO	2.7
10	L	1	MET	2.7
1	a	149	ALA	2.7
2	2	468	ALA	2.7
6	6	76	ALA	2.7
1	a	279	GLY	2.7
1	a	308	GLY	2.7
2	2	555	PRO	2.7
16	1	119	PRO	2.7
19	8	58	LYS	2.7
1	a	561	LEU	2.7
2	2	234	ALA	2.7
16	1	163	ILE	2.6
16	1	317	ILE	2.6
16	1	672	PHE	2.6
19	8	53	PRO	2.6
16	1	249	MET	2.6
1	a	340	LEU	2.6
2	2	475	LEU	2.6
14	e	9	VAL	2.6
1	a	159	TYR	2.6
1	a	635	PHE	2.6
2	2	385	PHE	2.6
2	2	498	ILE	2.6
19	8	61	PHE	2.6
6	F	113	LEU	2.6
6	f	53	LEU	2.6
9	K	55	LEU	2.6
2	2	605	GLN	2.6
5	5	53	ALA	2.6
1	a	348	TRP	2.6
9	K	18	TRP	2.6
1	a	381	ILE	2.6
1	A	570	PHE	2.6
16	1	144	PHE	2.6
1	a	204	LEU	2.6
6	6	131	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	k	20	LEU	2.6
15	k	10	GLN	2.6
1	a	521	ALA	2.6
1	a	416	TYR	2.6
16	1	100	TYR	2.6
2	B	501	GLY	2.6
5	5	7	ASP	2.6
10	l	153	ARG	2.6
16	1	29	GLY	2.6
2	B	244	PHE	2.6
1	a	562	VAL	2.6
2	2	642	VAL	2.6
16	1	372	ALA	2.6
19	8	12	SER	2.6
15	k	59	LYS	2.6
16	1	156	TYR	2.6
2	2	87	ILE	2.5
12	b	730	PHE	2.5
19	8	32	PHE	2.5
16	1	238	LEU	2.5
16	1	389	LEU	2.5
16	1	162	ALA	2.5
16	1	655	ALA	2.5
19	8	51	ALA	2.5
2	B	312	LEU	2.5
1	a	270	VAL	2.5
1	a	519	LYS	2.5
15	k	58	LYS	2.5
15	k	51	ALA	2.5
1	a	4	SER	2.5
2	2	470	TYR	2.5
5	5	23	GLY	2.5
2	2	699	ILE	2.5
6	6	75	ILE	2.5
2	2	494	TRP	2.5
1	a	672	PHE	2.5
2	2	452	LEU	2.5
9	K	20	LEU	2.5
16	1	707	LEU	2.5
1	a	68	VAL	2.5
2	2	282	VAL	2.5
1	a	367	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	1	688	SER	2.5
16	1	160	CYS	2.5
2	2	314	GLY	2.5
6	f	54	ILE	2.5
2	2	507	LEU	2.5
6	F	66	LEU	2.5
6	f	1	ALA	2.5
5	5	16	SER	2.5
15	k	44	THR	2.5
16	1	285	THR	2.5
16	1	631	THR	2.5
2	2	501	GLY	2.4
1	a	156	TYR	2.4
6	6	35	ILE	2.4
16	1	692	TYR	2.4
1	a	205	LEU	2.4
16	1	47	TRP	2.4
1	a	255	SER	2.4
2	2	487	GLY	2.4
12	b	259	GLY	2.4
1	A	721	ILE	2.4
1	a	207	LEU	2.4
16	1	430	LEU	2.4
6	6	52	HIS	2.4
9	K	39	PHE	2.4
2	B	229	ASN	2.4
2	2	230	TRP	2.4
12	b	603	VAL	2.4
9	K	13	PRO	2.4
17	4	106	GLU	2.4
6	6	129	GLY	2.4
17	4	135	GLY	2.4
16	1	713	ILE	2.4
2	2	320	LEU	2.4
8	J	1	MET	2.4
12	b	235	ALA	2.4
19	8	44	THR	2.4
1	A	6	PRO	2.4
17	4	126	PRO	2.4
1	A	235	ASP	2.4
1	a	637	GLN	2.4
5	5	68	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2	233	TYR	2.4
2	2	730	PHE	2.4
4	d	83	TYR	2.4
2	2	423	VAL	2.4
2	2	489	ALA	2.4
16	1	96	LYS	2.4
19	8	43	LYS	2.4
6	6	51	PRO	2.3
9	K	60	THR	2.3
14	e	18	TRP	2.4
1	a	580	GLY	2.3
1	a	146	LEU	2.3
2	2	255	LEU	2.3
2	2	312	LEU	2.3
2	2	482	ILE	2.3
2	2	536	LEU	2.3
15	k	25	ILE	2.3
6	6	2	ASP	2.3
16	1	158	LEU	2.3
1	a	1	MET	2.3
9	K	38	TYR	2.3
1	a	11	LYS	2.3
2	2	68	VAL	2.3
2	2	232	VAL	2.3
16	1	13	LYS	2.3
6	6	89	GLU	2.3
16	1	10	ALA	2.3
5	5	14	THR	2.3
1	a	41	GLY	2.3
1	a	408	GLY	2.3
10	L	106	GLY	2.3
19	8	37	GLY	2.3
1	A	481	ILE	2.3
2	2	213	LEU	2.3
2	2	524	LEU	2.3
2	2	628	LEU	2.3
8	j	1	MET	2.3
12	b	444	PHE	2.3
16	1	685	PHE	2.3
10	l	7	VAL	2.3
16	1	117	VAL	2.3
11	9	2	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	1	184	ALA	2.3
1	A	8	ARG	2.3
2	B	214	SER	2.3
13	c	78	GLY	2.3
1	a	93	HIS	2.3
1	a	298	LEU	2.3
10	l	155	LEU	2.3
3	3	54	CYS	2.3
1	a	668	TYR	2.3
8	7	33	TYR	2.3
16	1	521	ALA	2.3
19	8	40	ALA	2.3
1	a	286	GLY	2.3
2	2	199	ILE	2.3
12	b	643	TRP	2.3
16	1	146	LEU	2.3
6	F	2	ASP	2.3
19	8	46	LYS	2.3
1	a	402	VAL	2.3
6	6	102	VAL	2.3
15	k	22	VAL	2.3
1	a	107	PRO	2.3
1	a	374	PRO	2.3
2	2	229	ASN	2.2
12	b	326	ASN	2.2
1	a	153	THR	2.2
2	B	3	THR	2.2
12	b	611	THR	2.2
17	4	33	THR	2.2
1	a	191	GLN	2.2
12	b	501	GLY	2.2
2	2	543	LEU	2.2
2	2	723	ILE	2.2
15	k	43	LYS	2.2
16	1	638	SER	2.2
1	a	302	VAL	2.2
16	1	14	VAL	2.2
2	2	497	ALA	2.2
2	2	644	ALA	2.2
13	c	40	ALA	2.2
2	2	364	THR	2.2
2	B	495	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2	25	ILE	2.2
16	1	702	TRP	2.2
16	1	167	VAL	2.2
18	h	7	ALA	2.2
2	2	374	GLN	2.2
9	K	59	LYS	2.2
12	b	312	LEU	2.2
12	b	621	LEU	2.2
16	1	173	LEU	2.2
16	1	290	LEU	2.2
16	1	387	LEU	2.2
2	B	480	ASP	2.2
19	8	34	PHE	2.2
2	B	729	LYS	2.2
9	K	58	LYS	2.2
16	1	380	ALA	2.2
16	1	612	LYS	2.2
16	1	50	ASN	2.2
16	1	708	ASN	2.2
9	K	70	MET	2.2
1	a	261	THR	2.2
2	B	215	THR	2.2
1	A	492	LEU	2.2
2	B	213	LEU	2.2
2	B	310	GLY	2.2
2	2	704	LEU	2.2
5	E	32	GLY	2.2
14	e	20	GLY	2.2
15	k	62	GLY	2.2
16	1	280	GLY	2.2
16	1	689	GLY	2.2
16	1	744	LEU	2.2
19	8	23	GLY	2.2
2	2	115	ILE	2.2
19	8	21	SER	2.2
19	8	65	GLU	2.2
2	2	154	TRP	2.2
4	D	132	LYS	2.2
8	j	32	PHE	2.2
15	k	32	PHE	2.2
1	a	553	VAL	2.1
14	e	69	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	8	31	VAL	2.1
6	F	1	ALA	2.1
16	1	55	ALA	2.1
16	1	496	ALA	2.1
16	1	639	ALA	2.1
16	1	664	ALA	2.1
16	1	717	ALA	2.1
1	a	751	GLY	2.1
2	2	596	LEU	2.1
5	5	3	LEU	2.1
6	6	53	LEU	2.1
7	i	38	GLY	2.1
10	l	32	THR	2.1
1	a	125	ILE	2.1
2	2	226	PHE	2.1
2	2	617	PHE	2.1
16	1	256	PHE	2.1
16	1	257	ALA	2.1
1	a	567	ASN	2.1
2	2	260	GLY	2.1
2	2	278	LEU	2.1
4	d	68	LEU	2.1
6	6	73	LEU	2.1
16	1	204	LEU	2.1
2	B	243	ILE	2.1
12	b	567	ILE	2.1
1	a	145	TYR	2.1
1	a	341	TYR	2.1
2	2	43	TYR	2.1
16	1	180	TYR	2.1
16	1	374	PRO	2.1
2	2	284	PHE	2.1
2	2	392	PHE	2.1
4	d	104	PHE	2.1
6	6	98	MET	2.1
1	A	270	VAL	2.1
16	1	61	GLN	2.1
16	1	722	GLN	2.1
1	a	118	TRP	2.1
2	2	279	ALA	2.1
2	2	443	ALA	2.1
10	l	5	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	290	LEU	2.1
16	1	260	LEU	2.1
16	1	527	LEU	2.1
4	D	2	THR	2.1
16	1	346	THR	2.1
19	8	47	GLY	2.1
1	a	8	ARG	2.1
1	a	300	ILE	2.1
2	B	127	ILE	2.1
16	1	381	ILE	2.1
16	1	31	PRO	2.1
8	7	1	MET	2.1
16	1	635	PHE	2.1
19	8	42	GLN	2.1
20	0	29	PHE	2.1
1	a	114	ALA	2.1
1	a	353	ALA	2.1
15	k	78	ALA	2.1
2	2	369	LEU	2.1
2	2	427	LEU	2.1
6	F	117	LEU	2.1
10	L	157	ASN	2.1
16	1	147	TRP	2.1
1	A	499	PRO	2.1
1	a	31	PRO	2.1
2	2	511	PRO	2.1
4	d	1	MET	2.1
2	2	361	GLN	2.0
16	1	115	GLN	2.0
1	a	14	VAL	2.0
2	B	232	VAL	2.0
2	2	358	PHE	2.0
12	b	441	VAL	2.0
14	e	22	VAL	2.0
2	2	488	ALA	2.0
1	A	489	LEU	2.0
2	2	587	LEU	2.0
11	9	9	LEU	2.0
19	8	84	LEU	2.0
1	a	208	GLY	2.0
2	2	70	TRP	2.0
4	D	111	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	l	150	GLY	2.0
16	1	485	TRP	2.0
1	a	154	ASP	2.0
1	a	616	ASP	2.0
2	2	566	ASP	2.0
1	a	231	VAL	2.0
1	a	657	VAL	2.0
2	2	120	VAL	2.0
3	3	62	PHE	2.0
1	a	158	LEU	2.0
2	2	222	LEU	2.0
5	5	26	ALA	2.0
16	1	250	ALA	2.0
16	1	299	ALA	2.0
6	f	46	GLY	2.0
12	b	4	LYS	2.0
1	a	305	ILE	2.0
1	a	739	THR	2.0
2	2	252	THR	2.0
1	a	177	TRP	2.0
15	k	49	ASP	2.0
15	k	38	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	LHG	B	5006	49/49	0.43	0.21	84,117,143,146	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	LHG	6	5001	12/49	0.46	0.20	80,131,152,159	0
26	LMG	b	5007	55/55	0.50	0.21	76,97,115,116	0
27	ACT	B	7002	4/4	0.50	0.23	78,82,83,84	0
24	BCR	1	4019	40/40	0.51	0.25	106,122,142,143	0
21	CLA	6	1302	43/65	0.53	0.18	116,141,171,178	0
21	CLA	a	1113	50/65	0.53	0.22	116,145,155,159	0
31	SQD	F	5001	54/54	0.56	0.22	66,93,129,134	0
21	CLA	2	1240	41/65	0.58	0.17	131,137,146,150	0
24	BCR	2	4004	40/40	0.59	0.23	105,125,145,147	0
24	BCR	a	4019	40/40	0.59	0.26	98,114,155,155	0
21	CLA	7	1303	41/65	0.59	0.17	133,150,155,157	0
31	SQD	b	5006	54/54	0.60	0.18	46,81,138,143	0
25	LHG	a	5007	49/49	0.61	0.21	100,139,169,175	0
25	LHG	0	5004	49/49	0.61	0.20	55,96,124,136	0
21	CLA	B	1240	65/65	0.62	0.21	76,105,133,136	0
25	LHG	1	5005	49/49	0.63	0.22	90,126,165,169	0
27	ACT	B	7001	4/4	0.63	0.18	57,71,71,74	0
27	ACT	a	7001	4/4	0.63	0.15	128,130,130,131	0
21	CLA	j	1302	65/65	0.63	0.18	77,110,125,133	0
26	LMG	2	5005	55/55	0.63	0.21	105,127,150,153	0
25	LHG	F	5002	49/49	0.64	0.19	73,110,175,181	0
24	BCR	k	4001	40/40	0.64	0.17	119,152,167,168	0
21	CLA	J	1302	65/65	0.64	0.20	75,95,121,137	0
25	LHG	1	5007	49/49	0.65	0.17	80,102,149,154	0
25	LHG	2	5004	49/49	0.65	0.18	92,108,152,153	0
24	BCR	A	4019	40/40	0.65	0.19	72,84,114,114	0
21	CLA	2	1219	53/65	0.65	0.19	108,125,148,156	0
26	LMG	B	5005	55/55	0.65	0.25	71,110,133,137	0
21	CLA	k	1402	49/65	0.65	0.16	134,158,161,161	8
35	LMT	1	6001	35/35	0.65	0.17	76,127,136,141	0
25	LHG	l	5003	49/49	0.66	0.19	81,111,137,138	0
37	DGD	L	5004	66/66	0.66	0.18	42,87,116,121	0
21	CLA	7	1302	41/65	0.67	0.15	120,130,140,143	0
31	SQD	0	5005	54/54	0.67	0.18	59,91,141,148	0
26	LMG	b	5005	55/55	0.68	0.20	54,79,114,116	0
25	LHG	a	5005	49/49	0.69	0.17	51,107,175,183	0
21	CLA	j	1303	55/65	0.69	0.14	97,117,130,137	0
26	LMG	A	5008	55/55	0.69	0.20	72,119,146,146	0
35	LMT	l	6001	35/35	0.70	0.15	55,95,118,120	0
25	LHG	A	5006	49/49	0.70	0.19	44,81,137,147	0
24	BCR	8	4001	40/40	0.70	0.18	105,124,139,140	0
21	CLA	2	1218	65/65	0.71	0.17	91,133,158,162	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	7	4013	40/40	0.71	0.19	78,113,122,124	0
26	LMG	a	5004	55/55	0.71	0.21	85,112,130,136	0
21	CLA	f	1302	65/65	0.71	0.17	67,99,109,115	0
25	LHG	M	5001	49/49	0.71	0.18	51,97,144,149	0
21	CLA	1	1108	47/65	0.72	0.16	50,112,123,128	0
26	LMG	1	5004	55/55	0.72	0.17	83,97,112,118	0
21	CLA	J	1303	65/65	0.72	0.16	93,112,125,127	0
21	CLA	2	1232	45/65	0.73	0.17	101,128,147,151	0
21	CLA	2	1213	50/65	0.73	0.19	99,122,130,139	0
24	BCR	B	4018	40/40	0.73	0.23	64,85,115,121	0
25	LHG	A	5007	49/49	0.73	0.18	46,85,113,121	0
31	SQD	B	5008	54/54	0.74	0.17	61,86,107,113	0
24	BCR	2	4018	40/40	0.74	0.24	83,136,143,144	0
21	CLA	2	1217	52/65	0.74	0.17	99,130,138,139	0
31	SQD	f	5001	54/54	0.74	0.17	42,100,123,132	0
21	CLA	a	1120	55/65	0.75	0.15	98,124,129,138	0
25	LHG	A	5005	49/49	0.75	0.17	48,72,132,139	0
24	BCR	1	4001	40/40	0.75	0.21	90,109,136,137	0
30	ECH	2	4006	41/41	0.75	0.19	65,122,132,133	0
25	LHG	l	5001	49/49	0.75	0.18	64,92,141,144	0
26	LMG	K	5009	55/55	0.75	0.19	41,80,106,107	0
26	LMG	A	5002	50/55	0.76	0.17	40,72,99,106	0
25	LHG	l	5004	49/49	0.76	0.16	48,75,159,163	0
21	CLA	1	1134	65/65	0.76	0.17	89,105,120,125	0
24	BCR	b	4018	40/40	0.77	0.20	53,76,95,100	0
21	CLA	1	1120	65/65	0.77	0.17	85,102,126,128	0
24	BCR	6	4016	40/40	0.77	0.20	59,91,128,129	0
35	LMT	L	6001	35/35	0.77	0.15	55,79,90,97	0
24	BCR	l	4022	40/40	0.77	0.18	57,74,97,100	0
21	CLA	1	1109	65/65	0.77	0.17	72,109,120,122	0
21	CLA	2	1209	45/65	0.77	0.15	104,130,139,142	0
21	CLA	a	1115	65/65	0.78	0.21	89,133,152,154	0
26	LMG	a	5002	50/55	0.78	0.18	54,78,109,110	0
21	CLA	2	1216	50/65	0.78	0.16	91,127,138,139	0
21	CLA	2	1212	41/65	0.78	0.16	100,132,137,144	0
24	BCR	a	4002	40/40	0.78	0.22	108,123,141,142	0
26	LMG	1	5002	50/55	0.78	0.18	44,94,119,120	0
24	BCR	a	4003	40/40	0.78	0.22	81,121,142,146	0
21	CLA	B	1209	65/65	0.79	0.16	67,88,123,127	0
26	LMG	0	5001	55/55	0.79	0.18	34,74,99,107	0
21	CLA	2	1234	50/65	0.79	0.19	90,107,111,113	0
21	CLA	2	1231	46/65	0.79	0.17	84,122,128,129	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	6	1301	47/65	0.79	0.15	99,128,135,136	0
21	CLA	F	1302	65/65	0.80	0.14	70,93,105,114	0
21	CLA	a	1114	52/65	0.80	0.16	119,138,150,152	0
34	ZEX	7	4015	42/42	0.80	0.21	100,131,150,152	0
24	BCR	2	4005	40/40	0.80	0.22	81,113,134,136	0
21	CLA	b	1240	65/65	0.80	0.17	60,88,134,154	0
21	CLA	1	1114	45/65	0.80	0.14	107,117,125,129	0
21	CLA	k	1401	50/65	0.80	0.16	84,137,147,152	5
21	CLA	2	1235	53/65	0.81	0.17	82,112,122,123	0
24	BCR	j	4013	40/40	0.81	0.19	72,90,121,123	0
21	CLA	a	1110	59/65	0.81	0.21	77,109,156,159	0
24	BCR	B	4004	40/40	0.81	0.18	63,93,109,110	0
21	CLA	2	1230	47/65	0.81	0.15	89,114,127,129	0
24	BCR	a	4001	40/40	0.81	0.21	89,142,156,156	0
21	CLA	a	1118	65/65	0.81	0.16	102,119,142,150	0
21	CLA	B	1219	65/65	0.81	0.18	73,94,125,126	0
25	LHG	L	5005	49/49	0.81	0.17	46,75,102,104	0
25	LHG	0	5002	49/49	0.81	0.15	44,63,131,140	0
21	CLA	a	1108	57/65	0.81	0.16	91,124,129,130	0
27	ACT	A	7001	4/4	0.81	0.28	28,55,63,71	0
25	LHG	a	5003	49/49	0.81	0.17	76,96,106,109	0
21	CLA	1	1113	44/65	0.82	0.15	83,124,133,135	0
25	LHG	l	5002	49/49	0.82	0.16	65,87,148,157	0
21	CLA	a	1801	55/65	0.82	0.18	83,118,128,133	0
35	LMT	F	6001	35/35	0.82	0.12	57,88,112,115	0
21	CLA	2	1227	45/65	0.82	0.15	81,94,127,131	0
26	LMG	A	5004	48/55	0.82	0.20	37,84,102,107	0
31	SQD	L	5001	51/54	0.82	0.16	42,80,104,107	0
21	CLA	1	1105	50/65	0.82	0.15	96,116,123,126	0
21	CLA	a	1121	65/65	0.83	0.15	94,117,142,146	0
21	CLA	a	1125	65/65	0.83	0.18	64,91,106,111	0
21	CLA	1	1115	65/65	0.83	0.15	78,119,130,131	0
21	CLA	a	1111	65/65	0.83	0.19	76,106,131,133	0
21	CLA	a	1133	65/65	0.84	0.17	70,95,114,117	0
21	CLA	a	1134	49/65	0.84	0.16	73,118,128,132	0
21	CLA	a	1102	65/65	0.84	0.16	68,92,118,128	0
31	SQD	L	5002	54/54	0.84	0.16	33,61,95,99	0
21	CLA	a	1105	58/65	0.84	0.14	78,110,122,129	0
24	BCR	1	4007	40/40	0.84	0.17	55,73,127,132	0
24	BCR	a	4007	40/40	0.84	0.21	69,87,144,147	0
34	ZEX	J	4015	42/42	0.84	0.17	55,68,112,116	0
25	LHG	B	5004	49/49	0.84	0.18	73,87,96,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	a	4008	40/40	0.84	0.19	51,82,109,118	0
21	CLA	2	1222	50/65	0.84	0.19	69,105,119,122	0
21	CLA	2	1214	59/65	0.84	0.17	70,109,135,159	0
29	CL	2	6000	1/1	0.84	0.16	74,74,74,74	0
25	LHG	1	5003	49/49	0.84	0.17	62,83,96,99	0
24	BCR	L	4022	40/40	0.85	0.14	41,57,81,86	0
24	BCR	1	4012	40/40	0.85	0.19	100,112,124,125	0
21	CLA	b	1213	65/65	0.85	0.14	39,64,89,93	0
21	CLA	2	1208	60/65	0.85	0.16	63,88,138,142	0
24	BCR	2	4010	40/40	0.85	0.21	66,101,136,136	0
21	CLA	1	1112	50/65	0.85	0.13	83,109,122,126	0
21	CLA	2	1210	65/65	0.85	0.19	75,107,116,119	0
21	CLA	b	1219	60/65	0.85	0.17	33,66,132,132	0
21	CLA	B	1218	65/65	0.85	0.13	62,91,123,125	0
21	CLA	8	1401	45/65	0.85	0.12	83,101,137,143	3
21	CLA	8	1402	46/65	0.85	0.13	103,119,135,139	5
21	CLA	a	1122	65/65	0.85	0.17	61,95,108,113	0
21	CLA	2	1215	60/65	0.85	0.18	73,100,112,118	0
21	CLA	B	1217	65/65	0.85	0.13	64,93,113,116	0
24	BCR	1	4003	40/40	0.85	0.19	71,105,134,138	0
35	LMT	0	6001	35/35	0.85	0.12	51,72,84,90	0
24	BCR	K	4001	40/40	0.85	0.16	40,73,103,106	0
21	CLA	1	1139	65/65	0.86	0.16	75,115,124,125	0
21	CLA	2	1202	65/65	0.86	0.17	56,94,106,108	0
21	CLA	A	1113	65/65	0.86	0.13	41,64,105,111	0
21	CLA	f	1301	50/65	0.86	0.12	74,93,114,116	0
21	CLA	2	1221	65/65	0.86	0.17	84,95,132,137	0
21	CLA	1	1013	65/65	0.86	0.16	73,91,97,104	0
24	BCR	0	4022	40/40	0.86	0.16	41,60,87,92	0
25	LHG	b	5004	49/49	0.86	0.15	63,80,101,105	0
24	BCR	9	4021	40/40	0.86	0.18	58,80,116,118	0
21	CLA	B	1211	65/65	0.86	0.13	45,76,102,107	0
21	CLA	1	1118	65/65	0.86	0.14	79,103,130,134	0
30	ECH	B	4006	41/41	0.86	0.16	45,86,105,108	0
21	CLA	a	1112	65/65	0.86	0.18	74,129,135,137	0
21	CLA	B	1208	65/65	0.86	0.15	53,76,108,111	0
21	CLA	b	1227	65/65	0.87	0.15	58,73,120,124	0
24	BCR	2	4011	40/40	0.87	0.17	60,93,104,109	0
21	CLA	a	1011	65/65	0.87	0.16	40,58,71,96	0
21	CLA	1	1103	65/65	0.87	0.17	63,87,101,103	0
21	CLA	a	1116	60/65	0.87	0.18	79,99,109,110	0
23	SF4	C	3002	8/8	0.87	0.17	43,65,114,208	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	a	4012	40/40	0.87	0.18	66,95,106,110	0
21	CLA	B	1227	55/65	0.87	0.14	67,76,102,107	0
24	BCR	b	4014	40/40	0.87	0.17	59,79,88,92	0
21	CLA	1	1138	60/65	0.87	0.17	84,118,134,136	0
24	BCR	B	4005	40/40	0.87	0.14	45,78,102,103	0
34	ZEX	j	4015	42/42	0.87	0.16	51,97,113,117	0
26	LMG	2	5002	55/55	0.87	0.19	55,72,93,107	0
21	CLA	B	1232	50/65	0.87	0.13	81,92,105,108	0
24	BCR	J	4013	40/40	0.87	0.15	48,69,89,91	0
24	BCR	1	4002	40/40	0.87	0.18	89,100,119,123	0
21	CLA	1	1110	50/65	0.87	0.14	70,91,137,157	0
21	CLA	a	1107	50/65	0.87	0.14	68,88,108,112	0
21	CLA	B	1216	65/65	0.87	0.16	65,85,101,106	0
21	CLA	F	1301	65/65	0.88	0.14	53,77,121,124	0
21	CLA	1	1107	51/65	0.88	0.14	83,102,117,121	0
21	CLA	2	1225	65/65	0.88	0.15	52,92,111,114	0
21	CLA	a	1117	65/65	0.88	0.17	64,89,103,112	0
21	CLA	a	1101	65/65	0.88	0.15	50,83,91,100	0
21	CLA	2	1205	65/65	0.88	0.15	54,77,89,91	0
28	45D	h	4020	42/42	0.88	0.13	33,55,68,75	0
21	CLA	B	1213	65/65	0.88	0.17	58,80,112,120	0
25	LHG	1	5001	49/49	0.88	0.18	64,84,101,104	0
24	BCR	2	4014	40/40	0.88	0.22	78,113,132,136	0
21	CLA	a	1129	52/65	0.88	0.14	64,85,95,98	0
21	CLA	B	1228	65/65	0.88	0.16	44,66,113,122	0
21	CLA	2	1211	50/65	0.88	0.14	80,110,117,123	0
21	CLA	b	1231	65/65	0.88	0.13	50,69,93,98	0
21	CLA	b	1232	65/65	0.88	0.12	64,79,121,123	0
24	BCR	b	4004	40/40	0.88	0.13	36,60,76,87	0
21	CLA	1	1116	65/65	0.88	0.17	75,95,118,121	0
32	CA	2	6001	1/1	0.88	0.12	112,112,112,112	0
21	CLA	1	1117	65/65	0.88	0.17	57,99,112,123	0
24	BCR	f	4016	40/40	0.88	0.17	66,81,104,107	0
21	CLA	1	1102	55/65	0.88	0.15	50,81,117,120	0
21	CLA	b	1236	65/65	0.88	0.14	48,74,118,122	0
22	PQN	1	2001	33/33	0.88	0.18	67,88,108,108	0
23	SF4	A	3001	8/8	0.88	0.20	40,87,137,173	0
21	CLA	1	1124	56/65	0.88	0.14	44,66,87,93	0
21	CLA	1	1125	65/65	0.88	0.15	56,78,91,94	0
21	CLA	2	1220	45/65	0.88	0.14	114,124,128,132	0
21	CLA	B	1231	65/65	0.89	0.14	66,84,101,104	0
24	BCR	l	4019	40/40	0.89	0.14	29,44,54,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	1	1111	65/65	0.89	0.14	63,85,113,118	0
21	CLA	b	1235	65/65	0.89	0.13	45,80,93,97	0
21	CLA	a	1126	65/65	0.89	0.16	71,91,104,105	0
21	CLA	A	1134	65/65	0.89	0.14	25,57,107,111	0
21	CLA	A	1112	65/65	0.89	0.12	39,62,94,98	0
24	BCR	1	4008	40/40	0.89	0.17	49,69,93,95	0
21	CLA	B	1230	65/65	0.89	0.14	29,68,110,114	0
21	CLA	a	1136	65/65	0.89	0.12	44,73,87,100	0
30	ECH	b	4011	41/41	0.89	0.17	60,81,90,94	0
30	ECH	b	4006	41/41	0.89	0.13	32,47,97,99	0
30	ECH	m	4021	41/41	0.89	0.13	23,49,80,80	0
21	CLA	a	1139	65/65	0.89	0.15	64,86,103,105	0
21	CLA	A	1105	65/65	0.89	0.12	44,68,92,95	0
21	CLA	1	1121	55/65	0.89	0.14	58,96,124,128	0
21	CLA	a	1109	65/65	0.89	0.15	65,102,118,124	0
21	CLA	l	1501	65/65	0.89	0.14	48,69,110,117	0
21	CLA	1	1126	65/65	0.89	0.14	58,94,108,115	0
21	CLA	1	1128	65/65	0.89	0.16	62,79,99,113	0
21	CLA	b	1208	60/65	0.89	0.13	36,53,91,103	0
21	CLA	A	1114	65/65	0.89	0.12	56,75,111,116	0
34	ZEX	F	4016	42/42	0.89	0.15	46,72,98,103	0
21	CLA	B	1212	55/65	0.89	0.13	70,82,128,132	0
21	CLA	2	1201	65/65	0.89	0.14	61,77,86,90	0
21	CLA	2	1236	50/65	0.89	0.16	75,110,117,124	0
21	CLA	b	1222	65/65	0.89	0.14	38,54,114,118	0
24	BCR	b	4005	40/40	0.89	0.12	30,47,90,91	0
21	CLA	2	1203	65/65	0.89	0.15	57,88,101,105	0
21	CLA	A	1121	65/65	0.89	0.15	28,48,130,132	0
21	CLA	b	1228	65/65	0.89	0.16	58,73,117,121	0
21	CLA	a	1123	65/65	0.89	0.18	55,105,117,121	0
21	CLA	2	1226	55/65	0.90	0.16	55,70,91,97	0
21	CLA	a	1135	65/65	0.90	0.17	42,69,151,157	0
21	CLA	2	1228	45/65	0.90	0.13	53,67,126,132	0
24	BCR	B	4010	40/40	0.90	0.18	51,66,81,84	0
21	CLA	2	1229	65/65	0.90	0.14	83,109,124,136	0
24	BCR	B	4014	40/40	0.90	0.15	35,57,80,84	0
21	CLA	b	1220	65/65	0.90	0.12	48,64,100,103	0
21	CLA	A	1108	53/65	0.90	0.12	30,57,91,92	0
30	ECH	M	4021	41/41	0.90	0.12	45,61,74,81	0
21	CLA	K	1401	65/65	0.90	0.13	33,63,97,102	15
21	CLA	a	1128	65/65	0.90	0.16	59,86,97,102	0
30	ECH	i	4020	41/41	0.90	0.13	38,53,83,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	K	1402	65/65	0.90	0.13	50,71,111,115	10
24	BCR	2	4017	40/40	0.90	0.13	31,56,72,76	0
21	CLA	1	1133	65/65	0.90	0.15	73,87,99,107	0
21	CLA	a	1119	65/65	0.90	0.17	54,82,128,133	0
21	CLA	b	1209	65/65	0.90	0.13	40,57,100,107	0
24	BCR	h	4018	40/40	0.90	0.13	36,60,75,79	0
21	CLA	1	1801	56/65	0.90	0.13	62,76,106,112	0
21	CLA	a	1124	55/65	0.90	0.15	45,59,117,127	0
21	CLA	1	1101	65/65	0.90	0.16	58,88,120,123	0
21	CLA	1	1012	65/65	0.90	0.15	72,88,98,101	0
33	MG	B	6002	1/1	0.90	0.10	69,69,69,69	0
21	CLA	2	1237	65/65	0.90	0.12	30,51,61,76	0
22	PQN	a	2001	33/33	0.90	0.15	39,65,84,87	0
21	CLA	b	1218	65/65	0.90	0.12	46,66,101,102	0
26	LMG	b	5002	55/55	0.90	0.14	36,55,84,89	0
24	BCR	i	4018	40/40	0.90	0.14	29,52,63,69	0
21	CLA	1	1104	65/65	0.90	0.14	65,91,99,106	0
21	CLA	b	1230	65/65	0.90	0.15	53,86,120,125	0
24	BCR	A	4001	40/40	0.90	0.13	35,52,68,68	0
24	BCR	A	4003	40/40	0.90	0.14	32,53,89,91	0
25	LHG	a	5001	49/49	0.90	0.17	57,72,117,128	0
21	CLA	A	1139	65/65	0.91	0.12	43,59,83,91	0
21	CLA	1	1122	60/65	0.91	0.13	47,75,101,106	0
21	CLA	1	1123	65/65	0.91	0.14	49,86,107,115	0
21	CLA	A	1801	65/65	0.91	0.13	22,47,108,110	0
21	CLA	a	1127	65/65	0.91	0.17	50,80,108,110	0
21	CLA	A	1115	65/65	0.91	0.12	41,57,69,72	0
21	CLA	1	1127	65/65	0.91	0.16	64,86,112,118	0
21	CLA	b	1226	65/65	0.91	0.13	26,50,71,76	0
24	BCR	A	4002	40/40	0.91	0.15	33,60,75,82	0
21	CLA	B	1220	57/65	0.91	0.12	53,78,101,108	0
21	CLA	B	1222	55/65	0.91	0.13	50,68,84,89	0
21	CLA	1	1135	52/65	0.91	0.14	53,69,89,108	0
21	CLA	1	1137	51/65	0.91	0.11	48,65,76,87	0
21	CLA	A	1120	65/65	0.91	0.12	30,53,102,104	0
24	BCR	B	4017	40/40	0.91	0.13	22,44,56,57	0
21	CLA	2	1223	55/65	0.91	0.18	64,99,141,145	0
21	CLA	1	1140	65/65	0.91	0.14	60,77,119,120	0
21	CLA	B	1210	65/65	0.91	0.12	38,67,90,92	0
21	CLA	a	1103	65/65	0.91	0.18	49,67,130,133	0
21	CLA	A	1109	65/65	0.91	0.12	36,54,65,74	0
21	CLA	a	1106	65/65	0.91	0.17	58,95,106,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	2	1022	65/65	0.91	0.11	34,62,74,74	0
21	CLA	a	1130	65/65	0.91	0.13	52,68,111,119	0
26	LMG	B	5002	55/55	0.91	0.13	36,52,81,89	0
21	CLA	2	1023	65/65	0.91	0.13	46,60,68,82	0
24	BCR	0	4019	40/40	0.91	0.14	35,57,67,69	0
21	CLA	a	1138	65/65	0.91	0.13	50,77,85,90	0
21	CLA	A	1133	65/65	0.91	0.13	28,48,78,81	0
25	LHG	A	5003	49/49	0.91	0.16	29,62,101,107	0
21	CLA	b	1237	65/65	0.91	0.11	36,55,71,76	0
21	CLA	2	1204	65/65	0.91	0.13	35,67,89,91	0
21	CLA	A	1107	65/65	0.91	0.13	42,56,121,124	0
21	CLA	B	1214	65/65	0.91	0.15	48,81,89,92	0
21	CLA	A	1135	65/65	0.91	0.13	25,42,100,107	0
21	CLA	1	1106	65/65	0.92	0.16	49,91,119,122	0
21	CLA	b	1225	65/65	0.92	0.10	23,41,59,63	0
21	CLA	A	1011	65/65	0.92	0.11	20,37,61,79	0
21	CLA	a	1140	65/65	0.92	0.13	48,70,93,95	0
21	CLA	A	1118	65/65	0.92	0.12	38,52,84,89	0
21	CLA	b	1229	65/65	0.92	0.14	54,68,97,108	0
21	CLA	L	1501	65/65	0.92	0.12	33,51,91,94	0
21	CLA	2	1021	65/65	0.92	0.16	45,67,114,117	0
21	CLA	B	1234	65/65	0.92	0.13	39,73,95,100	0
21	CLA	b	1234	53/65	0.92	0.12	40,57,75,91	0
21	CLA	2	1239	65/65	0.92	0.11	39,57,93,104	0
21	CLA	B	1235	65/65	0.92	0.14	45,66,92,94	0
24	BCR	b	4010	40/40	0.92	0.13	41,58,68,71	0
24	BCR	b	4017	40/40	0.92	0.12	35,52,61,64	0
21	CLA	B	1224	65/65	0.92	0.12	28,52,78,87	0
21	CLA	b	1238	65/65	0.92	0.11	30,52,63,69	0
21	CLA	b	1021	65/65	0.92	0.12	36,52,66,72	0
21	CLA	2	1206	65/65	0.92	0.12	44,66,80,88	0
21	CLA	1	1119	65/65	0.92	0.14	53,75,92,112	0
21	CLA	a	1104	65/65	0.92	0.14	40,68,105,111	0
21	CLA	B	1225	65/65	0.92	0.11	41,61,70,76	0
21	CLA	b	1210	65/65	0.92	0.10	31,43,63,68	0
21	CLA	b	1211	65/65	0.92	0.12	29,46,98,103	0
21	CLA	b	1212	65/65	0.92	0.12	41,53,87,97	0
21	CLA	B	1226	65/65	0.92	0.12	31,51,70,79	0
23	SF4	C	3003	8/8	0.92	0.12	53,74,78,84	0
21	CLA	b	1216	65/65	0.92	0.11	41,57,91,102	0
21	CLA	b	1217	51/65	0.92	0.09	32,56,86,95	0
21	CLA	1	1011	65/65	0.92	0.12	38,62,88,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	A	4008	40/40	0.92	0.14	17,46,78,82	0
21	CLA	A	1122	60/65	0.92	0.11	25,42,70,83	0
24	BCR	A	4012	40/40	0.92	0.12	43,60,73,73	0
21	CLA	A	1126	65/65	0.92	0.10	28,48,62,75	0
21	CLA	B	1229	65/65	0.92	0.11	40,60,80,85	0
21	CLA	1	1136	65/65	0.92	0.10	46,66,77,83	0
21	CLA	a	1137	51/65	0.92	0.12	43,63,109,113	0
21	CLA	b	1224	65/65	0.92	0.12	33,48,83,87	0
21	CLA	2	1224	55/65	0.92	0.16	53,70,95,110	0
24	BCR	I	4018	40/40	0.92	0.11	24,45,59,67	0
21	CLA	a	1013	65/65	0.93	0.12	34,53,90,92	0
21	CLA	A	1124	65/65	0.93	0.11	23,35,118,122	0
21	CLA	A	1125	65/65	0.93	0.10	22,46,61,65	0
28	45D	B	4011	42/42	0.93	0.11	31,49,61,69	0
21	CLA	B	1237	65/65	0.93	0.10	21,34,54,61	0
21	CLA	1	1129	50/65	0.93	0.12	49,63,76,78	0
21	CLA	1	1132	65/65	0.93	0.10	23,48,63,71	0
21	CLA	a	1132	65/65	0.93	0.10	37,57,66,71	0
21	CLA	B	1202	65/65	0.93	0.12	32,54,66,69	0
24	BCR	L	4019	40/40	0.93	0.10	24,38,45,52	0
21	CLA	B	1236	50/65	0.93	0.12	44,63,96,101	0
21	CLA	b	1023	65/65	0.93	0.11	34,51,66,80	0
21	CLA	b	1203	65/65	0.93	0.10	25,45,60,64	0
21	CLA	b	1206	65/65	0.93	0.10	28,48,62,80	0
21	CLA	B	1204	65/65	0.93	0.10	32,50,67,83	0
21	CLA	0	1501	65/65	0.93	0.11	37,47,74,82	0
21	CLA	0	1502	65/65	0.93	0.11	32,49,77,84	0
21	CLA	0	1503	65/65	0.93	0.10	43,56,82,99	0
21	CLA	B	1207	65/65	0.93	0.11	28,39,61,68	0
22	PQN	b	2002	33/33	0.93	0.12	36,51,69,69	0
21	CLA	B	1221	65/65	0.93	0.13	50,62,95,98	0
21	CLA	A	1104	65/65	0.93	0.11	19,41,62,64	0
21	CLA	B	1223	65/65	0.93	0.14	54,67,78,95	0
21	CLA	A	1127	65/65	0.93	0.10	22,42,59,64	0
21	CLA	b	1214	65/65	0.93	0.14	33,49,89,98	0
21	CLA	A	1128	65/65	0.93	0.11	29,43,62,86	0
21	CLA	A	1129	58/65	0.93	0.13	20,42,92,96	0
24	BCR	A	4007	40/40	0.93	0.12	31,46,106,108	0
21	CLA	A	1110	65/65	0.93	0.14	30,47,124,127	0
21	CLA	A	1102	65/65	0.93	0.12	32,49,106,120	0
21	CLA	L	1503	65/65	0.93	0.12	35,54,82,87	0
36	EQ3	I	4020	42/42	0.93	0.09	24,37,48,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	A	1116	65/65	0.93	0.12	36,53,86,90	0
21	CLA	B	1023	65/65	0.94	0.08	21,33,45,55	0
21	CLA	B	1201	65/65	0.94	0.10	37,48,80,91	0
21	CLA	b	1215	65/65	0.94	0.10	28,48,68,83	0
21	CLA	A	1103	65/65	0.94	0.10	25,41,61,66	0
21	CLA	B	1203	65/65	0.94	0.10	33,50,69,75	0
21	CLA	A	1106	65/65	0.94	0.10	26,45,71,87	0
21	CLA	B	1205	65/65	0.94	0.10	34,43,69,74	0
21	CLA	l	1502	65/65	0.94	0.11	30,55,103,110	0
21	CLA	l	1503	65/65	0.94	0.13	31,54,99,101	0
21	CLA	B	1206	65/65	0.94	0.09	31,43,60,72	0
21	CLA	b	1221	65/65	0.94	0.11	31,50,85,99	0
21	CLA	a	1012	65/65	0.94	0.13	25,57,101,103	0
21	CLA	b	1223	65/65	0.94	0.11	33,55,83,86	0
22	PQN	A	2001	33/33	0.94	0.11	30,46,57,64	0
21	CLA	b	1022	65/65	0.94	0.11	37,49,59,65	0
21	CLA	A	1117	65/65	0.94	0.09	31,46,56,59	0
21	CLA	A	1137	65/65	0.94	0.10	24,38,111,116	0
22	PQN	2	2002	33/33	0.94	0.10	42,57,70,78	0
21	CLA	A	1138	65/65	0.94	0.10	46,61,68,73	0
21	CLA	A	1123	65/65	0.94	0.10	25,38,52,60	0
33	MG	b	6002	1/1	0.94	0.09	54,54,54,54	0
21	CLA	b	1204	65/65	0.94	0.10	26,40,78,108	0
21	CLA	b	1205	65/65	0.94	0.10	28,43,59,65	0
21	CLA	a	1131	65/65	0.94	0.10	36,58,68,71	0
21	CLA	b	1207	65/65	0.94	0.10	32,50,71,81	0
21	CLA	A	1101	65/65	0.94	0.11	32,50,68,74	0
21	CLA	A	1013	65/65	0.94	0.10	23,47,57,65	0
21	CLA	B	1022	65/65	0.94	0.09	19,36,44,51	0
21	CLA	b	1239	65/65	0.94	0.10	36,51,62,84	0
21	CLA	B	1215	65/65	0.94	0.13	33,57,92,99	0
21	CLA	A	1131	65/65	0.94	0.09	27,38,59,76	0
21	CLA	b	1201	65/65	0.94	0.10	30,44,81,84	0
21	CLA	A	1130	60/65	0.95	0.10	21,39,93,95	0
21	CLA	B	1238	65/65	0.95	0.08	17,35,46,56	0
25	LHG	A	5001	49/49	0.95	0.11	31,47,61,64	0
21	CLA	1	1131	65/65	0.95	0.10	35,47,69,74	0
21	CLA	b	1202	65/65	0.95	0.09	26,43,52,57	0
21	CLA	B	1239	65/65	0.95	0.10	11,39,59,85	0
21	CLA	A	1136	65/65	0.95	0.08	21,42,68,77	0
21	CLA	A	1119	65/65	0.95	0.09	27,39,52,56	0
21	CLA	A	1012	65/65	0.95	0.10	31,44,63,73	0

Continued on next page...

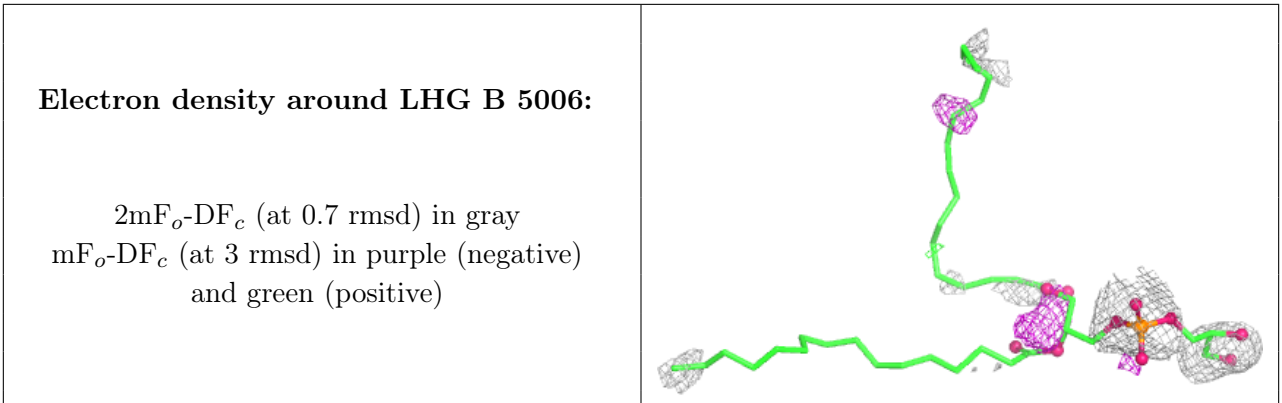
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	A	1111	65/65	0.95	0.12	31,48,81,86	0
21	CLA	A	1132	65/65	0.95	0.07	21,35,44,51	0
21	CLA	B	1021	65/65	0.95	0.09	30,42,53,61	0
21	CLA	A	1140	65/65	0.95	0.10	25,43,66,76	0
21	CLA	1	1130	55/65	0.95	0.10	29,53,83,95	0
21	CLA	2	1238	65/65	0.95	0.09	36,52,61,75	0
21	CLA	2	1207	56/65	0.95	0.10	29,46,78,86	0
32	CA	B	6001	1/1	0.96	0.05	80,80,80,80	0
23	SF4	1	3001	8/8	0.96	0.07	57,66,94,130	0
23	SF4	3	3002	8/8	0.96	0.09	65,73,110,240	0
22	PQN	B	2002	33/33	0.96	0.07	24,35,39,48	0
21	CLA	L	1502	65/65	0.96	0.09	21,36,98,103	0
29	CL	b	6000	1/1	0.97	0.09	53,53,53,53	0
23	SF4	c	3002	8/8	0.98	0.05	53,57,64,76	0
23	SF4	3	3003	8/8	0.98	0.07	75,88,175,321	0
32	CA	b	6001	1/1	0.98	0.04	61,61,61,61	0
23	SF4	c	3003	8/8	0.98	0.06	57,78,82,85	0
32	CA	0	1001	1/1	0.98	0.04	56,56,56,56	0
23	SF4	a	3001	8/8	0.98	0.04	61,65,75,77	0
32	CA	L	1001	1/1	0.99	0.03	44,44,44,44	0
29	CL	B	6000	1/1	0.99	0.03	36,36,36,36	0
32	CA	l	1001	1/1	0.99	0.03	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

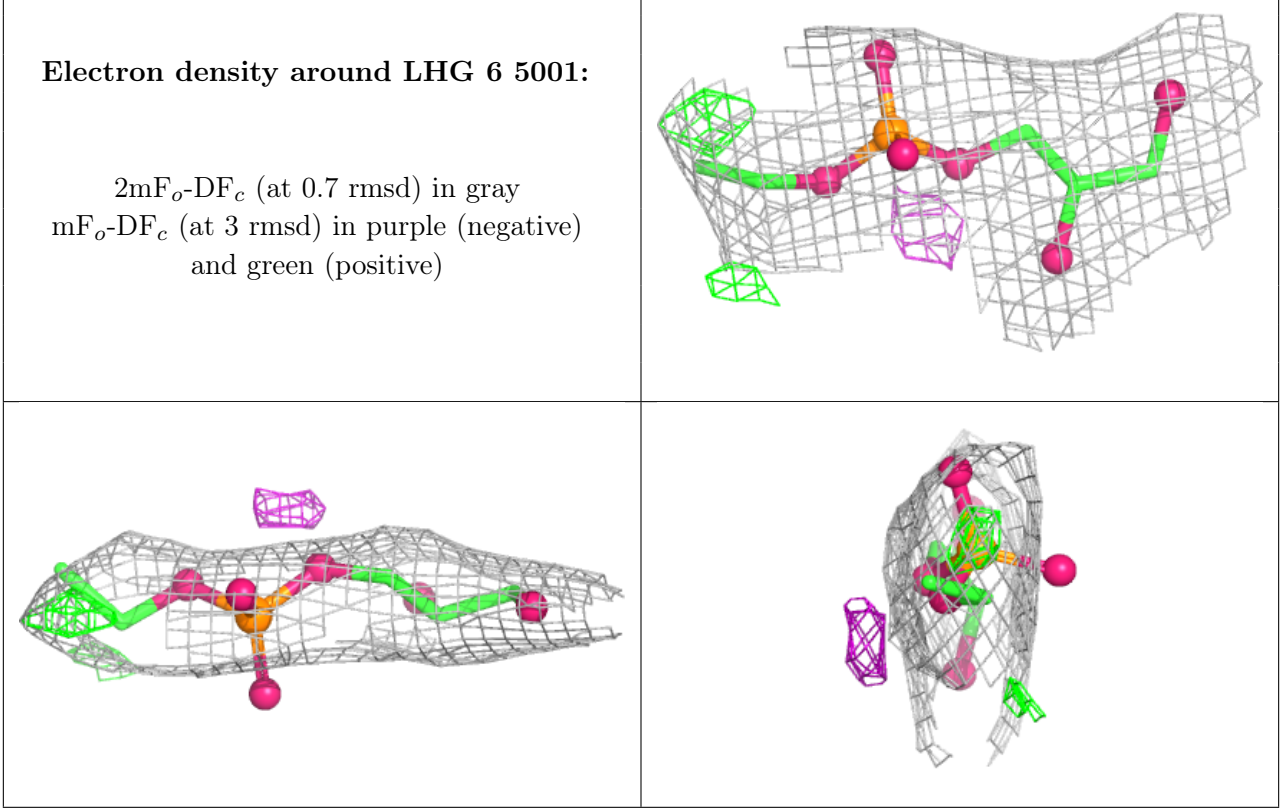
Electron density around LHG B 5006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



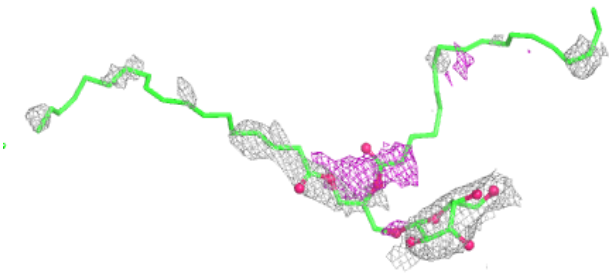
Electron density around LHG 6 5001:

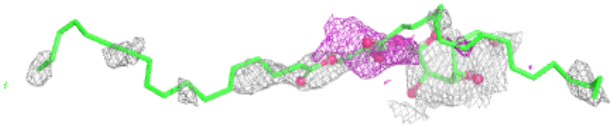
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

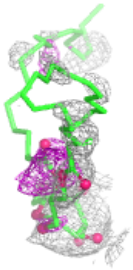


Electron density around LMG b 5007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



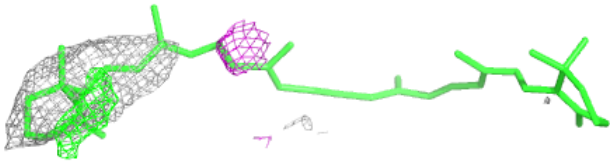


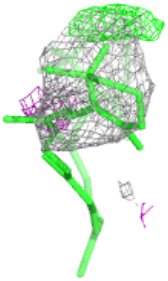


Electron density around BCR 1 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

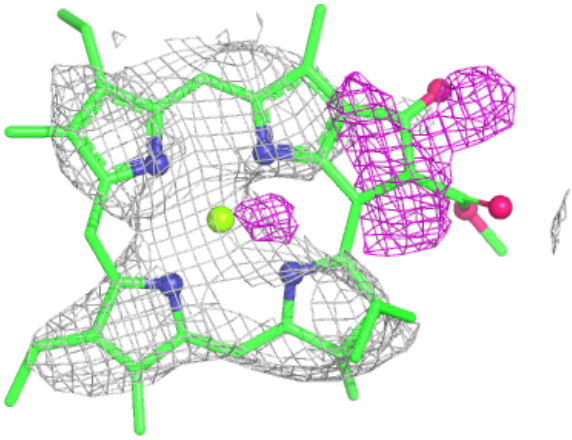


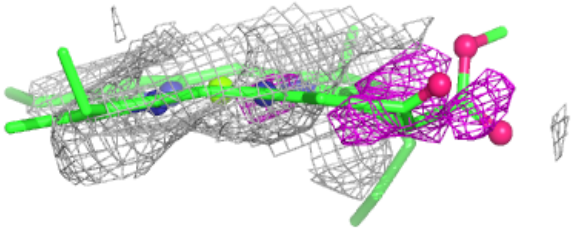


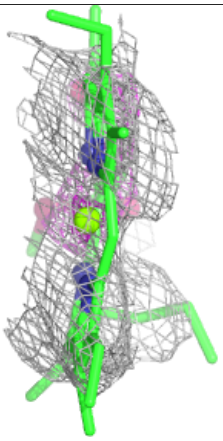


Electron density around CLA 6 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

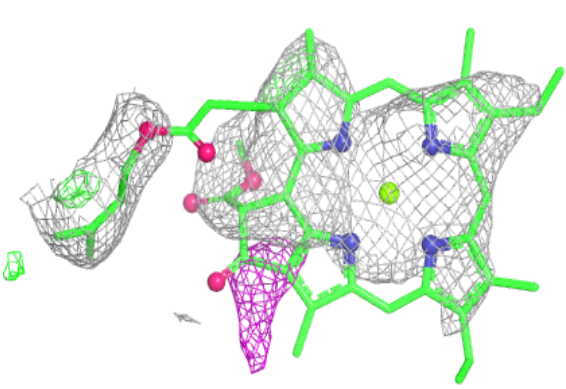


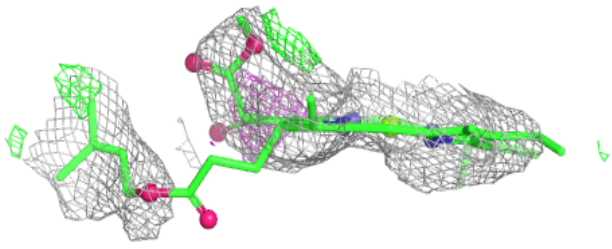


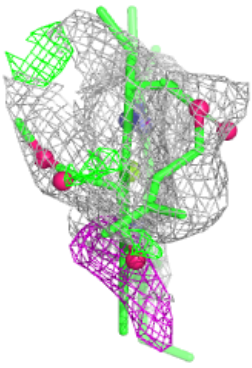


Electron density around CLA a 1113:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

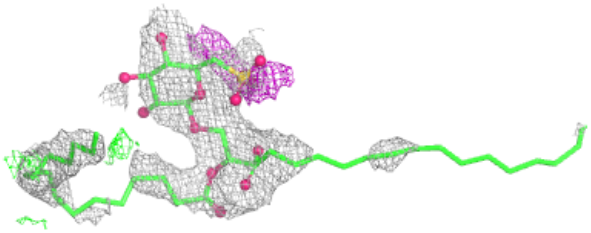


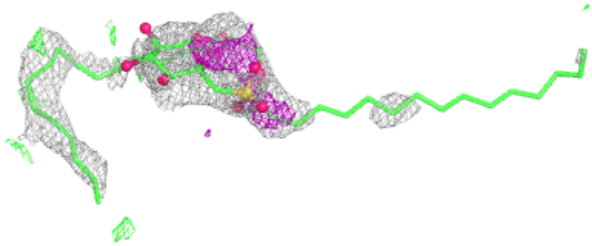


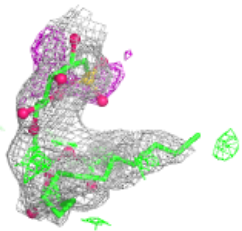


Electron density around SQD F 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

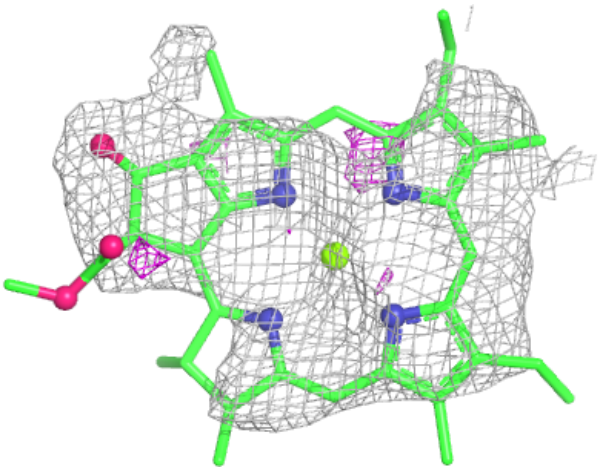


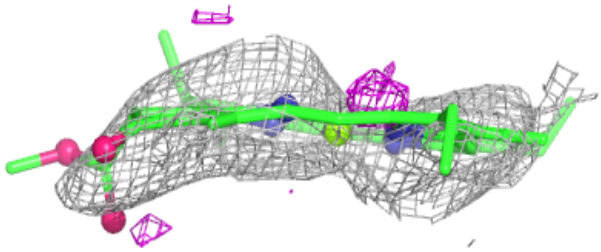


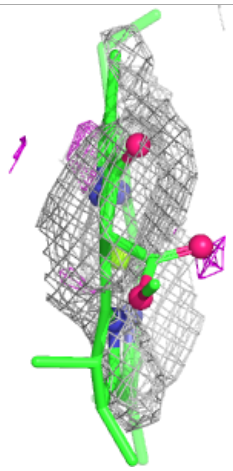


Electron density around CLA 2 1240:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

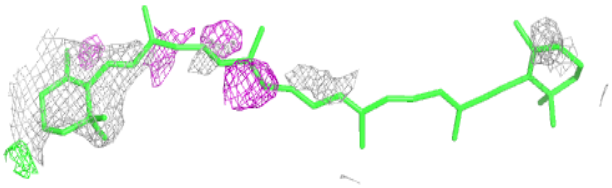


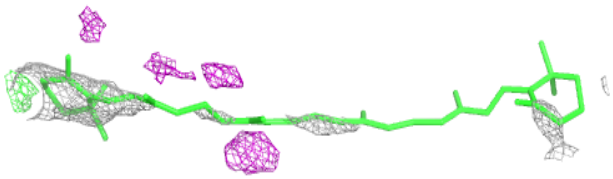


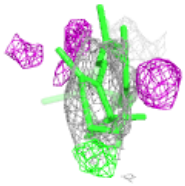


Electron density around BCR 2 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



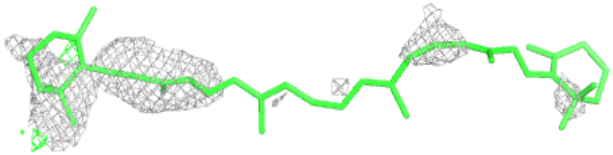


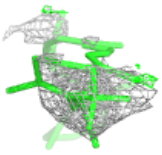


Electron density around BCR a 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

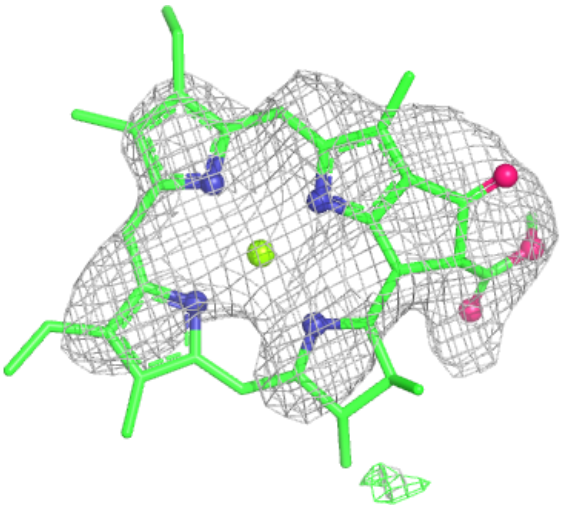


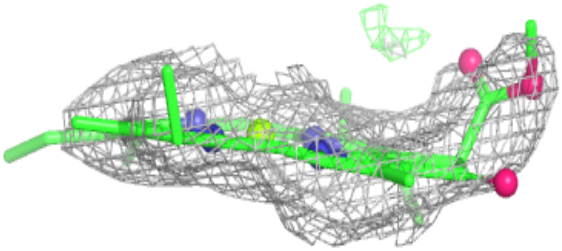


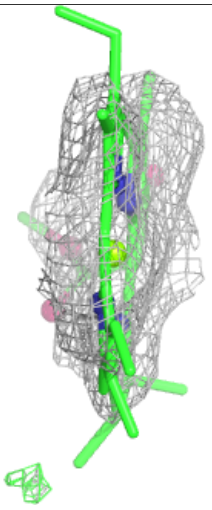


Electron density around CLA 7 1303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

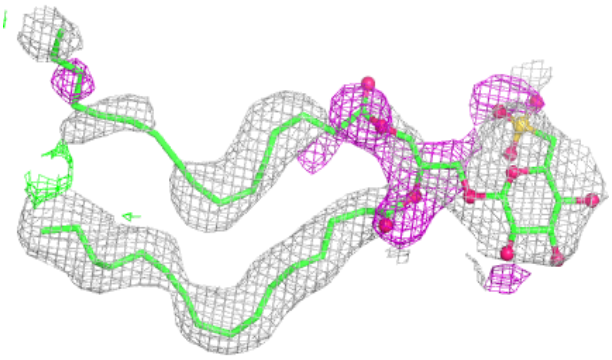


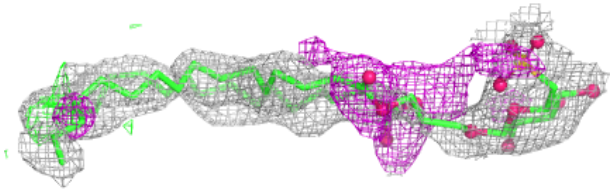


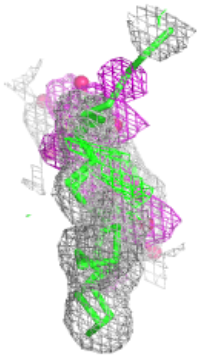


Electron density around SQD b 5006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

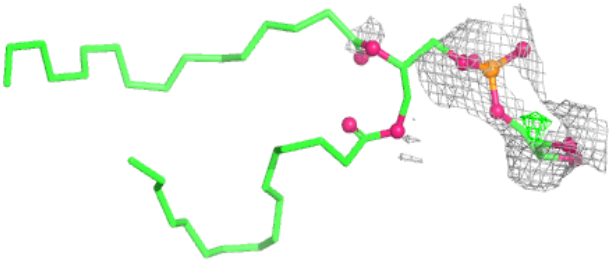


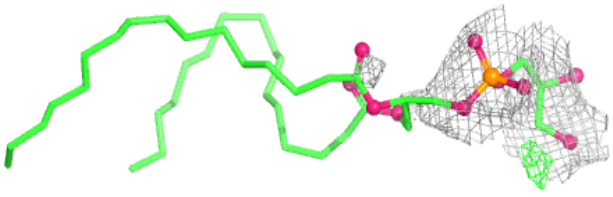


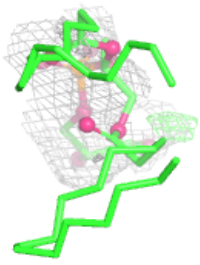


Electron density around LHG a 5007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



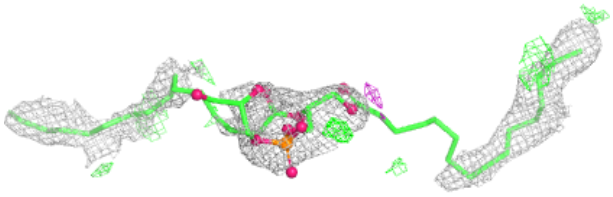


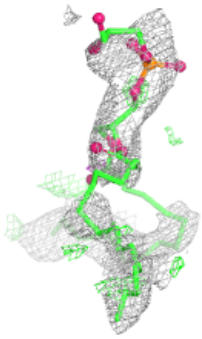


Electron density around LHG 0 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

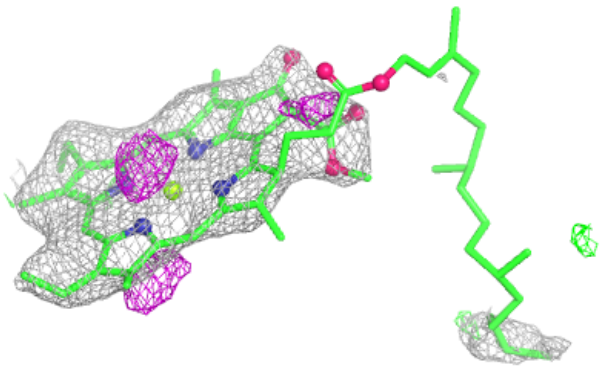


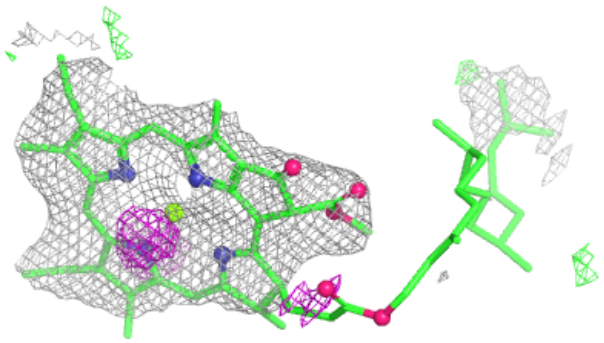


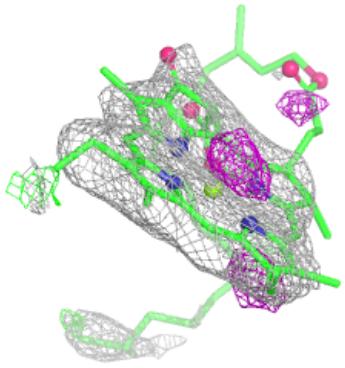


Electron density around CLA B 1240:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

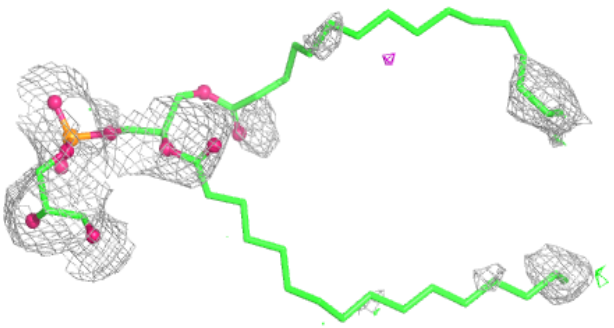


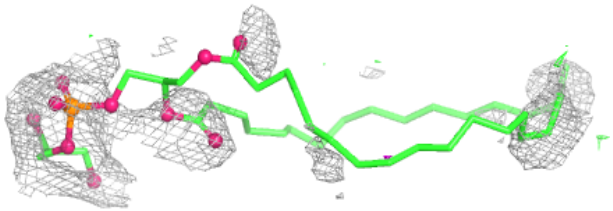


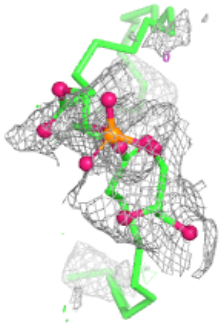


Electron density around LHG 1 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

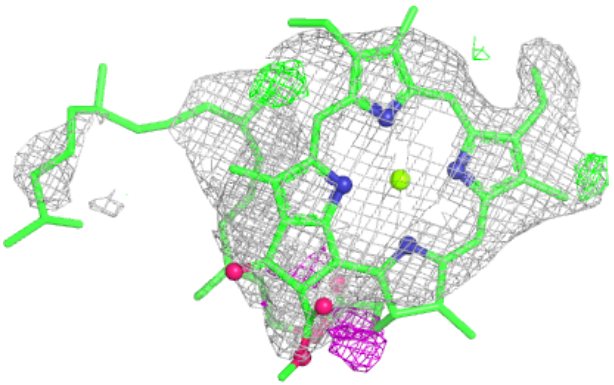


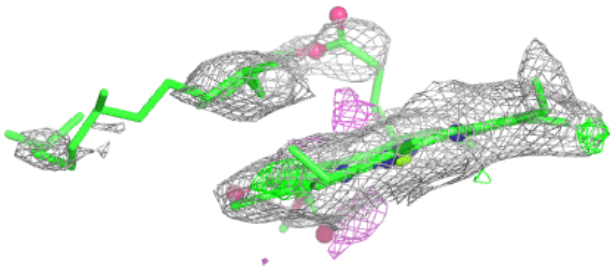




Electron density around CLA j 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



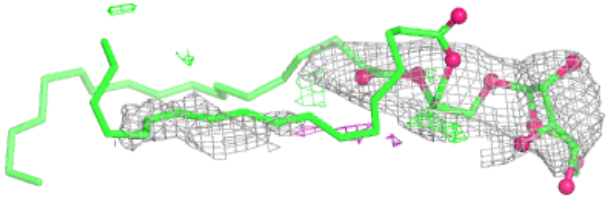


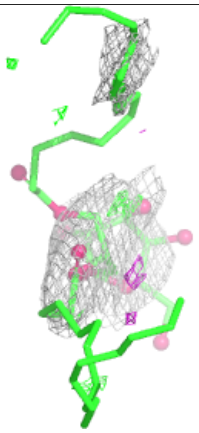


Electron density around LMG 2 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

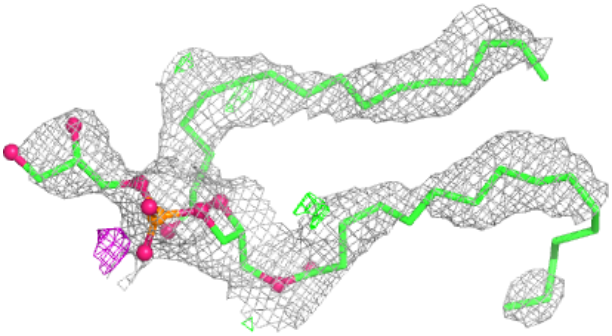


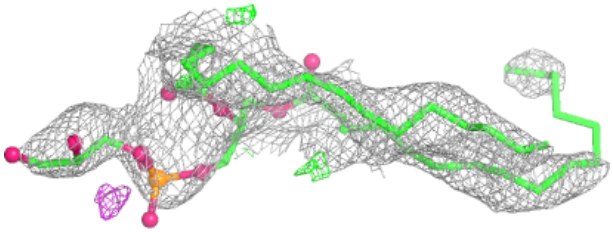


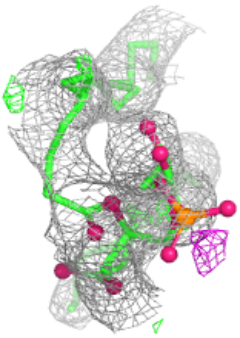


Electron density around LHG F 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

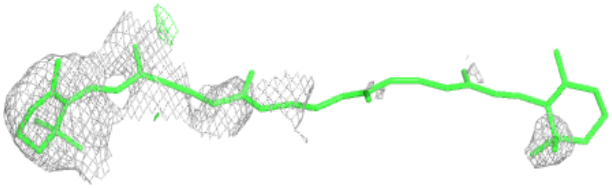


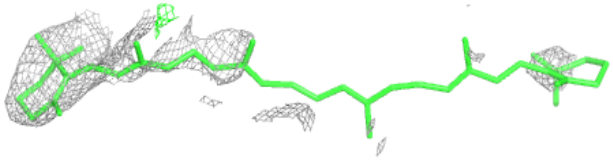


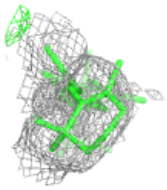


Electron density around BCR k 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

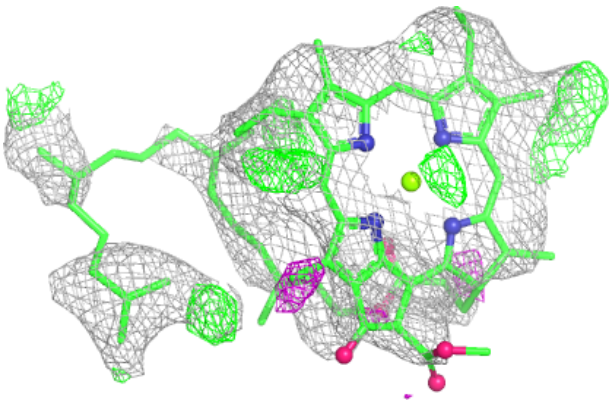


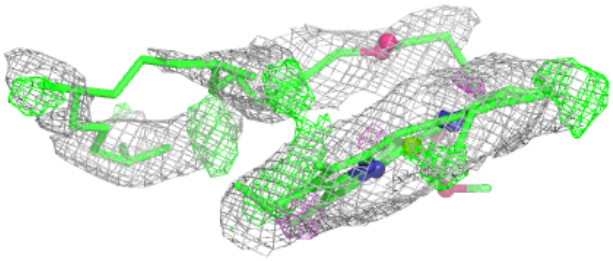


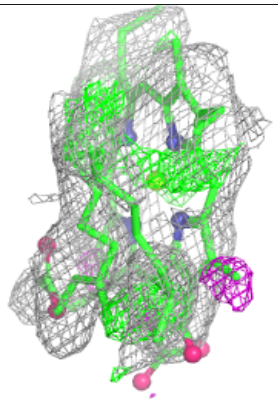


Electron density around CLA J 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

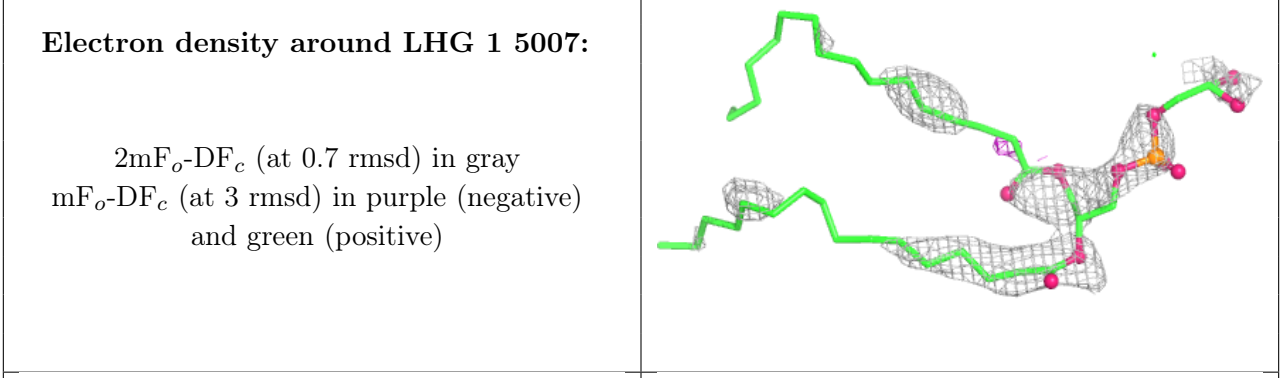


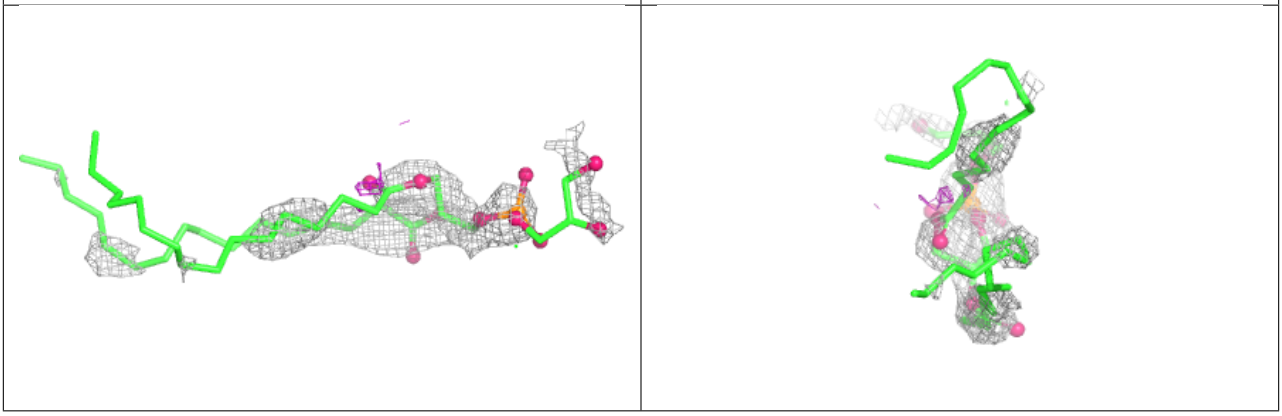




Electron density around LHG 1 5007:

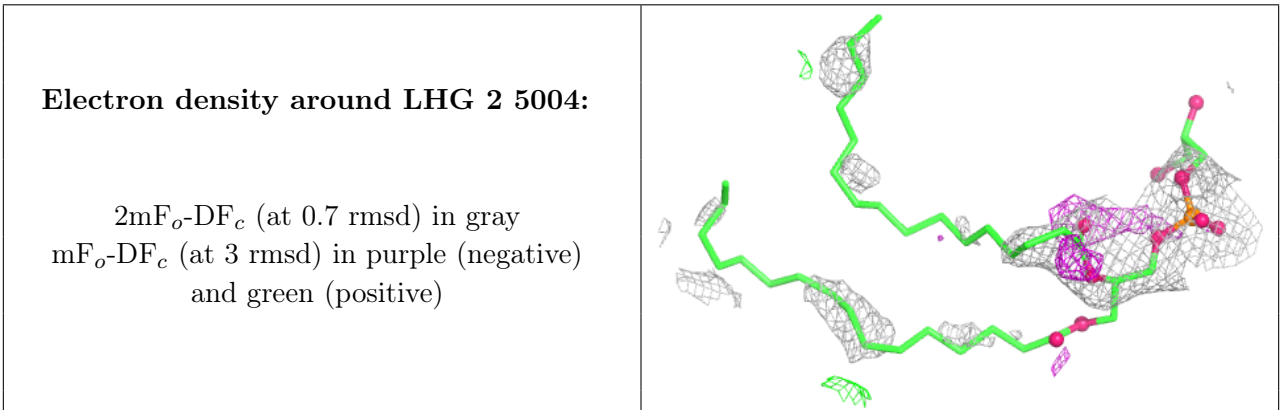
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

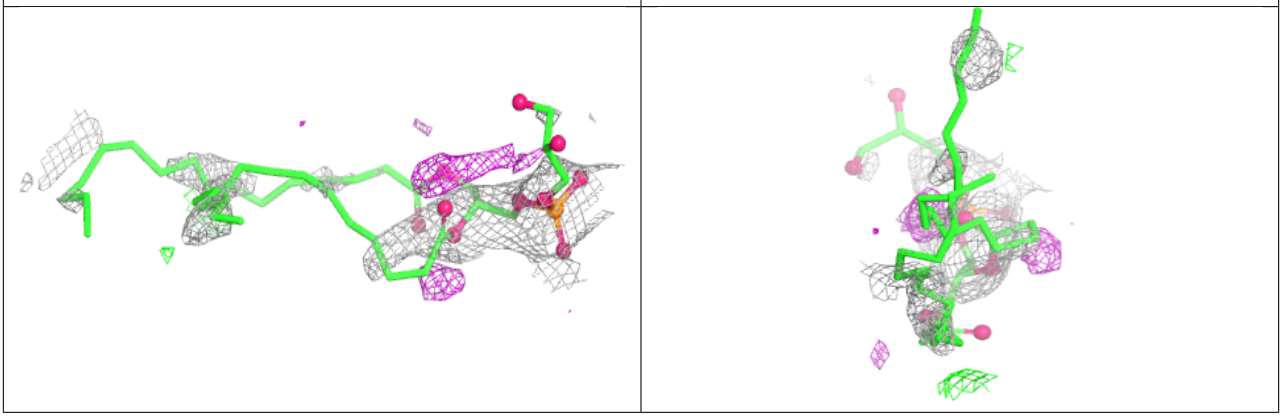




Electron density around LHG 2 5004:

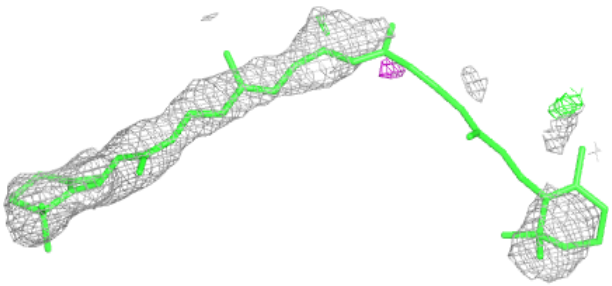
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

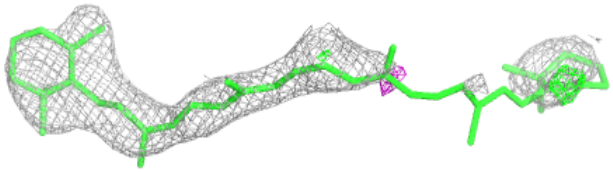


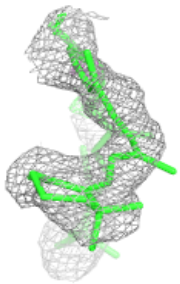


Electron density around BCR A 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

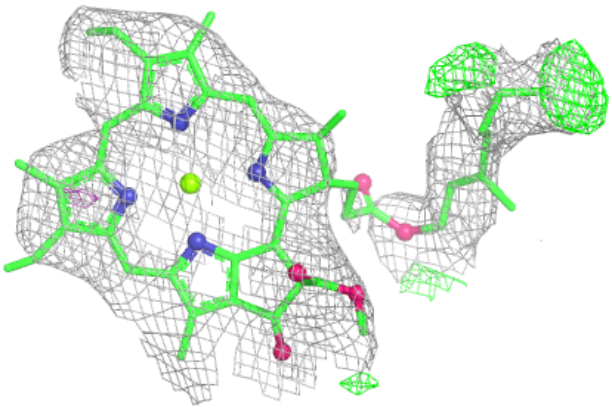


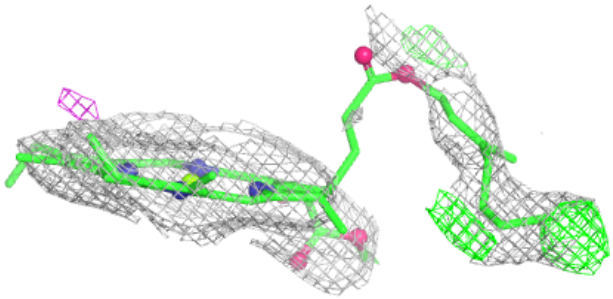




Electron density around CLA 2 1219:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

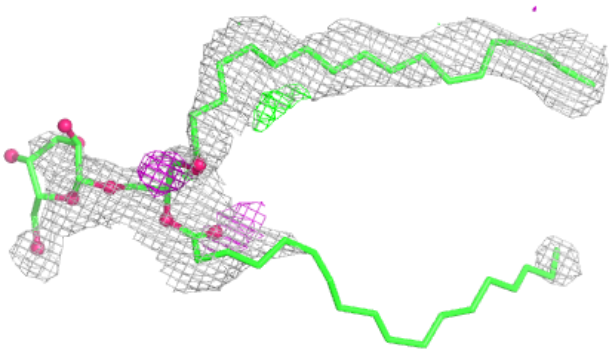


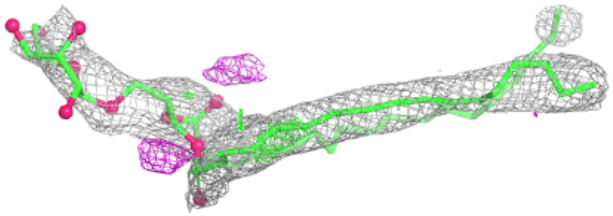


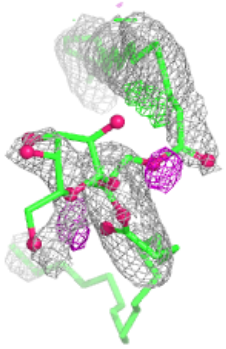


Electron density around LMG B 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

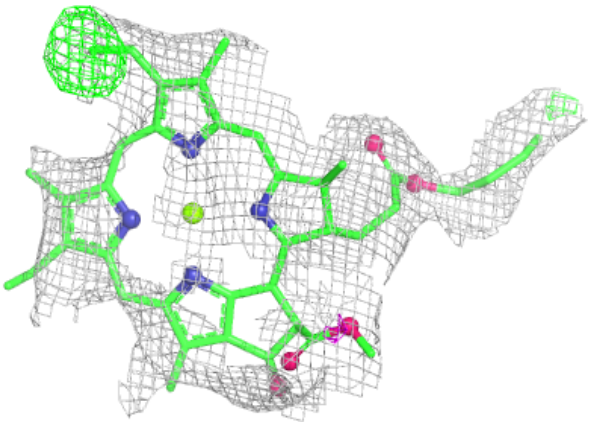


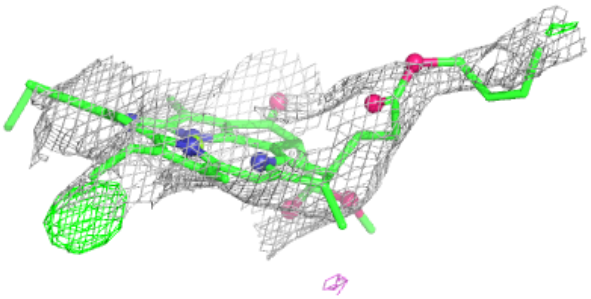


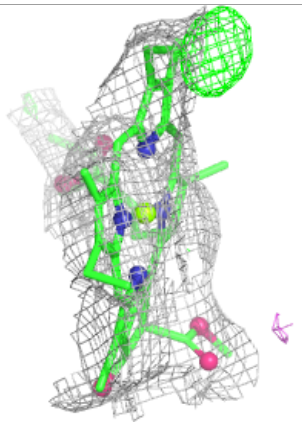


Electron density around CLA k 1402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

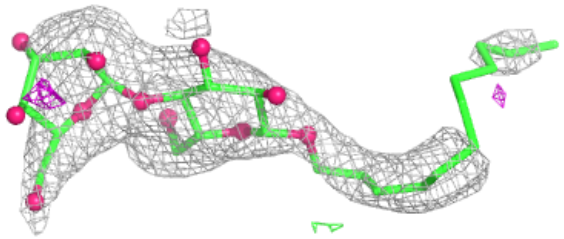


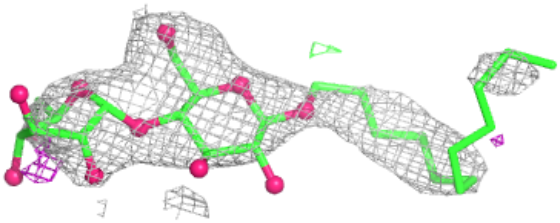


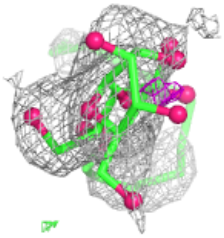


Electron density around LMT 1 6001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

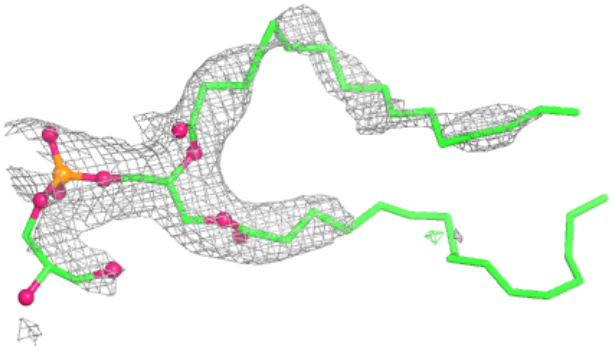


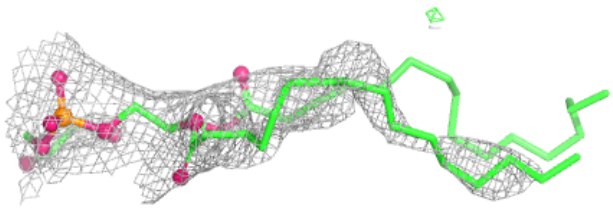


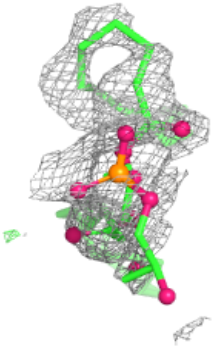


Electron density around LHG l 5003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

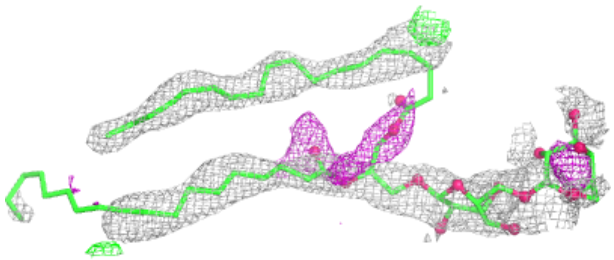


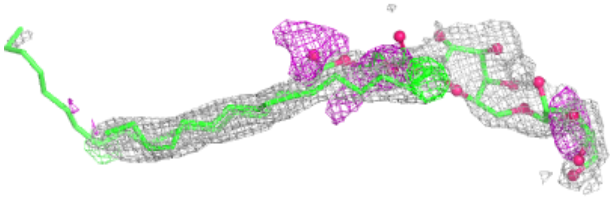


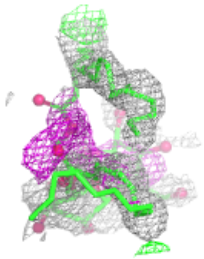


Electron density around DGD L 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

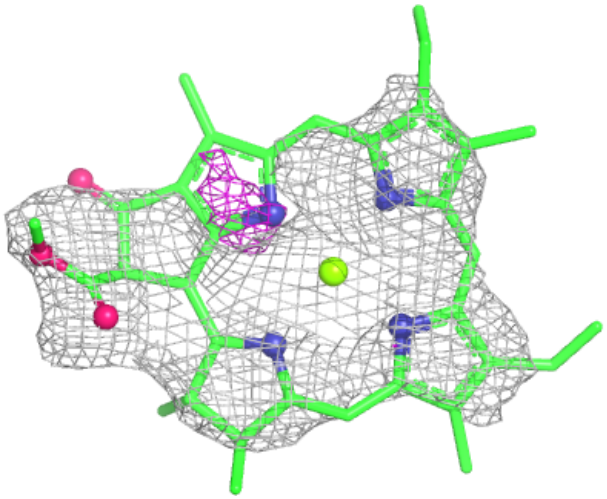


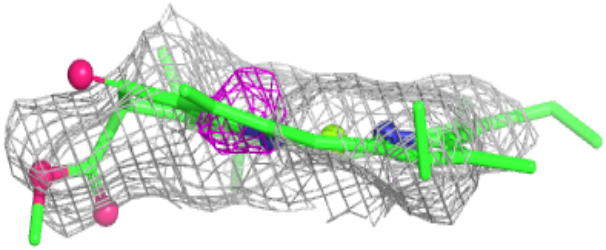


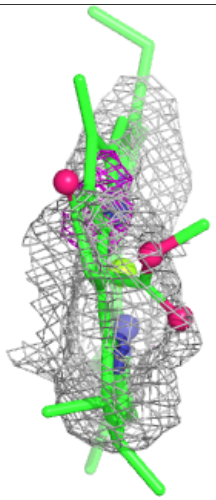


Electron density around CLA 7 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

