



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:09 am BST

PDB ID : 4L6V
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-06-13
Resolution : 3.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

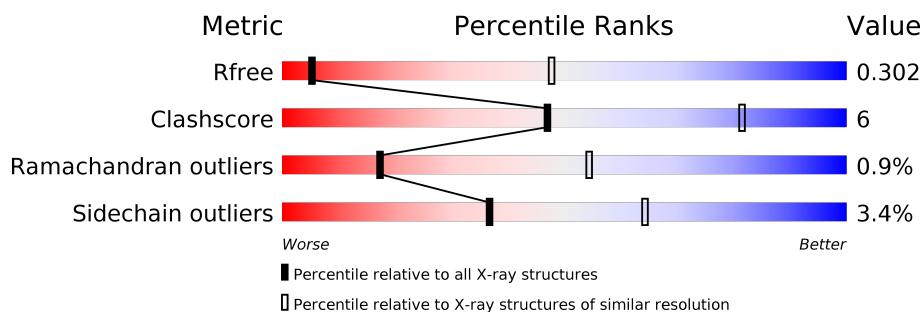
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.




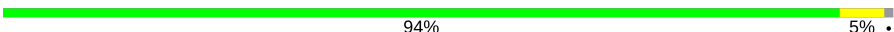












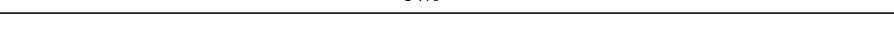

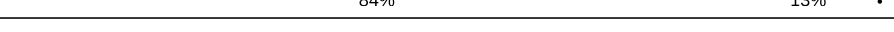
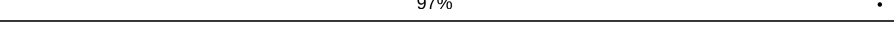
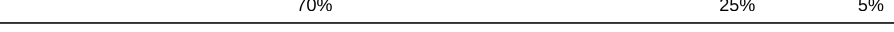



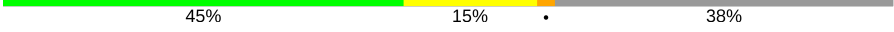
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	751	90% 8% .
1	A	751	86% 12% ..
1	a	751	96% ..
2	2	731	90% 9% .
2	B	731	87% 11% .
2	b	731	96% .
3	3	81	88% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	81	 84% 10% 5% .
3	c	81	 94% 5% .
4	4	141	 91% . . .
4	D	141	 88% 8% . .
4	d	141	 94% . .
5	5	74	 82% 7% . 8%
5	E	74	 84% 7% . 8%
5	e	74	 88% . 8%
6	6	125	 94% 6%
6	F	125	 90% 9% .
6	f	125	 98% .
7	8	157	 91% 5% .
7	L	157	 88% 8% . .
7	l	157	 94% . .
8	7	31	 81% 16% .
8	M	31	 84% 13% .
8	m	31	 97% .
9	9	40	 70% 25% 5%
9	I	40	 70% 25% 5%
9	i	40	 85% 10% 5%
10	0	128	 51% 10% . 38%
10	K	128	 45% 15% . 38%
10	k	128	 55% 8% 38%

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
11	CLA	0	1401	X	-	-	-
11	CLA	0	1402	X	-	-	-
11	CLA	1	1011	X	-	-	-
11	CLA	1	1012	X	-	-	-
11	CLA	1	1022	X	-	-	-
11	CLA	1	1101	X	-	-	-
11	CLA	1	1102	X	-	-	-
11	CLA	1	1103	X	-	-	-
11	CLA	1	1104	X	-	-	-
11	CLA	1	1105	X	-	-	-
11	CLA	1	1106	X	-	-	-
11	CLA	1	1107	X	-	-	-
11	CLA	1	1108	X	-	-	-
11	CLA	1	1109	X	-	-	-
11	CLA	1	1110	X	-	-	-
11	CLA	1	1111	X	-	-	-
11	CLA	1	1112	X	-	-	-
11	CLA	1	1113	X	-	-	-
11	CLA	1	1114	X	-	-	-
11	CLA	1	1115	X	-	-	-
11	CLA	1	1116	X	-	-	-
11	CLA	1	1117	X	-	-	-
11	CLA	1	1118	X	-	-	-
11	CLA	1	1119	X	-	-	-
11	CLA	1	1120	X	-	-	-
11	CLA	1	1121	X	-	-	-
11	CLA	1	1122	X	-	-	-
11	CLA	1	1123	X	-	-	-
11	CLA	1	1124	X	-	-	-
11	CLA	1	1125	X	-	-	-
11	CLA	1	1126	X	-	-	-
11	CLA	1	1127	X	-	-	-
11	CLA	1	1128	X	-	-	-
11	CLA	1	1129	X	-	-	-
11	CLA	1	1130	X	-	-	-
11	CLA	1	1131	X	-	-	-
11	CLA	1	1132	X	-	-	-
11	CLA	1	1133	X	-	-	-
11	CLA	1	1134	X	-	-	-
11	CLA	1	1135	X	-	-	-
11	CLA	1	1136	X	-	-	-
11	CLA	1	1137	X	-	-	-
11	CLA	1	1138	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	1	1139	X	-	-	-
11	CLA	1	1140	X	-	-	-
11	CLA	1	1237	X	-	-	-
11	CLA	1	1801	X	-	-	-
11	CLA	2	1013	X	-	-	-
11	CLA	2	1021	X	-	-	-
11	CLA	2	1023	X	-	-	-
11	CLA	2	1201	X	-	-	-
11	CLA	2	1202	X	-	-	-
11	CLA	2	1203	X	-	-	-
11	CLA	2	1204	X	-	-	-
11	CLA	2	1205	X	-	-	-
11	CLA	2	1206	X	-	-	-
11	CLA	2	1207	X	-	-	-
11	CLA	2	1208	X	-	-	-
11	CLA	2	1209	X	-	-	-
11	CLA	2	1210	X	-	-	-
11	CLA	2	1211	X	-	-	-
11	CLA	2	1212	X	-	-	-
11	CLA	2	1213	X	-	-	-
11	CLA	2	1214	X	-	-	-
11	CLA	2	1215	X	-	-	-
11	CLA	2	1216	X	-	-	-
11	CLA	2	1217	X	-	-	-
11	CLA	2	1218	X	-	-	-
11	CLA	2	1219	X	-	-	-
11	CLA	2	1220	X	-	-	-
11	CLA	2	1221	X	-	-	-
11	CLA	2	1222	X	-	-	-
11	CLA	2	1223	X	-	-	-
11	CLA	2	1224	X	-	-	-
11	CLA	2	1225	X	-	-	-
11	CLA	2	1226	X	-	-	-
11	CLA	2	1227	X	-	-	-
11	CLA	2	1228	X	-	-	-
11	CLA	2	1229	X	-	-	-
11	CLA	2	1230	X	-	-	-
11	CLA	2	1231	X	-	-	-
11	CLA	2	1232	X	-	-	-
11	CLA	2	1234	X	-	-	-
11	CLA	2	1235	X	-	-	-
11	CLA	2	1236	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	2	1238	X	-	-	-
11	CLA	2	1239	X	-	-	-
11	CLA	2	1240	X	-	-	-
11	CLA	8	1501	X	-	-	-
11	CLA	8	1502	X	-	-	-
11	CLA	8	1503	X	-	-	-
11	CLA	A	1011	X	-	-	-
11	CLA	A	1012	X	-	-	-
11	CLA	A	1022	X	-	-	-
11	CLA	A	1101	X	-	-	-
11	CLA	A	1102	X	-	-	-
11	CLA	A	1103	X	-	-	-
11	CLA	A	1104	X	-	-	-
11	CLA	A	1105	X	-	-	-
11	CLA	A	1106	X	-	-	-
11	CLA	A	1107	X	-	-	-
11	CLA	A	1108	X	-	-	-
11	CLA	A	1109	X	-	-	-
11	CLA	A	1110	X	-	-	-
11	CLA	A	1111	X	-	-	-
11	CLA	A	1112	X	-	-	-
11	CLA	A	1113	X	-	-	-
11	CLA	A	1114	X	-	-	-
11	CLA	A	1115	X	-	-	-
11	CLA	A	1116	X	-	-	-
11	CLA	A	1117	X	-	-	-
11	CLA	A	1118	X	-	-	-
11	CLA	A	1119	X	-	-	-
11	CLA	A	1120	X	-	-	-
11	CLA	A	1121	X	-	-	-
11	CLA	A	1122	X	-	-	-
11	CLA	A	1123	X	-	-	-
11	CLA	A	1124	X	-	-	-
11	CLA	A	1125	X	-	-	-
11	CLA	A	1126	X	-	-	-
11	CLA	A	1127	X	-	-	-
11	CLA	A	1128	X	-	-	-
11	CLA	A	1129	X	-	-	-
11	CLA	A	1130	X	-	-	-
11	CLA	A	1131	X	-	-	-
11	CLA	A	1132	X	-	-	-
11	CLA	A	1133	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	1134	X	-	-	-
11	CLA	A	1135	X	-	-	-
11	CLA	A	1136	X	-	-	-
11	CLA	A	1137	X	-	-	-
11	CLA	A	1138	X	-	-	-
11	CLA	A	1139	X	-	-	-
11	CLA	A	1140	X	-	-	-
11	CLA	A	1237	X	-	-	-
11	CLA	A	1801	X	-	-	-
11	CLA	B	1013	X	-	-	-
11	CLA	B	1021	X	-	-	-
11	CLA	B	1023	X	-	-	-
11	CLA	B	1201	X	-	-	-
11	CLA	B	1202	X	-	-	-
11	CLA	B	1203	X	-	-	-
11	CLA	B	1204	X	-	-	-
11	CLA	B	1205	X	-	-	-
11	CLA	B	1206	X	-	-	-
11	CLA	B	1207	X	-	-	-
11	CLA	B	1208	X	-	-	-
11	CLA	B	1209	X	-	-	-
11	CLA	B	1210	X	-	-	-
11	CLA	B	1211	X	-	-	-
11	CLA	B	1212	X	-	-	-
11	CLA	B	1213	X	-	-	-
11	CLA	B	1214	X	-	-	-
11	CLA	B	1215	X	-	-	-
11	CLA	B	1216	X	-	-	-
11	CLA	B	1217	X	-	-	-
11	CLA	B	1218	X	-	-	-
11	CLA	B	1219	X	-	-	-
11	CLA	B	1220	X	-	-	-
11	CLA	B	1221	X	-	-	-
11	CLA	B	1222	X	-	-	-
11	CLA	B	1223	X	-	-	-
11	CLA	B	1224	X	-	-	-
11	CLA	B	1225	X	-	-	-
11	CLA	B	1226	X	-	-	-
11	CLA	B	1227	X	-	-	-
11	CLA	B	1228	X	-	-	-
11	CLA	B	1229	X	-	-	-
11	CLA	B	1230	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1231	X	-	-	-
11	CLA	B	1232	X	-	-	-
11	CLA	B	1234	X	-	-	-
11	CLA	B	1235	X	-	-	-
11	CLA	B	1236	X	-	-	-
11	CLA	B	1238	X	-	-	-
11	CLA	B	1239	X	-	-	-
11	CLA	B	1240	X	-	-	-
11	CLA	K	1401	X	-	-	-
11	CLA	K	1402	X	-	-	-
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-
11	CLA	a	1011	X	-	-	-
11	CLA	a	1012	X	-	-	-
11	CLA	a	1022	X	-	-	-
11	CLA	a	1101	X	-	-	-
11	CLA	a	1102	X	-	-	-
11	CLA	a	1103	X	-	-	-
11	CLA	a	1104	X	-	-	-
11	CLA	a	1105	X	-	-	-
11	CLA	a	1106	X	-	-	-
11	CLA	a	1107	X	-	-	-
11	CLA	a	1108	X	-	-	-
11	CLA	a	1109	X	-	-	-
11	CLA	a	1110	X	-	-	-
11	CLA	a	1111	X	-	-	-
11	CLA	a	1112	X	-	-	-
11	CLA	a	1113	X	-	-	-
11	CLA	a	1114	X	-	-	-
11	CLA	a	1115	X	-	-	-
11	CLA	a	1116	X	-	-	-
11	CLA	a	1117	X	-	-	-
11	CLA	a	1118	X	-	-	-
11	CLA	a	1119	X	-	-	-
11	CLA	a	1120	X	-	-	-
11	CLA	a	1121	X	-	-	-
11	CLA	a	1122	X	-	-	-
11	CLA	a	1123	X	-	-	-
11	CLA	a	1124	X	-	-	-
11	CLA	a	1125	X	-	-	-
11	CLA	a	1126	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	a	1127	X	-	-	-
11	CLA	a	1128	X	-	-	-
11	CLA	a	1129	X	-	-	-
11	CLA	a	1130	X	-	-	-
11	CLA	a	1131	X	-	-	-
11	CLA	a	1132	X	-	-	-
11	CLA	a	1133	X	-	-	-
11	CLA	a	1134	X	-	-	-
11	CLA	a	1135	X	-	-	-
11	CLA	a	1136	X	-	-	-
11	CLA	a	1137	X	-	-	-
11	CLA	a	1138	X	-	-	-
11	CLA	a	1139	X	-	-	-
11	CLA	a	1140	X	-	-	-
11	CLA	a	1237	X	-	-	-
11	CLA	a	1801	X	-	-	-
11	CLA	b	1013	X	-	-	-
11	CLA	b	1021	X	-	-	-
11	CLA	b	1023	X	-	-	-
11	CLA	b	1201	X	-	-	-
11	CLA	b	1202	X	-	-	-
11	CLA	b	1203	X	-	-	-
11	CLA	b	1204	X	-	-	-
11	CLA	b	1205	X	-	-	-
11	CLA	b	1206	X	-	-	-
11	CLA	b	1207	X	-	-	-
11	CLA	b	1208	X	-	-	-
11	CLA	b	1209	X	-	-	-
11	CLA	b	1210	X	-	-	-
11	CLA	b	1211	X	-	-	-
11	CLA	b	1212	X	-	-	-
11	CLA	b	1213	X	-	-	-
11	CLA	b	1214	X	-	-	-
11	CLA	b	1215	X	-	-	-
11	CLA	b	1216	X	-	-	-
11	CLA	b	1217	X	-	-	-
11	CLA	b	1218	X	-	-	-
11	CLA	b	1219	X	-	-	-
11	CLA	b	1220	X	-	-	-
11	CLA	b	1221	X	-	-	-
11	CLA	b	1222	X	-	-	-
11	CLA	b	1223	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	b	1224	X	-	-	-
11	CLA	b	1225	X	-	-	-
11	CLA	b	1226	X	-	-	-
11	CLA	b	1227	X	-	-	-
11	CLA	b	1228	X	-	-	-
11	CLA	b	1229	X	-	-	-
11	CLA	b	1230	X	-	-	-
11	CLA	b	1231	X	-	-	-
11	CLA	b	1232	X	-	-	-
11	CLA	b	1234	X	-	-	-
11	CLA	b	1235	X	-	-	-
11	CLA	b	1236	X	-	-	-
11	CLA	b	1238	X	-	-	-
11	CLA	b	1239	X	-	-	-
11	CLA	b	1240	X	-	-	-
11	CLA	k	1401	X	-	-	-
11	CLA	k	1402	X	-	-	-
11	CLA	l	1501	X	-	-	-
11	CLA	l	1502	X	-	-	-
11	CLA	l	1503	X	-	-	-
13	SF4	3	3002	-	-	X	-
13	SF4	3	3003	-	-	X	-
13	SF4	A	3001	-	-	X	-
13	SF4	C	3002	-	-	X	-
13	SF4	C	3003	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 68370 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	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	b	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	2	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			

- 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	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 subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			
4	4	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	e	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	5	68	Total	C	N	O	0	0	0
			529	332	93	104			

- Molecule 6 is a protein called Fusion protein of Photosystem I subunit III and subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O	0	0	0
			676	420	126	130			
6	f	125	Total	C	N	O	0	0	0
			685	429	126	130			
6	6	125	Total	C	N	O	0	0	0
			685	429	126	130			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	CYS	-	LINKER	UNP L8AII8
F	42	SER	-	LINKER	UNP L8AII8
F	43	CYS	-	LINKER	UNP L8AII8
F	53	ILE	LEU	engineered mutation	UNP L8AII8
f	41	CYS	-	LINKER	UNP L8AII8
f	42	SER	-	LINKER	UNP L8AII8
f	43	CYS	-	LINKER	UNP L8AII8
f	53	ILE	LEU	engineered mutation	UNP L8AII8
6	41	CYS	-	LINKER	UNP L8AII8
6	42	SER	-	LINKER	UNP L8AII8
6	43	CYS	-	LINKER	UNP L8AII8
6	53	ILE	LEU	engineered mutation	UNP L8AII8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	l	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	8	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	m	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	7	31	Total	C	N	O	0	0	0
			235	157	36	42			

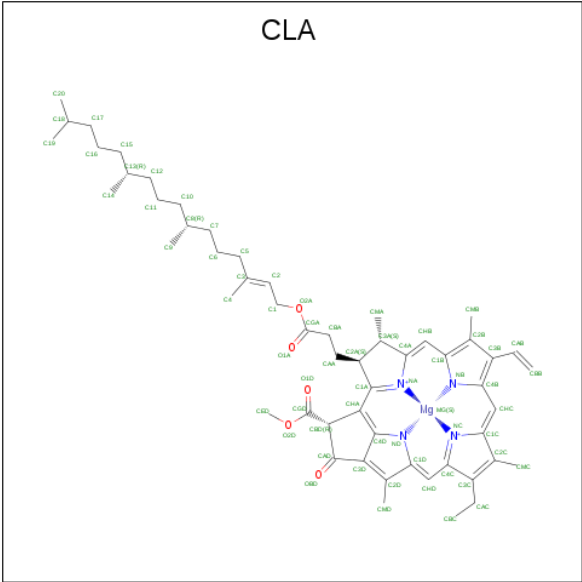
- Molecule 9 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	i	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	9	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	I	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	k	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	0	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	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
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	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
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	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
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	B	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
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	L	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
11	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	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
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	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
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	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
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	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
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	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
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

Continued on next page...

Continued from previous page...

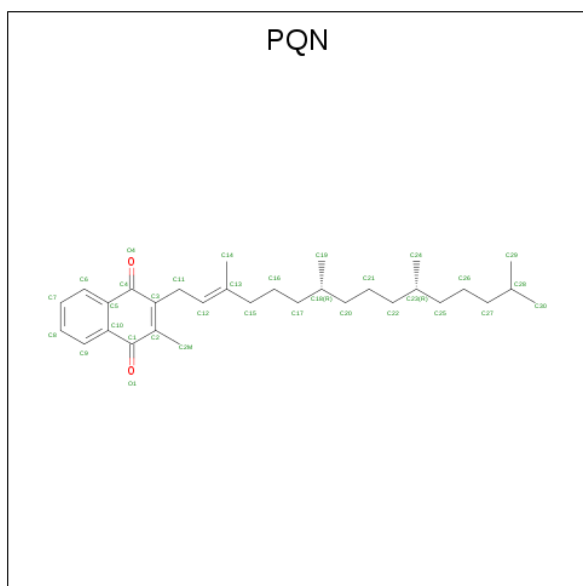
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



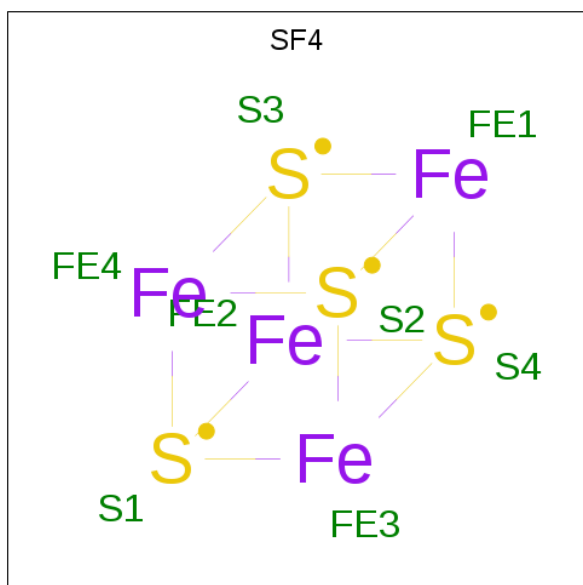
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

Continued on next page...

Continued from previous page...

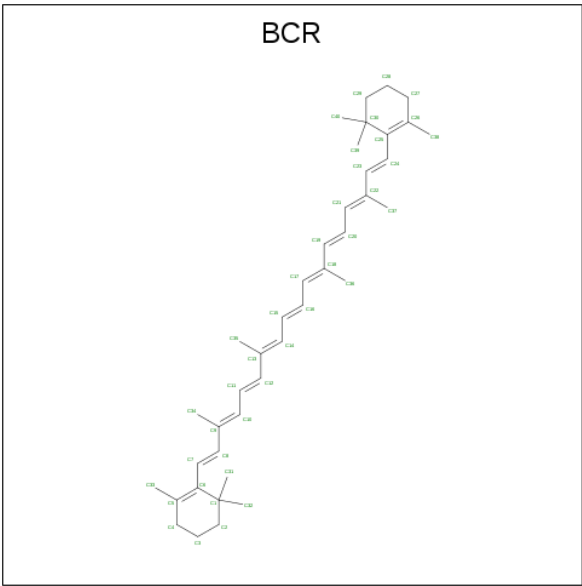
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	a	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	1	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	M	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

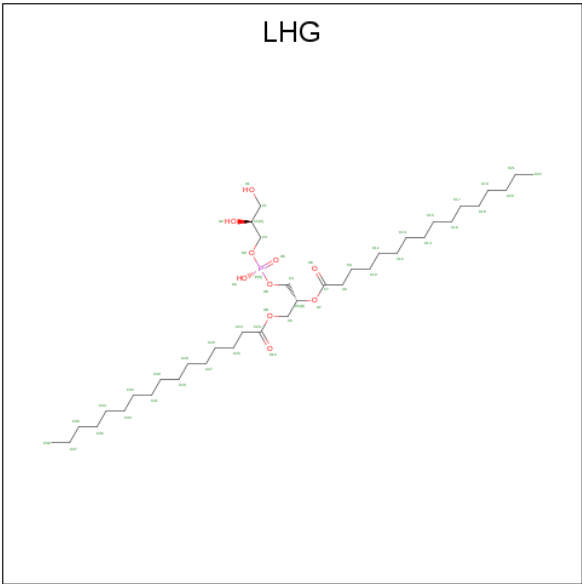
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	8	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

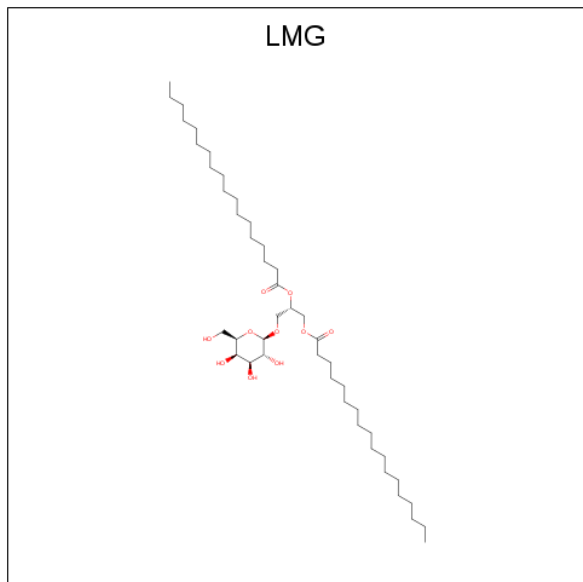
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O P 49 38 10 1	0	0
15	A	1	Total C O P 49 38 10 1	0	0
15	B	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	b	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	2	1	Total C O P 49 38 10 1	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

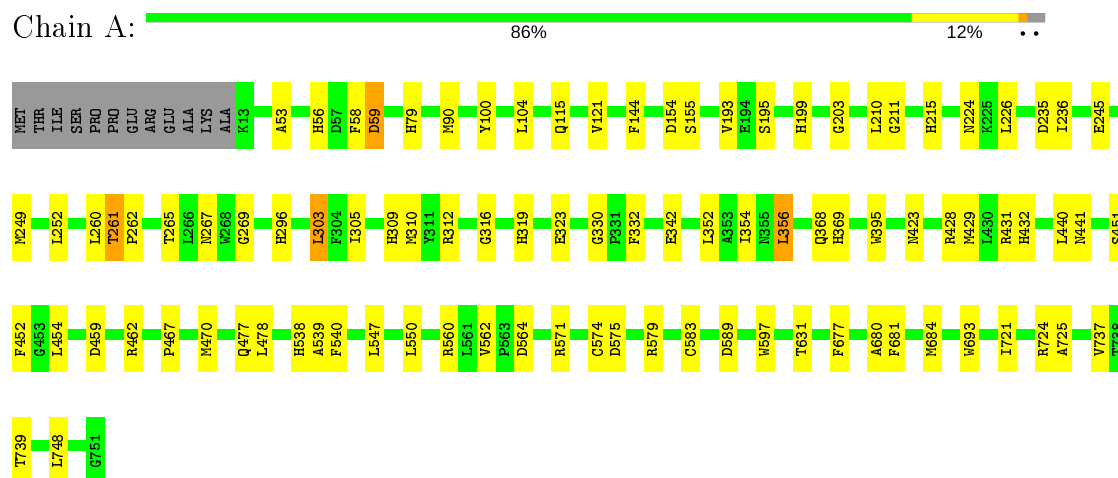


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

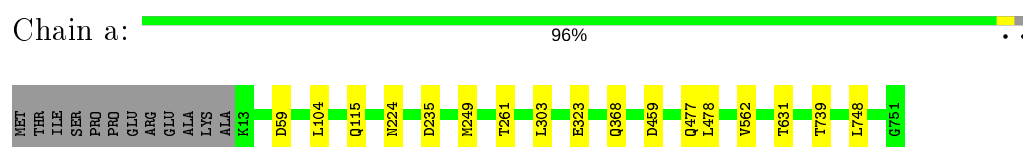
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

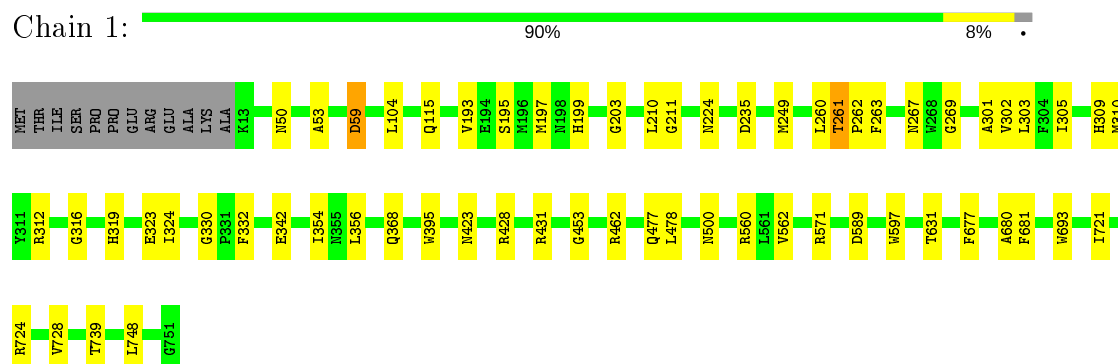
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

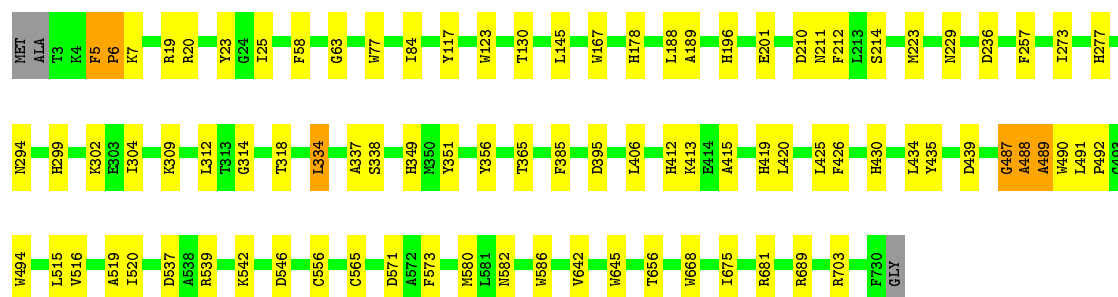


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  87% 11% .




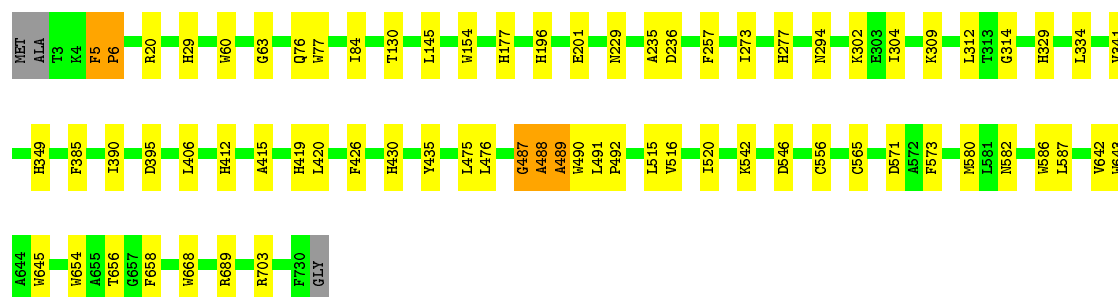
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  96% .




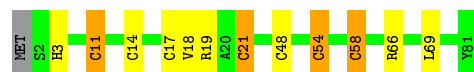
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  90% 9% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  84% 10% 5% .




- Molecule 3: Photosystem I iron-sulfur center

Chain c:  94% 5% .



- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  88% 9% .



- Molecule 4: Photosystem I subunit II

Chain D: 88% 8% ..



- Molecule 4: Photosystem I subunit II

Chain d: 94% ..



- Molecule 4: Photosystem I subunit II

Chain 4: 91% ..



- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 84% 7% 8% .



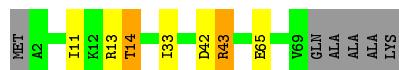
- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 88% 8% .



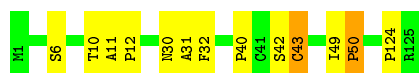
- Molecule 5: Photosystem I reaction center subunit IV

Chain 5: 82% 7% 8% .



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain F: 90% 9% .



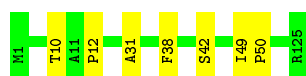
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain f: 98% .



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain 6: 94% 6%



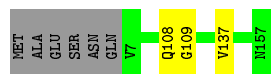
- Molecule 7: Photosystem I reaction center subunit XI

Chain L: 88% 8% . .



- Molecule 7: Photosystem I reaction center subunit XI

Chain l: 94% . .



- Molecule 7: Photosystem I reaction center subunit XI

Chain 8: 91% 5% .



- Molecule 8: Photosystem I reaction center subunit XII

Chain M: 84% 13% .

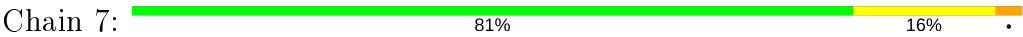


- Molecule 8: Photosystem I reaction center subunit XII

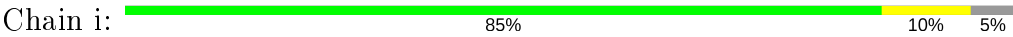
Chain m: 97% .



- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 9: Photosystem I subunit III



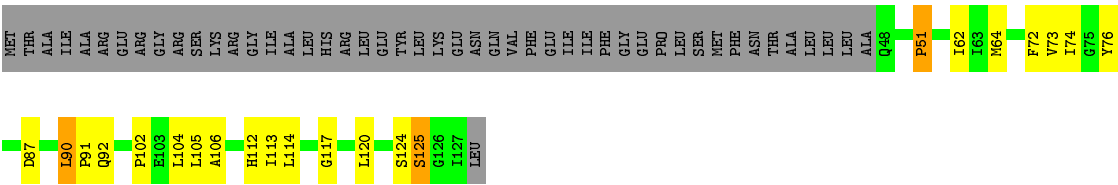
- Molecule 9: Photosystem I subunit III



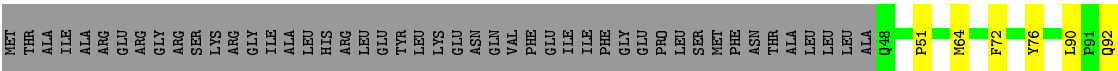
- Molecule 9: Photosystem I subunit III



- Molecule 10: Photosystem I reaction center subunit VIII

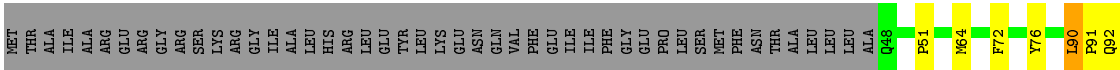


- Molecule 10: Photosystem I reaction center subunit VIII





- Molecule 10: Photosystem I reaction center subunit VIII



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 133.68Å 219.85Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 39.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-3.80) 71.5 (39.96-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.02 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2-1309, REFMAC 5.7.0032	Depositor
R, R_{free}	0.253 , 0.297 0.263 , 0.302	Depositor DCC
R_{free} test set	7809 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: LHG, SF4, CLA, PQN, BCR, LMG

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	1	0.22	0/5970	0.37	0/8138
1	A	0.23	0/5970	0.38	0/8138
1	a	0.22	0/5970	0.37	0/8138
2	2	0.23	0/5976	0.39	0/8173
2	B	0.24	0/5976	0.39	0/8173
2	b	0.23	0/5976	0.38	0/8173
3	3	0.28	0/610	0.44	0/826
3	C	0.24	0/610	0.46	0/826
3	c	0.25	0/610	0.43	0/826
4	4	0.23	0/1103	0.40	0/1487
4	D	0.23	0/1103	0.40	0/1487
4	d	0.23	0/1103	0.39	0/1487
5	5	0.23	0/538	0.45	0/729
5	E	0.24	0/538	0.43	0/729
5	e	0.23	0/538	0.42	0/729
6	6	0.23	0/700	0.43	0/976
6	F	0.24	0/690	0.47	0/963
6	f	0.23	0/700	0.43	0/976
7	8	0.23	0/1163	0.38	0/1580
7	L	0.23	0/1163	0.38	0/1580
7	l	0.23	0/1163	0.38	0/1580
8	7	0.26	0/238	0.38	0/323
8	M	0.26	0/238	0.39	0/323
8	m	0.25	0/238	0.38	0/323
9	9	0.25	0/308	0.42	0/421
9	I	0.24	0/308	0.41	0/421
9	i	0.25	0/308	0.43	0/421
10	0	0.22	0/504	0.48	0/688
10	K	0.24	0/504	0.45	0/688
10	k	0.23	0/504	0.45	0/688
All	All	0.23	0/51320	0.39	0/70010

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
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	5	PHE	Peptide
4	4	98	HIS	Peptide
2	B	5	PHE	Peptide
4	D	98	HIS	Peptide
6	F	40	PRO	Mainchain
2	b	5	PHE	Peptide
4	d	98	HIS	Peptide
10	k	125	SER	Peptide

5.2 Too-close contacts ⓘ

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	1	5772	0	5621	48	0
1	A	5772	0	5621	94	0
1	a	5772	0	5621	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	5765	0	5546	48	0
2	B	5765	0	5546	64	0
2	b	5765	0	5545	0	0
3	3	600	0	588	22	0
3	C	600	0	586	25	0
3	c	600	0	587	0	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	9	0
4	d	1079	0	1073	0	0
5	5	529	0	506	4	0
5	E	529	0	506	2	0
5	e	529	0	506	0	0
6	6	685	0	411	3	0
6	F	676	0	395	11	0
6	f	685	0	411	0	0
7	8	1133	0	1108	5	0
7	L	1133	0	1108	9	0
7	l	1133	0	1108	0	0
8	7	235	0	253	7	0
8	M	235	0	253	7	0
8	m	235	0	253	0	0
9	9	297	0	295	10	0
9	I	297	0	295	7	0
9	i	297	0	295	0	0
10	0	496	0	439	4	0
10	K	496	0	439	12	0
10	k	496	0	439	0	0
11	0	115	0	111	4	0
11	1	2546	0	2430	89	0
11	2	2313	0	2213	84	0
11	8	176	0	177	8	0
11	A	2546	0	2435	159	0
11	B	2313	0	2213	127	0
11	K	115	0	111	8	0
11	L	176	0	177	8	0
11	a	2546	0	2434	0	0
11	b	2313	0	2213	0	0
11	k	115	0	111	0	0
11	l	176	0	177	0	0
12	1	33	0	45	1	0
12	2	33	0	45	3	0
12	A	33	0	45	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	33	0	45	4	0
12	a	33	0	46	0	0
12	b	33	0	45	0	0
13	1	8	0	0	1	0
13	3	16	0	0	21	0
13	A	8	0	0	4	0
13	C	16	0	0	22	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	1	200	0	242	23	0
14	2	320	0	391	40	0
14	6	120	0	147	20	0
14	7	40	0	49	6	0
14	8	80	0	97	15	0
14	A	200	0	244	35	0
14	B	320	0	390	62	0
14	F	120	0	146	23	0
14	L	80	0	97	22	0
14	M	40	0	49	7	0
14	a	200	0	243	0	0
14	b	320	0	389	0	0
14	f	120	0	147	0	0
14	l	80	0	97	0	0
14	m	40	0	49	0	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	15	0
15	B	49	0	74	8	0
15	a	98	0	148	0	0
15	b	49	0	74	0	0
16	2	55	0	86	1	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	831	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 6.

All (831) 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)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:A:56:HIS:CG	11:A:1103:CLA:HBB2	3.55	1.62
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:C:58:CYS:SG	13:C:3003:SF4:FE1	1.08	1.57
3:C:11:CYS:SG	13:C:3003:SF4:FE3	0.82	1.54
3:C:14:CYS:SG	13:C:3003:SF4:FE2	1.31	1.44
1:A:56:HIS:CD2	11:A:1103:CLA:HBB2	2.63	1.40
1:A:56:HIS:CG	11:A:1103:CLA:CBB	3.92	1.36
3:C:54:CYS:SG	13:C:3002:SF4:FE3	1.22	1.29
3:3:58:CYS:SG	13:3:3003:SF4:FE1	1.23	1.29
3:3:14:CYS:SG	13:3:3003:SF4:FE2	1.29	1.23
3:C:48:CYS:SG	13:C:3002:SF4:S3	2.39	1.20
3:C:21:CYS:SG	13:C:3002:SF4:S1	2.57	1.06
3:3:51:CYS:SG	13:3:3002:SF4:FE1	1.45	1.06
3:3:58:CYS:SG	13:3:3003:SF4:S3	2.58	1.02
3:C:14:CYS:HG	13:C:3003:SF4:FE2	1.15	1.02
1:A:583:CYS:HG	13:A:3001:SF4:FE2	0.73	0.97
3:C:14:CYS:SG	13:C:3003:SF4:S4	3.10	0.96
3:C:54:CYS:HG	13:C:3002:SF4:FE3	0.67	0.93
2:2:586:TRP:CZ2	11:2:1021:CLA:H201	2.05	0.92
1:A:56:HIS:CD2	11:A:1103:CLA:CBB	3.27	0.92
3:3:48:CYS:HG	13:3:3002:SF4:FE4	0.83	0.91
3:3:51:CYS:HG	13:3:3002:SF4:FE1	0.65	0.91
11:B:1222:CLA:HBA1	11:B:1223:CLA:OBD	2.44	0.90
3:3:17:CYS:HG	13:3:3003:SF4:FE4	0.64	0.89
3:C:48:CYS:HG	13:C:3002:SF4:FE4	1.51	0.88
1:A:56:HIS:CB	11:A:1103:CLA:HBB2	4.57	0.88
14:B:4004:BCR:H23C	14:B:4004:BCR:H403	1.58	0.85
3:3:11:CYS:HG	13:3:3003:SF4:FE3	0.88	0.85
3:3:48:CYS:SG	13:3:3002:SF4:S1	2.75	0.84
14:F:4018:BCR:H14C	9:I:23:PRO:CG	2.08	0.83
3:3:17:CYS:SG	13:3:3003:SF4:FE4	1.71	0.82
11:A:1127:CLA:HHC	11:A:1127:CLA:HBB1	4.33	0.81
11:A:1123:CLA:HBB1	11:A:1123:CLA:HHC	1.63	0.81
3:C:48:CYS:SG	13:C:3002:SF4:S1	2.79	0.80
14:L:4019:BCR:HC8	14:L:4019:BCR:H321	1.62	0.80
11:A:1134:CLA:HHC	11:A:1134:CLA:HBB1	1.63	0.80
3:3:58:CYS:SG	13:3:3003:SF4:S2	2.80	0.80
1:1:395:TRP:CD1	11:1:1126:CLA:HAB	2.17	0.80
1:A:574:CYS:SG	13:A:3001:SF4:S3	2.87	0.79
1:A:56:HIS:ND1	11:A:1103:CLA:CBB	4.21	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1103:CLA:H51	11:A:1111:CLA:H12	2.31	0.79
11:A:1801:CLA:C1C	15:A:5003:LHG:HC31	2.38	0.79
11:A:1801:CLA:HHC	11:A:1801:CLA:HBB1	1.65	0.79
11:B:1227:CLA:HBC3	11:B:1227:CLA:HHD	1.65	0.78
14:2:4004:BCR:H403	14:2:4004:BCR:H23C	1.65	0.78
1:A:583:CYS:SG	13:A:3001:SF4:FE2	1.75	0.78
11:A:1140:CLA:HHC	11:A:1140:CLA:HBB1	1.67	0.77
3:C:58:CYS:SG	13:C:3003:SF4:S2	2.69	0.77
11:1:1107:CLA:HHC	11:1:1107:CLA:HBB1	1.67	0.77
3:3:11:CYS:SG	13:3:3003:SF4:S2	2.81	0.77
6:F:10:THR:CB	14:F:4013:BCR:H401	3.98	0.77
1:A:395:TRP:CD1	11:A:1126:CLA:HAB	2.20	0.77
11:1:1131:CLA:HAB	11:1:1132:CLA:HBB1	1.66	0.76
7:8:96:LEU:HG	14:8:4019:BCR:H24C	1.67	0.76
11:2:1231:CLA:HHC	11:2:1231:CLA:HBB1	1.65	0.76
1:A:354:ILE:HD11	14:A:4007:BCR:HC7	1.66	0.76
14:A:4001:BCR:H331	14:A:4002:BCR:H24C	1.66	0.76
14:B:4014:BCR:HC21	11:B:1229:CLA:HBB2	1.68	0.76
3:3:21:CYS:SG	13:3:3002:SF4:S1	2.78	0.75
11:A:1237:CLA:HHC	11:A:1237:CLA:HBB1	1.92	0.75
11:A:1128:CLA:HBB1	11:A:1128:CLA:HHC	3.40	0.75
14:B:4014:BCR:HC21	11:B:1229:CLA:CBB	2.17	0.74
1:A:193:VAL:CG1	11:A:1123:CLA:HHD	2.17	0.74
14:8:4019:BCR:H321	14:8:4019:BCR:HC8	1.69	0.74
11:A:1116:CLA:HHC	11:A:1116:CLA:HBB1	2.67	0.74
11:A:1129:CLA:HHC	11:A:1129:CLA:HBB1	1.70	0.74
11:B:1229:CLA:HHC	11:B:1229:CLA:HBB1	1.69	0.74
11:A:1125:CLA:HBB1	11:A:1125:CLA:HHC	4.18	0.74
14:A:4001:BCR:C33	14:A:4002:BCR:H24C	2.54	0.74
6:F:12:PRO:HG2	14:F:4013:BCR:H401	1.70	0.74
11:B:1214:CLA:HHC	11:B:1214:CLA:HBB1	2.25	0.74
11:A:1110:CLA:HHC	11:A:1110:CLA:HBB1	1.70	0.73
11:1:1125:CLA:HHD	11:1:1125:CLA:HBC2	1.70	0.73
1:A:56:HIS:CB	11:A:1103:CLA:CBB	4.84	0.73
11:A:1111:CLA:HBB1	11:A:1111:CLA:HHC	2.34	0.73
14:F:4018:BCR:H402	14:F:4020:BCR:H353	1.86	0.73
11:B:1021:CLA:HHC	11:B:1021:CLA:HBB1	4.13	0.73
14:2:4011:BCR:H23C	11:2:1230:CLA:HMC2	1.70	0.73
3:3:21:CYS:SG	13:3:3002:SF4:S3	2.80	0.73
11:K:1402:CLA:HHC	11:K:1402:CLA:HBB1	1.81	0.72
2:2:426:PHE:O	2:2:430:HIS:ND1	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1229:CLA:H201	11:B:1235:CLA:C15	2.20	0.72
2:B:656:THR:HA	11:B:1023:CLA:HAB	1.72	0.72
2:B:426:PHE:CE2	11:B:1235:CLA:HAB	3.29	0.72
11:1:1128:CLA:HBB1	11:1:1128:CLA:HHC	1.72	0.71
1:1:571:ARG:NH1	15:1:5001:LHG:O10	2.23	0.71
6:F:12:PRO:HB3	14:F:4013:BCR:H19C	6.28	0.71
14:F:4013:BCR:H392	14:F:4013:BCR:H23C	1.72	0.71
14:6:4013:BCR:H392	14:6:4013:BCR:H23C	1.72	0.71
14:6:4018:BCR:H14C	9:9:23:PRO:CG	2.21	0.71
11:A:1126:CLA:H42	14:B:4011:BCR:HC7	1.73	0.71
1:A:571:ARG:NH1	15:A:5001:LHG:O10	2.51	0.71
14:2:4009:BCR:H353	15:2:5004:LHG:H202	1.72	0.70
11:1:1106:CLA:H191	11:1:1109:CLA:H91	1.73	0.70
11:A:1101:CLA:H202	11:A:1126:CLA:H203	1.73	0.70
1:1:330:GLY:HA3	15:1:5003:LHG:HC32	1.72	0.70
1:A:330:GLY:HA3	15:A:5003:LHG:HC32	1.73	0.70
11:2:1220:CLA:HHD	11:2:1220:CLA:HBC2	1.73	0.70
11:A:1136:CLA:HHC	11:A:1136:CLA:HBB1	1.74	0.70
3:C:58:CYS:SG	13:C:3003:SF4:S3	2.05	0.70
2:2:309:LYS:O	15:2:5004:LHG:HC31	1.93	0.69
14:B:4010:BCR:HC41	11:B:1223:CLA:HMA3	1.94	0.69
14:1:4008:BCR:C8	11:1:1124:CLA:HAB	2.21	0.69
2:B:415:ALA:O	2:B:419:HIS:ND1	2.33	0.69
15:1:5001:LHG:H202	11:1:1128:CLA:H202	1.75	0.69
14:B:4006:BCR:H392	14:B:4006:BCR:H23C	1.97	0.69
11:1:1127:CLA:H71	11:1:1127:CLA:HMD2	1.75	0.68
2:B:309:LYS:O	15:B:5004:LHG:HC31	2.12	0.68
11:B:1238:CLA:H142	14:F:4020:BCR:HC8	1.75	0.68
11:L:1501:CLA:H43	14:L:4022:BCR:H14C	1.73	0.68
11:1:1104:CLA:HHC	11:1:1104:CLA:HBB1	1.74	0.68
11:1:1127:CLA:C7	11:1:1127:CLA:HMD2	2.24	0.68
11:1:1115:CLA:CHD	11:0:1401:CLA:HBA1	2.24	0.68
11:1:1012:CLA:C1B	11:2:1021:CLA:H203	2.24	0.68
14:A:4008:BCR:C8	11:A:1124:CLA:HAB	2.24	0.67
11:1:1110:CLA:HBB1	11:1:1110:CLA:HHC	1.76	0.67
11:1:1131:CLA:HAB	11:1:1132:CLA:CHB	2.25	0.67
4:D:82:ASP:N	4:D:82:ASP:OD1	2.28	0.67
7:L:96:LEU:HG	14:L:4019:BCR:H24C	1.80	0.67
11:1:1012:CLA:C2B	11:2:1021:CLA:H203	2.25	0.67
2:2:426:PHE:CE2	11:2:1235:CLA:HAB	2.29	0.67
11:B:1238:CLA:C14	14:F:4020:BCR:HC8	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4008:BCR:HC8	11:A:1124:CLA:HAB	1.83	0.67
1:A:681:PHE:HA	11:B:1013:CLA:HAB	1.75	0.67
2:B:23:TYR:CE2	16:B:5002:LMG:HC71	2.31	0.66
2:2:426:PHE:CD2	11:2:1235:CLA:HAB	2.31	0.66
14:B:4005:BCR:HC7	11:B:1209:CLA:HMC1	1.78	0.66
14:A:4003:BCR:H23C	14:A:4003:BCR:H403	1.78	0.66
11:B:1223:CLA:HHD	11:B:1223:CLA:HBC3	1.98	0.66
11:A:1104:CLA:HMD1	11:A:1106:CLA:H202	1.77	0.66
1:A:560:ARG:O	4:D:61:ARG:NH1	2.86	0.66
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC2	1.77	0.66
14:F:4018:BCR:H14C	9:I:23:PRO:HG3	1.77	0.66
14:B:4004:BCR:H14C	11:B:1217:CLA:HBB1	3.27	0.65
14:B:4009:BCR:H23C	11:B:1227:CLA:CBC	2.26	0.65
14:A:4007:BCR:H19C	11:A:1122:CLA:H43	1.76	0.65
2:B:426:PHE:O	2:B:430:HIS:ND1	2.37	0.65
6:F:12:PRO:CG	14:F:4013:BCR:H401	2.27	0.65
11:8:1501:CLA:HBA2	14:8:4022:BCR:H363	1.77	0.65
3:C:48:CYS:SG	13:C:3002:SF4:S2	2.95	0.65
2:B:546:ASP:OD2	3:C:66:ARG:NH1	2.29	0.65
15:1:5003:LHG:H302	11:1:1137:CLA:H102	1.79	0.65
8:M:16:LEU:CD2	14:M:4021:BCR:H19C	2.27	0.65
13:A:3001:SF4:S2	2:B:565:CYS:SG	2.95	0.64
14:B:4011:BCR:H23C	11:B:1230:CLA:HMC2	1.79	0.64
14:B:4017:BCR:HC7	11:B:1205:CLA:C10	3.64	0.64
14:1:4001:BCR:C33	14:1:4002:BCR:H24C	2.27	0.64
1:A:56:HIS:HB3	11:A:1103:CLA:CBB	4.61	0.64
1:1:312:ARG:NH2	1:1:316:GLY:O	2.29	0.64
11:B:1222:CLA:CBA	11:B:1223:CLA:OBD	3.05	0.64
14:A:4001:BCR:H333	14:A:4002:BCR:H24C	2.97	0.64
14:B:4010:BCR:H14C	11:B:1222:CLA:HMA1	2.17	0.64
16:2:5002:LMG:H202	11:2:1201:CLA:HBC1	1.80	0.64
3:3:14:CYS:SG	13:3:3003:SF4:S4	2.95	0.64
11:B:1222:CLA:CMB	11:B:1223:CLA:H202	2.28	0.64
11:B:1206:CLA:H43	14:F:4018:BCR:H342	2.56	0.63
10:K:102:PRO:O	10:K:106:ALA:N	2.30	0.63
14:2:4009:BCR:H23C	11:2:1227:CLA:HBC1	1.79	0.63
2:B:656:THR:CA	11:B:1023:CLA:HAB	2.28	0.63
11:A:1137:CLA:HAB	11:A:1129:CLA:CBB	2.29	0.63
1:A:597:TRP:HH2	11:A:1022:CLA:HAB	1.64	0.62
11:A:1132:CLA:H201	14:L:4022:BCR:H343	2.19	0.62
11:2:1212:CLA:HHC	11:2:1212:CLA:HBB1	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:TRP:CH2	11:A:1022:CLA:HAB	2.34	0.62
1:1:597:TRP:CH2	11:1:1022:CLA:HAB	2.34	0.62
11:A:1138:CLA:HHD	14:B:4014:BCR:C38	2.30	0.62
11:2:1212:CLA:HAB	11:2:1211:CLA:HMC1	1.82	0.62
11:1:1022:CLA:H172	14:2:4017:BCR:H343	1.82	0.62
13:1:3001:SF4:S2	2:2:565:CYS:SG	2.97	0.62
11:1:1112:CLA:CMC	11:1:1113:CLA:HAB	2.30	0.61
11:2:1206:CLA:H43	14:6:4018:BCR:H342	1.81	0.61
14:6:4018:BCR:H14C	9:9:23:PRO:HG3	1.82	0.61
11:A:1012:CLA:CHB	11:B:1021:CLA:H202	2.36	0.61
11:A:1125:CLA:CBC	11:A:1125:CLA:HHD	2.31	0.61
8:M:16:LEU:HD23	14:M:4021:BCR:H19C	1.87	0.61
11:A:1115:CLA:HHD	11:A:1115:CLA:HBC3	1.83	0.61
11:2:1206:CLA:H201	9:9:23:PRO:HA	1.83	0.61
14:A:4007:BCR:H352	11:A:1119:CLA:H71	2.32	0.61
11:1:1106:CLA:HBB1	11:1:1106:CLA:HHC	1.82	0.61
1:1:677:PHE:CG	14:2:4011:BCR:H363	2.35	0.61
1:A:677:PHE:CD1	14:B:4011:BCR:H363	2.35	0.61
11:1:1801:CLA:C1C	15:1:5003:LHG:HC31	2.31	0.60
11:1:1137:CLA:HAB	11:1:1129:CLA:CBB	2.32	0.60
2:2:520:ILE:HD13	11:2:1234:CLA:HAB	1.83	0.60
14:2:4017:BCR:H342	11:2:1205:CLA:C10	2.32	0.60
6:6:10:THR:CB	14:6:4013:BCR:H401	2.31	0.60
11:A:1131:CLA:H192	11:B:1023:CLA:H201	3.09	0.60
11:B:1225:CLA:C16	11:B:1211:CLA:HAB	2.44	0.60
11:L:1501:CLA:C4	14:L:4022:BCR:H14C	2.32	0.60
11:A:1119:CLA:HBC2	11:A:1119:CLA:HHD	1.82	0.60
1:1:597:TRP:HH2	11:1:1022:CLA:HAB	1.67	0.59
11:A:1126:CLA:C4	14:B:4011:BCR:HC7	2.54	0.59
2:2:312:LEU:HD23	15:2:5004:LHG:HC61	1.85	0.59
2:B:488:ALA:O	2:B:490:TRP:N	2.35	0.59
14:1:4008:BCR:HC8	11:1:1124:CLA:HAB	1.84	0.59
11:B:1210:CLA:HBC2	11:B:1210:CLA:HHD	1.85	0.59
7:L:41:ARG:NH2	7:L:52:GLU:OE2	2.35	0.59
14:2:4010:BCR:H14C	11:2:1222:CLA:HMA1	1.85	0.59
11:2:1214:CLA:H92	11:2:1231:CLA:O1A	2.03	0.59
2:B:188:LEU:HD21	14:B:4004:BCR:H331	1.85	0.59
14:A:4002:BCR:H14C	11:A:1112:CLA:HBB1	2.18	0.59
14:1:4007:BCR:H341	11:1:1123:CLA:HAB	1.86	0.58
2:2:312:LEU:HD22	15:2:5004:LHG:HC42	1.85	0.58
1:1:302:VAL:HG22	14:1:4001:BCR:H352	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1202:CLA:H202	11:B:1210:CLA:HMD1	1.84	0.58
11:B:1205:CLA:CGA	11:B:1205:CLA:C1A	2.82	0.58
3:C:21:CYS:SG	13:C:3002:SF4:S3	2.84	0.58
11:2:1231:CLA:C4C	11:2:1232:CLA:HAB	2.34	0.58
11:2:1205:CLA:HAB	11:2:1206:CLA:HAA2	1.85	0.58
2:B:63:GLY:HA3	11:B:1204:CLA:HAB	1.85	0.58
14:2:4014:BCR:HC21	11:2:1229:CLA:CBB	2.34	0.58
4:D:61:ARG:NH2	4:D:63:GLU:OE1	2.36	0.58
3:C:14:CYS:SG	13:C:3003:SF4:S3	3.20	0.58
11:2:1205:CLA:C1A	11:2:1205:CLA:CGA	2.81	0.58
11:A:1022:CLA:H172	14:B:4017:BCR:H343	1.85	0.58
8:7:16:LEU:HD23	14:7:4021:BCR:H19C	1.84	0.58
2:B:426:PHE:HE2	11:B:1235:CLA:HAB	2.93	0.58
2:B:299:HIS:NE2	11:B:1219:CLA:OBD	2.48	0.58
11:1:1133:CLA:HBB1	11:1:1133:CLA:HHC	1.86	0.57
14:2:4014:BCR:HC21	11:2:1229:CLA:HBB1	1.86	0.57
14:B:4005:BCR:H321	14:B:4005:BCR:HC8	1.86	0.57
11:2:1204:CLA:H2	14:6:4018:BCR:HC32	1.86	0.57
2:2:488:ALA:O	2:2:490:TRP:N	2.37	0.57
14:A:4007:BCR:HC41	11:A:1119:CLA:H191	1.86	0.57
14:2:4009:BCR:H23C	11:2:1227:CLA:CBC	2.34	0.57
11:A:1126:CLA:C4C	14:B:4011:BCR:HC42	2.34	0.57
14:F:4020:BCR:H333	7:L:87:ALA:HB3	2.25	0.57
14:1:4003:BCR:H321	14:1:4003:BCR:HC8	1.86	0.57
8:7:16:LEU:CD2	14:7:4021:BCR:H19C	2.35	0.57
14:2:4005:BCR:H321	14:2:4005:BCR:HC8	1.86	0.57
11:A:1138:CLA:HHC	11:A:1138:CLA:HBB1	1.87	0.57
11:2:1240:CLA:HHC	11:2:1240:CLA:HBB1	1.87	0.57
11:1:1106:CLA:H191	11:1:1109:CLA:C9	2.33	0.57
11:1:1115:CLA:C1D	11:0:1401:CLA:HBA1	2.35	0.56
14:6:4020:BCR:HC22	9:9:20:TRP:CD1	2.40	0.56
11:A:1131:CLA:H203	11:B:1023:CLA:H201	1.85	0.56
14:1:4008:BCR:H331	14:1:4008:BCR:C8	2.35	0.56
1:1:50:ASN:ND2	15:1:5001:LHG:HC12	2.21	0.56
5:5:13:ARG:NH1	5:5:65:GLU:OE2	2.39	0.56
14:B:4010:BCR:C19	11:B:1223:CLA:H111	5.12	0.56
14:2:4014:BCR:H333	11:2:1230:CLA:H51	1.87	0.56
11:8:1501:CLA:C4	14:8:4022:BCR:H14C	2.35	0.56
11:B:1224:CLA:HBC2	11:B:1224:CLA:HHD	1.86	0.56
14:B:4010:BCR:H23C	14:B:4010:BCR:H392	1.93	0.56
5:5:42:ASP:OD2	5:5:43:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ILE:O	2:B:277:HIS:ND1	2.39	0.56
12:2:2002:PQN:H302	11:2:1239:CLA:C1	2.36	0.55
11:B:1201:CLA:HMB2	14:M:4021:BCR:H333	1.88	0.55
3:3:11:CYS:SG	13:3:3003:SF4:S4	3.04	0.55
11:A:1114:CLA:HHC	11:A:1114:CLA:HBB1	1.89	0.55
1:A:395:TRP:NE1	11:A:1126:CLA:HAB	2.22	0.55
14:A:4003:BCR:H23C	14:A:4003:BCR:C40	2.36	0.55
11:L:1501:CLA:H41	14:L:4022:BCR:H14C	2.14	0.55
1:1:199:HIS:O	1:1:203:GLY:N	2.40	0.55
11:2:1227:CLA:HHD	11:2:1227:CLA:HBC3	1.88	0.55
14:1:4001:BCR:HC42	11:1:1113:CLA:HBB1	1.87	0.55
1:A:211:GLY:CA	14:A:4002:BCR:H363	2.38	0.55
11:B:1220:CLA:HBC2	11:B:1220:CLA:HHD	2.01	0.55
1:A:677:PHE:CG	14:B:4011:BCR:H363	2.59	0.55
10:K:120:LEU:HD13	11:K:1401:CLA:H11	2.39	0.55
2:2:645:TRP:CZ3	14:2:4017:BCR:HC21	2.41	0.55
1:A:560:ARG:NH2	4:D:15:THR:O	2.70	0.55
15:B:5004:LHG:HC82	15:B:5004:LHG:H262	1.88	0.55
11:A:1104:CLA:CMD	11:A:1106:CLA:H202	2.37	0.55
11:B:1208:CLA:HHC	11:B:1208:CLA:HBB1	2.90	0.55
2:B:5:PHE:CG	2:B:6:PRO:CD	2.90	0.55
3:C:54:CYS:SG	13:C:3002:SF4:S4	2.99	0.55
14:A:4008:BCR:H342	11:A:1124:CLA:CHC	2.37	0.54
11:1:1801:CLA:HBB1	11:1:1121:CLA:HAB	1.89	0.54
11:1:1106:CLA:C9	11:1:1128:CLA:H203	2.38	0.54
1:A:193:VAL:HG11	11:A:1123:CLA:HHD	1.89	0.54
11:0:1402:CLA:HBB1	11:0:1402:CLA:HHC	1.90	0.54
14:2:4017:BCR:H331	14:2:4017:BCR:C8	2.38	0.54
11:A:1801:CLA:HAB	11:A:1122:CLA:HHB	3.58	0.54
11:1:1101:CLA:H203	11:1:1140:CLA:H152	1.90	0.54
11:B:1228:CLA:HBB1	11:B:1228:CLA:HHC	3.84	0.54
14:B:4009:BCR:H321	14:B:4009:BCR:HC8	2.08	0.54
2:2:63:GLY:HA3	11:2:1204:CLA:HAB	1.90	0.54
1:A:571:ARG:HD2	15:A:5001:LHG:HC42	1.89	0.54
11:B:1221:CLA:CMB	11:B:1223:CLA:H8	2.43	0.54
2:B:130:THR:OG1	2:B:201:GLU:OE1	2.26	0.54
8:M:12:LEU:HD13	14:M:4021:BCR:H372	1.89	0.54
11:B:1238:CLA:O1A	14:L:4019:BCR:H363	2.08	0.54
2:B:349:HIS:ND1	11:B:1214:CLA:OBD	2.37	0.53
14:B:4017:BCR:H342	11:B:1205:CLA:C10	3.57	0.53
11:B:1222:CLA:HMB2	11:B:1223:CLA:H202	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:PHE:CE1	14:B:4005:BCR:H373	2.51	0.53
11:A:1101:CLA:C20	11:A:1126:CLA:H203	2.38	0.53
14:B:4010:BCR:C19	11:B:1223:CLA:H93	2.71	0.53
11:1:1137:CLA:HAB	11:1:1129:CLA:HBB2	1.91	0.53
14:1:4002:BCR:HC41	11:1:1103:CLA:H142	1.91	0.53
14:A:4008:BCR:H353	11:A:1119:CLA:H62	1.90	0.53
2:B:656:THR:N	11:B:1023:CLA:HAB	2.26	0.53
1:A:574:CYS:HB3	1:A:583:CYS:HA	1.90	0.53
11:B:1225:CLA:H162	11:B:1211:CLA:HAB	2.12	0.53
2:2:5:PHE:CG	2:2:6:PRO:CD	2.92	0.53
1:1:263:PHE:CE2	14:1:4001:BCR:H343	2.43	0.53
2:2:546:ASP:OD2	3:3:66:ARG:NH1	2.41	0.53
12:A:2001:PQN:H243	11:B:1013:CLA:H202	3.32	0.53
2:B:210:ASP:OD1	2:B:211:ASN:ND2	2.38	0.53
11:A:1112:CLA:CMC	11:A:1113:CLA:HAB	2.74	0.53
11:L:1501:CLA:H202	11:L:1503:CLA:C1	3.89	0.53
1:A:90:MET:HE1	11:A:1106:CLA:HBA2	2.54	0.52
1:A:332:PHE:HB2	15:A:5003:LHG:HC41	1.91	0.52
3:3:11:CYS:SG	13:3:3003:SF4:S1	3.07	0.52
1:A:681:PHE:CA	11:B:1013:CLA:HAB	2.39	0.52
8:M:16:LEU:HD21	14:M:4021:BCR:H19C	1.90	0.52
11:A:1106:CLA:HBB1	11:A:1106:CLA:HHC	2.72	0.52
11:B:1204:CLA:H93	14:F:4018:BCR:HC31	3.06	0.52
14:B:4006:BCR:H372	11:B:1225:CLA:H142	1.92	0.52
3:C:54:CYS:SG	13:C:3002:SF4:S2	3.08	0.52
7:L:55:MET:HB3	14:L:4022:BCR:H19C	1.92	0.52
11:A:1110:CLA:HAB	11:A:1118:CLA:H61	2.45	0.52
14:B:4010:BCR:H19C	11:B:1223:CLA:H111	4.82	0.52
2:2:349:HIS:ND1	11:2:1214:CLA:OBD	2.42	0.52
14:B:4017:BCR:H362	11:B:1023:CLA:H143	2.13	0.52
14:B:4009:BCR:C13	15:B:5004:LHG:H202	2.39	0.52
10:0:102:PRO:O	10:0:106:ALA:N	2.41	0.52
11:1:1801:CLA:HMA3	15:1:5003:LHG:HC62	1.92	0.52
1:1:560:ARG:NH2	4:4:15:THR:O	2.44	0.51
9:9:7:ALA:N	8:7:5:ASP:OD1	2.41	0.51
11:8:1503:CLA:HBC1	14:8:4022:BCR:H341	1.91	0.51
11:A:1112:CLA:HMC1	11:A:1113:CLA:HAB	2.53	0.51
11:B:1238:CLA:C2	14:L:4019:BCR:H363	3.31	0.51
11:B:1212:CLA:HAB	11:B:1211:CLA:HMC3	1.92	0.51
2:B:520:ILE:HD13	11:B:1234:CLA:HAB	1.92	0.51
2:B:413:LYS:NZ	6:F:124:PRO:O	2.69	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:ASN:O	6:F:32:PHE:N	2.43	0.51
15:B:5004:LHG:HC62	11:B:1220:CLA:HBB1	2.05	0.51
1:A:441:ASN:ND2	11:A:1237:CLA:OBD	3.30	0.51
14:B:4011:BCR:H392	14:B:4011:BCR:H23C	1.92	0.51
3:3:48:CYS:SG	13:3:3002:SF4:S3	2.99	0.51
2:B:337:ALA:HB2	14:B:4010:BCR:H372	1.93	0.51
1:1:193:VAL:CG1	11:1:1123:CLA:HHD	2.41	0.51
11:A:1125:CLA:HED1	11:A:1133:CLA:HAB	2.35	0.51
3:C:11:CYS:SG	13:C:3003:SF4:S4	2.63	0.51
14:2:4014:BCR:H23C	14:2:4014:BCR:H382	1.91	0.51
1:1:395:TRP:HD1	11:1:1126:CLA:HAB	1.71	0.51
2:2:668:TRP:CZ2	12:2:2002:PQN:H2M3	2.46	0.51
14:6:4020:BCR:HC22	9:9:20:TRP:NE1	2.26	0.51
14:A:4008:BCR:C8	14:A:4008:BCR:H331	2.41	0.51
2:B:571:ASP:OD1	2:B:703:ARG:NH2	2.44	0.51
14:2:4017:BCR:H362	11:2:1023:CLA:H111	1.93	0.51
7:8:41:ARG:NH2	7:8:52:GLU:OE2	2.41	0.51
1:A:56:HIS:CE1	11:A:1103:CLA:CBB	3.84	0.51
1:A:725:ALA:HB2	15:A:5001:LHG:HC62	1.91	0.51
5:E:12:LYS:NZ	5:E:67:GLU:OE1	2.39	0.51
11:A:1119:CLA:HBB1	11:A:1119:CLA:HHC	2.36	0.51
11:A:1012:CLA:H42	14:B:4011:BCR:H362	2.59	0.50
11:1:1112:CLA:HMC1	11:1:1113:CLA:HAB	1.92	0.50
14:2:4009:BCR:H353	15:2:5004:LHG:C20	2.40	0.50
11:8:1501:CLA:H41	14:8:4022:BCR:H14C	1.93	0.50
2:B:487:GLY:O	2:B:489:ALA:N	2.44	0.50
3:3:48:CYS:SG	13:3:3002:SF4:S2	3.08	0.50
11:L:1501:CLA:HBA2	14:L:4022:BCR:H363	1.94	0.50
11:L:1501:CLA:H202	11:L:1503:CLA:C2	2.86	0.50
11:2:1238:CLA:O1A	14:8:4019:BCR:H363	2.12	0.50
1:A:267:ASN:O	1:A:269:GLY:N	2.46	0.50
1:A:684:MET:HE2	1:A:693:TRP:CH2	2.46	0.50
11:B:1013:CLA:CGA	11:B:1013:CLA:H3A	2.42	0.50
1:A:538:HIS:ND1	11:A:1135:CLA:HAB	2.94	0.50
14:A:4003:BCR:H353	11:A:1111:CLA:C15	2.42	0.50
3:C:11:CYS:SG	13:C:3003:SF4:S2	2.17	0.50
6:F:12:PRO:CB	14:F:4013:BCR:H19C	6.16	0.50
11:B:1212:CLA:HBB1	11:B:1212:CLA:HHC	3.24	0.50
11:1:1011:CLA:HMB3	11:1:1012:CLA:HMD1	1.94	0.50
11:B:1226:CLA:HHC	11:B:1226:CLA:HBB1	1.94	0.50
3:C:11:CYS:SG	13:C:3003:SF4:S1	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:1130:CLA:HHC	11:1:1130:CLA:HBB1	1.94	0.49
11:1:1133:CLA:HHC	11:1:1133:CLA:CBB	2.42	0.49
1:1:354:ILE:HD11	14:1:4007:BCR:HC7	1.94	0.49
1:1:332:PHE:O	1:1:428:ARG:NH2	2.45	0.49
1:1:681:PHE:HA	11:2:1013:CLA:HAB	1.93	0.49
1:1:589:ASP:OD1	1:1:724:ARG:NH1	2.44	0.49
2:2:415:ALA:O	2:2:419:HIS:ND1	2.43	0.49
11:1:1127:CLA:H72	11:1:1127:CLA:HMD2	1.93	0.49
1:1:677:PHE:CD1	14:2:4011:BCR:H363	2.47	0.49
11:A:1138:CLA:HHD	14:B:4014:BCR:H381	1.94	0.49
1:A:199:HIS:O	1:A:203:GLY:N	2.44	0.49
11:1:1022:CLA:H203	11:2:1206:CLA:H51	1.94	0.49
11:1:1237:CLA:H3A	14:6:4020:BCR:H401	1.94	0.49
11:A:1106:CLA:CHC	11:A:1107:CLA:HMD2	2.42	0.49
11:B:1212:CLA:HAB	11:B:1211:CLA:CMC	2.43	0.49
7:8:137:VAL:HG23	14:8:4022:BCR:H403	1.93	0.49
11:B:1221:CLA:HMB2	11:B:1223:CLA:H8	2.17	0.49
11:2:1212:CLA:HHC	11:2:1212:CLA:CBB	2.43	0.49
6:6:12:PRO:CG	14:6:4013:BCR:H403	2.43	0.49
14:1:4007:BCR:H352	11:1:1119:CLA:H71	1.94	0.49
14:8:4019:BCR:H23C	14:8:4019:BCR:H392	1.94	0.49
11:A:1125:CLA:HBC3	11:A:1125:CLA:HHD	1.94	0.49
1:A:454:LEU:HD23	11:A:1132:CLA:HAB	1.95	0.49
10:K:90:LEU:CB	10:K:91:PRO:CD	2.91	0.49
2:2:312:LEU:CD2	15:2:5004:LHG:HC42	2.43	0.49
10:K:117:GLY:HA3	11:K:1401:CLA:C3B	2.64	0.49
1:1:267:ASN:O	1:1:269:GLY:N	2.45	0.48
14:2:4014:BCR:HC41	11:2:1229:CLA:CBB	2.43	0.48
2:B:334:LEU:HB3	14:B:4010:BCR:H401	3.41	0.48
11:A:1022:CLA:C17	14:B:4017:BCR:H343	2.43	0.48
11:1:1119:CLA:HMB2	11:1:1123:CLA:HMA3	1.95	0.48
14:2:4011:BCR:H321	14:2:4011:BCR:HC8	1.95	0.48
11:8:1501:CLA:H202	11:8:1503:CLA:H2	1.95	0.48
11:1:1106:CLA:H91	11:1:1106:CLA:H111	1.72	0.48
2:2:587:LEU:CD1	11:2:1234:CLA:HBB2	2.44	0.48
1:A:540:PHE:HE2	11:A:1022:CLA:HAB	2.41	0.48
11:2:1238:CLA:HBB1	11:2:1238:CLA:HHC	1.96	0.48
1:A:352:LEU:HD11	11:A:1128:CLA:HBB1	1.94	0.48
11:B:1223:CLA:HED1	11:B:1231:CLA:HAB	1.94	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:C8	2.44	0.48
1:A:540:PHE:CE2	11:A:1022:CLA:HAB	3.03	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HB2	11:A:1112:CLA:CHC	2.44	0.48
14:A:4007:BCR:H24C	11:A:1137:CLA:C9	2.43	0.48
1:1:195:SER:O	1:1:199:HIS:ND1	2.36	0.48
14:2:4005:BCR:H343	11:2:1209:CLA:HMC1	1.95	0.48
2:2:587:LEU:HD12	11:2:1234:CLA:HBB2	1.94	0.48
11:A:1131:CLA:HAB	11:A:1132:CLA:HMB2	1.95	0.48
11:1:1125:CLA:HHD	11:1:1125:CLA:CBC	2.42	0.48
15:A:5003:LHG:H02	15:A:5003:LHG:P	2.72	0.48
11:1:1128:CLA:H172	14:2:4011:BCR:H342	1.96	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:HC8	1.95	0.48
11:1:1106:CLA:H93	11:1:1128:CLA:H203	1.96	0.48
14:2:4010:BCR:H23C	14:2:4010:BCR:H392	1.95	0.48
11:A:1121:CLA:HHC	11:A:1121:CLA:HBB1	1.95	0.48
2:B:586:TRP:CE2	11:B:1021:CLA:H191	2.49	0.48
11:1:1107:CLA:H12	14:6:4013:BCR:H14C	1.96	0.48
11:A:1102:CLA:HAB	11:A:1104:CLA:CAD	2.44	0.48
1:1:681:PHE:N	11:2:1013:CLA:HAB	2.29	0.47
14:B:4004:BCR:H351	14:B:4004:BCR:H15C	1.60	0.47
14:B:4017:BCR:H15C	14:B:4017:BCR:H351	1.61	0.47
1:1:680:ALA:C	11:2:1013:CLA:HAB	2.34	0.47
1:A:121:VAL:HB	11:B:1230:CLA:HMD1	1.95	0.47
14:A:4007:BCR:H15C	14:A:4007:BCR:H351	1.64	0.47
14:1:4001:BCR:H332	14:1:4002:BCR:H24C	1.96	0.47
14:1:4007:BCR:H372	15:1:5003:LHG:H262	1.95	0.47
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.47	0.47
14:B:4009:BCR:H353	15:B:5004:LHG:H223	2.23	0.47
1:1:423:ASN:OD1	1:1:431:ARG:NH2	2.48	0.47
2:2:586:TRP:CE2	11:2:1021:CLA:H201	2.48	0.47
11:A:1138:CLA:HHD	14:B:4014:BCR:H383	1.96	0.47
14:A:4003:BCR:H402	11:A:1103:CLA:H72	2.39	0.47
1:A:429:MET:HA	1:A:432:HIS:CE1	2.50	0.47
14:B:4014:BCR:H15C	14:B:4014:BCR:H351	1.56	0.47
2:B:539:ARG:NH2	4:D:127:GLU:OE1	2.41	0.47
14:2:4010:BCR:H363	11:2:1222:CLA:C2B	2.44	0.47
6:F:42:SER:O	6:F:43:CYS:CB	2.63	0.47
11:B:1238:CLA:H2	14:L:4019:BCR:H363	3.26	0.47
11:1:1117:CLA:HAB	11:1:1117:CLA:C11	2.45	0.47
7:8:96:LEU:CG	14:8:4019:BCR:H24C	2.43	0.47
11:B:1207:CLA:HBB1	11:B:1207:CLA:HHC	2.47	0.47
11:B:1208:CLA:CBB	11:B:1208:CLA:HHC	2.98	0.47
14:B:4005:BCR:H343	11:B:1209:CLA:CMC	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4002:BCR:H15C	14:A:4002:BCR:H351	1.65	0.47
2:B:586:TRP:CD2	11:B:1021:CLA:H191	2.50	0.47
14:1:4001:BCR:H331	14:1:4002:BCR:H24C	1.96	0.47
14:2:4010:BCR:H351	14:2:4010:BCR:H15C	1.54	0.47
14:6:4018:BCR:H382	14:6:4018:BCR:H23C	1.96	0.47
14:B:4009:BCR:C14	15:B:5004:LHG:H202	2.45	0.47
11:2:1229:CLA:CAB	11:2:1230:CLA:HMB2	2.44	0.47
14:2:4006:BCR:H15C	14:2:4006:BCR:H351	1.72	0.47
14:2:4017:BCR:H15C	14:2:4017:BCR:H351	1.65	0.47
11:2:1238:CLA:H193	14:6:4018:BCR:H362	1.95	0.47
11:A:1137:CLA:HMB1	11:A:1137:CLA:HBB1	1.96	0.47
1:A:195:SER:O	1:A:199:HIS:ND1	2.44	0.47
11:B:1205:CLA:HAB	11:B:1206:CLA:HAA2	1.97	0.47
11:2:1013:CLA:CGA	11:2:1013:CLA:H3A	2.44	0.47
11:2:1223:CLA:HBB1	11:2:1231:CLA:HMA2	1.96	0.47
12:A:2001:PQN:C24	11:B:1013:CLA:H202	2.91	0.47
2:B:312:LEU:HD22	15:B:5004:LHG:HC42	2.17	0.47
8:7:26:SER:HB3	14:7:4021:BCR:HC41	1.97	0.47
11:A:1112:CLA:HBB1	11:A:1112:CLA:HHC	2.16	0.47
11:A:1136:CLA:HHC	11:A:1136:CLA:CBB	2.44	0.47
14:A:4007:BCR:HC41	11:A:1119:CLA:C19	2.45	0.47
11:B:1201:CLA:HAB	11:B:1203:CLA:CAD	2.84	0.47
11:2:1231:CLA:NC	11:2:1232:CLA:HAB	2.30	0.46
11:A:1114:CLA:CBB	11:A:1114:CLA:HHC	2.45	0.46
11:A:1133:CLA:HHC	11:A:1133:CLA:HBB1	4.19	0.46
11:1:1115:CLA:CBB	11:1:1115:CLA:HHC	2.45	0.46
11:2:1212:CLA:HAB	11:2:1211:CLA:CMC	2.45	0.46
11:A:1011:CLA:HBB1	11:A:1011:CLA:HMB1	1.97	0.46
1:A:589:ASP:OD1	1:A:724:ARG:NH1	2.55	0.46
11:A:1012:CLA:HMB3	11:B:1021:CLA:H203	1.96	0.46
11:B:1217:CLA:HBB1	11:B:1217:CLA:HHC	4.00	0.46
2:B:668:TRP:CZ2	12:B:2002:PQN:H2M3	2.50	0.46
11:1:1112:CLA:HBB1	11:1:1112:CLA:HHC	1.97	0.46
14:A:4001:BCR:H15C	14:A:4001:BCR:H351	1.54	0.46
2:B:642:VAL:HG22	11:B:1206:CLA:HHD	1.97	0.46
10:0:90:LEU:CB	10:0:91:PRO:CD	2.93	0.46
1:1:210:LEU:HB2	1:1:301:ALA:HB1	1.98	0.46
1:1:693:TRP:CZ2	12:1:2001:PQN:H2M3	2.50	0.46
14:F:4018:BCR:H14C	9:I:23:PRO:HG2	1.96	0.46
14:1:4001:BCR:H24C	10:0:110:PHE:HB2	1.97	0.46
1:1:342:GLU:OE1	1:1:342:GLU:N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4014:BCR:H15C	14:2:4014:BCR:H351	1.65	0.46
11:A:1138:CLA:HHC	11:A:1138:CLA:CBB	2.44	0.46
2:B:668:TRP:CH2	12:B:2002:PQN:H2M3	2.50	0.46
11:1:1105:CLA:C2	14:6:4013:BCR:H342	2.46	0.46
2:2:5:PHE:HB2	9:9:34:ILE:HA	1.98	0.46
1:A:330:GLY:N	15:A:5003:LHG:HC2	2.52	0.46
2:B:211:ASN:O	2:B:214:SER:OG	2.29	0.46
11:A:1125:CLA:HBC2	11:A:1125:CLA:HHD	1.99	0.46
14:B:4010:BCR:H332	11:B:1223:CLA:HED2	1.97	0.46
2:B:582:ASN:ND2	2:B:586:TRP:CZ2	2.83	0.46
11:B:1023:CLA:H193	14:F:4018:BCR:H19C	1.97	0.46
14:F:4020:BCR:HC42	7:L:87:ALA:HB1	1.96	0.46
11:A:1101:CLA:H8	11:A:1101:CLA:H52	2.75	0.46
1:A:369:HIS:ND1	11:A:1116:CLA:OBD	2.67	0.46
14:A:4003:BCR:C23	14:A:4003:BCR:H403	2.43	0.46
1:1:356:LEU:HD11	11:1:1128:CLA:CBB	2.46	0.46
11:8:1503:CLA:HMB1	11:8:1503:CLA:HBB1	1.97	0.46
11:1:1117:CLA:HAB	11:1:1117:CLA:H111	1.97	0.46
9:9:31:PHE:HB2	14:8:4019:BCR:H14C	1.97	0.46
2:B:117:TYR:HA	2:B:365:THR:HG22	2.09	0.46
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC1	1.99	0.46
14:F:4018:BCR:H24C	14:F:4018:BCR:H371	1.65	0.46
11:1:1101:CLA:HAB	11:1:1102:CLA:C2C	2.46	0.45
14:6:4013:BCR:H351	14:6:4013:BCR:H15C	1.62	0.45
11:A:1125:CLA:HAB	11:A:1133:CLA:HMA2	1.98	0.45
11:B:1210:CLA:HBB1	11:B:1210:CLA:HHC	2.09	0.45
11:A:1012:CLA:H43	14:B:4011:BCR:H362	1.97	0.45
10:K:62:ILE:HD12	11:K:1402:CLA:HMA1	1.98	0.45
11:1:1134:CLA:HBB1	11:1:1134:CLA:HHC	1.97	0.45
1:1:721:ILE:HG21	15:1:5001:LHG:HC42	1.97	0.45
2:2:668:TRP:CH2	12:2:2002:PQN:H2M3	2.51	0.45
1:A:53:ALA:HB2	15:A:5001:LHG:HC82	1.98	0.45
1:A:79:HIS:CD2	11:A:1103:CLA:HMA1	2.82	0.45
2:B:434:LEU:HD23	11:B:1230:CLA:HBB1	1.97	0.45
11:1:1237:CLA:HBA1	11:1:1237:CLA:CHA	2.45	0.45
11:A:1103:CLA:H51	11:A:1111:CLA:C1	2.94	0.45
11:A:1107:CLA:HAB	11:B:1230:CLA:HMD2	1.98	0.45
2:B:435:TYR:CE2	2:B:515:LEU:HB3	2.52	0.45
11:A:1117:CLA:H111	11:A:1117:CLA:HAB	3.44	0.45
11:A:1131:CLA:HAB	11:A:1132:CLA:HBB	1.98	0.45
2:B:519:ALA:HB1	11:B:1021:CLA:C19	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4017:BCR:H331	14:2:4017:BCR:HC8	1.99	0.45
14:A:4003:BCR:H402	14:A:4003:BCR:H23C	2.28	0.45
11:A:1104:CLA:H3A	11:A:1128:CLA:HAB	1.99	0.45
11:A:1102:CLA:HMA2	11:A:1109:CLA:HMD2	1.99	0.45
1:A:193:VAL:HG13	11:A:1123:CLA:HHD	1.98	0.45
11:B:1231:CLA:HHC	11:B:1231:CLA:HBB1	1.99	0.45
8:M:5:ASP:OD1	9:I:7:ALA:N	3.55	0.45
1:1:395:TRP:NE1	11:1:1126:CLA:HAB	2.32	0.45
1:1:203:GLY:HA2	11:1:1118:CLA:HBC1	1.97	0.45
1:A:79:HIS:CG	11:A:1103:CLA:HMA1	2.91	0.45
11:B:1222:CLA:HMB1	11:B:1223:CLA:H202	1.98	0.45
2:B:7:LYS:NZ	8:M:30:TYR:O	2.48	0.45
11:1:1101:CLA:H201	11:1:1012:CLA:H203	1.99	0.45
14:1:4008:BCR:H331	14:1:4008:BCR:HC8	1.98	0.45
2:2:130:THR:OG1	2:2:201:GLU:OE1	2.34	0.45
2:2:5:PHE:HB3	2:2:20:ARG:NH1	2.32	0.45
14:2:4017:BCR:H371	14:2:4017:BCR:H24C	1.78	0.45
2:2:487:GLY:O	2:2:489:ALA:N	2.50	0.45
1:A:721:ILE:HG21	15:A:5001:LHG:HC42	1.99	0.45
15:A:5003:LHG:H301	15:A:5003:LHG:H171	3.08	0.45
1:A:737:VAL:HG22	14:B:4011:BCR:H321	1.99	0.45
12:A:2001:PQN:H251	11:B:1013:CLA:H202	1.99	0.45
11:B:1215:CLA:CGA	11:B:1215:CLA:H3A	2.46	0.45
11:B:1228:CLA:CBB	11:B:1228:CLA:HHC	3.51	0.45
7:L:17:VAL:O	7:L:19:HIS:N	2.49	0.45
14:1:4007:BCR:C34	11:1:1123:CLA:HAB	2.45	0.45
14:6:4018:BCR:H351	14:6:4018:BCR:H15C	1.62	0.45
14:A:4003:BCR:H351	14:A:4003:BCR:H15C	1.64	0.45
1:A:681:PHE:N	11:B:1013:CLA:HAB	2.42	0.45
14:2:4009:BCR:H321	14:2:4009:BCR:HC8	1.99	0.45
14:2:4011:BCR:H15C	14:2:4011:BCR:H351	1.77	0.45
11:8:1501:CLA:HBB1	11:8:1501:CLA:HHC	1.98	0.45
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB2	1.97	0.45
11:L:1501:CLA:H202	11:L:1503:CLA:H2	2.31	0.44
1:1:59:ASP:N	1:1:59:ASP:OD1	2.50	0.44
11:A:1105:CLA:HHC	11:A:1105:CLA:CBB	2.84	0.44
11:L:1501:CLA:CBA	14:L:4022:BCR:H363	2.46	0.44
14:L:4019:BCR:H331	14:L:4019:BCR:HC7	1.58	0.44
4:4:3:GLU:HB3	4:4:4:LEU:H	1.61	0.44
1:A:59:ASP:N	1:A:59:ASP:OD1	2.49	0.44
2:B:25:ILE:HG12	14:L:4019:BCR:HC41	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4005:BCR:H351	14:2:4005:BCR:H15C	1.77	0.44
1:A:100:TYR:HA	1:A:144:PHE:CE2	2.53	0.44
11:A:1102:CLA:H203	11:A:1106:CLA:C14	2.48	0.44
11:B:1212:CLA:CBB	11:B:1212:CLA:HHC	3.15	0.44
14:B:4005:BCR:H351	14:B:4005:BCR:H15C	1.64	0.44
14:1:4007:BCR:H15C	14:1:4007:BCR:H351	1.56	0.44
11:2:1240:CLA:HHC	11:2:1240:CLA:CBB	2.47	0.44
5:5:13:ARG:O	5:5:14:THR:HB	2.18	0.44
6:6:49:ILE:CB	6:6:50:PRO:HD3	2.47	0.44
1:A:680:ALA:C	11:B:1013:CLA:HAB	2.74	0.44
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.61	0.44
9:I:10:LEU:HB2	9:I:11:PRO:HD3	2.02	0.44
11:2:1023:CLA:CGA	11:2:1023:CLA:H3A	2.47	0.44
1:A:203:GLY:HA2	11:A:1118:CLA:HBC1	1.98	0.44
11:A:1104:CLA:HBB	11:A:1128:CLA:HAB	1.99	0.44
11:B:1238:CLA:C1	14:L:4019:BCR:H363	2.69	0.44
2:2:312:LEU:HB2	15:2:5004:LHG:HC42	1.99	0.44
8:7:9:LEU:HD12	14:7:4021:BCR:H401	1.99	0.44
11:8:1501:CLA:H43	14:8:4022:BCR:H14C	1.99	0.44
11:A:1127:CLA:HMD2	11:A:1127:CLA:H71	2.00	0.44
2:B:338:SER:HB3	11:B:1221:CLA:H42	2.26	0.44
2:2:582:ASN:ND2	2:2:586:TRP:CZ2	2.86	0.44
11:A:1102:CLA:H142	11:A:1107:CLA:H202	2.00	0.44
1:A:356:LEU:HD11	11:A:1128:CLA:CBB	2.63	0.44
6:F:11:ALA:N	6:F:12:PRO:HD2	2.33	0.44
11:A:1104:CLA:HHD	11:A:1104:CLA:HBC3	2.00	0.44
11:A:1108:CLA:HBB1	11:A:1108:CLA:HHC	4.41	0.44
1:A:226:LEU:HD21	1:A:252:LEU:HD11	2.00	0.44
3:C:17:CYS:HB2	3:C:54:CYS:HB3	2.80	0.44
14:F:4018:BCR:H351	14:F:4018:BCR:H15C	1.63	0.44
6:F:49:ILE:CB	6:F:50:PRO:HD3	3.38	0.44
1:1:728:VAL:CG1	15:1:5001:LHG:H301	2.47	0.43
11:2:1205:CLA:CHA	11:2:1205:CLA:CGA	2.96	0.43
11:2:1210:CLA:H203	11:2:1225:CLA:C3D	2.48	0.43
14:A:4003:BCR:H23C	11:A:1103:CLA:H72	2.00	0.43
14:A:4001:BCR:H14C	11:A:1118:CLA:HBB1	2.75	0.43
1:A:440:LEU:HD23	1:A:547:LEU:HA	2.09	0.43
12:B:2002:PQN:H291	14:L:4019:BCR:HC8	3.20	0.43
14:F:4018:BCR:H14C	9:I:23:PRO:CB	2.48	0.43
1:1:500:ASN:ND2	11:1:1115:CLA:OBD	2.51	0.43
14:6:4020:BCR:H15C	14:6:4020:BCR:H351	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:17:VAL:O	7:8:19:HIS:N	2.48	0.43
11:A:1115:CLA:HBB1	11:A:1115:CLA:HHC	2.00	0.43
11:A:1133:CLA:CBB	11:A:1133:CLA:HHC	3.68	0.43
2:B:77:TRP:HA	2:B:84:ILE:HG21	2.00	0.43
11:1:1128:CLA:H201	11:1:1140:CLA:H2	2.00	0.43
11:A:1107:CLA:CBA	11:A:1107:CLA:HBD	2.66	0.43
11:A:1136:CLA:C1A	11:A:1136:CLA:CGA	2.96	0.43
1:A:354:ILE:CD1	14:A:4007:BCR:HC7	2.42	0.43
11:B:1238:CLA:H193	14:F:4018:BCR:H362	2.00	0.43
2:B:385:PHE:CZ	14:B:4010:BCR:H373	2.87	0.43
8:M:19:ALA:HB2	14:M:4021:BCR:H15C	2.26	0.43
11:1:1126:CLA:C4C	14:2:4011:BCR:HC42	2.48	0.43
14:1:4003:BCR:H371	11:1:1127:CLA:H62	2.01	0.43
14:A:4002:BCR:C14	11:A:1112:CLA:HBB1	2.48	0.43
11:A:1118:CLA:H3A	10:K:105:LEU:HD12	2.01	0.43
1:A:342:GLU:N	1:A:342:GLU:OE1	2.55	0.43
11:B:1201:CLA:HHC	11:B:1203:CLA:OBD	2.45	0.43
2:B:412:HIS:O	2:B:412:HIS:ND1	2.52	0.43
2:2:273:ILE:O	2:2:277:HIS:ND1	2.50	0.43
9:9:10:LEU:HB2	9:9:11:PRO:HD3	2.01	0.43
1:A:296:HIS:HE1	11:A:1117:CLA:C2B	2.31	0.43
11:B:1207:CLA:CBB	11:B:1207:CLA:HHC	2.71	0.43
4:D:98:HIS:CG	4:D:99:PRO:CD	3.01	0.43
11:B:1204:CLA:H92	14:M:4021:BCR:C14	2.48	0.43
11:1:1119:CLA:HMB1	11:1:1123:CLA:HED2	1.99	0.43
11:2:1207:CLA:HHC	11:2:1207:CLA:CBB	2.48	0.43
11:A:1125:CLA:CBB	11:A:1125:CLA:HHC	3.66	0.43
2:B:5:PHE:HB3	2:B:20:ARG:NH1	2.36	0.43
14:F:4020:BCR:H333	7:L:87:ALA:CB	3.07	0.43
11:A:1119:CLA:OBD	11:A:1121:CLA:HHD	2.41	0.43
11:A:1801:CLA:CHC	15:A:5003:LHG:HC31	2.85	0.43
11:B:1223:CLA:HBD	11:B:1223:CLA:HAA2	2.13	0.43
1:A:210:LEU:HD11	14:A:4001:BCR:HC8	2.01	0.43
11:A:1237:CLA:HHD	14:B:4017:BCR:H383	2.00	0.43
11:2:1239:CLA:HBB1	11:2:1239:CLA:HHC	2.00	0.43
1:A:550:LEU:HD11	11:A:1119:CLA:H202	3.41	0.43
11:A:1237:CLA:CBB	11:A:1237:CLA:HHC	2.48	0.43
1:A:303:LEU:HD22	11:A:1119:CLA:HMC1	2.01	0.43
1:A:330:GLY:HA3	15:A:5003:LHG:HC2	2.69	0.43
1:1:571:ARG:NE	15:1:5001:LHG:O5	2.51	0.43
1:A:564:ASP:N	1:A:564:ASP:OD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:LEU:N	2:B:492:PRO:CD	2.83	0.43
15:1:5001:LHG:C20	11:1:1128:CLA:H202	2.47	0.42
11:A:1104:CLA:HAB	11:A:1127:CLA:HMC2	2.69	0.42
1:A:261:THR:O	1:A:265:THR:N	2.48	0.42
14:A:4002:BCR:HC41	11:A:1103:CLA:H142	2.01	0.42
2:B:642:VAL:CG2	11:B:1206:CLA:HHD	2.49	0.42
1:A:269:GLY:HA3	10:K:51:PRO:HG3	2.01	0.42
11:2:1021:CLA:HBA1	11:2:1021:CLA:H3A	1.78	0.42
14:8:4022:BCR:H15C	14:8:4022:BCR:H351	1.66	0.42
1:A:312:ARG:NH2	1:A:316:GLY:O	2.52	0.42
11:B:1021:CLA:H3A	11:B:1021:CLA:HBA2	1.91	0.42
2:B:294:ASN:OD1	2:B:294:ASN:N	2.52	0.42
12:B:2002:PQN:H291	14:L:4019:BCR:H342	2.00	0.42
11:1:1103:CLA:H3A	11:1:1103:CLA:CGA	2.49	0.42
1:1:263:PHE:CZ	14:1:4001:BCR:H343	2.54	0.42
11:2:1206:CLA:CMB	11:2:1207:CLA:C1C	2.97	0.42
2:2:656:THR:HA	11:2:1023:CLA:HAB	2.01	0.42
5:E:13:ARG:O	5:E:14:THR:HB	2.18	0.42
10:0:110:PHE:HA	10:0:113:ILE:HG22	2.00	0.42
11:1:1134:CLA:O1A	11:0:1401:CLA:O1D	2.36	0.42
11:2:1207:CLA:H2A	11:2:1207:CLA:O2A	2.20	0.42
11:A:1801:CLA:NC	15:A:5003:LHG:HC31	2.93	0.42
10:K:120:LEU:HD13	11:K:1401:CLA:C1	2.97	0.42
11:2:1208:CLA:HHC	11:2:1208:CLA:CBB	2.50	0.42
2:2:177:HIS:CG	11:2:1210:CLA:HMC2	2.54	0.42
2:2:412:HIS:O	2:2:412:HIS:ND1	2.53	0.42
2:2:77:TRP:HA	2:2:84:ILE:HG21	2.01	0.42
14:8:4022:BCR:H371	14:8:4022:BCR:H24C	1.78	0.42
6:F:6:SER:O	6:F:10:THR:N	3.91	0.42
1:1:260:LEU:O	1:1:261:THR:OG1	2.31	0.42
11:2:1202:CLA:H141	11:2:1202:CLA:C17	2.49	0.42
2:2:385:PHE:CE2	14:2:4010:BCR:H373	2.55	0.42
2:2:435:TYR:CE2	2:2:515:LEU:HB3	2.55	0.42
4:4:77:LYS:HB2	4:4:78:PRO:HD3	2.00	0.42
11:B:1209:CLA:HHC	11:B:1209:CLA:CBB	2.57	0.42
14:B:4010:BCR:C20	11:B:1223:CLA:H91	3.84	0.42
1:1:262:PRO:O	1:1:267:ASN:N	2.49	0.42
1:1:305:ILE:O	1:1:309:HIS:ND1	2.53	0.42
2:2:294:ASN:N	2:2:294:ASN:OD1	2.52	0.42
2:2:642:VAL:HG12	2:2:643:TRP:N	2.35	0.42
1:A:211:GLY:HA2	14:A:4002:BCR:H363	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:TRP:CZ2	11:B:1208:CLA:HMA1	2.54	0.42
2:B:425:LEU:HB3	11:B:1229:CLA:CED	2.48	0.42
2:B:178:HIS:ND1	11:B:1221:CLA:O1D	2.53	0.42
14:B:4010:BCR:H351	14:B:4010:BCR:H15C	1.62	0.42
4:D:27:LYS:HG3	4:D:88:VAL:HG13	2.02	0.42
11:2:1207:CLA:HBB1	11:2:1207:CLA:HHC	2.01	0.42
1:A:395:TRP:HE1	11:A:1126:CLA:HAB	1.85	0.42
1:A:467:PRO:HA	1:A:470:MET:HG2	2.02	0.42
14:B:4010:BCR:HC21	11:B:1223:CLA:CMA	2.49	0.42
7:L:100:GLY:HA3	7:L:120:TRP:CD1	2.55	0.42
11:1:1237:CLA:C10	14:8:4019:BCR:H361	2.50	0.42
1:1:211:GLY:CA	14:1:4002:BCR:H363	2.50	0.42
1:1:681:PHE:CA	11:2:1013:CLA:HAB	2.49	0.42
11:2:1202:CLA:H142	11:2:1202:CLA:CAD	2.49	0.42
2:2:341:VAL:HG13	11:2:1222:CLA:HED1	2.01	0.42
4:4:98:HIS:CG	4:4:99:PRO:CD	3.03	0.42
11:A:1011:CLA:HBA2	11:A:1011:CLA:H3A	1.89	0.42
1:A:226:LEU:HD12	1:A:236:ILE:HG23	2.01	0.42
14:A:4003:BCR:C40	14:A:4003:BCR:C23	2.98	0.42
11:B:1201:CLA:HAC1	14:L:4019:BCR:HC32	2.01	0.42
14:B:4010:BCR:H332	11:B:1223:CLA:CED	2.50	0.42
2:B:212:PHE:CB	11:B:1211:CLA:HMD3	2.50	0.42
14:L:4019:BCR:HC8	14:L:4019:BCR:C32	2.46	0.42
11:1:1130:CLA:HHC	11:1:1130:CLA:CBB	2.50	0.42
11:2:1238:CLA:CBB	11:2:1238:CLA:HHC	2.49	0.42
11:A:1108:CLA:CBB	11:A:1108:CLA:HHC	3.89	0.42
11:B:1205:CLA:HAB	11:B:1206:CLA:O1A	3.77	0.42
2:B:189:ALA:HA	11:B:1212:CLA:HAB	2.02	0.42
11:A:1801:CLA:HBC2	11:A:1801:CLA:HMC1	2.00	0.41
11:B:1209:CLA:HHC	11:B:1209:CLA:HBB1	2.16	0.41
14:L:4022:BCR:H351	14:L:4022:BCR:H15C	1.75	0.41
14:F:4020:BCR:H351	14:F:4020:BCR:H15C	1.83	0.41
10:K:124:SER:O	10:K:125:SER:C	2.84	0.41
1:1:319:HIS:HB3	1:1:324:ILE:HD11	2.02	0.41
1:A:262:PRO:O	1:A:267:ASN:N	2.58	0.41
11:A:1801:CLA:C2C	15:A:5003:LHG:HC31	2.51	0.41
11:A:1118:CLA:H3A	10:K:105:LEU:CD1	2.50	0.41
11:1:1110:CLA:HAB	11:1:1118:CLA:H61	2.02	0.41
11:1:1106:CLA:H91	11:1:1128:CLA:H203	2.01	0.41
14:1:4007:BCR:H363	11:1:1122:CLA:H143	2.01	0.41
12:A:2001:PQN:H201	11:A:1101:CLA:H12	2.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1103:CLA:HBB1	11:A:1104:CLA:HBA1	4.61	0.41
11:A:1119:CLA:HMB2	11:A:1123:CLA:HMA3	2.02	0.41
1:A:305:ILE:O	1:A:309:HIS:ND1	2.55	0.41
1:A:681:PHE:HA	11:B:1013:CLA:CAB	2.58	0.41
11:B:1222:CLA:CAD	11:B:1234:CLA:HBB1	2.49	0.41
2:B:123:TRP:HA	2:B:356:TYR:CD1	2.56	0.41
9:I:15:ILE:HB	9:I:16:PRO:HD3	2.03	0.41
14:L:4019:BCR:C8	14:L:4019:BCR:H321	2.43	0.41
2:2:571:ASP:OD1	2:2:703:ARG:NH2	2.52	0.41
4:4:82:ASP:N	4:4:82:ASP:OD1	2.52	0.41
1:A:58:PHE:CD2	11:A:1103:CLA:HMC2	2.55	0.41
11:A:1138:CLA:C1A	11:A:1138:CLA:CGA	3.05	0.41
1:A:332:PHE:O	1:A:428:ARG:NH2	2.69	0.41
2:B:312:LEU:HB2	15:B:5004:LHG:HC42	2.21	0.41
1:1:721:ILE:CG2	15:1:5001:LHG:HC42	2.50	0.41
14:2:4004:BCR:H15C	14:2:4004:BCR:H351	1.67	0.41
2:2:491:LEU:N	2:2:492:PRO:CD	2.84	0.41
8:7:19:ALA:HB2	14:7:4021:BCR:C15	2.50	0.41
14:B:4005:BCR:H343	11:B:1209:CLA:HMC3	2.02	0.41
11:1:1137:CLA:HBB1	11:1:1137:CLA:HMB1	2.01	0.41
11:2:1201:CLA:HMB2	14:7:4021:BCR:H333	2.01	0.41
14:B:4010:BCR:C20	11:B:1223:CLA:C9	3.57	0.41
2:B:494:TRP:CE2	11:B:1231:CLA:HED2	3.33	0.41
4:D:77:LYS:HB2	4:D:78:PRO:HD3	2.02	0.41
10:K:73:VAL:HG13	10:K:74:ILE:N	2.36	0.41
14:2:4014:BCR:HC41	11:2:1229:CLA:HBB2	2.02	0.41
14:2:4017:BCR:H352	11:2:1239:CLA:HBA2	2.03	0.41
2:2:60:TRP:HA	11:2:1204:CLA:HBB2	2.02	0.41
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB1	2.01	0.41
11:B:1220:CLA:HHB	11:B:1240:CLA:HAB	2.93	0.41
10:K:120:LEU:CD1	11:K:1401:CLA:H11	2.97	0.41
1:1:453:GLY:C	11:1:1132:CLA:HAB	2.41	0.41
1:1:53:ALA:HB2	15:1:5001:LHG:HC91	2.03	0.41
2:2:154:TRP:CD1	8:7:28:GLU:HG3	2.56	0.41
11:2:1238:CLA:C19	14:6:4018:BCR:H362	2.51	0.41
11:A:1103:CLA:H111	11:A:1103:CLA:H71	2.20	0.41
11:A:1119:CLA:CBB	11:A:1119:CLA:HHC	2.73	0.41
14:A:4007:BCR:H341	11:A:1123:CLA:HAB	3.30	0.41
1:A:310:MET:O	1:A:319:HIS:N	2.72	0.41
2:B:645:TRP:CZ3	14:B:4017:BCR:HC21	2.56	0.41
2:B:413:LYS:NZ	2:B:537:ASP:OD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:310:MET:O	1:1:319:HIS:N	2.54	0.41
11:2:1202:CLA:H141	11:2:1202:CLA:H171	2.03	0.41
2:2:329:HIS:CE1	2:2:390:ILE:HG21	2.56	0.41
2:2:520:ILE:HG21	11:2:1234:CLA:HAB	2.03	0.41
11:A:1121:CLA:HHC	11:A:1121:CLA:CBB	2.53	0.41
1:A:575:ASP:OD2	1:A:579:ARG:NH1	2.53	0.41
14:B:4005:BCR:HC7	11:B:1209:CLA:CMC	2.47	0.41
11:1:1801:CLA:CMA	15:1:5003:LHG:HC62	2.51	0.41
11:2:1239:CLA:HHC	11:2:1239:CLA:CBB	2.51	0.41
11:A:1107:CLA:HBA1	11:A:1107:CLA:HBD	2.04	0.41
1:A:260:LEU:O	1:A:261:THR:OG1	2.32	0.41
11:B:1229:CLA:CAB	11:B:1230:CLA:HMB2	2.58	0.41
11:1:1106:CLA:CBB	11:1:1106:CLA:HHC	2.49	0.40
11:1:1012:CLA:CHB	11:2:1021:CLA:H203	2.51	0.40
11:1:1022:CLA:H203	11:2:1206:CLA:H62	2.03	0.40
11:1:1107:CLA:C1	14:6:4013:BCR:H14C	2.51	0.40
14:6:4018:BCR:H14C	9:9:23:PRO:HG2	2.00	0.40
1:A:154:ASP:OD1	1:A:155:SER:N	2.55	0.40
11:B:1207:CLA:O2A	11:B:1207:CLA:H2A	2.20	0.40
1:1:197:MET:HE3	11:1:1119:CLA:HMB3	2.02	0.40
14:2:4010:BCR:HC21	11:2:1223:CLA:CMA	2.51	0.40
2:2:476:LEU:HD12	11:2:1231:CLA:HED3	2.03	0.40
5:5:11:ILE:N	5:5:11:ILE:HD12	2.36	0.40
11:A:1112:CLA:HBC2	11:A:1112:CLA:HHH	2.03	0.40
1:A:539:ALA:HB1	11:A:1136:CLA:HMB3	2.03	0.40
1:A:684:MET:HE2	1:A:693:TRP:CZ2	2.56	0.40
2:B:19:ARG:HG2	2:B:23:TYR:CD1	2.56	0.40
2:B:656:THR:HA	11:B:1023:CLA:CAB	2.46	0.40
4:D:10:LYS:HG3	4:D:49:ILE:HD11	2.03	0.40
7:L:56:ALA:HA	14:L:4022:BCR:H15C	2.03	0.40
11:1:1111:CLA:CGA	11:1:1111:CLA:H3A	2.51	0.40
11:1:1801:CLA:H3A	11:1:1801:CLA:HBA2	1.93	0.40
11:2:1231:CLA:C4C	11:2:1232:CLA:CAB	2.99	0.40
11:A:1103:CLA:NC	11:A:1128:CLA:HMB3	2.51	0.40
1:A:451:SER:OG	1:A:452:PHE:N	2.55	0.40
11:B:1223:CLA:H111	11:B:1223:CLA:H93	3.77	0.40
11:K:1402:CLA:C1A	11:K:1402:CLA:CGA	3.00	0.40
11:K:1402:CLA:CBB	11:K:1402:CLA:HHC	2.49	0.40
11:1:1134:CLA:CBB	11:1:1134:CLA:HHC	2.50	0.40
1:1:728:VAL:HG13	15:1:5001:LHG:H301	2.04	0.40
2:2:29:HIS:ND1	11:2:1203:CLA:O1A	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:654:TRP:CH2	2:2:658:PHE:CZ	3.10	0.40
1:A:684:MET:HE2	12:A:2001:PQN:H2M3	2.03	0.40
11:B:1219:CLA:C1A	11:B:1219:CLA:CGA	4.44	0.40
2:B:223:MET:SD	2:B:223:MET:N	2.94	0.40
1:A:441:ASN:ND2	2:B:675:ILE:HG12	2.36	0.40
3:C:17:CYS:SG	3:C:18:VAL:N	3.19	0.40
2:2:475:LEU:HD13	11:2:1231:CLA:HHD	2.03	0.40
11:A:1011:CLA:HMB3	11:A:1012:CLA:HMD1	2.03	0.40
1:A:395:TRP:HD1	11:A:1126:CLA:HAB	1.79	0.40
11:A:1801:CLA:HBB1	11:A:1121:CLA:CAB	3.73	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	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	41	74
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	41	74
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	41	74
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	15	52
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	19	57
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	19	57
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	22	60
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	22	60
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	22	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	10	46
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	10	46
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	10	46
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	9	44
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	6	37
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	9	44
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	12	48
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	7	41
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	12	48
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	2	23
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	20
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	3	29
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	17	54

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR
2	b	6	PRO
4	d	99	PRO
1	1	261	THR
2	2	6	PRO
4	4	99	PRO
6	6	42	SER
10	K	92	GLN
10	K	125	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	k	92	GLN
10	0	92	GLN
2	B	488	ALA
2	B	489	ALA
5	E	14	THR
7	L	108	GLN
2	b	488	ALA
5	e	14	THR
6	f	42	SER
2	2	488	ALA
2	2	489	ALA
5	5	14	THR
7	8	108	GLN
10	K	90	LEU
10	k	90	LEU
10	0	90	LEU
10	0	126	GLY
2	B	556	CYS
6	F	31	ALA
2	b	489	ALA
2	b	556	CYS
7	l	108	GLN
2	2	314	GLY
2	2	487	GLY
2	2	556	CYS
1	A	115	GLN
2	B	314	GLY
2	B	487	GLY
7	L	109	GLY
1	a	115	GLN
2	b	487	GLY
6	f	31	ALA
1	1	115	GLN
6	6	31	ALA
10	k	51	PRO
6	F	50	PRO
2	2	235	ALA
2	b	314	GLY
7	l	109	GLY
7	8	109	GLY
10	K	51	PRO
10	K	87	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	0	51	PRO
7	L	18	GLY

5.3.2 Protein sidechains ⓘ

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	1	588/603 (98%)	573 (97%)	15 (3%)	46	69
1	A	588/603 (98%)	570 (97%)	18 (3%)	40	65
1	a	588/603 (98%)	573 (97%)	15 (3%)	46	69
2	2	582/583 (100%)	565 (97%)	17 (3%)	42	67
2	B	582/583 (100%)	562 (97%)	20 (3%)	37	64
2	b	582/583 (100%)	566 (97%)	16 (3%)	44	69
3	3	68/69 (99%)	65 (96%)	3 (4%)	28	57
3	C	68/69 (99%)	61 (90%)	7 (10%)	7	31
3	c	68/69 (99%)	64 (94%)	4 (6%)	19	51
4	4	113/116 (97%)	109 (96%)	4 (4%)	36	64
4	D	113/116 (97%)	111 (98%)	2 (2%)	59	77
4	d	113/116 (97%)	110 (97%)	3 (3%)	44	69
5	5	56/60 (93%)	54 (96%)	2 (4%)	35	63
5	E	56/60 (93%)	54 (96%)	2 (4%)	35	63
5	e	56/60 (93%)	54 (96%)	2 (4%)	35	63
6	6	21/106 (20%)	20 (95%)	1 (5%)	25	56
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	25	56
7	8	113/118 (96%)	113 (100%)	0	100	100
7	L	113/118 (96%)	112 (99%)	1 (1%)	78	88
7	l	113/118 (96%)	112 (99%)	1 (1%)	78	88
8	7	24/25 (96%)	23 (96%)	1 (4%)	30	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	M	24/25 (96%)	23 (96%)	1 (4%)	30	58
8	m	24/25 (96%)	23 (96%)	1 (4%)	30	58
9	9	31/32 (97%)	28 (90%)	3 (10%)	8	33
9	I	31/32 (97%)	27 (87%)	4 (13%)	4	23
9	i	31/32 (97%)	27 (87%)	4 (13%)	4	23
10	0	37/100 (37%)	30 (81%)	7 (19%)	1	10
10	K	37/100 (37%)	30 (81%)	7 (19%)	1	10
10	k	37/100 (37%)	31 (84%)	6 (16%)	2	15
All	All	4897/5436 (90%)	4729 (97%)	168 (3%)	37	64

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	104	LEU
1	A	224	ASN
1	A	235	ASP
1	A	245	GLU
1	A	249	MET
1	A	303	LEU
1	A	323	GLU
1	A	356	LEU
1	A	368	GLN
1	A	459	ASP
1	A	462	ARG
1	A	477	GLN
1	A	478	LEU
1	A	562	VAL
1	A	631	THR
1	A	739	THR
1	A	748	LEU
2	B	145	LEU
2	B	196	HIS
2	B	229	ASN
2	B	236	ASP
2	B	257	PHE
2	B	302	LYS
2	B	304	ILE
2	B	318	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	334	LEU
2	B	351	TYR
2	B	395	ASP
2	B	406	LEU
2	B	420	LEU
2	B	439	ASP
2	B	516	VAL
2	B	542	LYS
2	B	573	PHE
2	B	580	MET
2	B	681	ARG
2	B	689	ARG
3	C	3	HIS
3	C	11	CYS
3	C	19	ARG
3	C	21	CYS
3	C	54	CYS
3	C	58	CYS
3	C	69	LEU
4	D	73	ARG
4	D	82	ASP
5	E	33	ILE
5	E	43	ARG
7	L	96	LEU
8	M	5	ASP
1	a	59	ASP
1	a	104	LEU
1	a	224	ASN
1	a	235	ASP
1	a	249	MET
1	a	303	LEU
1	a	323	GLU
1	a	368	GLN
1	a	459	ASP
1	a	477	GLN
1	a	478	LEU
1	a	562	VAL
1	a	631	THR
1	a	739	THR
1	a	748	LEU
2	b	76	GLN
2	b	145	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	196	HIS
2	b	229	ASN
2	b	236	ASP
2	b	257	PHE
2	b	302	LYS
2	b	304	ILE
2	b	318	THR
2	b	334	LEU
2	b	406	LEU
2	b	420	LEU
2	b	516	VAL
2	b	542	LYS
2	b	573	PHE
2	b	689	ARG
3	c	21	CYS
3	c	58	CYS
3	c	66	ARG
3	c	69	LEU
4	d	73	ARG
4	d	82	ASP
4	d	107	LYS
5	e	33	ILE
5	e	43	ARG
6	f	38	PHE
9	i	1	MET
9	i	17	MET
9	i	21	LEU
9	i	30	LEU
7	l	137	VAL
8	m	5	ASP
1	1	59	ASP
1	1	104	LEU
1	1	224	ASN
1	1	235	ASP
1	1	249	MET
1	1	303	LEU
1	1	323	GLU
1	1	368	GLN
1	1	462	ARG
1	1	477	GLN
1	1	478	LEU
1	1	562	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	631	THR
1	1	739	THR
1	1	748	LEU
2	2	76	GLN
2	2	145	LEU
2	2	196	HIS
2	2	229	ASN
2	2	236	ASP
2	2	257	PHE
2	2	302	LYS
2	2	304	ILE
2	2	334	LEU
2	2	395	ASP
2	2	406	LEU
2	2	420	LEU
2	2	516	VAL
2	2	542	LYS
2	2	573	PHE
2	2	580	MET
2	2	689	ARG
3	3	58	CYS
3	3	66	ARG
3	3	69	LEU
4	4	3	GLU
4	4	73	ARG
4	4	82	ASP
4	4	107	LYS
5	5	33	ILE
5	5	43	ARG
6	6	38	PHE
9	9	1	MET
9	9	17	MET
9	9	30	LEU
8	7	5	ASP
10	K	64	MET
10	K	72	PHE
10	K	76	TYR
10	K	104	LEU
10	K	112	HIS
10	K	113	ILE
10	K	114	LEU
9	I	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	17	MET
9	I	21	LEU
9	I	30	LEU
10	k	64	MET
10	k	72	PHE
10	k	76	TYR
10	k	112	HIS
10	k	113	ILE
10	k	114	LEU
10	0	64	MET
10	0	72	PHE
10	0	76	TYR
10	0	104	LEU
10	0	112	HIS
10	0	113	ILE
10	0	114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS
1	A	432	HIS
1	A	608	HIS
2	B	34	HIS
2	B	373	HIS
2	B	437	HIS
2	B	582	ASN
1	a	224	ASN
1	a	296	HIS
1	a	432	HIS
2	b	34	HIS
2	b	437	HIS
2	b	582	ASN
1	1	76	HIS
1	1	224	ASN
1	1	296	HIS
1	1	432	HIS
1	1	488	HIS
1	1	608	HIS
2	2	34	HIS
2	2	317	HIS
2	2	373	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	437	HIS
2	2	582	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

357 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1218	-	36,53,73	2.83	14 (38%)	39,89,113	2.36	11 (28%)
11	CLA	a	1122	-	53,67,73	2.49	15 (28%)	59,105,113	2.37	16 (27%)
11	CLA	A	1101	-	59,73,73	2.32	15 (25%)	67,113,113	2.07	17 (25%)
11	CLA	b	1218	-	36,53,73	2.87	15 (41%)	39,89,113	2.30	9 (23%)
11	CLA	1	1801	15	46,60,73	2.67	15 (32%)	51,97,113	2.49	18 (35%)
11	CLA	A	1125	-	46,60,73	2.66	15 (32%)	51,97,113	2.60	19 (37%)
14	BCR	1	4008	-	41,41,41	2.72	6 (14%)	56,56,56	6.79	28 (50%)
11	CLA	b	1222	-	50,64,73	2.53	16 (32%)	56,102,113	2.49	18 (32%)
14	BCR	b	4010	-	41,41,41	2.79	6 (14%)	56,56,56	6.71	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1224	-	49,63,73	2.53	16 (32%)	55,101,113	2.46	17 (30%)
14	BCR	6	4020	-	41,41,41	2.86	7 (17%)	56,56,56	6.54	24 (42%)
11	CLA	K	1401	-	59,73,73	2.33	15 (25%)	67,113,113	2.22	18 (26%)
11	CLA	a	1124	-	49,63,73	2.56	16 (32%)	55,101,113	2.38	17 (30%)
11	CLA	1	1133	-	40,54,73	2.91	15 (37%)	44,90,113	2.36	13 (29%)
11	CLA	1	1139	-	44,58,73	2.72	16 (36%)	49,95,113	2.45	16 (32%)
15	LHG	1	5001	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
11	CLA	2	1208	-	36,53,73	2.86	14 (38%)	39,89,113	2.28	9 (23%)
11	CLA	1	1111	-	54,68,73	2.40	14 (25%)	61,107,113	2.32	20 (32%)
11	CLA	a	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.34	12 (27%)
14	BCR	a	4008	-	41,41,41	2.74	7 (17%)	56,56,56	6.57	29 (51%)
11	CLA	b	1213	-	59,73,73	2.35	16 (27%)	67,113,113	2.16	15 (22%)
15	LHG	a	5003	11	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	B	1210	-	59,73,73	2.35	15 (25%)	67,113,113	2.20	18 (26%)
14	BCR	b	4011	-	41,41,41	2.75	6 (14%)	56,56,56	6.79	25 (44%)
11	CLA	b	1240	-	36,53,73	2.89	15 (41%)	39,89,113	2.25	10 (25%)
11	CLA	a	1022	-	59,73,73	2.35	16 (27%)	67,113,113	2.16	16 (23%)
11	CLA	A	1120	-	40,54,73	2.91	16 (40%)	44,90,113	2.37	13 (29%)
11	CLA	8	1501	-	59,73,73	2.32	15 (25%)	67,113,113	2.25	18 (26%)
11	CLA	B	1216	-	59,73,73	2.34	15 (25%)	67,113,113	2.06	15 (22%)
11	CLA	B	1213	-	59,73,73	2.35	15 (25%)	67,113,113	2.15	16 (23%)
15	LHG	B	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.12	4 (7%)
11	CLA	1	1120	-	40,54,73	2.92	16 (40%)	44,90,113	2.39	13 (29%)
11	CLA	2	1217	-	41,55,73	2.77	15 (36%)	45,91,113	2.54	16 (35%)
13	SF4	3	3002	3	0,12,12	0.00	-	-		
14	BCR	2	4014	-	41,41,41	2.80	6 (14%)	56,56,56	6.44	23 (41%)
11	CLA	a	1237	-	49,63,73	2.55	15 (30%)	55,101,113	2.37	15 (27%)
14	BCR	b	4004	-	41,41,41	2.73	6 (14%)	56,56,56	6.57	26 (46%)
11	CLA	1	1108	-	36,53,73	2.88	15 (41%)	39,89,113	2.31	9 (23%)
14	BCR	1	4022	-	41,41,41	2.74	6 (14%)	56,56,56	6.41	26 (46%)
11	CLA	2	1204	-	59,73,73	2.34	15 (25%)	67,113,113	2.04	15 (22%)
11	CLA	B	1215	-	59,73,73	2.33	15 (25%)	67,113,113	2.31	17 (25%)
11	CLA	A	1133	-	40,54,73	2.87	15 (37%)	44,90,113	2.46	14 (31%)
14	BCR	7	4021	-	41,41,41	2.78	6 (14%)	56,56,56	6.61	21 (37%)
11	CLA	1	1138	-	40,54,73	2.88	15 (37%)	44,90,113	2.30	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	F	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.41	23 (41%)
11	CLA	b	1220	-	40,54,73	2.94	16 (40%)	44,90,113	2.35	13 (29%)
11	CLA	b	1216	-	59,73,73	2.36	16 (27%)	67,113,113	2.17	21 (31%)
11	CLA	b	1234	-	54,68,73	2.45	15 (27%)	61,107,113	2.28	16 (26%)
11	CLA	B	1207	-	59,73,73	2.31	14 (23%)	67,113,113	2.24	16 (23%)
14	BCR	B	4010	-	41,41,41	2.72	6 (14%)	56,56,56	6.41	26 (46%)
11	CLA	a	1103	-	59,73,73	2.36	16 (27%)	67,113,113	2.11	16 (23%)
11	CLA	1	1129	-	40,54,73	2.90	16 (40%)	44,90,113	2.40	12 (27%)
11	CLA	b	1239	-	40,54,73	2.90	15 (37%)	44,90,113	2.42	14 (31%)
11	CLA	1	1109	-	59,73,73	2.34	15 (25%)	67,113,113	2.17	16 (23%)
11	CLA	1	1132	-	59,73,73	2.32	15 (25%)	67,113,113	2.04	14 (20%)
11	CLA	A	1126	-	59,73,73	2.34	15 (25%)	67,113,113	2.21	17 (25%)
11	CLA	1	1103	-	59,73,73	2.32	15 (25%)	67,113,113	2.24	19 (28%)
14	BCR	a	4003	-	41,41,41	2.75	6 (14%)	56,56,56	6.20	26 (46%)
11	CLA	A	1109	11	59,73,73	2.36	15 (25%)	67,113,113	2.15	15 (22%)
11	CLA	B	1202	-	59,73,73	2.37	16 (27%)	67,113,113	2.15	15 (22%)
11	CLA	k	1402	-	44,58,73	2.73	15 (34%)	49,95,113	2.39	16 (32%)
11	CLA	B	1203	-	59,73,73	2.32	14 (23%)	67,113,113	2.07	14 (20%)
16	LMG	b	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.04	5 (7%)
11	CLA	8	1502	-	40,54,73	2.88	15 (37%)	44,90,113	2.44	14 (31%)
11	CLA	A	1119	-	59,73,73	2.31	15 (25%)	67,113,113	2.07	19 (28%)
11	CLA	A	1113	-	36,53,73	2.85	15 (41%)	39,89,113	2.36	12 (30%)
14	BCR	B	4011	-	41,41,41	2.81	7 (17%)	56,56,56	6.71	27 (48%)
11	CLA	L	1502	-	40,54,73	2.88	14 (35%)	44,90,113	2.40	12 (27%)
11	CLA	A	1131	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	18 (26%)
11	CLA	1	1022	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	a	1112	-	36,53,73	2.86	15 (41%)	39,89,113	2.27	11 (28%)
11	CLA	1	1123	-	59,73,73	2.35	16 (27%)	67,113,113	2.18	16 (23%)
11	CLA	a	1115	-	40,54,73	2.91	15 (37%)	44,90,113	2.26	13 (29%)
11	CLA	0	1401	-	59,73,73	2.33	15 (25%)	67,113,113	2.23	17 (25%)
11	CLA	b	1225	-	59,73,73	2.36	16 (27%)	67,113,113	2.12	15 (22%)
11	CLA	a	1012	-	59,73,73	2.37	16 (27%)	67,113,113	2.29	16 (23%)
11	CLA	1	1106	1	59,73,73	2.34	15 (25%)	67,113,113	2.08	17 (25%)
14	BCR	A	4001	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	A	1127	-	59,73,73	2.32	16 (27%)	67,113,113	2.18	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PQN	A	2001	-	34,34,34	1.65	2 (5%)	42,45,45	1.12	6 (14%)
11	CLA	A	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.27	12 (27%)
11	CLA	2	1221	-	48,62,73	2.59	16 (33%)	53,99,113	2.45	16 (30%)
11	CLA	B	1223	-	59,73,73	2.35	16 (27%)	67,113,113	2.24	19 (28%)
14	BCR	2	4011	-	41,41,41	2.80	6 (14%)	56,56,56	6.77	26 (46%)
11	CLA	a	1140	-	59,73,73	2.34	15 (25%)	67,113,113	2.16	16 (23%)
11	CLA	A	1134	1	40,54,73	2.89	15 (37%)	44,90,113	2.39	14 (31%)
11	CLA	1	1114	-	40,54,73	2.91	15 (37%)	44,90,113	2.34	12 (27%)
11	CLA	b	1235	-	54,68,73	2.47	16 (29%)	61,107,113	2.32	19 (31%)
11	CLA	a	1116	-	48,62,73	2.61	15 (31%)	53,99,113	2.32	16 (30%)
13	SF4	3	3003	-	0,12,12	0.00	-	-	-	-
11	CLA	A	1117	-	59,73,73	2.40	15 (25%)	67,113,113	2.10	16 (23%)
11	CLA	a	1119	-	59,73,73	2.32	15 (25%)	67,113,113	2.17	18 (26%)
11	CLA	B	1231	-	36,53,73	2.86	14 (38%)	39,89,113	2.52	14 (35%)
14	BCR	b	4014	-	41,41,41	2.74	6 (14%)	56,56,56	6.49	24 (42%)
13	SF4	a	3001	1,2	0,12,12	0.00	-	-	-	-
15	LHG	A	5003	11	48,48,48	0.95	2 (4%)	51,54,54	1.13	4 (7%)
11	CLA	2	1231	-	36,53,73	2.86	14 (38%)	39,89,113	2.48	15 (38%)
11	CLA	A	1128	-	59,73,73	2.31	14 (23%)	67,113,113	2.12	15 (22%)
11	CLA	B	1224	-	49,63,73	2.55	15 (30%)	55,101,113	2.44	16 (29%)
11	CLA	1	1137	-	59,73,73	2.35	15 (25%)	67,113,113	2.32	19 (28%)
14	BCR	f	4020	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	22 (39%)
11	CLA	1	1130	-	40,54,73	2.92	16 (40%)	44,90,113	2.24	11 (25%)
11	CLA	B	1206	2	59,73,73	2.30	15 (25%)	67,113,113	2.20	17 (25%)
14	BCR	b	4009	-	41,41,41	2.65	6 (14%)	56,56,56	6.93	25 (44%)
11	CLA	a	1102	11	59,73,73	2.34	16 (27%)	67,113,113	2.12	14 (20%)
15	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)
11	CLA	b	1219	-	49,63,73	2.60	15 (30%)	55,101,113	2.38	16 (29%)
11	CLA	a	1120	-	40,54,73	2.90	16 (40%)	44,90,113	2.47	13 (29%)
11	CLA	b	1230	-	52,66,73	2.53	16 (30%)	58,104,113	2.41	18 (31%)
11	CLA	0	1402	-	44,58,73	2.75	16 (36%)	49,95,113	2.35	12 (24%)
11	CLA	1	1124	-	49,63,73	2.56	16 (32%)	55,101,113	2.34	15 (27%)
14	BCR	A	4003	-	41,41,41	2.85	6 (14%)	56,56,56	6.29	24 (42%)
11	CLA	L	1503	-	59,73,73	2.30	14 (23%)	67,113,113	2.14	14 (20%)
11	CLA	B	1234	-	54,68,73	2.42	15 (27%)	61,107,113	2.32	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1106	1	59,73,73	2.34	16 (27%)	67,113,113	2.19	17 (25%)
11	CLA	2	1229	-	59,73,73	2.33	16 (27%)	67,113,113	2.11	16 (23%)
11	CLA	a	1801	15	46,60,73	2.68	15 (32%)	51,97,113	2.45	16 (31%)
11	CLA	B	1205	-	49,63,73	2.50	14 (28%)	55,101,113	2.56	15 (27%)
11	CLA	2	1201	-	48,62,73	2.60	15 (31%)	53,99,113	2.37	15 (28%)
11	CLA	a	1136	-	40,54,73	2.88	15 (37%)	44,90,113	2.35	11 (25%)
14	BCR	a	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.52	27 (48%)
11	CLA	2	1236	-	41,55,73	2.76	16 (39%)	45,91,113	2.52	13 (28%)
11	CLA	2	1219	-	49,63,73	2.61	16 (32%)	55,101,113	2.39	16 (29%)
11	CLA	1	1237	-	49,63,73	2.52	15 (30%)	55,101,113	2.33	18 (32%)
11	CLA	2	1212	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	12 (30%)
11	CLA	1	1135	-	45,59,73	2.68	16 (35%)	50,96,113	2.50	16 (32%)
11	CLA	1	1116	-	48,62,73	2.60	16 (33%)	53,99,113	2.36	17 (32%)
11	CLA	2	1232	-	36,53,73	2.87	15 (41%)	39,89,113	2.23	10 (25%)
14	BCR	L	4019	-	41,41,41	2.69	6 (14%)	56,56,56	6.58	25 (44%)
11	CLA	a	1117	-	59,73,73	2.36	15 (25%)	67,113,113	2.11	16 (23%)
11	CLA	b	1228	-	44,58,73	2.72	15 (34%)	49,95,113	2.43	14 (28%)
11	CLA	2	1227	-	36,53,73	2.84	14 (38%)	39,89,113	2.41	10 (25%)
11	CLA	A	1011	-	59,73,73	2.30	14 (23%)	67,113,113	2.24	18 (26%)
14	BCR	B	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.56	27 (48%)
11	CLA	b	1227	-	36,53,73	2.87	15 (41%)	39,89,113	2.45	12 (30%)
11	CLA	l	1501	7	59,73,73	2.35	16 (27%)	67,113,113	2.20	17 (25%)
11	CLA	a	1105	-	42,56,73	2.80	15 (35%)	46,92,113	2.49	14 (30%)
11	CLA	b	1201	-	48,62,73	2.60	15 (31%)	53,99,113	2.45	17 (32%)
11	CLA	B	1239	-	40,54,73	2.89	16 (40%)	44,90,113	2.38	11 (25%)
11	CLA	A	1237	-	49,63,73	2.55	15 (30%)	55,101,113	2.37	15 (27%)
11	CLA	B	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.38	12 (30%)
11	CLA	a	1118	-	55,69,73	2.39	14 (25%)	62,108,113	2.28	15 (24%)
11	CLA	A	1116	-	48,62,73	2.61	16 (33%)	53,99,113	2.34	17 (32%)
11	CLA	2	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.37	12 (30%)
11	CLA	k	1401	-	59,73,73	2.34	15 (25%)	67,113,113	2.23	18 (26%)
11	CLA	A	1022	-	59,73,73	2.32	15 (25%)	67,113,113	2.18	17 (25%)
14	BCR	M	4021	-	41,41,41	2.79	6 (14%)	56,56,56	6.58	21 (37%)
15	LHG	2	5004	11	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	2	1023	-	59,73,73	2.32	15 (25%)	67,113,113	2.34	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LHG	1	5003	11	48,48,48	0.96	2 (4%)	51,54,54	1.03	3 (5%)
11	CLA	b	1212	-	36,53,73	2.85	15 (41%)	39,89,113	2.43	9 (23%)
11	CLA	A	1106	1	59,73,73	2.33	15 (25%)	67,113,113	2.12	14 (20%)
14	BCR	a	4007	-	41,41,41	2.72	6 (14%)	56,56,56	6.74	25 (44%)
11	CLA	2	1238	-	59,73,73	2.35	16 (27%)	67,113,113	2.05	15 (22%)
11	CLA	a	1125	-	46,60,73	2.61	16 (34%)	51,97,113	2.34	16 (31%)
11	CLA	A	1801	15	46,60,73	2.70	15 (32%)	51,97,113	2.47	16 (31%)
11	CLA	b	1224	-	49,63,73	2.58	16 (32%)	55,101,113	2.41	16 (29%)
11	CLA	2	1214	-	53,67,73	2.46	15 (28%)	59,105,113	2.20	17 (28%)
11	CLA	B	1217	-	41,55,73	2.75	15 (36%)	45,91,113	2.45	13 (28%)
12	PQN	B	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.13	5 (11%)
14	BCR	2	4009	-	41,41,41	2.72	6 (14%)	56,56,56	6.76	25 (44%)
11	CLA	8	1503	-	59,73,73	2.37	16 (27%)	67,113,113	2.09	13 (19%)
13	SF4	c	3003	3	0,12,12	0.00	-	-	-	-
11	CLA	a	1133	-	40,54,73	2.89	15 (37%)	44,90,113	2.40	12 (27%)
11	CLA	a	1139	-	44,58,73	2.72	16 (36%)	49,95,113	2.49	15 (30%)
15	LHG	a	5001	-	48,48,48	0.96	2 (4%)	51,54,54	1.06	4 (7%)
11	CLA	a	1134	-	40,54,73	2.90	15 (37%)	44,90,113	2.38	15 (34%)
11	CLA	1	1127	-	59,73,73	2.36	15 (25%)	67,113,113	2.05	16 (23%)
11	CLA	1	1126	-	59,73,73	2.35	16 (27%)	67,113,113	2.17	19 (28%)
11	CLA	a	1107	1	59,73,73	2.32	15 (25%)	67,113,113	2.33	20 (29%)
14	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.31	24 (42%)
11	CLA	A	1129	-	40,54,73	2.88	15 (37%)	44,90,113	2.26	12 (27%)
11	CLA	K	1402	-	44,58,73	2.71	15 (34%)	49,95,113	2.37	14 (28%)
11	CLA	A	1115	-	40,54,73	2.91	16 (40%)	44,90,113	2.32	12 (27%)
14	BCR	B	4009	-	41,41,41	2.75	6 (14%)	56,56,56	6.71	22 (39%)
11	CLA	a	1113	-	36,53,73	2.87	15 (41%)	39,89,113	2.32	11 (28%)
11	CLA	a	1128	-	59,73,73	2.35	15 (25%)	67,113,113	2.15	17 (25%)
11	CLA	1	1122	-	53,67,73	2.48	16 (30%)	59,105,113	2.27	16 (27%)
11	CLA	a	1110	-	48,62,73	2.61	16 (33%)	53,99,113	2.36	17 (32%)
11	CLA	B	1212	-	36,53,73	2.87	15 (41%)	39,89,113	2.27	9 (23%)
11	CLA	L	1501	7	59,73,73	2.34	16 (27%)	67,113,113	2.11	15 (22%)
11	CLA	1	1140	-	59,73,73	2.36	16 (27%)	67,113,113	2.28	18 (26%)
14	BCR	b	4005	-	41,41,41	2.76	6 (14%)	56,56,56	6.58	25 (44%)
11	CLA	b	1215	-	59,73,73	2.36	15 (25%)	67,113,113	2.31	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	6	4018	-	41,41,41	2.87	7 (17%)	56,56,56	6.30	26 (46%)
11	CLA	A	1123	-	59,73,73	2.31	15 (25%)	67,113,113	2.24	17 (25%)
11	CLA	b	1226	-	59,73,73	2.32	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	a	1108	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	11 (28%)
11	CLA	2	1234	-	54,68,73	2.41	15 (27%)	61,107,113	2.23	16 (26%)
11	CLA	2	1213	-	59,73,73	2.40	16 (27%)	67,113,113	2.25	17 (25%)
13	SF4	1	3001	1,2	0,12,12	0.00	-	-		
14	BCR	b	4017	-	41,41,41	2.81	7 (17%)	56,56,56	6.66	28 (50%)
11	CLA	A	1130	-	40,54,73	2.90	16 (40%)	44,90,113	2.27	11 (25%)
11	CLA	B	1232	-	36,53,73	2.85	14 (38%)	39,89,113	2.37	10 (25%)
11	CLA	A	1012	-	59,73,73	2.34	16 (27%)	67,113,113	2.49	20 (29%)
11	CLA	A	1103	-	59,73,73	2.32	14 (23%)	67,113,113	2.11	17 (25%)
11	CLA	b	1238	-	59,73,73	2.34	15 (25%)	67,113,113	2.04	13 (19%)
11	CLA	a	1011	-	59,73,73	2.36	16 (27%)	67,113,113	2.26	17 (25%)
11	CLA	b	1204	-	59,73,73	2.32	15 (25%)	67,113,113	2.05	14 (20%)
11	CLA	b	1223	-	59,73,73	2.37	15 (25%)	67,113,113	2.10	17 (25%)
14	BCR	2	4005	-	41,41,41	2.73	6 (14%)	56,56,56	6.39	21 (37%)
11	CLA	b	1229	-	59,73,73	2.34	16 (27%)	67,113,113	2.07	17 (25%)
11	CLA	b	1023	-	59,73,73	2.31	15 (25%)	67,113,113	2.18	19 (28%)
11	CLA	a	1104	-	59,73,73	2.31	15 (25%)	67,113,113	2.12	18 (26%)
13	SF4	C	3003	3	0,12,12	0.00	-	-		
14	BCR	f	4013	-	41,41,41	2.76	6 (14%)	56,56,56	6.62	23 (41%)
14	BCR	2	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.83	28 (50%)
11	CLA	B	1222	-	50,64,73	2.58	15 (30%)	56,102,113	2.55	19 (33%)
14	BCR	A	4007	-	41,41,41	2.76	6 (14%)	56,56,56	6.80	22 (39%)
11	CLA	b	1232	-	36,53,73	2.88	15 (41%)	39,89,113	2.30	10 (25%)
11	CLA	A	1132	-	59,73,73	2.34	15 (25%)	67,113,113	2.24	14 (20%)
11	CLA	b	1231	-	36,53,73	2.85	15 (41%)	39,89,113	2.31	11 (28%)
13	SF4	C	3002	3	0,12,12	0.00	-	-		
14	BCR	A	4008	-	41,41,41	2.72	7 (17%)	56,56,56	6.70	30 (53%)
11	CLA	B	1236	-	41,55,73	2.71	15 (36%)	45,91,113	2.49	14 (31%)
11	CLA	l	1502	-	40,54,73	2.89	15 (37%)	44,90,113	2.43	13 (29%)
11	CLA	a	1126	-	59,73,73	2.36	15 (25%)	67,113,113	2.20	16 (23%)
11	CLA	B	1235	-	54,68,73	2.47	16 (29%)	61,107,113	2.24	13 (21%)
11	CLA	A	1104	-	59,73,73	2.27	14 (23%)	67,113,113	2.31	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1230	-	52,66,73	2.52	15 (28%)	58,104,113	2.38	18 (31%)
12	PQN	1	2001	-	34,34,34	1.66	2 (5%)	42,45,45	1.09	3 (7%)
11	CLA	2	1203	-	59,73,73	2.30	15 (25%)	67,113,113	2.15	18 (26%)
11	CLA	A	1137	-	59,73,73	2.36	16 (27%)	67,113,113	2.34	18 (26%)
11	CLA	1	1125	-	46,60,73	2.63	15 (32%)	51,97,113	2.41	18 (35%)
11	CLA	B	1021	-	59,73,73	2.28	15 (25%)	67,113,113	2.37	20 (29%)
11	CLA	A	1122	-	53,67,73	2.44	14 (26%)	59,105,113	2.38	17 (28%)
13	SF4	A	3001	1,2	0,12,12	0.00	-	-		
11	CLA	B	1221	-	48,62,73	2.58	16 (33%)	53,99,113	2.47	16 (30%)
14	BCR	1	4002	-	41,41,41	2.72	6 (14%)	56,56,56	6.93	23 (41%)
11	CLA	1	1101	-	59,73,73	2.32	15 (25%)	67,113,113	2.13	19 (28%)
12	PQN	a	2001	-	34,34,34	1.63	2 (5%)	42,45,45	1.04	4 (9%)
11	CLA	A	1138	-	40,54,73	2.86	15 (37%)	44,90,113	2.46	14 (31%)
11	CLA	b	1021	-	59,73,73	2.35	15 (25%)	67,113,113	2.32	23 (34%)
14	BCR	L	4022	-	41,41,41	2.69	6 (14%)	56,56,56	6.11	25 (44%)
11	CLA	2	1215	-	59,73,73	2.35	15 (25%)	67,113,113	2.33	19 (28%)
11	CLA	b	1207	-	59,73,73	2.32	15 (25%)	67,113,113	2.26	16 (23%)
14	BCR	1	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.55	27 (48%)
11	CLA	b	1214	-	53,67,73	2.46	16 (30%)	59,105,113	2.23	19 (32%)
11	CLA	1	1115	-	40,54,73	2.89	15 (37%)	44,90,113	2.41	12 (27%)
11	CLA	b	1013	-	59,73,73	2.35	15 (25%)	67,113,113	2.14	17 (25%)
11	CLA	1	1121	-	40,54,73	2.90	15 (37%)	44,90,113	2.37	13 (29%)
11	CLA	b	1217	-	41,55,73	2.78	16 (39%)	45,91,113	2.43	12 (26%)
14	BCR	8	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.65	24 (42%)
11	CLA	b	1205	-	49,63,73	2.53	15 (30%)	55,101,113	2.41	15 (27%)
11	CLA	A	1140	-	59,73,73	2.33	15 (25%)	67,113,113	2.24	16 (23%)
11	CLA	2	1225	-	59,73,73	2.34	15 (25%)	67,113,113	2.09	16 (23%)
11	CLA	a	1123	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	17 (25%)
11	CLA	B	1023	-	59,73,73	2.29	15 (25%)	67,113,113	2.23	20 (29%)
14	BCR	B	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	27 (48%)
11	CLA	b	1202	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	15 (22%)
11	CLA	2	1226	-	59,73,73	2.32	14 (23%)	67,113,113	2.22	16 (23%)
11	CLA	B	1238	-	59,73,73	2.32	14 (23%)	67,113,113	2.05	14 (20%)
11	CLA	A	1111	-	54,68,73	2.41	15 (27%)	61,107,113	2.22	16 (26%)
11	CLA	B	1204	-	59,73,73	2.30	14 (23%)	67,113,113	2.11	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1131	-	59,73,73	2.33	15 (25%)	67,113,113	2.15	18 (26%)
11	CLA	a	1135	-	45,59,73	2.67	15 (33%)	50,96,113	2.48	14 (28%)
11	CLA	1	1119	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	17 (25%)
14	BCR	B	4017	-	41,41,41	2.77	6 (14%)	56,56,56	6.60	31 (55%)
11	CLA	B	1226	-	59,73,73	2.30	14 (23%)	67,113,113	2.23	17 (25%)
11	CLA	A	1112	-	36,53,73	2.86	15 (41%)	39,89,113	2.41	11 (28%)
11	CLA	1	1118	-	55,69,73	2.39	15 (27%)	62,108,113	2.20	18 (29%)
11	CLA	2	1235	-	54,68,73	2.45	16 (29%)	61,107,113	2.22	20 (32%)
11	CLA	A	1124	-	49,63,73	2.56	15 (30%)	55,101,113	2.33	17 (30%)
11	CLA	1	1136	-	40,54,73	2.89	15 (37%)	44,90,113	2.32	11 (25%)
14	BCR	l	4019	-	41,41,41	2.75	6 (14%)	56,56,56	6.70	23 (41%)
11	CLA	2	1211	-	40,54,73	2.87	14 (35%)	44,90,113	2.38	12 (27%)
11	CLA	B	1214	-	53,67,73	2.45	16 (30%)	59,105,113	2.45	20 (33%)
11	CLA	B	1220	-	40,54,73	2.89	15 (37%)	44,90,113	2.24	11 (25%)
11	CLA	A	1136	-	40,54,73	2.88	15 (37%)	44,90,113	2.38	11 (25%)
11	CLA	a	1127	-	59,73,73	2.34	15 (25%)	67,113,113	2.28	20 (29%)
11	CLA	1	1110	-	48,62,73	2.60	15 (31%)	53,99,113	2.44	16 (30%)
14	BCR	F	4013	-	41,41,41	2.78	6 (14%)	56,56,56	6.78	21 (37%)
11	CLA	l	1503	-	59,73,73	2.33	16 (27%)	67,113,113	2.08	13 (19%)
11	CLA	A	1118	-	55,69,73	2.36	14 (25%)	62,108,113	2.31	15 (24%)
11	CLA	B	1218	-	36,53,73	2.86	14 (38%)	39,89,113	2.33	10 (25%)
14	BCR	8	4022	-	41,41,41	2.79	6 (14%)	56,56,56	6.49	31 (55%)
11	CLA	a	1132	-	59,73,73	2.35	16 (27%)	67,113,113	2.10	15 (22%)
11	CLA	1	1112	-	36,53,73	2.87	14 (38%)	39,89,113	2.35	13 (33%)
11	CLA	A	1139	-	44,58,73	2.71	16 (36%)	49,95,113	2.42	15 (30%)
11	CLA	2	1202	-	59,73,73	2.34	15 (25%)	67,113,113	2.14	17 (25%)
11	CLA	B	1208	-	36,53,73	2.87	14 (38%)	39,89,113	2.29	10 (25%)
11	CLA	B	1227	-	36,53,73	2.83	14 (38%)	39,89,113	2.53	12 (30%)
13	SF4	c	3002	3	0,12,12	0.00	-	-	-	-
11	CLA	1	1011	-	59,73,73	2.31	16 (27%)	67,113,113	2.52	18 (26%)
11	CLA	B	1228	-	44,58,73	2.73	15 (34%)	49,95,113	2.40	14 (28%)
11	CLA	B	1240	15	36,53,73	2.91	15 (41%)	39,89,113	2.32	11 (28%)
11	CLA	A	1135	-	45,59,73	2.66	15 (33%)	50,96,113	2.48	17 (34%)
11	CLA	1	1134	-	40,54,73	2.91	15 (37%)	44,90,113	2.35	13 (29%)
11	CLA	B	1219	-	49,63,73	2.57	16 (32%)	55,101,113	2.27	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1012	-	59,73,73	2.36	15 (25%)	67,113,113	2.39	20 (29%)
11	CLA	1	1104	-	59,73,73	2.32	15 (25%)	67,113,113	2.18	16 (23%)
11	CLA	2	1206	2	59,73,73	2.32	15 (25%)	67,113,113	2.16	16 (23%)
11	CLA	2	1240	15	36,53,73	2.88	14 (38%)	39,89,113	2.29	11 (28%)
11	CLA	2	1220	-	40,54,73	2.90	15 (37%)	44,90,113	2.35	12 (27%)
11	CLA	2	1239	-	40,54,73	2.93	15 (37%)	44,90,113	2.41	14 (31%)
11	CLA	A	1105	-	42,56,73	2.75	16 (38%)	46,92,113	2.39	14 (30%)
11	CLA	A	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.29	12 (27%)
11	CLA	A	1107	1	59,73,73	2.31	14 (23%)	67,113,113	2.21	18 (26%)
11	CLA	b	1208	-	36,53,73	2.88	14 (38%)	39,89,113	2.42	12 (30%)
11	CLA	a	1101	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	17 (25%)
16	LMG	B	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.07	4 (6%)
11	CLA	B	1013	-	59,73,73	2.32	15 (25%)	67,113,113	2.25	20 (29%)
11	CLA	B	1225	-	59,73,73	2.33	15 (25%)	67,113,113	2.11	17 (25%)
14	BCR	2	4010	-	41,41,41	2.84	6 (14%)	56,56,56	6.40	26 (46%)
14	BCR	1	4003	-	41,41,41	2.78	6 (14%)	56,56,56	6.39	27 (48%)
11	CLA	a	1111	-	54,68,73	2.40	16 (29%)	61,107,113	2.31	18 (29%)
11	CLA	2	1021	-	59,73,73	2.32	15 (25%)	67,113,113	2.32	20 (29%)
11	CLA	2	1223	-	59,73,73	2.35	16 (27%)	67,113,113	2.15	18 (26%)
11	CLA	B	1201	-	48,62,73	2.57	15 (31%)	53,99,113	2.49	18 (33%)
11	CLA	B	1211	-	40,54,73	2.86	15 (37%)	44,90,113	2.40	12 (27%)
14	BCR	a	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.59	26 (46%)
12	PQN	b	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.11	4 (9%)
12	PQN	2	2002	-	34,34,34	1.64	2 (5%)	42,45,45	1.08	6 (14%)
11	CLA	B	1230	-	52,66,73	2.50	15 (28%)	58,104,113	2.42	18 (31%)
11	CLA	b	1221	-	48,62,73	2.60	16 (33%)	53,99,113	2.51	17 (32%)
16	LMG	2	5002	-	55,55,55	0.91	2 (3%)	63,63,63	1.06	4 (6%)
11	CLA	b	1209	-	36,53,73	2.88	14 (38%)	39,89,113	2.38	11 (28%)
11	CLA	b	1203	-	59,73,73	2.34	16 (27%)	67,113,113	2.12	15 (22%)
11	CLA	2	1205	-	49,63,73	2.50	15 (30%)	55,101,113	2.46	14 (25%)
14	BCR	2	4004	-	41,41,41	2.71	6 (14%)	56,56,56	6.47	29 (51%)
14	BCR	b	4006	-	41,41,41	2.76	6 (14%)	56,56,56	6.93	27 (48%)
11	CLA	A	1108	-	36,53,73	2.85	14 (38%)	39,89,113	2.29	12 (30%)
14	BCR	1	4007	-	41,41,41	2.71	6 (14%)	56,56,56	6.67	26 (46%)
14	BCR	m	4021	-	41,41,41	2.84	6 (14%)	56,56,56	6.50	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	F	4018	-	41,41,41	2.91	7 (17%)	56,56,56	6.56	24 (42%)
11	CLA	1	1113	-	36,53,73	2.86	14 (38%)	39,89,113	2.34	10 (25%)
11	CLA	2	1210	-	59,73,73	2.31	15 (25%)	67,113,113	2.19	20 (29%)
11	CLA	a	1131	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	18 (26%)
11	CLA	1	1107	-	59,73,73	2.35	15 (25%)	67,113,113	2.21	15 (22%)
14	BCR	6	4013	-	41,41,41	2.69	6 (14%)	56,56,56	6.63	24 (42%)
11	CLA	a	1109	11	59,73,73	2.36	16 (27%)	67,113,113	2.16	16 (23%)
11	CLA	b	1236	-	41,55,73	2.76	16 (39%)	45,91,113	2.43	12 (26%)
14	BCR	B	4014	-	41,41,41	2.77	7 (17%)	56,56,56	6.29	25 (44%)
15	LHG	b	5004	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
14	BCR	2	4017	-	41,41,41	2.78	7 (17%)	56,56,56	6.54	29 (51%)
14	BCR	B	4005	-	41,41,41	2.79	7 (17%)	56,56,56	6.53	25 (44%)
11	CLA	a	1137	-	59,73,73	2.35	15 (25%)	67,113,113	2.24	18 (26%)
11	CLA	1	1105	-	42,56,73	2.77	15 (35%)	46,92,113	2.43	14 (30%)
11	CLA	2	1216	-	59,73,73	2.35	16 (27%)	67,113,113	2.20	16 (23%)
11	CLA	1	1102	-	59,73,73	2.36	16 (27%)	67,113,113	2.03	12 (17%)
11	CLA	b	1206	2	59,73,73	2.32	15 (25%)	67,113,113	2.18	18 (26%)
11	CLA	1	1117	-	59,73,73	2.35	15 (25%)	67,113,113	2.13	17 (25%)
11	CLA	A	1102	11	59,73,73	2.35	16 (27%)	67,113,113	2.17	18 (26%)
11	CLA	a	1129	-	40,54,73	2.89	15 (37%)	44,90,113	2.41	12 (27%)
11	CLA	2	1013	-	59,73,73	2.34	15 (25%)	67,113,113	2.20	18 (26%)
11	CLA	2	1207	-	59,73,73	2.31	15 (25%)	67,113,113	2.26	18 (26%)
11	CLA	b	1211	-	40,54,73	2.90	16 (40%)	44,90,113	2.37	13 (29%)
11	CLA	2	1228	-	44,58,73	2.71	16 (36%)	49,95,113	2.46	15 (30%)
11	CLA	a	1130	-	40,54,73	2.92	15 (37%)	44,90,113	2.28	13 (29%)
11	CLA	B	1229	-	59,73,73	2.33	15 (25%)	67,113,113	2.15	17 (25%)
14	BCR	f	4018	-	41,41,41	2.85	7 (17%)	56,56,56	6.36	24 (42%)
11	CLA	a	1138	-	40,54,73	2.89	15 (37%)	44,90,113	2.44	16 (36%)
11	CLA	b	1210	-	59,73,73	2.36	16 (27%)	67,113,113	2.13	20 (29%)
11	CLA	2	1222	-	50,64,73	2.54	16 (32%)	56,102,113	2.38	17 (30%)
11	CLA	A	1110	-	48,62,73	2.61	15 (31%)	53,99,113	2.46	16 (30%)
11	CLA	1	1128	-	59,73,73	2.33	15 (25%)	67,113,113	2.09	16 (23%)
11	CLA	a	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.38	13 (29%)