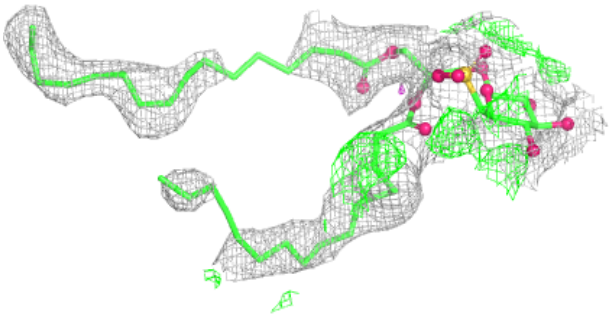


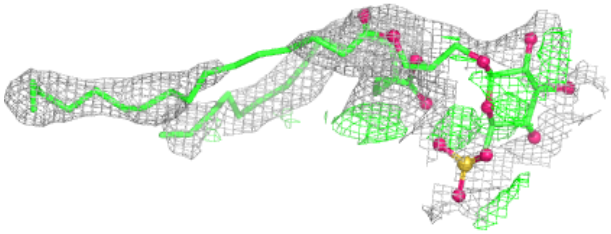


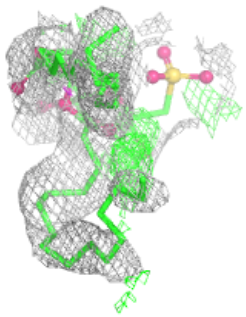


Electron density around SQD 0 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

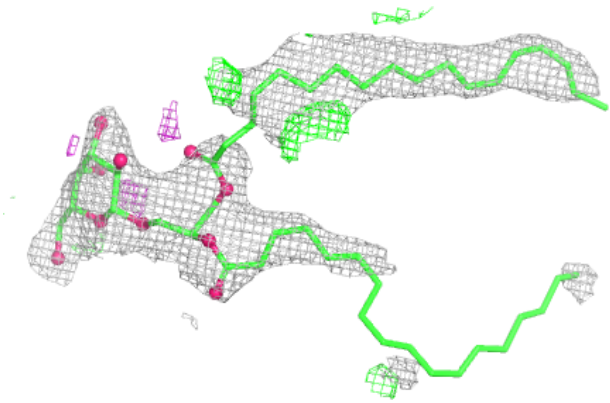


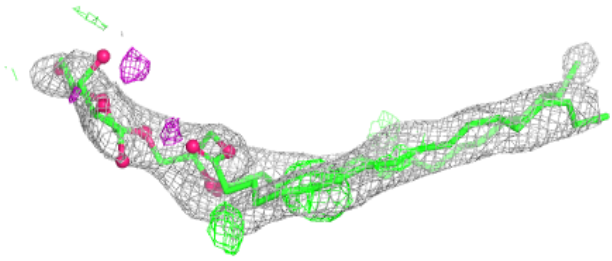


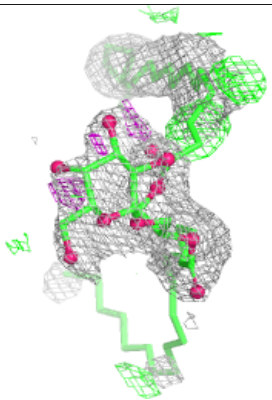


Electron density around LMG b 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

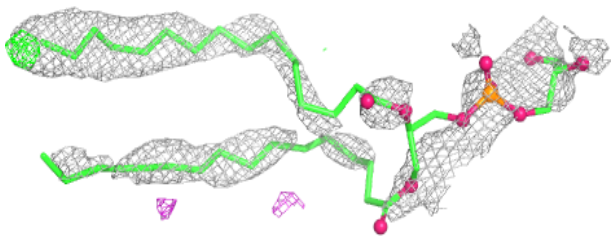


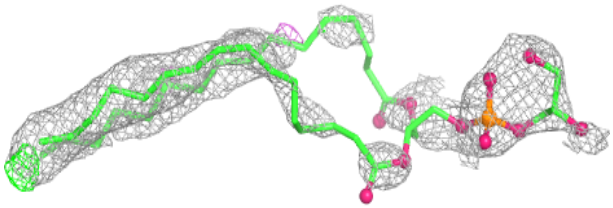


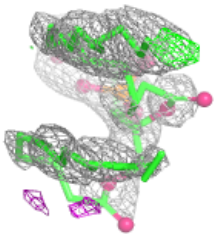


Electron density around LHG a 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

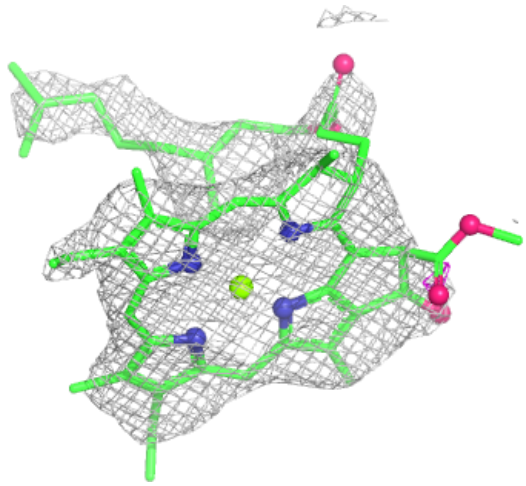


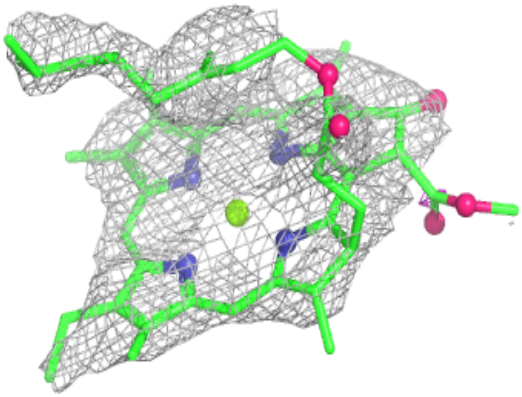


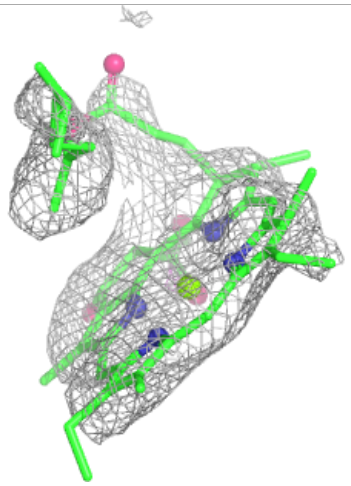


Electron density around CLA j 1303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

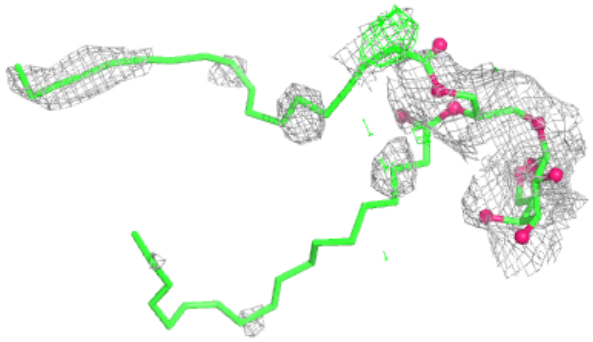


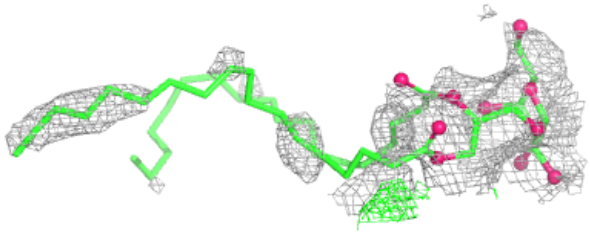


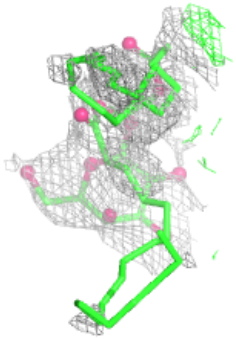


Electron density around LMG A 5008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

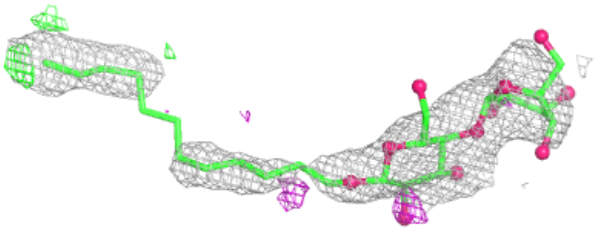


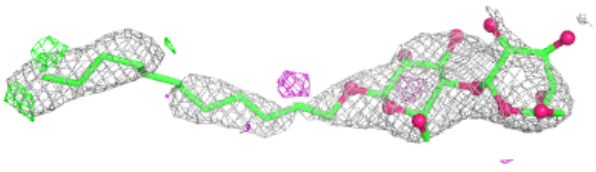


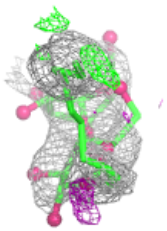


Electron density around LMT l 6001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

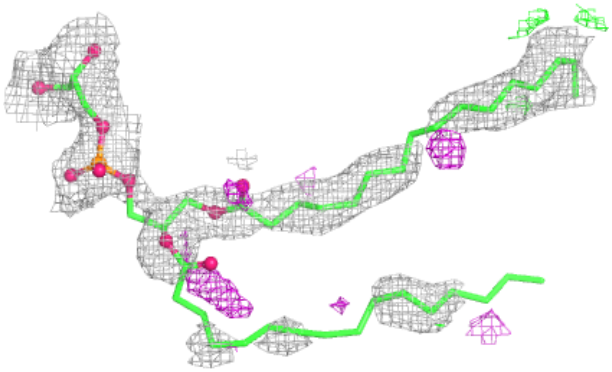


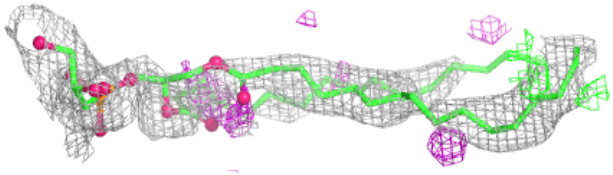


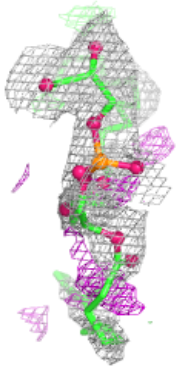


Electron density around LHG A 5006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

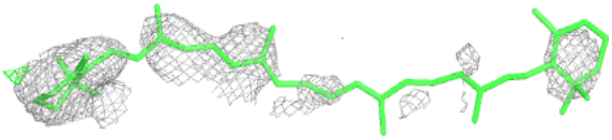


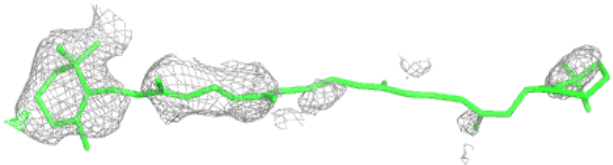


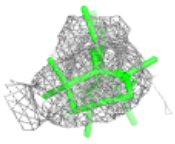


Electron density around BCR 8 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

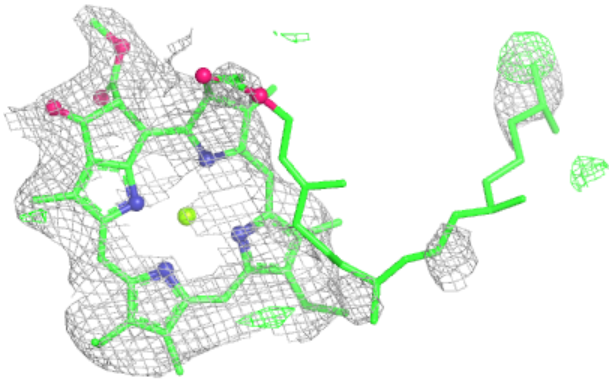


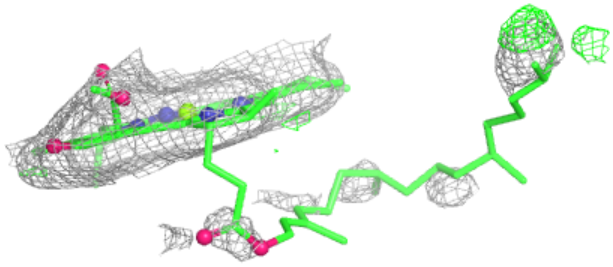


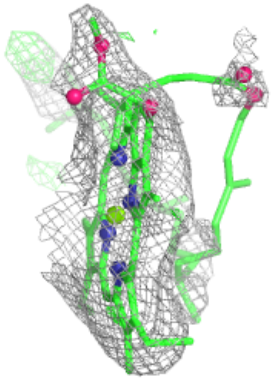


Electron density around CLA 2 1218:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

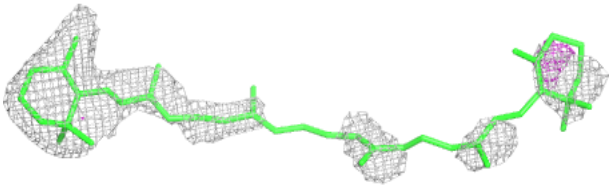


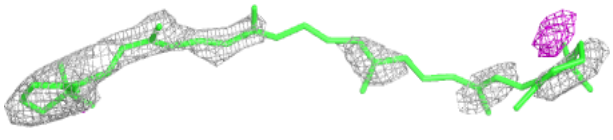


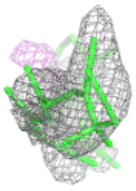


Electron density around BCR 7 4013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

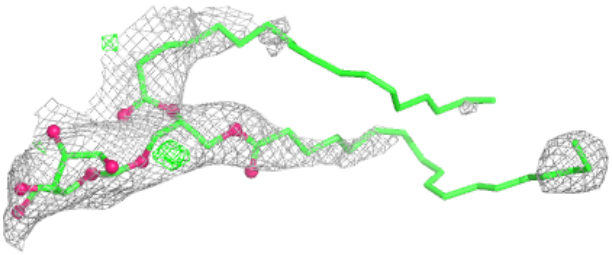


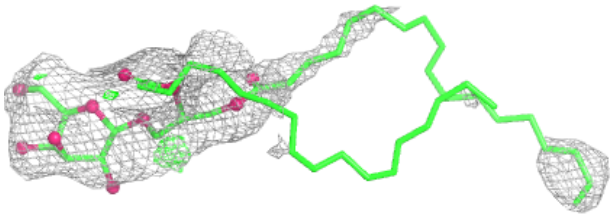


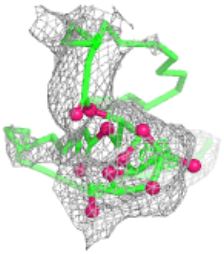


Electron density around LMG a 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

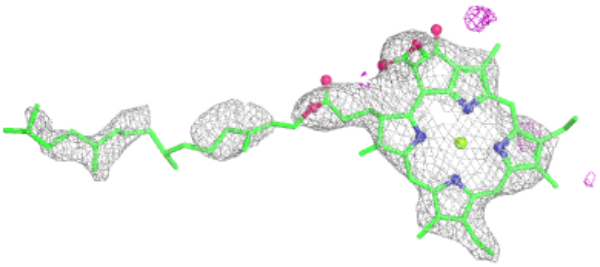


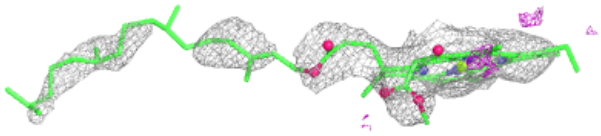


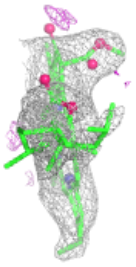


Electron density around CLA f 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

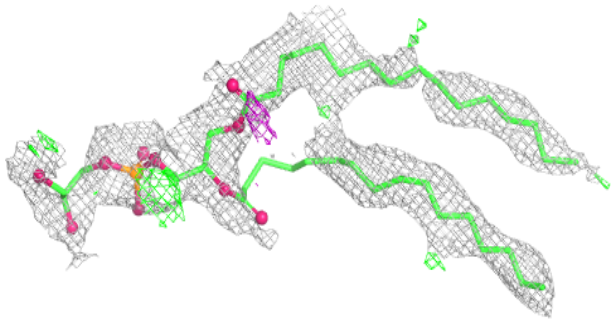


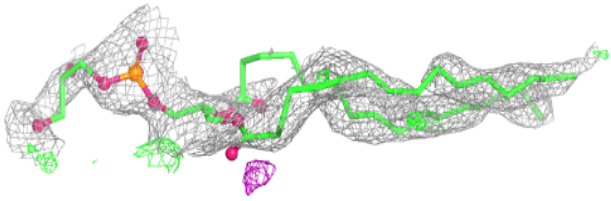


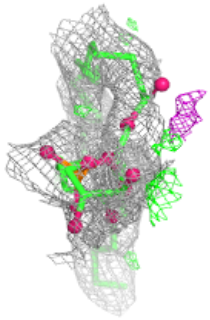


Electron density around LHG M 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

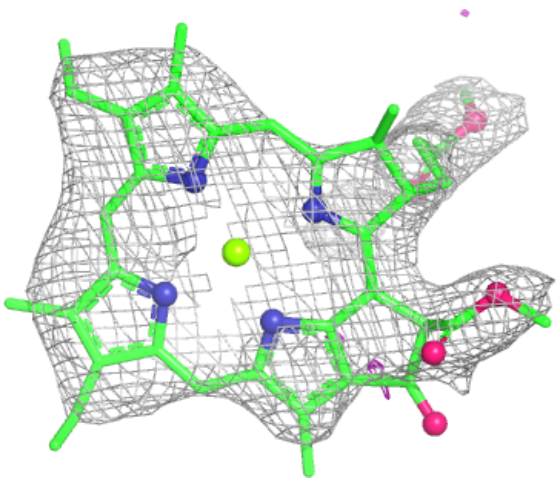


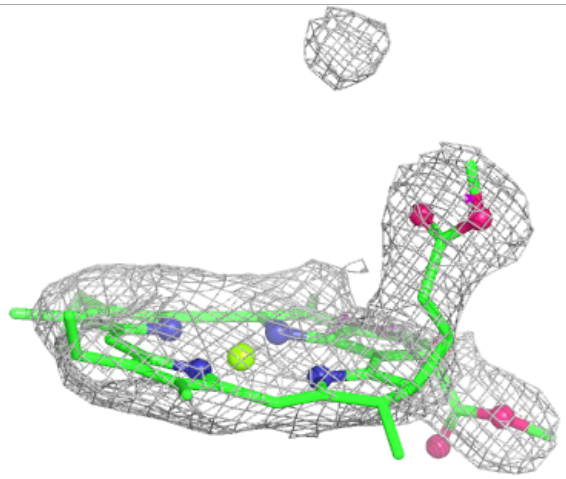


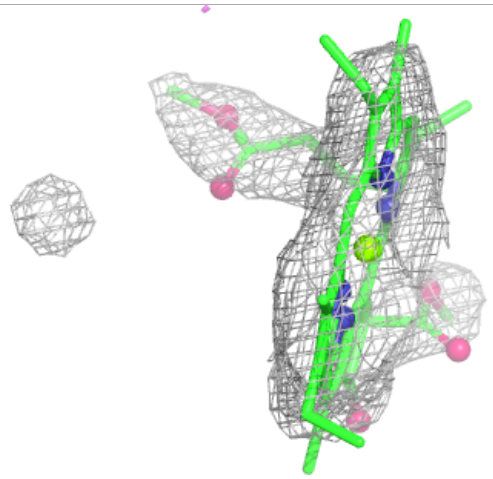


Electron density around CLA 1 1108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

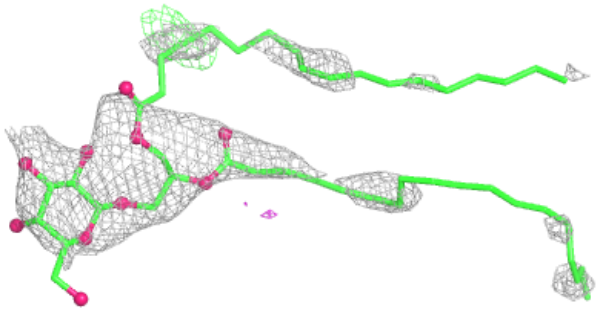


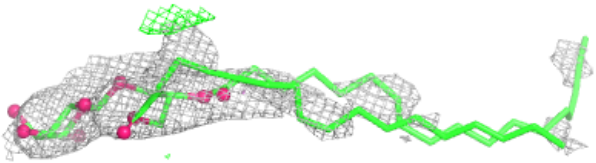


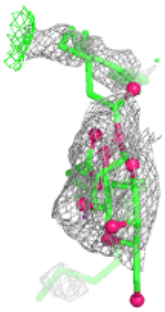


Electron density around LMG 1 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

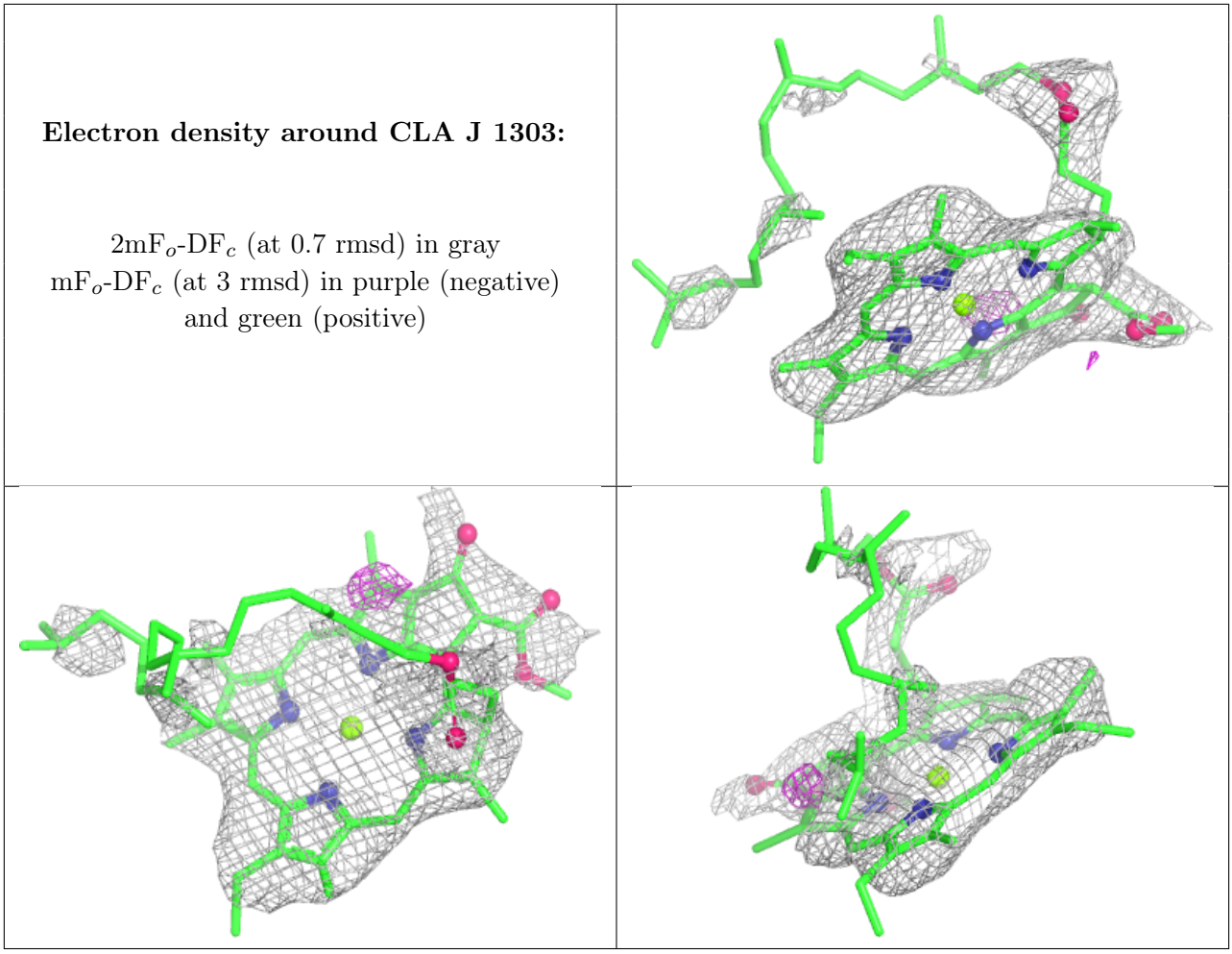






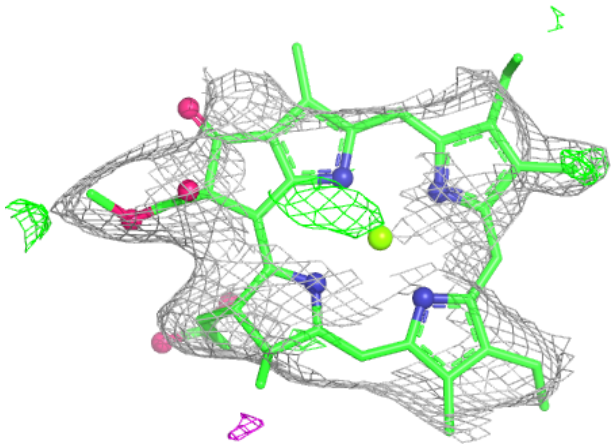
Electron density around CLA J 1303:

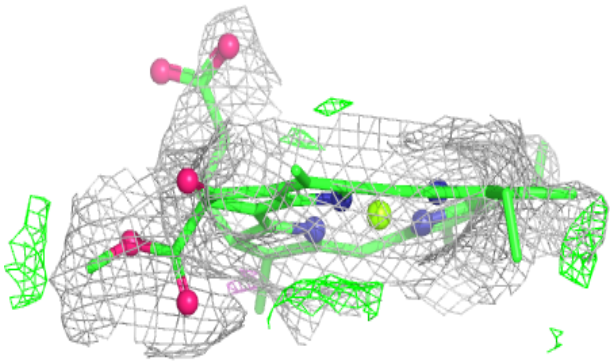
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

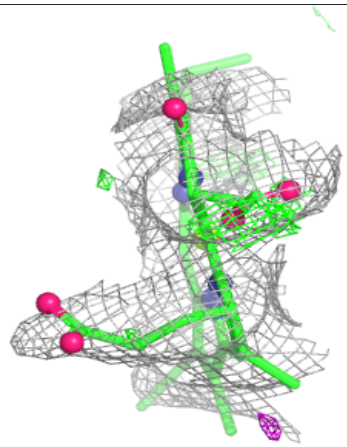


Electron density around CLA 2 1232:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

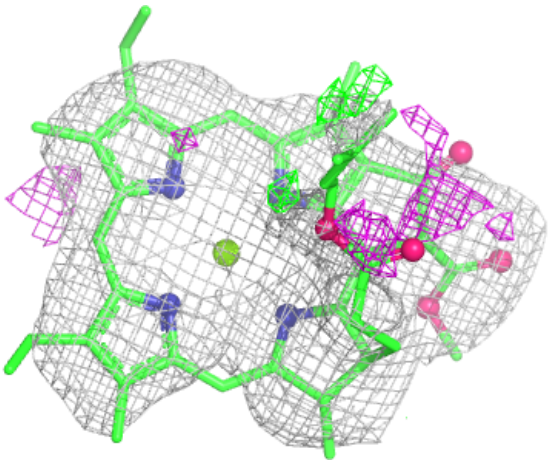


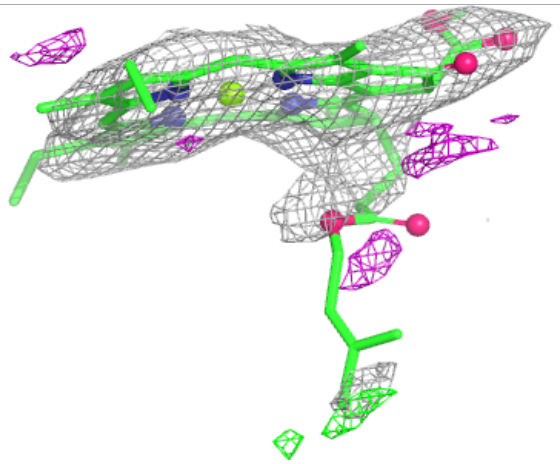


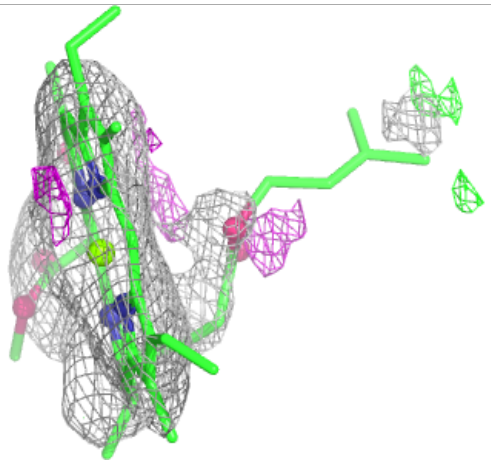


Electron density around CLA 2 1213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

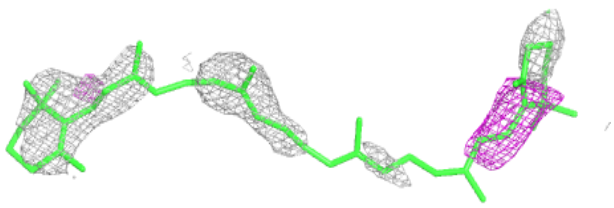


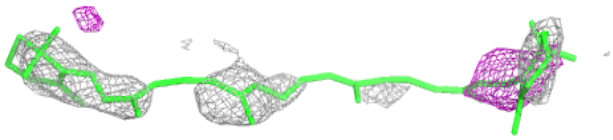


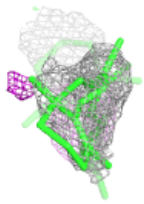


Electron density around BCR B 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

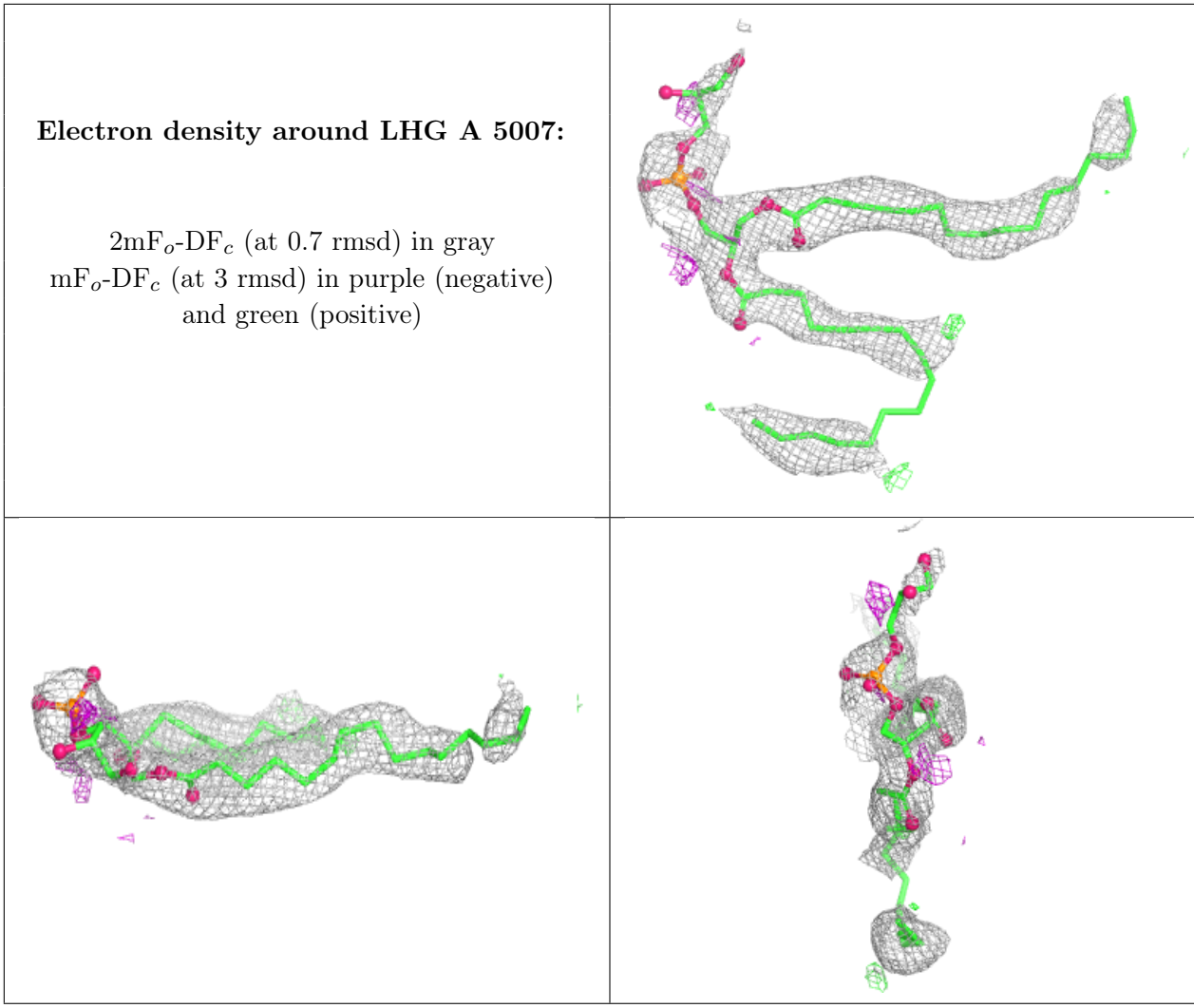






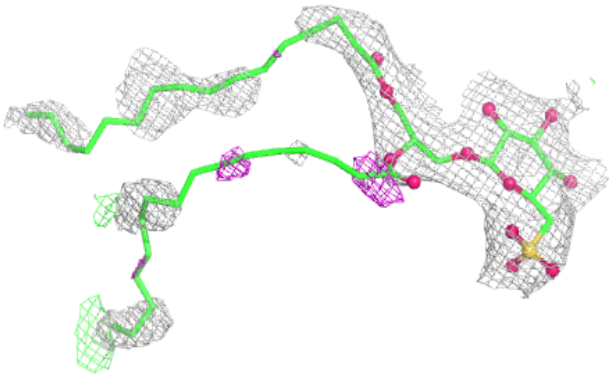
Electron density around LHG A 5007:

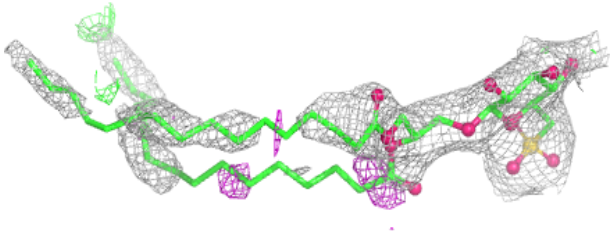
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

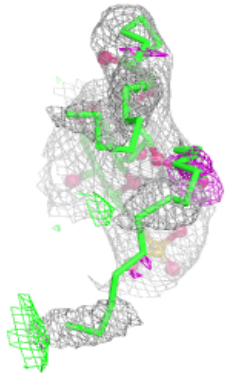


Electron density around SQD B 5008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

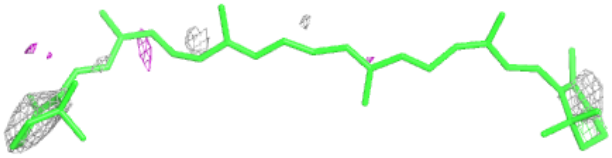




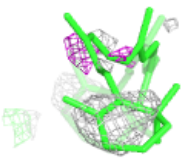


Electron density around BCR 2 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

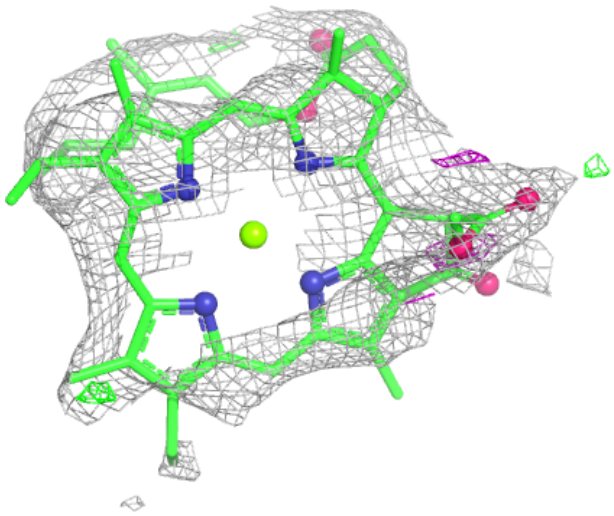


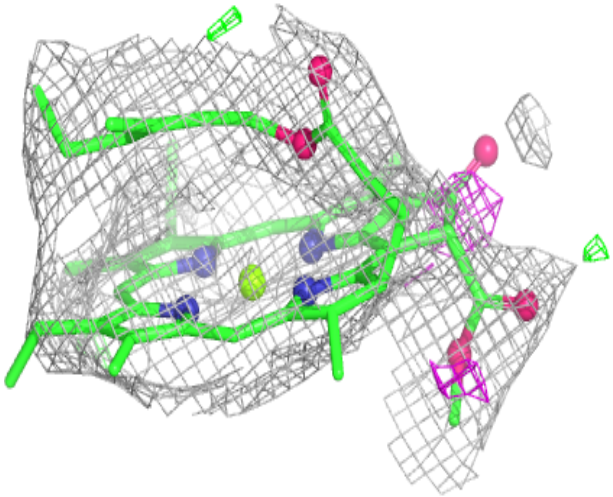


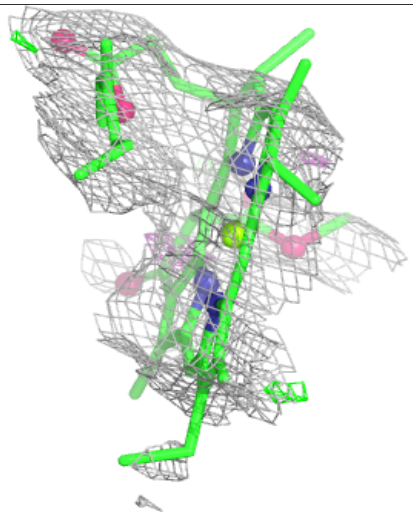


Electron density around CLA 2 1217:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

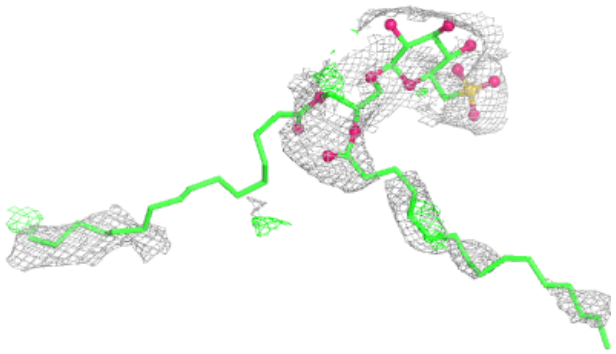


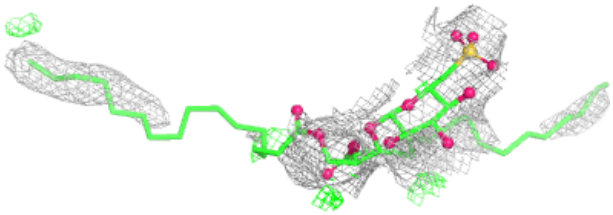




Electron density around SQD f 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

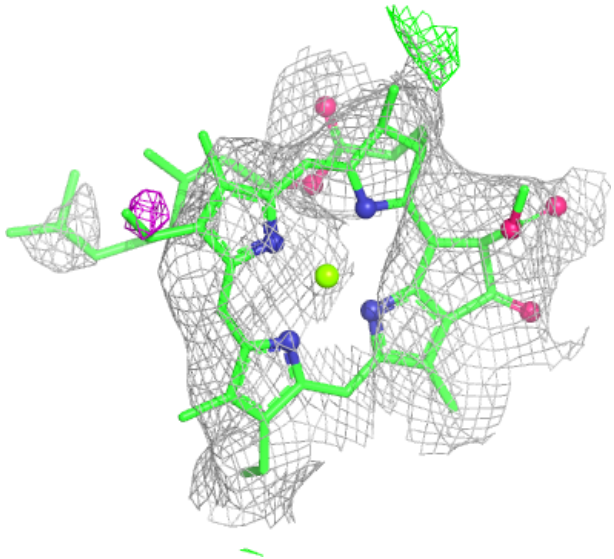


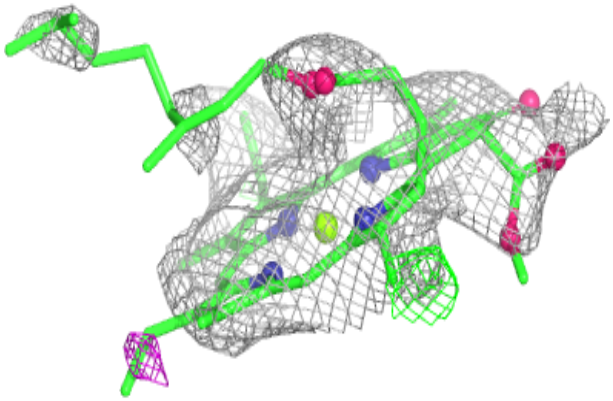


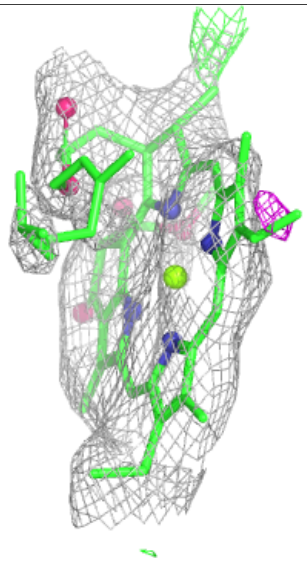


Electron density around CLA a 1120:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

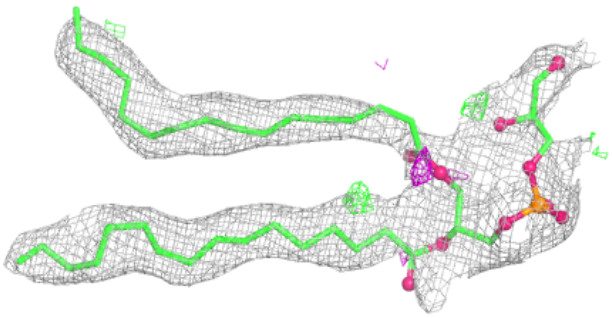


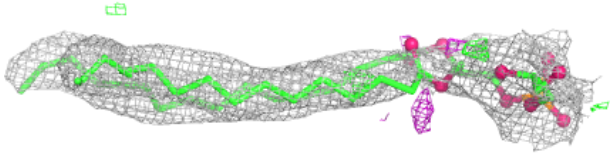


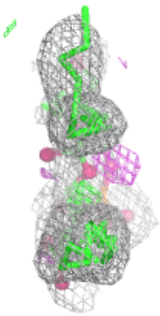


Electron density around LHG A 5005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

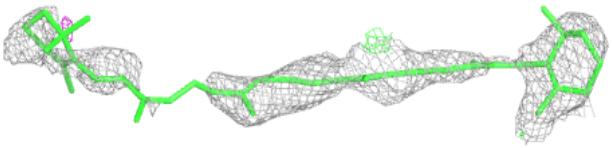


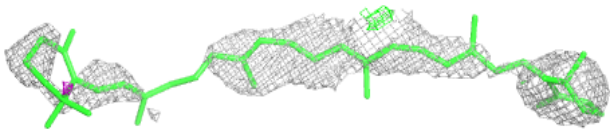


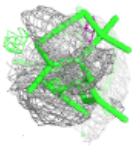


Electron density around BCR 1 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

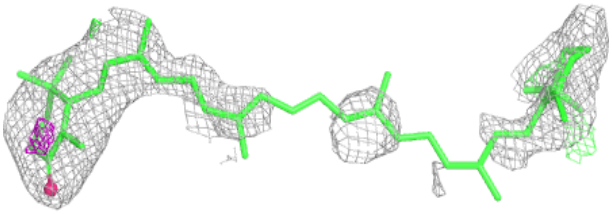


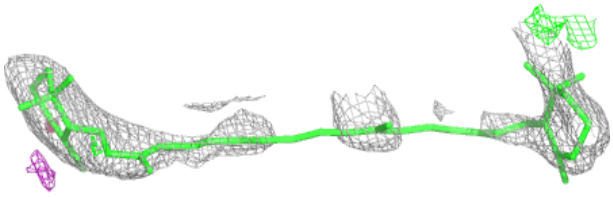


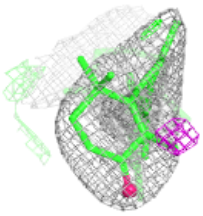


Electron density around ECH 2 4006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

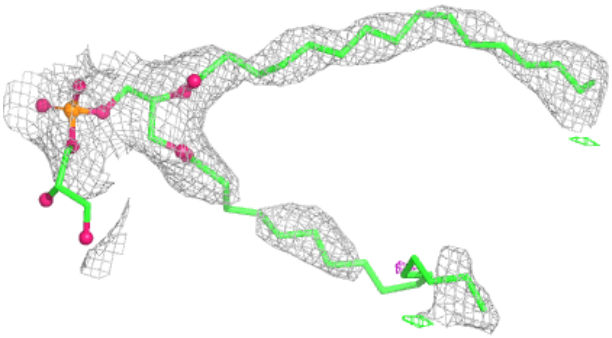


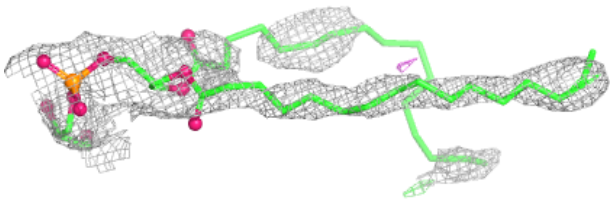


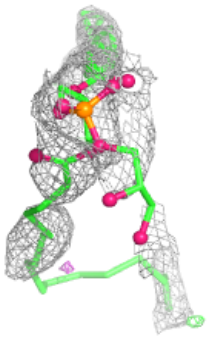


Electron density around LHG l 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

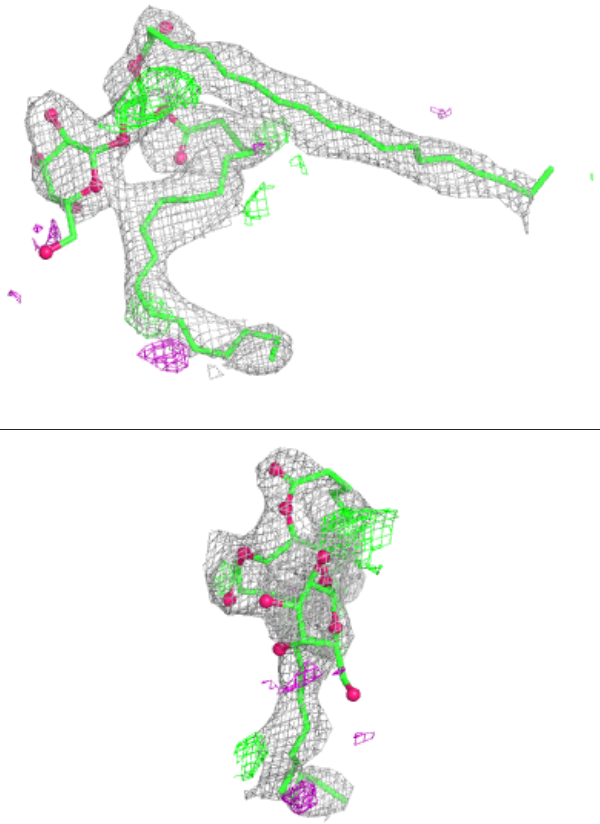






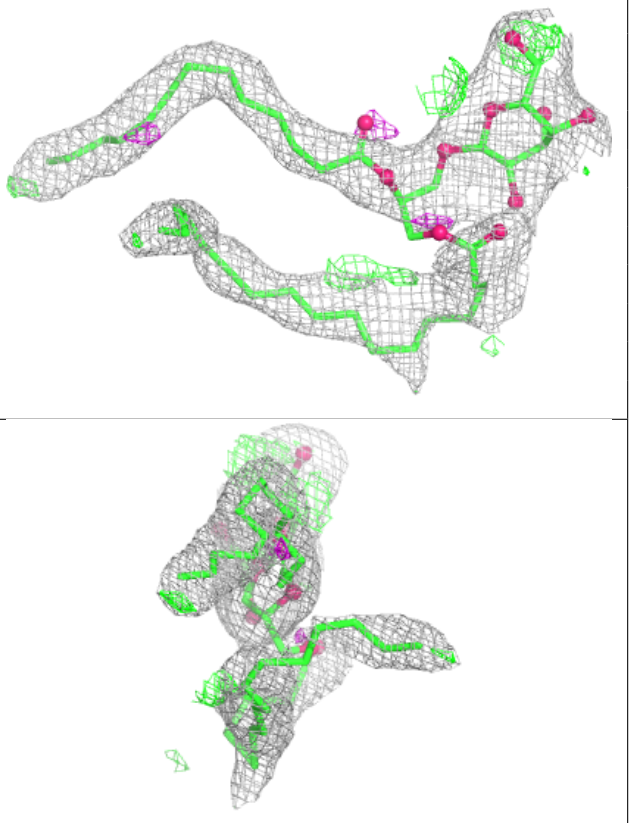
Electron density around LMG K 5009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



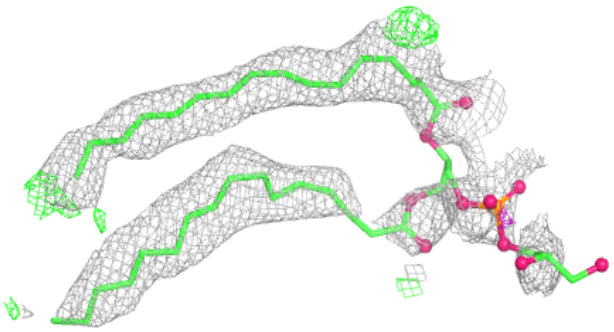
Electron density around LMG A 5002:

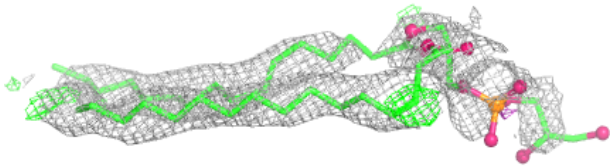
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG l 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

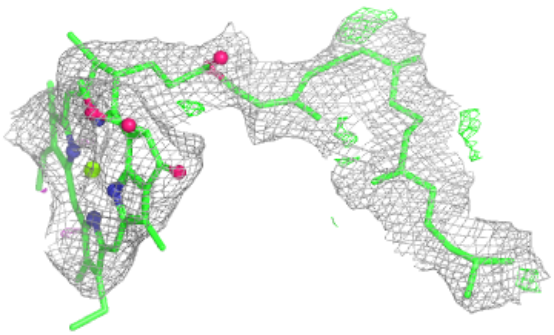


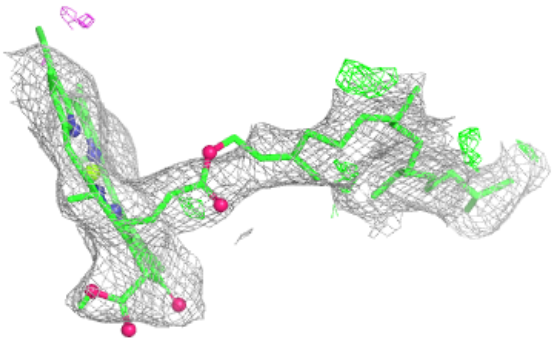


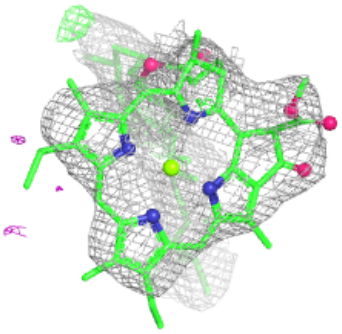


Electron density around CLA 1 1134:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

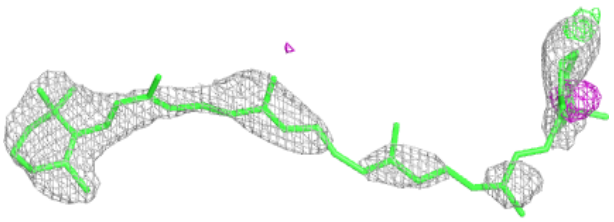


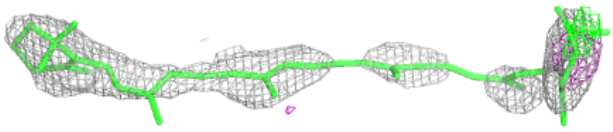


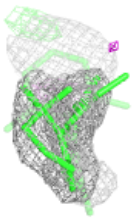


Electron density around BCR b 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

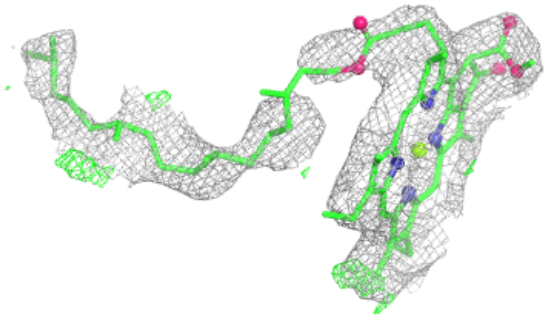


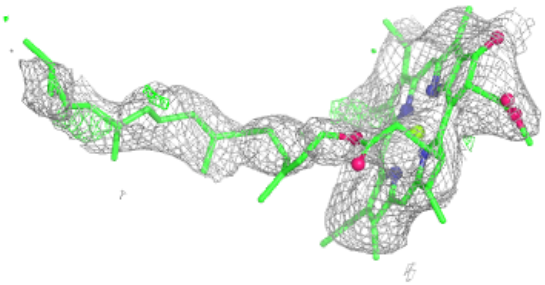


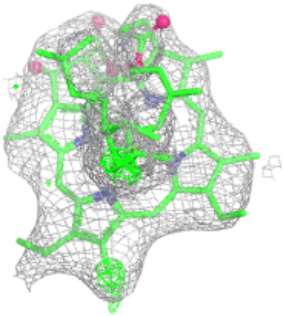


Electron density around CLA 1 1120:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

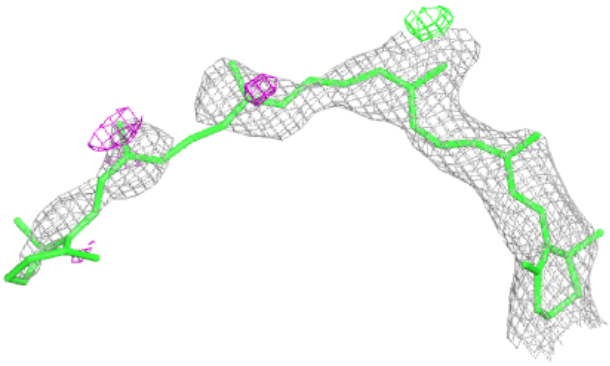


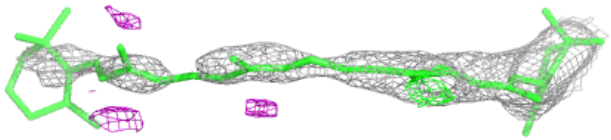


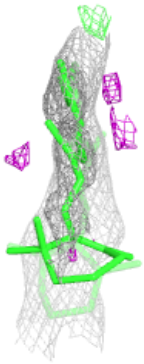


Electron density around BCR 6 4016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

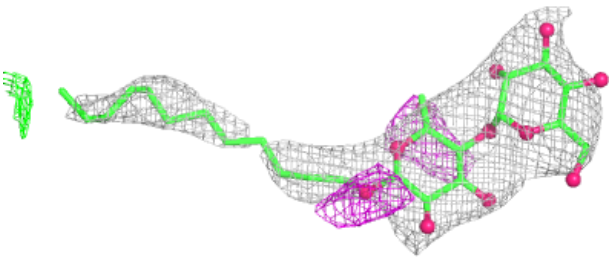


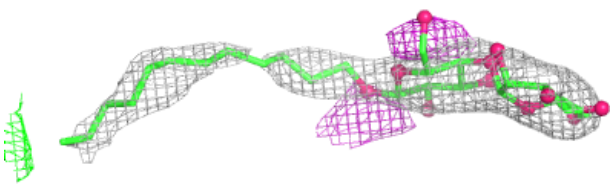


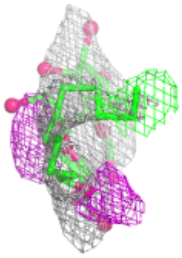


Electron density around LMT L 6001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

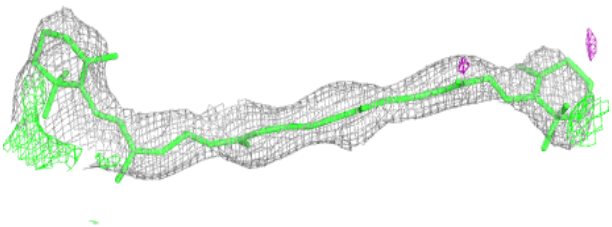


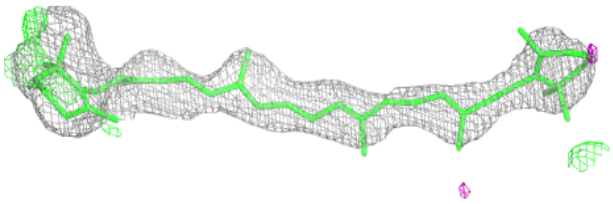


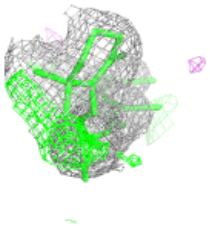


Electron density around BCR l 4022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

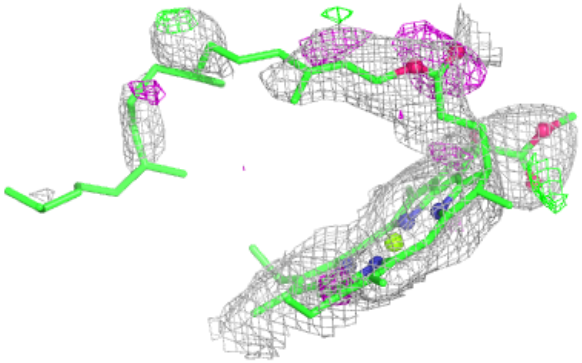


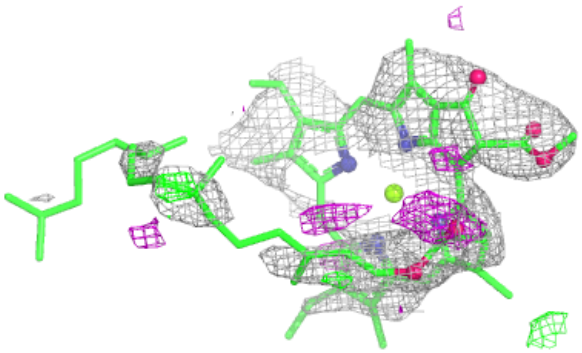


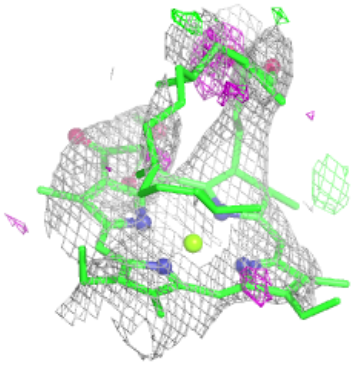


Electron density around CLA 1 1109:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

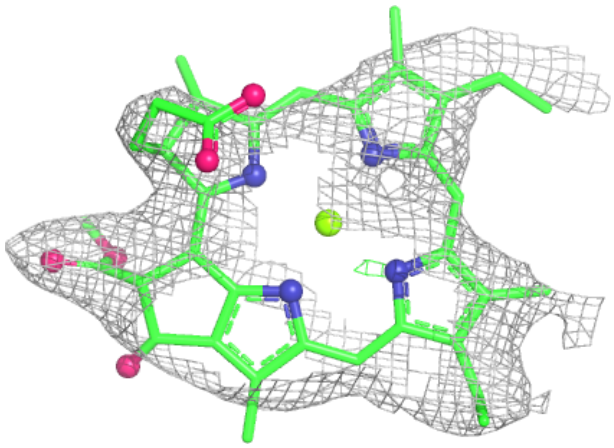


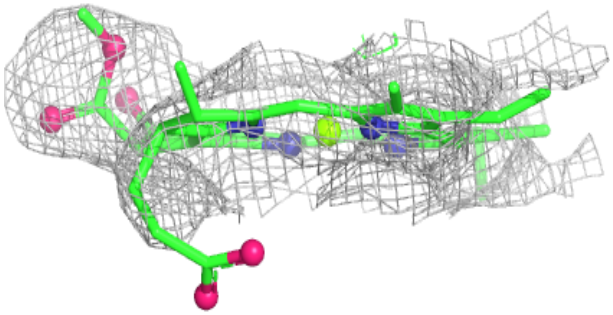


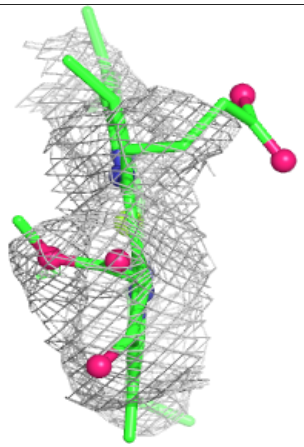


Electron density around CLA 2 1209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

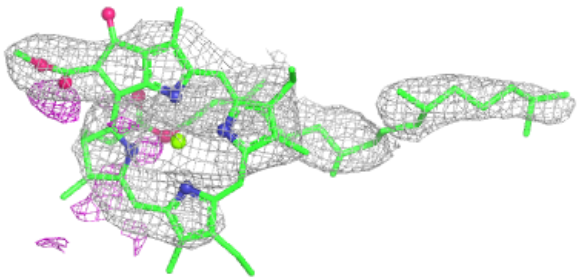


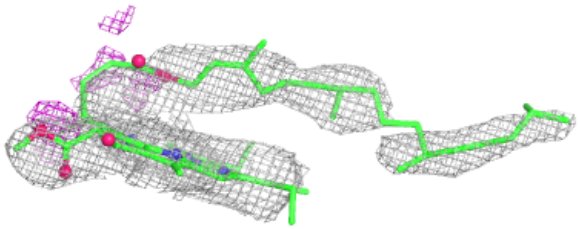


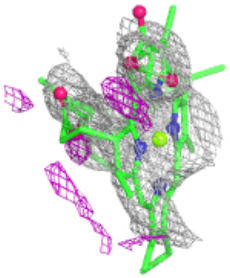


Electron density around CLA a 1115:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

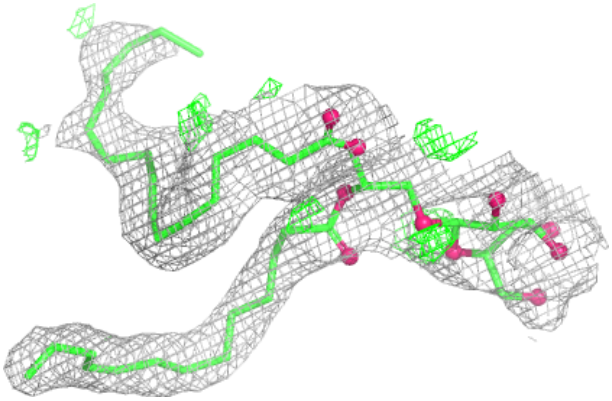


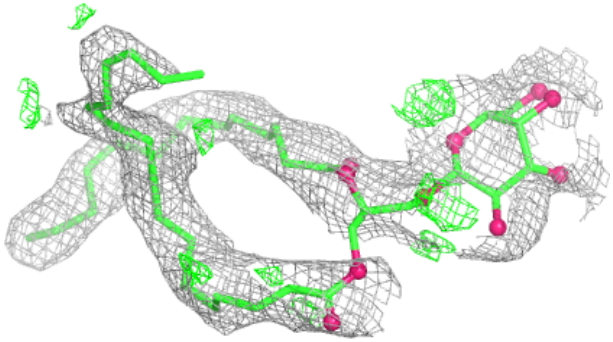


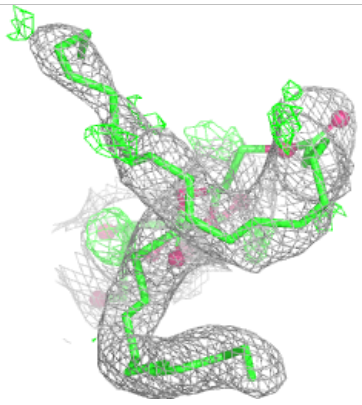


Electron density around LMG a 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

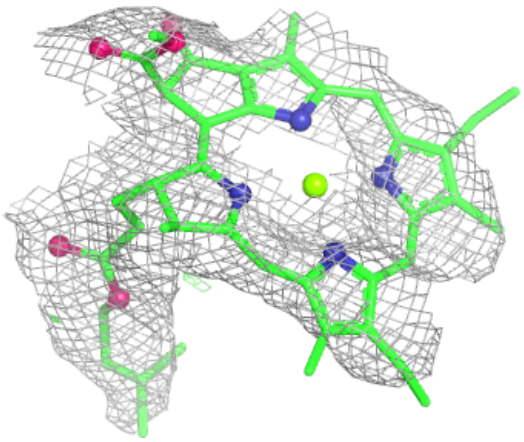


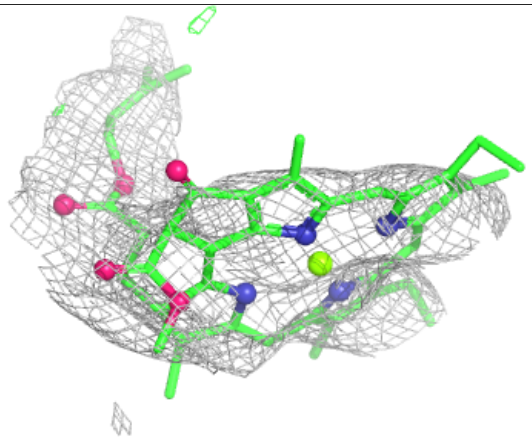


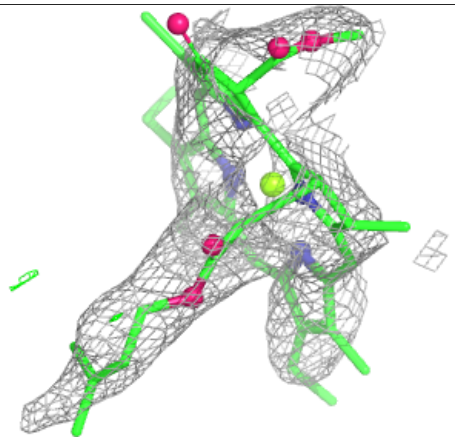


Electron density around CLA 2 1216:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

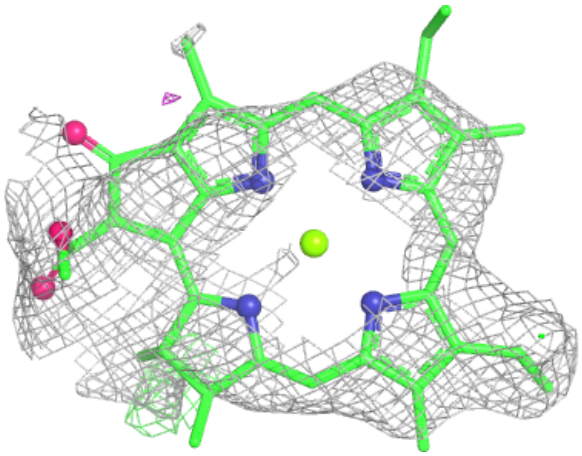


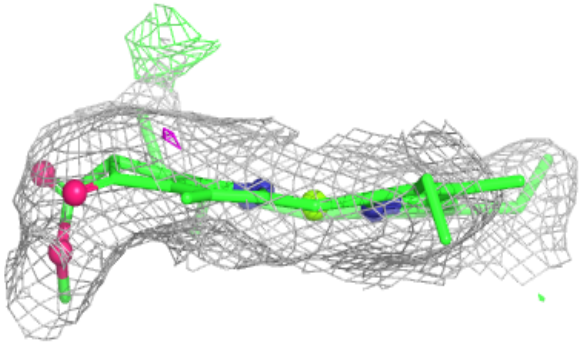


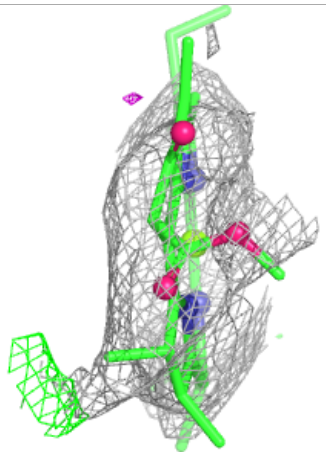


Electron density around CLA 2 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

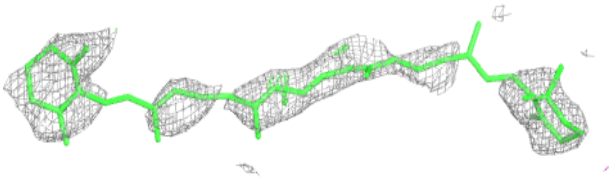


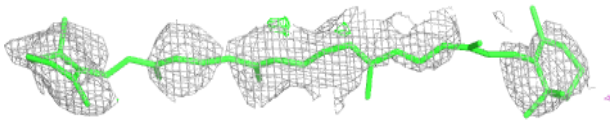


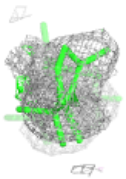


Electron density around BCR a 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

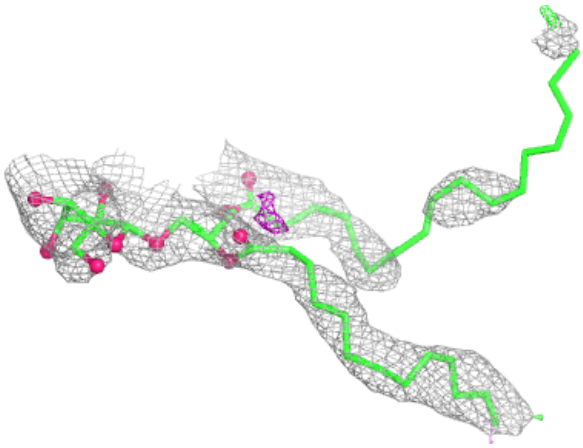


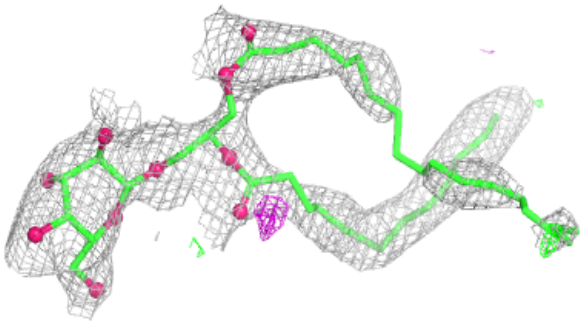


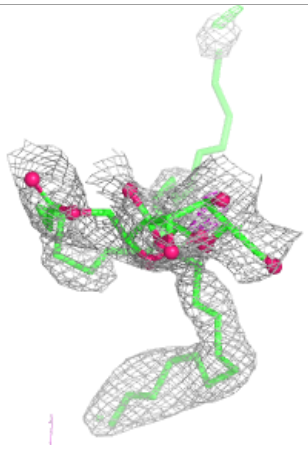


Electron density around LMG 1 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

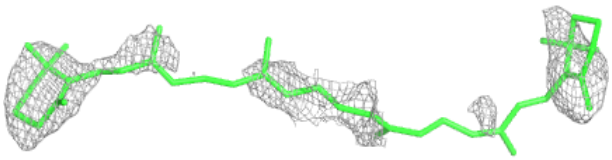


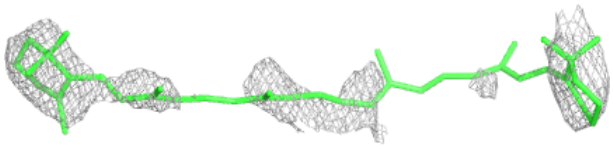


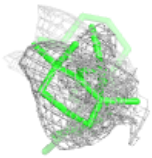


Electron density around BCR a 4003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

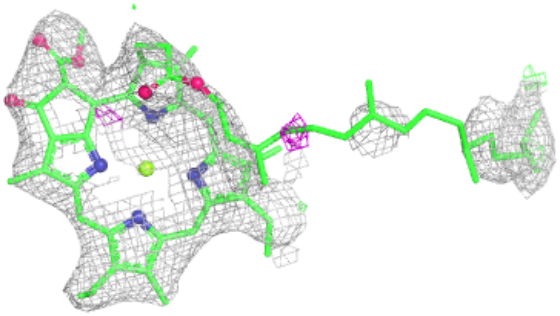


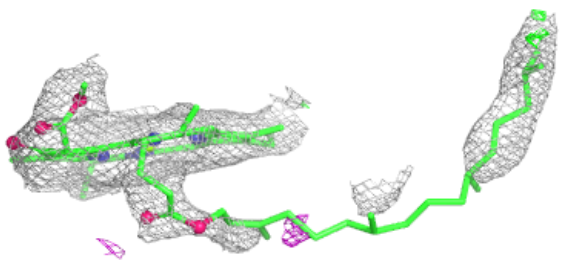


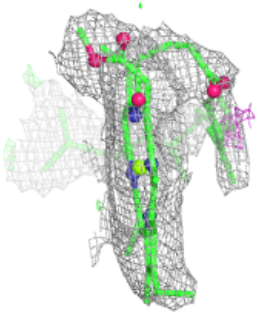


Electron density around CLA B 1209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

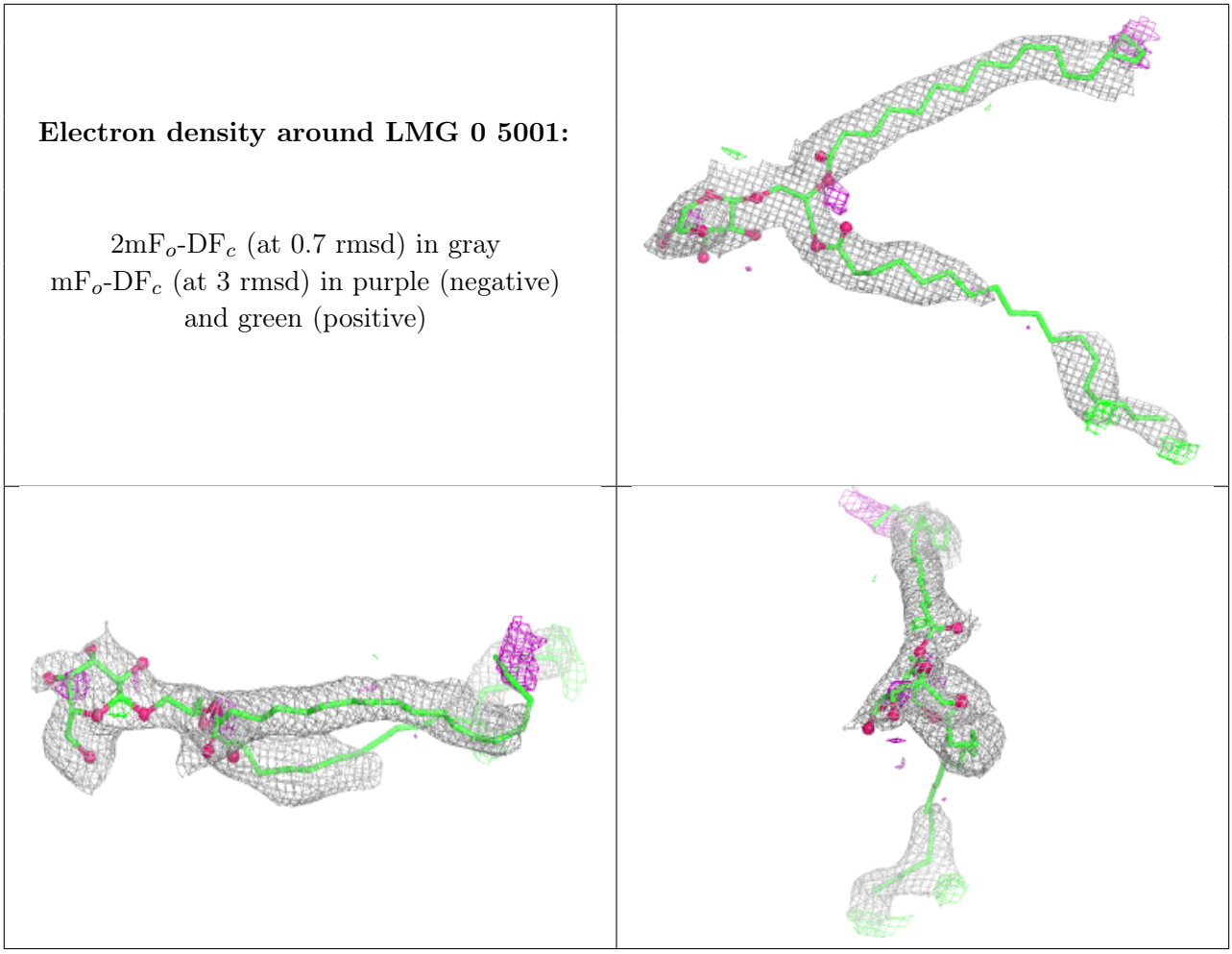






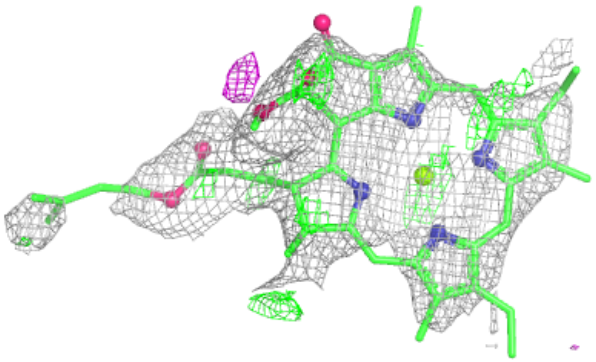
Electron density around LMG 0 5001:

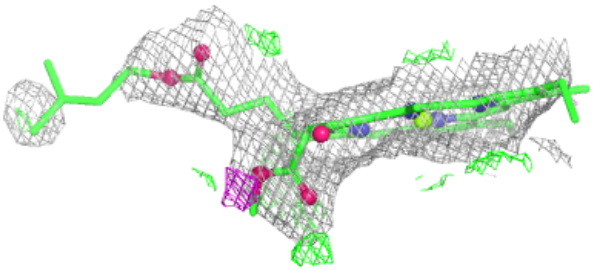
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

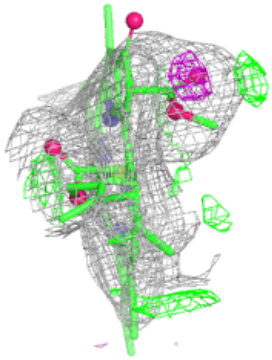


Electron density around CLA 2 1234:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

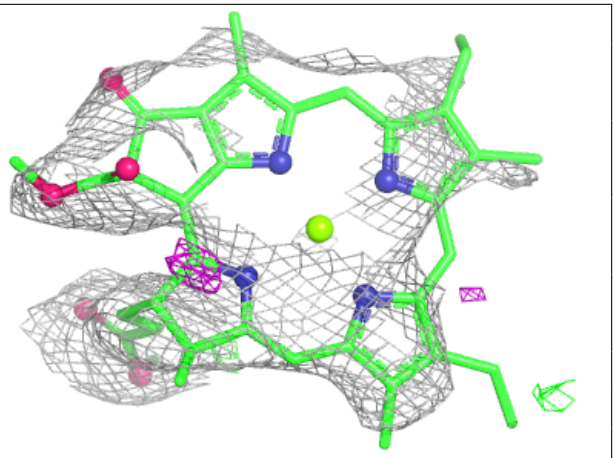


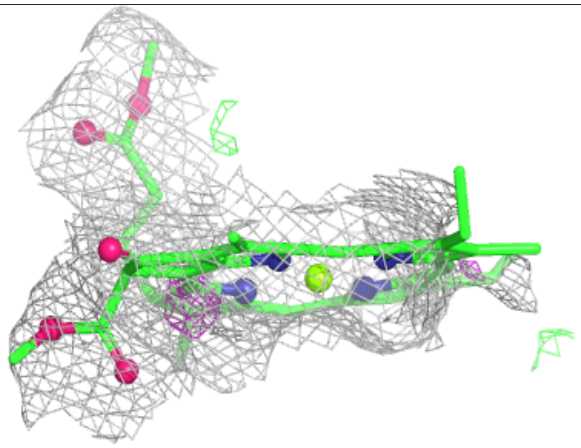


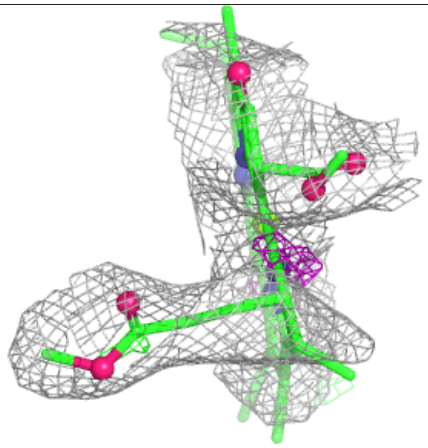


Electron density around CLA 2 1231:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

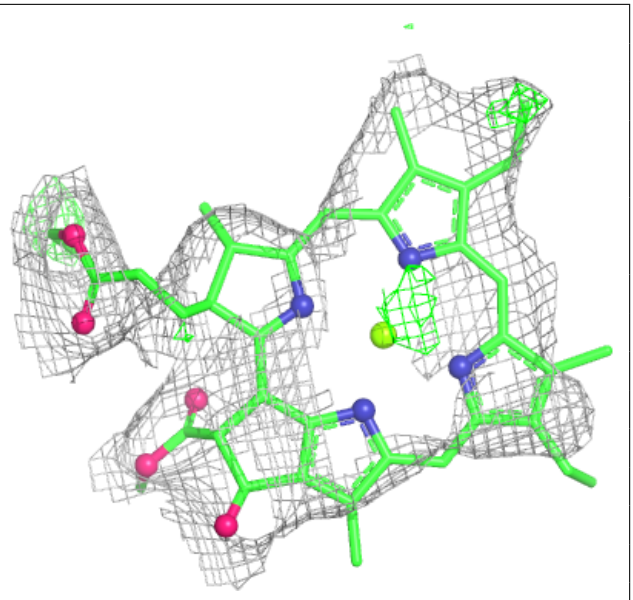


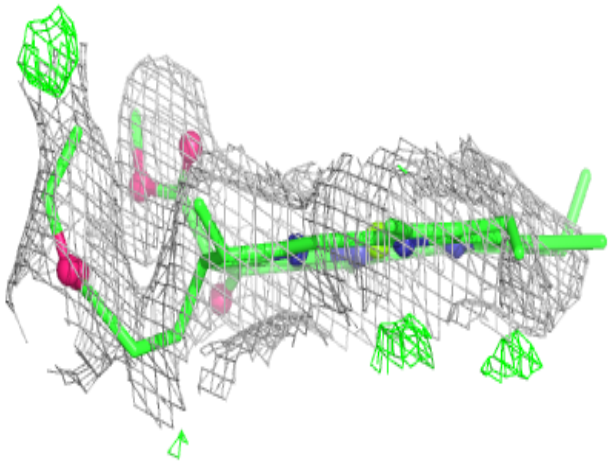




Electron density around CLA 6 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

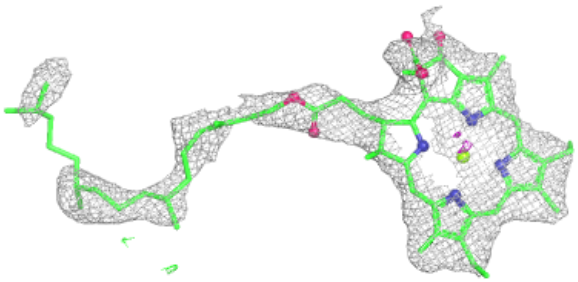


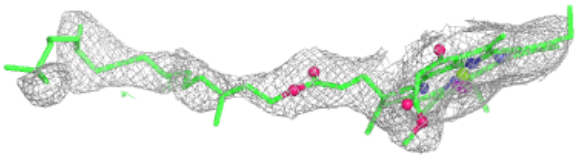


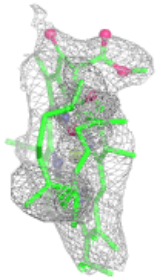


Electron density around CLA F 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

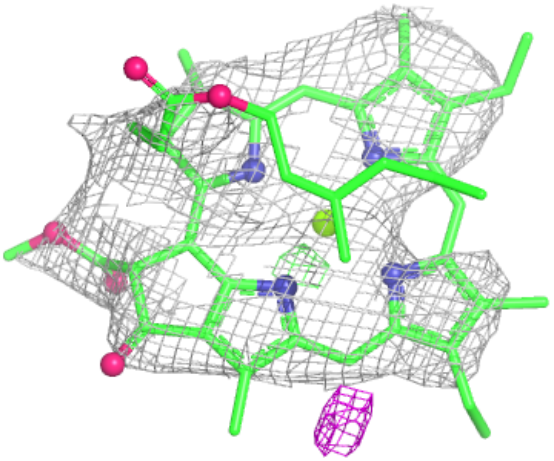


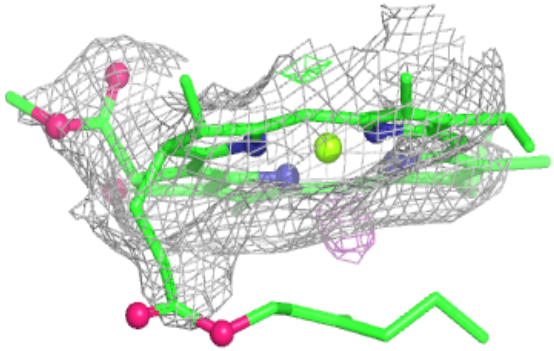


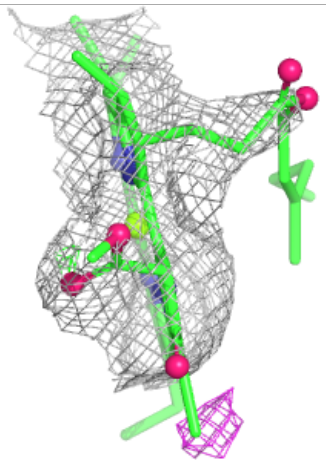


Electron density around CLA a 1114:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

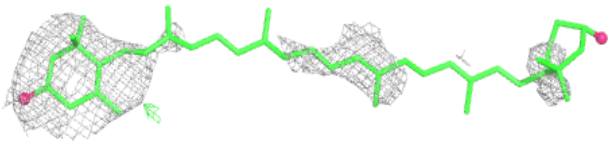


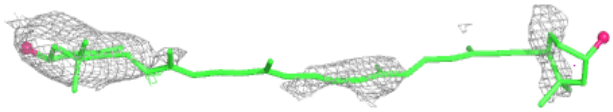


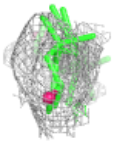


Electron density around ZEX 7 4015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

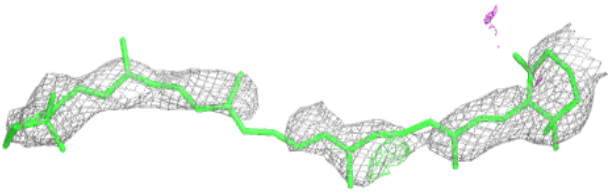


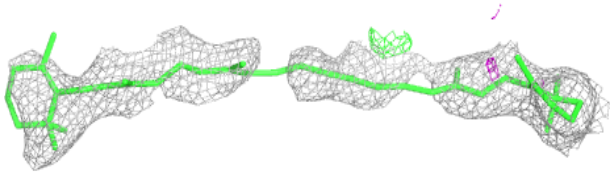


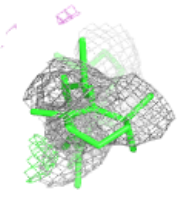


Electron density around BCR 2 4005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

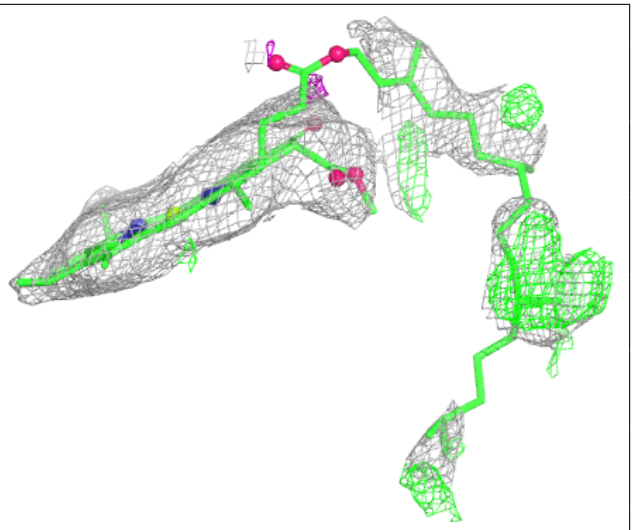


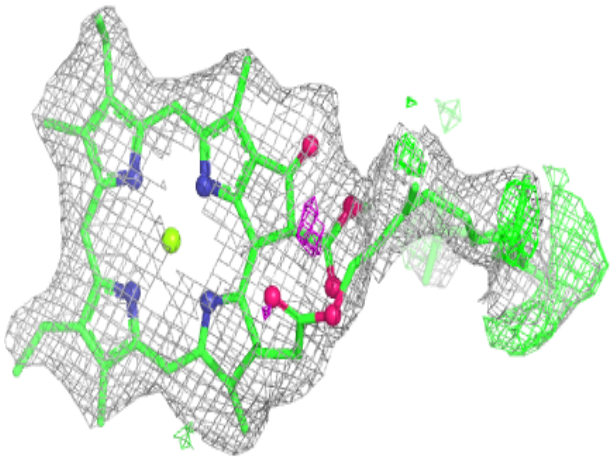


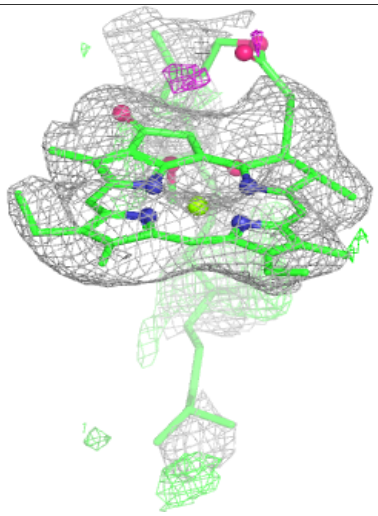


Electron density around CLA b 1240:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

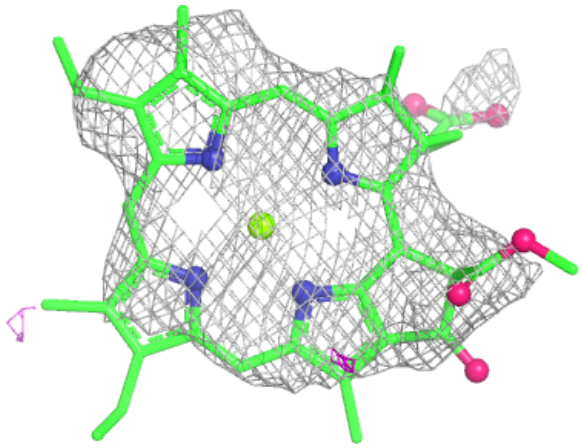


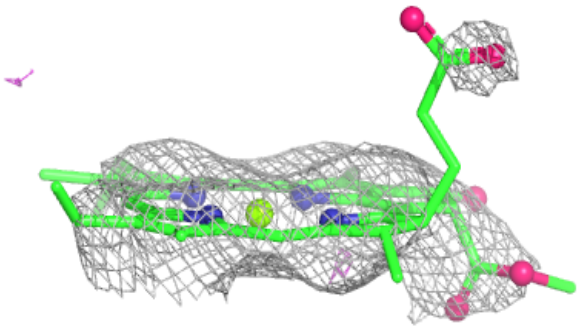




Electron density around CLA 1 1114:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

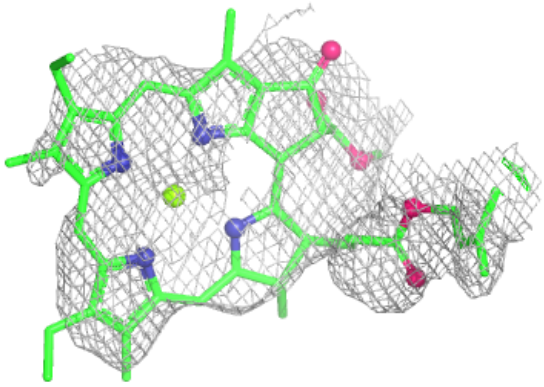


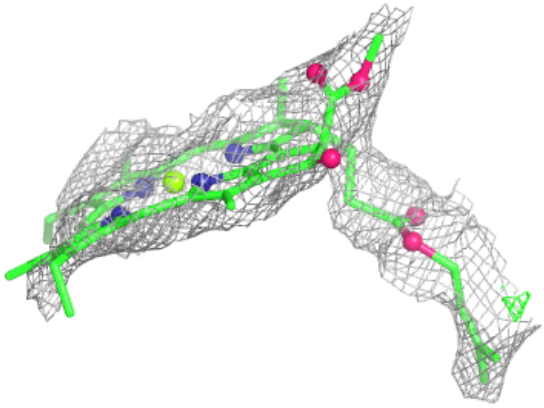


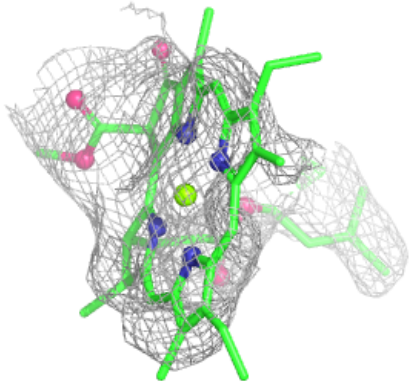


Electron density around CLA k 1401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

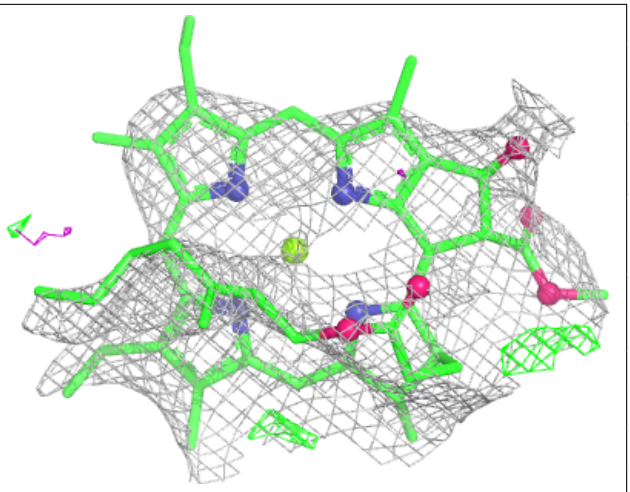


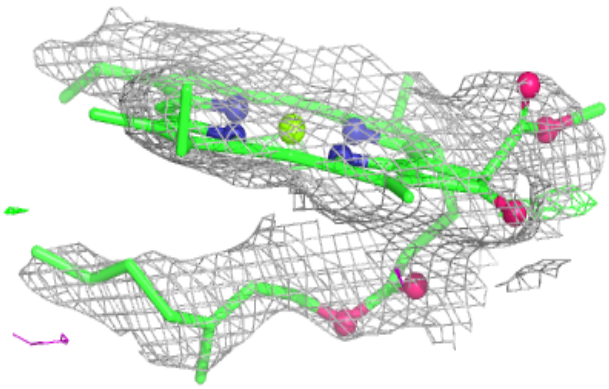


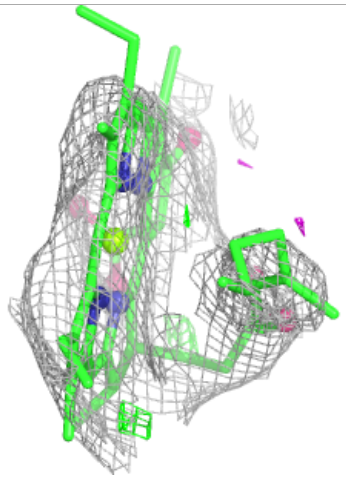


Electron density around CLA 2 1235:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

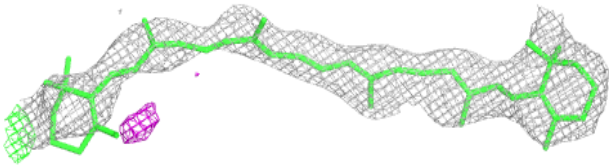


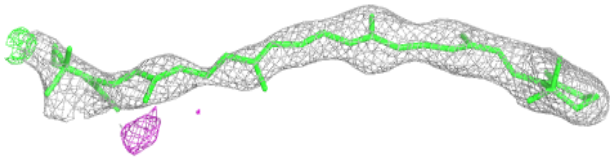


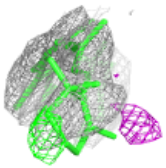


Electron density around BCR j 4013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

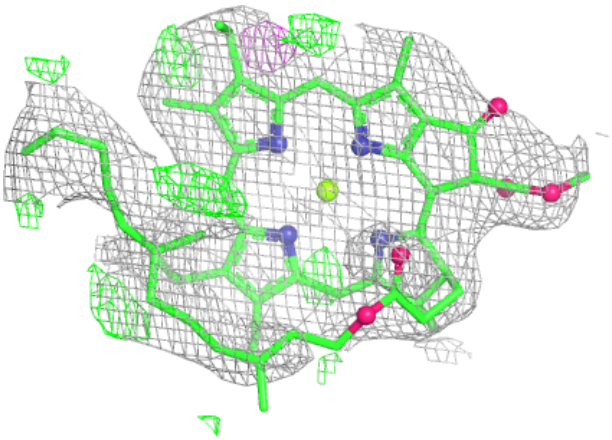


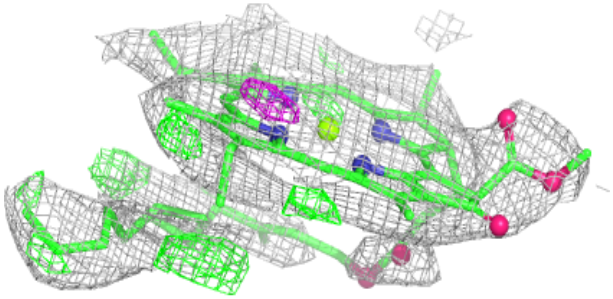


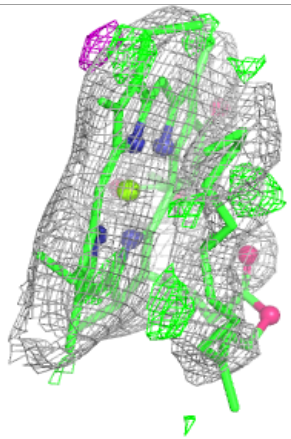


Electron density around CLA a 1110:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

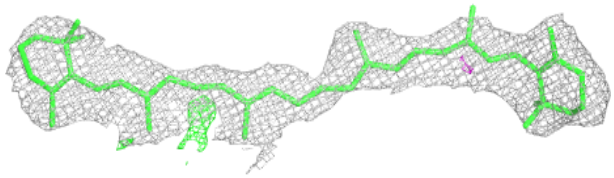


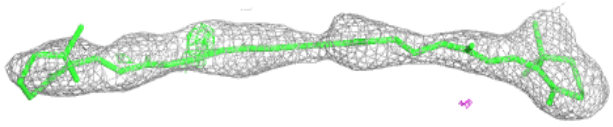


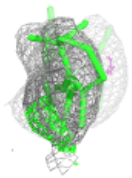


Electron density around BCR B 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

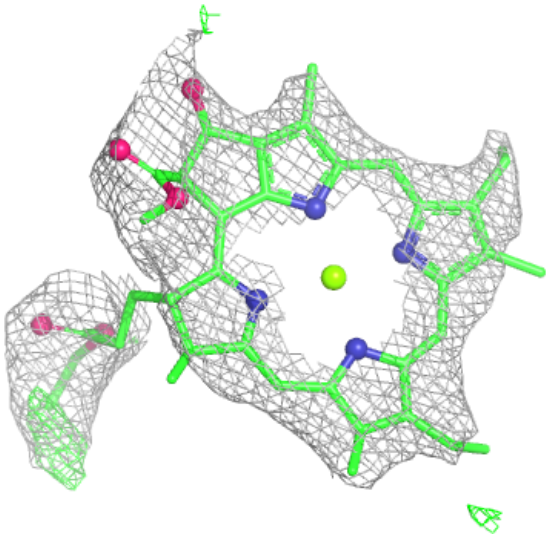


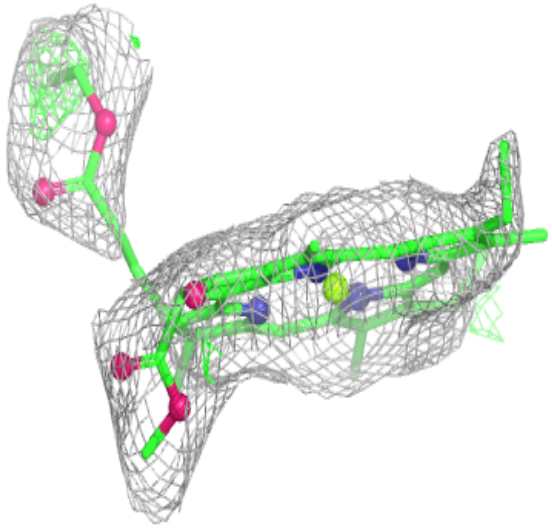


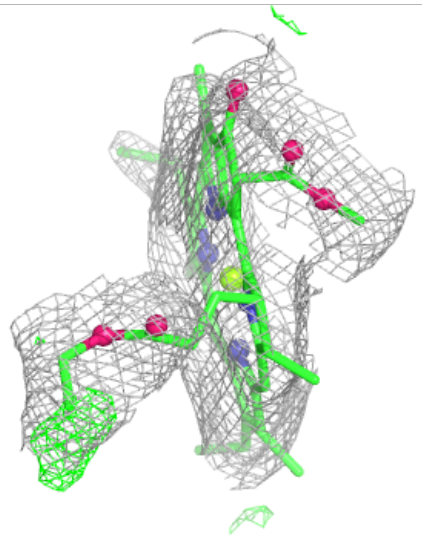


Electron density around CLA 2 1230:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

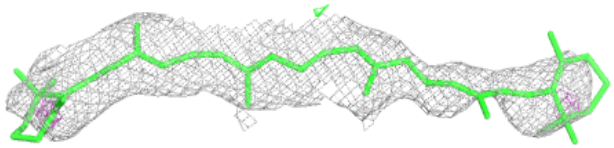


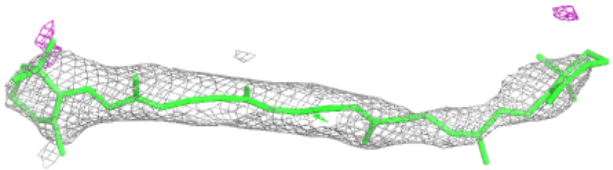


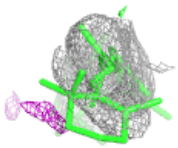


Electron density around BCR a 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

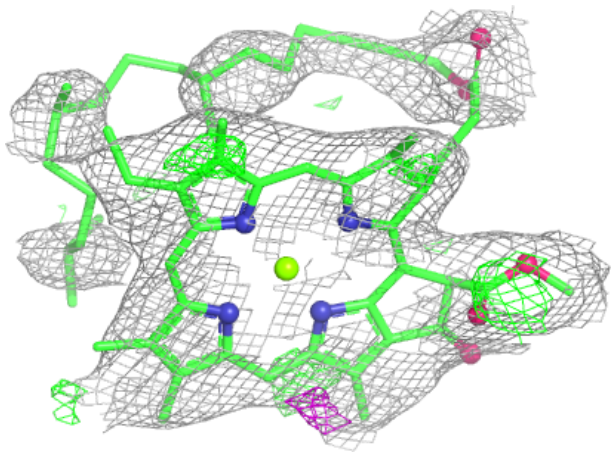


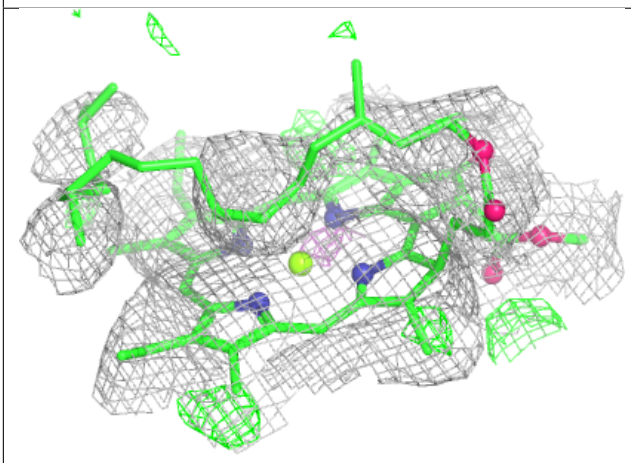


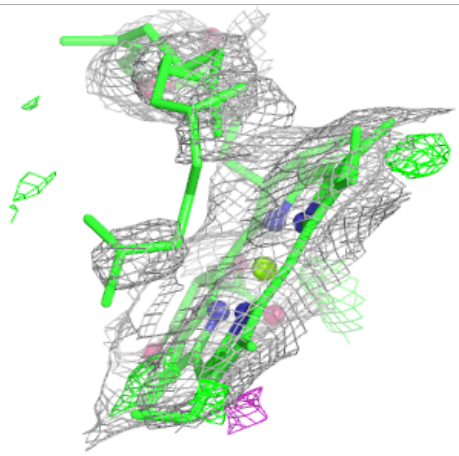


Electron density around CLA a 1118:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

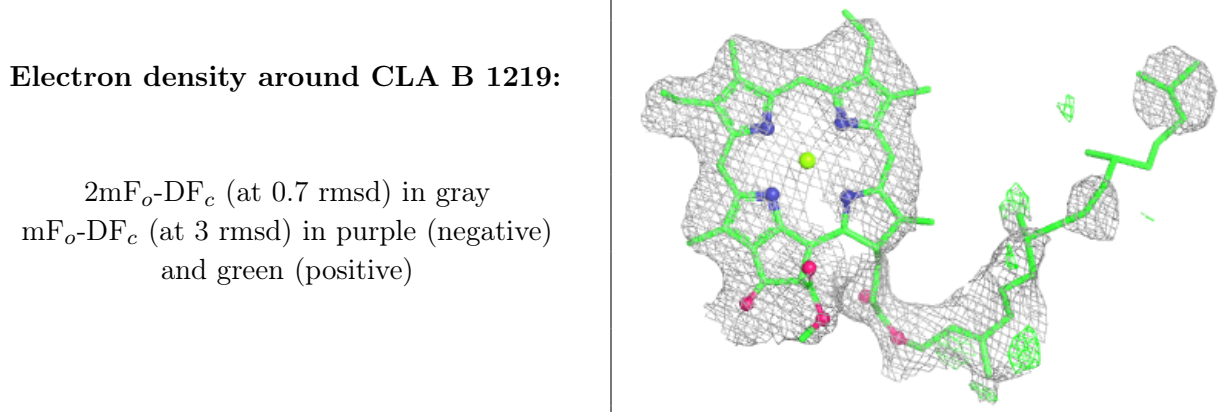






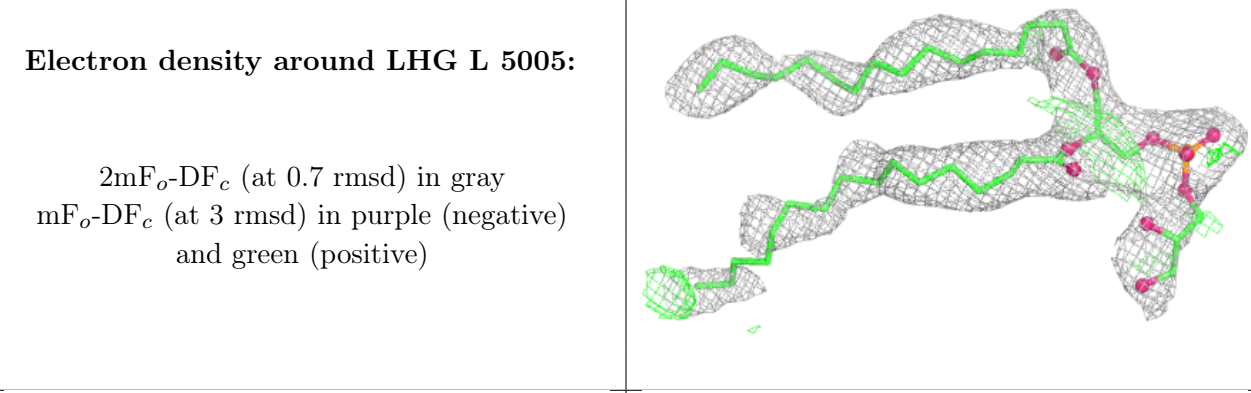
Electron density around CLA B 1219:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



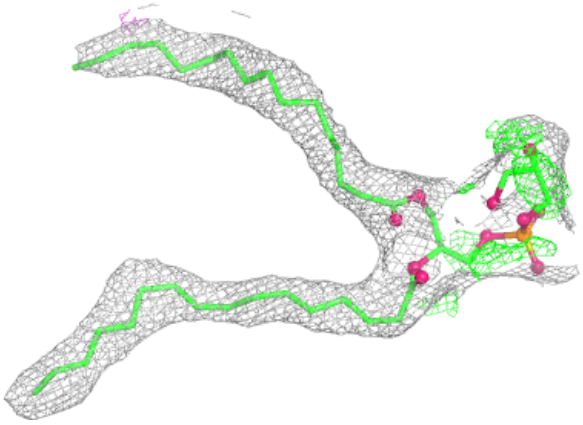
Electron density around LHG L 5005:

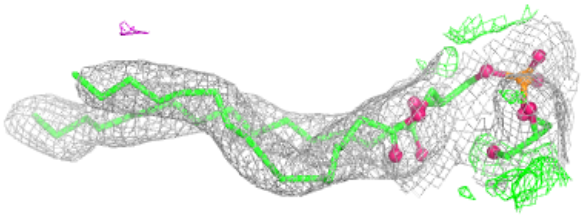
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

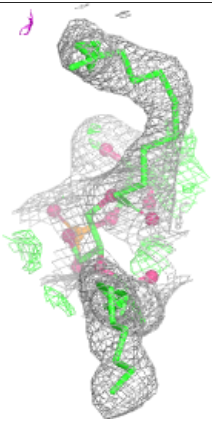


Electron density around LHG 0 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

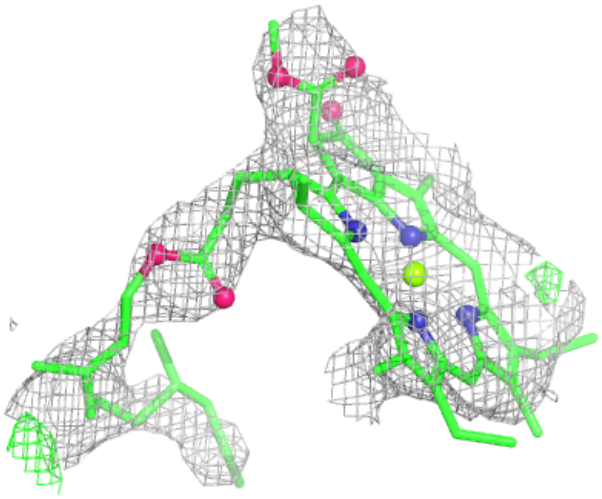


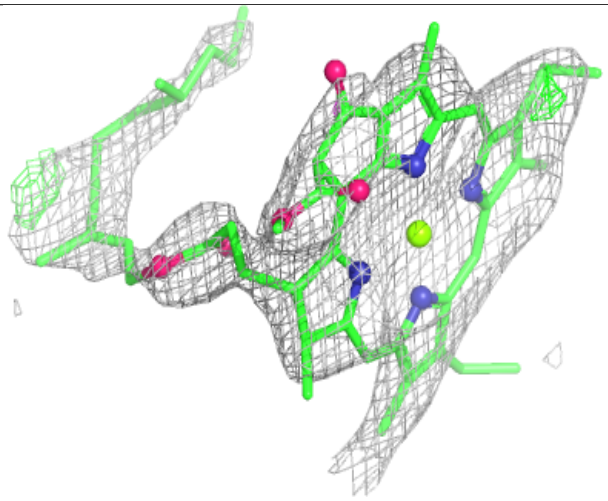


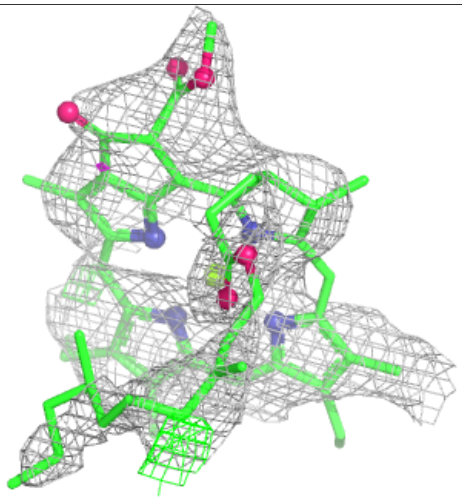


Electron density around CLA a 1108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

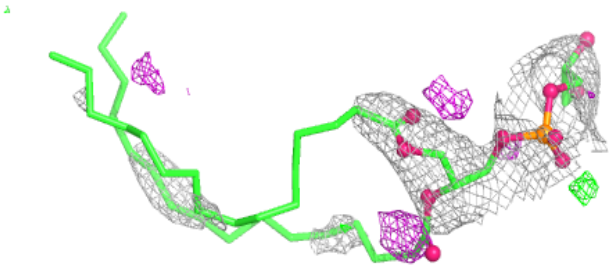


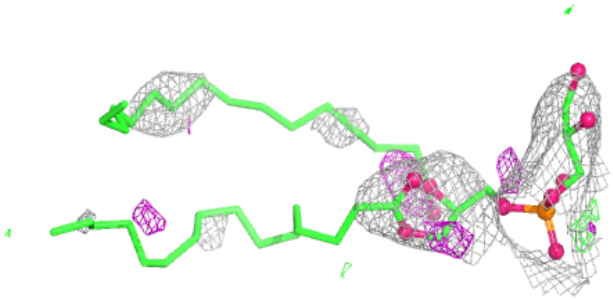


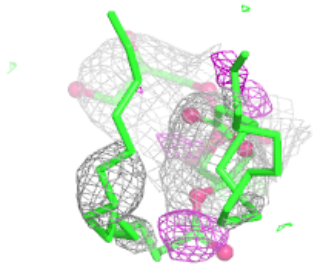


Electron density around LHG a 5003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

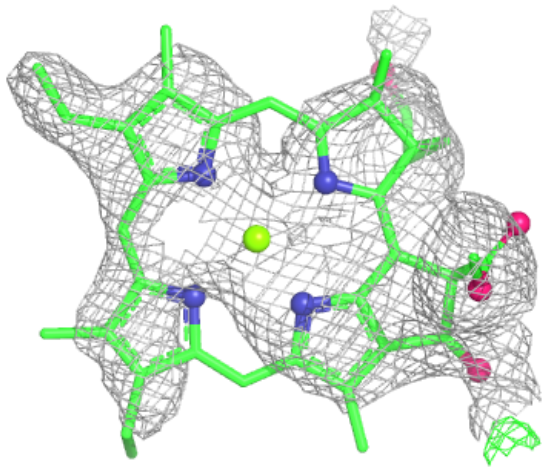


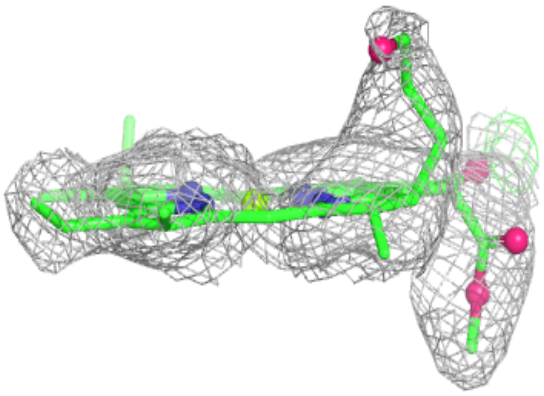


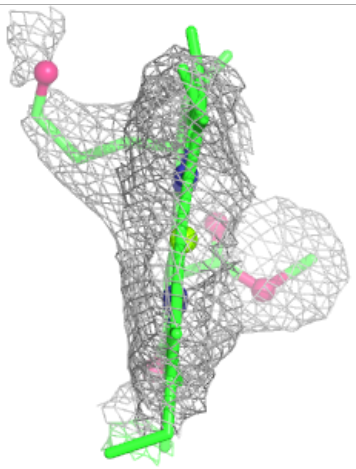


Electron density around CLA 1 1113:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

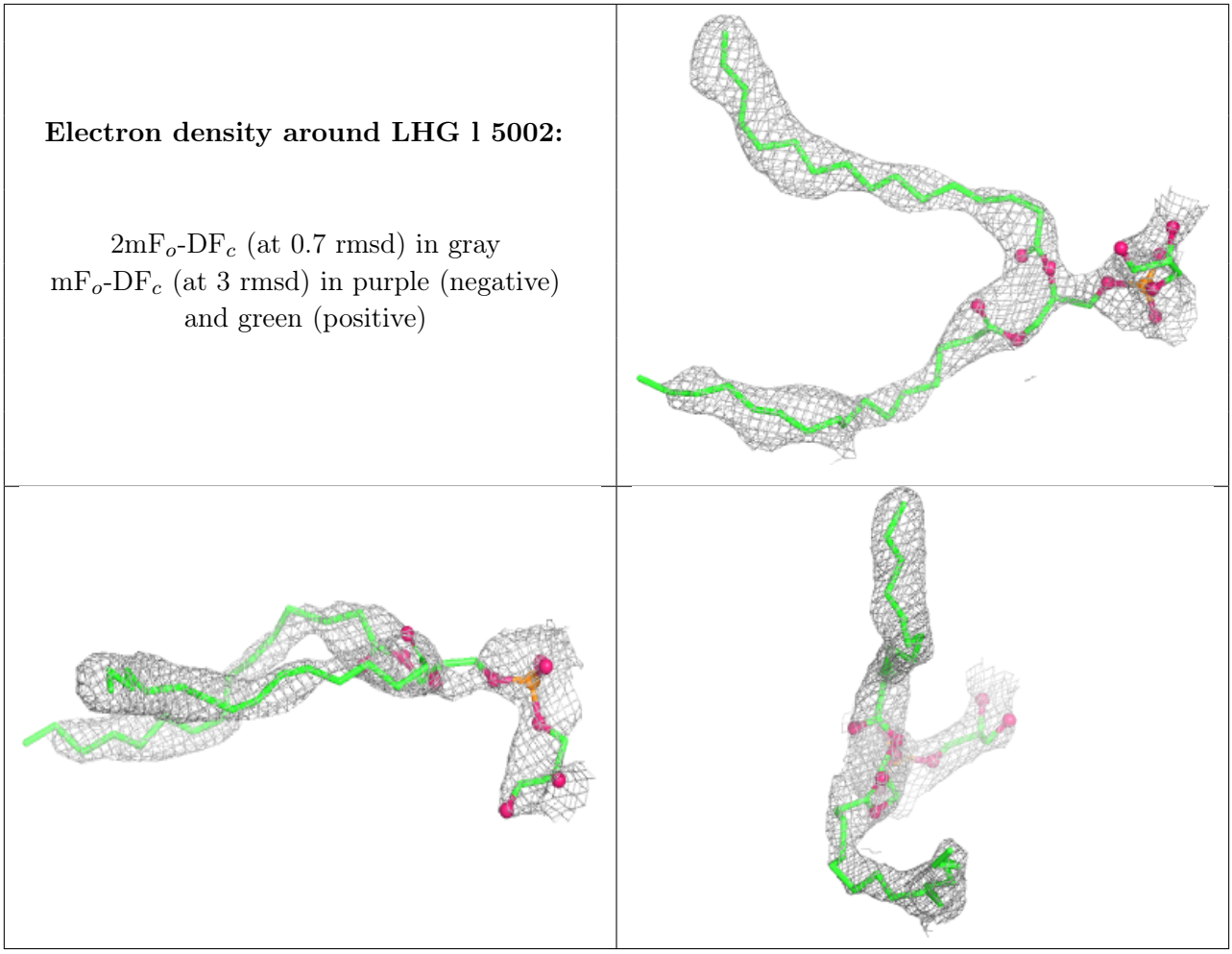






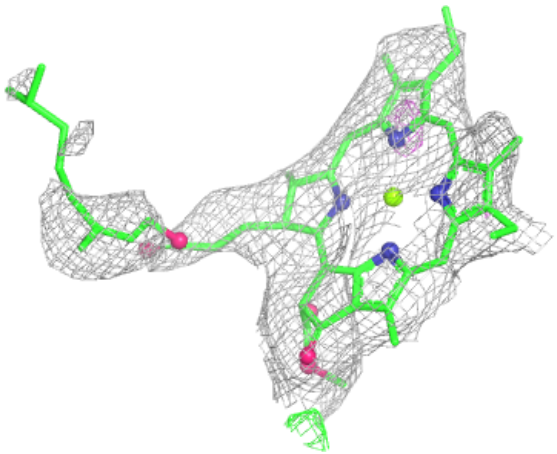
Electron density around LHG l 5002:

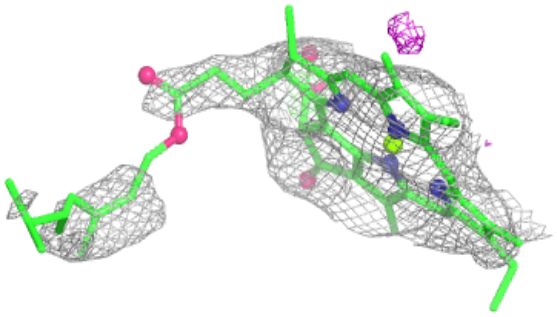
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

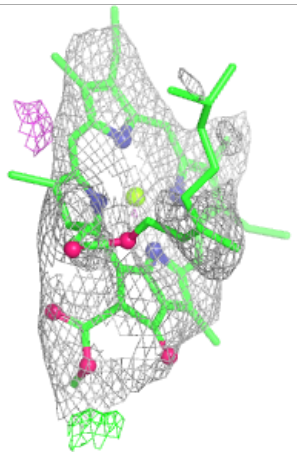


Electron density around CLA a 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

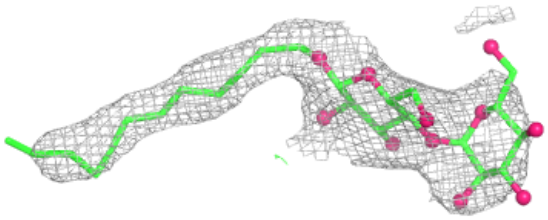


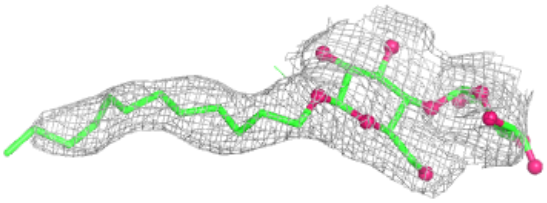


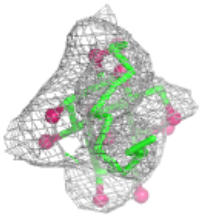


Electron density around LMT F 6001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

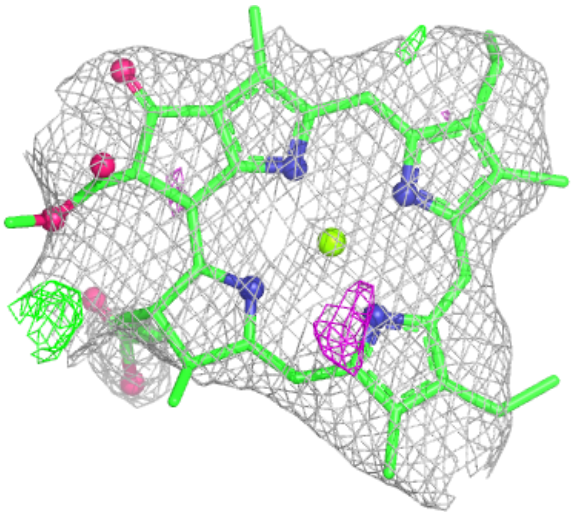


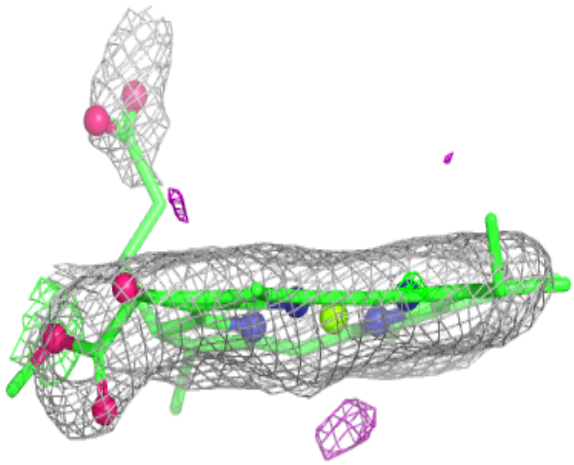


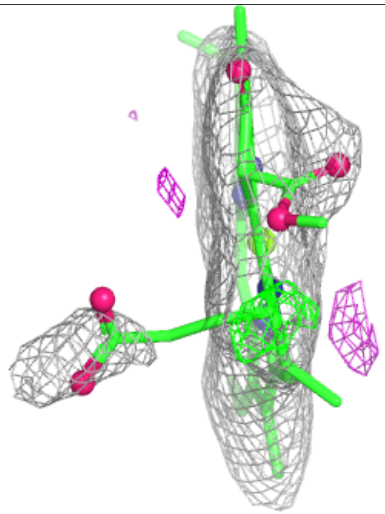


Electron density around CLA 2 1227:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

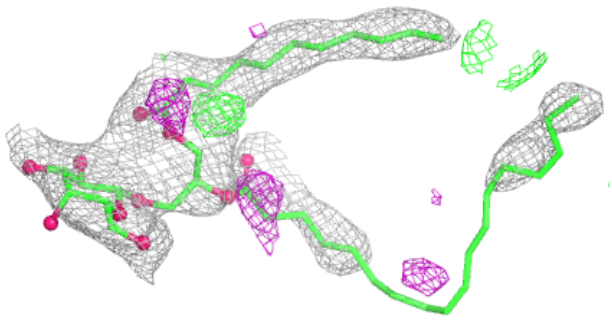


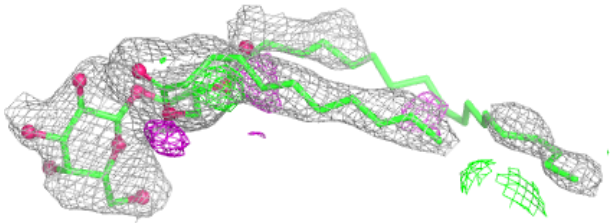


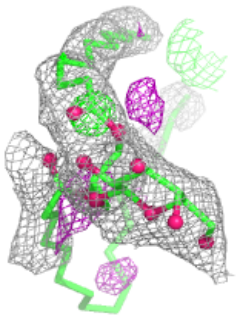


Electron density around LMG A 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

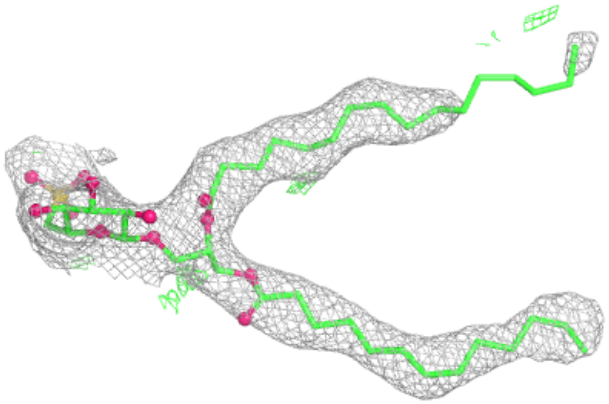


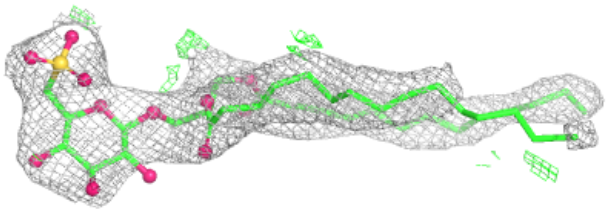


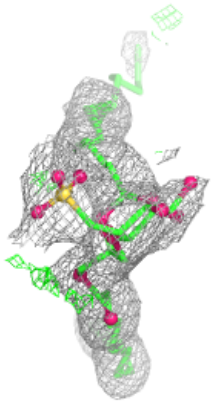


Electron density around SQD L 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

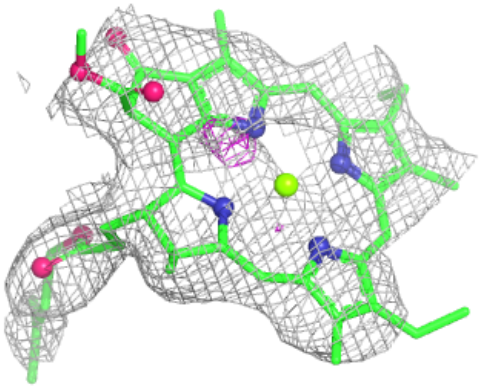


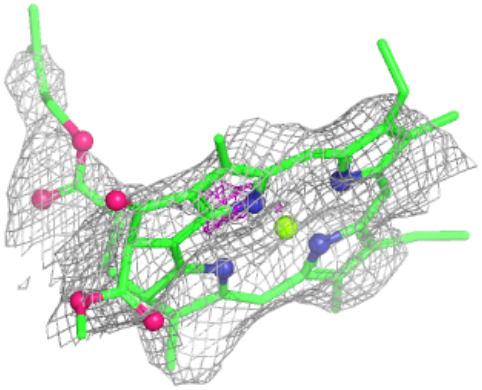


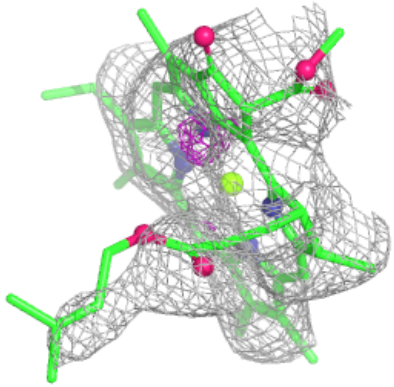


Electron density around CLA 1 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

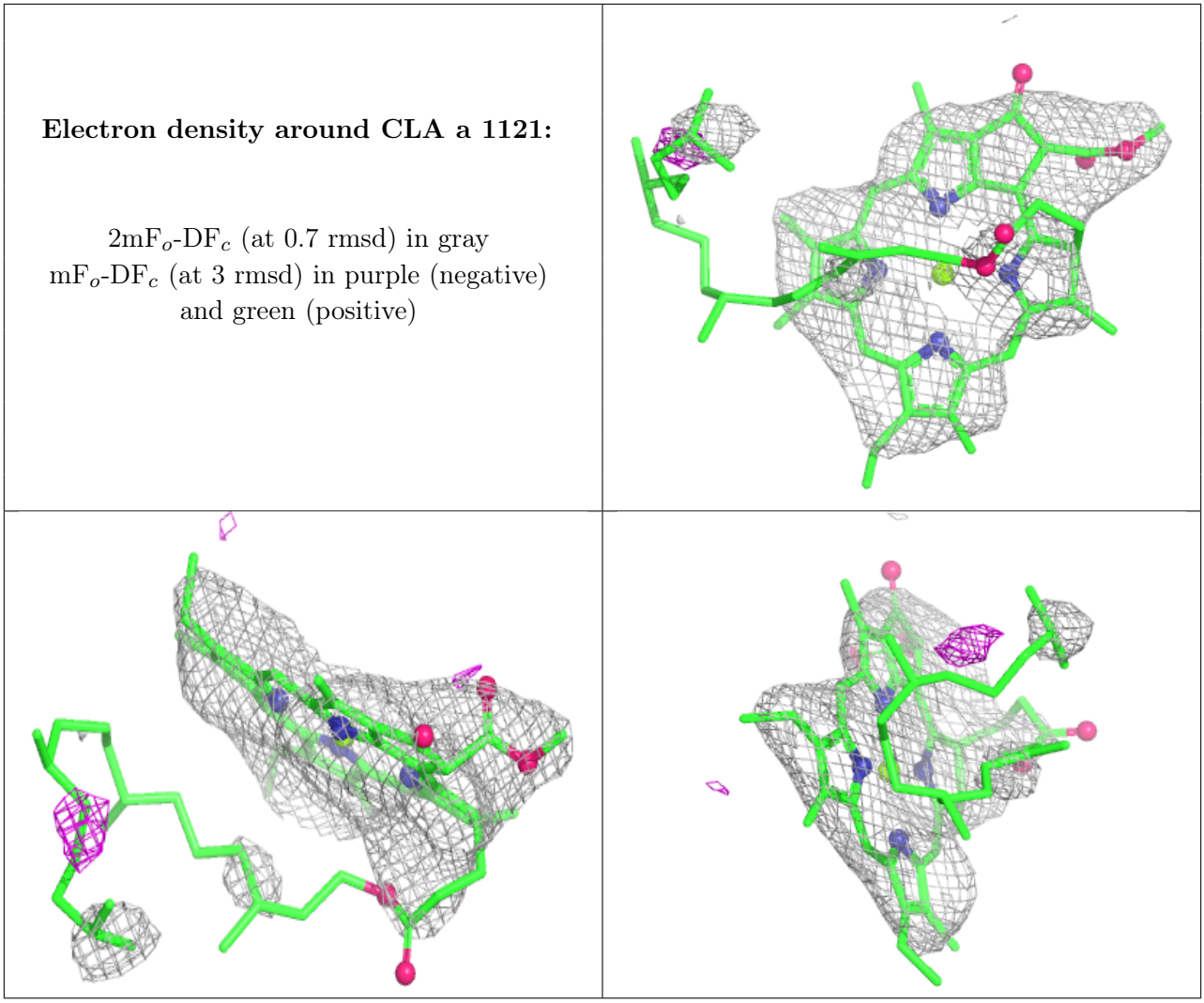






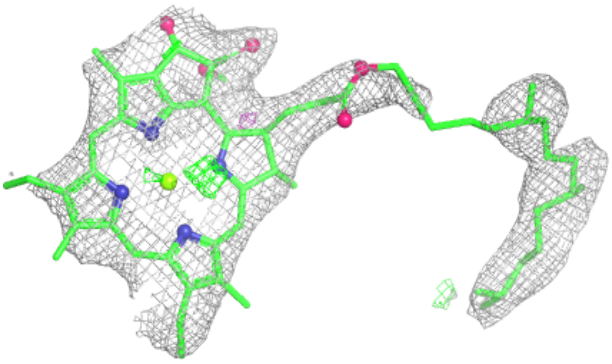
Electron density around CLA a 1121:

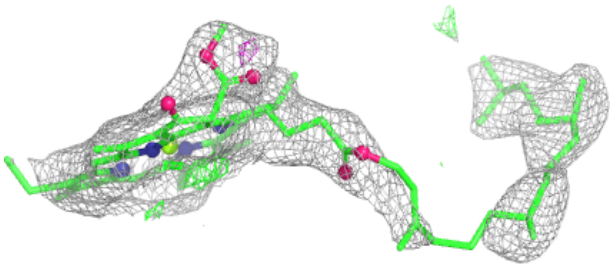
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

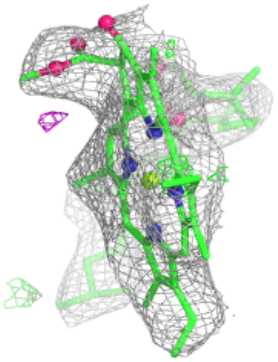


Electron density around CLA a 1125:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

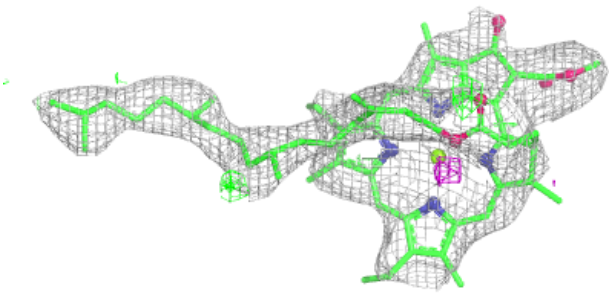


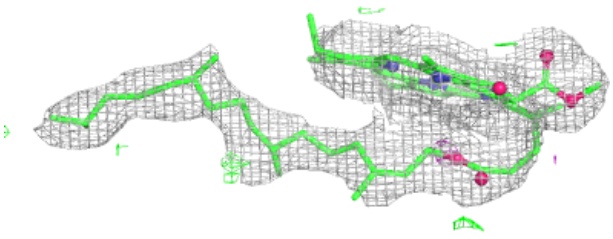


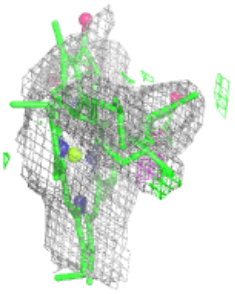


Electron density around CLA 1 1115:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

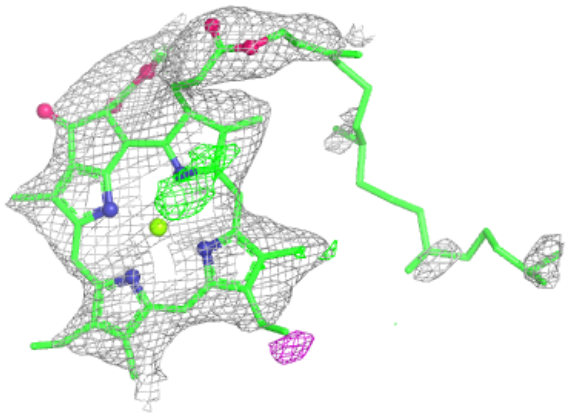


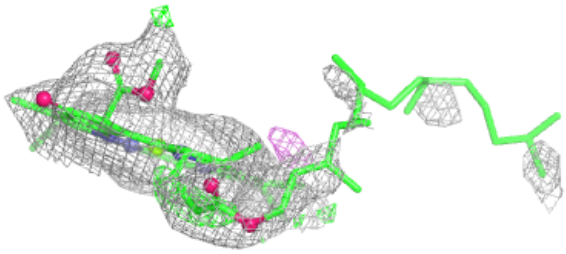


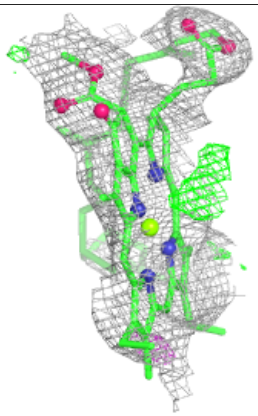


Electron density around CLA a 1111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

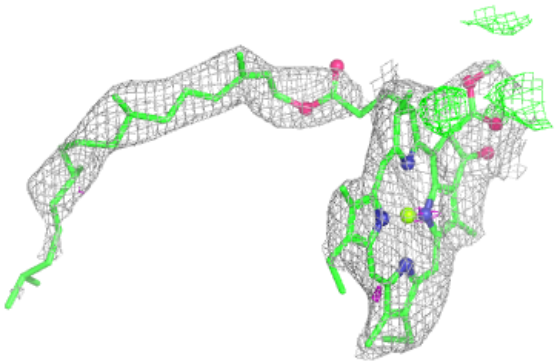


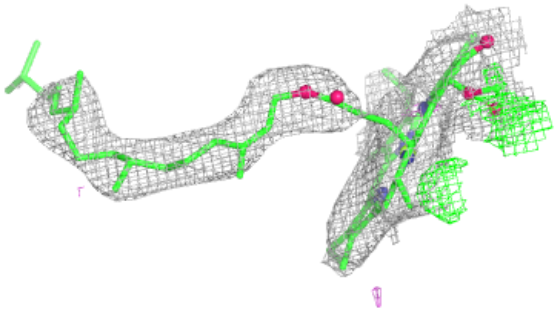


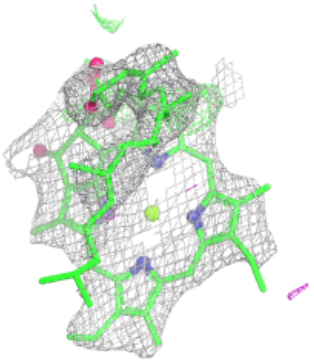


Electron density around CLA a 1133:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

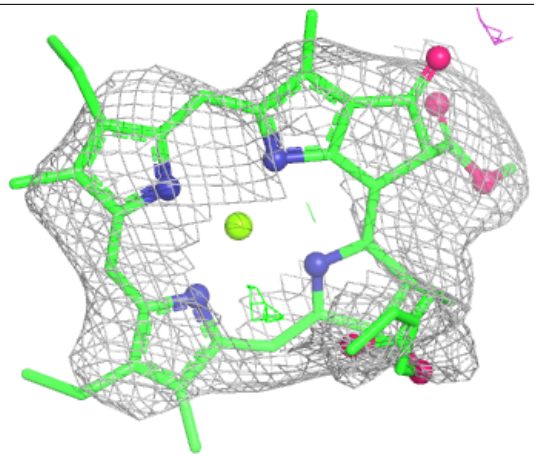


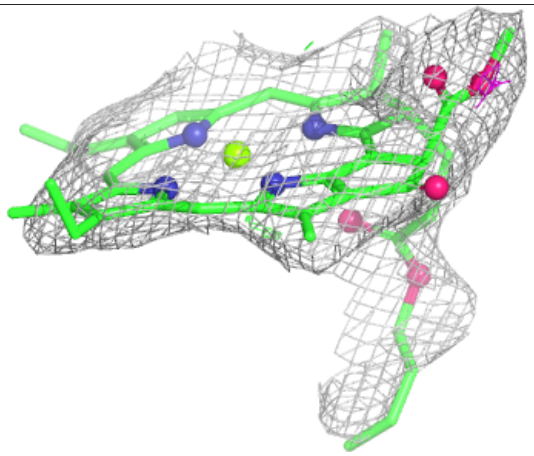


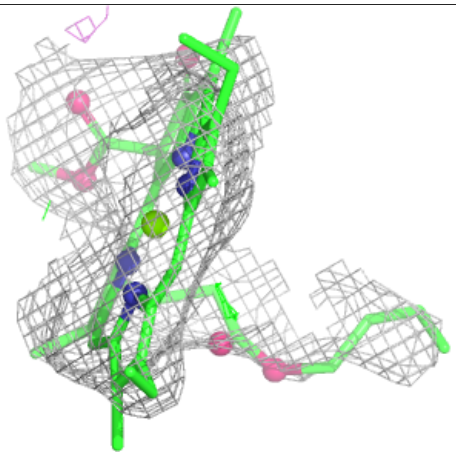


Electron density around CLA a 1134:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

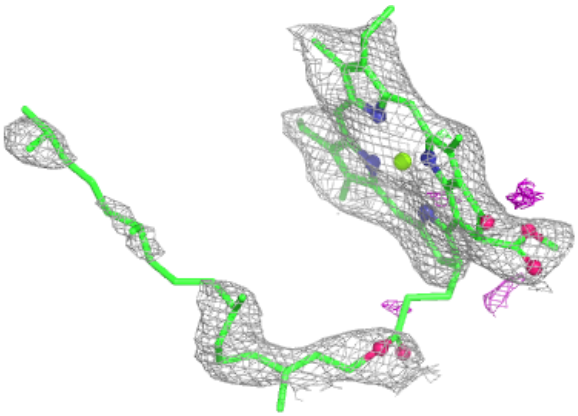


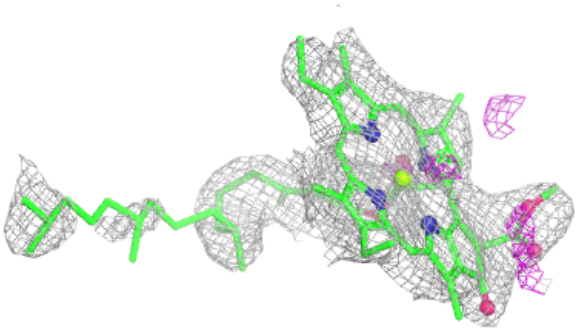


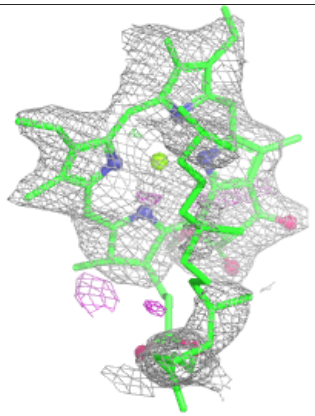


Electron density around CLA a 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

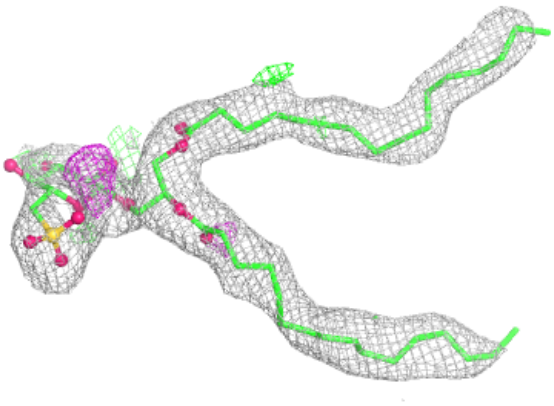


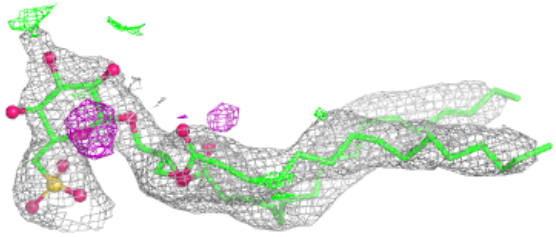


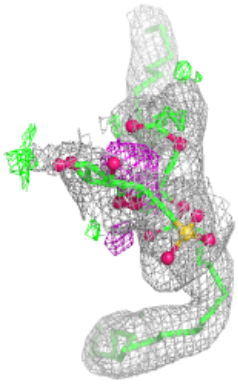


Electron density around SQD L 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

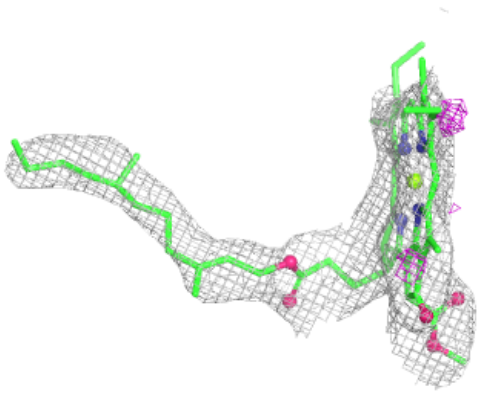


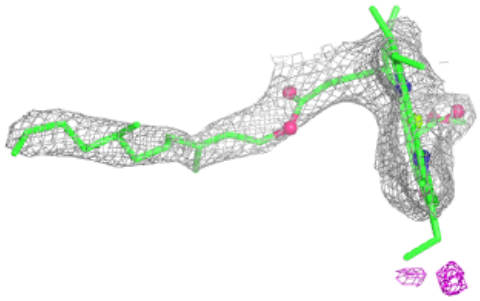


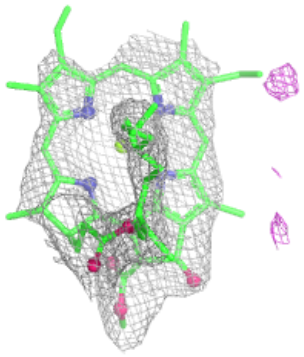


Electron density around CLA a 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

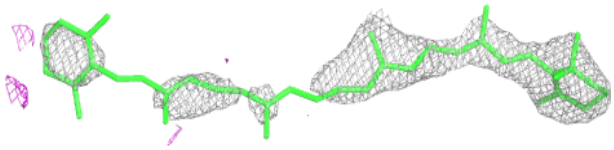


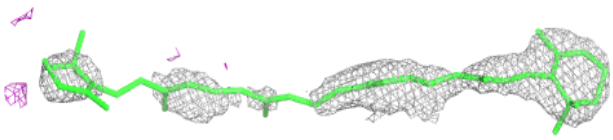


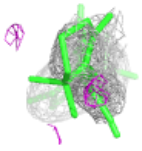


Electron density around BCR 1 4007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

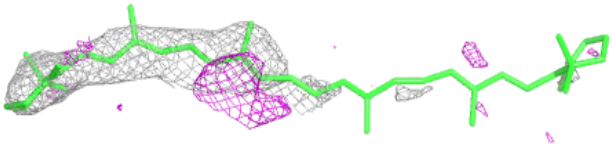


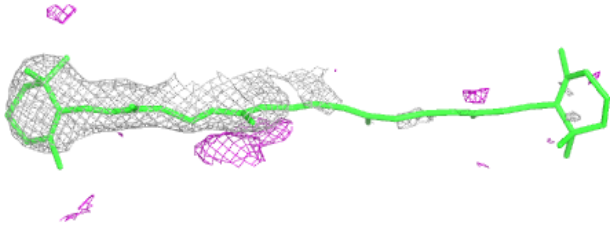


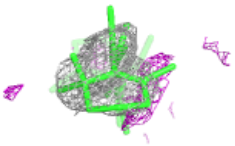


Electron density around BCR a 4007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

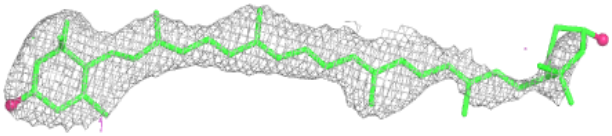


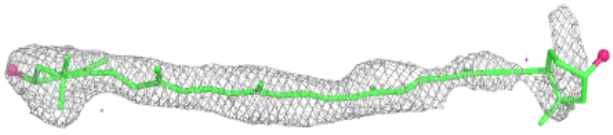


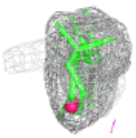


Electron density around ZEX J 4015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

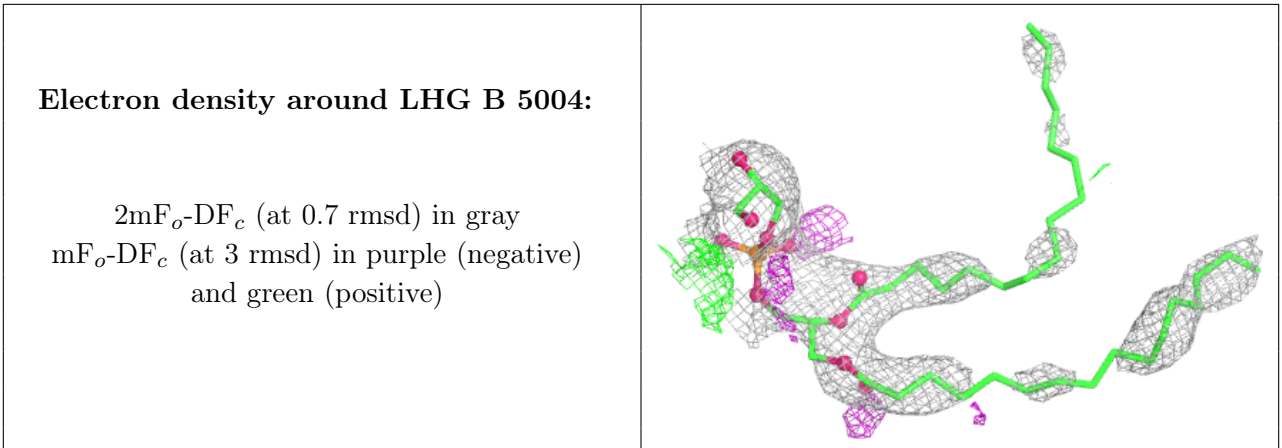






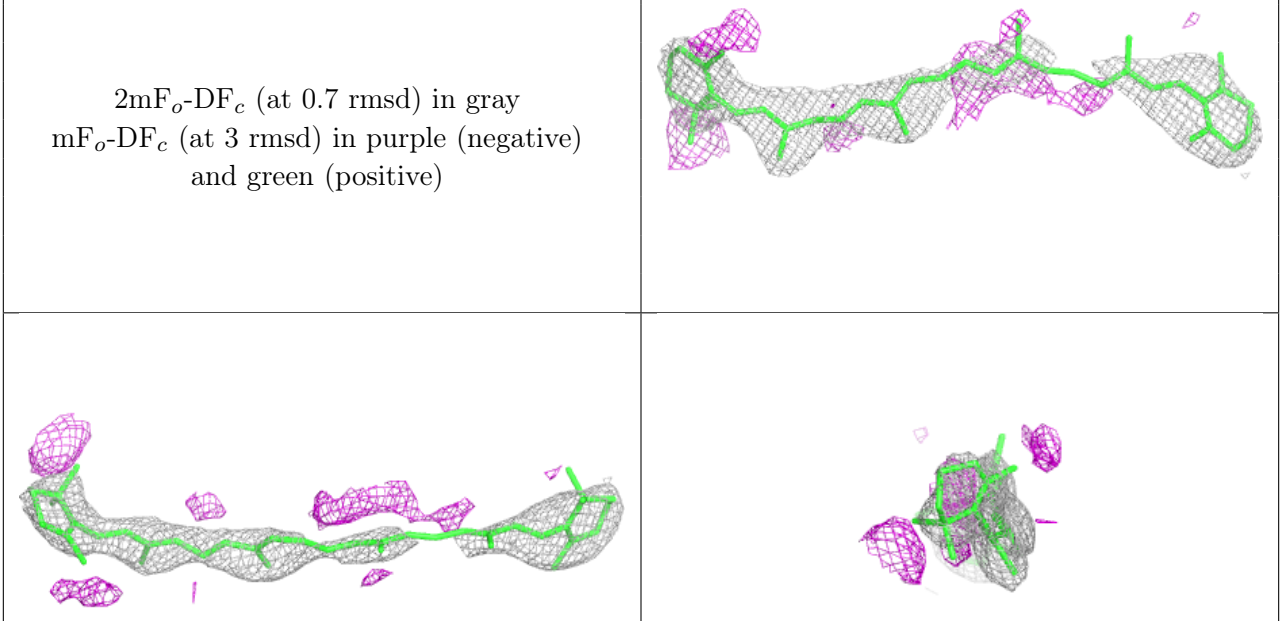
Electron density around LHG B 5004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



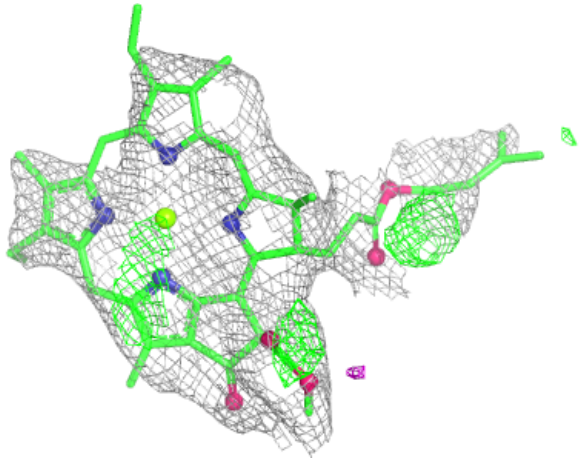
Electron density around BCR a 4008:

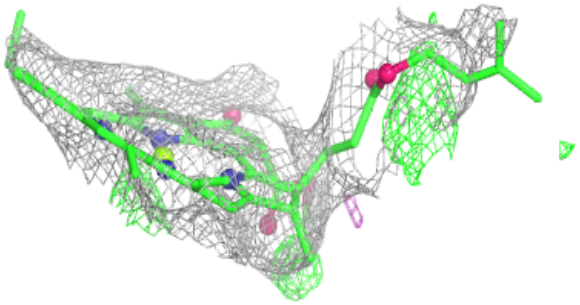
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

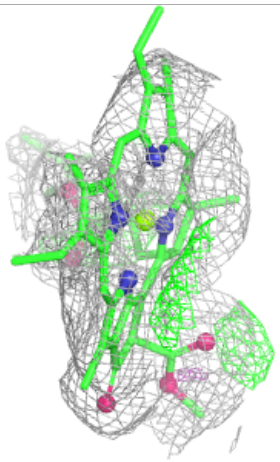


Electron density around CLA 2 1222:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

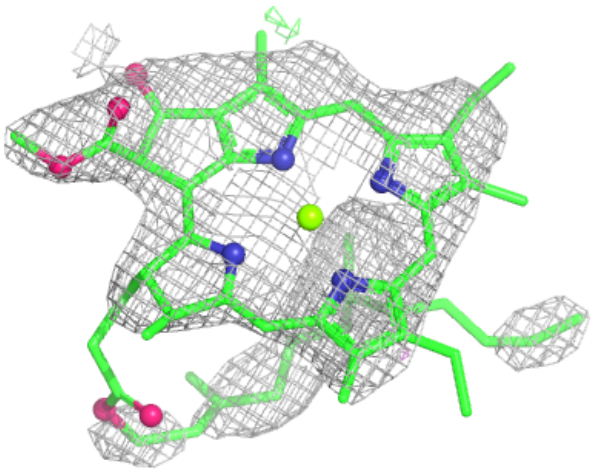


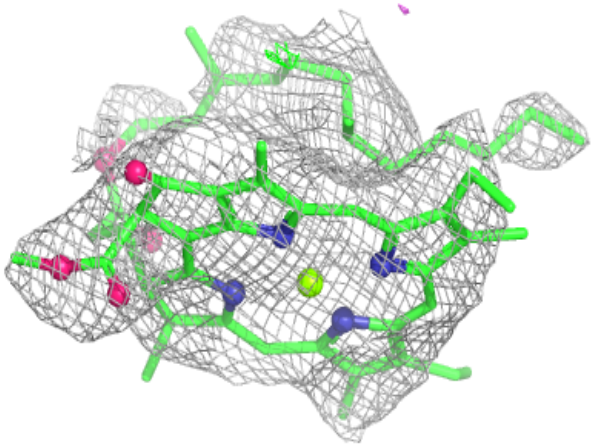


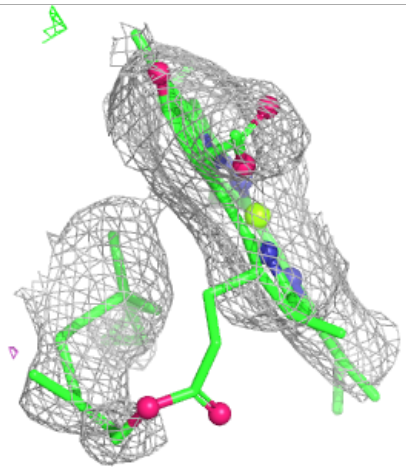


Electron density around CLA 2 1214:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

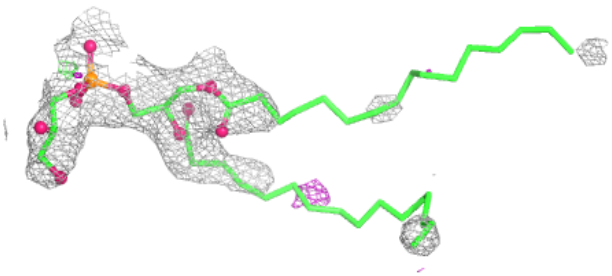


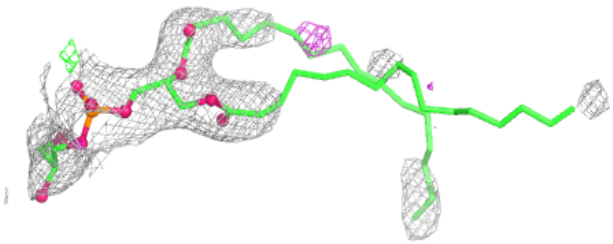


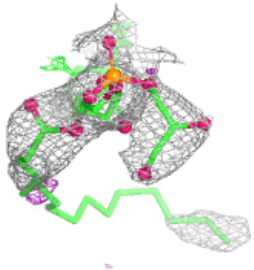


Electron density around LHG 1 5003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

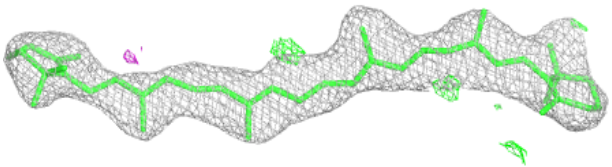


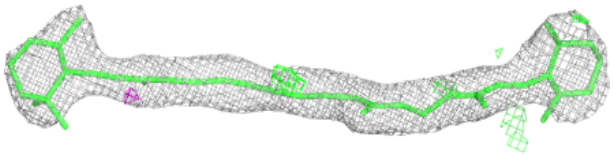


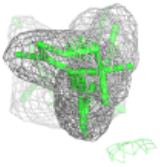


Electron density around BCR L 4022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

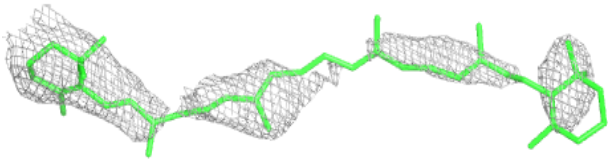


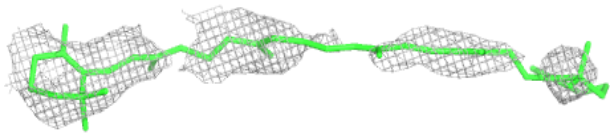


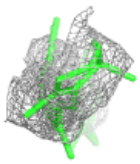


Electron density around BCR 1 4012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

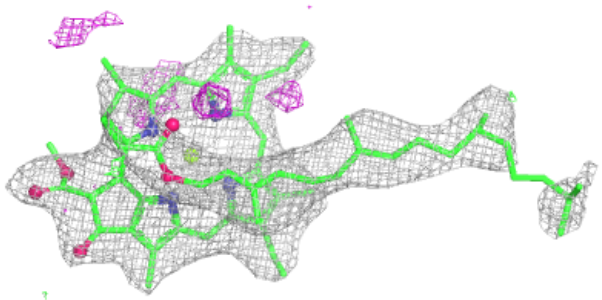


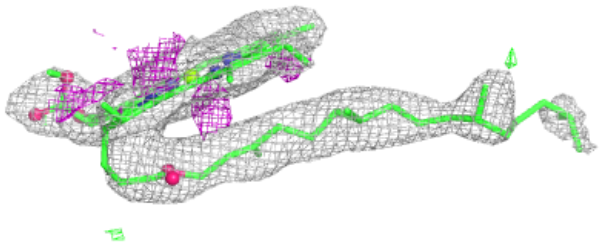


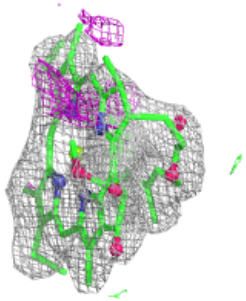


Electron density around CLA b 1213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

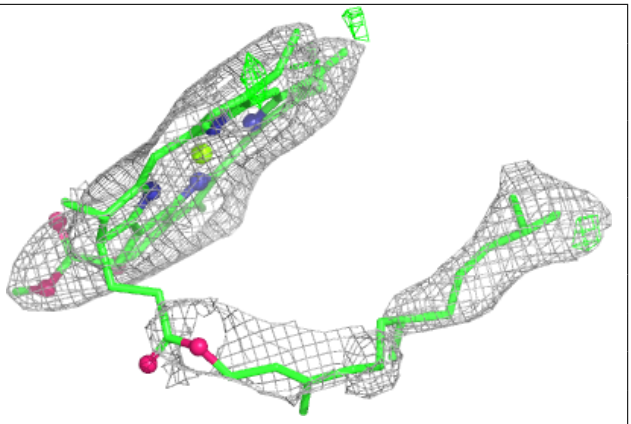


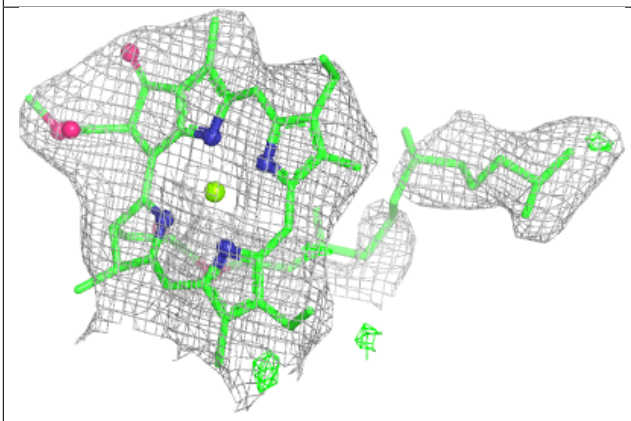


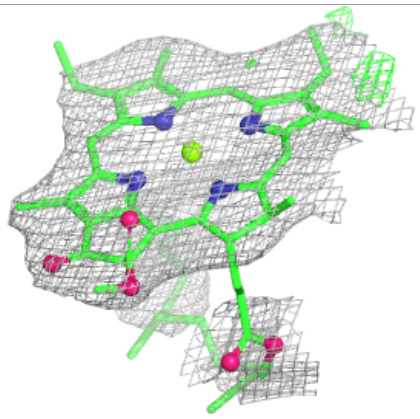


Electron density around CLA 2 1208:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

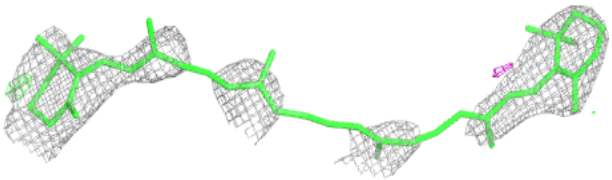


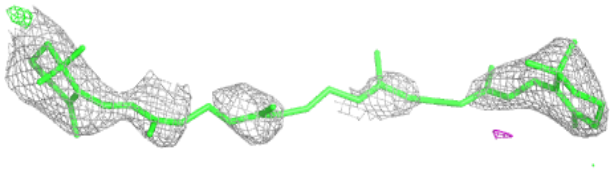


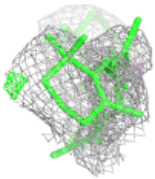


Electron density around BCR 2 4010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

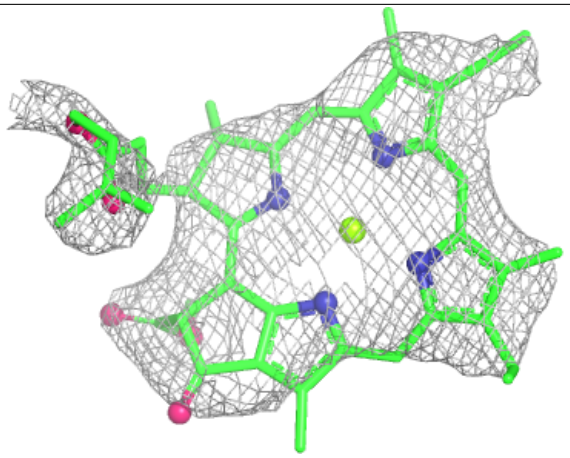


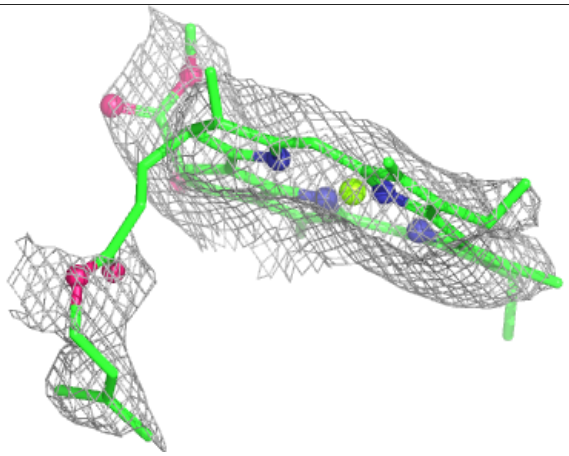


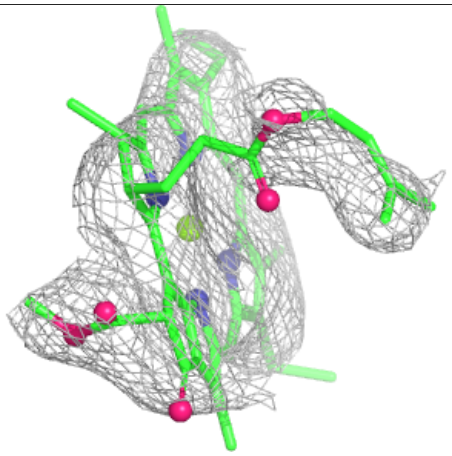


Electron density around CLA 1 1112:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

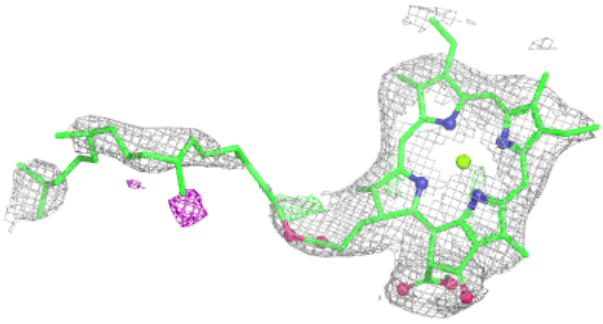


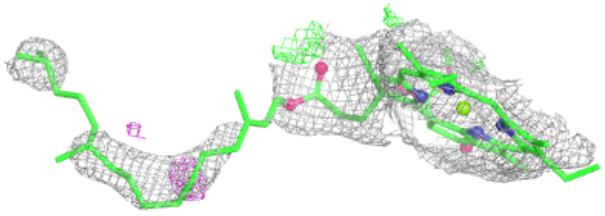


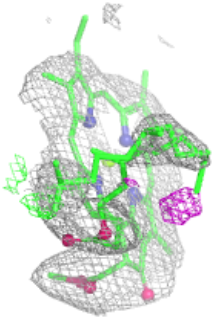


Electron density around CLA 2 1210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

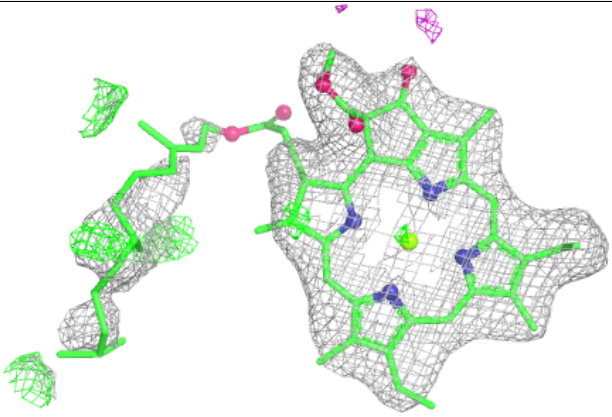


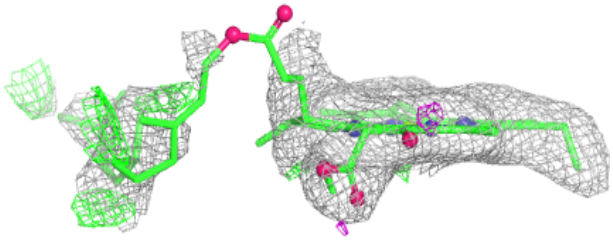


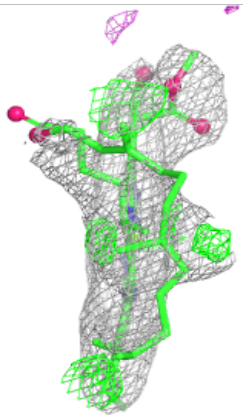


Electron density around CLA b 1219:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

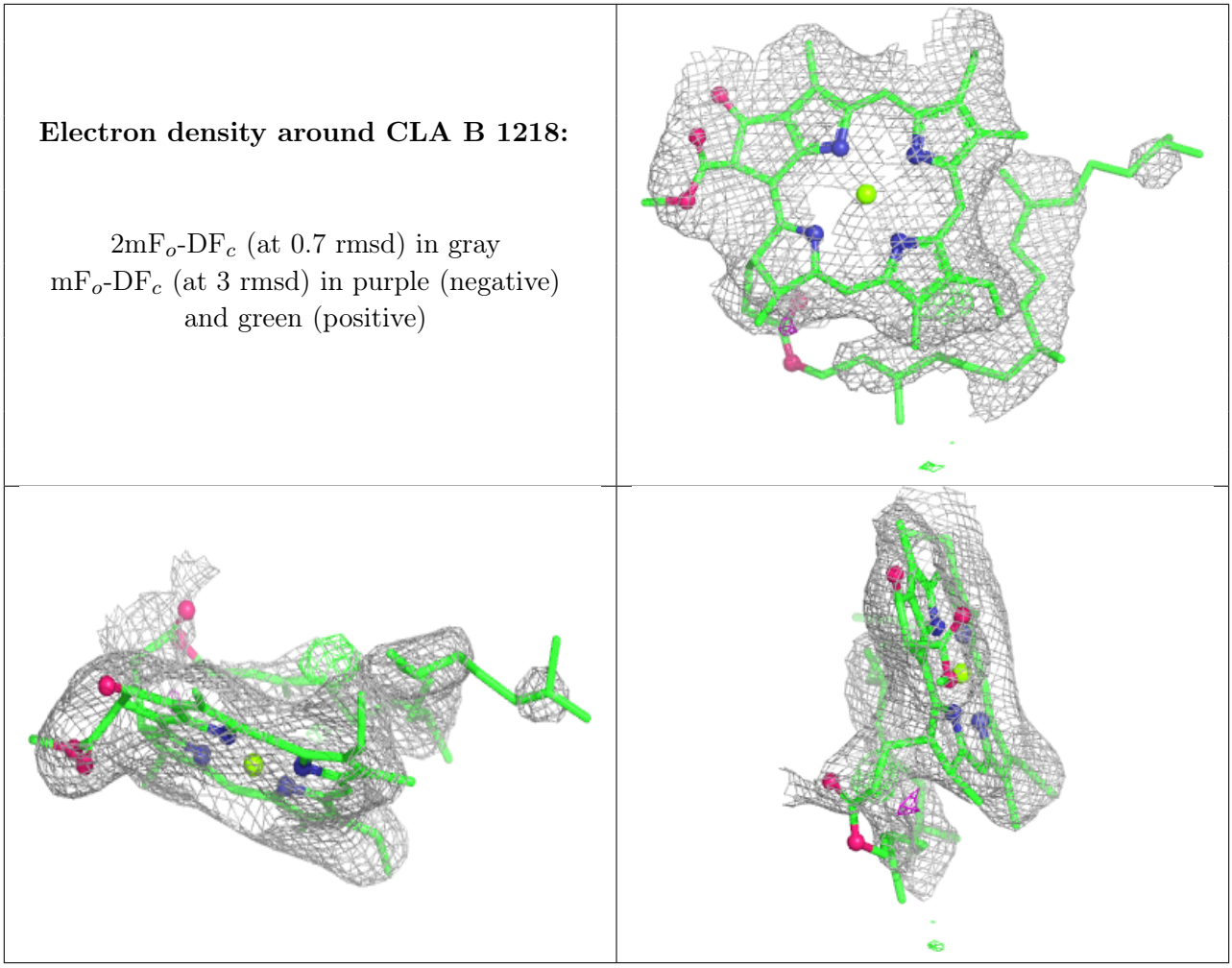






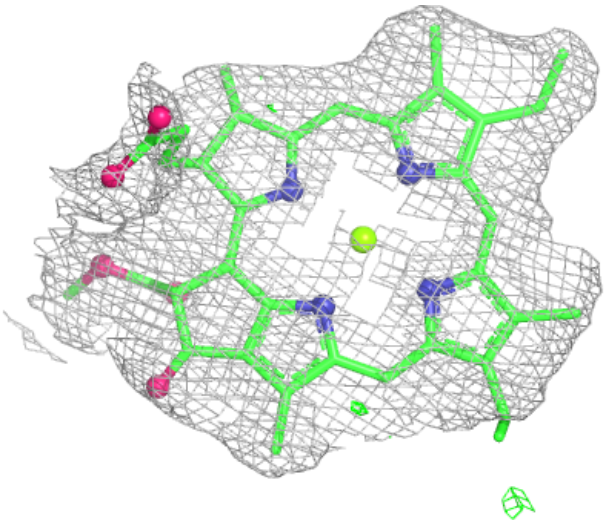
Electron density around CLA B 1218:

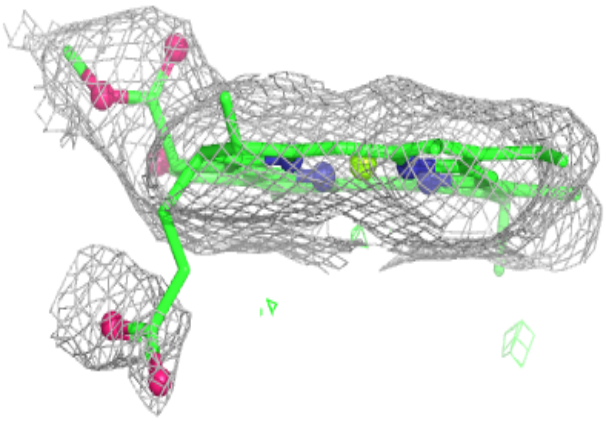
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

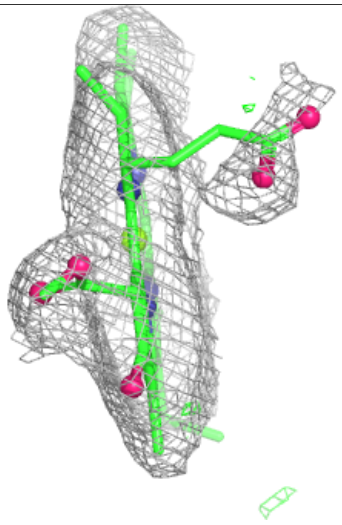


Electron density around CLA 8 1401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

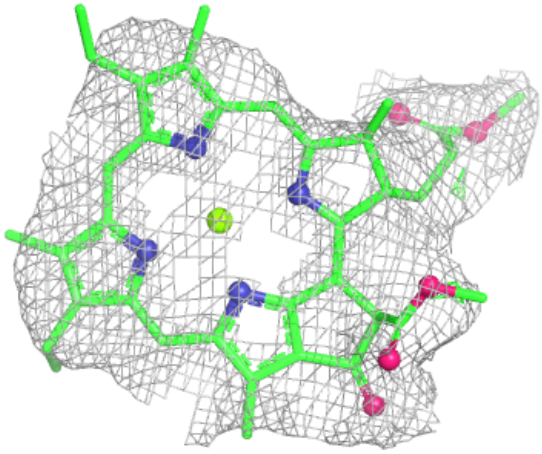


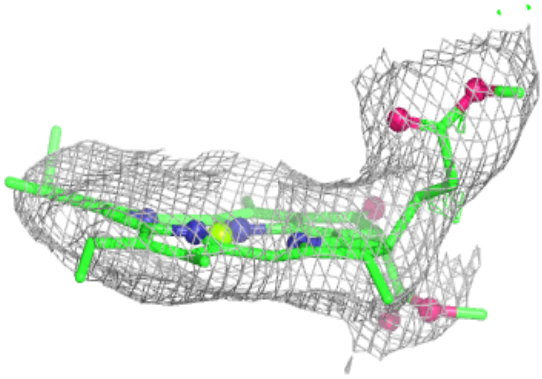


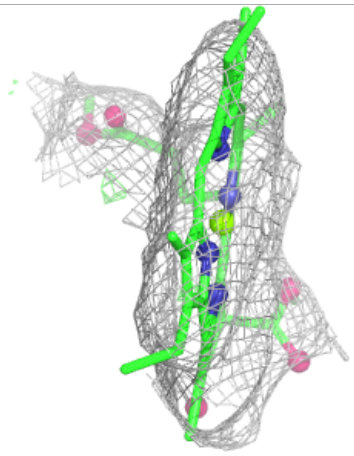


Electron density around CLA 8 1402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