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
11	CLA	2	1218	-	3/3/16/25	4/11/111/135	-
11	CLA	a	1122	-	3/3/18/25	14/30/128/135	-
11	CLA	A	1101	-	2/2/20/25	19/37/135/135	-
11	CLA	b	1218	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1801	15	3/3/17/25	13/22/120/135	-
11	CLA	A	1125	-	2/2/17/25	9/22/120/135	-
14	BCR	1	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1222	-	3/3/18/25	12/27/125/135	-
14	BCR	b	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1224	-	3/3/18/25	8/25/123/135	-
11	CLA	K	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	a	1124	-	3/3/18/25	8/25/123/135	-
11	CLA	1	1133	-	3/3/16/25	8/15/113/135	-
11	CLA	1	1139	-	3/3/17/25	10/19/117/135	-
15	LHG	1	5001	-	-	26/53/53/53	-
11	CLA	2	1208	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1111	-	3/3/19/25	18/31/129/135	-
11	CLA	a	1114	-	2/2/16/25	6/15/113/135	-
14	BCR	a	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	b	1213	-	3/3/20/25	13/37/135/135	-
15	LHG	a	5003	11	-	25/53/53/53	-
11	CLA	B	1210	-	3/3/20/25	27/37/135/135	-
14	BCR	b	4011	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1240	-	3/3/16/25	7/11/111/135	-
11	CLA	a	1022	-	2/2/20/25	12/37/135/135	-
11	CLA	A	1120	-	3/3/16/25	6/15/113/135	-
11	CLA	8	1501	-	3/3/20/25	18/37/135/135	-
11	CLA	B	1216	-	3/3/20/25	8/37/135/135	-
11	CLA	B	1213	-	3/3/20/25	18/37/135/135	-
15	LHG	B	5004	11	-	25/53/53/53	-
11	CLA	1	1120	-	3/3/16/25	9/15/113/135	-
11	CLA	2	1217	-	3/3/16/25	14/16/114/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	3	3002	3	-	-	0/6/5/5
14	BCR	2	4014	-	-	14/29/63/63	0/2/2/2
11	CLA	a	1237	-	3/3/18/25	10/25/123/135	-
14	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
11	CLA	1	1108	-	3/3/16/25	3/11/111/135	-
14	BCR	l	4022	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1204	-	2/2/20/25	11/37/135/135	-
11	CLA	B	1215	-	2/2/20/25	16/37/135/135	-
11	CLA	A	1133	-	3/3/16/25	4/15/113/135	-
14	BCR	7	4021	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1138	-	3/3/16/25	6/15/113/135	-
14	BCR	F	4020	-	-	12/29/63/63	0/2/2/2
11	CLA	b	1220	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1216	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1136	-	3/3/16/25	10/15/113/135	-
11	CLA	b	1234	-	3/3/19/25	16/31/129/135	-
11	CLA	B	1207	-	2/2/20/25	12/37/135/135	-
14	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1103	-	3/3/20/25	19/37/135/135	-
11	CLA	1	1129	-	3/3/16/25	6/15/113/135	-
11	CLA	b	1239	-	3/3/16/25	7/15/113/135	-
11	CLA	1	1109	-	2/2/20/25	15/37/135/135	-
11	CLA	1	1132	-	3/3/20/25	11/37/135/135	-
11	CLA	A	1126	-	3/3/20/25	12/37/135/135	-
11	CLA	1	1103	-	3/3/20/25	21/37/135/135	-
14	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
11	CLA	A	1109	11	2/2/20/25	13/37/135/135	-
11	CLA	B	1202	-	3/3/20/25	19/37/135/135	-
11	CLA	k	1402	-	3/3/17/25	7/19/117/135	-
11	CLA	B	1203	-	1/1/20/25	15/37/135/135	-
16	LMG	b	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	8	1502	-	3/3/16/25	4/15/113/135	-
11	CLA	A	1119	-	3/3/20/25	17/37/135/135	-
11	CLA	A	1113	-	3/3/16/25	5/11/111/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	L	1502	-	3/3/16/25	5/15/113/135	-
11	CLA	A	1131	-	2/2/20/25	15/37/135/135	-
11	CLA	1	1022	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1112	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1123	-	2/2/20/25	14/37/135/135	-
11	CLA	a	1115	-	2/2/16/25	6/15/113/135	-
11	CLA	0	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	b	1225	-	3/3/20/25	14/37/135/135	-
11	CLA	a	1012	-	2/2/20/25	20/37/135/135	-
11	CLA	1	1106	1	2/2/20/25	23/37/135/135	-
14	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1127	-	3/3/20/25	13/37/135/135	-
12	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
11	CLA	A	1114	-	3/3/16/25	7/15/113/135	-
11	CLA	2	1221	-	3/3/17/25	6/24/122/135	-
11	CLA	B	1223	-	2/2/20/25	9/37/135/135	-
14	BCR	2	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1140	-	3/3/20/25	14/37/135/135	-
11	CLA	A	1134	1	3/3/16/25	9/15/113/135	-
11	CLA	1	1114	-	3/3/16/25	10/15/113/135	-
11	CLA	b	1235	-	3/3/19/25	16/31/129/135	-
11	CLA	a	1116	-	3/3/17/25	9/24/122/135	-
13	SF4	3	3003	-	-	-	0/6/5/5
11	CLA	A	1117	-	3/3/20/25	13/37/135/135	-
11	CLA	a	1119	-	3/3/20/25	16/37/135/135	-
11	CLA	B	1231	-	3/3/16/25	7/11/111/135	-
14	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
13	SF4	a	3001	1,2	-	-	0/6/5/5
15	LHG	A	5003	11	-	31/53/53/53	-
11	CLA	2	1231	-	3/3/16/25	5/11/111/135	-
11	CLA	A	1128	-	3/3/20/25	12/37/135/135	-
11	CLA	B	1224	-	3/3/18/25	11/25/123/135	-
11	CLA	1	1137	-	3/3/20/25	18/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	f	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	1	1130	-	1/1/16/25	5/15/113/135	-
11	CLA	B	1206	2	2/2/20/25	13/37/135/135	-
14	BCR	b	4009	-	-	14/29/63/63	0/2/2/2
11	CLA	a	1102	11	3/3/20/25	13/37/135/135	-
15	LHG	A	5001	-	-	31/53/53/53	-
11	CLA	b	1219	-	3/3/18/25	8/25/123/135	-
11	CLA	a	1120	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1230	-	3/3/18/25	12/29/127/135	-
11	CLA	0	1402	-	3/3/17/25	5/19/117/135	-
11	CLA	1	1124	-	3/3/18/25	12/25/123/135	-
14	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
11	CLA	L	1503	-	2/2/20/25	13/37/135/135	-
11	CLA	B	1234	-	3/3/19/25	14/31/129/135	-
11	CLA	a	1106	1	3/3/20/25	19/37/135/135	-
11	CLA	2	1229	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1801	15	3/3/17/25	11/22/120/135	-
11	CLA	B	1205	-	3/3/18/25	9/25/123/135	-
11	CLA	2	1201	-	3/3/17/25	8/24/122/135	-
11	CLA	a	1136	-	3/3/16/25	6/15/113/135	-
14	BCR	a	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	2	1236	-	3/3/16/25	8/16/114/135	-
11	CLA	2	1219	-	3/3/18/25	12/25/123/135	-
11	CLA	1	1237	-	3/3/18/25	9/25/123/135	-
11	CLA	2	1212	-	3/3/16/25	3/11/111/135	-
11	CLA	A	1012	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1116	-	3/3/17/25	9/24/122/135	-
11	CLA	2	1232	-	2/2/16/25	3/11/111/135	-
14	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1117	-	3/3/20/25	18/37/135/135	-
11	CLA	b	1228	-	3/3/17/25	6/19/117/135	-
11	CLA	2	1227	-	2/2/16/25	6/11/111/135	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
11	CLA	b	1227	-	2/2/16/25	5/11/111/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	l	1501	7	2/2/20/25	16/37/135/135	-
11	CLA	a	1105	-	3/3/16/25	8/17/115/135	-
11	CLA	2	1235	-	3/3/19/25	17/31/129/135	-
11	CLA	b	1201	-	3/3/17/25	9/24/122/135	-
11	CLA	B	1239	-	3/3/16/25	10/15/113/135	-
11	CLA	A	1237	-	3/3/18/25	12/25/123/135	-
11	CLA	a	1134	-	3/3/16/25	8/15/113/135	-
11	CLA	a	1118	-	3/3/19/25	10/33/131/135	-
11	CLA	A	1116	-	3/3/17/25	8/24/122/135	-
11	CLA	2	1209	-	3/3/16/25	2/11/111/135	-
11	CLA	k	1401	-	3/3/20/25	19/37/135/135	-
11	CLA	A	1022	-	2/2/20/25	13/37/135/135	-
14	BCR	M	4021	-	-	8/29/63/63	0/2/2/2
15	LHG	2	5004	11	-	28/53/53/53	-
11	CLA	2	1023	-	3/3/20/25	15/37/135/135	-
15	LHG	1	5003	11	-	32/53/53/53	-
11	CLA	b	1212	-	3/3/16/25	5/11/111/135	-
11	CLA	A	1106	1	3/3/20/25	16/37/135/135	-
14	BCR	a	4007	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1238	-	3/3/20/25	12/37/135/135	-
11	CLA	a	1125	-	2/2/17/25	8/22/120/135	-
11	CLA	A	1801	15	3/3/17/25	14/22/120/135	-
11	CLA	b	1224	-	3/3/18/25	12/25/123/135	-
11	CLA	2	1214	-	3/3/18/25	11/30/128/135	-
11	CLA	B	1217	-	3/3/16/25	12/16/114/135	-
12	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
14	BCR	2	4009	-	-	15/29/63/63	0/2/2/2
11	CLA	8	1503	-	3/3/20/25	12/37/135/135	-
13	SF4	c	3003	3	-	-	0/6/5/5
14	BCR	6	4020	-	-	15/29/63/63	0/2/2/2
14	BCR	l	4019	-	-	17/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	30/53/53/53	-
11	CLA	B	1209	-	3/3/16/25	4/11/111/135	-
11	CLA	1	1127	-	3/3/20/25	15/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1126	-	3/3/20/25	20/37/135/135	-
11	CLA	a	1107	1	3/3/20/25	9/37/135/135	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1129	-	3/3/16/25	6/15/113/135	-
11	CLA	K	1402	-	3/3/17/25	8/19/117/135	-
11	CLA	A	1115	-	3/3/16/25	7/15/113/135	-
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
11	CLA	a	1113	-	3/3/16/25	4/11/111/135	-
11	CLA	a	1128	-	3/3/20/25	11/37/135/135	-
11	CLA	1	1122	-	3/3/18/25	18/30/128/135	-
11	CLA	a	1110	-	2/2/17/25	11/24/122/135	-
11	CLA	B	1212	-	3/3/16/25	5/11/111/135	-
11	CLA	L	1501	7	3/3/20/25	13/37/135/135	-
11	CLA	1	1140	-	3/3/20/25	15/37/135/135	-
14	BCR	b	4005	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1215	-	2/2/20/25	14/37/135/135	-
14	BCR	6	4018	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1123	-	2/2/20/25	17/37/135/135	-
11	CLA	b	1226	-	3/3/20/25	13/37/135/135	-
11	CLA	a	1108	-	3/3/16/25	2/11/111/135	-
11	CLA	2	1234	-	2/2/19/25	18/31/129/135	-
11	CLA	2	1213	-	3/3/20/25	18/37/135/135	-
13	SF4	1	3001	1,2	-	-	0/6/5/5
14	BCR	b	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	A	1130	-	2/2/16/25	5/15/113/135	-
11	CLA	B	1232	-	3/3/16/25	3/11/111/135	-
11	CLA	1	1135	-	2/2/17/25	9/21/119/135	-
11	CLA	A	1103	-	3/3/20/25	17/37/135/135	-
11	CLA	b	1238	-	3/3/20/25	12/37/135/135	-
11	CLA	a	1011	-	1/1/20/25	11/37/135/135	-
11	CLA	b	1204	-	2/2/20/25	16/37/135/135	-
11	CLA	b	1223	-	3/3/20/25	19/37/135/135	-
14	BCR	2	4005	-	-	9/29/63/63	0/2/2/2
11	CLA	b	1229	-	3/3/20/25	24/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1023	-	3/3/20/25	17/37/135/135	-
11	CLA	a	1104	-	3/3/20/25	15/37/135/135	-
13	SF4	C	3003	3	-	-	0/6/5/5
14	BCR	f	4013	-	-	17/29/63/63	0/2/2/2
14	BCR	2	4006	-	-	13/29/63/63	0/2/2/2
11	CLA	B	1222	-	3/3/18/25	15/27/125/135	-
14	BCR	A	4007	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1232	-	3/3/16/25	4/11/111/135	-
11	CLA	A	1132	-	3/3/20/25	16/37/135/135	-
11	CLA	b	1231	-	3/3/16/25	6/11/111/135	-
13	SF4	C	3002	3	-	-	0/6/5/5
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	B	1236	-	3/3/16/25	6/16/114/135	-
11	CLA	l	1502	-	3/3/16/25	3/15/113/135	-
11	CLA	a	1126	-	3/3/20/25	18/37/135/135	-
11	CLA	B	1235	-	3/3/19/25	14/31/129/135	-
11	CLA	A	1104	-	3/3/20/25	21/37/135/135	-
11	CLA	2	1230	-	2/2/18/25	7/29/127/135	-
12	PQN	1	2001	-	-	7/23/43/43	0/2/2/2
11	CLA	2	1203	-	3/3/20/25	17/37/135/135	-
11	CLA	A	1137	-	3/3/20/25	14/37/135/135	-
11	CLA	1	1125	-	2/2/17/25	9/22/120/135	-
11	CLA	B	1021	-	3/3/20/25	23/37/135/135	-
11	CLA	A	1122	-	3/3/18/25	8/30/128/135	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
11	CLA	B	1221	-	3/3/17/25	9/24/122/135	-
14	BCR	1	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1101	-	2/2/20/25	19/37/135/135	-
12	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
11	CLA	A	1138	-	3/3/16/25	2/15/113/135	-
11	CLA	b	1021	-	3/3/20/25	25/37/135/135	-
14	BCR	L	4022	-	-	12/29/63/63	0/2/2/2
11	CLA	2	1215	-	3/3/20/25	16/37/135/135	-
11	CLA	b	1207	-	2/2/20/25	16/37/135/135	-
14	BCR	1	4001	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1214	-	3/3/18/25	10/30/128/135	-
11	CLA	1	1115	-	2/2/16/25	4/15/113/135	-
11	CLA	b	1013	-	1/1/20/25	10/37/135/135	-
11	CLA	1	1121	-	2/2/16/25	6/15/113/135	-
11	CLA	b	1217	-	3/3/16/25	7/16/114/135	-
14	BCR	8	4019	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1205	-	3/3/18/25	8/25/123/135	-
11	CLA	A	1140	-	2/2/20/25	18/37/135/135	-
11	CLA	2	1225	-	3/3/20/25	10/37/135/135	-
11	CLA	a	1123	-	2/2/20/25	15/37/135/135	-
11	CLA	B	1023	-	3/3/20/25	15/37/135/135	-
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	b	1202	-	3/3/20/25	18/37/135/135	-
11	CLA	2	1226	-	3/3/20/25	12/37/135/135	-
11	CLA	B	1238	-	3/3/20/25	13/37/135/135	-
11	CLA	A	1111	-	3/3/19/25	16/31/129/135	-
11	CLA	B	1204	-	2/2/20/25	14/37/135/135	-
11	CLA	1	1131	-	2/2/20/25	20/37/135/135	-
11	CLA	a	1135	-	2/2/17/25	7/21/119/135	-
11	CLA	1	1119	-	3/3/20/25	18/37/135/135	-
14	BCR	B	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	B	1226	-	3/3/20/25	13/37/135/135	-
11	CLA	A	1112	-	3/3/16/25	6/11/111/135	-
11	CLA	1	1118	-	3/3/19/25	17/33/131/135	-
11	CLA	a	1133	-	3/3/16/25	4/15/113/135	-
11	CLA	A	1124	-	3/3/18/25	12/25/123/135	-
11	CLA	A	1011	-	2/2/20/25	17/37/135/135	-
11	CLA	a	1139	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1211	-	3/3/16/25	9/15/113/135	-
11	CLA	B	1214	-	3/3/18/25	13/30/128/135	-
11	CLA	B	1220	-	1/1/16/25	8/15/113/135	-
11	CLA	A	1136	-	3/3/16/25	6/15/113/135	-
11	CLA	a	1127	-	3/3/20/25	14/37/135/135	-
11	CLA	1	1110	-	2/2/17/25	14/24/122/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	F	4013	-	-	15/29/63/63	0/2/2/2
11	CLA	l	1503	-	2/2/20/25	16/37/135/135	-
11	CLA	A	1118	-	3/3/19/25	17/33/131/135	-
11	CLA	B	1218	-	3/3/16/25	3/11/111/135	-
14	BCR	8	4022	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1132	-	3/3/20/25	15/37/135/135	-
11	CLA	1	1112	-	3/3/16/25	3/11/111/135	-
11	CLA	A	1139	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1202	-	3/3/20/25	15/37/135/135	-
11	CLA	B	1208	-	2/2/16/25	5/11/111/135	-
11	CLA	B	1227	-	3/3/16/25	4/11/111/135	-
13	SF4	c	3002	3	-	-	0/6/5/5
11	CLA	1	1011	-	1/1/20/25	15/37/135/135	-
11	CLA	2	1013	-	1/1/20/25	14/37/135/135	-
11	CLA	B	1240	15	3/3/16/25	6/11/111/135	-
11	CLA	A	1135	-	3/3/17/25	8/21/119/135	-
11	CLA	1	1134	-	3/3/16/25	7/15/113/135	-
11	CLA	B	1219	-	3/3/18/25	10/25/123/135	-
11	CLA	1	1012	-	2/2/20/25	18/37/135/135	-
11	CLA	1	1104	-	2/2/20/25	14/37/135/135	-
11	CLA	2	1206	2	3/3/20/25	19/37/135/135	-
11	CLA	2	1240	15	3/3/16/25	3/11/111/135	-
11	CLA	2	1220	-	2/2/16/25	7/15/113/135	-
11	CLA	2	1239	-	3/3/16/25	12/15/113/135	-
11	CLA	A	1105	-	3/3/16/25	5/17/115/135	-
11	CLA	A	1121	-	3/3/16/25	5/15/113/135	-
11	CLA	A	1107	1	3/3/20/25	13/37/135/135	-
11	CLA	b	1208	-	3/3/16/25	2/11/111/135	-
11	CLA	a	1101	-	2/2/20/25	17/37/135/135	-
16	LMG	B	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	2	1228	-	3/3/17/25	3/19/117/135	-
11	CLA	B	1225	-	3/3/20/25	11/37/135/135	-
14	BCR	2	4010	-	-	11/29/63/63	0/2/2/2
14	BCR	1	4003	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1111	-	3/3/19/25	18/31/129/135	-
11	CLA	2	1021	-	3/3/20/25	21/37/135/135	-
11	CLA	2	1223	-	3/3/20/25	16/37/135/135	-
11	CLA	B	1201	-	3/3/17/25	8/24/122/135	-
11	CLA	B	1211	-	3/3/16/25	6/15/113/135	-
14	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
12	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
12	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	B	1230	-	2/2/18/25	8/29/127/135	-
11	CLA	b	1221	-	3/3/17/25	7/24/122/135	-
16	LMG	2	5002	-	-	30/50/70/70	0/1/1/1
11	CLA	b	1209	-	3/3/16/25	5/11/111/135	-
11	CLA	b	1203	-	3/3/20/25	12/37/135/135	-
11	CLA	2	1205	-	3/3/18/25	7/25/123/135	-
14	BCR	2	4004	-	-	10/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1108	-	3/3/16/25	3/11/111/135	-
14	BCR	1	4007	-	-	12/29/63/63	0/2/2/2
14	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
14	BCR	F	4018	-	-	5/29/63/63	0/2/2/2
11	CLA	1	1113	-	3/3/16/25	3/11/111/135	-
11	CLA	2	1210	-	3/3/20/25	15/37/135/135	-
11	CLA	a	1131	-	3/3/20/25	16/37/135/135	-
11	CLA	1	1107	-	3/3/20/25	14/37/135/135	-
14	BCR	6	4013	-	-	16/29/63/63	0/2/2/2
11	CLA	a	1109	11	2/2/20/25	19/37/135/135	-
11	CLA	b	1236	-	3/3/16/25	7/16/114/135	-
14	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
15	LHG	b	5004	-	-	26/53/53/53	-
14	BCR	2	4017	-	-	6/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
11	CLA	a	1137	-	3/3/20/25	12/37/135/135	-
11	CLA	1	1105	-	3/3/16/25	5/17/115/135	-
11	CLA	2	1216	-	3/3/20/25	17/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1102	-	3/3/20/25	15/37/135/135	-
11	CLA	b	1206	2	3/3/20/25	16/37/135/135	-
11	CLA	1	1117	-	3/3/20/25	16/37/135/135	-
11	CLA	A	1102	11	2/2/20/25	19/37/135/135	-
11	CLA	a	1129	-	3/3/16/25	7/15/113/135	-
11	CLA	B	1228	-	3/3/17/25	7/19/117/135	-
11	CLA	2	1207	-	1/1/20/25	13/37/135/135	-
11	CLA	b	1211	-	3/3/16/25	4/15/113/135	-
11	CLA	B	1013	-	2/2/20/25	18/37/135/135	-
11	CLA	a	1130	-	2/2/16/25	7/15/113/135	-
11	CLA	B	1229	-	2/2/20/25	24/37/135/135	-
14	BCR	f	4018	-	-	6/29/63/63	0/2/2/2
11	CLA	a	1138	-	3/3/16/25	8/15/113/135	-
11	CLA	b	1210	-	3/3/20/25	20/37/135/135	-
11	CLA	2	1222	-	3/3/18/25	11/27/125/135	-
11	CLA	A	1110	-	3/3/17/25	11/24/122/135	-
11	CLA	1	1128	-	3/3/20/25	13/37/135/135	-
11	CLA	a	1121	-	3/3/16/25	5/15/113/135	-