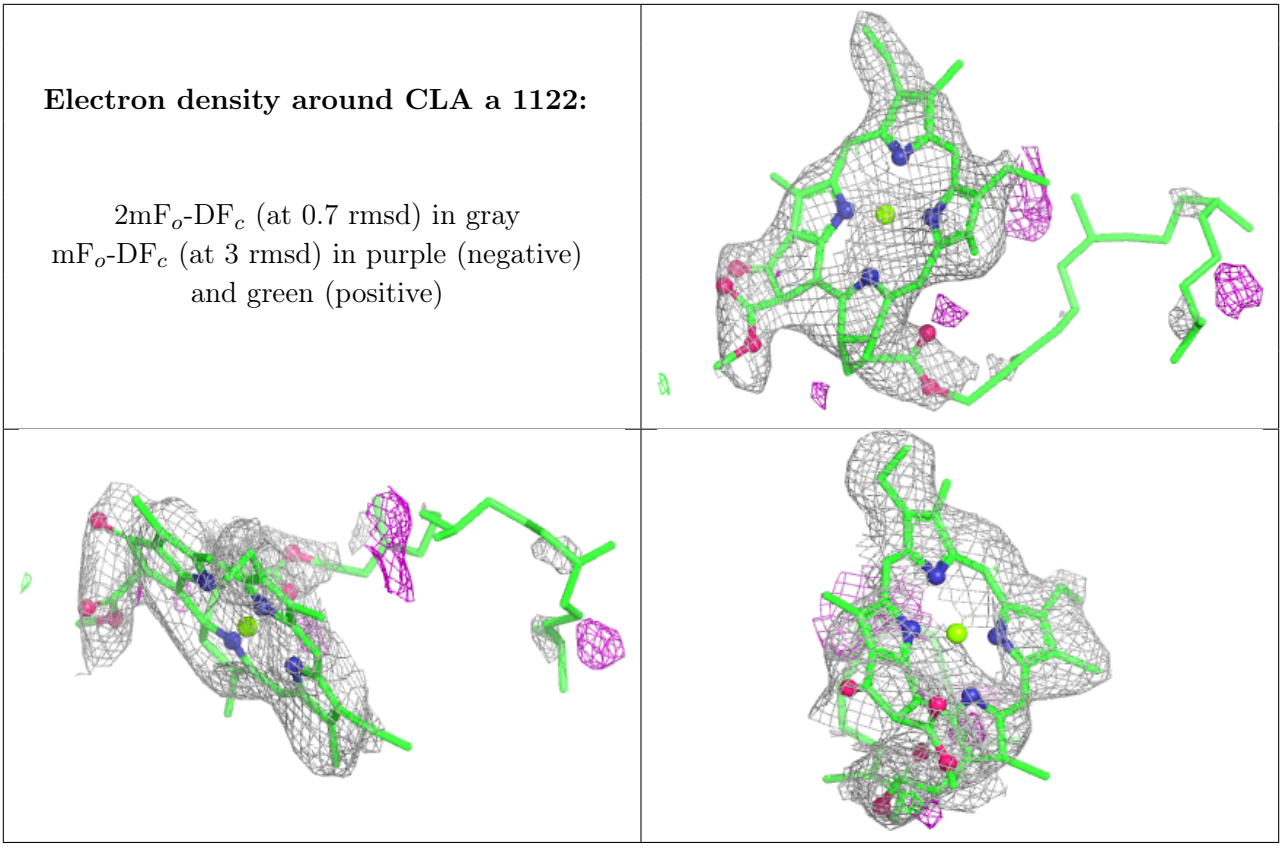






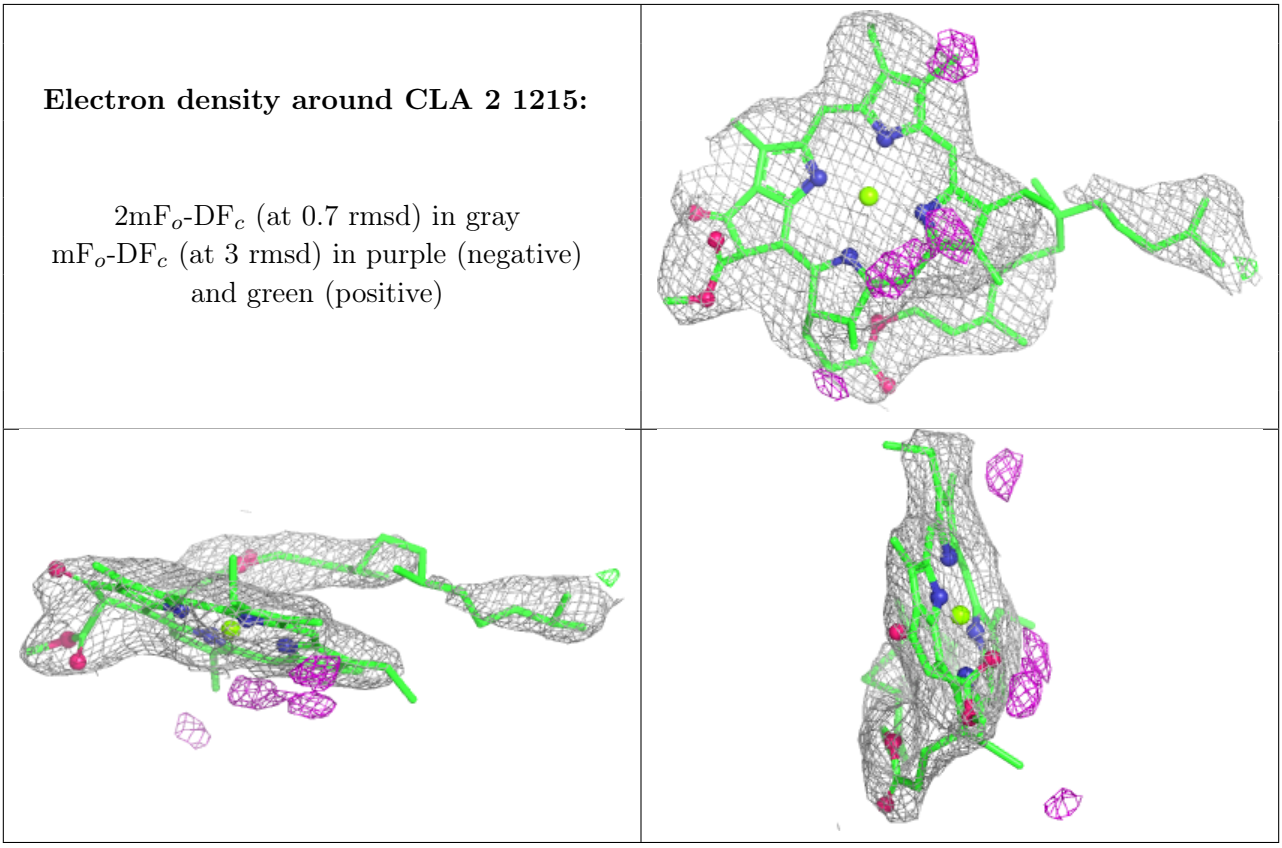
Electron density around CLA a 1122:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



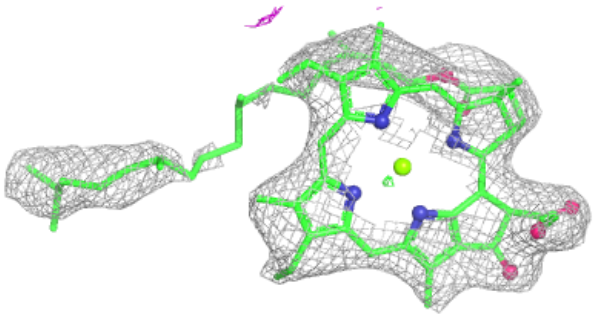
Electron density around CLA 2 1215:

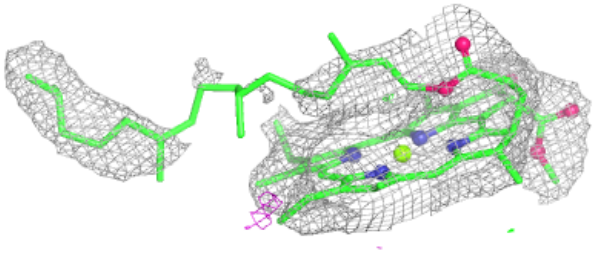
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 1217:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

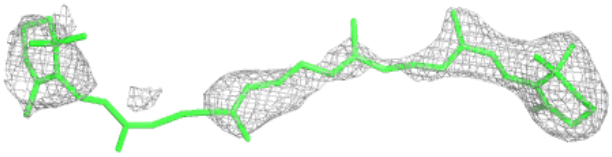


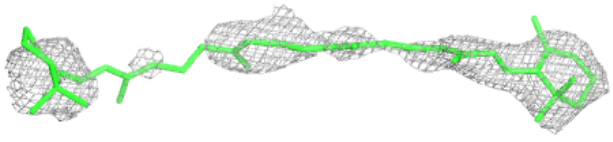


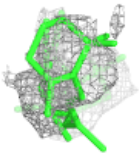


Electron density around BCR 1 4003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

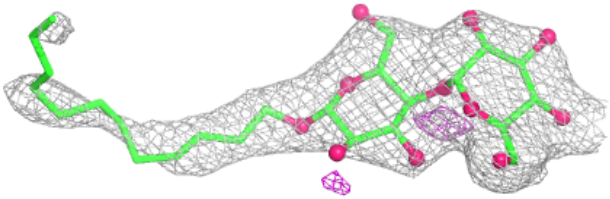


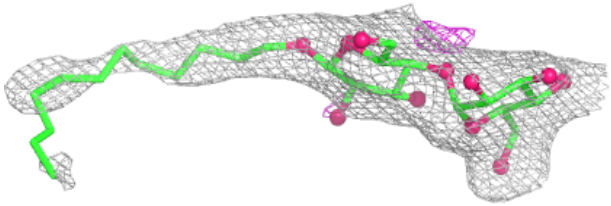


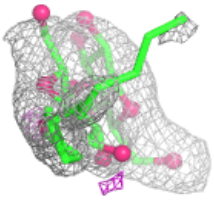


Electron density around LMT 0 6001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

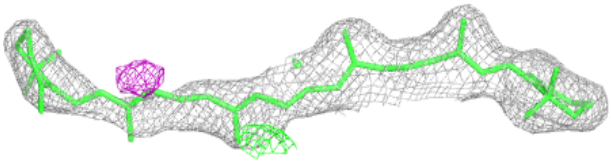


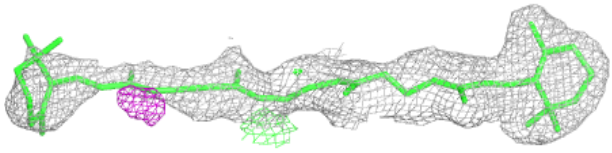


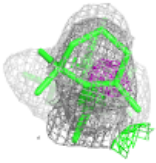


Electron density around BCR K 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



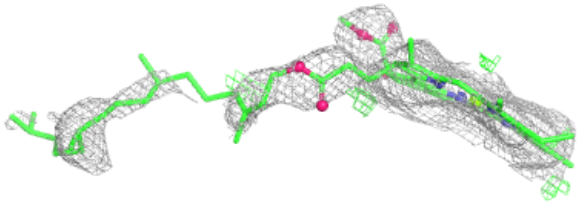


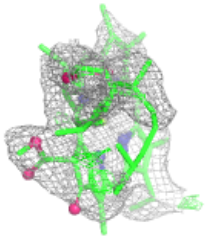


Electron density around CLA 1 1139:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

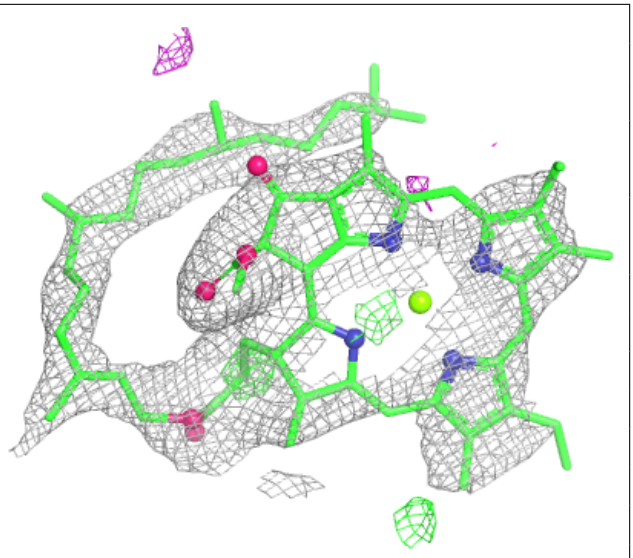


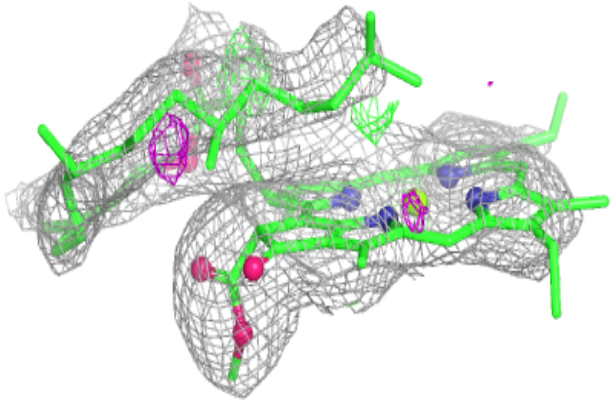


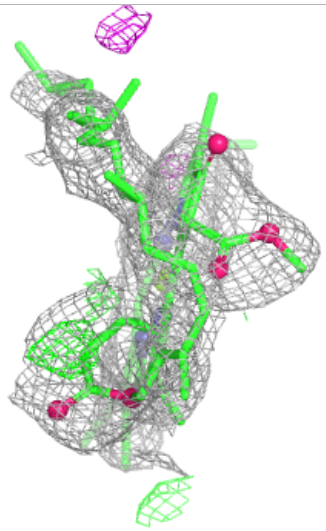


Electron density around CLA 2 1202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

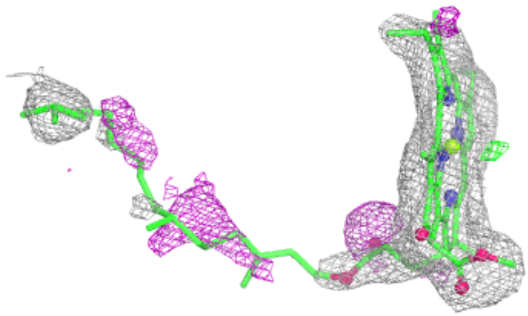


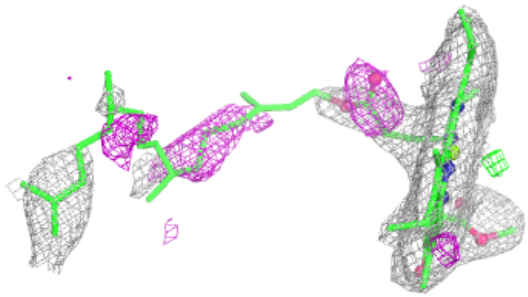


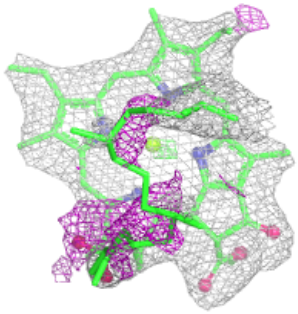


Electron density around CLA A 1113:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

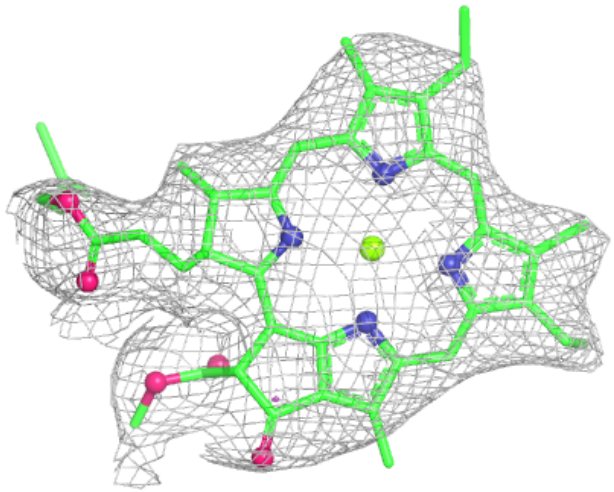


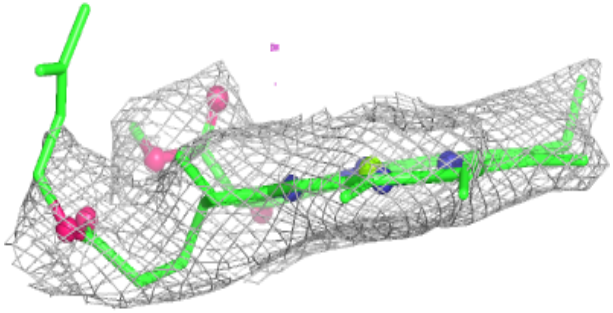


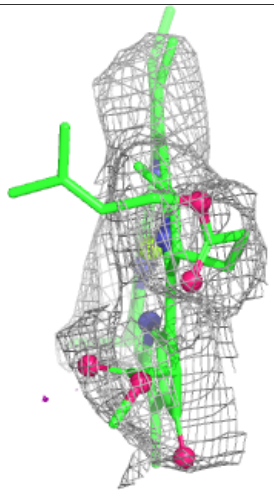


Electron density around CLA f 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

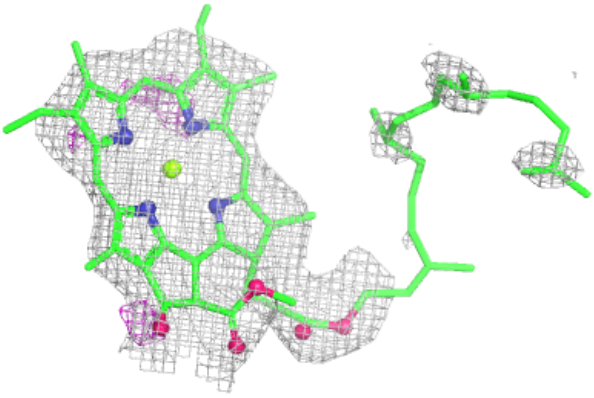


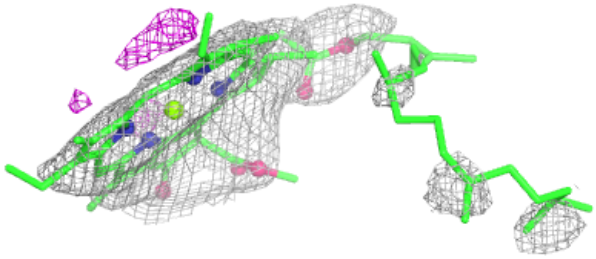


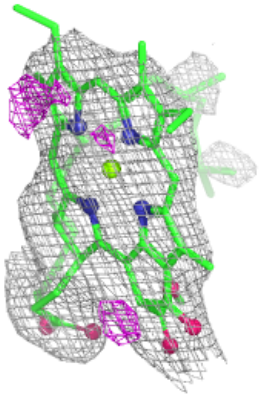


Electron density around CLA 2 1221:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

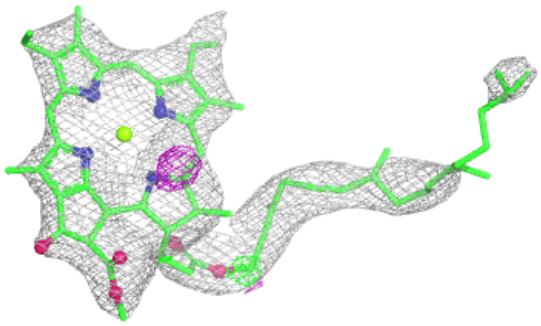


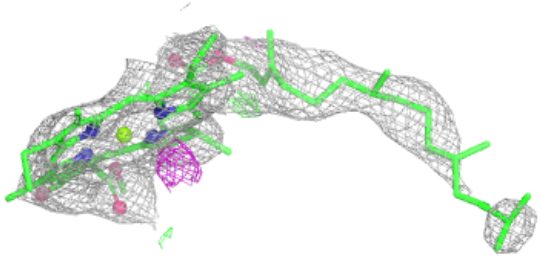




Electron density around CLA 1 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

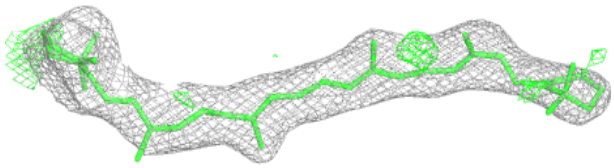


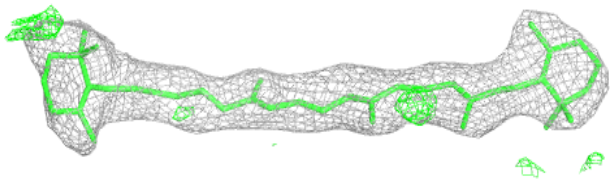


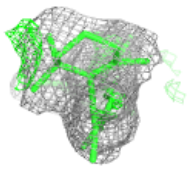


Electron density around BCR 0 4022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

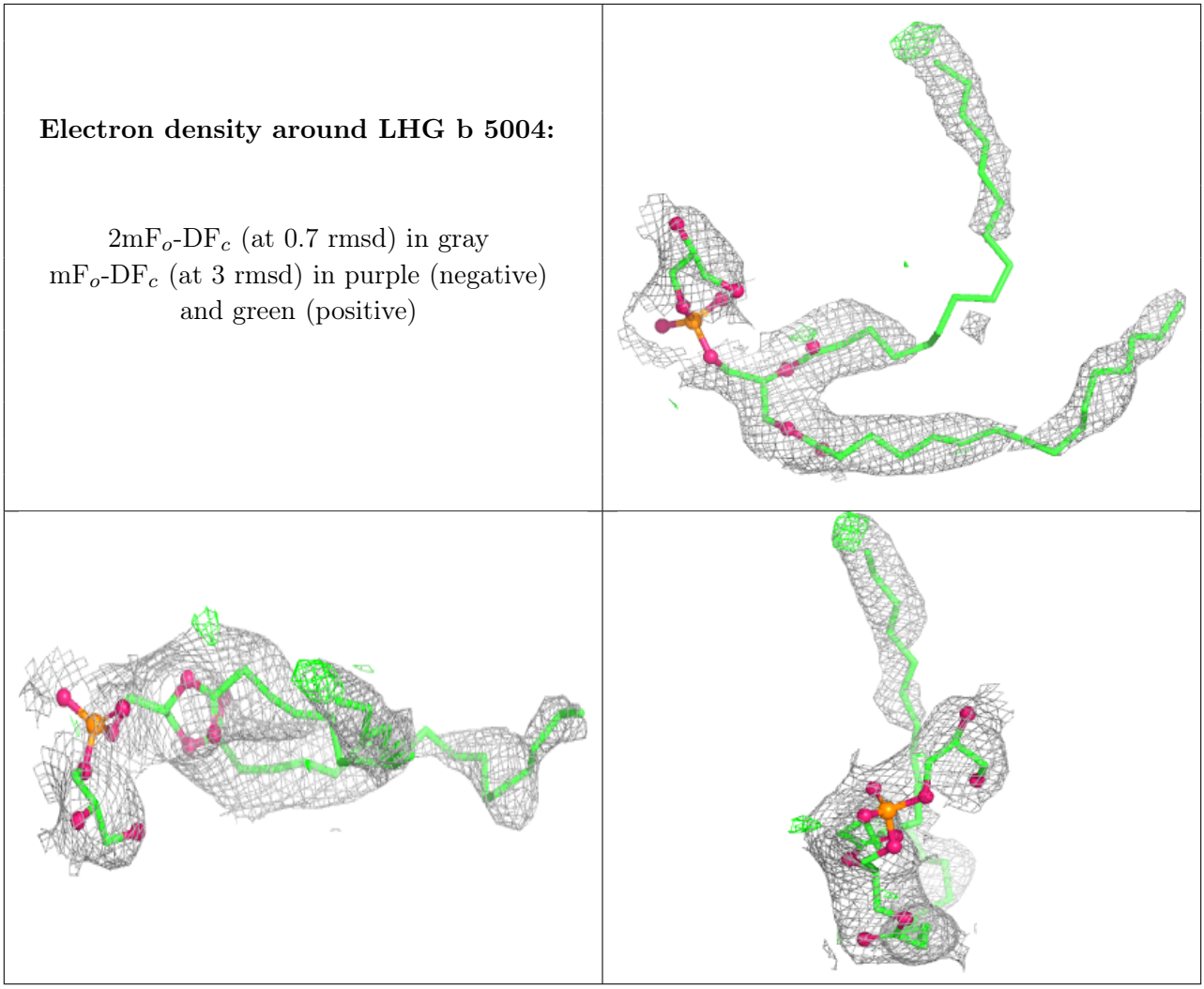






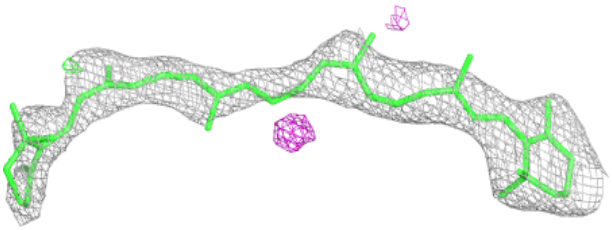
Electron density around LHG b 5004:

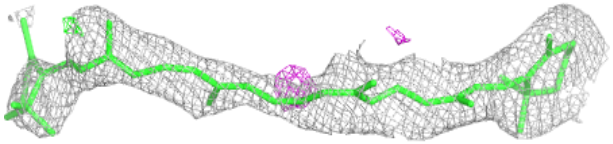
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

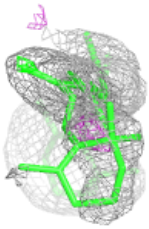


Electron density around BCR 9 4021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

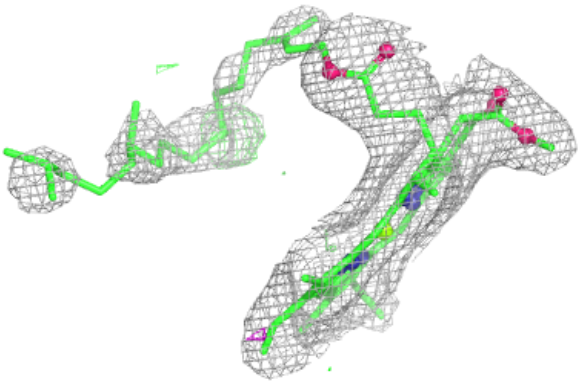


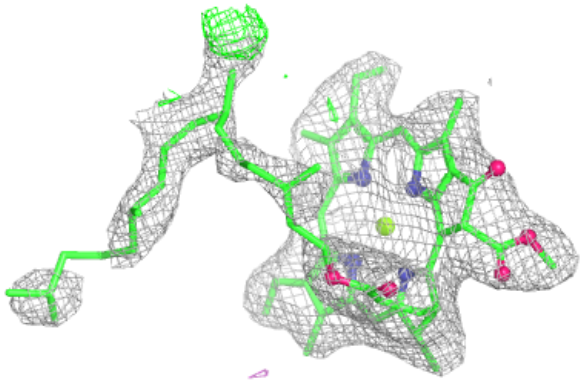


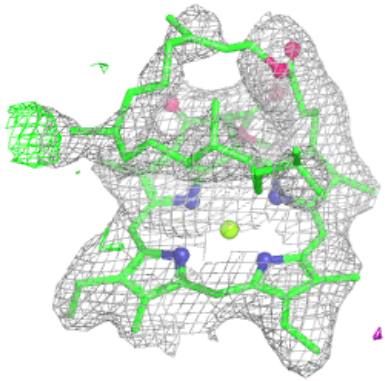


Electron density around CLA B 1211:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

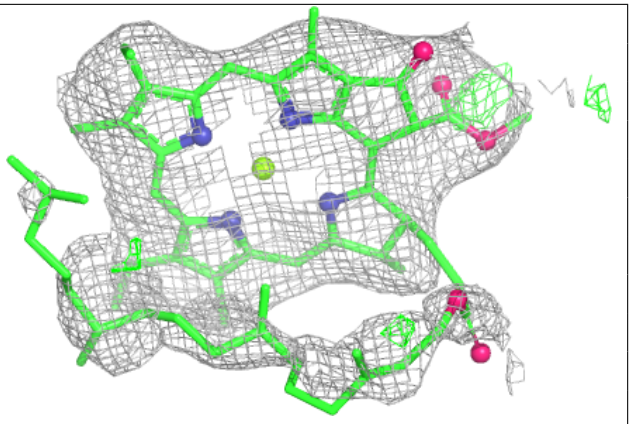


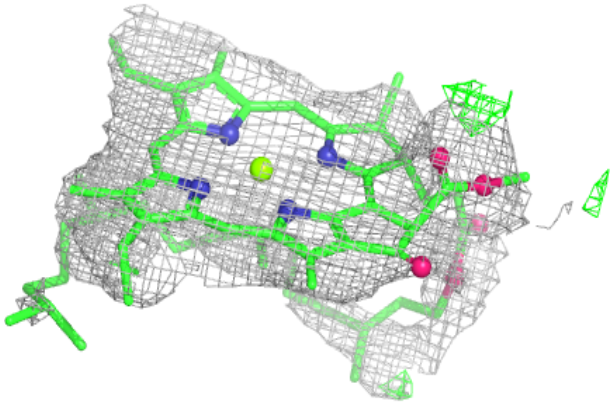


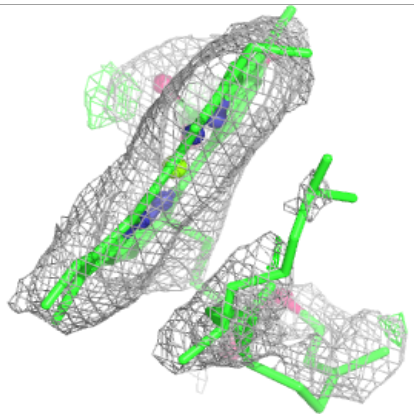


Electron density around CLA 1 1118:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

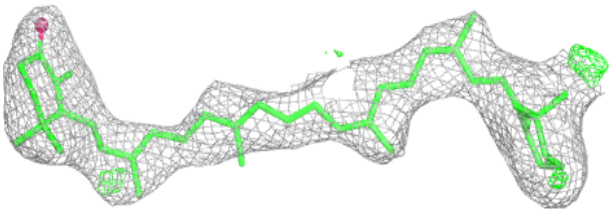


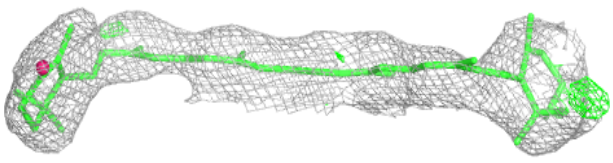


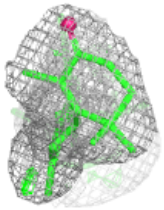


Electron density around ECH B 4006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

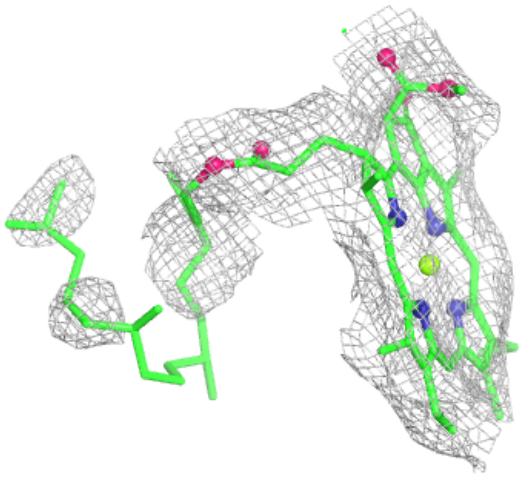


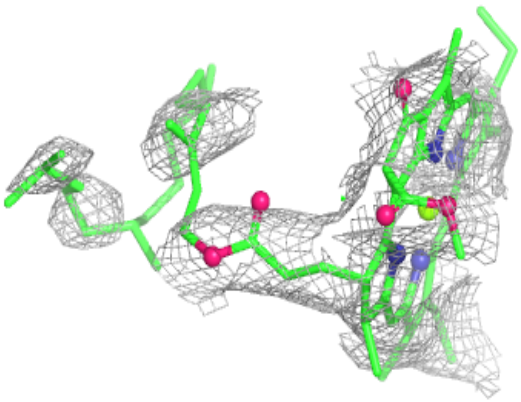


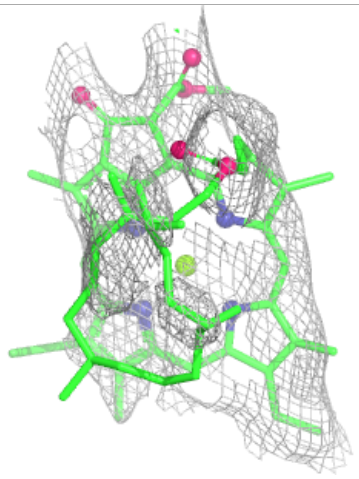


Electron density around CLA a 1112:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

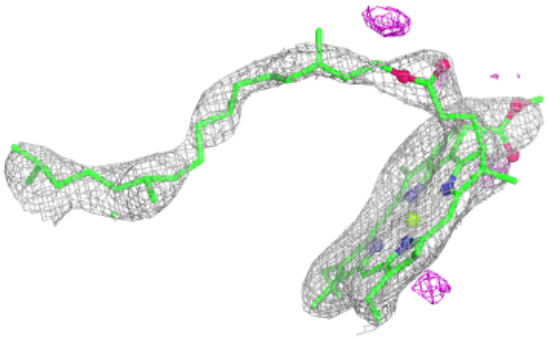


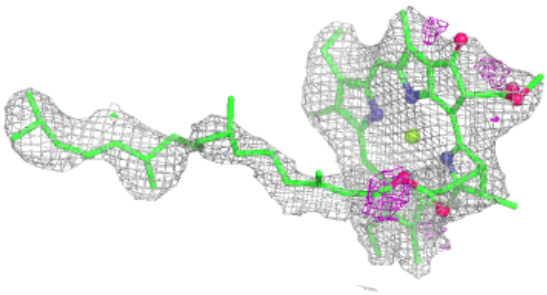


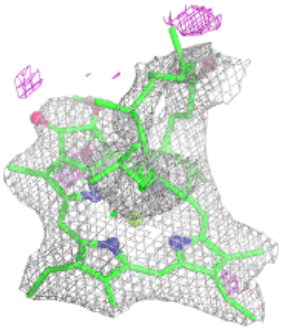


Electron density around CLA B 1208:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

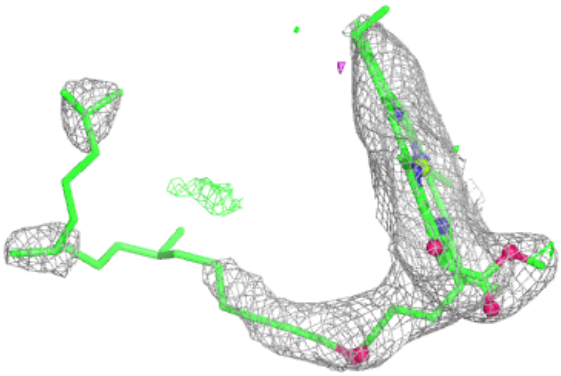


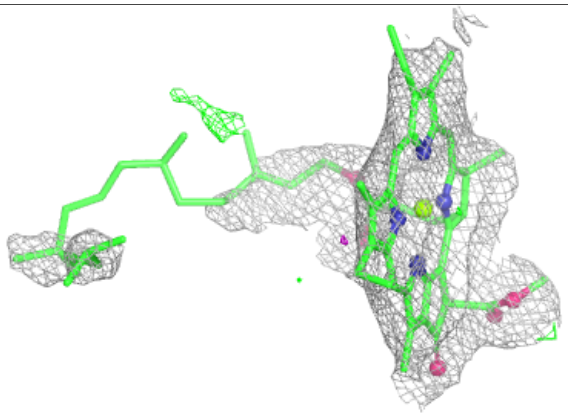


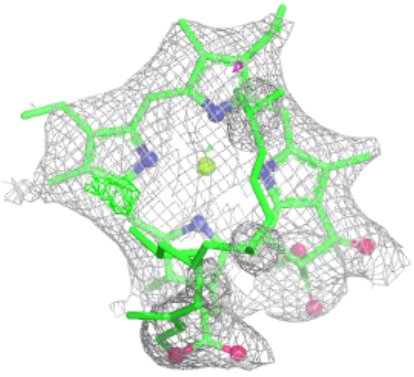


Electron density around CLA b 1227:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

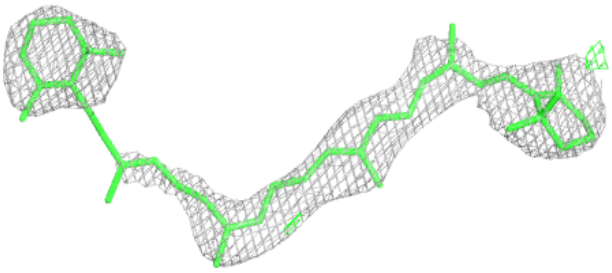


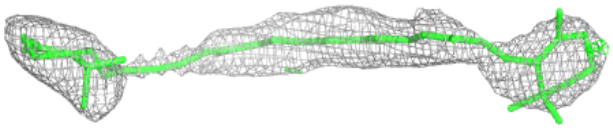


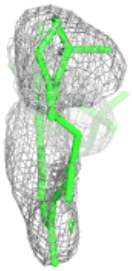


Electron density around BCR 2 4011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

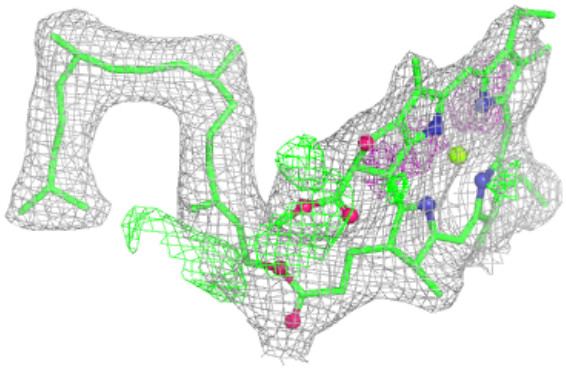


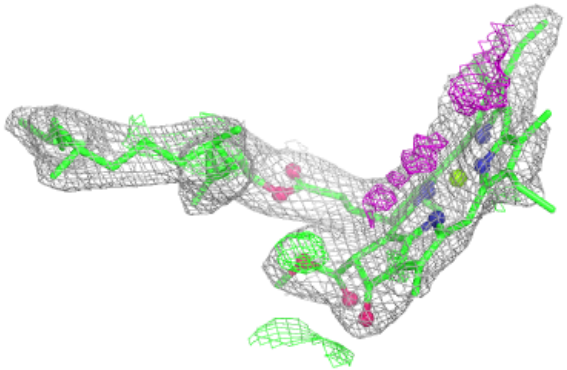


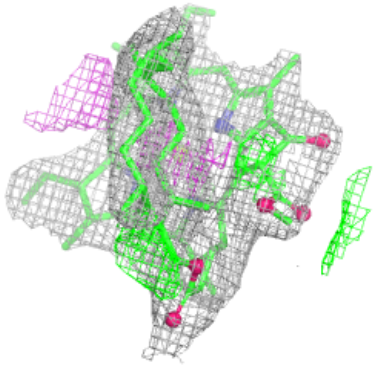


Electron density around CLA a 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

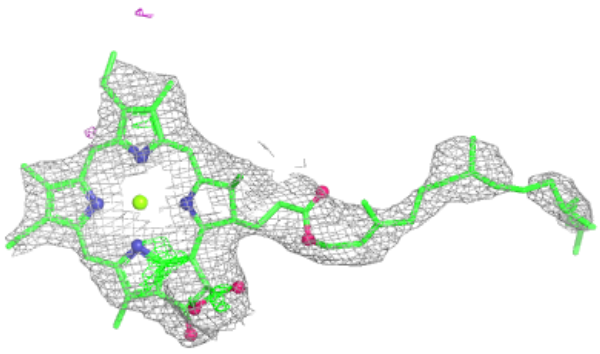


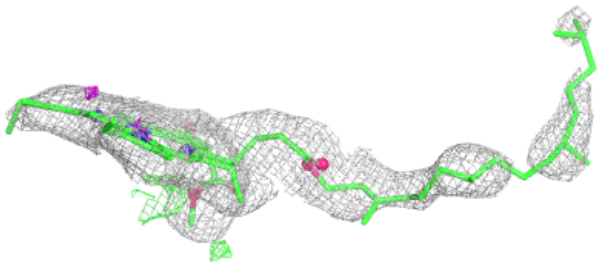


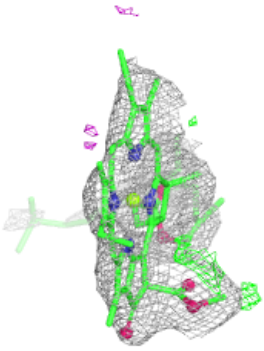


Electron density around CLA 1 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

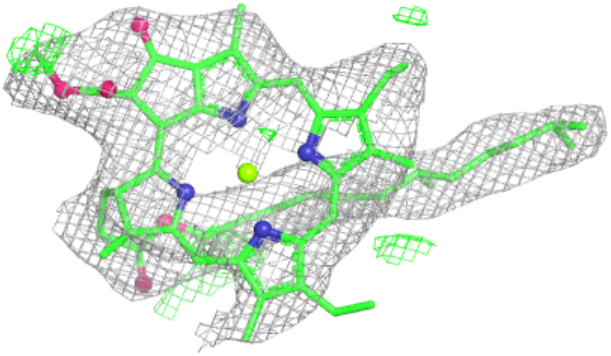


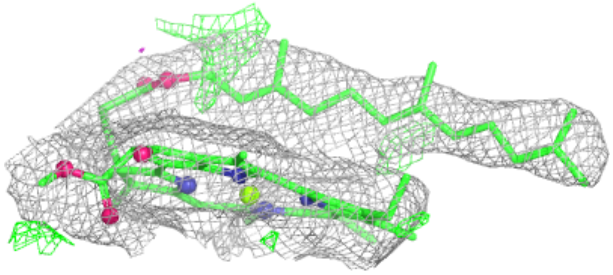


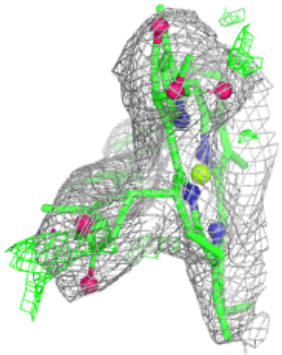


Electron density around CLA a 1116:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

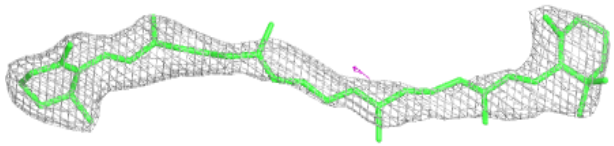


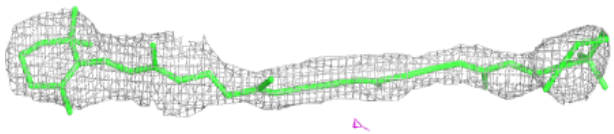


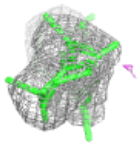


Electron density around BCR a 4012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

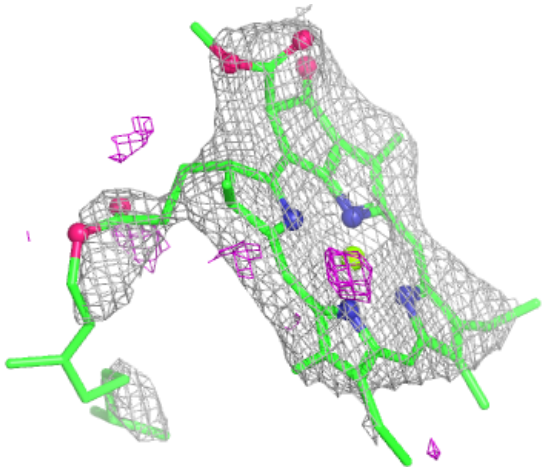


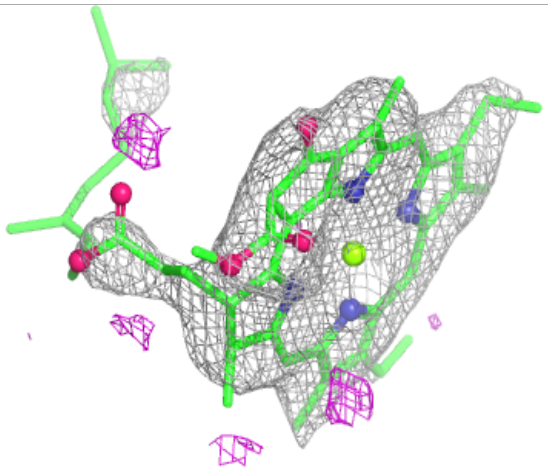


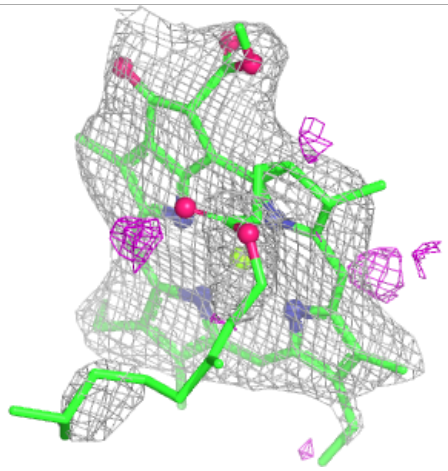


Electron density around CLA B 1227:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

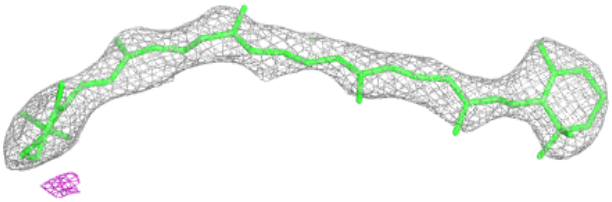


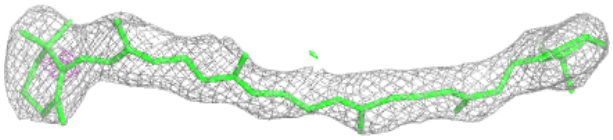


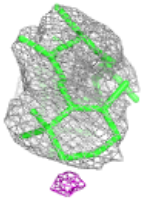


Electron density around BCR b 4014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

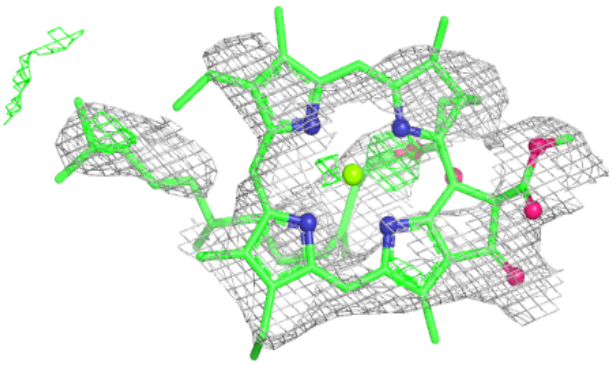


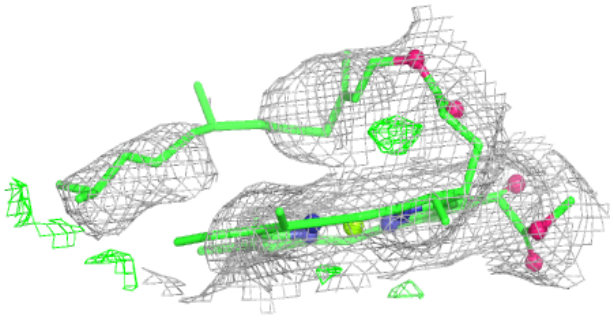


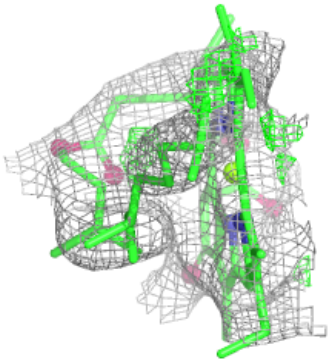


Electron density around CLA 1 1138:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

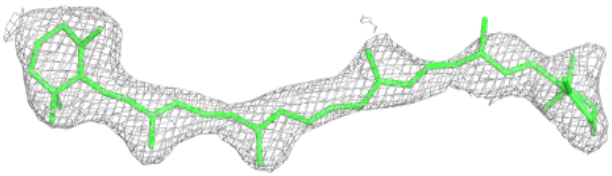


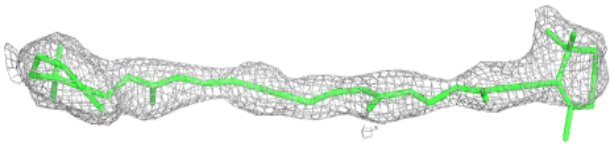


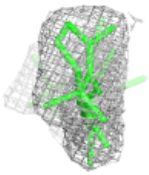


Electron density around BCR B 4005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

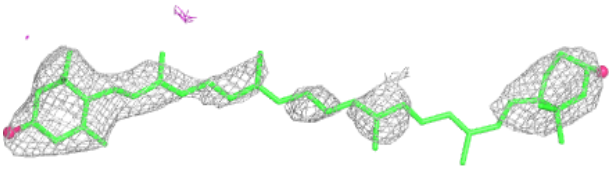


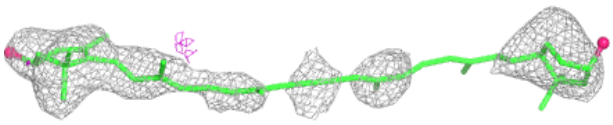


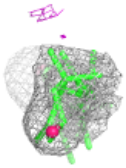


Electron density around ZEX j 4015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

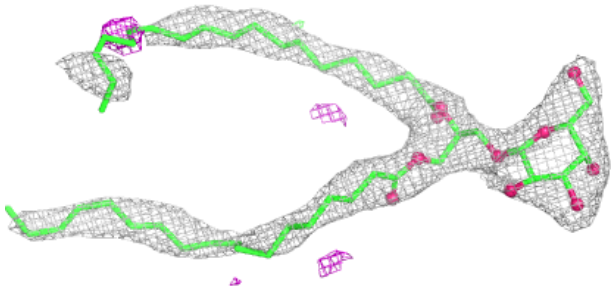


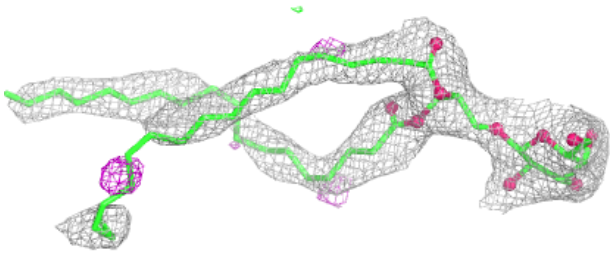


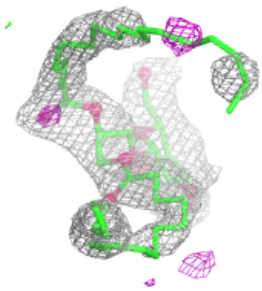


Electron density around LMG 2 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

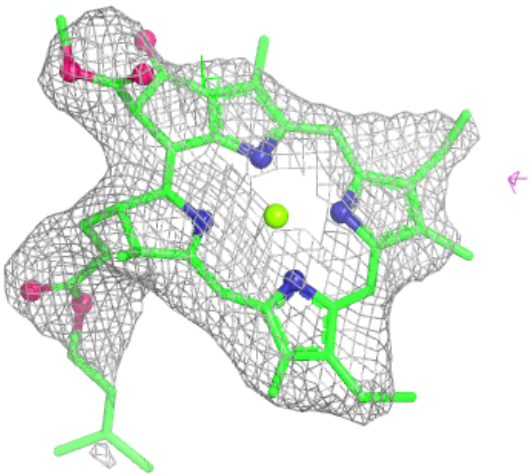


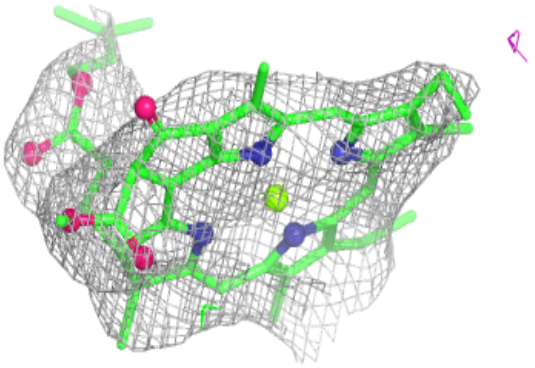


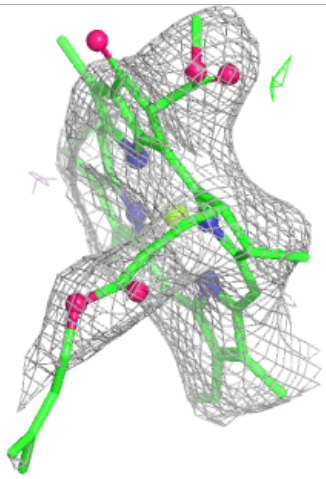


Electron density around CLA B 1232:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

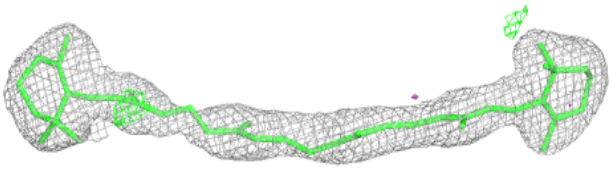


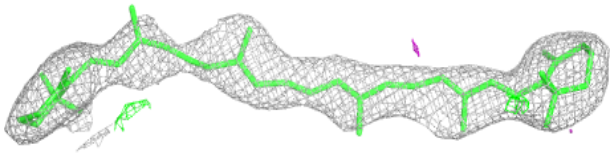


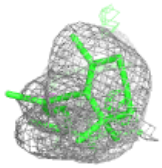


Electron density around BCR J 4013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

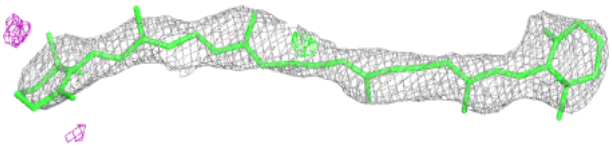


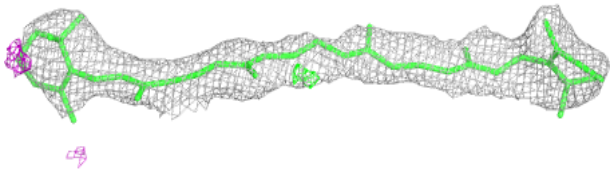


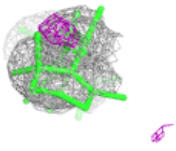


Electron density around BCR 1 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

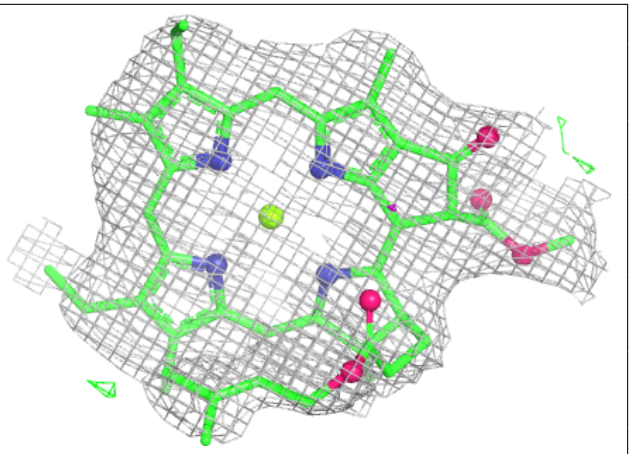


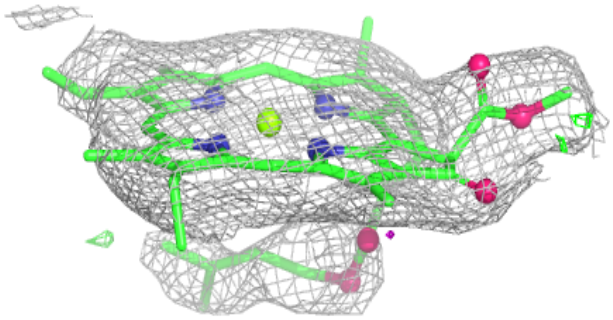


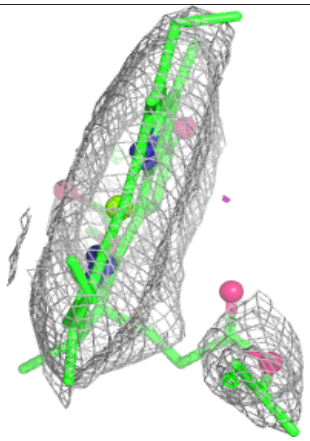


Electron density around CLA 1 1110:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

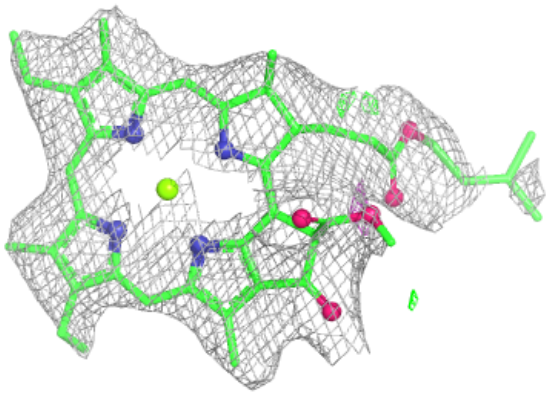


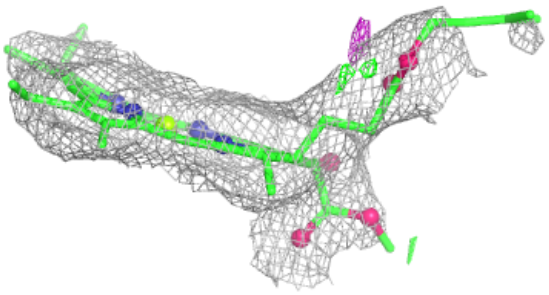


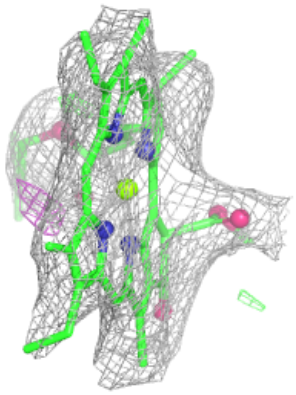


Electron density around CLA a 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

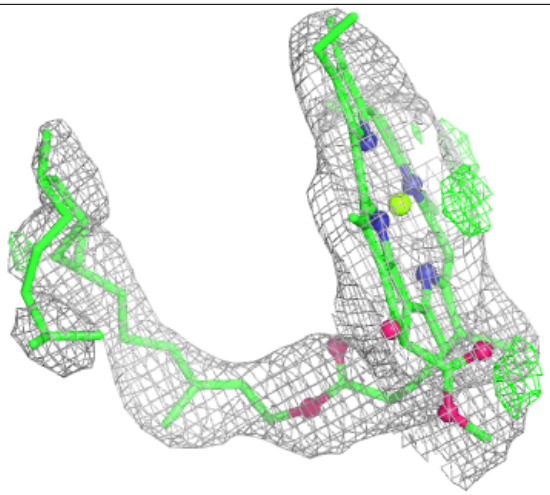


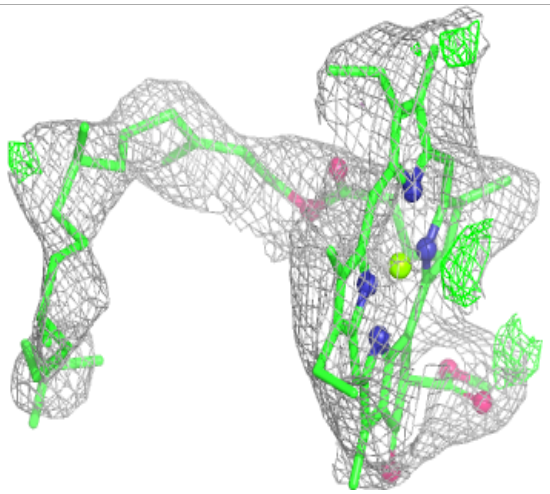


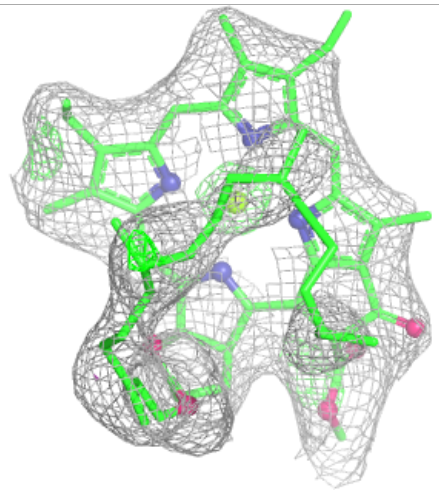


Electron density around CLA B 1216:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

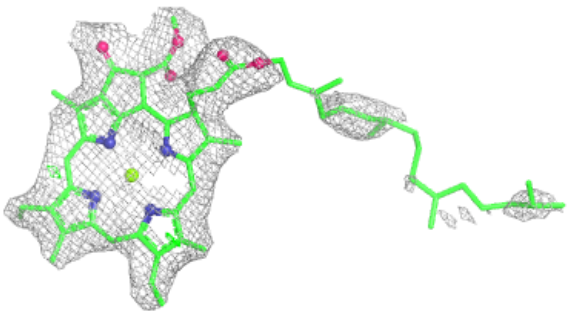


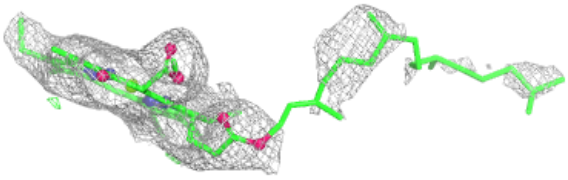


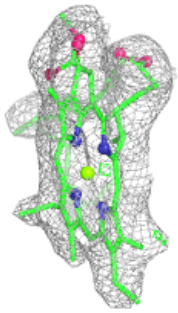


Electron density around CLA F 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

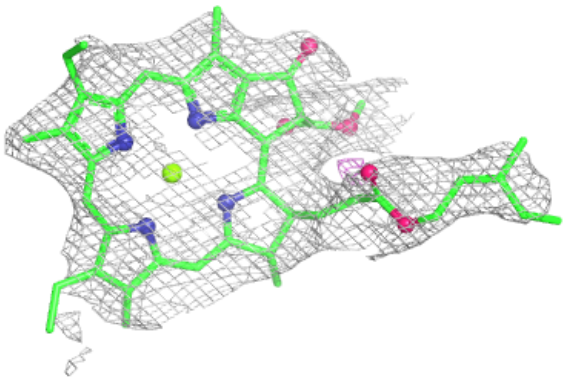


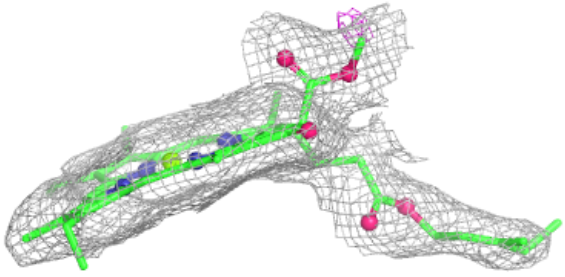


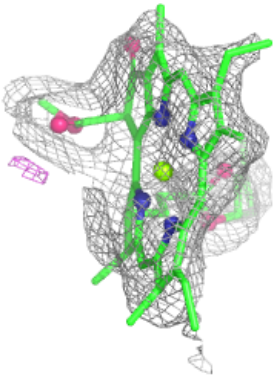


Electron density around CLA 1 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

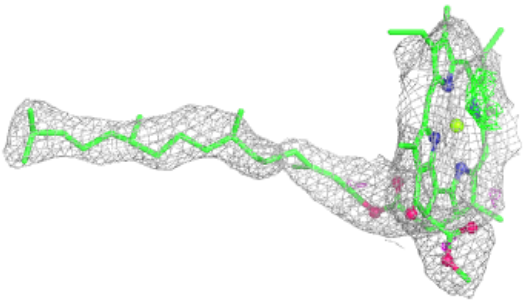


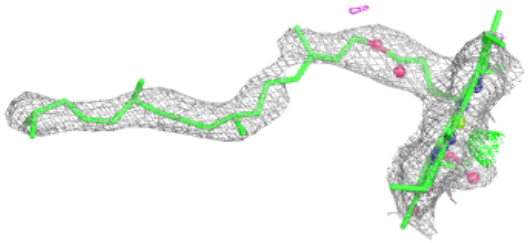


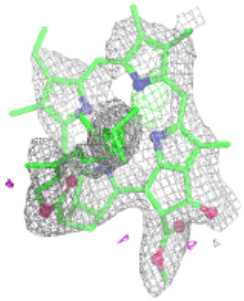


Electron density around CLA 2 1225:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

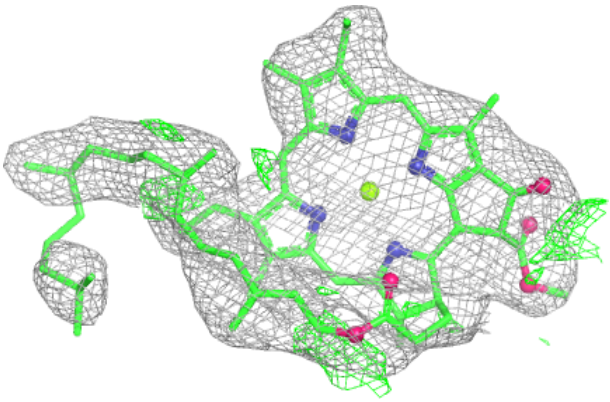


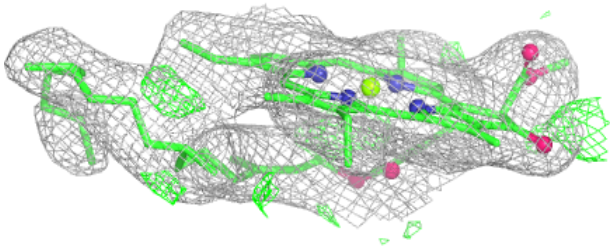


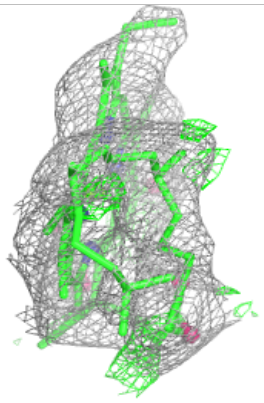


Electron density around CLA a 1117:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

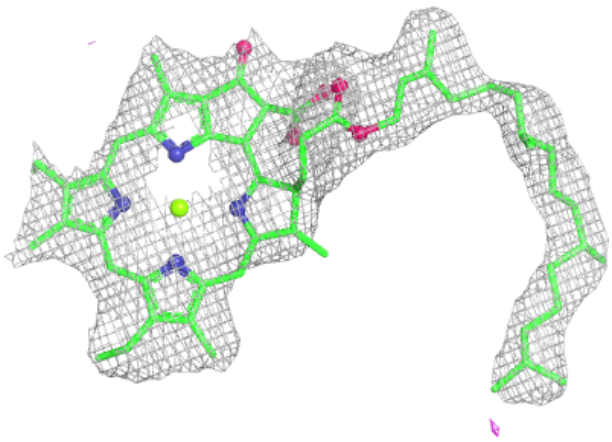


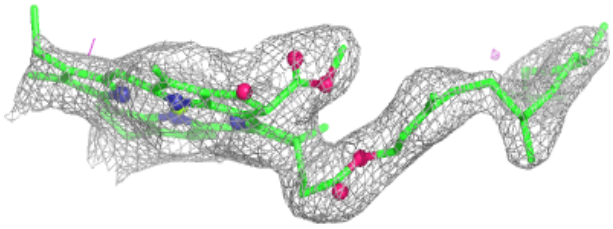


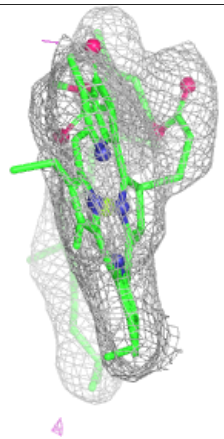


Electron density around CLA a 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

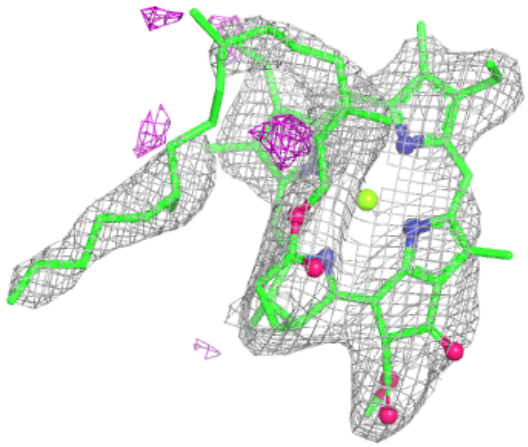


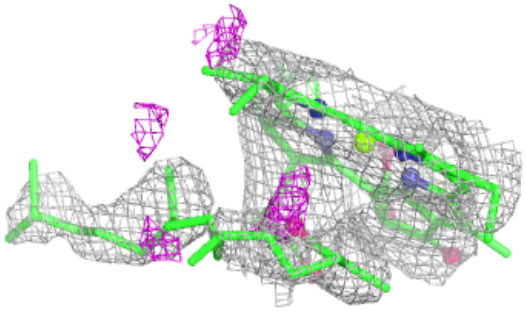


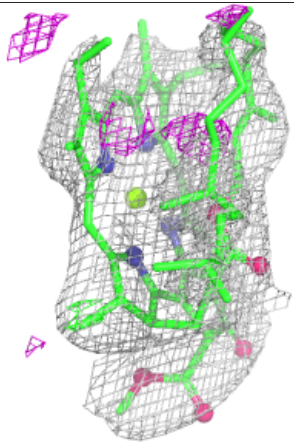


Electron density around CLA 2 1205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

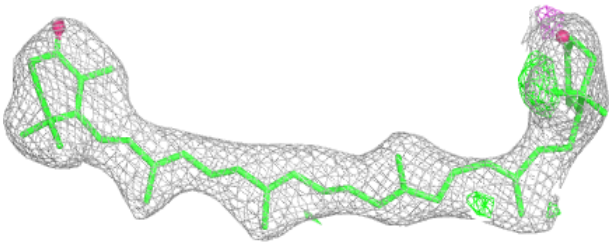


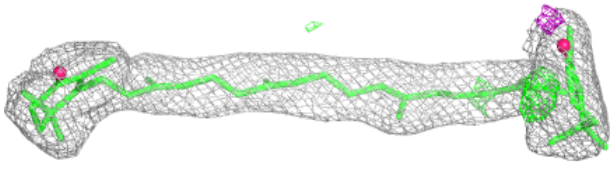


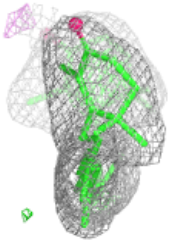


Electron density around 45D h 4020:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

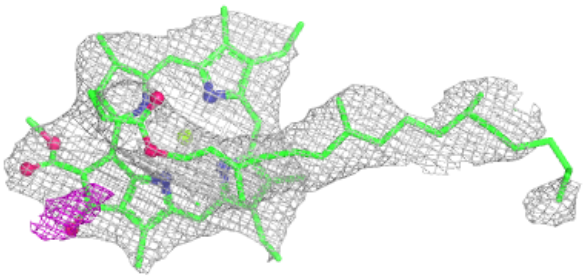


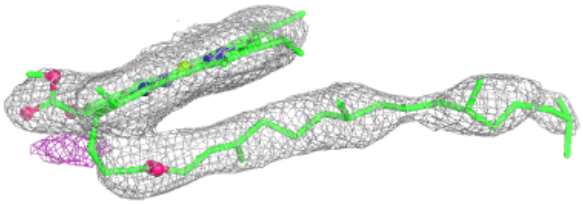


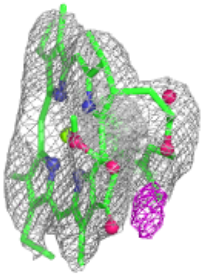


Electron density around CLA B 1213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

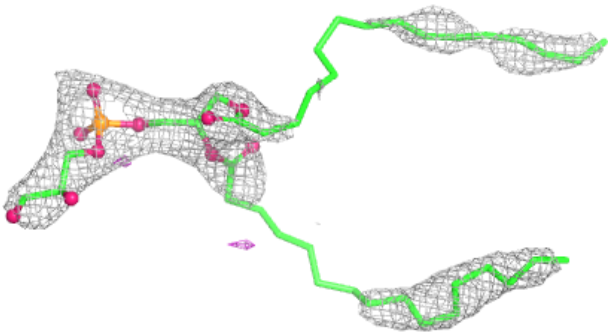


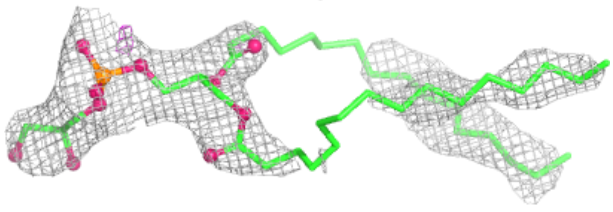


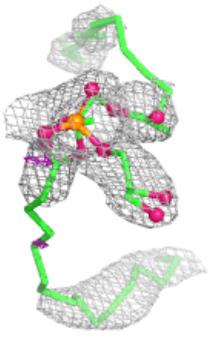


Electron density around LHG 1 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

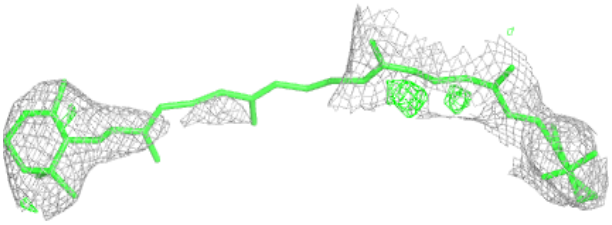


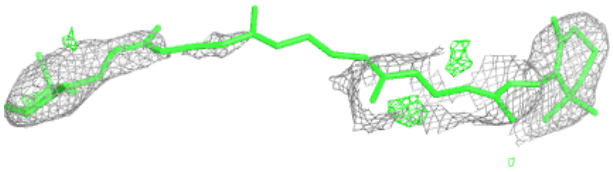


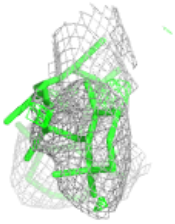


Electron density around BCR 2 4014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

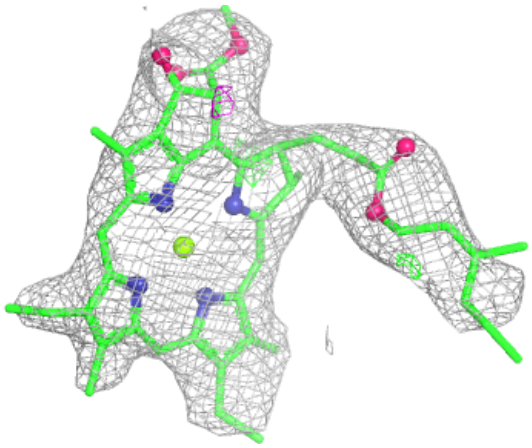


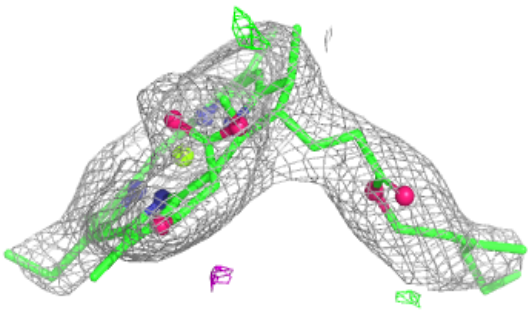


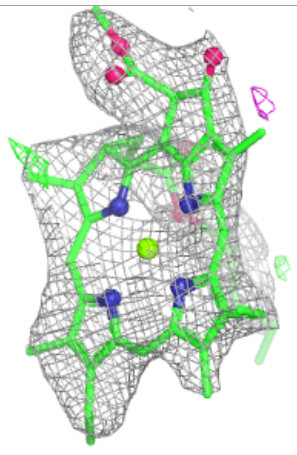


Electron density around CLA a 1129:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

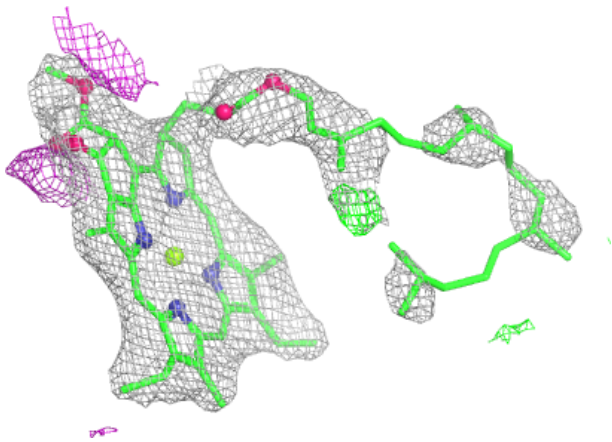


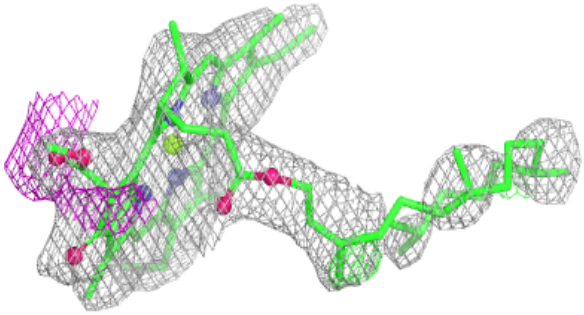


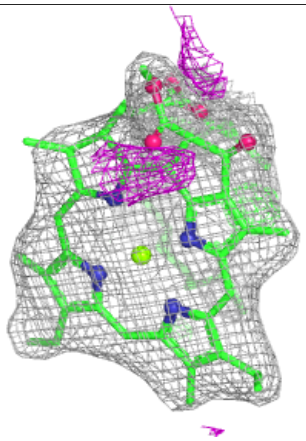


Electron density around CLA B 1228:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

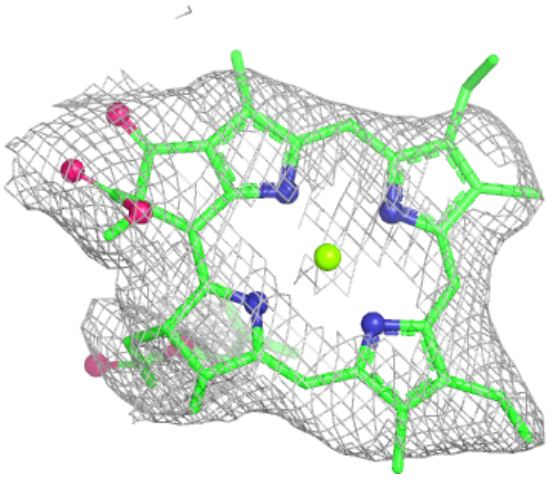


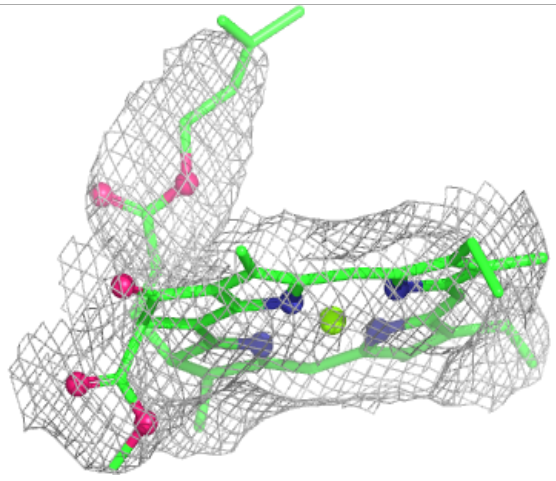


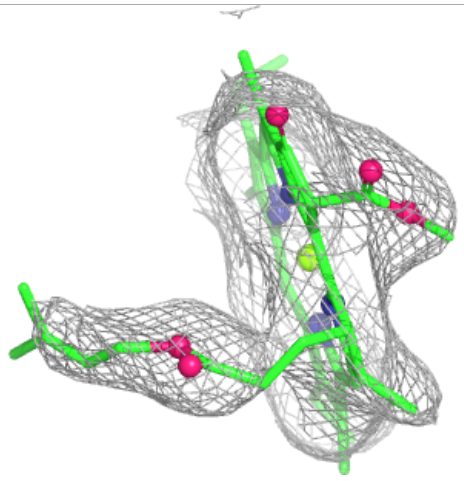


Electron density around CLA 2 1211:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

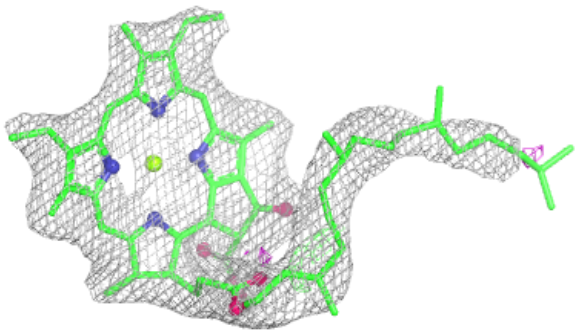


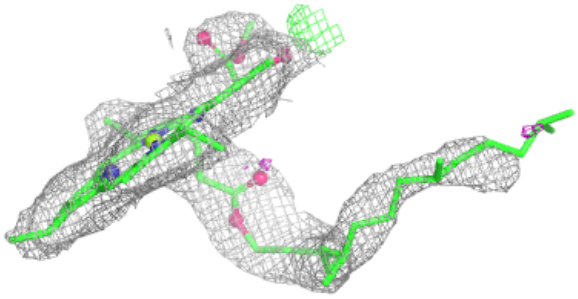


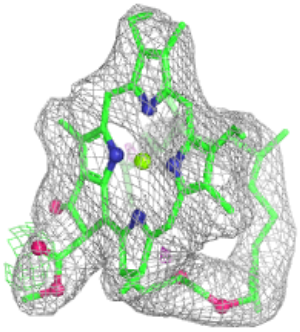


Electron density around CLA b 1231:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

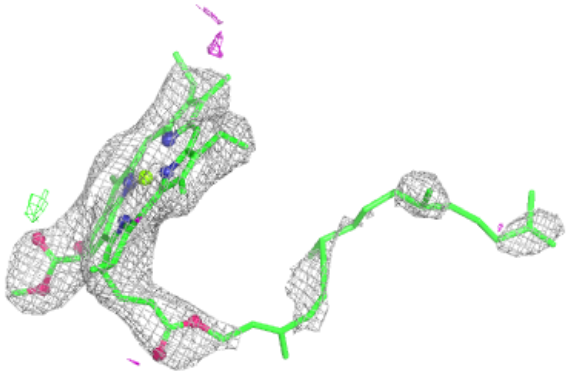


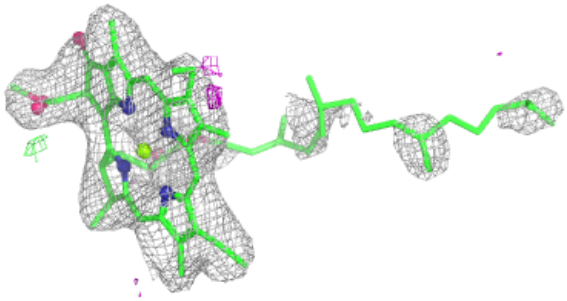


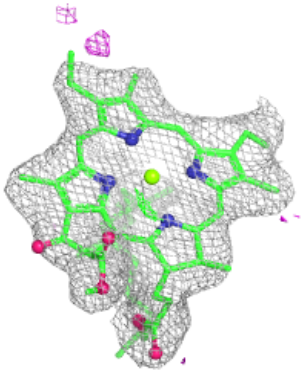


Electron density around CLA b 1232:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

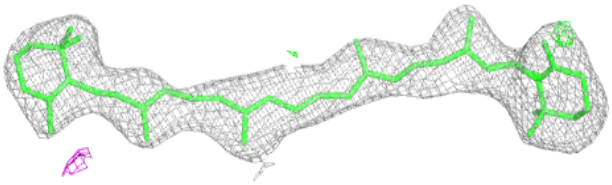


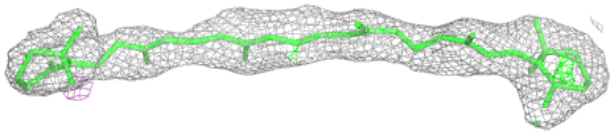


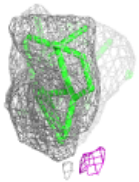


Electron density around BCR b 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

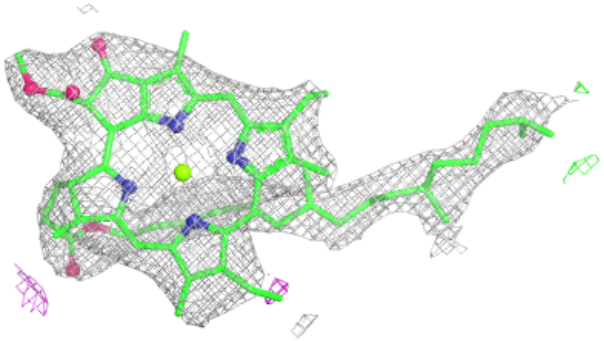


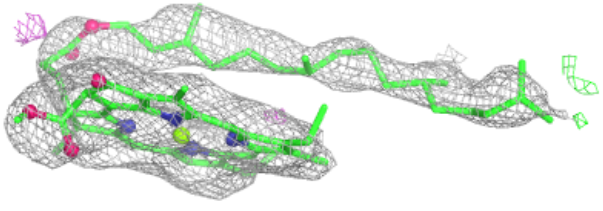


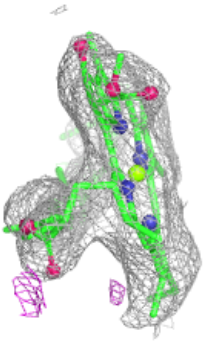


Electron density around CLA 1 1116:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

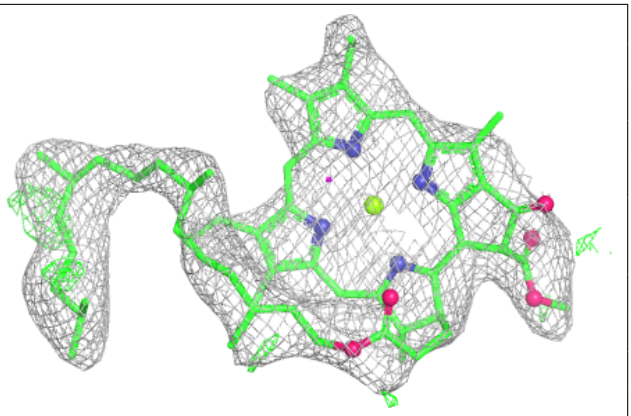


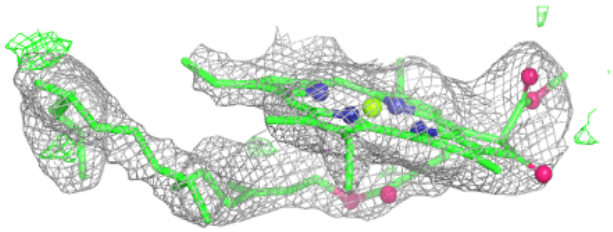


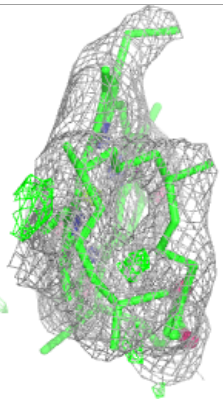


Electron density around CLA 1 1117:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

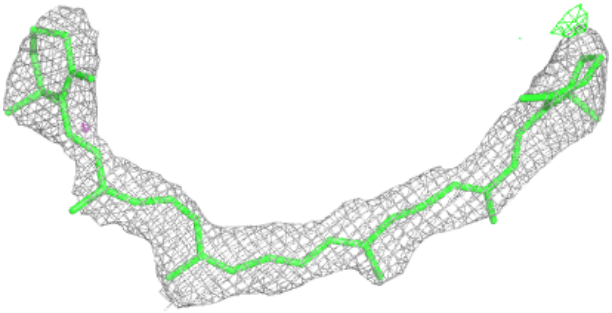


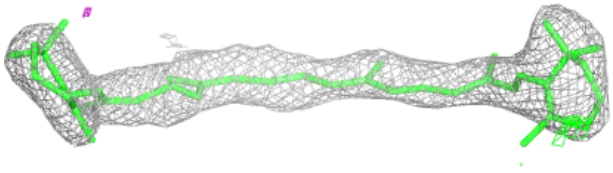


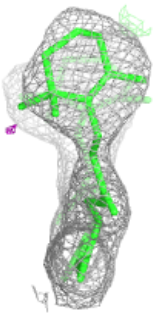


Electron density around BCR f 4016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

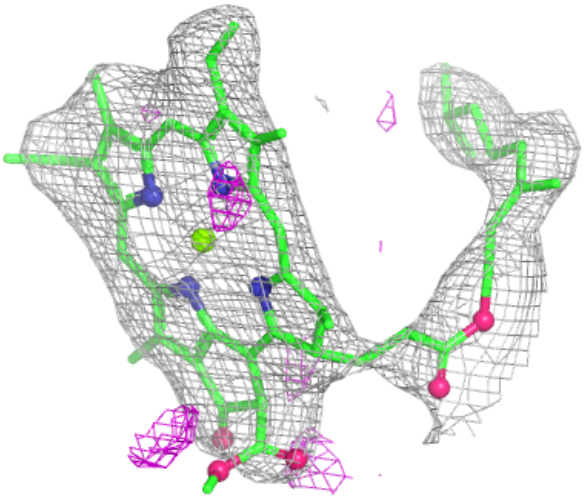


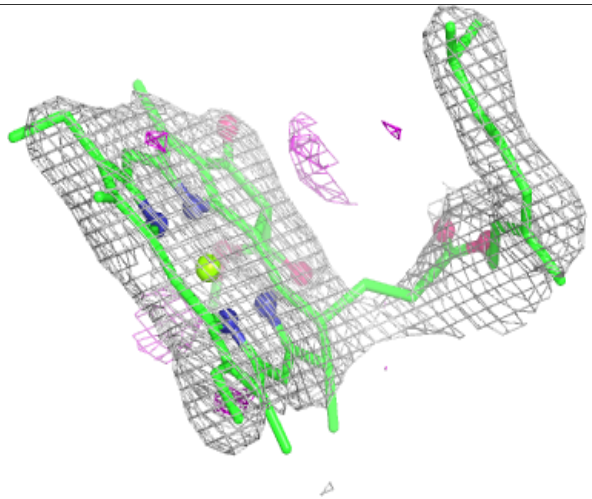


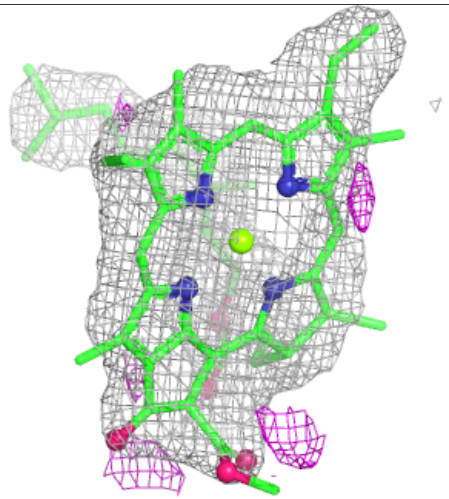


Electron density around CLA 1 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

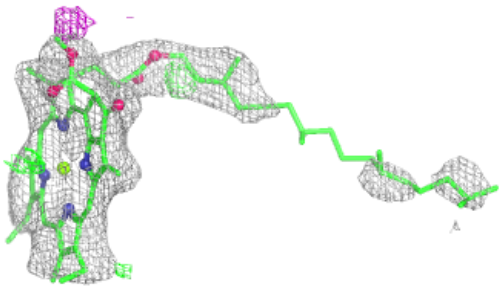


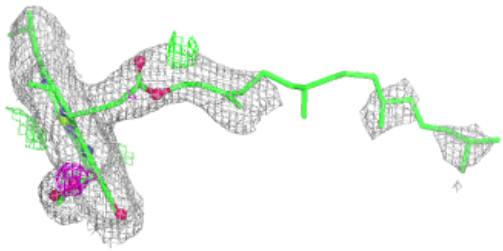


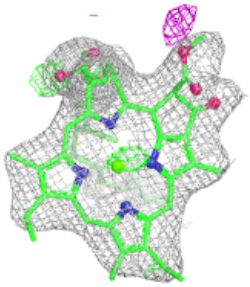


Electron density around CLA b 1236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

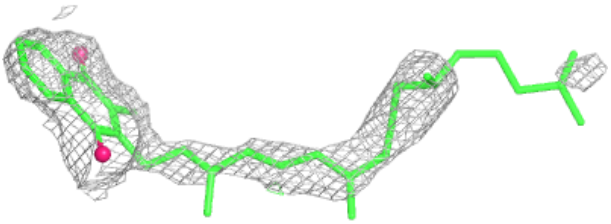


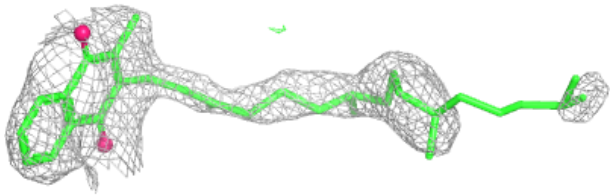


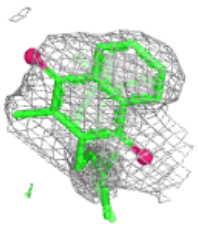


Electron density around PQN 1 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

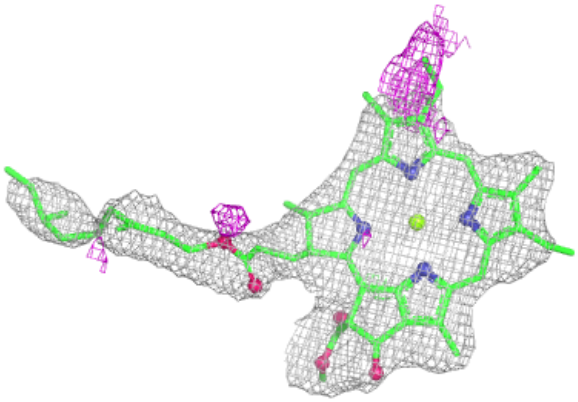


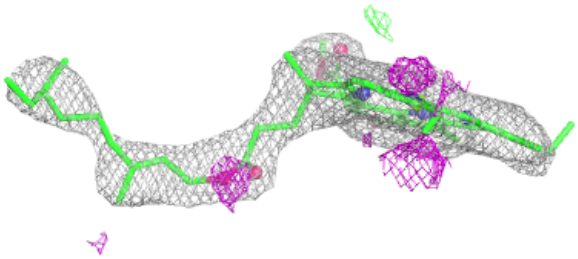


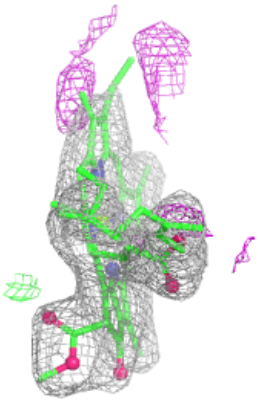


Electron density around CLA 1 1124:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

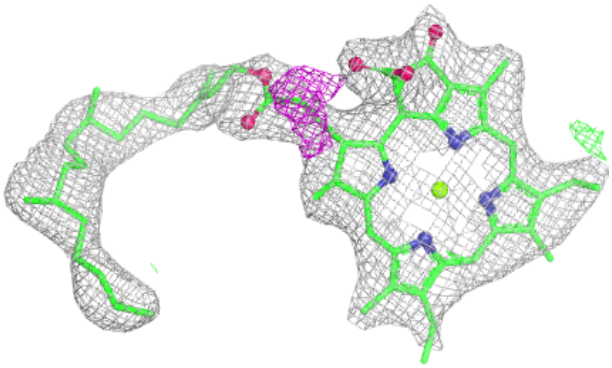


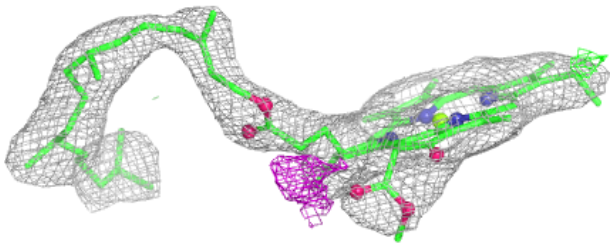




Electron density around CLA 1 1125:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

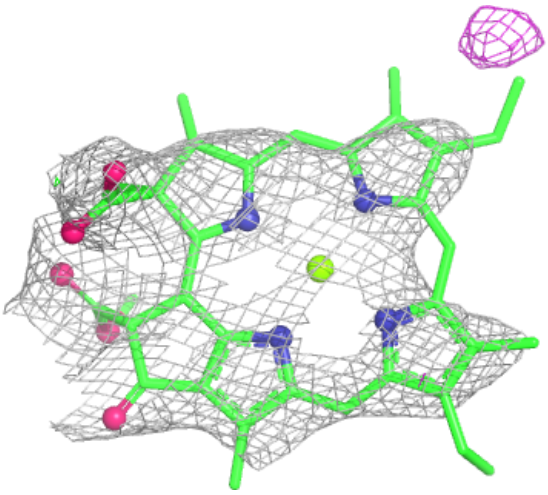


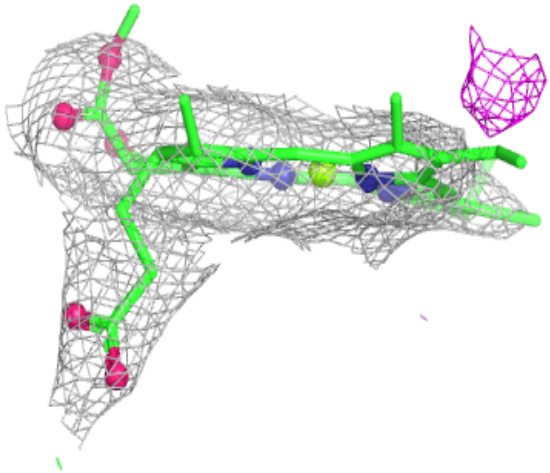


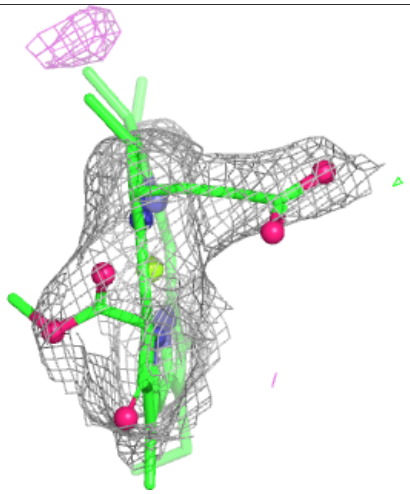


Electron density around CLA 2 1220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

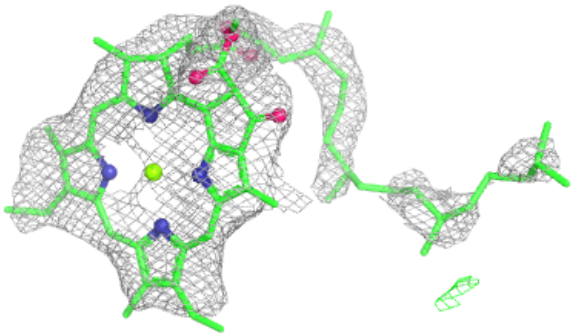


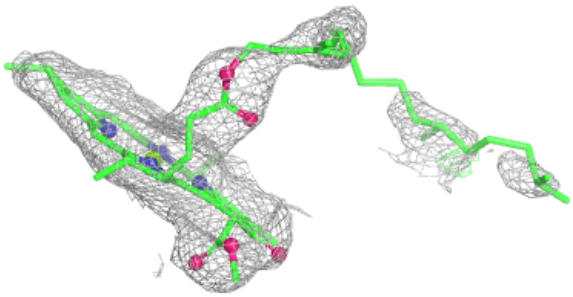


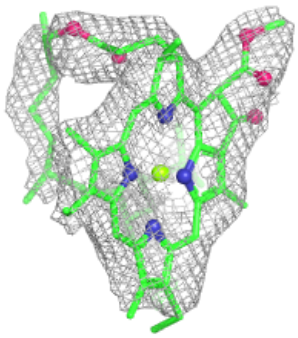


Electron density around CLA B 1231:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

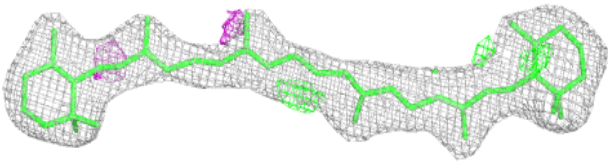


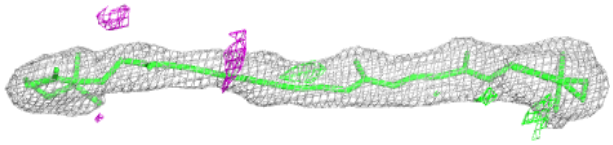


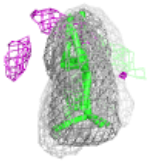


Electron density around BCR l 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

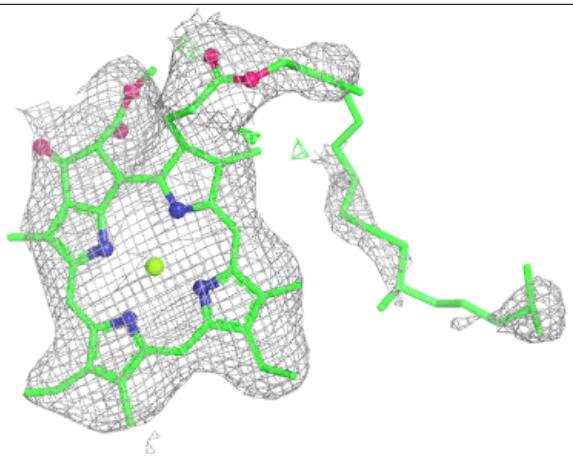


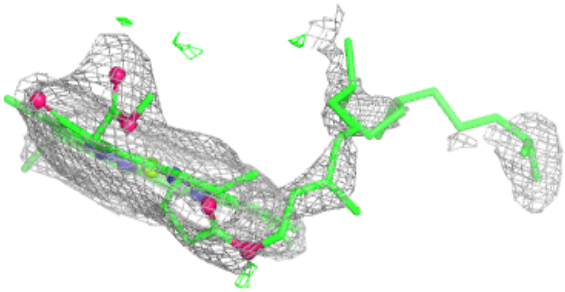


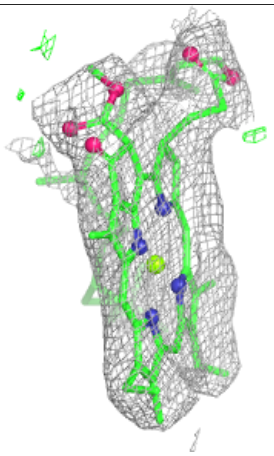


Electron density around CLA 1 1111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

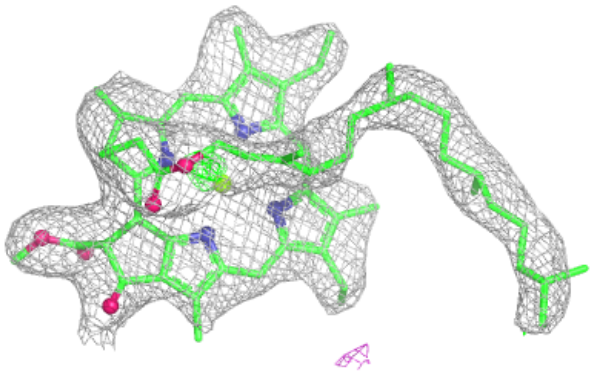


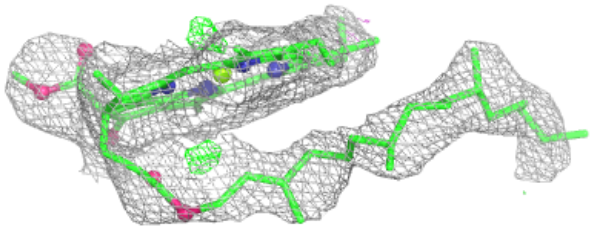


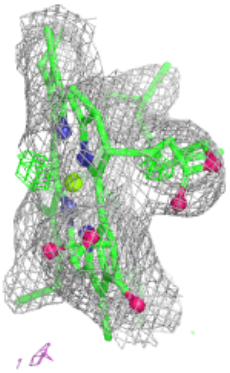


Electron density around CLA b 1235:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

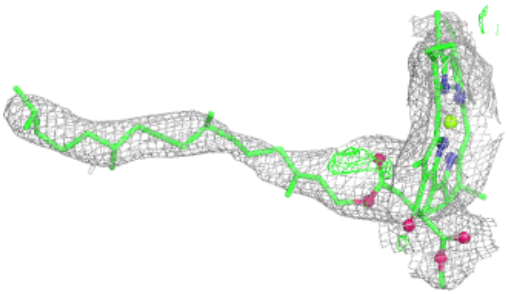


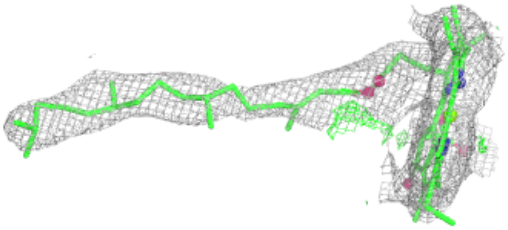


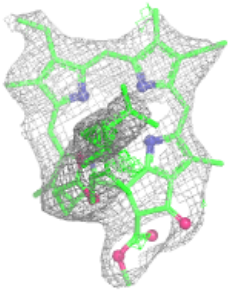


Electron density around CLA a 1126:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

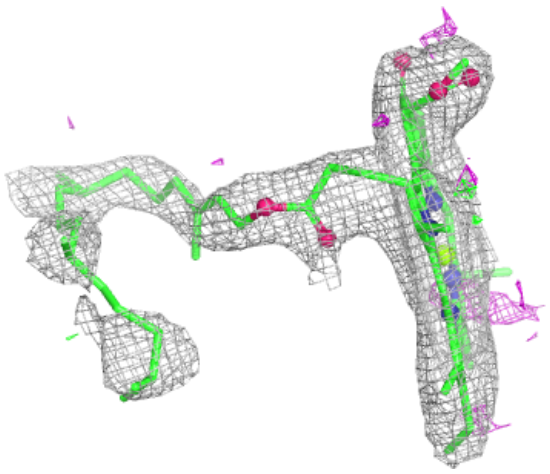


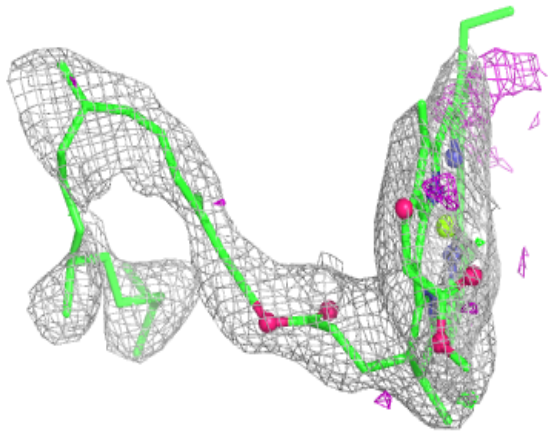


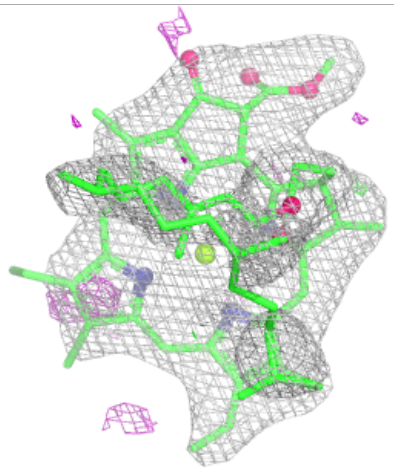


Electron density around CLA A 1134:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

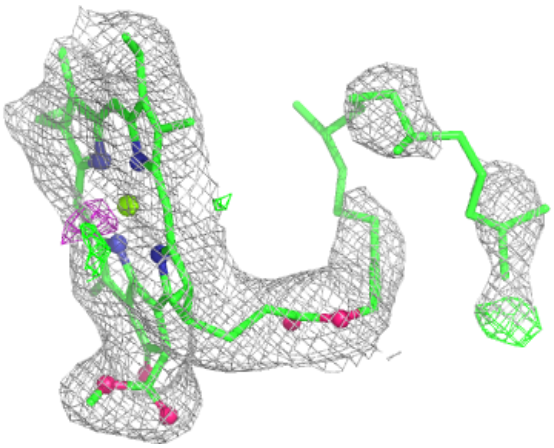


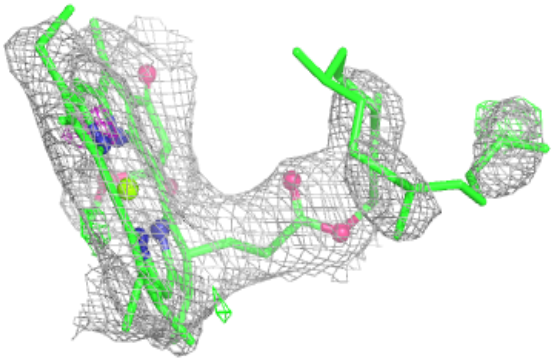


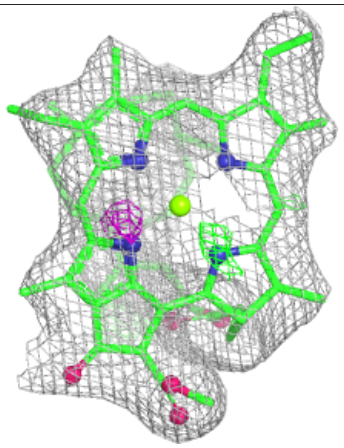


Electron density around CLA A 1112:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

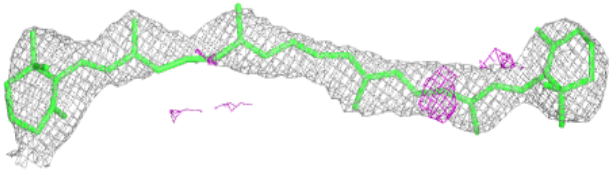


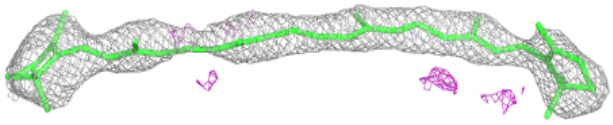


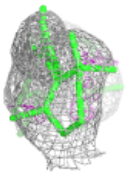


Electron density around BCR 1 4008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

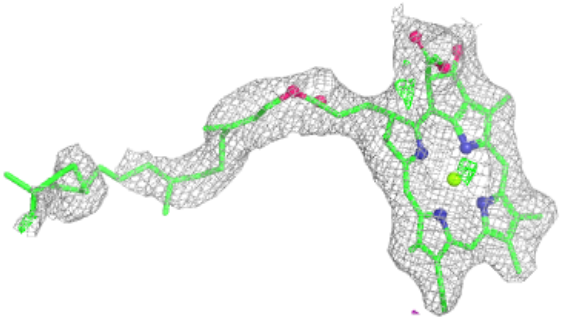


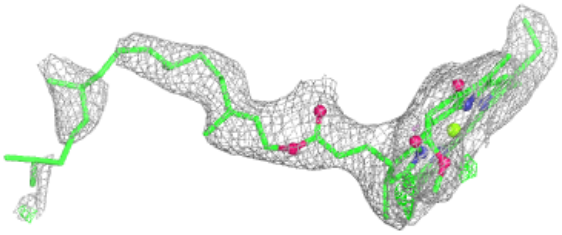


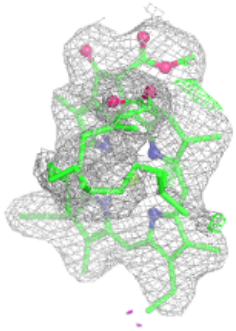


Electron density around CLA B 1230:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

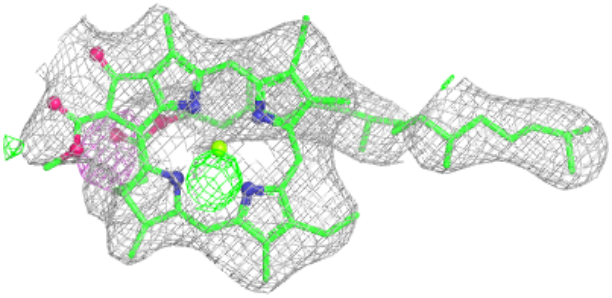


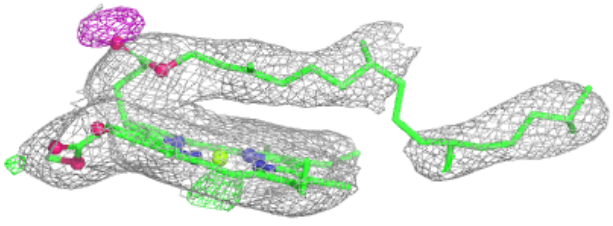




Electron density around CLA a 1136:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

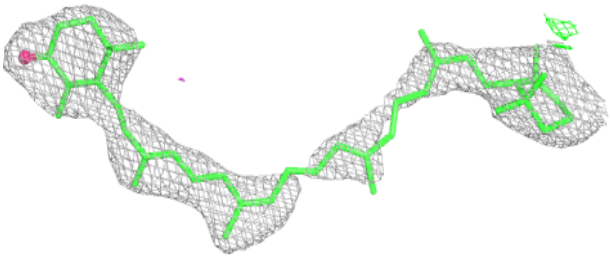


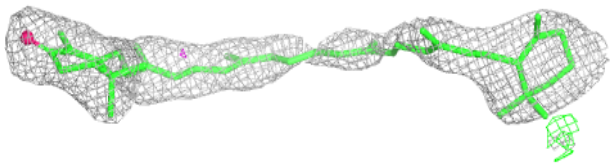


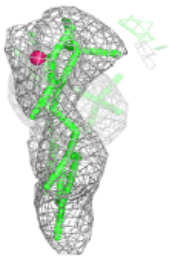


Electron density around ECH b 4011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

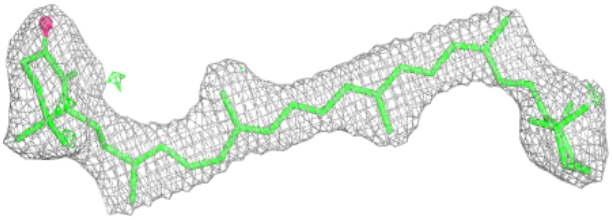


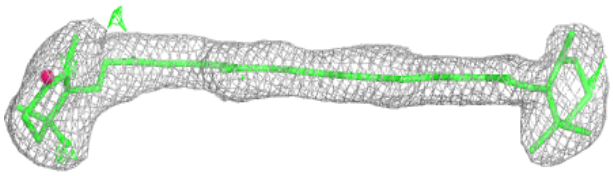


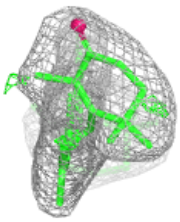


Electron density around ECH b 4006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

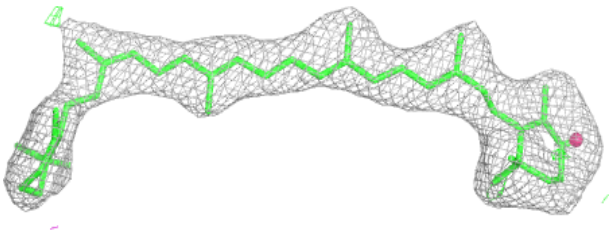


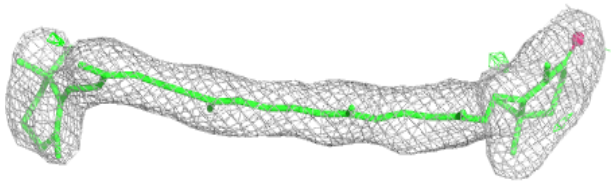




Electron density around ECH m 4021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

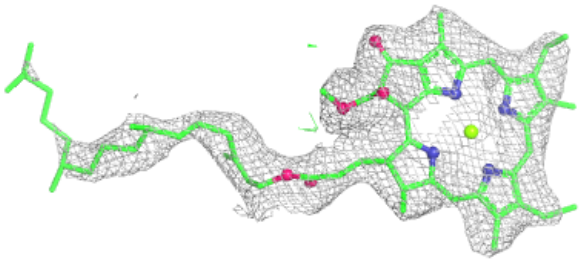


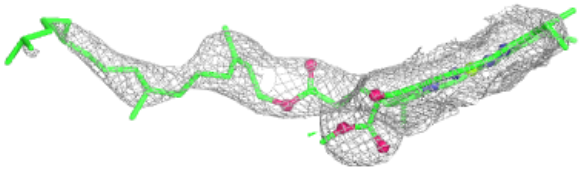


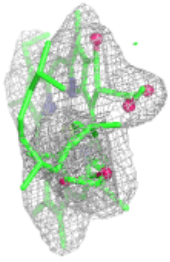


Electron density around CLA a 1139:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

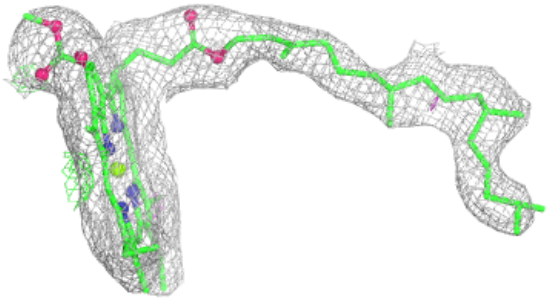


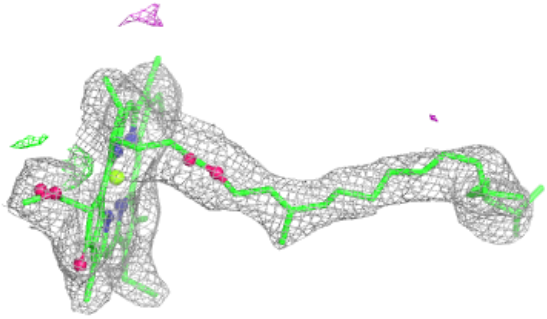


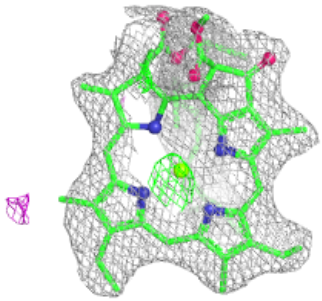


Electron density around CLA A 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

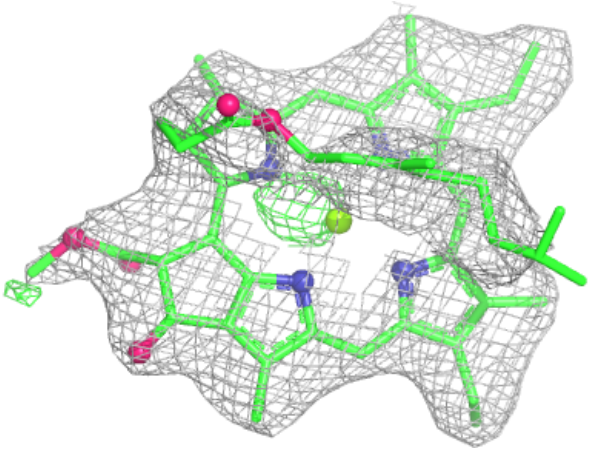


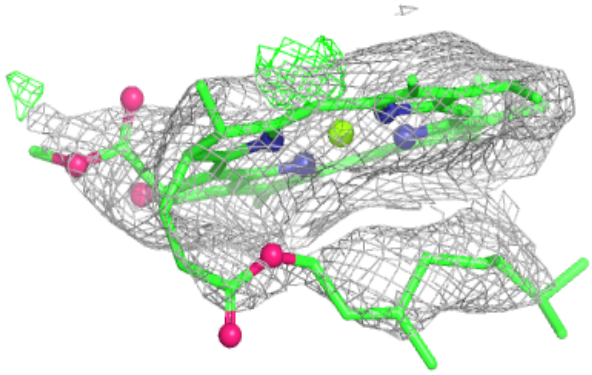


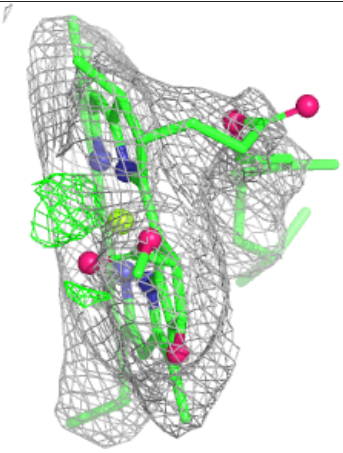


Electron density around CLA 1 1121:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

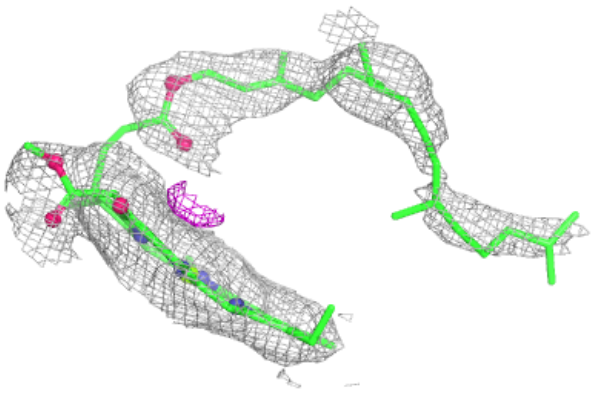


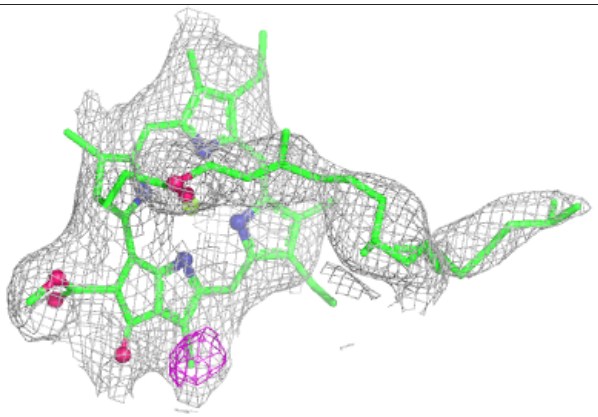


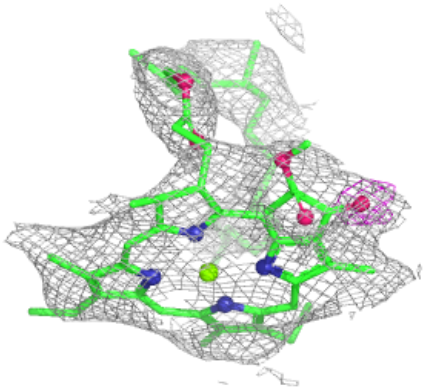


Electron density around CLA a 1109:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

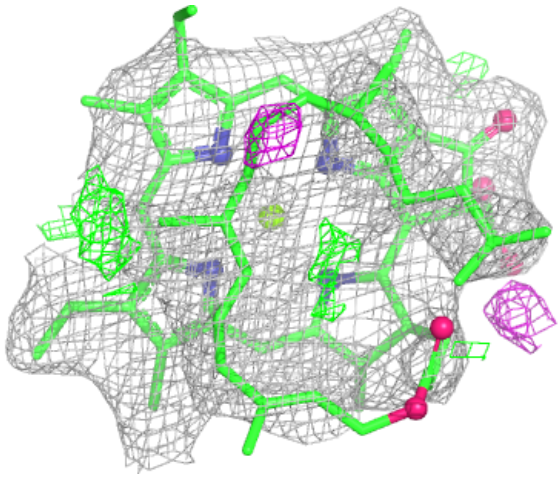


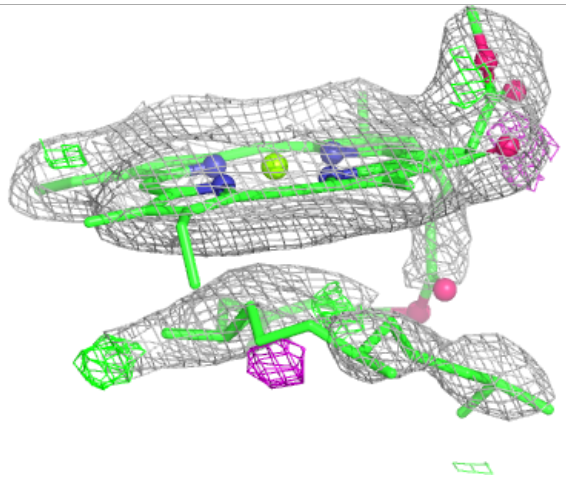


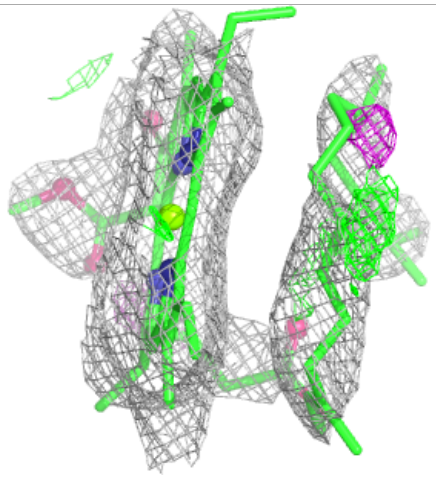


Electron density around CLA l 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

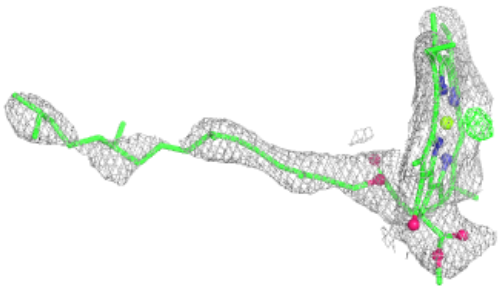


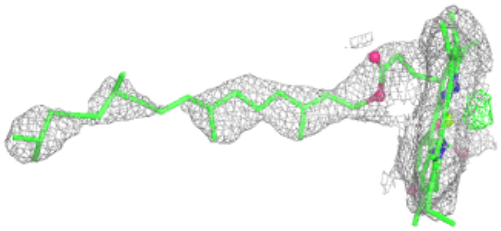


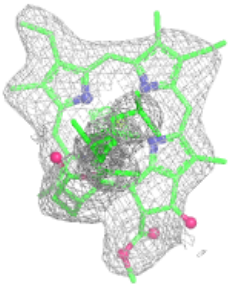


Electron density around CLA 1 1126:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

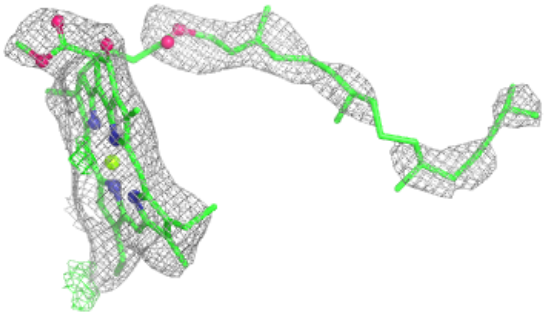


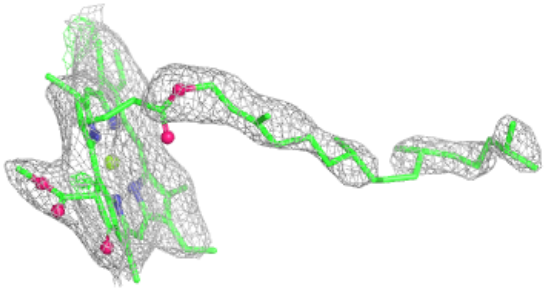


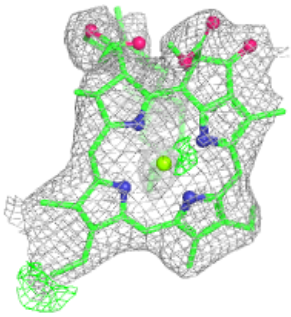


Electron density around CLA 1 1128:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

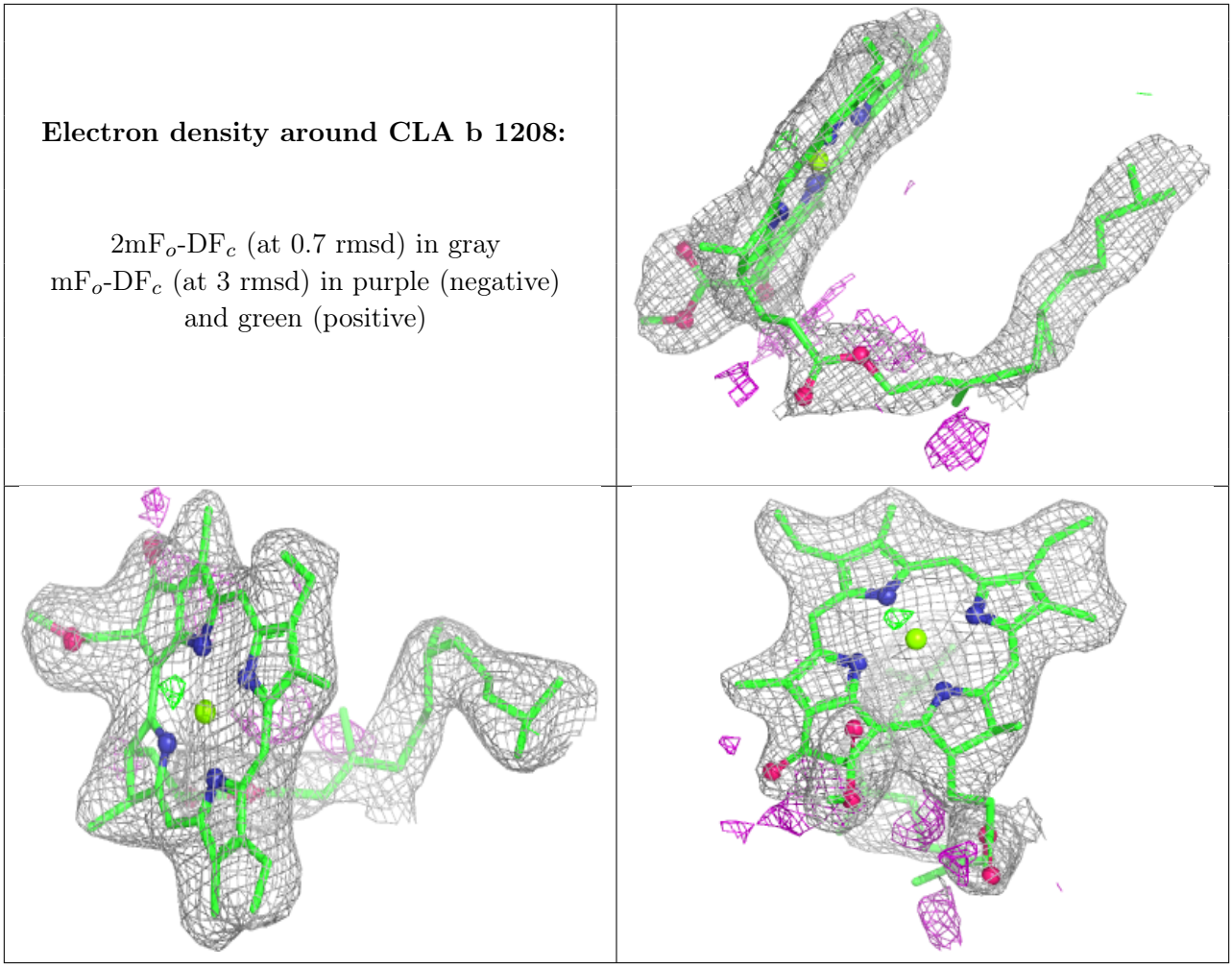






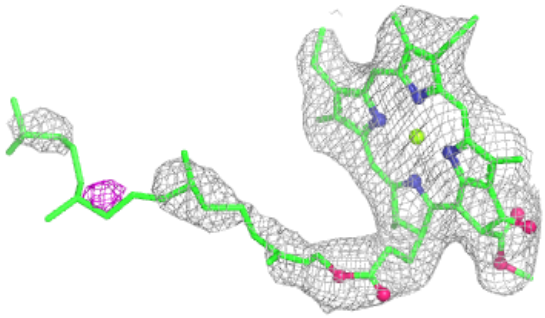
Electron density around CLA b 1208:

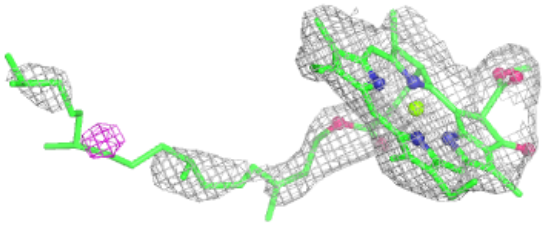
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

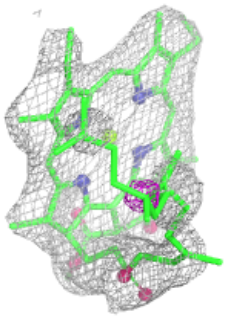


Electron density around CLA A 1114:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

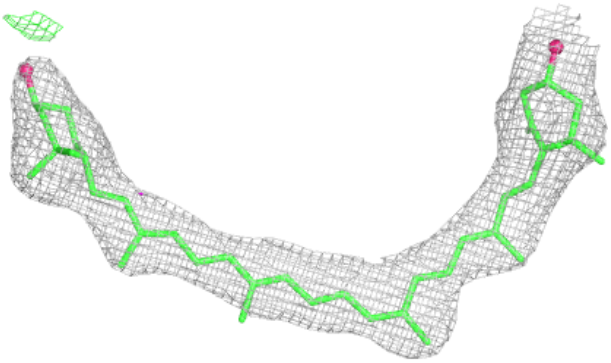


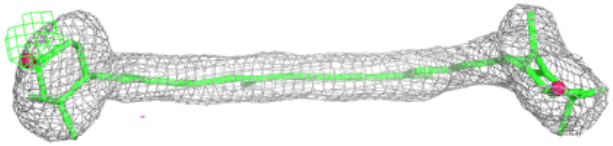


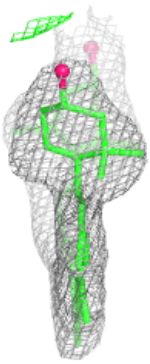


Electron density around ZEX F 4016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

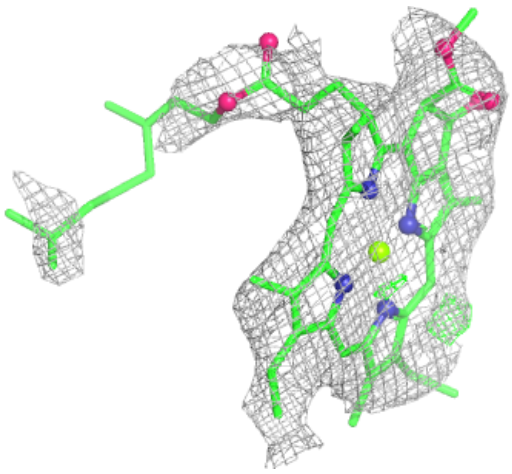


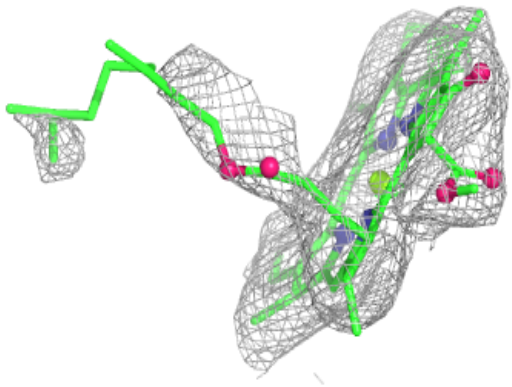


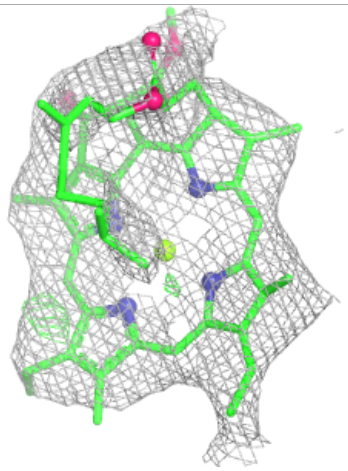


Electron density around CLA B 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

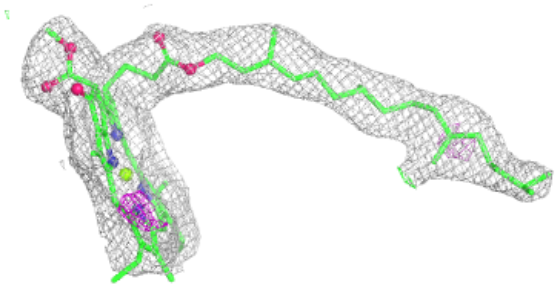


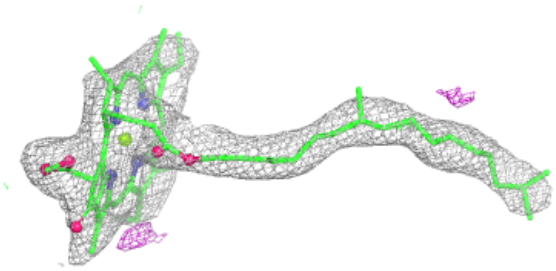


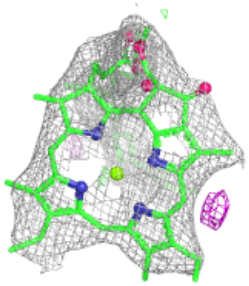


Electron density around CLA 2 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

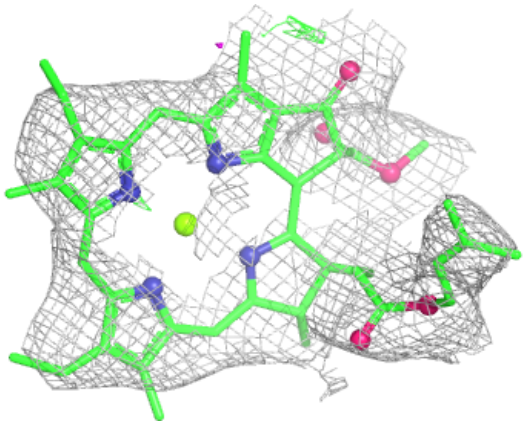


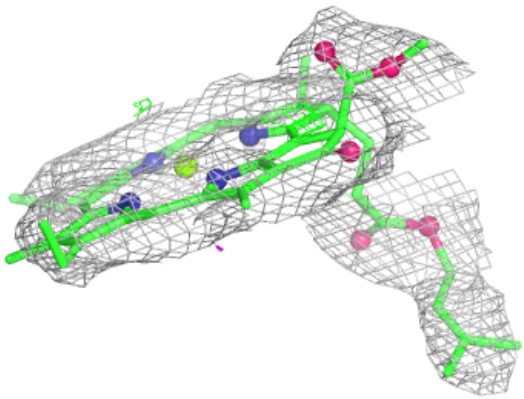


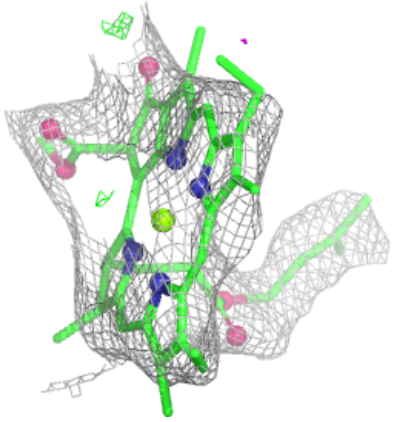


Electron density around CLA 2 1236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

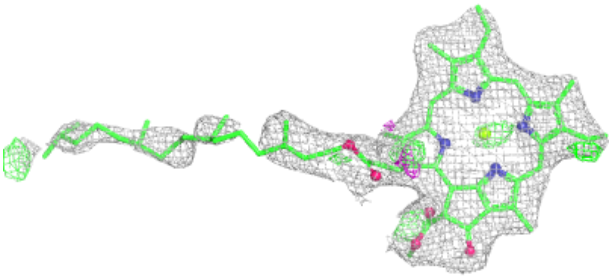




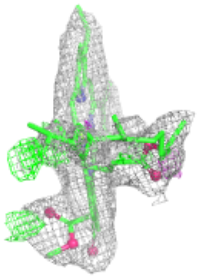


Electron density around CLA b 1222:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

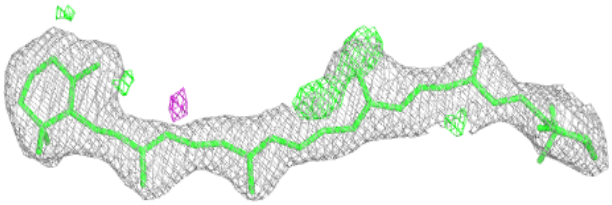


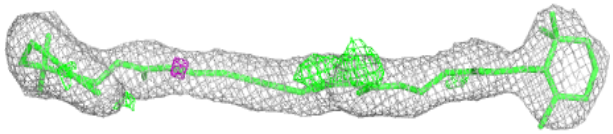


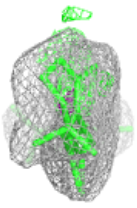


Electron density around BCR b 4005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

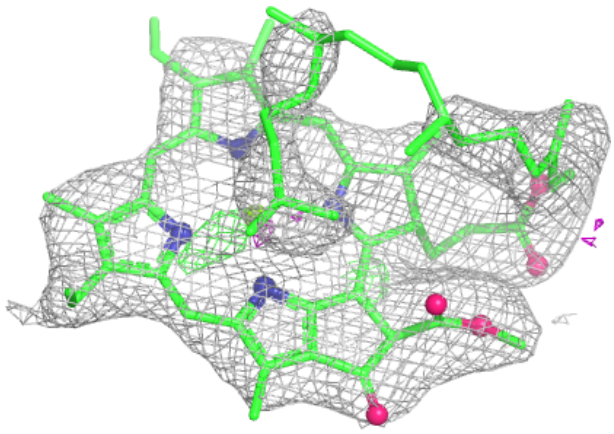


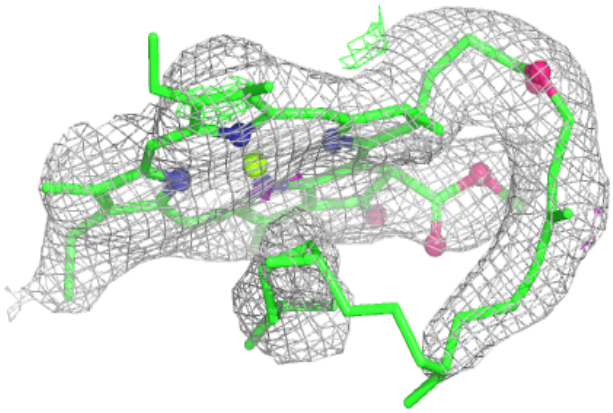


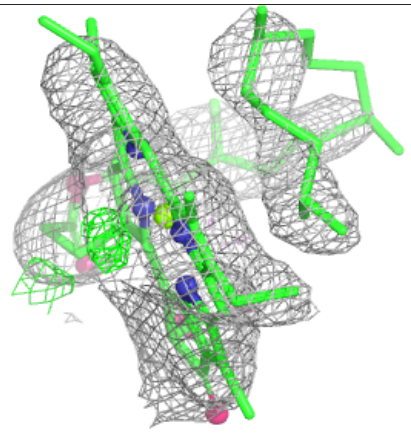


Electron density around CLA 2 1203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

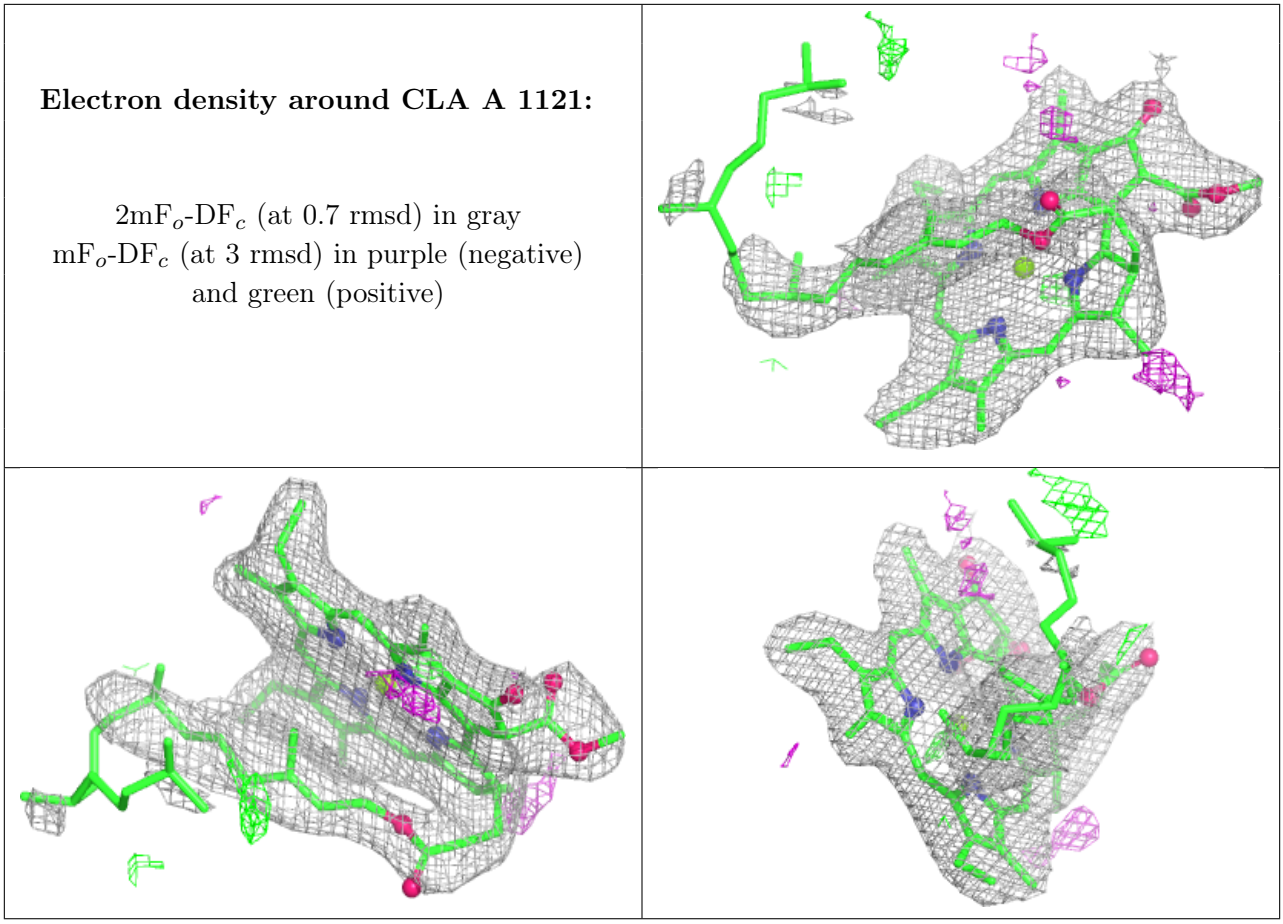






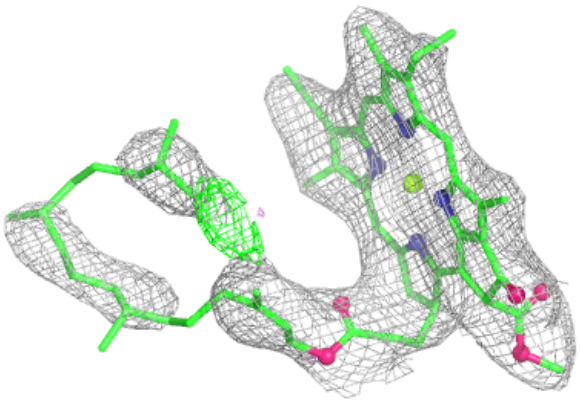
Electron density around CLA A 1121:

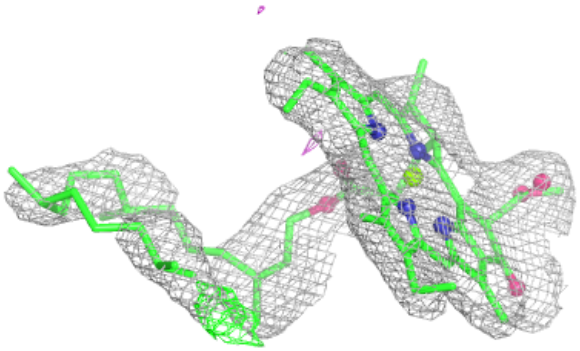
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

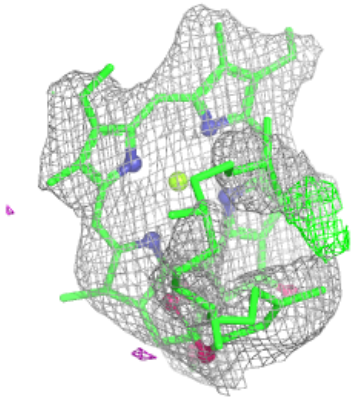


Electron density around CLA b 1228:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

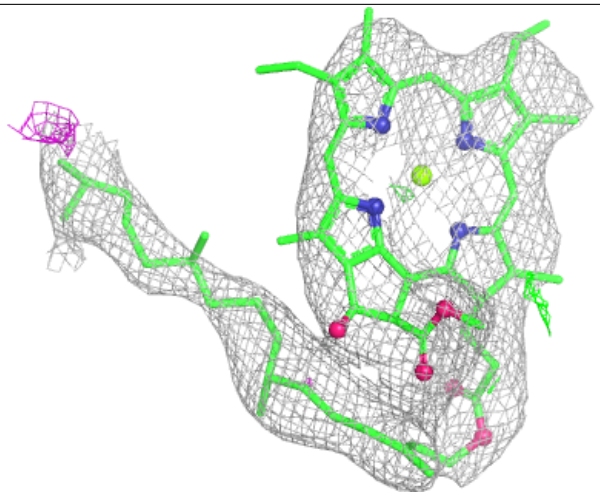


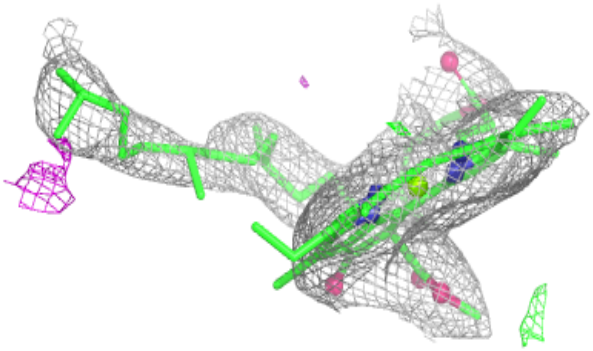


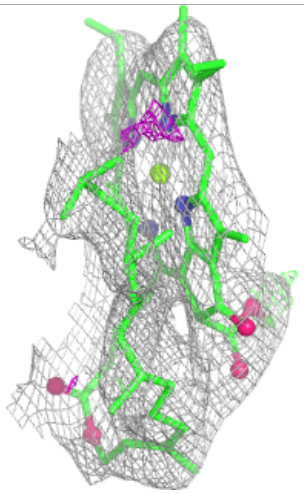


Electron density around CLA a 1123:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

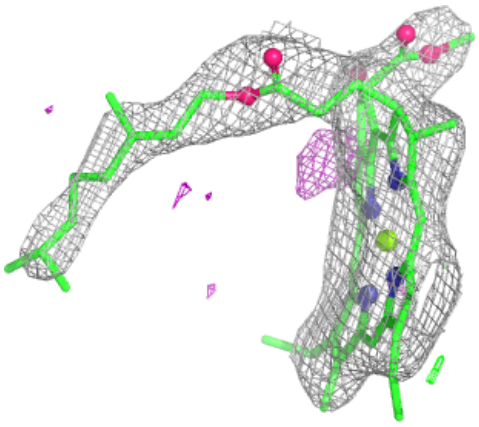


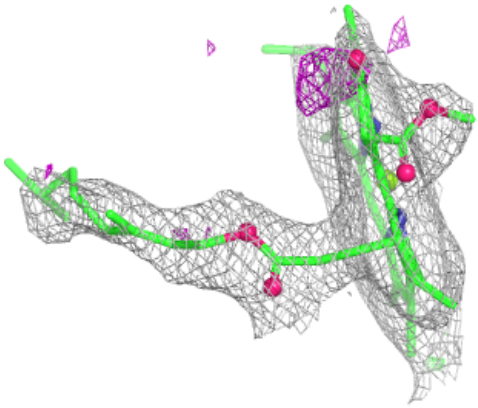


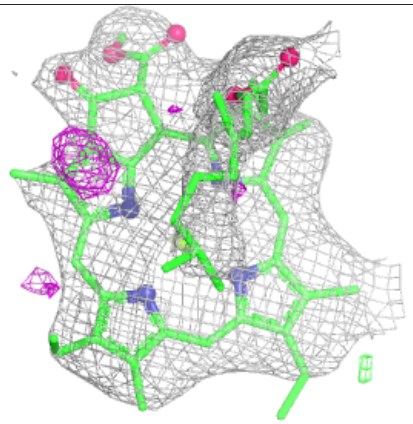


Electron density around CLA 2 1226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

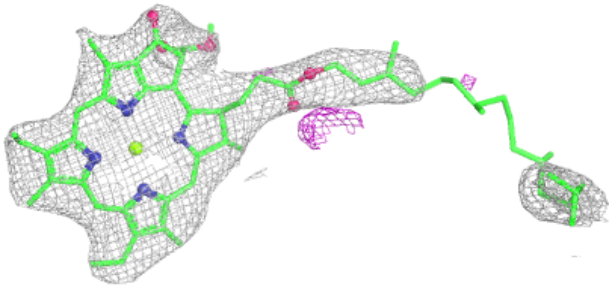


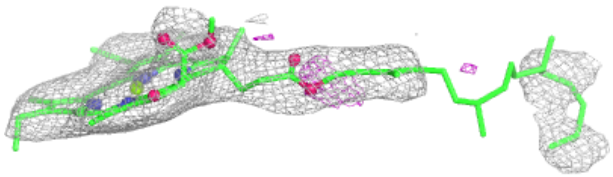


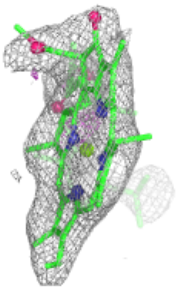


Electron density around CLA a 1135:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

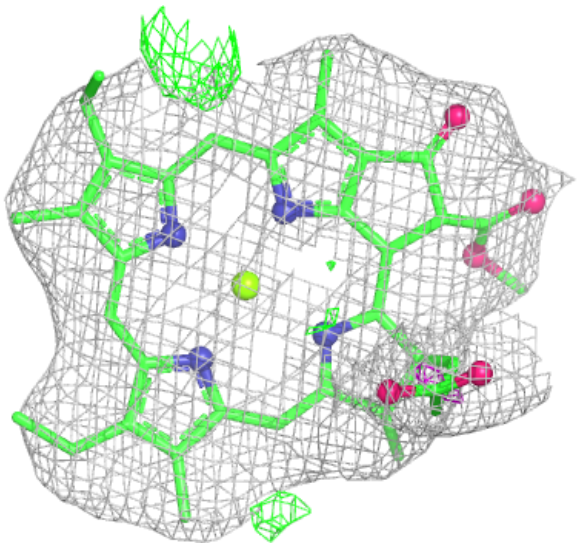


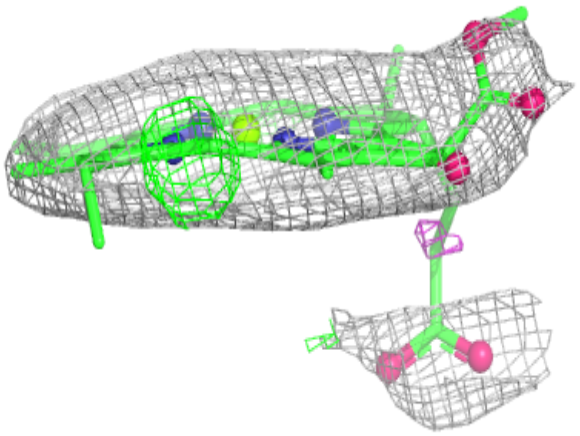


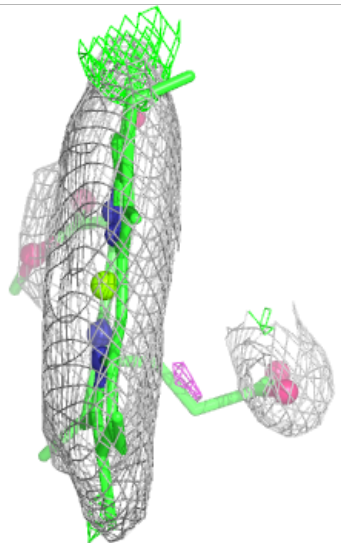


Electron density around CLA 2 1228:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

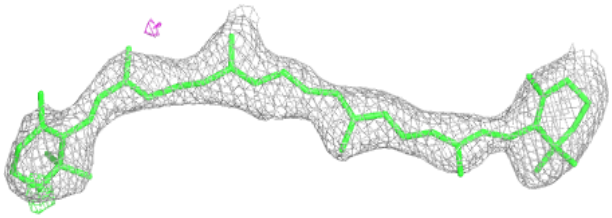


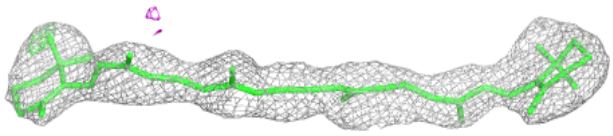


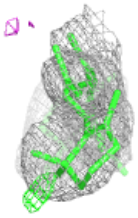


Electron density around BCR B 4010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

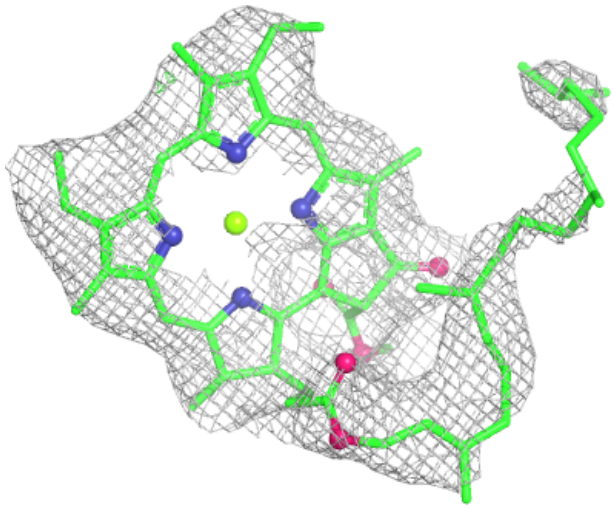


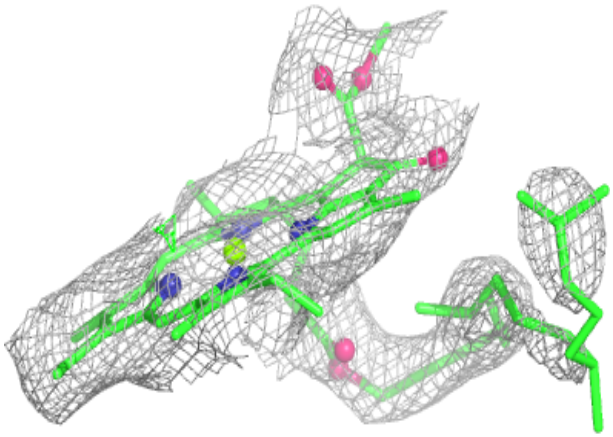


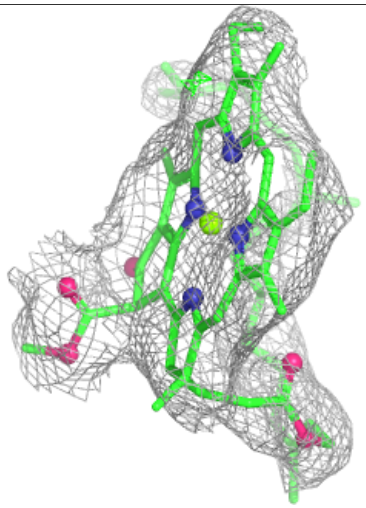


Electron density around CLA 2 1229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

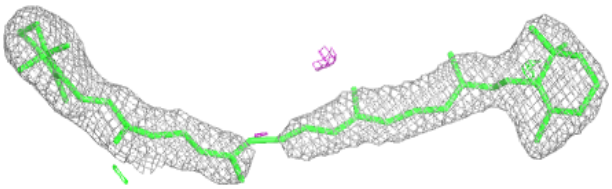


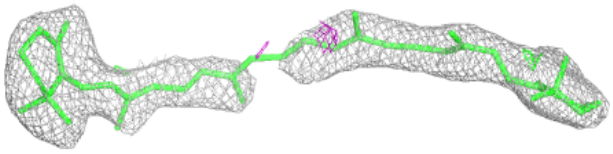


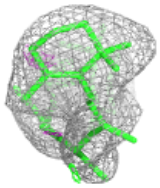


Electron density around BCR B 4014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

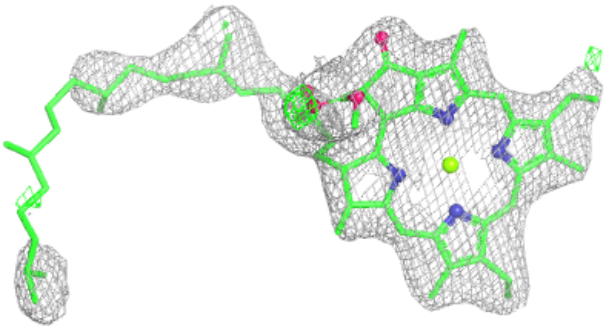


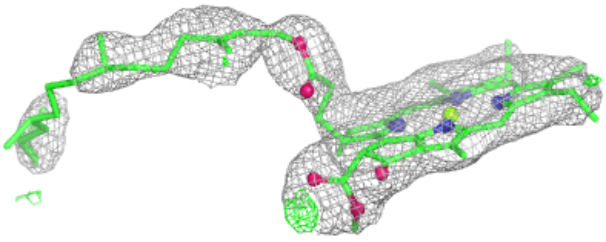


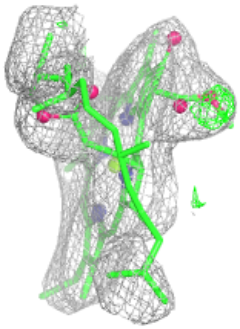


Electron density around CLA b 1220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

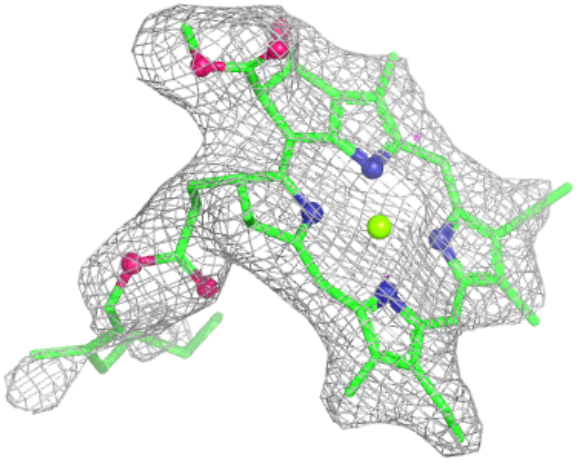


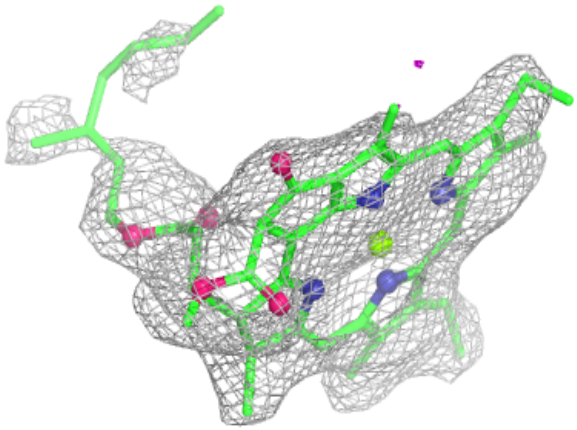


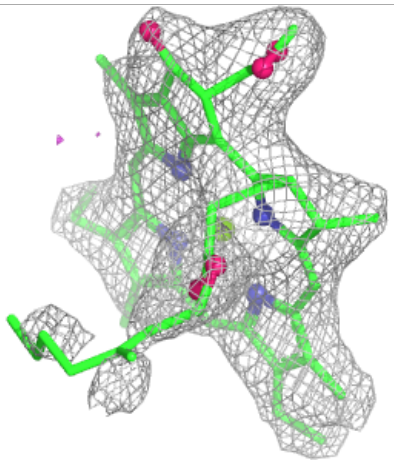


Electron density around CLA A 1108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

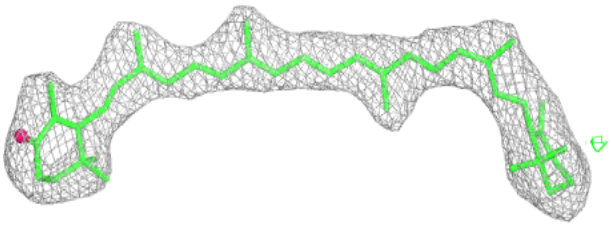


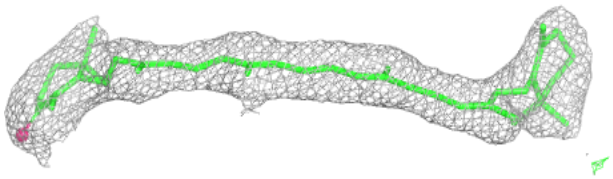


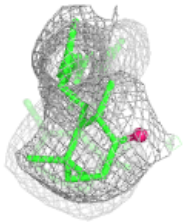


Electron density around ECH M 4021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

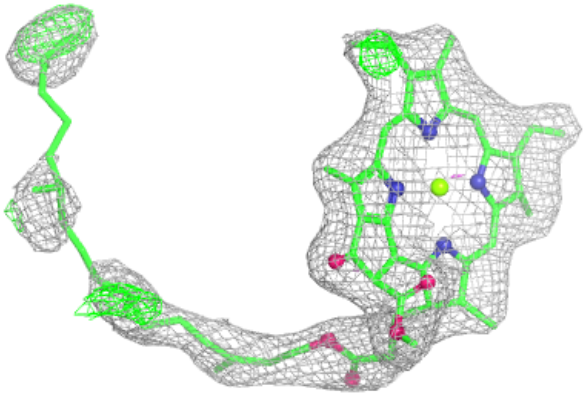


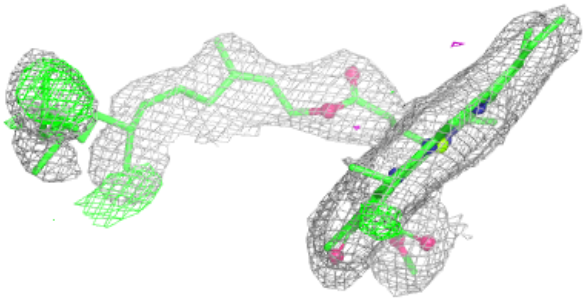


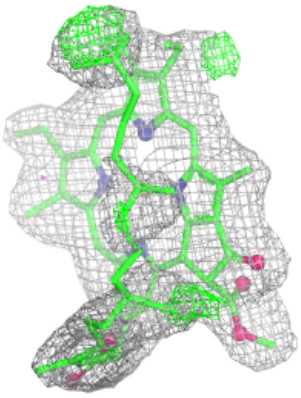


Electron density around CLA K 1401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

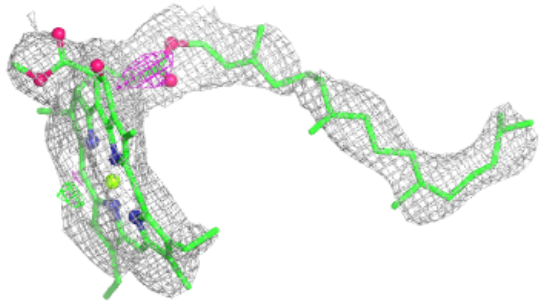


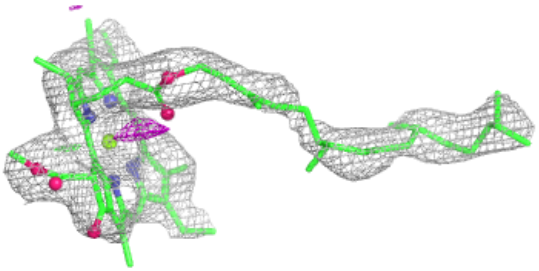


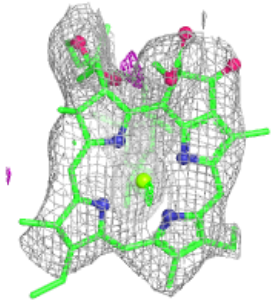


Electron density around CLA a 1128:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

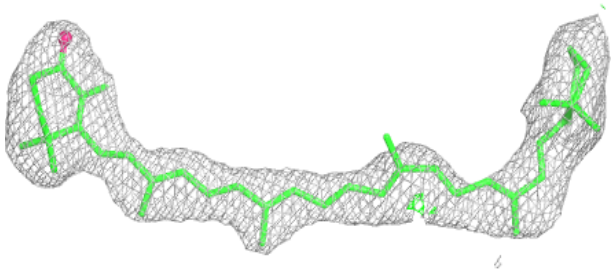


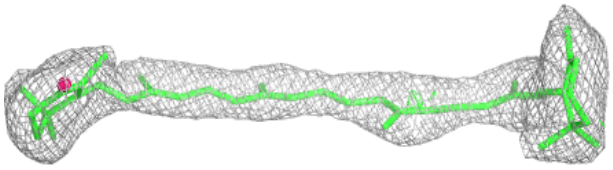


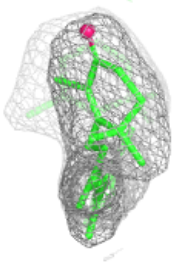


Electron density around ECH i 4020:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

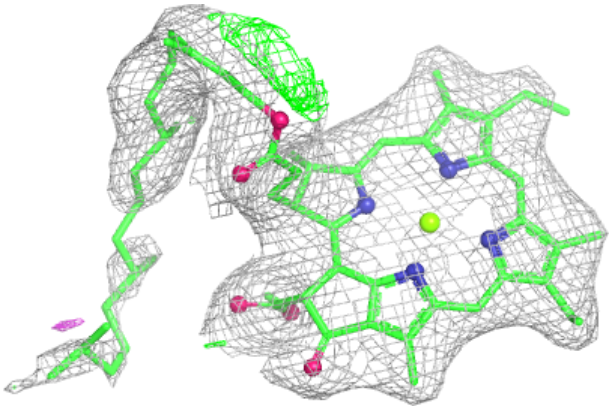


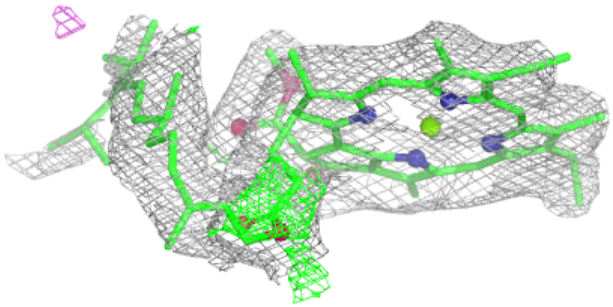


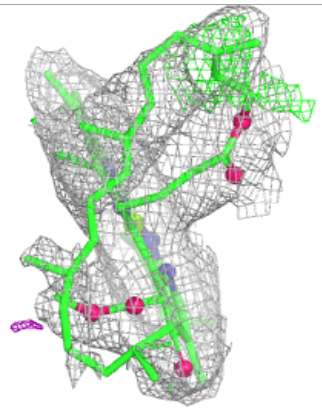


Electron density around CLA K 1402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

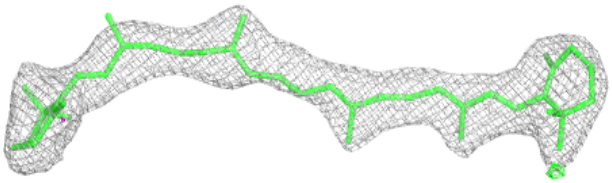


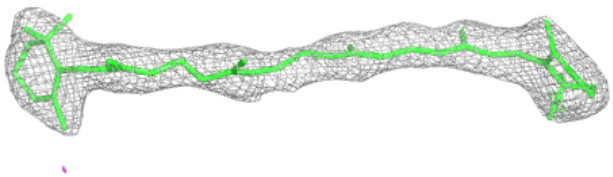


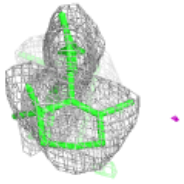


Electron density around BCR 2 4017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

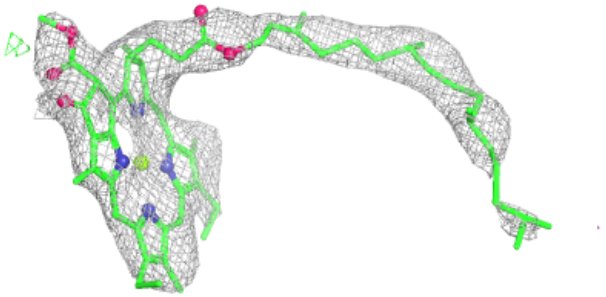


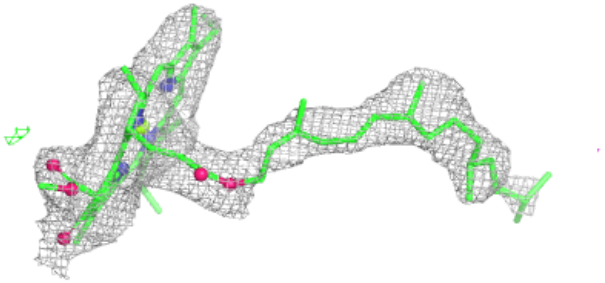


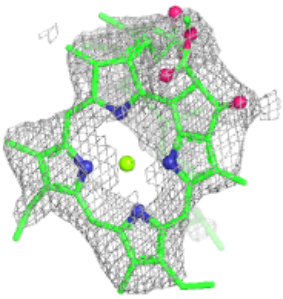


Electron density around CLA 1 1133:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

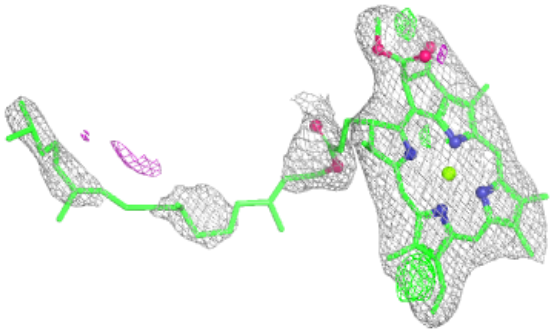


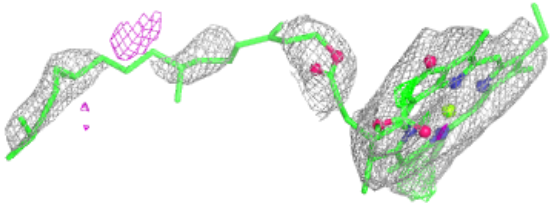


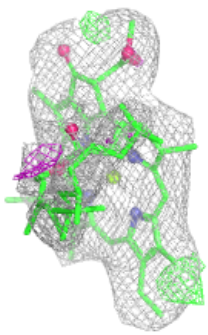


Electron density around CLA a 1119:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

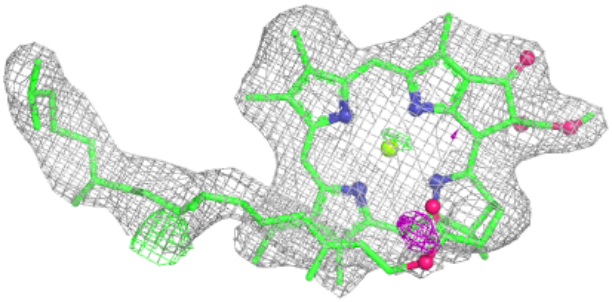


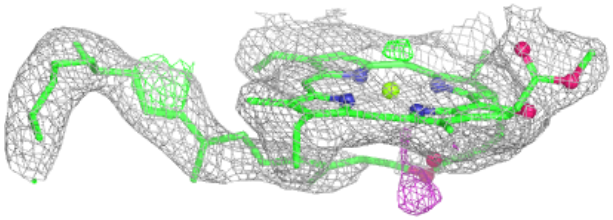


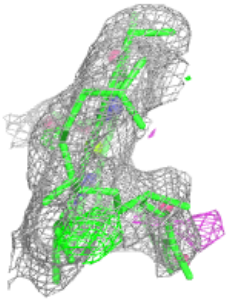


Electron density around CLA b 1209:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

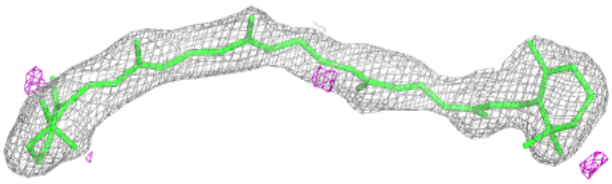


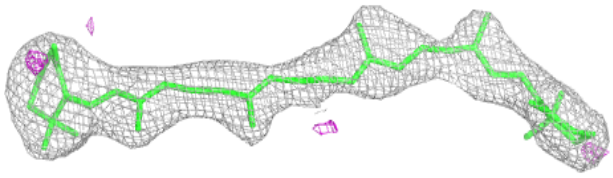


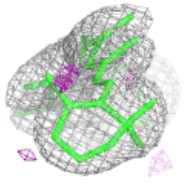


Electron density around BCR h 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

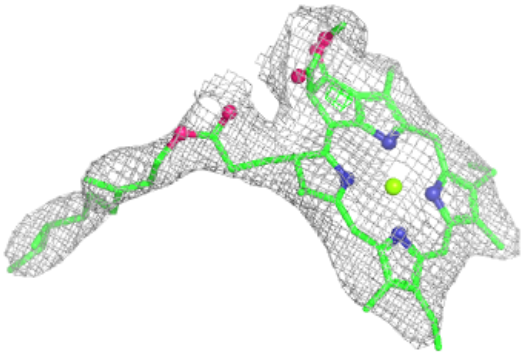


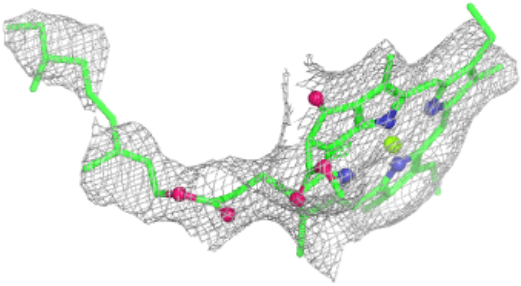


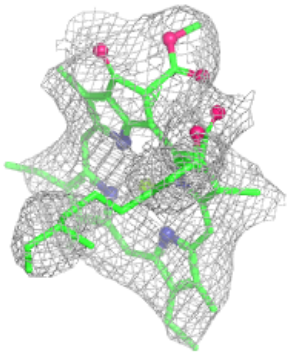


Electron density around CLA 1 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

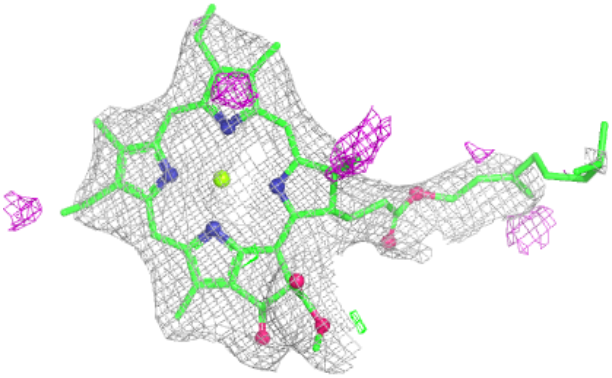


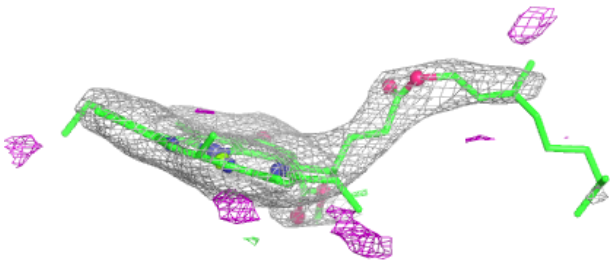


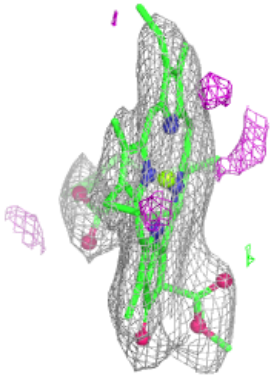


Electron density around CLA a 1124:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

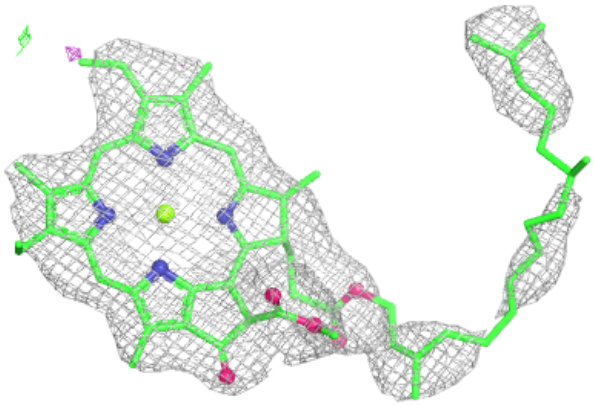


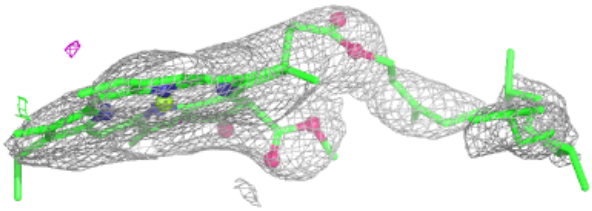


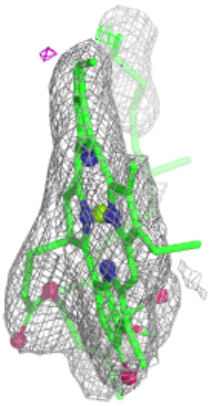


Electron density around CLA 1 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

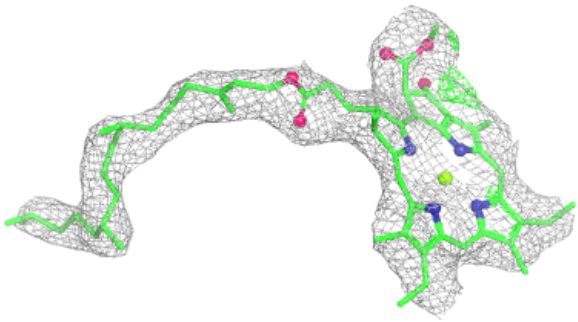


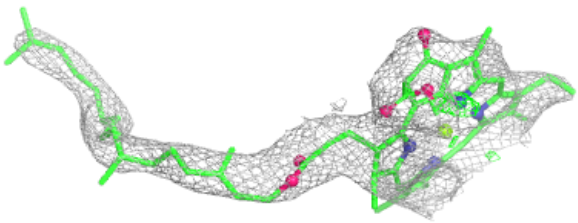


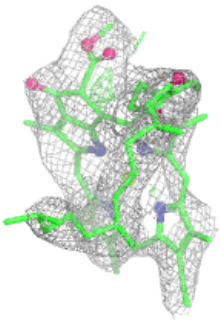


Electron density around CLA 1 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

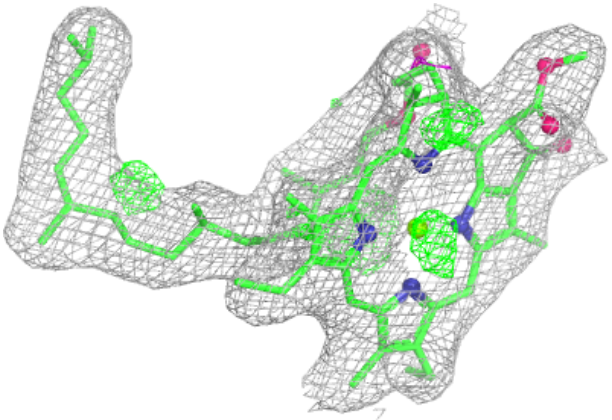


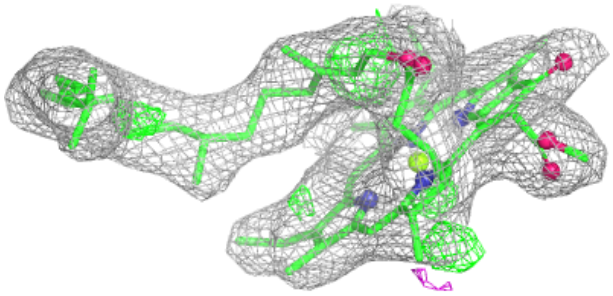


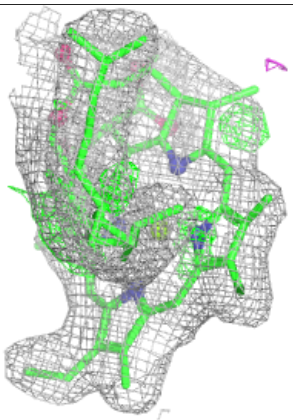


Electron density around CLA 2 1237:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