All (4528) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1125	CLA	MG-NA	9.70	2.29	2.06
11	a	1103	CLA	MG-NA	9.70	2.29	2.06
11	B	1223	CLA	MG-NA	9.65	2.29	2.06
11	b	1223	CLA	MG-NA	9.64	2.29	2.06
11	a	1139	CLA	MG-NA	9.64	2.29	2.06
11	1	1123	CLA	MG-NA	9.63	2.29	2.06
11	A	1120	CLA	MG-NA	9.63	2.29	2.06
11	b	1221	CLA	MG-NA	9.63	2.29	2.06
11	b	1220	CLA	MG-NA	9.61	2.29	2.06
11	1	1012	CLA	MG-NA	9.61	2.29	2.06
11	2	1216	CLA	MG-NA	9.61	2.29	2.06
11	1	1011	CLA	MG-NA	9.60	2.29	2.06
11	1	1120	CLA	MG-NA	9.59	2.29	2.06
11	2	1219	CLA	MG-NA	9.59	2.29	2.06
11	a	1012	CLA	MG-NA	9.59	2.29	2.06
11	b	1225	CLA	MG-NA	9.59	2.29	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1214	CLA	MG-NA	9.59	2.29	2.06
11	1	1110	CLA	MG-NA	9.59	2.29	2.06
11	b	1230	CLA	MG-NA	9.58	2.29	2.06
11	A	1110	CLA	MG-NA	9.58	2.29	2.06
11	a	1121	CLA	MG-NA	9.57	2.29	2.06
11	A	1112	CLA	MG-NA	9.57	2.29	2.06
11	1	1102	CLA	MG-NA	9.57	2.29	2.06
11	b	1234	CLA	MG-NA	9.57	2.29	2.06
11	1	1135	CLA	MG-NA	9.57	2.29	2.06
11	2	1232	CLA	MG-NA	9.56	2.29	2.06
11	A	1123	CLA	MG-NA	9.56	2.29	2.06
11	B	1240	CLA	MG-NA	9.55	2.29	2.06
11	a	1123	CLA	MG-NA	9.55	2.29	2.06
11	2	1212	CLA	MG-NA	9.55	2.29	2.06
11	2	1209	CLA	MG-NA	9.55	2.28	2.06
11	A	1114	CLA	MG-NA	9.54	2.28	2.06
11	2	1240	CLA	MG-NA	9.54	2.28	2.06
11	2	1221	CLA	MG-NA	9.54	2.28	2.06
11	b	1219	CLA	MG-NA	9.54	2.28	2.06
11	b	1021	CLA	MG-NA	9.54	2.28	2.06
11	b	1208	CLA	MG-NA	9.54	2.28	2.06
11	a	1022	CLA	MG-NA	9.54	2.28	2.06
11	2	1206	CLA	MG-NA	9.54	2.28	2.06
11	B	1209	CLA	MG-NA	9.53	2.28	2.06
11	1	1022	CLA	MG-NA	9.53	2.28	2.06
11	1	1140	CLA	MG-NA	9.53	2.28	2.06
11	1	1139	CLA	MG-NA	9.53	2.28	2.06
11	b	1240	CLA	MG-NA	9.52	2.28	2.06
11	a	1113	CLA	MG-NA	9.52	2.28	2.06
11	a	1011	CLA	MG-NA	9.52	2.28	2.06
11	2	1223	CLA	MG-NA	9.52	2.28	2.06
11	A	1134	CLA	MG-NA	9.52	2.28	2.06
11	b	1215	CLA	MG-NA	9.52	2.28	2.06
11	B	1220	CLA	MG-NA	9.51	2.28	2.06
11	1	1126	CLA	MG-NA	9.51	2.28	2.06
11	1	1115	CLA	MG-NA	9.51	2.28	2.06
11	b	1203	CLA	MG-NA	9.51	2.28	2.06
11	B	1221	CLA	MG-NA	9.50	2.28	2.06
11	a	1107	CLA	MG-NA	9.50	2.28	2.06
11	2	1239	CLA	MG-NA	9.50	2.28	2.06
11	A	1116	CLA	MG-NA	9.50	2.28	2.06
11	1	1121	CLA	MG-NA	9.50	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1503	CLA	MG-NA	9.50	2.28	2.06
11	B	1225	CLA	MG-NA	9.50	2.28	2.06
11	2	1220	CLA	MG-NA	9.50	2.28	2.06
11	a	1126	CLA	MG-NA	9.50	2.28	2.06
11	A	1801	CLA	MG-NA	9.50	2.28	2.06
11	1	1113	CLA	MG-NA	9.50	2.28	2.06
11	b	1224	CLA	MG-NA	9.50	2.28	2.06
11	k	1401	CLA	MG-NA	9.50	2.28	2.06
11	a	1125	CLA	MG-NA	9.50	2.28	2.06
11	L	1501	CLA	MG-NA	9.49	2.28	2.06
11	a	1120	CLA	MG-NA	9.49	2.28	2.06
11	2	1235	CLA	MG-NA	9.49	2.28	2.06
11	2	1222	CLA	MG-NA	9.49	2.28	2.06
11	a	1101	CLA	MG-NA	9.49	2.28	2.06
11	a	1801	CLA	MG-NA	9.49	2.28	2.06
11	b	1217	CLA	MG-NA	9.49	2.28	2.06
11	a	1105	CLA	MG-NA	9.49	2.28	2.06
11	b	1216	CLA	MG-NA	9.49	2.28	2.06
11	l	1501	CLA	MG-NA	9.48	2.28	2.06
11	a	1114	CLA	MG-NA	9.48	2.28	2.06
11	2	1225	CLA	MG-NA	9.48	2.28	2.06
11	A	1139	CLA	MG-NA	9.48	2.28	2.06
11	B	1231	CLA	MG-NA	9.48	2.28	2.06
11	b	1227	CLA	MG-NA	9.48	2.28	2.06
11	a	1115	CLA	MG-NA	9.48	2.28	2.06
11	b	1211	CLA	MG-NA	9.48	2.28	2.06
11	K	1401	CLA	MG-NA	9.48	2.28	2.06
11	2	1230	CLA	MG-NA	9.48	2.28	2.06
11	2	1231	CLA	MG-NA	9.47	2.28	2.06
11	B	1232	CLA	MG-NA	9.47	2.28	2.06
11	a	1127	CLA	MG-NA	9.47	2.28	2.06
11	B	1229	CLA	MG-NA	9.47	2.28	2.06
11	b	1235	CLA	MG-NA	9.47	2.28	2.06
11	A	1121	CLA	MG-NA	9.47	2.28	2.06
11	b	1239	CLA	MG-NA	9.47	2.28	2.06
11	0	1401	CLA	MG-NA	9.47	2.28	2.06
11	a	1108	CLA	MG-NA	9.47	2.28	2.06
11	b	1228	CLA	MG-NA	9.47	2.28	2.06
11	1	1127	CLA	MG-NA	9.47	2.28	2.06
11	a	1130	CLA	MG-NA	9.47	2.28	2.06
11	1	1801	CLA	MG-NA	9.46	2.28	2.06
11	B	1215	CLA	MG-NA	9.46	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1229	CLA	MG-NA	9.46	2.28	2.06
11	1	1134	CLA	MG-NA	9.46	2.28	2.06
11	b	1210	CLA	MG-NA	9.46	2.28	2.06
11	a	1112	CLA	MG-NA	9.46	2.28	2.06
11	1	1112	CLA	MG-NA	9.46	2.28	2.06
11	a	1140	CLA	MG-NA	9.46	2.28	2.06
11	1	1114	CLA	MG-NA	9.46	2.28	2.06
11	b	1232	CLA	MG-NA	9.46	2.28	2.06
11	B	1218	CLA	MG-NA	9.46	2.28	2.06
11	1	1103	CLA	MG-NA	9.46	2.28	2.06
11	1	1116	CLA	MG-NA	9.46	2.28	2.06
11	2	1213	CLA	MG-NA	9.45	2.28	2.06
11	b	1218	CLA	MG-NA	9.45	2.28	2.06
11	2	1202	CLA	MG-NA	9.45	2.28	2.06
11	b	1212	CLA	MG-NA	9.45	2.28	2.06
11	A	1140	CLA	MG-NA	9.45	2.28	2.06
11	1	1117	CLA	MG-NA	9.45	2.28	2.06
11	A	1124	CLA	MG-NA	9.45	2.28	2.06
11	1	1125	CLA	MG-NA	9.45	2.28	2.06
11	b	1204	CLA	MG-NA	9.45	2.28	2.06
11	A	1105	CLA	MG-NA	9.44	2.28	2.06
11	a	1109	CLA	MG-NA	9.44	2.28	2.06
11	a	1124	CLA	MG-NA	9.44	2.28	2.06
11	8	1502	CLA	MG-NA	9.44	2.28	2.06
11	2	1234	CLA	MG-NA	9.44	2.28	2.06
11	a	1133	CLA	MG-NA	9.44	2.28	2.06
11	B	1239	CLA	MG-NA	9.44	2.28	2.06
11	1	1108	CLA	MG-NA	9.44	2.28	2.06
11	A	1101	CLA	MG-NA	9.44	2.28	2.06
11	B	1222	CLA	MG-NA	9.44	2.28	2.06
11	1	1133	CLA	MG-NA	9.44	2.28	2.06
11	a	1135	CLA	MG-NA	9.44	2.28	2.06
11	a	1128	CLA	MG-NA	9.43	2.28	2.06
11	A	1131	CLA	MG-NA	9.43	2.28	2.06
11	B	1219	CLA	MG-NA	9.43	2.28	2.06
11	2	1204	CLA	MG-NA	9.43	2.28	2.06
11	b	1229	CLA	MG-NA	9.43	2.28	2.06
11	A	1012	CLA	MG-NA	9.43	2.28	2.06
11	2	1236	CLA	MG-NA	9.42	2.28	2.06
11	b	1231	CLA	MG-NA	9.42	2.28	2.06
11	A	1113	CLA	MG-NA	9.42	2.28	2.06
11	2	1228	CLA	MG-NA	9.42	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1116	CLA	MG-NA	9.42	2.28	2.06
11	1	1107	CLA	MG-NA	9.42	2.28	2.06
11	B	1234	CLA	MG-NA	9.42	2.28	2.06
11	1	1130	CLA	MG-NA	9.42	2.28	2.06
11	1	1137	CLA	MG-NA	9.42	2.28	2.06
11	2	1217	CLA	MG-NA	9.42	2.28	2.06
11	a	1102	CLA	MG-NA	9.41	2.28	2.06
11	b	1213	CLA	MG-NA	9.41	2.28	2.06
11	B	1210	CLA	MG-NA	9.41	2.28	2.06
11	b	1214	CLA	MG-NA	9.41	2.28	2.06
11	a	1117	CLA	MG-NA	9.41	2.28	2.06
11	A	1130	CLA	MG-NA	9.41	2.28	2.06
11	a	1131	CLA	MG-NA	9.41	2.28	2.06
11	1	1122	CLA	MG-NA	9.41	2.28	2.06
11	a	1110	CLA	MG-NA	9.41	2.28	2.06
11	2	1201	CLA	MG-NA	9.41	2.28	2.06
11	1	1124	CLA	MG-NA	9.41	2.28	2.06
11	l	1502	CLA	MG-NA	9.41	2.28	2.06
11	B	1228	CLA	MG-NA	9.41	2.28	2.06
11	b	1202	CLA	MG-NA	9.41	2.28	2.06
11	B	1213	CLA	MG-NA	9.40	2.28	2.06
11	B	1212	CLA	MG-NA	9.40	2.28	2.06
11	a	1132	CLA	MG-NA	9.40	2.28	2.06
11	a	1106	CLA	MG-NA	9.40	2.28	2.06
11	a	1134	CLA	MG-NA	9.40	2.28	2.06
11	l	1503	CLA	MG-NA	9.40	2.28	2.06
11	1	1129	CLA	MG-NA	9.40	2.28	2.06
11	2	1215	CLA	MG-NA	9.40	2.28	2.06
11	A	1129	CLA	MG-NA	9.40	2.28	2.06
11	a	1137	CLA	MG-NA	9.40	2.28	2.06
11	b	1206	CLA	MG-NA	9.39	2.28	2.06
11	2	1238	CLA	MG-NA	9.39	2.28	2.06
11	8	1501	CLA	MG-NA	9.39	2.28	2.06
11	1	1101	CLA	MG-NA	9.39	2.28	2.06
11	b	1222	CLA	MG-NA	9.39	2.28	2.06
11	a	1122	CLA	MG-NA	9.39	2.28	2.06
11	A	1107	CLA	MG-NA	9.39	2.28	2.06
11	2	1227	CLA	MG-NA	9.39	2.28	2.06
11	b	1236	CLA	MG-NA	9.39	2.28	2.06
11	A	1115	CLA	MG-NA	9.39	2.28	2.06
11	2	1218	CLA	MG-NA	9.39	2.28	2.06
11	a	1138	CLA	MG-NA	9.39	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1136	CLA	MG-NA	9.39	2.28	2.06
11	2	1224	CLA	MG-NA	9.38	2.28	2.06
11	b	1209	CLA	MG-NA	9.38	2.28	2.06
11	A	1102	CLA	MG-NA	9.38	2.28	2.06
11	B	1206	CLA	MG-NA	9.38	2.28	2.06
11	B	1235	CLA	MG-NA	9.38	2.28	2.06
11	L	1503	CLA	MG-NA	9.38	2.28	2.06
11	1	1131	CLA	MG-NA	9.38	2.28	2.06
11	0	1402	CLA	MG-NA	9.38	2.28	2.06
11	1	1119	CLA	MG-NA	9.38	2.28	2.06
11	1	1105	CLA	MG-NA	9.38	2.28	2.06
11	A	1011	CLA	MG-NA	9.38	2.28	2.06
11	A	1117	CLA	MG-NA	9.38	2.28	2.06
11	B	1230	CLA	MG-NA	9.37	2.28	2.06
11	b	1207	CLA	MG-NA	9.37	2.28	2.06
11	A	1127	CLA	MG-NA	9.37	2.28	2.06
11	B	1203	CLA	MG-NA	9.37	2.28	2.06
11	A	1022	CLA	MG-NA	9.37	2.28	2.06
11	B	1227	CLA	MG-NA	9.36	2.28	2.06
11	B	1214	CLA	MG-NA	9.36	2.28	2.06
11	1	1128	CLA	MG-NA	9.36	2.28	2.06
11	B	1208	CLA	MG-NA	9.36	2.28	2.06
11	B	1217	CLA	MG-NA	9.36	2.28	2.06
11	B	1202	CLA	MG-NA	9.36	2.28	2.06
11	b	1226	CLA	MG-NA	9.36	2.28	2.06
11	1	1132	CLA	MG-NA	9.36	2.28	2.06
11	b	1238	CLA	MG-NA	9.35	2.28	2.06
11	a	1119	CLA	MG-NA	9.35	2.28	2.06
11	A	1132	CLA	MG-NA	9.35	2.28	2.06
11	A	1126	CLA	MG-NA	9.34	2.28	2.06
11	L	1502	CLA	MG-NA	9.34	2.28	2.06
11	A	1135	CLA	MG-NA	9.34	2.28	2.06
11	2	1021	CLA	MG-NA	9.34	2.28	2.06
11	B	1207	CLA	MG-NA	9.33	2.28	2.06
11	A	1108	CLA	MG-NA	9.33	2.28	2.06
11	a	1237	CLA	MG-NA	9.33	2.28	2.06
11	A	1137	CLA	MG-NA	9.33	2.28	2.06
11	A	1136	CLA	MG-NA	9.33	2.28	2.06
11	2	1203	CLA	MG-NA	9.33	2.28	2.06
11	a	1111	CLA	MG-NA	9.33	2.28	2.06
11	A	1106	CLA	MG-NA	9.33	2.28	2.06
11	B	1224	CLA	MG-NA	9.32	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1013	CLA	MG-NA	9.32	2.28	2.06
11	A	1111	CLA	MG-NA	9.32	2.28	2.06
11	B	1205	CLA	MG-NA	9.31	2.28	2.06
11	1	1109	CLA	MG-NA	9.31	2.28	2.06
11	1	1106	CLA	MG-NA	9.31	2.28	2.06
11	2	1210	CLA	MG-NA	9.31	2.28	2.06
11	A	1103	CLA	MG-NA	9.31	2.28	2.06
11	a	1129	CLA	MG-NA	9.31	2.28	2.06
11	a	1104	CLA	MG-NA	9.30	2.28	2.06
11	B	1236	CLA	MG-NA	9.30	2.28	2.06
11	B	1216	CLA	MG-NA	9.30	2.28	2.06
11	1	1136	CLA	MG-NA	9.30	2.28	2.06
11	B	1226	CLA	MG-NA	9.29	2.28	2.06
11	b	1023	CLA	MG-NA	9.29	2.28	2.06
11	1	1104	CLA	MG-NA	9.29	2.28	2.06
11	1	1237	CLA	MG-NA	9.29	2.28	2.06
11	2	1226	CLA	MG-NA	9.29	2.28	2.06
11	B	1204	CLA	MG-NA	9.29	2.28	2.06
11	A	1109	CLA	MG-NA	9.29	2.28	2.06
11	2	1208	CLA	MG-NA	9.29	2.28	2.06
11	2	1013	CLA	MG-NA	9.28	2.28	2.06
11	A	1122	CLA	MG-NA	9.28	2.28	2.06
11	A	1138	CLA	MG-NA	9.28	2.28	2.06
11	K	1402	CLA	MG-NA	9.28	2.28	2.06
11	b	1205	CLA	MG-NA	9.28	2.28	2.06
11	B	1201	CLA	MG-NA	9.28	2.28	2.06
11	A	1133	CLA	MG-NA	9.27	2.28	2.06
11	k	1402	CLA	MG-NA	9.27	2.28	2.06
11	1	1118	CLA	MG-NA	9.27	2.28	2.06
11	A	1119	CLA	MG-NA	9.27	2.28	2.06
11	2	1207	CLA	MG-NA	9.26	2.28	2.06
11	B	1238	CLA	MG-NA	9.26	2.28	2.06
11	B	1023	CLA	MG-NA	9.26	2.28	2.06
11	1	1138	CLA	MG-NA	9.25	2.28	2.06
11	A	1237	CLA	MG-NA	9.24	2.28	2.06
11	B	1211	CLA	MG-NA	9.24	2.28	2.06
11	2	1205	CLA	MG-NA	9.24	2.28	2.06
11	b	1201	CLA	MG-NA	9.22	2.28	2.06
11	B	1021	CLA	MG-NA	9.22	2.28	2.06
11	A	1128	CLA	MG-NA	9.22	2.28	2.06
11	1	1111	CLA	MG-NA	9.20	2.28	2.06
11	2	1023	CLA	MG-NA	9.19	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1013	CLA	MG-NA	9.19	2.28	2.06
11	a	1118	CLA	MG-NA	9.19	2.28	2.06
11	2	1211	CLA	MG-NA	9.14	2.28	2.06
11	A	1118	CLA	MG-NA	9.10	2.27	2.06
11	A	1104	CLA	MG-NA	9.07	2.27	2.06
14	m	4021	BCR	C8-C9	-8.43	1.27	1.45
14	f	4013	BCR	C8-C9	-8.38	1.27	1.45
14	A	4003	BCR	C8-C9	-8.38	1.27	1.45
14	F	4013	BCR	C8-C9	-8.34	1.28	1.45
14	2	4011	BCR	C8-C9	-8.31	1.28	1.45
14	F	4018	BCR	C8-C9	-8.31	1.28	1.45
14	l	4019	BCR	C8-C9	-8.30	1.28	1.45
14	6	4018	BCR	C8-C9	-8.29	1.28	1.45
14	f	4018	BCR	C8-C9	-8.28	1.28	1.45
14	B	4011	BCR	C8-C9	-8.28	1.28	1.45
14	7	4021	BCR	C8-C9	-8.27	1.28	1.45
14	A	4003	BCR	C11-C10	-8.26	1.17	1.43
14	B	4004	BCR	C8-C9	-8.26	1.28	1.45
14	b	4006	BCR	C8-C9	-8.26	1.28	1.45
14	M	4021	BCR	C8-C9	-8.25	1.28	1.45
14	2	4014	BCR	C8-C9	-8.25	1.28	1.45
14	2	4010	BCR	C8-C9	-8.24	1.28	1.45
14	a	4008	BCR	C8-C9	-8.24	1.28	1.45
14	B	4006	BCR	C8-C9	-8.24	1.28	1.45
14	a	4003	BCR	C8-C9	-8.23	1.28	1.45
14	b	4010	BCR	C8-C9	-8.23	1.28	1.45
14	F	4018	BCR	C11-C10	-8.23	1.18	1.43
14	6	4013	BCR	C8-C9	-8.22	1.28	1.45
14	6	4020	BCR	C8-C9	-8.22	1.28	1.45
14	B	4010	BCR	C8-C9	-8.21	1.28	1.45
14	8	4019	BCR	C8-C9	-8.21	1.28	1.45
14	2	4005	BCR	C8-C9	-8.20	1.28	1.45
14	b	4014	BCR	C8-C9	-8.20	1.28	1.45
14	1	4003	BCR	C8-C9	-8.20	1.28	1.45
14	2	4010	BCR	C11-C10	-8.19	1.18	1.43
14	f	4020	BCR	C8-C9	-8.17	1.28	1.45
14	b	4005	BCR	C8-C9	-8.17	1.28	1.45
14	B	4005	BCR	C8-C9	-8.17	1.28	1.45
14	m	4021	BCR	C11-C10	-8.16	1.18	1.43
14	A	4001	BCR	C8-C9	-8.15	1.28	1.45
14	1	4008	BCR	C8-C9	-8.15	1.28	1.45
14	6	4020	BCR	C11-C10	-8.15	1.18	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	4020	BCR	C8-C9	-8.14	1.28	1.45
14	M	4021	BCR	C11-C10	-8.14	1.18	1.43
14	L	4022	BCR	C8-C9	-8.13	1.28	1.45
14	a	4002	BCR	C8-C9	-8.11	1.28	1.45
14	2	4009	BCR	C8-C9	-8.07	1.28	1.45
14	b	4017	BCR	C11-C10	-8.05	1.18	1.43
14	a	4007	BCR	C8-C9	-8.05	1.28	1.45
14	A	4002	BCR	C8-C9	-8.04	1.28	1.45
14	l	4022	BCR	C8-C9	-8.03	1.28	1.45
14	b	4010	BCR	C11-C10	-8.03	1.18	1.43
14	a	4001	BCR	C8-C9	-8.03	1.28	1.45
14	8	4022	BCR	C8-C9	-8.03	1.28	1.45
14	2	4006	BCR	C8-C9	-8.03	1.28	1.45
14	B	4009	BCR	C11-C10	-8.02	1.18	1.43
14	6	4018	BCR	C11-C10	-8.02	1.18	1.43
14	l	4019	BCR	C11-C10	-8.01	1.18	1.43
14	B	4004	BCR	C11-C10	-8.01	1.18	1.43
14	1	4001	BCR	C8-C9	-8.01	1.28	1.45
14	B	4011	BCR	C11-C10	-8.01	1.18	1.43
14	b	4011	BCR	C8-C9	-8.00	1.28	1.45
14	F	4013	BCR	C11-C10	-8.00	1.18	1.43
14	F	4020	BCR	C11-C10	-8.00	1.18	1.43
14	f	4020	BCR	C11-C10	-8.00	1.18	1.43
14	2	4011	BCR	C11-C10	-8.00	1.18	1.43
14	a	4008	BCR	C11-C10	-8.00	1.18	1.43
14	f	4013	BCR	C11-C10	-8.00	1.18	1.43
14	A	4007	BCR	C8-C9	-8.00	1.28	1.45
14	B	4014	BCR	C8-C9	-7.99	1.28	1.45
14	7	4021	BCR	C11-C10	-7.98	1.18	1.43
14	B	4009	BCR	C8-C9	-7.97	1.28	1.45
14	B	4017	BCR	C8-C9	-7.97	1.28	1.45
14	1	4003	BCR	C11-C10	-7.96	1.18	1.43
14	8	4022	BCR	C11-C10	-7.96	1.18	1.43
14	2	4004	BCR	C8-C9	-7.96	1.28	1.45
14	a	4002	BCR	C11-C10	-7.96	1.18	1.43
14	2	4017	BCR	C8-C9	-7.96	1.28	1.45
14	b	4004	BCR	C8-C9	-7.95	1.28	1.45
14	1	4007	BCR	C8-C9	-7.95	1.28	1.45
14	1	4002	BCR	C8-C9	-7.95	1.28	1.45
14	B	4005	BCR	C11-C10	-7.95	1.18	1.43
14	2	4017	BCR	C11-C10	-7.94	1.18	1.43
14	2	4014	BCR	C11-C10	-7.94	1.18	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	2001	PQN	C3-C2	7.93	1.49	1.35
14	b	4004	BCR	C11-C10	-7.93	1.18	1.43
14	L	4019	BCR	C8-C9	-7.93	1.28	1.45
14	f	4018	BCR	C11-C10	-7.92	1.18	1.43
14	A	4007	BCR	C11-C10	-7.92	1.18	1.43
14	F	4018	BCR	C10-C9	-7.92	1.25	1.35
14	1	4008	BCR	C11-C10	-7.91	1.18	1.43
14	b	4006	BCR	C11-C10	-7.91	1.18	1.43
14	b	4011	BCR	C11-C10	-7.91	1.18	1.43
14	b	4005	BCR	C11-C10	-7.90	1.19	1.43
14	B	4017	BCR	C11-C10	-7.89	1.19	1.43
14	2	4005	BCR	C11-C10	-7.88	1.19	1.43
14	l	4022	BCR	C11-C10	-7.88	1.19	1.43
14	a	4007	BCR	C11-C10	-7.87	1.19	1.43
12	B	2002	PQN	C3-C2	7.85	1.49	1.35
14	a	4003	BCR	C11-C10	-7.85	1.19	1.43
14	b	4009	BCR	C8-C9	-7.85	1.29	1.45
14	A	4008	BCR	C8-C9	-7.85	1.29	1.45
14	1	4001	BCR	C11-C10	-7.84	1.19	1.43
14	1	4007	BCR	C11-C10	-7.83	1.19	1.43
14	b	4014	BCR	C11-C10	-7.83	1.19	1.43
14	8	4019	BCR	C11-C10	-7.83	1.19	1.43
14	a	4001	BCR	C11-C10	-7.83	1.19	1.43
14	B	4006	BCR	C11-C10	-7.83	1.19	1.43
14	2	4009	BCR	C11-C10	-7.83	1.19	1.43
14	2	4004	BCR	C11-C10	-7.82	1.19	1.43
14	2	4006	BCR	C11-C10	-7.82	1.19	1.43
14	A	4001	BCR	C11-C10	-7.82	1.19	1.43
14	6	4013	BCR	C11-C10	-7.82	1.19	1.43
14	B	4010	BCR	C11-C10	-7.81	1.19	1.43
14	b	4017	BCR	C8-C9	-7.81	1.29	1.45
14	1	4002	BCR	C11-C10	-7.80	1.19	1.43
12	2	2002	PQN	C3-C2	7.79	1.49	1.35
14	A	4008	BCR	C11-C10	-7.79	1.19	1.43
14	m	4021	BCR	C10-C9	-7.78	1.25	1.35
12	A	2001	PQN	C3-C2	7.78	1.49	1.35
14	L	4019	BCR	C11-C10	-7.77	1.19	1.43
14	B	4014	BCR	C11-C10	-7.77	1.19	1.43
12	b	2002	PQN	C3-C2	7.75	1.49	1.35
12	a	2001	PQN	C3-C2	7.72	1.49	1.35
14	6	4018	BCR	C20-C21	-7.70	1.19	1.43
14	A	4002	BCR	C11-C10	-7.70	1.19	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	4009	BCR	C11-C10	-7.65	1.19	1.43
14	L	4022	BCR	C11-C10	-7.65	1.19	1.43
14	2	4014	BCR	C10-C9	-7.63	1.25	1.35
14	2	4010	BCR	C10-C9	-7.61	1.25	1.35
14	6	4018	BCR	C16-C17	-7.60	1.19	1.43
14	F	4018	BCR	C20-C21	-7.59	1.19	1.43
14	f	4018	BCR	C20-C21	-7.57	1.20	1.43
14	f	4018	BCR	C16-C17	-7.56	1.20	1.43
14	M	4021	BCR	C10-C9	-7.56	1.25	1.35
14	8	4022	BCR	C10-C9	-7.55	1.25	1.35
14	f	4013	BCR	C20-C21	-7.54	1.20	1.43
14	2	4017	BCR	C20-C21	-7.53	1.20	1.43
14	B	4017	BCR	C20-C21	-7.53	1.20	1.43
14	6	4020	BCR	C20-C21	-7.52	1.20	1.43
14	6	4020	BCR	C10-C9	-7.49	1.25	1.35
14	b	4017	BCR	C20-C21	-7.49	1.20	1.43
14	F	4018	BCR	C16-C17	-7.48	1.20	1.43
14	B	4004	BCR	C10-C9	-7.45	1.25	1.35
14	a	4003	BCR	C16-C17	-7.44	1.20	1.43
14	A	4003	BCR	C20-C21	-7.44	1.20	1.43
14	b	4017	BCR	C16-C17	-7.44	1.20	1.43
14	6	4020	BCR	C16-C17	-7.43	1.20	1.43
14	A	4003	BCR	C16-C17	-7.42	1.20	1.43
14	a	4003	BCR	C20-C21	-7.41	1.20	1.43
14	f	4013	BCR	C16-C17	-7.40	1.20	1.43
14	L	4022	BCR	C20-C21	-7.40	1.20	1.43
14	B	4014	BCR	C16-C17	-7.39	1.20	1.43
14	8	4022	BCR	C20-C21	-7.39	1.20	1.43
14	b	4017	BCR	C10-C9	-7.38	1.26	1.35
14	B	4014	BCR	C20-C21	-7.38	1.20	1.43
14	F	4020	BCR	C20-C21	-7.37	1.20	1.43
14	b	4010	BCR	C10-C9	-7.37	1.26	1.35
14	b	4006	BCR	C20-C21	-7.37	1.20	1.43
14	B	4005	BCR	C20-C21	-7.37	1.20	1.43
14	B	4011	BCR	C16-C17	-7.37	1.20	1.43
14	F	4013	BCR	C10-C9	-7.37	1.26	1.35
14	A	4001	BCR	C10-C9	-7.36	1.26	1.35
14	8	4019	BCR	C20-C21	-7.36	1.20	1.43
14	2	4011	BCR	C10-C9	-7.36	1.26	1.35
14	2	4010	BCR	C20-C21	-7.36	1.20	1.43
14	f	4018	BCR	C10-C9	-7.36	1.26	1.35
14	B	4004	BCR	C20-C21	-7.36	1.20	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4011	BCR	C20-C21	-7.36	1.20	1.43
14	f	4020	BCR	C16-C17	-7.35	1.20	1.43
14	m	4021	BCR	C16-C17	-7.35	1.20	1.43
14	f	4020	BCR	C20-C21	-7.34	1.20	1.43
14	2	4005	BCR	C20-C21	-7.33	1.20	1.43
14	B	4009	BCR	C20-C21	-7.33	1.20	1.43
14	F	4020	BCR	C10-C9	-7.32	1.26	1.35
14	l	4019	BCR	C20-C21	-7.32	1.20	1.43
14	6	4013	BCR	C20-C21	-7.32	1.20	1.43
14	A	4007	BCR	C10-C9	-7.32	1.26	1.35
14	B	4005	BCR	C10-C9	-7.32	1.26	1.35
14	2	4011	BCR	C20-C21	-7.31	1.20	1.43
14	B	4005	BCR	C16-C17	-7.31	1.20	1.43
14	6	4018	BCR	C10-C9	-7.31	1.26	1.35
14	b	4004	BCR	C20-C21	-7.31	1.20	1.43
14	1	4003	BCR	C20-C21	-7.31	1.20	1.43
14	1	4003	BCR	C10-C9	-7.30	1.26	1.35
14	A	4003	BCR	C10-C9	-7.30	1.26	1.35
14	l	4022	BCR	C20-C21	-7.30	1.20	1.43
14	a	4002	BCR	C20-C21	-7.30	1.20	1.43
14	b	4011	BCR	C20-C21	-7.30	1.20	1.43
14	f	4020	BCR	C10-C9	-7.30	1.26	1.35
14	2	4010	BCR	C16-C17	-7.30	1.20	1.43
14	2	4017	BCR	C16-C17	-7.30	1.20	1.43
14	b	4010	BCR	C20-C21	-7.29	1.20	1.43
14	a	4008	BCR	C20-C21	-7.29	1.20	1.43
14	B	4017	BCR	C16-C17	-7.29	1.20	1.43
14	A	4002	BCR	C10-C9	-7.29	1.26	1.35
14	B	4011	BCR	C10-C9	-7.29	1.26	1.35
14	a	4001	BCR	C20-C21	-7.28	1.20	1.43
14	7	4021	BCR	C20-C21	-7.28	1.20	1.43
14	F	4013	BCR	C20-C21	-7.27	1.20	1.43
14	2	4011	BCR	C16-C17	-7.27	1.20	1.43
14	2	4014	BCR	C16-C17	-7.26	1.20	1.43
14	A	4008	BCR	C20-C21	-7.26	1.20	1.43
14	b	4011	BCR	C16-C17	-7.26	1.21	1.43
14	6	4013	BCR	C16-C17	-7.26	1.21	1.43
14	1	4007	BCR	C20-C21	-7.26	1.21	1.43
14	A	4007	BCR	C16-C17	-7.26	1.21	1.43
14	L	4022	BCR	C16-C17	-7.26	1.21	1.43
14	1	4008	BCR	C20-C21	-7.26	1.21	1.43
14	8	4019	BCR	C10-C9	-7.26	1.26	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	4003	BCR	C16-C17	-7.25	1.21	1.43
14	F	4020	BCR	C16-C17	-7.25	1.21	1.43
14	2	4004	BCR	C20-C21	-7.25	1.21	1.43
14	a	4008	BCR	C16-C17	-7.25	1.21	1.43
14	b	4005	BCR	C20-C21	-7.25	1.21	1.43
14	b	4010	BCR	C16-C17	-7.25	1.21	1.43
14	8	4022	BCR	C16-C17	-7.25	1.21	1.43
14	A	4007	BCR	C20-C21	-7.24	1.21	1.43
14	A	4002	BCR	C20-C21	-7.24	1.21	1.43
14	B	4006	BCR	C20-C21	-7.24	1.21	1.43
14	7	4021	BCR	C16-C17	-7.23	1.21	1.43
14	1	4001	BCR	C20-C21	-7.23	1.21	1.43
14	m	4021	BCR	C20-C21	-7.23	1.21	1.43
14	B	4010	BCR	C20-C21	-7.22	1.21	1.43
14	A	4008	BCR	C16-C17	-7.22	1.21	1.43
14	7	4021	BCR	C10-C9	-7.22	1.26	1.35
14	2	4006	BCR	C20-C21	-7.22	1.21	1.43
14	B	4004	BCR	C16-C17	-7.21	1.21	1.43
14	a	4007	BCR	C20-C21	-7.21	1.21	1.43
14	b	4006	BCR	C16-C17	-7.20	1.21	1.43
14	1	4008	BCR	C16-C17	-7.20	1.21	1.43
14	A	4001	BCR	C20-C21	-7.20	1.21	1.43
14	b	4005	BCR	C16-C17	-7.20	1.21	1.43
14	a	4002	BCR	C10-C9	-7.19	1.26	1.35
14	A	4001	BCR	C16-C17	-7.19	1.21	1.43
14	b	4005	BCR	C10-C9	-7.19	1.26	1.35
14	b	4014	BCR	C16-C17	-7.18	1.21	1.43
14	1	4002	BCR	C20-C21	-7.18	1.21	1.43
14	B	4014	BCR	C10-C9	-7.18	1.26	1.35
14	2	4005	BCR	C16-C17	-7.18	1.21	1.43
14	2	4009	BCR	C20-C21	-7.17	1.21	1.43
14	a	4002	BCR	C16-C17	-7.17	1.21	1.43
14	2	4004	BCR	C16-C17	-7.17	1.21	1.43
14	a	4007	BCR	C16-C17	-7.17	1.21	1.43
14	1	4007	BCR	C16-C17	-7.17	1.21	1.43
14	l	4019	BCR	C16-C17	-7.16	1.21	1.43
14	1	4001	BCR	C16-C17	-7.16	1.21	1.43
14	F	4013	BCR	C16-C17	-7.16	1.21	1.43
14	l	4022	BCR	C16-C17	-7.15	1.21	1.43
14	B	4010	BCR	C16-C17	-7.15	1.21	1.43
14	M	4021	BCR	C20-C21	-7.15	1.21	1.43
14	8	4019	BCR	C16-C17	-7.14	1.21	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	4002	BCR	C16-C17	-7.14	1.21	1.43
14	L	4019	BCR	C20-C21	-7.14	1.21	1.43
14	A	4002	BCR	C16-C17	-7.14	1.21	1.43
14	M	4021	BCR	C16-C17	-7.13	1.21	1.43
14	B	4009	BCR	C16-C17	-7.13	1.21	1.43
14	2	4009	BCR	C16-C17	-7.12	1.21	1.43
14	B	4006	BCR	C16-C17	-7.12	1.21	1.43
14	b	4004	BCR	C16-C17	-7.12	1.21	1.43
14	b	4009	BCR	C20-C21	-7.12	1.21	1.43
14	2	4006	BCR	C16-C17	-7.11	1.21	1.43
14	b	4014	BCR	C20-C21	-7.10	1.21	1.43
14	a	4001	BCR	C16-C17	-7.10	1.21	1.43
14	L	4019	BCR	C16-C17	-7.09	1.21	1.43
14	B	4006	BCR	C10-C9	-7.09	1.26	1.35
14	2	4014	BCR	C20-C21	-7.09	1.21	1.43
14	l	4022	BCR	C10-C9	-7.08	1.26	1.35
14	b	4004	BCR	C10-C9	-7.07	1.26	1.35
14	B	4017	BCR	C10-C9	-7.06	1.26	1.35
14	b	4006	BCR	C10-C9	-7.06	1.26	1.35
14	2	4017	BCR	C10-C9	-7.06	1.26	1.35
14	a	4007	BCR	C10-C9	-7.04	1.26	1.35
14	a	4001	BCR	C10-C9	-7.02	1.26	1.35
14	b	4011	BCR	C10-C9	-7.01	1.26	1.35
14	B	4009	BCR	C10-C9	-7.00	1.26	1.35
14	b	4009	BCR	C16-C17	-6.98	1.21	1.43
14	2	4009	BCR	C10-C9	-6.96	1.26	1.35
14	L	4019	BCR	C10-C9	-6.94	1.26	1.35
14	1	4001	BCR	C10-C9	-6.94	1.26	1.35
14	2	4006	BCR	C10-C9	-6.94	1.26	1.35
14	1	4002	BCR	C10-C9	-6.93	1.26	1.35
14	b	4014	BCR	C10-C9	-6.89	1.26	1.35
14	1	4007	BCR	C10-C9	-6.87	1.26	1.35
14	A	4008	BCR	C10-C9	-6.82	1.26	1.35
14	l	4019	BCR	C10-C9	-6.82	1.26	1.35
14	2	4004	BCR	C10-C9	-6.81	1.26	1.35
14	2	4005	BCR	C10-C9	-6.76	1.26	1.35
14	B	4010	BCR	C10-C9	-6.66	1.27	1.35
14	b	4009	BCR	C10-C9	-6.63	1.27	1.35
11	a	1121	CLA	O2A-C1	6.57	1.60	1.45
11	a	1120	CLA	O2A-C1	6.51	1.60	1.45
11	2	1211	CLA	O2A-C1	6.51	1.60	1.45
11	A	1121	CLA	O2A-C1	6.48	1.60	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1130	CLA	O2A-C1	6.48	1.60	1.45
11	A	1134	CLA	O2A-C1	6.48	1.60	1.45
11	A	1129	CLA	O2A-C1	6.47	1.60	1.45
11	L	1502	CLA	O2A-C1	6.47	1.60	1.45
11	1	1134	CLA	O2A-C1	6.47	1.60	1.45
11	a	1130	CLA	O2A-C1	6.47	1.60	1.45
11	1	1133	CLA	O2A-C1	6.46	1.60	1.45
11	a	1133	CLA	O2A-C1	6.46	1.60	1.45
11	2	1239	CLA	O2A-C1	6.46	1.60	1.45
11	1	1121	CLA	O2A-C1	6.46	1.60	1.45
11	a	1138	CLA	O2A-C1	6.45	1.60	1.45
11	a	1115	CLA	O2A-C1	6.45	1.60	1.45
11	1	1136	CLA	O2A-C1	6.45	1.60	1.45
11	1	1138	CLA	O2A-C1	6.45	1.60	1.45
11	A	1120	CLA	O2A-C1	6.44	1.60	1.45
11	1	1120	CLA	O2A-C1	6.44	1.60	1.45
11	b	1220	CLA	O2A-C1	6.44	1.60	1.45
11	a	1114	CLA	O2A-C1	6.44	1.60	1.45
11	2	1220	CLA	O2A-C1	6.44	1.60	1.45
11	A	1138	CLA	O2A-C1	6.44	1.60	1.45
11	A	1114	CLA	O2A-C1	6.44	1.60	1.45
11	1	1114	CLA	O2A-C1	6.43	1.60	1.45
11	l	1502	CLA	O2A-C1	6.43	1.60	1.45
11	A	1130	CLA	O2A-C1	6.43	1.60	1.45
11	1	1115	CLA	O2A-C1	6.43	1.60	1.45
11	b	1211	CLA	O2A-C1	6.43	1.60	1.45
11	a	1129	CLA	O2A-C1	6.42	1.60	1.45
14	1	4008	BCR	C10-C9	-6.42	1.27	1.35
11	B	1211	CLA	O2A-C1	6.42	1.60	1.45
11	A	1136	CLA	O2A-C1	6.42	1.60	1.45
11	A	1115	CLA	O2A-C1	6.41	1.60	1.45
11	a	1136	CLA	O2A-C1	6.41	1.60	1.45
11	8	1502	CLA	O2A-C1	6.41	1.60	1.45
11	b	1239	CLA	O2A-C1	6.41	1.60	1.45
11	1	1129	CLA	O2A-C1	6.40	1.60	1.45
11	A	1133	CLA	O2A-C1	6.40	1.60	1.45
14	a	4003	BCR	C10-C9	-6.40	1.27	1.35
11	B	1239	CLA	O2A-C1	6.38	1.60	1.45
11	a	1134	CLA	O2A-C1	6.36	1.60	1.45
11	B	1220	CLA	O2A-C1	6.34	1.60	1.45
14	a	4008	BCR	C10-C9	-6.31	1.27	1.35
14	L	4022	BCR	C10-C9	-6.12	1.27	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	4013	BCR	C10-C9	-6.08	1.27	1.35
14	f	4013	BCR	C10-C9	-5.98	1.27	1.35
11	A	1126	CLA	CHC-C1C	5.67	1.49	1.35
11	A	1112	CLA	CHC-C1C	5.56	1.49	1.35
11	a	1126	CLA	CHC-C1C	5.52	1.49	1.35
11	A	1103	CLA	CHC-C1C	5.52	1.49	1.35
11	B	1202	CLA	CHC-C1C	5.50	1.49	1.35
11	B	1230	CLA	O2A-C1	5.49	1.61	1.46
11	a	1112	CLA	CHC-C1C	5.48	1.49	1.35
11	A	1106	CLA	O2A-C1	5.48	1.61	1.46
11	1	1106	CLA	O2A-C1	5.48	1.61	1.46
11	A	1117	CLA	CHC-C1C	5.48	1.49	1.35
11	2	1223	CLA	CHC-C1C	5.47	1.49	1.35
11	A	1116	CLA	CHC-C1C	5.47	1.49	1.35
11	A	1111	CLA	CHC-C1C	5.46	1.49	1.35
11	A	1117	CLA	O2A-C1	5.46	1.61	1.46
11	1	1126	CLA	CHC-C1C	5.46	1.49	1.35
11	b	1230	CLA	O2A-C1	5.46	1.61	1.46
11	b	1210	CLA	CHC-C1C	5.45	1.48	1.35
11	b	1221	CLA	CHC-C1C	5.45	1.48	1.35
11	a	1011	CLA	O2D-CGD	5.44	1.46	1.33
11	2	1213	CLA	CHC-C1C	5.43	1.48	1.35
11	B	1214	CLA	CHC-C1C	5.43	1.48	1.35
11	2	1235	CLA	CHC-C1C	5.43	1.48	1.35
11	a	1115	CLA	CHC-C1C	5.43	1.48	1.35
11	b	1213	CLA	CHC-C1C	5.43	1.48	1.35
11	b	1202	CLA	CHC-C1C	5.42	1.48	1.35
11	2	1207	CLA	O2A-C1	5.42	1.61	1.46
11	A	1137	CLA	CHC-C1C	5.42	1.48	1.35
11	1	1122	CLA	CHC-C1C	5.42	1.48	1.35
11	1	1107	CLA	O2A-C1	5.41	1.61	1.46
11	1	1111	CLA	CHC-C1C	5.41	1.48	1.35
11	a	1122	CLA	O2A-C1	5.41	1.61	1.46
11	2	1219	CLA	C3B-C2B	5.41	1.47	1.40
11	B	1212	CLA	CHC-C1C	5.40	1.48	1.35
11	2	1219	CLA	CHC-C1C	5.40	1.48	1.35
11	b	1236	CLA	CHC-C1C	5.40	1.48	1.35
11	a	1122	CLA	CHC-C1C	5.40	1.48	1.35
11	2	1204	CLA	CHC-C1C	5.39	1.48	1.35
11	2	1236	CLA	CHC-C1C	5.39	1.48	1.35
11	A	1115	CLA	CHC-C1C	5.38	1.48	1.35
11	a	1132	CLA	O2A-C1	5.38	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1214	CLA	CHC-C1C	5.38	1.48	1.35
11	A	1116	CLA	O2A-C1	5.38	1.61	1.46
11	2	1202	CLA	CHC-C1C	5.38	1.48	1.35
11	a	1801	CLA	CHC-C1C	5.38	1.48	1.35
11	B	1240	CLA	CHC-C1C	5.38	1.48	1.35
11	B	1208	CLA	CHC-C1C	5.38	1.48	1.35
11	0	1402	CLA	CHC-C1C	5.38	1.48	1.35
11	2	1210	CLA	CHC-C1C	5.37	1.48	1.35
11	1	1112	CLA	CHC-C1C	5.37	1.48	1.35
11	A	1022	CLA	CHC-C1C	5.37	1.48	1.35
11	a	1105	CLA	O2A-C1	5.37	1.61	1.46
11	2	1229	CLA	CHC-C1C	5.37	1.48	1.35
11	a	1116	CLA	CHC-C1C	5.37	1.48	1.35
11	8	1503	CLA	CHC-C1C	5.37	1.48	1.35
11	1	1129	CLA	CHC-C1C	5.36	1.48	1.35
11	B	1235	CLA	CHC-C1C	5.36	1.48	1.35
11	A	1113	CLA	CHC-C1C	5.36	1.48	1.35
11	B	1236	CLA	CHC-C1C	5.36	1.48	1.35
11	A	1132	CLA	O2A-C1	5.36	1.61	1.46
11	2	1013	CLA	CHC-C1C	5.36	1.48	1.35
11	B	1213	CLA	CHC-C1C	5.36	1.48	1.35
11	2	1201	CLA	O2A-C1	5.36	1.61	1.46
11	a	1104	CLA	CHC-C1C	5.36	1.48	1.35
11	A	1139	CLA	CHC-C1C	5.35	1.48	1.35
11	B	1223	CLA	CHC-C1C	5.35	1.48	1.35
11	k	1402	CLA	O2A-C1	5.35	1.61	1.46
11	A	1120	CLA	CHC-C1C	5.35	1.48	1.35
11	B	1224	CLA	CHC-C1C	5.35	1.48	1.35
11	1	1125	CLA	CHC-C1C	5.35	1.48	1.35
11	b	1235	CLA	CHC-C1C	5.35	1.48	1.35
11	A	1109	CLA	O2D-CGD	5.35	1.46	1.33
11	B	1222	CLA	C3B-C2B	5.35	1.47	1.40
11	2	1230	CLA	O2A-C1	5.35	1.61	1.46
11	A	1119	CLA	O2A-C1	5.34	1.61	1.46
11	a	1116	CLA	O2A-C1	5.34	1.61	1.46
11	2	1238	CLA	O2A-C1	5.34	1.61	1.46
11	a	1012	CLA	CHC-C1C	5.34	1.48	1.35
11	b	1226	CLA	CHC-C1C	5.34	1.48	1.35
11	b	1216	CLA	CHC-C1C	5.34	1.48	1.35
11	B	1013	CLA	CHC-C1C	5.34	1.48	1.35
11	B	1222	CLA	CHC-C1C	5.34	1.48	1.35
11	a	1127	CLA	O2D-CGD	5.34	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1022	CLA	CHC-C1C	5.34	1.48	1.35
11	a	1101	CLA	O2D-CGD	5.33	1.46	1.33
11	b	1240	CLA	CHC-C1C	5.33	1.48	1.35
11	2	1232	CLA	CHC-C1C	5.33	1.48	1.35
11	b	1013	CLA	CHC-C1C	5.33	1.48	1.35
11	k	1402	CLA	CHC-C1C	5.33	1.48	1.35
11	1	1138	CLA	O2D-CGD	5.33	1.46	1.33
11	1	1116	CLA	CHC-C1C	5.33	1.48	1.35
11	A	1108	CLA	CHC-C1C	5.33	1.48	1.35
11	b	1207	CLA	O2A-C1	5.33	1.61	1.46
11	b	1225	CLA	CHC-C1C	5.33	1.48	1.35
11	A	1107	CLA	CHC-C1C	5.33	1.48	1.35
11	B	1210	CLA	CHC-C1C	5.32	1.48	1.35
11	b	1231	CLA	CHC-C1C	5.32	1.48	1.35
11	L	1501	CLA	CHC-C1C	5.32	1.48	1.35
11	1	1108	CLA	CHC-C1C	5.32	1.48	1.35
11	B	1221	CLA	CHC-C1C	5.32	1.48	1.35
11	A	1133	CLA	O2D-CGD	5.32	1.46	1.33
11	1	1102	CLA	CHC-C1C	5.31	1.48	1.35
11	1	1801	CLA	O2A-C1	5.31	1.61	1.46
11	a	1137	CLA	O2A-C1	5.31	1.61	1.46
11	2	1218	CLA	CHC-C1C	5.31	1.48	1.35
11	a	1134	CLA	CHC-C1C	5.31	1.48	1.35
11	A	1137	CLA	C3B-C2B	5.31	1.47	1.40
11	l	1502	CLA	CHC-C1C	5.31	1.48	1.35
11	a	1117	CLA	O2A-C1	5.31	1.61	1.46
11	A	1801	CLA	O2A-C1	5.31	1.61	1.46
11	8	1502	CLA	CHC-C1C	5.31	1.48	1.35
11	b	1201	CLA	CHC-C1C	5.31	1.48	1.35
11	a	1801	CLA	O2A-C1	5.31	1.61	1.46
11	b	1224	CLA	CHC-C1C	5.30	1.48	1.35
11	b	1218	CLA	CHC-C1C	5.30	1.48	1.35
11	A	1012	CLA	CHC-C1C	5.30	1.48	1.35
11	l	1501	CLA	CHC-C1C	5.30	1.48	1.35
11	B	1217	CLA	CHC-C1C	5.30	1.48	1.35
11	0	1401	CLA	CHC-C1C	5.30	1.48	1.35
11	b	1211	CLA	CHC-C1C	5.30	1.48	1.35
11	a	1132	CLA	CHC-C1C	5.30	1.48	1.35
11	A	1122	CLA	CHC-C1C	5.30	1.48	1.35
11	a	1109	CLA	CHC-C1C	5.30	1.48	1.35
11	1	1130	CLA	CHC-C1C	5.29	1.48	1.35
11	1	1113	CLA	CHC-C1C	5.29	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1216	CLA	CHC-C1C	5.29	1.48	1.35
11	a	1117	CLA	CHC-C1C	5.29	1.48	1.35
11	1	1134	CLA	CHC-C1C	5.29	1.48	1.35
11	1	1137	CLA	CHC-C1C	5.29	1.48	1.35
11	A	1130	CLA	CHC-C1C	5.29	1.48	1.35
11	B	1207	CLA	O2A-C1	5.29	1.61	1.46
11	a	1124	CLA	CHC-C1C	5.29	1.48	1.35
11	1	1119	CLA	O2A-C1	5.28	1.61	1.46
11	b	1210	CLA	O2A-C1	5.28	1.61	1.46
11	2	1211	CLA	CHC-C1C	5.28	1.48	1.35
11	a	1111	CLA	CHC-C1C	5.28	1.48	1.35
11	2	1215	CLA	O2A-C1	5.28	1.61	1.46
11	A	1115	CLA	O2D-CGD	5.28	1.46	1.33
11	1	1121	CLA	O2D-CGD	5.28	1.46	1.33
11	a	1130	CLA	CHC-C1C	5.28	1.48	1.35
11	1	1117	CLA	O2A-C1	5.28	1.61	1.46
11	2	1216	CLA	CHC-C1C	5.28	1.48	1.35
11	a	1113	CLA	CHC-C1C	5.28	1.48	1.35
11	b	1203	CLA	CHC-C1C	5.28	1.48	1.35
11	a	1109	CLA	O2A-C1	5.28	1.61	1.46
11	a	1129	CLA	CHC-C1C	5.28	1.48	1.35
11	b	1013	CLA	O2A-C1	5.28	1.61	1.46
11	2	1230	CLA	O2D-CGD	5.28	1.46	1.33
11	2	1225	CLA	CHC-C1C	5.28	1.48	1.35
11	a	1140	CLA	O2A-C1	5.28	1.61	1.46
11	B	1221	CLA	O2A-C1	5.28	1.61	1.46
11	A	1801	CLA	C3C-C2C	5.27	1.47	1.36
11	A	1128	CLA	CHC-C1C	5.27	1.48	1.35
11	a	1118	CLA	O2A-C1	5.27	1.61	1.46
11	1	1119	CLA	CHC-C1C	5.27	1.48	1.35
11	A	1131	CLA	O2A-C1	5.27	1.61	1.46
11	2	1228	CLA	O2D-CGD	5.27	1.46	1.33
11	2	1221	CLA	CHC-C1C	5.27	1.48	1.35
11	A	1109	CLA	CHC-C1C	5.27	1.48	1.35
11	1	1136	CLA	CHC-C1C	5.27	1.48	1.35
11	B	1225	CLA	CHC-C1C	5.27	1.48	1.35
11	a	1237	CLA	O2A-C1	5.27	1.61	1.46
11	2	1222	CLA	CHC-C1C	5.27	1.48	1.35
11	2	1216	CLA	O2D-CGD	5.27	1.46	1.33
11	1	1106	CLA	CHC-C1C	5.27	1.48	1.35
11	b	1215	CLA	CHC-C1C	5.27	1.48	1.35
11	A	1121	CLA	CHC-C1C	5.27	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1108	CLA	O2D-CGD	5.27	1.46	1.33
11	A	1124	CLA	CHC-C1C	5.27	1.48	1.35
11	B	1213	CLA	O2D-CGD	5.27	1.46	1.33
11	b	1218	CLA	O2D-CGD	5.27	1.46	1.33
11	A	1102	CLA	O2A-C1	5.27	1.61	1.46
11	2	1023	CLA	O2D-CGD	5.26	1.46	1.33
11	B	1013	CLA	O2A-C1	5.26	1.61	1.46
11	1	1120	CLA	CHC-C1C	5.26	1.48	1.35
11	k	1401	CLA	CHC-C1C	5.26	1.48	1.35
11	B	1202	CLA	C3B-C2B	5.26	1.47	1.40
11	b	1224	CLA	O2D-CGD	5.26	1.46	1.33
11	1	1102	CLA	O2A-C1	5.26	1.61	1.46
11	b	1213	CLA	O2D-CGD	5.26	1.46	1.33
11	K	1401	CLA	CHC-C1C	5.26	1.48	1.35
11	1	1112	CLA	O2D-CGD	5.26	1.46	1.33
11	1	1121	CLA	CHC-C1C	5.26	1.48	1.35
11	a	1106	CLA	CHC-C1C	5.26	1.48	1.35
11	b	1021	CLA	O2D-CGD	5.26	1.46	1.33
11	A	1102	CLA	CHC-C1C	5.26	1.48	1.35
11	K	1402	CLA	O2A-C1	5.25	1.60	1.46
11	a	1102	CLA	O2A-C1	5.25	1.60	1.46
11	A	1127	CLA	CHC-C1C	5.25	1.48	1.35
11	A	1105	CLA	CHC-C1C	5.25	1.48	1.35
11	1	1012	CLA	O2A-C1	5.25	1.60	1.46
11	1	1801	CLA	CHC-C1C	5.25	1.48	1.35
11	b	1220	CLA	CHC-C1C	5.25	1.48	1.35
11	2	1209	CLA	CHC-C1C	5.25	1.48	1.35
11	B	1219	CLA	CHC-C1C	5.25	1.48	1.35
11	B	1239	CLA	CHC-C1C	5.25	1.48	1.35
11	a	1119	CLA	O2D-CGD	5.25	1.46	1.33
11	A	1101	CLA	CHC-C1C	5.25	1.48	1.35
11	b	1219	CLA	C3B-C2B	5.25	1.47	1.40
11	2	1239	CLA	O2D-CGD	5.25	1.46	1.33
11	b	1207	CLA	O2D-CGD	5.25	1.46	1.33
11	a	1128	CLA	O2A-C1	5.25	1.60	1.46
11	2	1226	CLA	CHC-C1C	5.25	1.48	1.35
11	b	1214	CLA	O2A-C1	5.25	1.60	1.46
11	A	1011	CLA	O2D-CGD	5.25	1.46	1.33
11	b	1201	CLA	C3B-C2B	5.25	1.47	1.40
11	1	1109	CLA	O2D-CGD	5.25	1.46	1.33
11	L	1502	CLA	CHC-C1C	5.25	1.48	1.35
11	a	1137	CLA	CHC-C1C	5.25	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1229	CLA	CHC-C1C	5.25	1.48	1.35
11	2	1230	CLA	CHC-C1C	5.25	1.48	1.35
11	2	1208	CLA	O2D-CGD	5.25	1.46	1.33
11	A	1118	CLA	O2A-C1	5.25	1.60	1.46
11	1	1118	CLA	CHC-C1C	5.25	1.48	1.35
11	a	1105	CLA	O2D-CGD	5.25	1.46	1.33
11	1	1127	CLA	CHC-C1C	5.24	1.48	1.35
11	1	1109	CLA	O2A-C1	5.24	1.60	1.46
11	1	1135	CLA	CHC-C1C	5.24	1.48	1.35
11	l	1503	CLA	CHC-C1C	5.24	1.48	1.35
11	2	1228	CLA	CHC-C1C	5.24	1.48	1.35
11	A	1119	CLA	O2D-CGD	5.24	1.46	1.33
11	2	1221	CLA	O2A-C1	5.24	1.60	1.46
11	A	1107	CLA	O2A-C1	5.24	1.60	1.46
11	b	1204	CLA	CHC-C1C	5.24	1.48	1.35
11	1	1135	CLA	O2A-C1	5.24	1.60	1.46
11	b	1219	CLA	O2D-CGD	5.24	1.46	1.33
11	1	1125	CLA	O2D-CGD	5.24	1.46	1.33
11	1	1140	CLA	O2A-C1	5.24	1.60	1.46
11	b	1209	CLA	CHC-C1C	5.24	1.48	1.35
11	A	1129	CLA	CHC-C1C	5.24	1.48	1.35
11	2	1204	CLA	O2D-CGD	5.24	1.46	1.33
11	1	1122	CLA	O2A-C1	5.24	1.60	1.46
11	A	1131	CLA	CHC-C1C	5.24	1.48	1.35
11	a	1108	CLA	CHC-C1C	5.24	1.48	1.35
11	B	1228	CLA	CHC-C1C	5.24	1.48	1.35
11	B	1235	CLA	O2A-C1	5.24	1.60	1.46
11	a	1115	CLA	O2D-CGD	5.24	1.46	1.33
11	a	1101	CLA	CHC-C1C	5.24	1.48	1.35
11	a	1139	CLA	O2D-CGD	5.24	1.46	1.33
11	1	1139	CLA	CHC-C1C	5.23	1.48	1.35
11	A	1104	CLA	CHC-C1C	5.23	1.48	1.35
11	1	1116	CLA	O2A-C1	5.23	1.60	1.46
11	b	1232	CLA	CHC-C1C	5.23	1.48	1.35
11	b	1238	CLA	CHC-C1C	5.23	1.48	1.35
11	B	1211	CLA	CHC-C1C	5.23	1.48	1.35
11	a	1114	CLA	O2D-CGD	5.23	1.46	1.33
11	A	1237	CLA	O2D-CGD	5.23	1.46	1.33
11	1	1124	CLA	CHC-C1C	5.23	1.48	1.35
11	1	1012	CLA	CHC-C1C	5.23	1.48	1.35
11	0	1402	CLA	O2A-C1	5.23	1.60	1.46
11	2	1231	CLA	CHC-C1C	5.23	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1226	CLA	CHC-C1C	5.23	1.48	1.35
11	A	1109	CLA	O2A-C1	5.23	1.60	1.46
11	b	1215	CLA	O2A-C1	5.23	1.60	1.46
11	2	1211	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1107	CLA	CHC-C1C	5.23	1.48	1.35
11	1	1110	CLA	CHC-C1C	5.23	1.48	1.35
11	a	1120	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1109	CLA	O2D-CGD	5.23	1.46	1.33
11	b	1217	CLA	CHC-C1C	5.23	1.48	1.35
11	B	1218	CLA	O2D-CGD	5.23	1.46	1.33
11	B	1230	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1123	CLA	CHC-C1C	5.23	1.48	1.35
11	1	1108	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1131	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1103	CLA	CHC-C1C	5.23	1.48	1.35
11	a	1140	CLA	CHC-C1C	5.23	1.48	1.35
11	b	1223	CLA	O2A-C1	5.23	1.60	1.46
11	a	1103	CLA	O2D-CGD	5.23	1.46	1.33
11	b	1228	CLA	O2A-C1	5.23	1.60	1.46
11	8	1503	CLA	O2D-CGD	5.23	1.46	1.33
11	b	1228	CLA	O2D-CGD	5.23	1.45	1.33
11	A	1116	CLA	O2D-CGD	5.23	1.45	1.33
11	a	1131	CLA	O2A-C1	5.22	1.60	1.46
11	B	1222	CLA	O2A-C1	5.22	1.60	1.46
11	B	1232	CLA	O2D-CGD	5.22	1.45	1.33
11	A	1135	CLA	O2A-C1	5.22	1.60	1.46
11	A	1135	CLA	CHC-C1C	5.22	1.48	1.35
11	A	1119	CLA	CHC-C1C	5.22	1.48	1.35
11	b	1227	CLA	CHC-C1C	5.22	1.48	1.35
11	a	1012	CLA	O2A-C1	5.22	1.60	1.46
11	1	1138	CLA	CHC-C1C	5.22	1.48	1.35
11	1	1136	CLA	O2D-CGD	5.22	1.45	1.33
11	1	1132	CLA	CHC-C1C	5.22	1.48	1.35
11	2	1023	CLA	CHC-C1C	5.22	1.48	1.35
11	1	1130	CLA	O2D-CGD	5.22	1.45	1.33
11	a	1106	CLA	O2A-C1	5.22	1.60	1.46
11	B	1235	CLA	O2D-CGD	5.22	1.45	1.33
11	1	1105	CLA	CHC-C1C	5.22	1.48	1.35
11	B	1219	CLA	O2D-CGD	5.22	1.45	1.33
11	2	1222	CLA	O2A-C1	5.22	1.60	1.46
11	1	1114	CLA	O2D-CGD	5.22	1.45	1.33
11	a	1126	CLA	O2D-CGD	5.22	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1139	CLA	O2D-CGD	5.22	1.45	1.33
11	2	1013	CLA	O2D-CGD	5.22	1.45	1.33
11	2	1013	CLA	O2A-C1	5.22	1.60	1.46
11	2	1223	CLA	O2A-C1	5.22	1.60	1.46
11	B	1238	CLA	CHC-C1C	5.22	1.48	1.35
11	a	1121	CLA	CHC-C1C	5.22	1.48	1.35
11	2	1213	CLA	C3C-C2C	5.22	1.47	1.36
11	1	1122	CLA	O2D-CGD	5.22	1.45	1.33
11	2	1021	CLA	O2D-CGD	5.22	1.45	1.33
11	B	1023	CLA	CHC-C1C	5.22	1.48	1.35
11	B	1207	CLA	CHC-C1C	5.22	1.48	1.35
11	b	1216	CLA	O2D-CGD	5.22	1.45	1.33
11	B	1209	CLA	CHC-C1C	5.21	1.48	1.35
11	b	1215	CLA	O2D-CGD	5.21	1.45	1.33
11	B	1217	CLA	O2D-CGD	5.21	1.45	1.33
11	1	1237	CLA	O2A-C1	5.21	1.60	1.46
11	2	1224	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1140	CLA	CHC-C1C	5.21	1.48	1.35
11	L	1501	CLA	O2A-C1	5.21	1.60	1.46
11	b	1230	CLA	CHC-C1C	5.21	1.48	1.35
11	b	1023	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1107	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1131	CLA	CHC-C1C	5.21	1.48	1.35
11	2	1021	CLA	CHC-C1C	5.21	1.48	1.35
11	a	1136	CLA	O2D-CGD	5.21	1.45	1.33
11	A	1122	CLA	O2A-C1	5.21	1.60	1.46
11	a	1102	CLA	O2D-CGD	5.21	1.45	1.33
11	a	1138	CLA	O2D-CGD	5.21	1.45	1.33
11	2	1217	CLA	CHC-C1C	5.21	1.48	1.35
11	A	1106	CLA	O2D-CGD	5.21	1.45	1.33
11	a	1102	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1101	CLA	CHC-C1C	5.21	1.48	1.35
11	A	1125	CLA	O2D-CGD	5.21	1.45	1.33
11	B	1226	CLA	O2A-C1	5.21	1.60	1.46
11	A	1140	CLA	O2D-CGD	5.21	1.45	1.33
11	2	1240	CLA	CHC-C1C	5.21	1.48	1.35
11	2	1205	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1133	CLA	O2D-CGD	5.21	1.45	1.33
11	b	1224	CLA	O2A-C1	5.21	1.60	1.46
11	1	1123	CLA	CHC-C1C	5.21	1.48	1.35
11	2	1208	CLA	CHC-C1C	5.21	1.48	1.35
11	1	1103	CLA	CHC-C1C	5.21	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1218	CLA	CHC-C1C	5.21	1.48	1.35
11	b	1206	CLA	O2D-CGD	5.21	1.45	1.33
11	A	1128	CLA	O2D-CGD	5.20	1.45	1.33
11	A	1136	CLA	O2D-CGD	5.20	1.45	1.33
11	a	1125	CLA	CHC-C1C	5.20	1.48	1.35
11	A	1237	CLA	O2A-C1	5.20	1.60	1.46
11	2	1236	CLA	O2D-CGD	5.20	1.45	1.33
11	2	1227	CLA	O2D-CGD	5.20	1.45	1.33
11	B	1208	CLA	O2D-CGD	5.20	1.45	1.33
11	1	1115	CLA	O2D-CGD	5.20	1.45	1.33
11	1	1128	CLA	O2D-CGD	5.20	1.45	1.33
11	B	1228	CLA	O2D-CGD	5.20	1.45	1.33
11	b	1021	CLA	CHC-C1C	5.20	1.48	1.35
11	A	1801	CLA	O2D-CGD	5.20	1.45	1.33
11	a	1130	CLA	O2D-CGD	5.20	1.45	1.33
11	a	1237	CLA	CHC-C1C	5.20	1.48	1.35
11	2	1023	CLA	O2A-C1	5.20	1.60	1.46
11	1	1101	CLA	O2D-CGD	5.20	1.45	1.33
11	2	1203	CLA	O2D-CGD	5.20	1.45	1.33
11	B	1219	CLA	O2A-C1	5.20	1.60	1.46
11	2	1220	CLA	O2D-CGD	5.20	1.45	1.33
11	A	1132	CLA	CHC-C1C	5.20	1.48	1.35
11	a	1138	CLA	CHC-C1C	5.20	1.48	1.35
11	k	1402	CLA	O2D-CGD	5.20	1.45	1.33
11	1	1113	CLA	O2D-CGD	5.20	1.45	1.33
11	a	1120	CLA	CHC-C1C	5.20	1.48	1.35
11	a	1128	CLA	CHC-C1C	5.20	1.48	1.35
11	2	1235	CLA	O2D-CGD	5.19	1.45	1.33
11	B	1214	CLA	O2D-CGD	5.19	1.45	1.33
11	a	1139	CLA	O2A-C1	5.19	1.60	1.46
11	A	1110	CLA	CHC-C1C	5.19	1.48	1.35
11	b	1235	CLA	O2D-CGD	5.19	1.45	1.33
11	b	1228	CLA	CHC-C1C	5.19	1.48	1.35
11	2	1202	CLA	O2D-CGD	5.19	1.45	1.33
11	A	1138	CLA	O2D-CGD	5.19	1.45	1.33
11	1	1119	CLA	O2D-CGD	5.19	1.45	1.33
11	b	1013	CLA	O2D-CGD	5.19	1.45	1.33
11	1	1105	CLA	O2D-CGD	5.19	1.45	1.33
11	a	1022	CLA	CHC-C1C	5.19	1.48	1.35
11	b	1209	CLA	O2D-CGD	5.19	1.45	1.33
11	a	1114	CLA	CHC-C1C	5.19	1.48	1.35
11	1	1139	CLA	O2D-CGD	5.19	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1131	CLA	CHC-C1C	5.19	1.48	1.35
11	b	1219	CLA	CHC-C1C	5.19	1.48	1.35
11	A	1237	CLA	CHC-C1C	5.19	1.48	1.35
11	A	1125	CLA	O2A-C1	5.19	1.60	1.46
11	A	1104	CLA	O2D-CGD	5.19	1.45	1.33
11	0	1401	CLA	O2D-CGD	5.19	1.45	1.33
11	b	1222	CLA	CHC-C1C	5.19	1.48	1.35
11	B	1223	CLA	O2A-C1	5.19	1.60	1.46
11	1	1237	CLA	CHC-C1C	5.18	1.48	1.35
11	B	1240	CLA	O2D-CGD	5.18	1.45	1.33
11	A	1102	CLA	O2D-CGD	5.18	1.45	1.33
11	2	1216	CLA	O2A-C1	5.18	1.60	1.46
11	b	1201	CLA	O2D-CGD	5.18	1.45	1.33
11	B	1203	CLA	CHC-C1C	5.18	1.48	1.35
11	2	1214	CLA	CHC-C1C	5.18	1.48	1.35
11	b	1230	CLA	O2D-CGD	5.18	1.45	1.33
11	b	1225	CLA	O2A-C1	5.18	1.60	1.46
11	2	1214	CLA	O2A-C1	5.18	1.60	1.46
11	a	1128	CLA	O2D-CGD	5.18	1.45	1.33
11	2	1213	CLA	O2D-CGD	5.18	1.45	1.33
11	b	1202	CLA	O2D-CGD	5.18	1.45	1.33
11	1	1104	CLA	CHC-C1C	5.18	1.48	1.35
11	b	1229	CLA	O2A-C1	5.18	1.60	1.46
11	2	1220	CLA	CHC-C1C	5.18	1.48	1.35
11	b	1205	CLA	O2A-C1	5.18	1.60	1.46
11	A	1140	CLA	O2A-C1	5.18	1.60	1.46
11	b	1235	CLA	C3B-C2B	5.18	1.47	1.40
11	A	1112	CLA	O2D-CGD	5.18	1.45	1.33
11	2	1215	CLA	O2D-CGD	5.18	1.45	1.33
11	l	1501	CLA	O2D-CGD	5.18	1.45	1.33
11	a	1123	CLA	O2D-CGD	5.18	1.45	1.33
11	A	1011	CLA	CHC-C1C	5.18	1.48	1.35
11	1	1137	CLA	O2A-C1	5.18	1.60	1.46
11	1	1117	CLA	O2D-CGD	5.18	1.45	1.33
11	1	1114	CLA	CHC-C1C	5.18	1.48	1.35
11	1	1111	CLA	O2A-C1	5.18	1.60	1.46
11	K	1401	CLA	O2D-CGD	5.18	1.45	1.33
11	b	1234	CLA	O2D-CGD	5.18	1.45	1.33
11	A	1126	CLA	O2D-CGD	5.18	1.45	1.33
11	K	1402	CLA	CHC-C1C	5.18	1.48	1.35
11	1	1117	CLA	CHC-C1C	5.18	1.48	1.35
11	B	1238	CLA	O2A-C1	5.18	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1228	CLA	O2A-C1	5.18	1.60	1.46
11	1	1118	CLA	O2A-C1	5.18	1.60	1.46
11	a	1129	CLA	O2D-CGD	5.18	1.45	1.33
11	a	1136	CLA	CHC-C1C	5.18	1.48	1.35
11	2	1206	CLA	O2A-C1	5.18	1.60	1.46
11	1	1118	CLA	O2D-CGD	5.18	1.45	1.33
11	A	1108	CLA	O2D-CGD	5.18	1.45	1.33
11	B	1225	CLA	O2A-C1	5.18	1.60	1.46
11	1	1105	CLA	O2A-C1	5.18	1.60	1.46
11	a	1110	CLA	CHC-C1C	5.18	1.48	1.35
11	k	1401	CLA	O2D-CGD	5.18	1.45	1.33
11	1	1134	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1216	CLA	O2D-CGD	5.17	1.45	1.33
11	2	1210	CLA	O2A-C1	5.17	1.60	1.46
11	A	1106	CLA	CHC-C1C	5.17	1.48	1.35
11	A	1801	CLA	CHC-C1C	5.17	1.48	1.35
11	1	1120	CLA	O2D-CGD	5.17	1.45	1.33
11	A	1123	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1204	CLA	O2D-CGD	5.17	1.45	1.33
11	b	1212	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1140	CLA	O2D-CGD	5.17	1.45	1.33
11	A	1124	CLA	O2D-CGD	5.17	1.45	1.33
11	b	1208	CLA	O2D-CGD	5.17	1.45	1.33
11	b	1240	CLA	O2D-CGD	5.17	1.45	1.33
11	a	1022	CLA	O2A-C1	5.17	1.60	1.46
11	b	1217	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1216	CLA	O2A-C1	5.17	1.60	1.46
11	1	1022	CLA	O2A-C1	5.17	1.60	1.46
11	b	1232	CLA	O2D-CGD	5.17	1.45	1.33
11	a	1110	CLA	O2A-C1	5.17	1.60	1.46
11	1	1106	CLA	O2D-CGD	5.17	1.45	1.33
11	b	1023	CLA	O2D-CGD	5.17	1.45	1.33
11	a	1012	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1220	CLA	CHC-C1C	5.17	1.48	1.35
11	b	1227	CLA	O2D-CGD	5.17	1.45	1.33
11	2	1228	CLA	O2A-C1	5.17	1.60	1.46
11	B	1210	CLA	O2D-CGD	5.17	1.45	1.33
11	a	1110	CLA	O2D-CGD	5.17	1.45	1.33
11	b	1205	CLA	O2D-CGD	5.17	1.45	1.33
11	8	1503	CLA	O2A-C1	5.16	1.60	1.46
11	b	1206	CLA	O2A-C1	5.16	1.60	1.46
11	B	1234	CLA	O2A-C1	5.16	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1215	CLA	CHC-C1C	5.16	1.48	1.35
11	b	1204	CLA	O2D-CGD	5.16	1.45	1.33
11	1	1801	CLA	O2D-CGD	5.16	1.45	1.33
11	b	1225	CLA	O2D-CGD	5.16	1.45	1.33
11	2	1219	CLA	O2D-CGD	5.16	1.45	1.33
11	2	1239	CLA	CHC-C1C	5.16	1.48	1.35
11	2	1203	CLA	O2A-C1	5.16	1.60	1.46
11	a	1116	CLA	O2D-CGD	5.16	1.45	1.33
11	a	1121	CLA	O2D-CGD	5.16	1.45	1.33
11	1	1129	CLA	O2D-CGD	5.16	1.45	1.33
11	2	1238	CLA	CHC-C1C	5.16	1.48	1.35
11	a	1133	CLA	O2D-CGD	5.16	1.45	1.33
11	a	1135	CLA	O2A-C1	5.16	1.60	1.46
11	b	1021	CLA	O2A-C1	5.16	1.60	1.46
11	1	1127	CLA	OBD-CAD	5.16	1.29	1.22
11	1	1126	CLA	O2D-CGD	5.16	1.45	1.33
11	b	1208	CLA	CHC-C1C	5.15	1.48	1.35
11	2	1235	CLA	O2A-C1	5.15	1.60	1.46
11	a	1118	CLA	O2D-CGD	5.15	1.45	1.33
11	l	1503	CLA	O2D-CGD	5.15	1.45	1.33
11	1	1104	CLA	O2D-CGD	5.15	1.45	1.33
11	B	1201	CLA	O2A-C1	5.15	1.60	1.46
11	0	1402	CLA	O2D-CGD	5.15	1.45	1.33
11	l	1501	CLA	O2A-C1	5.15	1.60	1.46
11	B	1229	CLA	O2A-C1	5.15	1.60	1.46
11	1	1022	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1128	CLA	O2A-C1	5.15	1.60	1.46
11	k	1401	CLA	O2A-C1	5.15	1.60	1.46
11	2	1234	CLA	O2D-CGD	5.15	1.45	1.33
11	a	1119	CLA	O2A-C1	5.15	1.60	1.46
11	2	1225	CLA	O2D-CGD	5.15	1.45	1.33
11	1	1127	CLA	O2D-CGD	5.15	1.45	1.33
11	8	1501	CLA	O2D-CGD	5.15	1.45	1.33
11	2	1217	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1114	CLA	O2D-CGD	5.15	1.45	1.33
11	B	1210	CLA	O2A-C1	5.15	1.60	1.46
11	8	1501	CLA	CHC-C1C	5.15	1.48	1.35
11	L	1501	CLA	O2D-CGD	5.15	1.45	1.33
11	a	1107	CLA	O2A-C1	5.15	1.60	1.46
11	1	1123	CLA	O2D-CGD	5.15	1.45	1.33
11	B	1223	CLA	O2D-CGD	5.15	1.45	1.33
11	a	1134	CLA	O2D-CGD	5.15	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1116	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1202	CLA	O2A-C1	5.14	1.60	1.46
11	A	1113	CLA	O2D-CGD	5.14	1.45	1.33
11	1	1132	CLA	O2A-C1	5.14	1.60	1.46
11	2	1203	CLA	CHC-C1C	5.14	1.48	1.35
11	A	1105	CLA	O2A-C1	5.14	1.60	1.46
11	B	1205	CLA	O2A-C1	5.14	1.60	1.46
11	A	1124	CLA	O2A-C1	5.14	1.60	1.46
11	A	1137	CLA	O2D-CGD	5.14	1.45	1.33
11	B	1224	CLA	O2A-C1	5.14	1.60	1.46
11	b	1216	CLA	O2A-C1	5.14	1.60	1.46
11	A	1136	CLA	CHC-C1C	5.14	1.48	1.35
11	a	1132	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1212	CLA	CHC-C1C	5.14	1.48	1.35
11	B	1204	CLA	CHC-C1C	5.14	1.48	1.35
11	1	1135	CLA	O2D-CGD	5.14	1.45	1.33
11	A	1012	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1213	CLA	O2A-C1	5.14	1.60	1.46
11	A	1131	CLA	O2D-CGD	5.14	1.45	1.33
11	1	1124	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1234	CLA	O2A-C1	5.14	1.60	1.46
11	2	1201	CLA	CHC-C1C	5.14	1.48	1.35
11	2	1209	CLA	O2D-CGD	5.14	1.45	1.33
11	B	1201	CLA	CHC-C1C	5.14	1.48	1.35
11	2	1232	CLA	O2D-CGD	5.14	1.45	1.33
11	B	1225	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1226	CLA	O2A-C1	5.13	1.60	1.46
11	a	1101	CLA	O2A-C1	5.13	1.60	1.46
11	A	1127	CLA	O2D-CGD	5.13	1.45	1.33
11	A	1130	CLA	O2D-CGD	5.13	1.45	1.33
11	1	1128	CLA	O2A-C1	5.13	1.60	1.46
11	1	1128	CLA	CHC-C1C	5.13	1.48	1.35
11	B	1206	CLA	O2A-C1	5.13	1.60	1.46
11	2	1212	CLA	O2D-CGD	5.13	1.45	1.33
11	a	1113	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1205	CLA	CHC-C1C	5.13	1.48	1.35
11	A	1126	CLA	O2A-C1	5.13	1.60	1.46
11	l	1503	CLA	O2A-C1	5.13	1.60	1.46
11	2	1218	CLA	O2D-CGD	5.13	1.45	1.33
11	a	1122	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1223	CLA	CHC-C1C	5.13	1.48	1.35
11	b	1219	CLA	O2A-C1	5.13	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1118	CLA	O2D-CGD	5.13	1.45	1.33
11	2	1215	CLA	CHC-C1C	5.13	1.48	1.35
11	K	1401	CLA	O2A-C1	5.13	1.60	1.46
11	a	1105	CLA	CHC-C1C	5.13	1.48	1.35
11	A	1117	CLA	C3B-C2B	5.12	1.47	1.40
11	b	1238	CLA	O2A-C1	5.12	1.60	1.46
11	a	1022	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1104	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1214	CLA	O2A-C1	5.12	1.60	1.46
11	B	1227	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1229	CLA	CHC-C1C	5.12	1.48	1.35
11	L	1503	CLA	O2A-C1	5.12	1.60	1.46
11	B	1222	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1135	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1112	CLA	O2D-CGD	5.12	1.45	1.33
11	A	1121	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1239	CLA	O2D-CGD	5.12	1.45	1.33
11	2	1240	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1213	CLA	O2A-C1	5.12	1.60	1.46
11	B	1206	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1220	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1118	CLA	CHC-C1C	5.12	1.48	1.35
11	L	1502	CLA	O2D-CGD	5.12	1.45	1.33
11	A	1132	CLA	O2D-CGD	5.12	1.45	1.33
11	A	1118	CLA	CHC-C1C	5.12	1.48	1.35
11	b	1222	CLA	O2A-C1	5.12	1.60	1.46
11	a	1117	CLA	O2D-CGD	5.12	1.45	1.33
11	2	1206	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1123	CLA	O2A-C1	5.12	1.60	1.46
11	B	1224	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1202	CLA	O2A-C1	5.12	1.60	1.46
11	1	1131	CLA	O2D-CGD	5.11	1.45	1.33
11	B	1209	CLA	O2D-CGD	5.11	1.45	1.33
11	1	1103	CLA	O2D-CGD	5.11	1.45	1.33
11	B	1202	CLA	O2D-CGD	5.11	1.45	1.33
11	b	1229	CLA	O2D-CGD	5.11	1.45	1.33
11	b	1222	CLA	O2D-CGD	5.11	1.45	1.33
11	2	1222	CLA	O2D-CGD	5.11	1.45	1.33
11	b	1023	CLA	O2A-C1	5.11	1.60	1.46
11	B	1215	CLA	O2D-CGD	5.11	1.45	1.33
11	B	1202	CLA	O2A-C1	5.11	1.60	1.46
11	b	1210	CLA	O2D-CGD	5.11	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1114	CLA	CHC-C1C	5.11	1.48	1.35
11	b	1214	CLA	O2D-CGD	5.11	1.45	1.33
11	2	1226	CLA	O2A-C1	5.11	1.60	1.46
11	a	1140	CLA	O2D-CGD	5.10	1.45	1.33
11	K	1402	CLA	O2D-CGD	5.10	1.45	1.33
11	b	1239	CLA	CHC-C1C	5.10	1.48	1.35
11	A	1137	CLA	O2A-C1	5.10	1.60	1.46
11	2	1214	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1224	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1234	CLA	O2A-C1	5.10	1.60	1.46
11	a	1127	CLA	CHC-C1C	5.10	1.48	1.35
11	a	1237	CLA	O2D-CGD	5.10	1.45	1.33
11	1	1107	CLA	O2D-CGD	5.10	1.45	1.33
11	a	1125	CLA	O2D-CGD	5.10	1.45	1.33
11	B	1239	CLA	O2D-CGD	5.10	1.45	1.33
11	0	1401	CLA	O2A-C1	5.10	1.60	1.46
11	1	1109	CLA	CHC-C1C	5.10	1.48	1.35
11	B	1231	CLA	CHC-C1C	5.10	1.48	1.35
11	2	1204	CLA	O2A-C1	5.10	1.60	1.46
11	A	1123	CLA	O2A-C1	5.10	1.60	1.46
11	a	1139	CLA	CHC-C1C	5.10	1.48	1.35
11	B	1212	CLA	O2D-CGD	5.10	1.45	1.33
11	B	1203	CLA	O2A-C1	5.09	1.60	1.46
11	a	1124	CLA	O2A-C1	5.09	1.60	1.46
11	2	1201	CLA	O2D-CGD	5.09	1.45	1.33
11	2	1226	CLA	O2D-CGD	5.09	1.45	1.33
11	2	1227	CLA	CHC-C1C	5.09	1.48	1.35
11	2	1229	CLA	O2A-C1	5.09	1.60	1.46
11	B	1021	CLA	CHC-C1C	5.09	1.48	1.35
11	a	1135	CLA	CHC-C1C	5.09	1.48	1.35
11	B	1211	CLA	O2D-CGD	5.09	1.45	1.33
11	A	1022	CLA	O2D-CGD	5.09	1.45	1.33
11	1	1237	CLA	O2D-CGD	5.09	1.45	1.33
11	B	1226	CLA	O2D-CGD	5.09	1.45	1.33
11	2	1229	CLA	O2D-CGD	5.09	1.45	1.33
11	B	1013	CLA	O2D-CGD	5.09	1.45	1.33
11	1	1104	CLA	O2A-C1	5.09	1.60	1.46
11	b	1213	CLA	O2A-C1	5.09	1.60	1.46
11	a	1011	CLA	O2A-C1	5.09	1.60	1.46
11	B	1221	CLA	O2D-CGD	5.09	1.45	1.33
11	L	1503	CLA	CHC-C1C	5.09	1.48	1.35
11	A	1120	CLA	O2D-CGD	5.09	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1134	CLA	O2D-CGD	5.09	1.45	1.33
11	l	1502	CLA	O2D-CGD	5.09	1.45	1.33
11	a	1011	CLA	CHC-C1C	5.08	1.48	1.35
11	B	1203	CLA	O2D-CGD	5.08	1.45	1.33
11	b	1221	CLA	O2D-CGD	5.08	1.45	1.33
11	2	1212	CLA	CHC-C1C	5.08	1.48	1.35
11	B	1021	CLA	O2D-CGD	5.08	1.45	1.33
11	a	1133	CLA	CHC-C1C	5.08	1.48	1.35
11	B	1234	CLA	O2D-CGD	5.08	1.45	1.33
11	a	1104	CLA	O2A-C1	5.08	1.60	1.46
11	a	1106	CLA	O2D-CGD	5.08	1.45	1.33
11	B	1236	CLA	O2D-CGD	5.08	1.45	1.33
11	B	1205	CLA	CHC-C1C	5.08	1.48	1.35
11	B	1207	CLA	O2D-CGD	5.08	1.45	1.33
11	1	1125	CLA	O2A-C1	5.08	1.60	1.46
11	1	1012	CLA	O2D-CGD	5.08	1.45	1.33
11	A	1129	CLA	O2D-CGD	5.08	1.45	1.33
11	A	1117	CLA	O2D-CGD	5.08	1.45	1.33
11	8	1501	CLA	O2A-C1	5.08	1.60	1.46
11	B	1023	CLA	O2A-C1	5.07	1.60	1.46
11	1	1801	CLA	C3C-C2C	5.07	1.47	1.36
11	2	1223	CLA	O2D-CGD	5.07	1.45	1.33
11	2	1207	CLA	O2D-CGD	5.07	1.45	1.33
11	2	1207	CLA	CHC-C1C	5.07	1.48	1.35
11	1	1137	CLA	O2D-CGD	5.07	1.45	1.33
11	b	1203	CLA	O2A-C1	5.07	1.60	1.46
11	B	1232	CLA	CHC-C1C	5.07	1.48	1.35
11	B	1201	CLA	O2D-CGD	5.07	1.45	1.33
11	A	1135	CLA	O2D-CGD	5.07	1.45	1.33
11	B	1204	CLA	O2A-C1	5.07	1.60	1.46
11	1	1111	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1221	CLA	O2A-C1	5.06	1.60	1.46
11	2	1234	CLA	CHC-C1C	5.06	1.47	1.35
11	a	1125	CLA	O2A-C1	5.06	1.60	1.46
11	b	1238	CLA	O2D-CGD	5.06	1.45	1.33
11	2	1210	CLA	O2D-CGD	5.06	1.45	1.33
11	A	1140	CLA	CHC-C1C	5.06	1.47	1.35
11	1	1110	CLA	O2A-C1	5.06	1.60	1.46
11	1	1011	CLA	O2A-C1	5.06	1.60	1.46
11	1	1011	CLA	O2D-CGD	5.06	1.45	1.33
11	A	1103	CLA	O2A-C1	5.06	1.60	1.46
11	1	1103	CLA	O2A-C1	5.06	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1110	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1236	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1211	CLA	O2D-CGD	5.06	1.45	1.33
11	1	1115	CLA	CHC-C1C	5.06	1.47	1.35
11	2	1238	CLA	O2D-CGD	5.05	1.45	1.33
11	a	1127	CLA	O2A-C1	5.05	1.60	1.46
11	B	1021	CLA	O2A-C1	5.05	1.60	1.46
11	a	1801	CLA	O2D-CGD	5.05	1.45	1.33
11	2	1206	CLA	CHC-C1C	5.05	1.47	1.35
11	1	1139	CLA	O2A-C1	5.05	1.60	1.46
11	2	1221	CLA	O2D-CGD	5.05	1.45	1.33
11	1	1133	CLA	CHC-C1C	5.05	1.47	1.35
11	2	1224	CLA	O2A-C1	5.05	1.60	1.46
11	1	1123	CLA	O2A-C1	5.04	1.60	1.46
11	A	1139	CLA	O2A-C1	5.04	1.60	1.46
11	B	1238	CLA	O2D-CGD	5.04	1.45	1.33
11	a	1137	CLA	O2D-CGD	5.04	1.45	1.33
11	1	1124	CLA	O2A-C1	5.04	1.60	1.46
11	A	1138	CLA	CHC-C1C	5.04	1.47	1.35
11	b	1234	CLA	CHC-C1C	5.04	1.47	1.35
11	A	1101	CLA	O2D-CGD	5.04	1.45	1.33
11	2	1021	CLA	O2A-C1	5.04	1.60	1.46
11	a	1103	CLA	O2A-C1	5.04	1.60	1.46
11	2	1225	CLA	O2A-C1	5.04	1.60	1.46
11	a	1124	CLA	O2D-CGD	5.04	1.45	1.33
11	A	1127	CLA	O2A-C1	5.03	1.60	1.46
11	b	1206	CLA	CHC-C1C	5.03	1.47	1.35
11	B	1205	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1101	CLA	O2A-C1	5.03	1.60	1.46
11	8	1503	CLA	C3B-C2B	5.03	1.47	1.40
11	2	1205	CLA	O2A-C1	5.03	1.60	1.46
11	L	1503	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1134	CLA	CHC-C1C	5.03	1.47	1.35
11	b	1201	CLA	O2A-C1	5.02	1.60	1.46
11	2	1205	CLA	O2D-CGD	5.02	1.45	1.33
11	B	1230	CLA	CHC-C1C	5.02	1.47	1.35
11	A	1103	CLA	O2D-CGD	5.02	1.45	1.33
11	A	1022	CLA	O2A-C1	5.02	1.60	1.46
11	a	1119	CLA	CHC-C1C	5.02	1.47	1.35
11	1	1102	CLA	O2D-CGD	5.02	1.45	1.33
11	B	1023	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1131	CLA	O2A-C1	5.01	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1110	CLA	O2A-C1	5.01	1.60	1.46
11	b	1226	CLA	O2D-CGD	5.01	1.45	1.33
11	A	1111	CLA	O2D-CGD	5.01	1.45	1.33
11	B	1220	CLA	O2D-CGD	5.01	1.45	1.33
11	B	1229	CLA	O2D-CGD	5.01	1.45	1.33
11	b	1223	CLA	C3B-C2B	5.01	1.47	1.40
11	a	1111	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1126	CLA	O2A-C1	5.01	1.60	1.46
11	b	1203	CLA	O2D-CGD	5.01	1.45	1.33
11	A	1104	CLA	O2A-C1	5.01	1.60	1.46
11	A	1012	CLA	O2A-C1	5.01	1.60	1.46
11	1	1011	CLA	CHC-C1C	5.00	1.47	1.35
11	a	1107	CLA	O2D-CGD	5.00	1.45	1.33
11	2	1219	CLA	O2A-C1	5.00	1.60	1.46
11	b	1235	CLA	O2A-C1	5.00	1.60	1.46
11	B	1227	CLA	CHC-C1C	4.99	1.47	1.35
11	b	1223	CLA	O2D-CGD	4.99	1.45	1.33
11	B	1215	CLA	O2A-C1	4.99	1.60	1.46
11	A	1011	CLA	O2A-C1	4.99	1.60	1.46
11	A	1105	CLA	O2D-CGD	4.98	1.45	1.33
12	A	2001	PQN	C10-C5	4.97	1.48	1.40
11	a	1011	CLA	C3B-C2B	4.97	1.47	1.40
11	B	1234	CLA	CHC-C1C	4.97	1.47	1.35
11	1	1132	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1207	CLA	CHC-C1C	4.96	1.47	1.35
11	A	1133	CLA	CHC-C1C	4.96	1.47	1.35
11	B	1206	CLA	CHC-C1C	4.96	1.47	1.35
11	A	1110	CLA	C3B-C2B	4.96	1.47	1.40
11	1	1127	CLA	O2A-C1	4.96	1.60	1.46
11	1	1126	CLA	O2A-C1	4.95	1.60	1.46
11	8	1502	CLA	O2D-CGD	4.95	1.45	1.33
11	A	1123	CLA	CHC-C1C	4.95	1.47	1.35
11	B	1240	CLA	C3B-C2B	4.95	1.47	1.40
12	b	2002	PQN	C10-C5	4.95	1.48	1.40
11	1	1101	CLA	O2A-C1	4.94	1.60	1.46
11	A	1012	CLA	C3D-C2D	4.92	1.48	1.39
11	b	1204	CLA	O2A-C1	4.92	1.60	1.46
11	B	1231	CLA	O2D-CGD	4.91	1.45	1.33
11	A	1110	CLA	O2D-CGD	4.91	1.45	1.33
11	2	1235	CLA	C3B-C2B	4.91	1.47	1.40
11	1	1137	CLA	C3B-C2B	4.91	1.47	1.40
11	A	1111	CLA	O2A-C1	4.91	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1240	CLA	C3C-C2C	4.91	1.47	1.36
12	a	2001	PQN	C10-C5	4.91	1.48	1.40
11	0	1402	CLA	C3B-C2B	4.90	1.47	1.40
11	A	1125	CLA	CHC-C1C	4.90	1.47	1.35
11	A	1122	CLA	O2D-CGD	4.90	1.45	1.33
11	A	1120	CLA	OBD-CAD	4.89	1.29	1.22
12	2	2002	PQN	C10-C5	4.89	1.48	1.40
11	a	1123	CLA	OBD-CAD	4.89	1.29	1.22
11	a	1801	CLA	C3C-C2C	4.89	1.47	1.36
11	K	1402	CLA	C3B-C2B	4.89	1.47	1.40
11	a	1111	CLA	O2A-C1	4.88	1.59	1.46
12	1	2001	PQN	C10-C5	4.88	1.48	1.40
12	B	2002	PQN	C10-C5	4.87	1.48	1.40
11	k	1402	CLA	C3B-C2B	4.86	1.47	1.40
11	2	1213	CLA	C3B-C2B	4.86	1.47	1.40
11	A	1119	CLA	C3C-C2C	4.86	1.47	1.36
11	a	1012	CLA	C3D-C2D	4.85	1.48	1.39
11	b	1231	CLA	O2D-CGD	4.85	1.45	1.33
11	b	1236	CLA	C3B-C2B	4.84	1.47	1.40
11	2	1209	CLA	OBD-CAD	4.84	1.29	1.22
11	a	1117	CLA	OBD-CAD	4.84	1.29	1.22
11	2	1202	CLA	OBD-CAD	4.83	1.29	1.22
11	A	1107	CLA	C3B-C2B	4.83	1.47	1.40
11	A	1109	CLA	OBD-CAD	4.83	1.29	1.22
11	a	1130	CLA	C3B-C2B	4.83	1.47	1.40
11	B	1222	CLA	OBD-CAD	4.82	1.29	1.22
11	b	1215	CLA	OBD-CAD	4.82	1.29	1.22
11	2	1222	CLA	OBD-CAD	4.82	1.29	1.22
11	b	1013	CLA	OBD-CAD	4.82	1.29	1.22
11	B	1205	CLA	OBD-CAD	4.82	1.29	1.22
11	2	1227	CLA	OBD-CAD	4.82	1.29	1.22
11	B	1210	CLA	OBD-CAD	4.81	1.29	1.22
11	B	1230	CLA	OBD-CAD	4.81	1.29	1.22
11	2	1201	CLA	OBD-CAD	4.81	1.29	1.22
11	B	1021	CLA	OBD-CAD	4.81	1.29	1.22
11	B	1213	CLA	OBD-CAD	4.81	1.29	1.22
11	b	1202	CLA	C3B-C2B	4.81	1.47	1.40
11	1	1108	CLA	OBD-CAD	4.81	1.29	1.22
11	A	1022	CLA	OBD-CAD	4.81	1.29	1.22
11	b	1231	CLA	OBD-CAD	4.81	1.29	1.22
11	2	1212	CLA	OBD-CAD	4.81	1.29	1.22
11	B	1212	CLA	OBD-CAD	4.81	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1139	CLA	OBD-CAD	4.80	1.29	1.22
11	2	1231	CLA	OBD-CAD	4.80	1.29	1.22
11	2	1213	CLA	OBD-CAD	4.80	1.29	1.22
11	1	1111	CLA	OBD-CAD	4.80	1.29	1.22
11	b	1225	CLA	OBD-CAD	4.80	1.29	1.22
11	B	1202	CLA	OBD-CAD	4.80	1.29	1.22
11	2	1211	CLA	OBD-CAD	4.80	1.29	1.22
11	a	1101	CLA	OBD-CAD	4.80	1.29	1.22
11	a	1137	CLA	C3B-C2B	4.80	1.47	1.40
11	a	1237	CLA	OBD-CAD	4.80	1.29	1.22
11	b	1023	CLA	OBD-CAD	4.80	1.29	1.22
11	b	1220	CLA	OBD-CAD	4.79	1.29	1.22
11	1	1114	CLA	OBD-CAD	4.79	1.29	1.22
11	0	1402	CLA	OBD-CAD	4.79	1.29	1.22
11	2	1232	CLA	OBD-CAD	4.79	1.29	1.22
11	1	1117	CLA	OBD-CAD	4.79	1.29	1.22
11	K	1402	CLA	C3C-C2C	4.79	1.46	1.36
11	l	1502	CLA	OBD-CAD	4.79	1.29	1.22
11	A	1125	CLA	C3B-C2B	4.79	1.47	1.40
11	A	1122	CLA	OBD-CAD	4.79	1.29	1.22
11	a	1114	CLA	OBD-CAD	4.79	1.29	1.22
11	2	1238	CLA	C3B-C2B	4.79	1.47	1.40
11	b	1230	CLA	OBD-CAD	4.79	1.29	1.22
11	a	1011	CLA	OBD-CAD	4.79	1.29	1.22
11	2	1021	CLA	OBD-CAD	4.79	1.29	1.22
11	1	1133	CLA	OBD-CAD	4.79	1.29	1.22
11	a	1104	CLA	OBD-CAD	4.78	1.29	1.22
11	a	1137	CLA	OBD-CAD	4.78	1.29	1.22
11	B	1231	CLA	OBD-CAD	4.78	1.29	1.22
11	2	1013	CLA	OBD-CAD	4.78	1.29	1.22
11	1	1012	CLA	C3D-C2D	4.78	1.48	1.39
11	A	1131	CLA	OBD-CAD	4.78	1.29	1.22
11	2	1240	CLA	OBD-CAD	4.78	1.29	1.22
11	B	1225	CLA	OBD-CAD	4.78	1.29	1.22
11	A	1117	CLA	OBD-CAD	4.78	1.29	1.22
11	2	1023	CLA	OBD-CAD	4.78	1.29	1.22
11	1	1011	CLA	OBD-CAD	4.78	1.29	1.22
11	b	1216	CLA	OBD-CAD	4.78	1.29	1.22
11	A	1116	CLA	OBD-CAD	4.78	1.29	1.22
11	B	1240	CLA	OBD-CAD	4.78	1.29	1.22
11	B	1201	CLA	OBD-CAD	4.78	1.29	1.22
11	2	1226	CLA	OBD-CAD	4.78	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1126	CLA	OBD-CAD	4.78	1.29	1.22
11	b	1232	CLA	OBD-CAD	4.78	1.29	1.22
11	A	1115	CLA	C3C-C2C	4.78	1.46	1.36
11	a	1126	CLA	OBD-CAD	4.78	1.29	1.22
11	2	1231	CLA	O2D-CGD	4.78	1.44	1.33
11	1	1129	CLA	OBD-CAD	4.78	1.29	1.22
11	1	1104	CLA	OBD-CAD	4.78	1.29	1.22
11	A	1138	CLA	OBD-CAD	4.78	1.29	1.22
11	A	1101	CLA	OBD-CAD	4.77	1.29	1.22
11	1	1130	CLA	OBD-CAD	4.77	1.29	1.22
11	A	1011	CLA	OBD-CAD	4.77	1.29	1.22
11	A	1135	CLA	OBD-CAD	4.77	1.29	1.22
11	A	1110	CLA	OBD-CAD	4.77	1.29	1.22
11	2	1239	CLA	OBD-CAD	4.77	1.29	1.22
11	1	1022	CLA	OBD-CAD	4.77	1.29	1.22
11	b	1207	CLA	OBD-CAD	4.77	1.29	1.22
11	b	1205	CLA	OBD-CAD	4.77	1.29	1.22
11	B	1013	CLA	OBD-CAD	4.77	1.29	1.22
11	a	1115	CLA	OBD-CAD	4.77	1.29	1.22
11	2	1215	CLA	OBD-CAD	4.77	1.29	1.22
11	A	1103	CLA	OBD-CAD	4.77	1.29	1.22
11	a	1129	CLA	OBD-CAD	4.77	1.29	1.22
11	a	1139	CLA	OBD-CAD	4.77	1.29	1.22
11	a	1110	CLA	OBD-CAD	4.77	1.29	1.22
11	2	1223	CLA	C3C-C2C	4.77	1.46	1.36
11	A	1117	CLA	C3C-C2C	4.77	1.46	1.36
11	b	1213	CLA	OBD-CAD	4.77	1.29	1.22
11	A	1111	CLA	OBD-CAD	4.77	1.29	1.22
11	B	1239	CLA	OBD-CAD	4.77	1.29	1.22
11	2	1208	CLA	OBD-CAD	4.76	1.29	1.22
11	B	1238	CLA	OBD-CAD	4.76	1.29	1.22
11	B	1229	CLA	OBD-CAD	4.76	1.29	1.22
11	1	1128	CLA	OBD-CAD	4.76	1.29	1.22
11	a	1012	CLA	OBD-CAD	4.76	1.29	1.22
11	b	1213	CLA	C3B-C2B	4.76	1.47	1.40
11	1	1103	CLA	OBD-CAD	4.76	1.29	1.22
11	A	1108	CLA	OBD-CAD	4.76	1.29	1.22
11	b	1229	CLA	C3C-C2C	4.76	1.46	1.36
11	B	1206	CLA	OBD-CAD	4.76	1.29	1.22
11	1	1140	CLA	OBD-CAD	4.76	1.29	1.22
11	b	1240	CLA	OBD-CAD	4.76	1.29	1.22
11	1	1107	CLA	OBD-CAD	4.76	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	0	1402	CLA	C3C-C2C	4.76	1.46	1.36
11	B	1228	CLA	C3C-C2C	4.76	1.46	1.36
11	b	1021	CLA	OBD-CAD	4.76	1.29	1.22
11	A	1801	CLA	OBD-CAD	4.76	1.29	1.22
11	a	1128	CLA	OBD-CAD	4.76	1.29	1.22
11	1	1130	CLA	C3C-C2C	4.76	1.46	1.36
11	k	1402	CLA	OBD-CAD	4.76	1.29	1.22
11	a	1134	CLA	OBD-CAD	4.76	1.29	1.22
11	a	1117	CLA	C3B-C2B	4.76	1.47	1.40
11	1	1116	CLA	OBD-CAD	4.76	1.29	1.22
11	1	1113	CLA	OBD-CAD	4.76	1.29	1.22
11	a	1113	CLA	OBD-CAD	4.76	1.28	1.22
11	b	1210	CLA	OBD-CAD	4.76	1.28	1.22
11	2	1230	CLA	OBD-CAD	4.75	1.28	1.22
11	2	1211	CLA	C3B-C2B	4.75	1.47	1.40
11	1	1107	CLA	C3B-C2B	4.75	1.47	1.40
11	b	1227	CLA	OBD-CAD	4.75	1.28	1.22
11	B	1226	CLA	OBD-CAD	4.75	1.28	1.22
11	2	1219	CLA	OBD-CAD	4.75	1.28	1.22
11	A	1107	CLA	OBD-CAD	4.75	1.28	1.22
11	1	1132	CLA	OBD-CAD	4.75	1.28	1.22
11	2	1229	CLA	OBD-CAD	4.75	1.28	1.22
11	1	1123	CLA	OBD-CAD	4.75	1.28	1.22
11	A	1104	CLA	C3C-C2C	4.75	1.46	1.36
11	1	1139	CLA	OBD-CAD	4.75	1.28	1.22
11	a	1105	CLA	OBD-CAD	4.75	1.28	1.22
11	a	1138	CLA	OBD-CAD	4.75	1.28	1.22
11	a	1237	CLA	C3B-C2B	4.75	1.47	1.40
11	b	1218	CLA	OBD-CAD	4.75	1.28	1.22
11	A	1132	CLA	OBD-CAD	4.75	1.28	1.22
11	1	1101	CLA	OBD-CAD	4.75	1.28	1.22
11	a	1115	CLA	C3B-C2B	4.75	1.47	1.40
11	B	1211	CLA	C3B-C2B	4.75	1.47	1.40
11	a	1116	CLA	OBD-CAD	4.75	1.28	1.22
11	b	1234	CLA	OBD-CAD	4.75	1.28	1.22
11	2	1221	CLA	OBD-CAD	4.75	1.28	1.22
11	B	1217	CLA	C3C-C2C	4.75	1.46	1.36
11	b	1220	CLA	C3C-C2C	4.75	1.46	1.36
11	b	1239	CLA	OBD-CAD	4.75	1.28	1.22
11	a	1112	CLA	OBD-CAD	4.74	1.28	1.22
11	2	1226	CLA	C3B-C2B	4.74	1.47	1.40
11	1	1120	CLA	OBD-CAD	4.74	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1135	CLA	OBD-CAD	4.74	1.28	1.22
11	b	1217	CLA	C3C-C2C	4.74	1.46	1.36
11	B	1203	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1133	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1128	CLA	C3C-C2C	4.74	1.46	1.36
11	1	1118	CLA	OBD-CAD	4.74	1.28	1.22
11	0	1401	CLA	OBD-CAD	4.74	1.28	1.22
11	A	1114	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1140	CLA	OBD-CAD	4.74	1.28	1.22
11	B	1223	CLA	C3C-C2C	4.74	1.46	1.36
11	b	1224	CLA	C3B-C2B	4.74	1.46	1.40
11	B	1219	CLA	C3B-C2B	4.74	1.46	1.40
11	a	1132	CLA	OBD-CAD	4.74	1.28	1.22
11	b	1208	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1111	CLA	OBD-CAD	4.74	1.28	1.22
11	1	1801	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1120	CLA	OBD-CAD	4.74	1.28	1.22
11	B	1204	CLA	OBD-CAD	4.74	1.28	1.22
11	A	1103	CLA	C3B-C2B	4.74	1.46	1.40
11	A	1133	CLA	OBD-CAD	4.74	1.28	1.22
11	A	1012	CLA	C3C-C2C	4.74	1.46	1.36
11	1	1112	CLA	OBD-CAD	4.74	1.28	1.22
11	1	1102	CLA	OBD-CAD	4.74	1.28	1.22
11	a	1120	CLA	C3C-C2C	4.74	1.46	1.36
11	b	1230	CLA	C3B-C2B	4.74	1.46	1.40
11	b	1212	CLA	OBD-CAD	4.74	1.28	1.22
11	b	1222	CLA	OBD-CAD	4.73	1.28	1.22
11	k	1401	CLA	OBD-CAD	4.73	1.28	1.22
11	B	1215	CLA	OBD-CAD	4.73	1.28	1.22
11	K	1401	CLA	OBD-CAD	4.73	1.28	1.22
11	l	1501	CLA	OBD-CAD	4.73	1.28	1.22
11	b	1229	CLA	OBD-CAD	4.73	1.28	1.22
11	b	1206	CLA	OBD-CAD	4.73	1.28	1.22
11	l	1503	CLA	OBD-CAD	4.73	1.28	1.22
11	2	1228	CLA	OBD-CAD	4.73	1.28	1.22
11	B	1218	CLA	OBD-CAD	4.73	1.28	1.22
11	a	1122	CLA	OBD-CAD	4.73	1.28	1.22
11	a	1105	CLA	C3B-C2B	4.73	1.46	1.40
11	1	1127	CLA	C3B-C2B	4.73	1.46	1.40
11	A	1121	CLA	C3B-C2B	4.73	1.46	1.40
11	b	1203	CLA	OBD-CAD	4.73	1.28	1.22
11	a	1108	CLA	C3B-C2B	4.73	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1103	CLA	C3C-C2C	4.73	1.46	1.36
11	B	1211	CLA	C3C-C2C	4.73	1.46	1.36
11	a	1108	CLA	OBD-CAD	4.73	1.28	1.22
11	A	1128	CLA	OBD-CAD	4.73	1.28	1.22
11	b	1201	CLA	OBD-CAD	4.73	1.28	1.22
11	2	1205	CLA	OBD-CAD	4.73	1.28	1.22
11	A	1107	CLA	O2D-CGD	4.73	1.44	1.33
11	a	1131	CLA	OBD-CAD	4.73	1.28	1.22
11	8	1501	CLA	OBD-CAD	4.73	1.28	1.22
11	B	1232	CLA	OBD-CAD	4.72	1.28	1.22
11	1	1110	CLA	OBD-CAD	4.72	1.28	1.22
11	b	1217	CLA	C3B-C2B	4.72	1.46	1.40
11	B	1230	CLA	C3B-C2B	4.72	1.46	1.40
11	1	1120	CLA	C3C-C2C	4.72	1.46	1.36
11	B	1224	CLA	OBD-CAD	4.72	1.28	1.22
11	a	1106	CLA	OBD-CAD	4.72	1.28	1.22
11	A	1112	CLA	OBD-CAD	4.72	1.28	1.22
11	a	1136	CLA	OBD-CAD	4.72	1.28	1.22
11	B	1224	CLA	C3B-C2B	4.72	1.46	1.40
11	2	1218	CLA	OBD-CAD	4.72	1.28	1.22
11	a	1102	CLA	OBD-CAD	4.72	1.28	1.22
11	1	1105	CLA	OBD-CAD	4.72	1.28	1.22
11	A	1126	CLA	OBD-CAD	4.72	1.28	1.22
11	A	1123	CLA	OBD-CAD	4.72	1.28	1.22
11	b	1220	CLA	C3B-C2B	4.72	1.46	1.40
11	b	1202	CLA	OBD-CAD	4.72	1.28	1.22
11	1	1135	CLA	C3C-C2C	4.72	1.46	1.36
11	2	1225	CLA	OBD-CAD	4.72	1.28	1.22
11	K	1402	CLA	OBD-CAD	4.72	1.28	1.22
11	b	1209	CLA	C3B-C2B	4.72	1.46	1.40
11	B	1208	CLA	OBD-CAD	4.72	1.28	1.22
11	2	1239	CLA	C3C-C2C	4.71	1.46	1.36
11	a	1110	CLA	C3B-C2B	4.71	1.46	1.40
11	2	1228	CLA	C3C-C2C	4.71	1.46	1.36
11	1	1128	CLA	C3C-C2C	4.71	1.46	1.36
11	b	1227	CLA	C3C-C2C	4.71	1.46	1.36
11	A	1130	CLA	OBD-CAD	4.71	1.28	1.22
11	B	1228	CLA	OBD-CAD	4.71	1.28	1.22
11	2	1206	CLA	OBD-CAD	4.71	1.28	1.22
11	2	1207	CLA	OBD-CAD	4.71	1.28	1.22
11	a	1135	CLA	C3C-C2C	4.71	1.46	1.36
11	B	1222	CLA	C3C-C2C	4.71	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1216	CLA	C3C-C2C	4.71	1.46	1.36
11	1	1122	CLA	OBD-CAD	4.71	1.28	1.22
11	B	1201	CLA	C3C-C2C	4.71	1.46	1.36
11	b	1228	CLA	C3C-C2C	4.71	1.46	1.36
11	B	1227	CLA	OBD-CAD	4.71	1.28	1.22
11	1	1134	CLA	OBD-CAD	4.71	1.28	1.22
11	a	1109	CLA	OBD-CAD	4.71	1.28	1.22
11	1	1136	CLA	OBD-CAD	4.70	1.28	1.22
11	A	1134	CLA	OBD-CAD	4.70	1.28	1.22
11	B	1209	CLA	OBD-CAD	4.70	1.28	1.22
11	A	1102	CLA	OBD-CAD	4.70	1.28	1.22
11	1	1122	CLA	C3B-C2B	4.70	1.46	1.40
11	B	1224	CLA	C3C-C2C	4.70	1.46	1.36
11	2	1204	CLA	OBD-CAD	4.70	1.28	1.22
11	a	1801	CLA	OBD-CAD	4.70	1.28	1.22
11	B	1236	CLA	C3C-C2C	4.70	1.46	1.36
11	a	1124	CLA	C3C-C2C	4.70	1.46	1.36
11	a	1126	CLA	C3B-C2B	4.70	1.46	1.40
11	A	1112	CLA	C3C-C2C	4.70	1.46	1.36
11	b	1226	CLA	C3C-C2C	4.70	1.46	1.36
11	A	1121	CLA	C3C-C2C	4.70	1.46	1.36
11	2	1219	CLA	C3C-C2C	4.70	1.46	1.36
11	A	1022	CLA	C3C-C2C	4.70	1.46	1.36
11	a	1022	CLA	C3D-C2D	4.70	1.47	1.39
11	1	1138	CLA	OBD-CAD	4.70	1.28	1.22
11	b	1209	CLA	OBD-CAD	4.70	1.28	1.22
11	1	1108	CLA	C3C-C2C	4.70	1.46	1.36
11	l	1502	CLA	C3B-C2B	4.70	1.46	1.40
11	1	1140	CLA	C3C-C2C	4.70	1.46	1.36
11	a	1130	CLA	OBD-CAD	4.70	1.28	1.22
11	L	1501	CLA	C3C-C2C	4.69	1.46	1.36
11	1	1012	CLA	C3C-C2C	4.69	1.46	1.36
11	b	1218	CLA	C3C-C2C	4.69	1.46	1.36
11	k	1402	CLA	C3C-C2C	4.69	1.46	1.36
11	2	1214	CLA	OBD-CAD	4.69	1.28	1.22
11	2	1230	CLA	C3B-C2B	4.69	1.46	1.40
11	A	1012	CLA	OBD-CAD	4.69	1.28	1.22
11	2	1210	CLA	OBD-CAD	4.69	1.28	1.22
11	A	1109	CLA	C3C-C2C	4.69	1.46	1.36
11	1	1106	CLA	OBD-CAD	4.69	1.28	1.22
11	B	1234	CLA	OBD-CAD	4.69	1.28	1.22
11	b	1021	CLA	C3C-C2C	4.69	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1134	CLA	C3B-C2B	4.69	1.46	1.40
11	a	1109	CLA	C3C-C2C	4.69	1.46	1.36
11	b	1223	CLA	OBD-CAD	4.69	1.28	1.22
11	a	1132	CLA	C3C-C2C	4.69	1.46	1.36
11	a	1113	CLA	C3B-C2B	4.69	1.46	1.40
11	b	1203	CLA	C3C-C2C	4.69	1.46	1.36
11	b	1221	CLA	OBD-CAD	4.69	1.28	1.22
11	1	1129	CLA	C3C-C2C	4.69	1.46	1.36
11	a	1110	CLA	C3C-C2C	4.69	1.46	1.36
11	2	1240	CLA	C3B-C2B	4.69	1.46	1.40
11	1	1139	CLA	C3C-C2C	4.69	1.46	1.36
11	1	1114	CLA	C3C-C2C	4.69	1.46	1.36
11	2	1212	CLA	C3B-C2B	4.68	1.46	1.40
11	b	1238	CLA	C3B-C2B	4.68	1.46	1.40
11	a	1118	CLA	OBD-CAD	4.68	1.28	1.22
11	1	1131	CLA	OBD-CAD	4.68	1.28	1.22
11	1	1115	CLA	C3B-C2B	4.68	1.46	1.40
11	L	1502	CLA	OBD-CAD	4.68	1.28	1.22
11	2	1238	CLA	OBD-CAD	4.68	1.28	1.22
11	A	1105	CLA	OBD-CAD	4.68	1.28	1.22
11	2	1236	CLA	C3B-C2B	4.68	1.46	1.40
11	B	1201	CLA	C3B-C2B	4.68	1.46	1.40
11	B	1235	CLA	OBD-CAD	4.68	1.28	1.22
11	b	1239	CLA	C3C-C2C	4.68	1.46	1.36
11	2	1235	CLA	OBD-CAD	4.68	1.28	1.22
11	b	1234	CLA	C3C-C2C	4.68	1.46	1.36
11	a	1121	CLA	OBD-CAD	4.68	1.28	1.22
11	a	1130	CLA	C3C-C2C	4.68	1.46	1.36
11	A	1124	CLA	OBD-CAD	4.68	1.28	1.22
11	B	1220	CLA	OBD-CAD	4.68	1.28	1.22
11	b	1235	CLA	C3C-C2C	4.68	1.46	1.36
11	a	1116	CLA	C3B-C2B	4.68	1.46	1.40
11	B	1208	CLA	C3C-C2C	4.68	1.46	1.36
11	1	1102	CLA	C3C-C2C	4.68	1.46	1.36
11	B	1207	CLA	OBD-CAD	4.68	1.28	1.22
11	1	1501	CLA	C3C-C2C	4.68	1.46	1.36
11	2	1226	CLA	C3C-C2C	4.68	1.46	1.36
11	A	1126	CLA	C3C-C2C	4.67	1.46	1.36
11	a	1101	CLA	C3C-C2C	4.67	1.46	1.36
11	2	1239	CLA	C3B-C2B	4.67	1.46	1.40
11	1	1109	CLA	OBD-CAD	4.67	1.28	1.22
11	A	1118	CLA	OBD-CAD	4.67	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1502	CLA	OBD-CAD	4.67	1.28	1.22
11	A	1130	CLA	C3C-C2C	4.67	1.46	1.36
11	L	1503	CLA	OBD-CAD	4.67	1.28	1.22
11	8	1503	CLA	OBD-CAD	4.67	1.28	1.22
11	A	1140	CLA	OBD-CAD	4.67	1.28	1.22
11	b	1224	CLA	C3C-C2C	4.67	1.46	1.36
11	b	1222	CLA	C3C-C2C	4.67	1.46	1.36
11	a	1022	CLA	OBD-CAD	4.67	1.28	1.22
11	1	1124	CLA	OBD-CAD	4.67	1.28	1.22
11	8	1502	CLA	C3C-C2C	4.67	1.46	1.36
11	b	1201	CLA	C3C-C2C	4.67	1.46	1.36
11	B	1202	CLA	C3C-C2C	4.67	1.46	1.36
11	2	1238	CLA	C3C-C2C	4.67	1.46	1.36
11	b	1235	CLA	OBD-CAD	4.67	1.28	1.22
11	A	1104	CLA	OBD-CAD	4.67	1.28	1.22
11	L	1501	CLA	OBD-CAD	4.67	1.28	1.22
11	b	1217	CLA	OBD-CAD	4.67	1.28	1.22
11	B	1216	CLA	C3C-C2C	4.67	1.46	1.36
11	2	1217	CLA	C3C-C2C	4.67	1.46	1.36
11	1	1119	CLA	OBD-CAD	4.67	1.28	1.22
11	1	1109	CLA	C3C-C2C	4.67	1.46	1.36
11	B	1210	CLA	C3B-C2B	4.67	1.46	1.40
11	2	1201	CLA	C3B-C2B	4.67	1.46	1.40
11	2	1229	CLA	C3C-C2C	4.67	1.46	1.36
11	A	1132	CLA	C3C-C2C	4.67	1.46	1.36
11	a	1106	CLA	C3C-C2C	4.67	1.46	1.36
11	B	1212	CLA	C3C-C2C	4.67	1.46	1.36
11	1	1104	CLA	C3C-C2C	4.66	1.46	1.36
11	B	1229	CLA	C3C-C2C	4.66	1.46	1.36
11	1	1119	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1224	CLA	OBD-CAD	4.66	1.28	1.22
11	b	1204	CLA	OBD-CAD	4.66	1.28	1.22
11	2	1232	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1113	CLA	C3B-C2B	4.66	1.46	1.40
11	A	1136	CLA	OBD-CAD	4.66	1.28	1.22
11	B	1211	CLA	OBD-CAD	4.66	1.28	1.22
11	2	1220	CLA	OBD-CAD	4.66	1.28	1.22
11	1	1113	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1211	CLA	C3B-C2B	4.66	1.46	1.40
11	B	1240	CLA	C3C-C2C	4.66	1.46	1.36
11	a	1129	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1101	CLA	C3C-C2C	4.66	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1133	CLA	C3C-C2C	4.66	1.46	1.36
11	B	1203	CLA	C3C-C2C	4.66	1.46	1.36
11	2	1224	CLA	OBD-CAD	4.66	1.28	1.22
11	b	1213	CLA	C3C-C2C	4.66	1.46	1.36
11	1	1137	CLA	C3C-C2C	4.66	1.46	1.36
11	1	1104	CLA	C3B-C2B	4.66	1.46	1.40
11	1	1136	CLA	C3C-C2C	4.66	1.46	1.36
11	B	1216	CLA	OBD-CAD	4.66	1.28	1.22
11	B	1235	CLA	C3B-C2B	4.66	1.46	1.40
11	1	1124	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1228	CLA	OBD-CAD	4.66	1.28	1.22
11	B	1213	CLA	C3C-C2C	4.66	1.46	1.36
11	1	1115	CLA	C3C-C2C	4.66	1.46	1.36
11	1	1022	CLA	C3C-C2C	4.65	1.46	1.36
11	1	1107	CLA	C3C-C2C	4.65	1.46	1.36
11	A	1113	CLA	OBD-CAD	4.65	1.28	1.22
11	a	1125	CLA	C3C-C2C	4.65	1.46	1.36
11	B	1235	CLA	C3C-C2C	4.65	1.46	1.36
11	B	1212	CLA	C3B-C2B	4.65	1.46	1.40
11	b	1238	CLA	C3C-C2C	4.65	1.46	1.36
11	B	1214	CLA	OBD-CAD	4.65	1.28	1.22
11	a	1124	CLA	OBD-CAD	4.65	1.28	1.22
11	a	1022	CLA	C3C-C2C	4.65	1.46	1.36
11	B	1023	CLA	OBD-CAD	4.65	1.28	1.22
11	b	1209	CLA	C3C-C2C	4.65	1.46	1.36
11	a	1106	CLA	C3B-C2B	4.65	1.46	1.40
11	A	1237	CLA	OBD-CAD	4.65	1.28	1.22
11	2	1216	CLA	OBD-CAD	4.64	1.28	1.22
11	2	1231	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1221	CLA	C3B-C2B	4.64	1.46	1.40
11	2	1201	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1102	CLA	C3C-C2C	4.64	1.46	1.36
11	2	1227	CLA	C3C-C2C	4.64	1.46	1.36
11	1	1130	CLA	C3B-C2B	4.64	1.46	1.40
11	L	1502	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1103	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1239	CLA	C3B-C2B	4.64	1.46	1.40
11	2	1204	CLA	C3C-C2C	4.64	1.46	1.36
11	b	1210	CLA	C3B-C2B	4.64	1.46	1.40
11	A	1128	CLA	C3C-C2C	4.64	1.46	1.36
11	2	1240	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1107	CLA	OBD-CAD	4.64	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1236	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1236	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1122	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1013	CLA	C3C-C2C	4.64	1.46	1.36
11	A	1124	CLA	C3C-C2C	4.64	1.46	1.36
11	2	1236	CLA	C3C-C2C	4.64	1.46	1.36
11	1	1109	CLA	C3B-C2B	4.64	1.46	1.40
11	A	1122	CLA	C3B-C2B	4.64	1.46	1.40
11	1	1131	CLA	C3B-C2B	4.64	1.46	1.40
11	B	1218	CLA	C3C-C2C	4.64	1.46	1.36
11	A	1129	CLA	OBD-CAD	4.64	1.28	1.22
11	2	1202	CLA	C3B-C2B	4.64	1.46	1.40
11	2	1220	CLA	C3B-C2B	4.64	1.46	1.40
11	a	1116	CLA	C3C-C2C	4.64	1.46	1.36
11	2	1208	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1219	CLA	OBD-CAD	4.63	1.28	1.22
11	B	1213	CLA	C3B-C2B	4.63	1.46	1.40
11	B	1227	CLA	C3C-C2C	4.63	1.46	1.36
11	A	1137	CLA	OBD-CAD	4.63	1.28	1.22
11	1	1125	CLA	C3C-C2C	4.63	1.46	1.36
11	A	1139	CLA	C3C-C2C	4.63	1.46	1.36
11	A	1106	CLA	OBD-CAD	4.63	1.28	1.22
11	2	1224	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1211	CLA	OBD-CAD	4.63	1.28	1.22
11	2	1231	CLA	C3C-C2C	4.63	1.46	1.36
11	8	1503	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1102	CLA	C3B-C2B	4.63	1.46	1.40
11	1	1116	CLA	C3C-C2C	4.63	1.46	1.36
11	a	1012	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1215	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1137	CLA	OBD-CAD	4.63	1.28	1.22
11	a	1115	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1225	CLA	C3B-C2B	4.63	1.46	1.40
11	B	1221	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1121	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1215	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1134	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1133	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1238	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1112	CLA	C3C-C2C	4.62	1.46	1.36
11	A	1127	CLA	C3B-C2B	4.62	1.46	1.40
11	1	1124	CLA	C3B-C2B	4.62	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1131	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1112	CLA	C3C-C2C	4.62	1.46	1.36
11	b	1021	CLA	C3B-C2B	4.62	1.46	1.40
11	a	1140	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1219	CLA	OBD-CAD	4.62	1.28	1.22
11	a	1137	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1105	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1121	CLA	OBD-CAD	4.62	1.28	1.22
11	a	1117	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1132	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1113	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1106	CLA	C3B-C2B	4.62	1.46	1.40
11	1	1134	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1119	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1140	CLA	C3B-C2B	4.61	1.46	1.40
11	2	1203	CLA	OBD-CAD	4.61	1.28	1.22
11	b	1211	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1108	CLA	C3B-C2B	4.61	1.46	1.40
11	B	1239	CLA	C3B-C2B	4.61	1.46	1.40
11	k	1401	CLA	C3C-C2C	4.61	1.46	1.36
11	b	1231	CLA	C3C-C2C	4.61	1.46	1.36
11	b	1214	CLA	OBD-CAD	4.61	1.28	1.22
11	a	1118	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1129	CLA	C3B-C2B	4.61	1.46	1.40
11	A	1133	CLA	C3C-C2C	4.61	1.46	1.36
11	2	1215	CLA	C3C-C2C	4.61	1.46	1.36
11	2	1013	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1110	CLA	C3C-C2C	4.61	1.46	1.36
11	2	1021	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1114	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1122	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1136	CLA	C3C-C2C	4.61	1.46	1.36
11	B	1228	CLA	C3B-C2B	4.61	1.46	1.40
11	B	1238	CLA	C3B-C2B	4.61	1.46	1.40
11	a	1135	CLA	C3B-C2B	4.61	1.46	1.40
11	A	1102	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1127	CLA	OBD-CAD	4.60	1.28	1.22
11	a	1131	CLA	C3B-C2B	4.60	1.46	1.40
11	A	1120	CLA	C3C-C2C	4.60	1.46	1.36
11	1	1127	CLA	C3C-C2C	4.60	1.46	1.36
11	1	1117	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1115	CLA	OBD-CAD	4.60	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1225	CLA	C3B-C2B	4.60	1.46	1.40
11	a	1131	CLA	C3C-C2C	4.60	1.46	1.36
11	b	1225	CLA	C3C-C2C	4.60	1.46	1.36
11	b	1222	CLA	C3B-C2B	4.60	1.46	1.40
11	B	1217	CLA	C3B-C2B	4.60	1.46	1.40
11	b	1207	CLA	C3B-C2B	4.60	1.46	1.40
11	1	1135	CLA	OBD-CAD	4.60	1.28	1.22
11	2	1234	CLA	OBD-CAD	4.60	1.28	1.22
11	L	1503	CLA	C3B-C2B	4.60	1.46	1.40
11	B	1209	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1224	CLA	C3B-C2B	4.60	1.46	1.40
11	A	1115	CLA	C3B-C2B	4.60	1.46	1.40
11	B	1220	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1237	CLA	C3B-C2B	4.60	1.46	1.40
11	8	1501	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1106	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1135	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1214	CLA	C3B-C2B	4.59	1.46	1.40
11	b	1232	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1129	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1021	CLA	C3C-C2C	4.59	1.46	1.36
11	2	1210	CLA	C3B-C2B	4.59	1.46	1.40
11	a	1122	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1237	CLA	C3B-C2B	4.59	1.46	1.40
11	B	1209	CLA	C3B-C2B	4.59	1.46	1.40
11	a	1118	CLA	C3B-C2B	4.59	1.46	1.40
11	2	1207	CLA	C3B-C2B	4.59	1.46	1.40
11	B	1013	CLA	C3D-C2D	4.59	1.47	1.39
11	a	1103	CLA	OBD-CAD	4.59	1.28	1.22
11	1	1118	CLA	C3B-C2B	4.59	1.46	1.40
11	b	1206	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1125	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1138	CLA	C3C-C2C	4.59	1.46	1.36
11	L	1502	CLA	C3B-C2B	4.59	1.46	1.40
11	8	1502	CLA	C3B-C2B	4.59	1.46	1.40
11	b	1238	CLA	OBD-CAD	4.59	1.28	1.22
11	2	1212	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1134	CLA	C3B-C2B	4.59	1.46	1.40
11	a	1105	CLA	C3C-C2C	4.59	1.46	1.36
11	b	1232	CLA	C3B-C2B	4.59	1.46	1.40
11	B	1239	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1136	CLA	C3C-C2C	4.59	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1121	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1221	CLA	OBD-CAD	4.59	1.28	1.22
11	a	1011	CLA	C3C-C2C	4.58	1.46	1.36
11	A	1113	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1209	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1104	CLA	C3C-C2C	4.58	1.46	1.36
11	b	1208	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1222	CLA	C3C-C2C	4.58	1.46	1.36
11	K	1401	CLA	C3C-C2C	4.58	1.46	1.36
11	A	1022	CLA	C3D-C2D	4.58	1.47	1.39
11	b	1230	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1225	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1208	CLA	C3B-C2B	4.58	1.46	1.40
11	1	1116	CLA	C3B-C2B	4.58	1.46	1.40
11	A	1137	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1139	CLA	C3B-C2B	4.58	1.46	1.40
11	B	1226	CLA	C3C-C2C	4.58	1.46	1.36
11	0	1401	CLA	C3C-C2C	4.58	1.46	1.36
11	l	1503	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1131	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1123	CLA	C3B-C2B	4.57	1.46	1.40
11	2	1218	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1223	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1110	CLA	C3C-C2C	4.57	1.46	1.36
11	B	1218	CLA	C3B-C2B	4.57	1.46	1.40
11	b	1204	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1136	CLA	C3B-C2B	4.57	1.46	1.40
11	1	1136	CLA	C3B-C2B	4.57	1.46	1.40
11	a	1127	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1101	CLA	C3B-C2B	4.57	1.46	1.40
11	2	1230	CLA	C3C-C2C	4.57	1.46	1.36
11	A	1127	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1125	CLA	C3B-C2B	4.56	1.46	1.40
11	a	1127	CLA	C3B-C2B	4.56	1.46	1.40
11	b	1240	CLA	C3B-C2B	4.56	1.46	1.40
11	a	1114	CLA	C3C-C2C	4.56	1.46	1.36
11	2	1211	CLA	C3C-C2C	4.56	1.46	1.36
11	b	1214	CLA	C3B-C2B	4.56	1.46	1.40
11	2	1216	CLA	C3C-C2C	4.56	1.46	1.36
11	2	1225	CLA	C3C-C2C	4.56	1.46	1.36
11	a	1108	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1135	CLA	C3B-C2B	4.55	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1124	CLA	C3B-C2B	4.55	1.46	1.40
11	b	1219	CLA	C3C-C2C	4.55	1.46	1.36
11	b	1236	CLA	OBD-CAD	4.55	1.28	1.22
11	l	1502	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1102	CLA	C3B-C2B	4.55	1.46	1.40
11	B	1219	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1138	CLA	C3B-C2B	4.55	1.46	1.40
11	B	1013	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1136	CLA	C3B-C2B	4.55	1.46	1.40
11	B	1231	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1214	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1126	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1208	CLA	C3B-C2B	4.55	1.46	1.40
11	2	1221	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1011	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1022	CLA	C3D-C2D	4.55	1.47	1.39
11	a	1134	CLA	C3B-C2B	4.54	1.46	1.40
11	1	1012	CLA	OBD-CAD	4.54	1.28	1.22
11	2	1228	CLA	C3B-C2B	4.54	1.46	1.40
11	A	1108	CLA	C3B-C2B	4.54	1.46	1.40
11	A	1011	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1122	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1107	CLA	C3B-C2B	4.54	1.46	1.40
11	b	1212	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1106	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1138	CLA	C3C-C2C	4.53	1.46	1.36
11	A	1105	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1101	CLA	C3C-C2C	4.53	1.46	1.36
11	b	1202	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1107	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1139	CLA	C3C-C2C	4.53	1.46	1.36
11	B	1231	CLA	C3B-C2B	4.53	1.46	1.40
11	b	1232	CLA	C3D-C2D	4.53	1.47	1.39
11	A	1108	CLA	C3C-C2C	4.53	1.46	1.36
11	A	1114	CLA	C3B-C2B	4.53	1.46	1.40
11	A	1237	CLA	C3C-C2C	4.53	1.46	1.36
11	B	1207	CLA	C3C-C2C	4.53	1.46	1.36
11	A	1107	CLA	C3C-C2C	4.53	1.46	1.36
11	2	1217	CLA	OBD-CAD	4.52	1.28	1.22
11	b	1215	CLA	C3D-C2D	4.52	1.47	1.39
11	b	1228	CLA	C3B-C2B	4.52	1.46	1.40
11	2	1209	CLA	C3B-C2B	4.52	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1221	CLA	C3B-C2B	4.52	1.46	1.40
11	B	1217	CLA	O2A-C1	4.52	1.61	1.46
11	a	1126	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1220	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1208	CLA	C3D-C2D	4.52	1.47	1.39
11	1	1125	CLA	OBD-CAD	4.52	1.28	1.22
11	1	1129	CLA	C3B-C2B	4.51	1.46	1.40
11	B	1221	CLA	C3B-C2B	4.51	1.46	1.40
11	B	1023	CLA	C3B-C2B	4.51	1.46	1.40
11	2	1222	CLA	C3B-C2B	4.51	1.46	1.40
11	b	1216	CLA	C3B-C2B	4.51	1.46	1.40
11	A	1127	CLA	C3D-C2D	4.51	1.47	1.39
11	A	1139	CLA	C3B-C2B	4.51	1.46	1.40
11	1	1111	CLA	C3B-C2B	4.51	1.46	1.40
11	A	1128	CLA	C3D-C2D	4.51	1.47	1.39
11	a	1801	CLA	C3B-C2B	4.51	1.46	1.40
11	2	1204	CLA	C3B-C2B	4.51	1.46	1.40
11	b	1023	CLA	C3C-C2C	4.51	1.46	1.36
11	1	1133	CLA	C3B-C2B	4.51	1.46	1.40
11	1	1138	CLA	C3B-C2B	4.51	1.46	1.40
11	1	1103	CLA	C3B-C2B	4.51	1.46	1.40
11	A	1134	CLA	C3C-C2C	4.51	1.46	1.36
11	b	1208	CLA	C3B-C2B	4.51	1.46	1.40
11	a	1140	CLA	C3B-C2B	4.51	1.46	1.40
11	2	1203	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1221	CLA	C3C-C2C	4.50	1.46	1.36
11	2	1202	CLA	C3C-C2C	4.50	1.46	1.36
11	B	1204	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1109	CLA	C3B-C2B	4.50	1.46	1.40
11	2	1021	CLA	C3B-C2B	4.50	1.46	1.40
11	A	1121	CLA	OBD-CAD	4.50	1.28	1.22
11	1	1120	CLA	C3B-C2B	4.50	1.46	1.40
11	a	1102	CLA	C3B-C2B	4.50	1.46	1.40
11	1	1112	CLA	C3B-C2B	4.50	1.46	1.40
11	2	1223	CLA	OBD-CAD	4.50	1.28	1.22
11	1	1503	CLA	C3B-C2B	4.50	1.46	1.40
11	1	1123	CLA	C3B-C2B	4.50	1.46	1.40
11	1	1140	CLA	C3B-C2B	4.50	1.46	1.40
11	A	1105	CLA	C3B-C2B	4.50	1.46	1.40
11	2	1212	CLA	C3D-C2D	4.50	1.47	1.39
11	B	1216	CLA	C3B-C2B	4.50	1.46	1.40
11	A	1130	CLA	C3B-C2B	4.50	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1220	CLA	C3B-C2B	4.50	1.46	1.40
11	1	1118	CLA	C3C-C2C	4.49	1.46	1.36
11	B	1232	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1117	CLA	C3D-C2D	4.49	1.47	1.39
11	2	1013	CLA	C3B-C2B	4.49	1.46	1.40
11	a	1119	CLA	C3B-C2B	4.49	1.46	1.40
11	A	1129	CLA	C3B-C2B	4.49	1.46	1.40
11	2	1205	CLA	C3B-C2B	4.49	1.46	1.40
11	b	1226	CLA	OBD-CAD	4.49	1.28	1.22
11	L	1503	CLA	C3C-C2C	4.49	1.46	1.36
11	b	1205	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1120	CLA	C3B-C2B	4.49	1.46	1.40
11	B	1217	CLA	OBD-CAD	4.48	1.28	1.22
11	A	1012	CLA	C3B-C2B	4.48	1.46	1.40
11	b	1204	CLA	C3B-C2B	4.48	1.46	1.40
11	a	1109	CLA	C3B-C2B	4.48	1.46	1.40
11	2	1230	CLA	C3D-C2D	4.48	1.47	1.39
11	A	1104	CLA	C3B-C2B	4.48	1.46	1.40
11	b	1205	CLA	C3B-C2B	4.48	1.46	1.40
11	A	1101	CLA	C3B-C2B	4.48	1.46	1.40
11	l	1501	CLA	C3B-C2B	4.48	1.46	1.40
11	1	1117	CLA	C3B-C2B	4.48	1.46	1.40
11	2	1217	CLA	C3B-C2B	4.48	1.46	1.40
11	1	1114	CLA	C3D-C2D	4.48	1.47	1.39
11	1	1012	CLA	C3B-C2B	4.47	1.46	1.40
11	B	1231	CLA	C3D-C2D	4.47	1.47	1.39
11	a	1120	CLA	C3B-C2B	4.47	1.46	1.40
11	B	1234	CLA	C3C-C2C	4.47	1.46	1.36
11	A	1116	CLA	C3B-C2B	4.47	1.46	1.40
11	2	1023	CLA	C3C-C2C	4.47	1.46	1.36
11	b	1219	CLA	C3D-C2D	4.47	1.47	1.39
11	b	1013	CLA	C3D-C2D	4.47	1.47	1.39
11	b	1013	CLA	C3B-C2B	4.47	1.46	1.40
11	a	1130	CLA	C3D-C2D	4.47	1.47	1.39
11	b	1227	CLA	C3B-C2B	4.46	1.46	1.40
11	b	1208	CLA	C3D-C2D	4.46	1.47	1.39
11	B	1230	CLA	C3D-C2D	4.46	1.47	1.39
11	B	1223	CLA	C3B-C2B	4.46	1.46	1.40
11	b	1214	CLA	C3C-C2C	4.46	1.46	1.36
11	a	1119	CLA	C3D-C2D	4.46	1.47	1.39
11	A	1102	CLA	C3D-C2D	4.46	1.47	1.39
11	B	1206	CLA	C3C-C2C	4.46	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1013	CLA	C3D-C2D	4.46	1.47	1.39
11	A	1131	CLA	C3B-C2B	4.46	1.46	1.40
11	1	1113	CLA	C3B-C2B	4.46	1.46	1.40
11	a	1128	CLA	C3D-C2D	4.46	1.47	1.39
11	1	1110	CLA	C3D-C2D	4.46	1.47	1.39
11	B	1013	CLA	C3B-C2B	4.46	1.46	1.40
11	2	1206	CLA	C3C-C2C	4.45	1.46	1.36
11	2	1217	CLA	O2A-C1	4.45	1.61	1.46
11	a	1109	CLA	C3D-C2D	4.45	1.47	1.39
11	2	1234	CLA	C3C-C2C	4.45	1.46	1.36
11	A	1131	CLA	C3D-C2D	4.45	1.47	1.39
11	1	1237	CLA	C3C-C2C	4.45	1.46	1.36
11	1	1126	CLA	C3B-C2B	4.45	1.46	1.40
11	A	1109	CLA	C3D-C2D	4.45	1.47	1.39
11	B	1236	CLA	O2A-C1	4.45	1.61	1.46
11	1	1117	CLA	C3D-C2D	4.45	1.47	1.39
11	b	1212	CLA	C3B-C2B	4.45	1.46	1.40
11	l	1503	CLA	C3D-C2D	4.45	1.47	1.39
11	A	1132	CLA	C3B-C2B	4.45	1.46	1.40
11	2	1223	CLA	C3B-C2B	4.45	1.46	1.40
11	2	1215	CLA	C3B-C2B	4.44	1.46	1.40
11	2	1205	CLA	C3C-C2C	4.44	1.46	1.36
11	b	1231	CLA	C3B-C2B	4.44	1.46	1.40
11	2	1023	CLA	C3D-C2D	4.44	1.47	1.39
11	a	1114	CLA	C3D-C2D	4.44	1.47	1.39
11	1	1120	CLA	C3D-C2D	4.44	1.47	1.39
11	A	1116	CLA	C3C-C2C	4.44	1.46	1.36
11	a	1121	CLA	C3B-C2B	4.44	1.46	1.40
11	A	1133	CLA	C3D-C2D	4.44	1.47	1.39
11	A	1103	CLA	C3C-C2C	4.44	1.46	1.36
11	2	1236	CLA	OBD-CAD	4.44	1.28	1.22
11	8	1501	CLA	C3B-C2B	4.44	1.46	1.40
11	a	1114	CLA	C3B-C2B	4.43	1.46	1.40
11	B	1225	CLA	C3B-C2B	4.43	1.46	1.40
11	b	1207	CLA	C3C-C2C	4.43	1.46	1.36
11	A	1140	CLA	C3C-C2C	4.43	1.46	1.36
11	k	1402	CLA	C3D-C2D	4.43	1.47	1.39
11	b	1218	CLA	C3B-C2B	4.43	1.46	1.40
11	a	1138	CLA	C3B-C2B	4.43	1.46	1.40
11	b	1210	CLA	C3C-C2C	4.43	1.46	1.36
11	2	1217	CLA	C3D-C2D	4.43	1.47	1.39
11	B	1205	CLA	C3C-C2C	4.43	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1110	CLA	C3D-C2D	4.43	1.47	1.39
11	2	1214	CLA	C3B-C2B	4.43	1.46	1.40
11	b	1228	CLA	C3D-C2D	4.43	1.47	1.39
11	B	1214	CLA	C3C-C2C	4.43	1.46	1.36
11	b	1229	CLA	C3D-C2D	4.43	1.47	1.39
11	b	1236	CLA	O2A-C1	4.42	1.61	1.46
11	b	1211	CLA	C3D-C2D	4.42	1.47	1.39
11	a	1111	CLA	C3B-C2B	4.42	1.46	1.40
11	a	1117	CLA	C3D-C2D	4.42	1.47	1.39
11	B	1209	CLA	C3D-C2D	4.42	1.47	1.39
11	1	1103	CLA	C3C-C2C	4.42	1.46	1.36
11	1	1137	CLA	C3D-C2D	4.42	1.47	1.39
11	2	1215	CLA	C3D-C2D	4.42	1.47	1.39
11	B	1232	CLA	C3D-C2D	4.42	1.47	1.39
11	B	1228	CLA	C3D-C2D	4.42	1.47	1.39
11	a	1132	CLA	C3D-C2D	4.41	1.47	1.39
11	1	1133	CLA	C3D-C2D	4.41	1.47	1.39
11	1	1128	CLA	C3D-C2D	4.41	1.47	1.39
11	B	1234	CLA	C3B-C2B	4.41	1.46	1.40
11	b	1023	CLA	C3B-C2B	4.41	1.46	1.40
11	b	1230	CLA	C3D-C2D	4.41	1.47	1.39
11	2	1236	CLA	C3D-C2D	4.41	1.47	1.39
11	A	1127	CLA	OBD-CAD	4.41	1.28	1.22
11	a	1112	CLA	C3B-C2B	4.41	1.46	1.40
11	B	1207	CLA	C3B-C2B	4.41	1.46	1.40
11	L	1501	CLA	C3B-C2B	4.41	1.46	1.40
11	1	1123	CLA	C3C-C2C	4.41	1.46	1.36
11	B	1212	CLA	C3D-C2D	4.41	1.47	1.39
11	a	1131	CLA	C3D-C2D	4.40	1.47	1.39
11	B	1215	CLA	C3B-C2B	4.40	1.46	1.40
11	B	1210	CLA	C3C-C2C	4.40	1.46	1.36
11	b	1238	CLA	C3D-C2D	4.40	1.47	1.39
11	1	1237	CLA	OBD-CAD	4.40	1.28	1.22
11	1	1105	CLA	C3D-C2D	4.40	1.47	1.39
11	1	1114	CLA	C3B-C2B	4.40	1.46	1.40
11	2	1235	CLA	C3C-C2C	4.40	1.46	1.36
11	1	1132	CLA	C3D-C2D	4.40	1.47	1.39
11	B	1229	CLA	C3D-C2D	4.40	1.47	1.39
11	2	1227	CLA	C3D-C2D	4.40	1.47	1.39
11	2	1204	CLA	C3D-C2D	4.40	1.47	1.39
11	B	1206	CLA	C3D-C2D	4.39	1.47	1.39
11	A	1106	CLA	C3D-C2D	4.39	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1130	CLA	C3D-C2D	4.39	1.47	1.39
11	a	1132	CLA	C3B-C2B	4.39	1.46	1.40
11	A	1114	CLA	C3D-C2D	4.39	1.47	1.39
11	b	1203	CLA	C3D-C2D	4.39	1.47	1.39
11	a	1133	CLA	C3D-C2D	4.39	1.47	1.39
11	1	1105	CLA	C3B-C2B	4.39	1.46	1.40
11	a	1119	CLA	OBD-CAD	4.39	1.28	1.22
11	B	1023	CLA	C3C-C2C	4.39	1.46	1.36
11	1	1121	CLA	C3B-C2B	4.39	1.46	1.40
15	A	5003	LHG	O8-C23	4.39	1.46	1.33
11	A	1135	CLA	C3D-C2D	4.39	1.47	1.39
11	l	1501	CLA	C3D-C2D	4.39	1.47	1.39
11	1	1126	CLA	C3D-C2D	4.39	1.47	1.39
11	2	1239	CLA	C3D-C2D	4.39	1.47	1.39
11	1	1110	CLA	C3B-C2B	4.38	1.46	1.40
11	a	1126	CLA	C3D-C2D	4.38	1.47	1.39
11	1	1101	CLA	C3D-C2D	4.38	1.47	1.39
11	a	1123	CLA	C3C-C2C	4.38	1.46	1.36
11	1	1801	CLA	C3D-C2D	4.38	1.47	1.39
11	A	1011	CLA	C3B-C2B	4.38	1.46	1.40
11	A	1118	CLA	C3C-C2C	4.38	1.46	1.36
11	1	1130	CLA	C3D-C2D	4.37	1.47	1.39
11	A	1123	CLA	C3C-C2C	4.37	1.46	1.36
11	2	1228	CLA	C3D-C2D	4.37	1.47	1.39
11	2	1021	CLA	C3D-C2D	4.37	1.47	1.39
11	2	1213	CLA	C3D-C2D	4.37	1.47	1.39
11	2	1236	CLA	O2A-C1	4.37	1.60	1.46
11	a	1102	CLA	C3D-C2D	4.37	1.47	1.39
11	a	1237	CLA	C3C-C2C	4.37	1.46	1.36
11	b	1218	CLA	C3D-C2D	4.37	1.47	1.39
11	B	1213	CLA	C3D-C2D	4.37	1.47	1.39
11	1	1109	CLA	C3D-C2D	4.37	1.47	1.39
11	K	1402	CLA	C3D-C2D	4.37	1.47	1.39
15	a	5001	LHG	O8-C23	4.36	1.46	1.33
11	B	1203	CLA	C3B-C2B	4.36	1.46	1.40
11	b	1206	CLA	C3D-C2D	4.36	1.47	1.39
11	a	1123	CLA	C3D-C2D	4.36	1.47	1.39
11	A	1111	CLA	C3D-C2D	4.36	1.47	1.39
11	l	1502	CLA	C3D-C2D	4.36	1.47	1.39
11	k	1401	CLA	C3B-C2B	4.36	1.46	1.40
11	2	1206	CLA	C3D-C2D	4.36	1.47	1.39
15	1	5003	LHG	O8-C23	4.36	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1135	CLA	C3B-C2B	4.36	1.46	1.40
11	A	1126	CLA	C3B-C2B	4.36	1.46	1.40
11	B	1235	CLA	C3D-C2D	4.36	1.47	1.39
11	2	1216	CLA	C3B-C2B	4.36	1.46	1.40
11	B	1223	CLA	OBD-CAD	4.36	1.28	1.22
11	2	1218	CLA	C3B-C2B	4.36	1.46	1.40
11	a	1122	CLA	C3D-C2D	4.36	1.47	1.39
11	1	1101	CLA	C3B-C2B	4.36	1.46	1.40
11	a	1133	CLA	C3B-C2B	4.36	1.46	1.40
11	B	1210	CLA	C3D-C2D	4.36	1.47	1.39
11	1	1119	CLA	C3D-C2D	4.36	1.47	1.39
11	a	1012	CLA	C3B-C2B	4.35	1.46	1.40
11	b	1204	CLA	C3D-C2D	4.35	1.47	1.39
11	A	1124	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1215	CLA	C3B-C2B	4.35	1.46	1.40
11	b	1229	CLA	C3B-C2B	4.35	1.46	1.40
11	a	1011	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1239	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1234	CLA	C3D-C2D	4.35	1.47	1.39
11	1	1123	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1226	CLA	C3B-C2B	4.35	1.46	1.40
11	A	1011	CLA	C3D-C2D	4.35	1.47	1.39
11	1	1122	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1234	CLA	C3B-C2B	4.35	1.46	1.40
11	1	1135	CLA	C3D-C2D	4.35	1.47	1.39
11	b	1203	CLA	C3B-C2B	4.35	1.46	1.40
11	a	1105	CLA	C3D-C2D	4.34	1.47	1.39
11	B	1215	CLA	C3D-C2D	4.34	1.47	1.39
11	2	1023	CLA	C3B-C2B	4.34	1.46	1.40
11	K	1401	CLA	C3B-C2B	4.34	1.46	1.40
11	8	1503	CLA	C3D-C2D	4.34	1.47	1.39
11	a	1101	CLA	C3D-C2D	4.34	1.47	1.39
11	2	1240	CLA	C3D-C2D	4.34	1.47	1.39
11	A	1116	CLA	C3D-C2D	4.34	1.47	1.39
11	A	1111	CLA	C3B-C2B	4.34	1.46	1.40
11	1	1119	CLA	C3B-C2B	4.34	1.46	1.40
11	A	1108	CLA	C3D-C2D	4.34	1.47	1.39
11	1	1138	CLA	C3D-C2D	4.34	1.47	1.39
11	a	1801	CLA	C3D-C2D	4.34	1.47	1.39
11	1	1115	CLA	OBD-CAD	4.34	1.28	1.22
11	A	1237	CLA	C3D-C2D	4.34	1.47	1.39
11	0	1401	CLA	C3B-C2B	4.34	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1230	CLA	C3C-C2C	4.34	1.45	1.36
11	2	1234	CLA	C3D-C2D	4.34	1.47	1.39
11	b	1217	CLA	C3D-C2D	4.34	1.47	1.39
11	b	1240	CLA	C3D-C2D	4.33	1.47	1.39
11	2	1238	CLA	C3D-C2D	4.33	1.47	1.39
11	1	1102	CLA	C3D-C2D	4.33	1.47	1.39
11	b	1214	CLA	C3D-C2D	4.33	1.47	1.39
11	2	1229	CLA	C3D-C2D	4.33	1.47	1.39
11	a	1137	CLA	C3D-C2D	4.33	1.47	1.39
11	A	1111	CLA	C3C-C2C	4.33	1.45	1.36
11	B	1204	CLA	C3D-C2D	4.33	1.47	1.39
11	B	1227	CLA	C3D-C2D	4.33	1.47	1.39
11	a	1128	CLA	C3B-C2B	4.33	1.46	1.40
11	B	1234	CLA	C3D-C2D	4.33	1.47	1.39
11	B	1206	CLA	C3B-C2B	4.33	1.46	1.40
11	a	1106	CLA	C3D-C2D	4.33	1.47	1.39
11	a	1022	CLA	C3B-C2B	4.33	1.46	1.40
11	2	1209	CLA	C3D-C2D	4.32	1.47	1.39
11	b	1023	CLA	C3D-C2D	4.32	1.47	1.39
11	B	1208	CLA	C3D-C2D	4.32	1.47	1.39
11	B	1239	CLA	C3D-C2D	4.32	1.47	1.39
11	1	1121	CLA	C3D-C2D	4.32	1.47	1.39
11	0	1402	CLA	C3D-C2D	4.32	1.47	1.39
11	a	1127	CLA	C3D-C2D	4.32	1.47	1.39
11	a	1134	CLA	C3D-C2D	4.32	1.47	1.39
11	8	1502	CLA	C3D-C2D	4.32	1.47	1.39
11	b	1212	CLA	C3D-C2D	4.32	1.47	1.39
11	B	1220	CLA	C3D-C2D	4.32	1.47	1.39
11	a	1129	CLA	C3D-C2D	4.32	1.47	1.39
11	b	1209	CLA	C3D-C2D	4.32	1.47	1.39
11	1	1118	CLA	C3D-C2D	4.32	1.47	1.39
11	b	1227	CLA	C3D-C2D	4.32	1.47	1.39
11	a	1104	CLA	C3B-C2B	4.32	1.46	1.40
11	2	1234	CLA	C3B-C2B	4.32	1.46	1.40
11	a	1139	CLA	C3B-C2B	4.31	1.46	1.40
11	8	1501	CLA	C3D-C2D	4.31	1.47	1.39
11	1	1139	CLA	C3D-C2D	4.31	1.47	1.39
11	A	1110	CLA	C3D-C2D	4.31	1.47	1.39
15	B	5004	LHG	O8-C23	4.31	1.45	1.33
11	a	1124	CLA	C3D-C2D	4.31	1.47	1.39
11	1	1132	CLA	C3B-C2B	4.31	1.46	1.40
11	1	1127	CLA	C3D-C2D	4.31	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1801	CLA	C3B-C2B	4.31	1.46	1.40
11	1	1112	CLA	C3D-C2D	4.31	1.47	1.39
11	B	1240	CLA	C3D-C2D	4.31	1.47	1.39
11	L	1503	CLA	C3D-C2D	4.31	1.47	1.39
11	2	1207	CLA	C3D-C2D	4.31	1.47	1.39
11	2	1207	CLA	C3C-C2C	4.30	1.45	1.36
11	a	1108	CLA	C3D-C2D	4.30	1.47	1.39
11	1	1131	CLA	C3D-C2D	4.30	1.47	1.39
11	2	1218	CLA	C3D-C2D	4.30	1.47	1.39
11	a	1103	CLA	C3D-C2D	4.30	1.47	1.39
11	2	1210	CLA	C3D-C2D	4.30	1.47	1.39
11	2	1232	CLA	C3D-C2D	4.30	1.47	1.39
11	A	1118	CLA	C3B-C2B	4.30	1.46	1.40
11	B	1219	CLA	C3D-C2D	4.30	1.47	1.39
11	B	1227	CLA	C3B-C2B	4.30	1.46	1.40
11	1	1134	CLA	C3D-C2D	4.29	1.47	1.39
15	1	5001	LHG	O8-C23	4.29	1.45	1.33
11	b	1216	CLA	C3D-C2D	4.29	1.47	1.39
11	1	1104	CLA	C3D-C2D	4.29	1.47	1.39
11	1	1140	CLA	C3D-C2D	4.29	1.47	1.39
11	b	1210	CLA	C3D-C2D	4.29	1.47	1.39
11	1	1113	CLA	C3D-C2D	4.29	1.47	1.39
11	b	1021	CLA	C3D-C2D	4.29	1.47	1.39
11	2	1211	CLA	C3D-C2D	4.29	1.47	1.39
11	b	1220	CLA	C3D-C2D	4.29	1.47	1.39
11	A	1801	CLA	C3D-C2D	4.29	1.47	1.39
11	1	1115	CLA	C3D-C2D	4.29	1.47	1.39
11	B	1216	CLA	C3D-C2D	4.29	1.47	1.39
11	A	1139	CLA	C3D-C2D	4.29	1.47	1.39
11	B	1229	CLA	C3B-C2B	4.29	1.46	1.40
11	L	1501	CLA	C3D-C2D	4.29	1.47	1.39
11	2	1203	CLA	C3B-C2B	4.29	1.46	1.40
11	a	1125	CLA	OBD-CAD	4.29	1.28	1.22
15	a	5003	LHG	O8-C23	4.29	1.45	1.33
11	A	1113	CLA	C3D-C2D	4.29	1.47	1.39
11	a	1112	CLA	C3D-C2D	4.28	1.47	1.39
16	2	5002	LMG	O8-C28	4.28	1.45	1.33
11	1	1108	CLA	C3D-C2D	4.28	1.47	1.39
11	a	1140	CLA	C3D-C2D	4.28	1.47	1.39
11	B	1021	CLA	C3B-C2B	4.28	1.46	1.40
11	B	1222	CLA	C3D-C2D	4.28	1.47	1.39
11	A	1125	CLA	C3D-C2D	4.28	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1136	CLA	C3D-C2D	4.28	1.47	1.39
11	A	1140	CLA	C3D-C2D	4.28	1.47	1.39
11	L	1502	CLA	C3D-C2D	4.28	1.47	1.39
11	b	1201	CLA	C3D-C2D	4.28	1.47	1.39
11	a	1104	CLA	C3D-C2D	4.28	1.47	1.39
11	1	1125	CLA	C3B-C2B	4.27	1.46	1.40
11	2	1235	CLA	C3D-C2D	4.27	1.47	1.39
11	A	1124	CLA	C3B-C2B	4.27	1.46	1.40
11	b	1205	CLA	C3D-C2D	4.27	1.47	1.39
11	B	1205	CLA	C3B-C2B	4.27	1.46	1.40
11	0	1401	CLA	C3D-C2D	4.26	1.47	1.39
11	B	1204	CLA	C3B-C2B	4.26	1.46	1.40
11	a	1113	CLA	C3D-C2D	4.26	1.47	1.39
15	2	5004	LHG	O8-C23	4.26	1.45	1.33
11	2	1220	CLA	C3D-C2D	4.26	1.47	1.39
11	b	1226	CLA	C3D-C2D	4.26	1.47	1.39
11	b	1217	CLA	O2A-C1	4.26	1.60	1.46
11	b	1222	CLA	C3D-C2D	4.26	1.47	1.39
11	a	1120	CLA	C3D-C2D	4.25	1.47	1.39
11	B	1021	CLA	C3D-C2D	4.25	1.47	1.39
15	b	5004	LHG	O8-C23	4.25	1.45	1.33
11	B	1202	CLA	C3D-C2D	4.25	1.47	1.39
11	b	1206	CLA	C3B-C2B	4.25	1.46	1.40
11	a	1111	CLA	C3C-C2C	4.25	1.45	1.36
11	A	1133	CLA	C3B-C2B	4.25	1.46	1.40
11	A	1119	CLA	C3D-C2D	4.25	1.47	1.39
11	2	1223	CLA	C3D-C2D	4.25	1.47	1.39
16	b	5002	LMG	O8-C28	4.25	1.45	1.33
11	b	1213	CLA	C3D-C2D	4.24	1.47	1.39
11	A	1121	CLA	C3D-C2D	4.24	1.47	1.39
11	A	1132	CLA	C3D-C2D	4.24	1.47	1.39
11	B	1214	CLA	C3D-C2D	4.24	1.47	1.39
15	2	5004	LHG	O7-C7	4.24	1.46	1.34
11	2	1221	CLA	C3D-C2D	4.24	1.47	1.39
11	a	1138	CLA	C3D-C2D	4.24	1.47	1.39
11	2	1227	CLA	C3B-C2B	4.24	1.46	1.40
11	1	1116	CLA	C3D-C2D	4.23	1.47	1.39
11	1	1124	CLA	C3D-C2D	4.23	1.47	1.39
11	K	1401	CLA	C3D-C2D	4.23	1.47	1.39
11	B	1232	CLA	C3B-C2B	4.23	1.46	1.40
11	A	1134	CLA	C3D-C2D	4.23	1.47	1.39
11	A	1115	CLA	C3D-C2D	4.23	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1023	CLA	C3D-C2D	4.23	1.47	1.39
11	k	1401	CLA	C3D-C2D	4.22	1.47	1.39
11	A	1138	CLA	C3D-C2D	4.22	1.47	1.39
11	2	1214	CLA	C3D-C2D	4.22	1.47	1.39
11	1	1125	CLA	C3D-C2D	4.22	1.47	1.39
11	a	1121	CLA	C3D-C2D	4.22	1.47	1.39
11	B	1238	CLA	C3D-C2D	4.22	1.47	1.39
11	b	1235	CLA	C3D-C2D	4.21	1.47	1.39
11	a	1237	CLA	C3D-C2D	4.21	1.47	1.39
11	a	1135	CLA	C3D-C2D	4.21	1.47	1.39
11	a	1118	CLA	C3D-C2D	4.21	1.47	1.39
11	1	1106	CLA	C3D-C2D	4.21	1.47	1.39
11	b	1231	CLA	C3D-C2D	4.21	1.47	1.39
11	B	1218	CLA	C3D-C2D	4.21	1.47	1.39
11	1	1136	CLA	C3D-C2D	4.21	1.47	1.39
11	2	1222	CLA	C3D-C2D	4.20	1.47	1.39
11	A	1129	CLA	C3D-C2D	4.20	1.47	1.39
11	1	1111	CLA	C3C-C2C	4.20	1.45	1.36
11	a	1139	CLA	C3D-C2D	4.20	1.47	1.39
11	2	1210	CLA	C3C-C2C	4.20	1.45	1.36
11	2	1203	CLA	C3D-C2D	4.20	1.47	1.39
11	a	1111	CLA	C3D-C2D	4.20	1.47	1.39
11	b	1221	CLA	C3D-C2D	4.20	1.47	1.39
11	a	1116	CLA	C3D-C2D	4.20	1.47	1.39
11	B	1221	CLA	C3D-C2D	4.20	1.47	1.39
11	1	1022	CLA	C3B-C2B	4.20	1.46	1.40
11	A	1120	CLA	C3D-C2D	4.20	1.47	1.39
11	A	1801	CLA	C3B-C2B	4.20	1.46	1.40
11	A	1138	CLA	C3C-C2C	4.19	1.45	1.36
11	B	1223	CLA	C3D-C2D	4.19	1.46	1.39
11	b	1223	CLA	C3D-C2D	4.19	1.46	1.39
15	B	5004	LHG	O7-C7	4.18	1.46	1.34
11	b	1207	CLA	C3D-C2D	4.18	1.46	1.39
11	A	1136	CLA	C3D-C2D	4.18	1.46	1.39
11	1	1011	CLA	C3B-C2B	4.18	1.46	1.40
11	2	1201	CLA	C3D-C2D	4.18	1.46	1.39
11	1	1128	CLA	C3B-C2B	4.18	1.46	1.40
11	1	1237	CLA	C3D-C2D	4.18	1.46	1.39
16	B	5002	LMG	O8-C28	4.18	1.45	1.33
11	b	1202	CLA	C3D-C2D	4.17	1.46	1.39
11	A	1105	CLA	C3D-C2D	4.17	1.46	1.39
11	b	1224	CLA	C3D-C2D	4.17	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1216	CLA	C3D-C2D	4.17	1.46	1.39
11	A	1122	CLA	C3D-C2D	4.17	1.46	1.39
11	B	1217	CLA	C3D-C2D	4.16	1.46	1.39
15	A	5001	LHG	O8-C23	4.16	1.45	1.33
15	a	5001	LHG	O7-C7	4.16	1.46	1.34
15	1	5001	LHG	O7-C7	4.16	1.46	1.34
11	A	1137	CLA	C3D-C2D	4.16	1.46	1.39
11	B	1203	CLA	C3D-C2D	4.16	1.46	1.39
11	A	1128	CLA	C3B-C2B	4.16	1.46	1.40
11	B	1205	CLA	C3D-C2D	4.15	1.46	1.39
11	1	1011	CLA	C3D-C2D	4.15	1.46	1.39
11	1	1129	CLA	C3D-C2D	4.15	1.46	1.39
11	2	1231	CLA	C3D-C2D	4.15	1.46	1.39
11	B	1225	CLA	C3D-C2D	4.15	1.46	1.39
11	a	1125	CLA	C3D-C2D	4.15	1.46	1.39
11	B	1226	CLA	C3B-C2B	4.15	1.46	1.40
11	B	1236	CLA	C3D-C2D	4.14	1.46	1.39
11	a	1115	CLA	C3D-C2D	4.14	1.46	1.39
11	A	1119	CLA	OBD-CAD	4.14	1.28	1.22
11	1	1103	CLA	C3D-C2D	4.14	1.46	1.39
11	2	1232	CLA	C3B-C2B	4.14	1.46	1.40
15	1	5003	LHG	O7-C7	4.14	1.46	1.34
11	1	1107	CLA	C3D-C2D	4.13	1.46	1.39
11	B	1207	CLA	C3D-C2D	4.13	1.46	1.39
11	A	1022	CLA	C3B-C2B	4.13	1.46	1.40
11	A	1123	CLA	C3D-C2D	4.12	1.46	1.39
11	A	1126	CLA	C3D-C2D	4.12	1.46	1.39
11	B	1226	CLA	C3D-C2D	4.12	1.46	1.39
11	1	1111	CLA	C3D-C2D	4.12	1.46	1.39
15	A	5001	LHG	O7-C7	4.12	1.45	1.34
11	A	1119	CLA	C3B-C2B	4.12	1.46	1.40
16	B	5002	LMG	O7-C10	4.12	1.45	1.34
11	B	1236	CLA	OBD-CAD	4.11	1.28	1.22
11	A	1118	CLA	C3D-C2D	4.11	1.46	1.39
11	2	1229	CLA	C3B-C2B	4.10	1.46	1.40
11	B	1201	CLA	C3D-C2D	4.10	1.46	1.39
11	A	1112	CLA	C3D-C2D	4.10	1.46	1.39
11	b	1225	CLA	C3D-C2D	4.10	1.46	1.39
11	2	1206	CLA	C3B-C2B	4.10	1.46	1.40
11	A	1106	CLA	C3B-C2B	4.09	1.46	1.40
16	2	5002	LMG	O7-C10	4.08	1.45	1.34
11	2	1219	CLA	C3D-C2D	4.08	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1107	CLA	C3D-C2D	4.08	1.46	1.39
11	2	1225	CLA	C3D-C2D	4.08	1.46	1.39
11	b	1236	CLA	C3D-C2D	4.07	1.46	1.39
11	A	1125	CLA	OBD-CAD	4.07	1.28	1.22
11	2	1202	CLA	C3D-C2D	4.07	1.46	1.39
15	b	5004	LHG	O7-C7	4.06	1.45	1.34
11	2	1205	CLA	C3D-C2D	4.06	1.46	1.39
11	A	1103	CLA	C3D-C2D	4.06	1.46	1.39
15	a	5003	LHG	O7-C7	4.04	1.45	1.34
11	A	1101	CLA	C3D-C2D	4.02	1.46	1.39
11	A	1104	CLA	C3D-C2D	4.01	1.46	1.39
11	A	1125	CLA	MG-NC	4.00	2.15	2.06
11	2	1226	CLA	C3D-C2D	4.00	1.46	1.39
15	A	5003	LHG	O7-C7	3.99	1.45	1.34
11	A	1112	CLA	C3B-C2B	3.98	1.45	1.40
11	a	1139	CLA	MG-NC	3.97	2.15	2.06
16	b	5002	LMG	O7-C10	3.97	1.45	1.34
11	A	1107	CLA	C3D-C2D	3.97	1.46	1.39
11	b	1230	CLA	MG-NC	3.95	2.15	2.06
11	1	1123	CLA	MG-NC	3.95	2.15	2.06
11	b	1220	CLA	MG-NC	3.94	2.15	2.06
11	2	1216	CLA	MG-NC	3.93	2.15	2.06
11	2	1224	CLA	C3D-C2D	3.93	1.46	1.39
11	b	1221	CLA	MG-NC	3.92	2.15	2.06
11	a	1012	CLA	MG-NC	3.90	2.15	2.06
11	a	1121	CLA	MG-NC	3.90	2.15	2.06
11	1	1110	CLA	MG-NC	3.88	2.15	2.06
11	2	1217	CLA	MG-NC	3.88	2.15	2.06
11	a	1123	CLA	MG-NC	3.88	2.15	2.06
11	2	1232	CLA	MG-NC	3.87	2.15	2.06
11	1	1012	CLA	MG-NC	3.86	2.15	2.06
11	b	1219	CLA	MG-NC	3.86	2.15	2.06
11	2	1239	CLA	MG-NC	3.86	2.15	2.06
11	a	1114	CLA	MG-NC	3.86	2.15	2.06
11	1	1102	CLA	MG-NC	3.85	2.15	2.06
11	A	1123	CLA	C3B-C2B	3.85	1.45	1.40
11	b	1223	CLA	MG-NC	3.85	2.15	2.06
11	2	1240	CLA	MG-NC	3.84	2.15	2.06
11	B	1224	CLA	C3D-C2D	3.84	1.46	1.39
11	A	1124	CLA	MG-NC	3.84	2.15	2.06
11	A	1114	CLA	MG-NC	3.83	2.15	2.06
11	b	1232	CLA	MG-NC	3.83	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1139	CLA	MG-NC	3.83	2.15	2.06
11	B	1232	CLA	MG-NC	3.83	2.15	2.06
11	A	1801	CLA	MG-NC	3.83	2.15	2.06
11	a	1022	CLA	MG-NC	3.83	2.15	2.06
11	b	1224	CLA	MG-NC	3.83	2.15	2.06
11	B	1240	CLA	MG-NC	3.83	2.15	2.06
11	b	1240	CLA	MG-NC	3.82	2.15	2.06
11	B	1223	CLA	MG-NC	3.82	2.15	2.06
11	2	1215	CLA	MG-NC	3.82	2.15	2.06
11	b	1225	CLA	MG-NC	3.82	2.15	2.06
11	1	1120	CLA	MG-NC	3.82	2.15	2.06
11	2	1231	CLA	MG-NC	3.82	2.15	2.06
11	b	1234	CLA	MG-NC	3.81	2.15	2.06
11	A	1131	CLA	MG-NC	3.81	2.15	2.06
11	A	1123	CLA	MG-NC	3.81	2.15	2.06
11	1	1022	CLA	MG-NC	3.81	2.15	2.06
11	1	1135	CLA	MG-NC	3.81	2.15	2.06
11	b	1210	CLA	MG-NC	3.81	2.15	2.06
11	2	1212	CLA	MG-NC	3.81	2.15	2.06
11	2	1230	CLA	MG-NC	3.80	2.15	2.06
11	2	1219	CLA	MG-NC	3.80	2.15	2.06
11	b	1208	CLA	MG-NC	3.80	2.15	2.06
11	B	1231	CLA	MG-NC	3.80	2.15	2.06
11	a	1113	CLA	MG-NC	3.80	2.15	2.06
11	A	1139	CLA	MG-NC	3.80	2.15	2.06
11	2	1206	CLA	MG-NC	3.80	2.15	2.06
11	b	1227	CLA	MG-NC	3.79	2.15	2.06
11	2	1220	CLA	MG-NC	3.79	2.15	2.06
11	2	1201	CLA	MG-NC	3.79	2.15	2.06
11	a	1101	CLA	MG-NC	3.79	2.15	2.06
11	a	1801	CLA	MG-NC	3.79	2.15	2.06
11	1	1133	CLA	MG-NC	3.79	2.15	2.06
11	a	1107	CLA	MG-NC	3.79	2.15	2.06
11	1	1140	CLA	MG-NC	3.79	2.15	2.06
11	1	1115	CLA	MG-NC	3.79	2.15	2.06
11	b	1239	CLA	MG-NC	3.78	2.15	2.06
11	b	1203	CLA	MG-NC	3.78	2.15	2.06
11	B	1222	CLA	MG-NC	3.78	2.15	2.06
11	1	1113	CLA	MG-NC	3.78	2.15	2.06
11	b	1021	CLA	MG-NC	3.78	2.15	2.06
11	a	1126	CLA	MG-NC	3.78	2.15	2.06
11	B	1220	CLA	MG-NC	3.78	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1209	CLA	MG-NC	3.78	2.15	2.06
11	a	1108	CLA	MG-NC	3.78	2.15	2.06
11	a	1135	CLA	MG-NC	3.78	2.15	2.06
11	0	1401	CLA	MG-NC	3.78	2.15	2.06
11	1	1114	CLA	MG-NC	3.77	2.15	2.06
11	b	1212	CLA	MG-NC	3.77	2.15	2.06
11	2	1223	CLA	MG-NC	3.77	2.15	2.06
11	A	1134	CLA	MG-NC	3.77	2.15	2.06
11	A	1110	CLA	MG-NC	3.77	2.15	2.06
11	8	1503	CLA	MG-NC	3.77	2.15	2.06
11	1	1101	CLA	MG-NC	3.77	2.15	2.06
11	B	1230	CLA	MG-NC	3.77	2.15	2.06
11	1	1011	CLA	MG-NC	3.77	2.15	2.06
11	b	1216	CLA	MG-NC	3.77	2.15	2.06
11	1	1129	CLA	MG-NC	3.76	2.15	2.06
11	b	1211	CLA	MG-NC	3.76	2.15	2.06
11	1	1108	CLA	MG-NC	3.76	2.15	2.06
11	a	1140	CLA	MG-NC	3.76	2.15	2.06
11	a	1102	CLA	MG-NC	3.76	2.15	2.06
11	A	1132	CLA	MG-NC	3.76	2.15	2.06
11	2	1229	CLA	MG-NC	3.76	2.15	2.06
11	L	1501	CLA	MG-NC	3.76	2.15	2.06
11	B	1225	CLA	MG-NC	3.76	2.15	2.06
11	2	1234	CLA	MG-NC	3.76	2.15	2.06
11	A	1102	CLA	MG-NC	3.76	2.15	2.06
11	1	1112	CLA	MG-NC	3.76	2.15	2.06
11	b	1235	CLA	MG-NC	3.76	2.15	2.06
11	B	1221	CLA	MG-NC	3.76	2.15	2.06
11	1	1134	CLA	MG-NC	3.75	2.15	2.06
11	K	1401	CLA	MG-NC	3.75	2.15	2.06
11	a	1120	CLA	MG-NC	3.75	2.15	2.06
11	a	1109	CLA	MG-NC	3.75	2.15	2.06
11	8	1501	CLA	MG-NC	3.75	2.15	2.06
11	a	1105	CLA	MG-NC	3.75	2.15	2.06
11	1	1125	CLA	MG-NC	3.75	2.15	2.06
11	A	1129	CLA	MG-NC	3.75	2.15	2.06
11	A	1127	CLA	MG-NC	3.75	2.15	2.06
11	A	1101	CLA	MG-NC	3.75	2.15	2.06
11	2	1213	CLA	MG-NC	3.75	2.15	2.06
11	B	1229	CLA	MG-NC	3.74	2.15	2.06
11	b	1222	CLA	MG-NC	3.74	2.15	2.06
11	2	1222	CLA	MG-NC	3.74	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1124	CLA	MG-NC	3.74	2.15	2.06
11	B	1227	CLA	MG-NC	3.74	2.15	2.06
11	b	1217	CLA	MG-NC	3.74	2.15	2.06
11	1	1131	CLA	MG-NC	3.74	2.15	2.06
11	B	1219	CLA	MG-NC	3.74	2.15	2.06
11	A	1112	CLA	MG-NC	3.74	2.15	2.06
11	1	1801	CLA	MG-NC	3.74	2.15	2.06
11	a	1127	CLA	MG-NC	3.74	2.15	2.06
11	2	1225	CLA	MG-NC	3.74	2.15	2.06
11	1	1121	CLA	MG-NC	3.74	2.15	2.06
11	a	1110	CLA	MG-NC	3.74	2.15	2.06
11	B	1234	CLA	MG-NC	3.73	2.15	2.06
11	B	1211	CLA	C3D-C2D	3.73	1.46	1.39
11	B	1235	CLA	MG-NC	3.73	2.15	2.06
11	l	1501	CLA	MG-NC	3.73	2.15	2.06
11	2	1227	CLA	MG-NC	3.73	2.15	2.06
11	k	1401	CLA	MG-NC	3.73	2.15	2.06
11	b	1213	CLA	MG-NC	3.73	2.15	2.06
11	B	1212	CLA	MG-NC	3.73	2.15	2.06
11	a	1112	CLA	MG-NC	3.73	2.15	2.06
11	A	1116	CLA	MG-NC	3.73	2.15	2.06
11	a	1133	CLA	MG-NC	3.72	2.15	2.06
11	b	1209	CLA	MG-NC	3.72	2.15	2.06
11	l	1502	CLA	MG-NC	3.72	2.15	2.06
11	2	1209	CLA	MG-NC	3.72	2.15	2.06
11	1	1116	CLA	MG-NC	3.72	2.15	2.06
11	1	1132	CLA	MG-NC	3.72	2.15	2.06
11	a	1106	CLA	MG-NC	3.72	2.15	2.06
11	1	1122	CLA	MG-NC	3.72	2.15	2.06
11	2	1221	CLA	MG-NC	3.72	2.15	2.06
11	1	1126	CLA	MG-NC	3.72	2.15	2.06
11	A	1121	CLA	MG-NC	3.71	2.15	2.06
11	b	1218	CLA	MG-NC	3.71	2.15	2.06
11	a	1115	CLA	MG-NC	3.71	2.15	2.06
11	8	1502	CLA	MG-NC	3.71	2.15	2.06
11	2	1235	CLA	MG-NC	3.71	2.15	2.06
11	2	1238	CLA	MG-NC	3.71	2.15	2.06
11	a	1137	CLA	MG-NC	3.71	2.15	2.06
11	A	1121	CLA	C1D-C2D	3.71	1.51	1.42
11	A	1109	CLA	C1D-C2D	3.70	1.51	1.42
11	a	1103	CLA	MG-NC	3.70	2.15	2.06
11	1	1124	CLA	MG-NC	3.70	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1011	CLA	MG-NC	3.70	2.15	2.06
11	1	1105	CLA	MG-NC	3.70	2.15	2.06
11	1	1117	CLA	MG-NC	3.69	2.15	2.06
11	b	1226	CLA	MG-NC	3.69	2.15	2.06
11	B	1210	CLA	MG-NC	3.69	2.15	2.06
11	b	1205	CLA	MG-NC	3.69	2.15	2.06
11	2	1228	CLA	MG-NC	3.69	2.15	2.06
11	2	1021	CLA	MG-NC	3.69	2.15	2.06
11	2	1236	CLA	MG-NC	3.69	2.15	2.06
11	b	1201	CLA	MG-NC	3.69	2.15	2.06
11	A	1113	CLA	MG-NC	3.68	2.15	2.06
11	1	1103	CLA	MG-NC	3.68	2.15	2.06
11	A	1012	CLA	MG-NC	3.68	2.15	2.06
11	a	1111	CLA	MG-NC	3.68	2.15	2.06
11	B	1215	CLA	MG-NC	3.68	2.15	2.06
11	B	1239	CLA	MG-NC	3.68	2.15	2.06
11	1	1107	CLA	MG-NC	3.68	2.15	2.06
11	a	1131	CLA	MG-NC	3.68	2.15	2.06
11	A	1126	CLA	MG-NC	3.68	2.15	2.06
11	b	1214	CLA	MG-NC	3.68	2.15	2.06
11	a	1117	CLA	MG-NC	3.67	2.15	2.06
11	a	1122	CLA	MG-NC	3.67	2.15	2.06
11	B	1217	CLA	MG-NC	3.67	2.15	2.06
11	A	1115	CLA	MG-NC	3.67	2.15	2.06
11	B	1202	CLA	MG-NC	3.67	2.15	2.06
11	a	1138	CLA	MG-NC	3.67	2.15	2.06
11	b	1204	CLA	MG-NC	3.67	2.15	2.06
11	2	1224	CLA	MG-NC	3.67	2.15	2.06
11	B	1206	CLA	MG-NC	3.67	2.15	2.06
11	l	1503	CLA	MG-NC	3.67	2.15	2.06
11	b	1207	CLA	MG-NC	3.67	2.15	2.06
11	A	1130	CLA	MG-NC	3.66	2.15	2.06
11	B	1224	CLA	MG-NC	3.66	2.15	2.06
11	A	1133	CLA	MG-NC	3.66	2.15	2.06
11	b	1229	CLA	MG-NC	3.66	2.15	2.06
11	b	1202	CLA	MG-NC	3.66	2.15	2.06
11	a	1134	CLA	MG-NC	3.66	2.15	2.06
11	b	1231	CLA	MG-NC	3.66	2.15	2.06
11	B	1214	CLA	MG-NC	3.66	2.15	2.06
11	a	1132	CLA	MG-NC	3.66	2.15	2.06
11	1	1137	CLA	MG-NC	3.66	2.15	2.06
11	a	1125	CLA	MG-NC	3.66	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1105	CLA	MG-NC	3.66	2.15	2.06
11	A	1137	CLA	MG-NC	3.66	2.15	2.06
11	B	1213	CLA	MG-NC	3.65	2.15	2.06
11	b	1238	CLA	MG-NC	3.65	2.14	2.06
11	A	1140	CLA	MG-NC	3.65	2.14	2.06
11	2	1225	CLA	C1D-C2D	3.65	1.50	1.42
11	2	1210	CLA	MG-NC	3.65	2.14	2.06
11	b	1228	CLA	MG-NC	3.65	2.14	2.06
11	a	1128	CLA	MG-NC	3.65	2.14	2.06
11	A	1106	CLA	MG-NC	3.64	2.14	2.06
11	1	1109	CLA	MG-NC	3.64	2.14	2.06
11	1	1130	CLA	MG-NC	3.64	2.14	2.06
11	B	1211	CLA	MG-NC	3.64	2.14	2.06
11	0	1402	CLA	MG-NC	3.64	2.14	2.06
11	2	1203	CLA	MG-NC	3.64	2.14	2.06
11	a	1129	CLA	MG-NC	3.64	2.14	2.06
11	B	1208	CLA	MG-NC	3.63	2.14	2.06
14	F	4018	BCR	C11-C12	-3.63	1.25	1.34
11	b	1215	CLA	MG-NC	3.63	2.14	2.06
11	a	1116	CLA	MG-NC	3.63	2.14	2.06
11	1	1136	CLA	MG-NC	3.63	2.14	2.06
11	B	1207	CLA	MG-NC	3.63	2.14	2.06
11	a	1130	CLA	MG-NC	3.63	2.14	2.06
11	L	1503	CLA	MG-NC	3.63	2.14	2.06
11	a	1237	CLA	MG-NC	3.63	2.14	2.06
11	A	1111	CLA	MG-NC	3.62	2.14	2.06
11	B	1216	CLA	C1D-C2D	3.62	1.50	1.42
11	2	1204	CLA	MG-NC	3.62	2.14	2.06
11	B	1226	CLA	MG-NC	3.62	2.14	2.06
11	B	1201	CLA	MG-NC	3.62	2.14	2.06
11	B	1203	CLA	MG-NC	3.62	2.14	2.06
11	b	1206	CLA	MG-NC	3.62	2.14	2.06
11	2	1208	CLA	MG-NC	3.62	2.14	2.06
11	A	1138	CLA	C1D-C2D	3.61	1.50	1.42
11	2	1023	CLA	MG-NC	3.61	2.14	2.06
11	B	1216	CLA	MG-NC	3.61	2.14	2.06
11	b	1023	CLA	MG-NC	3.61	2.14	2.06
11	b	1236	CLA	MG-NC	3.61	2.14	2.06
11	A	1136	CLA	MG-NC	3.61	2.14	2.06
11	B	1218	CLA	MG-NC	3.61	2.14	2.06
11	B	1205	CLA	MG-NC	3.61	2.14	2.06
11	1	1118	CLA	MG-NC	3.61	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1120	CLA	MG-NC	3.61	2.14	2.06
11	1	1128	CLA	MG-NC	3.61	2.14	2.06
11	B	1023	CLA	MG-NC	3.61	2.14	2.06
11	a	1109	CLA	C1D-C2D	3.60	1.50	1.42
11	1	1119	CLA	MG-NC	3.60	2.14	2.06
11	a	1136	CLA	MG-NC	3.60	2.14	2.06
11	B	1238	CLA	MG-NC	3.60	2.14	2.06
11	A	1237	CLA	MG-NC	3.60	2.14	2.06
11	b	1013	CLA	MG-NC	3.59	2.14	2.06
11	a	1118	CLA	MG-NC	3.59	2.14	2.06
11	B	1228	CLA	MG-NC	3.59	2.14	2.06
11	2	1202	CLA	MG-NC	3.59	2.14	2.06
11	A	1117	CLA	MG-NC	3.59	2.14	2.06
11	a	1119	CLA	MG-NC	3.59	2.14	2.06
11	a	1104	CLA	MG-NC	3.58	2.14	2.06
11	1	1127	CLA	MG-NC	3.58	2.14	2.06
11	A	1135	CLA	MG-NC	3.58	2.14	2.06
11	A	1107	CLA	MG-NC	3.57	2.14	2.06
11	A	1022	CLA	MG-NC	3.57	2.14	2.06
11	B	1228	CLA	C1D-C2D	3.57	1.50	1.42
11	B	1208	CLA	C1D-C2D	3.56	1.50	1.42
11	a	1138	CLA	C1D-C2D	3.56	1.50	1.42
11	k	1402	CLA	MG-NC	3.56	2.14	2.06
11	A	1138	CLA	MG-NC	3.56	2.14	2.06
11	2	1226	CLA	MG-NC	3.56	2.14	2.06
11	L	1502	CLA	MG-NC	3.55	2.14	2.06
11	B	1021	CLA	MG-NC	3.55	2.14	2.06
11	A	1108	CLA	MG-NC	3.55	2.14	2.06
11	a	1121	CLA	C1D-C2D	3.55	1.50	1.42
11	2	1214	CLA	MG-NC	3.55	2.14	2.06
11	2	1205	CLA	MG-NC	3.55	2.14	2.06
11	1	1237	CLA	MG-NC	3.54	2.14	2.06
11	2	1202	CLA	C1D-C2D	3.54	1.50	1.42
11	A	1109	CLA	MG-NC	3.54	2.14	2.06
11	A	1119	CLA	MG-NC	3.54	2.14	2.06
11	A	1108	CLA	C1D-C2D	3.53	1.50	1.42
11	2	1207	CLA	MG-NC	3.53	2.14	2.06
11	A	1011	CLA	MG-NC	3.53	2.14	2.06
11	2	1232	CLA	C1D-C2D	3.53	1.50	1.42
11	2	1213	CLA	C1D-C2D	3.53	1.50	1.42
11	b	1232	CLA	C1D-C2D	3.53	1.50	1.42
11	b	1231	CLA	C1D-C2D	3.53	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1114	CLA	C1D-C2D	3.53	1.50	1.42
11	2	1211	CLA	MG-NC	3.53	2.14	2.06
11	b	1238	CLA	C1D-C2D	3.52	1.50	1.42
11	b	1208	CLA	C1D-C2D	3.52	1.50	1.42
11	A	1128	CLA	MG-NC	3.52	2.14	2.06
11	1	1138	CLA	MG-NC	3.52	2.14	2.06
11	1	1104	CLA	MG-NC	3.52	2.14	2.06
11	1	1106	CLA	MG-NC	3.52	2.14	2.06
11	1	1105	CLA	C1D-C2D	3.52	1.50	1.42
11	A	1103	CLA	MG-NC	3.52	2.14	2.06
11	0	1402	CLA	C1D-C2D	3.52	1.50	1.42
11	B	1236	CLA	MG-NC	3.52	2.14	2.06
11	B	1218	CLA	C1D-C2D	3.51	1.50	1.42
11	b	1236	CLA	C1D-C2D	3.51	1.50	1.42
11	B	1215	CLA	C1D-C2D	3.51	1.50	1.42
11	1	1130	CLA	C1D-C2D	3.51	1.50	1.42
11	B	1013	CLA	MG-NC	3.51	2.14	2.06
11	1	1109	CLA	C1D-C2D	3.51	1.50	1.42
11	2	1209	CLA	C1D-C2D	3.50	1.50	1.42
11	1	1139	CLA	C1D-C2D	3.50	1.50	1.42
11	a	1134	CLA	C1D-C2D	3.50	1.50	1.42
11	a	1123	CLA	C1D-C2D	3.50	1.50	1.42
14	A	4003	BCR	C11-C12	-3.50	1.25	1.34
11	B	1204	CLA	MG-NC	3.50	2.14	2.06
11	B	1204	CLA	C1D-C2D	3.50	1.50	1.42
11	2	1013	CLA	MG-NC	3.50	2.14	2.06
11	a	1105	CLA	C1D-C2D	3.50	1.50	1.42
11	b	1218	CLA	C1D-C2D	3.50	1.50	1.42
11	1	1127	CLA	C1D-C2D	3.49	1.50	1.42
14	m	4021	BCR	C11-C12	-3.49	1.25	1.34
11	1	1121	CLA	C1D-C2D	3.49	1.50	1.42
11	1	1103	CLA	C1D-C2D	3.49	1.50	1.42
11	1	1134	CLA	C1D-C2D	3.49	1.50	1.42
11	1	1124	CLA	C1D-C2D	3.49	1.50	1.42
11	a	1130	CLA	C1D-C2D	3.49	1.50	1.42
11	b	1215	CLA	C1D-C2D	3.49	1.50	1.42
11	1	1237	CLA	C1D-C2D	3.49	1.50	1.42
11	B	1238	CLA	C1D-C2D	3.48	1.50	1.42
11	K	1402	CLA	MG-NC	3.48	2.14	2.06
11	A	1103	CLA	C1D-C2D	3.48	1.50	1.42
11	1	1119	CLA	C1D-C2D	3.48	1.50	1.42
11	B	1232	CLA	C1D-C2D	3.48	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1209	CLA	C1D-C2D	3.48	1.50	1.42
11	b	1240	CLA	C1D-C2D	3.48	1.50	1.42
11	k	1402	CLA	C1D-C2D	3.48	1.50	1.42
11	2	1204	CLA	C1D-C2D	3.48	1.50	1.42
11	b	1229	CLA	C1D-C2D	3.48	1.50	1.42
11	B	1203	CLA	C1D-C2D	3.47	1.50	1.42
11	l	1503	CLA	C1D-C2D	3.47	1.50	1.42
11	A	1120	CLA	C1D-C2D	3.47	1.50	1.42
11	a	1119	CLA	C1D-C2D	3.47	1.50	1.42
11	a	1116	CLA	C1D-C2D	3.47	1.50	1.42
11	A	1134	CLA	C1D-C2D	3.47	1.50	1.42
11	b	1239	CLA	C1D-C2D	3.47	1.50	1.42
11	a	1801	CLA	C1D-C2D	3.47	1.50	1.42
11	8	1503	CLA	C1D-C2D	3.47	1.50	1.42
11	A	1123	CLA	C1D-C2D	3.47	1.50	1.42
11	b	1235	CLA	C1D-C2D	3.46	1.50	1.42
11	1	1116	CLA	C1D-C2D	3.46	1.50	1.42
11	1	1138	CLA	C1D-C2D	3.46	1.50	1.42
11	1	1117	CLA	C1D-C2D	3.46	1.50	1.42
11	a	1114	CLA	C1D-C2D	3.46	1.50	1.42
11	B	1202	CLA	C1D-C2D	3.46	1.50	1.42
11	A	1118	CLA	MG-NC	3.46	2.14	2.06
11	A	1130	CLA	C1D-C2D	3.46	1.50	1.42
11	A	1117	CLA	C1D-C2D	3.46	1.50	1.42
11	1	1112	CLA	C1D-C2D	3.46	1.50	1.42
11	B	1220	CLA	C1D-C2D	3.46	1.50	1.42
11	a	1139	CLA	C1D-C2D	3.46	1.50	1.42
11	2	1223	CLA	C1D-C2D	3.46	1.50	1.42
11	a	1108	CLA	C1D-C2D	3.45	1.50	1.42
11	1	1101	CLA	C1D-C2D	3.45	1.50	1.42
11	B	1229	CLA	C1D-C2D	3.45	1.50	1.42
11	b	1204	CLA	C1D-C2D	3.45	1.50	1.42
11	A	1115	CLA	C1D-C2D	3.45	1.50	1.42
11	a	1101	CLA	C1D-C2D	3.45	1.50	1.42
11	b	1206	CLA	C1D-C2D	3.44	1.50	1.42
11	1	1106	CLA	C1D-C2D	3.44	1.50	1.42
11	a	1117	CLA	C1D-C2D	3.44	1.50	1.42
11	2	1013	CLA	C1D-C2D	3.44	1.50	1.42
11	2	1227	CLA	C1D-C2D	3.44	1.50	1.42
14	2	4014	BCR	C11-C12	-3.44	1.25	1.34
11	a	1124	CLA	C1D-C2D	3.44	1.50	1.42
11	2	1218	CLA	C1D-C2D	3.44	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1231	CLA	C1D-C2D	3.44	1.50	1.42
11	A	1104	CLA	MG-NC	3.44	2.14	2.06
11	2	1218	CLA	MG-NC	3.44	2.14	2.06
11	1	1108	CLA	C1D-C2D	3.44	1.50	1.42
11	A	1135	CLA	C1D-C2D	3.44	1.50	1.42
11	a	1112	CLA	C1D-C2D	3.43	1.50	1.42
11	b	1228	CLA	C1D-C2D	3.43	1.50	1.42
11	1	1123	CLA	C1D-C2D	3.43	1.50	1.42
11	A	1114	CLA	C1D-C2D	3.43	1.50	1.42
11	L	1503	CLA	C1D-C2D	3.43	1.50	1.42
11	1	1126	CLA	C1D-C2D	3.43	1.50	1.42
11	2	1239	CLA	C1D-C2D	3.43	1.50	1.42
11	A	1105	CLA	C1D-C2D	3.43	1.50	1.42
11	A	1106	CLA	C1D-C2D	3.43	1.50	1.42
11	b	1217	CLA	C1D-C2D	3.42	1.50	1.42
11	a	1103	CLA	C1D-C2D	3.42	1.50	1.42
11	a	1131	CLA	C1D-C2D	3.42	1.50	1.42
11	b	1227	CLA	C1D-C2D	3.42	1.50	1.42
11	B	1231	CLA	C1D-C2D	3.42	1.50	1.42
11	B	1235	CLA	C1D-C2D	3.42	1.50	1.42
11	B	1240	CLA	C1D-C2D	3.42	1.50	1.42
11	1	1133	CLA	C1D-C2D	3.42	1.50	1.42
11	a	1132	CLA	C1D-C2D	3.42	1.50	1.42
11	a	1133	CLA	C1D-C2D	3.42	1.50	1.42
11	2	1238	CLA	C1D-C2D	3.41	1.50	1.42
11	1	1110	CLA	C1D-C2D	3.41	1.50	1.42
11	b	1213	CLA	C1D-C2D	3.41	1.50	1.42
11	a	1136	CLA	C1D-C2D	3.41	1.50	1.42
14	6	4020	BCR	C11-C12	-3.41	1.25	1.34
11	b	1013	CLA	C1D-C2D	3.41	1.50	1.42
11	b	1202	CLA	C1D-C2D	3.41	1.50	1.42
11	a	1110	CLA	C1D-C2D	3.41	1.50	1.42
11	a	1137	CLA	C1D-C2D	3.41	1.50	1.42
11	1	1801	CLA	C1D-C2D	3.41	1.50	1.42
11	2	1215	CLA	C1D-C2D	3.41	1.50	1.42
11	A	1801	CLA	C1D-C2D	3.41	1.50	1.42
11	2	1222	CLA	C1D-C2D	3.41	1.50	1.42
11	k	1401	CLA	C1D-C2D	3.41	1.50	1.42
11	B	1213	CLA	C1D-C2D	3.41	1.50	1.42
11	2	1234	CLA	C1D-C2D	3.41	1.50	1.42
11	1	1104	CLA	C1D-C2D	3.41	1.50	1.42
11	2	1203	CLA	C1D-C2D	3.40	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1122	CLA	MG-NC	3.40	2.14	2.06
11	2	1229	CLA	C1D-C2D	3.40	1.50	1.42
11	1	1132	CLA	C1D-C2D	3.40	1.50	1.42
11	B	1212	CLA	C1D-C2D	3.40	1.50	1.42
11	B	1227	CLA	C1D-C2D	3.40	1.50	1.42
11	2	1210	CLA	C1D-C2D	3.40	1.50	1.42
11	1	1131	CLA	C1D-C2D	3.40	1.50	1.42
11	2	1228	CLA	C1D-C2D	3.40	1.50	1.42
11	B	1239	CLA	C1D-C2D	3.40	1.50	1.42
11	a	1104	CLA	C1D-C2D	3.40	1.50	1.42
11	A	1124	CLA	C1D-C2D	3.40	1.50	1.42
11	B	1209	CLA	C1D-C2D	3.40	1.50	1.42
11	A	1136	CLA	C1D-C2D	3.40	1.50	1.42
11	A	1119	CLA	C1D-C2D	3.40	1.50	1.42
11	B	1223	CLA	C1D-C2D	3.39	1.50	1.42
11	b	1211	CLA	C1D-C2D	3.39	1.50	1.42
11	1	1136	CLA	C1D-C2D	3.39	1.50	1.42
11	b	1210	CLA	C1D-C2D	3.39	1.50	1.42
11	A	1126	CLA	C1D-C2D	3.39	1.50	1.42
11	2	1214	CLA	C1D-C2D	3.39	1.50	1.42
11	1	1111	CLA	MG-NC	3.39	2.14	2.06
11	K	1401	CLA	C1D-C2D	3.38	1.50	1.42
11	b	1203	CLA	C1D-C2D	3.38	1.50	1.42
11	A	1102	CLA	C1D-C2D	3.38	1.50	1.42
11	a	1129	CLA	C1D-C2D	3.38	1.50	1.42
11	b	1214	CLA	C1D-C2D	3.38	1.50	1.42
11	a	1135	CLA	C1D-C2D	3.38	1.50	1.42
11	B	1234	CLA	C1D-C2D	3.38	1.50	1.42
11	2	1235	CLA	C1D-C2D	3.38	1.50	1.42
11	a	1102	CLA	C1D-C2D	3.38	1.50	1.42
11	A	1112	CLA	C1D-C2D	3.37	1.50	1.42
11	0	1401	CLA	C1D-C2D	3.37	1.50	1.42
11	A	1111	CLA	C1D-C2D	3.37	1.50	1.42
11	2	1208	CLA	C1D-C2D	3.37	1.50	1.42
11	A	1237	CLA	C1D-C2D	3.37	1.50	1.42
11	2	1240	CLA	C1D-C2D	3.37	1.50	1.42
11	a	1128	CLA	C1D-C2D	3.37	1.50	1.42
11	A	1131	CLA	C1D-C2D	3.36	1.50	1.42
11	L	1502	CLA	C1D-C2D	3.36	1.50	1.42
11	1	1102	CLA	C1D-C2D	3.36	1.50	1.42
11	1	1125	CLA	C1D-C2D	3.36	1.50	1.42
11	1	1115	CLA	C1D-C2D	3.36	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1219	CLA	C1D-C2D	3.36	1.50	1.42
11	1	1129	CLA	C1D-C2D	3.36	1.50	1.42
11	A	1139	CLA	C1D-C2D	3.36	1.50	1.42
14	6	4018	BCR	C11-C12	-3.35	1.25	1.34
11	b	1223	CLA	C1D-C2D	3.35	1.50	1.42
11	A	1137	CLA	C1D-C2D	3.35	1.50	1.42
14	M	4021	BCR	C11-C12	-3.35	1.25	1.34
11	K	1402	CLA	C1D-C2D	3.35	1.50	1.42
11	b	1216	CLA	C1D-C2D	3.35	1.50	1.42
11	A	1113	CLA	C1D-C2D	3.34	1.50	1.42
11	2	1224	CLA	C1D-C2D	3.34	1.50	1.42
11	b	1234	CLA	C1D-C2D	3.34	1.50	1.42
11	A	1125	CLA	C1D-C2D	3.34	1.50	1.42
11	B	1236	CLA	C1D-C2D	3.34	1.50	1.42
11	b	1212	CLA	C1D-C2D	3.34	1.50	1.42
14	2	4010	BCR	C11-C12	-3.34	1.26	1.34
11	2	1217	CLA	C1D-C2D	3.34	1.50	1.42
11	L	1501	CLA	C1D-C2D	3.33	1.50	1.42
11	1	1113	CLA	C1D-C2D	3.33	1.50	1.42
11	b	1222	CLA	C1D-C2D	3.33	1.50	1.42
11	A	1022	CLA	C1D-C2D	3.33	1.50	1.42
11	8	1501	CLA	C1D-C2D	3.33	1.50	1.42
11	2	1201	CLA	C1D-C2D	3.33	1.50	1.42
11	a	1113	CLA	C1D-C2D	3.33	1.50	1.42
11	B	1217	CLA	C1D-C2D	3.33	1.50	1.42
11	B	1219	CLA	C1D-C2D	3.33	1.50	1.42
11	1	1120	CLA	C1D-C2D	3.33	1.50	1.42
11	2	1236	CLA	C1D-C2D	3.33	1.50	1.42
11	a	1140	CLA	C1D-C2D	3.32	1.50	1.42
11	1	1128	CLA	C1D-C2D	3.32	1.50	1.42
11	A	1118	CLA	C1D-C2D	3.32	1.50	1.42
11	a	1111	CLA	C1D-C2D	3.32	1.50	1.42
11	1	1022	CLA	C1D-C2D	3.32	1.50	1.42
11	b	1224	CLA	C1D-C2D	3.32	1.50	1.42
11	A	1133	CLA	C1D-C2D	3.32	1.50	1.42
11	b	1023	CLA	C1D-C2D	3.32	1.50	1.42
11	b	1225	CLA	C1D-C2D	3.31	1.50	1.42
11	a	1120	CLA	C1D-C2D	3.31	1.50	1.42
11	b	1201	CLA	C1D-C2D	3.31	1.50	1.42
11	A	1101	CLA	C1D-C2D	3.30	1.50	1.42
11	1	1140	CLA	C1D-C2D	3.30	1.50	1.42
11	A	1116	CLA	C1D-C2D	3.30	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1132	CLA	C1D-C2D	3.30	1.50	1.42
11	B	1210	CLA	C1D-C2D	3.30	1.50	1.42
11	B	1207	CLA	C1D-C2D	3.30	1.50	1.42
11	A	1122	CLA	C1D-C2D	3.30	1.50	1.42
14	b	4017	BCR	C11-C12	-3.30	1.26	1.34
11	B	1214	CLA	C1D-C2D	3.29	1.50	1.42
11	B	1201	CLA	C1D-C2D	3.29	1.50	1.42
11	2	1220	CLA	C1D-C2D	3.29	1.50	1.42
14	2	4011	BCR	C11-C12	-3.29	1.26	1.34
11	B	1224	CLA	C1D-C2D	3.28	1.50	1.42
14	1	4003	BCR	C11-C12	-3.28	1.26	1.34
11	b	1226	CLA	C1D-C2D	3.28	1.50	1.42
14	B	4011	BCR	C11-C12	-3.28	1.26	1.34
11	2	1211	CLA	C1D-C2D	3.28	1.50	1.42
14	7	4021	BCR	C11-C12	-3.28	1.26	1.34
11	B	1206	CLA	C1D-C2D	3.28	1.50	1.42
14	f	4020	BCR	C11-C12	-3.27	1.26	1.34
11	a	1022	CLA	C1D-C2D	3.27	1.50	1.42
11	1	1137	CLA	C1D-C2D	3.27	1.50	1.42
11	1	1135	CLA	C1D-C2D	3.27	1.50	1.42
11	1	1122	CLA	C1D-C2D	3.27	1.50	1.42
11	a	1125	CLA	C1D-C2D	3.26	1.49	1.42
11	a	1107	CLA	C1D-C2D	3.26	1.49	1.42
11	A	1129	CLA	C1D-C2D	3.26	1.49	1.42
14	B	4004	BCR	C11-C12	-3.26	1.26	1.34
11	a	1122	CLA	C1D-C2D	3.26	1.49	1.42
11	a	1126	CLA	C1D-C2D	3.25	1.49	1.42
11	1	1111	CLA	C1D-C2D	3.25	1.49	1.42
11	A	1110	CLA	C1D-C2D	3.25	1.49	1.42
11	A	1140	CLA	C1D-C2D	3.25	1.49	1.42
14	B	4009	BCR	C11-C12	-3.24	1.26	1.34
14	b	4004	BCR	C11-C12	-3.24	1.26	1.34
11	B	1226	CLA	C1D-C2D	3.24	1.49	1.42
11	b	1219	CLA	C1D-C2D	3.24	1.49	1.42
11	2	1226	CLA	C1D-C2D	3.24	1.49	1.42
11	1	1107	CLA	C1D-C2D	3.24	1.49	1.42
11	A	1127	CLA	C1D-C2D	3.23	1.49	1.42
14	b	4010	BCR	C11-C12	-3.23	1.26	1.34
14	B	4005	BCR	C11-C12	-3.23	1.26	1.34
11	a	1118	CLA	C1D-C2D	3.23	1.49	1.42
11	a	1127	CLA	C1D-C2D	3.23	1.49	1.42
11	2	1207	CLA	C1D-C2D	3.23	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1237	CLA	C1D-C2D	3.23	1.49	1.42
11	l	1502	CLA	C1D-C2D	3.23	1.49	1.42
11	2	1206	CLA	C1D-C2D	3.22	1.49	1.42
14	A	4001	BCR	C11-C12	-3.22	1.26	1.34
14	b	4014	BCR	C11-C12	-3.22	1.26	1.34
11	l	1501	CLA	C1D-C2D	3.21	1.49	1.42
14	F	4020	BCR	C11-C12	-3.21	1.26	1.34
11	2	1212	CLA	C1D-C2D	3.21	1.49	1.42
11	A	1104	CLA	C1D-C2D	3.21	1.49	1.42
11	b	1220	CLA	C1D-C2D	3.21	1.49	1.42
11	2	1023	CLA	C1D-C2D	3.21	1.49	1.42
11	a	1106	CLA	C1D-C2D	3.21	1.49	1.42
11	A	1107	CLA	C1D-C2D	3.20	1.49	1.42
11	A	1128	CLA	C1D-C2D	3.20	1.49	1.42
11	a	1115	CLA	C1D-C2D	3.20	1.49	1.42
14	b	4005	BCR	C11-C12	-3.19	1.26	1.34
11	B	1225	CLA	C1D-C2D	3.18	1.49	1.42
11	B	1211	CLA	C1D-C2D	3.18	1.49	1.42
11	b	1021	CLA	C1D-C2D	3.18	1.49	1.42
14	a	4008	BCR	C11-C12	-3.18	1.26	1.34
14	f	4018	BCR	C11-C12	-3.18	1.26	1.34
11	8	1502	CLA	C1D-C2D	3.18	1.49	1.42
14	b	4011	BCR	C11-C12	-3.18	1.26	1.34
11	2	1221	CLA	C1D-C2D	3.17	1.49	1.42
14	A	4007	BCR	C11-C12	-3.17	1.26	1.34
11	b	1207	CLA	C1D-C2D	3.17	1.49	1.42
14	8	4022	BCR	C11-C12	-3.17	1.26	1.34
14	2	4017	BCR	C11-C12	-3.15	1.26	1.34
11	b	1221	CLA	C1D-C2D	3.15	1.49	1.42
14	1	4008	BCR	C11-C12	-3.15	1.26	1.34
11	b	1230	CLA	C1D-C2D	3.15	1.49	1.42
14	b	4006	BCR	C11-C12	-3.14	1.26	1.34
11	1	1011	CLA	C1D-C2D	3.14	1.49	1.42
14	l	4019	BCR	C11-C12	-3.14	1.26	1.34
14	F	4013	BCR	C11-C12	-3.14	1.26	1.34
11	B	1013	CLA	C1D-C2D	3.14	1.49	1.42
14	f	4013	BCR	C11-C12	-3.14	1.26	1.34
11	a	1011	CLA	C1D-C2D	3.13	1.49	1.42
11	a	1012	CLA	C1D-C2D	3.13	1.49	1.42
11	A	1011	CLA	C1D-C2D	3.12	1.49	1.42
11	2	1230	CLA	C1D-C2D	3.12	1.49	1.42
14	B	4017	BCR	C11-C12	-3.12	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1021	CLA	C1D-C2D	3.12	1.49	1.42
11	1	1118	CLA	C1D-C2D	3.11	1.49	1.42
11	2	1021	CLA	C1D-C2D	3.11	1.49	1.42
11	2	1216	CLA	C1D-C2D	3.11	1.49	1.42
14	2	4006	BCR	C11-C12	-3.09	1.26	1.34
14	l	4022	BCR	C11-C12	-3.09	1.26	1.34
14	a	4007	BCR	C11-C12	-3.09	1.26	1.34
14	B	4006	BCR	C11-C12	-3.08	1.26	1.34
14	L	4019	BCR	C11-C12	-3.08	1.26	1.34
11	B	1023	CLA	C1D-C2D	3.07	1.49	1.42
14	a	4001	BCR	C11-C12	-3.07	1.26	1.34
11	b	1205	CLA	C1D-C2D	3.07	1.49	1.42
14	2	4009	BCR	C11-C12	-3.06	1.26	1.34
14	a	4002	BCR	C11-C12	-3.06	1.26	1.34
14	2	4005	BCR	C11-C12	-3.05	1.26	1.34
14	1	4001	BCR	C11-C12	-3.05	1.26	1.34
14	a	4003	BCR	C11-C12	-3.05	1.26	1.34
14	2	4004	BCR	C11-C12	-3.03	1.26	1.34
14	1	4002	BCR	C11-C12	-3.03	1.26	1.34
14	L	4022	BCR	C11-C12	-3.02	1.26	1.34
11	B	1222	CLA	C1D-C2D	3.01	1.49	1.42
14	A	4008	BCR	C11-C12	-3.01	1.26	1.34
14	B	4010	BCR	C11-C12	-3.00	1.26	1.34
11	A	1126	CLA	C4B-CHC	3.00	1.49	1.41
14	1	4007	BCR	C11-C12	-2.99	1.26	1.34
14	B	4014	BCR	C11-C12	-2.99	1.26	1.34
11	A	1012	CLA	C1D-C2D	2.98	1.49	1.42
14	6	4013	BCR	C11-C12	-2.97	1.26	1.34
14	8	4019	BCR	C11-C12	-2.97	1.26	1.34
11	B	1221	CLA	C1D-C2D	2.96	1.49	1.42
11	1	1012	CLA	C1D-C2D	2.95	1.49	1.42
14	A	4002	BCR	C11-C12	-2.94	1.27	1.34
11	B	1230	CLA	C1D-C2D	2.94	1.49	1.42
11	A	1112	CLA	C4B-CHC	2.92	1.49	1.41
11	a	1126	CLA	C4B-CHC	2.92	1.49	1.41
11	A	1125	CLA	C4C-C3C	2.91	1.50	1.45
11	B	1205	CLA	C1D-C2D	2.91	1.49	1.42
11	2	1205	CLA	C1D-C2D	2.90	1.49	1.42
11	a	1115	CLA	C4B-CHC	2.90	1.49	1.41
11	1	1126	CLA	C4B-CHC	2.90	1.49	1.41
11	A	1115	CLA	C4B-CHC	2.89	1.49	1.41
11	a	1237	CLA	C1B-CHB	2.89	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1202	CLA	C4B-CHC	2.88	1.49	1.41
11	a	1112	CLA	C4B-CHC	2.88	1.49	1.41
11	A	1117	CLA	C4B-CHC	2.87	1.49	1.41
11	b	1210	CLA	C4B-CHC	2.86	1.49	1.41
14	b	4009	BCR	C11-C12	-2.86	1.27	1.34
11	2	1207	CLA	C1C-NC	-2.86	1.33	1.37
11	b	1202	CLA	C4B-CHC	2.86	1.48	1.41
11	b	1214	CLA	C4B-CHC	2.86	1.48	1.41
11	2	1223	CLA	C4B-CHC	2.85	1.48	1.41
11	2	1213	CLA	C4B-CHC	2.85	1.48	1.41
11	A	1116	CLA	C4B-CHC	2.85	1.48	1.41
11	0	1402	CLA	C4B-CHC	2.85	1.48	1.41
11	A	1103	CLA	C4B-CHC	2.85	1.48	1.41
11	A	1137	CLA	C4B-CHC	2.84	1.48	1.41
11	b	1221	CLA	C4B-CHC	2.84	1.48	1.41
11	2	1236	CLA	C4B-CHC	2.83	1.48	1.41
11	2	1219	CLA	C4B-CHC	2.83	1.48	1.41
11	a	1116	CLA	C4B-CHC	2.83	1.48	1.41
11	2	1235	CLA	C4B-CHC	2.82	1.48	1.41
11	A	1801	CLA	C1C-NC	-2.82	1.33	1.37
11	1	1111	CLA	C4B-CHC	2.82	1.48	1.41
11	B	1222	CLA	C4B-CHC	2.81	1.48	1.41
11	B	1214	CLA	C4B-CHC	2.81	1.48	1.41
11	2	1202	CLA	C4B-CHC	2.81	1.48	1.41
11	a	1104	CLA	C4B-CHC	2.81	1.48	1.41
11	A	1118	CLA	C1B-CHB	2.81	1.48	1.41
11	A	1101	CLA	C4B-CHC	2.81	1.48	1.41
11	B	1224	CLA	C4B-CHC	2.81	1.48	1.41
11	b	1223	CLA	C1B-CHB	2.81	1.48	1.41
11	b	1213	CLA	C4B-CHC	2.80	1.48	1.41
11	B	1240	CLA	C4B-CHC	2.80	1.48	1.41
11	1	1122	CLA	C4B-CHC	2.80	1.48	1.41
11	B	1235	CLA	C4B-CHC	2.80	1.48	1.41
11	A	1140	CLA	C1C-NC	-2.80	1.33	1.37
11	A	1111	CLA	C4B-CHC	2.80	1.48	1.41
11	B	1208	CLA	C4B-CHC	2.80	1.48	1.41
11	a	1111	CLA	C4B-CHC	2.80	1.48	1.41
11	a	1122	CLA	C4B-CHC	2.80	1.48	1.41
11	2	1202	CLA	C1B-CHB	2.79	1.48	1.41
11	b	1208	CLA	C1B-CHB	2.79	1.48	1.41
11	B	1236	CLA	C4B-CHC	2.79	1.48	1.41
11	2	1236	CLA	C1B-CHB	2.79	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1235	CLA	C4B-CHC	2.79	1.48	1.41
11	1	1125	CLA	C4B-CHC	2.78	1.48	1.41
11	A	1139	CLA	C4B-CHC	2.78	1.48	1.41
11	2	1205	CLA	C1B-CHB	2.78	1.48	1.41
11	A	1136	CLA	C1B-CHB	2.78	1.48	1.41
11	8	1503	CLA	C4B-CHC	2.77	1.48	1.41
11	A	1110	CLA	C1B-CHB	2.77	1.48	1.41
11	A	1801	CLA	C4C-C3C	2.77	1.49	1.45
11	2	1229	CLA	C4B-CHC	2.77	1.48	1.41
11	b	1236	CLA	C4B-CHC	2.77	1.48	1.41
11	1	1136	CLA	C1B-CHB	2.77	1.48	1.41
11	a	1133	CLA	C1B-CHB	2.77	1.48	1.41
11	2	1210	CLA	C4B-CHC	2.77	1.48	1.41
11	b	1013	CLA	C4B-CHC	2.77	1.48	1.41
11	2	1226	CLA	C1B-CHB	2.77	1.48	1.41
11	B	1234	CLA	C1B-CHB	2.77	1.48	1.41
11	B	1212	CLA	C4B-CHC	2.77	1.48	1.41
11	A	1132	CLA	C1B-CHB	2.77	1.48	1.41
11	b	1212	CLA	C1B-CHB	2.76	1.48	1.41
11	A	1105	CLA	C1B-CHB	2.76	1.48	1.41
11	b	1234	CLA	C1B-CHB	2.76	1.48	1.41
11	b	1226	CLA	C4B-CHC	2.76	1.48	1.41
11	A	1120	CLA	C4B-CHC	2.76	1.48	1.41
11	a	1132	CLA	C4B-CHC	2.75	1.48	1.41
11	2	1231	CLA	C4B-CHC	2.75	1.48	1.41
11	B	1227	CLA	C1B-CHB	2.75	1.48	1.41
11	8	1502	CLA	C4B-CHC	2.75	1.48	1.41
11	b	1218	CLA	C4B-CHC	2.75	1.48	1.41
11	2	1208	CLA	C1B-CHB	2.75	1.48	1.41
11	1	1112	CLA	C4B-CHC	2.75	1.48	1.41
11	a	1119	CLA	C1C-NC	-2.75	1.33	1.37
11	l	1502	CLA	C4B-CHC	2.75	1.48	1.41
11	b	1240	CLA	C4B-CHC	2.75	1.48	1.41
11	B	1223	CLA	C4B-CHC	2.75	1.48	1.41
11	b	1221	CLA	C1B-CHB	2.75	1.48	1.41
11	l	1501	CLA	C4B-CHC	2.74	1.48	1.41
11	b	1201	CLA	C4B-CHC	2.74	1.48	1.41
11	b	1216	CLA	C4B-CHC	2.74	1.48	1.41
11	A	1121	CLA	C4B-CHC	2.74	1.48	1.41
11	a	1111	CLA	C1B-CHB	2.74	1.48	1.41
11	A	1113	CLA	C4B-CHC	2.74	1.48	1.41
11	a	1125	CLA	C4B-CHC	2.74	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1130	CLA	C4B-CHC	2.74	1.48	1.41
11	B	1213	CLA	C1B-CHB	2.74	1.48	1.41
11	b	1211	CLA	C1B-CHB	2.74	1.48	1.41
11	1	1129	CLA	C4B-CHC	2.74	1.48	1.41
11	2	1232	CLA	C4B-CHC	2.74	1.48	1.41
11	1	1108	CLA	C4B-CHC	2.74	1.48	1.41
11	A	1125	CLA	C1B-CHB	2.74	1.48	1.41
11	1	1130	CLA	C4B-CHC	2.74	1.48	1.41
11	a	1136	CLA	C1B-CHB	2.73	1.48	1.41
11	1	1129	CLA	C1B-CHB	2.73	1.48	1.41
11	a	1115	CLA	C1B-CHB	2.73	1.48	1.41
11	a	1105	CLA	C1B-CHB	2.73	1.48	1.41
11	1	1107	CLA	C1B-CHB	2.73	1.48	1.41
11	b	1229	CLA	C4B-CHC	2.73	1.48	1.41
11	2	1216	CLA	C4B-CHC	2.73	1.48	1.41
11	L	1501	CLA	C4B-CHC	2.73	1.48	1.41
11	1	1134	CLA	C4B-CHC	2.73	1.48	1.41
11	A	1022	CLA	C4B-CHC	2.73	1.48	1.41
11	B	1232	CLA	C1B-CHB	2.73	1.48	1.41
11	1	1102	CLA	C4B-CHC	2.73	1.48	1.41
11	1	1116	CLA	C4B-CHC	2.73	1.48	1.41
11	1	1122	CLA	C1B-CHB	2.73	1.48	1.41
11	a	1114	CLA	C1B-CHB	2.72	1.48	1.41
11	a	1118	CLA	C1B-CHB	2.72	1.48	1.41
11	B	1013	CLA	C4B-CHC	2.72	1.48	1.41
11	1	1119	CLA	C4B-CHC	2.72	1.48	1.41
11	2	1204	CLA	C4B-CHC	2.72	1.48	1.41
11	1	1120	CLA	C4B-CHC	2.72	1.48	1.41
11	1	1114	CLA	C1B-CHB	2.72	1.48	1.41
11	B	1213	CLA	C4B-CHC	2.72	1.48	1.41
11	2	1213	CLA	C1B-CHB	2.72	1.48	1.41
11	b	1203	CLA	C4B-CHC	2.72	1.48	1.41
11	1	1113	CLA	C1B-CHB	2.72	1.48	1.41
11	b	1224	CLA	C4B-CHC	2.72	1.48	1.41
11	A	1140	CLA	C1B-CHB	2.72	1.48	1.41
11	B	1226	CLA	C4B-CHC	2.72	1.48	1.41
11	b	1231	CLA	C4B-CHC	2.72	1.48	1.41
11	B	1208	CLA	C1B-CHB	2.72	1.48	1.41
11	2	1205	CLA	C4B-CHC	2.72	1.48	1.41
11	a	1113	CLA	C1B-CHB	2.72	1.48	1.41
11	b	1207	CLA	C1C-NC	-2.71	1.33	1.37
11	1	1139	CLA	C4B-CHC	2.71	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1219	CLA	C1B-CHB	2.71	1.48	1.41
11	a	1121	CLA	C4B-CHC	2.71	1.48	1.41
11	a	1012	CLA	C4B-CHC	2.71	1.48	1.41
11	A	1114	CLA	C1B-CHB	2.71	1.48	1.41
11	a	1108	CLA	C1B-CHB	2.71	1.48	1.41
11	k	1402	CLA	C4B-CHC	2.71	1.48	1.41
11	l	1133	CLA	C1B-CHB	2.71	1.48	1.41
11	a	1106	CLA	C4B-CHC	2.71	1.48	1.41
11	a	1117	CLA	C4B-CHC	2.71	1.48	1.41
11	b	1238	CLA	C4B-CHC	2.71	1.48	1.41
11	b	1213	CLA	C1B-CHB	2.71	1.48	1.41
11	a	1113	CLA	C4B-CHC	2.71	1.48	1.41
11	B	1224	CLA	C1B-CHB	2.71	1.48	1.41
11	A	1107	CLA	C4B-CHC	2.71	1.48	1.41
11	l	1124	CLA	C4B-CHC	2.71	1.48	1.41
11	b	1216	CLA	C1B-CHB	2.71	1.48	1.41
11	a	1130	CLA	C4B-CHC	2.71	1.48	1.41
11	2	1013	CLA	C4B-CHC	2.71	1.48	1.41
11	2	1224	CLA	C1B-CHB	2.71	1.48	1.41
11	A	1108	CLA	C4B-CHC	2.71	1.48	1.41
11	a	1801	CLA	C4B-CHC	2.71	1.48	1.41
11	B	1218	CLA	C1B-CHB	2.71	1.48	1.41
11	2	1201	CLA	C1B-CHB	2.71	1.48	1.41
11	l	1107	CLA	C4B-CHC	2.71	1.48	1.41
11	a	1139	CLA	C1B-CHB	2.70	1.48	1.41
11	A	1127	CLA	C4B-CHC	2.70	1.48	1.41
11	B	1230	CLA	C1B-CHB	2.70	1.48	1.41
11	a	1134	CLA	C4B-CHC	2.70	1.48	1.41
11	A	1129	CLA	C4B-CHC	2.70	1.48	1.41
11	b	1232	CLA	C4B-CHC	2.70	1.48	1.41
11	b	1021	CLA	C4B-CHC	2.70	1.48	1.41
11	b	1220	CLA	C4B-CHC	2.70	1.48	1.41
11	b	1217	CLA	C4B-CHC	2.70	1.48	1.41
11	2	1216	CLA	C1B-CHB	2.70	1.48	1.41
11	l	1135	CLA	C4B-CHC	2.70	1.48	1.41
11	2	1238	CLA	C4B-CHC	2.70	1.48	1.41
11	l	1502	CLA	C1B-CHB	2.70	1.48	1.41
11	2	1230	CLA	C4B-CHC	2.70	1.48	1.41
11	b	1211	CLA	C4B-CHC	2.70	1.48	1.41
11	A	1109	CLA	C4B-CHC	2.70	1.48	1.41
11	B	1023	CLA	C4B-CHC	2.70	1.48	1.41
11	B	1210	CLA	C4B-CHC	2.70	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1124	CLA	C4B-CHC	2.70	1.48	1.41
11	2	1226	CLA	C4B-CHC	2.70	1.48	1.41
11	1	1131	CLA	C1B-CHB	2.70	1.48	1.41
11	L	1502	CLA	C4B-CHC	2.70	1.48	1.41
11	0	1402	CLA	C1B-CHB	2.69	1.48	1.41
11	1	1012	CLA	C1B-CHB	2.69	1.48	1.41
11	1	1137	CLA	C4B-CHC	2.69	1.48	1.41
11	b	1236	CLA	C1B-CHB	2.69	1.48	1.41
11	a	1129	CLA	C1B-CHB	2.69	1.48	1.41
11	B	1236	CLA	C1B-CHB	2.69	1.48	1.41
11	a	1137	CLA	C1B-CHB	2.69	1.48	1.41
11	2	1239	CLA	C1B-CHB	2.69	1.48	1.41
11	1	1136	CLA	C4B-CHC	2.69	1.48	1.41
11	1	1105	CLA	C4B-CHC	2.69	1.48	1.41
11	b	1224	CLA	C1B-CHB	2.69	1.48	1.41
11	b	1209	CLA	C1B-CHB	2.69	1.48	1.41
11	B	1230	CLA	C1C-NC	-2.69	1.33	1.37
11	a	1110	CLA	C4B-CHC	2.69	1.48	1.41
11	1	1108	CLA	C1B-CHB	2.69	1.48	1.41
11	1	1113	CLA	C4B-CHC	2.69	1.48	1.41
11	A	1131	CLA	C1B-CHB	2.69	1.48	1.41
11	A	1103	CLA	C1B-CHB	2.69	1.48	1.41
11	B	1216	CLA	C4B-CHC	2.69	1.48	1.41
11	2	1227	CLA	C1B-CHB	2.69	1.48	1.41
11	2	1211	CLA	C1B-CHB	2.69	1.48	1.41
11	A	1128	CLA	C1B-CHB	2.69	1.48	1.41
11	1	1138	CLA	C1B-CHB	2.69	1.48	1.41
11	A	1105	CLA	C4B-CHC	2.69	1.48	1.41
11	A	1102	CLA	C4B-CHC	2.69	1.48	1.41
11	K	1402	CLA	C1C-NC	-2.69	1.33	1.37
11	A	1012	CLA	C4B-CHC	2.68	1.48	1.41
11	1	1106	CLA	C1B-CHB	2.68	1.48	1.41
11	2	1023	CLA	C4B-CHC	2.68	1.48	1.41
11	a	1129	CLA	C4B-CHC	2.68	1.48	1.41
11	a	1108	CLA	C4B-CHC	2.68	1.48	1.41
11	1	1237	CLA	C1B-CHB	2.68	1.48	1.41
11	1	1022	CLA	C4B-CHC	2.68	1.48	1.41
11	B	1210	CLA	C1B-CHB	2.68	1.48	1.41
11	1	1127	CLA	C1B-CHB	2.68	1.48	1.41
11	B	1211	CLA	C1B-CHB	2.68	1.48	1.41
11	A	1131	CLA	C4B-CHC	2.68	1.48	1.41
11	B	1205	CLA	C1B-CHB	2.68	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1109	CLA	C4B-CHC	2.68	1.48	1.41
11	2	1212	CLA	C1B-CHB	2.68	1.48	1.41
11	b	1220	CLA	C1B-CHB	2.68	1.48	1.41
11	2	1222	CLA	C4B-CHC	2.68	1.48	1.41
11	2	1220	CLA	C1B-CHB	2.68	1.48	1.41
11	B	1211	CLA	C4B-CHC	2.68	1.48	1.41
11	B	1217	CLA	C4B-CHC	2.68	1.48	1.41
11	a	1137	CLA	C4B-CHC	2.68	1.48	1.41
11	A	1134	CLA	C1B-CHB	2.68	1.48	1.41
11	B	1239	CLA	C1B-CHB	2.68	1.48	1.41
11	1	1012	CLA	C4B-CHC	2.68	1.48	1.41
11	2	1240	CLA	C1B-CHB	2.68	1.48	1.41
11	a	1119	CLA	C1B-CHB	2.68	1.48	1.41
11	B	1219	CLA	C4B-CHC	2.68	1.48	1.41
11	A	1129	CLA	C1B-CHB	2.68	1.48	1.41
11	B	1203	CLA	C4B-CHC	2.68	1.48	1.41
11	b	1227	CLA	C1B-CHB	2.68	1.48	1.41
11	1	1104	CLA	C4B-CHC	2.68	1.48	1.41
11	1	1110	CLA	C4B-CHC	2.68	1.48	1.41
11	b	1239	CLA	C1B-CHB	2.67	1.48	1.41
11	A	1122	CLA	C1B-CHB	2.67	1.48	1.41
11	b	1226	CLA	C1B-CHB	2.67	1.48	1.41
11	b	1222	CLA	C4B-CHC	2.67	1.48	1.41
11	2	1228	CLA	C4B-CHC	2.67	1.48	1.41
11	B	1229	CLA	C1B-CHB	2.67	1.48	1.41
11	A	1104	CLA	C4B-CHC	2.67	1.48	1.41
11	A	1110	CLA	C4B-CHC	2.67	1.48	1.41
11	A	1124	CLA	C4B-CHC	2.67	1.48	1.41
11	A	1121	CLA	C1B-CHB	2.67	1.48	1.41
11	b	1212	CLA	C4B-CHC	2.67	1.48	1.41
11	B	1239	CLA	C4B-CHC	2.67	1.48	1.41
11	1	1115	CLA	C4B-CHC	2.67	1.48	1.41
11	a	1131	CLA	C4B-CHC	2.67	1.48	1.41
11	B	1210	CLA	C4C-C3C	2.67	1.49	1.45
11	1	1118	CLA	C4B-CHC	2.67	1.48	1.41
11	2	1239	CLA	C4B-CHC	2.67	1.48	1.41
11	b	1206	CLA	C1B-CHB	2.67	1.48	1.41
11	B	1206	CLA	C1B-CHB	2.67	1.48	1.41
11	2	1221	CLA	C4B-CHC	2.67	1.48	1.41
11	2	1023	CLA	C1C-NC	-2.66	1.33	1.37
11	2	1231	CLA	CHD-C4C	2.66	1.48	1.41
11	1	1127	CLA	C4B-CHC	2.66	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1122	CLA	C4B-CHC	2.66	1.48	1.41
11	b	1232	CLA	C1B-CHB	2.66	1.48	1.41
11	2	1240	CLA	C4B-CHC	2.66	1.48	1.41
11	b	1225	CLA	C4B-CHC	2.66	1.48	1.41
11	a	1117	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1140	CLA	C4B-CHC	2.66	1.48	1.41
11	A	1237	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1134	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1106	CLA	C4B-CHC	2.66	1.48	1.41
11	b	1227	CLA	C4B-CHC	2.66	1.48	1.41
11	2	1206	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1105	CLA	C1B-CHB	2.66	1.48	1.41
11	b	1218	CLA	C1B-CHB	2.66	1.48	1.41
11	a	1135	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1101	CLA	C4B-CHC	2.66	1.48	1.41
11	1	1131	CLA	C4B-CHC	2.66	1.48	1.41
11	B	1223	CLA	C1B-CHB	2.66	1.48	1.41
11	1	1116	CLA	C1B-CHB	2.66	1.48	1.41
11	B	1238	CLA	C1B-CHB	2.66	1.48	1.41
11	l	1503	CLA	C4B-CHC	2.66	1.48	1.41
11	1	1121	CLA	C4B-CHC	2.66	1.48	1.41
11	1	1118	CLA	C1B-CHB	2.66	1.48	1.41
11	b	1209	CLA	C4B-CHC	2.66	1.48	1.41
11	a	1131	CLA	C1B-CHB	2.65	1.48	1.41
11	A	1135	CLA	C4B-CHC	2.65	1.48	1.41
11	a	1140	CLA	C1B-CHB	2.65	1.48	1.41
11	a	1102	CLA	C4B-CHC	2.65	1.48	1.41
11	1	1121	CLA	C1B-CHB	2.65	1.48	1.41
11	A	1108	CLA	C1B-CHB	2.65	1.48	1.41
11	2	1234	CLA	C1B-CHB	2.65	1.48	1.41
11	B	1217	CLA	C1B-CHB	2.65	1.48	1.41
11	2	1211	CLA	C4B-CHC	2.65	1.48	1.41
11	1	1112	CLA	C1B-CHB	2.65	1.48	1.41
11	A	1130	CLA	C1B-CHB	2.65	1.48	1.41
11	a	1103	CLA	C4B-CHC	2.65	1.48	1.41
11	a	1140	CLA	C4B-CHC	2.65	1.48	1.41
11	b	1230	CLA	C1B-CHB	2.65	1.48	1.41
11	1	1801	CLA	C4B-CHC	2.65	1.48	1.41
11	a	1237	CLA	C4B-CHC	2.65	1.48	1.41
11	1	1128	CLA	C1B-CHB	2.65	1.48	1.41
11	A	1121	CLA	CHD-C4C	2.65	1.48	1.41
11	B	1228	CLA	C4B-CHC	2.65	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1218	CLA	C4B-CHC	2.65	1.48	1.41
11	2	1225	CLA	CHD-C4C	2.65	1.48	1.41
11	B	1207	CLA	C4B-CHC	2.65	1.48	1.41
11	2	1224	CLA	C4B-CHC	2.65	1.48	1.41
11	a	1126	CLA	C1B-CHB	2.65	1.48	1.41
11	A	1113	CLA	C1B-CHB	2.65	1.48	1.41
11	b	1228	CLA	C4B-CHC	2.65	1.48	1.41
11	2	1208	CLA	C4B-CHC	2.64	1.48	1.41
11	1	1140	CLA	C1B-CHB	2.64	1.48	1.41
11	B	1221	CLA	C4B-CHC	2.64	1.48	1.41
11	b	1208	CLA	C4B-CHC	2.64	1.48	1.41
11	b	1201	CLA	C1B-CHB	2.64	1.48	1.41
11	A	1801	CLA	C4B-CHC	2.64	1.48	1.41
11	A	1132	CLA	C4B-CHC	2.64	1.48	1.41
11	A	1104	CLA	C1B-CHB	2.64	1.48	1.41
11	A	1133	CLA	C1B-CHB	2.64	1.48	1.41
11	2	1217	CLA	C4B-CHC	2.64	1.48	1.41
11	2	1223	CLA	C1B-CHB	2.64	1.48	1.41
11	a	1120	CLA	C1B-CHB	2.64	1.48	1.41
11	L	1503	CLA	C1B-CHB	2.64	1.48	1.41
11	A	1137	CLA	C1B-CHB	2.64	1.48	1.41
11	1	1109	CLA	C1B-CHB	2.64	1.48	1.41
11	b	1240	CLA	C1B-CHB	2.64	1.48	1.41
11	B	1235	CLA	C1B-CHB	2.64	1.48	1.41
11	b	1204	CLA	C4B-CHC	2.64	1.48	1.41
11	a	1125	CLA	C1C-NC	-2.64	1.33	1.37
11	A	1115	CLA	C1B-CHB	2.63	1.48	1.41
11	A	1128	CLA	C4B-CHC	2.63	1.48	1.41
11	a	1128	CLA	C1B-CHB	2.63	1.48	1.41
11	a	1139	CLA	CHD-C4C	2.63	1.48	1.41
11	B	1219	CLA	C1B-CHB	2.63	1.48	1.41
11	B	1225	CLA	C4B-CHC	2.63	1.48	1.41
11	B	1231	CLA	C4C-C3C	2.63	1.49	1.45
11	a	1125	CLA	C1B-CHB	2.63	1.48	1.41
11	a	1123	CLA	C1B-CHB	2.63	1.48	1.41
11	A	1119	CLA	C1C-NC	-2.63	1.33	1.37
11	2	1218	CLA	C1B-CHB	2.63	1.48	1.41
11	A	1114	CLA	C4B-CHC	2.63	1.48	1.41
11	1	1137	CLA	C1B-CHB	2.63	1.48	1.41
11	A	1101	CLA	C1B-CHB	2.63	1.48	1.41
11	b	1235	CLA	C1B-CHB	2.63	1.48	1.41
11	2	1214	CLA	C1B-CHB	2.63	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1110	CLA	C1B-CHB	2.63	1.48	1.41
11	a	1107	CLA	C4B-CHC	2.63	1.48	1.41
11	a	1127	CLA	C1B-CHB	2.63	1.48	1.41
11	1	1123	CLA	C4B-CHC	2.63	1.48	1.41
11	A	1138	CLA	C1B-CHB	2.63	1.48	1.41
11	b	1204	CLA	C1B-CHB	2.63	1.48	1.41
11	k	1402	CLA	C1B-CHB	2.62	1.48	1.41
11	b	1207	CLA	C1B-CHB	2.62	1.48	1.41
11	K	1402	CLA	C1B-CHB	2.62	1.48	1.41
11	b	1023	CLA	C4B-CHC	2.62	1.48	1.41
11	a	1123	CLA	C4B-CHC	2.62	1.48	1.41
11	2	1217	CLA	C1B-CHB	2.62	1.48	1.41
11	A	1136	CLA	C4B-CHC	2.62	1.48	1.41
11	a	1122	CLA	C1B-CHB	2.62	1.48	1.41
11	2	1204	CLA	C1B-CHB	2.62	1.48	1.41
11	a	1120	CLA	C4B-CHC	2.62	1.48	1.41
11	B	1229	CLA	C4B-CHC	2.62	1.48	1.41
11	8	1503	CLA	C1B-CHB	2.62	1.48	1.41
11	2	1212	CLA	C4B-CHC	2.62	1.48	1.41
11	A	1133	CLA	C1C-NC	-2.62	1.33	1.37
11	a	1105	CLA	C4B-CHC	2.62	1.48	1.41
11	b	1229	CLA	C1B-CHB	2.62	1.48	1.41
11	b	1230	CLA	C4B-CHC	2.62	1.48	1.41
11	k	1401	CLA	C1B-CHB	2.62	1.48	1.41
11	a	1022	CLA	C4B-CHC	2.62	1.48	1.41
11	2	1230	CLA	C1C-NC	-2.62	1.33	1.37
11	1	1132	CLA	C4B-CHC	2.62	1.48	1.41
11	B	1203	CLA	C1B-CHB	2.62	1.48	1.41
11	B	1228	CLA	C1B-CHB	2.62	1.48	1.41
11	1	1128	CLA	C1C-NC	-2.62	1.33	1.37
11	b	1219	CLA	C4B-CHC	2.62	1.48	1.41
11	a	1136	CLA	C4B-CHC	2.62	1.48	1.41
11	B	1209	CLA	C1B-CHB	2.62	1.48	1.41
11	A	1140	CLA	C4B-CHC	2.62	1.48	1.41
11	2	1214	CLA	C4B-CHC	2.62	1.48	1.41
11	k	1401	CLA	C4B-CHC	2.62	1.48	1.41
11	2	1225	CLA	C4B-CHC	2.62	1.48	1.41
11	2	1210	CLA	C1B-CHB	2.62	1.48	1.41
11	2	1215	CLA	C1B-CHB	2.61	1.48	1.41
11	a	1114	CLA	C4B-CHC	2.61	1.48	1.41
11	a	1128	CLA	C4B-CHC	2.61	1.48	1.41
11	b	1215	CLA	C4B-CHC	2.61	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1101	CLA	C1B-CHB	2.61	1.48	1.41
11	b	1220	CLA	C4C-C3C	2.61	1.49	1.45
11	2	1220	CLA	C4B-CHC	2.61	1.48	1.41
11	B	1216	CLA	CHD-C4C	2.61	1.48	1.41
11	B	1023	CLA	C1C-NC	-2.61	1.33	1.37
11	1	1139	CLA	C1B-CHB	2.61	1.48	1.41
11	1	1103	CLA	C4B-CHC	2.61	1.48	1.41
11	A	1119	CLA	C4B-CHC	2.61	1.48	1.41
11	a	1109	CLA	CHD-C4C	2.61	1.48	1.41
11	2	1219	CLA	C1B-CHB	2.61	1.48	1.41
11	1	1119	CLA	C1B-CHB	2.61	1.48	1.41
11	a	1101	CLA	C1B-CHB	2.61	1.48	1.41
11	1	1117	CLA	C1B-CHB	2.61	1.48	1.41
11	B	1238	CLA	C4B-CHC	2.61	1.48	1.41
11	a	1128	CLA	C1C-NC	-2.61	1.33	1.37
11	b	1209	CLA	C4C-C3C	2.61	1.49	1.45
11	2	1232	CLA	C1B-CHB	2.61	1.48	1.41
11	B	1240	CLA	C1B-CHB	2.61	1.48	1.41
11	1	1123	CLA	C1B-CHB	2.61	1.48	1.41
11	B	1232	CLA	CHD-C4C	2.61	1.48	1.41
11	A	1109	CLA	CHD-C4C	2.60	1.48	1.41
11	K	1402	CLA	C4B-CHC	2.60	1.48	1.41
11	b	1208	CLA	CHD-C4C	2.60	1.48	1.41
11	K	1401	CLA	C4B-CHC	2.60	1.48	1.41
11	a	1118	CLA	C4B-CHC	2.60	1.48	1.41
11	b	1222	CLA	C1B-CHB	2.60	1.48	1.41
11	a	1012	CLA	C1B-CHB	2.60	1.48	1.41
11	b	1217	CLA	C1B-CHB	2.60	1.48	1.41
11	a	1138	CLA	CHD-C4C	2.60	1.48	1.41
11	B	1206	CLA	C1C-NC	-2.60	1.33	1.37
11	1	1114	CLA	C4B-CHC	2.60	1.48	1.41
11	b	1210	CLA	C1B-CHB	2.60	1.48	1.41
11	1	1135	CLA	C1B-CHB	2.60	1.48	1.41
11	L	1502	CLA	C1B-CHB	2.60	1.48	1.41
11	b	1202	CLA	C1B-CHB	2.60	1.48	1.41
11	2	1212	CLA	C1C-NC	-2.60	1.33	1.37
11	0	1401	CLA	C4B-CHC	2.60	1.48	1.41
11	1	1237	CLA	C4B-CHC	2.60	1.48	1.41
11	A	1120	CLA	CHD-C4C	2.60	1.48	1.41
11	2	1209	CLA	C4B-CHC	2.60	1.48	1.41
11	2	1215	CLA	C4B-CHC	2.60	1.48	1.41
11	A	1135	CLA	C1C-NC	-2.60	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1218	CLA	C4B-CHC	2.60	1.48	1.41
11	a	1139	CLA	C4C-C3C	2.60	1.49	1.45
11	1	1127	CLA	CHD-C4C	2.60	1.48	1.41
11	a	1130	CLA	C1B-CHB	2.60	1.48	1.41
11	a	1121	CLA	C1B-CHB	2.60	1.48	1.41
11	a	1109	CLA	C1B-CHB	2.59	1.48	1.41
11	B	1215	CLA	C4B-CHC	2.59	1.48	1.41
11	0	1401	CLA	C1B-CHB	2.59	1.48	1.41
11	A	1117	CLA	CHD-C4C	2.59	1.48	1.41
11	B	1231	CLA	CHD-C4C	2.59	1.48	1.41
11	b	1238	CLA	C1B-CHB	2.59	1.48	1.41
11	1	1133	CLA	C4C-C3C	2.59	1.49	1.45
11	8	1502	CLA	C1B-CHB	2.59	1.48	1.41
11	b	1205	CLA	C1B-CHB	2.59	1.48	1.41
11	K	1401	CLA	C1B-CHB	2.59	1.48	1.41
11	1	1115	CLA	C1B-CHB	2.59	1.48	1.41
11	1	1117	CLA	C4B-CHC	2.59	1.48	1.41
11	1	1133	CLA	C4B-CHC	2.59	1.48	1.41
11	A	1801	CLA	CHD-C4C	2.59	1.48	1.41
11	A	1109	CLA	C1B-CHB	2.59	1.48	1.41
11	B	1227	CLA	CHD-C4C	2.59	1.48	1.41
11	b	1021	CLA	C1B-CHB	2.59	1.48	1.41
11	a	1103	CLA	C1B-CHB	2.59	1.48	1.41
11	a	1101	CLA	C4B-CHC	2.59	1.48	1.41
11	B	1228	CLA	CHD-C4C	2.59	1.48	1.41
11	2	1230	CLA	C1B-CHB	2.59	1.48	1.41
11	1	1126	CLA	C1B-CHB	2.58	1.48	1.41
11	2	1235	CLA	C1B-CHB	2.58	1.48	1.41
11	A	1123	CLA	C1B-CHB	2.58	1.48	1.41
11	1	1115	CLA	C1C-NC	-2.58	1.34	1.37
11	A	1237	CLA	C4B-CHC	2.58	1.48	1.41
11	1	1120	CLA	C1B-CHB	2.58	1.48	1.41
11	b	1205	CLA	C4B-CHC	2.58	1.48	1.41
11	2	1021	CLA	C4B-CHC	2.58	1.48	1.41
11	B	1227	CLA	C4C-C3C	2.58	1.49	1.45
11	1	1130	CLA	C1B-CHB	2.58	1.48	1.41
11	B	1209	CLA	C4B-CHC	2.58	1.48	1.41
11	2	1221	CLA	C1B-CHB	2.58	1.48	1.41
11	k	1402	CLA	C1C-NC	-2.58	1.34	1.37
11	B	1234	CLA	C1C-NC	-2.58	1.34	1.37
11	2	1238	CLA	C1B-CHB	2.58	1.48	1.41
11	l	1501	CLA	C1B-CHB	2.58	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1226	CLA	C1B-CHB	2.58	1.48	1.41
11	b	1231	CLA	CHD-C4C	2.58	1.48	1.41
11	a	1130	CLA	CHD-C4C	2.58	1.48	1.41
11	a	1801	CLA	CHD-C4C	2.58	1.48	1.41
11	A	1011	CLA	C4B-CHC	2.58	1.48	1.41
11	A	1139	CLA	C1B-CHB	2.58	1.48	1.41
11	B	1212	CLA	C1B-CHB	2.58	1.48	1.41
11	2	1232	CLA	CHD-C4C	2.57	1.48	1.41
11	B	1205	CLA	C4B-CHC	2.57	1.48	1.41
11	a	1138	CLA	C4B-CHC	2.57	1.48	1.41
11	1	1128	CLA	C4B-CHC	2.57	1.48	1.41
11	B	1201	CLA	C1C-NC	-2.57	1.34	1.37
11	1	1011	CLA	C1B-CHB	2.57	1.48	1.41
11	B	1202	CLA	C1B-CHB	2.57	1.48	1.41
11	b	1214	CLA	C1B-CHB	2.57	1.48	1.41
11	2	1222	CLA	C1B-CHB	2.57	1.48	1.41
11	b	1013	CLA	CHD-C4C	2.57	1.48	1.41
11	1	1114	CLA	CHD-C4C	2.57	1.48	1.41
11	a	1127	CLA	C4C-C3C	2.57	1.49	1.45
11	a	1022	CLA	C1B-CHB	2.57	1.48	1.41
11	a	1107	CLA	C1B-CHB	2.57	1.48	1.41
11	B	1220	CLA	CHD-C4C	2.57	1.48	1.41
11	1	1109	CLA	C4B-CHC	2.57	1.48	1.41
11	B	1221	CLA	C1B-CHB	2.57	1.48	1.41
11	A	1118	CLA	C4B-CHC	2.57	1.48	1.41
11	B	1201	CLA	C4B-CHC	2.57	1.48	1.41
11	2	1228	CLA	C1B-CHB	2.57	1.48	1.41
11	B	1207	CLA	C1C-NC	-2.57	1.34	1.37
11	1	1103	CLA	C1B-CHB	2.57	1.48	1.41
11	A	1123	CLA	C4C-C3C	2.57	1.49	1.45
11	A	1102	CLA	CHD-C4C	2.57	1.48	1.41
11	b	1223	CLA	C4B-CHC	2.57	1.48	1.41
11	b	1232	CLA	CHD-C4C	2.57	1.48	1.41
11	A	1107	CLA	C1B-CHB	2.57	1.48	1.41
11	1	1138	CLA	C4B-CHC	2.57	1.48	1.41
11	A	1123	CLA	C1C-NC	-2.56	1.34	1.37
11	1	1124	CLA	C1B-CHB	2.56	1.48	1.41
11	1	1139	CLA	CHD-C4C	2.56	1.48	1.41
11	1	1101	CLA	CHD-C4C	2.56	1.48	1.41
11	A	1111	CLA	C1B-CHB	2.56	1.48	1.41
11	1	1801	CLA	C1C-NC	-2.56	1.34	1.37
11	b	1239	CLA	CHD-C4C	2.56	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1501	CLA	C4B-CHC	2.56	1.48	1.41
11	1	1109	CLA	CHD-C4C	2.56	1.48	1.41
11	B	1201	CLA	C1B-CHB	2.56	1.48	1.41
11	b	1206	CLA	CHD-C4C	2.56	1.48	1.41
11	B	1229	CLA	C1C-NC	-2.56	1.34	1.37
11	1	1022	CLA	C1B-CHB	2.56	1.48	1.41
11	2	1207	CLA	C4B-CHC	2.56	1.48	1.41
11	B	1220	CLA	C4B-CHC	2.56	1.48	1.41
11	a	1133	CLA	C4B-CHC	2.56	1.48	1.41
11	2	1209	CLA	C1B-CHB	2.56	1.48	1.41
11	A	1106	CLA	C4B-CHC	2.56	1.48	1.41
11	A	1124	CLA	CHD-C4C	2.55	1.48	1.41
11	2	1227	CLA	C4B-CHC	2.55	1.48	1.41
11	2	1203	CLA	C4B-CHC	2.55	1.48	1.41
11	A	1127	CLA	C1B-CHB	2.55	1.48	1.41
11	2	1013	CLA	CHD-C4C	2.55	1.48	1.41
11	1	1130	CLA	CHD-C4C	2.55	1.48	1.41
11	1	1121	CLA	CHD-C4C	2.55	1.48	1.41
11	b	1215	CLA	CHD-C4C	2.55	1.48	1.41
11	b	1228	CLA	C1B-CHB	2.55	1.48	1.41
11	1	1105	CLA	CHD-C4C	2.55	1.48	1.41
11	B	1215	CLA	C1B-CHB	2.55	1.48	1.41
11	2	1217	CLA	CHD-C4C	2.55	1.48	1.41
11	a	1123	CLA	CHD-C4C	2.55	1.48	1.41
11	2	1215	CLA	CHD-C4C	2.55	1.48	1.41
11	A	1120	CLA	C1B-CHB	2.55	1.48	1.41
11	1	1110	CLA	CHD-C4C	2.55	1.48	1.41
11	2	1203	CLA	C1B-CHB	2.55	1.48	1.41
11	b	1234	CLA	C1C-NC	-2.55	1.34	1.37
11	a	1105	CLA	CHD-C4C	2.55	1.48	1.41
11	1	1801	CLA	C1B-CHB	2.55	1.48	1.41
11	2	1214	CLA	C1C-NC	-2.55	1.34	1.37
11	A	1138	CLA	CHD-C4C	2.55	1.48	1.41
11	a	1134	CLA	C1B-CHB	2.54	1.48	1.41
11	A	1131	CLA	CHD-C4C	2.54	1.48	1.41
11	a	1110	CLA	CHD-C4C	2.54	1.48	1.41
11	B	1204	CLA	C1B-CHB	2.54	1.48	1.41
11	1	1104	CLA	C1B-CHB	2.54	1.48	1.41
11	2	1225	CLA	C1B-CHB	2.54	1.48	1.41
11	l	1503	CLA	C1B-CHB	2.54	1.48	1.41
11	a	1135	CLA	CHD-C4C	2.54	1.48	1.41
11	2	1229	CLA	C1B-CHB	2.54	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1227	CLA	CHD-C4C	2.54	1.48	1.41
11	1	1132	CLA	CHD-C4C	2.54	1.48	1.41
11	A	1112	CLA	C1B-CHB	2.54	1.48	1.41
11	b	1218	CLA	CHD-C4C	2.54	1.48	1.41
11	b	1215	CLA	C1B-CHB	2.54	1.48	1.41
11	a	1139	CLA	C4B-CHC	2.54	1.48	1.41
11	b	1203	CLA	C1B-CHB	2.54	1.48	1.41
11	1	1123	CLA	CHD-C4C	2.54	1.48	1.41
11	b	1209	CLA	CHD-C4C	2.54	1.48	1.41
11	A	1125	CLA	C1C-NC	-2.54	1.34	1.37
11	A	1237	CLA	C1C-NC	-2.54	1.34	1.37
11	2	1217	CLA	C4C-C3C	2.54	1.49	1.45
11	b	1228	CLA	CHD-C4C	2.54	1.48	1.41
11	b	1239	CLA	C4B-CHC	2.54	1.48	1.41
11	B	1218	CLA	C1C-NC	-2.54	1.34	1.37
11	B	1214	CLA	C1B-CHB	2.54	1.48	1.41
11	B	1216	CLA	C1B-CHB	2.53	1.48	1.41
11	B	1227	CLA	C1C-NC	-2.53	1.34	1.37
11	2	1202	CLA	CHD-C4C	2.53	1.48	1.41
11	B	1229	CLA	CHD-C4C	2.53	1.48	1.41
11	b	1225	CLA	C1B-CHB	2.53	1.48	1.41
11	A	1123	CLA	C4B-CHC	2.53	1.48	1.41
11	A	1125	CLA	CHD-C4C	2.53	1.48	1.41
11	2	1209	CLA	CHD-C4C	2.53	1.48	1.41
11	A	1122	CLA	C1C-NC	-2.53	1.34	1.37
11	B	1232	CLA	C4C-C3C	2.53	1.49	1.45
11	a	1134	CLA	CHD-C4C	2.53	1.48	1.41
11	1	1117	CLA	CHD-C4C	2.53	1.48	1.41
11	b	1229	CLA	CHD-C4C	2.53	1.48	1.41
11	2	1234	CLA	C4B-CHC	2.53	1.48	1.41
11	A	1138	CLA	C4B-CHC	2.53	1.48	1.41
11	B	1220	CLA	C1B-CHB	2.53	1.48	1.41
11	B	1228	CLA	C1C-NC	-2.53	1.34	1.37
11	A	1106	CLA	CHD-C4C	2.53	1.48	1.41
11	a	1116	CLA	C1B-CHB	2.53	1.48	1.41
11	L	1503	CLA	C4B-CHC	2.53	1.48	1.41
11	a	1103	CLA	CHD-C4C	2.53	1.48	1.41
11	1	1125	CLA	C1B-CHB	2.53	1.48	1.41
11	b	1217	CLA	CHD-C4C	2.53	1.48	1.41
11	a	1101	CLA	CHD-C4C	2.53	1.48	1.41
11	2	1209	CLA	C4C-C3C	2.53	1.49	1.45
11	B	1231	CLA	C4B-CHC	2.53	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1011	CLA	C4B-CHC	2.52	1.48	1.41
11	2	1201	CLA	CHD-C4C	2.52	1.48	1.41
11	A	1012	CLA	C1C-NC	-2.52	1.34	1.37
11	1	1131	CLA	CHD-C4C	2.52	1.48	1.41
11	A	1106	CLA	C1C-NC	-2.52	1.34	1.37
11	B	1207	CLA	C1B-CHB	2.52	1.48	1.41
11	a	1114	CLA	CHD-C4C	2.52	1.48	1.41
11	1	1132	CLA	C1B-CHB	2.52	1.48	1.41
11	A	1139	CLA	CHD-C4C	2.52	1.48	1.41
11	B	1225	CLA	C1B-CHB	2.52	1.48	1.41
11	b	1239	CLA	C1C-NC	-2.52	1.34	1.37
11	a	1112	CLA	CHD-C4C	2.52	1.48	1.41
11	1	1126	CLA	CHD-C4C	2.52	1.48	1.41
11	2	1239	CLA	CHD-C4C	2.52	1.48	1.41
11	2	1218	CLA	C1C-NC	-2.52	1.34	1.37
11	2	1227	CLA	CHD-C4C	2.52	1.48	1.41
11	8	1503	CLA	CHD-C4C	2.52	1.48	1.41
11	A	1115	CLA	CHD-C4C	2.52	1.48	1.41
11	B	1204	CLA	C4B-CHC	2.52	1.48	1.41
11	B	1230	CLA	C4B-CHC	2.52	1.48	1.41
11	B	1218	CLA	CHD-C4C	2.52	1.48	1.41
11	a	1131	CLA	CHD-C4C	2.52	1.48	1.41
11	a	1106	CLA	C1B-CHB	2.52	1.48	1.41
11	a	1138	CLA	C1B-CHB	2.52	1.48	1.41
11	2	1208	CLA	C1C-NC	-2.52	1.34	1.37
11	a	1140	CLA	CHD-C4C	2.52	1.48	1.41
11	a	1119	CLA	CHD-C4C	2.52	1.48	1.41
11	1	1106	CLA	CHD-C4C	2.51	1.48	1.41
11	A	1110	CLA	C1C-NC	-2.51	1.34	1.37
11	2	1201	CLA	C4B-CHC	2.51	1.48	1.41
11	A	1128	CLA	C1C-NC	-2.51	1.34	1.37
11	a	1132	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1121	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1124	CLA	C1C-NC	-2.51	1.34	1.37
11	2	1204	CLA	CHD-C4C	2.51	1.48	1.41
11	b	1240	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1119	CLA	C4B-CHC	2.51	1.48	1.41
11	b	1023	CLA	C1B-CHB	2.51	1.48	1.41
11	B	1203	CLA	C1C-NC	-2.51	1.34	1.37
11	1	1120	CLA	CHD-C4C	2.51	1.48	1.41
11	A	1132	CLA	CHD-C4C	2.51	1.48	1.41
11	B	1208	CLA	CHD-C4C	2.51	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1215	CLA	CHD-C4C	2.51	1.48	1.41
11	A	1126	CLA	CHD-C4C	2.51	1.48	1.41
11	2	1213	CLA	CHD-C4C	2.51	1.48	1.41
11	1	1115	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1127	CLA	C4B-CHC	2.51	1.48	1.41
11	a	1128	CLA	CHD-C4C	2.51	1.48	1.41
11	b	1238	CLA	CHD-C4C	2.51	1.48	1.41
11	1	1128	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1115	CLA	C1C-NC	-2.51	1.34	1.37
11	1	1107	CLA	C1C-NC	-2.51	1.34	1.37
11	2	1208	CLA	CHD-C4C	2.51	1.48	1.41
11	A	1118	CLA	CHD-C4C	2.51	1.48	1.41
11	a	1118	CLA	C1C-NC	-2.51	1.34	1.37
11	b	1234	CLA	C4C-C3C	2.51	1.49	1.45
11	A	1134	CLA	CHD-C4C	2.51	1.48	1.41
11	2	1214	CLA	CHD-C4C	2.51	1.48	1.41
11	1	1133	CLA	CHD-C4C	2.50	1.48	1.41
11	A	1134	CLA	C4B-CHC	2.50	1.48	1.41
11	2	1229	CLA	CHD-C4C	2.50	1.48	1.41
11	2	1222	CLA	CHD-C4C	2.50	1.48	1.41
11	1	1801	CLA	CHD-C4C	2.50	1.48	1.41
11	a	1102	CLA	C1B-CHB	2.50	1.47	1.41
11	B	1239	CLA	CHD-C4C	2.50	1.48	1.41
11	1	1102	CLA	C1B-CHB	2.50	1.47	1.41
11	A	1134	CLA	C4C-C3C	2.50	1.49	1.45
11	A	1119	CLA	CHD-C4C	2.50	1.48	1.41
11	L	1501	CLA	C1B-CHB	2.50	1.47	1.41
11	1	1116	CLA	CHD-C4C	2.50	1.48	1.41
11	A	1106	CLA	C1B-CHB	2.50	1.47	1.41
11	1	1110	CLA	C1B-CHB	2.50	1.47	1.41
11	B	1232	CLA	C4B-CHC	2.50	1.47	1.41
11	A	1123	CLA	CHD-C4C	2.50	1.48	1.41
11	b	1238	CLA	C1C-NC	-2.50	1.34	1.37
11	a	1801	CLA	C1B-CHB	2.50	1.47	1.41
11	2	1240	CLA	CHD-C4C	2.50	1.48	1.41
11	a	1138	CLA	C4C-C3C	2.50	1.49	1.45
11	a	1102	CLA	CHD-C4C	2.50	1.48	1.41
11	B	1222	CLA	C1B-CHB	2.50	1.47	1.41
11	1	1124	CLA	CHD-C4C	2.50	1.48	1.41
11	A	1130	CLA	CHD-C4C	2.50	1.48	1.41
11	1	1134	CLA	CHD-C4C	2.50	1.48	1.41
11	1	1106	CLA	C1C-NC	-2.50	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1204	CLA	CHD-C4C	2.50	1.48	1.41
11	b	1204	CLA	CHD-C4C	2.49	1.48	1.41
11	a	1135	CLA	C4B-CHC	2.49	1.47	1.41
11	A	1135	CLA	CHD-C4C	2.49	1.48	1.41
11	1	1102	CLA	CHD-C4C	2.49	1.48	1.41
11	A	1012	CLA	C1B-CHB	2.49	1.47	1.41
11	2	1234	CLA	CHD-C4C	2.49	1.48	1.41
11	2	1228	CLA	CHD-C4C	2.49	1.48	1.41
11	B	1209	CLA	C4C-C3C	2.49	1.49	1.45
11	a	1132	CLA	C1B-CHB	2.49	1.47	1.41
11	b	1216	CLA	CHD-C4C	2.49	1.48	1.41
11	B	1205	CLA	C1C-NC	-2.49	1.34	1.37
11	A	1129	CLA	C1C-NC	-2.49	1.34	1.37
11	a	1124	CLA	C1B-CHB	2.49	1.47	1.41
11	1	1138	CLA	C1C-NC	-2.49	1.34	1.37
11	l	1503	CLA	CHD-C4C	2.49	1.48	1.41
11	1	1112	CLA	CHD-C4C	2.49	1.48	1.41
11	a	1110	CLA	C1C-NC	-2.49	1.34	1.37
11	b	1225	CLA	CHD-C4C	2.49	1.48	1.41
11	A	1022	CLA	CHD-C4C	2.49	1.48	1.41
11	A	1114	CLA	C1C-NC	-2.49	1.34	1.37
11	1	1109	CLA	C1C-NC	-2.49	1.34	1.37
11	b	1236	CLA	CHD-C4C	2.49	1.48	1.41
11	B	1210	CLA	C1C-NC	-2.49	1.34	1.37
11	1	1111	CLA	C1C-NC	-2.49	1.34	1.37
11	B	1203	CLA	CHD-C4C	2.49	1.48	1.41
11	a	1011	CLA	C1B-CHB	2.49	1.47	1.41
11	a	1135	CLA	C4C-C3C	2.48	1.49	1.45
11	b	1209	CLA	C1C-NC	-2.48	1.34	1.37
11	A	1102	CLA	C1B-CHB	2.48	1.47	1.41
11	1	1119	CLA	CHD-C4C	2.48	1.48	1.41
11	B	1021	CLA	C4B-CHC	2.48	1.47	1.41
11	1	1133	CLA	C1C-NC	-2.48	1.34	1.37
11	b	1235	CLA	CHD-C4C	2.48	1.48	1.41
11	B	1202	CLA	CHD-C4C	2.48	1.48	1.41
11	B	1209	CLA	CHD-C4C	2.48	1.48	1.41
11	A	1114	CLA	CHD-C4C	2.48	1.48	1.41
11	b	1222	CLA	CHD-C4C	2.48	1.48	1.41
11	a	1117	CLA	CHD-C4C	2.48	1.48	1.41
11	1	1022	CLA	CHD-C4C	2.48	1.48	1.41
11	b	1201	CLA	CHD-C4C	2.48	1.48	1.41
11	b	1205	CLA	C1C-NC	-2.48	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1206	CLA	C1C-NC	-2.48	1.34	1.37
11	0	1402	CLA	CHD-C4C	2.48	1.48	1.41
11	2	1238	CLA	CHD-C4C	2.48	1.48	1.41
11	2	1220	CLA	C4C-C3C	2.48	1.49	1.45
11	B	1201	CLA	CHD-C4C	2.48	1.48	1.41
11	1	1103	CLA	CHD-C4C	2.48	1.48	1.41
11	a	1133	CLA	C4C-C3C	2.48	1.49	1.45
11	1	1125	CLA	CHD-C4C	2.48	1.48	1.41
11	1	1114	CLA	C4C-C3C	2.48	1.49	1.45
11	2	1218	CLA	CHD-C4C	2.48	1.48	1.41
11	B	1013	CLA	C1C-NC	-2.48	1.34	1.37
11	1	1125	CLA	C1C-NC	-2.47	1.34	1.37
11	b	1208	CLA	C4C-C3C	2.47	1.49	1.45
11	a	1112	CLA	C1B-CHB	2.47	1.47	1.41
11	b	1211	CLA	CHD-C4C	2.47	1.48	1.41
11	b	1023	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1136	CLA	C1C-NC	-2.47	1.34	1.37
11	a	1133	CLA	CHD-C4C	2.47	1.48	1.41
11	a	1135	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1116	CLA	C1B-CHB	2.47	1.47	1.41
11	B	1013	CLA	C1B-CHB	2.47	1.47	1.41
11	B	1023	CLA	C1B-CHB	2.47	1.47	1.41
11	2	1207	CLA	C1B-CHB	2.47	1.47	1.41
11	2	1238	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1108	CLA	CHD-C4C	2.47	1.48	1.41
11	A	1125	CLA	C4B-CHC	2.47	1.47	1.41
11	a	1137	CLA	CHD-C4C	2.47	1.48	1.41
11	2	1240	CLA	C1C-NC	-2.47	1.34	1.37
11	b	1230	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1138	CLA	C1C-NC	-2.47	1.34	1.37
11	2	1224	CLA	C1C-NC	-2.47	1.34	1.37
11	b	1207	CLA	C4B-CHC	2.47	1.47	1.41
11	2	1220	CLA	CHD-C4C	2.47	1.48	1.41
11	A	1117	CLA	C1B-CHB	2.47	1.47	1.41
11	b	1206	CLA	C4B-CHC	2.47	1.47	1.41
11	a	1136	CLA	C1C-NC	-2.47	1.34	1.37
11	1	1110	CLA	C4C-C3C	2.47	1.49	1.45
11	a	1124	CLA	CHD-C4C	2.47	1.48	1.41
11	1	1138	CLA	CHD-C4C	2.47	1.48	1.41
11	A	1110	CLA	CHD-C4C	2.47	1.48	1.41
11	A	1140	CLA	CHD-C4C	2.47	1.48	1.41
11	2	1206	CLA	CHD-C4C	2.47	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1021	CLA	C1C-NC	-2.47	1.34	1.37
11	B	1227	CLA	C4B-CHC	2.47	1.47	1.41
11	b	1213	CLA	CHD-C4C	2.46	1.48	1.41
11	B	1240	CLA	CHD-C4C	2.46	1.48	1.41
11	2	1227	CLA	C1C-NC	-2.46	1.34	1.37
11	B	1021	CLA	C1B-CHB	2.46	1.47	1.41
11	8	1501	CLA	C1C-NC	-2.46	1.34	1.37
11	8	1501	CLA	CHD-C4C	2.46	1.48	1.41
11	A	1133	CLA	C4B-CHC	2.46	1.47	1.41
11	2	1206	CLA	C4B-CHC	2.46	1.47	1.41
11	b	1234	CLA	CHD-C4C	2.46	1.48	1.41
11	2	1226	CLA	C1C-NC	-2.46	1.34	1.37
11	1	1117	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1116	CLA	CHD-C4C	2.46	1.48	1.41
11	A	1022	CLA	C1C-NC	-2.46	1.34	1.37
11	8	1501	CLA	C1B-CHB	2.46	1.47	1.41
11	b	1230	CLA	C4C-C3C	2.46	1.49	1.45
11	a	1237	CLA	C1C-NC	-2.46	1.34	1.37
11	b	1210	CLA	C4C-C3C	2.46	1.49	1.45
11	b	1212	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1108	CLA	CHD-C4C	2.46	1.48	1.41
11	B	1235	CLA	CHD-C4C	2.46	1.48	1.41
11	b	1220	CLA	CHD-C4C	2.46	1.48	1.41
11	B	1224	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1106	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1127	CLA	C1C-NC	-2.46	1.34	1.37
11	A	1108	CLA	C1C-NC	-2.46	1.34	1.37
11	b	1219	CLA	CHD-C4C	2.46	1.48	1.41
11	1	1125	CLA	C4C-C3C	2.46	1.49	1.45
11	a	1133	CLA	C1C-NC	-2.46	1.34	1.37
11	A	1124	CLA	C1C-NC	-2.45	1.34	1.37
11	A	1118	CLA	C1C-NC	-2.45	1.34	1.37
11	2	1206	CLA	C1C-NC	-2.45	1.34	1.37
11	k	1402	CLA	CHD-C4C	2.45	1.48	1.41
11	A	1119	CLA	C1B-CHB	2.45	1.47	1.41
11	A	1114	CLA	C4C-C3C	2.45	1.49	1.45
11	B	1212	CLA	CHD-C4C	2.45	1.48	1.41
11	2	1203	CLA	CHD-C4C	2.45	1.48	1.41
11	B	1206	CLA	CHD-C4C	2.45	1.48	1.41
11	A	1105	CLA	CHD-C4C	2.45	1.48	1.41
11	L	1503	CLA	CHD-C4C	2.45	1.48	1.41
11	1	1123	CLA	C4C-C3C	2.45	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1203	CLA	CHD-C4C	2.45	1.48	1.41
11	a	1116	CLA	C1C-NC	-2.45	1.34	1.37
11	B	1219	CLA	CHD-C4C	2.45	1.48	1.41
11	a	1136	CLA	CHD-C4C	2.45	1.48	1.41
11	1	1011	CLA	C4B-CHC	2.45	1.47	1.41
11	1	1111	CLA	C1B-CHB	2.45	1.47	1.41
11	B	1211	CLA	CHD-C4C	2.45	1.48	1.41
11	a	1127	CLA	CHD-C4C	2.45	1.48	1.41
11	L	1502	CLA	C1C-NC	-2.45	1.34	1.37
11	A	1119	CLA	C4C-C3C	2.45	1.49	1.45
11	a	1011	CLA	CHD-C4C	2.45	1.48	1.41
11	B	1228	CLA	C4C-C3C	2.45	1.49	1.45
11	a	1138	CLA	C1C-NC	-2.45	1.34	1.37
11	1	1012	CLA	C1C-NC	-2.45	1.34	1.37
11	a	1106	CLA	CHD-C4C	2.45	1.48	1.41
11	B	1226	CLA	C1C-NC	-2.45	1.34	1.37
11	2	1223	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1232	CLA	C1C-NC	-2.44	1.34	1.37
11	B	1234	CLA	C4B-CHC	2.44	1.47	1.41
11	B	1216	CLA	C4C-C3C	2.44	1.49	1.45
11	A	1133	CLA	C4C-C3C	2.44	1.49	1.45
11	0	1402	CLA	C1C-NC	-2.44	1.34	1.37
11	A	1107	CLA	C1C-NC	-2.44	1.34	1.37
11	2	1205	CLA	C1C-NC	-2.44	1.34	1.37
11	B	1234	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1215	CLA	C1C-NC	-2.44	1.34	1.37
11	b	1201	CLA	C1C-NC	-2.44	1.34	1.37
11	1	1237	CLA	CHD-C4C	2.44	1.48	1.41
11	A	1134	CLA	C1C-NC	-2.44	1.34	1.37
11	b	1217	CLA	C1C-NC	-2.44	1.34	1.37
11	A	1011	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1223	CLA	CHD-C4C	2.44	1.48	1.41
11	1	1129	CLA	CHD-C4C	2.44	1.48	1.41
11	b	1013	CLA	C1B-CHB	2.44	1.47	1.41
11	2	1240	CLA	C4C-C3C	2.44	1.49	1.45
11	1	1104	CLA	C1C-NC	-2.44	1.34	1.37
11	a	1022	CLA	CHD-C4C	2.44	1.48	1.41
11	2	1219	CLA	CHD-C4C	2.44	1.48	1.41
11	b	1239	CLA	C4C-C3C	2.44	1.49	1.45
11	A	1111	CLA	CHD-C4C	2.44	1.48	1.41
11	b	1226	CLA	CHD-C4C	2.44	1.48	1.41
11	1	1131	CLA	C1C-NC	-2.44	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1206	CLA	C4B-CHC	2.44	1.47	1.41
11	B	1013	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1225	CLA	CHD-C4C	2.43	1.48	1.41
11	A	1133	CLA	CHD-C4C	2.43	1.48	1.41
11	b	1021	CLA	CHD-C4C	2.43	1.48	1.41
11	1	1136	CLA	C1C-NC	-2.43	1.34	1.37
11	2	1201	CLA	C1C-NC	-2.43	1.34	1.37
11	2	1203	CLA	C1C-NC	-2.43	1.34	1.37
11	b	1212	CLA	CHD-C4C	2.43	1.48	1.41
11	b	1223	CLA	CHD-C4C	2.43	1.48	1.41
11	A	1237	CLA	CHD-C4C	2.43	1.48	1.41
11	2	1239	CLA	C4C-C3C	2.43	1.49	1.45
11	a	1104	CLA	C1B-CHB	2.43	1.47	1.41
11	1	1237	CLA	C1C-NC	-2.43	1.34	1.37
11	2	1021	CLA	CHD-C4C	2.43	1.48	1.41
11	b	1228	CLA	C1C-NC	-2.43	1.34	1.37
11	a	1134	CLA	C1C-NC	-2.43	1.34	1.37
11	1	1118	CLA	C1C-NC	-2.43	1.34	1.37
11	b	1216	CLA	C4C-C3C	2.43	1.49	1.45
11	b	1214	CLA	C1C-NC	-2.42	1.34	1.37
11	1	1105	CLA	C1C-NC	-2.42	1.34	1.37
11	1	1140	CLA	CHD-C4C	2.42	1.48	1.41
11	B	1238	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1113	CLA	CHD-C4C	2.42	1.48	1.41
11	A	1112	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1104	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1108	CLA	CHD-C4C	2.42	1.48	1.41
11	B	1217	CLA	CHD-C4C	2.42	1.48	1.41
11	b	1225	CLA	C4C-C3C	2.42	1.49	1.45
11	1	1104	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1113	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1801	CLA	C4C-C3C	2.42	1.49	1.45
11	b	1220	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1211	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1136	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1130	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1213	CLA	CHD-C4C	2.42	1.48	1.41
11	2	1239	CLA	C1C-NC	-2.42	1.34	1.37
11	2	1023	CLA	CHD-C4C	2.42	1.48	1.41
11	2	1215	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1216	CLA	C1C-NC	-2.42	1.34	1.37
11	1	1140	CLA	C1C-NC	-2.42	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1219	CLA	C1C-NC	-2.42	1.34	1.37
11	b	1234	CLA	C4B-CHC	2.42	1.47	1.41
11	K	1401	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1119	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1109	CLA	C1C-NC	-2.42	1.34	1.37
11	a	1105	CLA	C1C-NC	-2.42	1.34	1.37
11	2	1232	CLA	C4C-C3C	2.41	1.49	1.45
11	a	1120	CLA	CHD-C4C	2.41	1.48	1.41
11	A	1022	CLA	C1B-CHB	2.41	1.47	1.41
11	a	1130	CLA	C1C-NC	-2.41	1.34	1.37
11	B	1238	CLA	C1C-NC	-2.41	1.34	1.37
11	2	1210	CLA	C1C-NC	-2.41	1.34	1.37
11	B	1220	CLA	C4C-C3C	2.41	1.49	1.45
11	k	1401	CLA	CHD-C4C	2.41	1.48	1.41
11	b	1240	CLA	C1C-NC	-2.41	1.34	1.37
11	1	1136	CLA	CHD-C4C	2.41	1.48	1.41
11	A	1103	CLA	CHD-C4C	2.41	1.48	1.41
11	8	1502	CLA	C1C-NC	-2.41	1.34	1.37
11	1	1011	CLA	C1C-NC	-2.40	1.34	1.37
11	A	1124	CLA	C4C-C3C	2.40	1.49	1.45
11	2	1212	CLA	CHD-C4C	2.40	1.48	1.41
11	2	1217	CLA	C1C-NC	-2.40	1.34	1.37
11	0	1401	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1139	CLA	C4C-C3C	2.40	1.49	1.45
11	2	1201	CLA	C4C-C3C	2.40	1.49	1.45
11	k	1401	CLA	C1C-NC	-2.40	1.34	1.37
11	a	1129	CLA	CHD-C4C	2.40	1.48	1.41
11	B	1209	CLA	C1C-NC	-2.40	1.34	1.37
11	l	1501	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1132	CLA	C1C-NC	-2.40	1.34	1.37
11	2	1220	CLA	C1C-NC	-2.40	1.34	1.37
11	1	1118	CLA	CHD-C4C	2.40	1.48	1.41
11	A	1137	CLA	C1C-NC	-2.40	1.34	1.37
11	a	1118	CLA	CHD-C4C	2.40	1.48	1.41
11	b	1206	CLA	C4C-C3C	2.40	1.49	1.45
11	1	1127	CLA	C1C-NC	-2.40	1.34	1.37
11	A	1132	CLA	C1C-NC	-2.40	1.34	1.37
11	2	1216	CLA	C4C-C3C	2.40	1.49	1.45
11	2	1013	CLA	C1C-NC	-2.40	1.34	1.37
11	L	1502	CLA	CHD-C4C	2.40	1.48	1.41
11	A	1127	CLA	CHD-C4C	2.40	1.48	1.41
11	2	1231	CLA	C1B-CHB	2.40	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1213	CLA	C1C-NC	-2.39	1.34	1.37
11	2	1227	CLA	C4C-C3C	2.39	1.49	1.45
11	b	1224	CLA	CHD-C4C	2.39	1.48	1.41
11	a	1120	CLA	C1C-NC	-2.39	1.34	1.37
11	B	1239	CLA	C1C-NC	-2.39	1.34	1.37
11	b	1230	CLA	CHD-C4C	2.39	1.48	1.41
11	b	1204	CLA	C1C-NC	-2.39	1.34	1.37
11	A	1126	CLA	C1B-CHB	2.39	1.47	1.41
11	b	1214	CLA	CHD-C4C	2.39	1.48	1.41
11	b	1222	CLA	C1C-NC	-2.39	1.34	1.37
11	A	1801	CLA	C1B-CHB	2.39	1.47	1.41
11	a	1131	CLA	C1C-NC	-2.39	1.34	1.37
11	B	1207	CLA	CHD-C4C	2.39	1.47	1.41
11	L	1501	CLA	CHD-C4C	2.39	1.47	1.41
11	a	1125	CLA	CHD-C4C	2.39	1.47	1.41
11	b	1223	CLA	C1C-NC	-2.39	1.34	1.37
11	a	1022	CLA	C1C-NC	-2.38	1.34	1.37
11	B	1217	CLA	C1C-NC	-2.38	1.34	1.37
11	B	1204	CLA	C1C-NC	-2.38	1.34	1.37
11	A	1137	CLA	CHD-C4C	2.38	1.47	1.41
11	b	1023	CLA	CHD-C4C	2.38	1.47	1.41
11	a	1101	CLA	C1C-NC	-2.38	1.34	1.37
11	1	1122	CLA	CHD-C4C	2.38	1.47	1.41
11	1	1114	CLA	C1C-NC	-2.38	1.34	1.37
11	1	1135	CLA	C1C-NC	-2.38	1.34	1.37
11	1	1101	CLA	C1C-NC	-2.38	1.34	1.37
11	b	1231	CLA	C1B-CHB	2.38	1.47	1.41
11	a	1132	CLA	C1C-NC	-2.38	1.34	1.37
11	K	1401	CLA	C1C-NC	-2.38	1.34	1.37
11	0	1401	CLA	C1C-NC	-2.38	1.34	1.37
11	2	1207	CLA	CHD-C4C	2.38	1.47	1.41
11	1	1103	CLA	C1C-NC	-2.38	1.34	1.37
11	A	1117	CLA	C1C-NC	-2.38	1.34	1.37
11	b	1208	CLA	C1C-NC	-2.38	1.34	1.37
11	1	1135	CLA	CHD-C4C	2.38	1.47	1.41
11	K	1402	CLA	CHD-C4C	2.38	1.47	1.41
11	L	1501	CLA	C1C-NC	-2.38	1.34	1.37
11	1	1011	CLA	CHD-C4C	2.38	1.47	1.41
11	A	1124	CLA	C1B-CHB	2.38	1.47	1.41
11	a	1134	CLA	C4C-C3C	2.37	1.49	1.45
11	a	1111	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1210	CLA	CHD-C4C	2.37	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1223	CLA	C4C-C3C	2.37	1.49	1.45
11	a	1012	CLA	CHD-C4C	2.37	1.47	1.41
11	a	1122	CLA	CHD-C4C	2.37	1.47	1.41
11	a	1119	CLA	C4C-C3C	2.37	1.49	1.45
11	A	1120	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1231	CLA	C1C-NC	-2.37	1.34	1.37
11	A	1101	CLA	CHD-C4C	2.37	1.47	1.41
11	2	1216	CLA	CHD-C4C	2.37	1.47	1.41
11	1	1022	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1229	CLA	C4C-C3C	2.37	1.49	1.45
11	B	1221	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1021	CLA	CHD-C4C	2.37	1.47	1.41
11	b	1210	CLA	CHD-C4C	2.37	1.47	1.41
11	1	1137	CLA	CHD-C4C	2.37	1.47	1.41
11	1	1124	CLA	C1C-NC	-2.37	1.34	1.37
11	A	1128	CLA	CHD-C4C	2.37	1.47	1.41
11	2	1236	CLA	CHD-C4C	2.37	1.47	1.41
11	a	1140	CLA	C1C-NC	-2.37	1.34	1.37
11	a	1126	CLA	CHD-C4C	2.37	1.47	1.41
11	A	1104	CLA	CHD-C4C	2.37	1.47	1.41
11	b	1219	CLA	C1C-NC	-2.37	1.34	1.37
11	a	1117	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1231	CLA	C1B-CHB	2.37	1.47	1.41
11	a	1111	CLA	CHD-C4C	2.36	1.47	1.41
11	2	1234	CLA	C1C-NC	-2.36	1.34	1.37
11	2	1013	CLA	C1B-CHB	2.36	1.47	1.41
11	b	1232	CLA	C4C-C3C	2.36	1.49	1.45
11	a	1123	CLA	C4C-C3C	2.36	1.49	1.45
11	a	1122	CLA	C1C-NC	-2.36	1.34	1.37
11	a	1103	CLA	C1C-NC	-2.36	1.34	1.37
11	2	1210	CLA	CHD-C4C	2.36	1.47	1.41
14	f	4018	BCR	C30-C25	-2.36	1.50	1.53
11	b	1205	CLA	CHD-C4C	2.36	1.47	1.41
11	A	1127	CLA	C1C-NC	-2.36	1.34	1.37
11	B	1220	CLA	C1C-NC	-2.36	1.34	1.37
11	A	1105	CLA	C1C-NC	-2.36	1.34	1.37
11	a	1129	CLA	C1C-NC	-2.36	1.34	1.37
11	A	1110	CLA	C4C-C3C	2.36	1.49	1.45
11	a	1114	CLA	C1C-NC	-2.36	1.34	1.37
11	A	1104	CLA	C1C-NC	-2.36	1.34	1.37
11	A	1101	CLA	C1C-NC	-2.36	1.34	1.37
11	a	1137	CLA	C1C-NC	-2.36	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1202	CLA	CHD-C4C	2.36	1.47	1.41
11	2	1235	CLA	CHD-C4C	2.35	1.47	1.41
11	A	1011	CLA	C1B-CHB	2.35	1.47	1.41
11	2	1211	CLA	CHD-C4C	2.35	1.47	1.41
11	b	1227	CLA	C4C-C3C	2.35	1.49	1.45
11	b	1229	CLA	C1C-NC	-2.35	1.34	1.37
11	a	1126	CLA	C1C-C2C	2.35	1.49	1.44
11	2	1228	CLA	C1C-NC	-2.35	1.34	1.37
11	A	1116	CLA	CHD-C4C	2.35	1.47	1.41
11	a	1801	CLA	C1C-NC	-2.35	1.34	1.37
11	A	1115	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1222	CLA	C1C-NC	-2.35	1.34	1.37
11	A	1129	CLA	CHD-C4C	2.35	1.47	1.41
11	l	1501	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1214	CLA	CHD-C4C	2.35	1.47	1.41
11	b	1210	CLA	C1C-NC	-2.35	1.34	1.37
11	2	1204	CLA	C1C-NC	-2.35	1.34	1.37
11	b	1013	CLA	C1C-NC	-2.35	1.34	1.37
11	2	1202	CLA	C1C-NC	-2.35	1.34	1.37
11	a	1121	CLA	C4C-C3C	2.35	1.49	1.45
11	b	1218	CLA	C1C-NC	-2.35	1.34	1.37
11	L	1503	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1226	CLA	CHD-C4C	2.35	1.47	1.41
11	B	1236	CLA	C1C-NC	-2.34	1.34	1.37
11	B	1214	CLA	C1C-NC	-2.34	1.34	1.37
11	l	1503	CLA	C1C-NC	-2.34	1.34	1.37
11	b	1228	CLA	C4C-C3C	2.34	1.49	1.45
11	a	1113	CLA	C4C-C3C	2.34	1.49	1.45
11	1	1134	CLA	C4C-C3C	2.34	1.49	1.45
11	A	1135	CLA	C1B-CHB	2.34	1.47	1.41
11	a	1012	CLA	C1C-NC	-2.34	1.34	1.37
11	A	1131	CLA	C4C-C3C	2.34	1.49	1.45
11	2	1224	CLA	CHD-C4C	2.34	1.47	1.41
11	A	1113	CLA	CHD-C4C	2.34	1.47	1.41
11	2	1021	CLA	C1B-CHB	2.34	1.47	1.41
11	1	1137	CLA	C1C-NC	-2.34	1.34	1.37
11	a	1107	CLA	C1C-NC	-2.34	1.34	1.37
11	b	1224	CLA	C1C-NC	-2.34	1.34	1.37
11	2	1023	CLA	C4C-C3C	2.33	1.49	1.45
11	b	1203	CLA	C1C-NC	-2.33	1.34	1.37
11	1	1134	CLA	C1C-NC	-2.33	1.34	1.37
11	B	1222	CLA	CHD-C4C	2.33	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1110	CLA	C1C-NC	-2.33	1.34	1.37
11	a	1103	CLA	C4C-C3C	2.33	1.49	1.45
11	a	1105	CLA	C4C-C3C	2.33	1.49	1.45
11	A	1130	CLA	C1C-NC	-2.33	1.34	1.37
11	l	1502	CLA	C1C-NC	-2.33	1.34	1.37
11	1	1103	CLA	C4C-C3C	2.33	1.49	1.45
11	2	1225	CLA	C4C-C3C	2.33	1.49	1.45
11	A	1012	CLA	CHD-C4C	2.33	1.47	1.41
11	A	1103	CLA	C1C-NC	-2.33	1.34	1.37
11	a	1116	CLA	C4C-C3C	2.33	1.49	1.45
11	a	1130	CLA	C4C-C3C	2.33	1.49	1.45
11	1	1107	CLA	CHD-C4C	2.33	1.47	1.41
11	2	1209	CLA	C1C-NC	-2.33	1.34	1.37
11	2	1221	CLA	CHD-C4C	2.33	1.47	1.41
11	1	1120	CLA	C1C-NC	-2.32	1.34	1.37
11	1	1120	CLA	C4C-C3C	2.32	1.49	1.45
11	a	1114	CLA	C4C-C3C	2.32	1.49	1.45
11	2	1231	CLA	C4C-C3C	2.32	1.49	1.45
11	A	1121	CLA	C1C-NC	-2.32	1.34	1.37
11	2	1230	CLA	CHD-C4C	2.32	1.47	1.41
11	A	1011	CLA	C1C-NC	-2.32	1.34	1.37
11	2	1223	CLA	C1C-NC	-2.32	1.34	1.37
11	A	1111	CLA	C1C-NC	-2.32	1.34	1.37
11	1	1116	CLA	C4C-C3C	2.32	1.49	1.45
11	1	1108	CLA	C1C-NC	-2.32	1.34	1.37
11	2	1226	CLA	CHD-C4C	2.32	1.47	1.41
11	a	1108	CLA	C1C-NC	-2.32	1.34	1.37
11	a	1104	CLA	C1C-NC	-2.32	1.34	1.37
11	b	1207	CLA	CHD-C4C	2.32	1.47	1.41
11	1	1122	CLA	C1C-NC	-2.32	1.34	1.37
11	b	1215	CLA	C1C-NC	-2.32	1.34	1.37
11	b	1021	CLA	C4C-C3C	2.32	1.49	1.45
11	a	1115	CLA	CHD-C4C	2.31	1.47	1.41
11	2	1211	CLA	C1C-NC	-2.31	1.34	1.37
11	a	1107	CLA	CHD-C4C	2.31	1.47	1.41
11	A	1106	CLA	C4C-C3C	2.31	1.49	1.45
11	B	1202	CLA	C1C-NC	-2.31	1.34	1.37
11	a	1109	CLA	C4C-C3C	2.31	1.49	1.45
11	1	1121	CLA	C1C-NC	-2.31	1.34	1.37
11	A	1139	CLA	C1C-C2C	2.31	1.49	1.44
11	a	1124	CLA	C4C-C3C	2.31	1.49	1.45
11	2	1231	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)
11	b	1211	CLA	C4C-C3C	2.31	1.49	1.45
11	B	1206	CLA	C4C-C3C	2.31	1.49	1.45
11	a	1102	CLA	C1C-NC	-2.31	1.34	1.37
11	b	1211	CLA	C1C-NC	-2.31	1.34	1.37
11	2	1021	CLA	C4C-C3C	2.30	1.49	1.45
11	A	1140	CLA	C4C-C3C	2.30	1.49	1.45
11	B	1201	CLA	C4C-C3C	2.30	1.49	1.45
11	1	1129	CLA	C1C-NC	-2.30	1.34	1.37
11	8	1503	CLA	C1C-NC	-2.30	1.34	1.37
11	a	1011	CLA	C1C-NC	-2.30	1.34	1.37
11	b	1226	CLA	C1C-NC	-2.30	1.34	1.37
11	A	1131	CLA	C1C-NC	-2.30	1.34	1.37
11	1	1128	CLA	C4C-C3C	2.30	1.49	1.45
11	a	1110	CLA	C4C-C3C	2.30	1.49	1.45
11	k	1402	CLA	C4C-C3C	2.29	1.49	1.45
11	a	1121	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1131	CLA	C4C-C3C	2.29	1.49	1.45
11	2	1235	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1230	CLA	C4C-C3C	2.29	1.49	1.45
11	a	1108	CLA	C4C-C3C	2.29	1.49	1.45
11	2	1222	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1128	CLA	C4C-C3C	2.29	1.49	1.45
11	l	1502	CLA	CHD-C4C	2.29	1.47	1.41
11	2	1229	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1219	CLA	C1C-NC	-2.29	1.34	1.37
11	B	1223	CLA	C1C-NC	-2.29	1.34	1.37
11	B	1205	CLA	CHD-C4C	2.29	1.47	1.41
11	A	1102	CLA	C4C-C3C	2.28	1.49	1.45
11	1	1126	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1230	CLA	CHD-C4C	2.28	1.47	1.41
11	2	1219	CLA	C1C-C2C	2.28	1.49	1.44
11	B	1208	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1240	CLA	C1C-C2C	2.28	1.49	1.44
11	b	1021	CLA	C1C-NC	-2.28	1.34	1.37
11	A	1102	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1212	CLA	C1C-NC	-2.28	1.34	1.37
11	b	1231	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1225	CLA	C1C-NC	-2.28	1.34	1.37
11	2	1206	CLA	C4C-C3C	2.28	1.49	1.45
11	1	1123	CLA	C1C-NC	-2.28	1.34	1.37
11	1	1139	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1213	CLA	C1C-NC	-2.28	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1115	CLA	C1C-C2C	2.27	1.49	1.44
11	b	1231	CLA	C4C-C3C	2.27	1.49	1.45
11	1	1111	CLA	CHD-C4C	2.27	1.47	1.41
11	8	1502	CLA	CHD-C4C	2.27	1.47	1.41
11	a	1237	CLA	CHD-C4C	2.27	1.47	1.41
11	A	1136	CLA	C4C-C3C	2.27	1.49	1.45
11	b	1227	CLA	C1C-NC	-2.27	1.34	1.37
11	0	1401	CLA	C4C-C3C	2.27	1.49	1.45
11	A	1129	CLA	C4C-C3C	2.27	1.49	1.45
11	b	1215	CLA	C4C-C3C	2.27	1.49	1.45
11	a	1109	CLA	C1C-NC	-2.27	1.34	1.37
11	a	1112	CLA	C4C-C3C	2.27	1.49	1.45
11	A	1132	CLA	C4C-C3C	2.27	1.49	1.45
11	1	1102	CLA	C1C-C2C	2.27	1.49	1.44
11	2	1229	CLA	C4C-C3C	2.27	1.48	1.45
11	b	1202	CLA	C1C-NC	-2.27	1.34	1.37
11	B	1236	CLA	CHD-C4C	2.27	1.47	1.41
11	2	1021	CLA	C1C-NC	-2.27	1.34	1.37
11	A	1113	CLA	C1C-NC	-2.27	1.34	1.37
11	1	1801	CLA	C4C-C3C	2.26	1.48	1.45
14	6	4018	BCR	C30-C25	-2.26	1.50	1.53
11	B	1234	CLA	C4C-C3C	2.26	1.48	1.45
11	B	1023	CLA	CHD-C4C	2.26	1.47	1.41
11	A	1111	CLA	C4C-C3C	2.26	1.48	1.45
11	A	1135	CLA	C4C-C3C	2.26	1.48	1.45
11	2	1023	CLA	C1B-CHB	2.26	1.47	1.41
11	b	1221	CLA	CHD-C4C	2.26	1.47	1.41
11	2	1214	CLA	C4C-C3C	2.26	1.48	1.45
11	B	1240	CLA	C4C-C3C	2.26	1.48	1.45
11	A	1126	CLA	C1C-C2C	2.26	1.48	1.44
11	K	1401	CLA	C4C-C3C	2.26	1.48	1.45
11	2	1221	CLA	C1C-NC	-2.26	1.34	1.37
11	A	1120	CLA	C4C-C3C	2.25	1.48	1.45
11	2	1232	CLA	C1C-NC	-2.25	1.34	1.37
11	1	1012	CLA	CHD-C4C	2.25	1.47	1.41
11	A	1107	CLA	CHD-C4C	2.25	1.47	1.41
11	1	1127	CLA	C4C-C3C	2.25	1.48	1.45
11	2	1212	CLA	C4C-C3C	2.25	1.48	1.45
11	A	1122	CLA	CHD-C4C	2.25	1.47	1.41
11	b	1224	CLA	C4C-C3C	2.25	1.48	1.45
11	B	1224	CLA	CHD-C4C	2.25	1.47	1.41
11	b	1221	CLA	C1C-C2C	2.25	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1136	CLA	C4C-C3C	2.25	1.48	1.45
11	1	1106	CLA	C4C-C3C	2.25	1.48	1.45
11	1	1132	CLA	C4C-C3C	2.25	1.48	1.45
11	0	1402	CLA	C4C-C3C	2.25	1.48	1.45
11	1	1101	CLA	C4C-C3C	2.25	1.48	1.45
11	1	1121	CLA	C4C-C3C	2.25	1.48	1.45
11	2	1236	CLA	C1C-NC	-2.24	1.34	1.37
11	b	1219	CLA	C4C-C3C	2.24	1.48	1.45
11	1	1115	CLA	C4C-C3C	2.24	1.48	1.45
11	1	1113	CLA	C4C-C3C	2.24	1.48	1.45
11	1	1112	CLA	C4C-C3C	2.24	1.48	1.45
11	b	1240	CLA	C4C-C3C	2.24	1.48	1.45
11	b	1235	CLA	C1C-NC	-2.24	1.34	1.37
11	a	1139	CLA	C1C-NC	-2.24	1.34	1.37
11	k	1401	CLA	C4C-C3C	2.24	1.48	1.45
11	1	1109	CLA	C4C-C3C	2.24	1.48	1.45
11	B	1235	CLA	C1C-NC	-2.24	1.34	1.37
11	1	1113	CLA	C1C-NC	-2.24	1.34	1.37
11	B	1218	CLA	C4C-C3C	2.23	1.48	1.45
11	b	1225	CLA	C1C-NC	-2.23	1.34	1.37
11	b	1013	CLA	C4C-C3C	2.23	1.48	1.45
11	1	1105	CLA	C4C-C3C	2.23	1.48	1.45
11	b	1232	CLA	C1C-NC	-2.23	1.34	1.37
11	a	1102	CLA	C4C-C3C	2.23	1.48	1.45
11	B	1240	CLA	C1C-NC	-2.23	1.34	1.37
11	B	1222	CLA	C1C-C2C	2.23	1.48	1.44
11	b	1238	CLA	C4C-C3C	2.23	1.48	1.45
11	a	1113	CLA	C1C-NC	-2.23	1.34	1.37
11	2	1215	CLA	C4C-C3C	2.23	1.48	1.45
11	b	1218	CLA	C4C-C3C	2.22	1.48	1.45
11	1	1112	CLA	C1C-NC	-2.22	1.34	1.37
11	8	1501	CLA	C4C-C3C	2.22	1.48	1.45
11	2	1205	CLA	CHD-C4C	2.22	1.47	1.41
11	b	1216	CLA	C1C-NC	-2.22	1.34	1.37
11	B	1221	CLA	CHD-C4C	2.22	1.47	1.41
11	A	1116	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1238	CLA	C4C-C3C	2.22	1.48	1.45
11	B	1219	CLA	C4C-C3C	2.21	1.48	1.45
11	a	1106	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1117	CLA	C4C-C3C	2.21	1.48	1.45
11	1	1126	CLA	C1C-C2C	2.21	1.48	1.44
11	1	1129	CLA	C4C-C3C	2.21	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1116	CLA	C1C-NC	-2.21	1.34	1.37
11	2	1223	CLA	C1C-C2C	2.21	1.48	1.44
11	a	1022	CLA	C4C-C3C	2.21	1.48	1.45
11	2	1213	CLA	C4C-C3C	2.20	1.48	1.45
11	a	1126	CLA	C1C-NC	-2.20	1.34	1.37
11	B	1223	CLA	C4C-C3C	2.20	1.48	1.45
11	b	1235	CLA	C4C-C3C	2.20	1.48	1.45
11	B	1215	CLA	C4C-C3C	2.20	1.48	1.45
11	a	1011	CLA	C4C-C3C	2.20	1.48	1.45
11	a	1137	CLA	C4C-C3C	2.20	1.48	1.45
11	1	1022	CLA	C4C-C3C	2.20	1.48	1.45
11	1	1117	CLA	C4C-C3C	2.20	1.48	1.45
11	A	1138	CLA	C4C-C3C	2.20	1.48	1.45
11	a	1012	CLA	C1C-C2C	2.20	1.48	1.44
11	2	1216	CLA	C1C-NC	-2.20	1.34	1.37
11	1	1108	CLA	C4C-C3C	2.20	1.48	1.45
11	1	1012	CLA	C1C-C2C	2.19	1.48	1.44
11	8	1503	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1217	CLA	C4C-C3C	2.19	1.48	1.45
11	A	1112	CLA	C4C-C3C	2.19	1.48	1.45
11	A	1112	CLA	C1C-NC	-2.19	1.34	1.37
11	a	1140	CLA	C4C-C3C	2.19	1.48	1.45
11	A	1101	CLA	C1C-C2C	2.19	1.48	1.44
11	b	1213	CLA	C4C-C3C	2.19	1.48	1.45
11	a	1123	CLA	C1C-NC	-2.19	1.34	1.37
11	1	1130	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1102	CLA	C4C-C3C	2.18	1.48	1.45
14	6	4020	BCR	C30-C25	-2.18	1.50	1.53
11	b	1236	CLA	C1C-NC	-2.18	1.34	1.37
11	1	1237	CLA	C4C-C3C	2.18	1.48	1.45
11	1	1140	CLA	C4C-C3C	2.17	1.48	1.45
11	b	1214	CLA	C4C-C3C	2.17	1.48	1.45
11	a	1112	CLA	C1C-NC	-2.17	1.34	1.37
11	a	1115	CLA	C1C-C2C	2.17	1.48	1.44
11	2	1225	CLA	C1C-NC	-2.17	1.34	1.37
11	b	1222	CLA	C4C-C3C	2.17	1.48	1.45
11	1	1131	CLA	C4C-C3C	2.17	1.48	1.45
11	A	1116	CLA	C4C-C3C	2.17	1.48	1.45
11	A	1121	CLA	C4C-C3C	2.17	1.48	1.45
11	B	1230	CLA	C4C-C3C	2.17	1.48	1.45
11	A	1139	CLA	C1C-NC	-2.16	1.34	1.37
11	b	1207	CLA	C4C-C3C	2.16	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1101	CLA	C4C-C3C	2.16	1.48	1.45
11	B	1213	CLA	C4C-C3C	2.16	1.48	1.45
11	2	1234	CLA	C4C-C3C	2.16	1.48	1.45
11	A	1115	CLA	C4C-C3C	2.16	1.48	1.45
11	B	1214	CLA	C4C-C3C	2.16	1.48	1.45
11	b	1203	CLA	C1C-C2C	2.16	1.48	1.44
11	B	1235	CLA	C4C-C3C	2.16	1.48	1.45
11	b	1212	CLA	C4C-C3C	2.16	1.48	1.45
11	B	1236	CLA	C1C-C2C	2.16	1.48	1.44
11	1	1102	CLA	C1C-NC	-2.16	1.34	1.37
11	a	1136	CLA	C4C-C3C	2.15	1.48	1.45
11	B	1202	CLA	C4C-C3C	2.15	1.48	1.45
11	B	1225	CLA	C4C-C3C	2.15	1.48	1.45
14	2	4017	BCR	C30-C25	-2.15	1.50	1.53
11	b	1221	CLA	C1C-NC	-2.15	1.34	1.37
11	a	1120	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1104	CLA	C1C-C2C	2.15	1.48	1.44
11	l	1501	CLA	C1C-C2C	2.15	1.48	1.44
11	b	1226	CLA	C4C-C3C	2.15	1.48	1.45
14	B	4011	BCR	C1-C6	-2.15	1.50	1.53
11	a	1132	CLA	C4C-C3C	2.15	1.48	1.45
11	b	1202	CLA	C1C-C2C	2.14	1.48	1.44
11	b	1023	CLA	C4C-C3C	2.14	1.48	1.45
11	b	1213	CLA	C1C-NC	-2.14	1.34	1.37
11	A	1109	CLA	C4C-C3C	2.14	1.48	1.45
11	A	1127	CLA	C4C-C3C	2.14	1.48	1.45
11	A	1012	CLA	C4C-C3C	2.14	1.48	1.45
11	B	1212	CLA	C1C-C2C	2.14	1.48	1.44
11	a	1117	CLA	C4C-C3C	2.14	1.48	1.45
11	2	1210	CLA	C4C-C3C	2.14	1.48	1.45
11	B	1223	CLA	C1C-C2C	2.14	1.48	1.44
11	A	1112	CLA	C1C-C2C	2.14	1.48	1.44
11	2	1013	CLA	C4C-C3C	2.14	1.48	1.45
11	1	1107	CLA	C4C-C3C	2.13	1.48	1.45
11	2	1213	CLA	C1C-C2C	2.13	1.48	1.44
11	b	1229	CLA	C4C-C3C	2.13	1.48	1.45
11	1	1126	CLA	C4C-C3C	2.13	1.48	1.45
11	a	1012	CLA	C4C-C3C	2.13	1.48	1.45
11	2	1228	CLA	C4C-C3C	2.13	1.48	1.45
11	A	1116	CLA	C1C-C2C	2.12	1.48	1.44
11	1	1135	CLA	C1C-C2C	2.12	1.48	1.44
11	1	1124	CLA	C4C-C3C	2.12	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1203	CLA	C4C-C3C	2.12	1.48	1.45
11	B	1013	CLA	C4C-C3C	2.12	1.48	1.45
11	A	1137	CLA	C1C-C2C	2.11	1.48	1.44
11	K	1402	CLA	C4C-C3C	2.11	1.48	1.45
11	b	1204	CLA	C4C-C3C	2.11	1.48	1.45
11	1	1135	CLA	C4C-C3C	2.11	1.48	1.45
11	A	1130	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1218	CLA	C4C-C3C	2.11	1.48	1.45
11	b	1236	CLA	C1C-C2C	2.11	1.48	1.44
11	2	1229	CLA	C1C-C2C	2.11	1.48	1.44
11	1	1140	CLA	C1C-C2C	2.11	1.48	1.44
14	F	4018	BCR	C30-C25	-2.11	1.50	1.53
11	A	1108	CLA	C4C-C3C	2.11	1.48	1.45
11	B	1208	CLA	C1C-C2C	2.11	1.48	1.44
11	2	1224	CLA	C4C-C3C	2.10	1.48	1.45
11	1	1137	CLA	C4C-C3C	2.10	1.48	1.45
11	2	1207	CLA	C4C-C3C	2.10	1.48	1.45
11	2	1222	CLA	C4C-C3C	2.10	1.48	1.45
11	a	1011	CLA	C1A-CHA	2.10	1.51	1.43
11	a	1111	CLA	C4C-C3C	2.10	1.48	1.45
11	2	1235	CLA	C4C-C3C	2.10	1.48	1.45
11	A	1105	CLA	C4C-C3C	2.10	1.48	1.45
11	b	1212	CLA	C1C-C2C	2.10	1.48	1.44
11	1	1138	CLA	C4C-C3C	2.10	1.48	1.45
11	b	1221	CLA	C4C-C3C	2.10	1.48	1.45
11	b	1213	CLA	C1C-C2C	2.10	1.48	1.44
11	8	1502	CLA	C1C-C2C	2.10	1.48	1.44
11	2	1202	CLA	C4C-C3C	2.09	1.48	1.45
11	2	1236	CLA	C1C-C2C	2.09	1.48	1.44
14	b	4017	BCR	C30-C25	-2.09	1.50	1.53
11	1	1139	CLA	C1C-C2C	2.09	1.48	1.44
11	a	1107	CLA	C1A-CHA	2.09	1.51	1.43
11	b	1235	CLA	C1C-C2C	2.09	1.48	1.44
11	2	1235	CLA	C1C-C2C	2.09	1.48	1.44
11	B	1235	CLA	C1C-C2C	2.09	1.48	1.44
11	B	1224	CLA	C1C-C2C	2.09	1.48	1.44
11	2	1203	CLA	C4C-C3C	2.09	1.48	1.45
11	2	1221	CLA	C1C-C2C	2.09	1.48	1.44
11	2	1232	CLA	C1C-C2C	2.09	1.48	1.44
11	b	1240	CLA	C1C-C2C	2.09	1.48	1.44
11	1	1120	CLA	C1C-C2C	2.09	1.48	1.44
11	B	1212	CLA	C4C-C3C	2.09	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1224	CLA	C1C-C2C	2.08	1.48	1.44
11	A	1139	CLA	C4C-C3C	2.08	1.48	1.45
14	a	4008	BCR	C30-C25	-2.08	1.50	1.53
11	b	1217	CLA	C1C-C2C	2.08	1.48	1.44
11	A	1113	CLA	C4C-C3C	2.08	1.48	1.45
11	2	1216	CLA	C1C-C2C	2.08	1.48	1.44
11	B	1217	CLA	C1C-C2C	2.08	1.48	1.44
11	a	1122	CLA	C4C-C3C	2.08	1.48	1.45
11	2	1219	CLA	C4C-C3C	2.08	1.48	1.45
11	a	1111	CLA	C1C-C2C	2.08	1.48	1.44
11	1	1122	CLA	C4C-C3C	2.08	1.48	1.45
11	l	1502	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1102	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1113	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1232	CLA	C1C-C2C	2.07	1.48	1.44
11	1	1129	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1229	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1120	CLA	C1C-C2C	2.07	1.48	1.44
11	A	1022	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1121	CLA	C1C-C2C	2.07	1.48	1.44
11	1	1108	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1122	CLA	C1C-C2C	2.06	1.48	1.44
11	2	1222	CLA	C1C-C2C	2.06	1.48	1.44
11	b	1220	CLA	C1C-C2C	2.06	1.48	1.44
11	2	1208	CLA	C4C-C3C	2.06	1.48	1.45
11	l	1501	CLA	C4C-C3C	2.06	1.48	1.45
11	B	1221	CLA	C1C-C2C	2.06	1.48	1.44
11	b	1210	CLA	C1C-C2C	2.06	1.48	1.44
11	A	1126	CLA	C1C-NC	-2.06	1.34	1.37
11	1	1022	CLA	C1C-C2C	2.06	1.48	1.44
11	b	1214	CLA	C1C-C2C	2.06	1.48	1.44
11	a	1106	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1011	CLA	C4C-C3C	2.06	1.48	1.45
11	a	1112	CLA	C1C-C2C	2.06	1.48	1.44
11	2	1228	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1123	CLA	C1C-C2C	2.06	1.48	1.44
11	L	1501	CLA	C1C-C2C	2.06	1.48	1.44
11	a	1125	CLA	C4C-C3C	2.05	1.48	1.45
11	0	1402	CLA	C1C-C2C	2.05	1.48	1.44
14	A	4008	BCR	C30-C25	-2.05	1.50	1.53
11	b	1226	CLA	C1C-C2C	2.05	1.48	1.44
11	B	1021	CLA	C4C-C3C	2.05	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1130	CLA	C1C-C2C	2.05	1.48	1.44
11	A	1012	CLA	C1C-C2C	2.05	1.48	1.44
11	a	1123	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1221	CLA	C4C-C3C	2.05	1.48	1.45
11	a	1109	CLA	C1C-C2C	2.05	1.48	1.44
14	B	4014	BCR	C30-C25	-2.05	1.51	1.53
11	a	1103	CLA	C1C-C2C	2.05	1.48	1.44
11	b	1222	CLA	C1C-C2C	2.04	1.48	1.44
11	A	1237	CLA	C4C-C3C	2.04	1.48	1.45
11	B	1221	CLA	C4C-C3C	2.04	1.48	1.45
11	b	1227	CLA	C1C-C2C	2.04	1.48	1.44
11	B	1202	CLA	C1C-C2C	2.04	1.48	1.44
11	1	1119	CLA	C1C-C2C	2.04	1.48	1.44
11	B	1214	CLA	C1C-C2C	2.04	1.48	1.44
11	b	1236	CLA	C4C-C3C	2.04	1.48	1.45
11	A	1127	CLA	C1C-C2C	2.04	1.48	1.44
11	2	1205	CLA	C1C-C2C	2.04	1.48	1.44
11	1	1011	CLA	C1A-CHA	2.04	1.51	1.43
11	a	1129	CLA	C4C-C3C	2.04	1.48	1.45
11	A	1130	CLA	C1C-C2C	2.04	1.48	1.44
14	B	4005	BCR	C30-C25	-2.04	1.51	1.53
11	b	1216	CLA	C1C-C2C	2.04	1.48	1.44
11	b	1201	CLA	C4C-C3C	2.04	1.48	1.45
11	2	1238	CLA	C1C-C2C	2.04	1.48	1.44
11	2	1204	CLA	C1C-C2C	2.03	1.48	1.44
11	a	1110	CLA	C1C-C2C	2.03	1.48	1.44
11	1	1116	CLA	C1C-C2C	2.03	1.48	1.44
11	A	1113	CLA	C1C-C2C	2.03	1.48	1.44
11	a	1022	CLA	C1C-C2C	2.03	1.48	1.44
11	A	1102	CLA	C1C-C2C	2.03	1.48	1.44
11	2	1223	CLA	C4C-C3C	2.03	1.48	1.45
11	8	1503	CLA	C1C-C2C	2.03	1.48	1.44
11	l	1503	CLA	C4C-C3C	2.03	1.48	1.45
11	2	1224	CLA	C1C-C2C	2.03	1.48	1.44
11	A	1120	CLA	C1C-C2C	2.03	1.48	1.44
11	B	1023	CLA	C4C-C3C	2.03	1.48	1.45
11	B	1239	CLA	C4C-C3C	2.02	1.48	1.45
11	1	1118	CLA	C1C-C2C	2.02	1.48	1.44
11	a	1139	CLA	C1C-C2C	2.02	1.48	1.44
11	b	1205	CLA	C4C-C3C	2.02	1.48	1.45
11	b	1231	CLA	C1C-C2C	2.02	1.48	1.44
11	l	1503	CLA	C1C-C2C	2.02	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1124	CLA	C1C-C2C	2.02	1.48	1.44
11	A	1105	CLA	C1C-C2C	2.02	1.48	1.44
11	A	1137	CLA	C4C-C3C	2.02	1.48	1.45
11	B	1219	CLA	C1C-C2C	2.01	1.48	1.44
11	a	1132	CLA	C1C-C2C	2.01	1.48	1.44
11	b	1230	CLA	C1C-C2C	2.01	1.48	1.44
11	b	1218	CLA	C1C-C2C	2.01	1.48	1.44
11	b	1225	CLA	C1C-C2C	2.01	1.48	1.44
11	A	1121	CLA	C1C-C2C	2.01	1.48	1.44
11	L	1501	CLA	C4C-C3C	2.01	1.48	1.45
11	2	1236	CLA	C4C-C3C	2.01	1.48	1.45
11	a	1124	CLA	C1C-C2C	2.01	1.48	1.44
11	a	1125	CLA	C1C-C2C	2.01	1.48	1.44
11	B	1239	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1104	CLA	C1C-C2C	2.01	1.48	1.44
11	b	1211	CLA	C1C-C2C	2.00	1.48	1.44
11	B	1211	CLA	C4C-C3C	2.00	1.48	1.45
11	a	1237	CLA	C4C-C3C	2.00	1.48	1.45