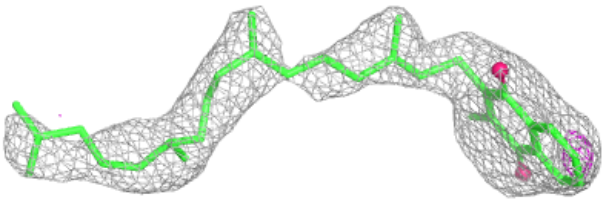


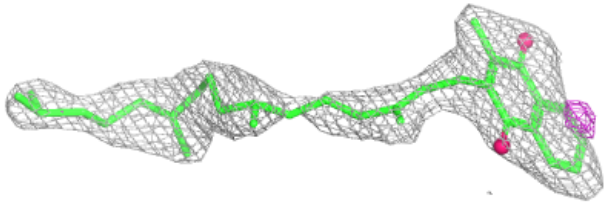


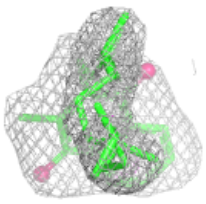


Electron density around PQN a 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

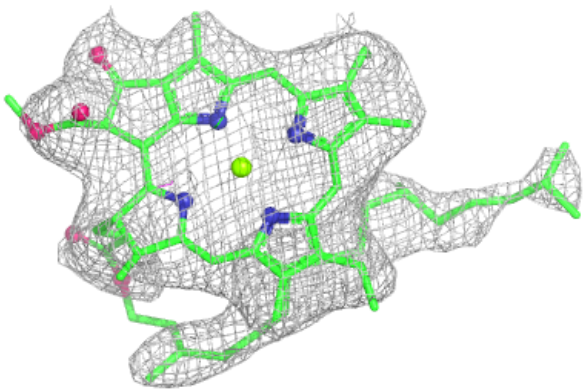


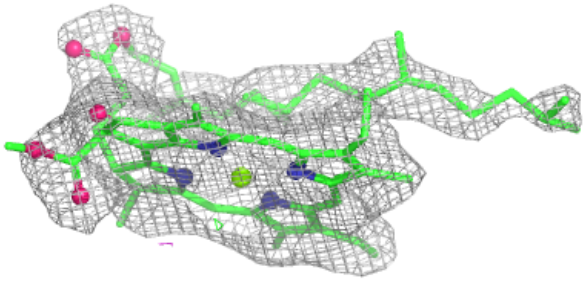


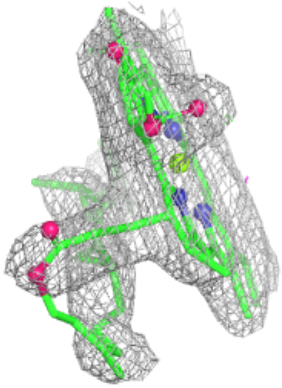


Electron density around CLA b 1218:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

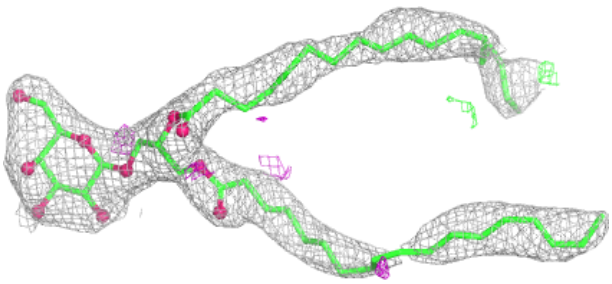


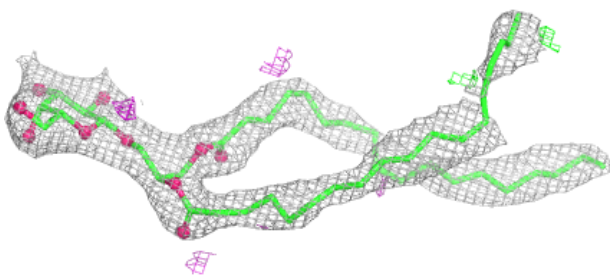


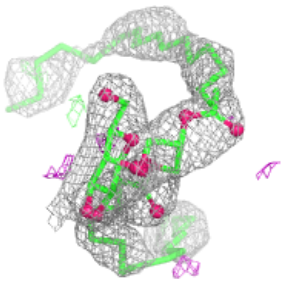


Electron density around LMG b 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

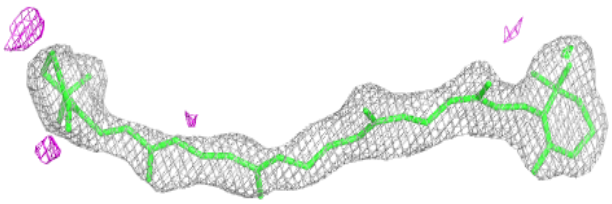


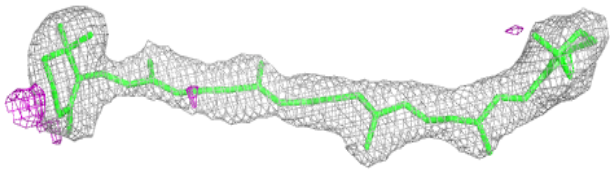


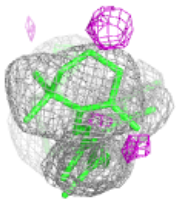


Electron density around BCR i 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

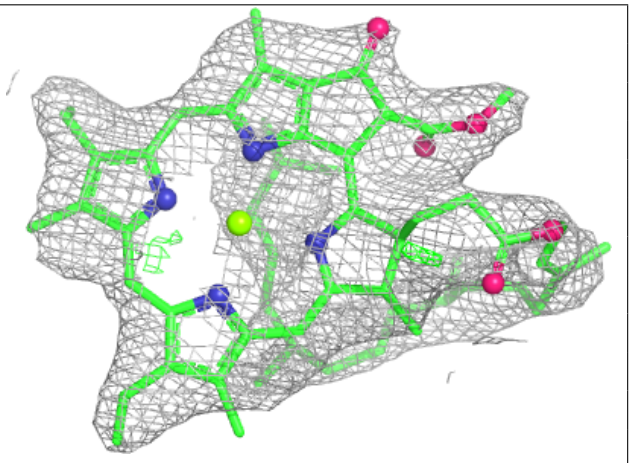


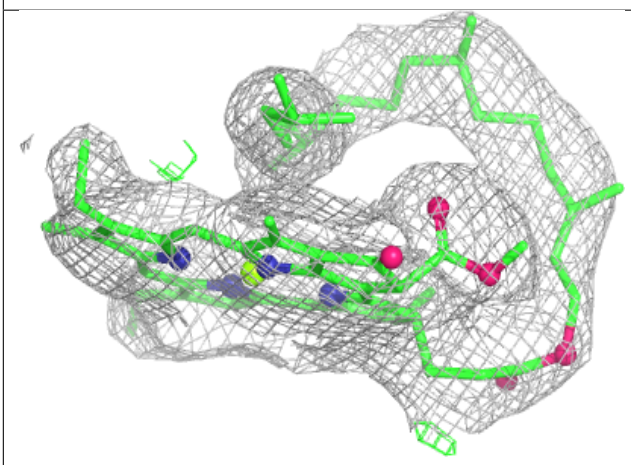


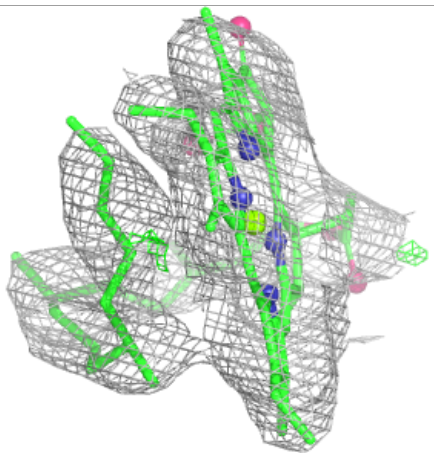


Electron density around CLA 1 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

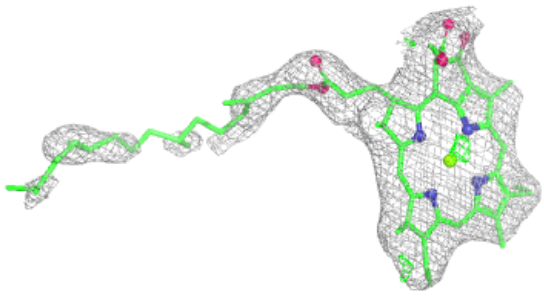


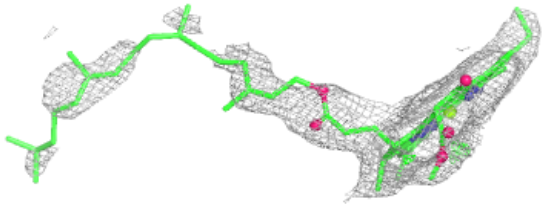


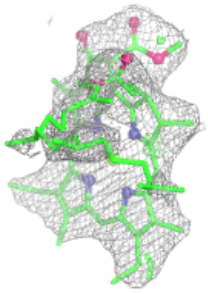


Electron density around CLA b 1230:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

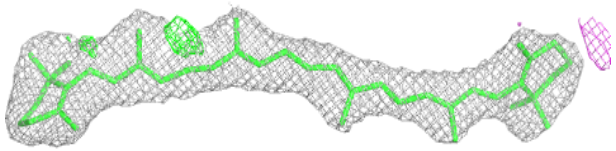


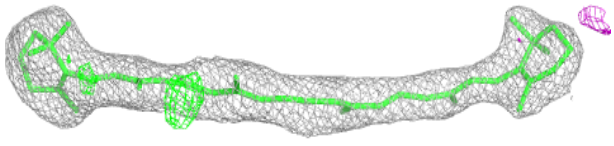


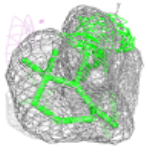


Electron density around BCR A 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

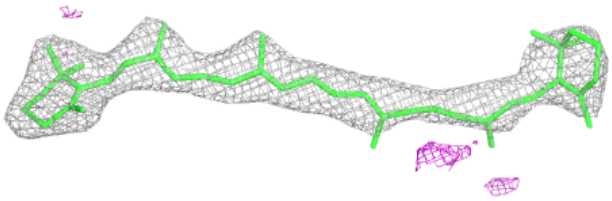


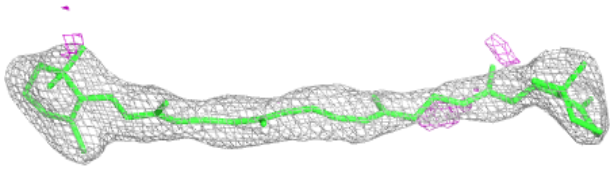


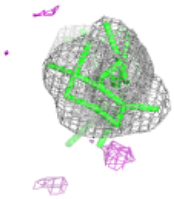


Electron density around BCR A 4003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

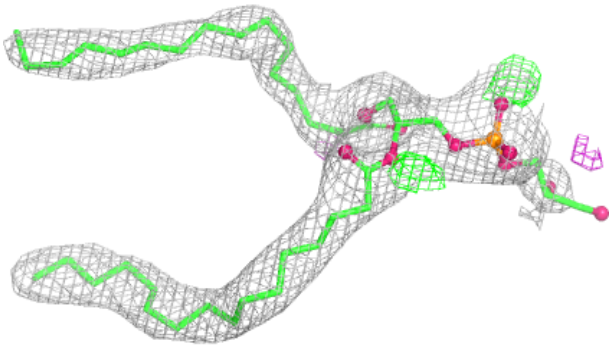


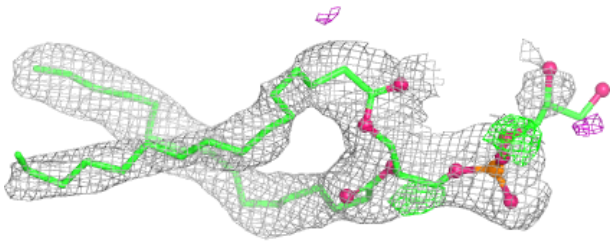


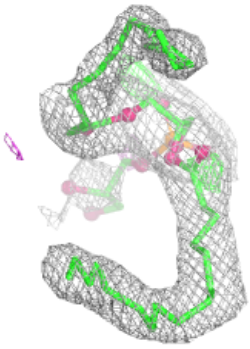


Electron density around LHG a 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

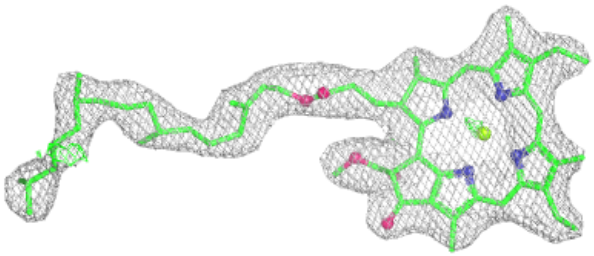


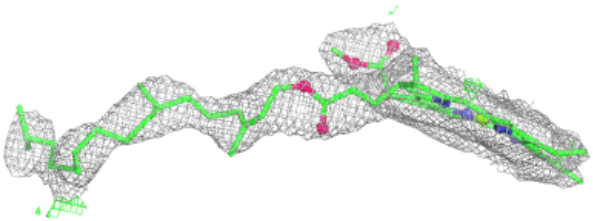


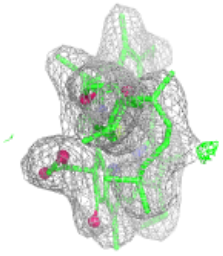


Electron density around CLA A 1139:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

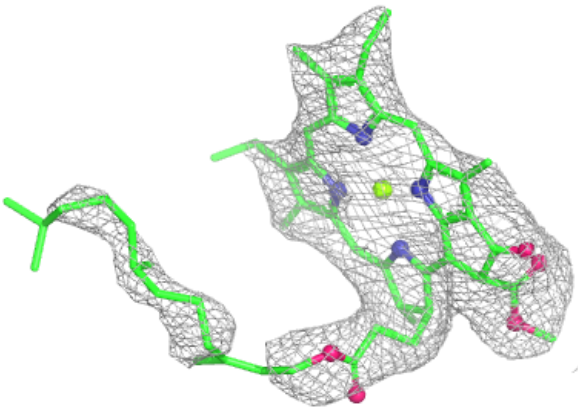


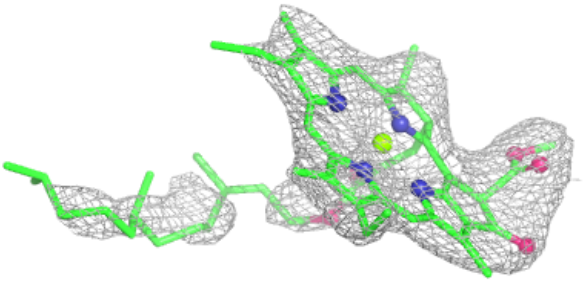


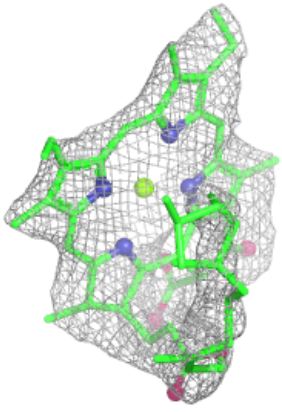


Electron density around CLA 1 1122:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

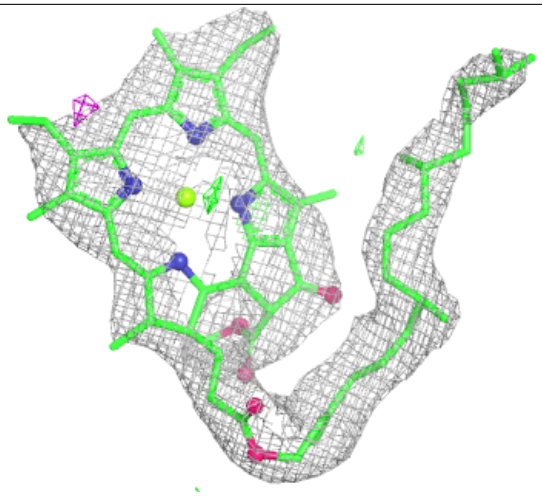


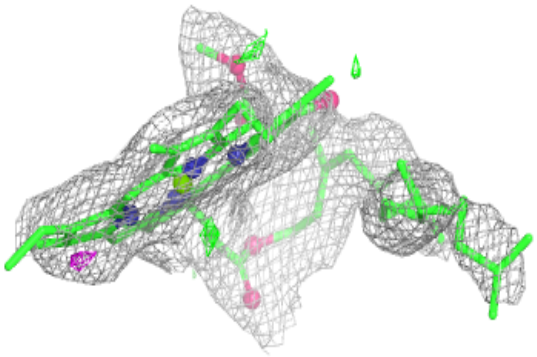


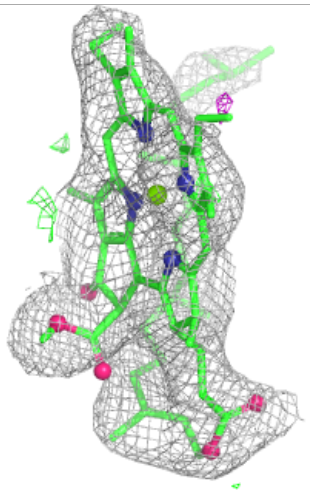


Electron density around CLA 1 1123:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

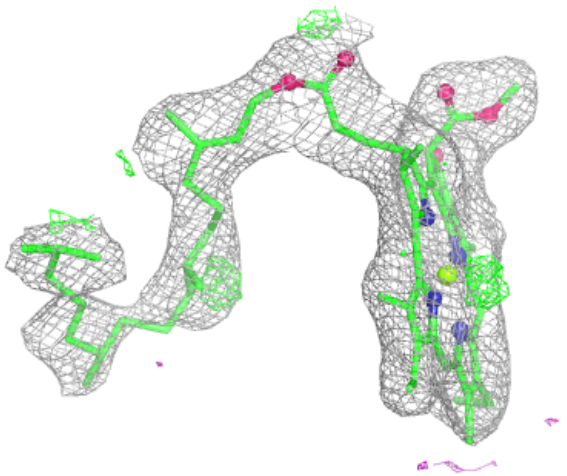




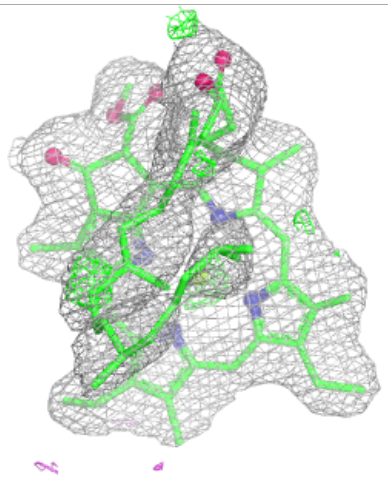


Electron density around CLA A 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

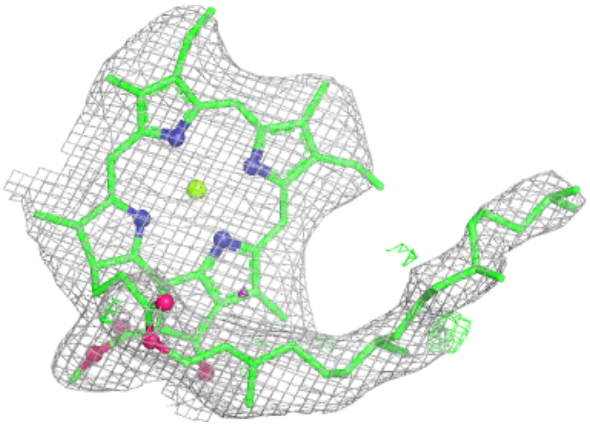


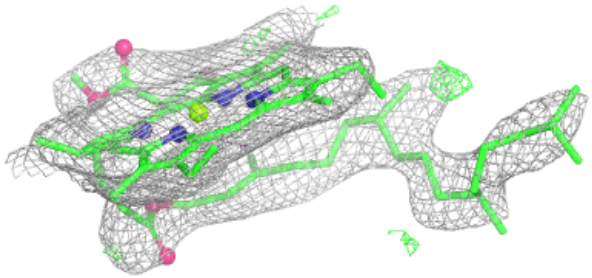


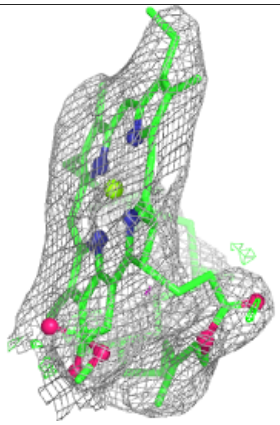


Electron density around CLA a 1127:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

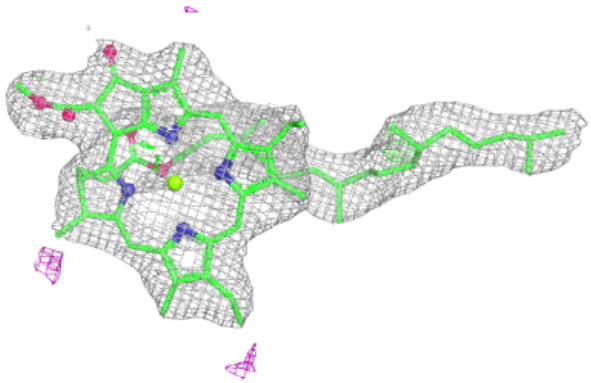


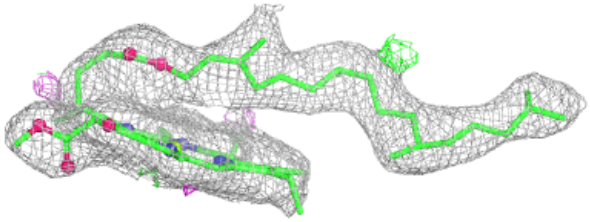


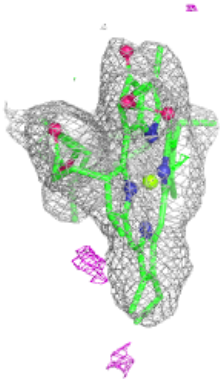


Electron density around CLA A 1115:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

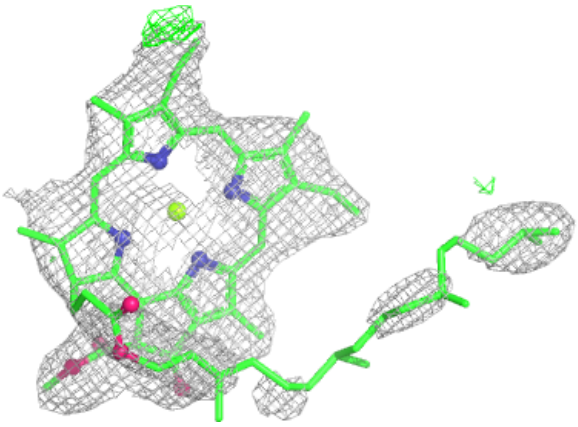


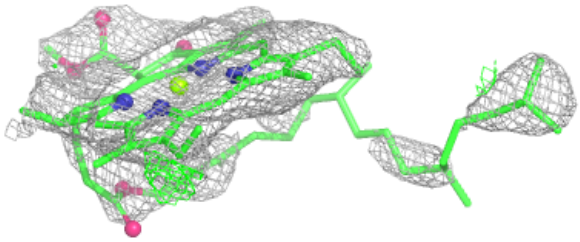


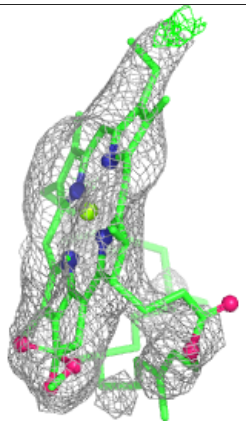


Electron density around CLA 1 1127:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

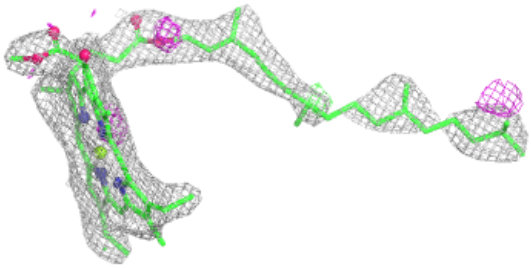


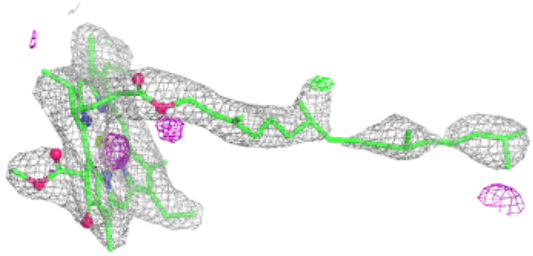


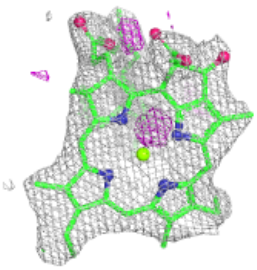


Electron density around CLA b 1226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

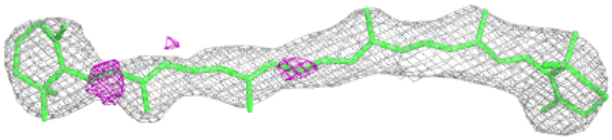


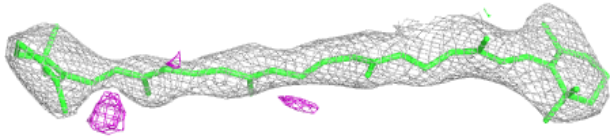


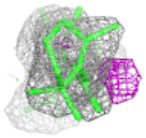


Electron density around BCR A 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

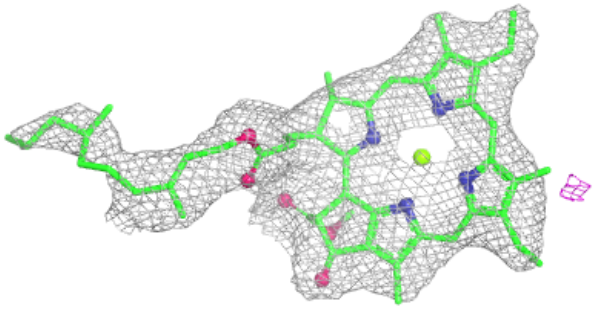


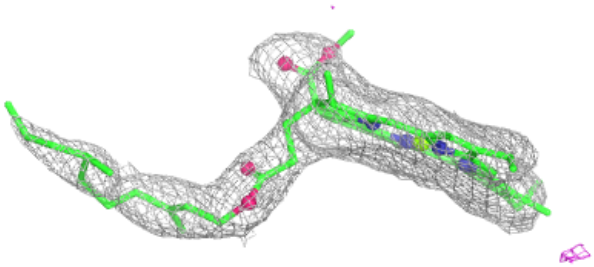


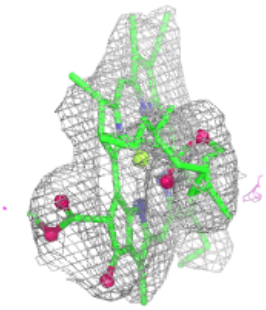


Electron density around CLA B 1220:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

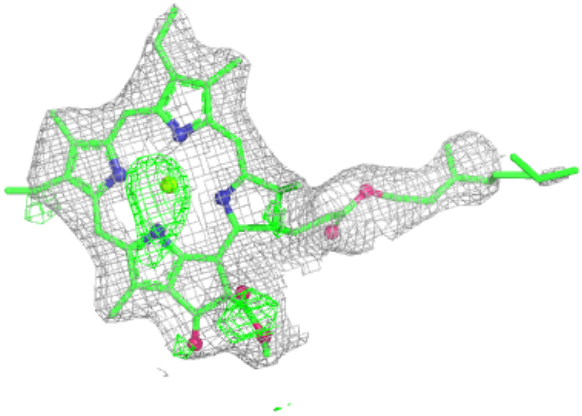


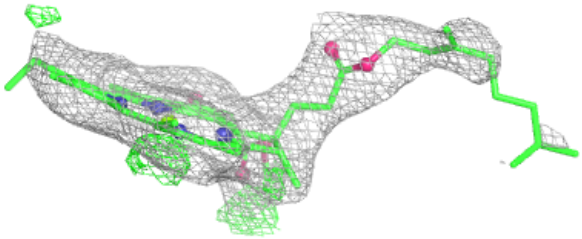


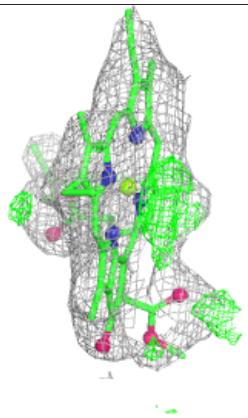


Electron density around CLA B 1222:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

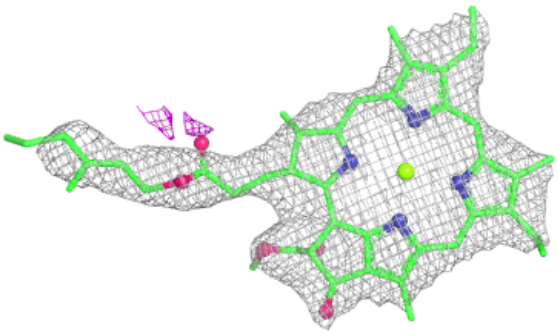


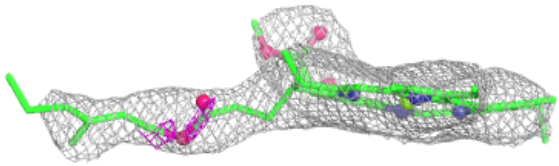


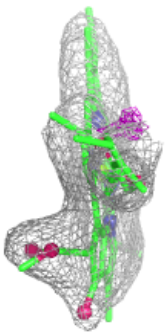


Electron density around CLA 1 1135:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

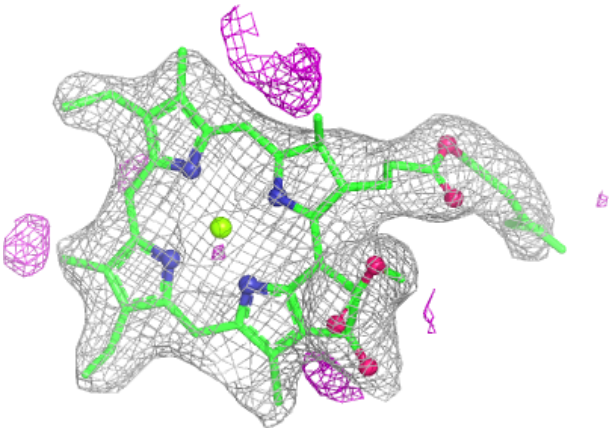


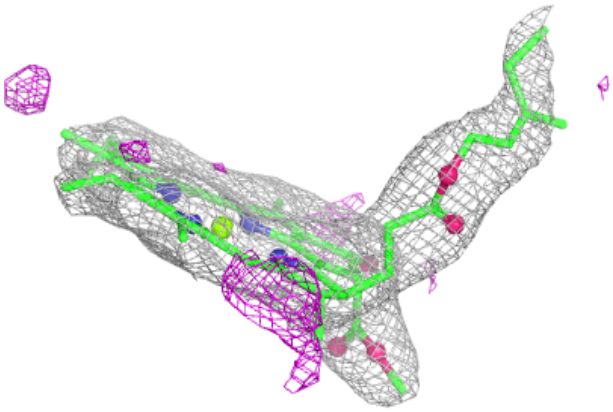


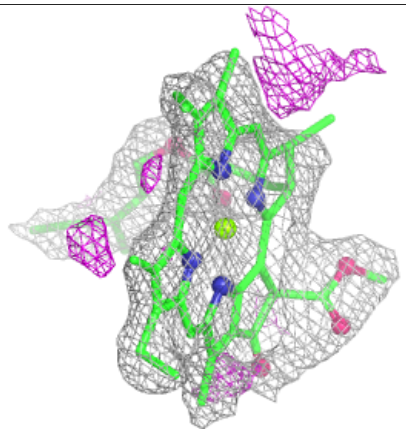


Electron density around CLA 1 1137:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

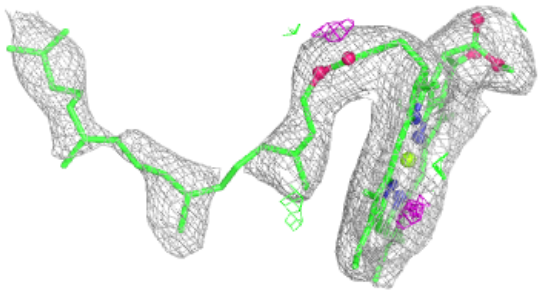


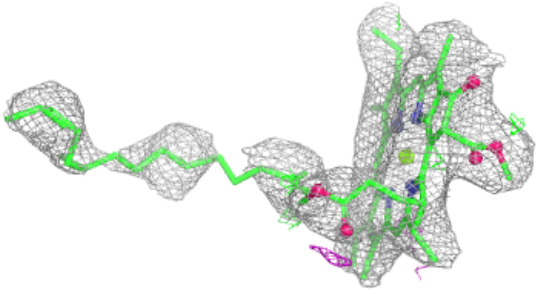


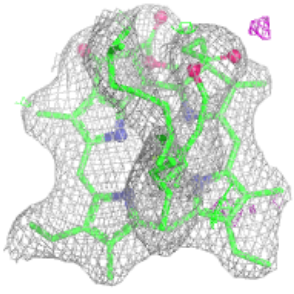


Electron density around CLA A 1120:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

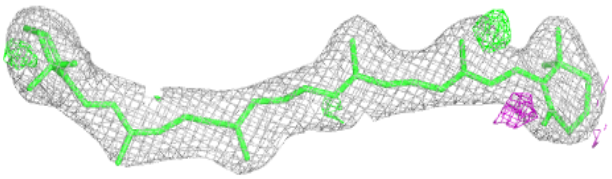


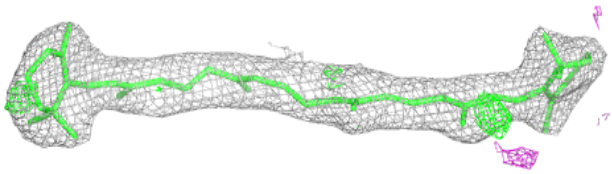


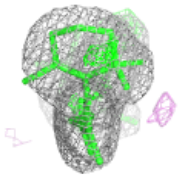


Electron density around BCR B 4017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

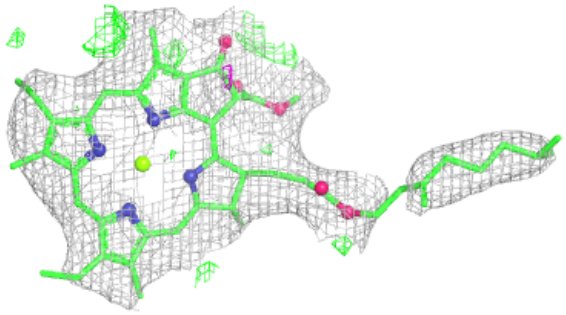


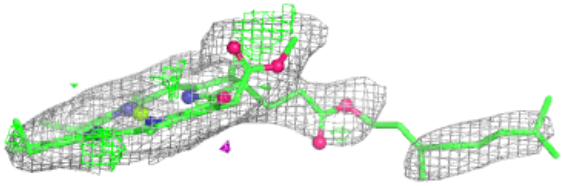


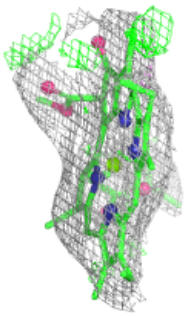


Electron density around CLA 2 1223:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

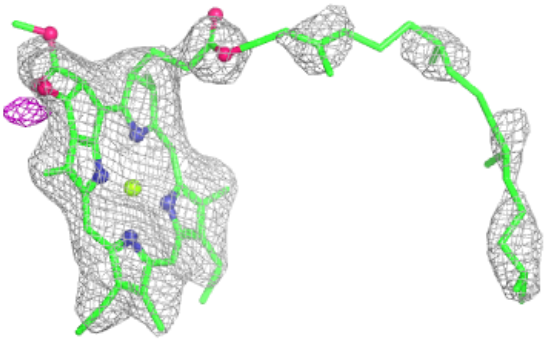


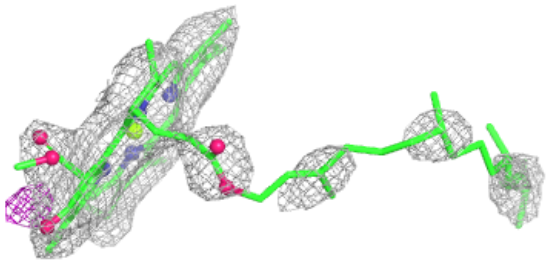


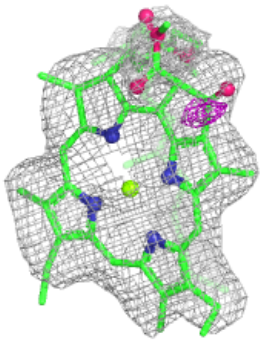


Electron density around CLA 1 1140:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

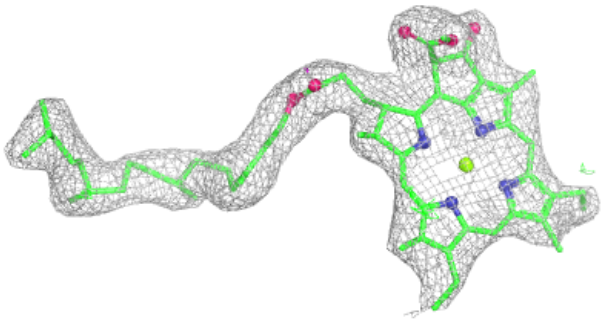


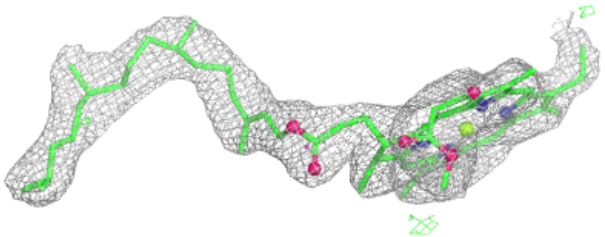


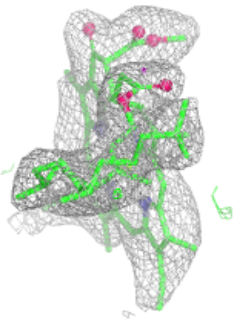


Electron density around CLA B 1210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

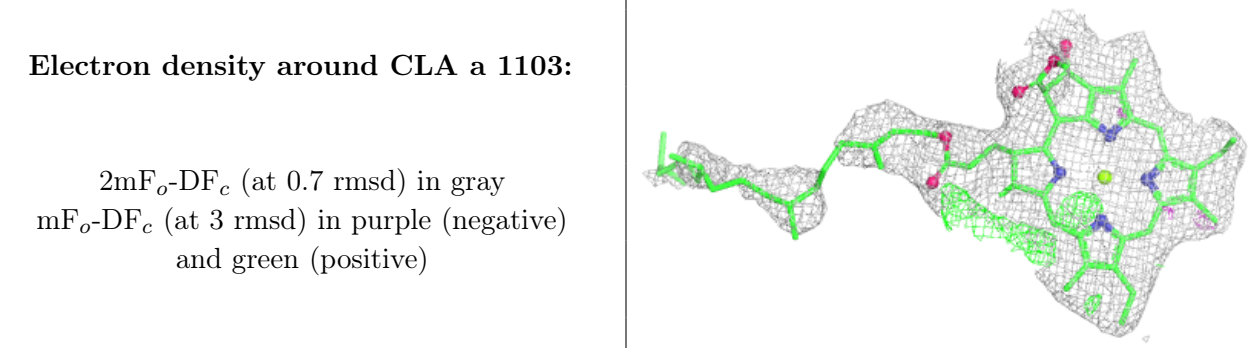






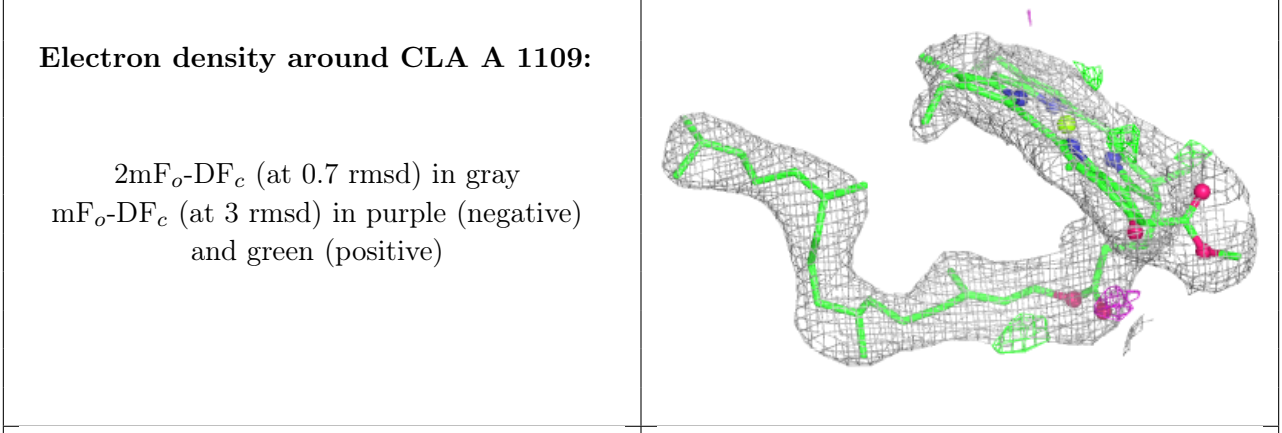
Electron density around CLA a 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



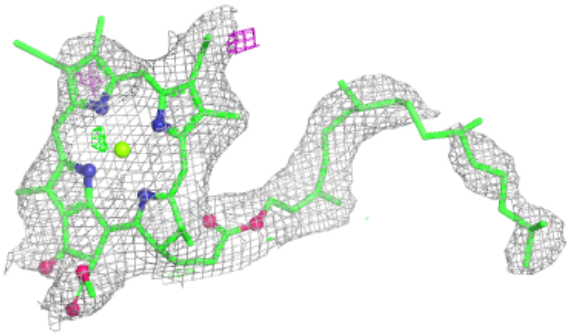
Electron density around CLA A 1109:

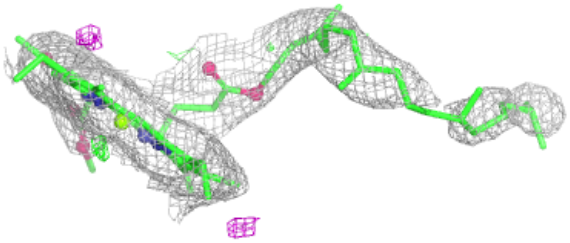
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

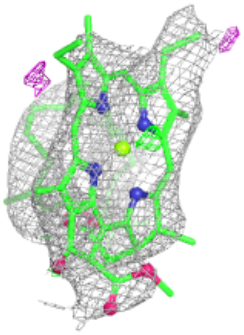


Electron density around CLA a 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

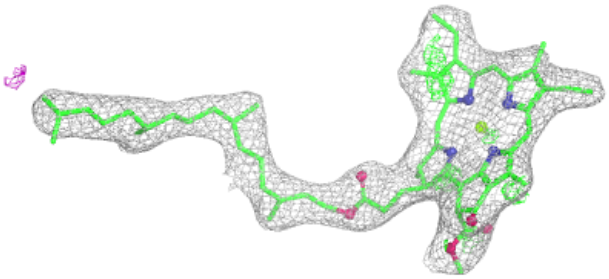


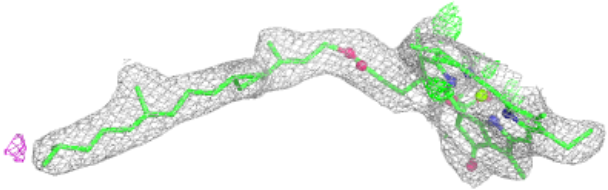


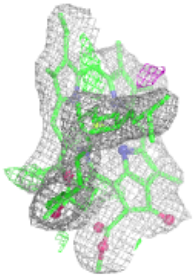


Electron density around CLA 2 1022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

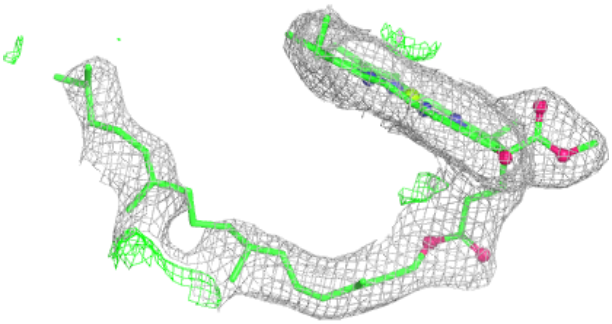


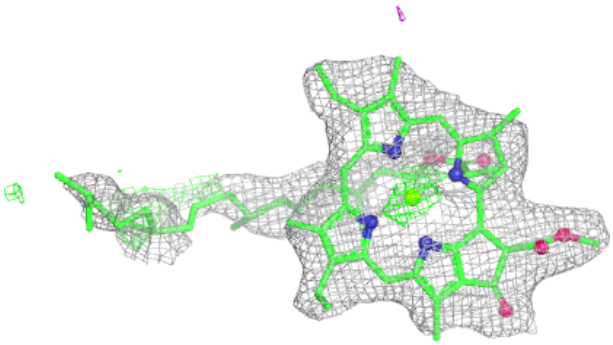


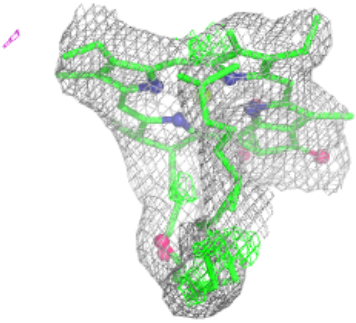


Electron density around CLA a 1130:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

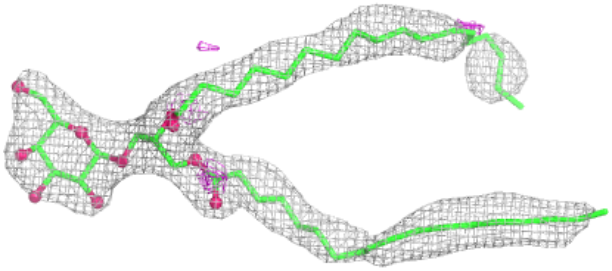


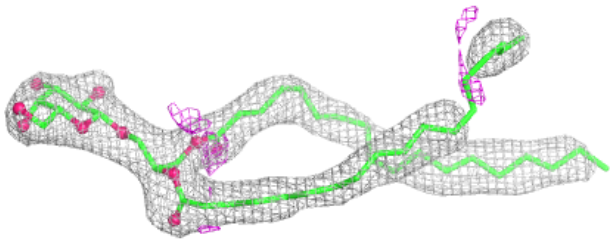


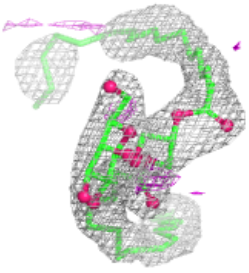


Electron density around LMG B 5002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

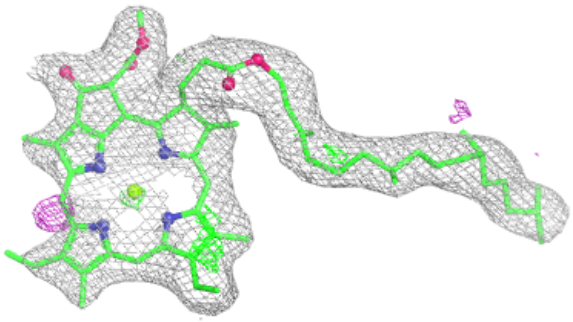


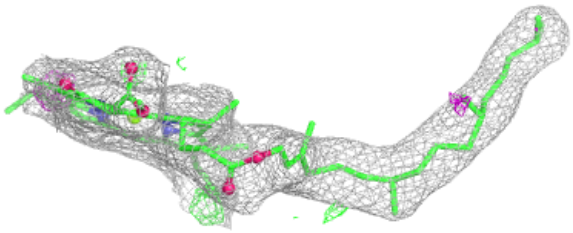


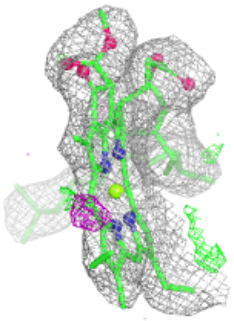


Electron density around CLA 2 1023:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

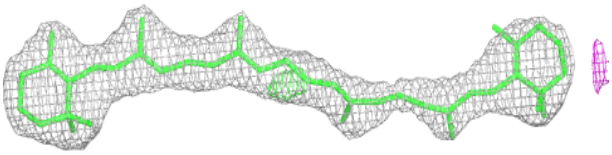


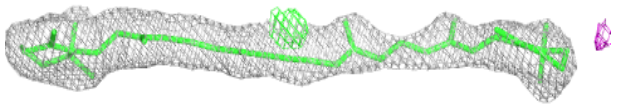


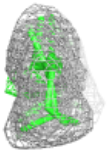


Electron density around BCR 0 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

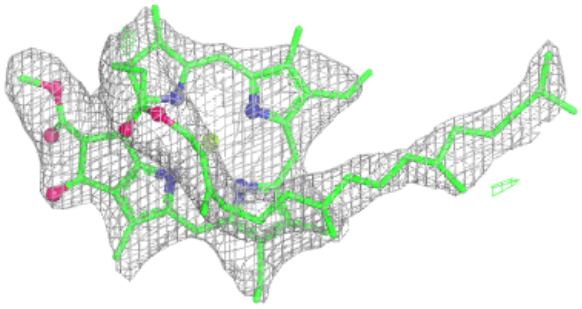


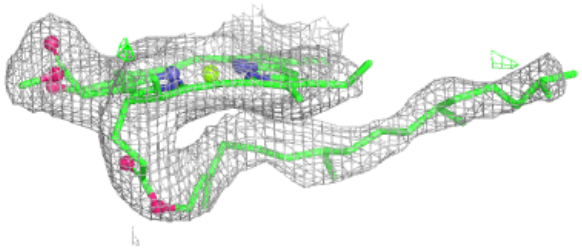


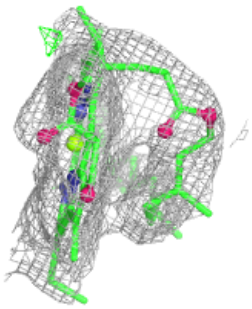


Electron density around CLA a 1138:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

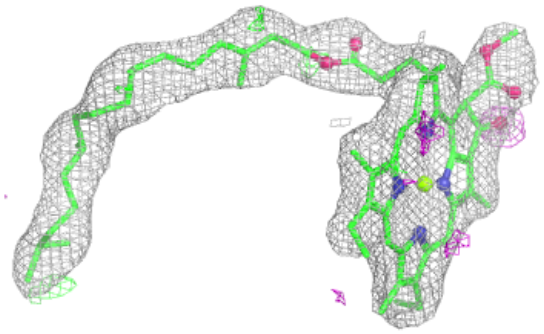


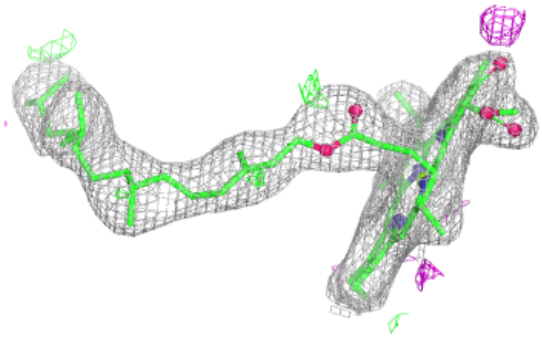


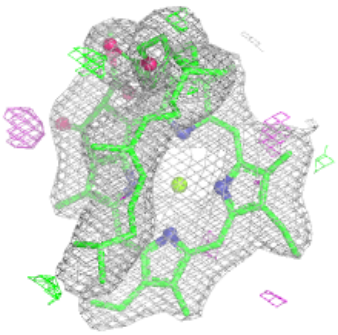


Electron density around CLA A 1133:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

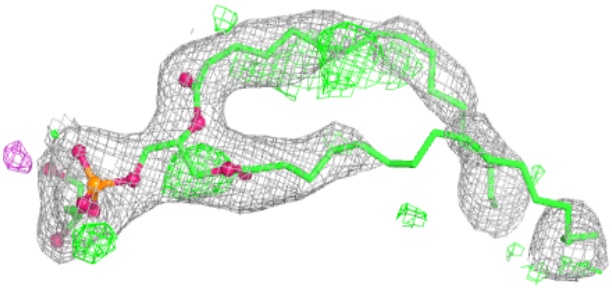


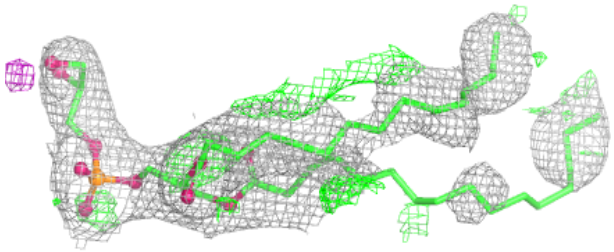


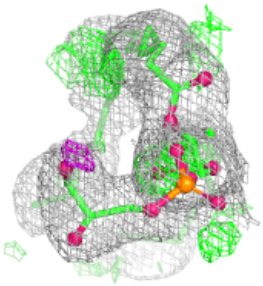


Electron density around LHG A 5003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

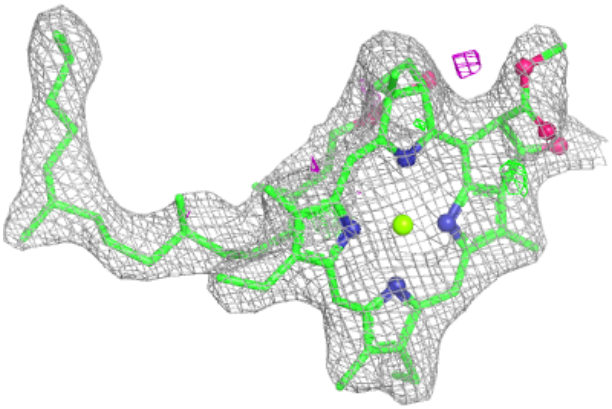


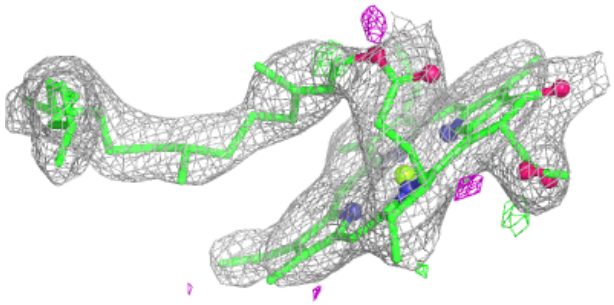


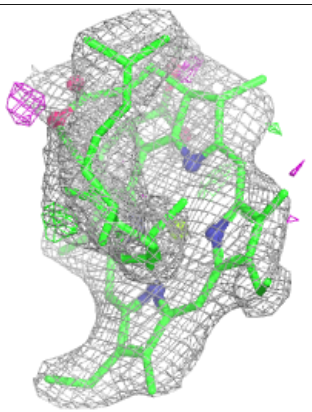


Electron density around CLA b 1237:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

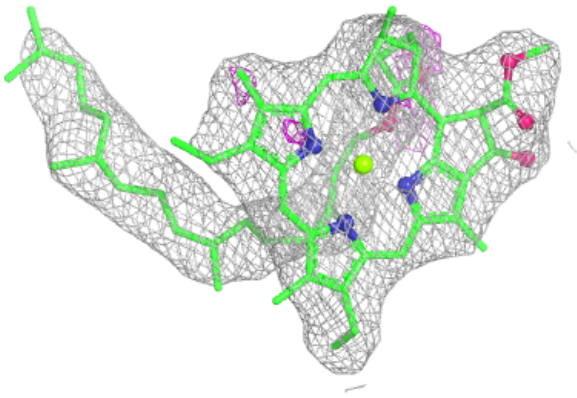


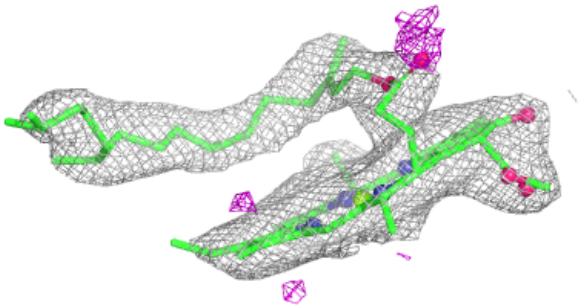




Electron density around CLA 2 1204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

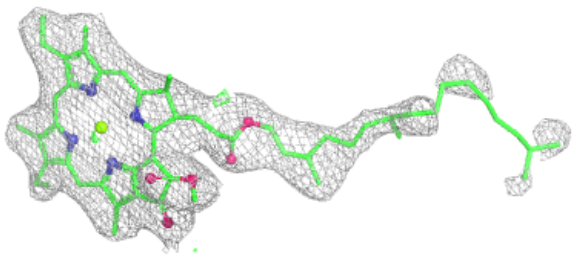


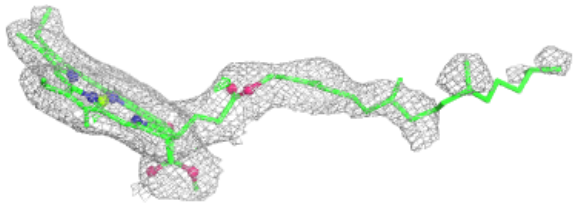


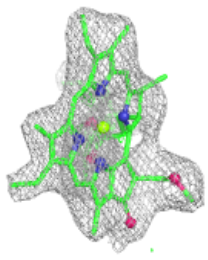


Electron density around CLA A 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

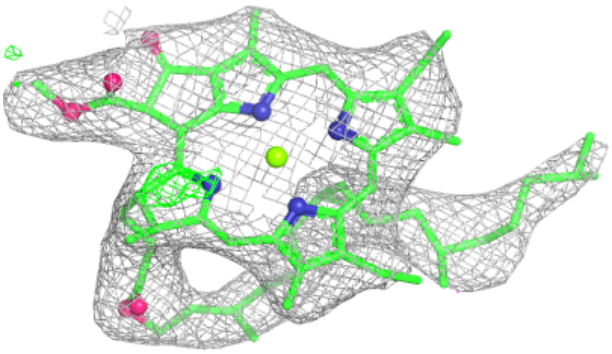


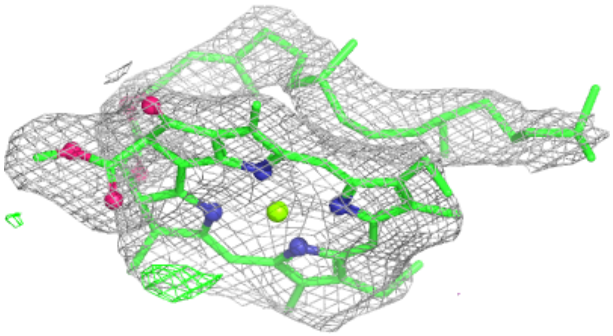


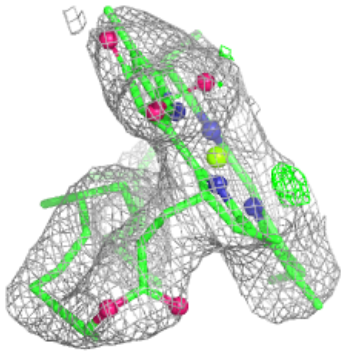


Electron density around CLA B 1214:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

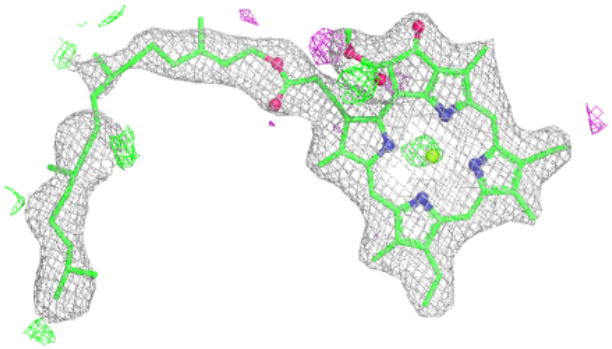


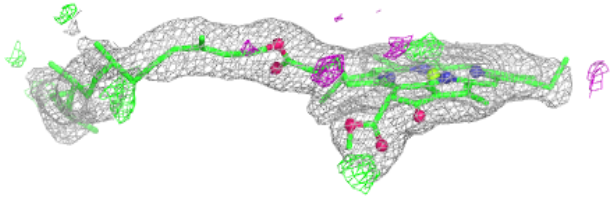


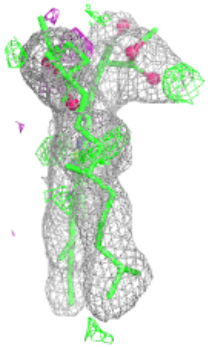


Electron density around CLA A 1135:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

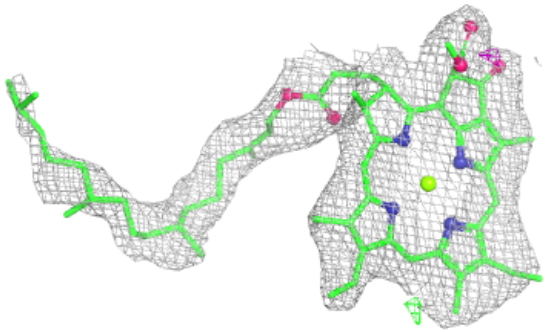


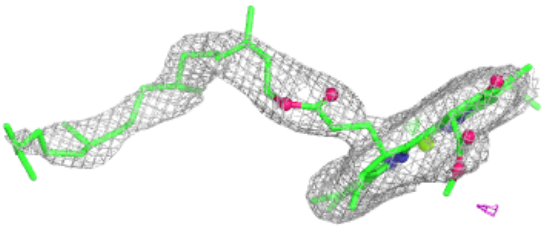


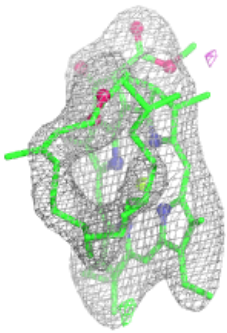


Electron density around CLA 1 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

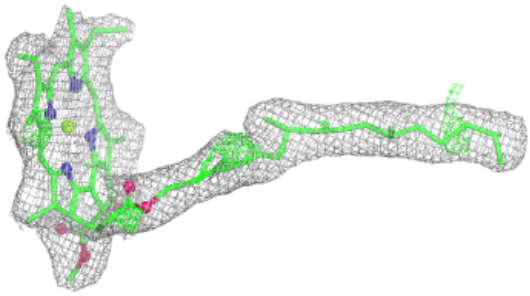


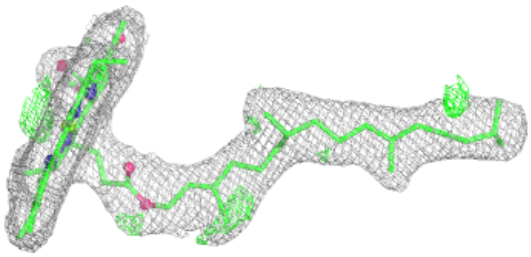


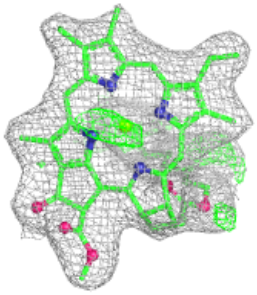


Electron density around CLA b 1225:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

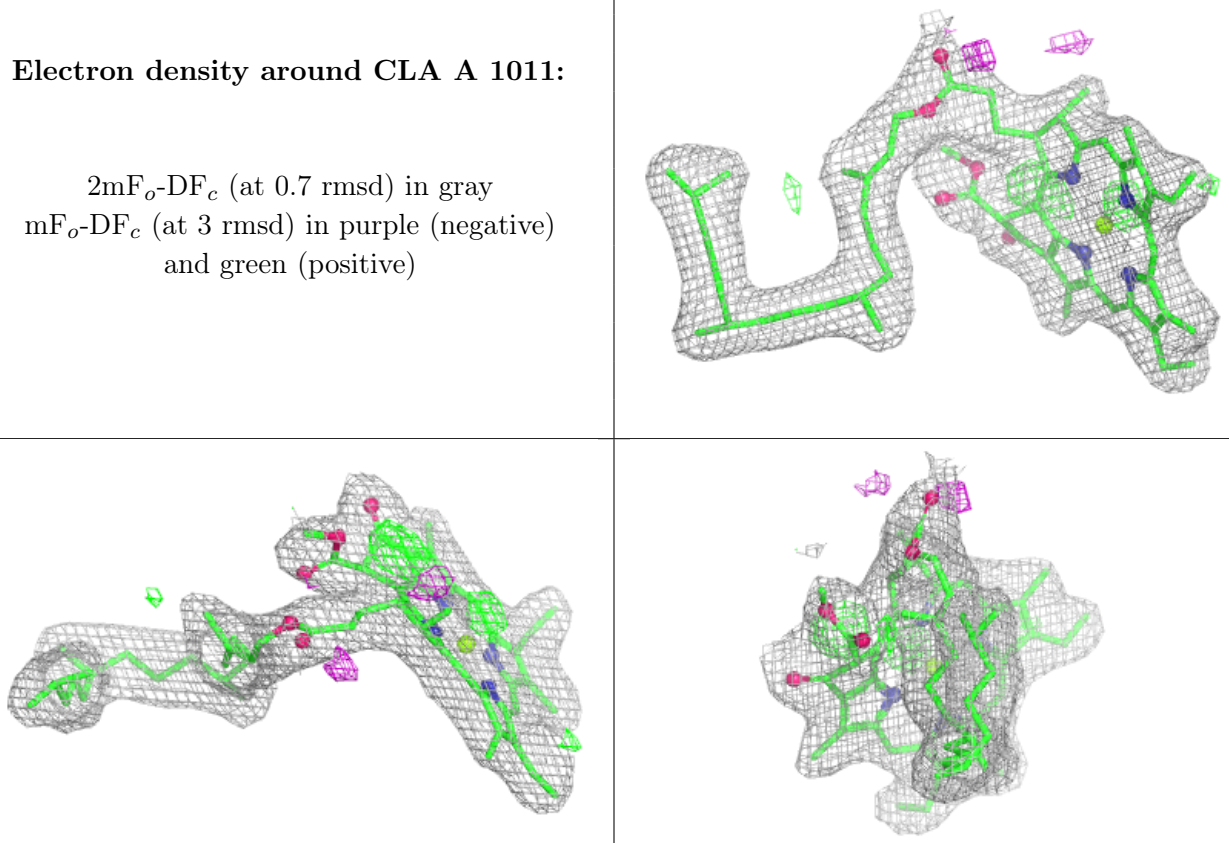






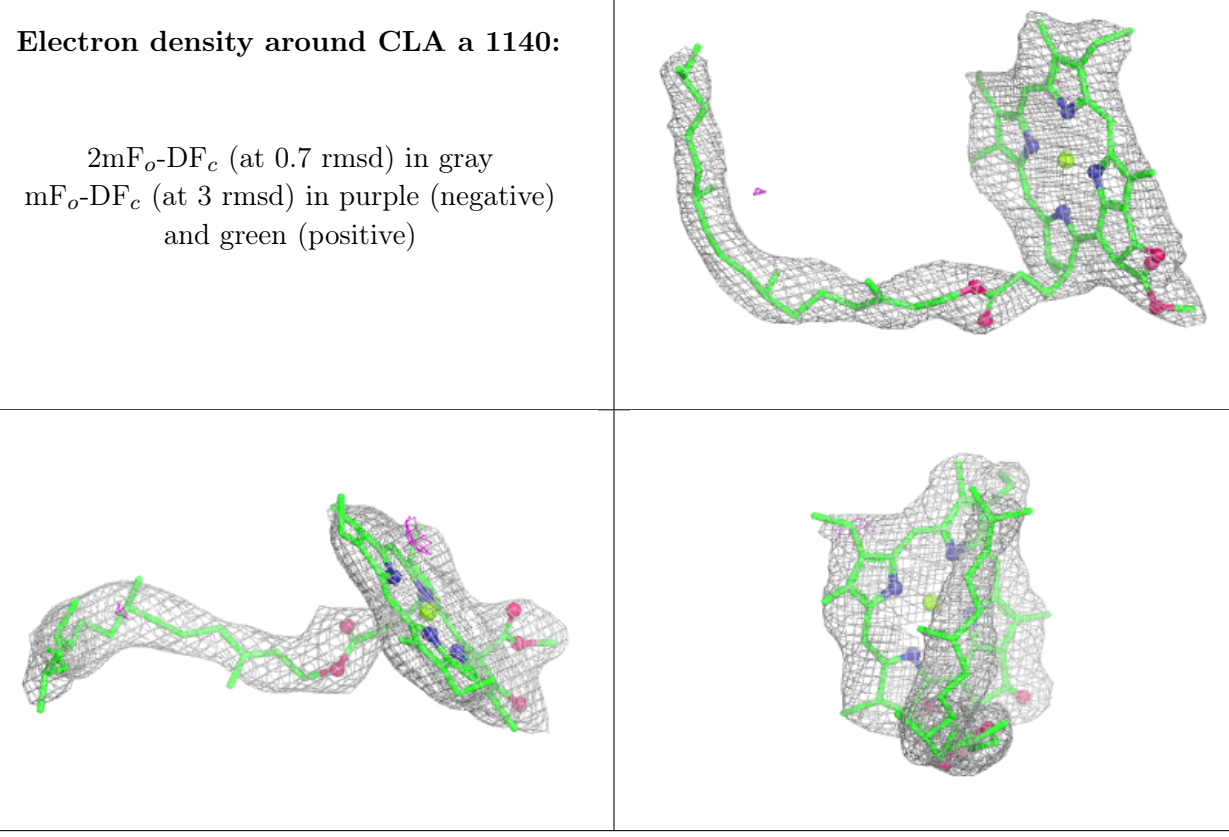
Electron density around CLA A 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



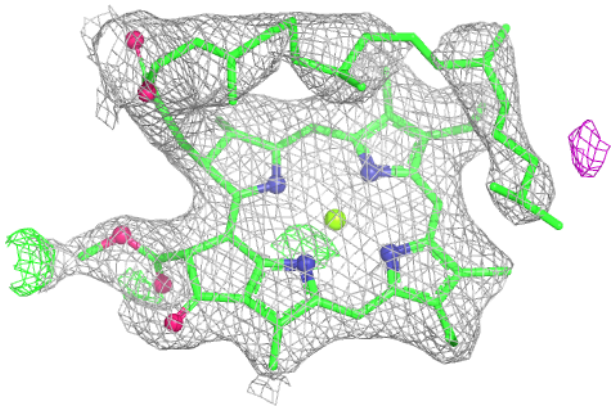
Electron density around CLA a 1140:

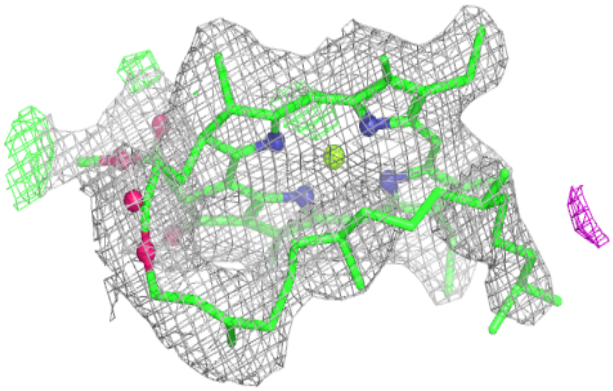
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

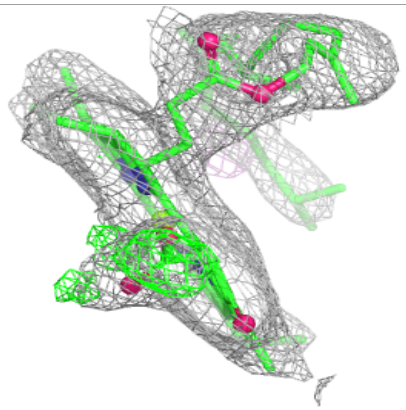


Electron density around CLA A 1118:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

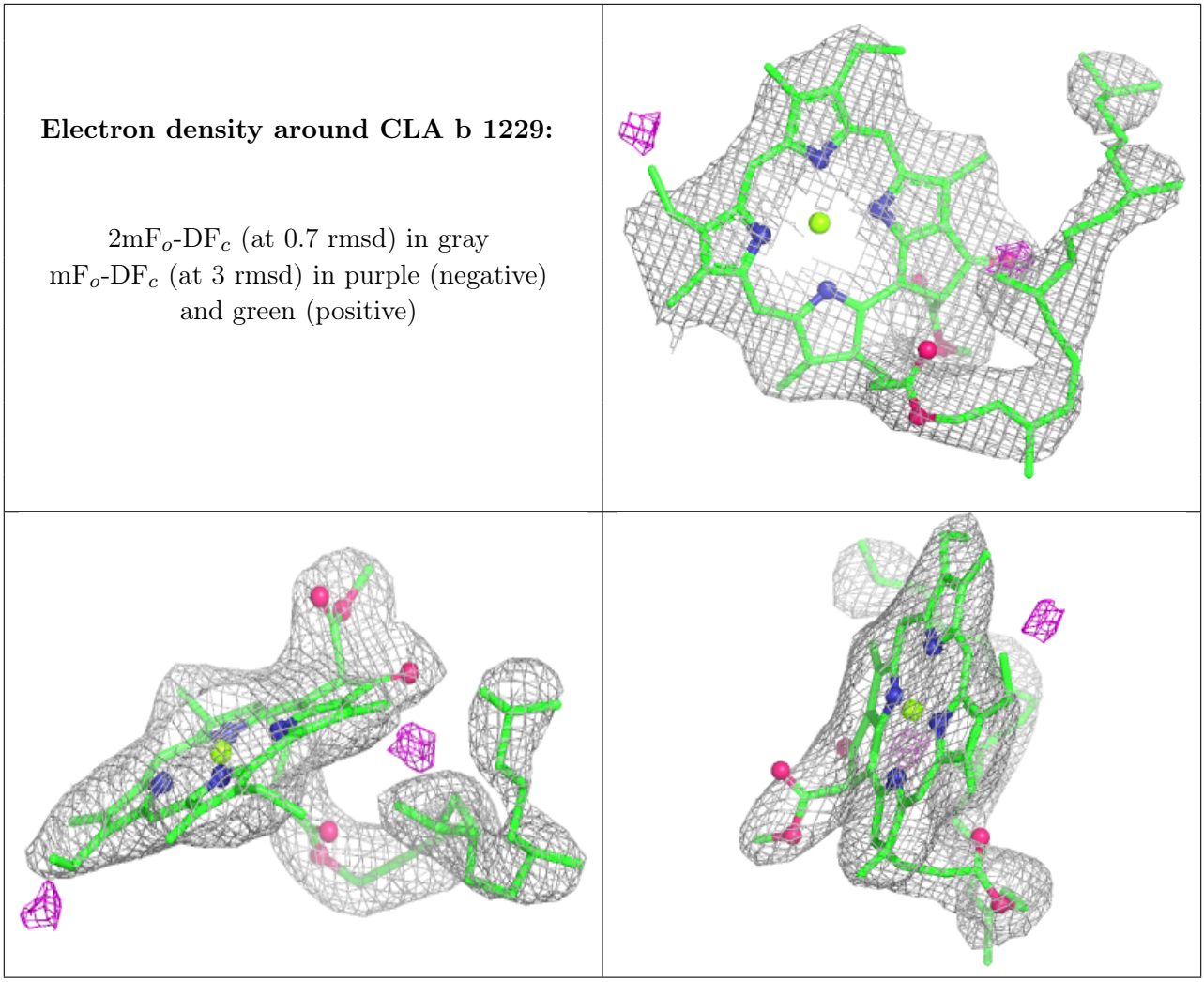






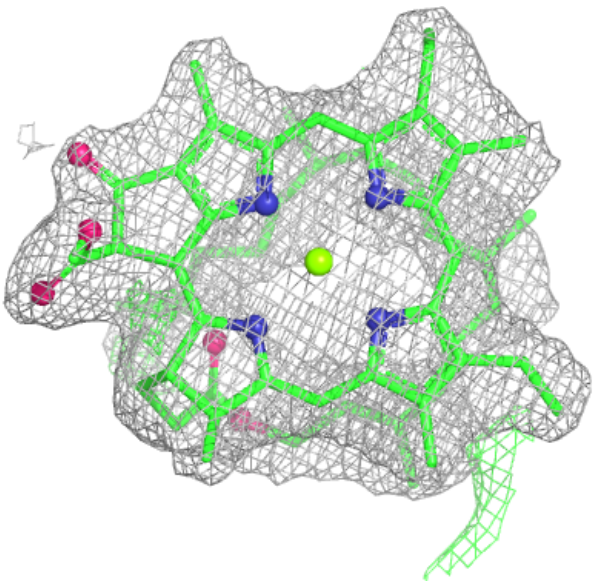
Electron density around CLA b 1229:

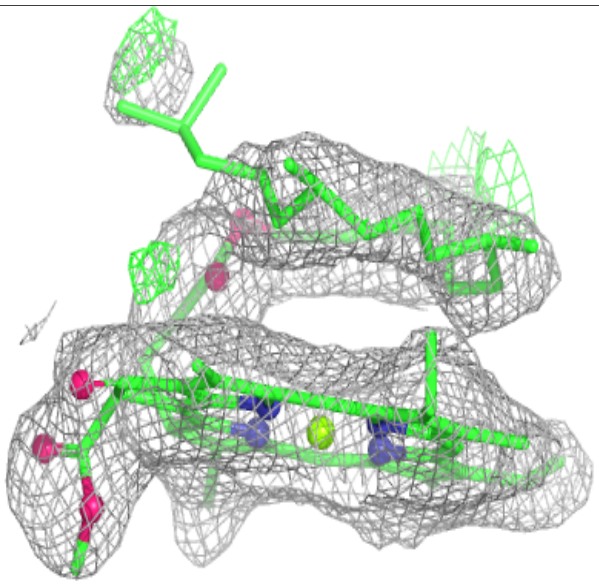
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

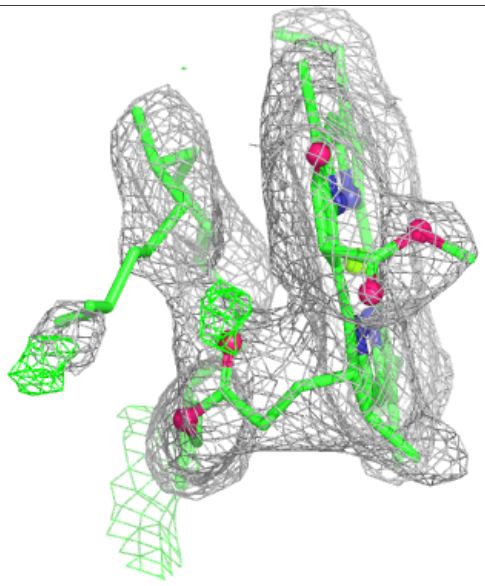


Electron density around CLA L 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

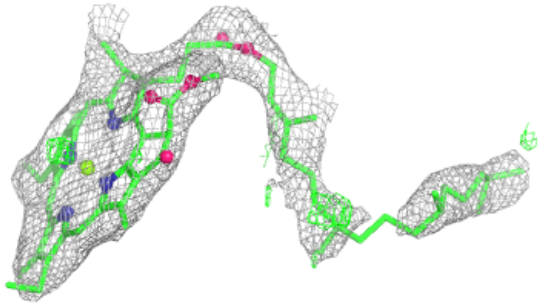


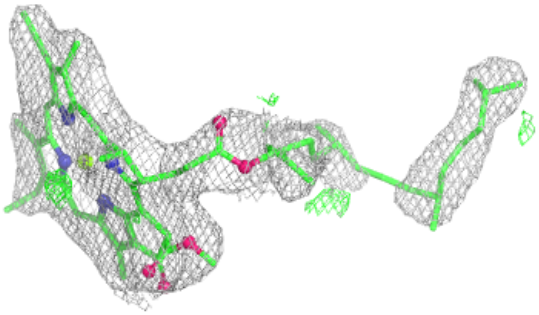


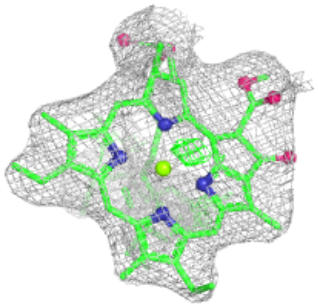


Electron density around CLA 2 1021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

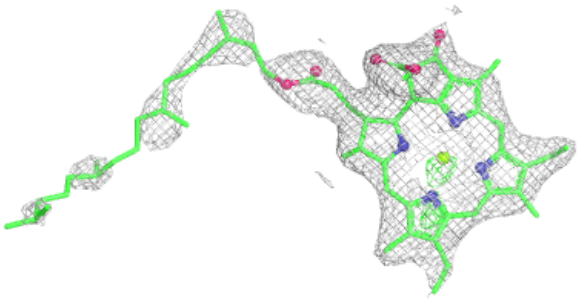


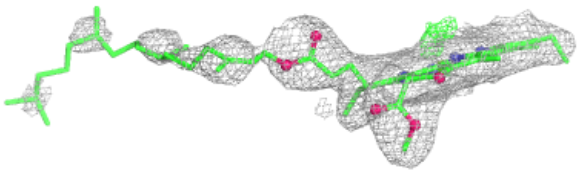


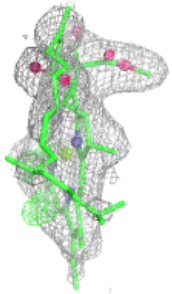


Electron density around CLA B 1234:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

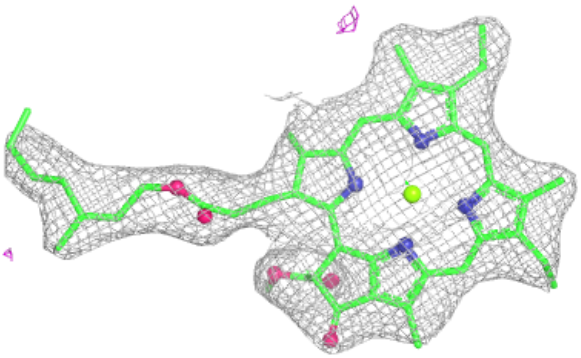


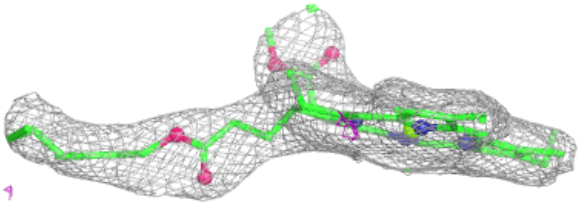


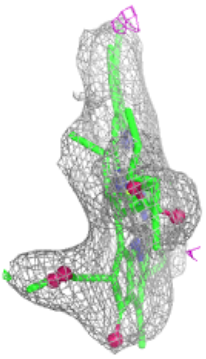


Electron density around CLA b 1234:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

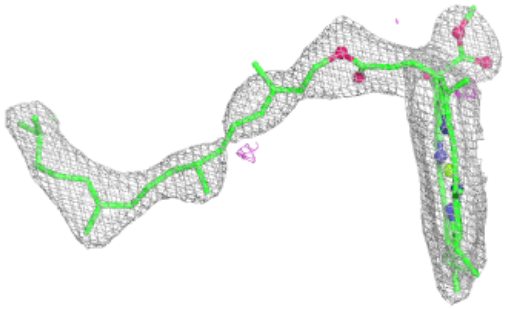


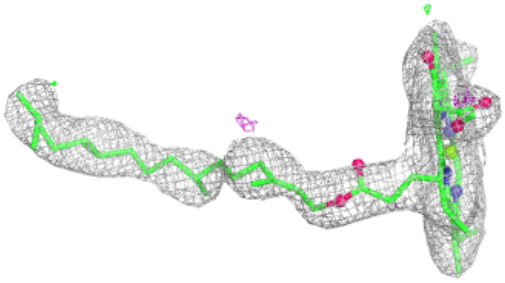


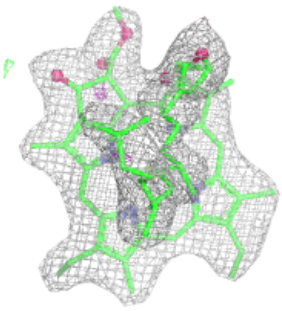


Electron density around CLA 2 1239:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

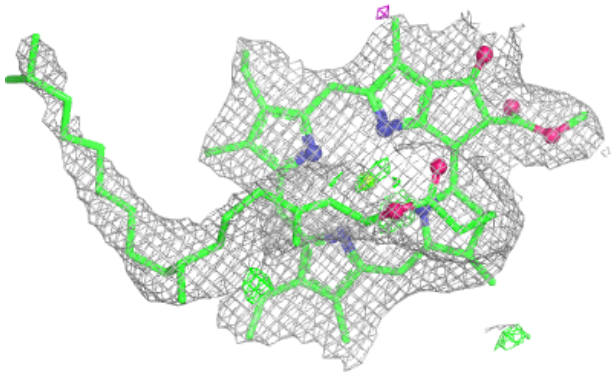


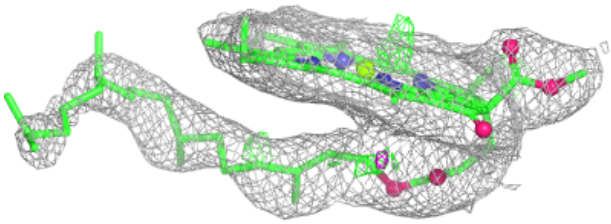


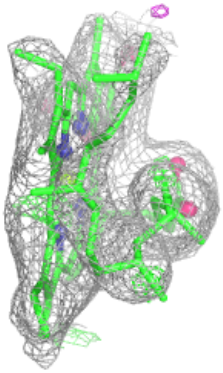


Electron density around CLA B 1235:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

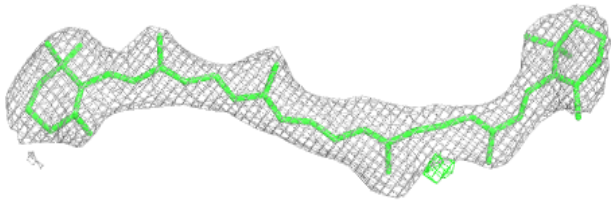


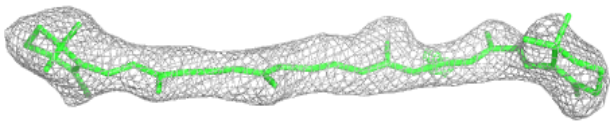


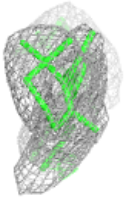


Electron density around BCR b 4010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



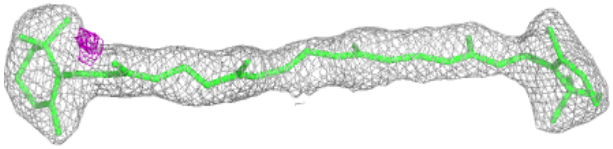




Electron density around BCR b 4017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

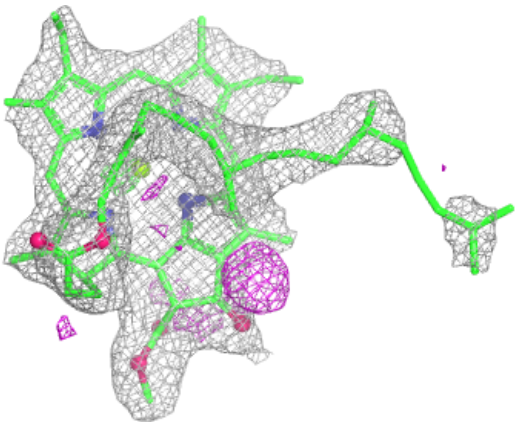


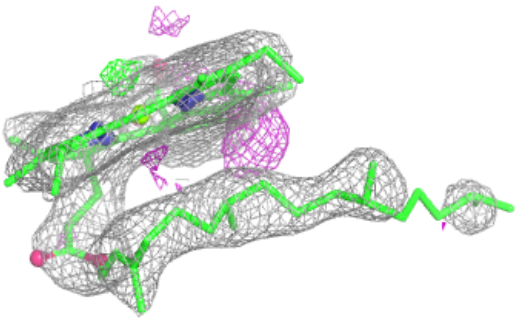


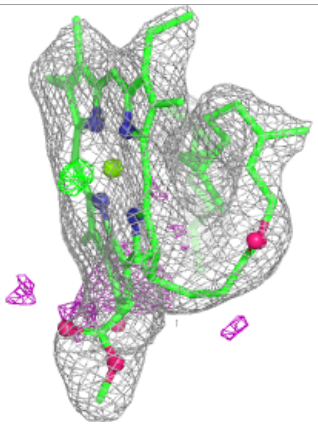


Electron density around CLA B 1224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

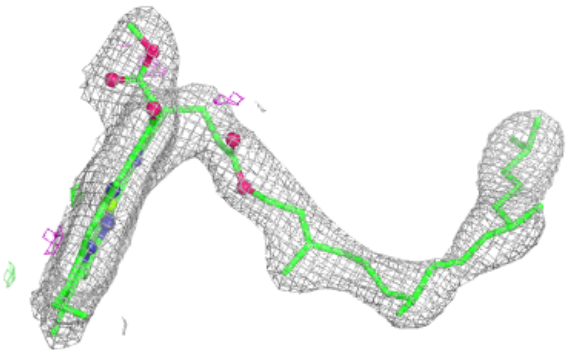


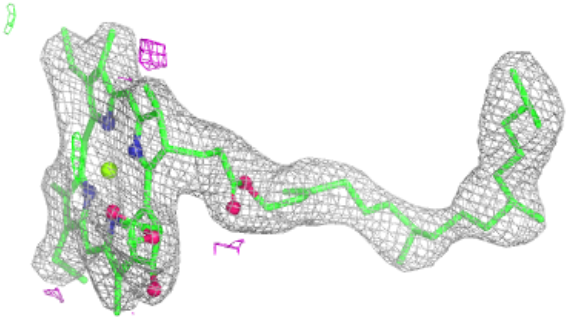


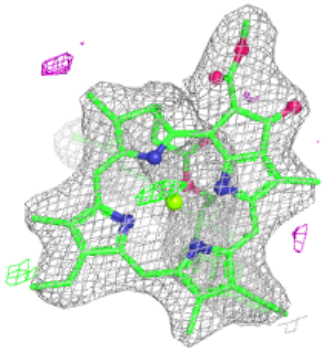


Electron density around CLA b 1238:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