All (5701) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4002	BCR	C16-C17-C18	28.55	168.05	127.31
14	b	4009	BCR	C16-C17-C18	27.86	167.07	127.31
14	6	4013	BCR	C20-C21-C22	26.01	164.43	127.31
14	F	4013	BCR	C20-C21-C22	25.73	164.03	127.31
14	f	4013	BCR	C20-C21-C22	25.36	163.51	127.31
14	l	4019	BCR	C20-C21-C22	24.80	162.70	127.31
14	b	4006	BCR	C20-C21-C22	24.66	162.51	127.31
14	8	4019	BCR	C20-C21-C22	24.42	162.16	127.31
14	B	4006	BCR	C20-C21-C22	24.38	162.10	127.31
14	1	4008	BCR	C20-C21-C22	24.11	161.72	127.31
14	2	4006	BCR	C20-C21-C22	24.08	161.67	127.31
14	B	4009	BCR	C16-C17-C18	23.84	161.34	127.31
14	A	4007	BCR	C20-C21-C22	23.50	160.84	127.31
14	2	4011	BCR	C16-C17-C18	23.47	160.81	127.31
14	A	4008	BCR	C20-C21-C22	23.32	160.59	127.31
14	b	4006	BCR	C16-C17-C18	23.23	160.47	127.31
14	2	4009	BCR	C16-C17-C18	23.20	160.42	127.31
14	f	4013	BCR	C16-C17-C18	23.12	160.30	127.31
14	a	4007	BCR	C20-C21-C22	22.98	160.10	127.31
14	b	4010	BCR	C16-C17-C18	22.94	160.05	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4008	BCR	C16-C17-C18	22.75	159.78	127.31
14	a	4008	BCR	C20-C21-C22	22.55	159.49	127.31
14	L	4019	BCR	C16-C17-C18	22.53	159.47	127.31
14	1	4002	BCR	C20-C21-C22	22.46	159.37	127.31
14	A	4007	BCR	C16-C17-C18	22.41	159.30	127.31
14	A	4002	BCR	C16-C17-C18	22.35	159.21	127.31
14	b	4017	BCR	C20-C21-C22	22.29	159.12	127.31
14	B	4009	BCR	C20-C21-C22	22.21	159.01	127.31
14	b	4010	BCR	C20-C21-C22	22.17	158.95	127.31
14	a	4002	BCR	C16-C17-C18	22.14	158.91	127.31
14	b	4011	BCR	C16-C17-C18	22.13	158.90	127.31
14	2	4017	BCR	C20-C21-C22	22.10	158.86	127.31
14	B	4011	BCR	C16-C17-C18	22.07	158.80	127.31
14	2	4009	BCR	C20-C21-C22	22.02	158.74	127.31
14	1	4007	BCR	C16-C17-C18	21.95	158.63	127.31
14	F	4013	BCR	C16-C17-C18	21.81	158.44	127.31
14	f	4020	BCR	C20-C21-C22	21.79	158.41	127.31
14	6	4013	BCR	C16-C17-C18	21.72	158.30	127.31
14	b	4011	BCR	C20-C21-C22	21.63	158.18	127.31
14	1	4007	BCR	C20-C21-C22	21.63	158.18	127.31
14	a	4007	BCR	C16-C17-C18	21.60	158.13	127.31
14	8	4019	BCR	C16-C17-C18	21.59	158.12	127.31
14	2	4017	BCR	C15-C16-C17	21.58	167.68	123.47
14	2	4005	BCR	C20-C21-C22	21.50	157.99	127.31
14	a	4008	BCR	C16-C17-C18	21.37	157.80	127.31
14	l	4019	BCR	C16-C17-C18	21.36	157.79	127.31
14	b	4004	BCR	C16-C17-C18	21.34	157.76	127.31
14	M	4021	BCR	C15-C16-C17	21.21	166.93	123.47
14	B	4006	BCR	C16-C17-C18	21.16	157.50	127.31
14	F	4020	BCR	C15-C16-C17	21.13	166.76	123.47
14	B	4004	BCR	C16-C17-C18	21.13	157.46	127.31
14	B	4010	BCR	C16-C17-C18	21.05	157.35	127.31
14	6	4020	BCR	C20-C21-C22	21.05	157.35	127.31
14	b	4014	BCR	C20-C21-C22	21.05	157.35	127.31
14	f	4018	BCR	C20-C21-C22	21.03	157.33	127.31
14	7	4021	BCR	C20-C21-C22	21.02	157.31	127.31
14	1	4001	BCR	C16-C17-C18	21.00	157.29	127.31
14	1	4003	BCR	C16-C17-C18	20.98	157.25	127.31
14	b	4005	BCR	C16-C17-C18	20.94	157.20	127.31
14	l	4022	BCR	C16-C17-C18	20.93	157.19	127.31
14	F	4018	BCR	C20-C21-C22	20.92	157.16	127.31
14	7	4021	BCR	C16-C17-C18	20.91	157.15	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4014	BCR	C16-C17-C18	20.90	157.13	127.31
14	b	4005	BCR	C20-C21-C22	20.86	157.08	127.31
14	F	4018	BCR	C16-C17-C18	20.82	157.02	127.31
14	f	4020	BCR	C15-C16-C17	20.81	166.11	123.47
14	2	4005	BCR	C16-C17-C18	20.81	157.01	127.31
14	B	4005	BCR	C20-C21-C22	20.78	156.97	127.31
14	b	4004	BCR	C20-C21-C22	20.77	156.95	127.31
14	6	4018	BCR	C20-C21-C22	20.74	156.91	127.31
14	a	4003	BCR	C16-C17-C18	20.73	156.90	127.31
14	A	4002	BCR	C20-C21-C22	20.71	156.87	127.31
14	M	4021	BCR	C20-C21-C22	20.70	156.85	127.31
14	8	4022	BCR	C16-C17-C18	20.69	156.84	127.31
14	6	4020	BCR	C16-C17-C18	20.65	156.78	127.31
14	B	4005	BCR	C16-C17-C18	20.61	156.72	127.31
14	B	4017	BCR	C20-C21-C22	20.60	156.71	127.31
14	a	4001	BCR	C16-C17-C18	20.57	156.67	127.31
14	a	4002	BCR	C20-C21-C22	20.54	156.63	127.31
14	b	4005	BCR	C15-C16-C17	20.48	165.43	123.47
14	L	4022	BCR	C16-C17-C18	20.48	156.54	127.31
14	B	4004	BCR	C20-C21-C22	20.48	156.53	127.31
14	2	4010	BCR	C16-C17-C18	20.47	156.53	127.31
14	2	4005	BCR	C15-C16-C17	20.47	165.41	123.47
14	2	4011	BCR	C20-C21-C22	20.45	156.50	127.31
14	m	4021	BCR	C20-C21-C22	20.44	156.48	127.31
14	B	4017	BCR	C15-C16-C17	20.37	165.20	123.47
14	B	4011	BCR	C20-C21-C22	20.32	156.31	127.31
14	2	4006	BCR	C16-C17-C18	20.31	156.30	127.31
14	m	4021	BCR	C15-C16-C17	20.24	164.94	123.47
14	f	4018	BCR	C16-C17-C18	20.19	156.13	127.31
14	2	4004	BCR	C16-C17-C18	20.19	156.12	127.31
14	A	4003	BCR	C16-C17-C18	20.16	156.09	127.31
14	2	4006	BCR	C15-C16-C17	20.07	164.59	123.47
14	f	4020	BCR	C16-C17-C18	20.02	155.88	127.31
14	7	4021	BCR	C15-C16-C17	20.00	164.44	123.47
14	B	4005	BCR	C15-C16-C17	19.97	164.39	123.47
14	2	4014	BCR	C16-C17-C18	19.97	155.82	127.31
14	B	4014	BCR	C15-C16-C17	19.93	164.31	123.47
14	L	4022	BCR	C15-C16-C17	19.89	164.22	123.47
14	8	4022	BCR	C20-C21-C22	19.87	155.67	127.31
14	6	4018	BCR	C16-C17-C18	19.86	155.66	127.31
14	m	4021	BCR	C16-C17-C18	19.85	155.64	127.31
14	f	4018	BCR	C15-C16-C17	19.84	164.12	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4001	BCR	C15-C16-C17	19.84	164.11	123.47
14	b	4017	BCR	C15-C16-C17	19.80	164.03	123.47
14	2	4004	BCR	C15-C16-C17	19.79	164.02	123.47
14	6	4018	BCR	C15-C16-C17	19.71	163.85	123.47
14	B	4017	BCR	C16-C17-C18	19.71	155.43	127.31
14	2	4004	BCR	C20-C21-C22	19.69	155.41	127.31
14	l	4022	BCR	C15-C16-C17	19.68	163.78	123.47
14	2	4014	BCR	C15-C16-C17	19.64	163.70	123.47
14	A	4001	BCR	C16-C17-C18	19.62	155.32	127.31
14	B	4014	BCR	C16-C17-C18	19.62	155.31	127.31
14	A	4003	BCR	C15-C16-C17	19.59	163.59	123.47
14	M	4021	BCR	C16-C17-C18	19.58	155.25	127.31
14	6	4020	BCR	C15-C16-C17	19.57	163.56	123.47
14	8	4022	BCR	C15-C16-C17	19.55	163.52	123.47
14	b	4014	BCR	C15-C16-C17	19.54	163.49	123.47
14	A	4008	BCR	C16-C17-C18	19.49	155.12	127.31
14	b	4009	BCR	C20-C21-C22	19.44	155.05	127.31
14	F	4020	BCR	C16-C17-C18	19.43	155.03	127.31
14	a	4003	BCR	C15-C16-C17	19.40	163.22	123.47
14	a	4001	BCR	C15-C16-C17	19.40	163.21	123.47
14	A	4008	BCR	C15-C16-C17	19.35	163.11	123.47
14	L	4022	BCR	C20-C21-C22	19.34	154.92	127.31
14	L	4019	BCR	C20-C21-C22	19.31	154.87	127.31
14	a	4001	BCR	C20-C21-C22	19.30	154.86	127.31
14	B	4009	BCR	C15-C16-C17	19.29	162.99	123.47
14	2	4014	BCR	C20-C21-C22	19.29	154.83	127.31
14	b	4017	BCR	C16-C17-C18	19.23	154.76	127.31
14	a	4007	BCR	C15-C16-C17	19.22	162.85	123.47
14	1	4001	BCR	C20-C21-C22	19.19	154.70	127.31
14	f	4013	BCR	C15-C16-C17	19.10	162.60	123.47
14	B	4006	BCR	C15-C16-C17	19.07	162.54	123.47
14	B	4004	BCR	C15-C16-C17	19.06	162.51	123.47
14	1	4001	BCR	C15-C16-C17	19.05	162.50	123.47
14	a	4003	BCR	C20-C21-C22	19.02	154.46	127.31
14	2	4010	BCR	C15-C16-C17	19.00	162.40	123.47
14	F	4018	BCR	C15-C16-C17	18.97	162.32	123.47
14	6	4013	BCR	C15-C16-C17	18.96	162.31	123.47
14	l	4022	BCR	C20-C21-C22	18.90	154.29	127.31
14	B	4010	BCR	C15-C16-C17	18.88	162.15	123.47
14	b	4004	BCR	C15-C16-C17	18.87	162.14	123.47
14	1	4003	BCR	C15-C16-C17	18.82	162.03	123.47
14	b	4011	BCR	C15-C16-C17	18.76	161.90	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4013	BCR	C15-C16-C17	18.75	161.88	123.47
14	A	4001	BCR	C20-C21-C22	18.68	153.97	127.31
14	a	4008	BCR	C15-C16-C17	18.67	161.73	123.47
14	1	4007	BCR	C15-C16-C17	18.64	161.66	123.47
14	F	4020	BCR	C20-C21-C22	18.62	153.88	127.31
14	A	4007	BCR	C15-C16-C17	18.60	161.57	123.47
14	2	4011	BCR	C15-C16-C17	18.52	161.42	123.47
14	B	4010	BCR	C20-C21-C22	18.44	153.63	127.31
14	2	4009	BCR	C15-C16-C17	18.27	160.90	123.47
14	B	4014	BCR	C20-C21-C22	18.26	153.36	127.31
14	b	4010	BCR	C15-C16-C17	18.13	160.61	123.47
14	b	4006	BCR	C15-C16-C17	18.12	160.59	123.47
14	B	4011	BCR	C15-C16-C17	17.92	160.18	123.47
14	1	4008	BCR	C15-C16-C17	17.82	159.98	123.47
14	L	4019	BCR	C15-C16-C17	17.81	159.95	123.47
14	L	4019	BCR	C10-C11-C12	17.66	178.32	123.22
14	2	4010	BCR	C20-C21-C22	17.63	152.47	127.31
14	2	4017	BCR	C16-C17-C18	17.56	152.38	127.31
14	1	4002	BCR	C10-C11-C12	17.53	177.91	123.22
14	8	4019	BCR	C15-C16-C17	17.53	159.37	123.47
14	B	4017	BCR	C10-C11-C12	17.51	177.86	123.22
14	l	4019	BCR	C15-C16-C17	17.42	159.16	123.47
14	2	4009	BCR	C10-C11-C12	17.39	177.49	123.22
14	F	4020	BCR	C10-C11-C12	17.38	177.45	123.22
14	1	4007	BCR	C10-C11-C12	17.38	177.44	123.22
14	1	4001	BCR	C10-C11-C12	17.37	177.43	123.22
14	f	4020	BCR	C10-C11-C12	17.37	177.41	123.22
14	l	4019	BCR	C10-C11-C12	17.35	177.36	123.22
14	B	4006	BCR	C10-C11-C12	17.32	177.28	123.22
14	7	4021	BCR	C10-C11-C12	17.32	177.26	123.22
14	b	4005	BCR	C10-C11-C12	17.32	177.26	123.22
14	6	4020	BCR	C10-C11-C12	17.27	177.12	123.22
14	B	4005	BCR	C10-C11-C12	17.26	177.09	123.22
14	a	4002	BCR	C15-C16-C17	17.26	158.82	123.47
14	2	4010	BCR	C10-C11-C12	17.18	176.83	123.22
14	A	4002	BCR	C15-C16-C17	17.12	158.55	123.47
14	b	4010	BCR	C10-C11-C12	17.12	176.63	123.22
14	m	4021	BCR	C10-C11-C12	17.11	176.62	123.22
14	2	4017	BCR	C10-C11-C12	17.11	176.60	123.22
14	B	4004	BCR	C10-C11-C12	17.09	176.55	123.22
14	F	4018	BCR	C10-C11-C12	17.07	176.48	123.22
14	2	4004	BCR	C10-C11-C12	17.04	176.40	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4004	BCR	C10-C11-C12	17.04	176.39	123.22
14	a	4002	BCR	C10-C11-C12	17.04	176.38	123.22
14	a	4007	BCR	C10-C11-C12	17.00	176.27	123.22
14	a	4001	BCR	C10-C11-C12	17.00	176.27	123.22
14	8	4022	BCR	C10-C11-C12	17.00	176.26	123.22
14	b	4017	BCR	C10-C11-C12	16.99	176.24	123.22
14	l	4022	BCR	C10-C11-C12	16.97	176.17	123.22
14	M	4021	BCR	C10-C11-C12	16.96	176.16	123.22
14	2	4014	BCR	C10-C11-C12	16.90	175.94	123.22
14	A	4008	BCR	C10-C11-C12	16.82	175.70	123.22
14	b	4006	BCR	C10-C11-C12	16.80	175.65	123.22
14	A	4007	BCR	C10-C11-C12	16.69	175.32	123.22
14	2	4006	BCR	C10-C11-C12	16.59	174.98	123.22
14	b	4009	BCR	C15-C16-C17	16.58	157.44	123.47
14	B	4010	BCR	C10-C11-C12	16.58	174.96	123.22
14	b	4009	BCR	C10-C11-C12	16.52	174.76	123.22
14	A	4003	BCR	C10-C11-C12	16.49	174.68	123.22
14	1	4003	BCR	C10-C11-C12	16.48	174.63	123.22
14	A	4003	BCR	C20-C21-C22	16.43	150.76	127.31
14	b	4011	BCR	C11-C10-C9	16.40	150.72	127.31
14	b	4014	BCR	C10-C11-C12	16.36	174.28	123.22
14	F	4013	BCR	C10-C11-C12	16.36	174.27	123.22
14	B	4009	BCR	C10-C11-C12	16.32	174.13	123.22
14	8	4019	BCR	C10-C11-C12	16.27	174.00	123.22
14	b	4011	BCR	C10-C11-C12	16.27	173.98	123.22
14	a	4008	BCR	C10-C11-C12	16.20	173.78	123.22
14	1	4008	BCR	C10-C11-C12	16.08	173.41	123.22
14	2	4011	BCR	C10-C11-C12	16.08	173.38	123.22
14	B	4011	BCR	C10-C11-C12	16.01	173.17	123.22
14	2	4005	BCR	C10-C11-C12	15.73	172.32	123.22
14	A	4001	BCR	C10-C11-C12	15.67	172.11	123.22
14	8	4019	BCR	C16-C15-C14	15.60	155.44	123.47
14	1	4003	BCR	C20-C21-C22	15.55	149.50	127.31
14	f	4018	BCR	C10-C11-C12	15.52	171.64	123.22
14	b	4009	BCR	C16-C15-C14	15.51	155.24	123.47
14	B	4014	BCR	C10-C11-C12	15.49	171.57	123.22
14	A	4002	BCR	C10-C11-C12	15.39	171.23	123.22
14	6	4013	BCR	C10-C11-C12	15.33	171.05	123.22
14	1	4008	BCR	C16-C15-C14	15.32	154.86	123.47
14	2	4009	BCR	C16-C15-C14	15.31	154.83	123.47
14	2	4011	BCR	C11-C10-C9	15.31	149.16	127.31
14	6	4018	BCR	C10-C11-C12	15.24	170.77	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	4019	BCR	C16-C15-C14	15.15	154.52	123.47
14	B	4011	BCR	C11-C10-C9	15.10	148.86	127.31
14	L	4019	BCR	C16-C15-C14	15.00	154.19	123.47
14	B	4009	BCR	C16-C15-C14	14.78	153.74	123.47
14	l	4002	BCR	C15-C16-C17	14.72	153.63	123.47
14	f	4013	BCR	C10-C11-C12	14.69	169.04	123.22
14	b	4010	BCR	C16-C15-C14	14.67	153.51	123.47
14	B	4011	BCR	C16-C15-C14	14.62	153.43	123.47
14	a	4003	BCR	C10-C11-C12	14.60	168.78	123.22
14	A	4007	BCR	C11-C10-C9	14.55	148.07	127.31
14	F	4013	BCR	C16-C15-C14	14.47	153.11	123.47
14	a	4008	BCR	C16-C15-C14	14.46	153.09	123.47
14	A	4008	BCR	C16-C15-C14	14.44	153.06	123.47
14	l	4001	BCR	C16-C15-C14	14.42	153.00	123.47
14	l	4003	BCR	C16-C15-C14	14.34	152.85	123.47
14	l	4007	BCR	C16-C15-C14	14.27	152.71	123.47
14	b	4006	BCR	C16-C15-C14	14.25	152.66	123.47
14	b	4005	BCR	C11-C10-C9	14.21	147.60	127.31
14	a	4002	BCR	C16-C15-C14	14.17	152.51	123.47
14	a	4007	BCR	C11-C10-C9	14.11	147.45	127.31
14	B	4010	BCR	C16-C15-C14	14.10	152.37	123.47
14	b	4004	BCR	C16-C15-C14	14.06	152.28	123.47
14	A	4003	BCR	C21-C20-C19	14.04	167.04	123.22
14	2	4010	BCR	C16-C15-C14	14.00	152.16	123.47
14	l	4003	BCR	C21-C20-C19	14.00	166.91	123.22
14	b	4017	BCR	C11-C10-C9	14.00	147.28	127.31
14	2	4006	BCR	C11-C10-C9	13.99	147.27	127.31
14	A	4001	BCR	C16-C15-C14	13.97	152.10	123.47
14	B	4006	BCR	C16-C15-C14	13.97	152.10	123.47
14	M	4021	BCR	C11-C10-C9	13.94	147.20	127.31
14	a	4001	BCR	C11-C10-C9	13.91	147.16	127.31
14	B	4004	BCR	C16-C15-C14	13.84	151.82	123.47
14	B	4017	BCR	C21-C20-C19	13.81	166.30	123.22
14	b	4009	BCR	C11-C10-C9	13.80	147.01	127.31
14	b	4009	BCR	C21-C20-C19	13.77	166.19	123.22
14	L	4022	BCR	C10-C11-C12	13.76	166.17	123.22
14	a	4001	BCR	C16-C15-C14	13.75	151.65	123.47
14	A	4007	BCR	C16-C15-C14	13.75	151.64	123.47
14	b	4006	BCR	C11-C10-C9	13.73	146.91	127.31
14	b	4014	BCR	C16-C15-C14	13.69	151.52	123.47
14	l	4001	BCR	C11-C10-C9	13.68	146.84	127.31
14	F	4020	BCR	C21-C20-C19	13.66	165.86	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4010	BCR	C21-C20-C19	13.66	165.84	123.22
14	2	4014	BCR	C16-C15-C14	13.64	151.42	123.47
14	1	4007	BCR	C11-C10-C9	13.64	146.77	127.31
14	B	4014	BCR	C21-C20-C19	13.63	165.75	123.22
14	l	4022	BCR	C21-C20-C19	13.61	165.70	123.22
14	A	4002	BCR	C16-C15-C14	13.60	151.33	123.47
14	A	4001	BCR	C21-C20-C19	13.59	165.62	123.22
14	6	4013	BCR	C16-C15-C14	13.55	151.24	123.47
14	B	4017	BCR	C11-C10-C9	13.54	146.63	127.31
14	L	4022	BCR	C21-C20-C19	13.53	165.44	123.22
14	b	4011	BCR	C16-C15-C14	13.52	151.18	123.47
14	a	4007	BCR	C16-C15-C14	13.52	151.17	123.47
14	B	4010	BCR	C21-C20-C19	13.48	165.30	123.22
14	8	4022	BCR	C21-C20-C19	13.44	165.15	123.22
14	2	4017	BCR	C21-C20-C19	13.42	165.10	123.22
14	2	4011	BCR	C16-C15-C14	13.42	150.96	123.47
14	B	4004	BCR	C11-C10-C9	13.36	146.38	127.31
14	B	4014	BCR	C16-C15-C14	13.36	150.85	123.47
14	7	4021	BCR	C16-C15-C14	13.33	150.77	123.47
14	2	4014	BCR	C21-C20-C19	13.31	164.74	123.22
14	a	4003	BCR	C16-C15-C14	13.30	150.73	123.47
14	a	4001	BCR	C21-C20-C19	13.30	164.71	123.22
14	2	4004	BCR	C16-C15-C14	13.28	150.67	123.47
14	F	4018	BCR	C16-C15-C14	13.25	150.62	123.47
14	f	4020	BCR	C11-C10-C9	13.23	146.20	127.31
14	A	4003	BCR	C16-C15-C14	13.18	150.48	123.47
14	F	4020	BCR	C11-C10-C9	13.18	146.12	127.31
14	8	4019	BCR	C21-C20-C19	13.12	164.17	123.22
14	1	4001	BCR	C21-C20-C19	13.12	164.16	123.22
14	b	4017	BCR	C16-C15-C14	13.11	150.33	123.47
14	2	4004	BCR	C21-C20-C19	13.11	164.13	123.22
14	a	4002	BCR	C21-C20-C19	13.10	164.09	123.22
14	B	4006	BCR	C11-C10-C9	13.08	145.98	127.31
14	8	4022	BCR	C16-C15-C14	13.06	150.22	123.47
14	b	4010	BCR	C11-C10-C9	13.04	145.93	127.31
14	2	4006	BCR	C16-C15-C14	13.03	150.17	123.47
14	2	4017	BCR	C11-C10-C9	13.03	145.91	127.31
14	f	4013	BCR	C16-C15-C14	13.03	150.16	123.47
14	B	4005	BCR	C16-C15-C14	13.02	150.15	123.47
14	6	4018	BCR	C21-C20-C19	13.00	163.78	123.22
14	m	4021	BCR	C21-C20-C19	12.99	163.75	123.22
14	L	4019	BCR	C21-C20-C19	12.98	163.73	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4003	BCR	C21-C20-C19	12.97	163.70	123.22
14	6	4020	BCR	C16-C15-C14	12.96	150.02	123.47
14	M	4021	BCR	C21-C20-C19	12.96	163.66	123.22
14	a	4002	BCR	C11-C10-C9	12.94	145.77	127.31
14	b	4004	BCR	C11-C10-C9	12.92	145.75	127.31
14	l	4019	BCR	C21-C20-C19	12.92	163.54	123.22
14	b	4017	BCR	C21-C20-C19	12.91	163.51	123.22
14	A	4001	BCR	C11-C10-C9	12.91	145.73	127.31
14	B	4017	BCR	C16-C15-C14	12.83	149.76	123.47
14	B	4004	BCR	C21-C20-C19	12.83	163.25	123.22
14	7	4021	BCR	C11-C10-C9	12.83	145.61	127.31
14	b	4005	BCR	C21-C20-C19	12.81	163.18	123.22
14	6	4018	BCR	C16-C15-C14	12.80	149.69	123.47
14	F	4018	BCR	C11-C10-C9	12.80	145.57	127.31
14	2	4011	BCR	C21-C20-C19	12.78	163.11	123.22
14	F	4018	BCR	C21-C20-C19	12.78	163.10	123.22
14	8	4022	BCR	C11-C10-C9	12.77	145.54	127.31
14	m	4021	BCR	C16-C15-C14	12.73	149.55	123.47
14	l	4022	BCR	C16-C15-C14	12.73	149.55	123.47
14	A	4008	BCR	C11-C10-C9	12.71	145.45	127.31
14	2	4009	BCR	C11-C10-C9	12.70	145.44	127.31
14	b	4014	BCR	C21-C20-C19	12.70	162.85	123.22
14	1	4002	BCR	C21-C20-C19	12.70	162.84	123.22
14	b	4005	BCR	C16-C15-C14	12.69	149.47	123.47
14	7	4021	BCR	C21-C20-C19	12.63	162.65	123.22
14	B	4005	BCR	C21-C20-C19	12.63	162.63	123.22
14	b	4004	BCR	C21-C20-C19	12.62	162.61	123.22
14	A	4002	BCR	C21-C20-C19	12.58	162.48	123.22
14	L	4022	BCR	C16-C15-C14	12.57	149.22	123.47
14	f	4020	BCR	C21-C20-C19	12.55	162.37	123.22
14	2	4005	BCR	C21-C20-C19	12.49	162.19	123.22
14	2	4005	BCR	C16-C15-C14	12.49	149.06	123.47
14	b	4011	BCR	C21-C20-C19	12.47	162.14	123.22
14	f	4018	BCR	C16-C15-C14	12.45	148.98	123.47
14	1	4002	BCR	C11-C10-C9	12.40	145.01	127.31
14	A	4007	BCR	C21-C20-C19	12.40	161.90	123.22
14	f	4018	BCR	C21-C20-C19	12.37	161.82	123.22
14	2	4004	BCR	C11-C10-C9	12.33	144.90	127.31
14	2	4010	BCR	C11-C10-C9	12.32	144.90	127.31
14	2	4006	BCR	C21-C20-C19	12.31	161.63	123.22
14	B	4009	BCR	C21-C20-C19	12.27	161.52	123.22
14	B	4011	BCR	C21-C20-C19	12.23	161.40	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4017	BCR	C16-C15-C14	12.21	148.49	123.47
14	M	4021	BCR	C16-C15-C14	12.19	148.44	123.47
14	1	4003	BCR	C11-C10-C9	12.18	144.69	127.31
14	f	4020	BCR	C16-C15-C14	12.16	148.38	123.47
14	a	4007	BCR	C21-C20-C19	12.15	161.12	123.22
14	2	4011	BCR	C11-C12-C13	12.13	160.51	126.42
14	B	4011	BCR	C11-C12-C13	12.09	160.38	126.42
14	6	4020	BCR	C21-C20-C19	12.06	160.86	123.22
14	2	4014	BCR	C11-C10-C9	12.02	144.46	127.31
14	B	4010	BCR	C11-C10-C9	12.00	144.44	127.31
14	F	4020	BCR	C16-C15-C14	11.91	147.88	123.47
14	B	4005	BCR	C11-C10-C9	11.89	144.27	127.31
14	1	4002	BCR	C16-C15-C14	11.87	147.78	123.47
14	B	4006	BCR	C21-C20-C19	11.85	160.19	123.22
14	2	4009	BCR	C21-C20-C19	11.83	160.13	123.22
14	M	4021	BCR	C11-C12-C13	11.78	159.50	126.42
14	b	4006	BCR	C21-C20-C19	11.72	159.78	123.22
14	a	4008	BCR	C21-C20-C19	11.71	159.75	123.22
14	2	4006	BCR	C11-C12-C13	11.69	159.24	126.42
14	b	4010	BCR	C21-C20-C19	11.61	159.44	123.22
14	l	4019	BCR	C11-C10-C9	11.58	143.84	127.31
14	b	4011	BCR	C11-C12-C13	11.55	158.87	126.42
14	b	4014	BCR	C11-C10-C9	11.53	143.77	127.31
14	m	4021	BCR	C11-C10-C9	11.53	143.76	127.31
14	1	4007	BCR	C21-C20-C19	11.52	159.18	123.22
14	1	4008	BCR	C21-C20-C19	11.51	159.15	123.22
14	F	4018	BCR	C11-C12-C13	11.47	158.65	126.42
14	b	4006	BCR	C11-C12-C13	11.45	158.57	126.42
14	l	4022	BCR	C11-C10-C9	11.35	143.50	127.31
14	F	4013	BCR	C11-C10-C9	11.31	143.45	127.31
14	f	4013	BCR	C21-C20-C19	11.30	158.47	123.22
14	A	4008	BCR	C21-C20-C19	11.28	158.43	123.22
14	B	4005	BCR	C11-C12-C13	11.25	158.03	126.42
14	1	4008	BCR	C11-C10-C9	11.20	143.29	127.31
14	6	4013	BCR	C21-C20-C19	11.13	157.96	123.22
14	1	4008	BCR	C11-C12-C13	11.06	157.50	126.42
14	A	4007	BCR	C11-C12-C13	11.06	157.48	126.42
14	F	4013	BCR	C21-C20-C19	11.04	157.68	123.22
14	b	4009	BCR	C11-C12-C13	11.01	157.33	126.42
14	1	4002	BCR	C11-C12-C13	11.00	157.31	126.42
14	a	4007	BCR	C11-C12-C13	10.97	157.23	126.42
14	B	4006	BCR	C11-C12-C13	10.95	157.17	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	m	4021	BCR	C11-C12-C13	10.91	157.06	126.42
14	a	4001	BCR	C11-C12-C13	10.88	156.97	126.42
14	6	4020	BCR	C11-C10-C9	10.86	142.80	127.31
14	F	4020	BCR	C11-C12-C13	10.85	156.89	126.42
14	7	4021	BCR	C11-C12-C13	10.83	156.84	126.42
14	a	4008	BCR	C11-C12-C13	10.82	156.82	126.42
14	a	4002	BCR	C11-C12-C13	10.78	156.70	126.42
14	B	4009	BCR	C11-C12-C13	10.78	156.69	126.42
14	B	4009	BCR	C11-C10-C9	10.66	142.53	127.31
14	1	4007	BCR	C11-C12-C13	10.64	156.32	126.42
14	2	4009	BCR	C11-C12-C13	10.60	156.19	126.42
14	B	4017	BCR	C11-C12-C13	10.60	156.18	126.42
14	1	4001	BCR	C11-C12-C13	10.58	156.13	126.42
14	L	4019	BCR	C11-C12-C13	10.48	155.84	126.42
14	L	4019	BCR	C11-C10-C9	10.44	142.21	127.31
14	2	4004	BCR	C11-C12-C13	10.43	155.72	126.42
14	8	4022	BCR	C11-C12-C13	10.40	155.64	126.42
14	b	4004	BCR	C11-C12-C13	10.40	155.62	126.42
14	l	4022	BCR	C11-C12-C13	10.34	155.47	126.42
14	l	4019	BCR	C11-C12-C13	10.33	155.44	126.42
14	6	4020	BCR	C11-C12-C13	10.26	155.24	126.42
14	B	4004	BCR	C11-C12-C13	10.25	155.20	126.42
14	2	4017	BCR	C11-C12-C13	10.22	155.13	126.42
14	B	4014	BCR	C11-C10-C9	10.17	141.83	127.31
14	2	4010	BCR	C11-C12-C13	10.13	154.88	126.42
14	2	4005	BCR	C11-C12-C13	10.07	154.71	126.42
14	A	4003	BCR	C11-C12-C13	10.06	154.68	126.42
14	b	4010	BCR	C11-C12-C13	10.05	154.66	126.42
14	A	4008	BCR	C11-C12-C13	10.04	154.62	126.42
14	f	4020	BCR	C11-C12-C13	10.03	154.60	126.42
14	A	4003	BCR	C11-C10-C9	10.01	141.60	127.31
14	b	4017	BCR	C11-C12-C13	9.99	154.49	126.42
14	8	4019	BCR	C11-C10-C9	9.99	141.56	127.31
14	B	4014	BCR	C11-C12-C13	9.99	154.47	126.42
14	B	4010	BCR	C11-C12-C13	9.97	154.44	126.42
14	f	4018	BCR	C11-C10-C9	9.94	141.50	127.31
14	2	4005	BCR	C11-C10-C9	9.92	141.47	127.31
14	8	4019	BCR	C11-C12-C13	9.71	153.70	126.42
14	A	4001	BCR	C11-C12-C13	9.61	153.41	126.42
14	a	4008	BCR	C11-C10-C9	9.59	141.00	127.31
14	A	4002	BCR	C11-C12-C13	9.47	153.02	126.42
14	F	4013	BCR	C11-C12-C13	9.39	152.80	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4003	BCR	C11-C12-C13	9.37	152.75	126.42
14	f	4018	BCR	C11-C12-C13	9.22	152.31	126.42
14	b	4014	BCR	C11-C12-C13	9.15	152.13	126.42
14	6	4018	BCR	C11-C12-C13	9.10	151.98	126.42
14	a	4003	BCR	C11-C12-C13	9.09	151.94	126.42
14	A	4007	BCR	C20-C19-C18	9.07	151.90	126.42
14	A	4002	BCR	C11-C10-C9	9.06	140.24	127.31
14	b	4005	BCR	C11-C12-C13	9.00	151.70	126.42
14	L	4022	BCR	C11-C12-C13	8.89	151.40	126.42
14	6	4013	BCR	C11-C12-C13	8.83	151.21	126.42
14	L	4019	BCR	C20-C19-C18	8.81	151.16	126.42
14	a	4007	BCR	C20-C19-C18	8.80	151.12	126.42
14	2	4009	BCR	C20-C19-C18	8.77	151.04	126.42
14	2	4014	BCR	C11-C12-C13	8.63	150.67	126.42
14	f	4013	BCR	C20-C19-C18	8.54	150.42	126.42
14	b	4006	BCR	C20-C19-C18	8.37	149.92	126.42
14	6	4013	BCR	C11-C10-C9	8.35	139.23	127.31
11	1	1011	CLA	O2D-CGD-CBD	8.33	126.06	111.27
14	6	4018	BCR	C11-C10-C9	8.31	139.17	127.31
14	b	4010	BCR	C20-C19-C18	8.25	149.60	126.42
14	1	4008	BCR	C20-C19-C18	8.17	149.38	126.42
14	6	4013	BCR	C20-C19-C18	8.17	149.38	126.42
14	1	4007	BCR	C20-C19-C18	8.02	148.94	126.42
14	f	4013	BCR	C11-C10-C9	8.00	138.73	127.31
14	B	4006	BCR	C20-C19-C18	7.96	148.79	126.42
14	B	4011	BCR	C20-C19-C18	7.94	148.71	126.42
14	a	4008	BCR	C20-C19-C18	7.91	148.65	126.42
14	b	4011	BCR	C20-C19-C18	7.86	148.50	126.42
14	F	4013	BCR	C20-C19-C18	7.82	148.40	126.42
14	6	4020	BCR	C20-C19-C18	7.82	148.39	126.42
14	b	4014	BCR	C20-C19-C18	7.79	148.29	126.42
14	A	4002	BCR	C20-C19-C18	7.77	148.24	126.42
14	B	4009	BCR	C20-C19-C18	7.67	147.97	126.42
14	7	4021	BCR	C20-C19-C18	7.67	147.97	126.42
11	1	1011	CLA	C4A-NA-C1A	7.64	110.14	106.71
11	B	1205	CLA	C4A-NA-C1A	7.64	110.14	106.71
14	f	4018	BCR	C20-C19-C18	7.59	147.75	126.42
14	M	4021	BCR	C20-C19-C18	7.58	147.70	126.42
14	2	4005	BCR	C20-C19-C18	7.57	147.69	126.42
14	2	4006	BCR	C20-C19-C18	7.53	147.56	126.42
14	B	4005	BCR	C20-C19-C18	7.49	147.47	126.42
14	a	4003	BCR	C11-C10-C9	7.47	137.97	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4005	BCR	C20-C19-C18	7.43	147.30	126.42
11	A	1801	CLA	C2C-C1C-NC	7.43	116.93	109.97
14	2	4011	BCR	C20-C19-C18	7.35	147.06	126.42
14	m	4021	BCR	C20-C19-C18	7.30	146.94	126.42
14	a	4002	BCR	C20-C19-C18	7.30	146.93	126.42
14	a	4003	BCR	C20-C19-C18	7.28	146.87	126.42
14	2	4014	BCR	C20-C19-C18	7.28	146.86	126.42
14	1	4001	BCR	C20-C19-C18	7.27	146.83	126.42
14	f	4020	BCR	C20-C19-C18	7.27	146.83	126.42
14	b	4004	BCR	C20-C19-C18	7.26	146.81	126.42
11	A	1133	CLA	C2C-C1C-NC	7.25	116.77	109.97
11	a	1011	CLA	C4A-NA-C1A	7.24	109.96	106.71
11	A	1125	CLA	C2C-C1C-NC	7.22	116.74	109.97
14	1	4003	BCR	C24-C23-C22	-7.21	115.34	126.23
14	l	4019	BCR	C20-C19-C18	7.21	146.67	126.42
11	A	1011	CLA	C4A-NA-C1A	7.19	109.94	106.71
11	a	1107	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	A	4008	BCR	C20-C19-C18	7.11	146.39	126.42
14	F	4018	BCR	C20-C19-C18	7.09	146.32	126.42
14	1	4002	BCR	C20-C19-C18	7.08	146.30	126.42
14	B	4004	BCR	C20-C19-C18	7.08	146.30	126.42
11	b	1239	CLA	C2C-C1C-NC	7.07	116.59	109.97
11	1	1133	CLA	C2C-C1C-NC	7.06	116.59	109.97
11	b	1207	CLA	C2C-C1C-NC	7.05	116.58	109.97
11	1	1011	CLA	C2C-C1C-NC	7.04	116.57	109.97
14	B	4010	BCR	C20-C19-C18	7.02	146.14	126.42
11	2	1205	CLA	O2D-CGD-CBD	7.02	123.74	111.27
11	A	1134	CLA	C2C-C1C-NC	7.01	116.54	109.97
11	a	1139	CLA	C2C-C1C-NC	7.01	116.54	109.97
11	a	1135	CLA	C2C-C1C-NC	6.99	116.52	109.97
11	A	1123	CLA	C2C-C1C-NC	6.98	116.51	109.97
11	b	1207	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	6	4018	BCR	C24-C23-C22	-6.97	115.70	126.23
11	2	1206	CLA	C2C-C1C-NC	6.95	116.48	109.97
11	2	1213	CLA	C2C-C1C-NC	6.94	116.47	109.97
11	a	1133	CLA	C2C-C1C-NC	6.94	116.47	109.97
14	a	4001	BCR	C20-C19-C18	6.93	145.89	126.42
14	2	4004	BCR	C20-C19-C18	6.93	145.89	126.42
11	B	1205	CLA	O2D-CGD-CBD	6.93	123.58	111.27
11	B	1234	CLA	C2C-C1C-NC	6.92	116.45	109.97
14	8	4019	BCR	C20-C19-C18	6.92	145.84	126.42
11	B	1206	CLA	C2C-C1C-NC	6.89	116.43	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	4019	BCR	C24-C23-C22	-6.88	115.83	126.23
11	B	1201	CLA	C4A-NA-C1A	6.88	109.80	106.71
11	B	1231	CLA	C2C-C1C-NC	6.87	116.41	109.97
11	L	1503	CLA	C2C-C1C-NC	6.87	116.41	109.97
11	B	1232	CLA	C2C-C1C-NC	6.86	116.40	109.97
11	b	1234	CLA	C2C-C1C-NC	6.86	116.40	109.97
11	1	1115	CLA	C2C-C1C-NC	6.86	116.39	109.97
11	a	1127	CLA	C2C-C1C-NC	6.83	116.38	109.97
11	B	1227	CLA	C2C-C1C-NC	6.83	116.37	109.97
11	B	1021	CLA	C2C-C1C-NC	6.82	116.36	109.97
11	b	1206	CLA	C2C-C1C-NC	6.78	116.33	109.97
14	2	4010	BCR	C20-C19-C18	6.78	145.47	126.42
11	A	1110	CLA	O2D-CGD-CBD	6.78	123.32	111.27
11	2	1239	CLA	C2C-C1C-NC	6.77	116.32	109.97
14	A	4001	BCR	C20-C19-C18	6.77	145.44	126.42
11	A	1114	CLA	C2C-C1C-NC	6.77	116.31	109.97
11	1	1111	CLA	C4A-NA-C1A	6.76	109.75	106.71
11	a	1011	CLA	C2C-C1C-NC	6.76	116.31	109.97
11	2	1207	CLA	C4A-NA-C1A	6.76	109.75	106.71
11	b	1219	CLA	C2C-C1C-NC	6.73	116.28	109.97
11	2	1212	CLA	C2C-C1C-NC	6.72	116.27	109.97
11	1	1107	CLA	C2C-C1C-NC	6.72	116.27	109.97
11	1	1110	CLA	C2C-C1C-NC	6.72	116.27	109.97
11	a	1103	CLA	C2C-C1C-NC	6.72	116.27	109.97
11	a	1118	CLA	C4A-NA-C1A	6.71	109.72	106.71
11	2	1205	CLA	C4A-NA-C1A	6.70	109.72	106.71
11	A	1237	CLA	C2C-C1C-NC	6.70	116.25	109.97
14	6	4018	BCR	C20-C19-C18	6.69	145.22	126.42
11	a	1114	CLA	C2C-C1C-NC	6.69	116.24	109.97
11	b	1021	CLA	C2C-C1C-NC	6.69	116.24	109.97
11	b	1208	CLA	C2C-C1C-NC	6.69	116.24	109.97
11	B	1221	CLA	O2D-CGD-CBD	6.69	123.15	111.27
11	1	1801	CLA	C2C-C1C-NC	6.68	116.23	109.97
11	A	1110	CLA	C2C-C1C-NC	6.68	116.23	109.97
11	2	1227	CLA	C2C-C1C-NC	6.68	116.23	109.97
11	a	1107	CLA	C2C-C1C-NC	6.67	116.22	109.97
11	2	1215	CLA	C2C-C1C-NC	6.66	116.21	109.97
11	1	1103	CLA	C4A-NA-C1A	6.66	109.70	106.71
11	B	1221	CLA	C4A-NA-C1A	6.66	109.70	106.71
11	a	1106	CLA	O2D-CGD-CBD	6.65	123.08	111.27
11	B	1229	CLA	C2C-C1C-NC	6.64	116.20	109.97
11	a	1119	CLA	C2C-C1C-NC	6.64	116.20	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1234	CLA	C2C-C1C-NC	6.64	116.19	109.97
14	1	4003	BCR	C20-C19-C18	6.64	145.07	126.42
11	2	1021	CLA	C2C-C1C-NC	6.64	116.19	109.97
11	B	1215	CLA	C2C-C1C-NC	6.63	116.19	109.97
11	B	1230	CLA	C2C-C1C-NC	6.63	116.18	109.97
11	a	1120	CLA	C4A-NA-C1A	6.62	109.68	106.71
11	B	1230	CLA	O2A-C1-C2	6.62	126.03	108.64
11	a	1101	CLA	C2C-C1C-NC	6.62	116.17	109.97
14	B	4014	BCR	C20-C19-C18	6.62	145.00	126.42
11	a	1105	CLA	C2C-C1C-NC	6.61	116.16	109.97
14	f	4018	BCR	C24-C23-C22	-6.60	116.26	126.23
11	1	1110	CLA	O2D-CGD-CBD	6.59	122.98	111.27
11	A	1132	CLA	O2D-CGD-CBD	6.59	122.98	111.27
11	B	1207	CLA	C4A-NA-C1A	6.59	109.67	106.71
11	2	1216	CLA	C2C-C1C-NC	6.59	116.14	109.97
11	2	1207	CLA	C2C-C1C-NC	6.59	116.14	109.97
11	B	1226	CLA	C2C-C1C-NC	6.58	116.14	109.97
11	a	1110	CLA	C2C-C1C-NC	6.58	116.13	109.97
11	a	1022	CLA	C2C-C1C-NC	6.57	116.13	109.97
11	1	1114	CLA	C2C-C1C-NC	6.57	116.13	109.97
11	1	1012	CLA	C2C-C1C-NC	6.57	116.13	109.97
11	B	1225	CLA	C2C-C1C-NC	6.57	116.13	109.97
11	b	1223	CLA	C2C-C1C-NC	6.56	116.12	109.97
11	b	1220	CLA	C2C-C1C-NC	6.56	116.12	109.97
14	b	4017	BCR	C20-C19-C18	6.56	144.85	126.42
11	a	1125	CLA	C2C-C1C-NC	6.56	116.12	109.97
11	B	1021	CLA	C4A-NA-C1A	6.56	109.66	106.71
11	1	1134	CLA	C2C-C1C-NC	6.56	116.11	109.97
11	A	1140	CLA	C2C-C1C-NC	6.56	116.11	109.97
11	B	1220	CLA	C2C-C1C-NC	6.56	116.11	109.97
11	b	1201	CLA	C4A-NA-C1A	6.56	109.65	106.71
11	A	1136	CLA	C2C-C1C-NC	6.55	116.11	109.97
11	b	1230	CLA	C2C-C1C-NC	6.55	116.11	109.97
11	k	1401	CLA	C2C-C1C-NC	6.54	116.10	109.97
11	a	1136	CLA	C2C-C1C-NC	6.54	116.10	109.97
11	A	1118	CLA	C4A-NA-C1A	6.54	109.64	106.71
11	2	1240	CLA	C2C-C1C-NC	6.53	116.09	109.97
11	B	1209	CLA	C2C-C1C-NC	6.53	116.09	109.97
11	2	1225	CLA	C2C-C1C-NC	6.52	116.08	109.97
11	b	1227	CLA	C2C-C1C-NC	6.52	116.08	109.97
11	1	1123	CLA	C2C-C1C-NC	6.52	116.08	109.97
11	a	1129	CLA	C2C-C1C-NC	6.51	116.08	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1121	CLA	C2C-C1C-NC	6.51	116.07	109.97
11	1	1237	CLA	C2C-C1C-NC	6.51	116.07	109.97
11	l	1503	CLA	C2C-C1C-NC	6.51	116.07	109.97
11	2	1221	CLA	C4A-NA-C1A	6.51	109.63	106.71
11	2	1209	CLA	C2C-C1C-NC	6.51	116.07	109.97
11	A	1106	CLA	C2C-C1C-NC	6.51	116.07	109.97
11	B	1206	CLA	C4A-NA-C1A	6.51	109.63	106.71
11	2	1224	CLA	C2C-C1C-NC	6.50	116.07	109.97
11	A	1131	CLA	C2C-C1C-NC	6.50	116.06	109.97
11	0	1401	CLA	C2C-C1C-NC	6.50	116.06	109.97
11	L	1502	CLA	C2C-C1C-NC	6.50	116.06	109.97
11	a	1237	CLA	C2C-C1C-NC	6.50	116.06	109.97
14	l	4022	BCR	C20-C19-C18	6.50	144.66	126.42
11	b	1211	CLA	C2C-C1C-NC	6.49	116.05	109.97
11	2	1217	CLA	C2C-C1C-NC	6.49	116.05	109.97
11	a	1237	CLA	C4A-NA-C1A	6.49	109.62	106.71
11	A	1104	CLA	C4A-NA-C1A	6.49	109.62	106.71
11	8	1501	CLA	C2C-C1C-NC	6.49	116.05	109.97
11	B	1205	CLA	C2C-C1C-NC	6.49	116.05	109.97
11	b	1225	CLA	C2C-C1C-NC	6.49	116.05	109.97
14	b	4017	BCR	C34-C9-C10	-6.48	113.84	122.92
11	B	1216	CLA	C2C-C1C-NC	6.48	116.04	109.97
11	b	1209	CLA	C2C-C1C-NC	6.48	116.04	109.97
11	A	1011	CLA	C2C-C1C-NC	6.47	116.04	109.97
11	1	1237	CLA	C4A-NA-C1A	6.47	109.62	106.71
11	K	1401	CLA	C2C-C1C-NC	6.47	116.03	109.97
11	a	1108	CLA	C2C-C1C-NC	6.47	116.03	109.97
11	1	1128	CLA	C2C-C1C-NC	6.46	116.03	109.97
11	b	1222	CLA	C2C-C1C-NC	6.46	116.02	109.97
11	b	1221	CLA	O2D-CGD-CBD	6.46	122.75	111.27
11	b	1205	CLA	C4A-NA-C1A	6.46	109.61	106.71
11	1	1121	CLA	C2C-C1C-NC	6.46	116.02	109.97
11	2	1201	CLA	C4A-NA-C1A	6.45	109.61	106.71
11	b	1212	CLA	C2C-C1C-NC	6.45	116.02	109.97
11	1	1132	CLA	C2C-C1C-NC	6.45	116.02	109.97
11	2	1226	CLA	C2C-C1C-NC	6.45	116.01	109.97
11	A	1132	CLA	C2C-C1C-NC	6.45	116.01	109.97
14	8	4022	BCR	C20-C19-C18	6.44	144.52	126.42
11	A	1129	CLA	C2C-C1C-NC	6.44	116.01	109.97
11	a	1137	CLA	C2C-C1C-NC	6.44	116.01	109.97
11	8	1501	CLA	C4A-NA-C1A	6.44	109.60	106.71
11	1	1101	CLA	C2C-C1C-NC	6.43	116.00	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1227	CLA	C4A-NA-C1A	6.43	109.60	106.71
11	a	1111	CLA	C4A-NA-C1A	6.43	109.60	106.71
11	a	1120	CLA	C2C-C1C-NC	6.43	115.99	109.97
11	1	1135	CLA	C2C-C1C-NC	6.43	115.99	109.97
11	A	1137	CLA	C2C-C1C-NC	6.42	115.99	109.97
11	1	1108	CLA	C2C-C1C-NC	6.42	115.98	109.97
11	b	1226	CLA	C2C-C1C-NC	6.42	115.98	109.97
11	a	1801	CLA	C2C-C1C-NC	6.41	115.98	109.97
14	7	4021	BCR	C7-C8-C9	-6.41	116.55	126.23
11	l	1502	CLA	C2C-C1C-NC	6.41	115.98	109.97
11	a	1124	CLA	C2C-C1C-NC	6.41	115.98	109.97
11	a	1012	CLA	C2C-C1C-NC	6.41	115.98	109.97
11	1	1137	CLA	O2D-CGD-CBD	6.41	122.65	111.27
11	8	1502	CLA	C2C-C1C-NC	6.41	115.97	109.97
11	1	1137	CLA	C2C-C1C-NC	6.41	115.97	109.97
11	1	1129	CLA	C2C-C1C-NC	6.40	115.97	109.97
11	2	1220	CLA	C2C-C1C-NC	6.40	115.97	109.97
11	B	1213	CLA	C2C-C1C-NC	6.40	115.97	109.97
11	a	1131	CLA	C2C-C1C-NC	6.40	115.97	109.97
11	2	1218	CLA	C4A-NA-C1A	6.40	109.58	106.71
11	2	1023	CLA	C2C-C1C-NC	6.39	115.96	109.97
11	B	1204	CLA	C4A-NA-C1A	6.39	109.58	106.71
11	A	1138	CLA	C4A-NA-C1A	6.39	109.58	106.71
11	1	1120	CLA	C2C-C1C-NC	6.39	115.96	109.97
11	a	1113	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	b	1203	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	1	1140	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	B	1201	CLA	O2D-CGD-CBD	6.38	122.61	111.27
11	a	1106	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	2	1201	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	2	1238	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	A	1135	CLA	C2C-C1C-NC	6.38	115.95	109.97
11	b	1216	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	2	1203	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	1	1138	CLA	C4A-NA-C1A	6.37	109.57	106.71
11	A	1140	CLA	C4A-NA-C1A	6.37	109.57	106.71
11	b	1205	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	A	1124	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	1	1104	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	1	1122	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	A	1237	CLA	C4A-NA-C1A	6.37	109.57	106.71
11	b	1212	CLA	C4A-NA-C1A	6.37	109.57	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1103	CLA	C2C-C1C-NC	6.37	115.94	109.97
11	a	1118	CLA	C2C-C1C-NC	6.36	115.93	109.97
14	A	4003	BCR	C20-C19-C18	6.36	144.29	126.42
11	A	1125	CLA	O2D-CGD-CBD	6.36	122.57	111.27
11	1	1139	CLA	C2C-C1C-NC	6.36	115.93	109.97
11	1	1106	CLA	C2C-C1C-NC	6.36	115.93	109.97
11	A	1130	CLA	C2C-C1C-NC	6.36	115.93	109.97
11	a	1128	CLA	C2C-C1C-NC	6.36	115.93	109.97
11	1	1113	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	B	1221	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	b	1023	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	A	1127	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	1	1109	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	B	1211	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	B	1239	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	B	1201	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	a	1134	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	1	1117	CLA	C2C-C1C-NC	6.35	115.92	109.97
11	B	1204	CLA	C2C-C1C-NC	6.34	115.92	109.97
14	L	4022	BCR	C11-C10-C9	6.34	136.36	127.31
11	b	1228	CLA	C2C-C1C-NC	6.33	115.91	109.97
11	b	1232	CLA	C2C-C1C-NC	6.33	115.90	109.97
14	2	4011	BCR	C7-C8-C9	-6.33	116.67	126.23
11	a	1123	CLA	C2C-C1C-NC	6.33	115.90	109.97
11	A	1102	CLA	C2C-C1C-NC	6.32	115.90	109.97
11	B	1222	CLA	O2D-CGD-CBD	6.32	122.50	111.27
11	B	1239	CLA	C4A-NA-C1A	6.32	109.55	106.71
11	b	1215	CLA	C2C-C1C-NC	6.32	115.89	109.97
11	A	1012	CLA	C2C-C1C-NC	6.32	115.89	109.97
11	b	1238	CLA	C2C-C1C-NC	6.32	115.89	109.97
11	2	1211	CLA	C2C-C1C-NC	6.32	115.89	109.97
11	b	1229	CLA	C2C-C1C-NC	6.32	115.89	109.97
11	b	1217	CLA	C2C-C1C-NC	6.31	115.89	109.97
11	1	1131	CLA	C2C-C1C-NC	6.31	115.89	109.97
11	A	1121	CLA	C2C-C1C-NC	6.31	115.89	109.97
11	2	1232	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	8	1503	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	B	1203	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	b	1204	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	2	1222	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	2	1221	CLA	C2C-C1C-NC	6.31	115.88	109.97
11	b	1224	CLA	C2C-C1C-NC	6.31	115.88	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1208	CLA	C2C-C1C-NC	6.30	115.88	109.97
11	1	1102	CLA	C2C-C1C-NC	6.30	115.87	109.97
11	2	1214	CLA	C2C-C1C-NC	6.30	115.87	109.97
11	a	1140	CLA	C2C-C1C-NC	6.30	115.87	109.97
14	B	4014	BCR	C7-C8-C9	-6.30	116.72	126.23
11	2	1219	CLA	C4A-NA-C1A	6.29	109.54	106.71
11	A	1138	CLA	C2C-C1C-NC	6.29	115.87	109.97
11	B	1228	CLA	C2C-C1C-NC	6.29	115.86	109.97
11	L	1501	CLA	C4A-NA-C1A	6.28	109.53	106.71
11	2	1224	CLA	C4A-NA-C1A	6.28	109.53	106.71
11	2	1230	CLA	C2C-C1C-NC	6.28	115.86	109.97
11	a	1102	CLA	C2C-C1C-NC	6.28	115.85	109.97
11	a	1130	CLA	C2C-C1C-NC	6.27	115.85	109.97
14	f	4013	BCR	C11-C12-C13	6.27	144.04	126.42
11	2	1230	CLA	O2A-C1-C2	6.26	125.09	108.64
11	2	1226	CLA	C4A-NA-C1A	6.26	109.52	106.71
11	B	1226	CLA	O2D-CGD-CBD	6.25	122.38	111.27
14	B	4011	BCR	C7-C8-C9	-6.25	116.79	126.23
14	L	4022	BCR	C20-C19-C18	6.25	143.97	126.42
11	1	1124	CLA	C2C-C1C-NC	6.24	115.82	109.97
11	1	1123	CLA	O2D-CGD-CBD	6.24	122.36	111.27
11	B	1211	CLA	C4D-C3D-CAD	6.24	111.95	108.47
11	B	1222	CLA	C2C-C1C-NC	6.23	115.81	109.97
11	K	1402	CLA	C2C-C1C-NC	6.23	115.81	109.97
11	2	1236	CLA	O2D-CGD-CBD	6.23	122.34	111.27
14	6	4020	BCR	C7-C8-C9	-6.23	116.82	126.23
11	1	1022	CLA	C2C-C1C-NC	6.22	115.80	109.97
11	B	1235	CLA	C2C-C1C-NC	6.22	115.80	109.97
11	A	1118	CLA	C2C-C1C-NC	6.22	115.80	109.97
11	L	1501	CLA	C2C-C1C-NC	6.22	115.80	109.97
14	A	4003	BCR	C24-C23-C22	-6.22	116.84	126.23
11	2	1213	CLA	O2D-CGD-CBD	6.22	122.31	111.27
11	1	1116	CLA	C2C-C1C-NC	6.21	115.79	109.97
11	b	1213	CLA	C2C-C1C-NC	6.21	115.79	109.97
11	L	1503	CLA	C4A-NA-C1A	6.21	109.50	106.71
11	a	1109	CLA	C2C-C1C-NC	6.21	115.79	109.97
11	b	1240	CLA	C2C-C1C-NC	6.21	115.79	109.97
11	1	1130	CLA	C2C-C1C-NC	6.21	115.78	109.97
11	2	1228	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	B	1240	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	A	1113	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	B	1207	CLA	C2C-C1C-NC	6.20	115.78	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	1501	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	A	1122	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	B	1223	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	1	1127	CLA	C2C-C1C-NC	6.19	115.78	109.97
11	B	1219	CLA	C2C-C1C-NC	6.19	115.77	109.97
11	B	1227	CLA	O2D-CGD-CBD	6.19	122.27	111.27
11	A	1101	CLA	C2C-C1C-NC	6.19	115.77	109.97
11	B	1214	CLA	O2D-CGD-CBD	6.19	122.27	111.27
11	1	1105	CLA	C2C-C1C-NC	6.19	115.77	109.97
11	B	1023	CLA	C2C-C1C-NC	6.18	115.77	109.97
11	a	1138	CLA	C2C-C1C-NC	6.18	115.77	109.97
11	2	1204	CLA	C2C-C1C-NC	6.18	115.76	109.97
11	B	1217	CLA	C2C-C1C-NC	6.18	115.76	109.97
11	A	1107	CLA	C2C-C1C-NC	6.18	115.76	109.97
14	b	4009	BCR	C20-C19-C18	6.18	143.77	126.42
11	A	1108	CLA	C2C-C1C-NC	6.17	115.75	109.97
11	b	1234	CLA	C4A-NA-C1A	6.17	109.48	106.71
11	b	1239	CLA	C4A-NA-C1A	6.17	109.48	106.71
11	2	1226	CLA	O2D-CGD-CBD	6.17	122.23	111.27
11	b	1222	CLA	O2D-CGD-CBD	6.17	122.23	111.27
11	b	1235	CLA	C2C-C1C-NC	6.17	115.75	109.97
11	B	1013	CLA	O2A-C1-C2	6.16	124.83	108.64
11	b	1218	CLA	C2C-C1C-NC	6.16	115.75	109.97
11	l	1501	CLA	C4A-NA-C1A	6.16	109.48	106.71
11	b	1206	CLA	C4A-NA-C1A	6.16	109.48	106.71
11	A	1105	CLA	C2C-C1C-NC	6.16	115.74	109.97
11	B	1236	CLA	C2C-C1C-NC	6.15	115.73	109.97
11	0	1402	CLA	C2C-C1C-NC	6.15	115.73	109.97
11	B	1210	CLA	C4A-NA-C1A	6.15	109.47	106.71
11	B	1238	CLA	C2C-C1C-NC	6.15	115.73	109.97
11	a	1129	CLA	C4A-NA-C1A	6.15	109.47	106.71
11	2	1231	CLA	C2C-C1C-NC	6.15	115.73	109.97
11	1	1011	CLA	C3D-CAD-CBD	-6.14	99.51	107.61
11	A	1012	CLA	OBD-CAD-CBD	-6.14	117.12	125.89
14	F	4020	BCR	C20-C19-C18	6.14	143.68	126.42
11	A	1102	CLA	C4A-NA-C1A	6.13	109.46	106.71
11	1	1112	CLA	C2C-C1C-NC	6.13	115.72	109.97
11	k	1402	CLA	C2C-C1C-NC	6.13	115.71	109.97
11	1	1136	CLA	C2C-C1C-NC	6.12	115.71	109.97
11	a	1116	CLA	C2C-C1C-NC	6.12	115.71	109.97
11	2	1211	CLA	C4A-NA-C1A	6.11	109.45	106.71
11	B	1224	CLA	C4A-NA-C1A	6.11	109.45	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1119	CLA	C2C-C1C-NC	6.11	115.70	109.97
11	2	1203	CLA	C4A-NA-C1A	6.11	109.45	106.71
11	1	1113	CLA	C4A-NA-C1A	6.11	109.45	106.71
11	a	1138	CLA	C4A-NA-C1A	6.11	109.45	106.71
11	b	1231	CLA	C2C-C1C-NC	6.11	115.69	109.97
11	1	1012	CLA	C4A-NA-C1A	6.11	109.45	106.71
11	b	1201	CLA	C2C-C1C-NC	6.10	115.69	109.97
11	2	1236	CLA	C2C-C1C-NC	6.09	115.68	109.97
14	A	4001	BCR	C24-C23-C22	-6.09	117.03	126.23
11	2	1229	CLA	C2C-C1C-NC	6.09	115.67	109.97
11	A	1132	CLA	C4A-NA-C1A	6.08	109.44	106.71
11	2	1227	CLA	C4A-NA-C1A	6.08	109.44	106.71
14	B	4014	BCR	C24-C23-C22	-6.07	117.06	126.23
11	B	1218	CLA	C2C-C1C-NC	6.07	115.66	109.97
11	k	1401	CLA	C4A-NA-C1A	6.05	109.43	106.71
11	0	1401	CLA	C4A-NA-C1A	6.05	109.43	106.71
11	B	1240	CLA	C4A-NA-C1A	6.05	109.43	106.71
11	a	1117	CLA	C2C-C1C-NC	6.05	115.64	109.97
11	b	1227	CLA	O2D-CGD-CBD	6.05	122.02	111.27
11	K	1401	CLA	C4A-NA-C1A	6.05	109.42	106.71
11	1	1140	CLA	C4A-NA-C1A	6.04	109.42	106.71
11	a	1132	CLA	C2C-C1C-NC	6.04	115.63	109.97
11	B	1238	CLA	C4A-NA-C1A	6.04	109.42	106.71
11	1	1138	CLA	C2C-C1C-NC	6.04	115.63	109.97
11	1	1125	CLA	C2C-C1C-NC	6.04	115.63	109.97
11	A	1128	CLA	C2C-C1C-NC	6.03	115.62	109.97
11	A	1104	CLA	C2C-C1C-NC	6.03	115.62	109.97
11	2	1202	CLA	C2C-C1C-NC	6.03	115.62	109.97
11	A	1107	CLA	C4A-NA-C1A	6.03	109.42	106.71
11	b	1231	CLA	C4A-NA-C1A	6.02	109.41	106.71
11	8	1502	CLA	C4A-NA-C1A	6.02	109.41	106.71
11	b	1221	CLA	C4A-NA-C1A	6.02	109.41	106.71
11	b	1236	CLA	C2C-C1C-NC	6.02	115.61	109.97
11	A	1119	CLA	C2C-C1C-NC	6.02	115.61	109.97
11	B	1208	CLA	C2C-C1C-NC	6.01	115.61	109.97
11	A	1139	CLA	C2C-C1C-NC	6.01	115.60	109.97
11	B	1212	CLA	C2C-C1C-NC	6.01	115.60	109.97
11	2	1208	CLA	C4A-NA-C1A	6.01	109.41	106.71
11	B	1234	CLA	C4A-NA-C1A	6.01	109.41	106.71
11	A	1120	CLA	C2C-C1C-NC	6.00	115.59	109.97
11	A	1109	CLA	C2C-C1C-NC	6.00	115.59	109.97
11	B	1224	CLA	C2C-C1C-NC	6.00	115.59	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1122	CLA	C2C-C1C-NC	6.00	115.59	109.97
11	B	1230	CLA	C4A-NA-C1A	5.99	109.40	106.71
11	1	1136	CLA	C4A-NA-C1A	5.99	109.40	106.71
11	A	1012	CLA	O2D-CGD-CBD	5.99	121.91	111.27
14	1	4003	BCR	C23-C22-C21	5.98	128.12	118.94
11	B	1235	CLA	O2A-C1-C2	5.98	124.35	108.64
11	a	1102	CLA	C4A-NA-C1A	5.98	109.39	106.71
11	a	1137	CLA	O2D-CGD-CBD	5.98	121.89	111.27
11	b	1219	CLA	C4A-NA-C1A	5.98	109.39	106.71
11	l	1502	CLA	C4A-NA-C1A	5.98	109.39	106.71
11	2	1205	CLA	C2C-C1C-NC	5.98	115.57	109.97
11	2	1206	CLA	C4A-NA-C1A	5.97	109.39	106.71
11	a	1138	CLA	O2D-CGD-CBD	5.97	121.88	111.27
11	A	1115	CLA	C2C-C1C-NC	5.97	115.57	109.97
11	A	1111	CLA	C4A-NA-C1A	5.97	109.39	106.71
11	A	1012	CLA	C4A-NA-C1A	5.96	109.39	106.71
11	8	1501	CLA	O2D-CGD-CBD	5.96	121.86	111.27
11	A	1110	CLA	C4A-NA-C1A	5.96	109.39	106.71
11	A	1103	CLA	C4A-NA-C1A	5.96	109.39	106.71
11	1	1129	CLA	O2D-CGD-CBD	5.96	121.85	111.27
11	A	1012	CLA	O2A-CGA-O1A	-5.95	108.56	123.59
11	A	1128	CLA	C4A-NA-C1A	5.95	109.38	106.71
11	1	1801	CLA	C4A-NA-C1A	5.95	109.38	106.71
11	L	1502	CLA	O2D-CGD-CBD	5.95	121.84	111.27
11	1	1118	CLA	C2C-C1C-NC	5.94	115.54	109.97
14	L	4022	BCR	C24-C23-C22	-5.94	117.26	126.23
11	1	1118	CLA	C4A-NA-C1A	5.93	109.37	106.71
11	b	1221	CLA	C2C-C1C-NC	5.93	115.53	109.97
11	A	1126	CLA	C4A-NA-C1A	5.93	109.37	106.71
11	K	1402	CLA	C4A-NA-C1A	5.93	109.37	106.71
11	a	1117	CLA	C4A-NA-C1A	5.93	109.37	106.71
11	B	1023	CLA	C4A-NA-C1A	5.92	109.37	106.71
11	L	1503	CLA	C1C-C2C-C3C	-5.92	100.73	106.96
11	b	1013	CLA	C2C-C1C-NC	5.92	115.52	109.97
11	B	1213	CLA	C4A-NA-C1A	5.91	109.36	106.71
11	b	1235	CLA	C4A-NA-C1A	5.91	109.36	106.71
11	b	1222	CLA	C4A-NA-C1A	5.91	109.36	106.71
11	A	1117	CLA	C2C-C1C-NC	5.90	115.50	109.97
11	A	1022	CLA	C2C-C1C-NC	5.90	115.50	109.97
11	2	1219	CLA	C2C-C1C-NC	5.90	115.50	109.97
11	a	1126	CLA	O2D-CGD-CBD	5.89	121.73	111.27
11	1	1108	CLA	C4A-NA-C1A	5.88	109.35	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1214	CLA	C4A-NA-C1A	5.88	109.35	106.71
11	B	1218	CLA	C4A-NA-C1A	5.88	109.35	106.71
11	a	1136	CLA	C4A-NA-C1A	5.87	109.34	106.71
11	b	1213	CLA	C4A-NA-C1A	5.87	109.34	106.71
11	A	1123	CLA	C4A-NA-C1A	5.87	109.34	106.71
11	1	1120	CLA	O2D-CGD-CBD	5.86	121.69	111.27
11	1	1135	CLA	C4A-NA-C1A	5.86	109.34	106.71
11	B	1202	CLA	C2C-C1C-NC	5.86	115.46	109.97
11	1	1121	CLA	C4A-NA-C1A	5.86	109.34	106.71
14	m	4021	BCR	C7-C8-C9	-5.85	117.39	126.23
11	A	1126	CLA	O2D-CGD-CBD	5.85	121.66	111.27
11	B	1206	CLA	C4D-C3D-CAD	5.85	111.73	108.47
11	A	1131	CLA	C4A-NA-C1A	5.85	109.33	106.71
11	1	1137	CLA	C4A-NA-C1A	5.85	109.33	106.71
11	B	1226	CLA	C4A-NA-C1A	5.85	109.33	106.71
11	a	1111	CLA	C2C-C1C-NC	5.85	115.45	109.97
11	b	1023	CLA	C4A-NA-C1A	5.85	109.33	106.71
14	F	4013	BCR	C15-C14-C13	-5.84	118.97	127.31
11	B	1231	CLA	C4A-NA-C1A	5.84	109.33	106.71
11	B	1214	CLA	C2C-C1C-NC	5.84	115.44	109.97
11	1	1104	CLA	C4A-NA-C1A	5.84	109.33	106.71
11	1	1107	CLA	C4A-NA-C1A	5.84	109.33	106.71
11	2	1013	CLA	C2C-C1C-NC	5.83	115.44	109.97
11	B	1225	CLA	C4D-C3D-CAD	5.83	111.72	108.47
11	B	1203	CLA	C4A-NA-C1A	5.83	109.33	106.71
11	2	1216	CLA	C4A-NA-C1A	5.83	109.33	106.71
11	A	1133	CLA	C4A-NA-C1A	5.83	109.33	106.71
11	2	1013	CLA	C4A-NA-C1A	5.83	109.33	106.71
11	2	1023	CLA	O2A-C1-C2	5.83	123.95	108.64
11	b	1224	CLA	C4A-NA-C1A	5.83	109.33	106.71
14	2	4017	BCR	C20-C19-C18	5.82	142.77	126.42
11	2	1222	CLA	O2D-CGD-CBD	5.82	121.61	111.27
11	1	1140	CLA	O2A-C1-C2	5.82	123.92	108.64
11	1	1502	CLA	O2D-CGD-CBD	5.82	121.60	111.27
11	b	1214	CLA	C2C-C1C-NC	5.81	115.42	109.97
11	2	1223	CLA	C2C-C1C-NC	5.81	115.41	109.97
14	F	4018	BCR	C24-C23-C22	-5.81	117.46	126.23
11	B	1023	CLA	O2A-C1-C2	5.80	123.89	108.64
11	2	1239	CLA	C4A-NA-C1A	5.80	109.31	106.71
11	A	1011	CLA	C1C-C2C-C3C	-5.80	100.86	106.96
11	a	1104	CLA	C2C-C1C-NC	5.80	115.41	109.97
11	B	1021	CLA	C1C-C2C-C3C	-5.80	100.86	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1210	CLA	C2C-C1C-NC	5.80	115.40	109.97
11	2	1220	CLA	C4A-NA-C1A	5.79	109.31	106.71
11	B	1207	CLA	O2D-CGD-CBD	5.79	121.55	111.27
11	2	1240	CLA	C4A-NA-C1A	5.78	109.30	106.71
11	2	1205	CLA	O2A-CGA-O1A	-5.78	109.01	123.59
11	L	1502	CLA	C4A-NA-C1A	5.78	109.30	106.71
11	a	1126	CLA	C4A-NA-C1A	5.78	109.30	106.71
11	b	1226	CLA	O2D-CGD-CBD	5.77	121.53	111.27
11	A	1112	CLA	C4A-NA-C1A	5.77	109.30	106.71
11	A	1137	CLA	C4A-NA-C1A	5.77	109.30	106.71
11	A	1116	CLA	C2C-C1C-NC	5.77	115.38	109.97
11	a	1112	CLA	C2C-C1C-NC	5.76	115.36	109.97
11	8	1502	CLA	O2D-CGD-CBD	5.75	121.49	111.27
11	B	1232	CLA	C4A-NA-C1A	5.75	109.29	106.71
11	b	1202	CLA	C4A-NA-C1A	5.75	109.29	106.71
11	A	1131	CLA	O2D-CGD-CBD	5.74	121.46	111.27
11	b	1210	CLA	C2C-C1C-NC	5.74	115.35	109.97
11	A	1105	CLA	C4A-NA-C1A	5.73	109.28	106.71
11	2	1217	CLA	C4A-NA-C1A	5.73	109.28	106.71
11	B	1222	CLA	C4A-NA-C1A	5.73	109.28	106.71
11	B	1013	CLA	C2C-C1C-NC	5.73	115.34	109.97
11	a	1012	CLA	O2D-CGD-CBD	5.73	121.45	111.27
11	b	1013	CLA	O2A-C1-C2	5.73	123.69	108.64
11	b	1230	CLA	O2D-CGD-CBD	5.73	121.44	111.27
11	2	1228	CLA	C4A-NA-C1A	5.73	109.28	106.71
11	B	1215	CLA	C4-C3-C5	5.72	124.90	115.27
11	B	1231	CLA	O2D-CGD-CBD	5.72	121.44	111.27
11	2	1235	CLA	C2C-C1C-NC	5.72	115.33	109.97
11	1	1126	CLA	C2C-C1C-NC	5.72	115.33	109.97
11	A	1134	CLA	C4A-NA-C1A	5.72	109.28	106.71
11	a	1114	CLA	C4A-NA-C1A	5.72	109.28	106.71
11	B	1224	CLA	O2D-CGD-CBD	5.72	121.43	111.27
11	2	1210	CLA	C2C-C1C-NC	5.71	115.32	109.97
11	1	1132	CLA	C4A-NA-C1A	5.71	109.27	106.71
11	B	1217	CLA	C4A-NA-C1A	5.71	109.27	106.71
11	1	1126	CLA	O2D-CGD-CBD	5.71	121.41	111.27
11	2	1229	CLA	C4A-NA-C1A	5.71	109.27	106.71
11	2	1023	CLA	C4A-NA-C1A	5.71	109.27	106.71
11	1	1125	CLA	O2D-CGD-CBD	5.70	121.40	111.27
11	a	1135	CLA	C4A-NA-C1A	5.70	109.27	106.71
11	A	1112	CLA	C2C-C1C-NC	5.70	115.31	109.97
11	a	1012	CLA	C4A-NA-C1A	5.70	109.27	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1111	CLA	C2C-C1C-NC	5.70	115.31	109.97
11	1	1120	CLA	C4A-NA-C1A	5.70	109.27	106.71
11	a	1136	CLA	O2D-CGD-CBD	5.70	121.39	111.27
11	A	1133	CLA	C1C-C2C-C3C	-5.70	100.97	106.96
11	1	1104	CLA	C1C-C2C-C3C	-5.70	100.97	106.96
11	a	1139	CLA	C1C-C2C-C3C	-5.70	100.97	106.96
11	B	1013	CLA	C4A-NA-C1A	5.69	109.26	106.71
11	a	1133	CLA	C4A-NA-C1A	5.69	109.26	106.71
11	2	1210	CLA	C4A-NA-C1A	5.68	109.26	106.71
11	a	1140	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	f	4013	BCR	C24-C23-C22	-5.68	117.66	126.23
11	2	1021	CLA	C4A-NA-C1A	5.68	109.26	106.71
11	b	1239	CLA	C1C-C2C-C3C	-5.68	100.99	106.96
11	a	1106	CLA	C4A-NA-C1A	5.67	109.26	106.71
11	1	1140	CLA	O2A-CGA-O1A	-5.67	109.28	123.59
11	1	1011	CLA	C1C-C2C-C3C	-5.67	100.99	106.96
11	l	1501	CLA	O2D-CGD-CBD	5.67	121.34	111.27
11	1	1124	CLA	C4A-NA-C1A	5.67	109.25	106.71
11	A	1104	CLA	O2D-CGD-CBD	5.66	121.33	111.27
14	1	4003	BCR	C37-C22-C21	-5.66	115.00	122.92
11	1	1123	CLA	C4A-NA-C1A	5.66	109.25	106.71
11	a	1116	CLA	O2D-CGD-CBD	5.66	121.32	111.27
11	a	1103	CLA	C1C-C2C-C3C	-5.66	101.01	106.96
11	1	1129	CLA	C4A-NA-C1A	5.65	109.25	106.71
11	A	1136	CLA	C4A-NA-C1A	5.65	109.25	106.71
11	A	1118	CLA	C1C-C2C-C3C	-5.65	101.02	106.96
11	b	1228	CLA	C4A-NA-C1A	5.65	109.25	106.71
11	b	1203	CLA	C4A-NA-C1A	5.65	109.25	106.71
11	2	1234	CLA	C4A-NA-C1A	5.64	109.24	106.71
11	a	1129	CLA	O2D-CGD-CBD	5.64	121.29	111.27
11	a	1115	CLA	C2C-C1C-NC	5.64	115.25	109.97
11	a	1133	CLA	O2D-CGD-CBD	5.64	121.28	111.27
11	a	1105	CLA	C4A-NA-C1A	5.64	109.24	106.71
11	2	1224	CLA	O2D-CGD-CBD	5.63	121.28	111.27
11	1	1112	CLA	O2D-CGD-CBD	5.63	121.27	111.27
11	1	1012	CLA	O2D-CGD-CBD	5.63	121.27	111.27
11	2	1213	CLA	C1C-C2C-C3C	-5.63	101.04	106.96
11	1	1116	CLA	C4A-NA-C1A	5.62	109.23	106.71
11	a	1113	CLA	C4A-NA-C1A	5.62	109.23	106.71
11	B	1236	CLA	C4A-NA-C1A	5.62	109.23	106.71
11	1	1134	CLA	C4A-NA-C1A	5.62	109.23	106.71
11	1	1012	CLA	O2A-CGA-O1A	-5.62	109.42	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1113	CLA	C4A-NA-C1A	5.62	109.23	106.71
11	b	1204	CLA	C4A-NA-C1A	5.61	109.23	106.71
11	2	1218	CLA	C2C-C1C-NC	5.61	115.23	109.97
11	a	1137	CLA	C4A-NA-C1A	5.61	109.23	106.71
14	B	4017	BCR	C20-C19-C18	5.61	142.16	126.42
11	l	1503	CLA	C1C-C2C-C3C	-5.60	101.06	106.96
11	B	1236	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
11	1	1102	CLA	C4A-NA-C1A	5.60	109.22	106.71
11	a	1126	CLA	C2C-C1C-NC	5.60	115.21	109.97
11	2	1231	CLA	O2D-CGD-CBD	5.60	121.21	111.27
11	A	1106	CLA	O2D-CGD-CBD	5.59	121.20	111.27
11	2	1221	CLA	O2D-CGD-CBD	5.59	121.20	111.27
11	a	1118	CLA	C1C-C2C-C3C	-5.59	101.08	106.96
11	2	1235	CLA	C4A-NA-C1A	5.59	109.22	106.71
11	B	1219	CLA	C4A-NA-C1A	5.59	109.22	106.71
11	1	1105	CLA	C4A-NA-C1A	5.59	109.22	106.71
11	1	1117	CLA	C4A-NA-C1A	5.59	109.22	106.71
11	1	1119	CLA	O2A-CGA-O1A	-5.58	109.50	123.59
11	A	1104	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
11	A	1801	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
11	2	1215	CLA	O2D-CGD-CBD	5.58	121.18	111.27
11	B	1205	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
11	2	1215	CLA	O2A-C1-C2	5.58	123.29	108.64
11	2	1231	CLA	C4A-NA-C1A	5.57	109.21	106.71
11	a	1139	CLA	C4A-NA-C1A	5.57	109.21	106.71
11	b	1211	CLA	O2D-CGD-CBD	5.57	121.16	111.27
11	1	1109	CLA	C4A-NA-C1A	5.57	109.21	106.71
11	a	1128	CLA	C4A-NA-C1A	5.57	109.21	106.71
11	A	1122	CLA	C4A-NA-C1A	5.57	109.21	106.71
11	a	1011	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
11	a	1124	CLA	O2D-CGD-CBD	5.56	121.15	111.27
11	B	1207	CLA	O2A-CGA-O1A	-5.56	109.56	123.59
11	1	1112	CLA	C4A-NA-C1A	5.56	109.21	106.71
11	2	1227	CLA	O2D-CGD-CBD	5.56	121.15	111.27
11	b	1220	CLA	C4A-NA-C1A	5.56	109.20	106.71
11	b	1207	CLA	O2A-CGA-O1A	-5.56	109.57	123.59
11	a	1108	CLA	C4A-NA-C1A	5.56	109.20	106.71
11	b	1209	CLA	C4A-NA-C1A	5.56	109.20	106.71
11	1	1101	CLA	O2D-CGD-CBD	5.56	121.14	111.27
11	a	1119	CLA	O2A-CGA-O1A	-5.55	109.57	123.59
11	A	1112	CLA	O2D-CGD-CBD	5.55	121.14	111.27
11	0	1402	CLA	C4A-NA-C1A	5.55	109.20	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1116	CLA	O2D-CGD-CBD	5.55	121.13	111.27
11	b	1021	CLA	C4A-NA-C1A	5.55	109.20	106.71
11	2	1218	CLA	O2D-CGD-CBD	5.55	121.13	111.27
11	A	1129	CLA	C4A-NA-C1A	5.55	109.20	106.71
14	2	4014	BCR	C24-C23-C22	-5.55	117.85	126.23
11	2	1210	CLA	O2D-CGD-CBD	5.55	121.12	111.27
11	1	1134	CLA	O2D-CGD-CBD	5.54	121.12	111.27
11	2	1204	CLA	O2D-CGD-CBD	5.54	121.11	111.27
14	A	4003	BCR	C7-C8-C9	-5.54	117.87	126.23
11	b	1221	CLA	C4-C3-C5	5.54	124.59	115.27
11	1	1133	CLA	C1C-C2C-C3C	-5.54	101.14	106.96
11	b	1202	CLA	C2C-C1C-NC	5.54	115.16	109.97
11	A	1112	CLA	C4D-C3D-CAD	5.53	111.56	108.47
11	B	1223	CLA	O2D-CGD-CBD	5.53	121.10	111.27
11	2	1206	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
11	2	1013	CLA	O2A-C1-C2	5.53	123.17	108.64
11	B	1234	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
11	A	1118	CLA	C4D-C3D-CAD	5.52	111.55	108.47
11	1	1115	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
14	a	4001	BCR	C24-C23-C22	-5.52	117.90	126.23
14	b	4017	BCR	C7-C8-C9	-5.52	117.90	126.23
11	A	1106	CLA	C4A-NA-C1A	5.51	109.18	106.71
11	A	1116	CLA	O2D-CGD-CBD	5.51	121.06	111.27
11	2	1215	CLA	C1C-C2C-C3C	-5.51	101.16	106.96
11	A	1109	CLA	C4A-NA-C1A	5.51	109.18	106.71
11	2	1230	CLA	C4A-NA-C1A	5.51	109.18	106.71
14	l	4022	BCR	C24-C23-C22	-5.51	117.91	126.23
11	B	1204	CLA	O2D-CGD-CBD	5.51	121.06	111.27
11	b	1227	CLA	C4A-NA-C1A	5.51	109.18	106.71
11	1	1131	CLA	C4A-NA-C1A	5.51	109.18	106.71
11	b	1217	CLA	C4A-NA-C1A	5.51	109.18	106.71
11	1	1801	CLA	O2D-CGD-CBD	5.50	121.05	111.27
11	l	1503	CLA	C4A-NA-C1A	5.50	109.18	106.71
11	a	1118	CLA	C4D-C3D-CAD	5.50	111.54	108.47
11	A	1102	CLA	O2D-CGD-CBD	5.50	121.04	111.27
11	b	1215	CLA	O2A-C1-C2	5.50	123.08	108.64
11	a	1110	CLA	O2D-CGD-CBD	5.50	121.04	111.27
11	B	1013	CLA	O2A-CGA-O1A	-5.50	109.72	123.59
11	2	1224	CLA	O2A-CGA-O1A	-5.49	109.73	123.59
11	B	1209	CLA	O2D-CGD-CBD	5.49	121.03	111.27
11	b	1212	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
11	B	1209	CLA	C4A-NA-C1A	5.49	109.17	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1131	CLA	C4A-NA-C1A	5.49	109.17	106.71
11	b	1023	CLA	O2A-C1-C2	5.49	123.06	108.64
11	2	1225	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
11	2	1207	CLA	O2A-CGA-O1A	-5.49	109.75	123.59
11	2	1236	CLA	C4A-NA-C1A	5.49	109.17	106.71
11	B	1224	CLA	O2A-CGA-O1A	-5.48	109.75	123.59
11	2	1211	CLA	O2D-CGD-CBD	5.48	121.01	111.27
11	a	1132	CLA	C4A-NA-C1A	5.48	109.17	106.71
11	b	1021	CLA	C1C-C2C-C3C	-5.48	101.20	106.96
11	b	1013	CLA	O2A-CGA-O1A	-5.48	109.77	123.59
11	A	1106	CLA	C1C-C2C-C3C	-5.48	101.20	106.96
11	a	1122	CLA	C4A-NA-C1A	5.48	109.17	106.71
11	B	1231	CLA	C1C-C2C-C3C	-5.47	101.20	106.96
11	A	1116	CLA	C4A-NA-C1A	5.47	109.17	106.71
11	b	1210	CLA	C4A-NA-C1A	5.47	109.17	106.71
11	B	1239	CLA	C1C-C2C-C3C	-5.47	101.21	106.96
11	a	1120	CLA	O2D-CGD-CBD	5.47	120.98	111.27
11	b	1222	CLA	C1C-C2C-C3C	-5.47	101.21	106.96
11	b	1236	CLA	C4A-NA-C1A	5.47	109.16	106.71
11	b	1224	CLA	O2D-CGD-CBD	5.46	120.98	111.27
11	A	1109	CLA	C1C-C2C-C3C	-5.46	101.21	106.96
11	2	1021	CLA	C1C-C2C-C3C	-5.46	101.21	106.96
11	A	1130	CLA	C4A-NA-C1A	5.46	109.16	106.71
11	A	1139	CLA	C4A-NA-C1A	5.46	109.16	106.71
11	B	1228	CLA	C4A-NA-C1A	5.46	109.16	106.71
11	a	1133	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
11	B	1204	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
11	L	1503	CLA	O2D-CGD-CBD	5.46	120.96	111.27
11	b	1203	CLA	C1C-C2C-C3C	-5.45	101.22	106.96
11	1	1801	CLA	C1C-C2C-C3C	-5.45	101.22	106.96
11	B	1203	CLA	C1C-C2C-C3C	-5.45	101.22	106.96
11	b	1230	CLA	C4A-NA-C1A	5.45	109.16	106.71
11	A	1115	CLA	C4A-NA-C1A	5.45	109.16	106.71
11	2	1013	CLA	O2A-CGA-O1A	-5.45	109.83	123.59
11	B	1208	CLA	C4A-NA-C1A	5.45	109.16	106.71
14	1	4008	BCR	C15-C14-C13	-5.45	119.53	127.31
11	2	1216	CLA	O2D-CGD-CBD	5.45	120.95	111.27
11	b	1227	CLA	C1C-C2C-C3C	-5.45	101.23	106.96
11	A	1134	CLA	C1C-C2C-C3C	-5.44	101.23	106.96
11	a	1105	CLA	C1C-C2C-C3C	-5.44	101.23	106.96
11	1	1102	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
11	1	1107	CLA	O2A-C1-C2	5.44	122.93	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	1503	CLA	O2D-CGD-CBD	5.44	120.93	111.27
11	A	1114	CLA	C4A-NA-C1A	5.43	109.15	106.71
11	2	1230	CLA	O2D-CGD-CBD	5.43	120.92	111.27
11	2	1225	CLA	O2D-CGD-CBD	5.43	120.92	111.27
11	1	1111	CLA	O2D-CGD-CBD	5.43	120.91	111.27
11	a	1237	CLA	C4D-C3D-CAD	5.43	111.50	108.47
11	b	1206	CLA	C4D-C3D-CAD	5.43	111.50	108.47
11	B	1232	CLA	C1C-C2C-C3C	-5.43	101.25	106.96
11	b	1219	CLA	C1C-C2C-C3C	-5.42	101.25	106.96
11	2	1023	CLA	O2A-CGA-O1A	-5.42	109.91	123.59
11	2	1205	CLA	C4D-C3D-CAD	5.42	111.49	108.47
11	a	1104	CLA	C4A-NA-C1A	5.42	109.14	106.71
11	b	1211	CLA	C4A-NA-C1A	5.42	109.14	106.71
11	1	1128	CLA	C4A-NA-C1A	5.42	109.14	106.71
11	b	1215	CLA	O2D-CGD-CBD	5.42	120.90	111.27
11	L	1502	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
11	l	1502	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
11	A	1138	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
11	2	1211	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
11	1	1101	CLA	C4A-NA-C1A	5.42	109.14	106.71
11	2	1219	CLA	C4D-C3D-CAD	5.42	111.49	108.47
11	A	1103	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	B	1214	CLA	C4D-C3D-CAD	5.42	111.49	108.47
11	2	1205	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
11	a	1129	CLA	C1C-C2C-C3C	-5.41	101.26	106.96
11	a	1115	CLA	C4A-NA-C1A	5.41	109.14	106.71
11	l	1501	CLA	O2A-CGA-O1A	-5.41	109.93	123.59
11	b	1214	CLA	O2D-CGD-CBD	5.41	120.88	111.27
11	1	1114	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	a	1101	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	2	1212	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	2	1217	CLA	O2D-CGD-CBD	5.41	120.88	111.27
11	a	1801	CLA	O2D-CGD-CBD	5.41	120.88	111.27
11	a	1109	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	a	1125	CLA	C4A-NA-C1A	5.41	109.14	106.71
11	2	1208	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	2	1227	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	b	1207	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
11	A	1101	CLA	C4A-NA-C1A	5.41	109.14	106.71
11	2	1222	CLA	C4A-NA-C1A	5.41	109.14	106.71
11	b	1239	CLA	O2D-CGD-CBD	5.40	120.87	111.27
11	B	1226	CLA	C1C-C2C-C3C	-5.40	101.28	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1235	CLA	O2D-CGD-CBD	5.40	120.87	111.27
11	b	1238	CLA	C4A-NA-C1A	5.40	109.14	106.71
11	b	1206	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
11	2	1226	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
11	a	1102	CLA	O2A-CGA-O1A	-5.40	109.96	123.59
11	a	1135	CLA	O2D-CGD-CBD	5.40	120.86	111.27
11	B	1224	CLA	C4D-C3D-CAD	5.40	111.48	108.47
11	A	1138	CLA	C4D-C3D-CAD	5.40	111.48	108.47
11	B	1211	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
11	8	1501	CLA	O2A-CGA-O1A	-5.39	109.98	123.59
11	b	1213	CLA	O2D-CGD-CBD	5.39	120.84	111.27
11	B	1234	CLA	O2A-CGA-O1A	-5.39	109.99	123.59
11	1	1122	CLA	C4A-NA-C1A	5.39	109.13	106.71
11	a	1114	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
11	a	1110	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
11	2	1234	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
11	2	1203	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
11	2	1224	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	A	1108	CLA	C4A-NA-C1A	5.38	109.13	106.71
11	a	1137	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	b	1202	CLA	O2D-CGD-CBD	5.38	120.83	111.27
11	B	1215	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	1	1107	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	2	1215	CLA	C4-C3-C5	5.38	124.32	115.27
11	2	1239	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	2	1222	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	1	1115	CLA	O2D-CGD-CBD	5.38	120.83	111.27
11	B	1223	CLA	C4D-C3D-CAD	5.38	111.47	108.47
11	B	1213	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	a	1135	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
11	1	1130	CLA	O2D-CGD-CBD	5.38	120.82	111.27
11	A	1126	CLA	C2C-C1C-NC	5.38	115.01	109.97
11	B	1021	CLA	O2A-CGA-O1A	-5.38	110.03	123.59
14	A	4008	BCR	C34-C9-C10	-5.37	115.40	122.92
11	b	1224	CLA	O2A-CGA-O1A	-5.37	110.04	123.59
11	1	1119	CLA	C4A-NA-C1A	5.37	109.12	106.71
11	a	1101	CLA	C4A-NA-C1A	5.37	109.12	106.71
11	1	1109	CLA	O2A-CGA-O1A	-5.37	110.04	123.59
11	A	1121	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
11	A	1114	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
11	1	1118	CLA	O2D-CGD-CBD	5.37	120.81	111.27
11	A	1123	CLA	C4D-C3D-CAD	5.37	111.46	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1130	CLA	O2D-CGD-CBD	5.36	120.80	111.27
11	2	1204	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
11	b	1229	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
11	b	1205	CLA	O2A-CGA-O1A	-5.36	110.06	123.59
11	A	1137	CLA	O2D-CGD-CBD	5.36	120.79	111.27
11	1	1135	CLA	O2D-CGD-CBD	5.36	120.79	111.27
11	A	1120	CLA	C4D-C3D-CAD	5.35	111.46	108.47
11	b	1209	CLA	O2D-CGD-CBD	5.35	120.78	111.27
14	a	4003	BCR	C24-C23-C22	-5.35	118.14	126.23
11	a	1127	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
11	B	1208	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
11	A	1135	CLA	O2A-CGA-O1A	-5.35	110.08	123.59
11	8	1501	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
11	a	1107	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
11	1	1131	CLA	O2D-CGD-CBD	5.35	120.77	111.27
11	A	1122	CLA	O2D-CGD-CBD	5.35	120.77	111.27
11	2	1238	CLA	C4A-NA-C1A	5.35	109.11	106.71
11	B	1227	CLA	C1C-C2C-C3C	-5.35	101.34	106.96
11	b	1235	CLA	O2D-CGD-CBD	5.35	120.77	111.27
11	a	1106	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	b	1208	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	A	1801	CLA	O2A-CGA-O1A	-5.34	110.11	123.59
11	1	1110	CLA	O2A-CGA-O1A	-5.34	110.11	123.59
14	1	4002	BCR	C33-C5-C6	-5.34	118.53	124.53
11	2	1238	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	A	1801	CLA	C4A-NA-C1A	5.34	109.11	106.71
11	a	1127	CLA	C4A-NA-C1A	5.34	109.11	106.71
11	a	1132	CLA	O2D-CGD-CBD	5.34	120.75	111.27
11	1	1108	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	1	1118	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	1	1134	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
11	b	1218	CLA	C4A-NA-C1A	5.34	109.11	106.71
11	a	1120	CLA	C1C-C2C-C3C	-5.34	101.35	106.96
11	8	1503	CLA	C4A-NA-C1A	5.33	109.10	106.71
11	A	1136	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
11	b	1236	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
11	1	1012	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
11	1	1103	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
11	a	1109	CLA	O2A-CGA-O1A	-5.33	110.14	123.59
11	A	1237	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
11	B	1230	CLA	O2D-CGD-CBD	5.33	120.74	111.27
11	b	1205	CLA	O2D-CGD-CBD	5.33	120.73	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1130	CLA	C1C-C2C-C3C	-5.33	101.36	106.96
11	1	1114	CLA	C4A-NA-C1A	5.32	109.10	106.71
11	B	1225	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	A	1110	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	B	1222	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	A	1237	CLA	O2A-C1-C2	5.32	122.62	108.64
11	2	1209	CLA	C4A-NA-C1A	5.32	109.10	106.71
11	B	1211	CLA	C4A-NA-C1A	5.32	109.10	106.71
11	a	1022	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	1	1109	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	1	1132	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	A	1102	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
11	b	1234	CLA	O2A-CGA-O1A	-5.32	110.17	123.59
11	B	1223	CLA	C4A-NA-C1A	5.32	109.10	106.71
11	2	1212	CLA	C4A-NA-C1A	5.32	109.10	106.71
11	B	1238	CLA	C1C-C2C-C3C	-5.32	101.37	106.96
11	B	1228	CLA	O2D-CGD-CBD	5.32	120.71	111.27
11	a	1125	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
11	A	1139	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
11	b	1229	CLA	C4A-NA-C1A	5.31	109.09	106.71
11	a	1112	CLA	O2D-CGD-CBD	5.31	120.71	111.27
11	a	1122	CLA	O2A-C1-C2	5.31	122.60	108.64
11	b	1213	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
11	b	1208	CLA	C4A-NA-C1A	5.31	109.09	106.71
11	1	1022	CLA	O2A-CGA-O1A	-5.31	110.19	123.59
11	1	1121	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
14	f	4013	BCR	C7-C8-C9	-5.31	118.21	126.23
11	b	1021	CLA	O2A-CGA-O1A	-5.31	110.19	123.59
11	b	1205	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
11	a	1104	CLA	O2D-CGD-CBD	5.31	120.70	111.27
11	b	1013	CLA	C4A-NA-C1A	5.30	109.09	106.71
11	1	1111	CLA	C2C-C1C-NC	5.30	114.94	109.97
11	A	1135	CLA	C4A-NA-C1A	5.30	109.09	106.71
11	1	1124	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
11	B	1235	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
11	A	1137	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
11	1	1137	CLA	O2A-CGA-O1A	-5.30	110.21	123.59
11	A	1022	CLA	OBD-CAD-CBD	-5.30	118.32	125.89
11	b	1215	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
11	A	1107	CLA	C4D-C3D-CAD	5.30	111.42	108.47
11	a	1121	CLA	C4A-NA-C1A	5.30	109.09	106.71
11	A	1137	CLA	O2A-CGA-O1A	-5.30	110.22	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1139	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
11	1	1129	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
11	B	1215	CLA	C4A-NA-C1A	5.30	109.09	106.71
11	2	1215	CLA	C4A-NA-C1A	5.30	109.09	106.71
11	a	1131	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
11	1	1117	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
11	L	1501	CLA	O2A-CGA-O1A	-5.29	110.23	123.59
11	1	1130	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
11	b	1235	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
11	2	1213	CLA	C4A-NA-C1A	5.29	109.08	106.71
11	B	1215	CLA	O2A-C1-C2	5.29	122.54	108.64
11	B	1217	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
11	a	1134	CLA	C4D-C3D-CAD	5.29	111.42	108.47
11	A	1124	CLA	C4A-NA-C1A	5.29	109.08	106.71
11	B	1205	CLA	O2A-CGA-O1A	-5.29	110.24	123.59
11	B	1225	CLA	C4A-NA-C1A	5.29	109.08	106.71
11	B	1021	CLA	O2D-CGD-CBD	5.29	120.66	111.27
11	k	1401	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
14	B	4017	BCR	C24-C23-C22	-5.28	118.25	126.23
11	A	1136	CLA	O2D-CGD-CBD	5.28	120.66	111.27
11	B	1235	CLA	C4A-NA-C1A	5.28	109.08	106.71
11	A	1111	CLA	O2D-CGD-CBD	5.28	120.65	111.27
11	a	1136	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
11	a	1237	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
11	b	1232	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
11	a	1134	CLA	C4A-NA-C1A	5.28	109.08	106.71
11	B	1216	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
11	1	1140	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
11	b	1204	CLA	O2D-CGD-CBD	5.28	120.64	111.27
14	2	4005	BCR	C24-C23-C22	-5.27	118.27	126.23
11	A	1135	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
11	a	1119	CLA	C4A-NA-C1A	5.27	109.08	106.71
11	A	1133	CLA	O2D-CGD-CBD	5.27	120.64	111.27
11	A	1137	CLA	C4D-C3D-CAD	5.27	111.41	108.47
11	0	1401	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
11	A	1118	CLA	O2D-CGD-CBD	5.27	120.63	111.27
11	a	1118	CLA	O2D-CGD-CBD	5.27	120.63	111.27
11	a	1121	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
11	a	1123	CLA	O2D-CGD-CBD	5.27	120.63	111.27
11	B	1023	CLA	O2A-CGA-O1A	-5.27	110.30	123.59
11	a	1237	CLA	O2A-C1-C2	5.27	122.47	108.64
11	1	1106	CLA	C1C-C2C-C3C	-5.27	101.42	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1226	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	a	1108	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	1	1119	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	a	1130	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	b	1204	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	A	1132	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	1	1131	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
11	b	1211	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
11	2	1221	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
11	1	1105	CLA	O2D-CGD-CBD	5.26	120.61	111.27
11	8	1503	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
11	1	1104	CLA	O2D-CGD-CBD	5.26	120.61	111.27
11	A	1140	CLA	O2D-CGD-CBD	5.25	120.60	111.27
11	K	1401	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	B	1206	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	1	1135	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
14	a	4008	BCR	C24-C23-C22	-5.25	118.30	126.23
11	b	1222	CLA	O2A-CGA-O1A	-5.25	110.34	123.59
11	2	1236	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	8	1502	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	a	1110	CLA	C4A-NA-C1A	5.25	109.06	106.71
11	a	1801	CLA	O2A-CGA-O1A	-5.25	110.35	123.59
11	A	1131	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	A	1115	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	b	1217	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
11	A	1102	CLA	O2A-CGA-O1A	-5.24	110.36	123.59
11	1	1103	CLA	C4D-C3D-CAD	5.24	111.39	108.47
11	2	1228	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
11	b	1218	CLA	O2D-CGD-CBD	5.24	120.58	111.27
11	b	1201	CLA	O2D-CGD-CBD	5.24	120.58	111.27
11	B	1212	CLA	O2D-CGD-CBD	5.24	120.58	111.27
11	b	1208	CLA	O2D-CGD-CBD	5.24	120.57	111.27
11	b	1225	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
11	1	1110	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
14	8	4022	BCR	C24-C23-C22	-5.23	118.33	126.23
11	A	1104	CLA	O2A-CGA-O1A	-5.23	110.38	123.59
11	b	1240	CLA	C4A-NA-C1A	5.23	109.06	106.71
11	B	1220	CLA	C4A-NA-C1A	5.23	109.06	106.71
11	a	1127	CLA	C4D-C3D-CAD	5.23	111.39	108.47
11	l	1501	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
11	b	1203	CLA	O2D-CGD-CBD	5.23	120.56	111.27
11	a	1102	CLA	C1C-C2C-C3C	-5.23	101.46	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1215	CLA	O2D-CGD-CBD	5.23	120.56	111.27
11	1	1111	CLA	O2A-C1-C2	5.23	122.38	108.64
11	a	1131	CLA	O2D-CGD-CBD	5.23	120.56	111.27
11	A	1123	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
11	b	1023	CLA	O2A-CGA-O1A	-5.23	110.40	123.59
11	1	1120	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
11	b	1232	CLA	C4A-NA-C1A	5.22	109.06	106.71
11	1	1137	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	A	1139	CLA	C4D-C3D-CAD	5.22	111.38	108.47
11	2	1214	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	2	1202	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	2	1231	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	a	1113	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	1	1136	CLA	O2D-CGD-CBD	5.22	120.54	111.27
11	b	1217	CLA	O2A-CGA-O1A	-5.22	110.42	123.59
11	2	1214	CLA	O2D-CGD-CBD	5.22	120.54	111.27
11	b	1228	CLA	O2D-CGD-CBD	5.22	120.54	111.27
11	a	1112	CLA	C4A-NA-C1A	5.22	109.05	106.71
11	A	1101	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
11	B	1229	CLA	C4A-NA-C1A	5.21	109.05	106.71
11	a	1139	CLA	C4D-C3D-CAD	5.21	111.38	108.47
11	b	1236	CLA	O2D-CGD-CBD	5.21	120.53	111.27
11	2	1224	CLA	C4D-C3D-CAD	5.21	111.38	108.47
14	b	4014	BCR	C24-C23-C22	-5.21	118.36	126.23
11	B	1229	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
11	2	1204	CLA	C4A-NA-C1A	5.21	109.05	106.71
11	b	1238	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
11	b	1201	CLA	C1C-C2C-C3C	-5.20	101.48	106.96
11	0	1402	CLA	O2A-CGA-O1A	-5.20	110.46	123.59
11	a	1119	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	A	1107	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	a	1012	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	a	1801	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	A	1105	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	a	1109	CLA	C4A-NA-C1A	5.20	109.04	106.71
11	a	1124	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	a	1134	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	B	1218	CLA	O2D-CGD-CBD	5.20	120.50	111.27
11	B	1202	CLA	O2A-CGA-O1A	-5.20	110.47	123.59
11	b	1216	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	b	1228	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
11	B	1239	CLA	O2D-CGD-CBD	5.19	120.50	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1105	CLA	O2D-CGD-CBD	5.19	120.50	111.27
11	a	1140	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
11	1	1022	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
11	B	1212	CLA	C4A-NA-C1A	5.19	109.04	106.71
11	A	1132	CLA	O2A-C1-C2	5.19	122.27	108.64
11	2	1229	CLA	O2D-CGD-CBD	5.19	120.48	111.27
11	1	1107	CLA	O2D-CGD-CBD	5.19	120.48	111.27
11	2	1225	CLA	C4A-NA-C1A	5.18	109.04	106.71
11	L	1501	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
11	1	1101	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
11	2	1223	CLA	C4A-NA-C1A	5.18	109.03	106.71
11	a	1122	CLA	O2A-CGA-O1A	-5.18	110.52	123.59
11	1	1135	CLA	C4-C3-C5	5.18	121.91	115.98
11	a	1107	CLA	C4D-C3D-CAD	5.18	111.36	108.47
11	2	1226	CLA	C4D-C3D-CAD	5.18	111.36	108.47
11	a	1022	CLA	OBD-CAD-CBD	-5.18	118.50	125.89
11	2	1223	CLA	O2D-CGD-CBD	5.18	120.47	111.27
11	B	1221	CLA	C1C-C2C-C3C	-5.18	101.52	106.96
11	1	1127	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
11	1	1139	CLA	C4D-C3D-CAD	5.17	111.36	108.47
11	1	1125	CLA	C4A-NA-C1A	5.17	109.03	106.71
11	1	1116	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
11	1	1123	CLA	C1C-C2C-C3C	-5.17	101.53	106.96
11	2	1225	CLA	C4D-C3D-CAD	5.16	111.35	108.47
11	B	1202	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	B	1212	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	a	1104	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	B	1240	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	B	1210	CLA	CAC-C3C-C4C	5.16	131.51	124.81
11	a	1123	CLA	C4A-NA-C1A	5.16	109.03	106.71
11	0	1402	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	b	1230	CLA	O2A-CGA-O1A	-5.16	110.57	123.59
14	A	4008	BCR	C15-C14-C13	-5.16	119.95	127.31
11	A	1127	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	2	1207	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
11	a	1140	CLA	O2D-CGD-CBD	5.16	120.43	111.27
11	B	1213	CLA	O2D-CGD-CBD	5.16	120.43	111.27
11	b	1214	CLA	C4A-NA-C1A	5.16	109.02	106.71
11	1	1126	CLA	C4A-NA-C1A	5.15	109.02	106.71
11	B	1202	CLA	O2D-CGD-CBD	5.15	120.43	111.27
11	B	1238	CLA	O2D-CGD-CBD	5.15	120.42	111.27
11	A	1122	CLA	O2A-CGA-O1A	-5.15	110.59	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1011	CLA	O2A-CGA-O1A	-5.15	110.59	123.59
11	2	1216	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
11	2	1238	CLA	O2D-CGD-CBD	5.15	120.42	111.27
11	b	1231	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
11	1	1237	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
11	2	1228	CLA	O2A-CGA-O1A	-5.15	110.60	123.59
11	1	1128	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
11	b	1226	CLA	C4A-NA-C1A	5.15	109.02	106.71
11	1	1113	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
11	1	1114	CLA	O2D-CGD-CBD	5.14	120.41	111.27
11	a	1128	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
11	B	1201	CLA	C4D-C3D-CAD	5.14	111.34	108.47
11	b	1218	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
11	a	1105	CLA	O2A-CGA-O1A	-5.14	110.62	123.59
11	1	1133	CLA	C4A-NA-C1A	5.14	109.02	106.71
11	A	1022	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
11	A	1103	CLA	C4D-C3D-CAD	5.13	111.33	108.47
14	1	4003	BCR	C15-C14-C13	-5.13	119.99	127.31
14	B	4005	BCR	C24-C23-C22	-5.13	118.48	126.23
11	a	1123	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
11	b	1216	CLA	O2D-CGD-CBD	5.13	120.38	111.27
11	A	1130	CLA	O2D-CGD-CBD	5.13	120.38	111.27
11	1	1115	CLA	C4A-NA-C1A	5.12	109.01	106.71
11	A	1120	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	b	1209	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	1	1105	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	1	1111	CLA	O2A-CGA-O1A	-5.12	110.66	123.59
11	0	1401	CLA	O2A-CGA-O1A	-5.12	110.66	123.59
11	B	1220	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	a	1132	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	A	1117	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	b	1023	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	1	1122	CLA	C1C-C2C-C3C	-5.12	101.57	106.96
11	8	1503	CLA	O2D-CGD-CBD	5.12	120.36	111.27
11	K	1401	CLA	O2A-CGA-O1A	-5.12	110.67	123.59
11	1	1012	CLA	O2A-C1-C2	5.12	122.09	108.64
11	1	1110	CLA	C4A-NA-C1A	5.12	109.01	106.71
11	1	1118	CLA	C4D-C3D-CAD	5.12	111.32	108.47
11	A	1011	CLA	O2A-CGA-O1A	-5.11	110.68	123.59
11	k	1401	CLA	O2A-CGA-O1A	-5.11	110.68	123.59
11	b	1232	CLA	O2D-CGD-CBD	5.11	120.35	111.27
11	A	1107	CLA	O2A-CGA-O1A	-5.11	110.69	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1110	CLA	O2A-CGA-O1A	-5.11	110.69	123.59
11	1	1102	CLA	O2A-CGA-O1A	-5.11	110.69	123.59
14	b	4011	BCR	C7-C8-C9	-5.11	118.52	126.23
11	b	1225	CLA	C4A-NA-C1A	5.11	109.00	106.71
11	1	1103	CLA	O2D-CGD-CBD	5.11	120.34	111.27
11	b	1225	CLA	C4D-C3D-CAD	5.11	111.32	108.47
11	b	1240	CLA	C1C-C2C-C3C	-5.11	101.59	106.96
11	b	1223	CLA	C4A-NA-C1A	5.10	109.00	106.71
11	A	1118	CLA	O2A-CGA-O1A	-5.10	110.71	123.59
11	A	1124	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
11	A	1113	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
11	b	1224	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
11	A	1012	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
11	k	1402	CLA	O2A-CGA-O1A	-5.10	110.72	123.59
11	1	1119	CLA	O2D-CGD-CBD	5.10	120.33	111.27
11	2	1232	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
14	b	4011	BCR	C34-C9-C10	-5.10	115.78	122.92
11	B	1207	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
11	b	1234	CLA	C1C-C2C-C3C	-5.09	101.60	106.96
11	b	1212	CLA	O2D-CGD-CBD	5.09	120.32	111.27
11	B	1224	CLA	C1C-C2C-C3C	-5.09	101.60	106.96
11	B	1236	CLA	O2D-CGD-CBD	5.09	120.31	111.27
14	f	4013	BCR	C15-C14-C13	-5.09	120.05	127.31
11	a	1117	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
11	A	1125	CLA	CAC-C3C-C4C	5.09	131.41	124.81
11	A	1128	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
14	6	4013	BCR	C7-C8-C9	-5.09	118.55	126.23
11	2	1217	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
11	B	1217	CLA	O2A-CGA-O1A	-5.09	110.76	123.59
11	2	1234	CLA	O2A-CGA-O1A	-5.08	110.76	123.59
11	2	1236	CLA	O2A-CGA-O1A	-5.08	110.76	123.59
11	1	1112	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
14	A	4003	BCR	C37-C22-C21	-5.08	115.81	122.92
11	1	1139	CLA	O2A-CGA-O1A	-5.08	110.77	123.59
11	B	1202	CLA	C4A-NA-C1A	5.08	108.99	106.71
11	A	1115	CLA	O2D-CGD-CBD	5.08	120.29	111.27
11	1	1127	CLA	O2A-CGA-O1A	-5.08	110.78	123.59
11	A	1111	CLA	O2A-CGA-O1A	-5.08	110.78	123.59
11	2	1240	CLA	C1C-C2C-C3C	-5.08	101.62	106.96
11	a	1101	CLA	O2D-CGD-CBD	5.07	120.29	111.27
11	2	1222	CLA	O2A-CGA-O1A	-5.07	110.79	123.59
11	b	1240	CLA	O2D-CGD-CBD	5.07	120.28	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	1402	CLA	C4A-NA-C1A	5.07	108.98	106.71
11	b	1202	CLA	C4D-C3D-CAD	5.07	111.30	108.47
11	2	1223	CLA	C4D-C3D-CAD	5.07	111.30	108.47
11	b	1215	CLA	O2A-CGA-O1A	-5.07	110.80	123.59
11	1	1129	CLA	C4D-C3D-CAD	5.07	111.30	108.47
11	A	1108	CLA	C1C-C2C-C3C	-5.07	101.63	106.96
11	a	1116	CLA	C4A-NA-C1A	5.06	108.98	106.71
11	A	1122	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
11	1	1116	CLA	O2A-CGA-O1A	-5.06	110.82	123.59
11	a	1022	CLA	C4A-NA-C1A	5.06	108.98	106.71
11	b	1021	CLA	O2D-CGD-CBD	5.06	120.26	111.27
11	2	1235	CLA	O2D-CGD-CBD	5.06	120.26	111.27
11	2	1239	CLA	O2D-CGD-CBD	5.06	120.26	111.27
11	B	1207	CLA	C4D-C3D-CAD	5.06	111.29	108.47
11	1	1105	CLA	C4D-C3D-CAD	5.06	111.29	108.47
11	2	1219	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
11	a	1137	CLA	O2A-CGA-O1A	-5.06	110.83	123.59
11	B	1209	CLA	C1C-C2C-C3C	-5.05	101.64	106.96
11	b	1223	CLA	C1C-C2C-C3C	-5.05	101.64	106.96
11	2	1229	CLA	C1C-C2C-C3C	-5.05	101.65	106.96
11	a	1122	CLA	C4D-C3D-CAD	5.05	111.29	108.47
11	a	1104	CLA	O2A-CGA-O1A	-5.05	110.85	123.59
11	a	1126	CLA	C4-C3-C5	5.05	123.76	115.27
11	a	1012	CLA	O2A-CGA-O1A	-5.05	110.85	123.59
11	a	1122	CLA	O2D-CGD-CBD	5.05	120.23	111.27
11	1	1106	CLA	O2A-CGA-O1A	-5.05	110.86	123.59
11	1	1124	CLA	O2A-CGA-O1A	-5.04	110.86	123.59
11	B	1210	CLA	O2A-CGA-O1A	-5.04	110.86	123.59
11	B	1222	CLA	O2A-CGA-O1A	-5.04	110.86	123.59
14	7	4021	BCR	C33-C5-C6	-5.04	118.87	124.53
11	B	1219	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
11	b	1225	CLA	O2D-CGD-CBD	5.04	120.22	111.27
11	B	1236	CLA	C4D-C3D-CAD	5.04	111.28	108.47
11	A	1123	CLA	O2D-CGD-CBD	5.04	120.22	111.27
11	2	1201	CLA	O2A-C1-C2	5.04	121.87	108.64
11	2	1209	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
11	A	1109	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
16	B	5002	LMG	O7-C10-C11	5.03	122.35	111.50
11	B	1226	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
11	B	1228	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
11	1	1011	CLA	O2A-CGA-O1A	-5.03	110.90	123.59
11	A	1125	CLA	C1C-C2C-C3C	-5.03	101.67	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1202	CLA	O2A-CGA-O1A	-5.03	110.91	123.59
11	A	1127	CLA	C4A-NA-C1A	5.03	108.97	106.71
11	a	1127	CLA	O2A-CGA-O1A	-5.03	110.91	123.59
11	B	1023	CLA	C4D-C3D-CAD	5.02	111.27	108.47
11	b	1219	CLA	O2A-CGA-O1A	-5.02	110.91	123.59
11	b	1238	CLA	O2D-CGD-CBD	5.02	120.19	111.27
11	b	1212	CLA	C4D-C3D-CAD	5.02	111.27	108.47
11	B	1232	CLA	O2D-CGD-CBD	5.02	120.19	111.27
11	1	1139	CLA	C4A-NA-C1A	5.02	108.96	106.71
11	2	1201	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
11	2	1216	CLA	O2A-CGA-O1A	-5.02	110.92	123.59
11	b	1201	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
11	1	1131	CLA	C4D-C3D-CAD	5.02	111.27	108.47
11	a	1121	CLA	C4D-C3D-CAD	5.02	111.27	108.47
11	1	1022	CLA	O2D-CGD-CBD	5.02	120.18	111.27
11	a	1119	CLA	O2D-CGD-CBD	5.02	120.18	111.27
11	B	1214	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
11	b	1203	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
11	a	1127	CLA	O2D-CGD-CBD	5.01	120.18	111.27
11	a	1124	CLA	O2A-CGA-O1A	-5.01	110.94	123.59
11	b	1236	CLA	O2A-CGA-O1A	-5.01	110.94	123.59
11	1	1105	CLA	O2A-CGA-O1A	-5.01	110.94	123.59
11	b	1215	CLA	C4-C3-C5	5.01	123.70	115.27
11	b	1210	CLA	O2D-CGD-CBD	5.01	120.17	111.27
11	A	1129	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
11	A	1127	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
11	1	1128	CLA	O2D-CGD-CBD	5.01	120.17	111.27
11	2	1021	CLA	O2A-CGA-CBA	5.01	127.62	111.91
11	B	1211	CLA	O2D-CGD-CBD	5.00	120.16	111.27
11	B	1223	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
11	a	1116	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
11	1	1133	CLA	O2D-CGD-CBD	5.00	120.15	111.27
11	a	1123	CLA	O2A-CGA-O1A	-5.00	110.98	123.59
11	1	1132	CLA	O2D-CGD-CBD	5.00	120.15	111.27
11	2	1218	CLA	C4D-C3D-CAD	4.99	111.25	108.47
11	2	1231	CLA	C4D-C3D-CAD	4.99	111.25	108.47
11	1	1801	CLA	O2A-CGA-O1A	-4.99	110.99	123.59
11	2	1232	CLA	C4A-NA-C1A	4.99	108.95	106.71
11	2	1202	CLA	C4A-NA-C1A	4.99	108.95	106.71
11	B	1230	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
11	2	1201	CLA	O2D-CGD-CBD	4.99	120.13	111.27
14	2	4014	BCR	C15-C14-C13	-4.99	120.19	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1113	CLA	C4D-C3D-CAD	4.99	111.25	108.47
11	a	1128	CLA	O2D-CGD-CBD	4.99	120.13	111.27
11	A	1136	CLA	C4D-C3D-CAD	4.98	111.25	108.47
11	B	1219	CLA	O2A-CGA-O1A	-4.98	111.02	123.59
14	M	4021	BCR	C33-C5-C6	-4.98	118.93	124.53
11	a	1111	CLA	C4D-C3D-CAD	4.98	111.25	108.47
11	b	1228	CLA	O2A-CGA-O1A	-4.98	111.02	123.59
11	2	1226	CLA	O2A-CGA-O1A	-4.98	111.02	123.59
11	B	1201	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
11	b	1216	CLA	C4D-C3D-CAD	4.97	111.24	108.47
11	l	1503	CLA	O2A-CGA-O1A	-4.97	111.04	123.59
11	1	1138	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
11	b	1215	CLA	C4A-NA-C1A	4.97	108.94	106.71
11	a	1101	CLA	O2A-CGA-O1A	-4.97	111.04	123.59
11	1	1107	CLA	C4D-C3D-CAD	4.97	111.24	108.47
11	1	1117	CLA	O2D-CGD-CBD	4.97	120.09	111.27
14	m	4021	BCR	C33-C5-C6	-4.97	118.95	124.53
11	2	1223	CLA	O2A-CGA-O1A	-4.97	111.06	123.59
14	b	4009	BCR	C19-C18-C17	4.97	126.56	118.94
11	2	1217	CLA	C4D-C3D-CAD	4.96	111.24	108.47
11	A	1140	CLA	O2A-CGA-O1A	-4.96	111.06	123.59
11	b	1223	CLA	O2A-CGA-O1A	-4.96	111.07	123.59
11	A	1124	CLA	O2A-CGA-O1A	-4.96	111.07	123.59
11	K	1402	CLA	O2A-CGA-O1A	-4.96	111.07	123.59
11	A	1140	CLA	C4D-C3D-CAD	4.96	111.24	108.47
11	K	1402	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
11	2	1220	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
11	b	1202	CLA	O2A-CGA-O1A	-4.96	111.08	123.59
11	A	1140	CLA	O2A-C1-C2	4.96	121.66	108.64
14	b	4006	BCR	C7-C8-C9	-4.96	118.75	126.23
11	2	1023	CLA	O2D-CGD-CBD	4.96	120.08	111.27
14	6	4020	BCR	C24-C23-C22	-4.95	118.75	126.23
11	b	1207	CLA	C4D-C3D-CAD	4.95	111.23	108.47
14	M	4021	BCR	C7-C8-C9	-4.95	118.75	126.23
14	7	4021	BCR	C38-C26-C25	-4.95	118.97	124.53
11	b	1230	CLA	O2A-C1-C2	4.95	121.63	108.64
14	6	4020	BCR	C34-C9-C10	-4.94	116.00	122.92
11	A	1121	CLA	C4A-NA-C1A	4.94	108.93	106.71
11	2	1201	CLA	C4D-C3D-CAD	4.94	111.23	108.47
11	1	1127	CLA	C4D-C3D-CAD	4.94	111.23	108.47
11	a	1138	CLA	C4D-C3D-CAD	4.94	111.23	108.47
11	1	1117	CLA	O2A-CGA-O1A	-4.94	111.12	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1021	CLA	O2D-CGD-CBD	4.94	120.05	111.27
11	A	1128	CLA	O2D-CGD-CBD	4.94	120.05	111.27
11	2	1206	CLA	O2D-CGD-CBD	4.94	120.04	111.27
14	1	4002	BCR	C36-C18-C17	-4.94	116.00	122.92
11	b	1230	CLA	C1C-C2C-C3C	-4.94	101.77	106.96
11	2	1023	CLA	C4D-C3D-CAD	4.94	111.22	108.47
11	B	1218	CLA	C1C-C2C-C3C	-4.94	101.77	106.96
11	L	1503	CLA	O2A-CGA-O1A	-4.94	111.14	123.59
11	A	1022	CLA	C4A-NA-C1A	4.93	108.92	106.71
11	k	1402	CLA	C1C-C2C-C3C	-4.93	101.77	106.96
11	a	1022	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
11	b	1220	CLA	C1C-C2C-C3C	-4.93	101.77	106.96
11	A	1135	CLA	O2A-C1-C2	4.93	121.59	108.64
11	A	1107	CLA	O2D-CGD-CBD	4.93	120.03	111.27
11	a	1108	CLA	C4D-C3D-CAD	4.93	111.22	108.47
11	B	1226	CLA	C4D-C3D-CAD	4.93	111.22	108.47
11	A	1122	CLA	C4D-C3D-CAD	4.92	111.22	108.47
14	2	4014	BCR	C7-C8-C9	-4.92	118.80	126.23
14	B	4004	BCR	C7-C8-C9	-4.92	118.80	126.23
11	a	1801	CLA	C4A-NA-C1A	4.92	108.92	106.71
11	A	1124	CLA	O2D-CGD-CBD	4.92	120.01	111.27
11	a	1122	CLA	C1C-C2C-C3C	-4.92	101.79	106.96
11	1	1136	CLA	C4D-C3D-CAD	4.92	111.21	108.47
11	A	1104	CLA	C4D-C3D-CAD	4.92	111.21	108.47
11	a	1139	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
11	1	1126	CLA	C4-C3-C5	4.92	123.54	115.27
11	b	1221	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
11	B	1216	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
11	b	1013	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
11	a	1115	CLA	O2D-CGD-CBD	4.91	120.00	111.27
11	2	1210	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
11	B	1222	CLA	C4-C3-C5	4.91	123.53	115.27
11	b	1216	CLA	C4A-NA-C1A	4.91	108.91	106.71
11	a	1117	CLA	O2D-CGD-CBD	4.91	119.99	111.27
11	B	1215	CLA	O2A-CGA-O1A	-4.91	111.21	123.59
11	a	1237	CLA	O2A-CGA-O1A	-4.91	111.21	123.59
11	B	1236	CLA	O2A-CGA-O1A	-4.90	111.21	123.59
11	a	1111	CLA	O2A-CGA-O1A	-4.90	111.22	123.59
11	a	1140	CLA	O2A-CGA-O1A	-4.90	111.22	123.59
11	b	1217	CLA	O2D-CGD-CBD	4.90	119.98	111.27
11	A	1126	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
11	2	1203	CLA	O2A-CGA-O1A	-4.90	111.22	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1116	CLA	C4D-C3D-CAD	4.90	111.20	108.47
11	1	1126	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
11	1	1139	CLA	O2D-CGD-CBD	4.90	119.97	111.27
11	b	1220	CLA	O2D-CGD-CBD	4.90	119.97	111.27
11	a	1116	CLA	O2A-CGA-O1A	-4.90	111.23	123.59
11	2	1023	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
11	a	1124	CLA	C4A-NA-C1A	4.90	108.91	106.71
11	1	1104	CLA	O2A-CGA-O1A	-4.89	111.24	123.59
11	2	1216	CLA	C4D-C3D-CAD	4.89	111.20	108.47
14	6	4018	BCR	C7-C8-C9	-4.89	118.84	126.23
11	2	1212	CLA	O2D-CGD-CBD	4.89	119.96	111.27
11	2	1221	CLA	O2A-C1-C2	4.89	121.49	108.64
11	1	1136	CLA	C1C-C2C-C3C	-4.89	101.81	106.96
11	2	1239	CLA	C4D-C3D-CAD	4.89	111.20	108.47
11	A	1140	CLA	C1C-C2C-C3C	-4.89	101.81	106.96
11	a	1125	CLA	O2A-CGA-O1A	-4.89	111.25	123.59
11	a	1138	CLA	C1C-C2C-C3C	-4.89	101.82	106.96
11	B	1216	CLA	C4A-NA-C1A	4.89	108.90	106.71
11	A	1119	CLA	C4A-NA-C1A	4.89	108.90	106.71
11	2	1013	CLA	C1C-C2C-C3C	-4.89	101.82	106.96
11	a	1140	CLA	C4D-C3D-CAD	4.89	111.20	108.47
11	1	1113	CLA	C4D-C3D-CAD	4.89	111.20	108.47
14	1	4007	BCR	C24-C23-C22	-4.89	118.85	126.23
11	8	1503	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
11	1	1022	CLA	OBD-CAD-CBD	-4.89	118.91	125.89
14	B	4004	BCR	C33-C5-C6	-4.88	119.04	124.53
11	a	1111	CLA	O2A-C1-C2	4.88	121.47	108.64
11	2	1207	CLA	C4D-C3D-CAD	4.88	111.19	108.47
11	A	1117	CLA	CMB-C2B-C3B	4.88	133.81	124.68
11	A	1122	CLA	O2A-C1-C2	4.88	121.46	108.64
11	1	1122	CLA	O2A-CGA-O1A	-4.88	111.28	123.59
11	a	1119	CLA	O2A-C1-C2	4.88	121.45	108.64
11	a	1132	CLA	O2A-C1-C2	4.88	121.45	108.64
11	b	1213	CLA	C4D-C3D-CAD	4.88	111.19	108.47
11	A	1117	CLA	O2A-CGA-O1A	-4.87	111.29	123.59
11	b	1226	CLA	O2A-CGA-O1A	-4.87	111.29	123.59
11	A	1124	CLA	O2A-C1-C2	4.87	121.44	108.64
11	2	1228	CLA	C4D-C3D-CAD	4.87	111.19	108.47
16	2	5002	LMG	O7-C10-C11	4.87	122.00	111.50
11	b	1202	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
11	b	1210	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
11	2	1219	CLA	CMB-C2B-C3B	4.87	133.78	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1105	CLA	C4D-C3D-CAD	4.87	111.18	108.47
11	A	1105	CLA	O2D-CGD-CBD	4.87	119.92	111.27
14	a	4002	BCR	C7-C8-C9	-4.87	118.88	126.23
11	2	1213	CLA	O2A-CGA-O1A	-4.87	111.31	123.59
11	A	1101	CLA	C4D-C3D-CAD	4.87	111.18	108.47
11	A	1120	CLA	O2D-CGD-CBD	4.86	119.91	111.27
11	B	1229	CLA	C4D-C3D-CAD	4.86	111.18	108.47
11	A	1125	CLA	C4A-NA-C1A	4.86	108.89	106.71
11	A	1117	CLA	O2D-CGD-CBD	4.86	119.90	111.27
11	A	1134	CLA	C4D-C3D-CAD	4.86	111.18	108.47
11	B	1023	CLA	C1C-C2C-C3C	-4.86	101.85	106.96
11	B	1228	CLA	O2A-CGA-O1A	-4.86	111.33	123.59
11	1	1124	CLA	C4D-C3D-CAD	4.86	111.18	108.47
11	a	1801	CLA	C4D-C3D-CAD	4.85	111.18	108.47
11	1	1101	CLA	O2A-CGA-O1A	-4.85	111.34	123.59
11	A	1120	CLA	C4A-NA-C1A	4.85	108.89	106.71
11	2	1229	CLA	O2A-CGA-O1A	-4.85	111.35	123.59
11	A	1138	CLA	O2D-CGD-CBD	4.85	119.88	111.27
11	a	1111	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
11	A	1116	CLA	O2A-CGA-O1A	-4.85	111.36	123.59
11	A	1103	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
11	L	1502	CLA	C4D-C3D-CAD	4.84	111.17	108.47
11	a	1118	CLA	O2A-CGA-O1A	-4.84	111.37	123.59
11	B	1216	CLA	O2D-CGD-CBD	4.84	119.87	111.27
11	0	1401	CLA	O2D-CGD-CBD	4.84	119.87	111.27
11	a	1112	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
11	B	1235	CLA	O2A-CGA-O1A	-4.84	111.37	123.59
11	2	1228	CLA	O2D-CGD-CBD	4.84	119.87	111.27
11	B	1213	CLA	C4D-C3D-CAD	4.84	111.17	108.47
11	a	1111	CLA	O2D-CGD-CBD	4.84	119.86	111.27
11	B	1222	CLA	CMB-C2B-C3B	4.83	133.72	124.68
11	B	1013	CLA	O2D-CGD-CBD	4.83	119.85	111.27
11	K	1401	CLA	O2D-CGD-CBD	4.83	119.85	111.27
11	2	1223	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
11	a	1112	CLA	C4D-C3D-CAD	4.83	111.16	108.47
11	B	1207	CLA	O2A-CGA-CBA	4.83	127.05	111.91
14	A	4002	BCR	C33-C5-C6	-4.83	119.11	124.53
11	2	1021	CLA	O2A-CGA-O1A	-4.83	111.41	123.59
11	k	1401	CLA	O2D-CGD-CBD	4.82	119.84	111.27
11	2	1207	CLA	O2D-CGD-CBD	4.82	119.84	111.27
11	2	1202	CLA	C4D-C3D-CAD	4.82	111.16	108.47
11	A	1121	CLA	C4D-C3D-CAD	4.82	111.16	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4004	BCR	C7-C8-C9	-4.82	118.95	126.23
14	2	4004	BCR	C33-C5-C6	-4.82	119.11	124.53
11	b	1201	CLA	C4D-C3D-CAD	4.82	111.16	108.47
11	B	1229	CLA	O2D-CGD-CBD	4.82	119.83	111.27
11	A	1237	CLA	O2A-CGA-O1A	-4.82	111.44	123.59
11	B	1231	CLA	C4D-C3D-CAD	4.82	111.16	108.47
11	2	1214	CLA	C4D-C3D-CAD	4.81	111.16	108.47
11	B	1223	CLA	O2A-CGA-O1A	-4.81	111.45	123.59
14	A	4008	BCR	C24-C23-C22	-4.81	118.96	126.23
14	b	4014	BCR	C7-C8-C9	-4.81	118.96	126.23
11	B	1021	CLA	O2A-CGA-CBA	4.81	127.01	111.91
11	A	1106	CLA	O2A-CGA-O1A	-4.81	111.45	123.59
11	A	1104	CLA	O2A-C1-C2	4.81	121.27	108.64
11	b	1213	CLA	O2A-CGA-O1A	-4.81	111.46	123.59
14	B	4010	BCR	C33-C5-C6	-4.81	119.13	124.53
11	2	1217	CLA	O2A-CGA-O1A	-4.80	111.47	123.59
11	2	1201	CLA	O2A-CGA-O1A	-4.80	111.47	123.59
11	B	1210	CLA	C4D-C3D-CAD	4.80	111.15	108.47
11	a	1116	CLA	C4D-C3D-CAD	4.80	111.15	108.47
11	A	1022	CLA	O2A-CGA-O1A	-4.80	111.48	123.59
14	A	4008	BCR	C33-C5-C6	-4.80	119.14	124.53
11	2	1222	CLA	C4D-C3D-CAD	4.80	111.14	108.47
11	A	1125	CLA	O2A-CGA-O1A	-4.80	111.49	123.59
11	2	1230	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
11	b	1234	CLA	O2D-CGD-CBD	4.79	119.78	111.27
11	b	1238	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
14	a	4007	BCR	C33-C5-C6	-4.79	119.15	124.53
11	2	1206	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
11	1	1106	CLA	O2A-C1-C2	4.79	121.22	108.64
11	A	1112	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
11	b	1207	CLA	O2A-CGA-CBA	4.79	126.92	111.91
11	B	1221	CLA	O2A-CGA-O1A	-4.78	111.52	123.59
11	a	1130	CLA	C4A-NA-C1A	4.78	108.86	106.71
14	2	4011	BCR	C34-C9-C10	-4.78	116.22	122.92
11	A	1132	CLA	C4D-C3D-CAD	4.78	111.13	108.47
11	a	1126	CLA	C1C-C2C-C3C	-4.78	101.94	106.96
11	a	1118	CLA	O2A-C1-C2	4.78	121.19	108.64
11	2	1221	CLA	C4D-C3D-CAD	4.77	111.13	108.47
11	B	1013	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
11	a	1121	CLA	O2D-CGD-CBD	4.77	119.75	111.27
11	2	1235	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
11	B	1214	CLA	C1C-C2C-C3C	-4.77	101.94	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1106	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
11	A	1123	CLA	O2A-C1-C2	4.77	121.17	108.64
11	B	1208	CLA	O2D-CGD-CBD	4.77	119.74	111.27
11	a	1117	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
11	a	1135	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
11	1	1114	CLA	C4D-C3D-CAD	4.77	111.13	108.47
11	b	1204	CLA	C4D-C3D-CAD	4.77	111.13	108.47
14	A	4002	BCR	C24-C23-C22	-4.77	119.03	126.23
11	k	1402	CLA	O2A-C1-C2	4.76	121.15	108.64
11	a	1113	CLA	O2D-CGD-CBD	4.76	119.73	111.27
14	F	4020	BCR	C33-C5-C6	-4.76	119.18	124.53
11	1	1106	CLA	C4D-C3D-CAD	4.76	111.12	108.47
11	B	1229	CLA	O2A-C1-C2	4.76	121.14	108.64
11	1	1118	CLA	O2A-CGA-O1A	-4.76	111.58	123.59
11	B	1234	CLA	C4D-C3D-CAD	4.75	111.12	108.47
11	2	1206	CLA	C4D-C3D-CAD	4.75	111.12	108.47
11	2	1207	CLA	O2A-CGA-CBA	4.75	126.82	111.91
11	a	1139	CLA	O2D-CGD-CBD	4.75	119.71	111.27
11	A	1139	CLA	O2A-CGA-O1A	-4.75	111.60	123.59
11	1	1126	CLA	O2A-CGA-O1A	-4.75	111.60	123.59
11	A	1116	CLA	C4D-C3D-CAD	4.75	111.12	108.47
14	A	4008	BCR	C7-C8-C9	-4.75	119.06	126.23
14	F	4018	BCR	C7-C8-C9	-4.75	119.06	126.23
14	2	4006	BCR	C1-C6-C5	-4.75	115.93	122.61
11	2	1209	CLA	O2D-CGD-CBD	4.74	119.70	111.27
11	B	1213	CLA	O2A-CGA-O1A	-4.74	111.62	123.59
11	A	1105	CLA	O2A-CGA-O1A	-4.74	111.62	123.59
11	b	1205	CLA	O2A-C1-C2	4.74	121.10	108.64
11	b	1223	CLA	O2A-C1-C2	4.74	121.10	108.64
11	1	1124	CLA	O2A-C1-C2	4.74	121.09	108.64
11	b	1216	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
11	2	1215	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
11	8	1502	CLA	C4D-C3D-CAD	4.74	111.11	108.47
11	2	1209	CLA	C4D-C3D-CAD	4.74	111.11	108.47
11	a	1103	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
14	b	4010	BCR	C7-C8-C9	-4.74	119.07	126.23
11	a	1126	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
11	1	1111	CLA	C4D-C3D-CAD	4.74	111.11	108.47
11	a	1115	CLA	C4D-C3D-CAD	4.73	111.11	108.47
11	a	1131	CLA	O2A-CGA-O1A	-4.73	111.64	123.59
11	b	1214	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
11	B	1202	CLA	CMB-C2B-C3B	4.73	133.53	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1138	CLA	O2D-CGD-CBD	4.73	119.68	111.27
11	b	1207	CLA	O2D-CGD-CBD	4.73	119.67	111.27
11	A	1128	CLA	O2A-CGA-O1A	-4.73	111.66	123.59
11	b	1209	CLA	C4D-C3D-CAD	4.73	111.11	108.47
11	K	1402	CLA	C4D-C3D-CAD	4.73	111.11	108.47
11	a	1110	CLA	O2A-CGA-O1A	-4.72	111.67	123.59
11	b	1222	CLA	C4D-C3D-CAD	4.72	111.10	108.47
11	B	1217	CLA	O2D-CGD-CBD	4.72	119.66	111.27
11	a	1135	CLA	O2A-C1-C2	4.72	121.04	108.64
11	A	1132	CLA	O2A-CGA-O1A	-4.72	111.68	123.59
11	b	1224	CLA	C4D-C3D-CAD	4.72	111.10	108.47
11	2	1219	CLA	O2A-CGA-O1A	-4.72	111.69	123.59
14	f	4020	BCR	C7-C8-C9	-4.71	119.11	126.23
11	b	1221	CLA	O2A-CGA-O1A	-4.71	111.70	123.59
14	b	4010	BCR	C38-C26-C25	-4.71	119.24	124.53
11	a	1114	CLA	O2D-CGD-CBD	4.71	119.64	111.27
11	A	1237	CLA	C4D-C3D-CAD	4.71	111.10	108.47
11	a	1107	CLA	O2D-CGD-CBD	4.71	119.64	111.27
11	1	1140	CLA	O2D-CGD-CBD	4.71	119.64	111.27
11	a	1103	CLA	O2D-CGD-CBD	4.71	119.63	111.27
14	f	4018	BCR	C7-C8-C9	-4.70	119.13	126.23
11	a	1126	CLA	O2A-C1-C2	4.70	120.99	108.64
14	F	4013	BCR	C24-C23-C22	-4.70	119.13	126.23
11	A	1115	CLA	C4D-C3D-CAD	4.70	111.09	108.47
11	A	1119	CLA	O2D-CGD-CBD	4.70	119.62	111.27
11	2	1236	CLA	C4D-C3D-CAD	4.70	111.09	108.47
11	b	1227	CLA	C4D-C3D-CAD	4.70	111.09	108.47
14	1	4007	BCR	C33-C5-C6	-4.70	119.25	124.53
11	A	1117	CLA	O2A-C1-C2	4.69	120.97	108.64
11	a	1110	CLA	C4D-C3D-CAD	4.69	111.09	108.47
11	b	1235	CLA	C4D-C3D-CAD	4.69	111.09	108.47
14	a	4002	BCR	C33-C5-C6	-4.69	119.26	124.53
11	1	1012	CLA	O2A-CGA-CBA	4.69	126.63	111.91
11	A	1022	CLA	O2D-CGD-CBD	4.69	119.61	111.27
11	l	1501	CLA	C4D-C3D-CAD	4.69	111.09	108.47
11	A	1116	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
11	B	1210	CLA	O2D-CGD-CBD	4.69	119.60	111.27
11	B	1238	CLA	C4D-C3D-CAD	4.69	111.08	108.47
11	L	1501	CLA	O2D-CGD-CBD	4.69	119.60	111.27
11	B	1225	CLA	O2A-CGA-O1A	-4.69	111.76	123.59
11	2	1203	CLA	C4D-C3D-CAD	4.68	111.08	108.47
11	1	1022	CLA	C4A-NA-C1A	4.68	108.81	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1128	CLA	O2A-CGA-O1A	-4.68	111.78	123.59
11	A	1135	CLA	C4D-C3D-CAD	4.68	111.08	108.47
11	L	1501	CLA	C4D-C3D-CAD	4.68	111.08	108.47
11	2	1225	CLA	O2A-CGA-O1A	-4.68	111.79	123.59
11	B	1205	CLA	C4D-C3D-CAD	4.68	111.08	108.47
11	a	1135	CLA	C4D-C3D-CAD	4.68	111.08	108.47
11	b	1230	CLA	C4-C3-C5	4.67	123.13	115.27
11	A	1121	CLA	O2D-CGD-CBD	4.67	119.57	111.27
11	1	1127	CLA	O2A-C1-C2	4.67	120.91	108.64
14	B	4005	BCR	C7-C8-C9	-4.67	119.18	126.23
11	b	1211	CLA	C4D-C3D-CAD	4.67	111.08	108.47
11	B	1203	CLA	O2A-CGA-O1A	-4.67	111.81	123.59
11	1	1123	CLA	O2A-CGA-O1A	-4.67	111.81	123.59
11	b	1013	CLA	O2D-CGD-CBD	4.67	119.56	111.27
11	b	1208	CLA	C4D-C3D-CAD	4.67	111.07	108.47
11	a	1102	CLA	O2D-CGD-CBD	4.67	119.56	111.27
11	2	1223	CLA	O2A-C1-C2	4.66	120.89	108.64
11	1	1108	CLA	C4D-C3D-CAD	4.66	111.07	108.47
11	1	1237	CLA	C4D-C3D-CAD	4.66	111.07	108.47
11	B	1021	CLA	C4D-C3D-CAD	4.66	111.07	108.47
11	1	1122	CLA	O2D-CGD-CBD	4.66	119.55	111.27
11	a	1127	CLA	O2A-C1-C2	4.66	120.88	108.64
11	b	1236	CLA	C4D-C3D-CAD	4.66	111.07	108.47
14	8	4019	BCR	C15-C14-C13	-4.65	120.67	127.31
11	1	1125	CLA	C1C-C2C-C3C	-4.65	102.06	106.96
11	2	1213	CLA	O2A-C1-C2	4.65	120.87	108.64
11	A	1801	CLA	C4D-C3D-CAD	4.65	111.06	108.47
11	A	1111	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
11	1	1012	CLA	C4-C3-C5	4.65	123.09	115.27
11	a	1129	CLA	C4D-C3D-CAD	4.65	111.06	108.47
11	B	1202	CLA	C4D-C3D-CAD	4.65	111.06	108.47
15	B	5004	LHG	O7-C7-C8	4.65	121.51	111.50
11	0	1402	CLA	O2D-CGD-CBD	4.64	119.52	111.27
11	b	1223	CLA	O2D-CGD-CBD	4.64	119.52	111.27
11	a	1115	CLA	C1C-C2C-C3C	-4.64	102.07	106.96
11	b	1215	CLA	C4D-C3D-CAD	4.64	111.06	108.47
11	l	1502	CLA	C4D-C3D-CAD	4.64	111.06	108.47
11	b	1226	CLA	C4D-C3D-CAD	4.64	111.06	108.47
11	a	1128	CLA	C4D-C3D-CAD	4.64	111.06	108.47
11	1	1107	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
11	B	1229	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
11	a	1106	CLA	C4D-C3D-CAD	4.64	111.06	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1239	CLA	C4D-C3D-CAD	4.63	111.05	108.47
11	1	1121	CLA	O2D-CGD-CBD	4.63	119.50	111.27
14	b	4005	BCR	C24-C23-C22	-4.63	119.23	126.23
11	1	1109	CLA	C4-C3-C5	4.63	123.06	115.27
11	a	1012	CLA	OBD-CAD-CBD	-4.63	119.28	125.89
11	A	1108	CLA	C4D-C3D-CAD	4.63	111.05	108.47
11	a	1011	CLA	O2A-CGA-CBA	4.63	126.43	111.91
11	1	1135	CLA	O2A-CGA-O1A	-4.63	111.91	123.59
11	1	1113	CLA	O2D-CGD-CBD	4.63	119.49	111.27
11	B	1214	CLA	O2A-C1-C2	4.63	120.80	108.64
11	B	1218	CLA	C4D-C3D-CAD	4.63	111.05	108.47
11	a	1120	CLA	C4D-C3D-CAD	4.62	111.05	108.47
11	1	1115	CLA	C4D-C3D-CAD	4.62	111.05	108.47
11	1	1117	CLA	O2A-C1-C2	4.62	120.78	108.64
11	1	1128	CLA	O2A-CGA-O1A	-4.62	111.93	123.59
11	1	1138	CLA	C4D-C3D-CAD	4.62	111.05	108.47
11	2	1202	CLA	O2D-CGD-CBD	4.62	119.47	111.27
11	b	1231	CLA	C4D-C3D-CAD	4.62	111.04	108.47
11	1	1121	CLA	C4D-C3D-CAD	4.62	111.04	108.47
11	a	1113	CLA	C4D-C3D-CAD	4.61	111.04	108.47
11	1	1131	CLA	O2A-CGA-O1A	-4.61	111.95	123.59
11	2	1220	CLA	CAC-C3C-C4C	4.61	130.79	124.81
11	a	1107	CLA	O2A-CGA-O1A	-4.61	111.96	123.59
11	B	1204	CLA	O2A-CGA-O1A	-4.61	111.96	123.59
11	A	1113	CLA	O2D-CGD-CBD	4.61	119.45	111.27
11	A	1126	CLA	O2A-C1-C2	4.61	120.74	108.64
11	1	1112	CLA	C4D-C3D-CAD	4.60	111.04	108.47
11	A	1801	CLA	O2A-CGA-CBA	4.60	126.35	111.91
11	A	1129	CLA	O2D-CGD-CBD	4.60	119.44	111.27
11	a	1801	CLA	O2A-CGA-CBA	4.60	126.34	111.91
14	A	4002	BCR	C38-C26-C25	-4.60	119.36	124.53
11	A	1127	CLA	C4D-C3D-CAD	4.60	111.03	108.47
11	2	1207	CLA	O2A-C1-C2	4.60	120.71	108.64
11	b	1222	CLA	C4-C3-C5	4.60	123.00	115.27
11	2	1221	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
11	a	1108	CLA	O2D-CGD-CBD	4.59	119.43	111.27
11	A	1137	CLA	O2A-C1-C2	4.59	120.70	108.64
11	A	1134	CLA	O2D-CGD-CBD	4.59	119.43	111.27
11	b	1213	CLA	C4-C3-C5	4.59	122.99	115.27
11	b	1206	CLA	O2D-CGD-CBD	4.59	119.42	111.27
11	A	1022	CLA	C4D-C3D-CAD	4.59	111.03	108.47
11	B	1206	CLA	O2A-CGA-O1A	-4.59	112.01	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1230	CLA	O2A-CGA-O1A	-4.59	112.01	123.59
11	a	1012	CLA	O2A-C1-C2	4.59	120.69	108.64
11	B	1217	CLA	O2A-CGA-CBA	4.58	126.30	111.91
11	k	1402	CLA	O2D-CGD-CBD	4.58	119.41	111.27
11	1	1125	CLA	O2A-CGA-O1A	-4.58	112.02	123.59
11	A	1126	CLA	O2A-CGA-O1A	-4.58	112.02	123.59
11	A	1012	CLA	O2A-CGA-CBA	4.58	126.29	111.91
11	b	1228	CLA	O2A-C1-C2	4.58	120.68	108.64
11	2	1218	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
11	2	1013	CLA	O2D-CGD-CBD	4.58	119.41	111.27
11	0	1402	CLA	C4D-C3D-CAD	4.58	111.02	108.47
11	B	1228	CLA	O2A-C1-C2	4.58	120.67	108.64
11	A	1109	CLA	C4D-C3D-CAD	4.57	111.02	108.47
14	f	4013	BCR	C38-C26-C25	-4.57	119.40	124.53
11	2	1204	CLA	O2A-CGA-O1A	-4.57	112.06	123.59
15	A	5003	LHG	O7-C7-C8	4.57	121.35	111.50
14	A	4007	BCR	C38-C26-C25	-4.57	119.40	124.53
11	A	1011	CLA	O2A-CGA-CBA	4.57	126.24	111.91
11	B	1239	CLA	C4D-C3D-CAD	4.57	111.02	108.47
11	2	1211	CLA	C4D-C3D-CAD	4.56	111.01	108.47
11	a	1140	CLA	O2A-C1-C2	4.56	120.62	108.64
11	b	1219	CLA	O2D-CGD-CBD	4.56	119.37	111.27
14	1	4002	BCR	C24-C23-C22	-4.56	119.35	126.23
11	b	1224	CLA	O2A-C1-C2	4.55	120.60	108.64
11	2	1232	CLA	C4D-C3D-CAD	4.55	111.01	108.47
11	b	1204	CLA	O2A-CGA-O1A	-4.55	112.10	123.59
11	b	1223	CLA	C4D-C3D-CAD	4.55	111.01	108.47
11	2	1021	CLA	C4D-C3D-CAD	4.55	111.01	108.47
11	a	1125	CLA	O2D-CGD-CBD	4.55	119.35	111.27
11	a	1103	CLA	C4D-C3D-CAD	4.55	111.01	108.47
11	a	1123	CLA	C4D-C3D-CAD	4.55	111.01	108.47
11	A	1126	CLA	C4D-C3D-CAD	4.55	111.00	108.47
11	1	1108	CLA	O2D-CGD-CBD	4.55	119.34	111.27
14	1	4008	BCR	C33-C5-C6	-4.55	119.42	124.53
11	1	1127	CLA	O2D-CGD-CBD	4.54	119.34	111.27
11	1	1133	CLA	C4D-C3D-CAD	4.54	111.00	108.47
11	2	1202	CLA	O2A-C1-C2	4.54	120.56	108.64
11	2	1234	CLA	O2A-C1-C2	4.54	120.56	108.64
11	1	1237	CLA	O2A-CGA-O1A	-4.54	112.14	123.59
11	B	1221	CLA	O2A-C1-C2	4.54	120.56	108.64
11	b	1219	CLA	CMB-C2B-C3B	4.54	133.16	124.68
11	A	1125	CLA	C4D-C3D-CAD	4.53	111.00	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1127	CLA	O2D-CGD-CBD	4.53	119.32	111.27
14	1	4002	BCR	C7-C8-C9	-4.53	119.39	126.23
14	2	4010	BCR	C7-C8-C9	-4.53	119.39	126.23
11	a	1107	CLA	C4-C3-C5	4.53	122.89	115.27
11	K	1402	CLA	O2D-CGD-CBD	4.53	119.31	111.27
11	B	1217	CLA	C4D-C3D-CAD	4.53	111.00	108.47
11	1	1122	CLA	C4D-C3D-CAD	4.53	111.00	108.47
11	B	1201	CLA	O2A-C1-C2	4.53	120.53	108.64
11	2	1208	CLA	O2D-CGD-CBD	4.53	119.31	111.27
11	k	1402	CLA	C4D-C3D-CAD	4.53	110.99	108.47
11	1	1109	CLA	O2D-CGD-CBD	4.53	119.31	111.27
14	l	4019	BCR	C15-C14-C13	-4.53	120.85	127.31
14	F	4013	BCR	C7-C8-C9	-4.52	119.40	126.23
14	A	4007	BCR	C33-C5-C6	-4.52	119.45	124.53
11	B	1227	CLA	C4D-C3D-CAD	4.52	110.99	108.47
11	2	1224	CLA	O2A-CGA-CBA	4.52	126.09	111.91
14	8	4019	BCR	C33-C5-C6	-4.52	119.45	124.53
14	B	4010	BCR	C7-C8-C9	-4.51	119.41	126.23
11	A	1123	CLA	O2A-CGA-O1A	-4.51	112.20	123.59
11	8	1501	CLA	C4D-C3D-CAD	4.51	110.98	108.47
11	b	1234	CLA	O2A-C1-C2	4.51	120.49	108.64
11	2	1240	CLA	O2D-CGD-CBD	4.51	119.28	111.27
11	1	1132	CLA	O2A-CGA-O1A	-4.51	112.22	123.59
11	b	1218	CLA	C4D-C3D-CAD	4.50	110.98	108.47
11	A	1114	CLA	C4D-C3D-CAD	4.50	110.98	108.47
14	6	4013	BCR	C38-C26-C25	-4.50	119.47	124.53
11	b	1235	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
11	b	1210	CLA	C4D-C3D-CAD	4.50	110.98	108.47
14	f	4020	BCR	C33-C5-C6	-4.50	119.47	124.53
11	1	1130	CLA	C4A-NA-C1A	4.50	108.73	106.71
11	A	1109	CLA	O2D-CGD-CBD	4.50	119.26	111.27
11	A	1131	CLA	O2A-C1-C2	4.50	120.46	108.64
11	B	1201	CLA	O2A-CGA-O1A	-4.50	112.24	123.59
11	b	1235	CLA	O2A-C1-C2	4.50	120.45	108.64
11	b	1220	CLA	C4D-C3D-CAD	4.49	110.98	108.47
11	B	1230	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
11	a	1105	CLA	C4D-C3D-CAD	4.49	110.97	108.47
11	1	1124	CLA	O2D-CGD-CBD	4.49	119.25	111.27
14	2	4010	BCR	C37-C22-C21	-4.49	116.64	122.92
11	b	1214	CLA	O2A-C1-C2	4.49	120.43	108.64
11	1	1137	CLA	C4-C3-C5	4.49	122.82	115.27
11	B	1235	CLA	C4D-C3D-CAD	4.48	110.97	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1103	CLA	O2A-CGA-O1A	-4.48	112.27	123.59
14	2	4010	BCR	C38-C26-C25	-4.48	119.49	124.53
11	b	1234	CLA	C4D-C3D-CAD	4.48	110.97	108.47
11	a	1137	CLA	O2A-C1-C2	4.48	120.41	108.64
14	b	4010	BCR	C33-C5-C6	-4.48	119.50	124.53
11	b	1214	CLA	O2A-CGA-O1A	-4.48	112.29	123.59
11	A	1119	CLA	O2A-CGA-O1A	-4.48	112.29	123.59
11	K	1401	CLA	O2A-CGA-CBA	4.48	125.96	111.91
11	0	1401	CLA	O2A-CGA-CBA	4.48	125.96	111.91
11	a	1103	CLA	O2A-C1-C2	4.48	120.40	108.64
11	2	1227	CLA	C4D-C3D-CAD	4.48	110.97	108.47
11	2	1210	CLA	C4D-C3D-CAD	4.48	110.97	108.47
11	a	1105	CLA	O2A-CGA-CBA	4.48	125.95	111.91
11	b	1225	CLA	O2A-CGA-O1A	-4.48	112.30	123.59
11	a	1011	CLA	CMB-C2B-C3B	4.47	133.05	124.68
11	k	1401	CLA	O2A-CGA-CBA	4.47	125.95	111.91
11	2	1238	CLA	O2A-CGA-O1A	-4.47	112.30	123.59
11	2	1235	CLA	C4D-C3D-CAD	4.47	110.96	108.47
11	1	1140	CLA	C4D-C3D-CAD	4.47	110.96	108.47
11	b	1229	CLA	C4D-C3D-CAD	4.47	110.96	108.47
11	A	1119	CLA	O2A-C1-C2	4.47	120.37	108.64
11	1	1111	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
11	1	1801	CLA	O2A-C1-C2	4.47	120.37	108.64
11	2	1229	CLA	C4D-C3D-CAD	4.46	110.96	108.47
14	1	4008	BCR	C34-C9-C10	-4.46	116.67	122.92
11	2	1203	CLA	O2A-C1-C2	4.46	120.36	108.64
11	b	1210	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
11	B	1205	CLA	O2A-C1-C2	4.46	120.36	108.64
11	a	1132	CLA	O2A-CGA-O1A	-4.46	112.33	123.59
11	B	1223	CLA	O2A-C1-C2	4.46	120.35	108.64
11	B	1214	CLA	C4-C3-C5	4.46	122.77	115.27
11	a	1117	CLA	O2A-C1-C2	4.46	120.35	108.64
11	A	1131	CLA	O2A-CGA-O1A	-4.46	112.35	123.59
11	a	1114	CLA	C4D-C3D-CAD	4.45	110.95	108.47
11	A	1012	CLA	O2A-C1-C2	4.45	120.34	108.64
11	2	1214	CLA	O2A-CGA-O1A	-4.45	112.36	123.59
11	A	1119	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
11	1	1137	CLA	O2A-CGA-CBA	4.45	125.88	111.91
11	b	1238	CLA	C4D-C3D-CAD	4.45	110.95	108.47
16	b	5002	LMG	O7-C10-C11	4.45	121.08	111.50
11	A	1137	CLA	O2A-CGA-CBA	4.45	125.86	111.91
11	B	1240	CLA	C4D-C3D-CAD	4.45	110.95	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	0	1401	CLA	O2A-C1-C2	4.44	120.32	108.64
11	K	1401	CLA	O2A-C1-C2	4.44	120.31	108.64
11	b	1217	CLA	O2A-CGA-CBA	4.44	125.84	111.91
11	k	1401	CLA	O2A-C1-C2	4.44	120.31	108.64
11	A	1022	CLA	O2A-C1-C2	4.44	120.31	108.64
14	6	4013	BCR	C33-C5-C6	-4.44	119.54	124.53
11	1	1135	CLA	O2A-C1-C2	4.44	120.30	108.64
14	L	4019	BCR	C33-C5-C6	-4.44	119.54	124.53
11	a	1022	CLA	O2D-CGD-CBD	4.44	119.16	111.27
11	a	1123	CLA	O2A-C1-C2	4.44	120.30	108.64
15	A	5001	LHG	O7-C7-C8	4.43	121.05	111.50
14	a	4003	BCR	C7-C8-C9	-4.43	119.54	126.23
11	1	1132	CLA	C4D-C3D-CAD	4.43	110.94	108.47
11	B	1238	CLA	O2A-CGA-O1A	-4.43	112.41	123.59
11	K	1402	CLA	O2A-C1-C2	4.43	120.28	108.64
11	A	1117	CLA	C4A-NA-C1A	4.43	108.70	106.71
11	a	1106	CLA	O2A-C1-C2	4.43	120.27	108.64
11	2	1023	CLA	O2A-CGA-CBA	4.43	125.80	111.91
11	B	1216	CLA	C4D-C3D-CAD	4.43	110.94	108.47
11	b	1230	CLA	O2A-CGA-CBA	4.42	125.79	111.91
11	B	1222	CLA	O2A-C1-C2	4.42	120.26	108.64
11	a	1124	CLA	C4D-C3D-CAD	4.42	110.94	108.47
11	b	1229	CLA	O2D-CGD-CBD	4.42	119.13	111.27
11	B	1234	CLA	O2A-CGA-CBA	4.42	125.78	111.91
11	a	1109	CLA	O2D-CGD-CBD	4.42	119.12	111.27
11	1	1102	CLA	C4D-C3D-CAD	4.42	110.93	108.47
14	a	4002	BCR	C24-C23-C22	-4.42	119.56	126.23
11	A	1137	CLA	CMB-C2B-C3B	4.42	132.94	124.68
11	b	1221	CLA	O2A-C1-C2	4.42	120.24	108.64
11	A	1122	CLA	O2A-CGA-CBA	4.42	125.77	111.91
11	a	1126	CLA	C4D-C3D-CAD	4.42	110.93	108.47
11	A	1012	CLA	C4-C3-C5	4.41	122.70	115.27
11	A	1111	CLA	O2A-C1-C2	4.41	120.23	108.64
14	2	4006	BCR	C38-C26-C25	-4.41	119.57	124.53
11	b	1219	CLA	C4D-C3D-CAD	4.41	110.93	108.47
11	2	1214	CLA	O2A-C1-C2	4.41	120.23	108.64
11	B	1219	CLA	O2D-CGD-CBD	4.41	119.10	111.27
11	1	1122	CLA	O2A-C1-C2	4.41	120.22	108.64
11	b	1205	CLA	C4D-C3D-CAD	4.41	110.93	108.47
11	A	1139	CLA	O2D-CGD-CBD	4.41	119.10	111.27
11	a	1102	CLA	C4D-C3D-CAD	4.40	110.92	108.47
11	B	1234	CLA	O2D-CGD-CBD	4.40	119.09	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1210	CLA	O2A-C1-C2	4.40	120.20	108.64
11	A	1109	CLA	O2A-CGA-CBA	4.40	125.72	111.91
11	A	1114	CLA	O2D-CGD-CBD	4.40	119.08	111.27
11	B	1013	CLA	O2A-CGA-CBA	4.40	125.71	111.91
14	2	4017	BCR	C19-C18-C17	4.40	125.69	118.94
11	A	1139	CLA	O2A-C1-C2	4.40	120.19	108.64
11	b	1229	CLA	O2A-CGA-O1A	-4.40	112.49	123.59
11	B	1224	CLA	O2A-CGA-CBA	4.40	125.71	111.91
11	a	1133	CLA	C4D-C3D-CAD	4.39	110.92	108.47
11	b	1023	CLA	O2D-CGD-CBD	4.39	119.07	111.27
11	b	1221	CLA	C4D-C3D-CAD	4.39	110.92	108.47
11	k	1401	CLA	C4D-C3D-CAD	4.39	110.92	108.47
11	1	1127	CLA	C4A-NA-C1A	4.39	108.68	106.71
14	F	4013	BCR	C38-C26-C25	-4.38	119.60	124.53
11	2	1222	CLA	O2A-C1-C2	4.38	120.16	108.64
11	b	1201	CLA	CMB-C2B-C3B	4.38	132.88	124.68
11	A	1133	CLA	C4D-C3D-CAD	4.38	110.91	108.47
11	0	1401	CLA	C4D-C3D-CAD	4.38	110.91	108.47
14	6	4020	BCR	C33-C5-C6	-4.38	119.61	124.53
11	1	1109	CLA	O2A-CGA-CBA	4.38	125.65	111.91
11	2	1220	CLA	C4D-C3D-CAD	4.38	110.91	108.47
11	A	1128	CLA	C4D-C3D-CAD	4.38	110.91	108.47
11	A	1106	CLA	O2A-C1-C2	4.37	120.13	108.64
14	A	4001	BCR	C15-C14-C13	-4.37	121.07	127.31
11	b	1206	CLA	O2A-CGA-O1A	-4.37	112.55	123.59
11	1	1137	CLA	C4D-C3D-CAD	4.37	110.91	108.47
11	B	1228	CLA	C4D-C3D-CAD	4.37	110.91	108.47
14	1	4002	BCR	C19-C18-C17	4.37	125.65	118.94
11	b	1231	CLA	O2D-CGD-CBD	4.37	119.03	111.27
11	a	1139	CLA	O2A-C1-C2	4.37	120.12	108.64
11	2	1238	CLA	C4D-C3D-CAD	4.37	110.91	108.47
14	6	4013	BCR	C24-C23-C22	-4.37	119.64	126.23
11	1	1106	CLA	O2D-CGD-CBD	4.37	119.03	111.27
11	B	1013	CLA	C4D-C3D-CAD	4.36	110.90	108.47
11	a	1102	CLA	O2A-CGA-CBA	4.36	125.60	111.91
11	a	1124	CLA	O2A-C1-C2	4.36	120.09	108.64
11	K	1401	CLA	C4D-C3D-CAD	4.36	110.90	108.47
11	1	1104	CLA	C4D-C3D-CAD	4.36	110.90	108.47
11	a	1122	CLA	O2A-CGA-CBA	4.35	125.57	111.91
11	2	1216	CLA	O2A-CGA-CBA	4.35	125.57	111.91
11	A	1110	CLA	C4D-C3D-CAD	4.35	110.90	108.47
11	A	1102	CLA	O2A-CGA-CBA	4.35	125.56	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1214	CLA	C4D-C3D-CAD	4.35	110.90	108.47
11	b	1236	CLA	O2A-CGA-CBA	4.35	125.56	111.91
11	2	1210	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
11	b	1210	CLA	O2A-C1-C2	4.35	120.06	108.64
14	2	4017	BCR	C24-C23-C22	-4.34	119.67	126.23
11	1	1125	CLA	C4D-C3D-CAD	4.34	110.89	108.47
11	b	1234	CLA	O2A-CGA-CBA	4.34	125.53	111.91
14	1	4001	BCR	C24-C23-C22	-4.34	119.68	126.23
11	a	1104	CLA	C4D-C3D-CAD	4.34	110.89	108.47
14	b	4014	BCR	C15-C14-C13	-4.34	121.12	127.31
11	b	1224	CLA	O2A-CGA-CBA	4.33	125.51	111.91
11	2	1210	CLA	O2A-C1-C2	4.33	120.01	108.64
11	B	1240	CLA	O2D-CGD-CBD	4.33	118.96	111.27
11	2	1013	CLA	O2A-CGA-CBA	4.33	125.49	111.91
11	B	1223	CLA	OBD-CAD-C3D	-4.33	120.80	127.98
11	1	1111	CLA	O2A-CGA-CBA	4.33	125.49	111.91
11	b	1206	CLA	O2A-C1-C2	4.33	120.01	108.64
11	A	1103	CLA	O2D-CGD-CBD	4.32	118.95	111.27
11	b	1228	CLA	C4D-C3D-CAD	4.32	110.88	108.47
11	a	1022	CLA	O2A-C1-C2	4.32	119.99	108.64
11	A	1126	CLA	C4-C3-C5	4.32	122.54	115.27
11	1	1022	CLA	O2A-C1-C2	4.32	119.99	108.64
11	A	1111	CLA	C4D-C3D-CAD	4.32	110.88	108.47
11	a	1109	CLA	C4-C3-C5	4.32	122.53	115.27
11	a	1137	CLA	O2A-CGA-CBA	4.32	125.45	111.91
11	b	1021	CLA	C4D-C3D-CAD	4.32	110.88	108.47
14	b	4010	BCR	C15-C14-C13	-4.31	121.15	127.31
11	1	1134	CLA	C4D-C3D-CAD	4.31	110.88	108.47
11	a	1109	CLA	C4D-C3D-CAD	4.31	110.88	108.47
11	2	1228	CLA	O2A-C1-C2	4.31	119.96	108.64
11	A	1103	CLA	O2A-CGA-O1A	-4.31	112.72	123.59
11	A	1801	CLA	O2D-CGD-CBD	4.31	118.92	111.27
11	A	1135	CLA	O2A-CGA-CBA	4.31	125.43	111.91
11	1	1123	CLA	O2A-C1-C2	4.31	119.95	108.64
11	b	1207	CLA	O2A-C1-C2	4.31	119.95	108.64
11	a	1109	CLA	O2A-C1-C2	4.30	119.95	108.64
11	1	1119	CLA	O2A-CGA-CBA	4.30	125.41	111.91
11	B	1221	CLA	C4D-C3D-CAD	4.30	110.87	108.47
11	a	1134	CLA	O2D-CGD-CBD	4.30	118.91	111.27
11	8	1503	CLA	C4D-C3D-CAD	4.30	110.87	108.47
11	L	1503	CLA	C4D-C3D-CAD	4.30	110.87	108.47
14	B	4006	BCR	C7-C8-C9	-4.30	119.74	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1232	CLA	O2D-CGD-CBD	4.30	118.90	111.27
11	a	1136	CLA	C4D-C3D-CAD	4.29	110.86	108.47
11	2	1215	CLA	C4D-C3D-CAD	4.29	110.86	108.47
11	B	1220	CLA	C4D-C3D-CAD	4.29	110.86	108.47
11	0	1402	CLA	O2A-C1-C2	4.29	119.91	108.64
11	B	1209	CLA	C4D-C3D-CAD	4.29	110.86	108.47
11	1	1128	CLA	C4D-C3D-CAD	4.29	110.86	108.47
11	2	1219	CLA	O2D-CGD-CBD	4.29	118.89	111.27
14	a	4002	BCR	C38-C26-C25	-4.29	119.72	124.53
11	B	1203	CLA	C4D-C3D-CAD	4.28	110.86	108.47
14	2	4006	BCR	C7-C8-C9	-4.28	119.76	126.23
11	b	1205	CLA	O2A-CGA-CBA	4.28	125.35	111.91
11	1	1123	CLA	C4D-C3D-CAD	4.28	110.86	108.47
11	2	1240	CLA	C4D-C3D-CAD	4.28	110.86	108.47
11	a	1101	CLA	O2A-C1-C2	4.28	119.88	108.64
14	A	4001	BCR	C1-C6-C5	-4.28	116.59	122.61
11	B	1215	CLA	C4D-C3D-CAD	4.27	110.85	108.47
11	B	1204	CLA	C4D-C3D-CAD	4.27	110.85	108.47
11	B	1208	CLA	C4D-C3D-CAD	4.27	110.85	108.47
11	B	1205	CLA	O2A-CGA-CBA	4.27	125.32	111.91
11	1	1103	CLA	O2A-C1-C2	4.27	119.86	108.64
11	2	1235	CLA	O2A-CGA-O1A	-4.27	112.81	123.59
11	b	1013	CLA	O2A-CGA-CBA	4.27	125.31	111.91
11	A	1106	CLA	C4D-C3D-CAD	4.26	110.85	108.47
11	1	1011	CLA	O2A-CGA-CBA	4.26	125.29	111.91
11	a	1012	CLA	C4-C3-C5	4.26	122.44	115.27
14	B	4011	BCR	C34-C9-C10	-4.26	116.95	122.92
11	1	1104	CLA	O2A-C1-C2	4.26	119.83	108.64
11	b	1222	CLA	O2A-CGA-CBA	4.26	125.28	111.91
15	a	5001	LHG	O7-C7-C8	4.26	120.68	111.50
11	B	1232	CLA	C4D-C3D-CAD	4.26	110.84	108.47
11	1	1120	CLA	C4D-C3D-CAD	4.26	110.84	108.47
11	A	1140	CLA	O2A-CGA-CBA	4.25	125.25	111.91
11	1	1125	CLA	CAC-C3C-C4C	4.25	130.33	124.81
11	b	1021	CLA	O2A-CGA-CBA	4.25	125.24	111.91
11	2	1203	CLA	O2D-CGD-CBD	4.25	118.81	111.27
14	b	4017	BCR	C24-C23-C22	-4.25	119.82	126.23
11	A	1107	CLA	O2A-C1-C2	4.25	119.79	108.64
11	a	1117	CLA	C4D-C3D-CAD	4.24	110.84	108.47
11	a	1131	CLA	O2A-C1-C2	4.24	119.78	108.64
11	A	1104	CLA	O2A-CGA-CBA	4.24	125.22	111.91
11	A	1128	CLA	O2A-C1-C2	4.24	119.78	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1108	CLA	O2D-CGD-CBD	4.24	118.80	111.27
11	2	1230	CLA	C4-C3-C5	4.24	122.40	115.27
11	0	1402	CLA	O2A-CGA-CBA	4.24	125.21	111.91
11	B	1224	CLA	O2A-C1-C2	4.24	119.77	108.64
11	a	1116	CLA	O2A-CGA-CBA	4.24	125.20	111.91
11	B	1021	CLA	C4-C3-C5	4.24	122.40	115.27
11	A	1116	CLA	O2A-CGA-CBA	4.24	125.20	111.91
11	1	1116	CLA	O2A-CGA-CBA	4.23	125.20	111.91
11	2	1206	CLA	O2A-C1-C2	4.23	119.76	108.64
14	A	4003	BCR	C23-C22-C21	4.23	125.44	118.94
11	2	1230	CLA	C4D-C3D-CAD	4.23	110.83	108.47
11	B	1219	CLA	C4D-C3D-CAD	4.23	110.83	108.47
11	2	1238	CLA	O2A-C1-C2	4.23	119.76	108.64
14	2	4009	BCR	C15-C14-C13	-4.23	121.27	127.31
14	L	4022	BCR	C33-C5-C6	-4.23	119.78	124.53
11	a	1131	CLA	C4D-C3D-CAD	4.23	110.83	108.47
11	a	1128	CLA	O2A-C1-C2	4.23	119.74	108.64
11	1	1126	CLA	O2A-C1-C2	4.22	119.73	108.64
11	A	1124	CLA	O2A-CGA-CBA	4.22	125.15	111.91
11	1	1101	CLA	C4D-C3D-CAD	4.22	110.82	108.47
14	F	4018	BCR	C34-C9-C10	-4.22	117.02	122.92
14	f	4018	BCR	C3-C4-C5	-4.21	106.55	114.08
11	A	1011	CLA	C1-C2-C3	-4.21	118.76	126.04
14	b	4004	BCR	C33-C5-C6	-4.21	119.80	124.53
11	2	1236	CLA	O2A-CGA-CBA	4.21	125.12	111.91
14	L	4022	BCR	C38-C26-C25	-4.21	119.80	124.53
15	1	5001	LHG	O7-C7-C8	4.21	120.57	111.50
11	1	1117	CLA	C4D-C3D-CAD	4.21	110.81	108.47
14	2	4014	BCR	C36-C18-C17	-4.20	117.04	122.92
11	A	1117	CLA	O2A-CGA-CBA	4.20	125.09	111.91
11	1	1128	CLA	O2A-C1-C2	4.20	119.67	108.64
11	b	1201	CLA	O2A-C1-C2	4.20	119.67	108.64
15	1	5003	LHG	O7-C7-C8	4.20	120.55	111.50
11	a	1127	CLA	O2A-CGA-CBA	4.19	125.07	111.91
11	A	1801	CLA	O2A-C1-C2	4.19	119.65	108.64
14	a	4003	BCR	C3-C4-C5	-4.19	106.60	114.08
11	A	1118	CLA	O2A-C1-C2	4.19	119.64	108.64
11	k	1402	CLA	O2A-CGA-CBA	4.19	125.05	111.91
11	2	1205	CLA	O2A-CGA-CBA	4.18	125.04	111.91
11	2	1213	CLA	C4-C3-C5	4.18	122.31	115.27
11	A	1124	CLA	C4D-C3D-CAD	4.18	110.80	108.47
11	a	1137	CLA	C4D-C3D-CAD	4.18	110.80	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1127	CLA	O2A-C1-C2	4.18	119.63	108.64
11	B	1230	CLA	C1-O2A-CGA	4.18	127.41	116.44
11	1	1110	CLA	O2A-CGA-CBA	4.18	125.02	111.91
11	1	1109	CLA	O2A-C1-C2	4.18	119.62	108.64
14	2	4010	BCR	C23-C22-C21	4.18	125.35	118.94
11	B	1207	CLA	O2A-C1-C2	4.18	119.61	108.64
11	a	1801	CLA	O2A-C1-C2	4.18	119.61	108.64
14	L	4019	BCR	C15-C14-C13	-4.18	121.35	127.31
14	l	4022	BCR	C38-C26-C25	-4.17	119.84	124.53
14	f	4018	BCR	C15-C14-C13	-4.17	121.36	127.31
14	m	4021	BCR	C28-C27-C26	-4.17	106.63	114.08
11	b	1240	CLA	C4D-C3D-CAD	4.17	110.80	108.47
11	l	1501	CLA	O2A-CGA-CBA	4.17	124.99	111.91
11	A	1109	CLA	O2A-C1-C2	4.17	119.59	108.64
11	2	1234	CLA	O2A-CGA-CBA	4.17	124.99	111.91
11	b	1230	CLA	C4D-C3D-CAD	4.16	110.79	108.47
11	A	1135	CLA	O2D-CGD-CBD	4.16	118.66	111.27
14	A	4007	BCR	C24-C23-C22	-4.16	119.95	126.23
14	b	4009	BCR	C38-C26-C25	-4.16	119.86	124.53
11	A	1101	CLA	O2A-CGA-O1A	-4.16	113.09	123.59
14	L	4019	BCR	C7-C8-C9	-4.16	119.95	126.23
11	1	1121	CLA	O2A-CGA-O1A	-4.16	110.11	123.14
15	b	5004	LHG	O7-C7-C8	4.16	120.46	111.50
11	1	1102	CLA	O2A-C1-C2	4.15	119.55	108.64
11	A	1022	CLA	OBD-CAD-C3D	-4.15	121.08	127.98
11	b	1217	CLA	C4D-C3D-CAD	4.15	110.79	108.47
11	B	1219	CLA	O2A-CGA-CBA	4.15	124.94	111.91
11	2	1229	CLA	O2A-C1-C2	4.15	119.55	108.64
14	6	4018	BCR	C3-C4-C5	-4.15	106.66	114.08
11	A	1118	CLA	O2A-CGA-CBA	4.15	124.93	111.91
11	2	1222	CLA	O2A-CGA-CBA	4.15	124.92	111.91
11	B	1228	CLA	O2A-CGA-CBA	4.15	124.92	111.91
11	A	1011	CLA	O2A-C1-C2	4.15	119.53	108.64
11	B	1230	CLA	C4D-C3D-CAD	4.14	110.78	108.47
14	a	4002	BCR	C34-C9-C10	-4.14	117.12	122.92
11	a	1022	CLA	OBD-CAD-C3D	-4.14	121.11	127.98
11	B	1222	CLA	O2A-CGA-CBA	4.14	124.90	111.91
11	a	1115	CLA	O2A-CGA-O1A	-4.13	110.19	123.14
11	8	1503	CLA	O2A-C1-C2	4.13	119.50	108.64
11	B	1234	CLA	O2A-C1-C2	4.13	119.49	108.64
11	b	1219	CLA	O2A-CGA-CBA	4.13	124.87	111.91
11	l	1503	CLA	C4D-C3D-CAD	4.13	110.77	108.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1012	CLA	OBD-CAD-CBD	-4.13	120.00	125.89
14	B	4010	BCR	C23-C22-C21	4.13	125.27	118.94
11	b	1214	CLA	O2A-CGA-CBA	4.13	124.86	111.91
11	A	1120	CLA	O2A-CGA-O1A	-4.13	110.21	123.14
11	1	1110	CLA	C4D-C3D-CAD	4.12	110.77	108.47
11	1	1801	CLA	O2A-CGA-CBA	4.12	124.85	111.91
11	a	1101	CLA	C4D-C3D-CAD	4.12	110.77	108.47
11	B	1210	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
11	8	1501	CLA	C4-C3-C5	4.12	122.20	115.27
11	b	1235	CLA	CMB-C2B-C3B	4.12	132.38	124.68
11	A	1119	CLA	C4D-C3D-CAD	4.12	110.77	108.47
11	1	1102	CLA	O2A-CGA-CBA	4.12	124.83	111.91
11	b	1021	CLA	C4-C3-C5	4.11	122.19	115.27
11	1	1102	CLA	O2D-CGD-CBD	4.11	118.58	111.27
11	2	1228	CLA	O2A-CGA-CBA	4.11	124.82	111.91
14	1	4001	BCR	C15-C14-C13	-4.11	121.44	127.31
11	1	1132	CLA	O2A-C1-C2	4.11	119.44	108.64
11	A	1111	CLA	O2A-CGA-CBA	4.11	124.81	111.91
11	b	1203	CLA	C4D-C3D-CAD	4.11	110.76	108.47
11	A	1127	CLA	O2A-CGA-CBA	4.11	124.79	111.91
11	b	1213	CLA	O2A-C1-C2	4.10	119.42	108.64
11	B	1202	CLA	O2A-C1-C2	4.10	119.42	108.64
11	B	1203	CLA	O2A-C1-C2	4.10	119.42	108.64
11	B	1212	CLA	C4D-C3D-CAD	4.10	110.76	108.47
11	A	1101	CLA	O2A-C1-C2	4.10	119.41	108.64
11	2	1021	CLA	C4-C3-C5	4.10	122.17	115.27
11	B	1222	CLA	C4D-C3D-CAD	4.10	110.75	108.47
11	B	1219	CLA	O2A-C1-C2	4.09	119.40	108.64
11	B	1226	CLA	O2A-CGA-CBA	4.09	124.76	111.91
11	A	1129	CLA	C4D-C3D-CAD	4.09	110.75	108.47
15	2	5004	LHG	O7-C7-C8	4.09	120.32	111.50
11	a	1125	CLA	O2A-C1-C2	4.09	119.39	108.64
11	A	1103	CLA	O2A-C1-C2	4.09	119.39	108.64
11	1	1022	CLA	OBD-CAD-C3D	-4.09	121.19	127.98
14	8	4019	BCR	C24-C23-C22	-4.09	120.06	126.23
11	B	1203	CLA	O2D-CGD-CBD	4.09	118.53	111.27
11	2	1234	CLA	O2D-CGD-CBD	4.09	118.53	111.27
11	A	1115	CLA	O2A-CGA-O1A	-4.09	110.33	123.14
14	f	4013	BCR	C33-C5-C6	-4.09	119.94	124.53
11	1	1106	CLA	C4A-NA-C1A	4.09	108.54	106.71
14	8	4019	BCR	C7-C8-C9	-4.08	120.07	126.23
11	B	1210	CLA	O2A-CGA-CBA	4.08	124.71	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1140	CLA	O2A-CGA-CBA	4.08	124.71	111.91
14	B	4014	BCR	C33-C5-C6	-4.08	119.95	124.53
11	1	1130	CLA	C4D-C3D-CAD	4.08	110.74	108.47
11	2	1013	CLA	C4D-C3D-CAD	4.08	110.74	108.47
14	a	4008	BCR	C15-C14-C13	-4.08	121.49	127.31
11	b	1223	CLA	O2A-CGA-CBA	4.07	124.69	111.91
11	b	1232	CLA	C4D-C3D-CAD	4.07	110.74	108.47
11	1	1137	CLA	O2A-C1-C2	4.07	119.33	108.64
11	2	1217	CLA	O2A-CGA-CBA	4.07	124.68	111.91
11	B	1023	CLA	O2D-CGD-CBD	4.07	118.50	111.27
11	b	1202	CLA	O2A-C1-C2	4.07	119.33	108.64
11	A	1109	CLA	C4-C3-C5	4.07	122.11	115.27
11	a	1111	CLA	O2A-CGA-CBA	4.07	124.67	111.91
11	b	1219	CLA	O2A-C1-C2	4.06	119.32	108.64
11	8	1503	CLA	CMB-C2B-C3B	4.06	132.28	124.68
11	1	1139	CLA	O2A-C1-C2	4.06	119.31	108.64
14	F	4020	BCR	C7-C8-C9	-4.06	120.10	126.23
11	b	1222	CLA	O2A-C1-C2	4.06	119.30	108.64
14	B	4011	BCR	C15-C14-C13	-4.06	121.52	127.31
11	b	1013	CLA	C4D-C3D-CAD	4.06	110.73	108.47
11	b	1229	CLA	O2A-C1-C2	4.06	119.29	108.64
14	F	4013	BCR	C33-C5-C6	-4.06	119.97	124.53
11	b	1225	CLA	O2A-C1-C2	4.06	119.29	108.64
11	a	1107	CLA	O2A-C1-C2	4.05	119.29	108.64
14	L	4019	BCR	C37-C22-C21	-4.05	117.25	122.92
11	1	1109	CLA	C4D-C3D-CAD	4.05	110.73	108.47
14	b	4006	BCR	C38-C26-C25	-4.05	119.98	124.53
14	l	4022	BCR	C37-C22-C21	-4.05	117.25	122.92
14	2	4010	BCR	C15-C14-C13	-4.04	121.54	127.31
11	2	1213	CLA	C4D-C3D-CAD	4.04	110.72	108.47
11	A	1110	CLA	O2A-CGA-CBA	4.04	124.59	111.91
11	1	1135	CLA	C4D-C3D-CAD	4.04	110.72	108.47
11	1	1117	CLA	O2A-CGA-CBA	4.04	124.59	111.91
14	1	4003	BCR	C7-C8-C9	-4.04	120.13	126.23
11	2	1224	CLA	O2A-C1-C2	4.04	119.25	108.64
11	b	1215	CLA	O2A-CGA-CBA	4.04	124.58	111.91
11	2	1204	CLA	C4D-C3D-CAD	4.03	110.72	108.47
11	1	1801	CLA	C4D-C3D-CAD	4.03	110.72	108.47
11	1	1237	CLA	O2D-CGD-CBD	4.02	118.42	111.27
11	A	1130	CLA	C4D-C3D-CAD	4.02	110.71	108.47
14	1	4007	BCR	C38-C26-C25	-4.02	120.01	124.53
14	b	4009	BCR	C36-C18-C17	-4.02	117.29	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1110	CLA	O2A-CGA-CBA	4.02	124.52	111.91
11	1	1119	CLA	C4D-C3D-CAD	4.02	110.71	108.47
14	6	4020	BCR	C38-C26-C27	4.02	121.33	113.62
11	2	1220	CLA	O2D-CGD-CBD	4.02	118.40	111.27
11	1	1126	CLA	C4D-C3D-CAD	4.01	110.71	108.47
11	l	1503	CLA	O2A-CGA-CBA	4.01	124.49	111.91
11	a	1120	CLA	O2A-CGA-O1A	-4.01	110.57	123.14
11	a	1012	CLA	C4D-C3D-CAD	4.01	110.70	108.47
14	b	4006	BCR	C33-C5-C4	4.01	121.31	113.62
11	a	1104	CLA	O2A-C1-C2	4.01	119.17	108.64
11	a	1012	CLA	O2A-CGA-CBA	4.01	124.48	111.91
11	B	1236	CLA	O2A-CGA-CBA	4.00	124.47	111.91
11	A	1102	CLA	O2A-C1-C2	4.00	119.15	108.64
15	a	5003	LHG	O7-C7-C8	4.00	120.13	111.50
14	6	4018	BCR	C15-C14-C13	-4.00	121.60	127.31
11	a	1124	CLA	O2A-CGA-CBA	4.00	124.45	111.91
11	2	1210	CLA	O2A-CGA-CBA	4.00	124.45	111.91
11	2	1239	CLA	O2A-CGA-O1A	-3.99	110.63	123.14
14	6	4018	BCR	C33-C5-C6	-3.99	120.05	124.53
11	B	1225	CLA	O2A-C1-C2	3.99	119.12	108.64
14	L	4022	BCR	C7-C8-C9	-3.99	120.21	126.23
11	1	1012	CLA	C4D-C3D-CAD	3.99	110.69	108.47
11	L	1501	CLA	O2A-CGA-CBA	3.98	124.41	111.91
11	A	1237	CLA	O2D-CGD-CBD	3.98	118.34	111.27
11	b	1023	CLA	C4D-C3D-CAD	3.98	110.69	108.47
11	a	1104	CLA	O2A-CGA-CBA	3.98	124.40	111.91
11	a	1109	CLA	O2A-CGA-CBA	3.98	124.39	111.91
14	B	4011	BCR	C28-C27-C26	-3.98	106.97	114.08
11	8	1502	CLA	O2A-CGA-O1A	-3.98	110.68	123.14
11	a	1119	CLA	C4D-C3D-CAD	3.98	110.69	108.47
11	a	1125	CLA	C4D-C3D-CAD	3.97	110.69	108.47
14	B	4006	BCR	C1-C6-C5	-3.97	117.02	122.61
11	B	1226	CLA	O2A-C1-C2	3.97	119.06	108.64
11	a	1119	CLA	O2A-CGA-CBA	3.96	124.35	111.91
11	a	1117	CLA	O2A-CGA-CBA	3.96	124.34	111.91
11	a	1237	CLA	O2D-CGD-CBD	3.95	118.29	111.27
14	1	4002	BCR	C38-C26-C25	-3.95	120.09	124.53
14	F	4018	BCR	C3-C4-C5	-3.95	107.02	114.08
11	b	1203	CLA	O2A-CGA-CBA	3.95	124.30	111.91
11	1	1139	CLA	C1-C2-C3	-3.95	120.37	126.75
14	a	4003	BCR	C37-C22-C21	-3.95	117.40	122.92
11	a	1140	CLA	O2A-CGA-CBA	3.94	124.29	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1116	CLA	O2A-C1-C2	3.94	119.00	108.64
11	1	1120	CLA	O2A-CGA-O1A	-3.94	110.78	123.14
11	A	1133	CLA	O2A-CGA-O1A	-3.94	110.79	123.14
11	a	1011	CLA	O2A-C1-C2	3.94	118.99	108.64
14	2	4014	BCR	C33-C5-C6	-3.94	120.11	124.53
11	a	1132	CLA	C4D-C3D-CAD	3.94	110.67	108.47
14	8	4022	BCR	C34-C9-C10	-3.93	117.41	122.92
14	l	4019	BCR	C33-C5-C6	-3.93	120.11	124.53
11	b	1210	CLA	O2A-CGA-CBA	3.93	124.25	111.91
11	2	1229	CLA	O2A-CGA-CBA	3.93	124.25	111.91
14	A	4003	BCR	C3-C4-C5	-3.93	107.06	114.08
11	A	1121	CLA	O2A-CGA-O1A	-3.93	110.83	123.14
11	1	1104	CLA	O2A-CGA-CBA	3.93	124.23	111.91
14	2	4014	BCR	C37-C22-C21	-3.93	117.42	122.92
14	2	4005	BCR	C7-C8-C9	-3.92	120.31	126.23
14	A	4001	BCR	C36-C18-C17	-3.92	117.43	122.92
11	B	1214	CLA	O2A-CGA-CBA	3.92	124.22	111.91
11	a	1134	CLA	O2A-CGA-O1A	-3.92	110.85	123.14
14	m	4021	BCR	C24-C23-C22	-3.92	120.31	126.23
11	1	1122	CLA	O2A-CGA-CBA	3.92	124.21	111.91
11	1	1124	CLA	O2A-CGA-CBA	3.92	124.21	111.91
11	a	1121	CLA	O2A-CGA-O1A	-3.92	110.86	123.14
11	2	1214	CLA	C4A-NA-C1A	3.92	108.47	106.71
11	1	1022	CLA	O2A-CGA-CBA	3.92	124.20	111.91
11	a	1116	CLA	O2A-C1-C2	3.92	118.93	108.64
11	2	1206	CLA	O2A-CGA-CBA	3.92	124.19	111.91
11	l	1501	CLA	C4-C3-C5	3.91	121.85	115.27
14	2	4006	BCR	C33-C5-C4	3.91	121.12	113.62
11	1	1237	CLA	O2A-C1-C2	3.91	118.91	108.64
11	a	1130	CLA	O2A-CGA-O1A	-3.91	110.89	123.14
11	B	1206	CLA	O2D-CGD-CBD	3.90	118.21	111.27
11	1	1011	CLA	O2A-C1-C2	3.90	118.89	108.64
11	L	1503	CLA	O2A-CGA-CBA	3.90	124.15	111.91
11	a	1110	CLA	O2A-C1-C2	3.90	118.88	108.64
11	B	1239	CLA	O2A-CGA-O1A	-3.90	110.92	123.14
11	B	1220	CLA	O2D-CGD-CBD	3.89	118.19	111.27
14	a	4007	BCR	C38-C26-C25	-3.89	120.16	124.53
11	B	1215	CLA	O2A-CGA-CBA	3.89	124.12	111.91
11	2	1212	CLA	C4D-C3D-CAD	3.89	110.64	108.47
11	A	1012	CLA	C4D-C3D-CAD	3.89	110.64	108.47
14	2	4017	BCR	C36-C18-C17	-3.89	117.48	122.92
11	2	1213	CLA	O2A-CGA-CBA	3.89	124.10	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1122	CLA	C4-C3-C5	3.89	121.81	115.27
11	8	1503	CLA	O2A-CGA-CBA	3.88	124.10	111.91
11	2	1220	CLA	O2A-CGA-O1A	-3.88	110.97	123.14
14	1	4019	BCR	C38-C26-C25	-3.88	120.17	124.53
11	2	1226	CLA	O2A-C1-C2	3.88	118.83	108.64
11	b	1023	CLA	O2A-CGA-CBA	3.88	124.08	111.91
14	A	4001	BCR	C37-C22-C21	-3.88	117.49	122.92
11	a	1133	CLA	O2A-CGA-O1A	-3.88	110.99	123.14
11	1	1134	CLA	O2A-CGA-O1A	-3.87	111.00	123.14
11	1	1237	CLA	C1-C2-C3	-3.87	119.35	126.04
11	a	1102	CLA	O2A-C1-C2	3.87	118.81	108.64
11	2	1021	CLA	O2A-C1-C2	3.87	118.80	108.64
11	2	1234	CLA	C4D-C3D-CAD	3.86	110.62	108.47
14	2	4006	BCR	C34-C9-C10	-3.86	117.51	122.92
11	A	1101	CLA	O2D-CGD-CBD	3.86	118.13	111.27
14	a	4003	BCR	C15-C14-C13	-3.86	121.80	127.31
11	B	1225	CLA	O2D-CGD-CBD	3.86	118.13	111.27
11	K	1402	CLA	O2A-CGA-CBA	3.86	124.02	111.91
11	1	1116	CLA	O2A-C1-C2	3.86	118.78	108.64
11	A	1012	CLA	OBD-CAD-C3D	-3.86	121.57	127.98
11	A	1117	CLA	C4D-C3D-CAD	3.86	110.62	108.47
11	B	1229	CLA	O2A-CGA-CBA	3.86	124.01	111.91
11	a	1130	CLA	C4D-C3D-CAD	3.86	110.62	108.47
11	b	1228	CLA	O2A-CGA-CBA	3.85	124.00	111.91
14	2	4011	BCR	C38-C26-C25	-3.85	120.20	124.53
11	b	1226	CLA	O2A-C1-C2	3.85	118.76	108.64
11	a	1139	CLA	O2A-CGA-CBA	3.85	124.00	111.91
11	1	1136	CLA	O2A-CGA-O1A	-3.85	111.07	123.14
11	A	1105	CLA	O2A-CGA-CBA	3.85	123.99	111.91
11	2	1226	CLA	O2A-CGA-CBA	3.85	123.99	111.91
11	1	1133	CLA	O2A-CGA-O1A	-3.85	111.08	123.14
11	1	1119	CLA	O2A-C1-C2	3.85	118.74	108.64
11	b	1210	CLA	CAC-C3C-C4C	3.84	129.80	124.81
11	2	1208	CLA	C4D-C3D-CAD	3.84	110.61	108.47
11	b	1202	CLA	O2A-CGA-CBA	3.84	123.96	111.91
11	a	1103	CLA	C4A-NA-C1A	3.84	108.43	106.71
11	a	1114	CLA	O2A-CGA-O1A	-3.84	111.10	123.14
11	b	1213	CLA	O2A-CGA-CBA	3.84	123.96	111.91
11	B	1230	CLA	C4-C3-C5	3.84	121.72	115.27
11	1	1127	CLA	O2A-CGA-CBA	3.83	123.94	111.91
14	f	4018	BCR	C33-C5-C6	-3.83	120.22	124.53
14	B	4009	BCR	C38-C26-C25	-3.83	120.22	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4006	BCR	C3-C4-C5	-3.83	107.24	114.08
11	1	1106	CLA	O2A-CGA-CBA	3.83	123.93	111.91
11	a	1103	CLA	O2A-CGA-CBA	3.83	123.92	111.91
11	a	1136	CLA	O2A-CGA-O1A	-3.82	111.15	123.14
11	B	1220	CLA	O2A-CGA-O1A	-3.82	111.15	123.14
11	2	1223	CLA	O2A-CGA-CBA	3.82	123.91	111.91
11	1	1140	CLA	C1-C2-C3	-3.82	119.43	126.04
14	A	4003	BCR	C15-C14-C13	-3.82	121.86	127.31
11	B	1202	CLA	O2A-CGA-CBA	3.82	123.89	111.91
11	b	1216	CLA	O2A-C1-C2	3.82	118.67	108.64
11	A	1129	CLA	O2A-CGA-O1A	-3.82	111.18	123.14
14	A	4001	BCR	C23-C22-C21	3.81	124.80	118.94
14	b	4017	BCR	C15-C14-C13	-3.81	121.87	127.31
11	A	1011	CLA	C4D-C3D-CAD	3.81	110.60	108.47
11	a	1118	CLA	O2A-CGA-CBA	3.81	123.88	111.91
14	l	4022	BCR	C33-C5-C6	-3.81	120.25	124.53
14	a	4007	BCR	C24-C23-C22	-3.81	120.48	126.23
14	l	4019	BCR	C24-C23-C22	-3.81	120.48	126.23
11	1	1131	CLA	O2A-C1-C2	3.81	118.65	108.64
11	A	1102	CLA	C4D-C3D-CAD	3.81	110.59	108.47
14	B	4009	BCR	C34-C9-C10	-3.81	117.59	122.92
11	A	1125	CLA	OBD-CAD-C3D	-3.80	121.67	127.98
14	F	4020	BCR	C38-C26-C25	-3.80	120.26	124.53
11	a	1138	CLA	O2A-CGA-O1A	-3.80	111.24	123.14
11	b	1239	CLA	O2A-CGA-O1A	-3.80	111.24	123.14
11	a	1129	CLA	O2A-CGA-O1A	-3.80	111.24	123.14
11	2	1202	CLA	O2A-CGA-CBA	3.80	123.82	111.91
14	b	4009	BCR	C37-C22-C21	-3.79	117.61	122.92
11	1	1139	CLA	O2A-CGA-CBA	3.79	123.80	111.91
14	B	4006	BCR	C38-C26-C25	-3.79	120.27	124.53
11	2	1235	CLA	O2A-CGA-CBA	3.79	123.79	111.91
11	A	1131	CLA	C4D-C3D-CAD	3.79	110.58	108.47
14	f	4020	BCR	C24-C23-C22	-3.79	120.52	126.23
14	A	4008	BCR	C38-C26-C27	3.79	120.89	113.62
14	a	4003	BCR	C38-C26-C25	-3.78	120.28	124.53
14	2	4014	BCR	C30-C25-C26	-3.78	117.28	122.61
14	2	4009	BCR	C38-C26-C25	-3.78	120.28	124.53
14	A	4008	BCR	C36-C18-C17	-3.78	117.62	122.92
11	8	1501	CLA	O2A-C1-C2	3.78	118.57	108.64
11	1	1118	CLA	O2A-CGA-CBA	3.78	123.77	111.91
11	A	1138	CLA	O2A-CGA-O1A	-3.77	111.31	123.14
14	B	4017	BCR	C19-C18-C17	3.77	124.73	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1136	CLA	O2A-CGA-O1A	-3.77	111.33	123.14
14	2	4010	BCR	C33-C5-C6	-3.77	120.30	124.53
11	1	1105	CLA	O2A-CGA-CBA	3.77	123.73	111.91
14	f	4020	BCR	C38-C26-C25	-3.77	120.30	124.53
14	1	4001	BCR	C1-C6-C5	-3.77	117.31	122.61
11	b	1220	CLA	O2A-CGA-O1A	-3.76	111.34	123.14
11	1	1101	CLA	O2A-CGA-CBA	3.76	123.72	111.91
11	b	1226	CLA	O2A-CGA-CBA	3.76	123.72	111.91
11	A	1106	CLA	O2A-CGA-CBA	3.76	123.72	111.91
11	2	1228	CLA	C1-C2-C3	-3.76	120.66	126.75
11	B	1206	CLA	O2A-CGA-CBA	3.76	123.72	111.91
11	A	1114	CLA	O2A-CGA-O1A	-3.76	111.35	123.14
11	A	1125	CLA	O2A-C1-C2	3.76	118.52	108.64
11	1	1138	CLA	O2A-CGA-O1A	-3.76	111.37	123.14
11	B	1213	CLA	O2A-C1-C2	3.75	118.50	108.64
11	A	1139	CLA	O2A-CGA-CBA	3.75	123.68	111.91
11	B	1023	CLA	O2A-CGA-CBA	3.75	123.67	111.91
11	B	1223	CLA	O2A-CGA-CBA	3.75	123.67	111.91
14	8	4019	BCR	C38-C26-C25	-3.75	120.32	124.53
14	1	4003	BCR	C3-C4-C5	-3.75	107.39	114.08
11	1	1110	CLA	O2A-C1-C2	3.75	118.48	108.64
14	B	4009	BCR	C15-C14-C13	-3.75	121.97	127.31
11	A	1134	CLA	O2A-CGA-O1A	-3.74	111.40	123.14
11	b	1216	CLA	O2A-CGA-CBA	3.74	123.66	111.91
11	b	1229	CLA	O2A-CGA-CBA	3.74	123.66	111.91
14	B	4014	BCR	C15-C14-C13	-3.74	121.97	127.31
11	1	1130	CLA	O2A-CGA-O1A	-3.74	111.41	123.14
14	F	4018	BCR	C15-C14-C13	-3.74	121.98	127.31
11	2	1219	CLA	O2A-CGA-CBA	3.72	123.59	111.91
11	a	1022	CLA	O2A-CGA-CBA	3.72	123.58	111.91
11	A	1132	CLA	O2A-CGA-CBA	3.72	123.58	111.91
11	1	1114	CLA	O2A-CGA-O1A	-3.72	111.49	123.14
14	L	4019	BCR	C23-C22-C21	3.71	124.64	118.94
11	a	1111	CLA	CMC-C2C-C1C	3.71	130.69	125.04
11	1	1107	CLA	O2A-CGA-CBA	3.71	123.55	111.91
11	2	1230	CLA	C1-O2A-CGA	3.71	126.17	116.44
14	a	4008	BCR	C33-C5-C4	3.70	120.73	113.62
11	A	1130	CLA	O2A-CGA-O1A	-3.70	111.54	123.14
14	B	4017	BCR	C7-C8-C9	-3.70	120.64	126.23
14	B	4014	BCR	C23-C22-C21	3.70	124.62	118.94
14	f	4018	BCR	C33-C5-C4	3.70	120.72	113.62
11	b	1211	CLA	O2A-CGA-O1A	-3.70	111.55	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1206	CLA	O2A-CGA-CBA	3.69	123.50	111.91
11	1	1129	CLA	O2A-CGA-O1A	-3.69	111.57	123.14
11	A	1110	CLA	O2A-C1-C2	3.69	118.33	108.64
11	A	1107	CLA	O2A-CGA-CBA	3.69	123.48	111.91
11	B	1013	CLA	C1-O2A-CGA	3.69	126.12	116.44
11	l	1502	CLA	O2A-CGA-O1A	-3.69	111.58	123.14
11	a	1137	CLA	C4-C3-C5	3.69	121.47	115.27
14	7	4021	BCR	C24-C23-C22	-3.69	120.67	126.23
11	a	1101	CLA	O2A-CGA-CBA	3.68	123.47	111.91
14	6	4013	BCR	C37-C22-C21	-3.68	117.76	122.92
11	b	1235	CLA	O2A-CGA-CBA	3.68	123.45	111.91
11	1	1115	CLA	O2A-CGA-O1A	-3.68	111.61	123.14
14	1	4001	BCR	C37-C22-C21	-3.68	117.77	122.92
11	a	1107	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
11	A	1128	CLA	O2A-CGA-CBA	3.68	123.44	111.91
14	B	4006	BCR	C3-C4-C5	-3.67	107.52	114.08
14	a	4008	BCR	C38-C26-C25	-3.67	120.40	124.53
11	L	1502	CLA	O2A-CGA-O1A	-3.67	111.63	123.14
14	B	4009	BCR	C7-C8-C9	-3.67	120.69	126.23
11	B	1216	CLA	O2A-CGA-CBA	3.67	123.43	111.91
14	a	4008	BCR	C38-C26-C27	3.67	120.67	113.62
11	2	1211	CLA	O2A-CGA-O1A	-3.67	111.63	123.14
14	1	4007	BCR	C15-C14-C13	-3.67	122.07	127.31
14	B	4004	BCR	C38-C26-C25	-3.67	120.41	124.53
14	2	4014	BCR	C23-C22-C21	3.67	124.57	118.94
14	2	4017	BCR	C34-C9-C10	-3.67	117.79	122.92
11	1	1135	CLA	O2A-CGA-CBA	3.67	123.41	111.91
14	6	4020	BCR	C15-C14-C13	-3.66	122.08	127.31
11	2	1216	CLA	O2A-C1-C2	3.66	118.26	108.64
14	F	4018	BCR	C38-C26-C25	-3.66	120.42	124.53
11	B	1213	CLA	O2A-CGA-CBA	3.65	123.37	111.91
11	b	1203	CLA	O2A-C1-C2	3.65	118.23	108.64
14	B	4011	BCR	C33-C5-C6	-3.65	120.43	124.53
11	B	1211	CLA	O2A-CGA-O1A	-3.65	111.70	123.14
11	2	1021	CLA	C1-C2-C3	-3.65	119.73	126.04
14	B	4017	BCR	C1-C6-C5	-3.65	117.47	122.61
14	1	4007	BCR	C7-C8-C9	-3.65	120.72	126.23
14	b	4014	BCR	C36-C18-C17	-3.65	117.82	122.92
11	A	1123	CLA	CAC-C3C-C4C	3.64	129.54	124.81
11	b	1220	CLA	CAC-C3C-C4C	3.64	129.53	124.81
11	1	1126	CLA	O2A-CGA-CBA	3.64	123.33	111.91
14	b	4011	BCR	C38-C26-C25	-3.64	120.44	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	4020	BCR	C38-C26-C25	-3.64	120.44	124.53
14	a	4001	BCR	C33-C5-C6	-3.64	120.44	124.53
11	2	1203	CLA	O2A-CGA-CBA	3.64	123.32	111.91
14	1	4008	BCR	C7-C8-C9	-3.63	120.74	126.23
11	a	1128	CLA	O2A-CGA-CBA	3.63	123.31	111.91
14	2	4009	BCR	C24-C23-C22	-3.63	120.75	126.23
11	8	1501	CLA	O2A-CGA-CBA	3.63	123.31	111.91
14	2	4004	BCR	C38-C26-C25	-3.63	120.45	124.53
11	1	1011	CLA	O1D-CGD-CBD	-3.63	117.06	124.48
14	b	4014	BCR	C33-C5-C6	-3.62	120.46	124.53
14	M	4021	BCR	C38-C26-C25	-3.62	120.46	124.53
11	A	1107	CLA	C4-C3-C5	3.62	121.36	115.27
11	2	1201	CLA	O2A-CGA-CBA	3.62	123.27	111.91
14	B	4005	BCR	C33-C5-C6	-3.62	120.47	124.53
11	1	1011	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
14	b	4017	BCR	C27-C26-C25	-3.62	117.48	122.73
14	1	4008	BCR	C33-C5-C4	3.62	120.56	113.62
14	2	4009	BCR	C33-C5-C6	-3.61	120.47	124.53
11	b	1021	CLA	O2A-C1-C2	3.61	118.13	108.64
14	m	4021	BCR	C36-C18-C17	-3.61	117.87	122.92
14	B	4010	BCR	C37-C22-C21	-3.61	117.87	122.92
11	a	1131	CLA	O2A-CGA-CBA	3.61	123.23	111.91
14	1	4001	BCR	C23-C22-C21	3.61	124.48	118.94
11	B	1203	CLA	O2A-CGA-CBA	3.61	123.23	111.91
14	1	4008	BCR	C38-C26-C27	3.60	120.54	113.62
11	A	1103	CLA	C1-C2-C3	-3.60	119.81	126.04
14	1	4003	BCR	C33-C5-C6	-3.60	120.48	124.53
14	F	4013	BCR	C23-C22-C21	3.60	124.47	118.94
14	B	4006	BCR	C33-C5-C4	3.60	120.53	113.62
14	2	4005	BCR	C33-C5-C6	-3.60	120.49	124.53
11	A	1138	CLA	CMC-C2C-C1C	3.60	130.52	125.04
14	b	4011	BCR	C38-C26-C27	3.60	120.53	113.62
11	A	1140	CLA	C4-C3-C5	3.60	121.32	115.27
14	a	4002	BCR	C38-C26-C27	3.59	120.52	113.62
14	m	4021	BCR	C38-C26-C27	3.59	120.52	113.62
14	a	4001	BCR	C37-C22-C21	-3.59	117.90	122.92
11	l	1503	CLA	O2A-C1-C2	3.58	118.05	108.64
11	l	1501	CLA	O2A-C1-C2	3.58	118.04	108.64
14	F	4018	BCR	C33-C5-C6	-3.58	120.51	124.53
14	A	4002	BCR	C7-C8-C9	-3.58	120.83	126.23
11	A	1139	CLA	CMC-C2C-C1C	3.58	130.49	125.04
11	B	1221	CLA	O2A-CGA-CBA	3.57	123.13	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4011	BCR	C33-C5-C6	-3.57	120.52	124.53
11	A	1104	CLA	C1-C2-C3	-3.57	119.87	126.04
11	1	1128	CLA	O2A-CGA-CBA	3.56	123.09	111.91
14	8	4022	BCR	C38-C26-C27	3.56	120.46	113.62
14	8	4022	BCR	C33-C5-C6	-3.56	120.53	124.53
11	b	1201	CLA	O2A-CGA-CBA	3.56	123.08	111.91
11	A	1022	CLA	O2A-CGA-CBA	3.56	123.08	111.91
14	B	4011	BCR	C38-C26-C27	3.56	120.45	113.62
14	B	4014	BCR	C36-C18-C17	-3.56	117.94	122.92
14	A	4003	BCR	C33-C5-C6	-3.56	120.53	124.53
11	1	1131	CLA	O2A-CGA-CBA	3.55	123.06	111.91
11	1	1103	CLA	O2A-CGA-CBA	3.55	123.06	111.91
14	a	4008	BCR	C34-C9-C10	-3.55	117.95	122.92
11	B	1216	CLA	O2A-C1-C2	3.55	117.97	108.64
14	f	4013	BCR	C23-C22-C21	3.55	124.39	118.94
14	2	4011	BCR	C33-C5-C6	-3.55	120.54	124.53
14	B	4010	BCR	C38-C26-C25	-3.55	120.55	124.53
14	b	4005	BCR	C15-C14-C13	-3.55	122.25	127.31
11	B	1240	CLA	CMB-C2B-C3B	3.54	131.31	124.68
14	B	4011	BCR	C24-C23-C22	-3.54	120.88	126.23
14	B	4014	BCR	C37-C22-C21	-3.54	117.96	122.92
11	a	1132	CLA	O2A-CGA-CBA	3.54	123.03	111.91
14	B	4004	BCR	C38-C26-C27	3.54	120.42	113.62
11	1	1123	CLA	O2A-CGA-CBA	3.54	123.02	111.91
14	a	4003	BCR	C33-C5-C6	-3.54	120.55	124.53
11	B	1206	CLA	O2A-C1-C2	3.54	117.94	108.64
11	B	1203	CLA	C4-C3-C5	3.54	121.22	115.27
14	b	4004	BCR	C38-C26-C27	3.54	120.41	113.62
14	A	4003	BCR	C38-C26-C25	-3.53	120.56	124.53
14	b	4017	BCR	C19-C18-C17	3.53	124.36	118.94
14	a	4003	BCR	C33-C5-C4	3.53	120.39	113.62
11	a	1135	CLA	O2A-CGA-CBA	3.53	122.97	111.91
14	b	4005	BCR	C33-C5-C6	-3.52	120.57	124.53
11	B	1021	CLA	CHB-C4A-NA	3.52	129.38	124.51
14	B	4010	BCR	C33-C5-C4	3.52	120.38	113.62
11	a	1122	CLA	C1-O2A-CGA	3.52	125.68	116.44
14	A	4001	BCR	C19-C18-C17	3.52	124.34	118.94
14	b	4009	BCR	C33-C5-C6	-3.52	120.58	124.53
11	L	1503	CLA	O2A-C1-C2	3.52	117.88	108.64
11	1	1121	CLA	O2A-CGA-CBA	3.52	126.13	112.23
11	A	1125	CLA	O2A-CGA-CBA	3.52	122.94	111.91
11	b	1238	CLA	O2A-CGA-CBA	3.52	122.94	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4009	BCR	C24-C23-C22	-3.51	120.92	126.23
11	2	1215	CLA	O2A-CGA-CBA	3.51	122.94	111.91
14	b	4005	BCR	C38-C26-C25	-3.51	120.58	124.53
11	A	1123	CLA	O2A-CGA-CBA	3.51	122.93	111.91
14	L	4019	BCR	C34-C9-C10	-3.51	118.01	122.92
11	b	1238	CLA	O2A-C1-C2	3.51	117.85	108.64
11	B	1230	CLA	O2A-CGA-CBA	3.51	122.91	111.91
14	L	4022	BCR	C33-C5-C4	3.50	120.35	113.62
14	B	4004	BCR	C15-C14-C13	-3.50	122.32	127.31
14	2	4006	BCR	C3-C4-C5	-3.50	107.84	114.08
11	B	1227	CLA	CAC-C3C-C4C	3.49	129.34	124.81
11	A	1126	CLA	O2A-CGA-CBA	3.49	122.87	111.91
14	M	4021	BCR	C34-C9-C10	-3.49	118.03	122.92
14	b	4004	BCR	C38-C26-C25	-3.49	120.61	124.53
11	a	1012	CLA	OBD-CAD-C3D	-3.49	122.19	127.98
14	L	4019	BCR	C38-C26-C25	-3.48	120.61	124.53
11	a	1106	CLA	O2A-CGA-CBA	3.48	122.84	111.91
11	a	1237	CLA	O2A-CGA-CBA	3.48	122.84	111.91
11	a	1105	CLA	O2A-C1-C2	3.48	121.25	109.49
14	b	4004	BCR	C15-C14-C13	-3.48	122.34	127.31
11	2	1225	CLA	O2A-C1-C2	3.48	117.78	108.64
11	a	1123	CLA	O2A-CGA-CBA	3.48	122.82	111.91
14	2	4017	BCR	C1-C6-C5	-3.48	117.72	122.61
14	2	4006	BCR	C4-C5-C6	-3.47	117.69	122.73
11	a	1128	CLA	C4-C3-C5	3.47	121.11	115.27
14	6	4018	BCR	C27-C26-C25	-3.47	117.70	122.73
11	2	1235	CLA	O2A-C1-C2	3.47	117.75	108.64
11	A	1101	CLA	O2A-CGA-CBA	3.47	122.78	111.91
14	b	4006	BCR	C1-C6-C5	-3.46	117.73	122.61
14	a	4008	BCR	C7-C8-C9	-3.46	121.00	126.23
14	M	4021	BCR	C36-C18-C17	-3.46	118.07	122.92
11	a	1132	CLA	C1-O2A-CGA	3.46	125.53	116.44
11	A	1138	CLA	CAC-C3C-C4C	3.46	129.30	124.81
14	2	4014	BCR	C27-C26-C25	-3.46	117.71	122.73
11	a	1120	CLA	O2A-CGA-CBA	3.45	125.88	112.23
14	B	4009	BCR	C33-C5-C6	-3.45	120.65	124.53
11	a	1107	CLA	O2A-CGA-CBA	3.45	122.75	111.91
14	b	4009	BCR	C15-C14-C13	-3.45	122.38	127.31
14	B	4017	BCR	C38-C26-C27	3.45	120.25	113.62
14	2	4004	BCR	C37-C22-C21	-3.45	118.09	122.92
11	a	1011	CLA	O2D-CGD-CBD	3.45	117.40	111.27
11	A	1124	CLA	C1-C2-C3	-3.45	120.08	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4017	BCR	C34-C9-C10	-3.45	118.09	122.92
11	B	1216	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	B	4006	BCR	C34-C9-C10	-3.44	118.10	122.92
11	a	1115	CLA	O2A-CGA-CBA	3.44	125.84	112.23
11	A	1131	CLA	O2A-CGA-CBA	3.43	122.68	111.91
11	A	1135	CLA	C1-C2-C3	-3.43	120.11	126.04
11	a	1124	CLA	C1-C2-C3	-3.43	120.11	126.04
11	b	1225	CLA	O2A-CGA-CBA	3.43	122.66	111.91
11	a	1126	CLA	O2A-CGA-CBA	3.43	122.66	111.91
14	A	4002	BCR	C34-C9-C10	-3.42	118.13	122.92
11	k	1401	CLA	C4-C3-C5	3.42	121.03	115.27
11	2	1215	CLA	C1-O2A-CGA	3.42	125.42	116.44
14	6	4013	BCR	C23-C22-C21	3.42	124.19	118.94
14	A	4008	BCR	C33-C5-C4	3.42	120.18	113.62
14	B	4009	BCR	C24-C23-C22	-3.42	121.07	126.23
11	K	1401	CLA	C4-C3-C5	3.42	121.02	115.27
11	a	1125	CLA	O2A-CGA-CBA	3.41	122.62	111.91
14	a	4008	BCR	C33-C5-C6	-3.41	120.70	124.53
11	1	1125	CLA	O2A-C1-C2	3.41	117.59	108.64
11	0	1401	CLA	C4-C3-C5	3.41	121.00	115.27
11	a	1022	CLA	C4D-C3D-CAD	3.41	110.37	108.47
14	B	4017	BCR	C27-C26-C25	-3.40	117.79	122.73
11	b	1204	CLA	O2A-CGA-CBA	3.40	122.58	111.91
11	b	1221	CLA	CMC-C2C-C1C	3.40	130.22	125.04
11	2	1238	CLA	O2A-CGA-CBA	3.40	122.57	111.91
14	a	4002	BCR	C37-C22-C21	-3.40	118.17	122.92
14	2	4004	BCR	C38-C26-C27	3.40	120.14	113.62
14	a	4001	BCR	C36-C18-C17	-3.39	118.18	122.92
14	b	4017	BCR	C38-C26-C27	3.39	120.12	113.62
11	2	1235	CLA	CMB-C2B-C3B	3.39	131.02	124.68
14	A	4008	BCR	C19-C18-C17	3.39	124.14	118.94
11	2	1013	CLA	C1-O2A-CGA	3.38	125.33	116.44
11	B	1201	CLA	O2A-CGA-CBA	3.38	122.52	111.91
11	2	1236	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
14	b	4011	BCR	C8-C9-C10	3.38	124.13	118.94
11	A	1137	CLA	C4-C3-C5	3.38	120.96	115.27
14	A	4003	BCR	C30-C25-C26	-3.38	117.85	122.61
14	2	4009	BCR	C3-C4-C5	-3.38	108.04	114.08
14	b	4009	BCR	C23-C22-C21	3.38	124.12	118.94
11	B	1235	CLA	O2A-CGA-CBA	3.38	122.50	111.91
14	A	4002	BCR	C38-C26-C27	3.37	120.10	113.62
11	b	1221	CLA	O2A-CGA-CBA	3.37	122.49	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1237	CLA	O2A-CGA-CBA	3.37	122.48	111.91
11	A	1011	CLA	CMB-C2B-C3B	3.37	130.98	124.68
11	A	1107	CLA	CAA-C2A-C3A	-3.37	103.56	112.78
14	b	4005	BCR	C38-C26-C27	3.37	120.08	113.62
11	a	1127	CLA	C1-C2-C3	-3.37	120.22	126.04
11	B	1021	CLA	O2A-C1-C2	3.37	117.48	108.64
11	a	1123	CLA	CMC-C2C-C1C	3.36	130.16	125.04
14	f	4013	BCR	C37-C22-C21	-3.36	118.21	122.92
11	b	1216	CLA	CMB-C2B-C3B	3.36	130.97	124.68
14	b	4017	BCR	C1-C6-C5	-3.36	117.88	122.61
14	1	4001	BCR	C36-C18-C17	-3.36	118.21	122.92
15	A	5003	LHG	C5-O7-C7	-3.36	109.52	117.79
11	b	1228	CLA	C1-C2-C3	-3.36	121.31	126.75
14	B	4006	BCR	C4-C5-C6	-3.36	117.85	122.73
11	B	1238	CLA	O2A-CGA-CBA	3.36	122.44	111.91
14	8	4022	BCR	C38-C26-C25	-3.36	120.76	124.53
14	b	4017	BCR	C33-C5-C4	3.35	120.06	113.62
11	a	1130	CLA	CMB-C2B-C3B	3.35	130.96	124.68
14	b	4004	BCR	C30-C25-C26	-3.35	117.89	122.61
11	2	1239	CLA	O2A-CGA-CBA	3.35	125.48	112.23
11	2	1234	CLA	C1-C2-C3	-3.35	120.24	126.04
11	k	1402	CLA	C1-C2-C3	-3.35	121.33	126.75
11	L	1501	CLA	O2A-C1-C2	3.35	117.44	108.64
11	2	1221	CLA	O2A-CGA-CBA	3.35	122.42	111.91
11	1	1022	CLA	C4D-C3D-CAD	3.35	110.34	108.47
14	B	4014	BCR	C38-C26-C27	3.35	120.05	113.62
11	B	1219	CLA	CMB-C2B-C3B	3.35	130.94	124.68
11	2	1202	CLA	C1-C2-C3	-3.34	120.26	126.04
11	a	1126	CLA	CMC-C2C-C1C	3.34	130.13	125.04
14	2	4011	BCR	C28-C27-C26	-3.34	108.11	114.08
11	2	1204	CLA	O2A-C1-C2	3.34	117.42	108.64
14	2	4014	BCR	C19-C18-C17	3.34	124.07	118.94
11	B	1206	CLA	OBD-CAD-C3D	-3.34	122.44	127.98
14	6	4018	BCR	C34-C9-C10	-3.34	118.25	122.92
11	A	1111	CLA	C1-C2-C3	-3.34	120.27	126.04
11	2	1210	CLA	C1-C2-C3	-3.34	120.27	126.04
14	2	4004	BCR	C33-C5-C4	3.34	120.02	113.62
11	2	1230	CLA	O2A-CGA-CBA	3.34	122.37	111.91
11	1	1102	CLA	CMC-C2C-C1C	3.33	130.12	125.04
11	2	1221	CLA	C4-C3-C5	3.33	120.88	115.27
14	b	4006	BCR	C4-C5-C6	-3.33	117.89	122.73
14	b	4011	BCR	C28-C27-C26	-3.33	108.13	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1107	CLA	C1-O2A-CGA	3.33	125.19	116.44
14	m	4021	BCR	C38-C26-C25	-3.33	120.79	124.53
11	1	1124	CLA	C1-C2-C3	-3.33	120.28	126.04
11	A	1127	CLA	C9-C8-C10	3.33	123.35	111.29
11	1	1101	CLA	O2A-C1-C2	3.33	117.38	108.64
11	A	1120	CLA	O2A-CGA-CBA	3.33	125.38	112.23
14	b	4006	BCR	C33-C5-C6	-3.33	120.79	124.53
11	2	1207	CLA	C1-O2A-CGA	3.32	125.17	116.44
11	a	1011	CLA	CHB-C4A-NA	3.32	129.11	124.51
11	b	1235	CLA	C9-C8-C7	3.32	123.32	111.29
11	A	1135	CLA	C4-C3-C5	3.32	119.78	115.98
14	2	4004	BCR	C34-C9-C10	-3.32	118.28	122.92
14	b	4006	BCR	C34-C9-C10	-3.31	118.28	122.92
11	A	1011	CLA	CHB-C4A-NA	3.31	129.09	124.51
11	A	1140	CLA	C1-C2-C3	-3.31	120.32	126.04
11	1	1125	CLA	O2A-CGA-CBA	3.31	122.29	111.91
11	B	1238	CLA	O2A-C1-C2	3.31	117.33	108.64
11	a	1139	CLA	CMC-C2C-C1C	3.31	130.08	125.04
11	a	1109	CLA	CMC-C2C-C1C	3.31	130.07	125.04
14	1	4001	BCR	C33-C5-C6	-3.30	120.82	124.53
11	2	1021	CLA	CHB-C4A-NA	3.30	129.08	124.51
11	B	1236	CLA	OBD-CAD-C3D	-3.30	122.50	127.98
14	a	4001	BCR	C23-C22-C21	3.30	124.00	118.94
11	B	1220	CLA	CAC-C3C-C4C	3.30	129.09	124.81
11	2	1023	CLA	C1-O2A-CGA	3.30	125.10	116.44
14	2	4010	BCR	C36-C18-C17	-3.29	118.31	122.92
11	1	1123	CLA	CMC-C2C-C1C	3.29	130.05	125.04
11	2	1235	CLA	CMC-C2C-C1C	3.29	130.05	125.04
11	B	1204	CLA	O2A-C1-C2	3.29	117.27	108.64
14	b	4009	BCR	C34-C9-C10	-3.28	118.32	122.92
11	2	1214	CLA	O2A-CGA-CBA	3.28	122.21	111.91
14	a	4002	BCR	C23-C22-C21	3.28	123.98	118.94
14	6	4020	BCR	C28-C27-C26	-3.28	108.22	114.08
11	A	1115	CLA	O2A-CGA-CBA	3.28	125.18	112.23
14	m	4021	BCR	C37-C22-C21	-3.27	118.34	122.92
11	1	1137	CLA	C4-C3-C2	-3.27	115.28	123.68
11	1	1105	CLA	O2A-C1-C2	3.27	120.55	109.49
14	a	4007	BCR	C7-C8-C9	-3.27	121.30	126.23
14	A	4003	BCR	C34-C9-C10	-3.27	118.35	122.92
11	B	1239	CLA	O2A-CGA-CBA	3.27	125.14	112.23
14	8	4022	BCR	C33-C5-C4	3.27	119.89	113.62
11	B	1236	CLA	O2A-C1-C2	3.26	120.41	108.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1012	CLA	C3C-C4C-NC	3.26	114.23	110.57
14	B	4014	BCR	C30-C25-C26	-3.26	118.02	122.61
14	2	4004	BCR	C7-C8-C9	-3.26	121.31	126.23
11	A	1125	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
14	A	4001	BCR	C4-C5-C6	-3.25	118.01	122.73
14	F	4013	BCR	C36-C18-C17	-3.25	118.37	122.92
11	1	1106	CLA	C1-O2A-CGA	3.25	124.97	116.44
11	1	1123	CLA	CAC-C3C-C4C	3.25	129.03	124.81
11	b	1236	CLA	O2A-C1-C2	3.25	120.36	108.42
11	A	1012	CLA	C9-C8-C10	3.25	123.06	111.29
11	1	1237	CLA	C4-C3-C5	3.25	120.73	115.27
14	L	4022	BCR	C34-C9-C10	-3.25	118.37	122.92
14	a	4003	BCR	C23-C22-C21	3.25	123.92	118.94
11	A	1111	CLA	CAC-C3C-C4C	3.25	129.02	124.81
11	2	1210	CLA	CAC-C3C-C4C	3.25	129.02	124.81
11	a	1123	CLA	CAC-C3C-C4C	3.24	129.02	124.81
11	B	1225	CLA	O2A-CGA-CBA	3.24	122.08	111.91
11	b	1013	CLA	C1-O2A-CGA	3.24	124.95	116.44
14	A	4001	BCR	C30-C25-C26	-3.24	118.05	122.61
11	b	1234	CLA	C1-C2-C3	-3.24	120.44	126.04
14	2	4009	BCR	C33-C5-C4	3.24	119.84	113.62
11	1	1120	CLA	O2A-CGA-CBA	3.24	125.02	112.23
14	L	4022	BCR	C38-C26-C27	3.23	119.83	113.62
11	a	1103	CLA	C4-C3-C5	3.23	120.71	115.27
11	1	1107	CLA	C4-C3-C5	3.23	120.71	115.27
11	A	1127	CLA	OBD-CAD-CBD	-3.23	121.28	125.89
11	B	1222	CLA	C4-C3-C2	-3.23	115.39	123.68
11	A	1012	CLA	C1-C2-C3	-3.23	120.46	126.04
14	1	4001	BCR	C35-C13-C14	-3.23	118.40	122.92
11	A	1118	CLA	CMC-C2C-C1C	3.23	129.95	125.04
11	2	1204	CLA	O2A-CGA-CBA	3.23	122.04	111.91
11	1	1137	CLA	CMB-C2B-C3B	3.23	130.71	124.68
11	b	1202	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
11	a	1127	CLA	CAC-C3C-C4C	3.22	128.99	124.81
14	b	4014	BCR	C38-C26-C27	3.22	119.80	113.62
14	2	4006	BCR	C23-C24-C25	-3.21	118.18	127.20
14	1	4003	BCR	C30-C25-C24	3.21	124.86	115.78
11	A	1105	CLA	CMC-C2C-C1C	3.21	129.93	125.04
14	L	4022	BCR	C37-C22-C21	-3.21	118.43	122.92
11	B	1204	CLA	O2A-CGA-CBA	3.21	121.97	111.91
14	2	4010	BCR	C33-C5-C4	3.20	119.77	113.62
11	2	1213	CLA	CAC-C3C-C2C	3.20	133.01	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1239	CLA	O2A-CGA-CBA	3.20	124.89	112.23
14	A	4008	BCR	C27-C26-C25	-3.20	118.08	122.73
11	A	1121	CLA	O2A-CGA-CBA	3.20	124.89	112.23
14	b	4009	BCR	C7-C8-C9	-3.20	121.40	126.23
12	B	2002	PQN	C24-C23-C25	3.20	122.86	111.29
11	A	1119	CLA	CMB-C2B-C3B	3.20	130.66	124.68
14	b	4017	BCR	C34-C9-C8	3.19	123.11	118.08
11	2	1217	CLA	CAC-C3C-C4C	3.19	128.95	124.81
14	b	4014	BCR	C30-C25-C26	-3.19	118.12	122.61
14	F	4020	BCR	C19-C18-C17	3.19	123.84	118.94
14	6	4018	BCR	C33-C5-C4	3.19	119.74	113.62
14	2	4010	BCR	C38-C26-C27	3.19	119.74	113.62
11	a	1137	CLA	C4-C3-C2	-3.19	115.50	123.68
11	2	1023	CLA	C4-C3-C5	3.19	120.63	115.27
11	b	1210	CLA	C1-C2-C3	-3.18	120.54	126.04
14	1	4002	BCR	C38-C26-C27	3.18	119.73	113.62
11	8	1502	CLA	O2A-CGA-CBA	3.18	124.80	112.23
11	1	1237	CLA	O2A-CGA-CBA	3.18	121.89	111.91
11	b	1207	CLA	C1-O2A-CGA	3.18	124.79	116.44
11	a	1011	CLA	C4D-C3D-CAD	3.18	110.24	108.47
11	a	1107	CLA	C4-C3-C2	-3.18	115.53	123.68
11	1	1103	CLA	C1-C2-C3	-3.18	120.55	126.04
14	b	4014	BCR	C38-C26-C25	-3.18	120.96	124.53
14	A	4003	BCR	C30-C25-C24	3.18	124.76	115.78
11	A	1011	CLA	O2D-CGD-CBD	3.18	116.91	111.27
14	2	4017	BCR	C34-C9-C8	3.17	123.08	118.08
11	a	1103	CLA	C11-C12-C13	-3.17	105.66	115.92
11	B	1205	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
11	A	1110	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
11	a	1121	CLA	O2A-CGA-CBA	3.17	124.75	112.23
14	2	4004	BCR	C30-C25-C26	-3.17	118.16	122.61
11	a	1121	CLA	CMC-C2C-C1C	3.17	129.86	125.04
14	B	4005	BCR	C38-C26-C27	3.16	119.70	113.62
14	A	4008	BCR	C35-C13-C14	-3.16	118.50	122.92
14	B	4010	BCR	C38-C26-C27	3.16	119.69	113.62
11	A	1132	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
14	f	4020	BCR	C36-C18-C17	-3.16	118.50	122.92
11	2	1213	CLA	C3C-C4C-NC	3.15	114.11	110.57
11	A	1107	CLA	CMB-C2B-C3B	3.15	130.58	124.68
11	1	1122	CLA	C9-C8-C10	3.15	122.71	111.29
11	1	1110	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	2	4009	BCR	C1-C6-C5	-3.15	118.17	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4011	BCR	C8-C9-C10	3.15	123.77	118.94
14	2	4004	BCR	C24-C23-C22	-3.15	121.48	126.23
11	b	1221	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	1	4008	BCR	C24-C23-C22	-3.15	121.48	126.23
11	a	1138	CLA	CAC-C3C-C4C	3.15	128.89	124.81
11	B	1214	CLA	C1-C2-C3	-3.15	120.60	126.04
14	1	4008	BCR	C30-C25-C26	-3.14	118.19	122.61
11	2	1205	CLA	CMC-C2C-C1C	3.14	129.82	125.04
11	a	1133	CLA	O2A-CGA-CBA	3.14	124.63	112.23
11	A	1119	CLA	O2A-CGA-CBA	3.14	121.75	111.91
11	1	1118	CLA	CMC-C2C-C1C	3.14	129.81	125.04
14	2	4010	BCR	C23-C24-C25	-3.14	118.40	127.20
14	B	4004	BCR	C30-C25-C26	-3.13	118.20	122.61
14	l	4022	BCR	C33-C5-C4	3.13	119.64	113.62
14	B	4009	BCR	C37-C22-C21	-3.13	118.53	122.92
14	2	4017	BCR	C38-C26-C27	3.13	119.64	113.62
14	B	4017	BCR	C15-C14-C13	-3.13	122.84	127.31
14	B	4010	BCR	C36-C18-C17	-3.13	118.54	122.92
11	2	1216	CLA	C9-C8-C10	3.13	122.63	111.29
11	2	1231	CLA	CMA-C3A-C4A	-3.13	103.36	111.77
14	L	4022	BCR	C3-C4-C5	-3.13	108.50	114.08
11	B	1231	CLA	CAC-C3C-C4C	3.12	128.86	124.81
14	2	4004	BCR	C36-C18-C17	-3.12	118.55	122.92
11	a	1237	CLA	CMC-C2C-C1C	3.12	129.79	125.04
11	l	1502	CLA	CMC-C2C-C1C	3.12	129.79	125.04
11	A	1139	CLA	C1-C2-C3	-3.12	121.70	126.75
14	A	4007	BCR	C34-C9-C8	3.12	122.99	118.08
14	b	4010	BCR	C28-C27-C26	-3.12	108.51	114.08
11	b	1223	CLA	CAC-C3C-C4C	3.12	128.86	124.81
11	2	1231	CLA	CMC-C2C-C1C	3.12	129.79	125.04
11	B	1221	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	A	4008	BCR	C38-C26-C25	-3.11	121.03	124.53
11	2	1236	CLA	O2A-C1-C2	3.11	119.86	108.42
14	F	4018	BCR	C33-C5-C4	3.11	119.59	113.62
14	b	4004	BCR	C34-C9-C10	-3.11	118.57	122.92
14	l	4022	BCR	C7-C8-C9	-3.11	121.54	126.23
14	l	4022	BCR	C38-C26-C27	3.11	119.58	113.62
11	b	1213	CLA	CMC-C2C-C1C	3.11	129.77	125.04
14	6	4020	BCR	C27-C26-C25	-3.10	118.22	122.73
11	a	1106	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
14	a	4001	BCR	C38-C26-C27	3.10	119.58	113.62
14	b	4010	BCR	C33-C5-C4	3.10	119.57	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4014	BCR	C33-C5-C4	3.10	119.57	113.62
14	B	4014	BCR	C33-C5-C4	3.10	119.57	113.62
11	8	1501	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
11	1	1111	CLA	CHB-C4A-NA	3.10	128.80	124.51
11	A	1119	CLA	C1-O2A-CGA	3.10	124.57	116.44
14	6	4018	BCR	C38-C26-C27	3.10	119.56	113.62
11	1	1140	CLA	C9-C8-C7	3.10	122.50	111.29
11	A	1115	CLA	CMC-C2C-C1C	3.09	129.75	125.04
14	1	4008	BCR	C27-C26-C25	-3.09	118.24	122.73
11	1	1115	CLA	OBD-CAD-C3D	-3.09	122.84	127.98
14	M	4021	BCR	C19-C18-C17	3.09	123.68	118.94
11	1	1137	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
11	2	1219	CLA	O2A-C1-C2	3.09	116.75	108.64
11	1	1119	CLA	C4-C3-C5	3.09	120.46	115.27
11	1	1126	CLA	CMC-C2C-C1C	3.08	129.74	125.04
14	8	4022	BCR	C37-C22-C21	-3.08	118.60	122.92
14	1	4002	BCR	C3-C4-C5	-3.08	108.57	114.08
11	a	1140	CLA	C1-O2A-CGA	3.08	124.53	116.44
14	b	4017	BCR	C4-C5-C6	-3.08	118.25	122.73
14	2	4017	BCR	C27-C26-C25	-3.08	118.26	122.73
11	A	1126	CLA	C9-C8-C10	3.08	122.45	111.29
11	2	1202	CLA	CMB-C2B-C3B	3.08	130.44	124.68
14	2	4011	BCR	C38-C26-C27	3.08	119.53	113.62
11	A	1126	CLA	CMB-C2B-C3B	3.07	130.43	124.68
14	2	4017	BCR	C33-C5-C4	3.07	119.52	113.62
11	8	1501	CLA	C1-C2-C3	-3.07	120.73	126.04
11	1	1118	CLA	O2A-C1-C2	3.07	116.71	108.64
11	b	1216	CLA	C9-C8-C10	3.07	122.42	111.29
11	a	1130	CLA	O2A-CGA-CBA	3.07	124.37	112.23
11	a	1114	CLA	O2A-CGA-CBA	3.07	124.37	112.23
11	A	1113	CLA	CMC-C2C-C1C	3.07	129.72	125.04
14	M	4021	BCR	C37-C22-C21	-3.07	118.63	122.92
11	l	1503	CLA	C4-C3-C5	3.07	120.43	115.27
14	B	4005	BCR	C36-C18-C17	-3.06	118.63	122.92
11	A	1237	CLA	C4-C3-C5	3.06	120.42	115.27
14	B	4017	BCR	C33-C5-C4	3.06	119.49	113.62
11	2	1023	CLA	CHB-C4A-NA	3.06	128.74	124.51
11	b	1204	CLA	O2A-C1-C2	3.06	116.67	108.64
14	F	4020	BCR	C23-C24-C25	-3.06	118.62	127.20
11	B	1217	CLA	O2A-C1-C2	3.06	119.65	108.42
11	1	1128	CLA	C9-C8-C7	3.05	122.36	111.29
11	2	1205	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1122	CLA	C4-C3-C5	3.05	120.41	115.27
14	F	4020	BCR	C24-C23-C22	-3.05	121.62	126.23
11	A	1116	CLA	CMC-C2C-C1C	3.05	129.69	125.04
14	b	4017	BCR	C36-C18-C17	-3.05	118.65	122.92
11	b	1232	CLA	CMC-C2C-C1C	3.05	129.69	125.04
11	2	1209	CLA	CAC-C3C-C4C	3.05	128.77	124.81
11	8	1502	CLA	C3C-C4C-NC	3.05	113.99	110.57
11	2	1220	CLA	O2A-CGA-CBA	3.05	124.27	112.23
11	a	1111	CLA	CAC-C3C-C4C	3.05	128.76	124.81
11	A	1126	CLA	CMC-C2C-C1C	3.04	129.68	125.04
11	B	1235	CLA	C1-O2A-CGA	3.04	124.43	116.44
11	1	1139	CLA	CMC-C2C-C1C	3.04	129.67	125.04
11	a	1012	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
11	a	1801	CLA	C1-O2A-CGA	3.04	124.43	116.44
11	a	1135	CLA	C1-C2-C3	-3.04	120.78	126.04
14	F	4020	BCR	C36-C18-C17	-3.04	118.66	122.92
11	A	1105	CLA	O2A-C1-C2	3.04	119.77	109.49
14	B	4014	BCR	C3-C4-C5	-3.04	108.65	114.08
11	A	1127	CLA	OBD-CAD-C3D	-3.04	122.94	127.98
11	b	1220	CLA	O2A-CGA-CBA	3.04	124.23	112.23
11	2	1217	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
14	B	4011	BCR	C33-C5-C4	3.03	119.44	113.62
14	1	4003	BCR	C36-C18-C17	-3.03	118.67	122.92
11	a	1012	CLA	CMC-C2C-C1C	3.03	129.66	125.04
11	2	1222	CLA	CMC-C2C-C1C	3.03	129.65	125.04
14	B	4011	BCR	C38-C26-C25	-3.03	121.13	124.53
14	F	4020	BCR	C38-C26-C27	3.03	119.44	113.62
14	b	4006	BCR	C37-C22-C21	-3.03	118.68	122.92
11	a	1106	CLA	C4-C3-C5	3.03	120.36	115.27
14	A	4002	BCR	C31-C1-C6	-3.03	105.39	110.30
11	b	1203	CLA	C9-C8-C7	3.03	122.25	111.29
14	f	4020	BCR	C38-C26-C27	3.03	119.43	113.62
14	2	4011	BCR	C37-C22-C21	-3.02	118.69	122.92
11	A	1103	CLA	O2A-CGA-CBA	3.02	121.40	111.91
14	2	4006	BCR	C36-C18-C17	-3.02	118.69	122.92
14	B	4004	BCR	C24-C23-C22	-3.02	121.67	126.23
14	1	4007	BCR	C33-C5-C4	3.02	119.42	113.62
11	A	1134	CLA	CAC-C3C-C4C	3.02	128.73	124.81
11	a	1135	CLA	C4-C3-C5	3.02	119.43	115.98
11	1	1132	CLA	O2A-CGA-CBA	3.02	121.37	111.91
11	a	1122	CLA	C4-C3-C5	3.01	120.34	115.27
14	1	4003	BCR	C30-C25-C26	-3.01	118.37	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1236	CLA	CMC-C2C-C1C	3.01	129.63	125.04
11	b	1212	CLA	CMC-C2C-C1C	3.01	129.63	125.04
11	A	1129	CLA	O2A-CGA-CBA	3.01	124.14	112.23
14	6	4020	BCR	C33-C5-C4	3.01	119.40	113.62
14	B	4014	BCR	C38-C26-C25	-3.01	121.15	124.53
11	A	1137	CLA	C4-C3-C2	-3.01	115.95	123.68
11	1	1012	CLA	C9-C8-C7	3.01	122.19	111.29
11	2	1221	CLA	C1-O2A-CGA	3.01	124.34	116.44
14	a	4008	BCR	C1-C6-C5	-3.01	118.38	122.61
14	7	4021	BCR	C37-C22-C21	-3.01	118.71	122.92
11	2	1224	CLA	C1-C2-C3	-3.01	120.84	126.04
14	a	4001	BCR	C19-C18-C17	3.00	123.55	118.94
14	A	4001	BCR	C38-C26-C27	3.00	119.39	113.62
11	a	1117	CLA	C9-C8-C7	3.00	122.17	111.29
14	A	4002	BCR	C37-C22-C21	-3.00	118.72	122.92
11	2	1219	CLA	C4-C3-C5	3.00	120.32	115.27
11	b	1214	CLA	C4-C3-C5	3.00	120.32	115.27
14	6	4020	BCR	C8-C9-C10	3.00	123.55	118.94
14	a	4002	BCR	C33-C5-C4	3.00	119.38	113.62
11	2	1235	CLA	C4-C3-C5	3.00	120.31	115.27
11	a	1126	CLA	CMB-C2B-C3B	3.00	130.28	124.68
11	a	1134	CLA	O2A-CGA-CBA	3.00	124.07	112.23
11	B	1201	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
14	B	4006	BCR	C23-C24-C25	-2.99	118.79	127.20
11	2	1217	CLA	O2A-C1-C2	2.99	119.42	108.42
11	B	1220	CLA	O2A-CGA-CBA	2.99	124.06	112.23
11	a	1126	CLA	C1-C2-C3	-2.99	120.87	126.04
11	A	1134	CLA	O2A-CGA-CBA	2.99	124.04	112.23
11	A	1120	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	1	4022	BCR	C34-C9-C10	-2.99	118.74	122.92
14	2	4006	BCR	C33-C5-C6	-2.99	121.17	124.53
11	a	1140	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	7	4021	BCR	C36-C18-C17	-2.98	118.74	122.92
11	1	1140	CLA	C4-C3-C5	2.98	120.29	115.27
11	b	1023	CLA	C1-C2-C3	-2.98	120.89	126.04
14	2	4010	BCR	C34-C9-C10	-2.98	118.75	122.92
14	b	4010	BCR	C38-C26-C27	2.98	119.34	113.62
12	b	2002	PQN	C24-C23-C25	2.98	122.09	111.29
11	2	1205	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
14	2	4017	BCR	C7-C8-C9	-2.98	121.73	126.23
14	2	4014	BCR	C3-C4-C5	-2.98	108.76	114.08
11	A	1126	CLA	C1-C2-C3	-2.98	120.89	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1221	CLA	C3C-C4C-NC	2.98	113.91	110.57
14	b	4005	BCR	C36-C18-C17	-2.98	118.75	122.92
14	f	4018	BCR	C38-C26-C25	-2.98	121.18	124.53
14	b	4004	BCR	C33-C5-C4	2.98	119.34	113.62
14	B	4005	BCR	C27-C26-C25	-2.98	118.41	122.73
11	1	1126	CLA	C9-C8-C10	2.98	122.07	111.29
11	B	1211	CLA	CMB-C2B-C3B	2.98	130.25	124.68
14	b	4014	BCR	C33-C5-C4	2.98	119.33	113.62
11	1	1103	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
11	2	1214	CLA	C1-C2-C3	-2.98	120.90	126.04
11	a	1111	CLA	C9-C8-C7	2.98	122.07	111.29
14	2	4004	BCR	C23-C22-C21	2.97	123.51	118.94
11	a	1137	CLA	C9-C8-C7	2.97	122.06	111.29
11	b	1203	CLA	CMC-C2C-C1C	2.97	129.57	125.04
11	1	1134	CLA	O2A-CGA-CBA	2.97	123.98	112.23
11	A	1137	CLA	CMC-C2C-C1C	2.97	129.56	125.04
11	A	1122	CLA	C1-O2A-CGA	2.97	124.24	116.44
14	1	4001	BCR	C38-C26-C25	-2.97	121.19	124.53
11	1	1112	CLA	CMC-C2C-C1C	2.97	129.56	125.04
14	B	4011	BCR	C27-C26-C25	-2.97	118.42	122.73
11	B	1214	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
11	1	1103	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	A	5001	LHG	C5-O7-C7	-2.97	110.49	117.79
14	1	4008	BCR	C23-C24-C25	-2.97	118.87	127.20
11	B	1209	CLA	CMB-C2B-C3B	2.96	130.22	124.68
11	B	1215	CLA	C4-C3-C2	-2.96	116.08	123.68
11	a	1128	CLA	C9-C8-C7	2.96	122.00	111.29
14	b	4004	BCR	C24-C23-C22	-2.96	121.77	126.23
11	1	1127	CLA	C1-C2-C3	-2.95	120.94	126.04
14	f	4020	BCR	C33-C5-C4	2.95	119.29	113.62
14	a	4002	BCR	C3-C4-C5	-2.95	108.80	114.08
11	A	1102	CLA	CMC-C2C-C1C	2.95	129.54	125.04
14	b	4017	BCR	C30-C25-C26	-2.95	118.46	122.61
11	b	1204	CLA	CMC-C2C-C1C	2.95	129.53	125.04
14	2	4017	BCR	C33-C5-C6	-2.95	121.22	124.53
11	B	1013	CLA	C9-C8-C10	2.95	121.97	111.29
11	a	1113	CLA	CMC-C2C-C1C	2.95	129.53	125.04
11	1	1133	CLA	O2A-CGA-CBA	2.95	123.89	112.23
14	2	4004	BCR	C19-C18-C17	2.95	123.46	118.94
14	1	4008	BCR	C38-C26-C25	-2.95	121.22	124.53
14	B	4011	BCR	C37-C22-C21	-2.95	118.80	122.92
14	1	4003	BCR	C38-C26-C25	-2.95	121.22	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1232	CLA	CAC-C3C-C4C	2.95	128.63	124.81
11	1	1123	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
11	a	1129	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
14	2	4006	BCR	C38-C26-C27	2.94	119.27	113.62
11	b	1221	CLA	C3C-C4C-NC	2.94	113.87	110.57
11	B	1204	CLA	CMC-C2C-C1C	2.94	129.52	125.04
11	B	1227	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
11	1	1012	CLA	OBD-CAD-C3D	-2.94	123.10	127.98
14	b	4004	BCR	C3-C4-C5	-2.94	108.83	114.08
11	B	1226	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
14	6	4018	BCR	C37-C22-C21	-2.93	118.81	122.92
11	b	1236	CLA	CMC-C2C-C1C	2.93	129.51	125.04
14	A	4008	BCR	C3-C4-C5	-2.93	108.84	114.08
14	8	4019	BCR	C19-C18-C17	2.93	123.44	118.94
14	a	4001	BCR	C15-C14-C13	-2.93	123.13	127.31
11	b	1217	CLA	O2A-C1-C2	2.93	119.19	108.42
11	a	1138	CLA	O2A-CGA-CBA	2.93	123.82	112.23
11	2	1216	CLA	CMC-C2C-C1C	2.93	129.50	125.04
11	1	1136	CLA	O2A-CGA-CBA	2.93	123.81	112.23
11	2	1211	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	F	4020	BCR	C28-C27-C26	-2.93	108.85	114.08
14	8	4019	BCR	C28-C27-C26	-2.93	108.85	114.08
11	2	1226	CLA	CMB-C2B-C3B	2.93	130.16	124.68
11	a	1125	CLA	C1-C2-C3	-2.93	120.98	126.04
11	1	1114	CLA	O2A-CGA-CBA	2.93	123.80	112.23
14	A	4003	BCR	C33-C5-C4	2.93	119.24	113.62
11	2	1234	CLA	CMC-C2C-C1C	2.93	129.50	125.04
14	B	4006	BCR	C36-C18-C17	-2.92	118.83	122.92
11	2	1201	CLA	C1-O2A-CGA	2.92	124.11	116.44
14	B	4006	BCR	C15-C14-C13	-2.92	123.14	127.31
11	b	1202	CLA	CMC-C2C-C1C	2.92	129.49	125.04
14	A	4008	BCR	C30-C25-C26	-2.92	118.50	122.61
11	A	1106	CLA	CMC-C2C-C1C	2.92	129.49	125.04
11	A	1137	CLA	OBD-CAD-C3D	-2.92	123.13	127.98
14	1	4007	BCR	C38-C26-C27	2.92	119.22	113.62
11	2	1013	CLA	CMB-C2B-C3B	2.92	130.14	124.68
11	2	1211	CLA	CMC-C2C-C1C	2.92	129.48	125.04
11	b	1236	CLA	CMB-C2B-C3B	2.92	130.14	124.68
14	2	4006	BCR	C8-C9-C10	2.92	123.42	118.94
11	B	1209	CLA	CAC-C3C-C4C	2.92	128.60	124.81
14	A	4003	BCR	C36-C18-C17	-2.92	118.84	122.92
11	a	1102	CLA	CMC-C2C-C1C	2.92	129.48	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1011	CLA	CHA-C1A-NA	-2.92	119.72	126.40
11	b	1211	CLA	CMC-C2C-C1C	2.92	129.48	125.04
14	1	4001	BCR	C38-C26-C27	2.91	119.22	113.62
11	B	1222	CLA	C3C-C4C-NC	2.91	113.84	110.57
11	a	1104	CLA	CMC-C2C-C1C	2.91	129.48	125.04
11	b	1234	CLA	CAC-C3C-C4C	2.91	128.59	124.81
11	b	1211	CLA	O2A-CGA-CBA	2.91	123.74	112.23
11	B	1231	CLA	CMB-C2B-C3B	2.91	130.12	124.68
11	a	1012	CLA	C3C-C4C-NC	2.91	113.83	110.57
11	1	1127	CLA	CMC-C2C-C1C	2.91	129.47	125.04
11	1	1125	CLA	CMC-C2C-C1C	2.91	129.47	125.04
11	b	1238	CLA	CMB-C2B-C3B	2.91	130.12	124.68
11	A	1137	CLA	C9-C8-C10	2.91	121.82	111.29
14	a	4001	BCR	C1-C6-C5	-2.91	118.52	122.61
11	A	1114	CLA	O2A-CGA-CBA	2.91	123.72	112.23
14	6	4013	BCR	C30-C25-C24	2.91	124.00	115.78
14	1	4003	BCR	C38-C26-C27	2.91	119.20	113.62
14	1	4003	BCR	C33-C5-C4	2.91	119.20	113.62
14	B	4017	BCR	C34-C9-C8	2.90	122.65	118.08
11	2	1225	CLA	CMB-C2B-C3B	2.90	130.11	124.68
11	2	1204	CLA	CMC-C2C-C1C	2.90	129.46	125.04
11	L	1502	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
11	2	1226	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
11	a	1137	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
11	A	1801	CLA	CMC-C2C-C3C	2.90	134.00	126.12
11	B	1239	CLA	CMC-C2C-C1C	2.90	129.46	125.04
11	A	1801	CLA	C3C-C4C-NC	2.90	113.83	110.57
11	A	1134	CLA	CMB-C2B-C3B	2.90	130.11	124.68
14	B	4010	BCR	C15-C14-C13	-2.90	123.17	127.31
11	2	1225	CLA	O2A-CGA-CBA	2.90	121.01	111.91
11	2	1235	CLA	C9-C8-C7	2.90	121.79	111.29
11	B	1212	CLA	CMC-C2C-C1C	2.90	129.45	125.04
11	1	1011	CLA	CHB-C4A-NA	2.90	128.52	124.51
11	b	1210	CLA	CMC-C2C-C1C	2.90	129.45	125.04
11	l	1502	CLA	C3C-C4C-NC	2.90	113.82	110.57
11	a	1126	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
11	B	1222	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
11	B	1224	CLA	C3C-C4C-NC	2.90	113.82	110.57
11	8	1502	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
14	F	4020	BCR	C33-C5-C4	2.90	119.18	113.62
11	1	1130	CLA	O2A-CGA-CBA	2.90	123.67	112.23
11	2	1231	CLA	CAC-C3C-C4C	2.89	128.56	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1122	CLA	CMC-C2C-C1C	2.89	129.45	125.04
11	2	1216	CLA	C3C-C4C-NC	2.89	113.82	110.57
11	1	1129	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
11	a	1138	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
11	b	1225	CLA	CMB-C2B-C3B	2.89	130.09	124.68
11	A	1109	CLA	CMC-C2C-C1C	2.89	129.44	125.04
14	B	4011	BCR	C8-C9-C10	2.89	123.38	118.94
11	a	1011	CLA	CED-O2D-CGD	2.89	122.47	115.94
11	A	1137	CLA	C3C-C4C-NC	2.89	113.81	110.57
11	B	1222	CLA	CMC-C2C-C1C	2.89	129.44	125.04
11	B	1236	CLA	CMC-C2C-C1C	2.89	129.44	125.04
11	1	1131	CLA	CMC-C2C-C1C	2.89	129.44	125.04
11	2	1204	CLA	C1-C2-C3	-2.89	121.05	126.04
11	b	1230	CLA	C3C-C4C-NC	2.89	113.81	110.57
14	2	4006	BCR	C19-C18-C17	2.89	123.37	118.94
11	a	1114	CLA	CMC-C2C-C1C	2.89	129.44	125.04
14	m	4021	BCR	C19-C18-C17	2.89	123.37	118.94
14	2	4004	BCR	C3-C4-C5	-2.89	108.92	114.08
11	2	1021	CLA	CMB-C2B-C3B	2.88	130.07	124.68
11	B	1205	CLA	C1-C2-C3	-2.88	121.06	126.04
14	B	4004	BCR	C37-C22-C21	-2.88	118.89	122.92
11	1	1102	CLA	CMB-C2B-C3B	2.88	130.07	124.68
11	l	1502	CLA	O2A-CGA-CBA	2.88	123.62	112.23
11	1	1105	CLA	CMC-C2C-C1C	2.88	129.43	125.04
11	a	1109	CLA	C9-C8-C10	2.88	121.72	111.29
14	2	4005	BCR	C38-C26-C27	2.88	119.14	113.62
11	2	1202	CLA	CMC-C2C-C1C	2.88	129.42	125.04
14	2	4006	BCR	C1-C6-C7	2.88	123.92	115.78
11	l	1503	CLA	CMC-C2C-C1C	2.88	129.42	125.04
11	A	1012	CLA	C3C-C4C-NC	2.88	113.80	110.57
11	1	1111	CLA	C9-C8-C7	2.88	121.71	111.29
11	B	1214	CLA	C9-C8-C7	2.88	121.71	111.29
11	A	1111	CLA	CMC-C2C-C1C	2.88	129.42	125.04
14	b	4010	BCR	C24-C23-C22	-2.88	121.89	126.23
14	B	4009	BCR	C38-C26-C27	2.88	119.14	113.62
15	2	5004	LHG	O8-C23-C24	2.87	120.93	111.91
14	A	4001	BCR	C7-C8-C9	-2.87	121.89	126.23
11	2	1235	CLA	CAC-C3C-C4C	2.87	128.54	124.81
14	2	4014	BCR	C38-C26-C27	2.87	119.13	113.62
11	2	1229	CLA	CMC-C2C-C1C	2.87	129.41	125.04
11	A	1012	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
11	1	1137	CLA	C9-C8-C10	2.87	121.69	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1122	CLA	C3C-C4C-NC	2.87	113.79	110.57
11	b	1222	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
11	a	1106	CLA	CMC-C2C-C1C	2.87	129.41	125.04
11	1	1126	CLA	CMB-C2B-C3B	2.87	130.04	124.68
14	b	4014	BCR	C37-C22-C21	-2.87	118.91	122.92
11	b	1218	CLA	CMC-C2C-C1C	2.87	129.41	125.04
11	A	1133	CLA	O2A-CGA-CBA	2.87	123.56	112.23
14	6	4013	BCR	C15-C14-C13	-2.87	123.22	127.31
11	B	1207	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	8	4019	BCR	C38-C26-C27	2.87	119.12	113.62
15	B	5004	LHG	C5-O7-C7	-2.86	110.74	117.79
11	2	1230	CLA	C3C-C4C-NC	2.86	113.78	110.57
11	A	1128	CLA	C1-C2-C3	-2.86	121.09	126.04
14	a	4008	BCR	C4-C5-C6	-2.86	118.57	122.73
11	A	1122	CLA	C3C-C4C-NC	2.86	113.78	110.57
11	B	1212	CLA	CMB-C2B-C3B	2.86	130.03	124.68
11	1	1115	CLA	O2A-CGA-CBA	2.86	123.55	112.23
15	1	5003	LHG	O8-C23-C24	2.86	120.89	111.91
11	2	1013	CLA	C9-C8-C10	2.86	121.65	111.29
14	F	4020	BCR	C34-C9-C10	-2.86	118.92	122.92
11	b	1202	CLA	CMB-C2B-C3B	2.86	130.03	124.68
11	2	1220	CLA	CMC-C2C-C1C	2.86	129.39	125.04
14	a	4003	BCR	C30-C25-C24	2.86	123.86	115.78
11	A	1011	CLA	C4-C3-C5	2.86	120.08	115.27
11	B	1201	CLA	CMB-C2B-C3B	2.86	130.02	124.68
14	b	4005	BCR	C37-C22-C21	-2.86	118.92	122.92
11	B	1235	CLA	CMC-C2C-C1C	2.86	129.39	125.04
11	b	1220	CLA	C3C-C4C-NC	2.86	113.77	110.57
11	A	1101	CLA	CMC-C2C-C1C	2.85	129.39	125.04
11	2	1223	CLA	OBD-CAD-C3D	-2.85	123.24	127.98
11	A	1127	CLA	CMC-C2C-C1C	2.85	129.38	125.04
11	a	1136	CLA	O2A-CGA-CBA	2.85	123.50	112.23
15	a	5001	LHG	O8-C23-C24	2.85	120.86	111.91
11	A	1130	CLA	O2A-CGA-CBA	2.85	123.50	112.23
11	2	1231	CLA	CMB-C2B-C3B	2.85	130.01	124.68
14	2	4009	BCR	C34-C9-C10	-2.85	118.93	122.92
11	b	1236	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
11	1	1101	CLA	CMC-C2C-C1C	2.85	129.38	125.04
11	2	1222	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
11	A	1135	CLA	CMC-C2C-C1C	2.85	129.37	125.04
11	1	1135	CLA	C3C-C4C-NC	2.85	113.76	110.57
15	A	5003	LHG	O8-C23-C24	2.84	120.83	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4004	BCR	C36-C18-C17	-2.84	118.94	122.92
11	b	1021	CLA	C1-O2A-CGA	2.84	123.90	116.44
11	2	1223	CLA	C3C-C4C-NC	2.84	113.76	110.57
11	B	1208	CLA	CMC-C2C-C1C	2.84	129.37	125.04
11	2	1223	CLA	C1-C2-C3	-2.84	121.13	126.04
14	b	4005	BCR	C30-C25-C26	-2.84	118.61	122.61
11	A	1136	CLA	O2A-CGA-CBA	2.84	123.46	112.23
11	a	1126	CLA	C3C-C4C-NC	2.84	113.75	110.57
14	8	4022	BCR	C3-C4-C5	-2.84	109.01	114.08
11	a	1112	CLA	CMC-C2C-C1C	2.84	129.36	125.04
11	B	1226	CLA	C9-C8-C7	2.84	121.57	111.29
11	a	1801	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
11	B	1209	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
11	1	1138	CLA	CED-O2D-CGD	2.84	122.36	115.94
14	B	4004	BCR	C33-C5-C4	2.84	119.07	113.62
14	A	4008	BCR	C8-C9-C10	2.84	123.30	118.94
11	a	1132	CLA	C1-C2-C3	-2.84	121.14	126.04
14	6	4013	BCR	C33-C5-C4	2.84	119.07	113.62
11	2	1225	CLA	CMC-C2C-C1C	2.84	129.36	125.04
11	1	1129	CLA	O2A-CGA-CBA	2.84	123.44	112.23
11	A	1801	CLA	C1-C2-C3	-2.83	121.14	126.04
11	A	1118	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
11	2	1205	CLA	O2A-C1-C2	2.83	116.08	108.64
11	2	1238	CLA	CMC-C2C-C1C	2.83	129.35	125.04
11	A	1135	CLA	CMB-C2B-C3B	2.83	129.98	124.68
14	b	4014	BCR	C3-C4-C5	-2.83	109.02	114.08
14	B	4010	BCR	C19-C18-C17	2.83	123.29	118.94
11	B	1207	CLA	C1-O2A-CGA	2.83	123.87	116.44
11	B	1238	CLA	C4-C3-C5	2.83	120.03	115.27
11	1	1111	CLA	CMC-C2C-C1C	2.83	129.35	125.04
11	1	1130	CLA	CMB-C2B-C3B	2.83	129.97	124.68
14	b	4011	BCR	C37-C22-C21	-2.83	118.96	122.92
14	2	4005	BCR	C36-C18-C17	-2.83	118.96	122.92
11	b	1219	CLA	CMC-C2C-C1C	2.83	129.34	125.04
11	1	1801	CLA	C3C-C4C-NC	2.83	113.74	110.57
11	a	1115	CLA	C3C-C4C-NC	2.83	113.74	110.57
11	2	1221	CLA	CMC-C2C-C1C	2.83	129.34	125.04
11	a	1105	CLA	C1-O2A-CGA	2.82	123.85	116.44
14	A	4007	BCR	C3-C4-C5	-2.82	109.04	114.08
11	A	1101	CLA	C3C-C4C-NC	2.82	113.74	110.57
14	f	4013	BCR	C33-C5-C4	2.82	119.04	113.62
11	k	1402	CLA	CMB-C2B-C3B	2.82	129.96	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1209	CLA	CAC-C3C-C4C	2.82	128.47	124.81
14	L	4022	BCR	C19-C18-C17	2.82	123.27	118.94
11	B	1224	CLA	C1-C2-C3	-2.82	121.17	126.04
11	a	1107	CLA	C3C-C4C-NC	2.82	113.73	110.57
11	1	1138	CLA	O2A-CGA-CBA	2.82	123.37	112.23
11	b	1227	CLA	CMC-C2C-C1C	2.82	129.33	125.04
15	1	5001	LHG	O8-C23-C24	2.82	120.75	111.91
11	B	1240	CLA	CMC-C2C-C1C	2.82	129.33	125.04
14	a	4003	BCR	C36-C18-C17	-2.82	118.98	122.92
11	1	1104	CLA	CMC-C2C-C1C	2.82	129.33	125.04
11	b	1235	CLA	C1-O2A-CGA	2.82	123.83	116.44
11	2	1221	CLA	C3C-C4C-NC	2.82	113.73	110.57
11	2	1213	CLA	CMB-C2B-C3B	2.82	129.95	124.68
11	b	1208	CLA	CMC-C2C-C1C	2.81	129.32	125.04
14	F	4013	BCR	C37-C22-C21	-2.81	118.98	122.92
11	B	1211	CLA	O2A-CGA-CBA	2.81	123.35	112.23
11	b	1231	CLA	CMC-C2C-C1C	2.81	129.32	125.04
11	B	1229	CLA	C1-C2-C3	-2.81	121.18	126.04
11	a	1121	CLA	CAC-C3C-C4C	2.81	128.46	124.81
11	2	1208	CLA	CMC-C2C-C1C	2.81	129.32	125.04
11	B	1223	CLA	C3C-C4C-NC	2.81	113.72	110.57
11	a	1134	CLA	CED-O2D-CGD	2.81	122.29	115.94
11	1	1133	CLA	CAC-C3C-C4C	2.81	128.45	124.81
11	K	1402	CLA	CMB-C2B-C3B	2.81	129.93	124.68
14	8	4019	BCR	C36-C18-C17	-2.81	118.99	122.92
11	l	1502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
11	2	1203	CLA	C4-C3-C5	2.80	119.99	115.27
11	A	1129	CLA	C3C-C4C-NC	2.80	113.72	110.57
14	M	4021	BCR	C24-C23-C22	-2.80	122.00	126.23
11	1	1012	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
11	b	1013	CLA	CMB-C2B-C3B	2.80	129.92	124.68
14	B	4010	BCR	C30-C25-C26	-2.80	118.67	122.61
11	B	1219	CLA	C1-C2-C3	-2.80	121.20	126.04
14	a	4007	BCR	C28-C27-C26	-2.80	109.08	114.08
14	b	4011	BCR	C24-C23-C22	-2.80	122.00	126.23
14	a	4003	BCR	C30-C25-C26	-2.80	118.67	122.61
11	b	1227	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
11	B	1235	CLA	CMB-C2B-C3B	2.80	129.91	124.68
11	1	1110	CLA	CMC-C2C-C1C	2.80	129.30	125.04
11	A	1101	CLA	C1-C2-C3	-2.80	121.20	126.04
11	b	1205	CLA	C1-C2-C3	-2.80	121.21	126.04
14	F	4013	BCR	C33-C5-C4	2.80	118.99	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1215	CLA	C4-C3-C2	-2.79	116.51	123.68
11	a	1124	CLA	CMB-C2B-C3B	2.79	129.91	124.68
14	a	4001	BCR	C7-C8-C9	-2.79	122.01	126.23
11	L	1503	CLA	CMC-C2C-C1C	2.79	129.29	125.04
11	a	1801	CLA	CMB-C2B-C3B	2.79	129.91	124.68
11	A	1022	CLA	CMB-C2B-C3B	2.79	129.90	124.68
11	1	1129	CLA	CMC-C2C-C1C	2.79	129.29	125.04
11	2	1210	CLA	C9-C8-C7	2.79	121.40	111.29
11	B	1210	CLA	C1-C2-C3	-2.79	121.22	126.04
11	2	1203	CLA	CMC-C2C-C1C	2.79	129.29	125.04
11	1	1132	CLA	C1-O2A-CGA	2.79	123.76	116.44
11	a	1123	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
11	2	1238	CLA	CMB-C2B-C3B	2.79	129.90	124.68
11	B	1225	CLA	CMC-C2C-C1C	2.79	129.28	125.04
11	B	1205	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
11	a	1105	CLA	CMC-C2C-C1C	2.79	129.28	125.04
14	b	4014	BCR	C23-C22-C21	2.79	123.22	118.94
14	l	4019	BCR	C36-C18-C17	-2.79	119.02	122.92
11	1	1106	CLA	CMC-C2C-C1C	2.79	129.28	125.04
11	b	1235	CLA	CMC-C2C-C1C	2.78	129.28	125.04
11	B	1210	CLA	C9-C8-C7	2.78	121.37	111.29
11	2	1210	CLA	CMB-C2B-C3B	2.78	129.88	124.68
14	B	4006	BCR	C37-C22-C21	-2.78	119.03	122.92
11	a	1137	CLA	CMB-C2B-C3B	2.78	129.88	124.68
14	a	4001	BCR	C38-C26-C25	-2.78	121.40	124.53
11	2	1224	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	1	4002	BCR	C33-C5-C4	2.78	118.96	113.62
11	1	1115	CLA	CMB-C2B-C3B	2.78	129.88	124.68
14	m	4021	BCR	C27-C26-C25	-2.78	118.69	122.73
11	B	1221	CLA	C4-C3-C5	2.78	119.95	115.27
11	b	1220	CLA	CMB-C2B-C3B	2.78	129.88	124.68
11	2	1023	CLA	OBD-CAD-C3D	-2.78	123.37	127.98
11	2	1214	CLA	CMC-C2C-C1C	2.78	129.27	125.04
11	a	1132	CLA	CMB-C2B-C3B	2.78	129.88	124.68
11	b	1224	CLA	C1-O2A-CGA	2.78	123.73	116.44
11	a	1107	CLA	CHB-C4A-NA	2.78	128.35	124.51
11	1	1125	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
11	A	1107	CLA	C4-C3-C2	-2.78	116.56	123.68
11	b	1228	CLA	CMB-C2B-C3B	2.78	129.87	124.68
11	B	1213	CLA	CMC-C2C-C1C	2.78	129.27	125.04
14	A	4001	BCR	C33-C5-C4	2.78	118.95	113.62
14	2	4009	BCR	C36-C18-C17	-2.78	119.03	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1137	CLA	C3C-C4C-NC	2.77	113.68	110.57
11	2	1219	CLA	C3C-C4C-NC	2.77	113.68	110.57
11	b	1224	CLA	C3C-C4C-NC	2.77	113.68	110.57
15	1	5001	LHG	C5-O7-C7	-2.77	110.96	117.79
11	A	1138	CLA	O2A-CGA-CBA	2.77	123.19	112.23
14	2	4011	BCR	C33-C5-C4	2.77	118.94	113.62
11	b	1215	CLA	C4-C3-C2	-2.77	116.57	123.68
11	A	1107	CLA	C3C-C4C-NC	2.77	113.68	110.57
11	1	1126	CLA	C1-C2-C3	-2.77	121.25	126.04
11	A	1116	CLA	C3C-C4C-NC	2.77	113.68	110.57
11	B	1230	CLA	C3C-C4C-NC	2.77	113.68	110.57
11	1	1106	CLA	C4-C3-C5	2.77	119.93	115.27
11	A	1132	CLA	C1-O2A-CGA	2.77	123.71	116.44
11	b	1217	CLA	CMB-C2B-C3B	2.77	129.86	124.68
11	0	1402	CLA	CMB-C2B-C3B	2.77	129.86	124.68
11	a	1129	CLA	O2A-CGA-CBA	2.77	123.16	112.23
14	2	4011	BCR	C24-C23-C22	-2.77	122.06	126.23
14	2	4017	BCR	C15-C14-C13	-2.77	123.36	127.31
14	B	4004	BCR	C36-C18-C17	-2.76	119.05	122.92
11	a	1119	CLA	C1-C2-C3	-2.76	121.26	126.04
14	l	4022	BCR	C23-C22-C21	2.76	123.18	118.94
11	1	1125	CLA	C4-C3-C5	2.76	119.92	115.27
11	2	1214	CLA	C1-O2A-CGA	2.76	123.69	116.44
11	1	1135	CLA	CMC-C2C-C1C	2.76	129.24	125.04
14	A	4002	BCR	C15-C14-C13	-2.76	123.37	127.31
11	a	1116	CLA	CMB-C2B-C3B	2.76	129.84	124.68
11	a	1103	CLA	CMC-C2C-C1C	2.76	129.24	125.04
11	1	1120	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
11	2	1232	CLA	CMC-C2C-C1C	2.76	129.24	125.04
11	A	1103	CLA	CMB-C2B-C3B	2.76	129.83	124.68
14	f	4018	BCR	C34-C9-C10	-2.76	119.06	122.92
11	1	1112	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
11	1	1012	CLA	C9-C8-C10	2.75	121.27	111.29
11	a	1237	CLA	C4-C3-C5	2.75	119.90	115.27
11	b	1211	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
11	a	1102	CLA	CMB-C2B-C3B	2.75	129.83	124.68
11	A	1103	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
11	a	1104	CLA	C4-C3-C5	2.75	119.90	115.27
11	L	1502	CLA	O2A-CGA-CBA	2.75	123.11	112.23
11	b	1214	CLA	C9-C8-C10	2.75	121.26	111.29
11	A	1112	CLA	CMC-C2C-C1C	2.75	129.23	125.04
11	b	1226	CLA	C9-C8-C7	2.75	121.25	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1111	CLA	C4-C3-C5	2.75	119.90	115.27
11	B	1223	CLA	OBD-CAD-CBD	-2.75	121.97	125.89
11	b	1231	CLA	CMB-C2B-C3B	2.75	129.82	124.68
14	f	4020	BCR	C3-C4-C5	-2.75	109.17	114.08
11	1	1116	CLA	CMC-C2C-C1C	2.75	129.22	125.04
11	2	1023	CLA	C9-C8-C7	2.75	121.25	111.29
11	1	1110	CLA	CAC-C3C-C4C	2.75	128.38	124.81
11	B	1203	CLA	CMC-C2C-C1C	2.75	129.22	125.04
14	A	4003	BCR	C38-C26-C27	2.75	118.89	113.62
14	a	4007	BCR	C38-C26-C27	2.75	118.89	113.62
14	b	4006	BCR	C23-C24-C25	-2.75	119.48	127.20
14	b	4004	BCR	C19-C18-C17	2.75	123.16	118.94
11	b	1214	CLA	C1-O2A-CGA	2.75	123.65	116.44
11	l	1501	CLA	C3C-C4C-NC	2.75	113.65	110.57
11	B	1023	CLA	C3C-C4C-NC	2.75	113.65	110.57
11	2	1226	CLA	C3C-C4C-NC	2.75	113.65	110.57
11	A	1113	CLA	C3C-C4C-NC	2.75	113.65	110.57
11	B	1226	CLA	CMC-C2C-C1C	2.75	129.22	125.04
11	b	1226	CLA	CMC-C2C-C1C	2.74	129.22	125.04
14	7	4021	BCR	C38-C26-C27	2.74	118.89	113.62
11	b	1222	CLA	C4-C3-C2	-2.74	116.65	123.68
11	A	1127	CLA	C3C-C4C-NC	2.74	113.64	110.57
14	f	4018	BCR	C36-C18-C17	-2.74	119.09	122.92
11	2	1228	CLA	CMB-C2B-C3B	2.74	129.80	124.68
11	2	1223	CLA	CMC-C2C-C1C	2.74	129.21	125.04
14	b	4011	BCR	C33-C5-C4	2.74	118.87	113.62
14	6	4013	BCR	C36-C18-C17	-2.74	119.09	122.92
11	l	1501	CLA	CMC-C2C-C1C	2.74	129.21	125.04
11	b	1226	CLA	C3C-C4C-NC	2.74	113.64	110.57
11	a	1118	CLA	CMC-C2C-C1C	2.74	129.21	125.04
11	A	1110	CLA	CMC-C2C-C1C	2.73	129.20	125.04
11	1	1104	CLA	C4-C3-C5	2.73	119.87	115.27
14	2	4011	BCR	C23-C24-C25	-2.73	119.52	127.20
11	1	1107	CLA	C3C-C4C-NC	2.73	113.64	110.57
11	8	1502	CLA	CMB-C2B-C3B	2.73	129.79	124.68
11	a	1127	CLA	OBD-CAD-C3D	-2.73	123.44	127.98
14	1	4008	BCR	C3-C4-C5	-2.73	109.20	114.08
11	l	1501	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
11	A	1118	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
11	1	1121	CLA	CMC-C2C-C1C	2.73	129.20	125.04
11	A	1124	CLA	CAC-C3C-C4C	2.73	128.35	124.81
14	1	4001	BCR	C33-C5-C4	2.73	118.86	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1021	CLA	CMC-C2C-C1C	2.73	129.20	125.04
15	A	5001	LHG	O8-C23-C24	2.73	120.48	111.91
11	A	1107	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
11	A	1119	CLA	CAC-C3C-C4C	2.73	128.35	124.81
14	b	4004	BCR	C37-C22-C21	-2.73	119.10	122.92
14	8	4022	BCR	C19-C18-C17	2.73	123.13	118.94
11	8	1503	CLA	CMC-C2C-C1C	2.73	129.19	125.04
11	1	1104	CLA	C9-C8-C7	2.73	121.17	111.29
11	A	1120	CLA	CMB-C2B-C3B	2.73	129.78	124.68
11	1	1124	CLA	CMB-C2B-C3B	2.73	129.78	124.68
11	a	1127	CLA	CED-O2D-CGD	2.73	122.11	115.94
14	B	4005	BCR	C3-C4-C5	-2.73	109.21	114.08
11	a	1140	CLA	C9-C8-C7	2.73	121.17	111.29
15	a	5003	LHG	O8-C23-C24	2.73	120.46	111.91
11	A	1127	CLA	CMB-C2B-C3B	2.73	129.78	124.68
11	1	1110	CLA	C4-C3-C5	2.73	119.86	115.27
11	a	1122	CLA	C3C-C4C-NC	2.73	113.63	110.57
14	6	4020	BCR	C23-C24-C25	-2.72	119.55	127.20
14	8	4022	BCR	C27-C26-C25	-2.72	118.78	122.73
11	A	1102	CLA	CMB-C2B-C3B	2.72	129.77	124.68
11	a	1120	CLA	C3C-C4C-NC	2.72	113.62	110.57
11	B	1234	CLA	CMC-C2C-C1C	2.72	129.19	125.04
11	b	1021	CLA	CBA-CAA-C2A	2.72	121.90	113.86
11	a	1131	CLA	C1-C2-C3	-2.72	121.33	126.04
11	b	1230	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
11	a	1127	CLA	C4-C3-C5	2.72	119.85	115.27
11	A	1112	CLA	C3C-C4C-NC	2.72	113.62	110.57
11	1	1108	CLA	CMC-C2C-C1C	2.72	129.18	125.04
11	B	1013	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
11	a	1122	CLA	CMB-C2B-C3B	2.72	129.76	124.68
11	a	1011	CLA	CMC-C2C-C1C	2.72	129.18	125.04
11	a	1022	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	B	4011	BCR	C35-C13-C12	2.72	122.36	118.08
11	2	1023	CLA	CAC-C3C-C4C	2.72	128.33	124.81
11	2	1238	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
11	a	1139	CLA	CAC-C3C-C4C	2.72	128.33	124.81
11	b	1225	CLA	CMC-C2C-C1C	2.72	129.17	125.04
11	b	1216	CLA	C1-C2-C3	-2.71	121.35	126.04
11	B	1013	CLA	CED-O2D-CGD	2.71	122.08	115.94
14	B	4005	BCR	C15-C14-C13	-2.71	123.44	127.31
11	B	1234	CLA	C1-C2-C3	-2.71	121.35	126.04
11	a	1125	CLA	C6-C5-C3	-2.71	110.18	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4001	BCR	C30-C25-C26	-2.71	118.79	122.61
11	1	1140	CLA	C1-O2A-CGA	2.71	123.56	116.44
11	B	1238	CLA	CMC-C2C-C1C	2.71	129.17	125.04
11	a	1131	CLA	CMC-C2C-C1C	2.71	129.17	125.04
11	A	1137	CLA	C9-C8-C7	2.71	121.11	111.29
11	1	1134	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
11	b	1208	CLA	CAC-C3C-C4C	2.71	128.33	124.81
14	1	4007	BCR	C37-C22-C21	-2.71	119.13	122.92
11	a	1134	CLA	CMC-C2C-C1C	2.71	129.17	125.04
14	2	4005	BCR	C38-C26-C25	-2.71	121.48	124.53
11	B	1214	CLA	CMC-C2C-C1C	2.71	129.16	125.04
11	A	1111	CLA	C4-C3-C5	2.71	119.83	115.27
11	b	1208	CLA	CAA-CBA-CGA	-2.71	107.77	113.59
11	B	1232	CLA	CMC-C2C-C1C	2.71	129.16	125.04
11	b	1215	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
11	A	1116	CLA	CMB-C2B-C3B	2.71	129.74	124.68
14	B	4011	BCR	C36-C18-C17	-2.71	119.13	122.92
11	1	1113	CLA	C3C-C4C-NC	2.71	113.61	110.57
14	B	4014	BCR	C27-C26-C25	-2.71	118.80	122.73
11	B	1213	CLA	C9-C8-C7	2.71	121.09	111.29
11	2	1212	CLA	CMC-C2C-C1C	2.71	129.16	125.04
11	2	1216	CLA	CMB-C2B-C3B	2.71	129.74	124.68
11	B	1023	CLA	C1-O2A-CGA	2.70	123.54	116.44
11	a	1133	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
14	1	4002	BCR	C31-C1-C6	-2.70	105.91	110.30
11	b	1021	CLA	CMB-C2B-C3B	2.70	129.74	124.68
11	a	1136	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
11	2	1207	CLA	OBD-CAD-C3D	-2.70	123.49	127.98
11	B	1023	CLA	CMB-C2B-C3B	2.70	129.73	124.68
11	b	1207	CLA	C3C-C4C-NC	2.70	113.60	110.57
16	2	5002	LMG	C8-O7-C10	-2.70	111.14	117.79
11	b	1226	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
11	b	1214	CLA	C1-C2-C3	-2.70	121.37	126.04
14	a	4001	BCR	C33-C5-C4	2.70	118.80	113.62
11	l	1503	CLA	CMB-C2B-C3B	2.70	129.73	124.68
14	m	4021	BCR	C15-C14-C13	-2.70	123.46	127.31
11	b	1209	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
11	1	1011	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
11	2	1211	CLA	O2A-CGA-CBA	2.70	122.90	112.23
11	b	1214	CLA	CMC-C2C-C1C	2.70	129.15	125.04
11	B	1219	CLA	CMC-C2C-C1C	2.70	129.15	125.04
11	2	1013	CLA	CHB-C4A-NA	2.70	128.24	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1226	CLA	C3C-C4C-NC	2.70	113.60	110.57
14	b	4006	BCR	C15-C14-C13	-2.70	123.46	127.31
11	b	1021	CLA	CED-O2D-CGD	2.70	122.04	115.94
14	a	4008	BCR	C30-C25-C26	-2.70	118.82	122.61
11	B	1225	CLA	C3C-C4C-NC	2.70	113.59	110.57
11	B	1206	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
11	a	1119	CLA	CMB-C2B-C3B	2.70	129.72	124.68
14	a	4008	BCR	C36-C18-C17	-2.69	119.15	122.92
11	1	1012	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	A	4002	BCR	C23-C22-C21	2.69	123.08	118.94
11	b	1230	CLA	CAC-C3C-C4C	2.69	128.31	124.81
11	2	1218	CLA	CMC-C2C-C1C	2.69	129.14	125.04
11	1	1134	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	a	4007	BCR	C36-C18-C17	-2.69	119.15	122.92
11	2	1023	CLA	CMB-C2B-C3B	2.69	129.72	124.68
11	b	1222	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	7	4021	BCR	C34-C9-C10	-2.69	119.15	122.92
11	a	1108	CLA	CMC-C2C-C1C	2.69	129.14	125.04
11	2	1224	CLA	C3C-C4C-NC	2.69	113.59	110.57
11	1	1109	CLA	C9-C8-C10	2.69	121.04	111.29
14	a	4003	BCR	C34-C9-C10	-2.69	119.15	122.92
14	L	4019	BCR	C8-C9-C10	2.69	123.07	118.94
11	A	1122	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
11	B	1240	CLA	C3C-C4C-NC	2.69	113.59	110.57
11	A	1136	CLA	CMC-C2C-C1C	2.69	129.13	125.04
11	b	1201	CLA	C1-C2-C3	-2.69	121.39	126.04
11	2	1214	CLA	CAA-CBA-CGA	-2.69	105.40	113.25
11	2	1226	CLA	C9-C8-C10	2.68	121.01	111.29
11	b	1223	CLA	C1-C2-C3	-2.68	121.40	126.04
11	b	1213	CLA	C4-C3-C2	-2.68	116.79	123.68
11	b	1213	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
11	A	1122	CLA	C9-C8-C10	2.68	121.01	111.29
11	2	1216	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
11	A	1237	CLA	C3C-C4C-NC	2.68	113.58	110.57
11	B	1207	CLA	C3C-C4C-NC	2.68	113.58	110.57
11	b	1023	CLA	C9-C8-C7	2.68	121.00	111.29
14	1	4001	BCR	C34-C9-C10	-2.68	119.17	122.92
11	2	1213	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
11	b	1216	CLA	CMC-C2C-C1C	2.68	129.12	125.04
11	b	1224	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	1	4007	BCR	C28-C27-C26	-2.68	109.29	114.08
11	L	1501	CLA	C3C-C4C-NC	2.68	113.58	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1202	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	B	4017	BCR	C36-C18-C17	-2.68	119.17	122.92
11	a	1110	CLA	CMC-C2C-C1C	2.68	129.12	125.04
11	2	1021	CLA	C9-C8-C7	2.68	120.99	111.29
14	B	4017	BCR	C4-C5-C6	-2.68	118.84	122.73
14	M	4021	BCR	C23-C22-C21	2.68	123.05	118.94
11	1	1115	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
11	a	1103	CLA	C1-C2-C3	-2.67	121.42	126.04
11	2	1212	CLA	CAA-CBA-CGA	-2.67	107.84	113.59
14	2	4006	BCR	C24-C23-C22	-2.67	122.20	126.23
11	A	1102	CLA	CHB-C4A-NA	2.67	128.21	124.51
11	2	1013	CLA	C4-C3-C5	2.67	119.76	115.27
11	B	1228	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
11	2	1221	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
11	2	1227	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
14	b	4010	BCR	C23-C24-C25	-2.67	119.71	127.20
11	B	1224	CLA	C4-C3-C5	2.67	119.76	115.27
11	a	1127	CLA	C9-C8-C10	2.67	120.95	111.29
11	1	1022	CLA	CMC-C2C-C1C	2.67	129.10	125.04
12	a	2001	PQN	C2M-C2-C3	-2.67	120.05	124.40
11	B	1231	CLA	CMC-C2C-C1C	2.66	129.10	125.04
11	b	1232	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
11	B	1023	CLA	C9-C8-C7	2.66	120.93	111.29
11	A	1137	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
11	A	1116	CLA	CAC-C3C-C4C	2.66	128.26	124.81
11	1	1140	CLA	C3C-C4C-NC	2.66	113.56	110.57
11	A	1110	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
14	b	4017	BCR	C8-C9-C10	2.66	123.02	118.94
12	b	2002	PQN	C2M-C2-C3	-2.66	120.06	124.40
11	1	1140	CLA	CMC-C2C-C1C	2.66	129.09	125.04
11	a	1140	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
11	1	1103	CLA	CMC-C2C-C1C	2.66	129.09	125.04
14	l	4019	BCR	C7-C8-C9	-2.66	122.22	126.23
11	A	1113	CLA	CMB-C2B-C3B	2.66	129.65	124.68
11	a	1125	CLA	C3C-C4C-NC	2.66	113.55	110.57
11	b	1223	CLA	C3C-C4C-NC	2.66	113.55	110.57
11	2	1206	CLA	CMC-C2C-C1C	2.66	129.09	125.04
11	B	1214	CLA	C3C-C4C-NC	2.66	113.55	110.57
11	B	1218	CLA	CMC-C2C-C1C	2.66	129.09	125.04
11	2	1207	CLA	CAC-C3C-C4C	2.66	128.26	124.81
11	l	1503	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
11	b	1225	CLA	CAC-C3C-C4C	2.66	128.25	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4006	BCR	C23-C22-C21	2.65	123.02	118.94
11	B	1224	CLA	CMC-C2C-C1C	2.65	129.08	125.04
11	1	1124	CLA	CMC-C2C-C1C	2.65	129.08	125.04
11	8	1501	CLA	CMB-C2B-C3B	2.65	129.65	124.68
11	A	1104	CLA	C4-C3-C5	2.65	119.73	115.27
11	a	1129	CLA	C3C-C4C-NC	2.65	113.55	110.57
11	a	1120	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	2	1230	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
14	m	4021	BCR	C34-C9-C10	-2.65	119.21	122.92
11	A	1103	CLA	C9-C8-C7	2.65	120.90	111.29
11	k	1401	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	B	1236	CLA	C3C-C4C-NC	2.65	113.55	110.57
11	2	1231	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	L	1501	CLA	C1-O2A-CGA	2.65	123.40	116.44
11	a	1125	CLA	CMC-C2C-C1C	2.65	129.08	125.04
11	1	1119	CLA	CMC-C2C-C1C	2.65	129.08	125.04
11	0	1401	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	2	1209	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
11	B	1204	CLA	C4-C3-C5	2.65	119.73	115.27
11	a	1132	CLA	CMC-C2C-C1C	2.65	129.07	125.04
11	b	1021	CLA	C9-C8-C7	2.65	120.89	111.29
11	1	1131	CLA	C9-C8-C10	2.65	120.89	111.29
11	A	1106	CLA	C1-O2A-CGA	2.65	123.39	116.44
11	1	1129	CLA	C3C-C4C-NC	2.65	113.54	110.57
14	a	4007	BCR	C3-C4-C5	-2.65	109.35	114.08
11	a	1022	CLA	C3C-C4C-NC	2.65	113.54	110.57
12	A	2001	PQN	C2M-C2-C3	-2.65	120.08	124.40
11	a	1110	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
11	2	1202	CLA	C4-C3-C5	2.65	119.72	115.27
11	2	1219	CLA	CMC-C2C-C1C	2.65	129.07	125.04
11	2	1230	CLA	CMB-C2B-C3B	2.65	129.63	124.68
11	1	1122	CLA	CMB-C2B-C3B	2.65	129.63	124.68
11	B	1013	CLA	CHB-C4A-NA	2.65	128.17	124.51
11	a	1124	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
11	1	1111	CLA	C1-O2A-CGA	2.64	123.38	116.44
11	1	1117	CLA	C1-C2-C3	-2.64	121.47	126.04
14	A	4001	BCR	C27-C26-C25	-2.64	118.89	122.73
11	K	1401	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
11	a	1117	CLA	CMC-C2C-C1C	2.64	129.06	125.04
11	A	1123	CLA	CMC-C2C-C1C	2.64	129.06	125.04
11	A	1103	CLA	CMC-C2C-C1C	2.64	129.06	125.04
11	a	1101	CLA	C4-C3-C2	-2.64	116.90	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1117	CLA	CMB-C2B-C3B	2.64	129.62	124.68
11	A	1104	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
14	6	4020	BCR	C3-C4-C5	-2.64	109.36	114.08
14	L	4019	BCR	C36-C18-C17	-2.64	119.22	122.92
11	2	1213	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
11	1	1011	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	m	4021	BCR	C23-C22-C21	2.64	122.99	118.94
11	B	1235	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
11	A	1109	CLA	CED-O2D-CGD	2.64	121.91	115.94
11	2	1211	CLA	C3C-C4C-NC	2.64	113.53	110.57
11	b	1238	CLA	CMC-C2C-C1C	2.64	129.06	125.04
14	B	4017	BCR	C1-C6-C7	2.64	123.24	115.78
11	A	1237	CLA	CMB-C2B-C3B	2.64	129.61	124.68
11	b	1214	CLA	CMB-C2B-C3B	2.64	129.61	124.68
11	k	1401	CLA	CMC-C2C-C1C	2.64	129.05	125.04
11	A	1104	CLA	C9-C8-C7	2.64	120.84	111.29
14	6	4020	BCR	C36-C18-C17	-2.63	119.23	122.92
11	1	1134	CLA	CMB-C2B-C3B	2.63	129.61	124.68
11	1	1101	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	b	4005	BCR	C3-C4-C5	-2.63	109.37	114.08
14	2	4010	BCR	C3-C4-C5	-2.63	109.38	114.08
11	b	1234	CLA	C3C-C4C-NC	2.63	113.52	110.57
14	B	4006	BCR	C38-C26-C27	2.63	118.67	113.62
11	8	1503	CLA	C4-C3-C5	2.63	119.70	115.27
11	A	1120	CLA	OBD-CAD-C3D	-2.63	123.61	127.98
14	B	4010	BCR	C3-C4-C5	-2.63	109.38	114.08
11	a	1112	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
11	B	1013	CLA	CMB-C2B-C3B	2.63	129.60	124.68
11	2	1240	CLA	CMB-C2B-C3B	2.63	129.60	124.68
11	B	1212	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	f	4020	BCR	C28-C27-C26	-2.63	109.38	114.08
11	1	1132	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	B	4017	BCR	C30-C25-C26	-2.63	118.91	122.61
14	L	4019	BCR	C38-C26-C27	2.63	118.66	113.62
14	A	4007	BCR	C15-C14-C13	-2.63	123.56	127.31
14	8	4022	BCR	C34-C9-C8	2.63	122.22	118.08
11	B	1221	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
14	A	4007	BCR	C36-C18-C17	-2.63	119.25	122.92
11	2	1215	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
11	b	1223	CLA	CMC-C2C-C1C	2.63	129.04	125.04
14	6	4018	BCR	C30-C25-C26	-2.63	118.92	122.61
14	6	4018	BCR	C36-C18-C17	-2.62	119.25	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1234	CLA	C4-C3-C5	2.62	119.69	115.27
11	1	1125	CLA	C3C-C4C-NC	2.62	113.51	110.57
11	A	1125	CLA	C6-C5-C3	-2.62	110.33	114.62
11	2	1212	CLA	CMB-C2B-C3B	2.62	129.59	124.68
11	a	1237	CLA	C3C-C4C-NC	2.62	113.51	110.57
14	2	4009	BCR	C23-C24-C25	-2.62	119.84	127.20
11	1	1130	CLA	CMC-C2C-C1C	2.62	129.03	125.04
11	b	1206	CLA	CAC-C3C-C4C	2.62	128.21	124.81
11	L	1502	CLA	C3C-C4C-NC	2.62	113.51	110.57
11	b	1201	CLA	C4-C3-C5	2.62	119.68	115.27
14	a	4008	BCR	C27-C26-C25	-2.62	118.93	122.73
11	b	1202	CLA	C3C-C4C-NC	2.62	113.51	110.57
11	a	1124	CLA	CED-O2D-CGD	2.62	121.86	115.94
11	2	1218	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
11	a	1130	CLA	CMC-C2C-C1C	2.62	129.03	125.04
14	B	4005	BCR	C37-C22-C21	-2.62	119.26	122.92
11	1	1117	CLA	C4-C3-C5	2.62	119.67	115.27
11	A	1125	CLA	CMB-C2B-C3B	2.62	129.57	124.68
11	b	1203	CLA	C4-C3-C5	2.62	119.67	115.27
11	A	1117	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
11	0	1401	CLA	CMC-C2C-C1C	2.62	129.02	125.04
11	a	1140	CLA	C1-C2-C3	-2.62	121.52	126.04
11	b	1240	CLA	C3C-C4C-NC	2.62	113.50	110.57
11	A	1121	CLA	CMB-C2B-C3B	2.62	129.57	124.68
11	A	1110	CLA	C4-C3-C5	2.61	119.67	115.27
11	A	1110	CLA	C1-C2-C3	-2.61	121.52	126.04
11	2	1201	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
11	A	1128	CLA	C3C-C4C-NC	2.61	113.50	110.57
11	b	1205	CLA	CMC-C2C-C1C	2.61	129.02	125.04
11	a	1117	CLA	C1-C2-C3	-2.61	121.53	126.04
11	B	1217	CLA	C3C-C4C-NC	2.61	113.50	110.57
11	B	1228	CLA	CMB-C2B-C3B	2.61	129.56	124.68
11	B	1023	CLA	OBD-CAD-C3D	-2.61	123.65	127.98
11	1	1120	CLA	CMC-C2C-C1C	2.61	129.01	125.04
11	K	1401	CLA	CMC-C2C-C1C	2.61	129.01	125.04
11	1	1110	CLA	C1-C2-C3	-2.61	121.53	126.04
15	B	5004	LHG	O8-C23-C24	2.61	120.10	111.91
11	1	1113	CLA	CMC-C2C-C1C	2.61	129.01	125.04
14	1	4003	BCR	C34-C9-C10	-2.61	119.27	122.92
11	a	1135	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
11	b	1214	CLA	C3C-C4C-NC	2.61	113.50	110.57
11	a	1106	CLA	O1D-CGD-CBD	-2.61	119.15	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1211	CLA	CMB-C2B-C3B	2.61	129.56	124.68
11	A	1131	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
11	2	1224	CLA	CMC-C2C-C1C	2.61	129.01	125.04
14	8	4019	BCR	C34-C9-C10	-2.61	119.27	122.92
11	b	1228	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
11	a	1108	CLA	CAC-C3C-C4C	2.61	128.19	124.81
11	A	1106	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
11	a	1123	CLA	C1-C2-C3	-2.60	121.54	126.04
11	1	1801	CLA	C1-O2A-CGA	2.60	123.28	116.44
16	2	5002	LMG	O8-C28-C29	2.60	120.08	111.91
11	b	1229	CLA	CMC-C2C-C1C	2.60	129.00	125.04
11	b	1239	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
11	b	1214	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
11	1	1115	CLA	CMC-C2C-C1C	2.60	129.00	125.04
14	1	4002	BCR	C34-C9-C10	-2.60	119.28	122.92
11	2	1210	CLA	C3C-C4C-NC	2.60	113.49	110.57
11	2	1214	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
11	a	1117	CLA	CMB-C2B-C3B	2.60	129.54	124.68
11	1	1801	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
11	1	1120	CLA	C3C-C4C-NC	2.60	113.49	110.57
11	A	1012	CLA	CMB-C2B-C3B	2.60	129.54	124.68
14	f	4018	BCR	C35-C13-C12	2.60	122.17	118.08
11	B	1206	CLA	CAC-C3C-C4C	2.60	128.18	124.81
11	a	1115	CLA	CMC-C2C-C1C	2.60	129.00	125.04
11	b	1215	CLA	CMC-C2C-C1C	2.60	129.00	125.04
14	B	4006	BCR	C33-C5-C6	-2.60	121.61	124.53
11	A	1111	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
11	1	1107	CLA	C4-C3-C2	-2.60	117.02	123.68
11	a	1101	CLA	CMC-C2C-C1C	2.60	128.99	125.04
11	1	1139	CLA	CAC-C3C-C4C	2.60	128.18	124.81
14	f	4020	BCR	C34-C9-C10	-2.60	119.29	122.92
11	b	1210	CLA	C3C-C4C-NC	2.59	113.48	110.57
11	b	1021	CLA	C9-C8-C10	2.59	120.69	111.29
11	A	1132	CLA	C1-C2-C3	-2.59	121.56	126.04
11	A	1139	CLA	CMB-C2B-C3B	2.59	129.53	124.68
11	a	1105	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
14	2	4010	BCR	C19-C18-C17	2.59	122.92	118.94
11	1	1118	CLA	OBD-CAD-C3D	-2.59	123.68	127.98
14	2	4011	BCR	C36-C18-C17	-2.59	119.29	122.92
11	B	1221	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	2	1204	CLA	C1-O2A-CGA	2.59	123.24	116.44
11	1	1130	CLA	O2D-CGD-O1D	-2.59	118.78	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1203	CLA	C9-C8-C7	2.59	120.67	111.29
11	A	1108	CLA	CMC-C2C-C1C	2.59	128.98	125.04
14	1	4007	BCR	C34-C9-C10	-2.59	119.30	122.92
11	B	1224	CLA	CMB-C2B-C3B	2.59	129.52	124.68
11	A	1011	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	a	1103	CLA	CMB-C2B-C3B	2.59	129.52	124.68
11	2	1223	CLA	C9-C8-C10	2.59	120.66	111.29
11	1	1114	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	1	1122	CLA	CMC-C2C-C1C	2.59	128.98	125.04
14	l	4022	BCR	C3-C4-C5	-2.58	109.46	114.08
14	b	4004	BCR	C27-C26-C25	-2.58	118.98	122.73
11	2	1210	CLA	CMC-C2C-C1C	2.58	128.97	125.04
11	A	1125	CLA	C3C-C4C-NC	2.58	113.47	110.57
11	1	1115	CLA	C3C-C4C-NC	2.58	113.47	110.57
14	b	4006	BCR	C38-C26-C27	2.58	118.58	113.62
11	a	1123	CLA	CMB-C2B-C3B	2.58	129.51	124.68
11	2	1236	CLA	C3C-C4C-NC	2.58	113.47	110.57
11	B	1221	CLA	C1-O2A-CGA	2.58	123.21	116.44
11	a	1134	CLA	CAC-C3C-C4C	2.58	128.16	124.81
11	a	1127	CLA	CMC-C2C-C1C	2.58	128.97	125.04
11	b	1204	CLA	C1-C2-C3	-2.58	121.58	126.04
11	1	1117	CLA	C9-C8-C7	2.58	120.63	111.29
14	f	4018	BCR	C37-C22-C21	-2.58	119.31	122.92
11	a	1118	CLA	OBD-CAD-C3D	-2.58	123.70	127.98
11	B	1219	CLA	C3C-C4C-NC	2.58	113.46	110.57
11	B	1204	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
11	A	1112	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
11	a	1122	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
11	b	1235	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
11	2	1217	CLA	OBD-CAD-C3D	-2.58	123.70	127.98
11	a	1137	CLA	CMC-C2C-C1C	2.57	128.96	125.04
11	B	1238	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
11	2	1207	CLA	CMC-C2C-C1C	2.57	128.96	125.04
11	L	1501	CLA	CMC-C2C-C1C	2.57	128.96	125.04
14	1	4001	BCR	C19-C18-C17	2.57	122.88	118.94
14	A	4002	BCR	C33-C5-C4	2.57	118.55	113.62
11	a	1011	CLA	C3C-C4C-NC	2.57	113.45	110.57
11	2	1240	CLA	C3C-C4C-NC	2.57	113.45	110.57
11	b	1223	CLA	C4-C3-C5	2.57	119.59	115.27
11	1	1118	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
11	A	1102	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	B	4014	BCR	C19-C18-C17	2.57	122.88	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1216	CLA	CAC-C3C-C4C	2.57	128.14	124.81
11	A	1115	CLA	CMB-C2B-C3B	2.57	129.48	124.68
11	2	1212	CLA	C3C-C4C-NC	2.57	113.45	110.57
11	A	1133	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
11	1	1801	CLA	CAC-C3C-C2C	2.57	131.92	127.53
14	B	4005	BCR	C35-C13-C12	2.57	122.12	118.08
11	1	1132	CLA	CMC-C2C-C1C	2.57	128.95	125.04
11	1	1108	CLA	C3C-C4C-NC	2.57	113.45	110.57
11	b	1208	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	b	4009	BCR	C3-C4-C5	-2.56	109.50	114.08
11	A	1131	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	b	1224	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	8	1501	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	2	1236	CLA	CMB-C2B-C3B	2.56	129.47	124.68
11	1	1125	CLA	C1-C2-C3	-2.56	121.61	126.04
11	2	1239	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	a	1129	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	A	1126	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
11	b	1213	CLA	CMB-C2B-C3B	2.56	129.47	124.68
14	b	4009	BCR	C33-C5-C4	2.56	118.54	113.62
11	b	1203	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
11	A	1122	CLA	CMC-C2C-C1C	2.56	128.94	125.04
14	B	4004	BCR	C34-C9-C10	-2.56	119.34	122.92
11	a	1131	CLA	C4-C3-C5	2.56	119.58	115.27
11	b	1219	CLA	C3C-C4C-NC	2.56	113.44	110.57
12	a	2001	PQN	C14-C13-C15	2.56	119.58	115.27
14	a	4007	BCR	C33-C5-C4	2.56	118.53	113.62
11	1	1114	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
11	a	1123	CLA	C9-C8-C10	2.56	120.56	111.29
11	A	1121	CLA	CMC-C2C-C1C	2.56	128.94	125.04
14	B	4017	BCR	C33-C5-C6	-2.56	121.66	124.53
11	B	1217	CLA	CMB-C2B-C3B	2.56	129.46	124.68
12	B	2002	PQN	C2M-C2-C3	-2.56	120.23	124.40
11	a	1115	CLA	CMB-C2B-C3B	2.56	129.46	124.68
11	1	1125	CLA	C6-C5-C3	-2.56	110.44	114.62
11	A	1118	CLA	C1-C2-C3	-2.56	121.62	126.04
11	B	1201	CLA	C1-O2A-CGA	2.56	123.15	116.44
14	a	4001	BCR	C27-C26-C25	-2.56	119.02	122.73
11	A	1101	CLA	C9-C8-C7	2.56	120.55	111.29
11	b	1023	CLA	C3C-C4C-NC	2.56	113.44	110.57
11	1	1012	CLA	CMB-C2B-C3B	2.56	129.46	124.68
11	B	1230	CLA	CMB-C2B-C3B	2.56	129.46	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1023	CLA	C1-O2A-CGA	2.55	123.15	116.44
11	1	1110	CLA	CMB-C2B-C3B	2.55	129.46	124.68
11	b	1021	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
11	b	1230	CLA	CMB-C2B-C3B	2.55	129.46	124.68
14	B	4005	BCR	C33-C5-C4	2.55	118.52	113.62
11	1	1131	CLA	CMB-C2B-C3B	2.55	129.45	124.68
11	B	1234	CLA	C4-C3-C5	2.55	119.56	115.27
11	a	1101	CLA	C3C-C4C-NC	2.55	113.43	110.57
11	B	1218	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
11	A	1012	CLA	CHB-C4A-NA	2.55	128.04	124.51
11	B	1210	CLA	CMB-C2B-C3B	2.55	129.45	124.68
11	a	1110	CLA	CMB-C2B-C3B	2.55	129.45	124.68
14	1	4002	BCR	C30-C25-C26	-2.55	119.02	122.61
11	b	1023	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	1	2001	PQN	C24-C23-C25	2.55	120.53	111.29
11	b	1217	CLA	CMC-C2C-C1C	2.55	128.92	125.04
11	A	1116	CLA	C4-C3-C5	2.55	119.56	115.27
14	b	4011	BCR	C27-C26-C25	-2.55	119.03	122.73
11	2	1209	CLA	CMB-C2B-C3B	2.55	129.45	124.68
11	B	1214	CLA	CAC-C3C-C4C	2.55	128.12	124.81
11	2	1226	CLA	C9-C8-C7	2.55	120.52	111.29
11	1	1107	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
11	a	1110	CLA	C1-C2-C3	-2.55	121.64	126.04
11	a	1107	CLA	C9-C8-C7	2.55	120.51	111.29
11	B	1212	CLA	C3C-C4C-NC	2.54	113.42	110.57
11	2	1213	CLA	CMC-C2C-C3C	2.54	133.02	126.12
11	2	1210	CLA	C4-C3-C5	2.54	119.55	115.27
11	b	1204	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
11	2	1013	CLA	CED-O2D-CGD	2.54	121.69	115.94
11	1	1104	CLA	C9-C8-C10	2.54	120.50	111.29
11	k	1401	CLA	CAA-C2A-C3A	2.54	119.74	112.78
11	1	1102	CLA	C3C-C4C-NC	2.54	113.42	110.57
11	A	1128	CLA	C9-C8-C7	2.54	120.50	111.29
11	b	1216	CLA	C4-C3-C5	2.54	119.55	115.27
14	b	4017	BCR	C33-C5-C6	-2.54	121.67	124.53
14	B	4004	BCR	C3-C4-C5	-2.54	109.54	114.08
14	A	4007	BCR	C37-C22-C21	-2.54	119.36	122.92
11	2	1235	CLA	C3C-C4C-NC	2.54	113.42	110.57
11	2	1220	CLA	CMB-C2B-C3B	2.54	129.43	124.68
11	A	1136	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
11	a	1116	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
11	B	1239	CLA	O2D-CGD-O1D	-2.54	118.87	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1210	CLA	CMB-C2B-C3B	2.54	129.43	124.68
11	b	1211	CLA	C3C-C4C-NC	2.54	113.42	110.57
11	A	1108	CLA	CMB-C2B-C3B	2.54	129.43	124.68
14	b	4006	BCR	C35-C13-C12	2.54	122.08	118.08
11	A	1130	CLA	CMB-C2B-C3B	2.54	129.43	124.68
11	2	1204	CLA	CMB-C2B-C3B	2.54	129.43	124.68
11	B	1223	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
11	2	1021	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
11	b	1203	CLA	CMB-C2B-C3B	2.54	129.42	124.68
11	B	1234	CLA	C9-C8-C10	2.54	120.47	111.29
11	A	1131	CLA	C1-C2-C3	-2.54	121.66	126.04
11	A	1119	CLA	C9-C8-C10	2.53	120.47	111.29
11	A	1104	CLA	C9-C8-C10	2.53	120.47	111.29
11	l	1501	CLA	C1-O2A-CGA	2.53	123.09	116.44
11	b	1216	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	a	1801	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	1	1103	CLA	CAC-C3C-C4C	2.53	128.10	124.81
11	A	1130	CLA	CMC-C2C-C1C	2.53	128.90	125.04
11	1	1135	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
11	1	1136	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
14	A	4001	BCR	C3-C4-C5	-2.53	109.55	114.08
11	B	1236	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
11	a	1121	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	B	1213	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	a	4003	BCR	C4-C5-C6	-2.53	119.06	122.73
11	B	1214	CLA	CMB-C2B-C3B	2.53	129.41	124.68
11	a	1113	CLA	C3C-C4C-NC	2.53	113.41	110.57
14	f	4018	BCR	C4-C5-C6	-2.53	119.06	122.73
11	b	1201	CLA	CMC-C2C-C1C	2.53	128.89	125.04
11	1	1136	CLA	CMC-C2C-C1C	2.53	128.89	125.04
11	b	1217	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	2	1228	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	A	1134	CLA	CED-O2D-CGD	2.53	121.66	115.94
11	1	1111	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	b	4011	BCR	C23-C24-C25	-2.53	120.10	127.20
11	a	1101	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
11	B	1228	CLA	C1-C2-C3	-2.53	122.66	126.75
12	2	2002	PQN	C2M-C2-C3	-2.53	120.28	124.40
11	2	1023	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	b	5004	LHG	O8-C23-C24	2.53	119.84	111.91
12	A	2001	PQN	C14-C13-C15	2.53	119.52	115.27
12	1	2001	PQN	C14-C13-C15	2.53	119.52	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1211	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	2	1235	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
11	a	1022	CLA	CMB-C2B-C3B	2.53	129.40	124.68
11	a	1111	CLA	C3C-C4C-NC	2.53	113.40	110.57
14	l	4019	BCR	C38-C26-C27	2.53	118.47	113.62
11	K	1401	CLA	CAA-C2A-C3A	2.52	119.69	112.78
11	B	1204	CLA	C1-O2A-CGA	2.52	123.07	116.44
11	A	1140	CLA	C3C-C4C-NC	2.52	113.40	110.57
11	A	1123	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
11	2	1207	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
11	b	1230	CLA	C1-O2A-CGA	2.52	123.07	116.44
11	B	1222	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
14	b	4005	BCR	C19-C18-C17	2.52	122.81	118.94
11	0	1401	CLA	CAA-C2A-C3A	2.52	119.69	112.78
11	B	1210	CLA	C3C-C4C-NC	2.52	113.40	110.57
11	1	1104	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
11	b	1240	CLA	CMC-C2C-C1C	2.52	128.88	125.04
11	1	1109	CLA	CMC-C2C-C1C	2.52	128.88	125.04
11	2	1229	CLA	C3C-C4C-NC	2.52	113.40	110.57
11	1	1103	CLA	C9-C8-C7	2.52	120.42	111.29
14	B	4017	BCR	C23-C24-C25	-2.52	120.12	127.20
11	B	1230	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
11	A	1140	CLA	CAC-C3C-C4C	2.52	128.08	124.81
14	b	4010	BCR	C3-C4-C5	-2.52	109.58	114.08
11	b	1211	CLA	CAC-C3C-C4C	2.52	128.08	124.81
11	2	1205	CLA	C3C-C4C-NC	2.52	113.40	110.57
11	B	1021	CLA	C9-C8-C7	2.52	120.41	111.29
11	b	1206	CLA	OBD-CAD-C3D	-2.52	123.80	127.98
11	B	1226	CLA	C1-C2-C3	-2.52	121.69	126.04
11	B	1231	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
11	2	1203	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
11	1	1140	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
14	1	4007	BCR	C3-C4-C5	-2.52	109.58	114.08
11	0	1402	CLA	CMC-C2C-C1C	2.52	128.87	125.04
11	2	1239	CLA	C3C-C4C-NC	2.52	113.39	110.57
14	l	4022	BCR	C29-C30-C25	-2.52	106.61	110.48
11	1	1110	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
11	2	1232	CLA	CAC-C3C-C4C	2.51	128.07	124.81
11	2	1225	CLA	CAC-C3C-C4C	2.51	128.07	124.81
11	b	1203	CLA	C3C-C4C-NC	2.51	113.39	110.57
11	B	1023	CLA	CMC-C2C-C1C	2.51	128.87	125.04
14	l	4022	BCR	C19-C18-C17	2.51	122.80	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1229	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
11	a	1131	CLA	CMB-C2B-C3B	2.51	129.38	124.68
11	a	1104	CLA	CMB-C2B-C3B	2.51	129.38	124.68
11	B	1201	CLA	C4-C3-C5	2.51	119.49	115.27
11	A	1102	CLA	C9-C8-C7	2.51	120.38	111.29
14	1	4001	BCR	C30-C25-C26	-2.51	119.08	122.61
14	6	4018	BCR	C28-C27-C26	-2.51	109.60	114.08
14	f	4018	BCR	C32-C1-C6	-2.51	106.23	110.30
11	b	1240	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
11	A	1132	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
14	a	4002	BCR	C30-C25-C26	-2.51	119.08	122.61
11	B	1023	CLA	CAC-C3C-C4C	2.51	128.06	124.81
11	a	1104	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
11	a	1132	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
11	a	1113	CLA	CMB-C2B-C3B	2.51	129.37	124.68
14	M	4021	BCR	C23-C24-C25	-2.51	120.17	127.20
11	l	1502	CLA	CMB-C2B-C3B	2.51	129.37	124.68
11	b	1226	CLA	C4-C3-C5	2.50	119.48	115.27
11	a	1118	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
11	b	1023	CLA	CMB-C2B-C3B	2.50	129.36	124.68
11	A	1110	CLA	C3C-C4C-NC	2.50	113.38	110.57
11	2	1217	CLA	C1-O2A-CGA	2.50	124.00	116.73
11	a	1103	CLA	CED-O2D-CGD	2.50	121.60	115.94
14	l	4019	BCR	C19-C18-C17	2.50	122.78	118.94
14	6	4013	BCR	C38-C26-C27	2.50	118.42	113.62
11	a	1114	CLA	CAC-C3C-C4C	2.50	128.06	124.81
11	A	1131	CLA	C3C-C4C-NC	2.50	113.38	110.57
14	A	4001	BCR	C38-C26-C25	-2.50	121.72	124.53
11	a	1103	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
11	A	1125	CLA	CMC-C2C-C1C	2.50	128.85	125.04
14	1	4008	BCR	C1-C6-C5	-2.50	119.09	122.61
11	1	1801	CLA	CMC-C2C-C3C	2.50	132.90	126.12
11	L	1503	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
11	b	1205	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
11	1	1117	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
11	L	1502	CLA	CMB-C2B-C3B	2.50	129.35	124.68
11	A	1103	CLA	CHB-C4A-NA	2.50	127.97	124.51
11	a	1130	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
11	1	1119	CLA	C9-C8-C10	2.50	120.34	111.29
11	2	1228	CLA	CMC-C2C-C1C	2.50	128.84	125.04
11	1	1127	CLA	CMB-C2B-C3B	2.50	129.35	124.68
11	a	1104	CLA	C3C-C4C-NC	2.50	113.37	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1212	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
11	2	1225	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
11	b	1202	CLA	CHB-C4A-NA	2.50	127.96	124.51
14	b	4011	BCR	C15-C14-C13	-2.50	123.75	127.31
11	A	1119	CLA	C3C-C4C-NC	2.50	113.37	110.57
11	a	1111	CLA	C1-C2-C3	-2.49	121.73	126.04
11	A	1130	CLA	C3C-C4C-NC	2.49	113.37	110.57
14	B	4004	BCR	C19-C18-C17	2.49	122.77	118.94
11	A	1124	CLA	CMC-C2C-C1C	2.49	128.84	125.04
11	b	1215	CLA	C9-C8-C10	2.49	120.32	111.29
11	A	1103	CLA	C1-O2A-CGA	2.49	122.99	116.44
11	1	1139	CLA	OBD-CAD-C3D	-2.49	123.84	127.98
11	2	1210	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
14	F	4018	BCR	C8-C9-C10	2.49	122.77	118.94
11	a	1119	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
11	a	1131	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
11	L	1503	CLA	C4-C3-C5	2.49	119.46	115.27
11	b	1232	CLA	CAC-C3C-C4C	2.49	128.04	124.81
14	f	4020	BCR	C19-C18-C17	2.49	122.76	118.94
11	2	1220	CLA	C3C-C4C-NC	2.49	113.36	110.57
11	2	1021	CLA	CMC-C2C-C1C	2.49	128.83	125.04
11	A	1139	CLA	C3C-C4C-NC	2.49	113.36	110.57
14	8	4022	BCR	C7-C8-C9	-2.49	122.47	126.23
11	A	1112	CLA	CHB-C4A-NA	2.49	127.95	124.51
11	a	1110	CLA	C4-C3-C5	2.49	119.46	115.27
11	1	1108	CLA	CMB-C2B-C3B	2.49	129.34	124.68
11	a	1102	CLA	C3C-C4C-NC	2.49	113.36	110.57
11	a	1105	CLA	CAC-C3C-C4C	2.49	128.04	124.81
11	a	1119	CLA	C9-C8-C10	2.49	120.30	111.29
11	2	1236	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
11	B	1238	CLA	CMB-C2B-C3B	2.49	129.33	124.68
14	F	4018	BCR	C37-C22-C21	-2.49	119.44	122.92
14	l	4019	BCR	C28-C27-C26	-2.49	109.64	114.08
11	k	1401	CLA	CHB-C4A-NA	2.49	127.95	124.51
11	1	1118	CLA	C1-O2A-CGA	2.49	122.97	116.44
11	2	1204	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
11	1	1135	CLA	CMB-C2B-C3B	2.49	129.33	124.68
11	b	1221	CLA	CMB-C2B-C3B	2.49	129.33	124.68
11	A	1110	CLA	CMB-C2B-C3B	2.49	129.33	124.68
11	a	1115	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
11	A	1237	CLA	CMC-C2C-C1C	2.48	128.82	125.04
11	A	1130	CLA	O2D-CGD-O1D	-2.48	118.98	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1232	CLA	C3C-C4C-NC	2.48	113.36	110.57
11	B	1203	CLA	C9-C8-C7	2.48	120.29	111.29
11	b	1229	CLA	C3C-C4C-NC	2.48	113.36	110.57
11	B	1201	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
11	b	1021	CLA	C3C-C4C-NC	2.48	113.35	110.57
14	B	4017	BCR	C3-C4-C5	-2.48	109.65	114.08
11	A	1101	CLA	CMB-C2B-C3B	2.48	129.32	124.68
11	B	1235	CLA	C3C-C4C-NC	2.48	113.35	110.57
11	2	1231	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	A	4007	BCR	C35-C13-C12	2.48	121.98	118.08
11	1	1105	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	l	4022	BCR	C35-C13-C12	2.48	121.98	118.08
11	B	1208	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
11	1	1109	CLA	C1-C2-C3	-2.48	121.76	126.04
11	B	1023	CLA	CHB-C4A-NA	2.48	127.94	124.51
11	A	1140	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
11	L	1501	CLA	CMB-C2B-C3B	2.48	129.31	124.68
11	a	1107	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
11	a	1138	CLA	CMC-C2C-C1C	2.48	128.81	125.04
11	2	1203	CLA	CED-O2D-CGD	2.48	121.54	115.94
11	2	1013	CLA	C1-C2-C3	-2.47	121.76	126.04
11	a	1121	CLA	CMB-C2B-C3B	2.47	129.31	124.68
11	A	1111	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	B	1210	CLA	C4-C3-C5	2.47	119.43	115.27
11	a	1125	CLA	C4-C3-C5	2.47	119.43	115.27
14	B	4005	BCR	C34-C9-C10	-2.47	119.46	122.92
11	A	1801	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
11	1	1132	CLA	C1-C2-C3	-2.47	121.77	126.04
11	a	1124	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	A	1128	CLA	C4-C3-C5	2.47	119.43	115.27
11	1	1111	CLA	CMB-C2B-C3B	2.47	129.30	124.68
11	1	1120	CLA	CMB-C2B-C3B	2.47	129.30	124.68
11	1	1119	CLA	CMB-C2B-C3B	2.47	129.30	124.68
11	K	1401	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	1	1022	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	a	1110	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	1	1112	CLA	C3C-C4C-NC	2.47	113.34	110.57
14	l	4022	BCR	C36-C18-C17	-2.47	119.46	122.92
11	a	1136	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	a	1137	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	8	1502	CLA	CMC-C2C-C1C	2.47	128.80	125.04
14	b	4005	BCR	C8-C7-C6	-2.47	120.27	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1114	CLA	CAC-C3C-C4C	2.47	128.01	124.81
11	1	1131	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
11	a	1105	CLA	CMB-C2B-C3B	2.47	129.30	124.68
12	A	2001	PQN	C24-C23-C22	2.47	120.23	111.29
14	B	4011	BCR	C23-C24-C25	-2.47	120.27	127.20
11	0	1401	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	B	1202	CLA	CMC-C2C-C1C	2.47	128.80	125.04
11	a	1104	CLA	C9-C8-C10	2.47	120.23	111.29
11	A	1117	CLA	C1-O2A-CGA	2.47	122.92	116.44
14	B	4006	BCR	C19-C18-C17	2.47	122.73	118.94
11	b	1232	CLA	CMB-C2B-C3B	2.47	129.29	124.68
11	2	1234	CLA	C3C-C4C-NC	2.47	113.34	110.57
11	1	1138	CLA	CMC-C2C-C1C	2.47	128.79	125.04
11	2	1239	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
11	B	1223	CLA	CMC-C2C-C1C	2.47	128.79	125.04
11	2	1206	CLA	C3C-C4C-NC	2.47	113.34	110.57
14	b	4010	BCR	C34-C9-C10	-2.47	119.47	122.92
11	a	1114	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	A	1109	CLA	CMB-C2B-C3B	2.46	129.29	124.68
11	2	1229	CLA	C9-C8-C7	2.46	120.21	111.29
11	k	1402	CLA	CMC-C2C-C1C	2.46	128.79	125.04
14	6	4018	BCR	C32-C1-C6	-2.46	106.31	110.30
11	B	1225	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	a	1138	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	1	1128	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
11	2	1222	CLA	C9-C8-C7	2.46	120.21	111.29
11	L	1503	CLA	C3C-C4C-NC	2.46	113.33	110.57
14	f	4020	BCR	C23-C24-C25	-2.46	120.29	127.20
11	2	1222	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	B	1229	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	8	1502	CLA	OBD-CAD-C3D	-2.46	123.89	127.98
14	f	4018	BCR	C38-C26-C27	2.46	118.34	113.62
11	a	1111	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
14	1	4001	BCR	C35-C13-C12	2.46	121.95	118.08
11	b	1218	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
11	1	1109	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	1	1237	CLA	CAC-C3C-C4C	2.46	128.00	124.81
11	1	1126	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	b	1220	CLA	CMC-C2C-C1C	2.46	128.78	125.04
11	A	1124	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
11	A	1115	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
14	A	4007	BCR	C33-C5-C4	2.46	118.33	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1126	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	1	1136	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	A	1108	CLA	C3C-C4C-NC	2.46	113.33	110.57
11	A	1133	CLA	CAC-C3C-C4C	2.46	128.00	124.81
11	B	1218	CLA	CMB-C2B-C3B	2.46	129.27	124.68
11	B	1215	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
11	a	1140	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	2	1023	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	8	1503	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
11	K	1402	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	b	1240	CLA	CMB-C2B-C3B	2.45	129.27	124.68
11	B	1204	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
14	b	4011	BCR	C1-C6-C5	-2.45	119.16	122.61
11	B	1215	CLA	CMB-C2B-C3B	2.45	129.27	124.68
11	a	1101	CLA	CMB-C2B-C3B	2.45	129.27	124.68
11	B	1213	CLA	C9-C8-C10	2.45	120.18	111.29
11	1	1119	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	1	1126	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
11	1	1117	CLA	CMC-C2C-C1C	2.45	128.77	125.04
11	b	1225	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
11	A	1135	CLA	CAC-C3C-C4C	2.45	127.99	124.81
14	B	4004	BCR	C27-C26-C25	-2.45	119.17	122.73
11	b	1021	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
11	2	1206	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
14	B	4010	BCR	C23-C24-C25	-2.45	120.32	127.20
11	K	1401	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	A	1140	CLA	C1-O2A-CGA	2.45	122.87	116.44
11	b	1210	CLA	C9-C8-C10	2.45	120.16	111.29
11	b	1201	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
11	b	1213	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	1	1110	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	2	1222	CLA	C3C-C4C-NC	2.45	113.32	110.57
11	1	1131	CLA	OBD-CAD-C3D	-2.45	123.92	127.98
11	B	1211	CLA	CMC-C2C-C1C	2.45	128.77	125.04
11	1	1107	CLA	CMC-C2C-C1C	2.45	128.77	125.04
11	a	1120	CLA	CHB-C4A-NA	2.45	127.90	124.51
11	A	1101	CLA	C6-C5-C3	-2.45	107.04	113.45
14	2	4006	BCR	C37-C22-C21	-2.45	119.49	122.92
11	B	1224	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
11	A	1124	CLA	CMB-C2B-C3B	2.45	129.26	124.68
14	8	4022	BCR	C36-C18-C17	-2.45	119.50	122.92
11	A	1126	CLA	O2D-CGD-O1D	-2.45	119.05	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1236	CLA	CMB-C2B-C3B	2.45	129.25	124.68
11	a	1119	CLA	C9-C8-C7	2.45	120.15	111.29
11	1	1121	CLA	C3C-C4C-NC	2.45	113.31	110.57
11	B	1224	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
14	2	4005	BCR	C19-C18-C17	2.45	122.69	118.94
11	1	1111	CLA	C3C-C4C-NC	2.44	113.31	110.57
11	A	1131	CLA	C9-C8-C10	2.44	120.14	111.29
11	1	1118	CLA	CMB-C2B-C3B	2.44	129.25	124.68
15	b	5004	LHG	C5-O7-C7	-2.44	111.78	117.79
11	B	1213	CLA	C3C-C4C-NC	2.44	113.31	110.57
11	B	1205	CLA	CMC-C2C-C1C	2.44	128.76	125.04
11	1	1104	CLA	CMB-C2B-C3B	2.44	129.25	124.68
11	A	1111	CLA	CMB-C2B-C3B	2.44	129.25	124.68
11	A	1104	CLA	CMC-C2C-C1C	2.44	128.76	125.04
11	B	1209	CLA	C3C-C4C-NC	2.44	113.31	110.57
14	L	4022	BCR	C35-C13-C12	2.44	121.92	118.08
11	1	1137	CLA	C9-C8-C7	2.44	120.13	111.29
11	A	1115	CLA	C3C-C4C-NC	2.44	113.31	110.57
11	a	1120	CLA	CMC-C2C-C1C	2.44	128.75	125.04
11	A	1127	CLA	C1-C2-C3	-2.44	121.82	126.04
11	1	1801	CLA	CMB-C2B-C3B	2.44	129.24	124.68
14	a	4007	BCR	C15-C14-C13	-2.44	123.83	127.31
11	a	1012	CLA	CMB-C2B-C3B	2.44	129.24	124.68
11	a	1109	CLA	CAC-C3C-C4C	2.44	127.97	124.81
14	L	4019	BCR	C7-C6-C5	-2.44	115.56	121.46
11	B	1216	CLA	C4-C3-C5	2.44	119.37	115.27
11	B	1220	CLA	CMB-C2B-C3B	2.44	129.24	124.68
11	B	1205	CLA	C3C-C4C-NC	2.44	113.30	110.57
14	m	4021	BCR	C33-C5-C4	2.44	118.30	113.62
11	B	1216	CLA	CAC-C3C-C4C	2.44	127.97	124.81
14	l	4019	BCR	C33-C5-C4	2.43	118.29	113.62
11	k	1401	CLA	C3C-C4C-NC	2.43	113.30	110.57
11	a	1135	CLA	C3C-C4C-NC	2.43	113.30	110.57
11	B	1220	CLA	CMC-C2C-C1C	2.43	128.75	125.04
11	A	1123	CLA	OBD-CAD-C3D	-2.43	123.94	127.98
14	B	4010	BCR	C30-C25-C24	2.43	122.66	115.78
14	B	4004	BCR	C30-C25-C24	2.43	122.66	115.78
11	a	1116	CLA	C3C-C4C-NC	2.43	113.30	110.57
11	B	1215	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	1	1133	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
14	2	4017	BCR	C1-C6-C7	2.43	122.66	115.78
11	A	1022	CLA	C4-C3-C5	2.43	119.36	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1222	CLA	C9-C8-C7	2.43	120.10	111.29
11	A	1124	CLA	C3C-C4C-NC	2.43	113.30	110.57
11	A	1114	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	A	1132	CLA	CMC-C2C-C1C	2.43	128.74	125.04
14	6	4018	BCR	C8-C7-C6	-2.43	120.38	127.20
11	B	1217	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	b	1224	CLA	C1-C2-C3	-2.43	121.84	126.04
11	B	1232	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	A	1022	CLA	C3C-C4C-NC	2.43	113.30	110.57
11	2	1214	CLA	CAC-C3C-C4C	2.43	127.96	124.81
11	B	1231	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	b	1225	CLA	C9-C8-C7	2.43	120.09	111.29
11	a	1116	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	2	1219	CLA	C1-C2-C3	-2.43	121.84	126.04
14	F	4018	BCR	C38-C26-C27	2.43	118.28	113.62
11	1	1109	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	2	1228	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	A	1128	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	b	1216	CLA	C9-C8-C7	2.43	120.08	111.29
11	A	1136	CLA	CAC-C3C-C4C	2.43	127.96	124.81
11	B	1226	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
11	a	1116	CLA	C1-O2A-CGA	2.42	122.81	116.44
11	B	1224	CLA	C1-O2A-CGA	2.42	122.81	116.44
11	1	1139	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
11	b	1222	CLA	CMB-C2B-C3B	2.42	129.21	124.68
11	a	1128	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
11	1	1101	CLA	C4-C3-C2	-2.42	117.46	123.68
11	0	1401	CLA	C3C-C4C-NC	2.42	113.29	110.57
11	2	1227	CLA	CMC-C2C-C1C	2.42	128.73	125.04
11	1	1101	CLA	C3C-C4C-NC	2.42	113.29	110.57
11	1	1122	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	a	4008	BCR	C37-C22-C21	-2.42	119.53	122.92
11	B	1013	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	B	1202	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a	5003	LHG	C5-O7-C7	-2.42	111.83	117.79
11	a	1011	CLA	C1-C2-C3	-2.42	121.86	126.04
11	b	1222	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	2	1021	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	b	1205	CLA	C4-C3-C5	2.42	119.34	115.27
11	b	1224	CLA	CMB-C2B-C3B	2.42	129.20	124.68
11	1	1137	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
11	2	1225	CLA	CMD-C2D-C3D	-2.42	120.16	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4008	BCR	C8-C7-C6	-2.42	120.41	127.20
14	B	4011	BCR	C32-C1-C6	-2.42	106.38	110.30
14	A	4008	BCR	C23-C24-C25	-2.42	120.42	127.20
11	A	1123	CLA	C4-C3-C5	2.42	119.34	115.27
11	B	1206	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	b	1212	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	1	1237	CLA	C3C-C4C-NC	2.42	113.28	110.57
11	a	1132	CLA	C3C-C4C-NC	2.42	113.28	110.57
14	A	4002	BCR	C3-C4-C5	-2.41	109.77	114.08
11	A	1118	CLA	C4-C3-C5	2.41	119.33	115.27
11	1	1123	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	1	1134	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	L	1502	CLA	CMC-C2C-C1C	2.41	128.72	125.04
11	l	1501	CLA	CMB-C2B-C3B	2.41	129.19	124.68
11	B	1214	CLA	OBD-CAD-C3D	-2.41	123.97	127.98
11	b	1222	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
11	8	1503	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	a	1133	CLA	CAC-C3C-C4C	2.41	127.94	124.81
11	1	1128	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	1	1126	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
11	B	1203	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	a	1106	CLA	C3C-C4C-NC	2.41	113.28	110.57
11	b	1214	CLA	CAC-C3C-C4C	2.41	127.94	124.81
11	B	1209	CLA	CMC-C2C-C1C	2.41	128.71	125.04
11	k	1402	CLA	C1-O2A-CGA	2.41	122.77	116.44
11	1	1801	CLA	C1-C2-C3	-2.41	121.88	126.04
14	8	4019	BCR	C35-C13-C14	-2.41	119.55	122.92
11	b	1225	CLA	C3C-C4C-NC	2.41	113.27	110.57
11	b	1227	CLA	C3C-C4C-NC	2.41	113.27	110.57
11	b	1221	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
11	2	1217	CLA	C3C-C4C-NC	2.41	113.27	110.57
11	b	1230	CLA	CMC-C2C-C1C	2.41	128.71	125.04
11	b	1206	CLA	C1-O2A-CGA	2.41	122.76	116.44
11	b	1021	CLA	C11-C10-C8	-2.41	108.14	115.92
11	2	1021	CLA	C9-C8-C10	2.41	120.01	111.29
11	A	1237	CLA	CED-O2D-CGD	2.41	121.38	115.94
14	a	4002	BCR	C30-C25-C24	2.41	122.58	115.78
11	b	1013	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	b	4014	BCR	C27-C26-C25	-2.40	119.24	122.73
11	A	1105	CLA	C3C-C4C-NC	2.40	113.27	110.57
14	1	4007	BCR	C36-C18-C17	-2.40	119.56	122.92
11	1	1123	CLA	O1D-CGD-CBD	-2.40	119.57	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1139	CLA	CMB-C2B-C3B	2.40	129.18	124.68
14	2	4017	BCR	C23-C24-C25	-2.40	120.45	127.20
11	2	1228	CLA	CED-O2D-CGD	2.40	121.37	115.94
14	2	4017	BCR	C30-C25-C26	-2.40	119.23	122.61
11	1	1011	CLA	CMC-C2C-C1C	2.40	128.70	125.04
11	B	1239	CLA	CMB-C2B-C3B	2.40	129.17	124.68
11	a	1125	CLA	CMB-C2B-C3B	2.40	129.17	124.68
11	b	1013	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
11	B	1203	CLA	CMB-C2B-C3B	2.40	129.17	124.68
11	a	1127	CLA	CMB-C2B-C3B	2.40	129.17	124.68
15	A	5003	LHG	O7-C7-O9	-2.40	117.90	123.70
11	a	1124	CLA	CMC-C2C-C1C	2.40	128.69	125.04
11	1	1101	CLA	C9-C8-C7	2.40	119.98	111.29
11	A	1105	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
14	b	4004	BCR	C28-C27-C26	-2.40	109.79	114.08
11	2	1013	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
14	a	4003	BCR	C38-C26-C27	2.40	118.22	113.62
14	7	4021	BCR	C33-C5-C4	2.40	118.22	113.62
11	A	1129	CLA	CAC-C3C-C4C	2.40	127.92	124.81
11	1	1022	CLA	CMB-C2B-C3B	2.40	129.16	124.68
11	B	1021	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	A	1129	CLA	CMC-C2C-C1C	2.40	128.69	125.04
11	2	1215	CLA	CMC-C2C-C1C	2.40	128.69	125.04
14	2	4017	BCR	C4-C5-C6	-2.39	119.25	122.73
11	2	1208	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
11	l	1503	CLA	C3C-C4C-NC	2.39	113.26	110.57
11	1	1137	CLA	CMC-C2C-C1C	2.39	128.69	125.04
11	a	1101	CLA	CED-O2D-CGD	2.39	121.35	115.94
11	1	1127	CLA	CAC-C3C-C4C	2.39	127.92	124.81
11	b	1215	CLA	CMB-C2B-C3B	2.39	129.16	124.68
11	b	1234	CLA	C4-C3-C5	2.39	119.30	115.27
11	1	1116	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
11	b	1207	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
11	a	1121	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
11	B	1229	CLA	CMC-C2C-C1C	2.39	128.68	125.04
11	B	1216	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
11	a	1109	CLA	C1-C2-C3	-2.39	121.91	126.04
11	1	1116	CLA	CMB-C2B-C3B	2.39	129.15	124.68
11	L	1501	CLA	C4-C3-C5	2.39	119.29	115.27
11	1	1135	CLA	C1-C2-C3	-2.39	121.91	126.04
11	0	1401	CLA	CBA-CAA-C2A	2.39	120.92	113.86
11	A	1133	CLA	C3C-C4C-NC	2.39	113.25	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1138	CLA	CMB-C2B-C3B	2.39	129.15	124.68
11	2	1239	CLA	CMB-C2B-C3B	2.39	129.15	124.68
11	b	1234	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
11	A	1117	CLA	C4-C3-C5	2.39	119.29	115.27
11	A	1132	CLA	C3C-C4C-NC	2.39	113.25	110.57
11	2	1221	CLA	CMB-C2B-C3B	2.39	129.15	124.68
11	B	1210	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
11	2	1223	CLA	C9-C8-C7	2.39	119.94	111.29
11	A	1109	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
11	1	1118	CLA	C4-C3-C5	2.39	119.29	115.27
14	2	4006	BCR	C29-C28-C27	2.39	116.71	111.38
11	a	1108	CLA	C3C-C4C-NC	2.39	113.25	110.57
14	B	4017	BCR	C37-C22-C21	-2.39	119.58	122.92
14	2	4011	BCR	C32-C1-C6	-2.39	106.43	110.30
11	a	1237	CLA	CAC-C3C-C4C	2.39	127.91	124.81
11	1	1011	CLA	CAA-C2A-C1A	2.39	119.80	111.97
11	1	1116	CLA	C3C-C4C-NC	2.39	113.25	110.57
11	a	1011	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
14	L	4019	BCR	C1-C6-C7	2.39	122.53	115.78
11	1	1119	CLA	C9-C8-C7	2.39	119.93	111.29
11	2	1207	CLA	C3C-C4C-NC	2.38	113.25	110.57
11	2	1201	CLA	CAC-C3C-C4C	2.38	127.90	124.81
11	B	1223	CLA	CMB-C2B-C3B	2.38	129.14	124.68
11	B	1229	CLA	C4-C3-C5	2.38	119.28	115.27
14	8	4022	BCR	C28-C27-C26	-2.38	109.82	114.08
14	b	4005	BCR	C33-C5-C4	2.38	118.19	113.62
11	A	1131	CLA	CAC-C3C-C4C	2.38	127.90	124.81
11	k	1401	CLA	CAC-C3C-C4C	2.38	127.90	124.81
11	2	1226	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
11	b	1220	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
14	2	4005	BCR	C37-C22-C21	-2.38	119.59	122.92
11	a	1136	CLA	CMC-C2C-C1C	2.38	128.66	125.04
11	K	1401	CLA	CBA-CAA-C2A	2.38	120.89	113.86
11	2	1234	CLA	C9-C8-C7	2.38	119.91	111.29
11	b	1238	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
11	a	1117	CLA	C4-C3-C5	2.38	119.28	115.27
11	k	1402	CLA	C3C-C4C-NC	2.38	113.24	110.57
11	A	1114	CLA	C3C-C4C-NC	2.38	113.24	110.57
11	B	1204	CLA	C1-C2-C3	-2.38	121.93	126.04
11	a	1108	CLA	CMB-C2B-C3B	2.38	129.13	124.68
11	b	1235	CLA	C3C-C4C-NC	2.38	113.24	110.57
11	a	1109	CLA	CMB-C2B-C3B	2.38	129.13	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1216	CLA	CMC-C2C-C1C	2.38	128.66	125.04
11	A	1107	CLA	CMC-C2C-C1C	2.38	128.66	125.04
11	b	1227	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
11	8	1501	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	2	4011	BCR	C23-C22-C21	2.38	122.59	118.94
11	b	1210	CLA	C1-O2A-CGA	2.38	122.68	116.44
11	1	1237	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
11	B	1234	CLA	CAC-C3C-C4C	2.38	127.89	124.81
14	1	4002	BCR	C35-C13-C12	2.38	121.82	118.08
11	B	1229	CLA	C9-C8-C10	2.38	119.89	111.29
11	2	1209	CLA	C3C-C4C-NC	2.38	113.23	110.57
11	a	1135	CLA	CMB-C2B-C3B	2.37	129.12	124.68
11	2	1240	CLA	CAC-C3C-C4C	2.37	127.89	124.81
14	F	4018	BCR	C32-C1-C6	-2.37	106.45	110.30
14	2	4006	BCR	C23-C22-C21	2.37	122.58	118.94
11	k	1401	CLA	CBA-CAA-C2A	2.37	120.87	113.86
11	2	1234	CLA	C9-C8-C10	2.37	119.89	111.29
11	B	1227	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
11	a	1113	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	b	1227	CLA	CMB-C2B-C3B	2.37	129.12	124.68
11	2	1224	CLA	C4-C3-C5	2.37	119.26	115.27
11	2	1227	CLA	CAC-C3C-C4C	2.37	127.89	124.81
14	2	4004	BCR	C15-C14-C13	-2.37	123.93	127.31
14	8	4019	BCR	C33-C5-C4	2.37	118.17	113.62
11	A	1122	CLA	CMB-C2B-C3B	2.37	129.11	124.68
11	a	1139	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	A	1237	CLA	CHB-C4A-NA	2.37	127.79	124.51
11	b	1206	CLA	CMB-C2B-C3B	2.37	129.11	124.68
11	A	1012	CLA	CMC-C2C-C1C	2.37	128.65	125.04
11	b	1218	CLA	C3C-C4C-NC	2.37	113.23	110.57
11	a	1117	CLA	C3C-C4C-NC	2.37	113.23	110.57
11	b	1013	CLA	C3C-C4C-NC	2.37	113.23	110.57
14	1	4001	BCR	C3-C4-C5	-2.37	109.85	114.08
11	B	1231	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
11	2	1217	CLA	CMC-C2C-C1C	2.37	128.65	125.04
11	A	1116	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
14	f	4020	BCR	C37-C22-C21	-2.37	119.61	122.92
11	2	1226	CLA	CMC-C2C-C1C	2.37	128.65	125.04
11	a	1106	CLA	C4-C3-C2	-2.37	117.60	123.68
11	1	1101	CLA	CAC-C3C-C4C	2.37	127.88	124.81
11	A	1011	CLA	CHA-C1A-NA	-2.37	120.98	126.40
11	b	1013	CLA	CED-O2D-CGD	2.37	121.29	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4007	BCR	C35-C13-C14	-2.37	119.61	122.92
11	A	1136	CLA	C3C-C4C-NC	2.37	113.22	110.57
11	a	1106	CLA	CMB-C2B-C3B	2.37	129.10	124.68
14	a	4007	BCR	C34-C9-C8	2.37	121.81	118.08
14	1	4003	BCR	C8-C7-C6	-2.37	120.56	127.20
14	2	4010	BCR	C30-C25-C26	-2.37	119.28	122.61
11	B	1215	CLA	C3C-C4C-NC	2.37	113.22	110.57
11	a	1112	CLA	C3C-C4C-NC	2.37	113.22	110.57
11	b	1201	CLA	C3C-C4C-NC	2.37	113.22	110.57
11	a	1133	CLA	C3C-C4C-NC	2.37	113.22	110.57
11	k	1402	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
14	b	4006	BCR	C23-C22-C21	2.36	122.57	118.94
11	B	1221	CLA	CHB-C4A-NA	2.36	127.78	124.51
11	B	1208	CLA	CMB-C2B-C3B	2.36	129.10	124.68
14	L	4019	BCR	C3-C4-C5	-2.36	109.86	114.08
11	1	1114	CLA	CAC-C3C-C4C	2.36	127.88	124.81
11	b	1206	CLA	CMC-C2C-C1C	2.36	128.64	125.04
11	b	1209	CLA	CHB-C4A-NA	2.36	127.78	124.51
11	b	1202	CLA	C4-C3-C5	2.36	119.25	115.27
11	a	1128	CLA	C3C-C4C-NC	2.36	113.22	110.57
11	2	1214	CLA	C4-C3-C5	2.36	119.24	115.27
11	K	1401	CLA	CAC-C3C-C4C	2.36	127.87	124.81
11	B	1234	CLA	C3C-C4C-NC	2.36	113.22	110.57
14	B	4005	BCR	C30-C25-C26	-2.36	119.29	122.61
14	L	4022	BCR	C23-C22-C21	2.36	122.56	118.94
11	b	1219	CLA	C1-C2-C3	-2.36	121.96	126.04
11	A	1122	CLA	C1-C2-C3	-2.36	121.96	126.04
11	b	1238	CLA	C3C-C4C-NC	2.36	113.22	110.57
11	b	1204	CLA	C3C-C4C-NC	2.36	113.22	110.57
11	a	1134	CLA	CMB-C2B-C3B	2.36	129.09	124.68
11	1	1116	CLA	C1-O2A-CGA	2.36	122.63	116.44
11	b	1209	CLA	CMB-C2B-C3B	2.36	129.09	124.68
11	a	1119	CLA	CAC-C3C-C4C	2.36	127.87	124.81
14	A	4001	BCR	C34-C9-C10	-2.36	119.62	122.92
11	b	1221	CLA	C1-O2A-CGA	2.36	122.63	116.44
11	A	1117	CLA	C9-C8-C10	2.36	119.83	111.29
11	a	1107	CLA	CMC-C2C-C1C	2.36	128.63	125.04
11	a	1113	CLA	CAC-C3C-C4C	2.36	127.87	124.81
11	A	1106	CLA	CHB-C4A-NA	2.36	127.77	124.51
11	a	1103	CLA	C3C-C4C-NC	2.36	113.21	110.57
11	b	1211	CLA	CMB-C2B-C3B	2.36	129.09	124.68
12	a	2001	PQN	C2M-C2-C1	2.36	120.17	116.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1219	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
11	2	1214	CLA	CMB-C2B-C3B	2.35	129.08	124.68
11	b	1216	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
11	A	1138	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
11	A	1022	CLA	CMC-C2C-C1C	2.35	128.62	125.04
14	b	4009	BCR	C1-C6-C5	-2.35	119.30	122.61
11	a	1127	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
11	a	1137	CLA	C1-O2A-CGA	2.35	122.62	116.44
11	b	1205	CLA	C3C-C4C-NC	2.35	113.21	110.57
14	B	4005	BCR	C38-C26-C25	-2.35	121.89	124.53
11	a	1128	CLA	C1-C2-C3	-2.35	121.97	126.04
11	1	1118	CLA	C3C-C4C-NC	2.35	113.21	110.57
14	2	4011	BCR	C35-C13-C12	2.35	121.78	118.08
11	1	1131	CLA	C3C-C4C-NC	2.35	113.21	110.57
14	a	4003	BCR	C29-C30-C25	-2.35	106.86	110.48
11	B	1229	CLA	CAC-C3C-C4C	2.35	127.86	124.81
14	1	4003	BCR	C19-C18-C17	2.35	122.55	118.94
11	A	1133	CLA	CHB-C4A-NA	2.35	127.76	124.51
11	a	1102	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
11	a	1801	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
14	a	4007	BCR	C23-C24-C25	-2.35	120.60	127.20
11	a	1102	CLA	C1-O2A-CGA	2.35	122.61	116.44
11	2	1224	CLA	CMB-C2B-C3B	2.35	129.07	124.68
11	2	1240	CLA	CMC-C2C-C1C	2.35	128.62	125.04
11	1	1123	CLA	C9-C8-C10	2.35	119.80	111.29
11	1	1139	CLA	C5-C3-C4	2.35	119.79	114.60
11	1	1125	CLA	CMB-C2B-C3B	2.35	129.07	124.68
14	a	4007	BCR	C37-C22-C21	-2.35	119.63	122.92
11	2	1223	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
11	B	1214	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
11	A	1128	CLA	CMC-C2C-C1C	2.35	128.61	125.04
11	B	1225	CLA	C1-O2A-CGA	2.35	122.60	116.44
11	b	1227	CLA	CAC-C3C-C4C	2.35	127.85	124.81
11	a	1123	CLA	C3C-C4C-NC	2.35	113.20	110.57
11	B	1214	CLA	CHB-C4A-NA	2.35	127.76	124.51
11	b	1229	CLA	C4-C3-C5	2.35	119.22	115.27
11	b	1217	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
11	A	1112	CLA	CAC-C3C-C4C	2.35	127.85	124.81
14	2	4014	BCR	C34-C9-C10	-2.34	119.64	122.92
11	0	1401	CLA	CAC-C3C-C4C	2.34	127.85	124.81
11	B	1229	CLA	C9-C8-C7	2.34	119.77	111.29
14	2	4004	BCR	C28-C27-C26	-2.34	109.90	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4014	BCR	C35-C13-C14	-2.34	119.64	122.92
11	l	1501	CLA	OBD-CAD-C3D	-2.34	124.09	127.98
11	A	1011	CLA	OBD-CAD-C3D	-2.34	124.09	127.98
14	b	4005	BCR	C27-C26-C25	-2.34	119.33	122.73
11	b	1023	CLA	C4-C3-C5	2.34	119.21	115.27
14	2	4009	BCR	C35-C13-C14	-2.34	119.65	122.92
14	b	4006	BCR	C1-C6-C7	2.34	122.39	115.78
15	1	5003	LHG	C5-O7-C7	-2.34	112.04	117.79
11	2	1201	CLA	CMC-C2C-C1C	2.34	128.60	125.04
11	0	1402	CLA	C3C-C4C-NC	2.34	113.19	110.57
11	1	1124	CLA	C3C-C4C-NC	2.34	113.19	110.57
11	b	1236	CLA	C3C-C4C-NC	2.34	113.19	110.57
11	1	1134	CLA	CAC-C3C-C4C	2.34	127.84	124.81
11	1	1116	CLA	O1D-CGD-CBD	-2.34	119.71	124.48
11	a	1124	CLA	C4-C3-C5	2.34	119.20	115.27
11	1	1130	CLA	C3C-C4C-NC	2.33	113.19	110.57
11	2	1201	CLA	C3C-C4C-NC	2.33	113.19	110.57
11	B	1201	CLA	C3C-C4C-NC	2.33	113.19	110.57
14	b	4010	BCR	C36-C18-C17	-2.33	119.65	122.92
11	a	1114	CLA	CMB-C2B-C3B	2.33	129.04	124.68
11	A	1123	CLA	C9-C8-C10	2.33	119.74	111.29
11	A	1133	CLA	CMB-C2B-C3B	2.33	129.04	124.68
11	2	1221	CLA	CHB-C4A-NA	2.33	127.74	124.51
11	b	1221	CLA	CAC-C3C-C4C	2.33	127.83	124.81
11	1	1106	CLA	C1-C2-C3	-2.33	122.02	126.04
11	1	1111	CLA	CAC-C3C-C4C	2.33	127.83	124.81
11	A	1138	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
11	b	1226	CLA	C1-C2-C3	-2.33	122.02	126.04
11	B	1217	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
11	b	1229	CLA	C9-C8-C7	2.33	119.72	111.29
11	1	1138	CLA	CMB-C2B-C3B	2.33	129.03	124.68
14	B	4017	BCR	C28-C27-C26	-2.33	109.92	114.08
11	b	1228	CLA	C3C-C4C-NC	2.33	113.18	110.57
11	a	1127	CLA	C3C-C4C-NC	2.33	113.18	110.57
11	2	1212	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
12	2	2002	PQN	C24-C23-C25	2.33	119.72	111.29
11	b	1215	CLA	C9-C8-C7	2.33	119.71	111.29
11	2	1207	CLA	CHB-C4A-NA	2.32	127.73	124.51
11	B	1202	CLA	C1-O2A-CGA	2.32	122.54	116.44
11	1	1132	CLA	C3C-C4C-NC	2.32	113.18	110.57
11	a	1138	CLA	CED-O2D-CGD	2.32	121.19	115.94
11	B	1238	CLA	C3C-C4C-NC	2.32	113.18	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1210	CLA	CMC-C2C-C1C	2.32	128.58	125.04
11	a	1131	CLA	CAC-C3C-C4C	2.32	127.82	124.81
11	A	1108	CLA	CED-O2D-CGD	2.32	121.19	115.94
11	B	1239	CLA	C3C-C4C-NC	2.32	113.18	110.57
11	A	1107	CLA	CHB-C4A-NA	2.32	127.72	124.51
11	a	1114	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
11	A	1116	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
11	B	1223	CLA	C1-C2-C3	-2.32	122.03	126.04
11	A	1117	CLA	CMC-C2C-C1C	2.32	128.57	125.04
11	A	1104	CLA	CMB-C2B-C3B	2.32	129.02	124.68
15	a	5001	LHG	C5-O7-C7	-2.32	112.08	117.79
11	b	1210	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
11	a	1118	CLA	CMB-C2B-C3B	2.32	129.02	124.68
11	2	1218	CLA	C3C-C4C-NC	2.32	113.17	110.57
11	a	1107	CLA	CMB-C2B-C3B	2.32	129.02	124.68
11	A	1134	CLA	CMC-C2C-C1C	2.32	128.57	125.04
11	8	1501	CLA	C3C-C4C-NC	2.32	113.17	110.57
14	8	4022	BCR	C23-C24-C25	-2.32	120.69	127.20
11	b	1234	CLA	CMB-C2B-C3B	2.32	129.02	124.68
11	b	1210	CLA	C4-C3-C5	2.32	119.17	115.27
14	2	4005	BCR	C27-C26-C25	-2.32	119.37	122.73
11	a	1108	CLA	CED-O2D-CGD	2.32	121.18	115.94
11	B	1021	CLA	CMC-C2C-C1C	2.32	128.57	125.04
11	2	1213	CLA	C4-C3-C2	-2.32	117.73	123.68
14	f	4018	BCR	C8-C7-C6	-2.32	120.70	127.20
14	B	4010	BCR	C24-C23-C22	-2.32	122.73	126.23
11	a	1122	CLA	CAC-C3C-C4C	2.32	127.81	124.81
11	1	1129	CLA	CMB-C2B-C3B	2.32	129.01	124.68
11	A	1105	CLA	CMB-C2B-C3B	2.32	129.01	124.68
11	B	1218	CLA	C3C-C4C-NC	2.32	113.17	110.57
11	1	1132	CLA	CMB-C2B-C3B	2.31	129.01	124.68
11	a	1106	CLA	CHB-C4A-NA	2.31	127.71	124.51
11	2	1238	CLA	C3C-C4C-NC	2.31	113.17	110.57
14	L	4022	BCR	C36-C18-C17	-2.31	119.68	122.92
12	A	2001	PQN	C24-C23-C25	2.31	119.67	111.29
11	a	1131	CLA	C3C-C4C-NC	2.31	113.17	110.57
11	B	1211	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
11	1	1801	CLA	CHB-C4A-NA	2.31	127.71	124.51
12	1	2001	PQN	C2M-C2-C3	-2.31	120.63	124.40
11	b	1223	CLA	CMB-C2B-C3B	2.31	129.00	124.68
11	b	1224	CLA	CAC-C3C-C4C	2.31	127.81	124.81
11	B	1230	CLA	CAC-C3C-C4C	2.31	127.81	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1208	CLA	C3C-C4C-NC	2.31	113.16	110.57
11	A	1120	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
11	b	1224	CLA	C4-C3-C5	2.31	119.16	115.27
11	A	1135	CLA	C3C-C4C-NC	2.31	113.16	110.57
11	1	1138	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
11	A	1012	CLA	C5-C3-C2	-2.31	116.44	121.12
11	a	1116	CLA	CAC-C3C-C4C	2.31	127.81	124.81
11	B	1229	CLA	C1-O2A-CGA	2.31	122.50	116.44
11	b	1229	CLA	C9-C8-C10	2.31	119.65	111.29
11	2	1217	CLA	CMB-C2B-C3B	2.31	129.00	124.68
11	1	1011	CLA	CMB-C2B-C3B	2.31	128.99	124.68
11	1	1127	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
11	A	1140	CLA	OBD-CAD-C3D	-2.31	124.15	127.98
14	B	4009	BCR	C3-C4-C5	-2.30	109.96	114.08
16	B	5002	LMG	O7-C10-O9	-2.30	118.13	123.70
11	a	1126	CLA	C4-C3-C2	-2.30	117.77	123.68
11	a	1130	CLA	CAC-C3C-C4C	2.30	127.80	124.81
11	2	1021	CLA	CHA-C1A-NA	-2.30	121.13	126.40
11	b	1219	CLA	C4-C3-C5	2.30	119.14	115.27
11	1	1119	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
11	B	1219	CLA	CAC-C3C-C4C	2.30	127.80	124.81
12	b	2002	PQN	C11-C12-C13	-2.30	122.96	126.79
11	a	1127	CLA	C6-C5-C3	-2.30	107.42	113.45
11	A	1801	CLA	C1-O2A-CGA	2.30	122.48	116.44
14	1	4007	BCR	C34-C9-C8	2.30	121.70	118.08
14	B	4009	BCR	C33-C5-C4	2.30	118.03	113.62
11	b	1228	CLA	CMC-C2C-C1C	2.30	128.54	125.04
11	1	1104	CLA	C1-C2-C3	-2.30	122.07	126.04
11	1	1237	CLA	CBA-CAA-C2A	2.30	120.65	113.86
11	k	1401	CLA	C1-O2A-CGA	2.30	122.48	116.44
11	2	1013	CLA	C3C-C4C-NC	2.30	113.15	110.57
11	A	1134	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
11	b	1021	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	a	1139	CLA	C1-C2-C3	-2.30	123.03	126.75
11	2	1207	CLA	CMB-C2B-C3B	2.30	128.98	124.68
11	A	1113	CLA	OBD-CAD-C3D	-2.30	124.17	127.98
11	1	1108	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
11	1	1237	CLA	CMB-C2B-C3B	2.30	128.97	124.68
11	b	1226	CLA	CMB-C2B-C3B	2.30	128.97	124.68
11	b	1219	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
11	1	1126	CLA	CAC-C3C-C4C	2.30	127.79	124.81
14	A	4002	BCR	C35-C13-C14	-2.30	119.71	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1102	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	K	1401	CLA	C1-O2A-CGA	2.30	122.47	116.44
11	0	1401	CLA	C1-O2A-CGA	2.30	122.47	116.44
11	1	1105	CLA	CAC-C3C-C4C	2.30	127.79	124.81
11	A	1123	CLA	C3C-C4C-NC	2.30	113.14	110.57
11	A	1131	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
11	a	1134	CLA	C3C-C4C-NC	2.29	113.14	110.57
11	A	1135	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	2	1023	CLA	C11-C10-C8	-2.29	108.51	115.92
11	B	1021	CLA	C9-C8-C10	2.29	119.59	111.29
11	8	1501	CLA	CAC-C3C-C4C	2.29	127.78	124.81
11	A	1139	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
11	A	1116	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	a	1112	CLA	CAC-C3C-C4C	2.29	127.78	124.81
11	1	1128	CLA	C1-C2-C3	-2.29	122.08	126.04
14	8	4019	BCR	C1-C6-C7	2.29	122.25	115.78
11	b	1225	CLA	C1-O2A-CGA	2.29	122.45	116.44
11	2	1238	CLA	C1-O2A-CGA	2.29	122.45	116.44
11	1	1140	CLA	CMB-C2B-C3B	2.29	128.96	124.68
11	A	1133	CLA	CMC-C2C-C1C	2.29	128.52	125.04
11	a	1116	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
11	B	1213	CLA	CMB-C2B-C3B	2.29	128.96	124.68
14	2	4004	BCR	C27-C26-C25	-2.29	119.41	122.73
11	A	1127	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
14	2	4009	BCR	C7-C8-C9	-2.29	122.78	126.23
11	a	1118	CLA	C1-C2-C3	-2.29	122.09	126.04
14	A	4002	BCR	C36-C18-C17	-2.29	119.72	122.92
14	f	4013	BCR	C3-C4-C5	-2.29	110.00	114.08
11	A	1104	CLA	C3C-C4C-NC	2.29	113.13	110.57
11	A	1118	CLA	OBD-CAD-C3D	-2.29	124.19	127.98
14	B	4017	BCR	C38-C26-C25	-2.28	121.96	124.53
14	A	4008	BCR	C28-C27-C26	-2.28	110.00	114.08
11	b	1235	CLA	C11-C10-C8	-2.28	108.54	115.92
11	B	1234	CLA	C6-C7-C8	-2.28	108.54	115.92
14	a	4008	BCR	C35-C13-C14	-2.28	119.72	122.92
14	a	4001	BCR	C35-C13-C14	-2.28	119.72	122.92
11	B	1207	CLA	CMC-C2C-C1C	2.28	128.51	125.04
11	2	1214	CLA	C3C-C4C-NC	2.28	113.13	110.57
11	A	1119	CLA	C1-C2-C3	-2.28	122.10	126.04
11	2	1209	CLA	OBD-CAD-C3D	-2.28	124.19	127.98
11	a	1101	CLA	C9-C8-C7	2.28	119.55	111.29
14	F	4020	BCR	C31-C1-C6	-2.28	106.60	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4008	BCR	C3-C4-C5	-2.28	110.01	114.08
11	b	1216	CLA	CAC-C3C-C4C	2.28	127.77	124.81
11	B	1219	CLA	C4-C3-C5	2.28	119.10	115.27
14	F	4013	BCR	C40-C30-C25	-2.28	106.60	110.30
11	1	1133	CLA	CMB-C2B-C3B	2.28	128.94	124.68
11	b	1232	CLA	C3C-C4C-NC	2.28	113.12	110.57
11	A	1102	CLA	C3C-C4C-NC	2.28	113.12	110.57
11	1	1101	CLA	C4-C3-C5	2.28	119.10	115.27
11	1	1128	CLA	C4-C3-C5	2.28	119.10	115.27
11	a	1117	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
11	A	1129	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
11	b	1216	CLA	C6-C7-C8	-2.28	108.56	115.92
14	B	4004	BCR	C28-C27-C26	-2.28	110.01	114.08
11	1	1122	CLA	CED-O2D-CGD	2.28	121.08	115.94
11	1	1121	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
11	b	1229	CLA	C1-O2A-CGA	2.27	122.41	116.44
11	1	1101	CLA	C9-C8-C10	2.27	119.53	111.29
11	b	1204	CLA	CMB-C2B-C3B	2.27	128.93	124.68
14	F	4018	BCR	C36-C18-C17	-2.27	119.74	122.92
11	b	1208	CLA	C3C-C4C-NC	2.27	113.12	110.57
14	b	4017	BCR	C3-C4-C5	-2.27	110.02	114.08
11	1	1131	CLA	CAC-C3C-C4C	2.27	127.76	124.81
11	1	1106	CLA	C3C-C4C-NC	2.27	113.12	110.57
11	a	1131	CLA	C9-C8-C7	2.27	119.51	111.29
11	a	1135	CLA	CAC-C3C-C4C	2.27	127.75	124.81
11	1	1106	CLA	CMB-C2B-C3B	2.27	128.92	124.68
11	1	1114	CLA	CMB-C2B-C3B	2.27	128.92	124.68
11	a	1109	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
11	1	1139	CLA	C3C-C4C-NC	2.27	113.11	110.57
11	2	1204	CLA	C3C-C4C-NC	2.27	113.11	110.57
11	B	1214	CLA	C9-C8-C10	2.27	119.50	111.29
16	2	5002	LMG	O7-C10-O9	-2.27	118.22	123.70
11	B	1220	CLA	C3C-C4C-NC	2.27	113.11	110.57
11	1	1137	CLA	OBD-CAD-C3D	-2.27	124.22	127.98
14	a	4003	BCR	C8-C7-C6	-2.27	120.84	127.20
11	1	1123	CLA	CMB-C2B-C3B	2.27	128.92	124.68
14	a	4002	BCR	C15-C14-C13	-2.27	124.08	127.31
11	1	1136	CLA	CAC-C3C-C4C	2.27	127.75	124.81
11	1	1133	CLA	C3C-C4C-NC	2.27	113.11	110.57
11	b	1235	CLA	CHB-C4A-NA	2.27	127.64	124.51
11	2	1230	CLA	CAC-C3C-C4C	2.27	127.75	124.81
16	b	5002	LMG	O7-C10-O9	-2.27	118.23	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1104	CLA	C3C-C4C-NC	2.26	113.11	110.57
11	B	1227	CLA	CMC-C2C-C1C	2.26	128.49	125.04
11	A	1125	CLA	C1-O2A-CGA	2.26	122.38	116.44
11	B	1206	CLA	C4-C3-C5	2.26	119.08	115.27
11	A	1109	CLA	C9-C8-C7	2.26	119.49	111.29
11	A	1120	CLA	CAC-C3C-C4C	2.26	127.75	124.81
11	a	1111	CLA	CHB-C4A-NA	2.26	127.64	124.51
11	B	1215	CLA	C11-C10-C8	-2.26	108.61	115.92
11	2	1209	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	a	1128	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	1	1103	CLA	CMB-C2B-C3B	2.26	128.91	124.68
11	b	1023	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
11	B	1228	CLA	C3C-C4C-NC	2.26	113.11	110.57
11	2	1201	CLA	CMB-C2B-C3B	2.26	128.90	124.68
11	a	1131	CLA	C9-C8-C10	2.26	119.47	111.29
11	b	1231	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	L	1503	CLA	CMB-C2B-C3B	2.26	128.90	124.68
11	A	1022	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
11	1	1120	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
11	b	1229	CLA	CMB-C2B-C3B	2.26	128.90	124.68
11	b	1239	CLA	CAC-C3C-C4C	2.26	127.74	124.81
11	A	1012	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
11	b	1207	CLA	CMC-C2C-C1C	2.26	128.47	125.04
11	A	1119	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
14	6	4013	BCR	C30-C25-C26	-2.26	119.44	122.61
11	1	1127	CLA	C3C-C4C-NC	2.26	113.10	110.57
11	B	1210	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
11	B	1201	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	1	1107	CLA	CMB-C2B-C3B	2.26	128.90	124.68
11	L	1501	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
11	A	1119	CLA	C4C-C3C-C2C	-2.25	103.61	106.90
14	a	4001	BCR	C35-C13-C12	2.25	121.63	118.08
11	b	1231	CLA	C3C-C4C-NC	2.25	113.10	110.57
11	a	1011	CLA	CHA-C1A-NA	-2.25	121.24	126.40
11	2	1225	CLA	C4-C3-C5	2.25	119.06	115.27
11	A	1110	CLA	CAC-C3C-C4C	2.25	127.73	124.81
11	b	1222	CLA	CHB-C4A-NA	2.25	127.62	124.51
11	2	1208	CLA	C3C-C4C-NC	2.25	113.09	110.57
11	1	1105	CLA	C3C-C4C-NC	2.25	113.09	110.57
11	A	1108	CLA	CHB-C4A-NA	2.25	127.62	124.51
11	b	1202	CLA	C1-C2-C3	-2.25	122.15	126.04
14	l	4022	BCR	C30-C25-C26	-2.25	119.44	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1102	CLA	C9-C8-C10	2.25	119.44	111.29
14	8	4019	BCR	C37-C22-C21	-2.25	119.77	122.92
11	a	1140	CLA	C4-C3-C5	2.25	119.06	115.27
14	2	4010	BCR	C35-C13-C14	-2.25	119.77	122.92
14	a	4008	BCR	C34-C9-C8	2.25	121.62	118.08
11	1	1116	CLA	CAC-C3C-C4C	2.25	127.73	124.81
11	1	1128	CLA	C11-C12-C13	-2.25	108.65	115.92
11	B	1202	CLA	C3C-C4C-NC	2.25	113.09	110.57
11	B	1021	CLA	C3C-C4C-NC	2.25	113.09	110.57
11	b	1218	CLA	CMB-C2B-C3B	2.25	128.88	124.68
11	A	1101	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
14	b	4004	BCR	C30-C25-C24	2.25	122.14	115.78
11	A	1131	CLA	CMB-C2B-C3B	2.25	128.88	124.68
11	2	1203	CLA	C3C-C4C-NC	2.25	113.09	110.57
11	2	1210	CLA	C11-C10-C8	-2.25	108.66	115.92
12	2	2002	PQN	C2M-C2-C1	2.24	119.99	116.27
11	b	1206	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
14	1	4008	BCR	C28-C27-C26	-2.24	110.07	114.08
11	0	1402	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
11	1	1106	CLA	CAC-C3C-C4C	2.24	127.72	124.81
11	2	1206	CLA	CAC-C3C-C4C	2.24	127.72	124.81
11	B	1222	CLA	C9-C8-C7	2.24	119.41	111.29
11	a	1129	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	A	1104	CLA	C6-C5-C3	-2.24	107.58	113.45
11	B	1021	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
11	2	1215	CLA	C3C-C4C-NC	2.24	113.08	110.57
11	1	1113	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
11	2	1215	CLA	CMB-C2B-C3B	2.24	128.87	124.68
14	A	4003	BCR	C19-C18-C17	2.24	122.38	118.94
11	2	1222	CLA	C4-C3-C2	-2.24	117.93	123.68
11	B	1204	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
11	a	1128	CLA	C11-C10-C8	-2.24	108.68	115.92
11	A	1121	CLA	CMD-C2D-C3D	-2.24	120.49	124.68
11	a	1122	CLA	C9-C8-C7	2.24	119.40	111.29
11	a	1140	CLA	CMB-C2B-C3B	2.24	128.87	124.68
11	1	1127	CLA	C4-C3-C5	2.24	119.03	115.27
11	B	1231	CLA	OBD-CAD-C3D	-2.24	124.27	127.98
11	A	1111	CLA	C3C-C4C-NC	2.24	113.08	110.57
11	B	1206	CLA	CMC-C2C-C1C	2.24	128.45	125.04
11	2	1211	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	B	1229	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
11	2	1204	CLA	O1D-CGD-CBD	-2.24	119.91	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1235	CLA	C9-C8-C10	2.24	119.39	111.29
11	b	1215	CLA	C3C-C4C-NC	2.24	113.08	110.57
11	B	1206	CLA	CED-O2D-CGD	2.24	120.99	115.94
11	A	1139	CLA	CED-O2D-CGD	2.24	120.99	115.94
11	a	1107	CLA	C9-C8-C10	2.24	119.39	111.29
11	B	1219	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
14	a	4001	BCR	C3-C4-C5	-2.24	110.09	114.08
14	A	4008	BCR	C1-C6-C7	2.23	122.10	115.78
11	2	1210	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
11	A	1135	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
11	b	1235	CLA	C9-C8-C10	2.23	119.38	111.29
11	a	1133	CLA	CMC-C2C-C1C	2.23	128.44	125.04
14	7	4021	BCR	C19-C18-C17	2.23	122.37	118.94
11	a	1137	CLA	C9-C8-C10	2.23	119.37	111.29
11	b	1226	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
14	m	4021	BCR	C23-C24-C25	-2.23	120.94	127.20
11	2	1240	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
11	a	1129	CLA	CMB-C2B-C3B	2.23	128.85	124.68
14	B	4010	BCR	C34-C9-C10	-2.23	119.80	122.92
14	b	4009	BCR	C8-C9-C10	2.23	122.36	118.94
14	2	4004	BCR	C30-C25-C24	2.23	122.08	115.78
11	a	1012	CLA	C1-O2A-CGA	2.23	122.29	116.44
11	2	1223	CLA	CMB-C2B-C3B	2.23	128.84	124.68
14	B	4011	BCR	C1-C6-C5	-2.23	119.48	122.61
14	2	4005	BCR	C33-C5-C4	2.23	117.89	113.62
14	7	4021	BCR	C23-C24-C25	-2.23	120.95	127.20
11	A	1105	CLA	CED-O2D-CGD	2.23	120.97	115.94
11	B	1223	CLA	C4-C3-C5	2.23	119.01	115.27
12	B	2002	PQN	C11-C12-C13	-2.22	123.09	126.79
11	2	1212	CLA	CAC-C3C-C4C	2.22	127.70	124.81
11	a	1138	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
14	B	4009	BCR	C36-C18-C17	-2.22	119.81	122.92
14	l	4019	BCR	C37-C22-C21	-2.22	119.81	122.92
11	B	1221	CLA	CMB-C2B-C3B	2.22	128.84	124.68
11	1	1118	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
11	a	1119	CLA	C3C-C4C-NC	2.22	113.06	110.57
14	6	4018	BCR	C35-C13-C12	2.22	121.58	118.08
11	2	1226	CLA	C1-C2-C3	-2.22	122.20	126.04
11	k	1402	CLA	CAC-C3C-C4C	2.22	127.69	124.81
14	2	4004	BCR	C34-C9-C8	2.22	121.57	118.08
11	a	1137	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
11	1	1133	CLA	CMC-C2C-C1C	2.22	128.42	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1134	CLA	CHB-C4A-NA	2.22	127.58	124.51
11	A	1119	CLA	OBD-CAD-C3D	-2.22	124.30	127.98
14	a	4001	BCR	C34-C9-C10	-2.22	119.82	122.92
14	A	4002	BCR	C34-C9-C8	2.22	121.57	118.08
11	A	1102	CLA	CAC-C3C-C4C	2.22	127.69	124.81
11	a	1125	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	a	1134	CLA	OBD-CAD-C3D	-2.22	124.30	127.98
11	a	1119	CLA	C4-C3-C5	2.22	119.00	115.27
11	1	1116	CLA	C4-C3-C5	2.22	119.00	115.27
11	b	1013	CLA	CMC-C2C-C1C	2.22	128.41	125.04
11	2	1212	CLA	CED-O2D-CGD	2.22	120.95	115.94
11	a	1104	CLA	C9-C8-C7	2.22	119.31	111.29
11	A	1125	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
11	A	1116	CLA	C1-O2A-CGA	2.21	122.25	116.44
11	2	1203	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	A	1102	CLA	C1-O2A-CGA	2.21	122.25	116.44
11	A	1121	CLA	C3C-C4C-NC	2.21	113.05	110.57
14	L	4019	BCR	C35-C13-C14	-2.21	119.82	122.92
11	2	1215	CLA	C9-C8-C7	2.21	119.30	111.29
11	1	1124	CLA	C4-C3-C5	2.21	118.99	115.27
11	b	1239	CLA	CMB-C2B-C3B	2.21	128.81	124.68
11	1	1129	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
11	2	1219	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	B	1201	CLA	C1-C2-C3	-2.21	122.22	126.04
11	b	1215	CLA	CAC-C3C-C4C	2.21	127.68	124.81
11	a	1120	CLA	CMB-C2B-C3B	2.21	128.81	124.68
11	2	1208	CLA	CMB-C2B-C3B	2.21	128.81	124.68
11	B	1230	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	B	1023	CLA	C4-C3-C5	2.21	118.99	115.27
11	B	1228	CLA	CAC-C3C-C4C	2.21	127.67	124.81
11	2	1021	CLA	CAC-C3C-C4C	2.21	127.67	124.81
11	2	1227	CLA	C3C-C4C-NC	2.21	113.05	110.57
11	1	1022	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
11	A	1115	CLA	CAC-C3C-C4C	2.21	127.67	124.81
11	b	1209	CLA	C3C-C4C-NC	2.21	113.05	110.57
11	2	1229	CLA	C4-C3-C5	2.21	118.98	115.27
11	2	1205	CLA	C4-C3-C5	2.21	118.98	115.27
11	1	1117	CLA	C3C-C4C-NC	2.21	113.05	110.57
11	a	1104	CLA	C1-C2-C3	-2.21	122.23	126.04
11	B	1013	CLA	OBD-CAD-C3D	-2.21	124.32	127.98
11	1	1237	CLA	CHB-C4A-NA	2.20	127.56	124.51
11	b	1013	CLA	C4-C3-C5	2.20	118.98	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1108	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
11	b	1207	CLA	CED-O2D-CGD	2.20	120.92	115.94
11	A	1109	CLA	C9-C8-C10	2.20	119.27	111.29
11	a	1105	CLA	C3C-C4C-NC	2.20	113.04	110.57
11	A	1103	CLA	C3C-C4C-NC	2.20	113.04	110.57
11	B	1207	CLA	OBD-CAD-C3D	-2.20	124.32	127.98
11	2	1021	CLA	CED-O2D-CGD	2.20	120.92	115.94
11	B	1230	CLA	CMC-C2C-C1C	2.20	128.39	125.04
11	A	1129	CLA	CMB-C2B-C3B	2.20	128.80	124.68
14	B	4005	BCR	C23-C24-C25	-2.20	121.02	127.20
14	l	4022	BCR	C30-C25-C24	2.20	122.01	115.78
11	b	1219	CLA	CAC-C3C-C4C	2.20	127.67	124.81
11	A	1140	CLA	CMB-C2B-C3B	2.20	128.79	124.68
11	1	1122	CLA	C1-O2A-CGA	2.20	122.21	116.44
11	1	1237	CLA	CMC-C2C-C1C	2.20	128.39	125.04
14	2	4005	BCR	C3-C4-C5	-2.20	110.15	114.08
12	b	2002	PQN	C2M-C2-C1	2.20	119.91	116.27
11	L	1501	CLA	CHB-C4A-NA	2.20	127.55	124.51
11	b	1231	CLA	CAC-C3C-C4C	2.20	127.66	124.81
11	2	1202	CLA	C1-O2A-CGA	2.20	122.21	116.44
11	A	1108	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
11	a	1237	CLA	C1-O2A-CGA	2.20	122.21	116.44
11	b	1021	CLA	C5-C3-C2	-2.20	116.67	121.12
11	A	1801	CLA	CAC-C3C-C2C	2.20	131.29	127.53
14	b	4017	BCR	C37-C22-C21	-2.20	119.85	122.92
14	2	4009	BCR	C8-C7-C6	-2.20	121.03	127.20
11	a	1101	CLA	C9-C8-C10	2.20	119.24	111.29
11	2	1203	CLA	CMB-C2B-C3B	2.20	128.78	124.68
14	2	4010	BCR	C30-C25-C24	2.19	121.99	115.78
14	B	4005	BCR	C19-C18-C17	2.19	122.31	118.94
14	b	4010	BCR	C35-C13-C14	-2.19	119.85	122.92
11	b	1205	CLA	CMB-C2B-C3B	2.19	128.78	124.68
11	b	1235	CLA	C4-C3-C5	2.19	118.96	115.27
11	B	1238	CLA	C1-O2A-CGA	2.19	122.19	116.44
11	A	1104	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
14	F	4020	BCR	C3-C4-C5	-2.19	110.16	114.08
11	b	1207	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	a	1118	CLA	C3C-C4C-NC	2.19	113.03	110.57
11	B	1226	CLA	CMB-C2B-C3B	2.19	128.78	124.68
11	L	1502	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
11	A	1113	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
11	a	1022	CLA	C1-O2A-CGA	2.19	122.19	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	4022	BCR	C1-C6-C5	-2.19	119.53	122.61
11	b	1239	CLA	C3C-C4C-NC	2.19	113.03	110.57
11	2	1206	CLA	CMB-C2B-C3B	2.19	128.78	124.68
11	A	1113	CLA	CAC-C3C-C4C	2.19	127.65	124.81
14	1	4003	BCR	C27-C26-C25	-2.19	119.55	122.73
14	b	4017	BCR	C23-C24-C25	-2.19	121.05	127.20
11	b	1210	CLA	C9-C8-C7	2.19	119.22	111.29
11	1	1112	CLA	CAC-C3C-C4C	2.19	127.65	124.81
11	A	1134	CLA	C3C-C4C-NC	2.19	113.03	110.57
11	2	1217	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	1	4002	BCR	C37-C22-C21	-2.19	119.86	122.92
14	a	4002	BCR	C36-C18-C17	-2.19	119.86	122.92
14	2	4005	BCR	C30-C25-C26	-2.19	119.53	122.61
11	a	1011	CLA	C4-C3-C5	2.19	118.95	115.27
11	b	1212	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
11	B	1205	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	B	1223	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
11	1	1140	CLA	C4-C3-C2	-2.18	118.08	123.68
11	1	1116	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	1	4008	BCR	C36-C18-C17	-2.18	119.87	122.92
11	B	1209	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	a	1111	CLA	C9-C8-C10	2.18	119.19	111.29
11	B	1205	CLA	C4-C3-C5	2.18	118.94	115.27
11	2	1223	CLA	C4-C3-C5	2.18	118.94	115.27
11	B	1013	CLA	C1-C2-C3	-2.18	122.28	126.04
14	l	4019	BCR	C8-C7-C6	-2.18	121.08	127.20
11	1	1124	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
11	2	1215	CLA	C6-C5-C3	2.18	119.17	113.45
11	A	1022	CLA	C1-O2A-CGA	2.18	122.16	116.44
14	2	4011	BCR	C1-C6-C5	-2.18	119.55	122.61
16	b	5002	LMG	O8-C28-C29	2.18	118.73	111.91
11	B	1225	CLA	OBD-CAD-C3D	-2.18	124.37	127.98
11	a	1117	CLA	C1-O2A-CGA	2.18	122.15	116.44
14	1	4008	BCR	C30-C25-C24	2.17	121.93	115.78
14	2	4004	BCR	C1-C6-C5	-2.17	119.55	122.61
11	1	1105	CLA	OBD-CAD-C3D	-2.17	124.37	127.98
11	b	1230	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
11	B	1021	CLA	CHA-C1A-NA	-2.17	121.42	126.40
11	B	1013	CLA	CMC-C2C-C1C	2.17	128.35	125.04
14	f	4013	BCR	C40-C30-C25	-2.17	106.78	110.30
11	1	1112	CLA	CED-O2D-CGD	2.17	120.85	115.94
11	a	1112	CLA	CMB-C2B-C3B	2.17	128.74	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1236	CLA	C1-O2A-CGA	2.17	123.03	116.73
11	a	1111	CLA	C11-C10-C8	-2.17	108.90	115.92
11	A	1131	CLA	C4-C3-C5	2.17	118.92	115.27
11	l	1502	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
11	1	1022	CLA	C11-C10-C8	-2.17	108.91	115.92
11	B	1207	CLA	CHB-C4A-NA	2.17	127.51	124.51
11	1	1114	CLA	C3C-C4C-NC	2.17	113.00	110.57
11	2	1239	CLA	OBD-CAD-C3D	-2.17	124.38	127.98
11	2	1210	CLA	C1-O2A-CGA	2.17	122.13	116.44
11	A	1106	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
14	8	4022	BCR	C4-C5-C6	-2.17	119.58	122.73
14	B	4004	BCR	C23-C22-C21	2.17	122.27	118.94
14	1	4001	BCR	C27-C26-C25	-2.17	119.59	122.73
11	a	1136	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
14	8	4022	BCR	C35-C13-C14	-2.17	119.89	122.92
11	2	1202	CLA	C3C-C4C-NC	2.17	113.00	110.57
11	A	1121	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
11	A	1131	CLA	C1-O2A-CGA	2.16	122.12	116.44
11	B	1228	CLA	C1-O2A-CGA	2.16	122.12	116.44
11	a	1138	CLA	CMD-C2D-C3D	-2.16	120.63	124.68
14	B	4006	BCR	C35-C13-C14	-2.16	119.89	122.92
11	b	1215	CLA	C1-O2A-CGA	2.16	122.12	116.44
11	A	1127	CLA	CED-O2D-CGD	2.16	120.83	115.94
15	A	5001	LHG	O7-C7-O9	-2.16	118.48	123.70
11	2	1235	CLA	CHB-C4A-NA	2.16	127.50	124.51
11	a	1131	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	a	4007	BCR	C31-C1-C6	-2.16	106.79	110.30
11	B	1234	CLA	C9-C8-C7	2.16	119.12	111.29
11	1	1117	CLA	C9-C8-C10	2.16	119.12	111.29
11	b	1228	CLA	C1-O2A-CGA	2.16	122.11	116.44
11	B	1216	CLA	C3C-C4C-NC	2.16	113.00	110.57
11	a	1126	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
11	A	1112	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
11	A	1103	CLA	C9-C8-C10	2.16	119.12	111.29
14	L	4022	BCR	C29-C30-C25	-2.16	107.16	110.48
11	B	1234	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
14	b	4006	BCR	C28-C27-C26	-2.16	110.22	114.08
14	2	4017	BCR	C38-C26-C25	-2.16	122.10	124.53
11	A	1011	CLA	C3C-C4C-NC	2.16	112.99	110.57
11	a	1022	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
16	B	5002	LMG	O8-C28-C29	2.16	118.68	111.91
14	F	4018	BCR	C8-C7-C6	-2.16	121.14	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4001	BCR	C35-C13-C14	-2.16	119.90	122.92
11	1	1111	CLA	C4-C3-C5	2.16	118.90	115.27
11	b	1021	CLA	CAC-C3C-C4C	2.16	127.61	124.81
11	1	1119	CLA	C7-C6-C5	-2.16	107.50	113.36
14	M	4021	BCR	C38-C26-C27	2.16	117.76	113.62
14	B	4017	BCR	C35-C13-C12	2.16	121.47	118.08
14	6	4018	BCR	C29-C30-C25	-2.16	107.16	110.48
14	b	4006	BCR	C8-C7-C6	-2.16	121.15	127.20
11	A	1801	CLA	CMB-C2B-C3B	2.15	128.71	124.68
11	A	1127	CLA	CAC-C3C-C4C	2.15	127.60	124.81
14	f	4013	BCR	C35-C13-C12	2.15	121.47	118.08
11	L	1503	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
11	B	1232	CLA	C3C-C4C-NC	2.15	112.98	110.57
11	a	1130	CLA	C3C-C4C-NC	2.15	112.98	110.57
11	b	1203	CLA	CHB-C4A-NA	2.15	127.49	124.51
11	B	1219	CLA	CED-O2D-CGD	2.15	120.80	115.94
14	L	4022	BCR	C34-C9-C8	2.15	121.46	118.08
11	A	1120	CLA	C3C-C4C-NC	2.15	112.98	110.57
11	A	1124	CLA	CHB-C4A-NA	2.15	127.48	124.51
11	A	1801	CLA	C4C-C3C-C2C	-2.15	103.77	106.90
11	a	1139	CLA	C1-O2A-CGA	2.15	122.08	116.44
11	b	1216	CLA	CED-O2D-CGD	2.15	120.79	115.94
14	b	4005	BCR	C28-C27-C26	-2.15	110.25	114.08
11	2	1218	CLA	CMB-C2B-C3B	2.14	128.69	124.68
11	2	1240	CLA	CAA-CBA-CGA	-2.14	108.98	113.59
14	B	4011	BCR	C23-C22-C21	2.14	122.23	118.94
11	A	1117	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
11	2	1216	CLA	C9-C8-C7	2.14	119.06	111.29
11	1	1022	CLA	C4-C3-C5	2.14	118.88	115.27
11	1	1138	CLA	C3C-C4C-NC	2.14	112.97	110.57
11	B	1222	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	8	4022	BCR	C35-C13-C12	2.14	121.45	118.08
14	2	4017	BCR	C37-C22-C21	-2.14	119.92	122.92
11	2	1229	CLA	C9-C8-C10	2.14	119.05	111.29
11	1	1121	CLA	CMB-C2B-C3B	2.14	128.69	124.68
14	f	4013	BCR	C30-C25-C24	2.14	121.84	115.78
11	B	1215	CLA	C9-C8-C10	2.14	119.05	111.29
11	2	1234	CLA	CAC-C3C-C4C	2.14	127.59	124.81
11	2	1215	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
11	1	1012	CLA	C5-C3-C2	-2.14	116.79	121.12
11	2	1228	CLA	C5-C3-C4	2.14	119.33	114.60
14	a	4008	BCR	C23-C24-C25	-2.14	121.19	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1134	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
11	A	1101	CLA	C9-C8-C10	2.14	119.03	111.29
11	1	1103	CLA	CED-O2D-CGD	2.14	120.77	115.94
11	K	1402	CLA	C1-C2-C3	-2.14	123.30	126.75
14	7	4021	BCR	C35-C13-C12	2.14	121.44	118.08
14	8	4022	BCR	C23-C22-C21	2.14	122.22	118.94
12	2	2002	PQN	C14-C13-C15	2.14	118.86	115.27
11	a	1139	CLA	C3C-C4C-NC	2.13	112.97	110.57
11	2	1207	CLA	CAA-C2A-C1A	2.13	118.97	111.97
11	2	1222	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
16	B	5002	LMG	C8-O7-C10	-2.13	112.54	117.79
11	1	1106	CLA	CED-O2D-CGD	2.13	120.76	115.94
11	b	1215	CLA	OBD-CAD-C3D	-2.13	124.44	127.98
11	B	1201	CLA	CMC-C2C-C1C	2.13	128.29	125.04
11	A	1114	CLA	CMB-C2B-C3B	2.13	128.67	124.68
11	B	1226	CLA	C4-C3-C5	2.13	118.86	115.27
14	1	4008	BCR	C35-C13-C14	-2.13	119.94	122.92
11	2	1225	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
11	B	1225	CLA	C4-C3-C5	2.13	118.85	115.27
11	2	1209	CLA	CHB-C4A-NA	2.13	127.45	124.51
11	1	1140	CLA	C9-C8-C10	2.13	119.00	111.29
15	2	5004	LHG	C5-O7-C7	-2.13	112.55	117.79
11	A	1126	CLA	C9-C8-C7	2.13	119.00	111.29
11	a	1110	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
11	B	1227	CLA	CHC-C1C-C2C	-2.13	120.84	126.72
11	b	1229	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
12	A	2001	PQN	C2M-C2-C1	2.13	119.79	116.27
11	2	1218	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
11	A	1102	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
11	B	1213	CLA	C4-C3-C5	2.12	118.84	115.27
11	2	1231	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
14	l	4019	BCR	C34-C9-C10	-2.12	119.95	122.92
12	B	2002	PQN	C2M-C2-C1	2.12	119.79	116.27
11	b	1210	CLA	CHB-C4A-NA	2.12	127.45	124.51
11	b	1208	CLA	OBD-CAD-C3D	-2.12	124.46	127.98
14	B	4017	BCR	C35-C13-C14	-2.12	119.95	122.92
15	B	5004	LHG	O7-C7-O9	-2.12	118.58	123.70
11	b	1234	CLA	CMC-C2C-C1C	2.12	128.27	125.04
11	2	1231	CLA	CAA-CBA-CGA	-2.12	109.03	113.59
11	2	1203	CLA	C1-O2A-CGA	2.12	122.01	116.44
11	B	1225	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	b	1206	CLA	CHC-C1C-C2C	-2.12	120.86	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1208	CLA	CED-O2D-CGD	2.12	120.73	115.94
11	B	1021	CLA	C1-C2-C3	-2.12	122.38	126.04
11	2	1239	CLA	CED-O2D-CGD	2.12	120.73	115.94
11	a	1801	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	b	1219	CLA	CED-O2D-CGD	2.12	120.73	115.94
14	8	4022	BCR	C30-C25-C24	2.12	121.77	115.78
11	A	1138	CLA	CED-O2D-CGD	2.12	120.72	115.94
11	b	1201	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	2	1221	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
11	a	1124	CLA	C10-C8-C9	2.12	120.26	110.51
11	2	1231	CLA	C3C-C4C-NC	2.12	112.94	110.57
14	6	4013	BCR	C35-C13-C12	2.11	121.41	118.08
11	B	1203	CLA	CHB-C4A-NA	2.11	127.44	124.51
11	B	1211	CLA	CMD-C2D-C3D	-2.11	120.72	124.68
11	B	1204	CLA	C3C-C4C-NC	2.11	112.94	110.57
11	2	1235	CLA	CED-O2D-CGD	2.11	120.72	115.94
11	1	1128	CLA	CMC-C2C-C1C	2.11	128.26	125.04
11	a	1133	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
14	F	4020	BCR	C34-C9-C8	2.11	121.41	118.08
11	b	1201	CLA	CED-O2D-CGD	2.11	120.71	115.94
14	A	4008	BCR	C37-C22-C21	-2.11	119.97	122.92
11	2	1224	CLA	CHB-C4A-NA	2.11	127.43	124.51
11	B	1217	CLA	CHB-C4A-NA	2.11	127.43	124.51
11	l	1501	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
11	2	1229	CLA	CAC-C3C-C4C	2.11	127.55	124.81
11	B	1225	CLA	C6-C5-C3	-2.11	107.92	113.45
11	A	1137	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
16	b	5002	LMG	C7-O1-C1	-2.11	109.62	113.74
11	2	1238	CLA	C1-C2-C3	-2.11	122.39	126.04
11	1	1103	CLA	C3C-C4C-NC	2.11	112.94	110.57
11	1	1101	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
11	2	1230	CLA	CED-O2D-CGD	2.11	120.70	115.94
11	b	1206	CLA	C3C-C4C-NC	2.11	112.94	110.57
11	1	1131	CLA	C9-C8-C7	2.11	118.92	111.29
11	A	1114	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
14	2	4006	BCR	C35-C13-C12	2.11	121.40	118.08
14	2	4010	BCR	C1-C6-C5	-2.11	119.65	122.61
11	A	1125	CLA	C4-C3-C5	2.11	118.81	115.27
14	A	4008	BCR	C1-C6-C5	-2.11	119.65	122.61
11	b	1221	CLA	C4-C3-C2	-2.11	118.28	123.68
11	2	1235	CLA	C1-C2-C3	-2.11	122.40	126.04
11	a	1124	CLA	O1D-CGD-CBD	-2.10	120.18	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1105	CLA	CAC-C3C-C4C	2.10	127.54	124.81
11	2	1202	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
11	a	1127	CLA	C10-C8-C7	2.10	123.19	112.13
14	1	4008	BCR	C1-C6-C7	2.10	121.73	115.78
11	A	1119	CLA	C9-C8-C7	2.10	118.91	111.29
11	B	1021	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
11	2	1230	CLA	CHB-C4A-NA	2.10	127.42	124.51
11	B	1223	CLA	C1-O2A-CGA	2.10	121.96	116.44
14	1	4001	BCR	C8-C7-C6	-2.10	121.30	127.20
11	2	1232	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
14	f	4013	BCR	C38-C26-C27	2.10	117.65	113.62
11	1	1111	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
11	b	1235	CLA	CAC-C3C-C4C	2.10	127.53	124.81
11	1	1125	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
11	a	1112	CLA	CHB-C4A-NA	2.10	127.42	124.51
11	1	1101	CLA	CMB-C2B-C3B	2.10	128.61	124.68
11	B	1230	CLA	CED-O2D-CGD	2.10	120.69	115.94
11	2	1202	CLA	CED-O2D-CGD	2.10	120.68	115.94
11	1	1801	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
11	2	1230	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
12	2	2002	PQN	C11-C12-C13	-2.10	123.30	126.79
11	2	1220	CLA	CED-O2D-CGD	2.10	120.68	115.94
11	b	1215	CLA	C1-C2-C3	-2.10	122.42	126.04
11	b	1230	CLA	CHB-C4A-NA	2.10	127.41	124.51
11	A	1011	CLA	CED-O2D-CGD	2.10	120.68	115.94
11	A	1139	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
11	2	1205	CLA	C1-O2A-CGA	2.10	121.94	116.44
11	A	1118	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	a	1134	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
14	2	4009	BCR	C4-C5-C6	-2.09	119.69	122.73
11	B	1206	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
11	1	1137	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	1	1117	CLA	C1-O2A-CGA	2.09	121.93	116.44
11	B	1207	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
12	a	2001	PQN	C11-C12-C13	-2.09	123.31	126.79
11	B	1210	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	A	4007	BCR	C34-C9-C10	-2.09	120.00	122.92
11	a	1237	CLA	CED-O2D-CGD	2.09	120.66	115.94
11	1	1131	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
11	b	1239	CLA	CMC-C2C-C1C	2.09	128.22	125.04
11	1	1127	CLA	CED-O2D-CGD	2.09	120.66	115.94
11	a	1125	CLA	OBD-CAD-C3D	-2.09	124.51	127.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1227	CLA	C3C-C4C-NC	2.09	112.91	110.57
14	1	4003	BCR	C35-C13-C14	-2.09	120.00	122.92
11	A	1117	CLA	C3C-C4C-NC	2.09	112.91	110.57
11	2	1210	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	l	1501	CLA	C4-C3-C2	-2.08	118.33	123.68
11	a	1139	CLA	CMB-C2B-C3B	2.08	128.58	124.68
11	b	1226	CLA	C1-O2A-CGA	2.08	121.91	116.44
14	b	4011	BCR	C1-C6-C7	2.08	121.67	115.78
14	b	4006	BCR	C8-C9-C10	2.08	122.14	118.94
11	A	1128	CLA	C9-C8-C10	2.08	118.83	111.29
14	F	4013	BCR	C30-C25-C24	2.08	121.67	115.78
11	b	1229	CLA	CED-O2D-CGD	2.08	120.64	115.94
11	B	1201	CLA	CAC-C3C-C4C	2.08	127.51	124.81
11	A	1123	CLA	C9-C8-C7	2.08	118.83	111.29
11	1	1126	CLA	C4-C3-C2	-2.08	118.34	123.68
14	1	4008	BCR	C8-C9-C10	2.08	122.13	118.94
11	2	1201	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	a	1104	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	2	1227	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
11	2	1238	CLA	CAC-C3C-C4C	2.08	127.51	124.81
14	b	4010	BCR	C37-C22-C21	-2.08	120.01	122.92
14	b	4009	BCR	C1-C6-C7	2.08	121.66	115.78
14	b	4017	BCR	C28-C27-C26	-2.08	110.37	114.08
11	1	1011	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
11	a	1101	CLA	C4-C3-C5	2.08	118.76	115.27
14	2	4017	BCR	C35-C13-C14	-2.08	120.02	122.92
11	b	1208	CLA	CMB-C2B-C3B	2.08	128.56	124.68
11	2	1234	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
11	A	1106	CLA	C3C-C4C-NC	2.07	112.90	110.57
11	a	1138	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	b	1206	CLA	C4-C3-C5	2.07	118.76	115.27
11	b	1023	CLA	C9-C8-C10	2.07	118.80	111.29
11	a	1116	CLA	C4-C3-C5	2.07	118.76	115.27
11	b	1220	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
11	8	1502	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	a	1130	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
14	B	4014	BCR	C31-C1-C6	-2.07	106.94	110.30
11	1	1113	CLA	CAC-C3C-C4C	2.07	127.50	124.81
11	a	1022	CLA	C4-C3-C5	2.07	118.75	115.27
14	L	4019	BCR	C28-C27-C26	-2.07	110.38	114.08
11	1	1012	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	1	1106	CLA	C7-C6-C5	-2.07	107.74	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1234	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
11	a	1106	CLA	C1-O2A-CGA	2.07	121.87	116.44
11	B	1231	CLA	C3C-C4C-NC	2.07	112.89	110.57
14	M	4021	BCR	C33-C5-C4	2.07	117.59	113.62
11	b	1023	CLA	CMC-C2C-C1C	2.07	128.19	125.04
11	B	1206	CLA	C1-O2A-CGA	2.07	121.87	116.44
11	b	1239	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
14	b	4009	BCR	C35-C13-C14	-2.07	120.03	122.92
11	B	1207	CLA	CMB-C2B-C3B	2.07	128.54	124.68
11	1	1112	CLA	CMB-C2B-C3B	2.07	128.54	124.68
11	B	1023	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
11	A	1133	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
11	1	1128	CLA	CMB-C2B-C3B	2.07	128.54	124.68
11	a	1123	CLA	C4-C3-C5	2.07	118.75	115.27
11	B	1223	CLA	C9-C8-C7	2.06	118.77	111.29
11	2	1224	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
11	a	1110	CLA	CAC-C3C-C4C	2.06	127.49	124.81
11	2	1023	CLA	C1-C2-C3	-2.06	122.47	126.04
11	2	1232	CLA	CMB-C2B-C3B	2.06	128.54	124.68
11	A	1022	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	8	4022	BCR	C30-C25-C26	-2.06	119.71	122.61
11	A	1135	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
11	8	1501	CLA	C4-C3-C2	-2.06	118.39	123.68
11	a	1107	CLA	C1-O2A-CGA	2.06	121.85	116.44
11	a	1115	CLA	CAC-C3C-C4C	2.06	127.48	124.81
14	1	4007	BCR	C31-C1-C6	-2.06	106.96	110.30
14	1	4007	BCR	C23-C22-C21	2.06	122.10	118.94
11	2	1215	CLA	C9-C8-C10	2.06	118.75	111.29
11	b	1204	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
11	B	1231	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
11	2	1207	CLA	C11-C10-C8	-2.06	109.27	115.92
11	1	1112	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
14	1	4007	BCR	C23-C24-C25	-2.06	121.42	127.20
11	2	1216	CLA	C4-C3-C5	2.06	118.73	115.27
11	b	1023	CLA	CAC-C3C-C4C	2.06	127.48	124.81
11	a	1128	CLA	CMB-C2B-C3B	2.06	128.53	124.68
14	a	4002	BCR	C28-C27-C26	-2.06	110.41	114.08
11	2	1222	CLA	C1-O2A-CGA	2.06	121.84	116.44
11	A	1138	CLA	CMD-C2D-C3D	-2.06	120.83	124.68
11	B	1222	CLA	C1-O2A-CGA	2.05	121.83	116.44
14	b	4010	BCR	C1-C6-C5	-2.05	119.72	122.61
11	b	1213	CLA	CAC-C3C-C4C	2.05	127.47	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1013	CLA	CAC-C3C-C4C	2.05	127.47	124.81
11	a	1128	CLA	C1-O2A-CGA	2.05	121.83	116.44
14	a	4007	BCR	C35-C13-C12	2.05	121.31	118.08
11	2	1223	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
11	1	1109	CLA	CED-O2D-CGD	2.05	120.58	115.94
11	A	1011	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
11	b	1238	CLA	C11-C10-C8	-2.05	109.29	115.92
11	a	1118	CLA	C4-C3-C5	2.05	118.72	115.27
11	A	1108	CLA	CAC-C3C-C4C	2.05	127.47	124.81
11	B	1232	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
16	b	5002	LMG	C8-O7-C10	-2.05	112.74	117.79
11	B	1225	CLA	CBA-CAA-C2A	2.05	119.91	113.86
11	a	1119	CLA	CMC-C2C-C1C	2.05	128.16	125.04
11	b	1206	CLA	CHB-C4A-NA	2.05	127.34	124.51
11	1	1111	CLA	CHA-C1A-NA	-2.05	121.71	126.40
14	b	4005	BCR	C7-C8-C9	-2.05	123.14	126.23
11	a	1237	CLA	CMB-C2B-C3B	2.05	128.51	124.68
11	a	1121	CLA	CMD-C2D-C3D	-2.05	120.85	124.68
11	B	1234	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
14	A	4008	BCR	C34-C9-C8	2.05	121.30	118.08
11	A	1101	CLA	CED-O2D-CGD	2.05	120.57	115.94
11	A	1124	CLA	CED-O2D-CGD	2.05	120.57	115.94
11	1	1102	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
14	a	4002	BCR	C27-C26-C25	-2.04	119.76	122.73
14	A	4007	BCR	C8-C7-C6	-2.04	121.46	127.20
11	k	1402	CLA	C5-C3-C4	2.04	119.12	114.60
11	a	1110	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
11	2	1235	CLA	C6-C5-C3	-2.04	108.09	113.45
11	A	1124	CLA	C6-C5-C3	-2.04	108.10	113.45
11	1	1113	CLA	CHB-C4A-NA	2.04	127.34	124.51
14	B	4010	BCR	C27-C26-C25	-2.04	119.77	122.73
11	1	1125	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
11	1	1022	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
14	F	4013	BCR	C1-C6-C5	-2.04	119.74	122.61
11	2	1218	CLA	CHB-C4A-NA	2.04	127.33	124.51
11	1	1133	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
11	a	1132	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
11	2	1229	CLA	C1-C2-C3	-2.04	122.51	126.04
14	a	4002	BCR	C8-C9-C10	2.04	122.07	118.94
11	1	1103	CLA	C11-C12-C13	-2.04	109.32	115.92
11	B	1219	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	2	4011	BCR	C19-C18-C17	2.04	122.07	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1209	CLA	CMC-C2C-C1C	2.04	128.15	125.04
11	a	1123	CLA	C9-C8-C7	2.04	118.68	111.29
11	B	1218	CLA	CAC-C3C-C4C	2.04	127.46	124.81
11	1	1124	CLA	CHB-C4A-NA	2.04	127.33	124.51
11	b	1205	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
14	2	4017	BCR	C3-C4-C5	-2.04	110.44	114.08
11	B	1202	CLA	C4-C3-C5	2.04	118.70	115.27
11	1	1131	CLA	C4-C3-C5	2.04	118.70	115.27
11	2	1206	CLA	C1-C2-C3	-2.04	122.52	126.04
11	A	1237	CLA	C1-O2A-CGA	2.04	121.79	116.44
11	b	1223	CLA	C1-O2A-CGA	2.04	121.79	116.44
11	1	1109	CLA	CAC-C3C-C4C	2.04	127.45	124.81
14	a	4007	BCR	C34-C9-C10	-2.04	120.07	122.92
11	2	1023	CLA	CED-O2D-CGD	2.04	120.54	115.94
11	B	1222	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	B	1215	CLA	C9-C8-C7	2.03	118.66	111.29
11	2	1206	CLA	C4-C3-C5	2.03	118.69	115.27
11	B	1023	CLA	C11-C10-C8	-2.03	109.34	115.92
11	2	1203	CLA	CAC-C3C-C4C	2.03	127.45	124.81
14	b	4011	BCR	C32-C1-C6	-2.03	107.00	110.30
11	2	1202	CLA	CMD-C2D-C3D	-2.03	120.87	124.68
11	B	1021	CLA	CHC-C1C-C2C	-2.03	121.09	126.72
11	A	1122	CLA	C9-C8-C7	2.03	118.66	111.29
11	b	1240	CLA	CAC-C3C-C4C	2.03	127.45	124.81
11	b	1231	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
11	1	1135	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
11	1	1101	CLA	CED-O2D-CGD	2.03	120.53	115.94
11	A	1104	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	1	1126	CLA	C9-C8-C7	2.03	118.65	111.29
11	b	1227	CLA	OBD-CAD-C3D	-2.03	124.61	127.98
11	2	1213	CLA	C7-C6-C5	-2.03	107.84	113.36
11	8	1502	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
14	B	4004	BCR	C23-C24-C25	-2.03	121.50	127.20
14	b	4004	BCR	C23-C22-C21	2.03	122.06	118.94
11	b	1214	CLA	C9-C8-C7	2.03	118.64	111.29
11	1	1119	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
14	2	4004	BCR	C1-C6-C7	2.03	121.52	115.78
11	2	1239	CLA	CAC-C3C-C4C	2.03	127.44	124.81
11	B	1226	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	1	1112	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	1	1801	CLA	C4-C3-C5	2.03	118.68	115.27
14	B	4006	BCR	C29-C30-C25	2.03	113.60	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1120	CLA	CHB-C4A-NA	2.03	127.32	124.51
14	f	4013	BCR	C36-C18-C17	-2.03	120.08	122.92
11	2	1219	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
15	1	5001	LHG	O7-C7-O9	-2.03	118.81	123.70
15	a	5001	LHG	O7-C7-O9	-2.03	118.81	123.70
11	1	1103	CLA	C1-O2A-CGA	2.03	121.76	116.44
11	1	1134	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
11	1	1121	CLA	CHB-C4A-NA	2.03	127.31	124.51
11	B	1209	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
14	L	4022	BCR	C23-C24-C25	-2.02	121.52	127.20
11	a	1801	CLA	C1-C2-C3	-2.02	122.54	126.04
11	b	1216	CLA	C1-O2A-CGA	2.02	121.75	116.44
14	6	4013	BCR	C24-C25-C26	-2.02	116.56	121.46
11	b	1230	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
11	1	1135	CLA	C1-O2A-CGA	2.02	121.75	116.44
11	B	1234	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
11	A	1104	CLA	C11-C12-C13	-2.02	109.38	115.92
14	b	4014	BCR	C19-C18-C17	2.02	122.04	118.94
11	2	1206	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
14	F	4018	BCR	C40-C30-C25	-2.02	107.02	110.30
11	A	1123	CLA	CMD-C2D-C3D	-2.02	120.90	124.68
11	b	1223	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
11	B	1240	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
14	B	4009	BCR	C23-C22-C21	2.02	122.04	118.94
12	A	2001	PQN	C11-C12-C13	-2.02	123.43	126.79
11	K	1402	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
14	a	4008	BCR	C1-C6-C7	2.02	121.49	115.78
11	2	1225	CLA	C3C-C4C-NC	2.02	112.84	110.57
11	a	1120	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
11	B	1230	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
11	1	1121	CLA	CED-O2D-CGD	2.02	120.50	115.94
12	2	2002	PQN	C25-C23-C22	2.02	122.75	112.13
12	B	2002	PQN	C14-C13-C15	2.02	118.67	115.27
14	8	4022	BCR	C1-C6-C5	-2.02	119.77	122.61
11	A	1107	CLA	CHA-C1A-NA	-2.02	121.78	126.40
11	1	1123	CLA	C4-C3-C5	2.02	118.67	115.27
11	b	1013	CLA	C1-C2-C3	-2.02	122.55	126.04
11	8	1501	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
11	2	1222	CLA	CHB-C4A-NA	2.02	127.30	124.51
11	a	1119	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
11	A	1107	CLA	C1-O2A-CGA	2.02	121.73	116.44
11	K	1402	CLA	CHB-C4A-NA	2.02	127.30	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1107	CLA	CHA-C1A-NA	-2.02	121.78	126.40
11	B	1023	CLA	OBD-CAD-CBD	-2.02	123.02	125.89
11	a	1113	CLA	CHB-C4A-NA	2.01	127.30	124.51
11	b	1222	CLA	C6-C7-C8	-2.01	109.41	115.92
14	l	4019	BCR	C35-C13-C14	-2.01	120.10	122.92
11	l	1502	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
11	A	1113	CLA	CHB-C4A-NA	2.01	127.30	124.51
14	6	4020	BCR	C35-C13-C12	2.01	121.25	118.08
14	A	4007	BCR	C7-C8-C9	-2.01	123.19	126.23
11	a	1104	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
14	B	4009	BCR	C23-C24-C25	-2.01	121.55	127.20
11	b	1214	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
11	a	1109	CLA	C3C-C4C-NC	2.01	112.83	110.57
14	8	4019	BCR	C8-C9-C10	2.01	122.03	118.94
14	b	4014	BCR	C8-C7-C6	-2.01	121.55	127.20
11	A	1125	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
11	b	1207	CLA	CAC-C3C-C4C	2.01	127.42	124.81
11	1	1012	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
11	b	1210	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
11	k	1401	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	6	4013	BCR	C35-C13-C14	-2.01	120.11	122.92
11	K	1402	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
11	b	1201	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
11	1	1118	CLA	CHB-C4A-NA	2.01	127.29	124.51
11	2	1230	CLA	CMC-C2C-C1C	2.01	128.10	125.04
11	b	1239	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
11	2	1231	CLA	CMD-C2D-C3D	-2.01	120.92	124.68
11	B	1013	CLA	C4-C3-C5	2.01	118.65	115.27
11	1	1237	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
11	2	1013	CLA	CMC-C2C-C1C	2.01	128.10	125.04
14	B	4006	BCR	C1-C6-C7	2.01	121.46	115.78
11	2	1224	CLA	C1-O2A-CGA	2.01	121.71	116.44
11	a	1115	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
11	b	1223	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
11	B	1240	CLA	CAC-C3C-C4C	2.01	127.41	124.81
11	B	1240	CLA	CHB-C4A-NA	2.01	127.29	124.51
14	A	4001	BCR	C8-C7-C6	-2.01	121.57	127.20
11	1	1118	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
11	b	1211	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
11	K	1401	CLA	CHA-C1A-NA	-2.01	121.80	126.40
11	B	1213	CLA	C4-C3-C2	-2.00	118.53	123.68
14	b	4005	BCR	C23-C24-C25	-2.00	121.57	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4009	BCR	C37-C22-C21	-2.00	120.11	122.92
11	b	1216	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
11	1	1111	CLA	C9-C8-C10	2.00	118.55	111.29
11	B	1227	CLA	CHB-C4A-NA	2.00	127.28	124.51
14	2	4009	BCR	C28-C27-C26	-2.00	110.50	114.08
11	B	1216	CLA	CED-O2D-CGD	2.00	120.46	115.94
11	a	1138	CLA	C3C-C4C-NC	2.00	112.81	110.57
11	b	1207	CLA	C16-C15-C13	-2.00	109.45	115.92
11	a	1801	CLA	CMC-C2C-C3C	2.00	131.55	126.12
11	1	1105	CLA	CMB-C2B-C3B	2.00	128.42	124.68
11	A	1119	CLA	CED-O2D-CGD	2.00	120.46	115.94