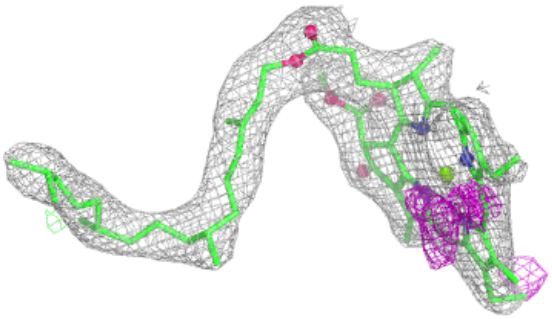


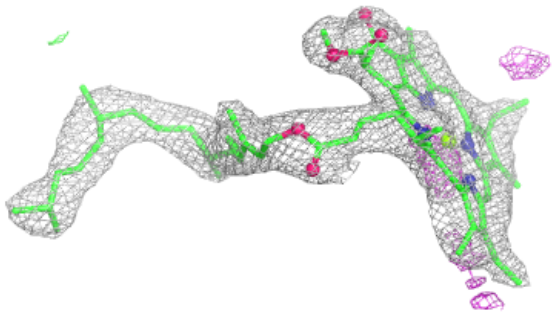


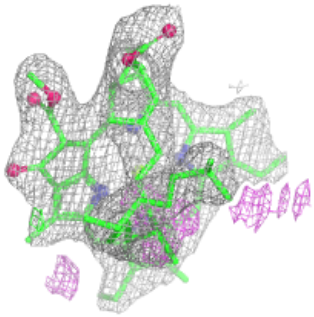


Electron density around CLA b 1021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

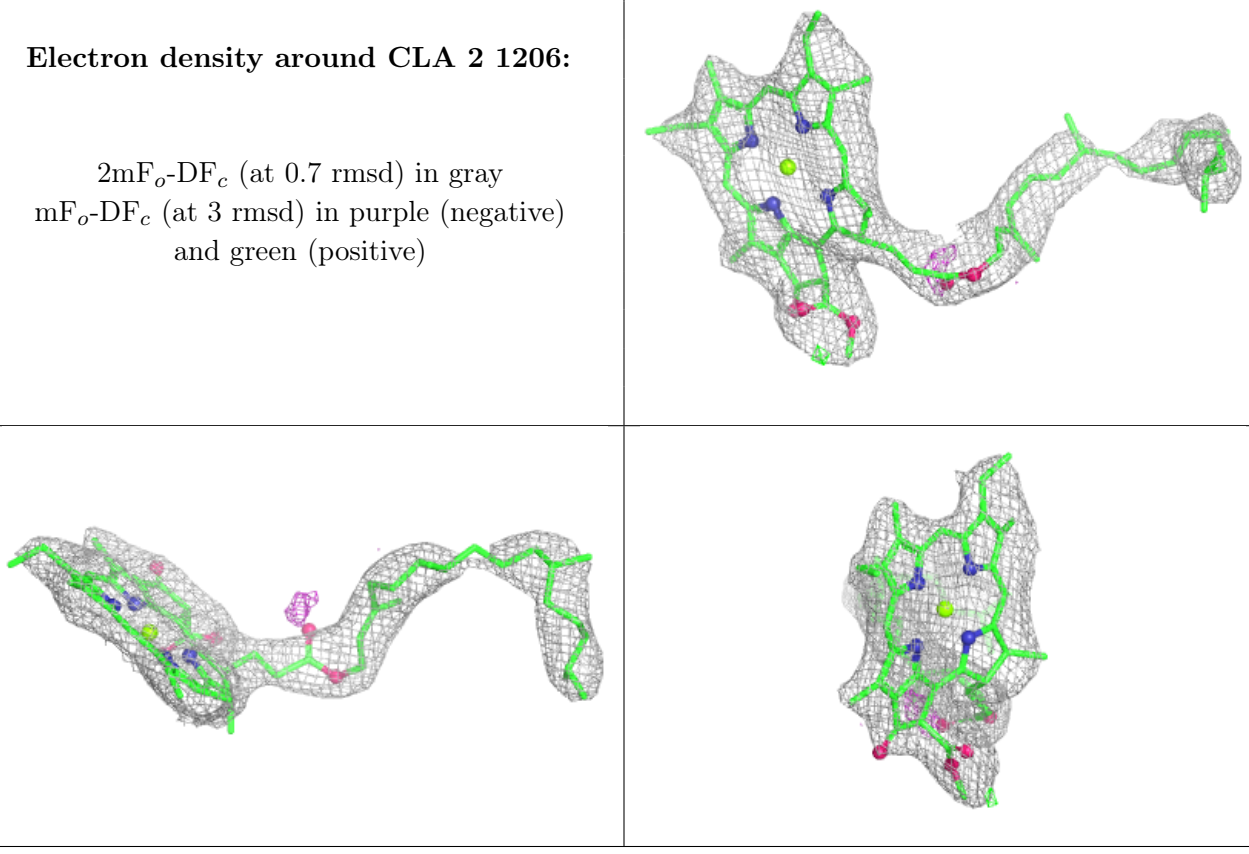






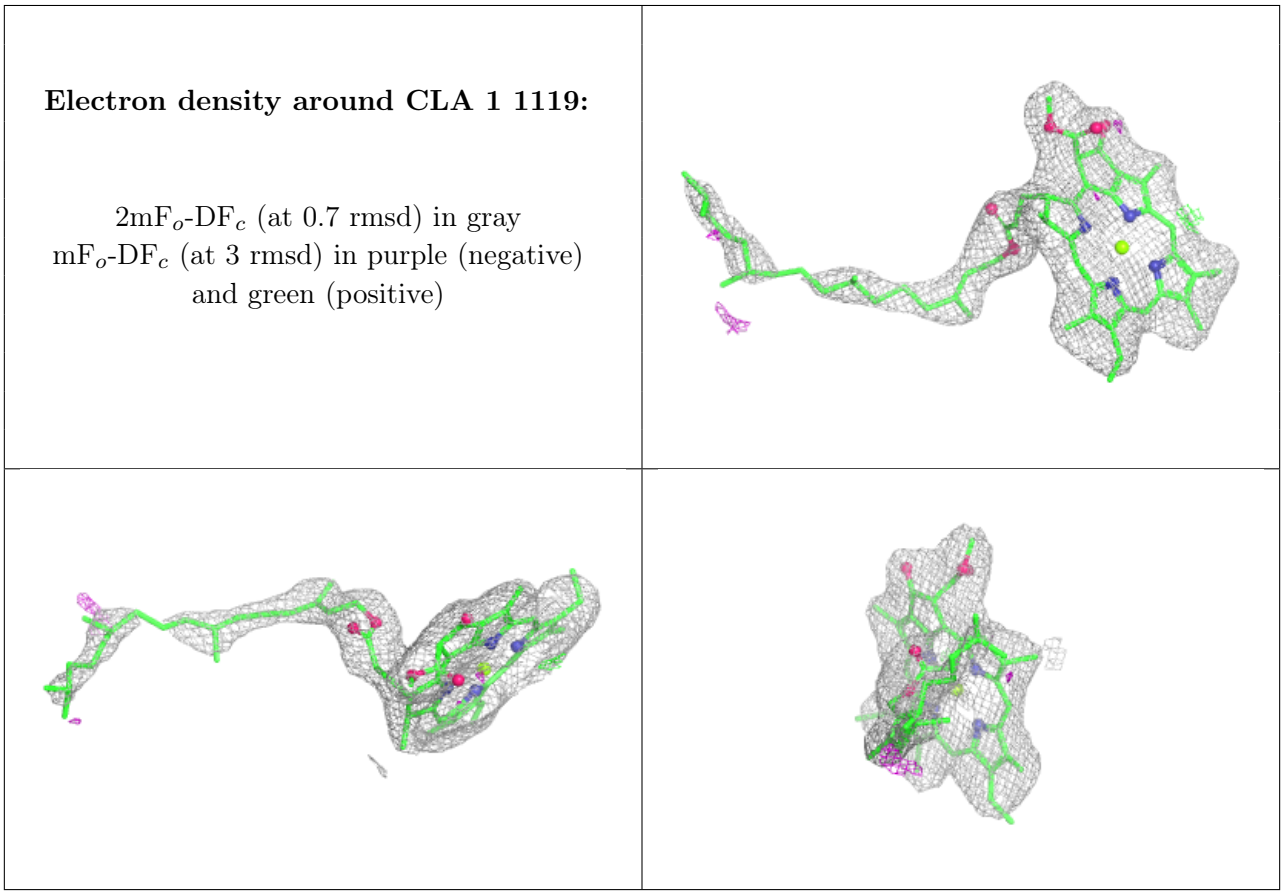
Electron density around CLA 2 1206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



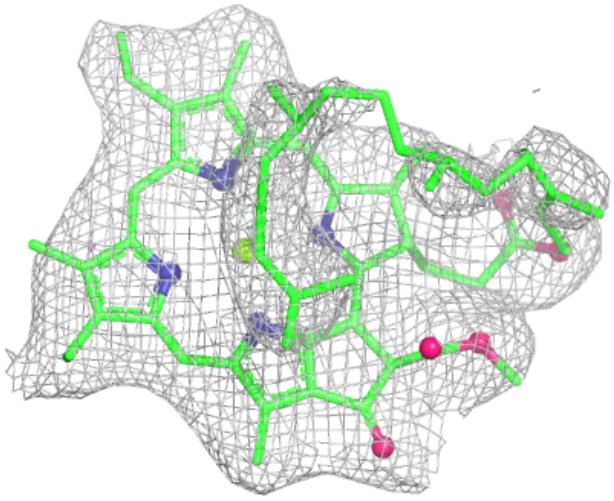
Electron density around CLA 1 1119:

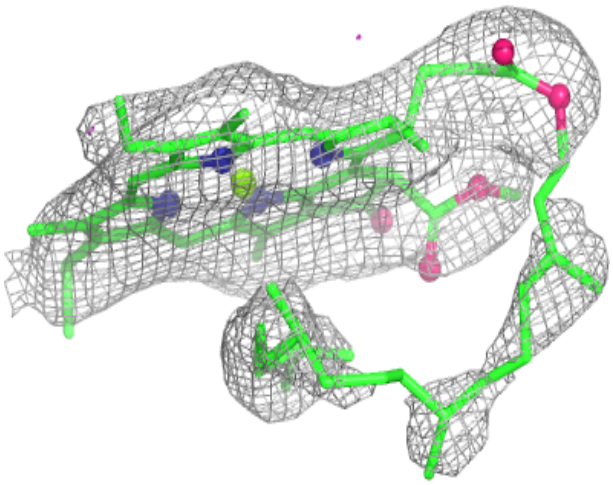
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

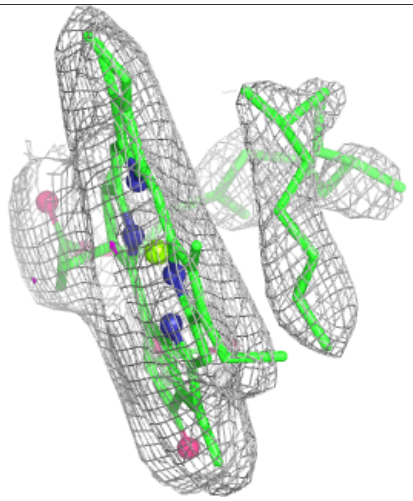


Electron density around CLA a 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

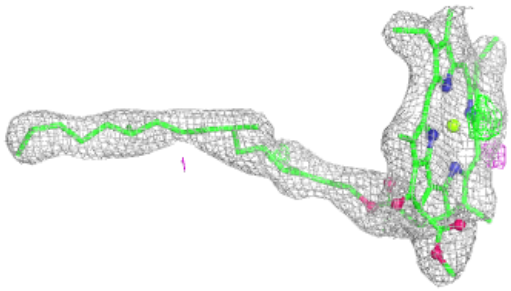


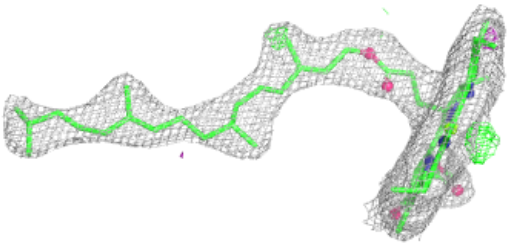


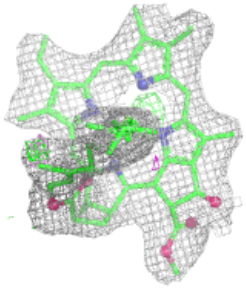


Electron density around CLA B 1225:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

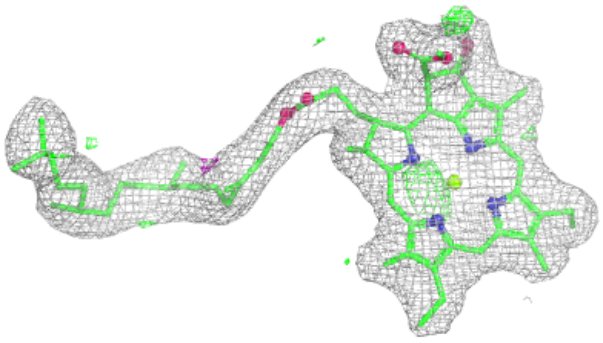


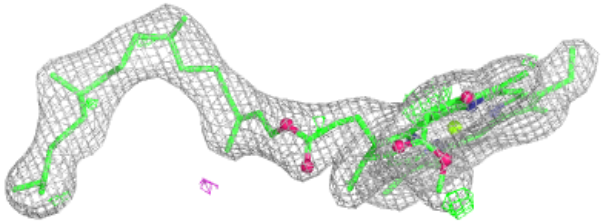


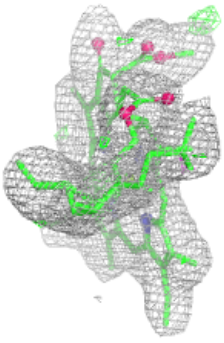


Electron density around CLA b 1210:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

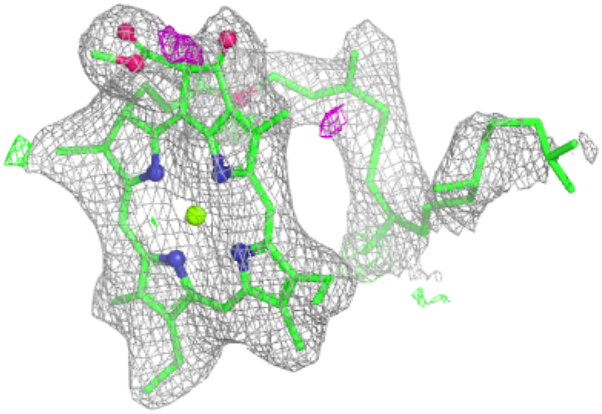


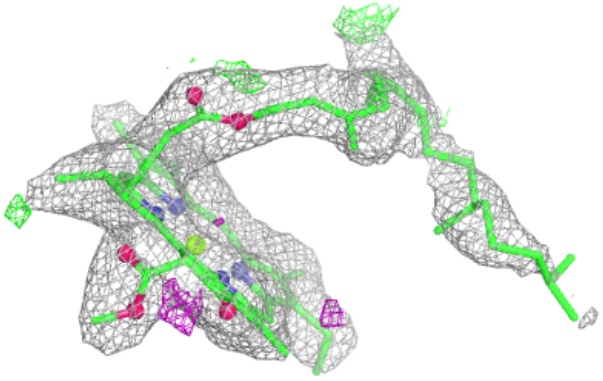


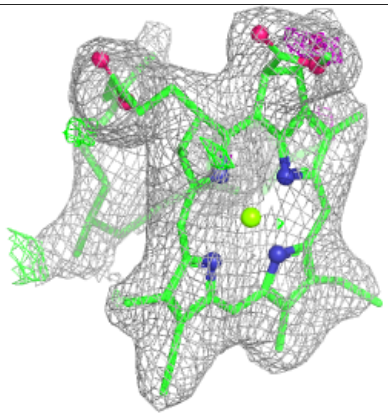


Electron density around CLA b 1211:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

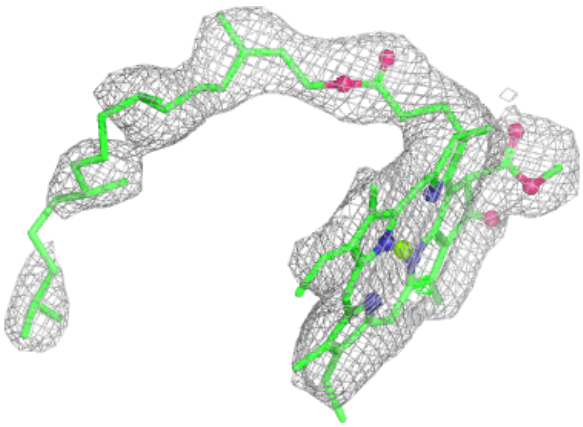


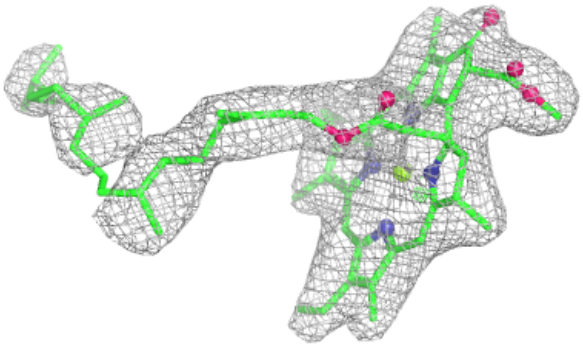


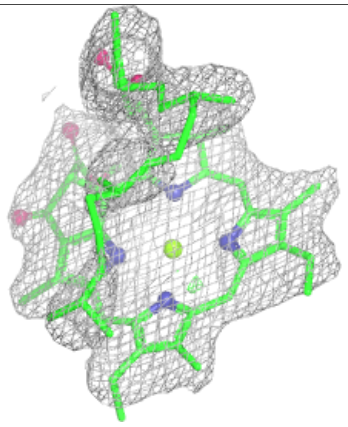


Electron density around CLA b 1212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

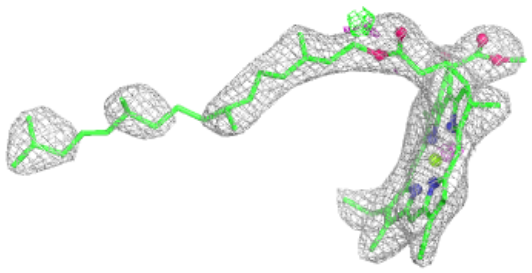


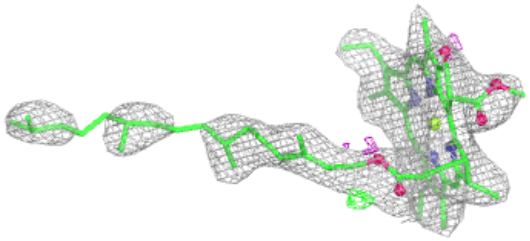


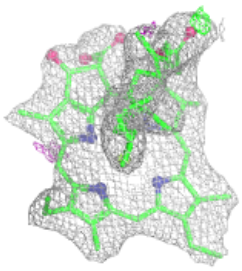


Electron density around CLA B 1226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

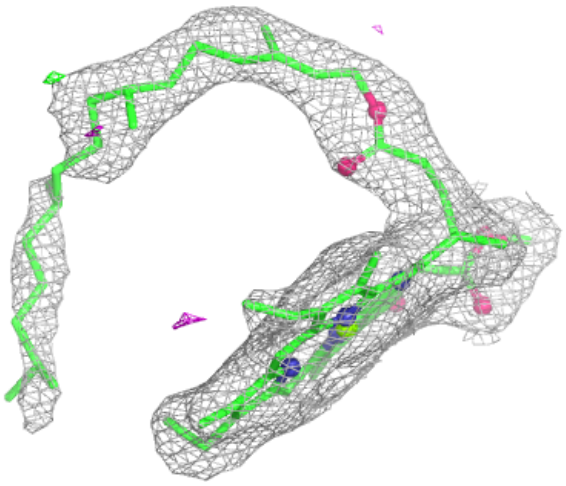


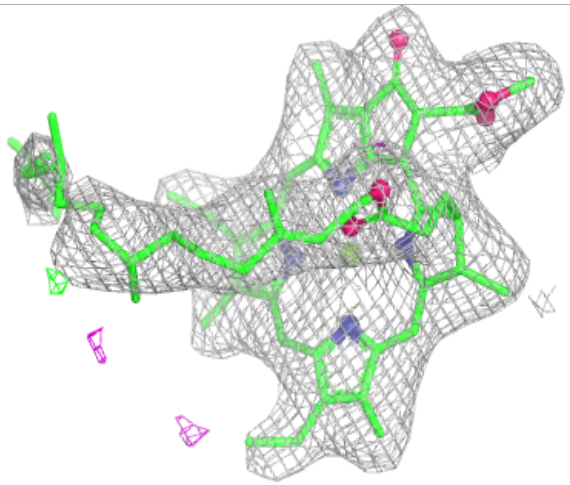


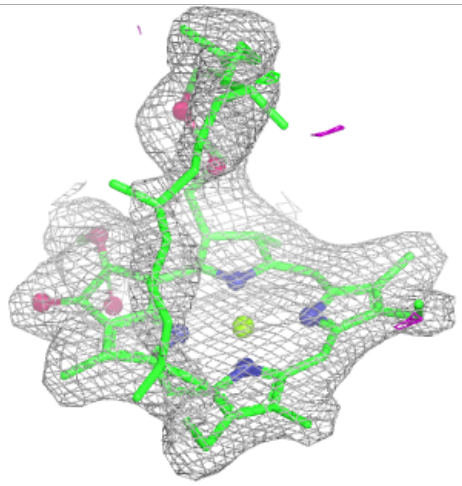


Electron density around CLA b 1216:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

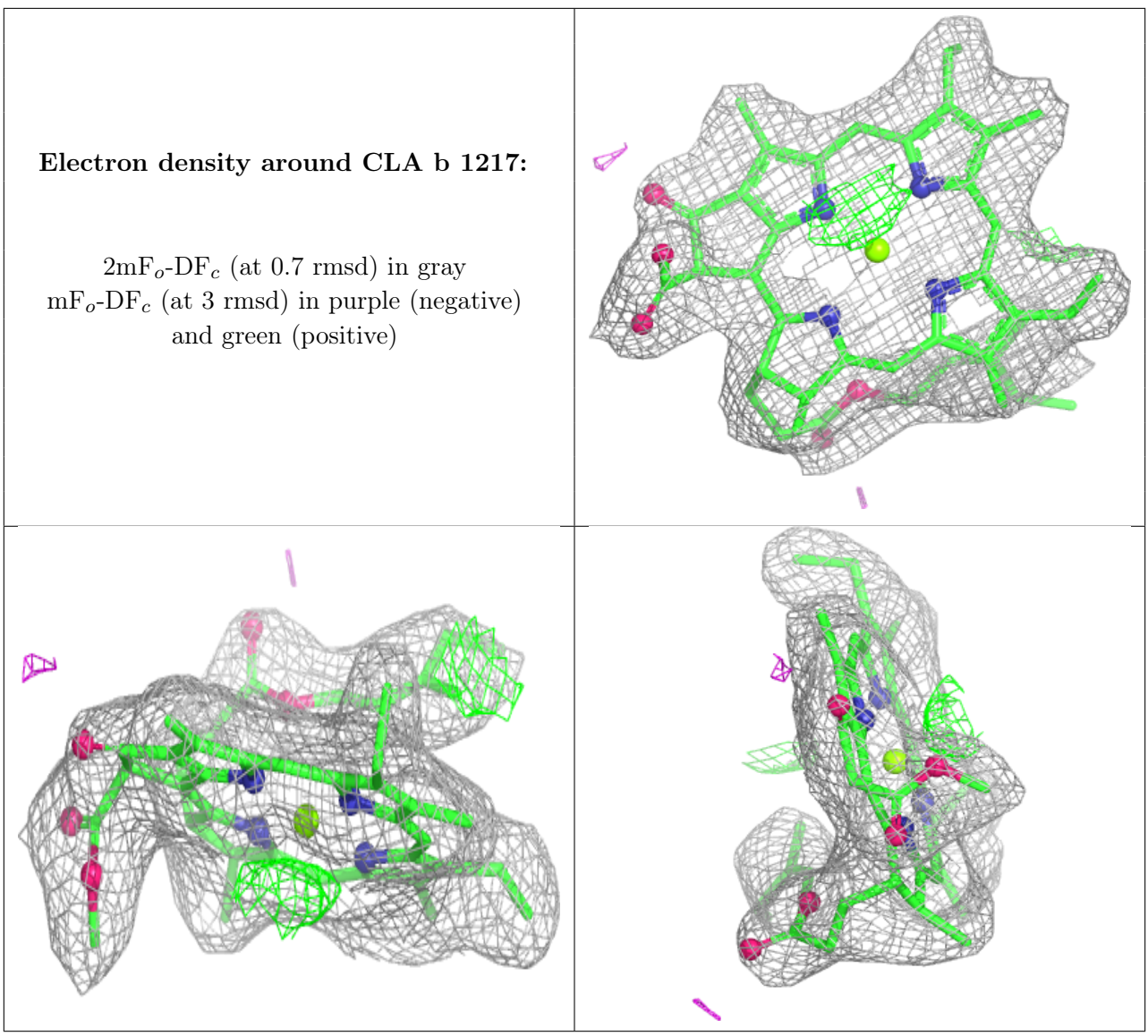






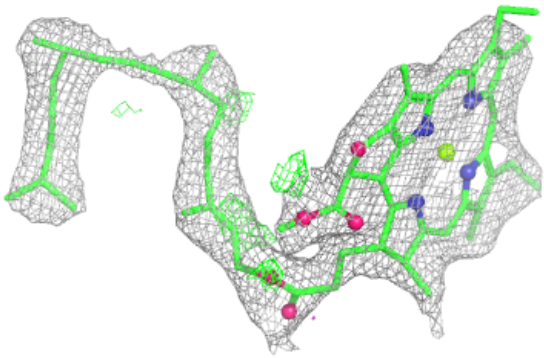
Electron density around CLA b 1217:

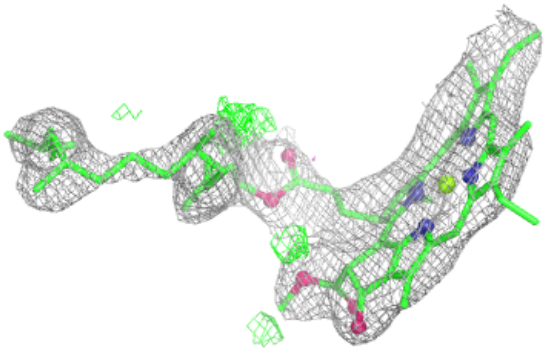
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

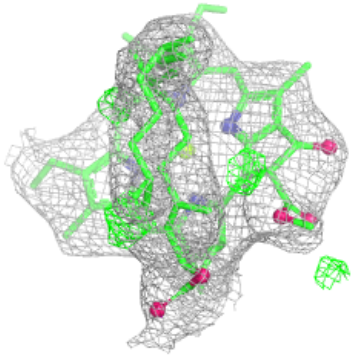


Electron density around CLA 1 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

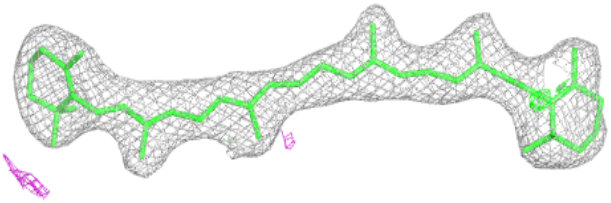


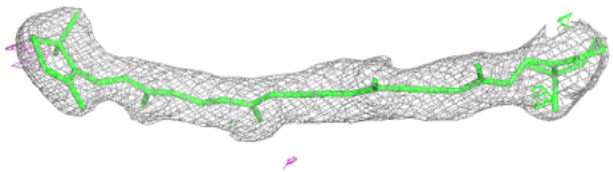


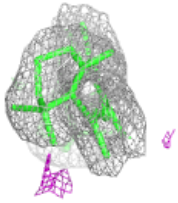


Electron density around BCR A 4008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

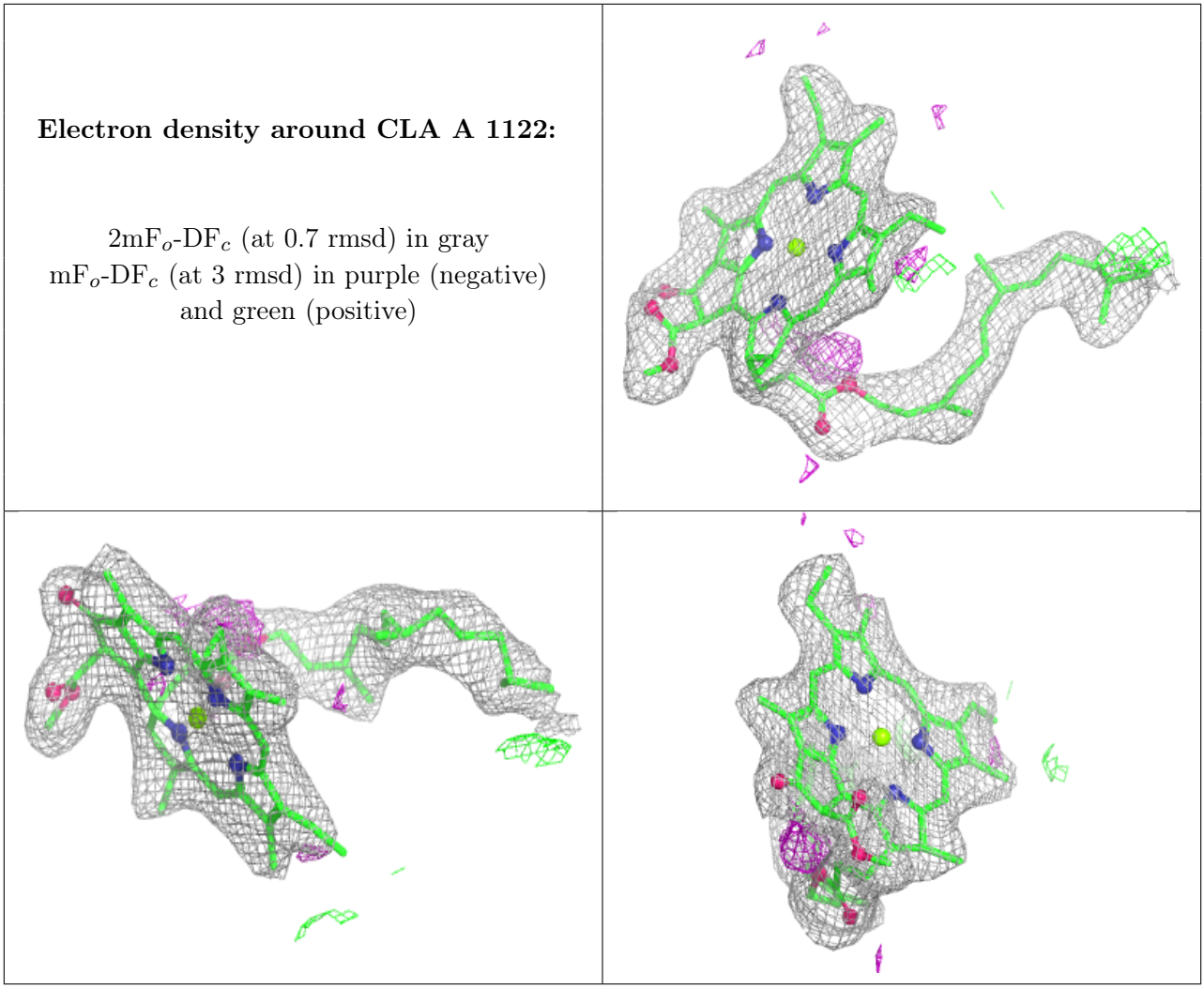






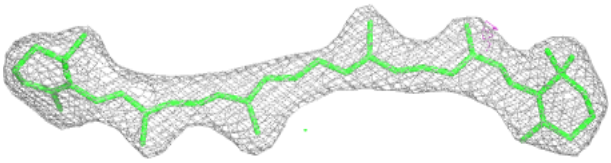
Electron density around CLA A 1122:

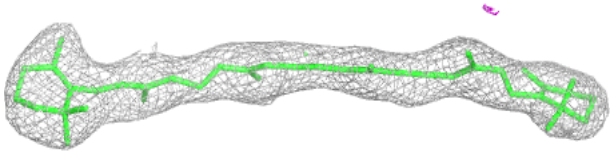
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

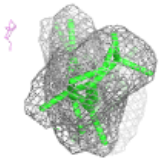


Electron density around BCR A 4012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

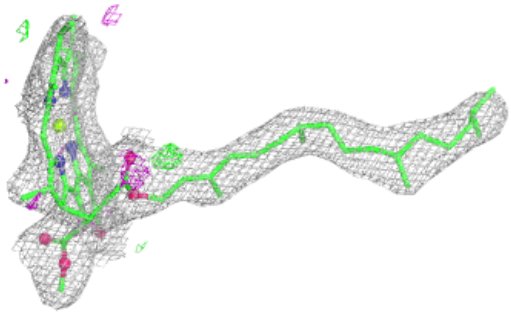


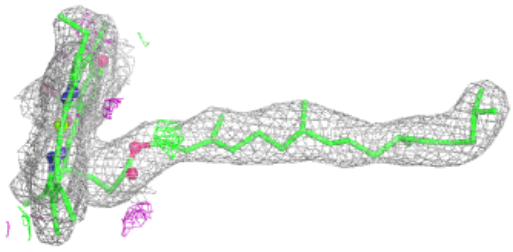


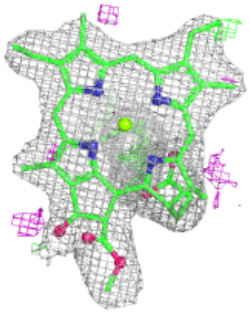


Electron density around CLA A 1126:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

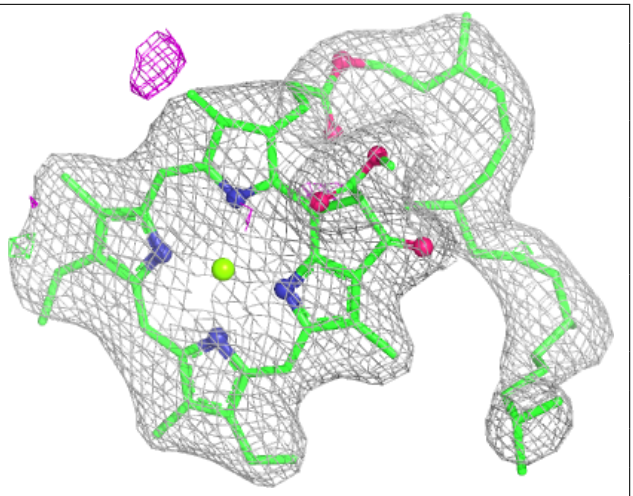


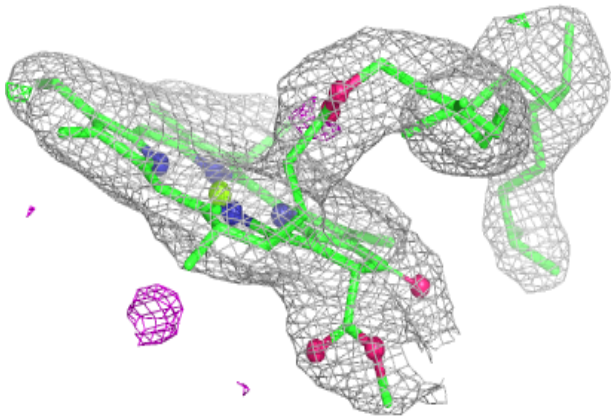


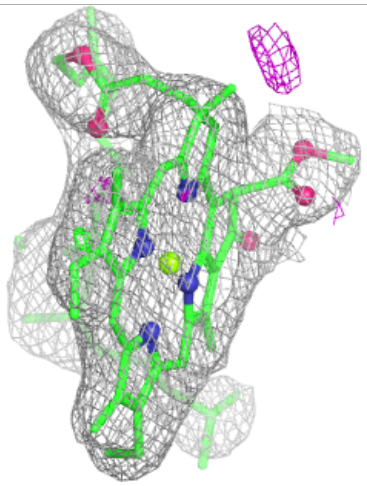


Electron density around CLA B 1229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

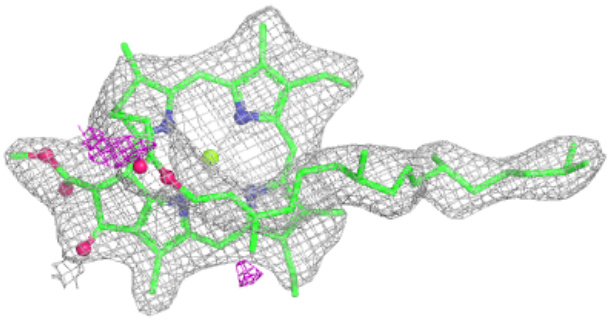


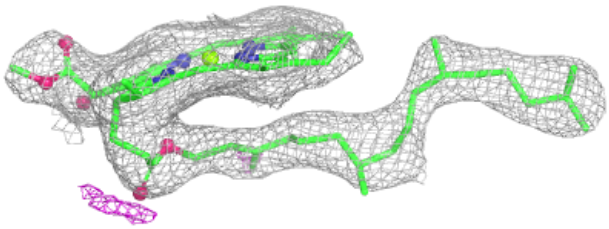


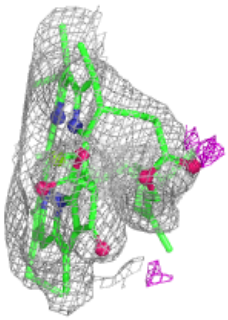


Electron density around CLA 1 1136:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

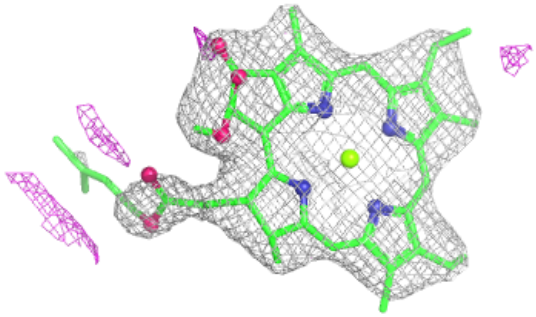


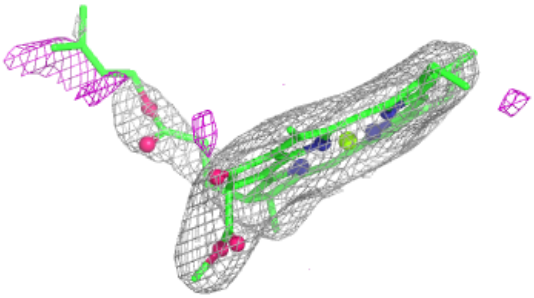


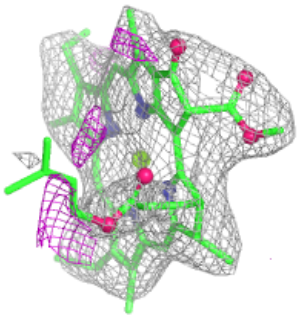


Electron density around CLA a 1137:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

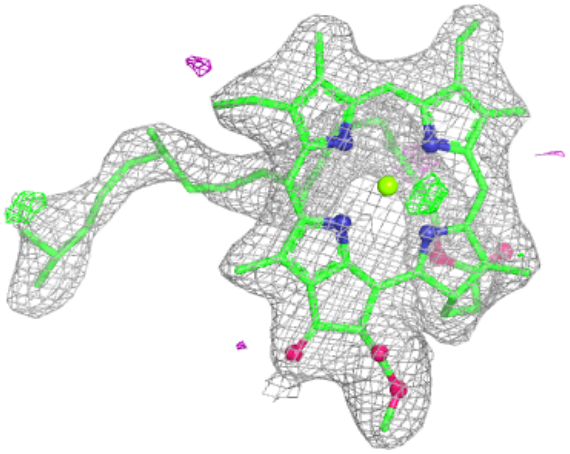


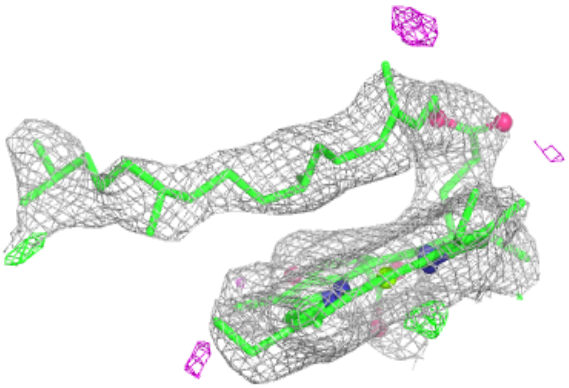


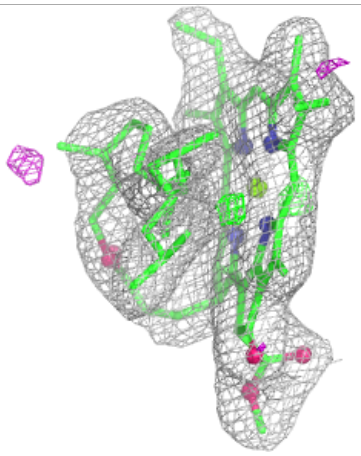


Electron density around CLA b 1224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

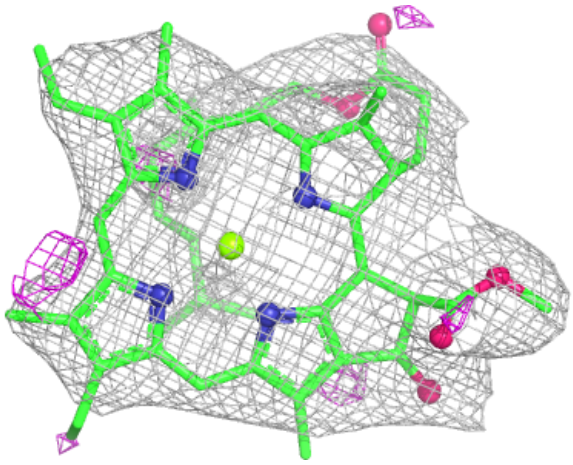


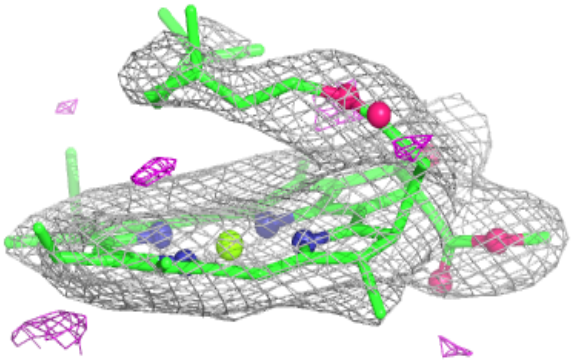


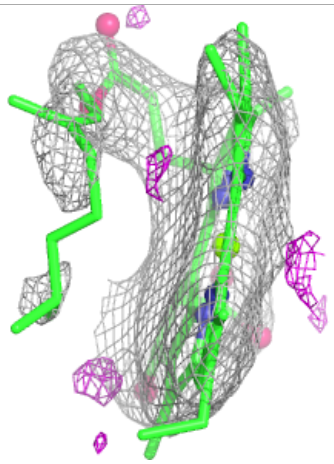


Electron density around CLA 2 1224:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

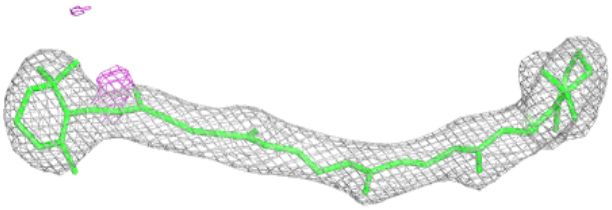


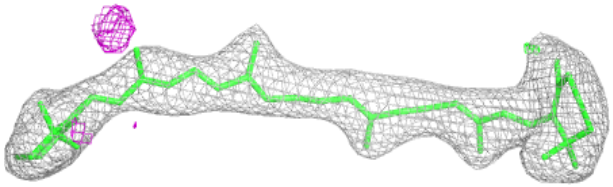


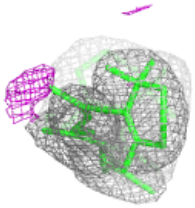


Electron density around BCR I 4018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

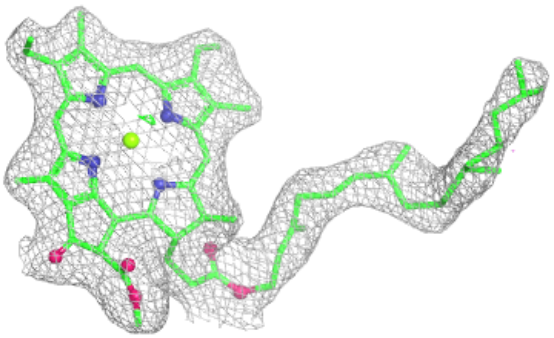


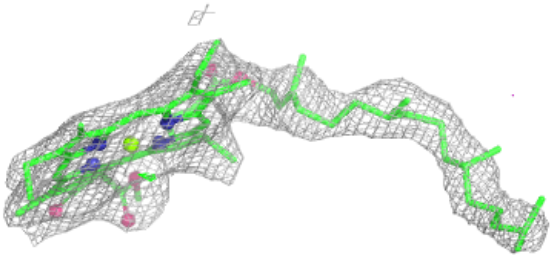


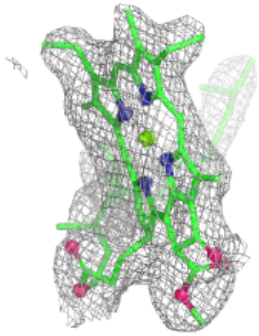


Electron density around CLA a 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

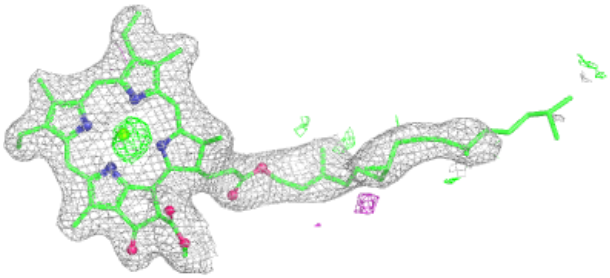


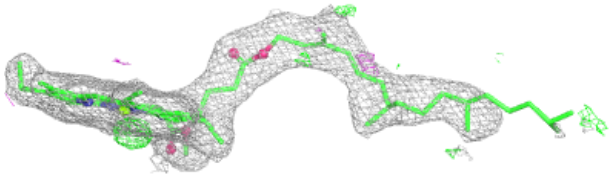


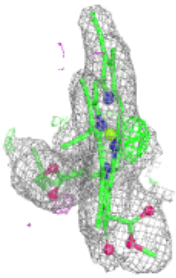


Electron density around CLA A 1124:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

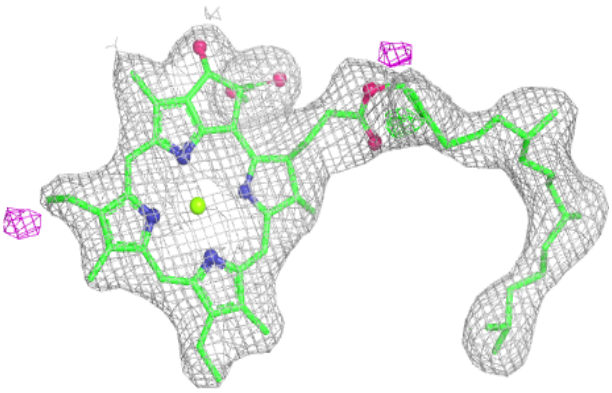


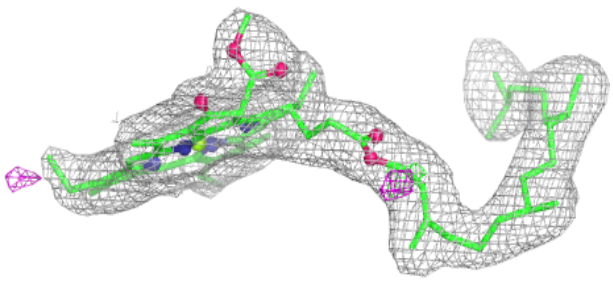


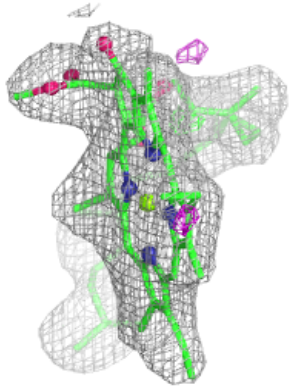


Electron density around CLA A 1125:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

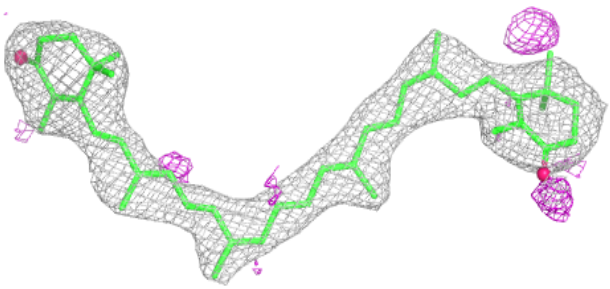


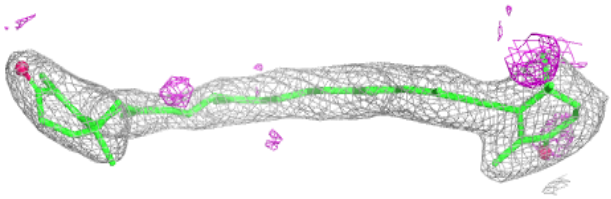


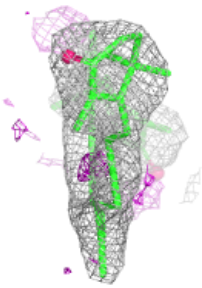


Electron density around 45D B 4011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

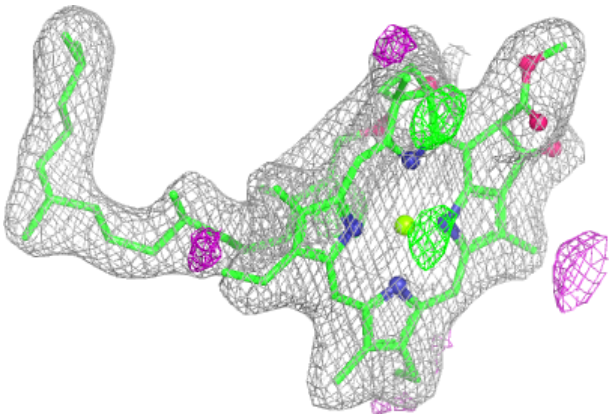


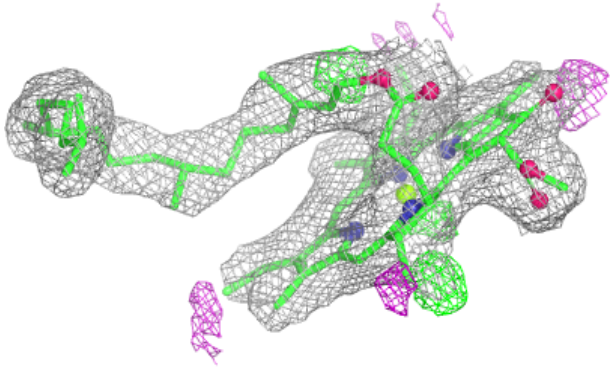




Electron density around CLA B 1237:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

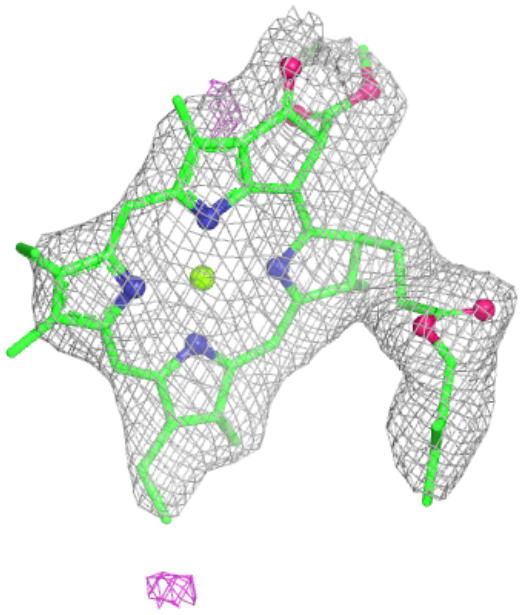


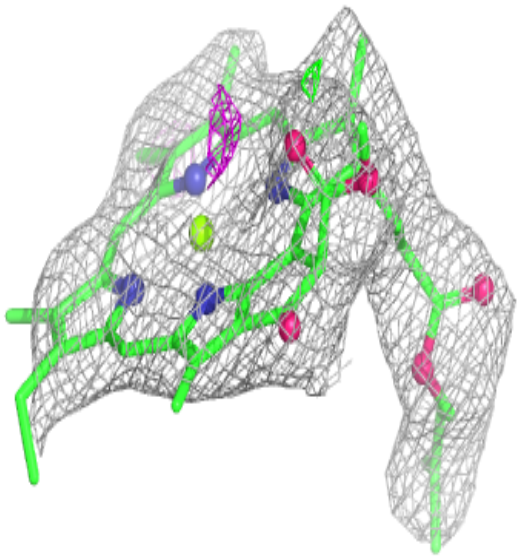


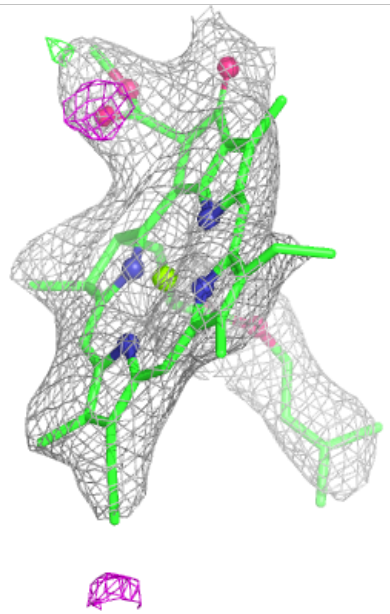


Electron density around CLA 1 1129:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

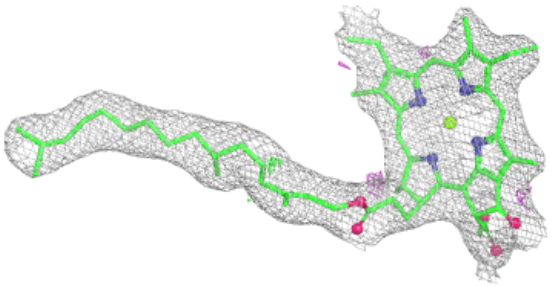


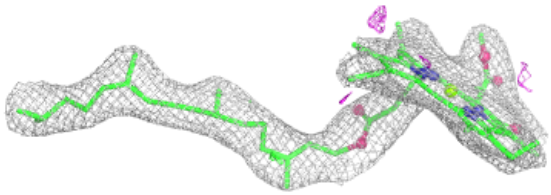


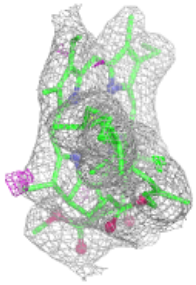


Electron density around CLA 1 1132:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

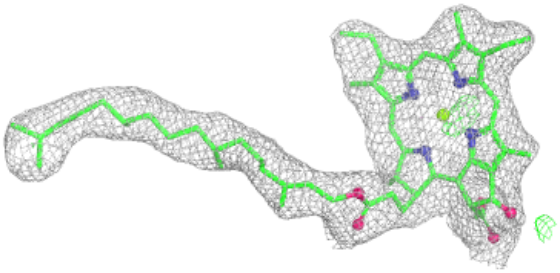


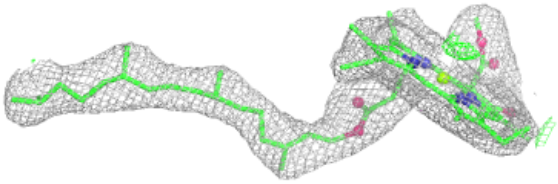


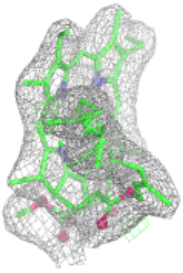


Electron density around CLA a 1132:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

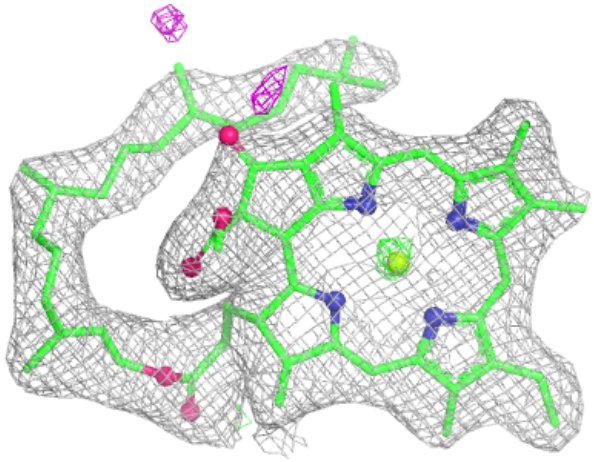


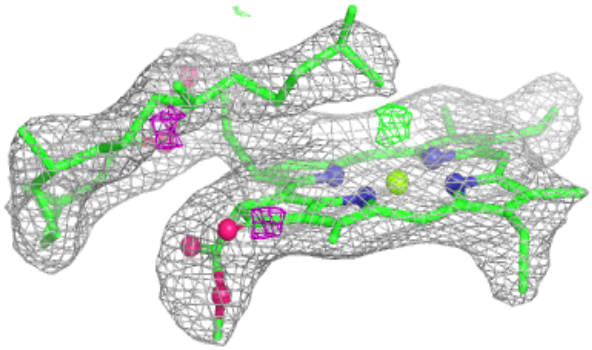


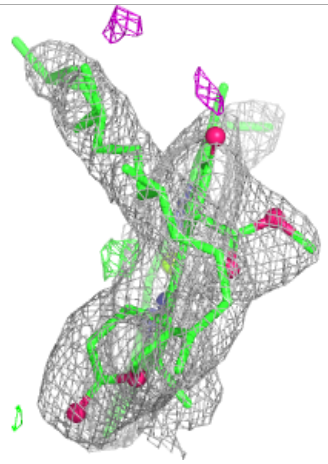


Electron density around CLA B 1202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

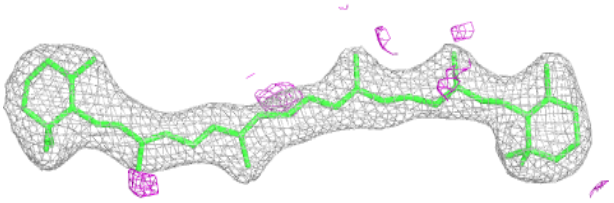


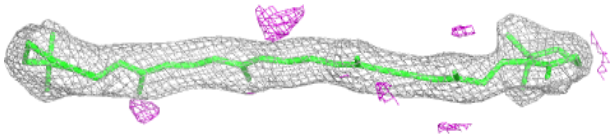


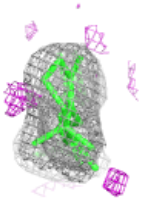


Electron density around BCR L 4019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

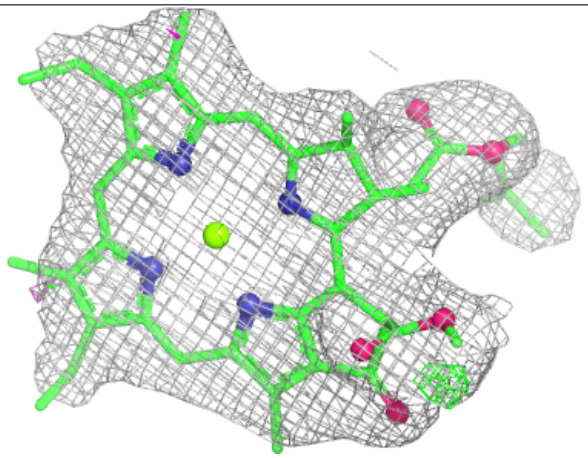


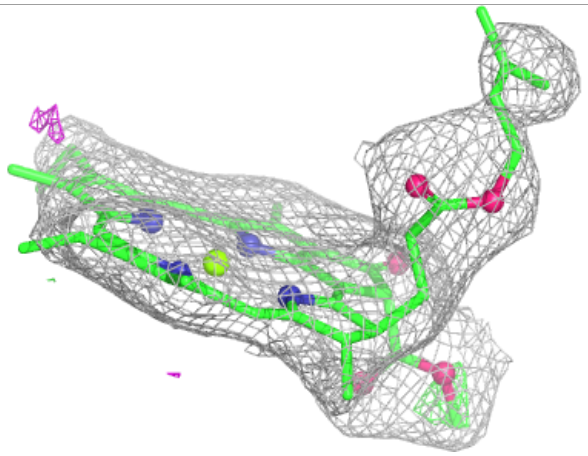


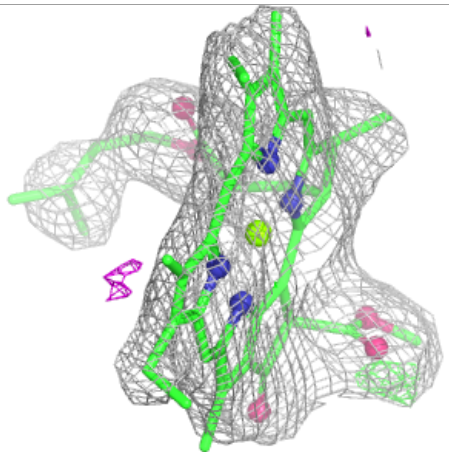


Electron density around CLA B 1236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

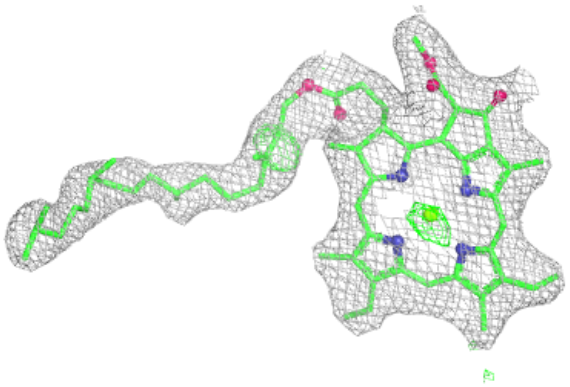


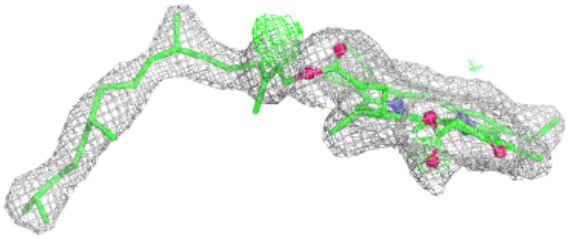


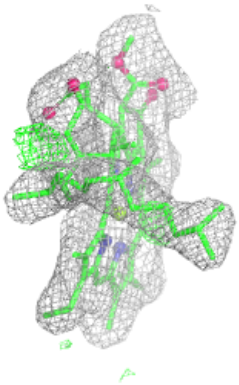


Electron density around CLA b 1023:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

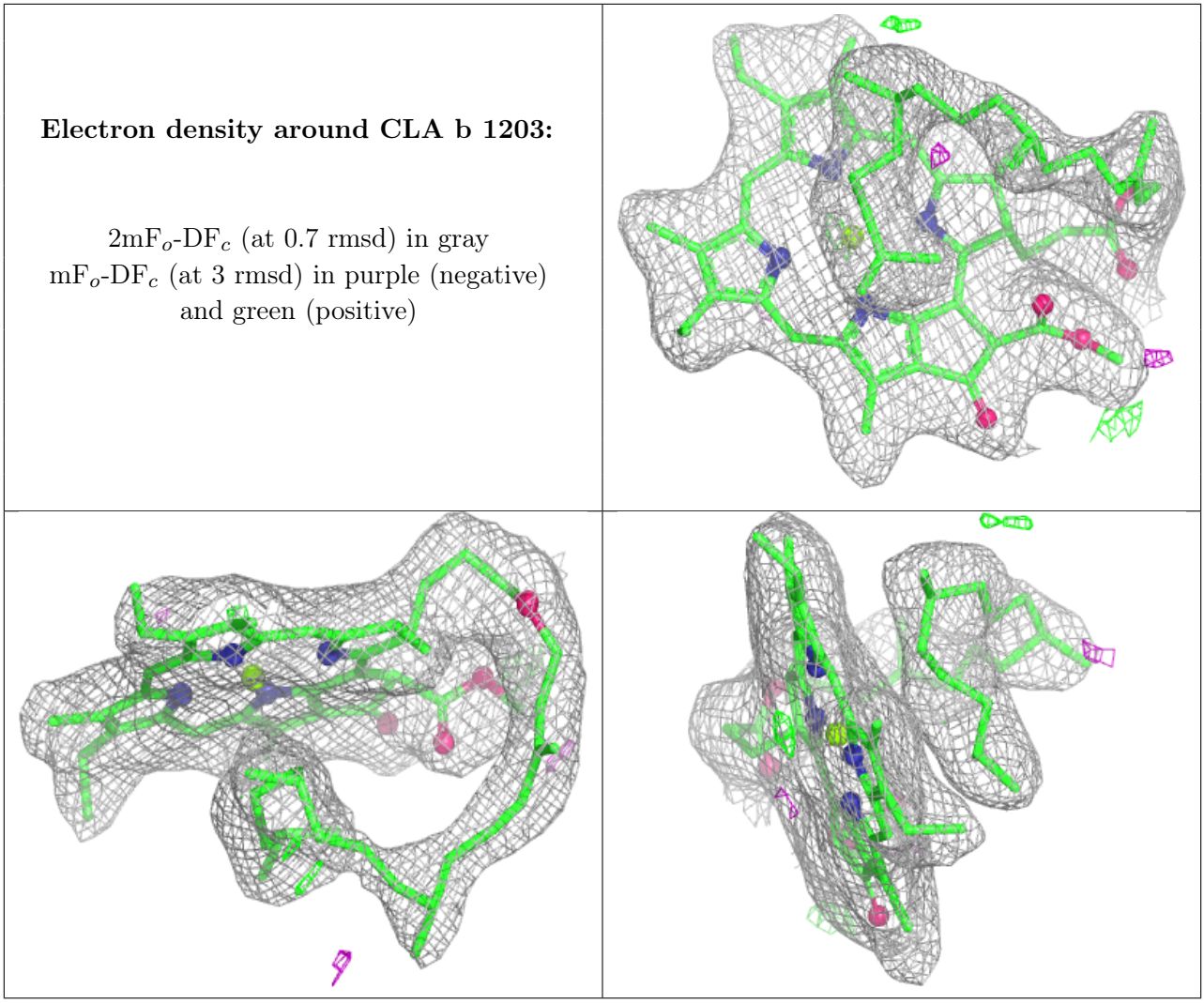






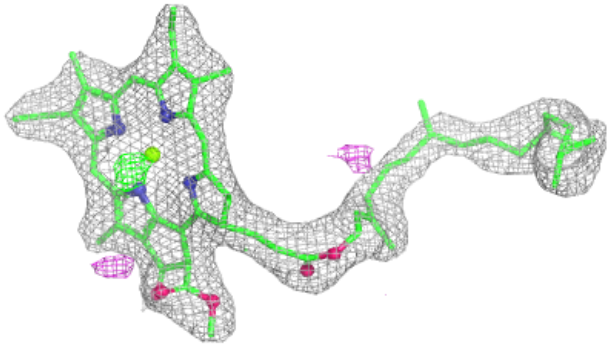
Electron density around CLA b 1203:

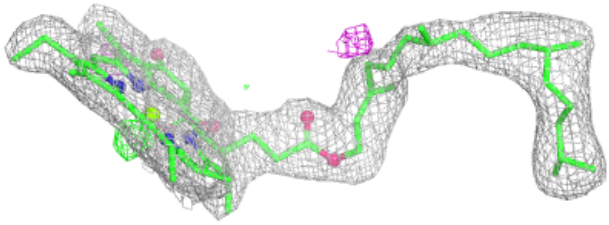
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

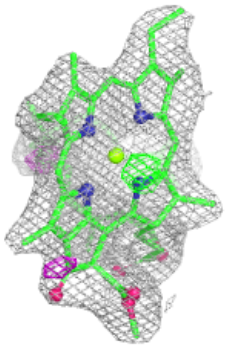


Electron density around CLA b 1206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

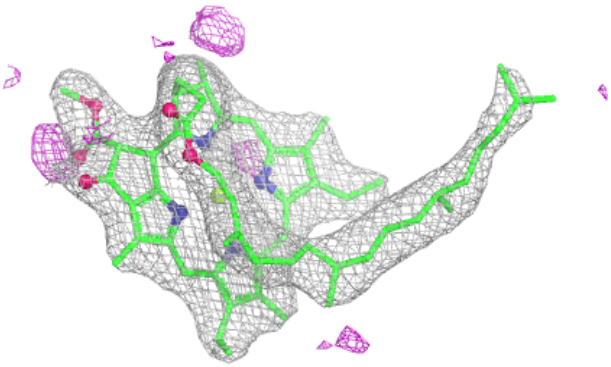


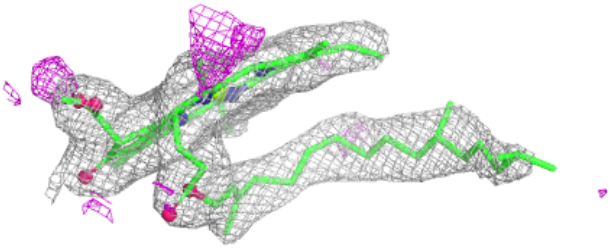


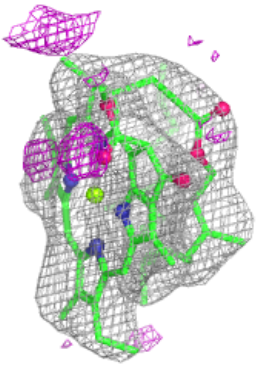


Electron density around CLA B 1204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

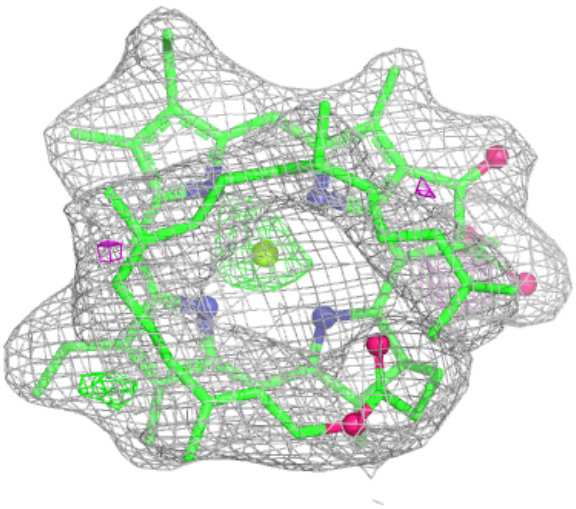


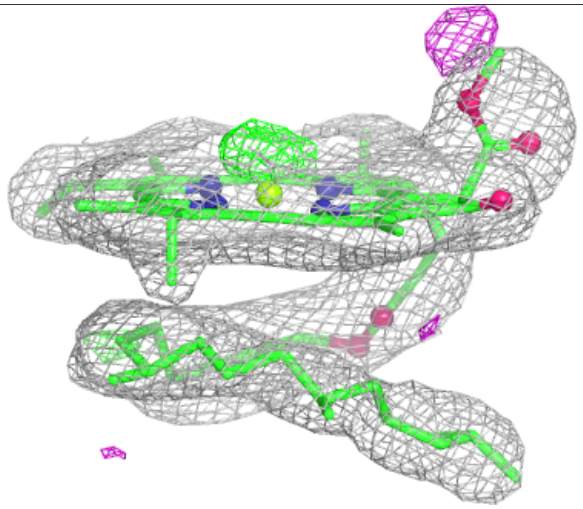


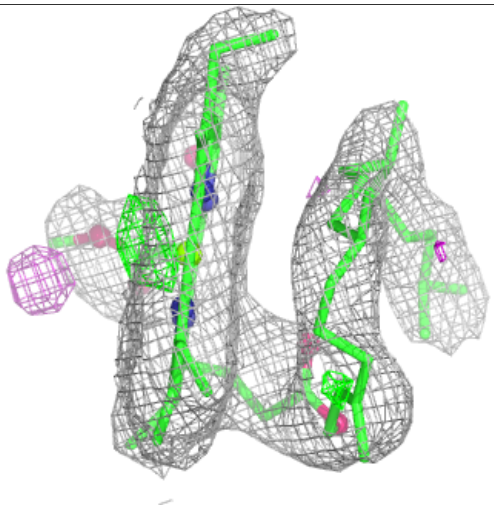


Electron density around CLA 0 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

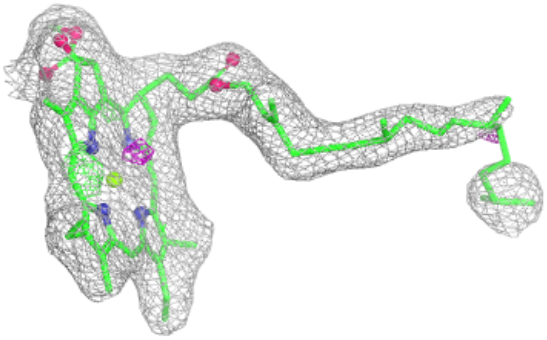


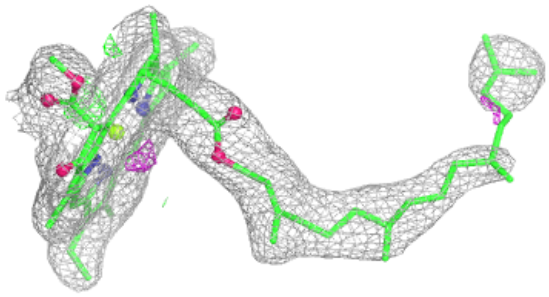


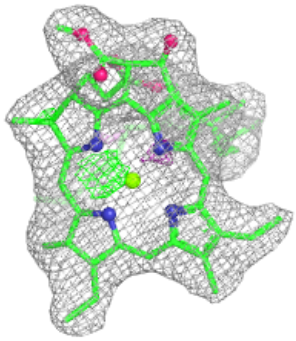


Electron density around CLA 0 1502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

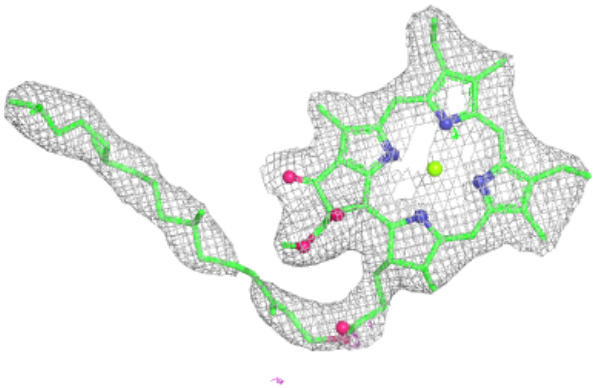


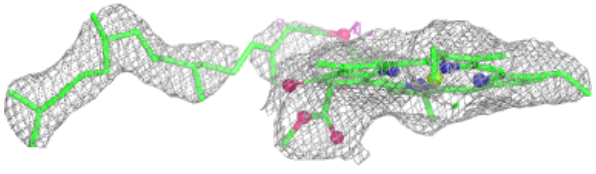




Electron density around CLA 0 1503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

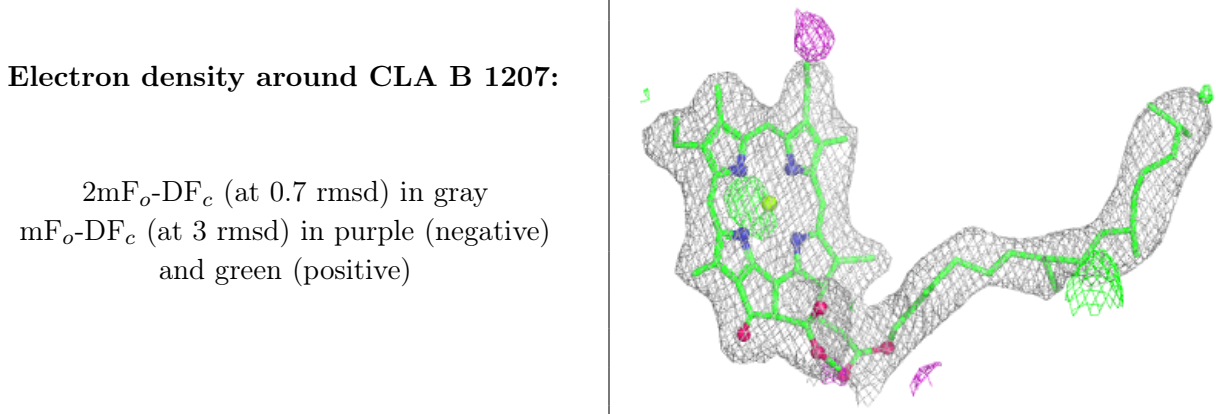






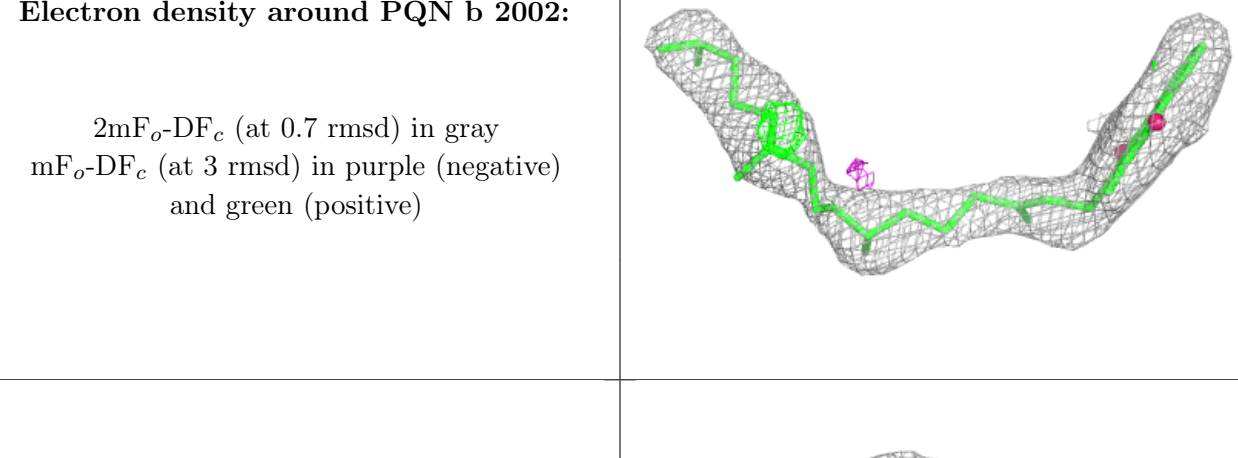
Electron density around CLA B 1207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



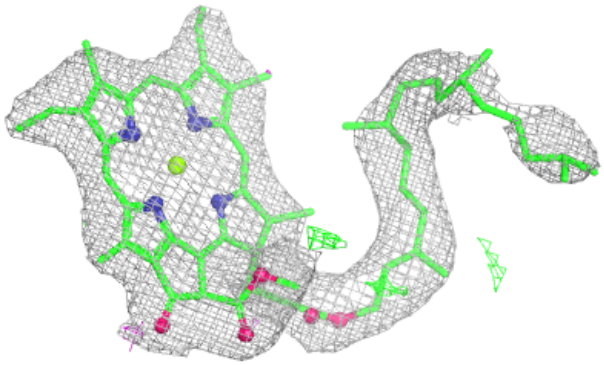
Electron density around PQN b 2002:

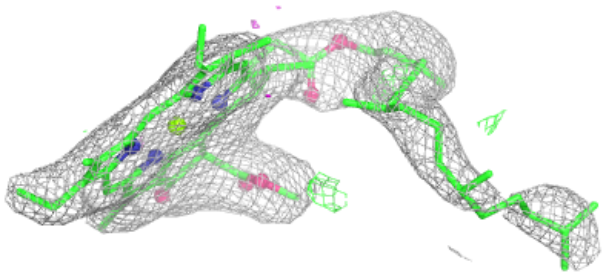
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

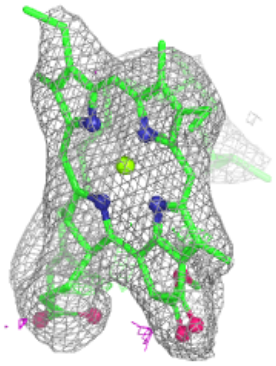


Electron density around CLA B 1221:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

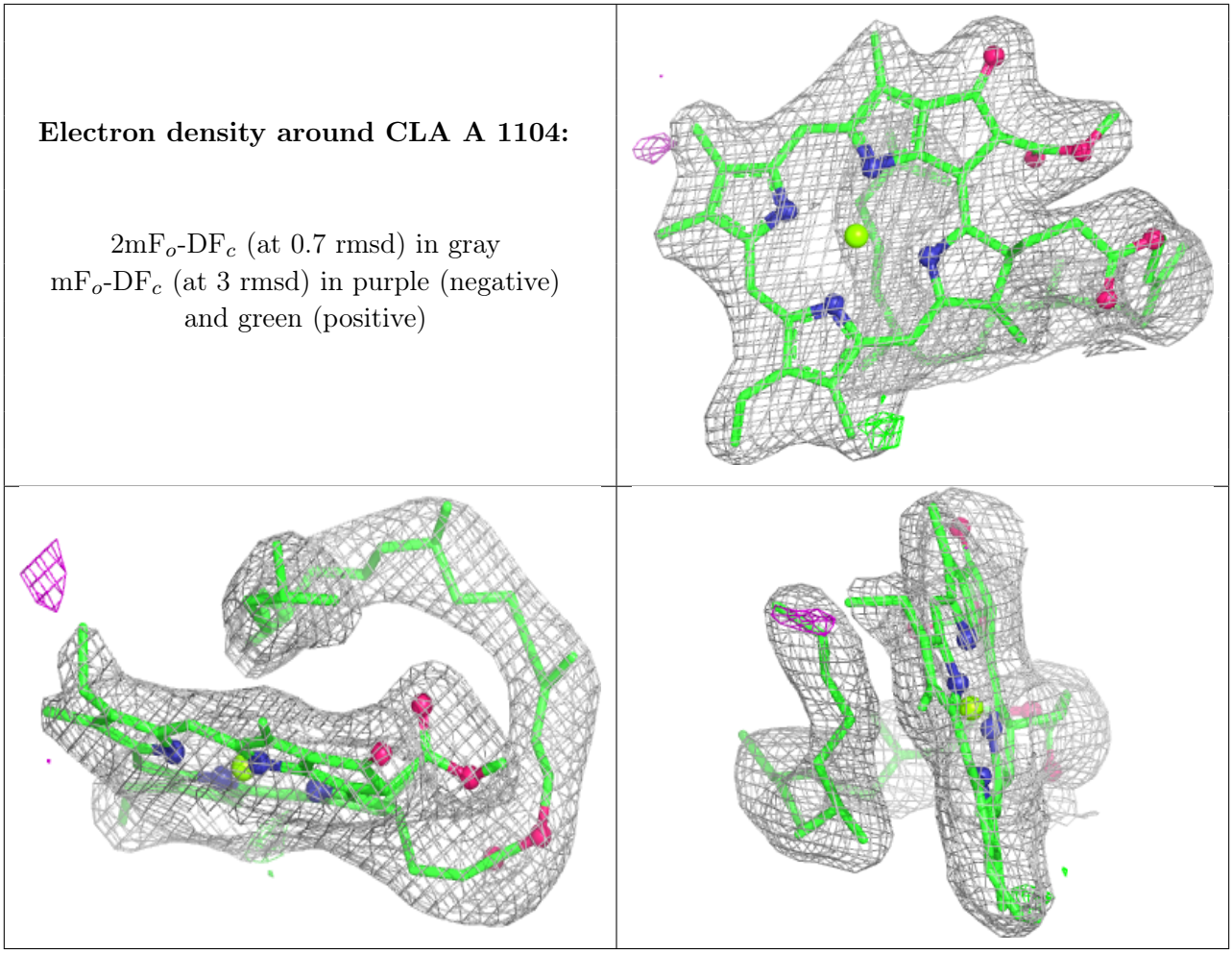






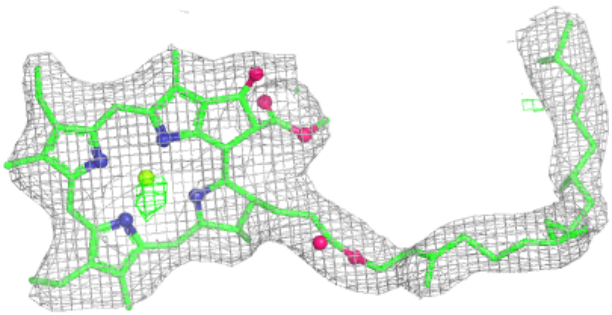
Electron density around CLA A 1104:

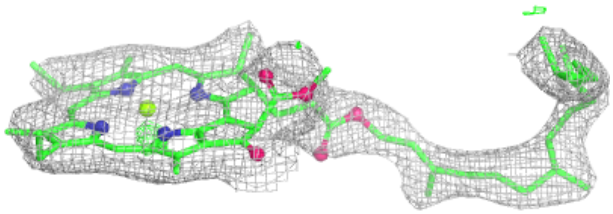
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

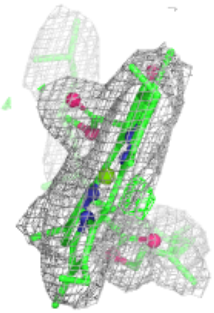


Electron density around CLA B 1223:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

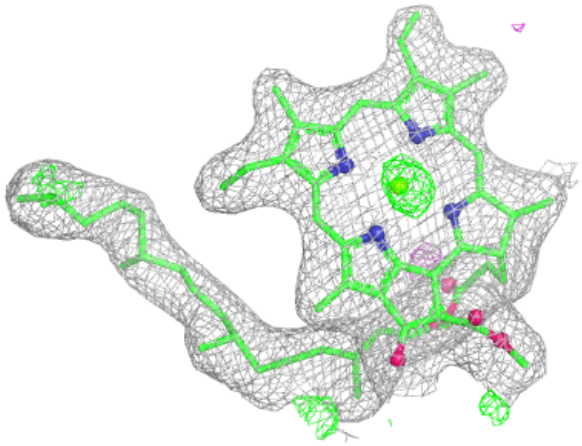


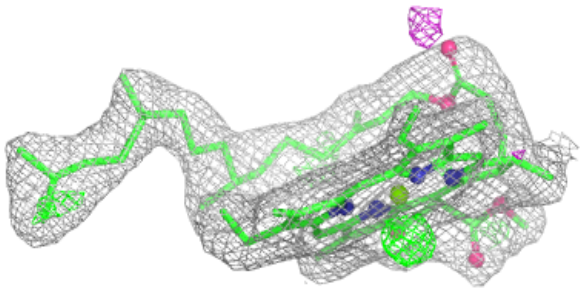


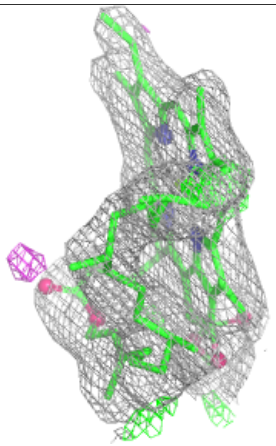


Electron density around CLA A 1127:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

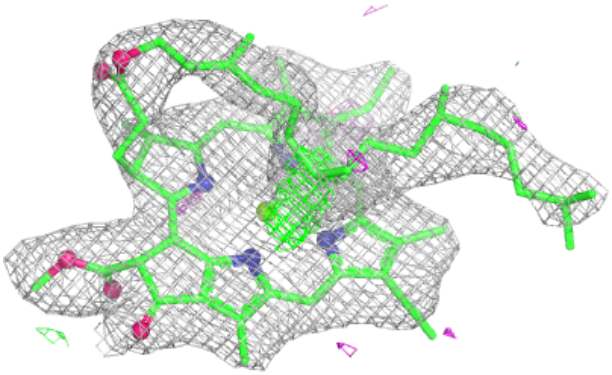


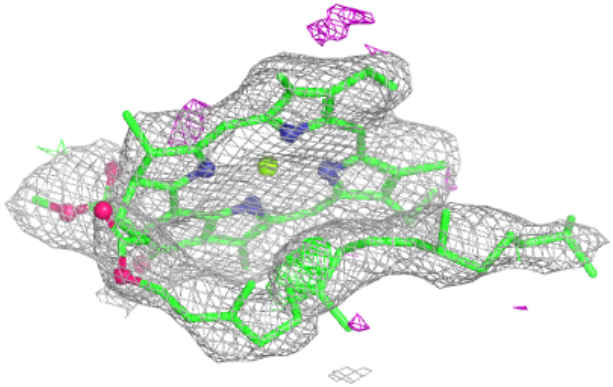


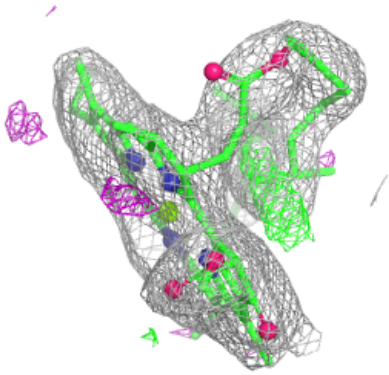


Electron density around CLA b 1214:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

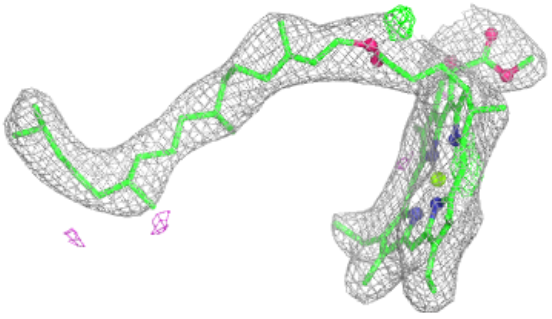


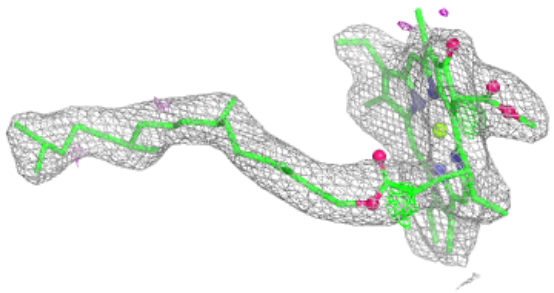


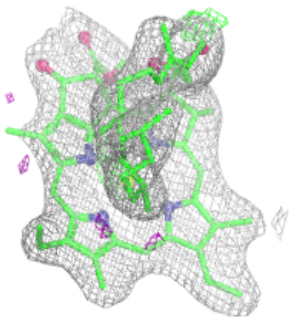


Electron density around CLA A 1128:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

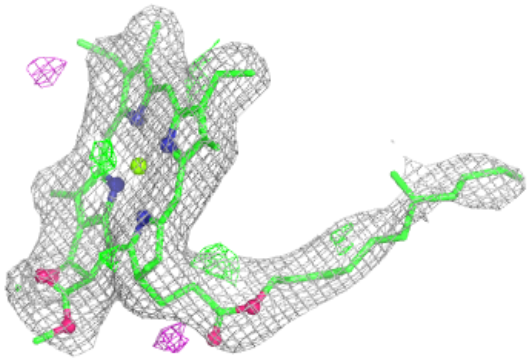


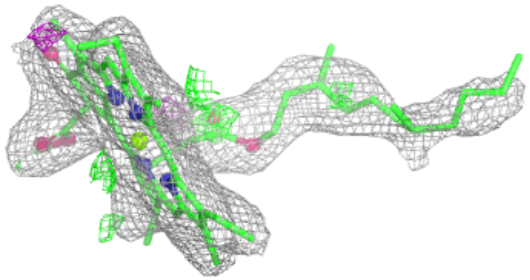


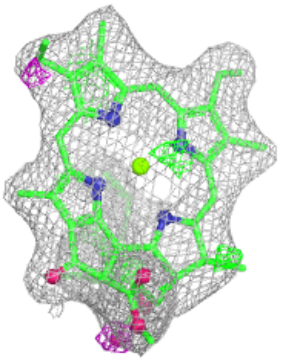


Electron density around CLA A 1129:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