All (748) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	2	1218	CLA	NC
11	2	1218	CLA	ND
11	2	1218	CLA	NA
11	a	1122	CLA	NC
11	a	1122	CLA	ND
11	a	1122	CLA	NA
11	A	1101	CLA	ND
11	A	1101	CLA	NA
11	b	1218	CLA	NC
11	b	1218	CLA	ND
11	b	1218	CLA	NA
11	1	1801	CLA	NC
11	1	1801	CLA	ND
11	1	1801	CLA	NA
11	A	1125	CLA	ND
11	A	1125	CLA	NA
11	b	1222	CLA	NC
11	b	1222	CLA	ND
11	b	1222	CLA	NA
11	2	1224	CLA	NC
11	2	1224	CLA	NA
11	2	1224	CLA	ND
11	K	1401	CLA	NC
11	K	1401	CLA	NA
11	K	1401	CLA	ND
11	a	1124	CLA	NC
11	a	1124	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	a	1124	CLA	NA
11	1	1133	CLA	NC
11	1	1133	CLA	ND
11	1	1133	CLA	NA
11	1	1139	CLA	NC
11	1	1139	CLA	ND
11	1	1139	CLA	NA
11	2	1208	CLA	NC
11	2	1208	CLA	ND
11	2	1208	CLA	NA
11	1	1111	CLA	NC
11	1	1111	CLA	NA
11	1	1111	CLA	ND
11	a	1114	CLA	ND
11	a	1114	CLA	NA
11	b	1213	CLA	NC
11	b	1213	CLA	ND
11	b	1213	CLA	NA
11	B	1210	CLA	NC
11	B	1210	CLA	ND
11	B	1210	CLA	NA
11	b	1240	CLA	NC
11	b	1240	CLA	ND
11	b	1240	CLA	NA
11	a	1022	CLA	ND
11	a	1022	CLA	NA
11	A	1120	CLA	NC
11	A	1120	CLA	ND
11	A	1120	CLA	NA
11	8	1501	CLA	NC
11	8	1501	CLA	ND
11	8	1501	CLA	NA
11	B	1216	CLA	NC
11	B	1216	CLA	ND
11	B	1216	CLA	NA
11	B	1213	CLA	NC
11	B	1213	CLA	ND
11	B	1213	CLA	NA
11	1	1120	CLA	NC
11	1	1120	CLA	ND
11	1	1120	CLA	NA
11	2	1217	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	2	1217	CLA	ND
11	2	1217	CLA	NA
11	K	1402	CLA	NC
11	K	1402	CLA	ND
11	K	1402	CLA	NA
11	1	1108	CLA	NC
11	1	1108	CLA	ND
11	1	1108	CLA	NA
11	2	1204	CLA	ND
11	2	1204	CLA	NA
11	B	1215	CLA	ND
11	B	1215	CLA	NA
11	A	1133	CLA	NC
11	A	1133	CLA	ND
11	A	1133	CLA	NA
11	1	1138	CLA	NC
11	1	1138	CLA	ND
11	1	1138	CLA	NA
11	b	1220	CLA	NC
11	b	1220	CLA	ND
11	b	1220	CLA	NA
11	b	1216	CLA	NC
11	b	1216	CLA	NA
11	b	1216	CLA	ND
11	b	1234	CLA	NC
11	b	1234	CLA	ND
11	b	1234	CLA	NA
11	B	1207	CLA	ND
11	B	1207	CLA	NA
11	a	1103	CLA	NC
11	a	1103	CLA	NA
11	a	1103	CLA	ND
11	1	1129	CLA	NC
11	1	1129	CLA	ND
11	1	1129	CLA	NA
11	b	1239	CLA	NC
11	b	1239	CLA	ND
11	b	1239	CLA	NA
11	1	1109	CLA	NC
11	1	1109	CLA	NA
11	1	1132	CLA	NC
11	1	1132	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	1	1132	CLA	NA
11	A	1126	CLA	NC
11	A	1126	CLA	ND
11	A	1126	CLA	NA
11	1	1103	CLA	NC
11	1	1103	CLA	ND
11	1	1103	CLA	NA
11	A	1109	CLA	NC
11	A	1109	CLA	NA
11	B	1202	CLA	NC
11	B	1202	CLA	NA
11	B	1202	CLA	ND
11	k	1402	CLA	NC
11	k	1402	CLA	ND
11	k	1402	CLA	NA
11	B	1203	CLA	NA
11	8	1502	CLA	NC
11	8	1502	CLA	ND
11	8	1502	CLA	NA
11	A	1119	CLA	NC
11	A	1119	CLA	ND
11	A	1119	CLA	NA
11	A	1113	CLA	NC
11	A	1113	CLA	NA
11	A	1113	CLA	ND
11	L	1502	CLA	NC
11	L	1502	CLA	ND
11	L	1502	CLA	NA
11	A	1131	CLA	ND
11	A	1131	CLA	NA
11	1	1022	CLA	NC
11	1	1022	CLA	ND
11	1	1022	CLA	NA
11	a	1112	CLA	NC
11	a	1112	CLA	ND
11	a	1112	CLA	NA
11	1	1123	CLA	ND
11	1	1123	CLA	NA
11	a	1115	CLA	NC
11	a	1115	CLA	NA
11	0	1401	CLA	NC
11	0	1401	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	0	1401	CLA	ND
11	b	1225	CLA	NC
11	b	1225	CLA	ND
11	b	1225	CLA	NA
11	a	1012	CLA	ND
11	a	1012	CLA	NA
11	1	1106	CLA	ND
11	1	1106	CLA	NA
11	A	1127	CLA	NC
11	A	1127	CLA	ND
11	A	1127	CLA	NA
11	A	1114	CLA	NC
11	A	1114	CLA	ND
11	A	1114	CLA	NA
11	2	1221	CLA	NC
11	2	1221	CLA	NA
11	2	1221	CLA	ND
11	B	1223	CLA	ND
11	B	1223	CLA	NA
11	a	1140	CLA	NC
11	a	1140	CLA	ND
11	a	1140	CLA	NA
11	A	1134	CLA	NC
11	A	1134	CLA	ND
11	A	1134	CLA	NA
11	1	1114	CLA	NC
11	1	1114	CLA	ND
11	1	1114	CLA	NA
11	b	1235	CLA	NC
11	b	1235	CLA	NA
11	b	1235	CLA	ND
11	a	1116	CLA	NC
11	a	1116	CLA	ND
11	a	1116	CLA	NA
11	A	1117	CLA	NC
11	A	1117	CLA	ND
11	A	1117	CLA	NA
11	a	1119	CLA	NC
11	a	1119	CLA	ND
11	a	1119	CLA	NA
11	B	1231	CLA	NC
11	B	1231	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	B	1231	CLA	NA
11	2	1231	CLA	NC
11	2	1231	CLA	ND
11	2	1231	CLA	NA
11	A	1128	CLA	NC
11	A	1128	CLA	ND
11	A	1128	CLA	NA
11	B	1224	CLA	NC
11	B	1224	CLA	NA
11	B	1224	CLA	ND
11	1	1137	CLA	NC
11	1	1137	CLA	NA
11	1	1137	CLA	ND
11	1	1130	CLA	NA
11	B	1206	CLA	ND
11	B	1206	CLA	NA
11	a	1102	CLA	NC
11	a	1102	CLA	ND
11	a	1102	CLA	NA
11	b	1219	CLA	NC
11	b	1219	CLA	ND
11	b	1219	CLA	NA
11	a	1120	CLA	NC
11	a	1120	CLA	ND
11	a	1120	CLA	NA
11	b	1230	CLA	NC
11	b	1230	CLA	ND
11	b	1230	CLA	NA
11	0	1402	CLA	NC
11	0	1402	CLA	ND
11	0	1402	CLA	NA
11	1	1124	CLA	NC
11	1	1124	CLA	ND
11	1	1124	CLA	NA
11	L	1503	CLA	ND
11	L	1503	CLA	NA
11	B	1234	CLA	NC
11	B	1234	CLA	ND
11	B	1234	CLA	NA
11	a	1106	CLA	NC
11	a	1106	CLA	ND
11	a	1106	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	2	1229	CLA	NC
11	2	1229	CLA	ND
11	2	1229	CLA	NA
11	a	1801	CLA	NC
11	a	1801	CLA	ND
11	a	1801	CLA	NA
11	B	1205	CLA	NC
11	B	1205	CLA	ND
11	B	1205	CLA	NA
11	2	1201	CLA	NC
11	2	1201	CLA	ND
11	2	1201	CLA	NA
11	a	1136	CLA	NC
11	a	1136	CLA	NA
11	a	1136	CLA	ND
11	2	1236	CLA	NC
11	2	1236	CLA	ND
11	2	1236	CLA	NA
11	2	1219	CLA	NC
11	2	1219	CLA	ND
11	2	1219	CLA	NA
11	1	1237	CLA	NC
11	1	1237	CLA	ND
11	1	1237	CLA	NA
11	2	1212	CLA	NC
11	2	1212	CLA	ND
11	2	1212	CLA	NA
11	1	1135	CLA	ND
11	1	1135	CLA	NA
11	1	1116	CLA	NC
11	1	1116	CLA	ND
11	1	1116	CLA	NA
11	2	1232	CLA	ND
11	2	1232	CLA	NA
11	a	1117	CLA	NC
11	a	1117	CLA	ND
11	a	1117	CLA	NA
11	b	1228	CLA	NC
11	b	1228	CLA	ND
11	b	1228	CLA	NA
11	2	1227	CLA	NC
11	2	1227	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	A	1011	CLA	NC
11	A	1011	CLA	NA
11	b	1227	CLA	NC
11	b	1227	CLA	NA
11	l	1501	CLA	NC
11	l	1501	CLA	NA
11	a	1105	CLA	NC
11	a	1105	CLA	ND
11	a	1105	CLA	NA
11	2	1235	CLA	NC
11	2	1235	CLA	ND
11	2	1235	CLA	NA
11	b	1201	CLA	NC
11	b	1201	CLA	ND
11	b	1201	CLA	NA
11	B	1239	CLA	NC
11	B	1239	CLA	ND
11	B	1239	CLA	NA
11	A	1237	CLA	NC
11	A	1237	CLA	ND
11	A	1237	CLA	NA
11	B	1209	CLA	NC
11	B	1209	CLA	ND
11	B	1209	CLA	NA
11	a	1118	CLA	NC
11	a	1118	CLA	ND
11	a	1118	CLA	NA
11	A	1116	CLA	NC
11	A	1116	CLA	ND
11	A	1116	CLA	NA
11	2	1209	CLA	NC
11	2	1209	CLA	ND
11	2	1209	CLA	NA
11	k	1401	CLA	NC
11	k	1401	CLA	NA
11	k	1401	CLA	ND
11	A	1022	CLA	ND
11	A	1022	CLA	NA
11	1	1136	CLA	NC
11	1	1136	CLA	NA
11	1	1136	CLA	ND
11	b	1212	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	b	1212	CLA	ND
11	b	1212	CLA	NA
11	A	1106	CLA	NC
11	A	1106	CLA	ND
11	A	1106	CLA	NA
11	2	1238	CLA	NC
11	2	1238	CLA	ND
11	2	1238	CLA	NA
11	a	1139	CLA	NC
11	a	1139	CLA	ND
11	a	1139	CLA	NA
11	a	1125	CLA	ND
11	a	1125	CLA	NA
11	A	1801	CLA	NC
11	A	1801	CLA	ND
11	A	1801	CLA	NA
11	b	1224	CLA	NC
11	b	1224	CLA	ND
11	b	1224	CLA	NA
11	2	1214	CLA	NC
11	2	1214	CLA	ND
11	2	1214	CLA	NA
11	B	1217	CLA	NC
11	B	1217	CLA	ND
11	B	1217	CLA	NA
11	8	1503	CLA	NC
11	8	1503	CLA	ND
11	8	1503	CLA	NA
11	B	1204	CLA	ND
11	B	1204	CLA	NA
11	a	1134	CLA	NC
11	a	1134	CLA	NA
11	a	1134	CLA	ND
11	1	1127	CLA	NC
11	1	1127	CLA	ND
11	1	1127	CLA	NA
11	1	1126	CLA	NC
11	1	1126	CLA	ND
11	1	1126	CLA	NA
11	a	1107	CLA	NC
11	a	1107	CLA	ND
11	a	1107	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	A	1129	CLA	NC
11	A	1129	CLA	ND
11	A	1129	CLA	NA
11	a	1237	CLA	NC
11	a	1237	CLA	ND
11	a	1237	CLA	NA
11	A	1115	CLA	NC
11	A	1115	CLA	ND
11	A	1115	CLA	NA
11	a	1113	CLA	NC
11	a	1113	CLA	ND
11	a	1113	CLA	NA
11	a	1128	CLA	NC
11	a	1128	CLA	ND
11	a	1128	CLA	NA
11	1	1122	CLA	NC
11	1	1122	CLA	ND
11	1	1122	CLA	NA
11	a	1110	CLA	ND
11	a	1110	CLA	NA
11	B	1212	CLA	NC
11	B	1212	CLA	ND
11	B	1212	CLA	NA
11	L	1501	CLA	NC
11	L	1501	CLA	ND
11	L	1501	CLA	NA
11	1	1140	CLA	NC
11	1	1140	CLA	ND
11	1	1140	CLA	NA
11	b	1215	CLA	ND
11	b	1215	CLA	NA
11	A	1123	CLA	ND
11	A	1123	CLA	NA
11	b	1226	CLA	NC
11	b	1226	CLA	ND
11	b	1226	CLA	NA
11	a	1108	CLA	NC
11	a	1108	CLA	ND
11	a	1108	CLA	NA
11	2	1234	CLA	ND
11	2	1234	CLA	NA
11	2	1213	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	2	1213	CLA	ND
11	2	1213	CLA	NA
11	A	1130	CLA	ND
11	A	1130	CLA	NA
11	B	1232	CLA	NC
11	B	1232	CLA	ND
11	B	1232	CLA	NA
11	A	1012	CLA	NC
11	A	1012	CLA	ND
11	A	1012	CLA	NA
11	A	1103	CLA	NC
11	A	1103	CLA	NA
11	A	1103	CLA	ND
11	b	1238	CLA	NC
11	b	1238	CLA	ND
11	b	1238	CLA	NA
11	a	1011	CLA	NA
11	b	1204	CLA	ND
11	b	1204	CLA	NA
11	b	1223	CLA	NC
11	b	1223	CLA	ND
11	b	1223	CLA	NA
11	b	1229	CLA	NC
11	b	1229	CLA	ND
11	b	1229	CLA	NA
11	b	1023	CLA	NC
11	b	1023	CLA	ND
11	b	1023	CLA	NA
11	a	1104	CLA	NC
11	a	1104	CLA	ND
11	a	1104	CLA	NA
11	B	1222	CLA	NC
11	B	1222	CLA	ND
11	B	1222	CLA	NA
11	b	1232	CLA	NC
11	b	1232	CLA	ND
11	b	1232	CLA	NA
11	A	1132	CLA	NC
11	A	1132	CLA	ND
11	A	1132	CLA	NA
11	b	1231	CLA	NC
11	b	1231	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	b	1231	CLA	NA
11	B	1236	CLA	NC
11	B	1236	CLA	ND
11	B	1236	CLA	NA
11	l	1502	CLA	NC
11	l	1502	CLA	ND
11	l	1502	CLA	NA
11	a	1126	CLA	NC
11	a	1126	CLA	ND
11	a	1126	CLA	NA
11	B	1235	CLA	NC
11	B	1235	CLA	ND
11	B	1235	CLA	NA
11	A	1104	CLA	NC
11	A	1104	CLA	ND
11	A	1104	CLA	NA
11	2	1230	CLA	NC
11	2	1230	CLA	NA
11	2	1203	CLA	NC
11	2	1203	CLA	ND
11	2	1203	CLA	NA
11	A	1137	CLA	NC
11	A	1137	CLA	NA
11	A	1137	CLA	ND
11	1	1125	CLA	ND
11	1	1125	CLA	NA
11	B	1021	CLA	NC
11	B	1021	CLA	NA
11	B	1021	CLA	ND
11	A	1122	CLA	NC
11	A	1122	CLA	ND
11	A	1122	CLA	NA
11	B	1221	CLA	NC
11	B	1221	CLA	NA
11	B	1221	CLA	ND
11	1	1101	CLA	ND
11	1	1101	CLA	NA
11	A	1138	CLA	NC
11	A	1138	CLA	ND
11	A	1138	CLA	NA
11	b	1021	CLA	NC
11	b	1021	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	b	1021	CLA	NA
11	2	1215	CLA	NC
11	2	1215	CLA	ND
11	2	1215	CLA	NA
11	b	1207	CLA	ND
11	b	1207	CLA	NA
11	b	1214	CLA	NC
11	b	1214	CLA	ND
11	b	1214	CLA	NA
11	1	1115	CLA	ND
11	1	1115	CLA	NA
11	b	1013	CLA	NA
11	1	1121	CLA	ND
11	1	1121	CLA	NA
11	b	1217	CLA	NC
11	b	1217	CLA	ND
11	b	1217	CLA	NA
11	b	1205	CLA	NC
11	b	1205	CLA	ND
11	b	1205	CLA	NA
11	A	1140	CLA	ND
11	A	1140	CLA	NA
11	2	1225	CLA	NC
11	2	1225	CLA	ND
11	2	1225	CLA	NA
11	a	1123	CLA	ND
11	a	1123	CLA	NA
11	B	1023	CLA	NC
11	B	1023	CLA	ND
11	B	1023	CLA	NA
11	b	1202	CLA	NC
11	b	1202	CLA	NA
11	b	1202	CLA	ND
11	2	1226	CLA	NC
11	2	1226	CLA	ND
11	2	1226	CLA	NA
11	B	1238	CLA	NC
11	B	1238	CLA	ND
11	B	1238	CLA	NA
11	A	1111	CLA	NC
11	A	1111	CLA	ND
11	A	1111	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	1	1131	CLA	ND
11	1	1131	CLA	NA
11	a	1135	CLA	ND
11	a	1135	CLA	NA
11	1	1119	CLA	NC
11	1	1119	CLA	ND
11	1	1119	CLA	NA
11	B	1226	CLA	NC
11	B	1226	CLA	ND
11	B	1226	CLA	NA
11	A	1112	CLA	NC
11	A	1112	CLA	NA
11	A	1112	CLA	ND
11	1	1118	CLA	NC
11	1	1118	CLA	ND
11	1	1118	CLA	NA
11	a	1133	CLA	NC
11	a	1133	CLA	ND
11	a	1133	CLA	NA
11	A	1124	CLA	NC
11	A	1124	CLA	ND
11	A	1124	CLA	NA
11	2	1023	CLA	NC
11	2	1023	CLA	NA
11	2	1023	CLA	ND
11	2	1211	CLA	NC
11	2	1211	CLA	ND
11	2	1211	CLA	NA
11	B	1214	CLA	NC
11	B	1214	CLA	ND
11	B	1214	CLA	NA
11	B	1220	CLA	NA
11	A	1136	CLA	NC
11	A	1136	CLA	ND
11	A	1136	CLA	NA
11	a	1127	CLA	NC
11	a	1127	CLA	ND
11	a	1127	CLA	NA
11	1	1110	CLA	ND
11	1	1110	CLA	NA
11	l	1503	CLA	ND
11	l	1503	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	A	1118	CLA	NC
11	A	1118	CLA	ND
11	A	1118	CLA	NA
11	B	1218	CLA	NC
11	B	1218	CLA	ND
11	B	1218	CLA	NA
11	a	1132	CLA	NC
11	a	1132	CLA	ND
11	a	1132	CLA	NA
11	1	1112	CLA	NC
11	1	1112	CLA	ND
11	1	1112	CLA	NA
11	A	1139	CLA	NC
11	A	1139	CLA	ND
11	A	1139	CLA	NA
11	2	1202	CLA	NC
11	2	1202	CLA	NA
11	2	1202	CLA	ND
11	B	1208	CLA	ND
11	B	1208	CLA	NA
11	B	1227	CLA	NC
11	B	1227	CLA	ND
11	B	1227	CLA	NA
11	1	1011	CLA	NA
11	B	1228	CLA	NC
11	B	1228	CLA	ND
11	B	1228	CLA	NA
11	B	1240	CLA	NC
11	B	1240	CLA	ND
11	B	1240	CLA	NA
11	A	1135	CLA	NC
11	A	1135	CLA	ND
11	A	1135	CLA	NA
11	1	1134	CLA	NC
11	1	1134	CLA	NA
11	1	1134	CLA	ND
11	B	1219	CLA	NC
11	B	1219	CLA	ND
11	B	1219	CLA	NA
11	1	1012	CLA	ND
11	1	1012	CLA	NA
11	1	1104	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	1	1104	CLA	NA
11	2	1206	CLA	NC
11	2	1206	CLA	ND
11	2	1206	CLA	NA
11	2	1240	CLA	NC
11	2	1240	CLA	ND
11	2	1240	CLA	NA
11	2	1220	CLA	ND
11	2	1220	CLA	NA
11	2	1239	CLA	NC
11	2	1239	CLA	ND
11	2	1239	CLA	NA
11	A	1105	CLA	NC
11	A	1105	CLA	ND
11	A	1105	CLA	NA
11	A	1121	CLA	NC
11	A	1121	CLA	ND
11	A	1121	CLA	NA
11	A	1107	CLA	NC
11	A	1107	CLA	ND
11	A	1107	CLA	NA
11	b	1208	CLA	NC
11	b	1208	CLA	ND
11	b	1208	CLA	NA
11	a	1101	CLA	ND
11	a	1101	CLA	NA
11	B	1013	CLA	NC
11	B	1013	CLA	NA
11	B	1225	CLA	NC
11	B	1225	CLA	ND
11	B	1225	CLA	NA
11	a	1111	CLA	NC
11	a	1111	CLA	ND
11	a	1111	CLA	NA
11	2	1021	CLA	NC
11	2	1021	CLA	ND
11	2	1021	CLA	NA
11	2	1223	CLA	NC
11	2	1223	CLA	ND
11	2	1223	CLA	NA
11	B	1201	CLA	NC
11	B	1201	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	B	1201	CLA	NA
11	B	1211	CLA	NC
11	B	1211	CLA	ND
11	B	1211	CLA	NA
11	B	1230	CLA	NC
11	B	1230	CLA	NA
11	b	1221	CLA	NC
11	b	1221	CLA	NA
11	b	1221	CLA	ND
11	b	1209	CLA	NC
11	b	1209	CLA	ND
11	b	1209	CLA	NA
11	b	1203	CLA	NC
11	b	1203	CLA	ND
11	b	1203	CLA	NA
11	2	1205	CLA	NC
11	2	1205	CLA	ND
11	2	1205	CLA	NA
11	A	1108	CLA	NC
11	A	1108	CLA	ND
11	A	1108	CLA	NA
11	1	1113	CLA	NC
11	1	1113	CLA	ND
11	1	1113	CLA	NA
11	2	1210	CLA	NC
11	2	1210	CLA	ND
11	2	1210	CLA	NA
11	a	1131	CLA	NC
11	a	1131	CLA	ND
11	a	1131	CLA	NA
11	1	1107	CLA	NC
11	1	1107	CLA	ND
11	1	1107	CLA	NA
11	a	1109	CLA	NC
11	a	1109	CLA	NA
11	b	1236	CLA	NC
11	b	1236	CLA	NA
11	b	1236	CLA	ND
11	a	1137	CLA	NC
11	a	1137	CLA	NA
11	a	1137	CLA	ND
11	1	1105	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	1	1105	CLA	ND
11	1	1105	CLA	NA
11	2	1216	CLA	NC
11	2	1216	CLA	ND
11	2	1216	CLA	NA
11	1	1102	CLA	NC
11	1	1102	CLA	ND
11	1	1102	CLA	NA
11	b	1206	CLA	NC
11	b	1206	CLA	ND
11	b	1206	CLA	NA
11	1	1117	CLA	NC
11	1	1117	CLA	ND
11	1	1117	CLA	NA
11	A	1102	CLA	ND
11	A	1102	CLA	NA
11	a	1129	CLA	NC
11	a	1129	CLA	ND
11	a	1129	CLA	NA
11	2	1013	CLA	NA
11	2	1207	CLA	NA
11	b	1211	CLA	NC
11	b	1211	CLA	ND
11	b	1211	CLA	NA
11	2	1228	CLA	NC
11	2	1228	CLA	ND
11	2	1228	CLA	NA
11	a	1130	CLA	NC
11	a	1130	CLA	NA
11	B	1229	CLA	ND
11	B	1229	CLA	NA
11	a	1138	CLA	NC
11	a	1138	CLA	ND
11	a	1138	CLA	NA
11	b	1210	CLA	NC
11	b	1210	CLA	ND
11	b	1210	CLA	NA
11	2	1222	CLA	NC
11	2	1222	CLA	ND
11	2	1222	CLA	NA
11	A	1110	CLA	NC
11	A	1110	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
11	A	1110	CLA	NA
11	1	1128	CLA	NC
11	1	1128	CLA	ND
11	1	1128	CLA	NA
11	a	1121	CLA	NC
11	a	1121	CLA	ND
11	a	1121	CLA	NA

All (4167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	1122	CLA	C2-C1-O2A-CGA
11	a	1122	CLA	CHA-CBD-CGD-O1D
11	a	1122	CLA	CHA-CBD-CGD-O2D
11	A	1101	CLA	C3A-C2A-CAA-CBA
11	A	1101	CLA	C2-C1-O2A-CGA
11	1	1801	CLA	C1A-C2A-CAA-CBA
11	1	1801	CLA	C3A-C2A-CAA-CBA
11	1	1801	CLA	CBA-CGA-O2A-C1
11	1	1801	CLA	O1A-CGA-O2A-C1
11	A	1125	CLA	C2C-C3C-CAC-CBC
11	A	1125	CLA	C4C-C3C-CAC-CBC
14	1	4008	BCR	C7-C8-C9-C34
14	1	4008	BCR	C11-C10-C9-C8
14	1	4008	BCR	C11-C10-C9-C34
14	1	4008	BCR	C10-C11-C12-C13
14	1	4008	BCR	C11-C12-C13-C14
14	1	4008	BCR	C11-C12-C13-C35
14	1	4008	BCR	C21-C22-C23-C24
14	1	4008	BCR	C37-C22-C23-C24
11	b	1222	CLA	C11-C10-C8-C7
14	b	4010	BCR	C11-C10-C9-C8
14	b	4010	BCR	C11-C10-C9-C34
14	b	4010	BCR	C19-C20-C21-C22
14	b	4010	BCR	C23-C24-C25-C26
14	b	4010	BCR	C23-C24-C25-C30
11	2	1224	CLA	CBD-CGD-O2D-CED
11	K	1401	CLA	C3A-C2A-CAA-CBA
11	K	1401	CLA	CAD-CBD-CGD-O1D
11	K	1401	CLA	CAD-CBD-CGD-O2D
11	K	1401	CLA	CBD-CGD-O2D-CED
11	a	1124	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1124	CLA	CBD-CGD-O2D-CED
11	1	1139	CLA	CBD-CGD-O2D-CED
15	1	5001	LHG	C4-O6-P-O4
11	2	1208	CLA	CBD-CGD-O2D-CED
11	1	1111	CLA	CBD-CGD-O2D-CED
11	a	1114	CLA	CBD-CGD-O2D-CED
14	a	4008	BCR	C7-C8-C9-C10
14	a	4008	BCR	C7-C8-C9-C34
14	a	4008	BCR	C11-C10-C9-C8
14	a	4008	BCR	C11-C10-C9-C34
14	a	4008	BCR	C10-C11-C12-C13
14	a	4008	BCR	C11-C12-C13-C14
14	a	4008	BCR	C11-C12-C13-C35
14	a	4008	BCR	C21-C22-C23-C24
14	a	4008	BCR	C37-C22-C23-C24
11	b	1213	CLA	C4-C3-C5-C6
15	a	5003	LHG	C3-O3-P-O5
15	a	5003	LHG	C3-O3-P-O6
15	a	5003	LHG	C4-O6-P-O3
15	a	5003	LHG	C4-O6-P-O4
15	a	5003	LHG	C4-O6-P-O5
11	B	1210	CLA	CHA-CBD-CGD-O1D
11	B	1210	CLA	CHA-CBD-CGD-O2D
11	B	1210	CLA	CAD-CBD-CGD-O1D
11	B	1210	CLA	CBD-CGD-O2D-CED
14	b	4011	BCR	C1-C6-C7-C8
14	b	4011	BCR	C5-C6-C7-C8
14	b	4011	BCR	C7-C8-C9-C10
14	b	4011	BCR	C7-C8-C9-C34
14	b	4011	BCR	C17-C18-C19-C20
14	b	4011	BCR	C36-C18-C19-C20
14	b	4011	BCR	C23-C24-C25-C26
14	b	4011	BCR	C23-C24-C25-C30
11	b	1240	CLA	C1A-C2A-CAA-CBA
11	b	1240	CLA	C3A-C2A-CAA-CBA
11	b	1240	CLA	C2A-CAA-CBA-CGA
11	b	1240	CLA	CHA-CBD-CGD-O1D
11	b	1240	CLA	CHA-CBD-CGD-O2D
11	a	1022	CLA	CBD-CGD-O2D-CED
11	A	1120	CLA	C3A-C2A-CAA-CBA
11	8	1501	CLA	C1A-C2A-CAA-CBA
11	8	1501	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	8	1501	CLA	CHA-CBD-CGD-O1D
11	8	1501	CLA	CHA-CBD-CGD-O2D
11	8	1501	CLA	CAD-CBD-CGD-O1D
11	1	1120	CLA	C1A-C2A-CAA-CBA
11	1	1120	CLA	C3A-C2A-CAA-CBA
11	2	1217	CLA	C1A-C2A-CAA-CBA
11	2	1217	CLA	C3A-C2A-CAA-CBA
11	2	1217	CLA	CHA-CBD-CGD-O1D
11	2	1217	CLA	CHA-CBD-CGD-O2D
11	2	1217	CLA	CAD-CBD-CGD-O1D
11	2	1217	CLA	CAD-CBD-CGD-O2D
14	2	4014	BCR	C11-C10-C9-C8
14	2	4014	BCR	C11-C10-C9-C34
14	2	4014	BCR	C9-C10-C11-C12
14	2	4014	BCR	C17-C18-C19-C20
14	2	4014	BCR	C36-C18-C19-C20
14	2	4014	BCR	C21-C22-C23-C24
14	2	4014	BCR	C37-C22-C23-C24
11	K	1402	CLA	C1A-C2A-CAA-CBA
11	K	1402	CLA	CBD-CGD-O2D-CED
14	b	4004	BCR	C11-C10-C9-C8
14	b	4004	BCR	C11-C10-C9-C34
14	l	4022	BCR	C7-C8-C9-C10
14	l	4022	BCR	C7-C8-C9-C34
14	l	4022	BCR	C11-C10-C9-C8
14	l	4022	BCR	C11-C10-C9-C34
14	l	4022	BCR	C17-C18-C19-C20
14	l	4022	BCR	C36-C18-C19-C20
14	l	4022	BCR	C21-C22-C23-C24
14	l	4022	BCR	C37-C22-C23-C24
11	2	1204	CLA	CHA-CBD-CGD-O1D
11	2	1204	CLA	CHA-CBD-CGD-O2D
11	B	1215	CLA	C1A-C2A-CAA-CBA
11	B	1215	CLA	C3A-C2A-CAA-CBA
11	B	1215	CLA	CBD-CGD-O2D-CED
14	7	4021	BCR	C11-C10-C9-C8
14	7	4021	BCR	C11-C10-C9-C34
14	7	4021	BCR	C10-C11-C12-C13
14	7	4021	BCR	C21-C22-C23-C24
14	7	4021	BCR	C37-C22-C23-C24
11	1	1138	CLA	CHA-CBD-CGD-O1D
11	1	1138	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	F	4020	BCR	C7-C8-C9-C10
14	F	4020	BCR	C7-C8-C9-C34
14	F	4020	BCR	C11-C10-C9-C8
14	F	4020	BCR	C11-C10-C9-C34
14	F	4020	BCR	C10-C11-C12-C13
14	F	4020	BCR	C21-C22-C23-C24
14	F	4020	BCR	C37-C22-C23-C24
11	b	1220	CLA	CHA-CBD-CGD-O1D
11	b	1220	CLA	CHA-CBD-CGD-O2D
11	b	1220	CLA	CBD-CGD-O2D-CED
11	b	1216	CLA	CHA-CBD-CGD-O1D
11	b	1216	CLA	CHA-CBD-CGD-O2D
11	b	1234	CLA	CHA-CBD-CGD-O1D
11	b	1234	CLA	CHA-CBD-CGD-O2D
11	b	1234	CLA	CAD-CBD-CGD-O1D
14	B	4010	BCR	C7-C8-C9-C10
14	B	4010	BCR	C7-C8-C9-C34
14	B	4010	BCR	C11-C10-C9-C8
14	B	4010	BCR	C11-C10-C9-C34
14	B	4010	BCR	C10-C11-C12-C13
14	B	4010	BCR	C17-C18-C19-C20
14	B	4010	BCR	C36-C18-C19-C20
14	B	4010	BCR	C23-C24-C25-C26
11	a	1103	CLA	C2-C1-O2A-CGA
11	a	1103	CLA	CHA-CBD-CGD-O1D
11	a	1103	CLA	CHA-CBD-CGD-O2D
11	a	1103	CLA	CAD-CBD-CGD-O1D
11	a	1103	CLA	CAD-CBD-CGD-O2D
11	1	1129	CLA	CBA-CGA-O2A-C1
11	b	1239	CLA	CBA-CGA-O2A-C1
11	1	1109	CLA	C2-C3-C5-C6
11	1	1109	CLA	C4-C3-C5-C6
11	1	1132	CLA	C2A-CAA-CBA-CGA
11	1	1132	CLA	CHA-CBD-CGD-O1D
11	1	1132	CLA	CHA-CBD-CGD-O2D
11	A	1126	CLA	CBD-CGD-O2D-CED
11	A	1126	CLA	C2-C3-C5-C6
11	A	1126	CLA	C4-C3-C5-C6
11	1	1103	CLA	C1A-C2A-CAA-CBA
11	1	1103	CLA	C3A-C2A-CAA-CBA
11	1	1103	CLA	CAD-CBD-CGD-O1D
11	1	1103	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	4003	BCR	C10-C11-C12-C13
14	a	4003	BCR	C21-C22-C23-C24
14	a	4003	BCR	C23-C24-C25-C26
14	a	4003	BCR	C23-C24-C25-C30
11	B	1202	CLA	C3A-C2A-CAA-CBA
11	B	1202	CLA	CHA-CBD-CGD-O1D
11	B	1202	CLA	CHA-CBD-CGD-O2D
11	B	1202	CLA	CAD-CBD-CGD-O1D
11	B	1202	CLA	CAD-CBD-CGD-O2D
11	k	1402	CLA	CHA-CBD-CGD-O1D
11	k	1402	CLA	CHA-CBD-CGD-O2D
11	k	1402	CLA	CBD-CGD-O2D-CED
11	B	1203	CLA	C6-C7-C8-C9
11	A	1113	CLA	C2A-CAA-CBA-CGA
11	A	1113	CLA	CBD-CGD-O2D-CED
14	B	4011	BCR	C1-C6-C7-C8
14	B	4011	BCR	C5-C6-C7-C8
14	B	4011	BCR	C11-C10-C9-C8
14	B	4011	BCR	C11-C10-C9-C34
14	B	4011	BCR	C23-C24-C25-C26
14	B	4011	BCR	C23-C24-C25-C30
11	A	1131	CLA	C1A-C2A-CAA-CBA
11	A	1131	CLA	C3A-C2A-CAA-CBA
11	A	1131	CLA	CHA-CBD-CGD-O1D
11	A	1131	CLA	CBD-CGD-O2D-CED
11	1	1022	CLA	CHA-CBD-CGD-O1D
11	1	1022	CLA	CHA-CBD-CGD-O2D
11	1	1022	CLA	CBD-CGD-O2D-CED
11	1	1123	CLA	C2-C1-O2A-CGA
11	0	1401	CLA	C3A-C2A-CAA-CBA
11	0	1401	CLA	CAD-CBD-CGD-O1D
11	0	1401	CLA	CAD-CBD-CGD-O2D
11	0	1401	CLA	CBD-CGD-O2D-CED
11	b	1225	CLA	C6-C7-C8-C9
11	a	1012	CLA	CHA-CBD-CGD-O1D
11	a	1012	CLA	CAD-CBD-CGD-O1D
11	a	1012	CLA	CAD-CBD-CGD-O2D
11	a	1012	CLA	C2-C3-C5-C6
11	a	1012	CLA	C4-C3-C5-C6
11	1	1106	CLA	C1A-C2A-CAA-CBA
11	1	1106	CLA	C3A-C2A-CAA-CBA
11	1	1106	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1106	CLA	CHA-CBD-CGD-O2D
11	1	1106	CLA	C2-C3-C5-C6
11	1	1106	CLA	C4-C3-C5-C6
11	A	1114	CLA	CBA-CGA-O2A-C1
11	A	1114	CLA	CBD-CGD-O2D-CED
14	2	4011	BCR	C1-C6-C7-C8
14	2	4011	BCR	C5-C6-C7-C8
14	2	4011	BCR	C11-C10-C9-C8
14	2	4011	BCR	C11-C10-C9-C34
14	2	4011	BCR	C21-C22-C23-C24
14	2	4011	BCR	C23-C24-C25-C26
11	a	1140	CLA	CBD-CGD-O2D-CED
11	A	1134	CLA	CHA-CBD-CGD-O1D
11	A	1134	CLA	CHA-CBD-CGD-O2D
11	1	1114	CLA	CHA-CBD-CGD-O1D
11	1	1114	CLA	CHA-CBD-CGD-O2D
11	b	1235	CLA	CBD-CGD-O2D-CED
11	a	1116	CLA	C3A-C2A-CAA-CBA
11	a	1116	CLA	CBD-CGD-O2D-CED
11	A	1117	CLA	CBD-CGD-O2D-CED
11	a	1119	CLA	C2-C1-O2A-CGA
11	a	1119	CLA	CBD-CGD-O2D-CED
11	B	1231	CLA	CBD-CGD-O2D-CED
14	b	4014	BCR	C11-C10-C9-C8
14	b	4014	BCR	C11-C10-C9-C34
14	b	4014	BCR	C10-C11-C12-C13
14	b	4014	BCR	C11-C12-C13-C35
15	A	5003	LHG	O1-C1-C2-C3
15	A	5003	LHG	C3-O3-P-O5
15	A	5003	LHG	C4-O6-P-O4
15	A	5003	LHG	C4-O6-P-O5
11	2	1231	CLA	CHA-CBD-CGD-O1D
11	2	1231	CLA	CHA-CBD-CGD-O2D
11	A	1128	CLA	C6-C7-C8-C9
11	1	1137	CLA	C2-C1-O2A-CGA
11	1	1137	CLA	CBD-CGD-O2D-CED
14	f	4020	BCR	C7-C8-C9-C34
14	f	4020	BCR	C11-C10-C9-C8
14	f	4020	BCR	C11-C10-C9-C34
14	f	4020	BCR	C10-C11-C12-C13
14	f	4020	BCR	C37-C22-C23-C24
14	f	4020	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1130	CLA	CBA-CGA-O2A-C1
14	b	4009	BCR	C1-C6-C7-C8
14	b	4009	BCR	C5-C6-C7-C8
14	b	4009	BCR	C7-C8-C9-C10
14	b	4009	BCR	C7-C8-C9-C34
14	b	4009	BCR	C11-C10-C9-C8
14	b	4009	BCR	C11-C10-C9-C34
14	b	4009	BCR	C10-C11-C12-C13
14	b	4009	BCR	C21-C22-C23-C24
14	b	4009	BCR	C37-C22-C23-C24
14	b	4009	BCR	C23-C24-C25-C30
11	a	1102	CLA	C1A-C2A-CAA-CBA
11	a	1102	CLA	C3A-C2A-CAA-CBA
11	a	1102	CLA	CBD-CGD-O2D-CED
15	A	5001	LHG	O1-C1-C2-C3
15	A	5001	LHG	C1-C2-C3-O3
15	A	5001	LHG	C4-O6-P-O5
15	A	5001	LHG	O7-C5-C6-O8
11	a	1120	CLA	C3A-C2A-CAA-CBA
11	b	1230	CLA	C2-C1-O2A-CGA
11	b	1230	CLA	C4-C3-C5-C6
11	0	1402	CLA	CBD-CGD-O2D-CED
14	A	4003	BCR	C10-C11-C12-C13
11	L	1503	CLA	C2-C1-O2A-CGA
11	a	1106	CLA	CHA-CBD-CGD-O1D
11	a	1106	CLA	CHA-CBD-CGD-O2D
11	2	1229	CLA	C2-C1-O2A-CGA
11	2	1229	CLA	CHA-CBD-CGD-O1D
11	2	1229	CLA	CHA-CBD-CGD-O2D
11	a	1801	CLA	C1A-C2A-CAA-CBA
11	a	1801	CLA	C3A-C2A-CAA-CBA
11	a	1801	CLA	CBA-CGA-O2A-C1
11	a	1801	CLA	O1A-CGA-O2A-C1
11	a	1801	CLA	CBD-CGD-O2D-CED
11	B	1205	CLA	CHA-CBD-CGD-O1D
11	B	1205	CLA	CHA-CBD-CGD-O2D
11	2	1201	CLA	CHA-CBD-CGD-O1D
11	2	1201	CLA	CHA-CBD-CGD-O2D
11	2	1201	CLA	CAD-CBD-CGD-O1D
11	a	1136	CLA	CBA-CGA-O2A-C1
14	a	4001	BCR	C11-C10-C9-C8
14	a	4001	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	4001	BCR	C10-C11-C12-C13
11	2	1236	CLA	CHA-CBD-CGD-O1D
11	2	1236	CLA	CHA-CBD-CGD-O2D
11	2	1236	CLA	CAD-CBD-CGD-O1D
11	2	1219	CLA	C1A-C2A-CAA-CBA
11	2	1219	CLA	C3A-C2A-CAA-CBA
11	1	1237	CLA	C1A-C2A-CAA-CBA
11	1	1237	CLA	CBD-CGD-O2D-CED
11	1	1135	CLA	CHA-CBD-CGD-O1D
11	1	1135	CLA	CHA-CBD-CGD-O2D
11	1	1135	CLA	C2-C3-C5-C6
11	1	1135	CLA	C4-C3-C5-C6
11	1	1116	CLA	C3A-C2A-CAA-CBA
11	1	1116	CLA	CBD-CGD-O2D-CED
11	2	1232	CLA	CBD-CGD-O2D-CED
14	L	4019	BCR	C10-C11-C12-C13
14	L	4019	BCR	C23-C24-C25-C26
14	L	4019	BCR	C23-C24-C25-C30
11	2	1227	CLA	C2A-CAA-CBA-CGA
11	A	1011	CLA	C1A-C2A-CAA-CBA
11	A	1011	CLA	C3A-C2A-CAA-CBA
11	A	1011	CLA	CBD-CGD-O2D-CED
14	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C11-C10-C9-C34
11	a	1105	CLA	C2-C1-O2A-CGA
11	a	1105	CLA	CBD-CGD-O2D-CED
11	2	1235	CLA	CHA-CBD-CGD-O1D
11	2	1235	CLA	CHA-CBD-CGD-O2D
11	b	1201	CLA	CBD-CGD-O2D-CED
11	B	1239	CLA	CBA-CGA-O2A-C1
11	B	1239	CLA	CHA-CBD-CGD-O1D
11	B	1239	CLA	CHA-CBD-CGD-O2D
11	A	1237	CLA	C1A-C2A-CAA-CBA
11	A	1237	CLA	CHA-CBD-CGD-O1D
11	A	1237	CLA	CHA-CBD-CGD-O2D
11	A	1237	CLA	O2A-C1-C2-C3
11	B	1209	CLA	C1A-C2A-CAA-CBA
11	B	1209	CLA	C3A-C2A-CAA-CBA
11	a	1118	CLA	CBD-CGD-O2D-CED
11	A	1116	CLA	C3A-C2A-CAA-CBA
11	A	1116	CLA	CBD-CGD-O2D-CED
11	k	1401	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	k	1401	CLA	CAD-CBD-CGD-O1D
11	k	1401	CLA	CAD-CBD-CGD-O2D
11	k	1401	CLA	CBD-CGD-O2D-CED
11	A	1022	CLA	C2-C1-O2A-CGA
11	A	1022	CLA	CBD-CGD-O2D-CED
14	M	4021	BCR	C5-C6-C7-C8
14	M	4021	BCR	C11-C10-C9-C8
14	M	4021	BCR	C11-C10-C9-C34
14	M	4021	BCR	C21-C22-C23-C24
14	M	4021	BCR	C37-C22-C23-C24
15	2	5004	LHG	C3-O3-P-O4
15	2	5004	LHG	C4-O6-P-O4
15	2	5004	LHG	C8-C7-O7-C5
15	1	5003	LHG	O1-C1-C2-C3
15	1	5003	LHG	C3-O3-P-O5
15	1	5003	LHG	C4-O6-P-O3
15	1	5003	LHG	C4-O6-P-O4
15	1	5003	LHG	C4-O6-P-O5
11	b	1212	CLA	CBD-CGD-O2D-CED
11	A	1106	CLA	C3A-C2A-CAA-CBA
11	A	1106	CLA	CHA-CBD-CGD-O1D
11	A	1106	CLA	CHA-CBD-CGD-O2D
14	a	4007	BCR	C7-C8-C9-C10
14	a	4007	BCR	C7-C8-C9-C34
14	a	4007	BCR	C23-C24-C25-C26
14	a	4007	BCR	C23-C24-C25-C30
11	a	1125	CLA	CBD-CGD-O2D-CED
11	b	1224	CLA	CBA-CGA-O2A-C1
11	b	1224	CLA	CHA-CBD-CGD-O1D
11	b	1224	CLA	CHA-CBD-CGD-O2D
11	b	1224	CLA	CBD-CGD-O2D-CED
11	B	1217	CLA	C3A-C2A-CAA-CBA
11	B	1217	CLA	CHA-CBD-CGD-O1D
11	B	1217	CLA	CHA-CBD-CGD-O2D
11	B	1217	CLA	CAD-CBD-CGD-O1D
14	2	4009	BCR	C1-C6-C7-C8
14	2	4009	BCR	C5-C6-C7-C8
14	2	4009	BCR	C7-C8-C9-C10
14	2	4009	BCR	C7-C8-C9-C34
14	2	4009	BCR	C11-C10-C9-C8
14	2	4009	BCR	C11-C10-C9-C34
14	2	4009	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	2	4009	BCR	C15-C16-C17-C18
14	2	4009	BCR	C21-C22-C23-C24
14	2	4009	BCR	C37-C22-C23-C24
14	2	4009	BCR	C23-C24-C25-C30
11	8	1503	CLA	C2-C1-O2A-CGA
14	6	4020	BCR	C7-C8-C9-C10
14	6	4020	BCR	C7-C8-C9-C34
14	6	4020	BCR	C11-C10-C9-C8
14	6	4020	BCR	C11-C10-C9-C34
14	6	4020	BCR	C9-C10-C11-C12
14	6	4020	BCR	C10-C11-C12-C13
14	6	4020	BCR	C21-C22-C23-C24
14	6	4020	BCR	C37-C22-C23-C24
15	a	5001	LHG	O1-C1-C2-O2
15	a	5001	LHG	O1-C1-C2-C3
15	a	5001	LHG	C3-O3-P-O6
15	a	5001	LHG	C4-O6-P-O5
15	a	5001	LHG	O7-C5-C6-O8
11	a	1134	CLA	C3A-C2A-CAA-CBA
11	a	1134	CLA	CHA-CBD-CGD-O1D
11	a	1134	CLA	CHA-CBD-CGD-O2D
11	1	1126	CLA	CBD-CGD-O2D-CED
11	1	1126	CLA	C2-C3-C5-C6
11	1	1126	CLA	C4-C3-C5-C6
11	a	1107	CLA	C2-C3-C5-C6
11	a	1107	CLA	C4-C3-C5-C6
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C11-C10-C9-C8
14	A	4002	BCR	C11-C10-C9-C34
14	A	4002	BCR	C10-C11-C12-C13
14	A	4002	BCR	C23-C24-C25-C26
14	A	4002	BCR	C23-C24-C25-C30
11	a	1237	CLA	C1A-C2A-CAA-CBA
11	a	1237	CLA	O2A-C1-C2-C3
14	B	4009	BCR	C5-C6-C7-C8
14	B	4009	BCR	C11-C12-C13-C14
14	B	4009	BCR	C11-C12-C13-C35
14	B	4009	BCR	C13-C14-C15-C16
14	B	4009	BCR	C21-C22-C23-C24
14	B	4009	BCR	C37-C22-C23-C24
11	a	1113	CLA	CBD-CGD-O2D-CED
11	1	1122	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1122	CLA	CHA-CBD-CGD-O2D
11	L	1501	CLA	C1A-C2A-CAA-CBA
11	1	1140	CLA	C2-C1-O2A-CGA
11	1	1140	CLA	C6-C7-C8-C9
14	b	4005	BCR	C5-C6-C7-C8
14	b	4005	BCR	C11-C10-C9-C8
14	b	4005	BCR	C11-C10-C9-C34
14	b	4005	BCR	C9-C10-C11-C12
14	b	4005	BCR	C10-C11-C12-C13
14	b	4005	BCR	C11-C12-C13-C14
14	b	4005	BCR	C11-C12-C13-C35
14	b	4005	BCR	C37-C22-C23-C24
11	b	1215	CLA	C1A-C2A-CAA-CBA
11	b	1215	CLA	C3A-C2A-CAA-CBA
11	b	1215	CLA	CHA-CBD-CGD-O1D
11	b	1215	CLA	CHA-CBD-CGD-O2D
14	6	4018	BCR	C11-C10-C9-C8
14	6	4018	BCR	C11-C10-C9-C34
14	6	4018	BCR	C11-C12-C13-C14
14	6	4018	BCR	C11-C12-C13-C35
14	6	4018	BCR	C21-C22-C23-C24
14	6	4018	BCR	C23-C24-C25-C26
11	A	1123	CLA	C2-C1-O2A-CGA
11	2	1234	CLA	C1A-C2A-CAA-CBA
11	2	1234	CLA	CHA-CBD-CGD-O1D
11	2	1234	CLA	CHA-CBD-CGD-O2D
11	2	1234	CLA	CAD-CBD-CGD-O1D
11	2	1213	CLA	C2-C3-C5-C6
11	2	1213	CLA	C4-C3-C5-C6
11	2	1213	CLA	C6-C7-C8-C9
14	b	4017	BCR	C11-C10-C9-C8
14	b	4017	BCR	C11-C10-C9-C34
14	b	4017	BCR	C10-C11-C12-C13
14	b	4017	BCR	C11-C12-C13-C14
14	b	4017	BCR	C11-C12-C13-C35
11	B	1232	CLA	C2A-CAA-CBA-CGA
11	B	1232	CLA	CBD-CGD-O2D-CED
11	A	1012	CLA	CHA-CBD-CGD-O1D
11	A	1012	CLA	CHA-CBD-CGD-O2D
11	A	1012	CLA	C4-C3-C5-C6
11	A	1103	CLA	C3A-C2A-CAA-CBA
11	A	1103	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1103	CLA	CAD-CBD-CGD-O2D
11	b	1238	CLA	CBD-CGD-O2D-CED
11	a	1011	CLA	C1A-C2A-CAA-CBA
11	a	1011	CLA	C3A-C2A-CAA-CBA
11	a	1011	CLA	CBD-CGD-O2D-CED
11	b	1204	CLA	CHA-CBD-CGD-O1D
11	b	1204	CLA	CHA-CBD-CGD-O2D
11	b	1223	CLA	CHA-CBD-CGD-O1D
11	b	1223	CLA	CHA-CBD-CGD-O2D
11	b	1223	CLA	CAD-CBD-CGD-O1D
14	2	4005	BCR	C1-C6-C7-C8
14	2	4005	BCR	C5-C6-C7-C8
14	2	4005	BCR	C7-C8-C9-C10
14	2	4005	BCR	C7-C8-C9-C34
14	2	4005	BCR	C37-C22-C23-C24
11	b	1229	CLA	C2-C1-O2A-CGA
11	b	1023	CLA	C6-C7-C8-C9
11	a	1104	CLA	C1A-C2A-CAA-CBA
11	a	1104	CLA	CBD-CGD-O2D-CED
14	f	4013	BCR	C5-C6-C7-C8
14	f	4013	BCR	C11-C10-C9-C8
14	f	4013	BCR	C11-C10-C9-C34
14	f	4013	BCR	C21-C22-C23-C24
14	f	4013	BCR	C23-C24-C25-C26
14	f	4013	BCR	C23-C24-C25-C30
14	2	4006	BCR	C11-C10-C9-C8
14	2	4006	BCR	C11-C10-C9-C34
14	2	4006	BCR	C23-C24-C25-C26
14	2	4006	BCR	C23-C24-C25-C30
11	B	1222	CLA	C2-C3-C5-C6
11	B	1222	CLA	C4-C3-C5-C6
14	A	4007	BCR	C10-C11-C12-C13
14	A	4007	BCR	C21-C22-C23-C24
14	A	4007	BCR	C37-C22-C23-C24
11	b	1232	CLA	CBD-CGD-O2D-CED
11	A	1132	CLA	CHA-CBD-CGD-O2D
14	A	4008	BCR	C7-C8-C9-C10
14	A	4008	BCR	C7-C8-C9-C34
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
11	B	1236	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1126	CLA	CHA-CBD-CGD-O1D
11	a	1126	CLA	CHA-CBD-CGD-O2D
11	a	1126	CLA	CBD-CGD-O2D-CED
11	B	1235	CLA	CHA-CBD-CGD-O1D
11	A	1104	CLA	CBD-CGD-O2D-CED
11	2	1203	CLA	C2-C1-O2A-CGA
11	A	1137	CLA	CHA-CBD-CGD-O1D
11	A	1137	CLA	CHA-CBD-CGD-O2D
11	1	1125	CLA	C4C-C3C-CAC-CBC
11	B	1021	CLA	CHA-CBD-CGD-O1D
11	B	1021	CLA	CHA-CBD-CGD-O2D
11	B	1021	CLA	CBD-CGD-O2D-CED
11	A	1122	CLA	CBA-CGA-O2A-C1
11	A	1122	CLA	C2-C3-C5-C6
11	A	1122	CLA	C4-C3-C5-C6
14	1	4002	BCR	C7-C8-C9-C10
14	1	4002	BCR	C7-C8-C9-C34
14	1	4002	BCR	C11-C10-C9-C8
14	1	4002	BCR	C11-C10-C9-C34
14	1	4002	BCR	C9-C10-C11-C12
14	1	4002	BCR	C17-C18-C19-C20
14	1	4002	BCR	C36-C18-C19-C20
14	1	4002	BCR	C23-C24-C25-C26
14	1	4002	BCR	C23-C24-C25-C30
11	1	1101	CLA	C2-C1-O2A-CGA
11	A	1138	CLA	CHA-CBD-CGD-O1D
11	A	1138	CLA	CHA-CBD-CGD-O2D
11	b	1021	CLA	C1A-C2A-CAA-CBA
11	b	1021	CLA	C3A-C2A-CAA-CBA
11	b	1021	CLA	CHA-CBD-CGD-O1D
11	b	1021	CLA	CHA-CBD-CGD-O2D
11	b	1021	CLA	CBD-CGD-O2D-CED
11	b	1021	CLA	O1D-CGD-O2D-CED
14	L	4022	BCR	C11-C10-C9-C8
14	L	4022	BCR	C11-C10-C9-C34
14	L	4022	BCR	C10-C11-C12-C13
14	L	4022	BCR	C11-C12-C13-C35
14	L	4022	BCR	C17-C18-C19-C20
14	L	4022	BCR	C36-C18-C19-C20
14	L	4022	BCR	C21-C22-C23-C24
14	L	4022	BCR	C37-C22-C23-C24
11	2	1215	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1215	CLA	C4-C3-C5-C6
14	1	4001	BCR	C7-C8-C9-C10
14	1	4001	BCR	C7-C8-C9-C34
14	1	4001	BCR	C11-C10-C9-C8
14	1	4001	BCR	C11-C10-C9-C34
14	1	4001	BCR	C10-C11-C12-C13
11	b	1214	CLA	CBD-CGD-O2D-CED
11	b	1013	CLA	CBD-CGD-O2D-CED
11	1	1121	CLA	C3A-C2A-CAA-CBA
11	1	1121	CLA	CBA-CGA-O2A-C1
11	b	1217	CLA	C1A-C2A-CAA-CBA
11	b	1217	CLA	C3A-C2A-CAA-CBA
14	8	4019	BCR	C7-C8-C9-C10
14	8	4019	BCR	C7-C8-C9-C34
14	8	4019	BCR	C9-C10-C11-C12
14	8	4019	BCR	C11-C12-C13-C14
14	8	4019	BCR	C11-C12-C13-C35
14	8	4019	BCR	C19-C20-C21-C22
14	8	4019	BCR	C37-C22-C23-C24
14	8	4019	BCR	C23-C24-C25-C26
14	8	4019	BCR	C23-C24-C25-C30
11	b	1205	CLA	CHA-CBD-CGD-O2D
11	2	1225	CLA	C1A-C2A-CAA-CBA
11	2	1225	CLA	C3A-C2A-CAA-CBA
11	a	1123	CLA	C2-C1-O2A-CGA
11	B	1023	CLA	C2-C1-O2A-CGA
11	B	1023	CLA	CBD-CGD-O2D-CED
11	B	1023	CLA	C6-C7-C8-C9
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C23-C24-C25-C26
14	B	4006	BCR	C23-C24-C25-C30
11	b	1202	CLA	C1A-C2A-CAA-CBA
11	b	1202	CLA	C3A-C2A-CAA-CBA
11	b	1202	CLA	CAD-CBD-CGD-O1D
11	b	1202	CLA	CAD-CBD-CGD-O2D
11	1	1119	CLA	C2-C1-O2A-CGA
11	1	1119	CLA	CHA-CBD-CGD-O1D
11	1	1119	CLA	CHA-CBD-CGD-O2D
11	1	1119	CLA	CBD-CGD-O2D-CED
14	B	4017	BCR	C11-C10-C9-C8
14	B	4017	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	4017	BCR	C9-C10-C11-C12
14	B	4017	BCR	C10-C11-C12-C13
11	B	1226	CLA	CHA-CBD-CGD-O1D
11	B	1226	CLA	CHA-CBD-CGD-O2D
11	A	1112	CLA	C1A-C2A-CAA-CBA
11	A	1112	CLA	C3A-C2A-CAA-CBA
11	a	1133	CLA	CBA-CGA-O2A-C1
11	A	1124	CLA	C2-C1-O2A-CGA
11	2	1023	CLA	CHA-CBD-CGD-O1D
11	2	1023	CLA	CHA-CBD-CGD-O2D
11	2	1023	CLA	CBD-CGD-O2D-CED
11	2	1023	CLA	O2A-C1-C2-C3
14	l	4019	BCR	C1-C6-C7-C8
14	l	4019	BCR	C5-C6-C7-C8
14	l	4019	BCR	C11-C10-C9-C8
14	l	4019	BCR	C11-C10-C9-C34
14	l	4019	BCR	C10-C11-C12-C13
14	l	4019	BCR	C11-C12-C13-C14
14	l	4019	BCR	C11-C12-C13-C35
14	l	4019	BCR	C23-C24-C25-C26
14	l	4019	BCR	C23-C24-C25-C30
11	2	1211	CLA	CBA-CGA-O2A-C1
11	2	1211	CLA	CHA-CBD-CGD-O1D
11	2	1211	CLA	CHA-CBD-CGD-O2D
11	2	1211	CLA	CAD-CBD-CGD-O1D
11	B	1214	CLA	C2-C3-C5-C6
11	B	1214	CLA	C4-C3-C5-C6
11	a	1127	CLA	C11-C10-C8-C9
11	1	1110	CLA	CHA-CBD-CGD-O1D
11	1	1110	CLA	CHA-CBD-CGD-O2D
14	F	4013	BCR	C1-C6-C7-C8
14	F	4013	BCR	C5-C6-C7-C8
14	F	4013	BCR	C11-C10-C9-C8
14	F	4013	BCR	C11-C10-C9-C34
14	F	4013	BCR	C11-C12-C13-C35
11	l	1503	CLA	C2-C1-O2A-CGA
11	A	1118	CLA	CHA-CBD-CGD-O1D
11	A	1118	CLA	CHA-CBD-CGD-O2D
11	A	1118	CLA	CAD-CBD-CGD-O1D
14	8	4022	BCR	C11-C10-C9-C8
14	8	4022	BCR	C11-C10-C9-C34
14	8	4022	BCR	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	8	4022	BCR	C36-C18-C19-C20
11	A	1139	CLA	C1A-C2A-CAA-CBA
11	A	1139	CLA	C3A-C2A-CAA-CBA
11	A	1139	CLA	CBD-CGD-O2D-CED
11	2	1202	CLA	C3A-C2A-CAA-CBA
11	B	1208	CLA	CBD-CGD-O2D-CED
11	1	1011	CLA	CHA-CBD-CGD-O2D
11	B	1228	CLA	CBD-CGD-O2D-CED
11	B	1240	CLA	C1A-C2A-CAA-CBA
11	B	1240	CLA	CBD-CGD-O2D-CED
11	1	1134	CLA	CHA-CBD-CGD-O1D
11	1	1134	CLA	CHA-CBD-CGD-O2D
11	1	1104	CLA	C1A-C2A-CAA-CBA
11	1	1104	CLA	CBD-CGD-O2D-CED
11	2	1206	CLA	CHA-CBD-CGD-O1D
11	2	1206	CLA	CBD-CGD-O2D-CED
11	2	1240	CLA	CBD-CGD-O2D-CED
11	2	1239	CLA	C1A-C2A-CAA-CBA
11	2	1239	CLA	C3A-C2A-CAA-CBA
11	2	1239	CLA	CHA-CBD-CGD-O1D
11	2	1239	CLA	CHA-CBD-CGD-O2D
11	2	1239	CLA	CBD-CGD-O2D-CED
11	A	1105	CLA	CBD-CGD-O2D-CED
11	A	1121	CLA	CBD-CGD-O2D-CED
11	A	1107	CLA	C1A-C2A-CAA-CBA
11	A	1107	CLA	C2-C3-C5-C6
11	A	1107	CLA	C4-C3-C5-C6
11	a	1101	CLA	C1A-C2A-CAA-CBA
11	a	1101	CLA	C2-C1-O2A-CGA
11	B	1013	CLA	CBD-CGD-O2D-CED
11	B	1225	CLA	C1A-C2A-CAA-CBA
11	B	1225	CLA	C3A-C2A-CAA-CBA
11	B	1225	CLA	C11-C10-C8-C7
14	2	4010	BCR	C7-C8-C9-C10
14	2	4010	BCR	C7-C8-C9-C34
14	2	4010	BCR	C11-C10-C9-C8
14	2	4010	BCR	C11-C10-C9-C34
14	2	4010	BCR	C9-C10-C11-C12
14	2	4010	BCR	C23-C24-C25-C26
14	2	4010	BCR	C23-C24-C25-C30
14	1	4003	BCR	C1-C6-C7-C8
14	1	4003	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	1	4003	BCR	C11-C10-C9-C8
14	1	4003	BCR	C11-C10-C9-C34
14	1	4003	BCR	C10-C11-C12-C13
11	2	1021	CLA	C3A-C2A-CAA-CBA
11	2	1021	CLA	CHA-CBD-CGD-O1D
11	2	1021	CLA	CBD-CGD-O2D-CED
11	2	1021	CLA	O1D-CGD-O2D-CED
11	B	1211	CLA	CBA-CGA-O2A-C1
14	a	4002	BCR	C7-C8-C9-C10
14	a	4002	BCR	C7-C8-C9-C34
14	a	4002	BCR	C11-C10-C9-C8
14	a	4002	BCR	C11-C10-C9-C34
14	a	4002	BCR	C11-C12-C13-C35
14	a	4002	BCR	C17-C18-C19-C20
14	a	4002	BCR	C36-C18-C19-C20
14	a	4002	BCR	C21-C22-C23-C24
14	a	4002	BCR	C23-C24-C25-C26
14	a	4002	BCR	C23-C24-C25-C30
11	B	1230	CLA	C2-C1-O2A-CGA
11	B	1230	CLA	C2-C3-C5-C6
11	b	1209	CLA	C2A-CAA-CBA-CGA
11	b	1203	CLA	C6-C7-C8-C9
11	2	1205	CLA	CHA-CBD-CGD-O1D
11	2	1205	CLA	CHA-CBD-CGD-O2D
14	2	4004	BCR	C7-C8-C9-C10
14	2	4004	BCR	C7-C8-C9-C34
14	2	4004	BCR	C11-C10-C9-C8
14	2	4004	BCR	C11-C10-C9-C34
14	2	4004	BCR	C10-C11-C12-C13
14	2	4004	BCR	C21-C22-C23-C24
14	2	4004	BCR	C37-C22-C23-C24
14	b	4006	BCR	C1-C6-C7-C8
14	b	4006	BCR	C11-C10-C9-C8
14	b	4006	BCR	C11-C10-C9-C34
14	b	4006	BCR	C11-C12-C13-C14
14	b	4006	BCR	C11-C12-C13-C35
14	b	4006	BCR	C23-C24-C25-C26
14	b	4006	BCR	C23-C24-C25-C30
11	A	1108	CLA	C1A-C2A-CAA-CBA
11	A	1108	CLA	C3A-C2A-CAA-CBA
14	1	4007	BCR	C7-C8-C9-C10
14	1	4007	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	1	4007	BCR	C11-C10-C9-C8
14	1	4007	BCR	C11-C10-C9-C34
14	1	4007	BCR	C10-C11-C12-C13
14	1	4007	BCR	C19-C20-C21-C22
14	1	4007	BCR	C23-C24-C25-C26
14	m	4021	BCR	C11-C10-C9-C8
14	m	4021	BCR	C11-C10-C9-C34
14	m	4021	BCR	C10-C11-C12-C13
14	F	4018	BCR	C11-C10-C9-C8
14	F	4018	BCR	C11-C10-C9-C34
14	F	4018	BCR	C10-C11-C12-C13
11	1	1113	CLA	CBD-CGD-O2D-CED
11	a	1131	CLA	CBD-CGD-O2D-CED
11	1	1107	CLA	C1A-C2A-CAA-CBA
11	1	1107	CLA	CBD-CGD-O2D-CED
14	6	4013	BCR	C11-C10-C9-C8
14	6	4013	BCR	C11-C10-C9-C34
14	6	4013	BCR	C21-C22-C23-C24
14	6	4013	BCR	C37-C22-C23-C24
11	a	1109	CLA	CBD-CGD-O2D-CED
11	a	1109	CLA	C2-C3-C5-C6
11	a	1109	CLA	C4-C3-C5-C6
14	B	4014	BCR	C11-C10-C9-C8
14	B	4014	BCR	C11-C10-C9-C34
14	B	4014	BCR	C10-C11-C12-C13
14	B	4014	BCR	C17-C18-C19-C20
14	B	4014	BCR	C36-C18-C19-C20
15	b	5004	LHG	C3-O3-P-O4
15	b	5004	LHG	C4-O6-P-O3
14	2	4017	BCR	C11-C10-C9-C8
14	2	4017	BCR	C11-C10-C9-C34
14	2	4017	BCR	C10-C11-C12-C13
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C21-C22-C23-C24
14	B	4005	BCR	C37-C22-C23-C24
11	a	1137	CLA	C2-C1-O2A-CGA
11	a	1137	CLA	C11-C10-C8-C9
11	1	1105	CLA	C2A-CAA-CBA-CGA
11	2	1216	CLA	C2-C1-O2A-CGA
11	2	1216	CLA	CBD-CGD-O2D-CED
11	1	1102	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1102	CLA	C3A-C2A-CAA-CBA
11	1	1102	CLA	CBD-CGD-O2D-CED
11	A	1102	CLA	C1A-C2A-CAA-CBA
11	A	1102	CLA	C3A-C2A-CAA-CBA
11	A	1102	CLA	O1A-CGA-O2A-C1
11	A	1102	CLA	CBD-CGD-O2D-CED
11	a	1129	CLA	CBA-CGA-O2A-C1
11	a	1129	CLA	CHA-CBD-CGD-O1D
11	b	1211	CLA	CBD-CGD-O2D-CED
14	f	4018	BCR	C11-C10-C9-C8
14	f	4018	BCR	C11-C10-C9-C34
14	f	4018	BCR	C11-C12-C13-C14
14	f	4018	BCR	C11-C12-C13-C35
11	a	1138	CLA	CBD-CGD-O2D-CED
11	2	1222	CLA	CHA-CBD-CGD-O2D
11	A	1110	CLA	CBA-CGA-O2A-C1
11	A	1110	CLA	O1A-CGA-O2A-C1
11	1	1128	CLA	CBD-CGD-O2D-CED
11	1	1128	CLA	C6-C7-C8-C9
11	A	1801	CLA	C4C-C3C-CAC-CBC
11	1	1125	CLA	C2C-C3C-CAC-CBC
11	2	1220	CLA	C2C-C3C-CAC-CBC
11	1	1133	CLA	O1D-CGD-O2D-CED
11	B	1210	CLA	O1D-CGD-O2D-CED
11	a	1022	CLA	O1D-CGD-O2D-CED
11	1	1108	CLA	O1D-CGD-O2D-CED
11	1	1109	CLA	O1D-CGD-O2D-CED
11	A	1109	CLA	O1D-CGD-O2D-CED
11	a	1108	CLA	O1D-CGD-O2D-CED
11	a	1011	CLA	O1D-CGD-O2D-CED
11	B	1023	CLA	O1D-CGD-O2D-CED
11	A	1105	CLA	O1D-CGD-O2D-CED
11	a	1121	CLA	O1D-CGD-O2D-CED
11	1	1801	CLA	C4C-C3C-CAC-CBC
11	B	1210	CLA	C2C-C3C-CAC-CBC
11	A	1801	CLA	C2C-C3C-CAC-CBC
11	a	1124	CLA	O1D-CGD-O2D-CED
11	1	1139	CLA	O1D-CGD-O2D-CED
11	2	1208	CLA	O1D-CGD-O2D-CED
11	b	1240	CLA	O1D-CGD-O2D-CED
11	K	1402	CLA	O1D-CGD-O2D-CED
11	b	1220	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1216	CLA	O1D-CGD-O2D-CED
11	A	1113	CLA	O1D-CGD-O2D-CED
11	1	1022	CLA	O1D-CGD-O2D-CED
11	A	1114	CLA	O1D-CGD-O2D-CED
11	B	1231	CLA	O1D-CGD-O2D-CED
11	2	1219	CLA	O1D-CGD-O2D-CED
11	2	1232	CLA	O1D-CGD-O2D-CED
11	A	1011	CLA	O1D-CGD-O2D-CED
11	a	1139	CLA	O1D-CGD-O2D-CED
11	A	1801	CLA	O1D-CGD-O2D-CED
11	A	1130	CLA	O1D-CGD-O2D-CED
11	A	1104	CLA	O1D-CGD-O2D-CED
11	B	1021	CLA	O1D-CGD-O2D-CED
11	1	1121	CLA	O1D-CGD-O2D-CED
11	A	1139	CLA	O1D-CGD-O2D-CED
11	B	1208	CLA	O1D-CGD-O2D-CED
11	B	1240	CLA	O1D-CGD-O2D-CED
11	B	1219	CLA	O1D-CGD-O2D-CED
11	1	1104	CLA	O1D-CGD-O2D-CED
11	A	1121	CLA	O1D-CGD-O2D-CED
11	A	1107	CLA	O1D-CGD-O2D-CED
11	1	1113	CLA	O1D-CGD-O2D-CED
11	a	1131	CLA	O1D-CGD-O2D-CED
11	a	1109	CLA	O1D-CGD-O2D-CED
11	1	1102	CLA	O1D-CGD-O2D-CED
11	a	1138	CLA	O1D-CGD-O2D-CED
11	b	1210	CLA	O1D-CGD-O2D-CED
11	2	1218	CLA	CBD-CGD-O2D-CED
11	b	1218	CLA	CBD-CGD-O2D-CED
11	1	1133	CLA	CBD-CGD-O2D-CED
11	b	1240	CLA	CBD-CGD-O2D-CED
11	1	1108	CLA	CBD-CGD-O2D-CED
11	1	1138	CLA	CBD-CGD-O2D-CED
11	b	1216	CLA	CBD-CGD-O2D-CED
11	b	1234	CLA	CBD-CGD-O2D-CED
11	b	1239	CLA	CBD-CGD-O2D-CED
11	1	1109	CLA	CBD-CGD-O2D-CED
11	1	1103	CLA	CBD-CGD-O2D-CED
11	A	1109	CLA	CBD-CGD-O2D-CED
11	b	1225	CLA	CBD-CGD-O2D-CED
11	1	1114	CLA	CBD-CGD-O2D-CED
11	2	1231	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1128	CLA	CBD-CGD-O2D-CED
11	B	1224	CLA	CBD-CGD-O2D-CED
11	1	1130	CLA	CBD-CGD-O2D-CED
11	b	1219	CLA	CBD-CGD-O2D-CED
11	L	1503	CLA	CBD-CGD-O2D-CED
11	a	1106	CLA	CBD-CGD-O2D-CED
11	2	1219	CLA	CBD-CGD-O2D-CED
11	2	1212	CLA	CBD-CGD-O2D-CED
11	1	1135	CLA	CBD-CGD-O2D-CED
11	a	1117	CLA	CBD-CGD-O2D-CED
11	b	1228	CLA	CBD-CGD-O2D-CED
11	l	1501	CLA	CBD-CGD-O2D-CED
11	B	1239	CLA	CBD-CGD-O2D-CED
11	1	1136	CLA	CBD-CGD-O2D-CED
11	2	1238	CLA	CBD-CGD-O2D-CED
11	a	1139	CLA	CBD-CGD-O2D-CED
11	A	1801	CLA	CBD-CGD-O2D-CED
11	8	1503	CLA	CBD-CGD-O2D-CED
11	a	1107	CLA	CBD-CGD-O2D-CED
11	B	1212	CLA	CBD-CGD-O2D-CED
11	1	1140	CLA	CBD-CGD-O2D-CED
11	A	1123	CLA	CBD-CGD-O2D-CED
11	a	1108	CLA	CBD-CGD-O2D-CED
11	2	1234	CLA	CBD-CGD-O2D-CED
11	A	1130	CLA	CBD-CGD-O2D-CED
11	A	1103	CLA	CBD-CGD-O2D-CED
11	b	1023	CLA	CBD-CGD-O2D-CED
11	B	1222	CLA	CBD-CGD-O2D-CED
11	A	1132	CLA	CBD-CGD-O2D-CED
11	1	1101	CLA	CBD-CGD-O2D-CED
11	b	1207	CLA	CBD-CGD-O2D-CED
11	1	1121	CLA	CBD-CGD-O2D-CED
11	b	1205	CLA	CBD-CGD-O2D-CED
11	2	1225	CLA	CBD-CGD-O2D-CED
11	B	1238	CLA	CBD-CGD-O2D-CED
11	1	1131	CLA	CBD-CGD-O2D-CED
11	A	1112	CLA	CBD-CGD-O2D-CED
11	a	1127	CLA	CBD-CGD-O2D-CED
11	l	1503	CLA	CBD-CGD-O2D-CED
11	A	1118	CLA	CBD-CGD-O2D-CED
11	B	1219	CLA	CBD-CGD-O2D-CED
11	A	1107	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1101	CLA	CBD-CGD-O2D-CED
11	a	1111	CLA	CBD-CGD-O2D-CED
11	2	1223	CLA	CBD-CGD-O2D-CED
11	b	1209	CLA	CBD-CGD-O2D-CED
11	b	1206	CLA	CBD-CGD-O2D-CED
11	1	1117	CLA	CBD-CGD-O2D-CED
11	2	1013	CLA	CBD-CGD-O2D-CED
11	a	1130	CLA	CBD-CGD-O2D-CED
11	b	1210	CLA	CBD-CGD-O2D-CED
11	2	1222	CLA	CBD-CGD-O2D-CED
11	a	1121	CLA	CBD-CGD-O2D-CED
11	2	1224	CLA	O1A-CGA-O2A-C1
11	B	1224	CLA	O1A-CGA-O2A-C1
11	1	1237	CLA	O1A-CGA-O2A-C1
11	b	1224	CLA	O1A-CGA-O2A-C1
11	1	1122	CLA	O1A-CGA-O2A-C1
11	L	1501	CLA	O1A-CGA-O2A-C1
11	1	1140	CLA	O1A-CGA-O2A-C1
11	b	1223	CLA	O1A-CGA-O2A-C1
11	A	1122	CLA	O1A-CGA-O2A-C1
11	1	1104	CLA	O1A-CGA-O2A-C1
11	B	1013	CLA	O1A-CGA-O2A-C1
11	1	1102	CLA	O1A-CGA-O2A-C1
11	2	1013	CLA	O1A-CGA-O2A-C1
11	A	1120	CLA	O1A-CGA-O2A-C1
11	1	1130	CLA	O1A-CGA-O2A-C1
11	A	1129	CLA	O1A-CGA-O2A-C1
11	A	1130	CLA	O1A-CGA-O2A-C1
11	a	1133	CLA	O1A-CGA-O2A-C1
11	B	1211	CLA	O1A-CGA-O2A-C1
11	B	1227	CLA	C2C-C3C-CAC-CBC
11	2	1220	CLA	C4C-C3C-CAC-CBC
11	b	1236	CLA	C2-C1-O2A-CGA
11	a	1114	CLA	O1D-CGD-O2D-CED
11	k	1402	CLA	O1D-CGD-O2D-CED
11	2	1231	CLA	O1D-CGD-O2D-CED
11	b	1219	CLA	O1D-CGD-O2D-CED
11	0	1402	CLA	O1D-CGD-O2D-CED
11	a	1117	CLA	O1D-CGD-O2D-CED
11	a	1125	CLA	O1D-CGD-O2D-CED
11	a	1107	CLA	O1D-CGD-O2D-CED
11	a	1113	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1023	CLA	O1D-CGD-O2D-CED
11	a	1104	CLA	O1D-CGD-O2D-CED
11	b	1214	CLA	O1D-CGD-O2D-CED
11	1	1131	CLA	O1D-CGD-O2D-CED
11	2	1023	CLA	O1D-CGD-O2D-CED
11	2	1240	CLA	O1D-CGD-O2D-CED
11	a	1111	CLA	O1D-CGD-O2D-CED
11	A	1120	CLA	CBA-CGA-O2A-C1
11	L	1502	CLA	CBA-CGA-O2A-C1
11	A	1129	CLA	CBA-CGA-O2A-C1
11	A	1115	CLA	CBA-CGA-O2A-C1
11	A	1130	CLA	CBA-CGA-O2A-C1
11	1	1801	CLA	C2C-C3C-CAC-CBC
11	B	1210	CLA	C4C-C3C-CAC-CBC
11	2	1236	CLA	C2-C1-O2A-CGA
11	K	1401	CLA	O1D-CGD-O2D-CED
11	1	1111	CLA	O1D-CGD-O2D-CED
11	1	1103	CLA	O1D-CGD-O2D-CED
11	0	1401	CLA	O1D-CGD-O2D-CED
11	a	1140	CLA	O1D-CGD-O2D-CED
11	a	1119	CLA	O1D-CGD-O2D-CED
11	A	1128	CLA	O1D-CGD-O2D-CED
11	L	1503	CLA	O1D-CGD-O2D-CED
11	b	1201	CLA	O1D-CGD-O2D-CED
11	a	1118	CLA	O1D-CGD-O2D-CED
11	A	1116	CLA	O1D-CGD-O2D-CED
11	k	1401	CLA	O1D-CGD-O2D-CED
11	A	1022	CLA	O1D-CGD-O2D-CED
11	b	1224	CLA	O1D-CGD-O2D-CED
11	8	1503	CLA	O1D-CGD-O2D-CED
11	1	1140	CLA	O1D-CGD-O2D-CED
11	b	1238	CLA	O1D-CGD-O2D-CED
11	b	1232	CLA	O1D-CGD-O2D-CED
11	a	1126	CLA	O1D-CGD-O2D-CED
11	b	1013	CLA	O1D-CGD-O2D-CED
11	1	1119	CLA	O1D-CGD-O2D-CED
11	B	1228	CLA	O1D-CGD-O2D-CED
11	2	1206	CLA	O1D-CGD-O2D-CED
11	B	1013	CLA	O1D-CGD-O2D-CED
11	1	1107	CLA	O1D-CGD-O2D-CED
11	2	1216	CLA	O1D-CGD-O2D-CED
11	b	1211	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1224	CLA	CBA-CGA-O2A-C1
11	B	1224	CLA	CBA-CGA-O2A-C1
11	1	1237	CLA	CBA-CGA-O2A-C1
11	B	1013	CLA	CBA-CGA-O2A-C1
11	1	1102	CLA	CBA-CGA-O2A-C1
11	A	1102	CLA	CBA-CGA-O2A-C1
11	2	1013	CLA	CBA-CGA-O2A-C1
11	a	1122	CLA	CBD-CGD-O2D-CED
11	1	1801	CLA	CBD-CGD-O2D-CED
11	B	1213	CLA	CBD-CGD-O2D-CED
11	1	1120	CLA	CBD-CGD-O2D-CED
11	2	1217	CLA	CBD-CGD-O2D-CED
11	a	1103	CLA	CBD-CGD-O2D-CED
11	b	1230	CLA	CBD-CGD-O2D-CED
11	B	1234	CLA	CBD-CGD-O2D-CED
11	B	1209	CLA	CBD-CGD-O2D-CED
11	A	1106	CLA	CBD-CGD-O2D-CED
11	2	1230	CLA	CBD-CGD-O2D-CED
11	2	1203	CLA	CBD-CGD-O2D-CED
11	2	1215	CLA	CBD-CGD-O2D-CED
11	A	1140	CLA	CBD-CGD-O2D-CED
11	b	1202	CLA	CBD-CGD-O2D-CED
11	a	1135	CLA	CBD-CGD-O2D-CED
11	B	1226	CLA	CBD-CGD-O2D-CED
11	A	1136	CLA	CBD-CGD-O2D-CED
11	B	1218	CLA	CBD-CGD-O2D-CED
11	a	1132	CLA	CBD-CGD-O2D-CED
11	1	1112	CLA	CBD-CGD-O2D-CED
11	b	1208	CLA	CBD-CGD-O2D-CED
11	B	1201	CLA	CBD-CGD-O2D-CED
11	a	1122	CLA	O1A-CGA-O2A-C1
11	K	1401	CLA	O1A-CGA-O2A-C1
11	1	1111	CLA	O1A-CGA-O2A-C1
11	1	1109	CLA	O1A-CGA-O2A-C1
11	0	1401	CLA	O1A-CGA-O2A-C1
11	a	1140	CLA	O1A-CGA-O2A-C1
11	a	1102	CLA	O1A-CGA-O2A-C1
11	L	1503	CLA	O1A-CGA-O2A-C1
11	b	1228	CLA	O1A-CGA-O2A-C1
11	l	1501	CLA	O1A-CGA-O2A-C1
11	A	1237	CLA	O1A-CGA-O2A-C1
11	k	1401	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1801	CLA	O1A-CGA-O2A-C1
11	a	1237	CLA	O1A-CGA-O2A-C1
11	b	1023	CLA	O1A-CGA-O2A-C1
11	b	1021	CLA	O1A-CGA-O2A-C1
11	b	1013	CLA	O1A-CGA-O2A-C1
11	a	1123	CLA	O1A-CGA-O2A-C1
11	2	1226	CLA	O1A-CGA-O2A-C1
11	2	1023	CLA	O1A-CGA-O2A-C1
11	1	1110	CLA	O1A-CGA-O2A-C1
11	l	1503	CLA	O1A-CGA-O2A-C1
11	A	1118	CLA	O1A-CGA-O2A-C1
11	B	1228	CLA	O1A-CGA-O2A-C1
11	2	1021	CLA	O1A-CGA-O2A-C1
11	2	1228	CLA	O1A-CGA-O2A-C1
11	b	1239	CLA	O1A-CGA-O2A-C1
11	a	1115	CLA	O1A-CGA-O2A-C1
11	A	1114	CLA	O1A-CGA-O2A-C1
11	A	1115	CLA	O1A-CGA-O2A-C1
11	1	1121	CLA	O1A-CGA-O2A-C1
11	2	1211	CLA	O1A-CGA-O2A-C1
11	A	1121	CLA	O1A-CGA-O2A-C1
11	a	1130	CLA	O1A-CGA-O2A-C1
11	a	1121	CLA	O1A-CGA-O2A-C1
11	B	1215	CLA	O1D-CGD-O2D-CED
11	A	1131	CLA	O1D-CGD-O2D-CED
11	a	1102	CLA	O1D-CGD-O2D-CED
11	a	1801	CLA	O1D-CGD-O2D-CED
11	1	1116	CLA	O1D-CGD-O2D-CED
11	B	1232	CLA	O1D-CGD-O2D-CED
11	2	1239	CLA	O1D-CGD-O2D-CED
11	1	1128	CLA	O1D-CGD-O2D-CED
11	2	1213	CLA	C2C-C3C-CAC-CBC
11	B	1236	CLA	C2-C1-O2A-CGA
11	2	1224	CLA	O1D-CGD-O2D-CED
11	b	1235	CLA	O1D-CGD-O2D-CED
11	a	1116	CLA	O1D-CGD-O2D-CED
11	A	1117	CLA	O1D-CGD-O2D-CED
11	1	1237	CLA	O1D-CGD-O2D-CED
11	a	1105	CLA	O1D-CGD-O2D-CED
11	b	1212	CLA	O1D-CGD-O2D-CED
11	1	1126	CLA	O1D-CGD-O2D-CED
11	A	1102	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1213	CLA	C4C-C3C-CAC-CBC
11	A	1125	CLA	CBD-CGD-O2D-CED
11	a	1112	CLA	CBD-CGD-O2D-CED
11	a	1136	CLA	CBD-CGD-O2D-CED
11	2	1227	CLA	CBD-CGD-O2D-CED
11	b	1227	CLA	CBD-CGD-O2D-CED
11	A	1237	CLA	CBD-CGD-O2D-CED
11	A	1115	CLA	CBD-CGD-O2D-CED
11	1	1115	CLA	CBD-CGD-O2D-CED
11	2	1220	CLA	CBD-CGD-O2D-CED
11	B	1230	CLA	CBD-CGD-O2D-CED
11	1	1138	CLA	O1D-CGD-O2D-CED
11	A	1126	CLA	O1D-CGD-O2D-CED
11	1	1137	CLA	O1D-CGD-O2D-CED
11	B	1236	CLA	O1D-CGD-O2D-CED
11	1	1117	CLA	O1D-CGD-O2D-CED
15	2	5004	LHG	O9-C7-O7-C5
11	a	1125	CLA	O1A-CGA-O2A-C1
11	2	1203	CLA	O1A-CGA-O2A-C1
11	A	1124	CLA	O1A-CGA-O2A-C1
11	1	1120	CLA	CBA-CGA-O2A-C1
11	a	1115	CLA	CBA-CGA-O2A-C1
11	a	1134	CLA	CBA-CGA-O2A-C1
11	A	1121	CLA	CBA-CGA-O2A-C1
11	b	1211	CLA	CBA-CGA-O2A-C1
11	a	1130	CLA	CBA-CGA-O2A-C1
11	a	1121	CLA	CBA-CGA-O2A-C1
11	B	1227	CLA	C4C-C3C-CAC-CBC
11	1	1120	CLA	O1A-CGA-O2A-C1
11	L	1502	CLA	O1A-CGA-O2A-C1
11	A	1134	CLA	O1A-CGA-O2A-C1
11	a	1134	CLA	O1A-CGA-O2A-C1
11	1	1115	CLA	O1A-CGA-O2A-C1
11	1	1134	CLA	O1A-CGA-O2A-C1
11	b	1211	CLA	O1A-CGA-O2A-C1
11	2	1222	CLA	O1D-CGD-O2D-CED
11	B	1216	CLA	C3-C5-C6-C7
11	A	1119	CLA	C3-C5-C6-C7
11	1	1022	CLA	C3-C5-C6-C7
11	B	1223	CLA	C3-C5-C6-C7
11	a	1140	CLA	C3-C5-C6-C7
11	a	1119	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1206	CLA	C3-C5-C6-C7
11	L	1503	CLA	C3-C5-C6-C7
11	a	1117	CLA	C3-C5-C6-C7
11	A	1022	CLA	C3-C5-C6-C7
12	B	2002	PQN	C13-C15-C16-C17
11	a	1237	CLA	C3-C5-C6-C7
11	a	1110	CLA	C3-C5-C6-C7
11	L	1501	CLA	C3-C5-C6-C7
11	2	1234	CLA	C3-C5-C6-C7
11	a	1011	CLA	C3-C5-C6-C7
11	b	1223	CLA	C3-C5-C6-C7
11	B	1235	CLA	C3-C5-C6-C7
11	2	1215	CLA	C3-C5-C6-C7
11	b	1207	CLA	C3-C5-C6-C7
11	l	1503	CLA	C3-C5-C6-C7
11	2	1202	CLA	C3-C5-C6-C7
11	a	1131	CLA	C3-C5-C6-C7
11	1	1117	CLA	C3-C5-C6-C7
11	b	1210	CLA	C3-C5-C6-C7
11	a	1122	CLA	CBA-CGA-O2A-C1
11	K	1401	CLA	CBA-CGA-O2A-C1
11	1	1109	CLA	CBA-CGA-O2A-C1
11	0	1401	CLA	CBA-CGA-O2A-C1
11	a	1119	CLA	CBA-CGA-O2A-C1
11	a	1102	CLA	CBA-CGA-O2A-C1
11	0	1402	CLA	CBA-CGA-O2A-C1
11	L	1503	CLA	CBA-CGA-O2A-C1
11	l	1501	CLA	CBA-CGA-O2A-C1
11	k	1401	CLA	CBA-CGA-O2A-C1
11	a	1237	CLA	CBA-CGA-O2A-C1
11	1	1122	CLA	CBA-CGA-O2A-C1
11	L	1501	CLA	CBA-CGA-O2A-C1
11	1	1140	CLA	CBA-CGA-O2A-C1
11	b	1223	CLA	CBA-CGA-O2A-C1
11	B	1021	CLA	CBA-CGA-O2A-C1
11	b	1021	CLA	CBA-CGA-O2A-C1
11	b	1013	CLA	CBA-CGA-O2A-C1
11	2	1226	CLA	CBA-CGA-O2A-C1
11	B	1226	CLA	CBA-CGA-O2A-C1
11	1	1110	CLA	CBA-CGA-O2A-C1
11	l	1503	CLA	CBA-CGA-O2A-C1
11	A	1118	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1104	CLA	CBA-CGA-O2A-C1
11	2	1021	CLA	CBA-CGA-O2A-C1
11	2	1216	CLA	CBA-CGA-O2A-C1
11	A	1011	CLA	C5-C6-C7-C8
11	1	1114	CLA	O1D-CGD-O2D-CED
11	B	1239	CLA	O1D-CGD-O2D-CED
11	b	1207	CLA	O1D-CGD-O2D-CED
11	a	1127	CLA	O1D-CGD-O2D-CED
11	2	1204	CLA	CBD-CGD-O2D-CED
11	B	1203	CLA	CBD-CGD-O2D-CED
11	B	1211	CLA	CBD-CGD-O2D-CED
11	8	1503	CLA	O1A-CGA-O2A-C1
11	a	1104	CLA	O1A-CGA-O2A-C1
11	1	1125	CLA	O1A-CGA-O2A-C1
11	a	1136	CLA	O1A-CGA-O2A-C1
11	B	1239	CLA	O1A-CGA-O2A-C1
11	a	1129	CLA	O1A-CGA-O2A-C1
11	A	1134	CLA	CBA-CGA-O2A-C1
11	a	1120	CLA	CBA-CGA-O2A-C1
11	1	1115	CLA	CBA-CGA-O2A-C1
11	1	1134	CLA	CBA-CGA-O2A-C1
11	A	1109	CLA	C4-C3-C5-C6
11	l	1501	CLA	C4-C3-C5-C6
11	B	1230	CLA	C4-C3-C5-C6
11	A	1109	CLA	C2-C3-C5-C6
11	A	1012	CLA	C2-C3-C5-C6
11	2	1215	CLA	C2-C3-C5-C6
11	A	1133	CLA	CBD-CGD-O2D-CED
11	B	1206	CLA	CBD-CGD-O2D-CED
11	b	1215	CLA	CBD-CGD-O2D-CED
11	1	1118	CLA	CBD-CGD-O2D-CED
11	B	1220	CLA	CBD-CGD-O2D-CED
11	B	1227	CLA	CBD-CGD-O2D-CED
11	2	1207	CLA	CBD-CGD-O2D-CED
11	b	1222	CLA	C2A-CAA-CBA-CGA
11	a	1012	CLA	C2A-CAA-CBA-CGA
11	a	1140	CLA	C2A-CAA-CBA-CGA
11	b	1228	CLA	C2A-CAA-CBA-CGA
11	2	1214	CLA	C2A-CAA-CBA-CGA
11	a	1110	CLA	C2A-CAA-CBA-CGA
11	b	1223	CLA	C2A-CAA-CBA-CGA
11	B	1222	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1101	CLA	C2A-CAA-CBA-CGA
11	b	1021	CLA	C2A-CAA-CBA-CGA
11	b	1214	CLA	C2A-CAA-CBA-CGA
11	2	1225	CLA	C2A-CAA-CBA-CGA
11	A	1135	CLA	C2A-CAA-CBA-CGA
11	A	1107	CLA	C2A-CAA-CBA-CGA
11	2	1222	CLA	C2A-CAA-CBA-CGA
11	A	1101	CLA	O1A-CGA-O2A-C1
11	a	1118	CLA	O1A-CGA-O2A-C1
11	A	1103	CLA	O1D-CGD-O2D-CED
11	1	1237	CLA	C3-C5-C6-C7
11	A	1011	CLA	C3-C5-C6-C7
11	A	1106	CLA	C3-C5-C6-C7
11	B	1222	CLA	C3-C5-C6-C7
11	B	1238	CLA	C3-C5-C6-C7
11	1	1118	CLA	C3-C5-C6-C7
11	2	1210	CLA	C3-C5-C6-C7
11	b	1206	CLA	C3-C5-C6-C7
11	1	1111	CLA	CBA-CGA-O2A-C1
11	b	1234	CLA	CBA-CGA-O2A-C1
11	1	1103	CLA	CBA-CGA-O2A-C1
11	k	1402	CLA	CBA-CGA-O2A-C1
11	1	1123	CLA	CBA-CGA-O2A-C1
11	a	1140	CLA	CBA-CGA-O2A-C1
11	b	1219	CLA	CBA-CGA-O2A-C1
11	1	1124	CLA	CBA-CGA-O2A-C1
11	b	1228	CLA	CBA-CGA-O2A-C1
11	a	1105	CLA	CBA-CGA-O2A-C1
11	A	1237	CLA	CBA-CGA-O2A-C1
11	a	1125	CLA	CBA-CGA-O2A-C1
11	A	1801	CLA	CBA-CGA-O2A-C1
11	b	1226	CLA	CBA-CGA-O2A-C1
11	2	1213	CLA	CBA-CGA-O2A-C1
11	b	1023	CLA	CBA-CGA-O2A-C1
11	A	1104	CLA	CBA-CGA-O2A-C1
11	1	1101	CLA	CBA-CGA-O2A-C1
11	a	1123	CLA	CBA-CGA-O2A-C1
11	1	1119	CLA	CBA-CGA-O2A-C1
11	A	1124	CLA	CBA-CGA-O2A-C1
11	2	1023	CLA	CBA-CGA-O2A-C1
11	B	1228	CLA	CBA-CGA-O2A-C1
11	B	1219	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1107	CLA	CBA-CGA-O2A-C1
11	a	1101	CLA	CBA-CGA-O2A-C1
11	2	1228	CLA	CBA-CGA-O2A-C1
11	B	1229	CLA	CBA-CGA-O2A-C1
11	b	1220	CLA	C2C-C3C-CAC-CBC
11	a	1801	CLA	C2C-C3C-CAC-CBC
11	B	1224	CLA	O1D-CGD-O2D-CED
11	1	1135	CLA	O1D-CGD-O2D-CED
11	2	1234	CLA	O1D-CGD-O2D-CED
11	B	1205	CLA	CBD-CGD-O2D-CED
11	b	1236	CLA	CBD-CGD-O2D-CED
11	b	1218	CLA	O1D-CGD-O2D-CED
11	b	1239	CLA	O1D-CGD-O2D-CED
11	1	1130	CLA	O1D-CGD-O2D-CED
11	a	1106	CLA	O1D-CGD-O2D-CED
11	1	1136	CLA	O1D-CGD-O2D-CED
11	B	1212	CLA	O1D-CGD-O2D-CED
11	B	1222	CLA	O1D-CGD-O2D-CED
11	a	1101	CLA	O1D-CGD-O2D-CED
11	a	1119	CLA	O1A-CGA-O2A-C1
11	b	1219	CLA	O1A-CGA-O2A-C1
11	2	1213	CLA	O1A-CGA-O2A-C1
11	1	1101	CLA	O1A-CGA-O2A-C1
11	B	1226	CLA	O1A-CGA-O2A-C1
11	a	1127	CLA	O1A-CGA-O2A-C1
11	2	1216	CLA	O1A-CGA-O2A-C1
11	2	1232	CLA	C2A-CAA-CBA-CGA
11	b	1232	CLA	C2A-CAA-CBA-CGA
11	1	1129	CLA	O1A-CGA-O2A-C1
11	a	1120	CLA	O1A-CGA-O2A-C1
11	l	1501	CLA	O1D-CGD-O2D-CED
11	2	1225	CLA	O1D-CGD-O2D-CED
11	b	1206	CLA	O1D-CGD-O2D-CED
11	a	1130	CLA	O1D-CGD-O2D-CED
14	b	4004	BCR	C9-C10-C11-C12
14	L	4019	BCR	C15-C16-C17-C18
14	a	4007	BCR	C19-C20-C21-C22
14	2	4009	BCR	C13-C14-C15-C16
14	A	4002	BCR	C15-C16-C17-C18
14	f	4013	BCR	C9-C10-C11-C12
14	A	4007	BCR	C19-C20-C21-C22
14	8	4019	BCR	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	4002	BCR	C15-C16-C17-C18
11	1	1129	CLA	CBD-CGD-O2D-CED
11	1	1106	CLA	CBD-CGD-O2D-CED
11	2	1235	CLA	CBD-CGD-O2D-CED
11	a	1237	CLA	CBD-CGD-O2D-CED
11	B	1235	CLA	CBD-CGD-O2D-CED
11	A	1124	CLA	CBD-CGD-O2D-CED
11	A	1135	CLA	CBD-CGD-O2D-CED
11	b	1203	CLA	CBD-CGD-O2D-CED
11	2	1013	CLA	O1D-CGD-O2D-CED
15	1	5001	LHG	O2-C2-C3-O3
15	a	5003	LHG	O2-C2-C3-O3
15	A	5003	LHG	O2-C2-C3-O3
15	A	5001	LHG	O2-C2-C3-O3
11	b	1216	CLA	C3-C5-C6-C7
11	B	1202	CLA	C3-C5-C6-C7
11	b	1235	CLA	C3-C5-C6-C7
11	1	1124	CLA	C3-C5-C6-C7
11	1	1501	CLA	C3-C5-C6-C7
11	2	1238	CLA	C3-C5-C6-C7
11	8	1503	CLA	C3-C5-C6-C7
11	2	1203	CLA	C3-C5-C6-C7
11	2	1225	CLA	C3-C5-C6-C7
11	A	1107	CLA	C3-C5-C6-C7
11	1	1107	CLA	C3-C5-C6-C7
11	A	1110	CLA	C3-C5-C6-C7
11	A	1101	CLA	CBA-CGA-O2A-C1
11	a	1124	CLA	CBA-CGA-O2A-C1
11	K	1402	CLA	CBA-CGA-O2A-C1
11	B	1202	CLA	CBA-CGA-O2A-C1
11	A	1127	CLA	CBA-CGA-O2A-C1
11	1	1137	CLA	CBA-CGA-O2A-C1
11	a	1118	CLA	CBA-CGA-O2A-C1
11	8	1503	CLA	CBA-CGA-O2A-C1
11	a	1104	CLA	CBA-CGA-O2A-C1
11	2	1203	CLA	CBA-CGA-O2A-C1
11	A	1111	CLA	CBA-CGA-O2A-C1
11	A	1105	CLA	CBA-CGA-O2A-C1
11	a	1131	CLA	CBA-CGA-O2A-C1
11	1	1123	CLA	O1A-CGA-O2A-C1
11	0	1402	CLA	O1A-CGA-O2A-C1
11	a	1105	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1226	CLA	O1A-CGA-O2A-C1
11	A	1104	CLA	O1A-CGA-O2A-C1
11	A	1140	CLA	O1A-CGA-O2A-C1
11	a	1135	CLA	O1A-CGA-O2A-C1
11	a	1109	CLA	O1A-CGA-O2A-C1
11	2	1218	CLA	O1D-CGD-O2D-CED
11	b	1234	CLA	O1D-CGD-O2D-CED
11	2	1238	CLA	O1D-CGD-O2D-CED
11	A	1123	CLA	O1D-CGD-O2D-CED
11	A	1112	CLA	O1D-CGD-O2D-CED
11	l	1503	CLA	O1D-CGD-O2D-CED
11	2	1223	CLA	O1D-CGD-O2D-CED
16	B	5002	LMG	C11-C10-O7-C8
11	b	1223	CLA	C2C-C3C-CAC-CBC
11	b	1205	CLA	O1D-CGD-O2D-CED
11	1	1136	CLA	CBA-CGA-O2A-C1
11	a	1133	CLA	CBD-CGD-O2D-CED
11	B	1214	CLA	CBD-CGD-O2D-CED
11	1	1105	CLA	CBD-CGD-O2D-CED
11	k	1402	CLA	O1A-CGA-O2A-C1
11	B	1021	CLA	O1A-CGA-O2A-C1
11	1	1101	CLA	O1D-CGD-O2D-CED
11	B	1238	CLA	O1D-CGD-O2D-CED
11	b	1217	CLA	C2-C1-O2A-CGA
11	b	1231	CLA	CBD-CGD-O2D-CED
11	2	1226	CLA	CBD-CGD-O2D-CED
11	b	1224	CLA	C3-C5-C6-C7
11	2	1206	CLA	C3-C5-C6-C7
12	2	2002	PQN	C13-C15-C16-C17
11	A	1109	CLA	CBA-CGA-O2A-C1
11	1	1125	CLA	CBA-CGA-O2A-C1
11	A	1140	CLA	CBA-CGA-O2A-C1
11	a	1135	CLA	CBA-CGA-O2A-C1
11	a	1127	CLA	CBA-CGA-O2A-C1
11	a	1109	CLA	CBA-CGA-O2A-C1
11	b	1225	CLA	O1D-CGD-O2D-CED
11	A	1118	CLA	O1D-CGD-O2D-CED
16	2	5002	LMG	O6-C5-C6-O5
11	b	1234	CLA	O1A-CGA-O2A-C1
11	1	1103	CLA	O1A-CGA-O2A-C1
11	B	1202	CLA	O1A-CGA-O2A-C1
11	A	1127	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1137	CLA	O1A-CGA-O2A-C1
11	1	1124	CLA	O1A-CGA-O2A-C1
11	A	1111	CLA	O1A-CGA-O2A-C1
11	B	1219	CLA	O1A-CGA-O2A-C1
11	A	1107	CLA	O1A-CGA-O2A-C1
11	a	1101	CLA	O1A-CGA-O2A-C1
11	B	1229	CLA	O1A-CGA-O2A-C1
11	l	1502	CLA	CBA-CGA-O2A-C1
11	b	1222	CLA	C4-C3-C5-C6
11	B	1215	CLA	C4-C3-C5-C6
11	b	1215	CLA	C4-C3-C5-C6
11	a	1126	CLA	C4-C3-C5-C6
11	B	1021	CLA	C4-C3-C5-C6
11	1	1012	CLA	C4-C3-C5-C6
11	b	1221	CLA	C4-C3-C5-C6
11	1	1107	CLA	C4-C3-C5-C6
11	b	1222	CLA	C2-C3-C5-C6
11	b	1213	CLA	C2-C3-C5-C6
11	B	1215	CLA	C2-C3-C5-C6
11	b	1230	CLA	C2-C3-C5-C6
11	l	1501	CLA	C2-C3-C5-C6
11	b	1215	CLA	C2-C3-C5-C6
11	a	1126	CLA	C2-C3-C5-C6
11	2	1230	CLA	C2-C3-C5-C6
11	1	1012	CLA	C2-C3-C5-C6
11	b	1221	CLA	C2-C3-C5-C6
11	1	1134	CLA	C2A-CAA-CBA-CGA
11	a	1121	CLA	C2A-CAA-CBA-CGA
11	A	1119	CLA	C2C-C3C-CAC-CBC
16	b	5002	LMG	O6-C5-C6-O5
11	a	1124	CLA	O1A-CGA-O2A-C1
11	1	1119	CLA	O1A-CGA-O2A-C1
11	a	1131	CLA	O1A-CGA-O2A-C1
11	b	1228	CLA	O1D-CGD-O2D-CED
11	b	1209	CLA	O1D-CGD-O2D-CED
11	a	1801	CLA	C4C-C3C-CAC-CBC
11	b	1227	CLA	C2C-C3C-CAC-CBC
11	1	1139	CLA	CBA-CGA-O2A-C1
16	b	5002	LMG	C29-C28-O8-C9
11	b	1202	CLA	CBA-CGA-O2A-C1
11	1	1011	CLA	CBA-CGA-O2A-C1
11	2	1205	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1222	CLA	CBA-CGA-O2A-C1
11	2	1212	CLA	O1D-CGD-O2D-CED
11	a	1103	CLA	O1D-CGD-O2D-CED
11	A	1132	CLA	O1D-CGD-O2D-CED
11	2	1203	CLA	O1D-CGD-O2D-CED
11	b	1202	CLA	O1D-CGD-O2D-CED
11	B	1218	CLA	O1D-CGD-O2D-CED
11	K	1402	CLA	O1A-CGA-O2A-C1
11	1	1011	CLA	O1A-CGA-O2A-C1
11	A	1105	CLA	O1A-CGA-O2A-C1
11	2	1205	CLA	O1A-CGA-O2A-C1
15	b	5004	LHG	C8-C7-O7-C5
11	b	1210	CLA	C2C-C3C-CAC-CBC
11	2	1217	CLA	O1D-CGD-O2D-CED
11	A	1106	CLA	O1D-CGD-O2D-CED
11	A	1140	CLA	O1D-CGD-O2D-CED
11	A	1136	CLA	O1D-CGD-O2D-CED
11	b	1208	CLA	O1D-CGD-O2D-CED
11	A	1115	CLA	C2C-C3C-CAC-CBC
15	1	5001	LHG	C1-C2-C3-O3
15	B	5004	LHG	C1-C2-C3-O3
16	B	5002	LMG	O9-C10-O7-C8
11	1	1139	CLA	O1A-CGA-O2A-C1
11	A	1109	CLA	O1A-CGA-O2A-C1
16	b	5002	LMG	O10-C28-O8-C9
11	a	1111	CLA	O1A-CGA-O2A-C1
11	2	1201	CLA	C3-C5-C6-C7
12	b	2002	PQN	C13-C15-C16-C17
11	1	1801	CLA	O1D-CGD-O2D-CED
11	B	1234	CLA	O1D-CGD-O2D-CED
11	b	1222	CLA	CBA-CGA-O2A-C1
11	B	1213	CLA	CBA-CGA-O2A-C1
11	B	1207	CLA	CBA-CGA-O2A-C1
11	A	1131	CLA	CBA-CGA-O2A-C1
11	b	1230	CLA	CBA-CGA-O2A-C1
11	B	1234	CLA	CBA-CGA-O2A-C1
11	2	1236	CLA	CBA-CGA-O2A-C1
11	A	1011	CLA	CBA-CGA-O2A-C1
11	A	1022	CLA	CBA-CGA-O2A-C1
11	a	1128	CLA	CBA-CGA-O2A-C1
11	A	1123	CLA	CBA-CGA-O2A-C1
11	a	1011	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1222	CLA	CBA-CGA-O2A-C1
11	B	1236	CLA	CBA-CGA-O2A-C1
11	b	1207	CLA	CBA-CGA-O2A-C1
11	b	1217	CLA	CBA-CGA-O2A-C1
11	B	1023	CLA	CBA-CGA-O2A-C1
11	B	1238	CLA	CBA-CGA-O2A-C1
11	1	1131	CLA	CBA-CGA-O2A-C1
11	2	1202	CLA	CBA-CGA-O2A-C1
11	2	1206	CLA	CBA-CGA-O2A-C1
11	a	1111	CLA	CBA-CGA-O2A-C1
16	2	5002	LMG	C29-C28-O8-C9
11	b	1203	CLA	CBA-CGA-O2A-C1
11	a	1137	CLA	CBA-CGA-O2A-C1
11	1	1128	CLA	CBA-CGA-O2A-C1
11	a	1103	CLA	C8-C10-C11-C12
11	2	1203	CLA	C10-C11-C12-C13
11	2	1214	CLA	CBD-CGD-O2D-CED
11	B	1226	CLA	O1D-CGD-O2D-CED
14	B	4004	BCR	C9-C10-C11-C12
11	1	1126	CLA	C8-C10-C11-C12
11	b	1217	CLA	O1A-CGA-O2A-C1
11	1	1136	CLA	O1A-CGA-O2A-C1
11	1	1132	CLA	C10-C11-C12-C13
11	A	1109	CLA	C5-C6-C7-C8
11	B	1021	CLA	C13-C15-C16-C17
11	A	1140	CLA	C8-C10-C11-C12
11	a	1132	CLA	C5-C6-C7-C8
11	1	1011	CLA	C5-C6-C7-C8
11	2	1223	CLA	C8-C10-C11-C12
11	1	1102	CLA	C13-C15-C16-C17
15	1	5003	LHG	O2-C2-C3-O3
15	B	5004	LHG	C23-C24-C25-C26
15	B	5004	LHG	O7-C5-C6-O8
11	B	1207	CLA	O1A-CGA-O2A-C1
11	B	1234	CLA	O1A-CGA-O2A-C1
11	a	1128	CLA	O1A-CGA-O2A-C1
11	A	1123	CLA	O1A-CGA-O2A-C1
11	B	1023	CLA	O1A-CGA-O2A-C1
11	2	1202	CLA	O1A-CGA-O2A-C1
16	2	5002	LMG	O10-C28-O8-C9
11	1	1137	CLA	C4-C3-C5-C6
11	2	1230	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	2	5002	LMG	C4-C5-C6-O5
11	B	1021	CLA	C2-C3-C5-C6
11	K	1401	CLA	C11-C12-C13-C14
11	1	1111	CLA	C6-C7-C8-C9
11	a	1022	CLA	C6-C7-C8-C9
11	B	1213	CLA	C6-C7-C8-C9
11	B	1213	CLA	C11-C10-C8-C9
11	b	1216	CLA	C11-C10-C8-C9
11	b	1234	CLA	C11-C10-C8-C9
11	1	1109	CLA	C11-C12-C13-C14
11	A	1126	CLA	C6-C7-C8-C9
11	A	1126	CLA	C11-C10-C8-C9
11	1	1103	CLA	C6-C7-C8-C9
11	B	1202	CLA	C6-C7-C8-C9
11	1	1022	CLA	C6-C7-C8-C9
11	1	1022	CLA	C14-C13-C15-C16
11	0	1401	CLA	C11-C12-C13-C14
11	a	1012	CLA	C11-C10-C8-C9
11	1	1106	CLA	C11-C10-C8-C9
11	A	1127	CLA	C11-C10-C8-C9
11	a	1140	CLA	C6-C7-C8-C9
11	b	1235	CLA	C6-C7-C8-C9
11	1	1137	CLA	C6-C7-C8-C9
11	1	1137	CLA	C11-C10-C8-C9
11	a	1102	CLA	C6-C7-C8-C9
11	a	1117	CLA	C6-C7-C8-C9
11	A	1011	CLA	C11-C10-C8-C9
11	l	1501	CLA	C11-C12-C13-C14
11	k	1401	CLA	C11-C12-C13-C14
11	A	1022	CLA	C6-C7-C8-C9
11	2	1214	CLA	C11-C10-C8-C9
12	B	2002	PQN	C24-C23-C25-C26
11	B	1204	CLA	C11-C12-C13-C14
11	1	1127	CLA	C11-C10-C8-C9
11	1	1126	CLA	C11-C10-C8-C9
11	a	1128	CLA	C6-C7-C8-C9
11	1	1122	CLA	C11-C10-C8-C9
11	L	1501	CLA	C6-C7-C8-C9
11	b	1226	CLA	C6-C7-C8-C9
11	b	1226	CLA	C11-C12-C13-C14
11	A	1012	CLA	C11-C10-C8-C9
11	b	1023	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1132	CLA	C11-C10-C8-C9
11	2	1203	CLA	C6-C7-C8-C9
11	A	1137	CLA	C6-C7-C8-C9
11	A	1137	CLA	C11-C10-C8-C9
11	b	1214	CLA	C11-C10-C8-C9
11	A	1140	CLA	C6-C7-C8-C9
11	B	1023	CLA	C11-C12-C13-C14
11	2	1226	CLA	C6-C7-C8-C9
11	B	1226	CLA	C6-C7-C8-C9
11	2	1023	CLA	C6-C7-C8-C9
11	a	1132	CLA	C11-C10-C8-C9
11	1	1011	CLA	C11-C10-C8-C9
11	1	1012	CLA	C6-C7-C8-C9
11	1	1012	CLA	C11-C10-C8-C9
12	b	2002	PQN	C24-C23-C25-C26
12	2	2002	PQN	C24-C23-C25-C26
11	2	1210	CLA	C11-C12-C13-C14
11	a	1109	CLA	C11-C12-C13-C14
11	2	1216	CLA	C11-C10-C8-C9
11	1	1102	CLA	C6-C7-C8-C9
11	2	1013	CLA	C11-C10-C8-C9
11	2	1013	CLA	C11-C12-C13-C14
11	1	1120	CLA	O1D-CGD-O2D-CED
11	B	1209	CLA	O1D-CGD-O2D-CED
11	a	1132	CLA	O1D-CGD-O2D-CED
11	B	1204	CLA	C15-C16-C17-C18
11	1	1140	CLA	C8-C10-C11-C12
11	2	1023	CLA	C10-C11-C12-C13
11	A	1801	CLA	C2A-CAA-CBA-CGA
11	b	1238	CLA	C2A-CAA-CBA-CGA
11	B	1219	CLA	C2A-CAA-CBA-CGA
11	a	1109	CLA	C2A-CAA-CBA-CGA
14	b	4010	BCR	C7-C8-C9-C34
14	2	4014	BCR	C11-C12-C13-C35
14	b	4004	BCR	C7-C8-C9-C34
14	7	4021	BCR	C7-C8-C9-C34
14	a	4003	BCR	C7-C8-C9-C34
14	a	4003	BCR	C11-C12-C13-C35
14	a	4003	BCR	C37-C22-C23-C24
14	B	4011	BCR	C7-C8-C9-C34
14	B	4011	BCR	C37-C22-C23-C24
14	A	4001	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	4001	BCR	C37-C22-C23-C24
14	2	4011	BCR	C7-C8-C9-C34
14	2	4011	BCR	C37-C22-C23-C24
14	b	4014	BCR	C7-C8-C9-C34
14	b	4014	BCR	C36-C18-C19-C20
14	b	4014	BCR	C37-C22-C23-C24
14	f	4020	BCR	C11-C12-C13-C35
14	A	4003	BCR	C7-C8-C9-C34
14	A	4003	BCR	C37-C22-C23-C24
14	a	4001	BCR	C7-C8-C9-C34
14	L	4019	BCR	C11-C12-C13-C35
14	L	4019	BCR	C37-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C34
14	M	4021	BCR	C7-C8-C9-C34
14	6	4020	BCR	C11-C12-C13-C35
14	A	4002	BCR	C37-C22-C23-C24
14	B	4009	BCR	C7-C8-C9-C34
14	b	4005	BCR	C7-C8-C9-C34
14	6	4018	BCR	C7-C8-C9-C34
14	6	4018	BCR	C37-C22-C23-C24
14	f	4013	BCR	C37-C22-C23-C24
14	2	4006	BCR	C7-C8-C9-C34
14	2	4006	BCR	C37-C22-C23-C24
14	A	4008	BCR	C37-C22-C23-C24
14	1	4002	BCR	C37-C22-C23-C24
14	B	4006	BCR	C7-C8-C9-C34
14	B	4006	BCR	C37-C22-C23-C24
14	B	4017	BCR	C7-C8-C9-C34
14	l	4019	BCR	C7-C8-C9-C34
14	F	4013	BCR	C7-C8-C9-C34
14	1	4003	BCR	C11-C12-C13-C35
14	a	4002	BCR	C37-C22-C23-C24
14	b	4006	BCR	C7-C8-C9-C34
14	b	4006	BCR	C37-C22-C23-C24
14	1	4007	BCR	C37-C22-C23-C24
14	m	4021	BCR	C37-C22-C23-C24
14	F	4018	BCR	C7-C8-C9-C34
14	2	4017	BCR	C7-C8-C9-C34
14	B	4005	BCR	C7-C8-C9-C34
14	f	4018	BCR	C7-C8-C9-C34
14	1	4008	BCR	C7-C8-C9-C10
14	b	4010	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	4011	BCR	C21-C22-C23-C24
14	2	4014	BCR	C11-C12-C13-C14
14	b	4004	BCR	C7-C8-C9-C10
14	a	4003	BCR	C7-C8-C9-C10
14	a	4003	BCR	C11-C12-C13-C14
14	B	4011	BCR	C7-C8-C9-C10
14	B	4011	BCR	C21-C22-C23-C24
14	A	4001	BCR	C21-C22-C23-C24
14	2	4011	BCR	C7-C8-C9-C10
14	b	4014	BCR	C7-C8-C9-C10
14	b	4014	BCR	C11-C12-C13-C14
14	b	4014	BCR	C17-C18-C19-C20
14	b	4014	BCR	C21-C22-C23-C24
14	f	4020	BCR	C7-C8-C9-C10
14	f	4020	BCR	C21-C22-C23-C24
14	A	4003	BCR	C21-C22-C23-C24
14	a	4001	BCR	C7-C8-C9-C10
14	L	4019	BCR	C7-C8-C9-C10
14	L	4019	BCR	C21-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C10
14	M	4021	BCR	C7-C8-C9-C10
14	a	4007	BCR	C21-C22-C23-C24
14	6	4020	BCR	C11-C12-C13-C14
14	A	4002	BCR	C21-C22-C23-C24
14	B	4009	BCR	C7-C8-C9-C10
14	6	4018	BCR	C7-C8-C9-C10
14	f	4013	BCR	C7-C8-C9-C10
14	f	4013	BCR	C11-C12-C13-C14
14	2	4006	BCR	C21-C22-C23-C24
14	1	4002	BCR	C21-C22-C23-C24
14	1	4001	BCR	C21-C22-C23-C24
14	8	4019	BCR	C21-C22-C23-C24
14	B	4006	BCR	C7-C8-C9-C10
14	B	4006	BCR	C21-C22-C23-C24
14	l	4019	BCR	C7-C8-C9-C10
14	F	4013	BCR	C7-C8-C9-C10
14	F	4013	BCR	C11-C12-C13-C14
14	b	4006	BCR	C7-C8-C9-C10
14	b	4006	BCR	C21-C22-C23-C24
14	1	4007	BCR	C21-C22-C23-C24
14	m	4021	BCR	C21-C22-C23-C24
14	F	4018	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	4005	BCR	C7-C8-C9-C10
11	B	1220	CLA	C2C-C3C-CAC-CBC
11	A	1131	CLA	O1A-CGA-O2A-C1
11	2	1236	CLA	O1A-CGA-O2A-C1
11	1	1131	CLA	O1A-CGA-O2A-C1
11	b	1203	CLA	O1A-CGA-O2A-C1
11	B	1210	CLA	C8-C10-C11-C12
12	B	2002	PQN	C20-C21-C22-C23
11	A	1012	CLA	C15-C16-C17-C18
11	b	1021	CLA	C13-C15-C16-C17
11	b	1013	CLA	C13-C15-C16-C17
11	2	1206	CLA	C8-C10-C11-C12
11	1	1112	CLA	O1D-CGD-O2D-CED
11	B	1201	CLA	O1D-CGD-O2D-CED
11	a	1138	CLA	CBA-CGA-O2A-C1
16	b	5002	LMG	C4-C5-C6-O5
11	2	1215	CLA	O1D-CGD-O2D-CED
11	B	1203	CLA	C3-C5-C6-C7
11	A	1237	CLA	C3-C5-C6-C7
11	2	1238	CLA	CBA-CGA-O2A-C1
16	B	5002	LMG	C29-C28-O8-C9
11	1	1132	CLA	C15-C16-C17-C18
11	1	1103	CLA	C8-C10-C11-C12
11	B	1203	CLA	C10-C11-C12-C13
11	1	1123	CLA	C13-C15-C16-C17
11	1	1106	CLA	C8-C10-C11-C12
11	a	1107	CLA	C8-C10-C11-C12
12	1	2001	PQN	C20-C21-C22-C23
11	b	1214	CLA	C5-C6-C7-C8
11	B	1226	CLA	C15-C16-C17-C18
11	b	1203	CLA	C13-C15-C16-C17
15	A	5003	LHG	C7-C8-C9-C10
11	b	1229	CLA	CBD-CGD-O2D-CED
11	a	1122	CLA	C8-C10-C11-C12
11	A	1131	CLA	C10-C11-C12-C13
11	1	1106	CLA	C15-C16-C17-C18
12	A	2001	PQN	C15-C16-C17-C18
11	L	1503	CLA	C15-C16-C17-C18
11	b	1238	CLA	C10-C11-C12-C13
11	b	1238	CLA	C13-C15-C16-C17
11	b	1207	CLA	C15-C16-C17-C18
11	1	1118	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1214	CLA	C5-C6-C7-C8
11	A	1118	CLA	C10-C11-C12-C13
12	2	2002	PQN	C23-C25-C26-C27
11	1	1102	CLA	C15-C16-C17-C18
11	A	1102	CLA	C10-C11-C12-C13
11	b	1207	CLA	O1A-CGA-O2A-C1
11	a	1137	CLA	O1A-CGA-O2A-C1
15	a	5003	LHG	C23-C24-C25-C26
15	B	5004	LHG	C7-C8-C9-C10
15	A	5003	LHG	C23-C24-C25-C26
15	2	5004	LHG	C23-C24-C25-C26
15	1	5003	LHG	C7-C8-C9-C10
15	1	5003	LHG	C23-C24-C25-C26
15	b	5004	LHG	C23-C24-C25-C26
11	b	1204	CLA	CBD-CGD-O2D-CED
11	b	1216	CLA	C15-C16-C17-C18
11	1	1103	CLA	C15-C16-C17-C18
11	B	1203	CLA	C15-C16-C17-C18
12	A	2001	PQN	C23-C25-C26-C27
11	1	1127	CLA	C10-C11-C12-C13
11	B	1235	CLA	C5-C6-C7-C8
12	1	2001	PQN	C18-C20-C21-C22
11	B	1021	CLA	C5-C6-C7-C8
11	b	1207	CLA	C8-C10-C11-C12
11	A	1111	CLA	C5-C6-C7-C8
11	a	1111	CLA	C10-C11-C12-C13
11	2	1021	CLA	C5-C6-C7-C8
11	a	1131	CLA	C10-C11-C12-C13
11	a	1110	CLA	CBA-CGA-O2A-C1
11	b	1220	CLA	C4C-C3C-CAC-CBC
11	B	1213	CLA	O1D-CGD-O2D-CED
11	b	1230	CLA	O1D-CGD-O2D-CED
11	a	1135	CLA	O1D-CGD-O2D-CED
16	B	5002	LMG	O6-C5-C6-O5
11	a	1022	CLA	C2-C1-O2A-CGA
11	1	1103	CLA	C2-C1-O2A-CGA
11	1	1022	CLA	C2-C1-O2A-CGA
11	b	1235	CLA	C2-C1-O2A-CGA
11	1	1124	CLA	C2-C1-O2A-CGA
11	2	1214	CLA	C2-C1-O2A-CGA
11	1	1122	CLA	C2-C1-O2A-CGA
11	b	1023	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1104	CLA	C2-C1-O2A-CGA
11	A	1104	CLA	C2-C1-O2A-CGA
11	2	1230	CLA	C2-C1-O2A-CGA
11	b	1013	CLA	C2-C1-O2A-CGA
11	A	1139	CLA	C2-C1-O2A-CGA
11	2	1223	CLA	C2-C1-O2A-CGA
11	b	1203	CLA	C2-C1-O2A-CGA
11	A	1022	CLA	C15-C16-C17-C18
11	1	1131	CLA	C5-C6-C7-C8
11	1	1118	CLA	C10-C11-C12-C13
11	B	1013	CLA	C13-C15-C16-C17
11	1	1110	CLA	CBD-CGD-O2D-CED
11	B	1224	CLA	C2C-C3C-CAC-CBC
11	B	1240	CLA	C2A-CAA-CBA-CGA
11	A	1109	CLA	C8-C10-C11-C12
11	B	1229	CLA	C13-C15-C16-C17
11	a	1136	CLA	O1D-CGD-O2D-CED
11	1	1115	CLA	O1D-CGD-O2D-CED
11	b	1222	CLA	C6-C7-C8-C10
11	B	1203	CLA	C11-C10-C8-C7
11	b	1225	CLA	C11-C10-C8-C7
11	A	1117	CLA	C11-C10-C8-C7
11	a	1102	CLA	C6-C7-C8-C10
11	L	1503	CLA	C6-C7-C8-C10
11	2	1214	CLA	C11-C10-C8-C7
11	8	1503	CLA	C6-C7-C8-C10
11	A	1103	CLA	C11-C10-C8-C7
11	A	1103	CLA	C11-C12-C13-C15
11	A	1104	CLA	C12-C13-C15-C16
12	a	2001	PQN	C21-C22-C23-C25
11	b	1013	CLA	C6-C7-C8-C10
11	1	1131	CLA	C11-C12-C13-C15
11	1	1131	CLA	C12-C13-C15-C16
11	1	1119	CLA	C6-C7-C8-C10
11	B	1214	CLA	C11-C10-C8-C7
11	a	1127	CLA	C6-C7-C8-C10
11	l	1503	CLA	C6-C7-C8-C10
11	A	1107	CLA	C6-C7-C8-C10
11	B	1013	CLA	C6-C7-C8-C10
12	2	2002	PQN	C21-C22-C23-C25
11	a	1109	CLA	C6-C7-C8-C10
11	1	1102	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1013	CLA	C6-C7-C8-C10
11	b	1230	CLA	O1A-CGA-O2A-C1
11	A	1022	CLA	O1A-CGA-O2A-C1
11	B	1222	CLA	O1A-CGA-O2A-C1
11	2	1222	CLA	O1A-CGA-O2A-C1
11	1	1128	CLA	O1A-CGA-O2A-C1
14	b	4014	BCR	C9-C10-C11-C12
14	f	4020	BCR	C9-C10-C11-C12
14	B	4009	BCR	C15-C16-C17-C18
14	b	4017	BCR	C9-C10-C11-C12
14	A	4008	BCR	C9-C10-C11-C12
14	8	4019	BCR	C15-C16-C17-C18
11	A	1119	CLA	C2A-CAA-CBA-CGA
11	1	1124	CLA	C2A-CAA-CBA-CGA
11	a	1123	CLA	C2A-CAA-CBA-CGA
11	B	1238	CLA	C2A-CAA-CBA-CGA
11	B	1214	CLA	C2A-CAA-CBA-CGA
11	2	1021	CLA	C2A-CAA-CBA-CGA
11	a	1122	CLA	O1D-CGD-O2D-CED
11	A	1125	CLA	O1D-CGD-O2D-CED
11	2	1227	CLA	O1D-CGD-O2D-CED
11	b	1227	CLA	O1D-CGD-O2D-CED
11	A	1237	CLA	O1D-CGD-O2D-CED
11	A	1115	CLA	O1D-CGD-O2D-CED
11	2	1230	CLA	O1D-CGD-O2D-CED
11	2	1220	CLA	O1D-CGD-O2D-CED
11	B	1230	CLA	O1D-CGD-O2D-CED
11	b	1213	CLA	C10-C11-C12-C13
11	2	1204	CLA	C5-C6-C7-C8
11	B	1202	CLA	C8-C10-C11-C12
11	2	1229	CLA	C8-C10-C11-C12
11	1	1140	CLA	C10-C11-C12-C13
11	b	1229	CLA	C8-C10-C11-C12
12	a	2001	PQN	C15-C16-C17-C18
11	b	1203	CLA	C10-C11-C12-C13
11	b	1222	CLA	O1A-CGA-O2A-C1
11	b	1202	CLA	O1A-CGA-O2A-C1
11	2	1206	CLA	O1A-CGA-O2A-C1
11	1	1125	CLA	CBD-CGD-O2D-CED
16	b	5002	LMG	O6-C1-O1-C7
11	A	1119	CLA	C5-C6-C7-C8
11	b	1225	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	8	1503	CLA	C15-C16-C17-C18
11	a	1128	CLA	C10-C11-C12-C13
11	A	1123	CLA	C13-C15-C16-C17
11	2	1213	CLA	C13-C15-C16-C17
11	1	1101	CLA	C10-C11-C12-C13
11	B	1227	CLA	O1D-CGD-O2D-CED
14	b	4004	BCR	C10-C11-C12-C13
14	a	4007	BCR	C10-C11-C12-C13
14	B	4009	BCR	C10-C11-C12-C13
14	6	4013	BCR	C10-C11-C12-C13
15	B	5004	LHG	O2-C2-C3-O3
15	2	5004	LHG	O2-C2-C3-O3
15	b	5004	LHG	O2-C2-C3-O3
15	b	5004	LHG	O9-C7-O7-C5
11	A	1117	CLA	C3-C5-C6-C7
11	K	1401	CLA	C5-C6-C7-C8
11	B	1203	CLA	C13-C15-C16-C17
11	0	1401	CLA	C5-C6-C7-C8
11	a	1140	CLA	C15-C16-C17-C18
11	1	1137	CLA	C13-C15-C16-C17
11	2	1235	CLA	C8-C10-C11-C12
11	k	1401	CLA	C5-C6-C7-C8
11	A	1123	CLA	C10-C11-C12-C13
11	a	1104	CLA	C5-C6-C7-C8
11	A	1104	CLA	C8-C10-C11-C12
11	2	1203	CLA	C13-C15-C16-C17
11	1	1012	CLA	C5-C6-C7-C8
11	1	1104	CLA	C5-C6-C7-C8
11	2	1210	CLA	C8-C10-C11-C12
11	a	1137	CLA	C8-C10-C11-C12
11	b	1213	CLA	CBA-CGA-O2A-C1
11	8	1501	CLA	CBA-CGA-O2A-C1
11	B	1211	CLA	O1D-CGD-O2D-CED
11	B	1213	CLA	O1A-CGA-O2A-C1
11	B	1236	CLA	O1A-CGA-O2A-C1
15	b	5004	LHG	C7-C8-C9-C10
11	K	1401	CLA	C15-C16-C17-C18
11	b	1213	CLA	C13-C15-C16-C17
11	0	1401	CLA	C15-C16-C17-C18
11	2	1219	CLA	C5-C6-C7-C8
11	k	1401	CLA	C15-C16-C17-C18
11	a	1123	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1023	CLA	C13-C15-C16-C17
11	l	1503	CLA	C5-C6-C7-C8
11	1	1011	CLA	C10-C11-C12-C13
11	1	1012	CLA	C13-C15-C16-C17
11	a	1101	CLA	C10-C11-C12-C13
12	b	2002	PQN	C20-C21-C22-C23
11	2	1205	CLA	C5-C6-C7-C8
11	a	1131	CLA	C5-C6-C7-C8
11	a	1137	CLA	C5-C6-C7-C8
11	2	1216	CLA	C13-C15-C16-C17
11	1	1117	CLA	C5-C6-C7-C8
11	B	1229	CLA	C10-C11-C12-C13
11	2	1204	CLA	O1D-CGD-O2D-CED
11	a	1112	CLA	O1D-CGD-O2D-CED
11	B	1206	CLA	O1D-CGD-O2D-CED
16	B	5002	LMG	C4-C5-C6-O5
11	a	1012	CLA	CBD-CGD-O2D-CED
11	b	1226	CLA	CBD-CGD-O2D-CED
11	B	1221	CLA	CBD-CGD-O2D-CED
11	A	1011	CLA	O1A-CGA-O2A-C1
11	a	1011	CLA	O1A-CGA-O2A-C1
11	B	1238	CLA	O1A-CGA-O2A-C1
16	B	5002	LMG	O10-C28-O8-C9
11	b	1223	CLA	C4C-C3C-CAC-CBC
11	A	1119	CLA	C10-C11-C12-C13
11	a	1012	CLA	C8-C10-C11-C12
11	1	1106	CLA	C5-C6-C7-C8
11	a	1106	CLA	C5-C6-C7-C8
11	A	1106	CLA	C5-C6-C7-C8
11	b	1023	CLA	C13-C15-C16-C17
11	a	1104	CLA	C8-C10-C11-C12
11	A	1104	CLA	C5-C6-C7-C8
11	2	1203	CLA	C15-C16-C17-C18
11	b	1214	CLA	C8-C10-C11-C12
11	1	1119	CLA	C13-C15-C16-C17
11	l	1503	CLA	C8-C10-C11-C12
11	A	1107	CLA	C8-C10-C11-C12
11	a	1101	CLA	C8-C10-C11-C12
11	a	1137	CLA	C15-C16-C17-C18
15	1	5001	LHG	C4-O6-P-O3
15	A	5003	LHG	C4-O6-P-O3
15	2	5004	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	2	5004	LHG	C4-O6-P-O3
15	a	5001	LHG	C4-O6-P-O3
11	8	1501	CLA	C3-C5-C6-C7
11	b	1216	CLA	CBA-CGA-O2A-C1
11	1	1118	CLA	CBA-CGA-O2A-C1
11	A	1139	CLA	CBA-CGA-O2A-C1
11	b	1236	CLA	CBA-CGA-O2A-C1
11	1	1105	CLA	CBA-CGA-O2A-C1
11	2	1207	CLA	CBA-CGA-O2A-C1
11	1	1118	CLA	O1D-CGD-O2D-CED
11	A	1111	CLA	CBD-CGD-O2D-CED
11	1	1109	CLA	C15-C16-C17-C18
11	a	1012	CLA	C5-C6-C7-C8
11	a	1117	CLA	C5-C6-C7-C8
11	a	1128	CLA	C5-C6-C7-C8
11	A	1123	CLA	C8-C10-C11-C12
11	1	1104	CLA	C8-C10-C11-C12
11	B	1203	CLA	O1D-CGD-O2D-CED
11	B	1220	CLA	O1D-CGD-O2D-CED
15	a	5003	LHG	C1-C2-C3-O3
15	A	5003	LHG	C1-C2-C3-O3
15	2	5004	LHG	C1-C2-C3-O3
15	b	5004	LHG	C1-C2-C3-O3
11	a	1122	CLA	C4-C3-C5-C6
11	2	1226	CLA	C4-C3-C5-C6
11	b	1235	CLA	C10-C11-C12-C13
12	a	2001	PQN	C25-C26-C27-C28
11	b	1021	CLA	C5-C6-C7-C8
11	2	1215	CLA	C8-C10-C11-C12
11	A	1140	CLA	C5-C6-C7-C8
11	a	1110	CLA	O1A-CGA-O2A-C1
11	K	1401	CLA	C2A-CAA-CBA-CGA
11	A	1126	CLA	C2A-CAA-CBA-CGA
11	A	1109	CLA	C2A-CAA-CBA-CGA
11	0	1401	CLA	C2A-CAA-CBA-CGA
11	b	1201	CLA	C2A-CAA-CBA-CGA
11	k	1401	CLA	C2A-CAA-CBA-CGA
11	A	1140	CLA	C2A-CAA-CBA-CGA
11	a	1101	CLA	C2A-CAA-CBA-CGA
11	A	1125	CLA	CBA-CGA-O2A-C1
11	a	1103	CLA	CBA-CGA-O2A-C1
11	A	1119	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1127	CLA	CBA-CGA-O2A-C1
11	A	1108	CLA	C2A-CAA-CBA-CGA
11	2	1226	CLA	C5-C6-C7-C8
11	b	1227	CLA	C4C-C3C-CAC-CBC
14	b	4011	BCR	C19-C20-C21-C22
15	a	5003	LHG	C13-C14-C15-C16
16	b	5002	LMG	C34-C35-C36-C37
11	b	1236	CLA	O1D-CGD-O2D-CED
15	B	5004	LHG	C8-C7-O7-C5
11	a	1140	CLA	C10-C11-C12-C13
11	A	1132	CLA	C5-C6-C7-C8
14	a	4003	BCR	C11-C10-C9-C34
14	A	4001	BCR	C11-C10-C9-C34
14	a	4007	BCR	C11-C10-C9-C34
14	A	4007	BCR	C11-C10-C9-C34
14	B	4005	BCR	C11-C10-C9-C34
11	B	1205	CLA	C3-C5-C6-C7
15	B	5004	LHG	C13-C14-C15-C16
16	b	5002	LMG	C38-C39-C40-C41
15	A	5001	LHG	C28-C29-C30-C31
16	2	5002	LMG	C36-C37-C38-C39
11	2	1235	CLA	O1D-CGD-O2D-CED
11	B	1213	CLA	C16-C17-C18-C19
11	B	1206	CLA	C16-C17-C18-C20
11	l	1501	CLA	C16-C17-C18-C19
11	b	1238	CLA	C16-C17-C18-C19
11	b	1023	CLA	C16-C17-C18-C19
11	a	1126	CLA	C16-C17-C18-C19
11	B	1021	CLA	C16-C17-C18-C20
11	b	1021	CLA	C16-C17-C18-C20
11	B	1226	CLA	C16-C17-C18-C20
11	2	1206	CLA	C16-C17-C18-C20
11	A	1128	CLA	CBA-CGA-O2A-C1
15	A	5003	LHG	C29-C30-C31-C32
16	2	5002	LMG	C13-C14-C15-C16
11	A	1133	CLA	O1D-CGD-O2D-CED
11	b	1215	CLA	O1D-CGD-O2D-CED
11	2	1207	CLA	O1D-CGD-O2D-CED
15	B	5004	LHG	O9-C7-O7-C5
11	l	1501	CLA	C5-C6-C7-C8
12	a	2001	PQN	C18-C20-C21-C22
11	1	1011	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1119	CLA	C4C-C3C-CAC-CBC
15	2	5004	LHG	C11-C10-C9-C8
15	1	5003	LHG	C29-C30-C31-C32
16	B	5002	LMG	C14-C15-C16-C17
16	B	5002	LMG	C35-C36-C37-C38
15	b	5004	LHG	C15-C16-C17-C18
15	1	5001	LHG	C28-C29-C30-C31
11	2	1201	CLA	C2C-C3C-CAC-CBC
15	a	5001	LHG	C18-C19-C20-C21
11	1	1110	CLA	C5-C6-C7-C8
11	B	1205	CLA	O1D-CGD-O2D-CED
16	b	5002	LMG	C2-C1-O1-C7
14	A	4001	BCR	C11-C10-C9-C8
14	a	4007	BCR	C11-C10-C9-C8
14	A	4007	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C8
11	2	1229	CLA	CBA-CGA-O2A-C1
11	b	1238	CLA	CBA-CGA-O2A-C1
11	2	1201	CLA	C5-C6-C7-C8
15	b	5004	LHG	C31-C32-C33-C34
11	l	1502	CLA	O1A-CGA-O2A-C1
11	8	1503	CLA	C8-C10-C11-C12
11	b	1204	CLA	C15-C16-C17-C18
11	1	1101	CLA	C8-C10-C11-C12
11	a	1123	CLA	C8-C10-C11-C12
11	B	1023	CLA	C10-C11-C12-C13
11	1	1128	CLA	C5-C6-C7-C8
11	A	1125	CLA	O1A-CGA-O2A-C1
11	A	1139	CLA	O1A-CGA-O2A-C1
11	b	1236	CLA	O1A-CGA-O2A-C1
11	1	1106	CLA	C16-C17-C18-C19
12	A	2001	PQN	C26-C27-C28-C29
11	A	1117	CLA	C16-C17-C18-C20
11	1	1137	CLA	C16-C17-C18-C20
11	a	1117	CLA	C16-C17-C18-C20
11	b	1224	CLA	C6-C7-C8-C10
11	b	1204	CLA	C16-C17-C18-C19
11	B	1021	CLA	C16-C17-C18-C19
11	1	1101	CLA	C16-C17-C18-C19
11	1	1011	CLA	C16-C17-C18-C19
11	b	1206	CLA	C16-C17-C18-C20
11	A	1102	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1207	CLA	C16-C17-C18-C20
11	a	1801	CLA	C4-C3-C5-C6
15	a	5001	LHG	C11-C12-C13-C14
11	a	1801	CLA	C2-C3-C5-C6
11	B	1216	CLA	C6-C7-C8-C9
11	A	1128	CLA	C14-C13-C15-C16
11	L	1503	CLA	C6-C7-C8-C9
11	a	1117	CLA	C11-C12-C13-C14
12	a	2001	PQN	C24-C23-C25-C26
11	1	1012	CLA	C14-C13-C15-C16
11	B	1225	CLA	C11-C10-C8-C9
12	b	2002	PQN	C16-C17-C18-C19
11	a	1109	CLA	C6-C7-C8-C9
11	2	1207	CLA	C11-C10-C8-C9
11	1	1129	CLA	O1D-CGD-O2D-CED
11	A	1135	CLA	O1D-CGD-O2D-CED
15	B	5004	LHG	C16-C17-C18-C19
15	B	5004	LHG	C34-C35-C36-C37
16	b	5002	LMG	C11-C12-C13-C14
16	b	5002	LMG	C13-C14-C15-C16
16	b	5002	LMG	C36-C37-C38-C39
15	A	5001	LHG	C11-C12-C13-C14
15	a	5001	LHG	C29-C30-C31-C32
16	B	5002	LMG	C29-C30-C31-C32
16	B	5002	LMG	C37-C38-C39-C40
11	B	1238	CLA	C5-C6-C7-C8
11	2	1239	CLA	CBA-CGA-O2A-C1
11	2	1238	CLA	C2A-CAA-CBA-CGA
11	B	1229	CLA	C2A-CAA-CBA-CGA
11	b	1213	CLA	O1A-CGA-O2A-C1
11	a	1103	CLA	O1A-CGA-O2A-C1
11	2	1238	CLA	O1A-CGA-O2A-C1
11	1	1118	CLA	O1A-CGA-O2A-C1
14	b	4011	BCR	C37-C22-C23-C24
14	2	4014	BCR	C7-C8-C9-C34
14	A	4003	BCR	C11-C12-C13-C35
14	a	4001	BCR	C37-C22-C23-C24
14	L	4019	BCR	C7-C8-C9-C34
14	a	4007	BCR	C37-C22-C23-C24
14	f	4013	BCR	C7-C8-C9-C34
14	f	4013	BCR	C11-C12-C13-C35
14	1	4001	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	4006	BCR	C11-C12-C13-C35
14	l	4019	BCR	C37-C22-C23-C24
14	F	4013	BCR	C37-C22-C23-C24
14	2	4010	BCR	C37-C22-C23-C24
14	1	4003	BCR	C7-C8-C9-C34
14	1	4003	BCR	C37-C22-C23-C24
14	m	4021	BCR	C7-C8-C9-C34
14	6	4013	BCR	C7-C8-C9-C34
14	6	4013	BCR	C11-C12-C13-C35
14	B	4014	BCR	C7-C8-C9-C34
14	B	4014	BCR	C11-C12-C13-C35
14	B	4014	BCR	C37-C22-C23-C24
11	a	1116	CLA	C5-C6-C7-C8
15	B	5004	LHG	O1-C1-C2-C3
14	2	4014	BCR	C7-C8-C9-C10
14	7	4021	BCR	C7-C8-C9-C10
14	A	4001	BCR	C7-C8-C9-C10
14	A	4003	BCR	C7-C8-C9-C10
14	A	4003	BCR	C11-C12-C13-C14
14	a	4001	BCR	C21-C22-C23-C24
14	2	4009	BCR	C11-C12-C13-C14
14	b	4005	BCR	C7-C8-C9-C10
14	2	4006	BCR	C7-C8-C9-C10
14	l	4019	BCR	C21-C22-C23-C24
14	F	4013	BCR	C21-C22-C23-C24
14	2	4010	BCR	C21-C22-C23-C24
14	1	4003	BCR	C7-C8-C9-C10
14	1	4003	BCR	C21-C22-C23-C24
14	m	4021	BCR	C7-C8-C9-C10
14	6	4013	BCR	C7-C8-C9-C10
14	6	4013	BCR	C11-C12-C13-C14
14	B	4014	BCR	C7-C8-C9-C10
14	B	4014	BCR	C11-C12-C13-C14
14	B	4014	BCR	C21-C22-C23-C24
14	f	4018	BCR	C7-C8-C9-C10
11	b	1202	CLA	C3-C5-C6-C7
11	1	1022	CLA	C15-C16-C17-C18
12	B	2002	PQN	C15-C16-C17-C18
11	B	1204	CLA	C8-C10-C11-C12
11	a	1128	CLA	C13-C15-C16-C17
11	2	1023	CLA	C13-C15-C16-C17
11	A	1118	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	5004	LHG	C9-C10-C11-C12
11	a	1237	CLA	O1D-CGD-O2D-CED
15	1	5001	LHG	C18-C19-C20-C21
11	b	1239	CLA	C2C-C3C-CAC-CBC
16	b	5002	LMG	C40-C41-C42-C43
15	A	5003	LHG	C24-C25-C26-C27
15	2	5004	LHG	C15-C16-C17-C18
11	2	1224	CLA	C6-C7-C8-C10
11	B	1206	CLA	C16-C17-C18-C19
11	l	1501	CLA	C16-C17-C18-C20
11	a	1126	CLA	C16-C17-C18-C20
11	A	1137	CLA	C16-C17-C18-C19
11	A	1137	CLA	C16-C17-C18-C20
11	b	1021	CLA	C16-C17-C18-C19
11	2	1206	CLA	C16-C17-C18-C19
11	8	1501	CLA	C5-C6-C7-C8
11	A	1127	CLA	C15-C16-C17-C18
11	b	1235	CLA	C5-C6-C7-C8
11	2	1229	CLA	C10-C11-C12-C13
11	b	1226	CLA	C13-C15-C16-C17
11	1	1107	CLA	C8-C10-C11-C12
15	2	5004	LHG	C11-C12-C13-C14
11	A	1122	CLA	C10-C11-C12-C13
11	8	1502	CLA	CBA-CGA-O2A-C1
11	2	1211	CLA	CBD-CGD-O2D-CED
15	1	5001	LHG	C11-C12-C13-C14
11	1	1116	CLA	C5-C6-C7-C8
15	1	5003	LHG	C30-C31-C32-C33
11	b	1210	CLA	C4C-C3C-CAC-CBC
11	8	1501	CLA	C8-C10-C11-C12
11	L	1503	CLA	C8-C10-C11-C12
11	a	1011	CLA	C8-C10-C11-C12
11	8	1501	CLA	O1A-CGA-O2A-C1
11	b	1216	CLA	O1A-CGA-O2A-C1
11	1	1127	CLA	O1A-CGA-O2A-C1
11	2	1207	CLA	O1A-CGA-O2A-C1
11	2	1214	CLA	C10-C11-C12-C13
11	A	1115	CLA	C4C-C3C-CAC-CBC
11	1	1106	CLA	O1D-CGD-O2D-CED
11	b	1201	CLA	CBA-CGA-O2A-C1
16	2	5002	LMG	C14-C15-C16-C17
15	b	5004	LHG	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1139	CLA	C3A-C2A-CAA-CBA
11	B	1210	CLA	C3A-C2A-CAA-CBA
11	1	1237	CLA	C3A-C2A-CAA-CBA
11	A	1237	CLA	C3A-C2A-CAA-CBA
11	a	1139	CLA	C3A-C2A-CAA-CBA
11	2	1234	CLA	C3A-C2A-CAA-CBA
11	a	1104	CLA	C3A-C2A-CAA-CBA
11	A	1104	CLA	C3A-C2A-CAA-CBA
11	1	1101	CLA	C3A-C2A-CAA-CBA
11	a	1123	CLA	C3A-C2A-CAA-CBA
11	1	1131	CLA	C3A-C2A-CAA-CBA
11	B	1240	CLA	C3A-C2A-CAA-CBA
11	A	1135	CLA	C3A-C2A-CAA-CBA
11	1	1104	CLA	C3A-C2A-CAA-CBA
11	a	1101	CLA	C3A-C2A-CAA-CBA
11	2	1210	CLA	C3A-C2A-CAA-CBA
11	a	1131	CLA	C3A-C2A-CAA-CBA
11	1	1107	CLA	C3A-C2A-CAA-CBA
11	a	1102	CLA	C10-C11-C12-C13
11	b	1023	CLA	C10-C11-C12-C13
11	b	1013	CLA	C8-C10-C11-C12
14	l	4019	BCR	C15-C16-C17-C18
16	b	5002	LMG	C21-C22-C23-C24
11	B	1235	CLA	O1D-CGD-O2D-CED
11	b	1023	CLA	C16-C17-C18-C20
11	b	1207	CLA	C16-C17-C18-C19
11	b	1207	CLA	C16-C17-C18-C20
11	B	1226	CLA	C16-C17-C18-C19
11	2	1207	CLA	C16-C17-C18-C19
16	b	5002	LMG	C17-C18-C19-C20
11	a	1105	CLA	O2A-C1-C2-C3
11	A	1124	CLA	O1D-CGD-O2D-CED
15	1	5001	LHG	C26-C27-C28-C29
11	2	1223	CLA	C3-C5-C6-C7
11	1	1103	CLA	C4-C3-C5-C6
11	b	1225	CLA	CBA-CGA-O2A-C1
11	1	1103	CLA	C2-C3-C5-C6
11	a	1115	CLA	C2A-CAA-CBA-CGA
11	A	1115	CLA	C2A-CAA-CBA-CGA
15	A	5003	LHG	O1-C1-C2-O2
15	A	5001	LHG	O1-C1-C2-O2
11	a	1110	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1203	CLA	O1D-CGD-O2D-CED
11	A	1119	CLA	O1A-CGA-O2A-C1
11	b	1201	CLA	O1A-CGA-O2A-C1
11	1	1105	CLA	O1A-CGA-O2A-C1
11	A	1126	CLA	C16-C17-C18-C19
11	b	1204	CLA	C16-C17-C18-C20
16	B	5002	LMG	C13-C14-C15-C16
11	B	1216	CLA	C13-C15-C16-C17
11	2	1217	CLA	C2C-C3C-CAC-CBC
11	b	1229	CLA	C3-C5-C6-C7
11	A	1124	CLA	C3-C5-C6-C7
15	a	5003	LHG	C28-C29-C30-C31
15	B	5004	LHG	C28-C29-C30-C31
11	A	1101	CLA	C5-C6-C7-C8
11	1	1109	CLA	C8-C10-C11-C12
11	a	1138	CLA	O1A-CGA-O2A-C1
16	2	5002	LMG	C21-C22-C23-C24
11	K	1401	CLA	C2-C1-O2A-CGA
11	B	1203	CLA	C2-C1-O2A-CGA
11	A	1131	CLA	C2-C1-O2A-CGA
11	0	1401	CLA	C2-C1-O2A-CGA
11	2	1221	CLA	C2-C1-O2A-CGA
11	B	1223	CLA	C2-C1-O2A-CGA
11	A	1117	CLA	C2-C1-O2A-CGA
11	a	1117	CLA	C2-C1-O2A-CGA
11	2	1235	CLA	C2-C1-O2A-CGA
11	k	1401	CLA	C2-C1-O2A-CGA
11	1	1126	CLA	C2-C1-O2A-CGA
11	a	1126	CLA	C2-C1-O2A-CGA
11	B	1221	CLA	C2-C1-O2A-CGA
11	b	1021	CLA	C2-C1-O2A-CGA
11	2	1215	CLA	C2-C1-O2A-CGA
11	2	1023	CLA	C2-C1-O2A-CGA
11	1	1104	CLA	C2-C1-O2A-CGA
11	B	1013	CLA	C2-C1-O2A-CGA
11	1	1107	CLA	C2-C1-O2A-CGA
11	1	1117	CLA	C2-C1-O2A-CGA
11	B	1229	CLA	C2-C1-O2A-CGA
15	1	5003	LHG	C18-C19-C20-C21
16	B	5002	LMG	C21-C22-C23-C24
11	a	1022	CLA	C15-C16-C17-C18
11	1	1012	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1210	CLA	C8-C10-C11-C12
11	2	1229	CLA	O1A-CGA-O2A-C1
16	b	5002	LMG	C14-C15-C16-C17
16	2	5002	LMG	C32-C33-C34-C35
11	1	1106	CLA	C16-C17-C18-C20
11	b	1238	CLA	C16-C17-C18-C20
11	1	1101	CLA	C16-C17-C18-C20
11	B	1210	CLA	C3-C5-C6-C7
14	2	4014	BCR	C23-C24-C25-C26
14	2	4014	BCR	C23-C24-C25-C30
14	l	4022	BCR	C23-C24-C25-C26
14	l	4022	BCR	C23-C24-C25-C30
14	7	4021	BCR	C1-C6-C7-C8
14	7	4021	BCR	C5-C6-C7-C8
14	7	4021	BCR	C23-C24-C25-C26
14	7	4021	BCR	C23-C24-C25-C30
14	B	4010	BCR	C23-C24-C25-C30
14	a	4003	BCR	C1-C6-C7-C8
14	a	4003	BCR	C5-C6-C7-C8
14	A	4001	BCR	C1-C6-C7-C8
14	A	4001	BCR	C5-C6-C7-C8
14	2	4011	BCR	C23-C24-C25-C30
14	f	4020	BCR	C23-C24-C25-C26
14	b	4009	BCR	C23-C24-C25-C26
14	A	4003	BCR	C1-C6-C7-C8
14	A	4003	BCR	C5-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C30
14	M	4021	BCR	C1-C6-C7-C8
14	6	4020	BCR	C23-C24-C25-C26
14	6	4020	BCR	C23-C24-C25-C30
14	B	4009	BCR	C1-C6-C7-C8
14	B	4009	BCR	C23-C24-C25-C26
14	B	4009	BCR	C23-C24-C25-C30
14	b	4005	BCR	C1-C6-C7-C8
14	6	4018	BCR	C23-C24-C25-C30
14	f	4013	BCR	C1-C6-C7-C8
14	2	4006	BCR	C1-C6-C7-C8
14	2	4006	BCR	C5-C6-C7-C8
14	A	4007	BCR	C23-C24-C25-C26
14	A	4007	BCR	C23-C24-C25-C30
14	1	4001	BCR	C1-C6-C7-C8
14	1	4001	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	8	4019	BCR	C1-C6-C7-C8
14	8	4019	BCR	C5-C6-C7-C8
14	B	4006	BCR	C1-C6-C7-C8
14	B	4006	BCR	C5-C6-C7-C8
14	2	4004	BCR	C23-C24-C25-C26
14	2	4004	BCR	C23-C24-C25-C30
14	1	4007	BCR	C23-C24-C25-C30
14	m	4021	BCR	C1-C6-C7-C8
14	m	4021	BCR	C5-C6-C7-C8
14	6	4013	BCR	C1-C6-C7-C8
14	6	4013	BCR	C5-C6-C7-C8
15	A	5003	LHG	C32-C33-C34-C35
15	a	5001	LHG	C14-C15-C16-C17
11	1	1105	CLA	O1D-CGD-O2D-CED
11	2	1219	CLA	CBA-CGA-O2A-C1
11	2	1225	CLA	CBA-CGA-O2A-C1
11	a	1140	CLA	C13-C15-C16-C17
11	b	1203	CLA	C8-C10-C11-C12
11	a	1109	CLA	C15-C16-C17-C18
15	1	5001	LHG	C12-C13-C14-C15
15	a	5001	LHG	C31-C32-C33-C34
16	B	5002	LMG	C39-C40-C41-C42
11	B	1223	CLA	C15-C16-C17-C18
11	a	1127	CLA	C15-C16-C17-C18
11	A	1137	CLA	C4-C3-C5-C6
11	B	1210	CLA	C11-C10-C8-C7
11	8	1501	CLA	C12-C13-C15-C16
11	B	1216	CLA	C6-C7-C8-C10
11	B	1215	CLA	C6-C7-C8-C10
11	1	1109	CLA	C6-C7-C8-C10
11	1	1103	CLA	C11-C10-C8-C7
11	1	1022	CLA	C11-C10-C8-C7
11	A	1117	CLA	C6-C7-C8-C10
11	a	1106	CLA	C6-C7-C8-C10
11	a	1106	CLA	C11-C10-C8-C7
11	a	1117	CLA	C11-C12-C13-C15
11	a	1118	CLA	C11-C10-C8-C7
11	a	1128	CLA	C11-C10-C8-C7
11	L	1501	CLA	C12-C13-C15-C16
11	A	1123	CLA	C11-C10-C8-C7
11	b	1226	CLA	C11-C12-C13-C15
11	2	1234	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1103	CLA	C2-C3-C5-C6
11	a	1011	CLA	C6-C7-C8-C10
11	b	1229	CLA	C11-C10-C8-C7
11	b	1023	CLA	C11-C12-C13-C15
11	a	1104	CLA	C6-C7-C8-C10
11	a	1104	CLA	C11-C10-C8-C7
11	B	1222	CLA	C6-C7-C8-C10
11	A	1104	CLA	C11-C10-C8-C7
12	1	2001	PQN	C21-C22-C23-C25
11	2	1203	CLA	C11-C10-C8-C7
11	b	1021	CLA	C6-C7-C8-C10
11	a	1123	CLA	C11-C10-C8-C7
11	2	1226	CLA	C2-C3-C5-C6
11	1	1012	CLA	C12-C13-C15-C16
11	a	1101	CLA	C12-C13-C15-C16
11	2	1021	CLA	C11-C10-C8-C7
12	b	2002	PQN	C16-C17-C18-C20
11	2	1210	CLA	C6-C7-C8-C10
11	2	1210	CLA	C11-C12-C13-C15
11	1	1107	CLA	C2-C3-C5-C6
11	1	1107	CLA	C6-C7-C8-C10
11	1	1107	CLA	C11-C10-C8-C7
11	b	1206	CLA	C12-C13-C15-C16
11	1	1117	CLA	C11-C10-C8-C7
11	2	1207	CLA	C11-C10-C8-C7
11	B	1229	CLA	C11-C10-C8-C7
11	b	1210	CLA	C11-C10-C8-C7
11	a	1103	CLA	C3-C5-C6-C7
11	1	1109	CLA	C3-C5-C6-C7
11	A	1116	CLA	C3-C5-C6-C7
11	2	1222	CLA	C3-C5-C6-C7
11	A	1128	CLA	O1A-CGA-O2A-C1
11	b	1238	CLA	O1A-CGA-O2A-C1
11	A	1011	CLA	C10-C11-C12-C13
11	A	1137	CLA	C5-C6-C7-C8
14	a	4008	BCR	C9-C10-C11-C12
14	A	4001	BCR	C9-C10-C11-C12
14	F	4013	BCR	C9-C10-C11-C12
14	8	4022	BCR	C9-C10-C11-C12
11	B	1207	CLA	C16-C17-C18-C19
11	1	1137	CLA	C16-C17-C18-C19
11	b	1206	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	2	5002	LMG	O9-C10-O7-C8
11	B	1210	CLA	CBA-CGA-O2A-C1
11	1	1135	CLA	CBA-CGA-O2A-C1
11	2	1234	CLA	CBA-CGA-O2A-C1
11	2	1221	CLA	C5-C6-C7-C8
16	B	5002	LMG	C11-C12-C13-C14
16	B	5002	LMG	C41-C42-C43-C44
11	A	1134	CLA	C2A-CAA-CBA-CGA
11	2	1226	CLA	O1D-CGD-O2D-CED
11	B	1210	CLA	C15-C16-C17-C18
11	a	1022	CLA	C13-C15-C16-C17
11	A	1022	CLA	C10-C11-C12-C13
11	A	1104	CLA	C13-C15-C16-C17
11	B	1225	CLA	C13-C15-C16-C17
11	A	1102	CLA	C13-C15-C16-C17
11	1	1128	CLA	C15-C16-C17-C18
15	1	5001	LHG	C25-C26-C27-C28
15	A	5003	LHG	C18-C19-C20-C21
15	a	5003	LHG	C31-C32-C33-C34
11	A	1124	CLA	C2C-C3C-CAC-CBC
15	b	5004	LHG	C16-C17-C18-C19
11	A	1131	CLA	C5-C6-C7-C8
11	b	1202	CLA	C15-C16-C17-C18
15	1	5003	LHG	C33-C34-C35-C36
11	1	1122	CLA	C2C-C3C-CAC-CBC
11	1	1127	CLA	C3-C5-C6-C7
11	b	1203	CLA	C3-C5-C6-C7
11	a	1133	CLA	O1D-CGD-O2D-CED
15	1	5001	LHG	C16-C17-C18-C19
15	B	5004	LHG	C11-C12-C13-C14
11	b	1225	CLA	O1A-CGA-O2A-C1
11	A	1119	CLA	C16-C17-C18-C20
11	B	1224	CLA	C6-C7-C8-C10
11	B	1204	CLA	C5-C6-C7-C8
16	b	5002	LMG	C11-C10-O7-C8
15	a	5001	LHG	C8-C7-O7-C5
16	2	5002	LMG	C11-C10-O7-C8
15	a	5001	LHG	C28-C29-C30-C31
11	2	1204	CLA	C8-C10-C11-C12
11	B	1238	CLA	C8-C10-C11-C12
15	1	5003	LHG	C14-C15-C16-C17
15	2	5004	LHG	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1106	CLA	C13-C15-C16-C17
11	b	1205	CLA	C5-C6-C7-C8
15	1	5001	LHG	O7-C5-C6-O8
15	1	5003	LHG	O7-C5-C6-O8
16	B	5002	LMG	O7-C8-C9-O8
15	2	5004	LHG	C16-C17-C18-C19
11	a	1117	CLA	C16-C17-C18-C19
11	1	1011	CLA	C16-C17-C18-C20
11	1	1117	CLA	C16-C17-C18-C20
11	A	1102	CLA	C16-C17-C18-C20
15	b	5004	LHG	C28-C29-C30-C31
11	A	1128	CLA	C10-C11-C12-C13
11	1	1122	CLA	C4-C3-C5-C6
11	A	1103	CLA	C4-C3-C5-C6
11	1	1133	CLA	CBA-CGA-O2A-C1
11	a	1122	CLA	C2-C3-C5-C6
11	1	1801	CLA	C2-C3-C5-C6
11	1	1137	CLA	C2-C3-C5-C6
11	8	1501	CLA	C14-C13-C15-C16
11	B	1215	CLA	C6-C7-C8-C9
11	1	1109	CLA	C6-C7-C8-C9
11	1	1103	CLA	C11-C10-C8-C9
11	A	1109	CLA	C6-C7-C8-C9
11	B	1203	CLA	C11-C10-C8-C9
11	1	1022	CLA	C11-C10-C8-C9
11	A	1117	CLA	C11-C10-C8-C9
11	a	1118	CLA	C11-C10-C8-C9
11	8	1503	CLA	C6-C7-C8-C9
11	L	1501	CLA	C14-C13-C15-C16
11	A	1103	CLA	C11-C10-C8-C9
11	A	1103	CLA	C11-C12-C13-C14
11	a	1011	CLA	C6-C7-C8-C9
11	b	1229	CLA	C6-C7-C8-C9
11	a	1126	CLA	C11-C12-C13-C14
11	A	1104	CLA	C14-C13-C15-C16
12	1	2001	PQN	C21-C22-C23-C24
11	2	1203	CLA	C11-C10-C8-C9
11	1	1131	CLA	C6-C7-C8-C9
11	1	1131	CLA	C14-C13-C15-C16
11	1	1119	CLA	C14-C13-C15-C16
11	a	1101	CLA	C14-C13-C15-C16
11	B	1013	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1216	CLA	C6-C7-C8-C9
16	2	5002	LMG	C18-C19-C20-C21
11	1	1111	CLA	C2A-CAA-CBA-CGA
11	1	1106	CLA	C2A-CAA-CBA-CGA
11	1	1118	CLA	C2A-CAA-CBA-CGA
11	a	1127	CLA	C2A-CAA-CBA-CGA
16	b	5002	LMG	C31-C32-C33-C34
15	2	5004	LHG	C13-C14-C15-C16
11	1	1113	CLA	C2A-CAA-CBA-CGA
14	b	4010	BCR	C37-C22-C23-C24
14	A	4002	BCR	C36-C18-C19-C20
11	B	1210	CLA	C13-C15-C16-C17
11	a	1140	CLA	C8-C10-C11-C12
11	a	1109	CLA	C5-C6-C7-C8
11	b	1234	CLA	C2C-C3C-CAC-CBC
16	2	5002	LMG	C39-C40-C41-C42
14	b	4010	BCR	C21-C22-C23-C24
14	b	4005	BCR	C21-C22-C23-C24
14	2	4005	BCR	C21-C22-C23-C24
14	L	4022	BCR	C11-C12-C13-C14
14	a	4002	BCR	C11-C12-C13-C14
11	2	1219	CLA	O1A-CGA-O2A-C1
11	2	1218	CLA	C1A-C2A-CAA-CBA
11	A	1101	CLA	C1A-C2A-CAA-CBA
11	K	1401	CLA	C1A-C2A-CAA-CBA
11	1	1139	CLA	C1A-C2A-CAA-CBA
11	2	1208	CLA	C1A-C2A-CAA-CBA
11	a	1114	CLA	C1A-C2A-CAA-CBA
11	b	1213	CLA	C1A-C2A-CAA-CBA
11	A	1120	CLA	C1A-C2A-CAA-CBA
11	B	1213	CLA	C1A-C2A-CAA-CBA
11	b	1216	CLA	C1A-C2A-CAA-CBA
11	1	1132	CLA	C1A-C2A-CAA-CBA
11	A	1109	CLA	C1A-C2A-CAA-CBA
11	B	1202	CLA	C1A-C2A-CAA-CBA
11	k	1402	CLA	C1A-C2A-CAA-CBA
11	A	1119	CLA	C1A-C2A-CAA-CBA
11	0	1401	CLA	C1A-C2A-CAA-CBA
11	b	1225	CLA	C1A-C2A-CAA-CBA
11	A	1114	CLA	C1A-C2A-CAA-CBA
11	1	1114	CLA	C1A-C2A-CAA-CBA
11	a	1116	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1117	CLA	C1A-C2A-CAA-CBA
11	a	1119	CLA	C1A-C2A-CAA-CBA
11	B	1231	CLA	C1A-C2A-CAA-CBA
11	a	1120	CLA	C1A-C2A-CAA-CBA
11	0	1402	CLA	C1A-C2A-CAA-CBA
11	a	1106	CLA	C1A-C2A-CAA-CBA
11	2	1236	CLA	C1A-C2A-CAA-CBA
11	1	1116	CLA	C1A-C2A-CAA-CBA
11	a	1117	CLA	C1A-C2A-CAA-CBA
11	A	1116	CLA	C1A-C2A-CAA-CBA
11	k	1401	CLA	C1A-C2A-CAA-CBA
11	A	1106	CLA	C1A-C2A-CAA-CBA
11	a	1139	CLA	C1A-C2A-CAA-CBA
11	B	1217	CLA	C1A-C2A-CAA-CBA
11	a	1134	CLA	C1A-C2A-CAA-CBA
11	a	1128	CLA	C1A-C2A-CAA-CBA
11	a	1110	CLA	C1A-C2A-CAA-CBA
11	B	1212	CLA	C1A-C2A-CAA-CBA
11	2	1213	CLA	C1A-C2A-CAA-CBA
11	A	1130	CLA	C1A-C2A-CAA-CBA
11	A	1103	CLA	C1A-C2A-CAA-CBA
11	b	1229	CLA	C1A-C2A-CAA-CBA
11	b	1232	CLA	C1A-C2A-CAA-CBA
11	B	1236	CLA	C1A-C2A-CAA-CBA
11	A	1104	CLA	C1A-C2A-CAA-CBA
11	A	1137	CLA	C1A-C2A-CAA-CBA
11	1	1101	CLA	C1A-C2A-CAA-CBA
11	2	1215	CLA	C1A-C2A-CAA-CBA
11	1	1121	CLA	C1A-C2A-CAA-CBA
11	a	1123	CLA	C1A-C2A-CAA-CBA
11	1	1131	CLA	C1A-C2A-CAA-CBA
11	1	1119	CLA	C1A-C2A-CAA-CBA
11	2	1211	CLA	C1A-C2A-CAA-CBA
11	1	1110	CLA	C1A-C2A-CAA-CBA
11	2	1202	CLA	C1A-C2A-CAA-CBA
11	A	1135	CLA	C1A-C2A-CAA-CBA
11	A	1121	CLA	C1A-C2A-CAA-CBA
11	2	1021	CLA	C1A-C2A-CAA-CBA
11	B	1211	CLA	C1A-C2A-CAA-CBA
11	a	1131	CLA	C1A-C2A-CAA-CBA
11	a	1109	CLA	C1A-C2A-CAA-CBA
11	b	1236	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1117	CLA	C1A-C2A-CAA-CBA
11	A	1110	CLA	C1A-C2A-CAA-CBA
11	1	1128	CLA	C1A-C2A-CAA-CBA
11	A	1126	CLA	C16-C17-C18-C20
11	A	1119	CLA	C16-C17-C18-C19
12	A	2001	PQN	C26-C27-C28-C30
11	A	1117	CLA	C16-C17-C18-C19
11	2	1229	CLA	C16-C17-C18-C19
11	B	1205	CLA	C6-C7-C8-C10
16	b	5002	LMG	O9-C10-O7-C8
15	a	5001	LHG	O9-C7-O7-C5
14	b	4009	BCR	C9-C10-C11-C12
14	l	4019	BCR	C9-C10-C11-C12
11	A	1119	CLA	C8-C10-C11-C12
11	a	1126	CLA	C8-C10-C11-C12
11	1	1107	CLA	C15-C16-C17-C18
11	b	1210	CLA	C15-C16-C17-C18
15	a	5003	LHG	C26-C27-C28-C29
15	A	5001	LHG	C24-C25-C26-C27
11	B	1213	CLA	C3-C5-C6-C7
11	b	1201	CLA	C3-C5-C6-C7
11	a	1119	CLA	C13-C15-C16-C17
11	a	1117	CLA	C8-C10-C11-C12
11	B	1229	CLA	C8-C10-C11-C12
11	a	1126	CLA	CBA-CGA-O2A-C1
15	a	5001	LHG	O6-C4-C5-C6
11	2	1239	CLA	C2C-C3C-CAC-CBC
11	b	1223	CLA	C5-C6-C7-C8
11	1	1125	CLA	C3-C5-C6-C7
15	A	5003	LHG	C10-C11-C12-C13
11	B	1220	CLA	C4C-C3C-CAC-CBC
11	A	1114	CLA	C2C-C3C-CAC-CBC
15	1	5001	LHG	C7-C8-C9-C10
11	1	1801	CLA	C4-C3-C5-C6
16	B	5002	LMG	C19-C20-C21-C22
11	b	1223	CLA	C15-C16-C17-C18
11	a	1131	CLA	C15-C16-C17-C18
11	B	1210	CLA	O1A-CGA-O2A-C1
11	2	1234	CLA	O1A-CGA-O2A-C1
11	2	1225	CLA	O1A-CGA-O2A-C1
15	2	5004	LHG	C31-C32-C33-C34
11	1	1129	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1106	CLA	C2A-CAA-CBA-CGA
11	B	1213	CLA	C16-C17-C18-C20
11	a	1119	CLA	C16-C17-C18-C20
11	A	1011	CLA	C16-C17-C18-C19
11	A	1111	CLA	C3-C5-C6-C7
15	B	5004	LHG	C4-C5-C6-O8
16	b	5002	LMG	O1-C7-C8-C9
15	A	5001	LHG	C4-C5-C6-O8
16	2	5002	LMG	O1-C7-C8-C9
15	b	5004	LHG	C4-C5-C6-O8
15	b	5004	LHG	C19-C20-C21-C22
11	A	1123	CLA	C5-C6-C7-C8
11	2	1214	CLA	O1D-CGD-O2D-CED
11	b	1229	CLA	O1D-CGD-O2D-CED
15	2	5004	LHG	O8-C23-C24-C25
11	1	1138	CLA	CBA-CGA-O2A-C1
11	a	1012	CLA	C10-C11-C12-C13
11	2	1216	CLA	C5-C6-C7-C8
16	2	5002	LMG	C24-C25-C26-C27
15	1	5003	LHG	O1-C1-C2-O2
11	1	1122	CLA	C11-C12-C13-C14
11	a	1106	CLA	C13-C15-C16-C17
11	2	1201	CLA	C4C-C3C-CAC-CBC
15	2	5004	LHG	C35-C36-C37-C38
15	a	5003	LHG	C35-C36-C37-C38
11	1	1114	CLA	C2C-C3C-CAC-CBC
11	2	1227	CLA	C2C-C3C-CAC-CBC
16	2	5002	LMG	C16-C17-C18-C19
11	b	1231	CLA	O1D-CGD-O2D-CED
11	b	1216	CLA	C13-C15-C16-C17
11	1	1140	CLA	C5-C6-C7-C8
11	a	1137	CLA	C13-C15-C16-C17
11	2	1013	CLA	C13-C15-C16-C17
11	2	1204	CLA	C4-C3-C5-C6
15	A	5003	LHG	C26-C27-C28-C29
15	a	5003	LHG	C7-C8-C9-C10
11	b	1229	CLA	C16-C17-C18-C19
15	b	5004	LHG	C11-C12-C13-C14
11	B	1202	CLA	CBD-CGD-O2D-CED
11	1	1123	CLA	C8-C10-C11-C12
11	A	1012	CLA	C8-C10-C11-C12
11	A	1140	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1207	CLA	C10-C11-C12-C13
11	A	1116	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	C42-C43-C44-C45
11	b	1204	CLA	O1D-CGD-O2D-CED
11	B	1214	CLA	O1D-CGD-O2D-CED
11	A	1101	CLA	C13-C15-C16-C17
11	A	1117	CLA	C5-C6-C7-C8
11	1	1137	CLA	C8-C10-C11-C12
11	a	1139	CLA	C2-C1-O2A-CGA
11	A	1801	CLA	C2-C1-O2A-CGA
11	B	1235	CLA	C2-C1-O2A-CGA
11	b	1221	CLA	C2-C1-O2A-CGA
11	2	1013	CLA	C2-C1-O2A-CGA
11	2	1213	CLA	CBD-CGD-O2D-CED
11	A	1012	CLA	C3-C5-C6-C7
11	B	1013	CLA	C3-C5-C6-C7
15	2	5004	LHG	C28-C29-C30-C31
16	B	5002	LMG	C31-C32-C33-C34
16	2	5002	LMG	C23-C24-C25-C26
11	B	1204	CLA	CBA-CGA-O2A-C1
11	B	1225	CLA	CBA-CGA-O2A-C1
11	1	1135	CLA	O1A-CGA-O2A-C1
11	2	1211	CLA	O1D-CGD-O2D-CED
11	1	1117	CLA	C16-C17-C18-C19
11	a	1012	CLA	O1D-CGD-O2D-CED
11	b	1222	CLA	C5-C6-C7-C8
11	8	1501	CLA	C15-C16-C17-C18
11	a	1109	CLA	C13-C15-C16-C17
14	a	4003	BCR	C11-C10-C9-C8
11	A	1140	CLA	C2C-C3C-CAC-CBC
15	b	5004	LHG	O7-C5-C6-O8
15	a	5003	LHG	C15-C16-C17-C18
11	a	1125	CLA	C2C-C3C-CAC-CBC
11	1	1127	CLA	C4-C3-C5-C6
11	a	1123	CLA	C4-C3-C5-C6
12	2	2002	PQN	C15-C16-C17-C18
11	a	1122	CLA	C11-C10-C8-C7
11	A	1101	CLA	C6-C7-C8-C10
11	K	1401	CLA	C6-C7-C8-C10
11	K	1401	CLA	C11-C10-C8-C7
11	b	1234	CLA	C11-C10-C8-C7
11	B	1207	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1103	CLA	C11-C12-C13-C15
11	A	1109	CLA	C6-C7-C8-C10
11	B	1202	CLA	C6-C7-C8-C10
11	A	1131	CLA	C11-C10-C8-C7
11	1	1022	CLA	C6-C7-C8-C10
11	1	1123	CLA	C11-C10-C8-C7
11	0	1401	CLA	C6-C7-C8-C10
11	0	1401	CLA	C11-C10-C8-C7
11	1	1106	CLA	C6-C7-C8-C10
11	A	1127	CLA	C11-C12-C13-C15
12	A	2001	PQN	C21-C22-C23-C25
12	A	2001	PQN	C22-C23-C25-C26
11	a	1119	CLA	C11-C10-C8-C7
11	1	1137	CLA	C6-C7-C8-C10
11	a	1117	CLA	C11-C10-C8-C7
11	k	1401	CLA	C6-C7-C8-C10
11	k	1401	CLA	C11-C10-C8-C7
11	1	1126	CLA	C11-C12-C13-C15
11	1	1140	CLA	C12-C13-C15-C16
11	b	1215	CLA	C11-C10-C8-C7
11	b	1226	CLA	C11-C10-C8-C7
11	2	1213	CLA	C6-C7-C8-C10
11	b	1223	CLA	C12-C13-C15-C16
11	b	1023	CLA	C11-C10-C8-C7
11	A	1132	CLA	C11-C10-C8-C7
11	a	1126	CLA	C11-C12-C13-C15
11	B	1021	CLA	C12-C13-C15-C16
11	1	1101	CLA	C6-C7-C8-C10
11	b	1021	CLA	C12-C13-C15-C16
11	2	1215	CLA	C11-C10-C8-C7
11	2	1225	CLA	C11-C12-C13-C15
11	B	1023	CLA	C11-C10-C8-C7
11	B	1023	CLA	C11-C12-C13-C15
11	B	1238	CLA	C11-C12-C13-C15
11	A	1111	CLA	C11-C10-C8-C7
11	1	1131	CLA	C11-C10-C8-C7
11	1	1119	CLA	C12-C13-C15-C16
11	a	1127	CLA	C11-C10-C8-C7
11	l	1503	CLA	C12-C13-C15-C16
11	A	1118	CLA	C11-C10-C8-C7
11	A	1118	CLA	C11-C12-C13-C15
11	1	1011	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1206	CLA	C12-C13-C15-C16
11	2	1223	CLA	C6-C7-C8-C10
11	2	1210	CLA	C11-C10-C8-C7
11	a	1137	CLA	C11-C10-C8-C7
11	A	1102	CLA	C6-C7-C8-C10
11	b	1210	CLA	C6-C7-C8-C10
11	2	1222	CLA	C6-C7-C8-C10
11	B	1215	CLA	CAA-CBA-CGA-O2A
11	B	1239	CLA	CAA-CBA-CGA-O2A
11	A	1101	CLA	C14-C13-C15-C16
11	b	1216	CLA	C6-C7-C8-C9
11	B	1207	CLA	C6-C7-C8-C9
11	1	1123	CLA	C6-C7-C8-C9
11	1	1106	CLA	C11-C12-C13-C14
11	A	1127	CLA	C11-C12-C13-C14
11	B	1223	CLA	C6-C7-C8-C9
11	b	1235	CLA	C11-C10-C8-C9
11	B	1206	CLA	C11-C10-C8-C9
11	a	1106	CLA	C11-C10-C8-C9
11	2	1229	CLA	C6-C7-C8-C9
11	2	1229	CLA	C11-C12-C13-C14
11	2	1235	CLA	C11-C10-C8-C9
11	1	1126	CLA	C11-C12-C13-C14
11	1	1140	CLA	C11-C10-C8-C9
11	A	1123	CLA	C6-C7-C8-C9
11	B	1021	CLA	C11-C10-C8-C9
11	B	1021	CLA	C14-C13-C15-C16
11	A	1122	CLA	C6-C7-C8-C9
12	a	2001	PQN	C21-C22-C23-C24
11	b	1021	CLA	C11-C10-C8-C9
11	b	1021	CLA	C14-C13-C15-C16
11	2	1215	CLA	C6-C7-C8-C9
11	b	1214	CLA	C6-C7-C8-C9
11	A	1140	CLA	C14-C13-C15-C16
11	B	1238	CLA	C11-C12-C13-C14
11	1	1119	CLA	C11-C12-C13-C14
11	B	1214	CLA	C6-C7-C8-C9
11	a	1127	CLA	C6-C7-C8-C9
11	l	1503	CLA	C6-C7-C8-C9
11	A	1118	CLA	C11-C10-C8-C9
11	A	1118	CLA	C11-C12-C13-C14
11	2	1206	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1107	CLA	C6-C7-C8-C9
11	a	1111	CLA	C11-C10-C8-C9
11	b	1203	CLA	C11-C10-C8-C9
11	a	1131	CLA	C6-C7-C8-C9
11	1	1107	CLA	C11-C10-C8-C9
11	a	1109	CLA	C11-C10-C8-C9
11	b	1206	CLA	C14-C13-C15-C16
11	B	1229	CLA	C6-C7-C8-C9
11	B	1229	CLA	C11-C12-C13-C14
11	a	1139	CLA	CBA-CGA-O2A-C1
11	a	1114	CLA	CBA-CGA-O2A-C1
11	a	1124	CLA	C2A-CAA-CBA-CGA
11	1	1237	CLA	C2A-CAA-CBA-CGA
11	A	1124	CLA	C2A-CAA-CBA-CGA
11	1	1012	CLA	C2A-CAA-CBA-CGA
11	a	1111	CLA	C2A-CAA-CBA-CGA
11	1	1110	CLA	O1D-CGD-O2D-CED
11	B	1204	CLA	O1A-CGA-O2A-C1
11	B	1225	CLA	O1A-CGA-O2A-C1
14	b	4004	BCR	C37-C22-C23-C24
14	B	4010	BCR	C37-C22-C23-C24
14	B	4004	BCR	C37-C22-C23-C24
11	B	1207	CLA	C16-C17-C18-C20
11	2	1229	CLA	C16-C17-C18-C20
11	B	1221	CLA	C5-C6-C7-C8
11	b	1226	CLA	O1D-CGD-O2D-CED
14	b	4004	BCR	C21-C22-C23-C24
14	B	4010	BCR	C21-C22-C23-C24
14	B	4004	BCR	C21-C22-C23-C24
14	A	4002	BCR	C7-C8-C9-C10
14	B	4017	BCR	C7-C8-C9-C10
14	2	4017	BCR	C7-C8-C9-C10
11	B	1215	CLA	C3-C5-C6-C7
11	1	1110	CLA	C3-C5-C6-C7
11	B	1206	CLA	C8-C10-C11-C12
11	a	1118	CLA	C8-C10-C11-C12
11	1	1012	CLA	C15-C16-C17-C18
12	b	2002	PQN	C15-C16-C17-C18
11	B	1224	CLA	C4C-C3C-CAC-CBC
11	B	1217	CLA	CBA-CGA-O2A-C1
11	1	1126	CLA	CBA-CGA-O2A-C1
16	B	5002	LMG	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1239	CLA	C4C-C3C-CAC-CBC
11	B	1214	CLA	C10-C11-C12-C13
11	2	1229	CLA	CAA-CBA-CGA-O2A
11	8	1502	CLA	O1A-CGA-O2A-C1
11	b	1205	CLA	C6-C7-C8-C9
11	2	1238	CLA	C10-C11-C12-C13
12	2	2002	PQN	C18-C20-C21-C22
15	A	5001	LHG	O6-C4-C5-C6
15	2	5004	LHG	O6-C4-C5-C6
11	1	1131	CLA	C3-C5-C6-C7
15	b	5004	LHG	C9-C10-C11-C12
15	b	5004	LHG	C13-C14-C15-C16
15	2	5004	LHG	C26-C27-C28-C29
14	2	4005	BCR	C10-C11-C12-C13
11	1	1111	CLA	C10-C11-C12-C13
11	a	1102	CLA	C15-C16-C17-C18
11	a	1106	CLA	C8-C10-C11-C12
11	A	1102	CLA	C15-C16-C17-C18
11	B	1221	CLA	O1D-CGD-O2D-CED
11	a	1022	CLA	C4-C3-C5-C6
11	B	1207	CLA	C4-C3-C5-C6
11	a	1103	CLA	C4-C3-C5-C6
11	A	1022	CLA	C4-C3-C5-C6
11	2	1207	CLA	C4-C3-C5-C6
11	2	1204	CLA	C2-C3-C5-C6
11	a	1103	CLA	C2-C3-C5-C6
11	1	1127	CLA	C2-C3-C5-C6
11	a	1123	CLA	C2-C3-C5-C6
12	B	2002	PQN	C18-C20-C21-C22
11	1	1125	CLA	O1D-CGD-O2D-CED
11	a	1119	CLA	C16-C17-C18-C19
11	A	1128	CLA	C13-C15-C16-C17
11	b	1202	CLA	C8-C10-C11-C12
15	A	5003	LHG	C24-C23-O8-C6
11	A	1106	CLA	CBA-CGA-O2A-C1
11	A	1137	CLA	CBA-CGA-O2A-C1
11	2	1210	CLA	CBA-CGA-O2A-C1
15	a	5003	LHG	C2-C3-O3-P
15	A	5003	LHG	C2-C3-O3-P
11	a	1126	CLA	O1A-CGA-O2A-C1
11	b	1225	CLA	C3A-C2A-CAA-CBA
11	a	1106	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1801	CLA	C3A-C2A-CAA-CBA
11	L	1501	CLA	C3A-C2A-CAA-CBA
11	B	1021	CLA	C3A-C2A-CAA-CBA
11	1	1118	CLA	C3A-C2A-CAA-CBA
11	B	1214	CLA	C3A-C2A-CAA-CBA
11	B	1219	CLA	C3A-C2A-CAA-CBA
14	b	4010	BCR	C9-C10-C11-C12
14	B	4010	BCR	C9-C10-C11-C12
14	6	4020	BCR	C19-C20-C21-C22
14	1	4003	BCR	C19-C20-C21-C22
14	a	4002	BCR	C19-C20-C21-C22
14	b	4006	BCR	C19-C20-C21-C22
11	1	1110	CLA	C6-C7-C8-C9
11	1	1128	CLA	C8-C10-C11-C12
11	A	1011	CLA	C16-C17-C18-C20
11	B	1013	CLA	C16-C17-C18-C20
16	b	5002	LMG	C29-C30-C31-C32
11	1	1111	CLA	C5-C6-C7-C8
11	2	1204	CLA	C10-C11-C12-C13
11	b	1207	CLA	C13-C15-C16-C17
11	2	1206	CLA	C13-C15-C16-C17
11	a	1111	CLA	C5-C6-C7-C8
15	1	5001	LHG	C4-C5-C6-O8
15	1	5003	LHG	C4-C5-C6-O8
15	a	5001	LHG	C4-C5-C6-O8
16	B	5002	LMG	C7-C8-C9-O8
11	b	1201	CLA	C5-C6-C7-C8
11	A	1011	CLA	O2A-C1-C2-C3
11	b	1023	CLA	O2A-C1-C2-C3
11	B	1013	CLA	O2A-C1-C2-C3
15	1	5001	LHG	C10-C11-C12-C13
11	1	1122	CLA	C4C-C3C-CAC-CBC
11	B	1214	CLA	C8-C10-C11-C12
11	1	1131	CLA	C16-C17-C18-C20
11	A	1022	CLA	C2-C3-C5-C6
15	A	5001	LHG	C19-C20-C21-C22
11	a	1106	CLA	C3-C5-C6-C7
11	b	1217	CLA	C2A-CAA-CBA-CGA
11	B	1201	CLA	C2A-CAA-CBA-CGA
11	2	1216	CLA	C2A-CAA-CBA-CGA
11	a	1109	CLA	C8-C10-C11-C12
15	2	5004	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1132	CLA	CBA-CGA-O2A-C1
11	A	1112	CLA	C2C-C3C-CAC-CBC
11	a	1139	CLA	O1A-CGA-O2A-C1
11	A	1237	CLA	C6-C7-C8-C9
11	2	1238	CLA	C5-C6-C7-C8
11	L	1503	CLA	C5-C6-C7-C8
11	2	1238	CLA	C8-C10-C11-C12
11	1	1101	CLA	C5-C6-C7-C8
11	B	1217	CLA	O1A-CGA-O2A-C1
11	2	1239	CLA	O1A-CGA-O2A-C1
16	b	5002	LMG	O1-C7-C8-O7
16	2	5002	LMG	O1-C7-C8-O7
11	B	1216	CLA	CBA-CGA-O2A-C1
11	B	1021	CLA	CAA-CBA-CGA-O2A
15	A	5001	LHG	C11-C10-C9-C8
15	b	5004	LHG	C26-C27-C28-C29
14	l	4019	BCR	C19-C20-C21-C22
11	B	1205	CLA	C6-C7-C8-C9
11	B	1234	CLA	C2-C1-O2A-CGA
11	a	1110	CLA	C2-C1-O2A-CGA
11	A	1111	CLA	O1D-CGD-O2D-CED
11	a	1022	CLA	C2-C3-C5-C6
15	a	5003	LHG	C18-C19-C20-C21
11	1	1103	CLA	C11-C12-C13-C14
11	a	1140	CLA	C11-C10-C8-C9
11	2	1235	CLA	C6-C7-C8-C9
11	2	1238	CLA	C11-C12-C13-C14
12	B	2002	PQN	C21-C22-C23-C24
11	1	1127	CLA	C11-C12-C13-C14
11	1	1122	CLA	C6-C7-C8-C9
11	b	1215	CLA	C6-C7-C8-C9
11	2	1234	CLA	C11-C10-C8-C9
11	A	1103	CLA	C6-C7-C8-C9
11	b	1238	CLA	C11-C10-C8-C9
11	B	1021	CLA	C6-C7-C8-C9
11	1	1101	CLA	C11-C10-C8-C9
11	b	1021	CLA	C11-C12-C13-C14
11	a	1123	CLA	C6-C7-C8-C9
11	b	1202	CLA	C14-C13-C15-C16
11	2	1226	CLA	C11-C10-C8-C9
11	1	1118	CLA	C6-C7-C8-C9
11	1	1011	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1101	CLA	C11-C10-C8-C9
11	a	1111	CLA	C6-C7-C8-C9
11	2	1021	CLA	C6-C7-C8-C9
11	2	1223	CLA	C11-C10-C8-C9
12	b	2002	PQN	C21-C22-C23-C24
11	a	1137	CLA	C6-C7-C8-C9
11	A	1102	CLA	C11-C10-C8-C9
15	a	5003	LHG	C16-C17-C18-C19
16	b	5002	LMG	C32-C33-C34-C35
11	2	1213	CLA	O1D-CGD-O2D-CED
11	A	1127	CLA	C13-C15-C16-C17
11	A	1128	CLA	C5-C6-C7-C8
11	A	1103	CLA	C8-C10-C11-C12
11	b	1223	CLA	C10-C11-C12-C13
11	1	1012	CLA	C10-C11-C12-C13
11	1	1117	CLA	C8-C10-C11-C12
15	A	5001	LHG	C2-C3-O3-P
11	B	1224	CLA	C2A-CAA-CBA-CGA
11	b	1013	CLA	C2A-CAA-CBA-CGA
11	b	1229	CLA	C16-C17-C18-C20
14	F	4020	BCR	C23-C24-C25-C26
14	F	4020	BCR	C23-C24-C25-C30
14	A	4003	BCR	C23-C24-C25-C26
14	2	4009	BCR	C23-C24-C25-C26
14	A	4008	BCR	C5-C6-C7-C8
14	b	4006	BCR	C5-C6-C7-C8
14	m	4021	BCR	C23-C24-C25-C26
14	m	4021	BCR	C23-C24-C25-C30
14	6	4013	BCR	C23-C24-C25-C26
11	B	1206	CLA	C13-C15-C16-C17
11	2	1202	CLA	C15-C16-C17-C18
16	B	5002	LMG	C42-C43-C44-C45
11	L	1503	CLA	CAA-CBA-CGA-O2A
14	B	4011	BCR	C36-C18-C19-C20
14	f	4020	BCR	C11-C12-C13-C14
14	L	4019	BCR	C11-C12-C13-C14
14	A	4002	BCR	C17-C18-C19-C20
14	A	4008	BCR	C21-C22-C23-C24
11	b	1204	CLA	C10-C11-C12-C13
11	1	1131	CLA	C15-C16-C17-C18
11	B	1013	CLA	C10-C11-C12-C13
11	a	1111	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1224	CLA	C6-C7-C8-C9
11	1	1124	CLA	C6-C7-C8-C9
11	A	1104	CLA	C16-C17-C18-C20
11	A	1140	CLA	C3-C5-C6-C7
15	1	5003	LHG	O6-C4-C5-C6
11	B	1217	CLA	CAA-CBA-CGA-O2A
15	A	5001	LHG	C14-C15-C16-C17
11	A	1129	CLA	C2C-C3C-CAC-CBC
11	A	1101	CLA	C12-C13-C15-C16
11	B	1210	CLA	C6-C7-C8-C10
11	B	1215	CLA	C11-C10-C8-C7
11	B	1215	CLA	C12-C13-C15-C16
11	B	1207	CLA	C2-C3-C5-C6
11	A	1126	CLA	C12-C13-C15-C16
11	A	1119	CLA	C11-C10-C8-C7
11	A	1131	CLA	C6-C7-C8-C10
11	a	1012	CLA	C11-C10-C8-C7
11	1	1106	CLA	C11-C12-C13-C15
12	A	2001	PQN	C17-C18-C20-C21
11	a	1119	CLA	C12-C13-C15-C16
11	A	1128	CLA	C11-C10-C8-C7
11	B	1206	CLA	C11-C10-C8-C7
11	B	1206	CLA	C12-C13-C15-C16
11	B	1234	CLA	C6-C7-C8-C10
11	B	1234	CLA	C11-C10-C8-C7
11	2	1229	CLA	C11-C10-C8-C7
11	2	1229	CLA	C11-C12-C13-C15
11	1	1501	CLA	C11-C12-C13-C15
11	2	1235	CLA	C6-C7-C8-C10
11	A	1022	CLA	C6-C7-C8-C10
11	2	1238	CLA	C11-C12-C13-C15
11	1	1127	CLA	C11-C12-C13-C15
11	1	1126	CLA	C6-C7-C8-C10
11	L	1501	CLA	C6-C7-C8-C10
11	L	1501	CLA	C11-C10-C8-C7
11	2	1234	CLA	C11-C10-C8-C7
11	A	1012	CLA	C6-C7-C8-C10
11	b	1238	CLA	C11-C10-C8-C7
11	b	1204	CLA	C12-C13-C15-C16
11	b	1223	CLA	C11-C12-C13-C15
11	b	1229	CLA	C11-C12-C13-C15
11	A	1132	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1235	CLA	C11-C10-C8-C7
11	B	1021	CLA	C11-C12-C13-C15
11	b	1021	CLA	C11-C12-C13-C15
11	A	1140	CLA	C6-C7-C8-C10
11	A	1140	CLA	C12-C13-C15-C16
11	b	1202	CLA	C12-C13-C15-C16
11	1	1119	CLA	C11-C12-C13-C15
11	B	1226	CLA	C6-C7-C8-C10
11	1	1118	CLA	C6-C7-C8-C10
11	A	1118	CLA	C6-C7-C8-C10
11	a	1132	CLA	C12-C13-C15-C16
11	1	1104	CLA	C11-C10-C8-C7
11	a	1101	CLA	C6-C7-C8-C10
11	a	1111	CLA	C6-C7-C8-C10
12	b	2002	PQN	C22-C23-C25-C26
12	2	2002	PQN	C22-C23-C25-C26
11	a	1131	CLA	C11-C10-C8-C7
11	a	1109	CLA	C11-C12-C13-C15
11	1	1117	CLA	C6-C7-C8-C10
11	2	1207	CLA	C2-C3-C5-C6
11	B	1229	CLA	C11-C12-C13-C15
11	a	1117	CLA	C15-C16-C17-C18
14	2	4011	BCR	C19-C20-C21-C22
14	f	4020	BCR	C19-C20-C21-C22
14	A	4003	BCR	C9-C10-C11-C12
14	A	4002	BCR	C19-C20-C21-C22
14	2	4006	BCR	C19-C20-C21-C22
14	2	4004	BCR	C19-C20-C21-C22
14	2	4017	BCR	C9-C10-C11-C12
11	A	1012	CLA	CBA-CGA-O2A-C1
11	b	1229	CLA	CBA-CGA-O2A-C1
15	2	5004	LHG	C30-C31-C32-C33
11	2	1213	CLA	C10-C11-C12-C13
11	b	1202	CLA	C10-C11-C12-C13
11	A	1116	CLA	C6-C7-C8-C9
14	2	4005	BCR	C11-C10-C9-C34
14	8	4019	BCR	C20-C21-C22-C37
11	a	1022	CLA	C3-C5-C6-C7
11	b	1225	CLA	C3-C5-C6-C7
11	B	1226	CLA	C3-C5-C6-C7
11	b	1235	CLA	CBA-CGA-O2A-C1
11	B	1222	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1101	CLA	CAD-CBD-CGD-O2D
11	A	1125	CLA	CAD-CBD-CGD-O2D
11	b	1213	CLA	CAD-CBD-CGD-O2D
11	B	1210	CLA	CAD-CBD-CGD-O2D
11	8	1501	CLA	CAD-CBD-CGD-O2D
11	b	1234	CLA	CAD-CBD-CGD-O2D
11	8	1502	CLA	CAD-CBD-CGD-O2D
11	B	1223	CLA	CAD-CBD-CGD-O2D
11	a	1140	CLA	CAD-CBD-CGD-O2D
11	b	1219	CLA	CAD-CBD-CGD-O2D
11	1	1124	CLA	CAD-CBD-CGD-O2D
11	2	1219	CLA	CAD-CBD-CGD-O2D
11	2	1227	CLA	CAD-CBD-CGD-O2D
11	A	1011	CLA	CAD-CBD-CGD-O2D
11	a	1105	CLA	CAD-CBD-CGD-O2D
11	A	1801	CLA	CAD-CBD-CGD-O2D
11	B	1217	CLA	CAD-CBD-CGD-O2D
11	a	1128	CLA	CAD-CBD-CGD-O2D
11	1	1140	CLA	CAD-CBD-CGD-O2D
11	A	1123	CLA	CAD-CBD-CGD-O2D
11	2	1234	CLA	CAD-CBD-CGD-O2D
11	2	1211	CLA	CAD-CBD-CGD-O2D
11	B	1211	CLA	CAD-CBD-CGD-O2D
11	1	1117	CLA	CAD-CBD-CGD-O2D
11	B	1229	CLA	CAD-CBD-CGD-O2D
11	a	1138	CLA	CAD-CBD-CGD-O2D
15	a	5001	LHG	C16-C17-C18-C19
15	A	5001	LHG	C35-C36-C37-C38
11	b	1234	CLA	C4-C3-C5-C6
11	B	1013	CLA	C16-C17-C18-C19
15	B	5004	LHG	C30-C31-C32-C33
11	1	1109	CLA	C5-C6-C7-C8
15	1	5003	LHG	C10-C11-C12-C13
16	B	5002	LMG	O1-C7-C8-C9
11	1	1116	CLA	O1A-CGA-O2A-C1
11	A	1012	CLA	O1A-CGA-O2A-C1
15	1	5001	LHG	C8-C7-O7-C5
15	a	5001	LHG	C33-C34-C35-C36
15	A	5003	LHG	O6-C4-C5-O7
15	1	5003	LHG	O6-C4-C5-O7
11	A	1117	CLA	C8-C10-C11-C12
11	2	1223	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1210	CLA	C13-C15-C16-C17
11	1	1118	CLA	CAA-CBA-CGA-O2A
15	1	5003	LHG	C15-C16-C17-C18
11	b	1234	CLA	C8-C10-C11-C12
11	b	1238	CLA	C15-C16-C17-C18
15	B	5004	LHG	C31-C32-C33-C34
11	A	1114	CLA	C4C-C3C-CAC-CBC
15	1	5003	LHG	C1-C2-C3-O3
11	b	1222	CLA	CHA-CBD-CGD-O1D
11	b	1222	CLA	CHA-CBD-CGD-O2D
11	A	1120	CLA	CHA-CBD-CGD-O1D
11	A	1131	CLA	CHA-CBD-CGD-O2D
11	B	1231	CLA	CHA-CBD-CGD-O1D
11	B	1231	CLA	CHA-CBD-CGD-O2D
11	b	1230	CLA	CHA-CBD-CGD-O1D
11	b	1230	CLA	CHA-CBD-CGD-O2D
11	A	1129	CLA	CHA-CBD-CGD-O1D
11	A	1129	CLA	CHA-CBD-CGD-O2D
11	A	1123	CLA	CHA-CBD-CGD-O1D
11	b	1226	CLA	CHA-CBD-CGD-O1D
11	b	1226	CLA	CHA-CBD-CGD-O2D
11	B	1222	CLA	CHA-CBD-CGD-O1D
11	B	1222	CLA	CHA-CBD-CGD-O2D
11	A	1132	CLA	CHA-CBD-CGD-O1D
11	b	1231	CLA	CHA-CBD-CGD-O1D
11	b	1231	CLA	CHA-CBD-CGD-O2D
11	B	1235	CLA	CHA-CBD-CGD-O2D
11	2	1230	CLA	CHA-CBD-CGD-O1D
11	2	1230	CLA	CHA-CBD-CGD-O2D
11	B	1221	CLA	CHA-CBD-CGD-O1D
11	B	1221	CLA	CHA-CBD-CGD-O2D
11	b	1207	CLA	CHA-CBD-CGD-O1D
11	b	1205	CLA	CHA-CBD-CGD-O1D
11	A	1111	CLA	CHA-CBD-CGD-O1D
11	A	1111	CLA	CHA-CBD-CGD-O2D
11	a	1135	CLA	CHA-CBD-CGD-O1D
11	a	1135	CLA	CHA-CBD-CGD-O2D
11	a	1132	CLA	CHA-CBD-CGD-O1D
11	a	1132	CLA	CHA-CBD-CGD-O2D
11	2	1202	CLA	CHA-CBD-CGD-O1D
11	2	1202	CLA	CHA-CBD-CGD-O2D
11	1	1011	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1012	CLA	CHA-CBD-CGD-O1D
11	1	1012	CLA	CHA-CBD-CGD-O2D
11	2	1206	CLA	CHA-CBD-CGD-O2D
11	a	1101	CLA	CHA-CBD-CGD-O1D
11	a	1111	CLA	CHA-CBD-CGD-O1D
11	a	1111	CLA	CHA-CBD-CGD-O2D
11	a	1129	CLA	CHA-CBD-CGD-O2D
11	b	1210	CLA	CHA-CBD-CGD-O1D
11	2	1222	CLA	CHA-CBD-CGD-O1D
11	A	1110	CLA	CHA-CBD-CGD-O1D
11	A	1110	CLA	CHA-CBD-CGD-O2D
11	A	1106	CLA	O1A-CGA-O2A-C1
11	1	1126	CLA	O1A-CGA-O2A-C1
11	A	1137	CLA	O1A-CGA-O2A-C1
11	a	1132	CLA	O1A-CGA-O2A-C1
11	2	1210	CLA	O1A-CGA-O2A-C1
11	2	1239	CLA	C4C-C3C-CAC-CBC
11	B	1221	CLA	C6-C7-C8-C9
16	B	5002	LMG	O1-C7-C8-O7
16	2	5002	LMG	O7-C8-C9-O8
11	B	1229	CLA	C15-C16-C17-C18
15	A	5003	LHG	O10-C23-O8-C6
11	b	1229	CLA	O1A-CGA-O2A-C1
15	B	5004	LHG	C26-C27-C28-C29
11	B	1202	CLA	C13-C15-C16-C17
11	a	1109	CLA	C10-C11-C12-C13
11	2	1229	CLA	C4-C3-C5-C6
11	A	1801	CLA	C4-C3-C5-C6
11	B	1219	CLA	C4-C3-C5-C6
11	A	1801	CLA	C2-C3-C5-C6
11	B	1219	CLA	C2-C3-C5-C6
11	1	1116	CLA	CBA-CGA-O2A-C1
15	A	5001	LHG	C17-C18-C19-C20
15	1	5001	LHG	O9-C7-O7-C5
11	B	1013	CLA	C15-C16-C17-C18
11	B	1215	CLA	C14-C13-C15-C16
11	B	1207	CLA	C11-C12-C13-C14
11	1	1132	CLA	C14-C13-C15-C16
11	A	1126	CLA	C14-C13-C15-C16
11	A	1131	CLA	C6-C7-C8-C9
11	A	1127	CLA	C6-C7-C8-C9
11	B	1206	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1215	CLA	C14-C13-C15-C16
11	b	1229	CLA	C14-C13-C15-C16
11	A	1132	CLA	C14-C13-C15-C16
11	2	1215	CLA	C14-C13-C15-C16
11	b	1202	CLA	C11-C10-C8-C9
11	2	1023	CLA	C11-C10-C8-C9
11	a	1132	CLA	C14-C13-C15-C16
11	2	1021	CLA	C11-C12-C13-C14
11	1	1128	CLA	C11-C10-C8-C9
15	1	5001	LHG	C30-C31-C32-C33
15	b	5004	LHG	C34-C35-C36-C37
11	B	1216	CLA	O1A-CGA-O2A-C1
11	B	1202	CLA	O1D-CGD-O2D-CED
11	1	1131	CLA	C10-C11-C12-C13
11	A	1101	CLA	C16-C17-C18-C20
11	1	1131	CLA	C16-C17-C18-C19
11	b	1023	CLA	C2A-CAA-CBA-CGA
14	A	4007	BCR	C7-C8-C9-C34
12	2	2002	PQN	C20-C21-C22-C23
16	b	5002	LMG	C15-C16-C17-C18
14	B	4006	BCR	C11-C12-C13-C14
14	1	4003	BCR	C11-C12-C13-C14
11	B	1210	CLA	C1A-C2A-CAA-CBA
11	B	1216	CLA	C1A-C2A-CAA-CBA
11	A	1128	CLA	C1A-C2A-CAA-CBA
11	1	1130	CLA	C1A-C2A-CAA-CBA
11	b	1212	CLA	C1A-C2A-CAA-CBA
11	A	1801	CLA	C1A-C2A-CAA-CBA
11	1	1122	CLA	C1A-C2A-CAA-CBA
11	b	1231	CLA	C1A-C2A-CAA-CBA
11	1	1118	CLA	C1A-C2A-CAA-CBA
11	B	1214	CLA	C1A-C2A-CAA-CBA
11	A	1118	CLA	C1A-C2A-CAA-CBA
11	a	1132	CLA	C1A-C2A-CAA-CBA
11	B	1208	CLA	C1A-C2A-CAA-CBA
11	B	1219	CLA	C1A-C2A-CAA-CBA
11	a	1129	CLA	C1A-C2A-CAA-CBA
11	a	1130	CLA	C1A-C2A-CAA-CBA
11	B	1229	CLA	C1A-C2A-CAA-CBA
11	1	1139	CLA	C2-C1-O2A-CGA
14	b	4004	BCR	C19-C20-C21-C22
14	f	4013	BCR	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	B	5004	LHG	C4-O6-P-O3
11	1	1114	CLA	CBA-CGA-O2A-C1
11	1	1123	CLA	C4-C3-C5-C6
11	2	1021	CLA	C4-C3-C5-C6
11	l	1503	CLA	CAA-CBA-CGA-O2A
15	1	5003	LHG	C2-C3-O3-P
15	a	5001	LHG	C2-C3-O3-P
11	2	1229	CLA	C2-C3-C5-C6
11	1	1122	CLA	C2-C3-C5-C6
11	A	1137	CLA	C2-C3-C5-C6
15	2	5004	LHG	C3-O3-P-O5
15	a	5001	LHG	C3-O3-P-O4
15	a	5001	LHG	C4-O6-P-O4
15	b	5004	LHG	C4-O6-P-O4
11	2	1224	CLA	C6-C7-C8-C9
11	1	1111	CLA	C11-C12-C13-C14
15	a	5003	LHG	O6-C4-C5-C6
15	A	5003	LHG	O6-C4-C5-C6
11	B	1222	CLA	C5-C6-C7-C8
15	1	5003	LHG	C35-C36-C37-C38
11	2	1235	CLA	C10-C11-C12-C13
11	b	1235	CLA	O1A-CGA-O2A-C1
11	A	1237	CLA	C6-C7-C8-C10
11	b	1224	CLA	C6-C7-C8-C9
11	2	1213	CLA	C16-C17-C18-C20
11	A	1104	CLA	C16-C17-C18-C19
11	L	1502	CLA	CAD-CBD-CGD-O1D
11	a	1120	CLA	CAD-CBD-CGD-O1D
11	a	1118	CLA	CAD-CBD-CGD-O1D
11	b	1212	CLA	CAD-CBD-CGD-O1D
11	A	1129	CLA	CAD-CBD-CGD-O1D
11	B	1212	CLA	CAD-CBD-CGD-O1D
11	A	1012	CLA	CAD-CBD-CGD-O1D
11	1	1125	CLA	CAD-CBD-CGD-O1D
11	b	1207	CLA	CAD-CBD-CGD-O1D
11	A	1111	CLA	CAD-CBD-CGD-O1D
11	2	1202	CLA	CAD-CBD-CGD-O1D
11	1	1011	CLA	CAD-CBD-CGD-O1D
11	A	1135	CLA	CAD-CBD-CGD-O1D
11	1	1012	CLA	CAD-CBD-CGD-O1D
11	a	1111	CLA	CAD-CBD-CGD-O1D
11	b	1236	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1129	CLA	CAD-CBD-CGD-O1D
11	2	1207	CLA	CAD-CBD-CGD-O1D
11	b	1210	CLA	CAD-CBD-CGD-O1D
11	2	1223	CLA	C5-C6-C7-C8
15	1	5001	LHG	C11-C10-C9-C8
11	b	1222	CLA	C3-C5-C6-C7
11	a	1120	CLA	C2C-C3C-CAC-CBC
11	A	1123	CLA	C16-C17-C18-C20
11	l	1503	CLA	C16-C17-C18-C20
11	b	1204	CLA	C4-C3-C5-C6
11	A	1132	CLA	C4-C3-C5-C6
11	K	1401	CLA	C11-C12-C13-C15
11	1	1111	CLA	C11-C10-C8-C7
15	a	5003	LHG	O6-C4-C5-O7
11	B	1213	CLA	C11-C10-C8-C7
11	B	1213	CLA	C12-C13-C15-C16
11	a	1103	CLA	C11-C12-C13-C15
11	A	1109	CLA	C11-C10-C8-C7
11	1	1022	CLA	C12-C13-C15-C16
11	0	1401	CLA	C11-C12-C13-C15
11	a	1012	CLA	C11-C12-C13-C15
11	A	1128	CLA	C12-C13-C15-C16
15	A	5001	LHG	O6-C4-C5-O7
11	a	1117	CLA	C6-C7-C8-C10
11	A	1011	CLA	C11-C10-C8-C7
11	k	1401	CLA	C11-C12-C13-C15
11	A	1106	CLA	C11-C12-C13-C15
12	B	2002	PQN	C22-C23-C25-C26
15	a	5001	LHG	O6-C4-C5-O7
11	1	1126	CLA	C11-C10-C8-C7
11	1	1126	CLA	C12-C13-C15-C16
11	b	1215	CLA	C12-C13-C15-C16
11	a	1104	CLA	C11-C12-C13-C15
11	2	1215	CLA	C12-C13-C15-C16
11	b	1214	CLA	C11-C10-C8-C7
11	2	1226	CLA	C6-C7-C8-C10
11	1	1119	CLA	C11-C10-C8-C7
11	B	1226	CLA	C11-C10-C8-C7
11	2	1021	CLA	C11-C12-C13-C15
11	2	1021	CLA	C12-C13-C15-C16
11	2	1216	CLA	C11-C10-C8-C7
11	1	1102	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1102	CLA	C11-C12-C13-C15
16	2	5002	LMG	C30-C31-C32-C33
11	A	1110	CLA	C5-C6-C7-C8
11	2	1202	CLA	C8-C10-C11-C12
11	2	1217	CLA	CAA-CBA-CGA-O2A
11	1	1114	CLA	C4C-C3C-CAC-CBC
11	B	1234	CLA	C8-C10-C11-C12
11	B	1205	CLA	C5-C6-C7-C8
11	b	1224	CLA	C2C-C3C-CAC-CBC
16	2	5002	LMG	C11-C12-C13-C14
11	2	1217	CLA	C4C-C3C-CAC-CBC
11	2	1235	CLA	C5-C6-C7-C8
11	1	1122	CLA	CBD-CGD-O2D-CED
11	1	1133	CLA	O1A-CGA-O2A-C1
11	2	1224	CLA	C2A-CAA-CBA-CGA
11	b	1224	CLA	C2A-CAA-CBA-CGA
11	B	1023	CLA	C2A-CAA-CBA-CGA
11	A	1111	CLA	C2A-CAA-CBA-CGA
11	a	1123	CLA	C16-C17-C18-C20
11	b	1239	CLA	CAA-CBA-CGA-O2A
11	A	1801	CLA	CAA-CBA-CGA-O2A
11	2	1217	CLA	O1A-CGA-O2A-C1
11	b	1229	CLA	CAA-CBA-CGA-O2A
11	2	1221	CLA	C6-C7-C8-C9
11	1	1122	CLA	O1D-CGD-O2D-CED
15	1	5003	LHG	C24-C23-O8-C6
11	1	1111	CLA	C11-C10-C8-C9
11	8	1501	CLA	C11-C10-C8-C9
11	A	1119	CLA	C6-C7-C8-C9
11	a	1012	CLA	C11-C12-C13-C14
12	A	2001	PQN	C19-C18-C20-C21
11	a	1119	CLA	C14-C13-C15-C16
11	a	1106	CLA	C6-C7-C8-C9
11	L	1501	CLA	C11-C10-C8-C9
11	1	1140	CLA	C14-C13-C15-C16
11	b	1229	CLA	C11-C12-C13-C14
11	a	1104	CLA	C11-C10-C8-C9
11	B	1222	CLA	C6-C7-C8-C9
11	B	1235	CLA	C11-C10-C8-C9
11	A	1104	CLA	C11-C10-C8-C9
11	B	1021	CLA	C11-C12-C13-C14
11	b	1021	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1013	CLA	C6-C7-C8-C9
11	2	1225	CLA	C11-C12-C13-C14
11	1	1131	CLA	C11-C12-C13-C14
11	A	1118	CLA	C6-C7-C8-C9
11	1	1104	CLA	C6-C7-C8-C9
11	2	1210	CLA	C11-C10-C8-C9
11	1	1107	CLA	C6-C7-C8-C9
11	1	1117	CLA	C6-C7-C8-C9
11	b	1210	CLA	C11-C10-C8-C9
11	2	1204	CLA	O1A-CGA-O2A-C1
11	A	1102	CLA	C3-C5-C6-C7
11	1	1127	CLA	C16-C17-C18-C20
11	a	1131	CLA	C13-C15-C16-C17
11	B	1239	CLA	C2C-C3C-CAC-CBC
11	b	1209	CLA	C2C-C3C-CAC-CBC
11	a	1131	CLA	C2C-C3C-CAC-CBC
11	l	1503	CLA	C2A-CAA-CBA-CGA
16	B	5002	LMG	C12-C13-C14-C15
11	1	1138	CLA	O1A-CGA-O2A-C1
14	1	4008	BCR	C18-C19-C20-C21
14	b	4010	BCR	C18-C19-C20-C21
14	a	4008	BCR	C18-C19-C20-C21
14	L	4019	BCR	C18-C19-C20-C21
14	a	4007	BCR	C18-C19-C20-C21
14	f	4013	BCR	C18-C19-C20-C21
14	A	4007	BCR	C18-C19-C20-C21
14	A	4008	BCR	C18-C19-C20-C21
14	F	4013	BCR	C18-C19-C20-C21
14	1	4007	BCR	C18-C19-C20-C21
14	6	4013	BCR	C18-C19-C20-C21
11	1	1126	CLA	C13-C15-C16-C17
11	b	1229	CLA	C15-C16-C17-C18
11	1	1102	CLA	C10-C11-C12-C13
16	b	5002	LMG	O7-C10-C11-C12
11	8	1503	CLA	CAA-CBA-CGA-O2A
11	B	1223	CLA	C2C-C3C-CAC-CBC
11	B	1220	CLA	CBA-CGA-O2A-C1
11	b	1229	CLA	C10-C11-C12-C13
11	2	1224	CLA	C2C-C3C-CAC-CBC
15	A	5001	LHG	C30-C31-C32-C33
11	A	1011	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	C9-C8-O7-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	B	1013	CLA	C2A-CAA-CBA-CGA
11	2	1013	CLA	C2A-CAA-CBA-CGA
15	a	5003	LHG	C10-C11-C12-C13
15	A	5001	LHG	C16-C17-C18-C19
11	1	1801	CLA	C2-C1-O2A-CGA
11	b	1213	CLA	C2-C1-O2A-CGA
11	b	1216	CLA	C2-C1-O2A-CGA
11	A	1011	CLA	C2-C1-O2A-CGA
11	1	1127	CLA	C2-C1-O2A-CGA
11	b	1214	CLA	C2-C1-O2A-CGA
11	B	1214	CLA	C2-C1-O2A-CGA
11	B	1228	CLA	C2-C1-O2A-CGA
11	B	1201	CLA	C2-C1-O2A-CGA
11	a	1109	CLA	C2-C1-O2A-CGA
11	1	1102	CLA	C2-C1-O2A-CGA
11	A	1102	CLA	C2-C1-O2A-CGA
11	b	1210	CLA	C2-C1-O2A-CGA
11	1	1116	CLA	CAA-CBA-CGA-O2A
11	a	1117	CLA	O1A-CGA-O2A-C1
11	a	1111	CLA	C3-C5-C6-C7
11	b	1221	CLA	C3-C5-C6-C7
11	A	1140	CLA	C4C-C3C-CAC-CBC
11	a	1116	CLA	C2C-C3C-CAC-CBC
15	A	5003	LHG	C17-C18-C19-C20
14	B	4004	BCR	C19-C20-C21-C22
14	a	4002	BCR	C9-C10-C11-C12
15	1	5003	LHG	O10-C23-O8-C6
11	2	1215	CLA	CAA-CBA-CGA-O2A
11	a	1103	CLA	C5-C6-C7-C8
11	A	1132	CLA	C10-C11-C12-C13
11	B	1203	CLA	C4-C3-C5-C6
11	a	1132	CLA	C4-C3-C5-C6
11	b	1206	CLA	C4-C3-C5-C6
11	B	1223	CLA	O1D-CGD-O2D-CED
14	A	4008	BCR	C1-C6-C7-C8
11	1	1123	CLA	C2-C3-C5-C6
11	a	1140	CLA	C5-C6-C7-C8
11	a	1115	CLA	C2C-C3C-CAC-CBC
11	1	1012	CLA	C16-C17-C18-C19
11	1	1139	CLA	C2A-CAA-CBA-CGA
11	1	1127	CLA	C2A-CAA-CBA-CGA
11	A	1132	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	4009	BCR	C16-C17-C18-C19
14	2	4005	BCR	C11-C10-C9-C8
15	A	5003	LHG	O7-C5-C6-O8
11	a	1117	CLA	CBA-CGA-O2A-C1
15	1	5001	LHG	C3-O3-P-O6
15	A	5003	LHG	C3-O3-P-O6
15	A	5001	LHG	C3-O3-P-O6
15	A	5001	LHG	C4-O6-P-O3
15	1	5003	LHG	C3-O3-P-O6
11	2	1202	CLA	C13-C15-C16-C17
15	A	5001	LHG	C25-C26-C27-C28
15	A	5001	LHG	C29-C30-C31-C32
15	a	5003	LHG	C34-C35-C36-C37
11	b	1209	CLA	C4C-C3C-CAC-CBC
16	2	5002	LMG	C7-C8-C9-O8
11	B	1235	CLA	C4-C3-C5-C6
11	B	1229	CLA	C4-C3-C5-C6
11	b	1234	CLA	C2-C3-C5-C6
11	1	1132	CLA	C12-C13-C15-C16
11	1	1106	CLA	C12-C13-C15-C16
11	B	1223	CLA	C6-C7-C8-C10
11	b	1229	CLA	C12-C13-C15-C16
12	1	2001	PQN	C13-C15-C16-C17
11	b	1222	CLA	C6-C7-C8-C9
11	a	1119	CLA	C6-C7-C8-C9
11	1	1126	CLA	C6-C7-C8-C9
11	A	1123	CLA	C11-C10-C8-C9
11	2	1234	CLA	C6-C7-C8-C9
11	b	1223	CLA	C11-C12-C13-C14
11	b	1223	CLA	C14-C13-C15-C16
11	A	1111	CLA	C11-C10-C8-C9
11	l	1503	CLA	C14-C13-C15-C16
11	2	1021	CLA	C11-C10-C8-C9
11	A	1102	CLA	C11-C12-C13-C14
11	B	1229	CLA	C11-C10-C8-C9
14	A	4003	BCR	C19-C20-C21-C22
14	B	4006	BCR	C19-C20-C21-C22
14	l	4019	BCR	C13-C14-C15-C16
11	B	1240	CLA	C2C-C3C-CAC-CBC
15	a	5001	LHG	C30-C31-C32-C33
11	2	1217	CLA	CBA-CGA-O2A-C1
11	A	1101	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1204	CLA	CBA-CGA-O2A-C1
11	b	1215	CLA	CAA-CBA-CGA-O2A
11	1	1022	CLA	C10-C11-C12-C13
11	2	1210	CLA	C15-C16-C17-C18
11	A	1134	CLA	C2C-C3C-CAC-CBC
11	1	1134	CLA	C2C-C3C-CAC-CBC
11	2	1240	CLA	C2A-CAA-CBA-CGA
11	b	1204	CLA	C2-C3-C5-C6
11	2	1021	CLA	C2-C3-C5-C6
11	2	1213	CLA	C16-C17-C18-C19
11	A	1132	CLA	CBA-CGA-O2A-C1
11	a	1114	CLA	O1A-CGA-O2A-C1
15	1	5003	LHG	C12-C13-C14-C15
11	2	1235	CLA	O1A-CGA-O2A-C1
11	B	1223	CLA	CBD-CGD-O2D-CED
11	2	1235	CLA	CBA-CGA-O2A-C1
11	A	1012	CLA	C2A-CAA-CBA-CGA
11	1	1111	CLA	C11-C12-C13-C15
14	B	4011	BCR	C19-C20-C21-C22
14	L	4022	BCR	C19-C20-C21-C22
14	1	4001	BCR	C9-C10-C11-C12
11	b	1220	CLA	CBA-CGA-O2A-C1
14	F	4013	BCR	C10-C11-C12-C13
16	b	5002	LMG	C30-C31-C32-C33
11	A	1124	CLA	C6-C7-C8-C9
11	a	1237	CLA	C4-C3-C5-C6
16	2	5002	LMG	C37-C38-C39-C40
11	b	1210	CLA	O1A-CGA-O2A-C1
11	B	1202	CLA	C15-C16-C17-C18
11	1	1119	CLA	C8-C10-C11-C12
15	B	5004	LHG	C35-C36-C37-C38
11	B	1210	CLA	C2-C1-O2A-CGA
11	1	1109	CLA	C2-C1-O2A-CGA
11	b	1225	CLA	C2-C1-O2A-CGA
11	a	1116	CLA	C2-C1-O2A-CGA
11	1	1116	CLA	C2-C1-O2A-CGA
11	a	1128	CLA	C2-C1-O2A-CGA
11	A	1111	CLA	C2-C1-O2A-CGA
11	B	1201	CLA	C2C-C3C-CAC-CBC
11	b	1225	CLA	C2A-CAA-CBA-CGA
11	B	1204	CLA	C2A-CAA-CBA-CGA
15	2	5004	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1124	CLA	CBD-CGD-O2D-CED
15	2	5004	LHG	O10-C23-C24-C25
11	1	1140	CLA	C3-C5-C6-C7
11	2	1209	CLA	C3A-C2A-CAA-CBA
11	2	1214	CLA	C3A-C2A-CAA-CBA
11	a	1237	CLA	C3A-C2A-CAA-CBA
11	2	1216	CLA	C3A-C2A-CAA-CBA
11	1	1124	CLA	C6-C7-C8-C10
11	a	1111	CLA	C11-C12-C13-C15
11	A	1124	CLA	C4C-C3C-CAC-CBC
14	7	4021	BCR	C19-C20-C21-C22
14	a	4003	BCR	C19-C20-C21-C22
11	B	1204	CLA	C13-C15-C16-C17
11	b	1235	CLA	C4-C3-C5-C6
11	2	1219	CLA	C4-C3-C5-C6
11	8	1501	CLA	O1D-CGD-O2D-CED
11	1	1103	CLA	CAA-CBA-CGA-O2A
11	b	1213	CLA	C11-C10-C8-C9
11	B	1210	CLA	C6-C7-C8-C9
11	a	1103	CLA	C6-C7-C8-C9
11	1	1109	CLA	C11-C10-C8-C9
11	B	1202	CLA	C11-C12-C13-C14
11	b	1229	CLA	C11-C10-C8-C9
11	B	1235	CLA	C6-C7-C8-C9
12	1	2001	PQN	C24-C23-C25-C26
11	a	1123	CLA	C11-C10-C8-C9
11	2	1206	CLA	C11-C12-C13-C14
11	2	1021	CLA	C14-C13-C15-C16
11	a	1106	CLA	C16-C17-C18-C20
11	l	1503	CLA	C16-C17-C18-C19
15	1	5001	LHG	C27-C28-C29-C30
11	2	1214	CLA	C8-C10-C11-C12
11	2	1203	CLA	C5-C6-C7-C8
15	a	5003	LHG	C25-C26-C27-C28
11	a	1130	CLA	C2C-C3C-CAC-CBC
14	b	4011	BCR	C16-C17-C18-C36
14	F	4020	BCR	C20-C21-C22-C37
14	2	4011	BCR	C16-C17-C18-C36
14	f	4020	BCR	C20-C21-C22-C37
14	b	4009	BCR	C16-C17-C18-C36
14	6	4020	BCR	C20-C21-C22-C37
14	f	4013	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	2	4006	BCR	C20-C21-C22-C37
14	1	4002	BCR	C16-C17-C18-C36
14	B	4006	BCR	C20-C21-C22-C37
14	F	4013	BCR	C20-C21-C22-C37
14	b	4006	BCR	C20-C21-C22-C37
14	6	4013	BCR	C20-C21-C22-C37
11	B	1222	CLA	C2C-C3C-CAC-CBC
11	a	1801	CLA	C2A-CAA-CBA-CGA
11	2	1228	CLA	C2A-CAA-CBA-CGA
11	1	1108	CLA	C2A-CAA-CBA-CGA
11	1	1237	CLA	O2A-C1-C2-C3
11	2	1013	CLA	O2A-C1-C2-C3
14	a	4001	BCR	C36-C18-C19-C20
14	B	4004	BCR	C36-C18-C19-C20
15	a	5001	LHG	C11-C10-C9-C8
11	1	1132	CLA	C13-C15-C16-C17
16	2	5002	LMG	C7-C8-O7-C10
11	B	1234	CLA	C4-C3-C5-C6
11	1	1123	CLA	C1A-C2A-CAA-CBA
11	1	1137	CLA	C1A-C2A-CAA-CBA
11	B	1234	CLA	C1A-C2A-CAA-CBA
11	2	1209	CLA	C1A-C2A-CAA-CBA
11	2	1214	CLA	C1A-C2A-CAA-CBA
11	b	1226	CLA	C1A-C2A-CAA-CBA
11	B	1021	CLA	C1A-C2A-CAA-CBA
11	2	1210	CLA	C1A-C2A-CAA-CBA
11	a	1137	CLA	C1A-C2A-CAA-CBA
11	B	1207	CLA	C11-C12-C13-C15
11	B	1203	CLA	C2-C3-C5-C6
11	1	1123	CLA	C6-C7-C8-C10
11	a	1102	CLA	C11-C10-C8-C7
11	2	1238	CLA	C11-C10-C8-C7
11	b	1204	CLA	C11-C10-C8-C7
11	a	1126	CLA	C12-C13-C15-C16
11	A	1104	CLA	C11-C12-C13-C15
11	2	1215	CLA	C6-C7-C8-C10
11	1	1104	CLA	C11-C12-C13-C15
11	2	1206	CLA	C11-C10-C8-C7
11	b	1206	CLA	C11-C10-C8-C7
14	F	4020	BCR	C19-C20-C21-C22
11	1	1139	CLA	C2C-C3C-CAC-CBC
11	B	1201	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	B	5002	LMG	C16-C17-C18-C19
11	1	1136	CLA	C2A-CAA-CBA-CGA
11	2	1023	CLA	C2A-CAA-CBA-CGA
11	a	1129	CLA	C2A-CAA-CBA-CGA
11	1	1106	CLA	C13-C15-C16-C17
11	A	1012	CLA	C5-C6-C7-C8
11	2	1210	CLA	C13-C15-C16-C17
15	1	5001	LHG	C24-C25-C26-C27
16	B	5002	LMG	C15-C16-C17-C18
11	2	1223	CLA	CBA-CGA-O2A-C1
11	b	1221	CLA	C6-C7-C8-C9
15	1	5001	LHG	C13-C14-C15-C16
11	1	1119	CLA	C16-C17-C18-C20
11	B	1229	CLA	C16-C17-C18-C19
11	A	1125	CLA	C4-C3-C5-C6
16	2	5002	LMG	C20-C21-C22-C23
11	b	1203	CLA	C5-C6-C7-C8
11	A	1132	CLA	C2-C3-C5-C6
11	1	1111	CLA	C8-C10-C11-C12
12	1	2001	PQN	C15-C16-C17-C18
11	2	1203	CLA	C8-C10-C11-C12
14	b	4011	BCR	C16-C17-C18-C19
14	F	4020	BCR	C20-C21-C22-C23
14	2	4011	BCR	C16-C17-C18-C19
14	f	4020	BCR	C20-C21-C22-C23
14	6	4020	BCR	C20-C21-C22-C23
14	f	4013	BCR	C20-C21-C22-C23
14	1	4002	BCR	C16-C17-C18-C19
14	B	4006	BCR	C20-C21-C22-C23
14	F	4013	BCR	C20-C21-C22-C23
14	b	4006	BCR	C20-C21-C22-C23
14	6	4013	BCR	C20-C21-C22-C23
11	a	1118	CLA	C5-C6-C7-C8
14	2	4014	BCR	C13-C14-C15-C16
14	7	4021	BCR	C9-C10-C11-C12
14	B	4010	BCR	C19-C20-C21-C22
14	b	4005	BCR	C13-C14-C15-C16
14	A	4007	BCR	C9-C10-C11-C12
14	2	4010	BCR	C19-C20-C21-C22
14	1	4007	BCR	C9-C10-C11-C12
11	A	1132	CLA	O1A-CGA-O2A-C1
11	1	1012	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1227	CLA	C4C-C3C-CAC-CBC
15	a	5001	LHG	C25-C26-C27-C28
15	1	5001	LHG	C19-C20-C21-C22
11	a	1106	CLA	C4-C3-C5-C6
11	2	1234	CLA	C4-C3-C5-C6
11	b	1229	CLA	C4-C3-C5-C6
11	b	1207	CLA	C4-C3-C5-C6
11	1	1118	CLA	C4-C3-C5-C6
11	b	1234	CLA	C2-C1-O2A-CGA
11	b	1201	CLA	C2-C1-O2A-CGA
11	a	1111	CLA	C2-C1-O2A-CGA
11	b	1235	CLA	C2-C3-C5-C6
11	B	1234	CLA	C2-C3-C5-C6
11	2	1219	CLA	C2-C3-C5-C6
11	B	1229	CLA	C2-C3-C5-C6
11	a	1011	CLA	CAA-CBA-CGA-O2A
11	0	1401	CLA	C14-C13-C15-C16
11	b	1230	CLA	C6-C7-C8-C9
11	a	1107	CLA	C6-C7-C8-C9
11	b	1223	CLA	C11-C10-C8-C9
11	1	1117	CLA	C11-C12-C13-C14
11	2	1013	CLA	C6-C7-C8-C9
11	B	1229	CLA	C14-C13-C15-C16
11	A	1116	CLA	CAA-CBA-CGA-O1A
11	B	1212	CLA	C2A-CAA-CBA-CGA
11	1	1127	CLA	C13-C15-C16-C17
15	B	5004	LHG	C2-C3-O3-P
11	1	1114	CLA	O1A-CGA-O2A-C1
15	A	5003	LHG	C12-C13-C14-C15
11	1	1124	CLA	O1D-CGD-O2D-CED
11	B	1207	CLA	C15-C16-C17-C18
11	l	1501	CLA	C2C-C3C-CAC-CBC
15	1	5003	LHG	C9-C10-C11-C12
14	1	4008	BCR	C1-C6-C7-C8
14	b	4004	BCR	C23-C24-C25-C30
14	L	4019	BCR	C5-C6-C7-C8
14	L	4022	BCR	C23-C24-C25-C30
14	6	4013	BCR	C23-C24-C25-C30
11	a	1106	CLA	C10-C11-C12-C13
11	1	1117	CLA	C15-C16-C17-C18
15	b	5004	LHG	C35-C36-C37-C38
15	1	5003	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1213	CLA	C5-C6-C7-C8
15	A	5003	LHG	C33-C34-C35-C36
11	B	1239	CLA	CAA-CBA-CGA-O1A
14	1	4001	BCR	C19-C20-C21-C22
11	A	1127	CLA	C4-C3-C5-C6
11	b	1223	CLA	C4-C3-C5-C6
11	b	1021	CLA	C4-C3-C5-C6
11	2	1202	CLA	C4-C3-C5-C6
11	A	1124	CLA	C6-C7-C8-C10
11	B	1225	CLA	C10-C11-C12-C13
11	B	1235	CLA	C2-C3-C5-C6
11	a	1132	CLA	C2-C3-C5-C6
11	b	1206	CLA	C2-C3-C5-C6
11	B	1217	CLA	C2C-C3C-CAC-CBC
11	a	1012	CLA	C15-C16-C17-C18
11	a	1117	CLA	C10-C11-C12-C13
11	A	1104	CLA	C2C-C3C-CAC-CBC
11	8	1503	CLA	C5-C6-C7-C8
11	B	1219	CLA	C5-C6-C7-C8
11	B	1021	CLA	CAA-CBA-CGA-O1A
11	B	1210	CLA	C16-C17-C18-C19
11	a	1116	CLA	C4C-C3C-CAC-CBC
11	1	1104	CLA	C13-C15-C16-C17
11	1	1133	CLA	C4C-C3C-CAC-CBC
11	A	1127	CLA	C2A-CAA-CBA-CGA
11	a	1125	CLA	C2A-CAA-CBA-CGA
11	2	1223	CLA	O1A-CGA-O2A-C1
11	A	1106	CLA	C4-C3-C5-C6
11	B	1204	CLA	C4-C3-C5-C6
11	A	1123	CLA	C4-C3-C5-C6
11	A	1111	CLA	C4-C3-C5-C6
11	a	1127	CLA	C4-C3-C5-C6
11	B	1225	CLA	C4-C3-C5-C6
11	2	1229	CLA	CAA-CBA-CGA-O1A
11	a	1022	CLA	C6-C7-C8-C10
11	8	1501	CLA	C11-C10-C8-C7
11	b	1230	CLA	C6-C7-C8-C10
11	B	1021	CLA	C6-C7-C8-C10
11	A	1122	CLA	C11-C10-C8-C7
11	b	1207	CLA	C2-C3-C5-C6
11	b	1202	CLA	C11-C10-C8-C7
11	1	1011	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1206	CLA	C11-C12-C13-C15
11	1	1128	CLA	C11-C10-C8-C7
11	B	1213	CLA	C5-C6-C7-C8
15	B	5004	LHG	O1-C1-C2-O2
14	a	4001	BCR	C9-C10-C11-C12
11	1	1124	CLA	CAA-CBA-CGA-O2A
15	A	5001	LHG	C13-C14-C15-C16
15	1	5003	LHG	C19-C20-C21-C22
11	a	1132	CLA	C13-C15-C16-C17
11	a	1124	CLA	CAA-CBA-CGA-O2A
11	B	1235	CLA	CAA-CBA-CGA-O2A
11	b	1021	CLA	CAA-CBA-CGA-O2A
11	1	1110	CLA	CAA-CBA-CGA-O2A
15	a	5001	LHG	C35-C36-C37-C38
11	a	1131	CLA	C4C-C3C-CAC-CBC
11	b	1210	CLA	CBA-CGA-O2A-C1
14	b	4011	BCR	C11-C10-C9-C34
11	1	1133	CLA	C2C-C3C-CAC-CBC
15	1	5001	LHG	C35-C36-C37-C38
11	B	1210	CLA	C4-C3-C5-C6
11	A	1119	CLA	C4-C3-C5-C6
11	1	1022	CLA	C4-C3-C5-C6
11	b	1224	CLA	C4-C3-C5-C6
11	1	1110	CLA	C4-C3-C5-C6
11	B	1013	CLA	C4-C3-C5-C6
11	a	1137	CLA	C4-C3-C5-C6
11	A	1110	CLA	C4-C3-C5-C6
11	2	1202	CLA	C2-C3-C5-C6
11	A	1101	CLA	C11-C10-C8-C9
11	K	1401	CLA	C14-C13-C15-C16
11	B	1210	CLA	C11-C10-C8-C9
11	B	1213	CLA	C14-C13-C15-C16
11	a	1103	CLA	C11-C12-C13-C14
11	1	1123	CLA	C11-C10-C8-C9
11	1	1106	CLA	C6-C7-C8-C9
11	1	1106	CLA	C14-C13-C15-C16
12	A	2001	PQN	C24-C23-C25-C26
11	a	1102	CLA	C11-C10-C8-C9
11	k	1401	CLA	C14-C13-C15-C16
11	A	1022	CLA	C14-C13-C15-C16
11	A	1106	CLA	C11-C12-C13-C14
11	B	1204	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1126	CLA	C14-C13-C15-C16
11	a	1107	CLA	C11-C10-C8-C9
11	b	1204	CLA	C14-C13-C15-C16
11	a	1104	CLA	C11-C12-C13-C14
11	A	1104	CLA	C11-C12-C13-C14
11	1	1104	CLA	C11-C12-C13-C14
11	1	1102	CLA	C11-C12-C13-C14
11	2	1222	CLA	C6-C7-C8-C9
15	A	5001	LHG	C33-C34-C35-C36
11	B	1201	CLA	C4C-C3C-CAC-CBC
11	K	1402	CLA	C3A-C2A-CAA-CBA
11	1	1123	CLA	C3A-C2A-CAA-CBA
11	B	1234	CLA	C3A-C2A-CAA-CBA
11	l	1501	CLA	C3A-C2A-CAA-CBA
11	2	1223	CLA	C3A-C2A-CAA-CBA
11	b	1234	CLA	C4C-C3C-CAC-CBC
11	2	1214	CLA	C11-C12-C13-C14
11	1	1134	CLA	C4C-C3C-CAC-CBC
11	B	1203	CLA	O1A-CGA-O2A-C1
11	a	1122	CLA	CAA-CBA-CGA-O2A
11	B	1202	CLA	CAA-CBA-CGA-O2A
11	2	1235	CLA	CAA-CBA-CGA-O2A
11	2	1213	CLA	CAA-CBA-CGA-O2A
11	2	1218	CLA	CAD-CBD-CGD-O2D
11	b	1218	CLA	CAD-CBD-CGD-O2D
11	1	1129	CLA	CAD-CBD-CGD-O2D
11	A	1117	CLA	CAD-CBD-CGD-O2D
11	2	1201	CLA	CAD-CBD-CGD-O2D
11	2	1236	CLA	CAD-CBD-CGD-O2D
11	2	1212	CLA	CAD-CBD-CGD-O2D
11	a	1110	CLA	CAD-CBD-CGD-O2D
11	L	1501	CLA	CAD-CBD-CGD-O2D
11	b	1223	CLA	CAD-CBD-CGD-O2D
11	A	1118	CLA	CAD-CBD-CGD-O2D
11	B	1218	CLA	CAD-CBD-CGD-O2D
11	1	1112	CLA	CAD-CBD-CGD-O2D
15	A	5001	LHG	O9-C7-O7-C5
11	a	1134	CLA	C2C-C3C-CAC-CBC
11	8	1501	CLA	CBD-CGD-O2D-CED
11	1	1139	CLA	C4C-C3C-CAC-CBC
11	B	1239	CLA	C4C-C3C-CAC-CBC
11	B	1210	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a	5001	LHG	O7-C7-C8-C9
11	2	1216	CLA	CAA-CBA-CGA-O2A
11	b	1206	CLA	CAA-CBA-CGA-O2A
11	a	1101	CLA	C15-C16-C17-C18
11	1	1111	CLA	C4-C3-C5-C6
11	B	1206	CLA	C4-C3-C5-C6
11	a	1110	CLA	C4-C3-C5-C6
11	b	1205	CLA	C4-C3-C5-C6
11	A	1125	CLA	C2-C3-C5-C6
11	1	1110	CLA	C2-C3-C5-C6
11	1	1801	CLA	CAA-CBA-CGA-O2A
11	B	1225	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	C17-C18-C19-C20
14	B	4011	BCR	C17-C18-C19-C20
14	a	4001	BCR	C17-C18-C19-C20
14	B	4004	BCR	C17-C18-C19-C20
14	A	4007	BCR	C7-C8-C9-C10
11	1	1111	CLA	CAA-CBA-CGA-O2A
11	a	1116	CLA	CAA-CBA-CGA-O2A
11	b	1219	CLA	CAA-CBA-CGA-O2A
11	1	1131	CLA	CAA-CBA-CGA-O2A
11	1	1011	CLA	CAA-CBA-CGA-O2A
11	A	1103	CLA	O2A-C1-C2-C3
11	2	1021	CLA	O2A-C1-C2-C3
11	B	1229	CLA	O2A-C1-C2-C3
11	2	1217	CLA	C2A-CAA-CBA-CGA
11	1	1137	CLA	C15-C16-C17-C18
11	2	1206	CLA	CAA-CBA-CGA-O2A
11	1	1133	CLA	CHA-CBD-CGD-O1D
11	1	1133	CLA	CHA-CBD-CGD-O2D
11	1	1111	CLA	CHA-CBD-CGD-O1D
11	1	1111	CLA	CHA-CBD-CGD-O2D
11	a	1022	CLA	CHA-CBD-CGD-O1D
11	a	1022	CLA	CHA-CBD-CGD-O2D
11	A	1120	CLA	CHA-CBD-CGD-O2D
11	K	1402	CLA	CHA-CBD-CGD-O2D
11	B	1215	CLA	CHA-CBD-CGD-O1D
11	B	1215	CLA	CHA-CBD-CGD-O2D
11	A	1133	CLA	CHA-CBD-CGD-O1D
11	A	1133	CLA	CHA-CBD-CGD-O2D
11	1	1103	CLA	CHA-CBD-CGD-O1D
11	1	1103	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	1113	CLA	CHA-CBD-CGD-O1D
11	A	1113	CLA	CHA-CBD-CGD-O2D
11	L	1502	CLA	CHA-CBD-CGD-O1D
11	a	1115	CLA	CHA-CBD-CGD-O1D
11	a	1115	CLA	CHA-CBD-CGD-O2D
11	b	1225	CLA	CHA-CBD-CGD-O1D
11	b	1225	CLA	CHA-CBD-CGD-O2D
11	a	1012	CLA	CHA-CBD-CGD-O2D
11	A	1127	CLA	CHA-CBD-CGD-O1D
11	A	1127	CLA	CHA-CBD-CGD-O2D
11	2	1221	CLA	CHA-CBD-CGD-O1D
11	2	1221	CLA	CHA-CBD-CGD-O2D
11	b	1235	CLA	CHA-CBD-CGD-O1D
11	b	1235	CLA	CHA-CBD-CGD-O2D
11	a	1119	CLA	CHA-CBD-CGD-O1D
11	a	1119	CLA	CHA-CBD-CGD-O2D
11	B	1224	CLA	CHA-CBD-CGD-O1D
11	B	1224	CLA	CHA-CBD-CGD-O2D
11	1	1137	CLA	CHA-CBD-CGD-O1D
11	1	1137	CLA	CHA-CBD-CGD-O2D
11	a	1120	CLA	CHA-CBD-CGD-O1D
11	a	1120	CLA	CHA-CBD-CGD-O2D
11	b	1227	CLA	CHA-CBD-CGD-O1D
11	b	1201	CLA	CHA-CBD-CGD-O2D
11	a	1118	CLA	CHA-CBD-CGD-O1D
11	1	1136	CLA	CHA-CBD-CGD-O1D
11	1	1136	CLA	CHA-CBD-CGD-O2D
11	b	1212	CLA	CHA-CBD-CGD-O1D
11	B	1204	CLA	CHA-CBD-CGD-O1D
11	B	1204	CLA	CHA-CBD-CGD-O2D
11	1	1126	CLA	CHA-CBD-CGD-O1D
11	1	1126	CLA	CHA-CBD-CGD-O2D
11	a	1113	CLA	CHA-CBD-CGD-O1D
11	a	1113	CLA	CHA-CBD-CGD-O2D
11	2	1213	CLA	CHA-CBD-CGD-O2D
11	A	1103	CLA	CHA-CBD-CGD-O1D
11	A	1103	CLA	CHA-CBD-CGD-O2D
11	b	1229	CLA	CHA-CBD-CGD-O1D
11	b	1229	CLA	CHA-CBD-CGD-O2D
11	b	1023	CLA	CHA-CBD-CGD-O1D
11	b	1023	CLA	CHA-CBD-CGD-O2D
11	l	1502	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	2	1203	CLA	CHA-CBD-CGD-O1D
11	2	1203	CLA	CHA-CBD-CGD-O2D
11	1	1125	CLA	CHA-CBD-CGD-O1D
11	1	1101	CLA	CHA-CBD-CGD-O2D
11	b	1207	CLA	CHA-CBD-CGD-O2D
11	a	1123	CLA	CHA-CBD-CGD-O2D
11	B	1023	CLA	CHA-CBD-CGD-O1D
11	B	1023	CLA	CHA-CBD-CGD-O2D
11	2	1226	CLA	CHA-CBD-CGD-O2D
11	A	1112	CLA	CHA-CBD-CGD-O1D
11	1	1118	CLA	CHA-CBD-CGD-O2D
11	A	1136	CLA	CHA-CBD-CGD-O1D
11	A	1136	CLA	CHA-CBD-CGD-O2D
11	a	1127	CLA	CHA-CBD-CGD-O1D
11	a	1127	CLA	CHA-CBD-CGD-O2D
11	B	1208	CLA	CHA-CBD-CGD-O1D
11	B	1208	CLA	CHA-CBD-CGD-O2D
11	A	1135	CLA	CHA-CBD-CGD-O1D
11	2	1220	CLA	CHA-CBD-CGD-O1D
11	2	1220	CLA	CHA-CBD-CGD-O2D
11	a	1101	CLA	CHA-CBD-CGD-O2D
11	B	1013	CLA	CHA-CBD-CGD-O1D
11	B	1013	CLA	CHA-CBD-CGD-O2D
11	2	1021	CLA	CHA-CBD-CGD-O2D
11	2	1223	CLA	CHA-CBD-CGD-O2D
11	B	1230	CLA	CHA-CBD-CGD-O1D
11	B	1230	CLA	CHA-CBD-CGD-O2D
11	b	1221	CLA	CHA-CBD-CGD-O1D
11	b	1221	CLA	CHA-CBD-CGD-O2D
11	2	1210	CLA	CHA-CBD-CGD-O2D
11	2	1216	CLA	CHA-CBD-CGD-O1D
11	2	1216	CLA	CHA-CBD-CGD-O2D
11	b	1206	CLA	CHA-CBD-CGD-O1D
11	b	1206	CLA	CHA-CBD-CGD-O2D
11	A	1102	CLA	CHA-CBD-CGD-O1D
11	A	1102	CLA	CHA-CBD-CGD-O2D
11	b	1210	CLA	CHA-CBD-CGD-O2D
11	a	1131	CLA	C4-C3-C5-C6
15	A	5003	LHG	O7-C7-C8-C9
11	b	1204	CLA	CAA-CBA-CGA-O2A
11	2	1202	CLA	CAA-CBA-CGA-O2A
11	1	1022	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	1110	CLA	C2-C3-C5-C6
11	b	1205	CLA	C2-C3-C5-C6
11	A	1110	CLA	C2-C3-C5-C6
11	a	1135	CLA	C2C-C3C-CAC-CBC
14	b	4011	BCR	C11-C10-C9-C8
14	2	4006	BCR	C20-C21-C22-C23
11	A	1101	CLA	CAA-CBA-CGA-O2A
11	K	1401	CLA	CAA-CBA-CGA-O2A
11	0	1401	CLA	CAA-CBA-CGA-O2A
15	A	5003	LHG	O8-C23-C24-C25
11	k	1401	CLA	CAA-CBA-CGA-O2A
11	2	1239	CLA	CAA-CBA-CGA-O2A
15	a	5003	LHG	O7-C5-C6-O8
15	2	5004	LHG	O7-C5-C6-O8
11	b	1226	CLA	C5-C6-C7-C8
11	A	1134	CLA	C4C-C3C-CAC-CBC
11	1	1136	CLA	C4C-C3C-CAC-CBC
11	a	1130	CLA	C4C-C3C-CAC-CBC
11	b	1216	CLA	CAA-CBA-CGA-O2A
15	A	5001	LHG	O7-C7-C8-C9
11	1	1136	CLA	CAA-CBA-CGA-O2A
11	A	1111	CLA	CAA-CBA-CGA-O2A
11	A	1136	CLA	CAA-CBA-CGA-O2A
11	A	1131	CLA	C2A-CAA-CBA-CGA
11	2	1216	CLA	C16-C17-C18-C20
11	A	1101	CLA	C15-C16-C17-C18
11	B	1203	CLA	CBA-CGA-O2A-C1
16	b	5002	LMG	C12-C13-C14-C15
16	2	5002	LMG	O7-C10-C11-C12
11	2	1221	CLA	C4-C3-C5-C6
11	1	1132	CLA	C2C-C3C-CAC-CBC
11	B	1201	CLA	O1A-CGA-O2A-C1
11	B	1210	CLA	C2-C3-C5-C6
11	A	1119	CLA	C2-C3-C5-C6
11	a	1102	CLA	C11-C12-C13-C15
11	A	1123	CLA	C2-C3-C5-C6
11	2	1023	CLA	C11-C10-C8-C7
11	1	1012	CLA	C11-C10-C8-C7
11	2	1223	CLA	C12-C13-C15-C16
11	B	1229	CLA	C12-C13-C15-C16
11	A	1132	CLA	C16-C17-C18-C20
15	B	5004	LHG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	A	5003	LHG	C9-C10-C11-C12
15	b	5004	LHG	C32-C33-C34-C35
15	a	5001	LHG	O8-C23-C24-C25
11	b	1210	CLA	CAA-CBA-CGA-O2A
11	B	1231	CLA	C2C-C3C-CAC-CBC
11	a	1122	CLA	C6-C7-C8-C9
11	l	1501	CLA	C14-C13-C15-C16
11	a	1128	CLA	C11-C10-C8-C9
11	a	1126	CLA	C14-C13-C15-C16
11	B	1238	CLA	C11-C10-C8-C9
11	1	1128	CLA	C11-C12-C13-C14
14	b	4014	BCR	C13-C14-C15-C16
14	2	4009	BCR	C19-C20-C21-C22
11	b	1213	CLA	C2C-C3C-CAC-CBC
11	B	1238	CLA	C15-C16-C17-C18
11	a	1111	CLA	C11-C12-C13-C14
11	2	1013	CLA	C16-C17-C18-C20
11	2	1235	CLA	CAA-CBA-CGA-O1A
11	b	1021	CLA	CAA-CBA-CGA-O1A
11	2	1206	CLA	CAA-CBA-CGA-O1A
11	b	1206	CLA	CAA-CBA-CGA-O1A
11	2	1215	CLA	C13-C15-C16-C17
16	2	5002	LMG	C34-C35-C36-C37
11	1	1801	CLA	CAA-CBA-CGA-O1A
11	2	1021	CLA	C10-C11-C12-C13
11	b	1219	CLA	C6-C7-C8-C10
11	1	1119	CLA	C16-C17-C18-C19
11	B	1231	CLA	C4C-C3C-CAC-CBC
15	B	5004	LHG	C15-C16-C17-C18
11	L	1502	CLA	C2C-C3C-CAC-CBC
11	1	1126	CLA	C2C-C3C-CAC-CBC
11	B	1204	CLA	C2-C3-C5-C6
11	a	1237	CLA	C2-C3-C5-C6
11	2	1234	CLA	C2-C3-C5-C6
11	a	1127	CLA	C2-C3-C5-C6
11	a	1124	CLA	CAA-CBA-CGA-O1A
14	A	4007	BCR	C11-C12-C13-C14
11	a	1110	CLA	C2C-C3C-CAC-CBC
11	b	1220	CLA	C1A-C2A-CAA-CBA
11	a	1103	CLA	C1A-C2A-CAA-CBA
11	1	1022	CLA	C1A-C2A-CAA-CBA
11	a	1012	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1235	CLA	C1A-C2A-CAA-CBA
11	b	1230	CLA	C1A-C2A-CAA-CBA
11	1	1135	CLA	C1A-C2A-CAA-CBA
11	2	1235	CLA	C1A-C2A-CAA-CBA
11	2	1223	CLA	C1A-C2A-CAA-CBA
11	B	1230	CLA	C1A-C2A-CAA-CBA
11	B	1229	CLA	C16-C17-C18-C20
11	1	1111	CLA	CAA-CBA-CGA-O1A
11	2	1216	CLA	CAA-CBA-CGA-O1A
11	A	1127	CLA	C2-C1-O2A-CGA
11	b	1202	CLA	C13-C15-C16-C17
11	B	1202	CLA	CAA-CBA-CGA-O1A
15	A	5003	LHG	O10-C23-C24-C25
11	1	1124	CLA	CAA-CBA-CGA-O1A
11	L	1503	CLA	CAA-CBA-CGA-O1A
11	B	1235	CLA	CAA-CBA-CGA-O1A
11	1	1118	CLA	CAA-CBA-CGA-O1A
11	B	1217	CLA	C2-C1-O2A-CGA
11	A	1137	CLA	CAA-CBA-CGA-O2A
15	1	5003	LHG	C24-C25-C26-C27
11	2	1205	CLA	CBD-CGD-O2D-CED
15	b	5004	LHG	C3-O3-P-O6
11	B	1215	CLA	CAA-CBA-CGA-O1A
11	b	1219	CLA	CAA-CBA-CGA-O1A
11	2	1239	CLA	CAA-CBA-CGA-O1A
11	a	1126	CLA	C13-C15-C16-C17
11	b	1213	CLA	C4C-C3C-CAC-CBC
11	B	1220	CLA	O1A-CGA-O2A-C1
11	a	1122	CLA	CAA-CBA-CGA-O1A
15	A	5003	LHG	O9-C7-C8-C9
11	1	1136	CLA	CAA-CBA-CGA-O1A
11	1	1110	CLA	CAA-CBA-CGA-O1A
11	b	1021	CLA	C2-C3-C5-C6
11	b	1231	CLA	C2A-CAA-CBA-CGA
15	A	5001	LHG	C4-O6-P-O4
15	b	5004	LHG	C3-O3-P-O5
11	B	1210	CLA	CAA-CBA-CGA-O1A
11	2	1213	CLA	CAA-CBA-CGA-O1A
11	2	1202	CLA	CAA-CBA-CGA-O1A
11	b	1210	CLA	CAA-CBA-CGA-O1A
11	B	1205	CLA	CAA-CBA-CGA-O2A
15	B	5004	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	4004	BCR	C23-C24-C25-C26
14	L	4019	BCR	C1-C6-C7-C8
14	L	4022	BCR	C23-C24-C25-C26
11	B	1216	CLA	C15-C16-C17-C18
15	a	5001	LHG	O9-C7-C8-C9
11	b	1204	CLA	CAA-CBA-CGA-O1A
11	1	1131	CLA	CAA-CBA-CGA-O1A
11	B	1225	CLA	CAA-CBA-CGA-O1A
11	1	1140	CLA	CAA-CBA-CGA-O2A
11	A	1122	CLA	CAA-CBA-CGA-O2A
11	1	1101	CLA	CAA-CBA-CGA-O2A
11	A	1105	CLA	CAA-CBA-CGA-O2A
11	b	1215	CLA	C8-C10-C11-C12
11	B	1217	CLA	C2A-CAA-CBA-CGA
11	B	1221	CLA	C2A-CAA-CBA-CGA
11	2	1235	CLA	C2C-C3C-CAC-CBC
11	a	1125	CLA	C4C-C3C-CAC-CBC
11	A	1124	CLA	CAA-CBA-CGA-O2A
11	A	1104	CLA	C10-C11-C12-C13
15	A	5001	LHG	O9-C7-C8-C9
11	b	1229	CLA	C2-C3-C5-C6
11	1	1120	CLA	CAD-CBD-CGD-O1D
11	K	1402	CLA	CAD-CBD-CGD-O1D
11	a	1112	CLA	CAD-CBD-CGD-O1D
11	2	1231	CLA	CAD-CBD-CGD-O1D
11	B	1234	CLA	CAD-CBD-CGD-O1D
11	l	1501	CLA	CAD-CBD-CGD-O1D
11	a	1125	CLA	CAD-CBD-CGD-O1D
11	a	1104	CLA	CAD-CBD-CGD-O1D
11	A	1104	CLA	CAD-CBD-CGD-O1D
11	2	1203	CLA	CAD-CBD-CGD-O1D
11	B	1221	CLA	CAD-CBD-CGD-O1D
11	b	1217	CLA	CAD-CBD-CGD-O1D
11	B	1023	CLA	CAD-CBD-CGD-O1D
11	B	1220	CLA	CAD-CBD-CGD-O1D
11	A	1135	CLA	C2-C3-C5-C6
11	2	1220	CLA	CAD-CBD-CGD-O1D
11	b	1206	CLA	CAD-CBD-CGD-O1D
11	a	1138	CLA	CAD-CBD-CGD-O1D
11	2	1222	CLA	CAD-CBD-CGD-O1D
11	A	1111	CLA	CAA-CBA-CGA-O1A
16	B	5002	LMG	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	1	1114	CLA	CAA-CBA-CGA-O2A
11	1	1122	CLA	CAA-CBA-CGA-O2A
11	A	1110	CLA	CAA-CBA-CGA-O2A
12	A	2001	PQN	C20-C21-C22-C23
11	1	1122	CLA	C5-C6-C7-C8
11	2	1023	CLA	C8-C10-C11-C12
11	A	1101	CLA	C6-C7-C8-C9
11	A	1119	CLA	C11-C12-C13-C14
11	b	1204	CLA	C11-C10-C8-C9
11	1	1101	CLA	C14-C13-C15-C16
11	b	1207	CLA	C6-C7-C8-C9
11	A	1140	CLA	C11-C12-C13-C14
11	2	1206	CLA	C11-C10-C8-C9
11	1	1102	CLA	C11-C10-C8-C9
11	b	1206	CLA	C11-C10-C8-C9
11	a	1126	CLA	C2C-C3C-CAC-CBC
12	B	2002	PQN	C25-C26-C27-C28
11	a	1114	CLA	CAA-CBA-CGA-O2A
15	a	5003	LHG	O8-C23-C24-C25
11	B	1213	CLA	CAA-CBA-CGA-O2A
11	a	1012	CLA	CAA-CBA-CGA-O2A
11	A	1134	CLA	CAA-CBA-CGA-O2A
11	a	1136	CLA	CAA-CBA-CGA-O2A
15	1	5003	LHG	O8-C23-C24-C25
11	A	1140	CLA	CAA-CBA-CGA-O2A
11	B	1228	CLA	CAA-CBA-CGA-O2A
11	B	1229	CLA	CAA-CBA-CGA-O2A
11	b	1210	CLA	C10-C11-C12-C13
11	A	1101	CLA	CAA-CBA-CGA-O1A
16	b	5002	LMG	C23-C24-C25-C26
11	1	1120	CLA	CAA-CBA-CGA-O2A
11	a	1105	CLA	CAA-CBA-CGA-O2A
11	2	1234	CLA	CAA-CBA-CGA-O2A
11	2	1205	CLA	CAA-CBA-CGA-O2A
11	a	1138	CLA	CAA-CBA-CGA-O2A
11	B	1207	CLA	C10-C11-C12-C13
11	B	1234	CLA	C10-C11-C12-C13
11	L	1501	CLA	C5-C6-C7-C8
15	2	5004	LHG	C14-C15-C16-C17
11	K	1401	CLA	CAA-CBA-CGA-O1A
11	b	1216	CLA	CAA-CBA-CGA-O1A
11	a	1012	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	k	1401	CLA	CAA-CBA-CGA-O1A
11	B	1213	CLA	C4-C3-C5-C6
11	2	1223	CLA	C10-C11-C12-C13
11	B	1210	CLA	C12-C13-C15-C16
11	a	1103	CLA	C11-C10-C8-C7
11	1	1132	CLA	C11-C10-C8-C7
11	1	1123	CLA	C12-C13-C15-C16
11	1	1106	CLA	C11-C10-C8-C7
11	a	1106	CLA	C2-C3-C5-C6
11	A	1106	CLA	C11-C10-C8-C7
11	B	1204	CLA	C11-C12-C13-C15
11	1	1127	CLA	C11-C10-C8-C7
11	a	1107	CLA	C3A-C2A-CAA-CBA
11	1	1122	CLA	C6-C7-C8-C10
11	A	1012	CLA	C11-C10-C8-C7
11	B	1238	CLA	C11-C10-C8-C7
11	a	1132	CLA	C11-C10-C8-C7
11	A	1107	CLA	C3A-C2A-CAA-CBA
11	1	1117	CLA	C11-C12-C13-C15
11	2	1013	CLA	C11-C12-C13-C15
11	B	1229	CLA	C6-C7-C8-C10
11	1	1128	CLA	C11-C12-C13-C15
11	0	1401	CLA	CAA-CBA-CGA-O1A
11	A	1140	CLA	CAA-CBA-CGA-O1A
11	A	1136	CLA	CAA-CBA-CGA-O1A
11	8	1502	CLA	CAA-CBA-CGA-O2A
11	2	1219	CLA	CAA-CBA-CGA-O2A
11	b	1228	CLA	CAA-CBA-CGA-O2A
11	2	1210	CLA	CAA-CBA-CGA-O2A
11	2	1207	CLA	CAA-CBA-CGA-O2A
15	a	5001	LHG	C7-C8-C9-C10
14	A	4001	BCR	C17-C18-C19-C20
14	2	4010	BCR	C17-C18-C19-C20
11	1	1120	CLA	CAA-CBA-CGA-O1A
11	2	1219	CLA	CAA-CBA-CGA-O1A
11	A	1137	CLA	CAA-CBA-CGA-O1A
11	B	1228	CLA	CAA-CBA-CGA-O1A
14	1	4022	BCR	C19-C20-C21-C22
14	8	4022	BCR	C19-C20-C21-C22
15	1	5001	LHG	O8-C23-C24-C25
11	b	1235	CLA	CAA-CBA-CGA-O2A
11	1	1127	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	b	1214	CLA	CAA-CBA-CGA-O2A
11	2	1226	CLA	C8-C10-C11-C12
11	1	1118	CLA	C5-C6-C7-C8
11	A	1134	CLA	CAA-CBA-CGA-O1A
15	A	5001	LHG	C8-C7-O7-C5
11	A	1126	CLA	C8-C10-C11-C12
11	B	1203	CLA	C5-C6-C7-C8
11	B	1206	CLA	O1A-CGA-O2A-C1
11	B	1220	CLA	CAA-CBA-CGA-O2A
11	a	1107	CLA	C15-C16-C17-C18
11	B	1213	CLA	CAA-CBA-CGA-O1A
11	1	1101	CLA	CAA-CBA-CGA-O1A
11	A	1110	CLA	CAA-CBA-CGA-O1A
11	B	1213	CLA	C2A-CAA-CBA-CGA
11	A	1106	CLA	C16-C17-C18-C20
11	a	1134	CLA	C4C-C3C-CAC-CBC
11	A	1101	CLA	C8-C10-C11-C12
11	a	1136	CLA	CAA-CBA-CGA-O1A
11	a	1138	CLA	CAA-CBA-CGA-O1A
11	b	1202	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