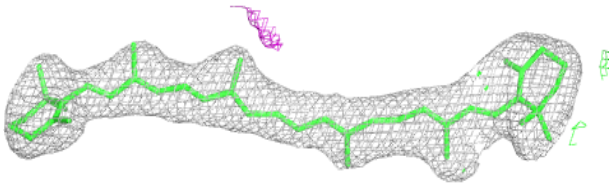


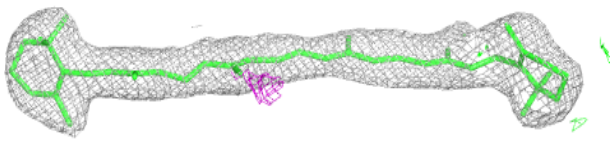


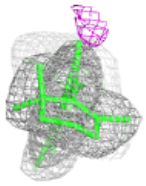


Electron density around BCR A 4007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

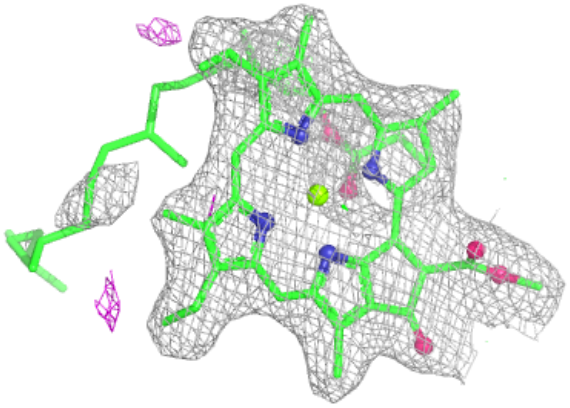


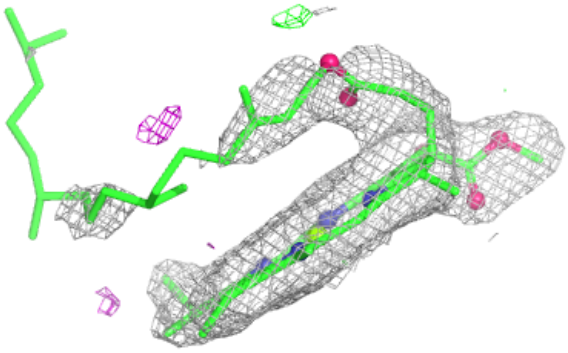


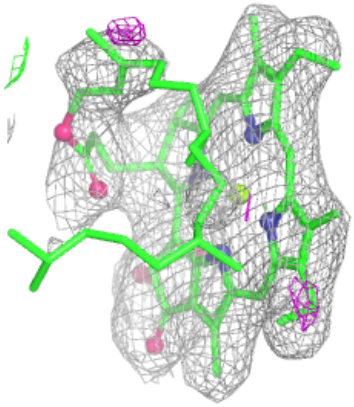


Electron density around CLA A 1110:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

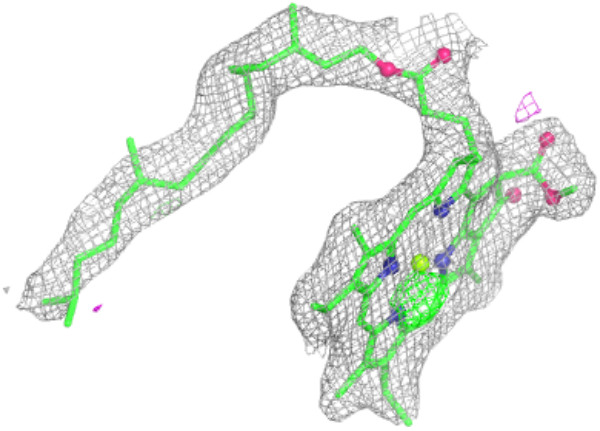


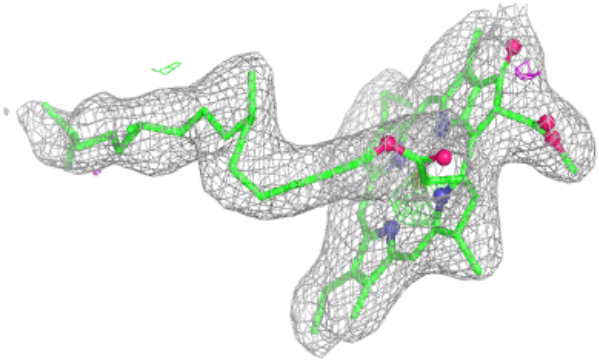


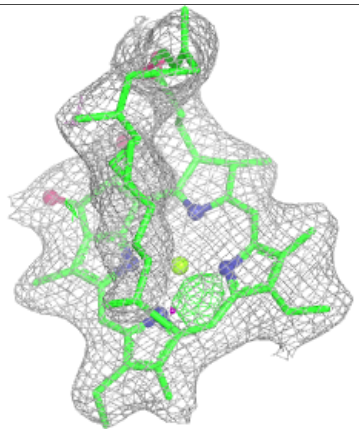


Electron density around CLA A 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

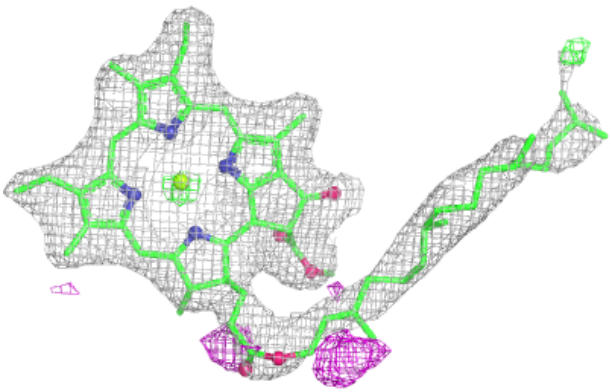


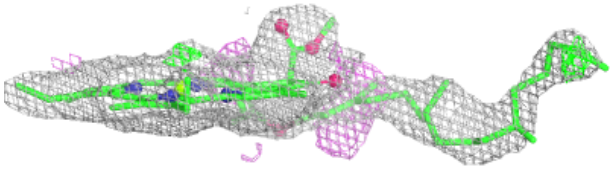


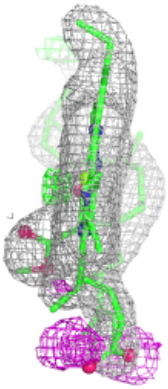


Electron density around CLA L 1503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

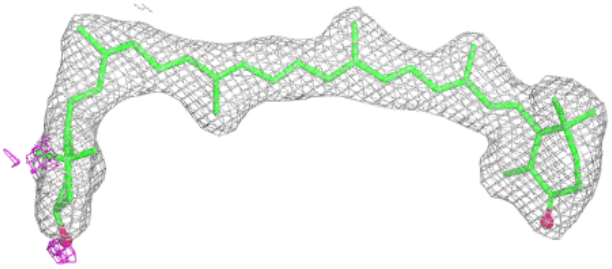


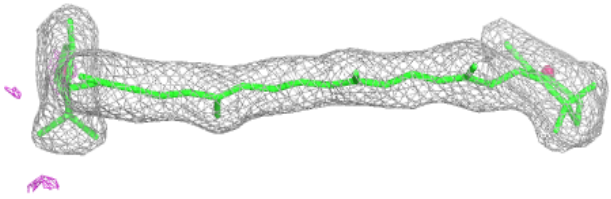


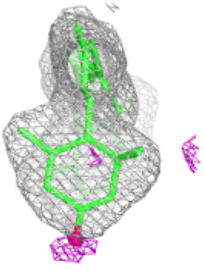


Electron density around EQ3 I 4020:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

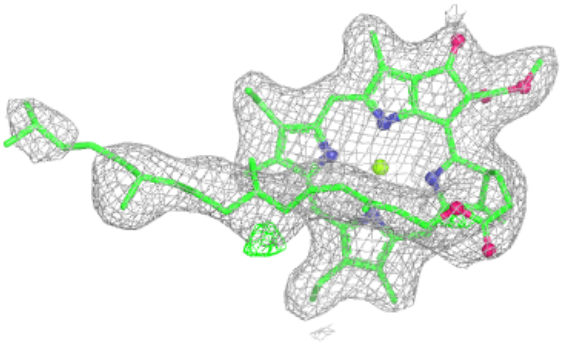


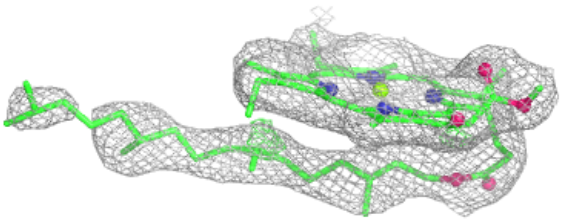




Electron density around CLA A 1116:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

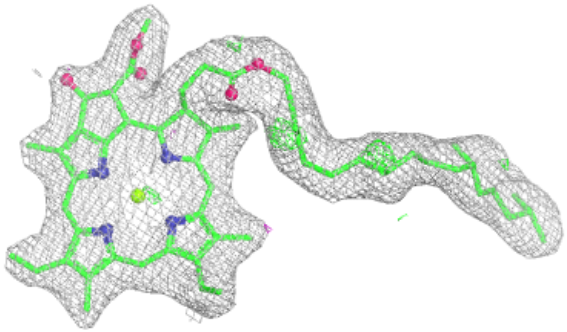


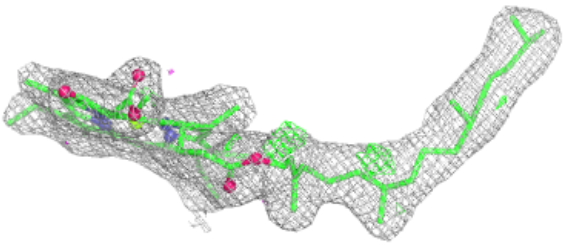




Electron density around CLA B 1023:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

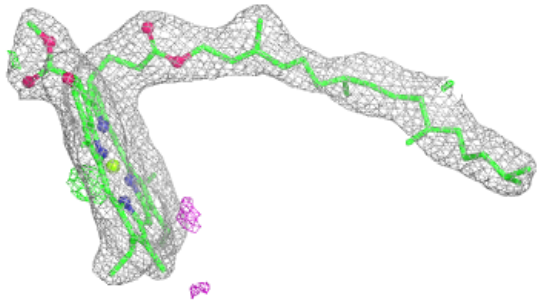


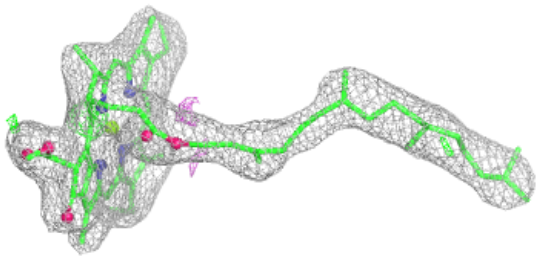


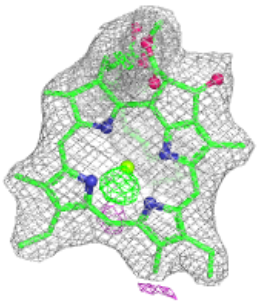


Electron density around CLA B 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

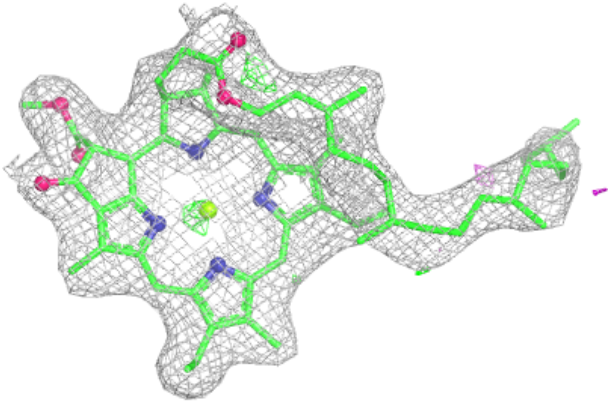


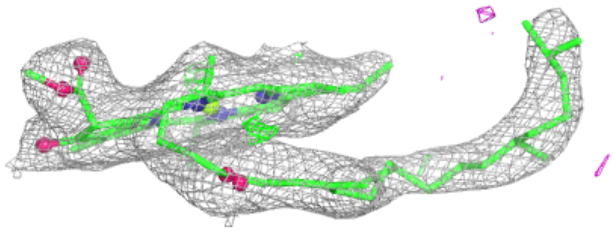


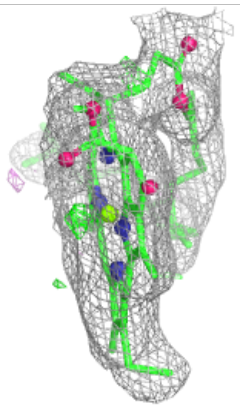


Electron density around CLA b 1215:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

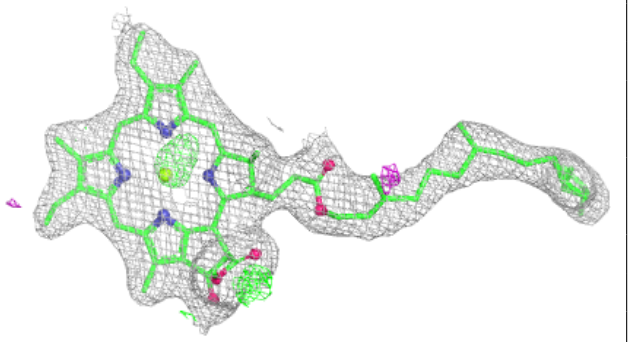


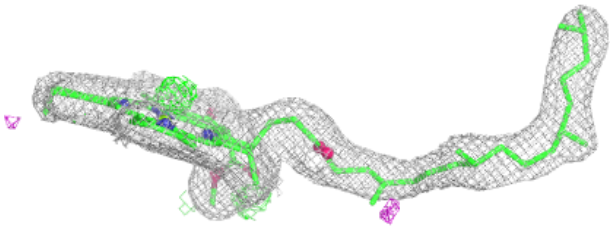


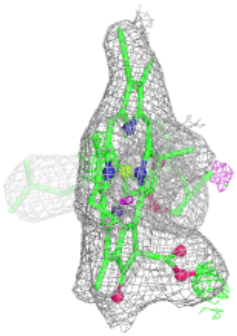


Electron density around CLA A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

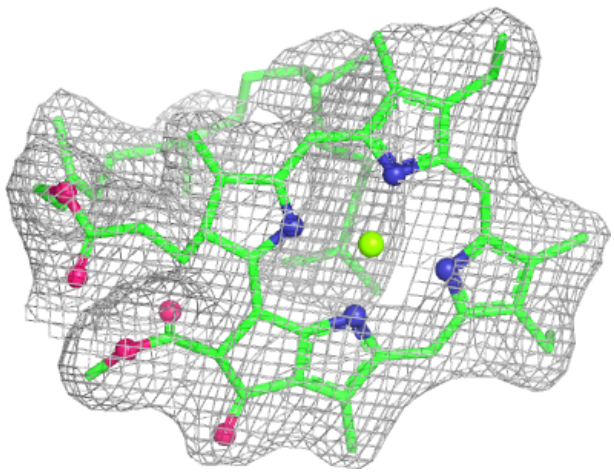


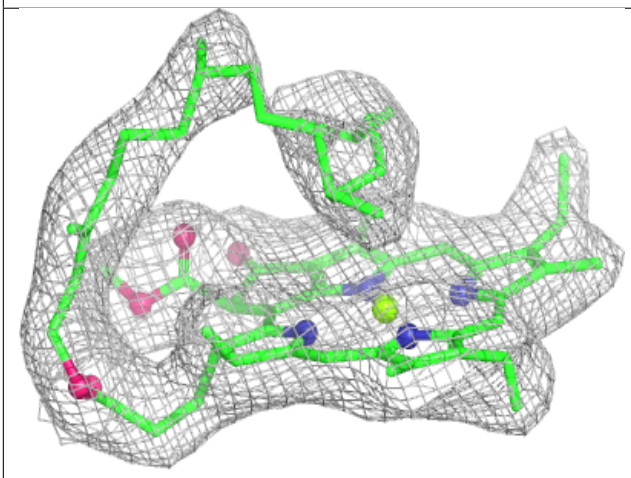


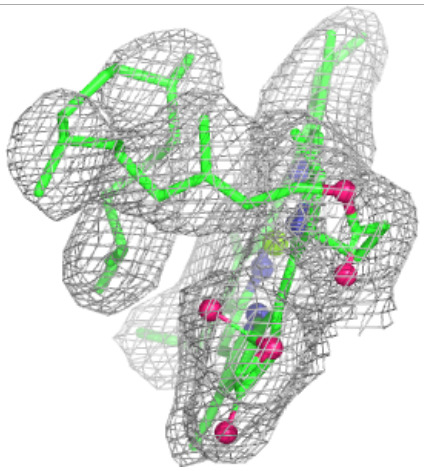


Electron density around CLA B 1203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

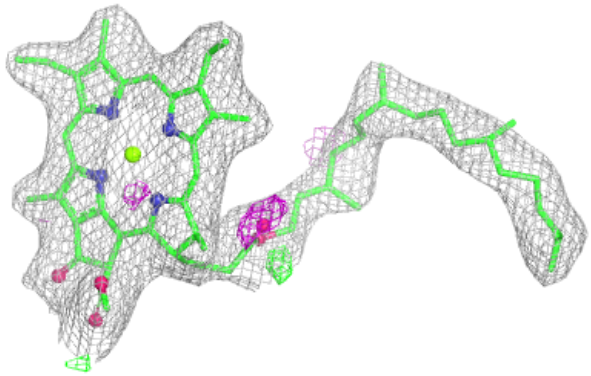


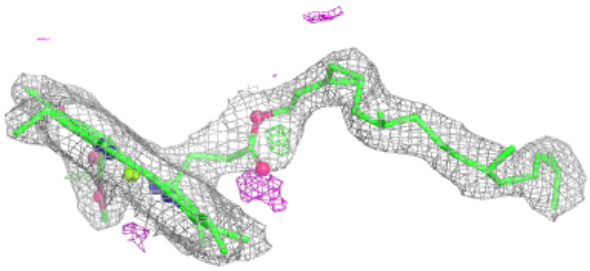


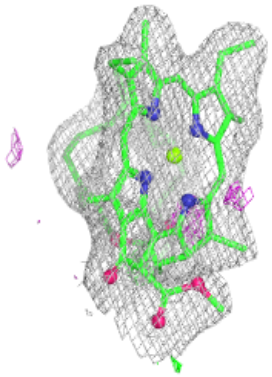


Electron density around CLA A 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

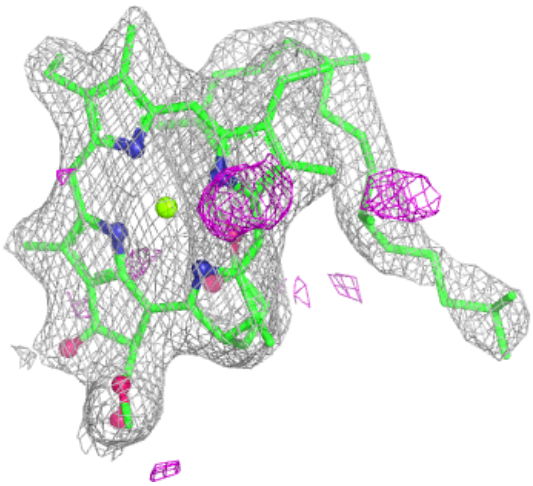


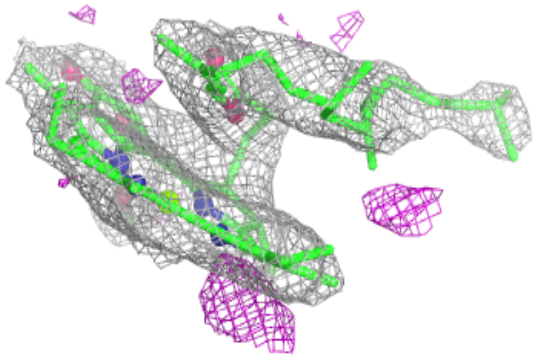


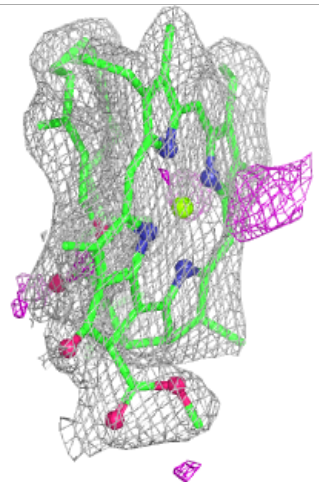


Electron density around CLA B 1205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

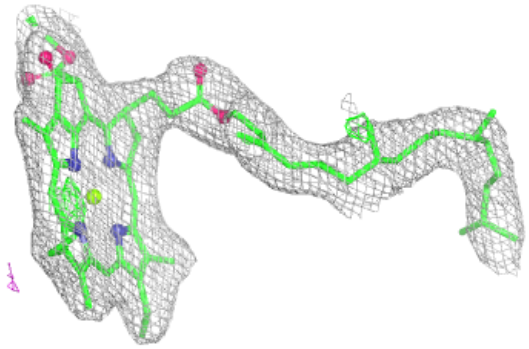


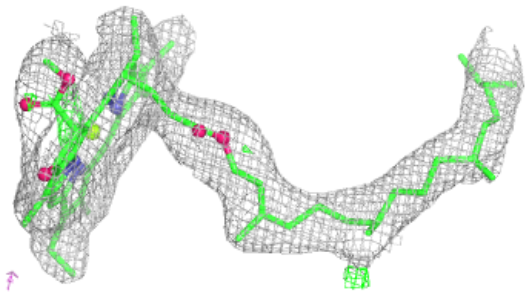


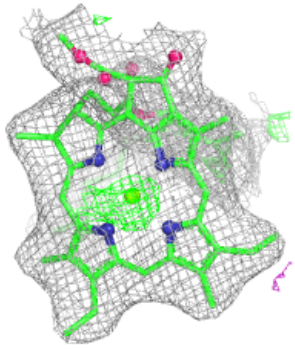


Electron density around CLA l 1502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

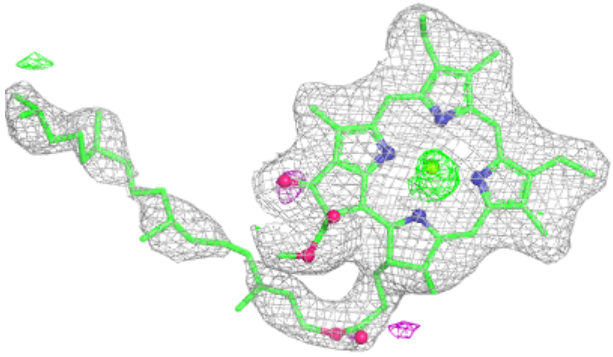


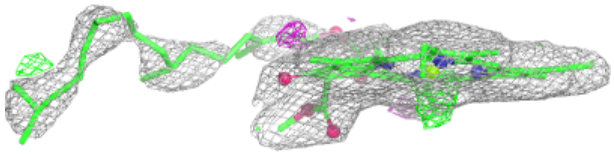


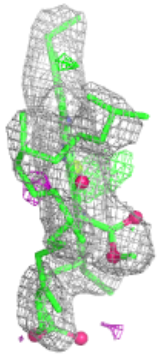


Electron density around CLA l 1503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

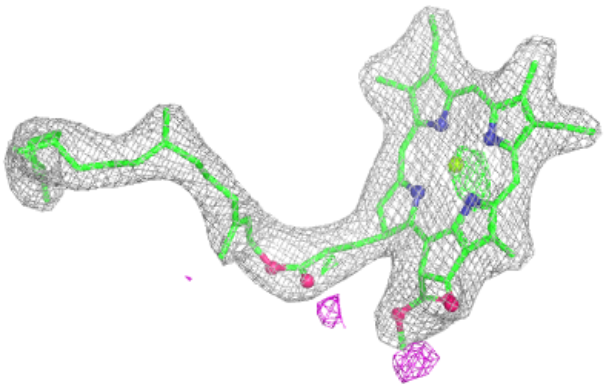


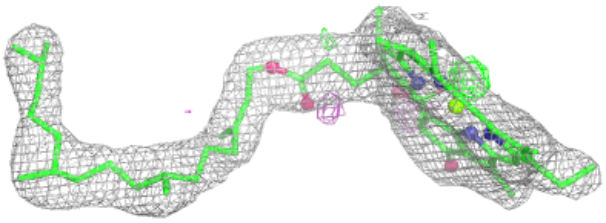


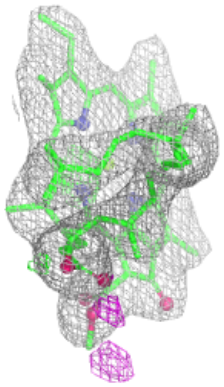


Electron density around CLA B 1206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

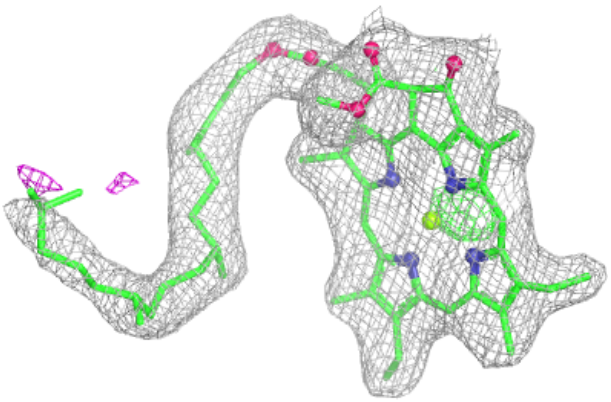


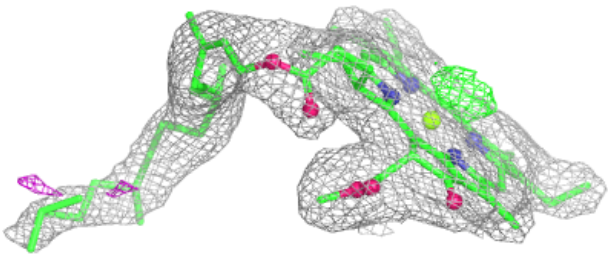


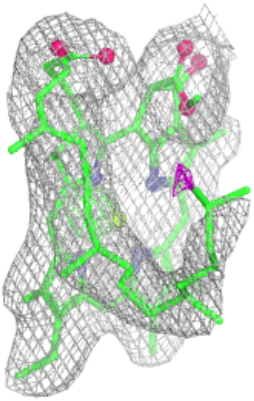


Electron density around CLA b 1221:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

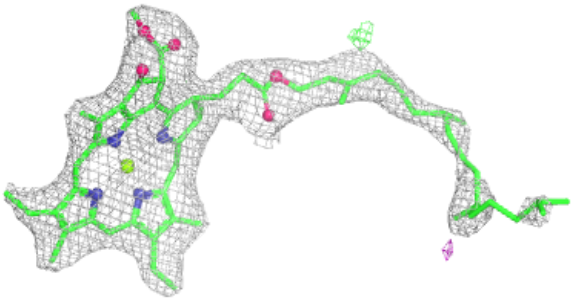


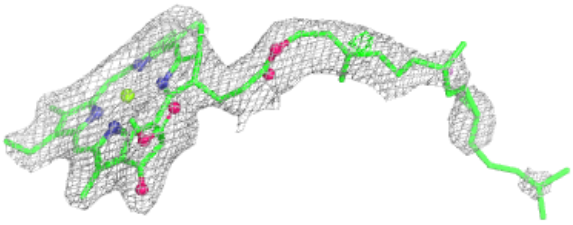


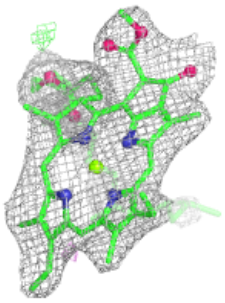


Electron density around CLA a 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

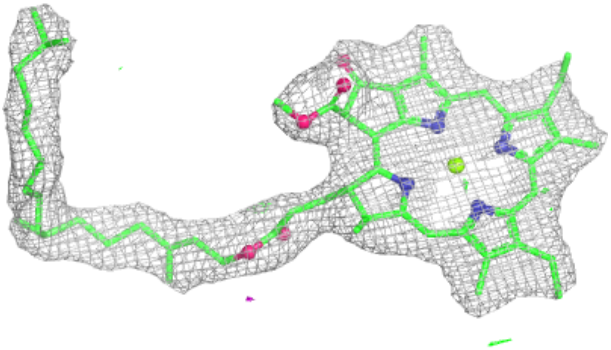


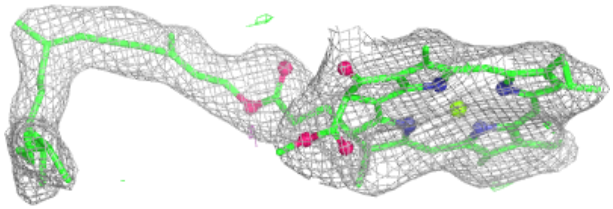


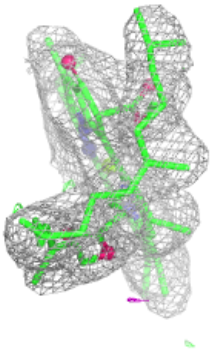


Electron density around CLA b 1223:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

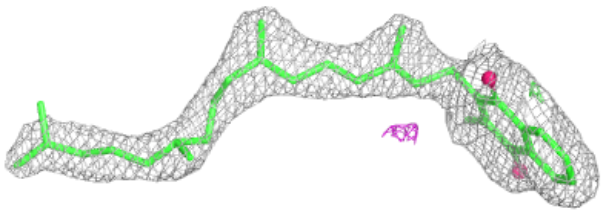


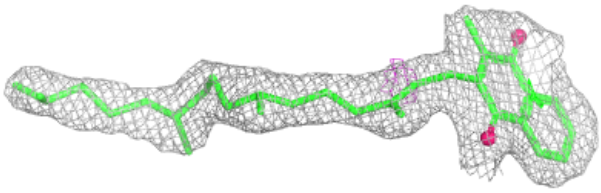


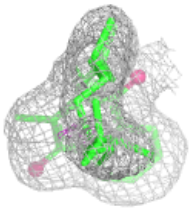


Electron density around PQN A 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

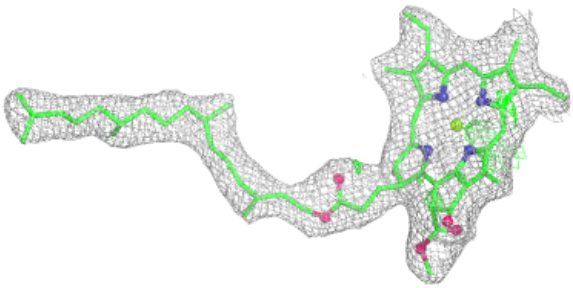


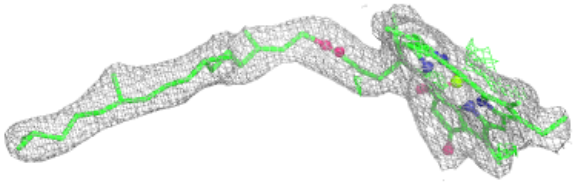


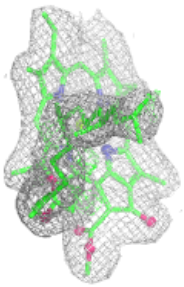


Electron density around CLA b 1022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

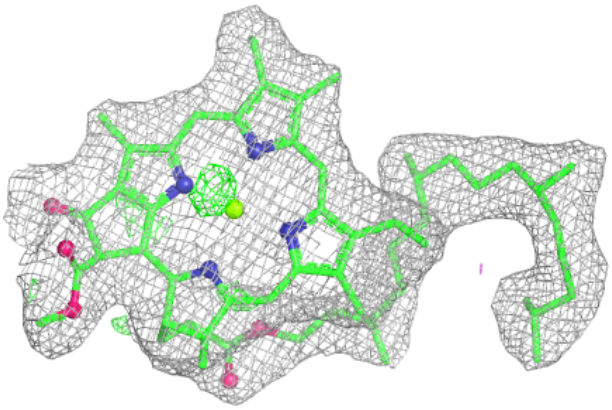


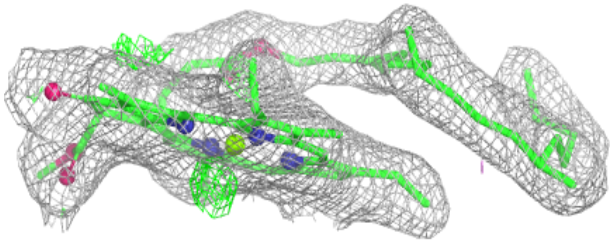


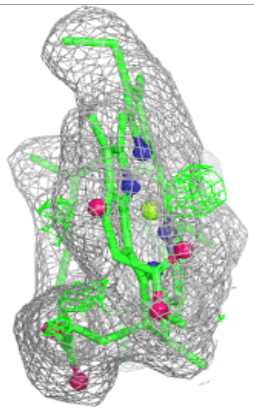


Electron density around CLA A 1117:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

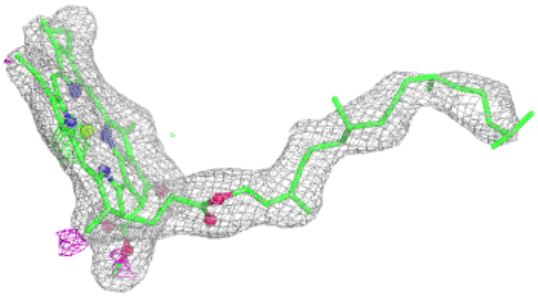


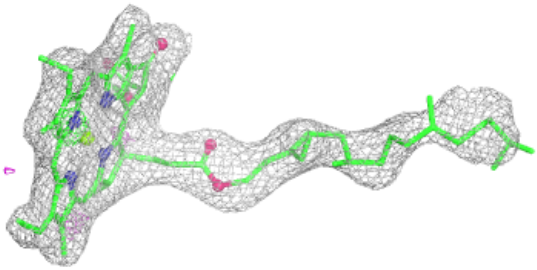


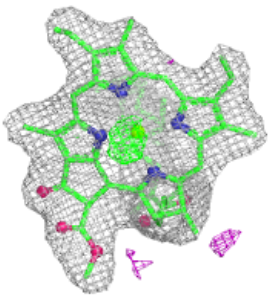


Electron density around CLA A 1137:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

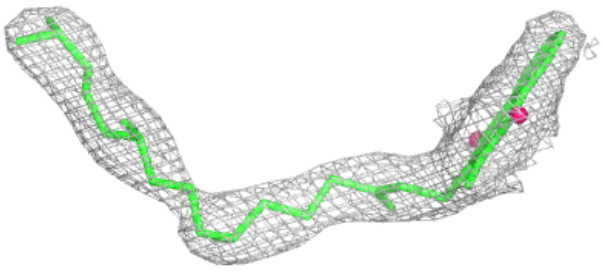


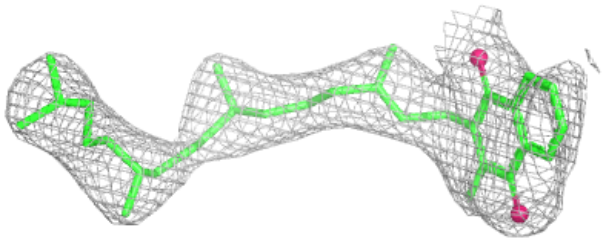


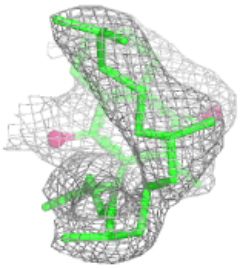


Electron density around PQN 2 2002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

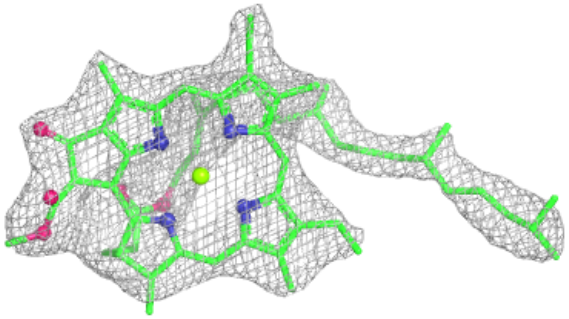


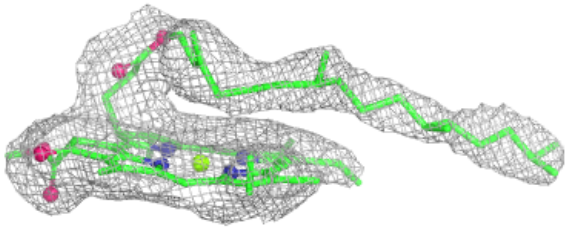


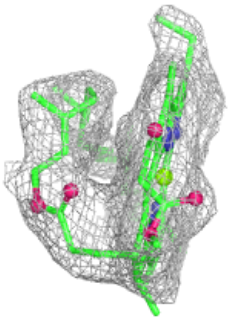


Electron density around CLA A 1138:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

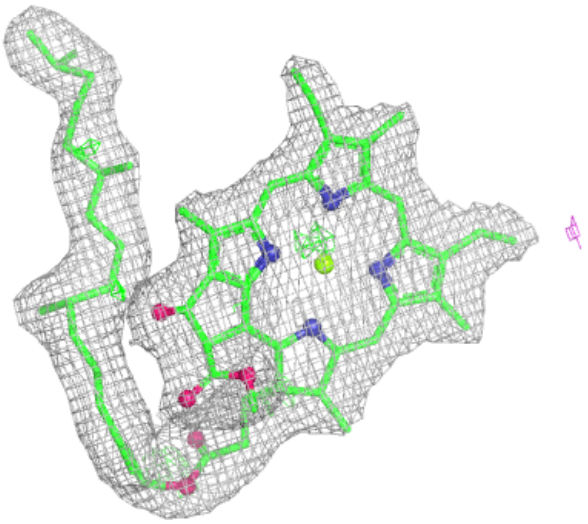


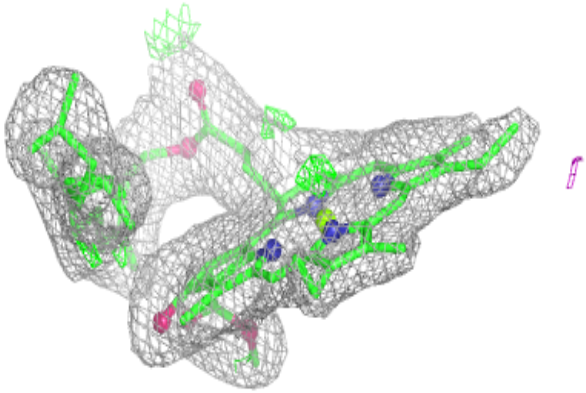


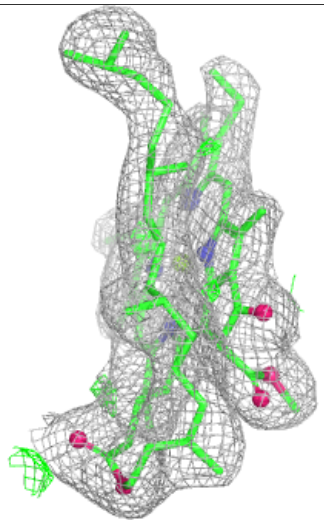


Electron density around CLA A 1123:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

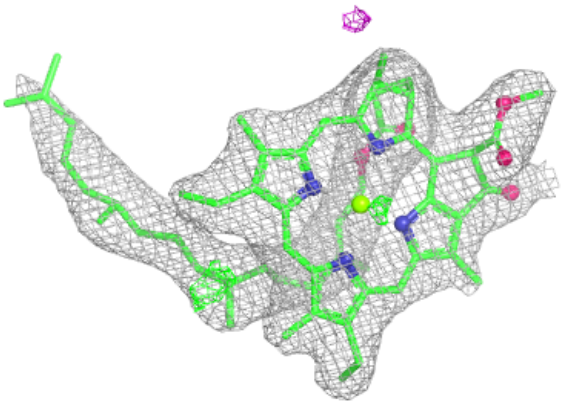


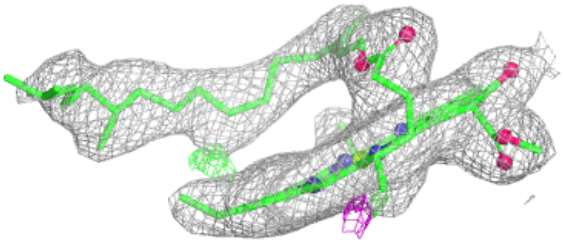


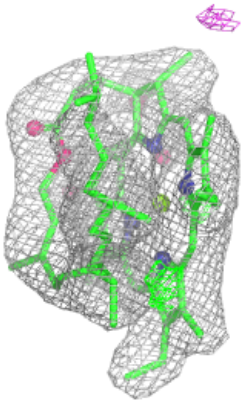


Electron density around CLA b 1204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

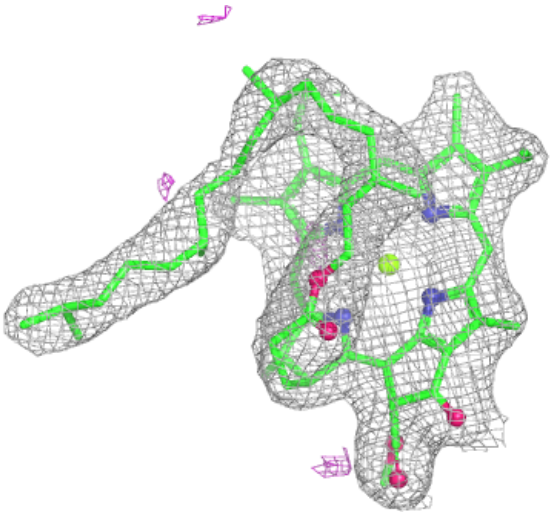


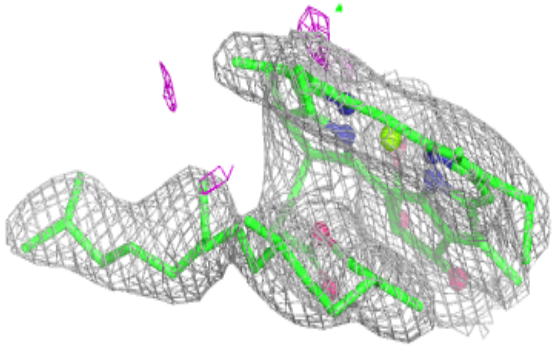




Electron density around CLA b 1205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

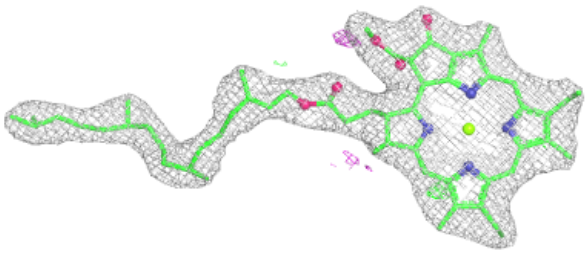


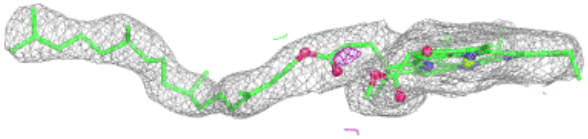


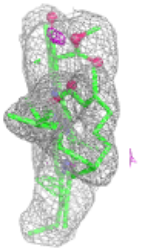


Electron density around CLA a 1131:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

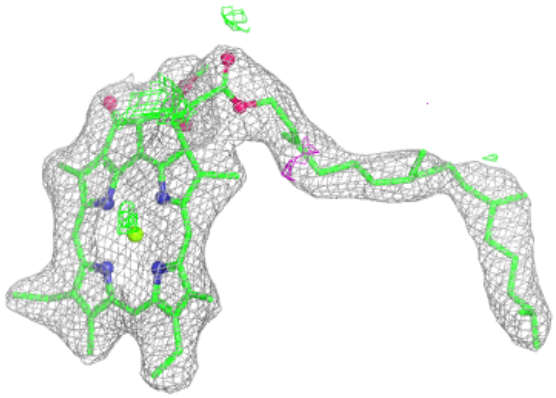


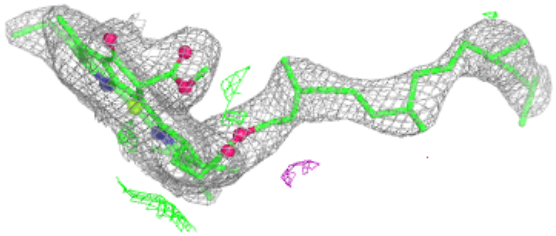


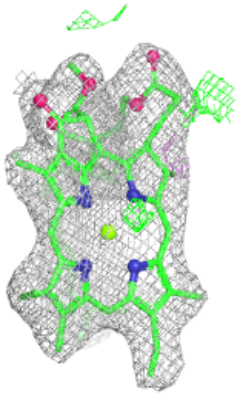


Electron density around CLA b 1207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

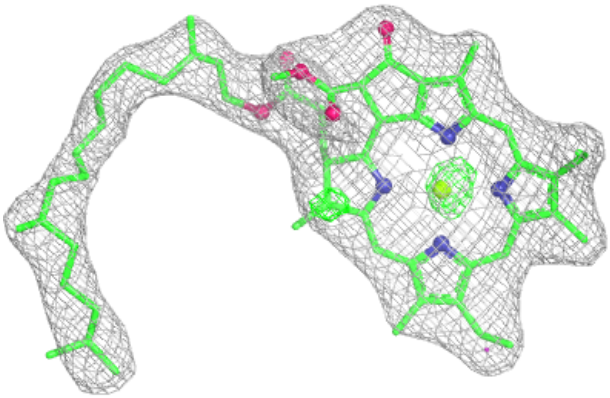


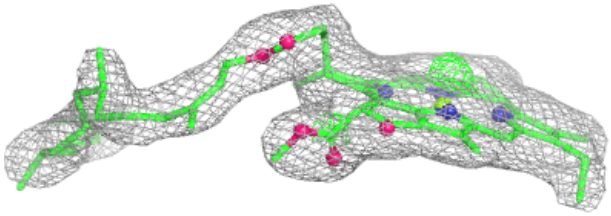


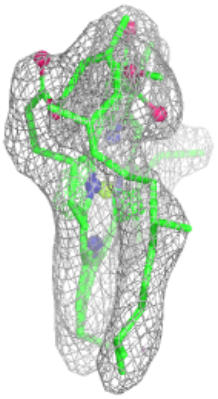


Electron density around CLA A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

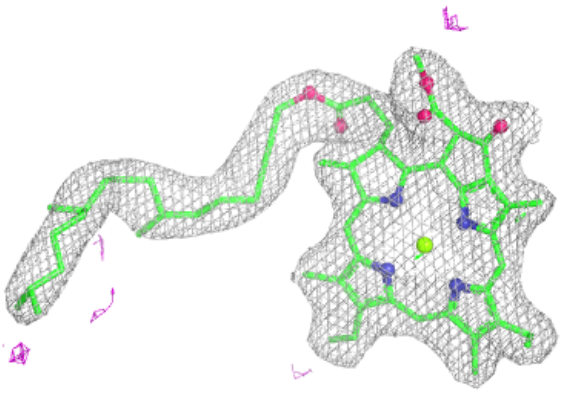


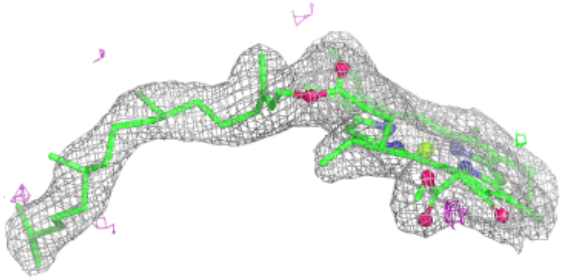


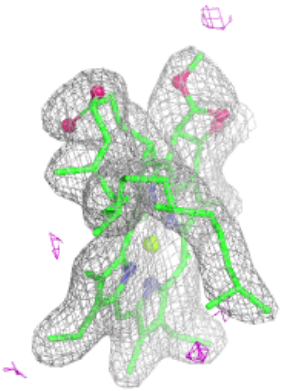


Electron density around CLA A 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

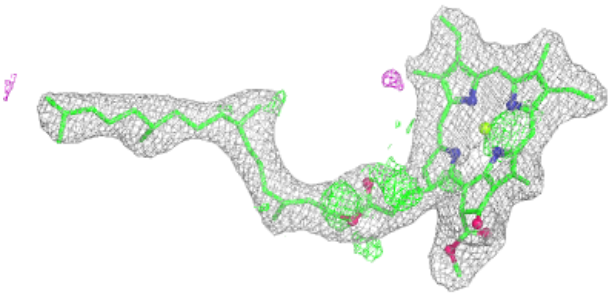


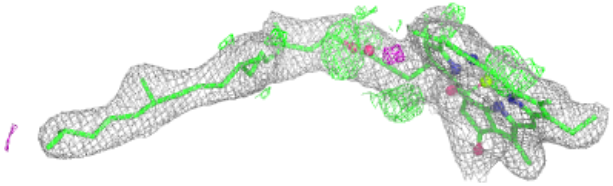


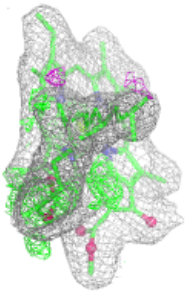


Electron density around CLA B 1022:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

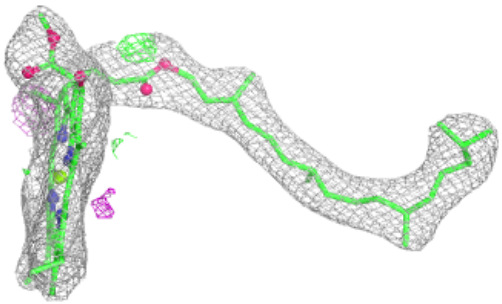


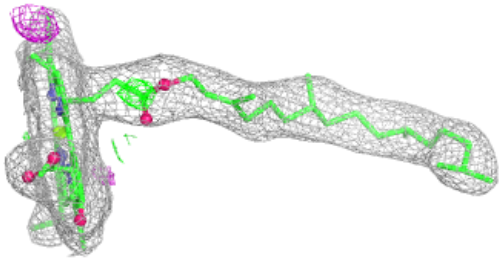


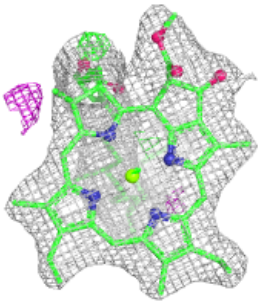


Electron density around CLA b 1239:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

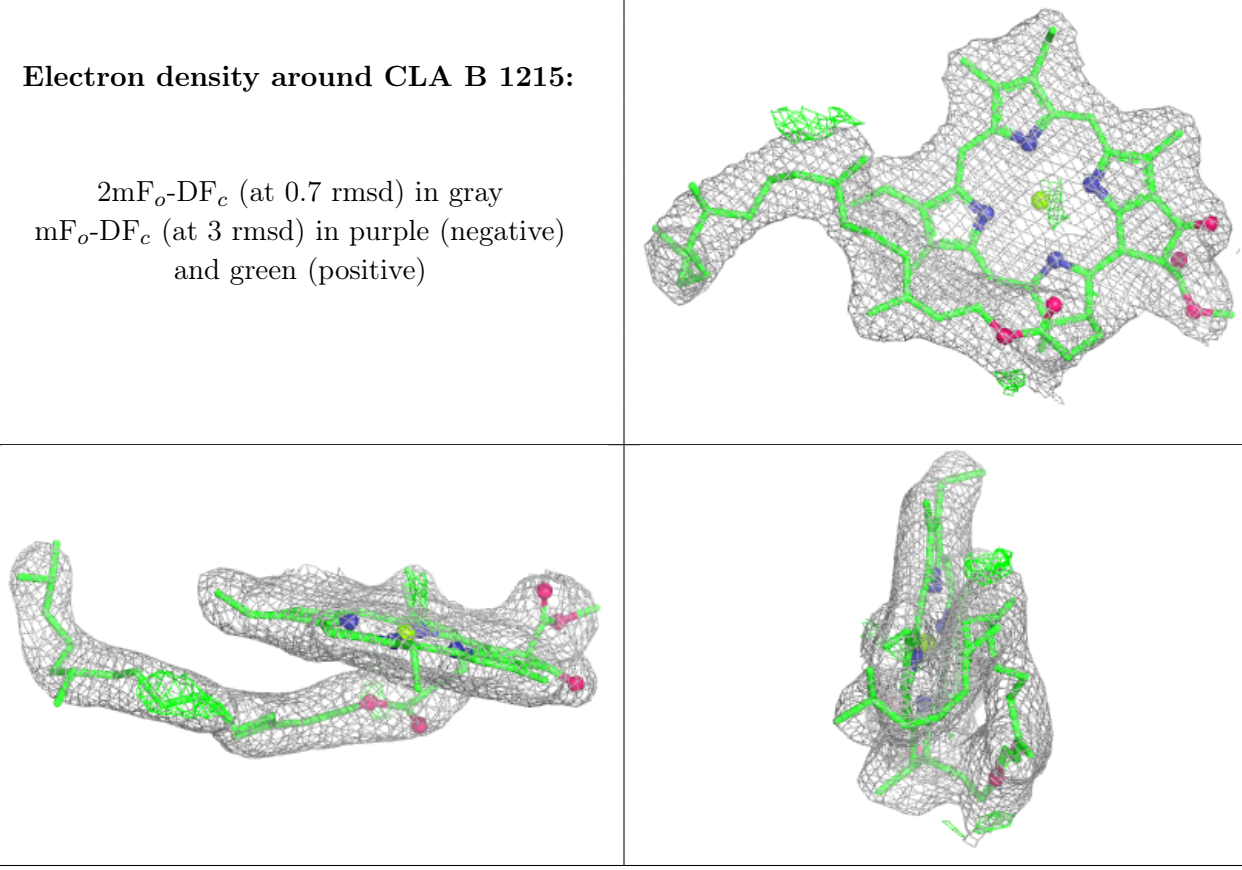






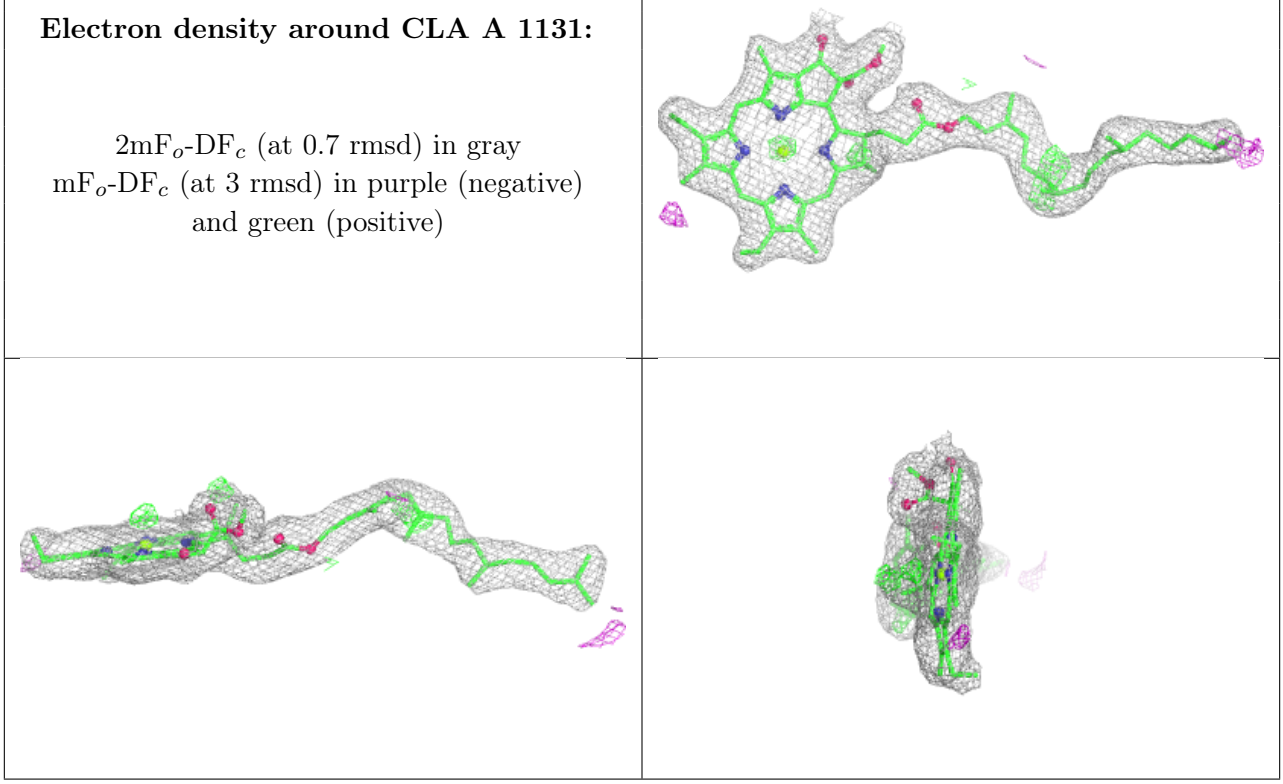
Electron density around CLA B 1215:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



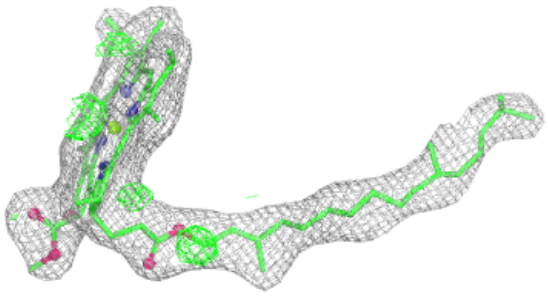
Electron density around CLA A 1131:

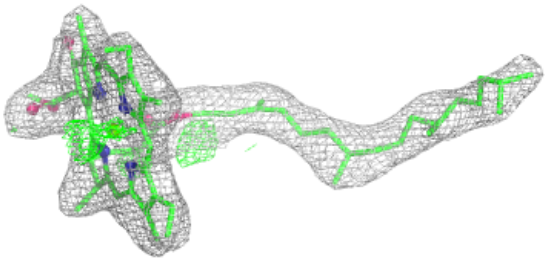
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

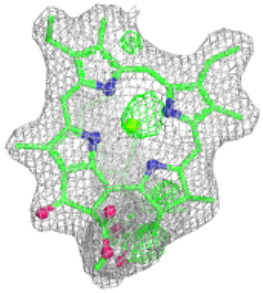


Electron density around CLA b 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

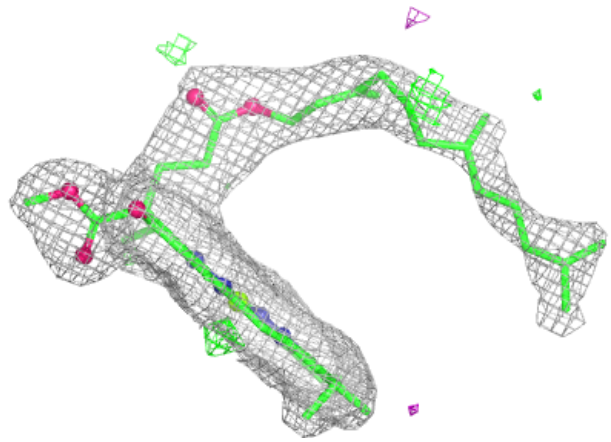


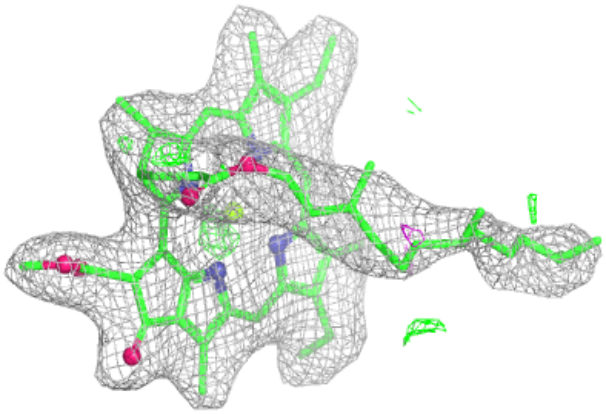


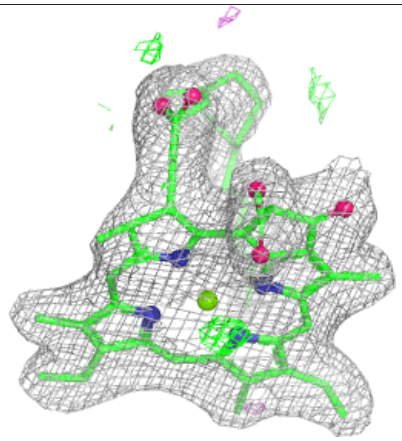


Electron density around CLA A 1130:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

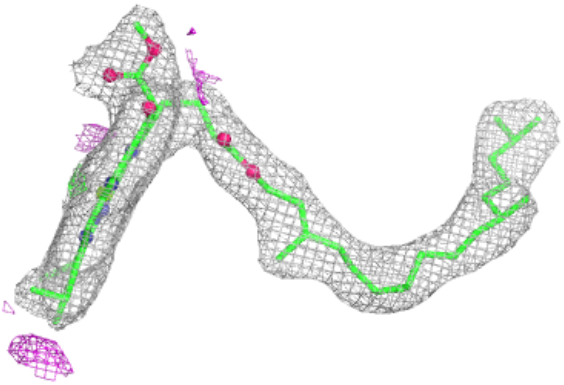


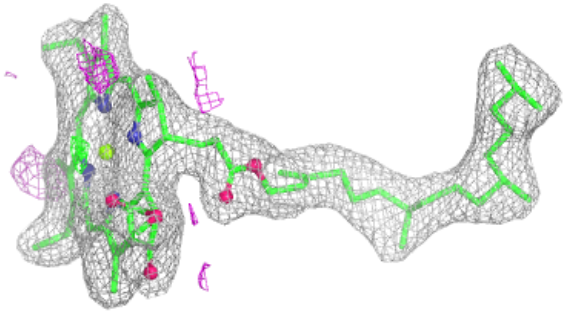


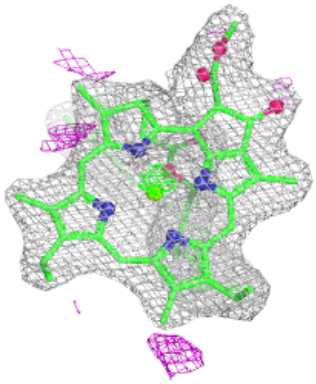


Electron density around CLA B 1238:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

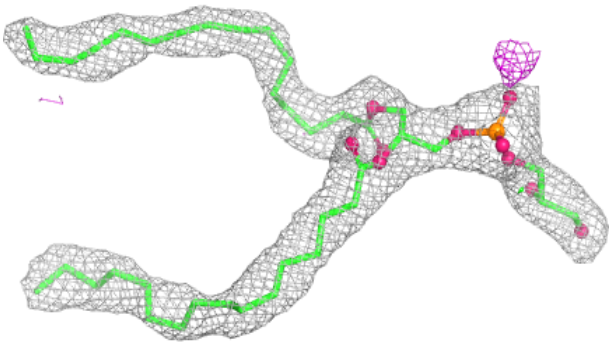


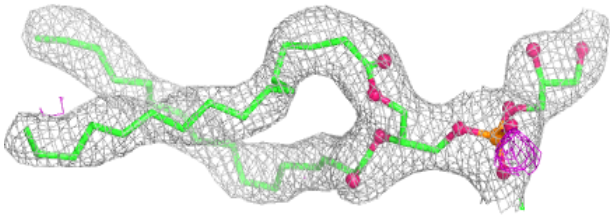


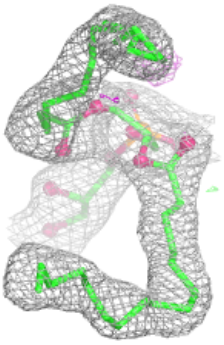


Electron density around LHG A 5001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

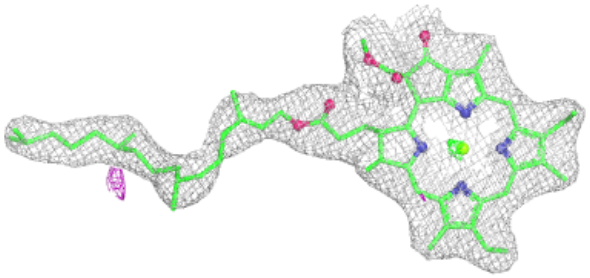


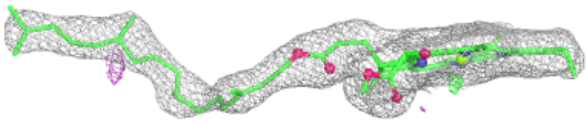


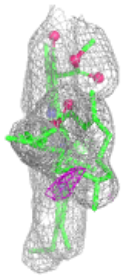


Electron density around CLA 1 1131:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

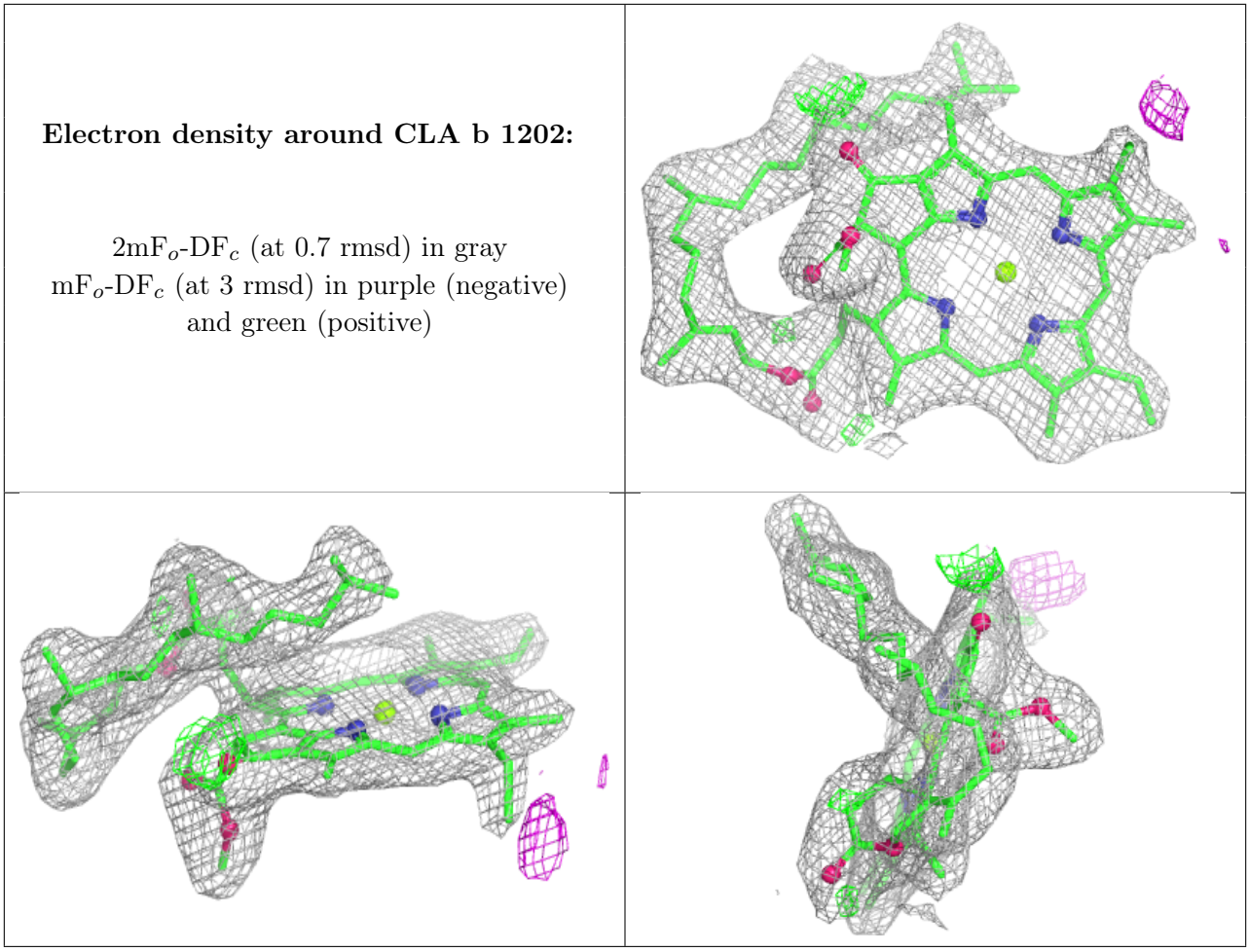






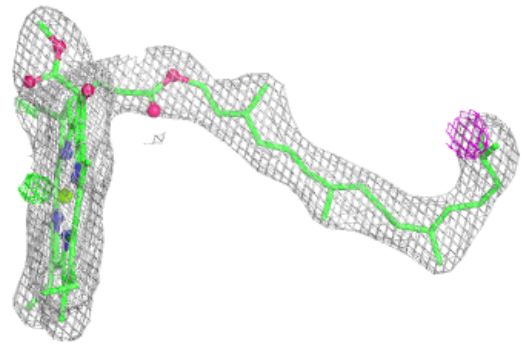
Electron density around CLA b 1202:

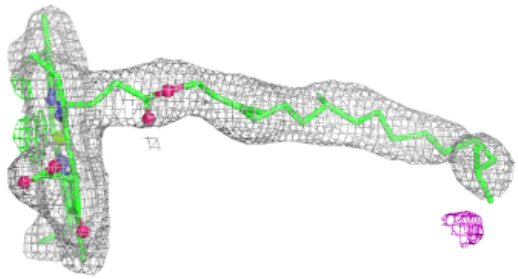
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

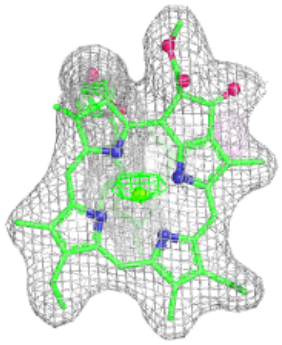


Electron density around CLA B 1239:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

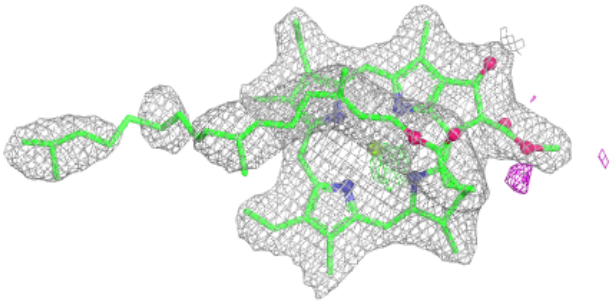


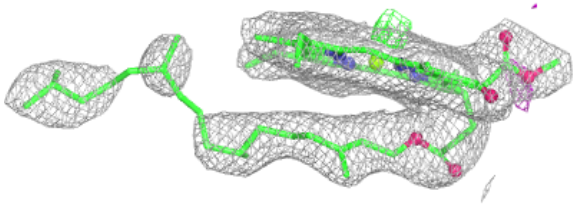


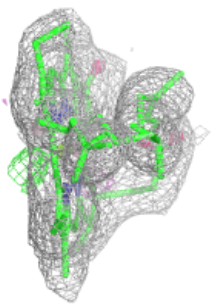


Electron density around CLA A 1136:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

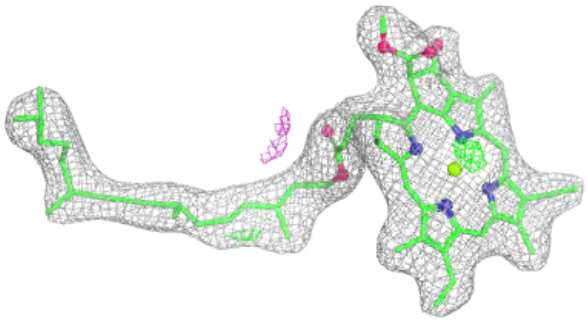


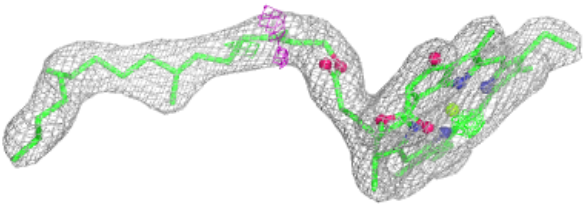




Electron density around CLA A 1119:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

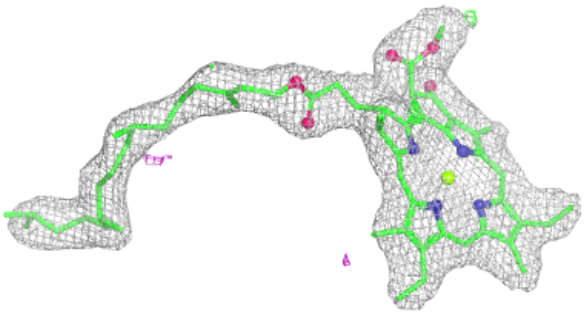


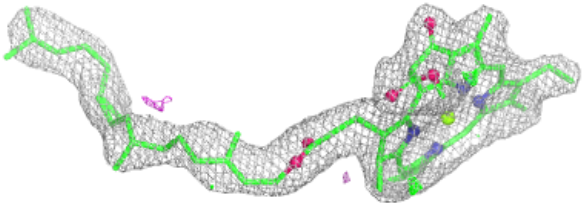


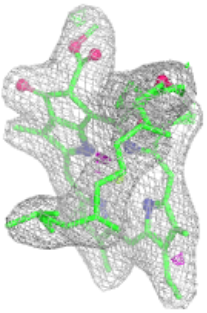


Electron density around CLA A 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

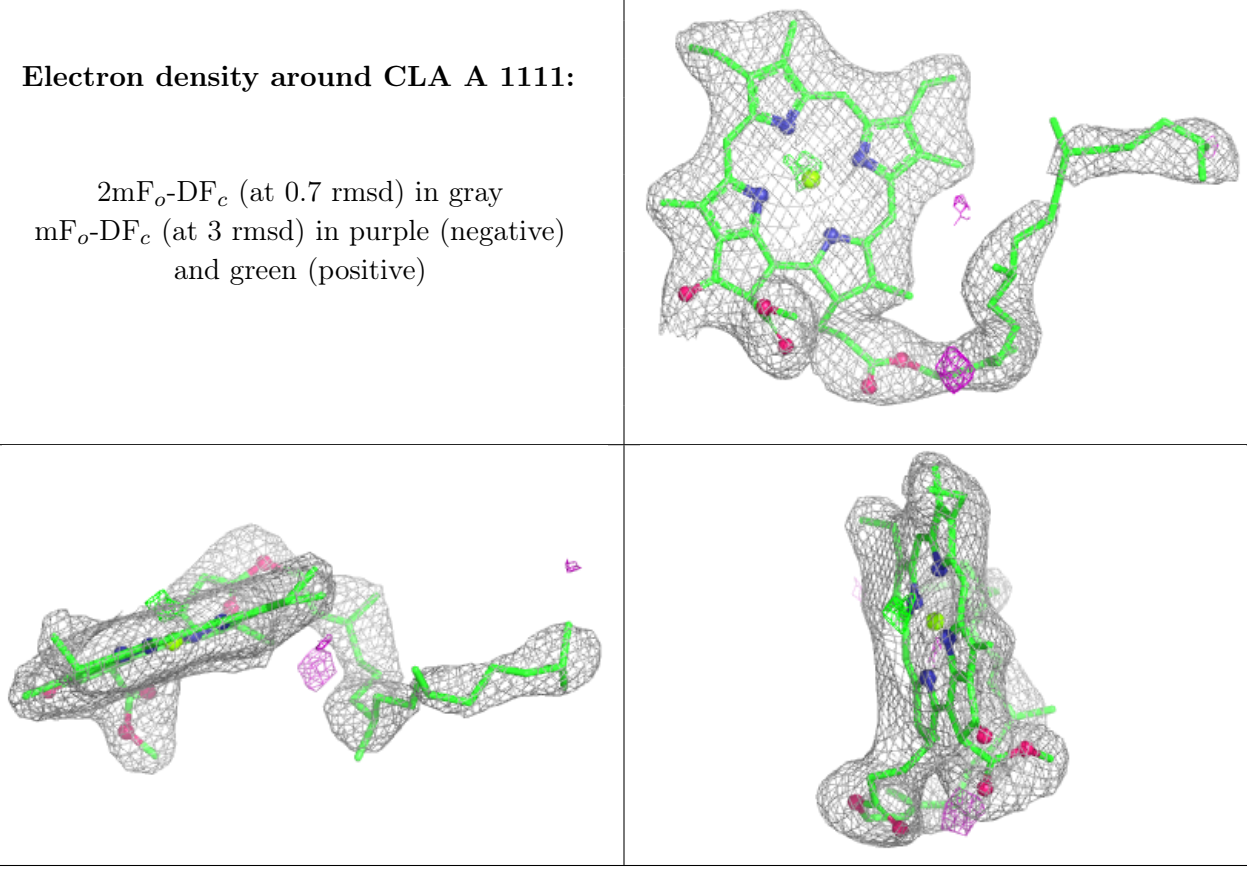






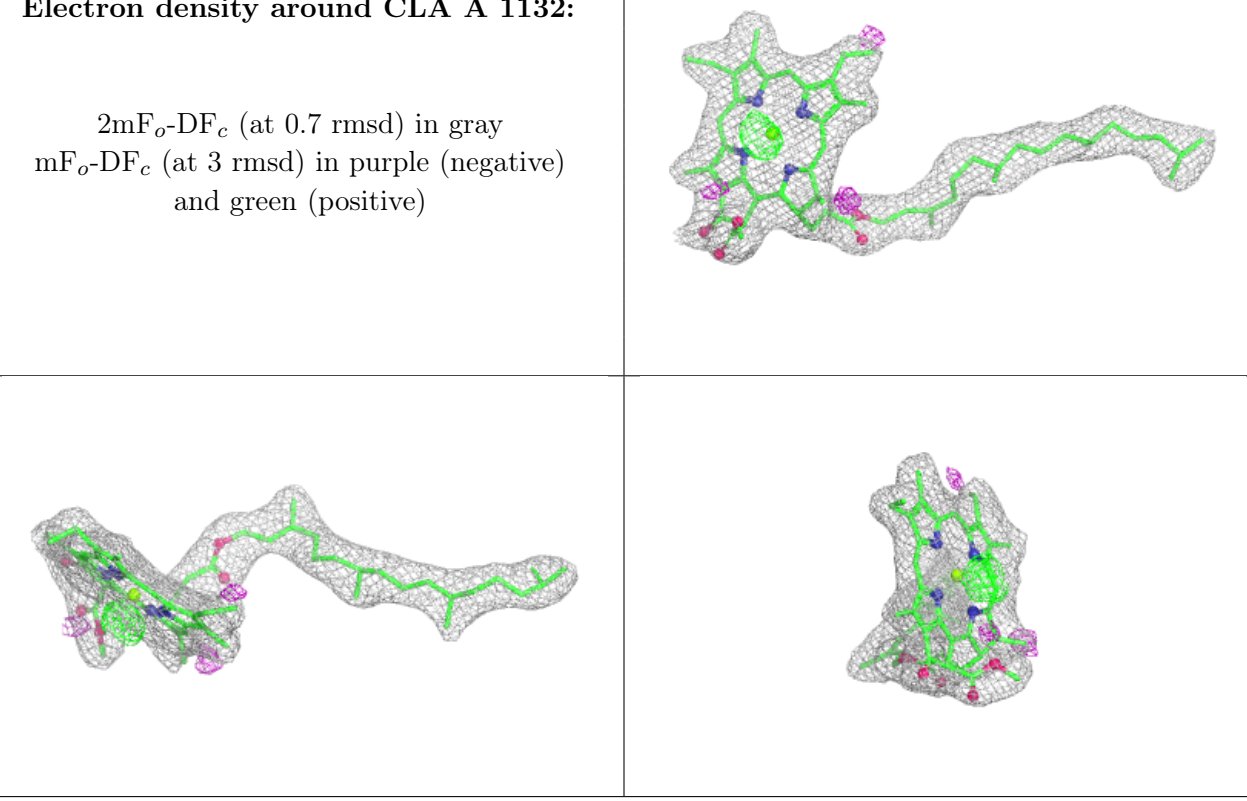
Electron density around CLA A 1111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



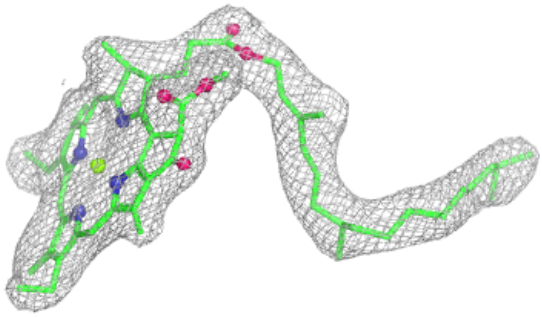
Electron density around CLA A 1132:

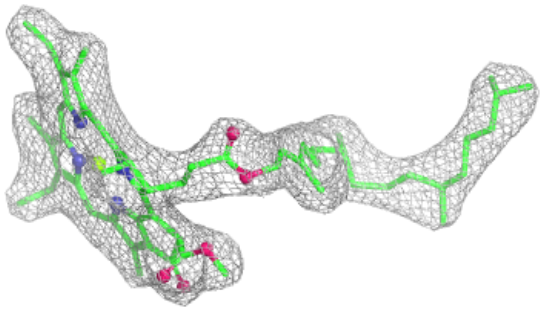
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

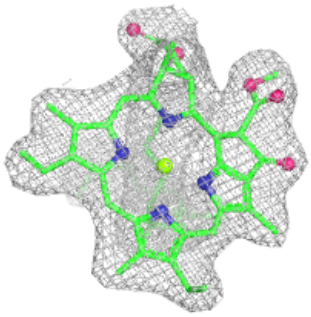


Electron density around CLA B 1021:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

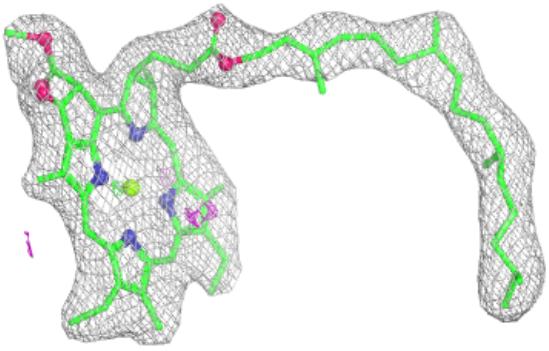


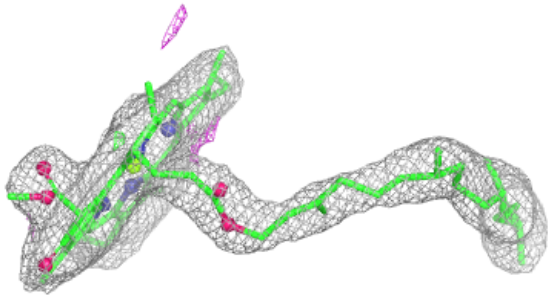


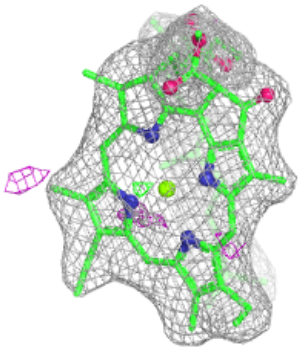


Electron density around CLA A 1140:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

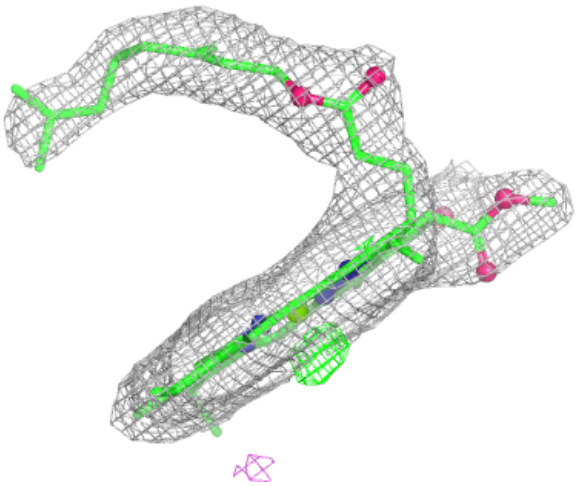


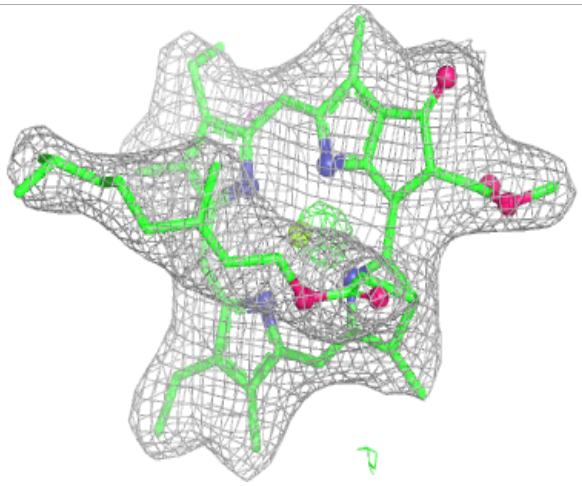


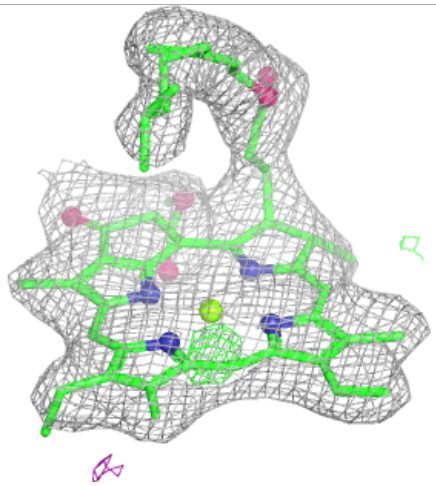


Electron density around CLA 1 1130:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

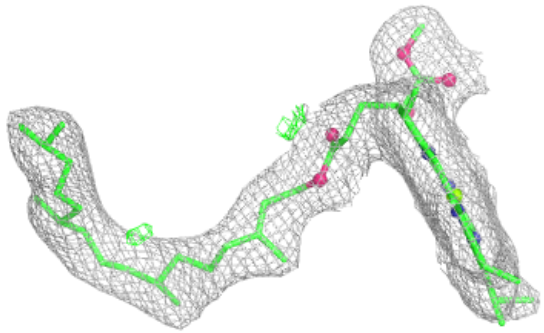


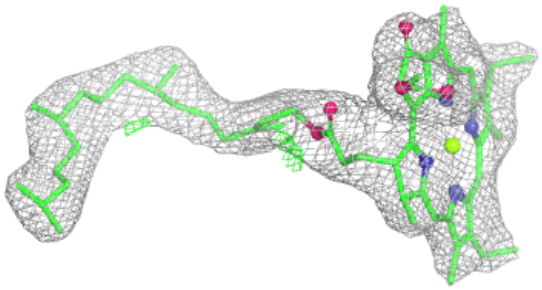


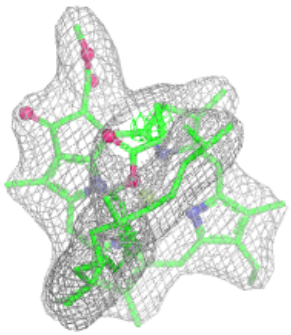


Electron density around CLA 2 1238:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

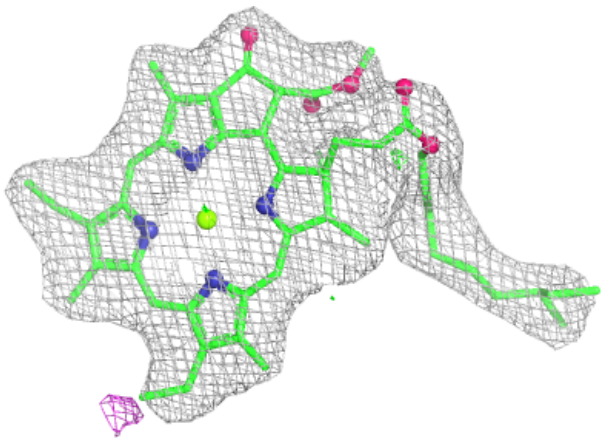


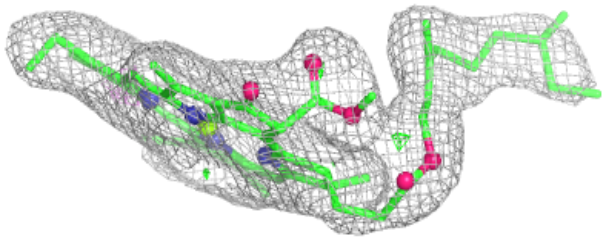


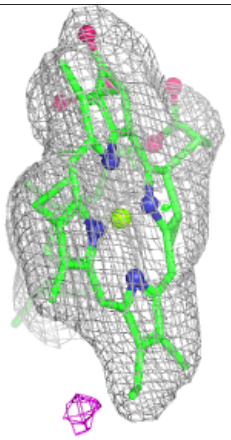


Electron density around CLA 2 1207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

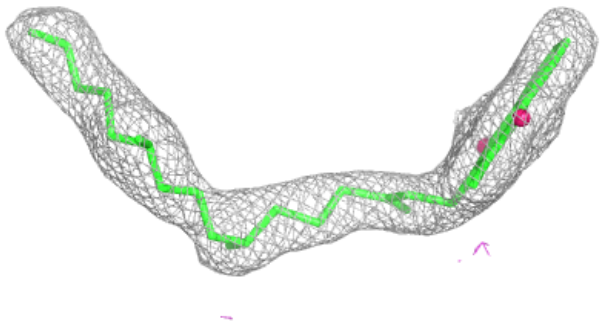


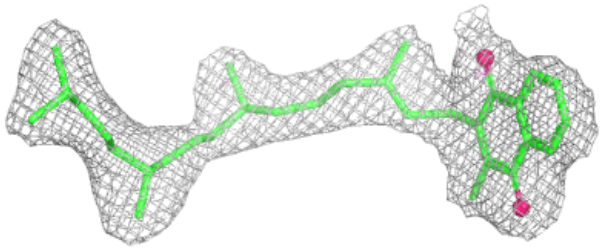


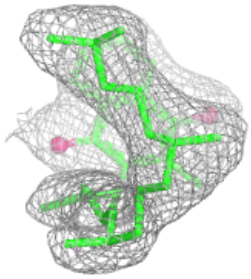


Electron density around PQN B 2002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

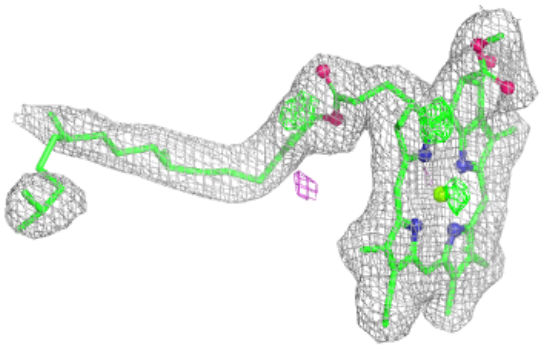


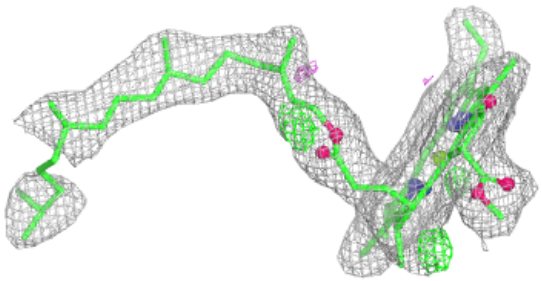


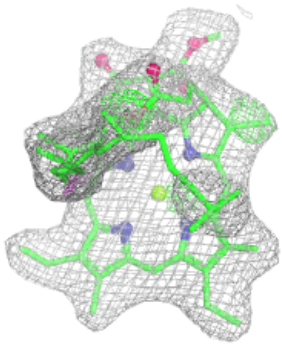


Electron density around CLA L 1502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.