208 monomers are involved in 696 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1101	CLA	4	0
11	1	1801	CLA	5	0
11	A	1125	CLA	7	0
14	1	4008	BCR	4	0
14	6	4020	BCR	4	0
11	K	1401	CLA	4	0
11	1	1133	CLA	2	0
15	1	5001	LHG	10	0
11	2	1208	CLA	1	0
11	1	1111	CLA	1	0
11	B	1210	CLA	3	0
11	8	1501	CLA	6	0
15	B	5004	LHG	8	0
13	3	3002	SF4	9	0
14	2	4014	BCR	7	0
11	2	1204	CLA	3	0
11	B	1215	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1133	CLA	4	0
14	7	4021	BCR	6	0
14	F	4020	BCR	7	0
11	B	1207	CLA	3	0
14	B	4010	BCR	15	0
11	1	1129	CLA	2	0
11	1	1109	CLA	2	0
11	1	1132	CLA	3	0
11	A	1126	CLA	9	0
11	1	1103	CLA	2	0
11	A	1109	CLA	1	0
11	B	1202	CLA	1	0
11	B	1203	CLA	2	0
11	A	1119	CLA	11	0
11	A	1113	CLA	2	0
14	B	4011	BCR	10	0
11	A	1131	CLA	4	0
11	1	1022	CLA	5	0
11	1	1123	CLA	5	0
11	0	1401	CLA	3	0
11	1	1106	CLA	8	0
14	A	4001	BCR	6	0
11	A	1127	CLA	3	0
12	A	2001	PQN	5	0
11	A	1114	CLA	2	0
11	B	1223	CLA	20	0
14	2	4011	BCR	7	0
11	A	1134	CLA	1	0
13	3	3003	SF4	12	0
11	A	1117	CLA	2	0
11	B	1231	CLA	3	0
15	A	5003	LHG	10	0
11	2	1231	CLA	8	0
11	A	1128	CLA	6	0
11	B	1224	CLA	1	0
11	1	1137	CLA	4	0
11	1	1130	CLA	2	0
11	B	1206	CLA	5	0
15	A	5001	LHG	5	0
11	0	1402	CLA	1	0
11	1	1124	CLA	2	0
14	A	4003	BCR	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	1503	CLA	3	0
11	B	1234	CLA	2	0
11	2	1229	CLA	5	0
11	B	1205	CLA	5	0
11	2	1201	CLA	2	0
11	1	1237	CLA	3	0
11	2	1212	CLA	4	0
11	2	1232	CLA	3	0
14	L	4019	BCR	13	0
11	2	1227	CLA	3	0
11	A	1011	CLA	3	0
14	B	4004	BCR	4	0
11	A	1237	CLA	4	0
11	B	1209	CLA	6	0
11	A	1116	CLA	2	0
11	2	1209	CLA	1	0
11	A	1022	CLA	6	0
14	M	4021	BCR	7	0
15	2	5004	LHG	7	0
11	2	1023	CLA	3	0
15	1	5003	LHG	6	0
11	A	1106	CLA	6	0
11	2	1238	CLA	5	0
11	A	1801	CLA	8	0
11	2	1214	CLA	2	0
11	B	1217	CLA	2	0
12	B	2002	PQN	4	0
14	2	4009	BCR	5	0
11	8	1503	CLA	3	0
11	1	1127	CLA	4	0
11	1	1126	CLA	4	0
14	A	4002	BCR	9	0
11	A	1129	CLA	4	0
11	K	1402	CLA	4	0
11	A	1115	CLA	2	0
14	B	4009	BCR	7	0
11	1	1122	CLA	1	0
11	B	1212	CLA	5	0
11	L	1501	CLA	8	0
11	1	1140	CLA	2	0
14	6	4018	BCR	9	0
11	A	1123	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	2	1234	CLA	4	0
13	1	3001	SF4	1	0
11	A	1012	CLA	5	0
11	A	1103	CLA	20	0
14	2	4005	BCR	3	0
13	C	3003	SF4	11	0
14	2	4006	BCR	1	0
11	B	1222	CLA	7	0
14	A	4007	BCR	9	0
11	A	1132	CLA	4	0
13	C	3002	SF4	11	0
14	A	4008	BCR	5	0
11	B	1235	CLA	3	0
11	A	1104	CLA	8	0
11	2	1230	CLA	3	0
12	1	2001	PQN	1	0
11	2	1203	CLA	1	0
11	A	1137	CLA	5	0
11	1	1125	CLA	2	0
11	B	1021	CLA	7	0
11	A	1122	CLA	2	0
13	A	3001	SF4	4	0
11	B	1221	CLA	4	0
14	1	4002	BCR	5	0
11	1	1101	CLA	3	0
11	A	1138	CLA	6	0
14	L	4022	BCR	9	0
14	1	4001	BCR	8	0
11	1	1115	CLA	4	0
11	1	1121	CLA	1	0
14	8	4019	BCR	7	0
11	A	1140	CLA	1	0
11	2	1225	CLA	1	0
11	B	1023	CLA	8	0
14	B	4006	BCR	3	0
11	B	1238	CLA	7	0
11	A	1111	CLA	4	0
11	B	1204	CLA	3	0
11	1	1131	CLA	2	0
11	1	1119	CLA	4	0
14	B	4017	BCR	10	0
11	B	1226	CLA	1	0

Continued on next page...

Continued from previous page...

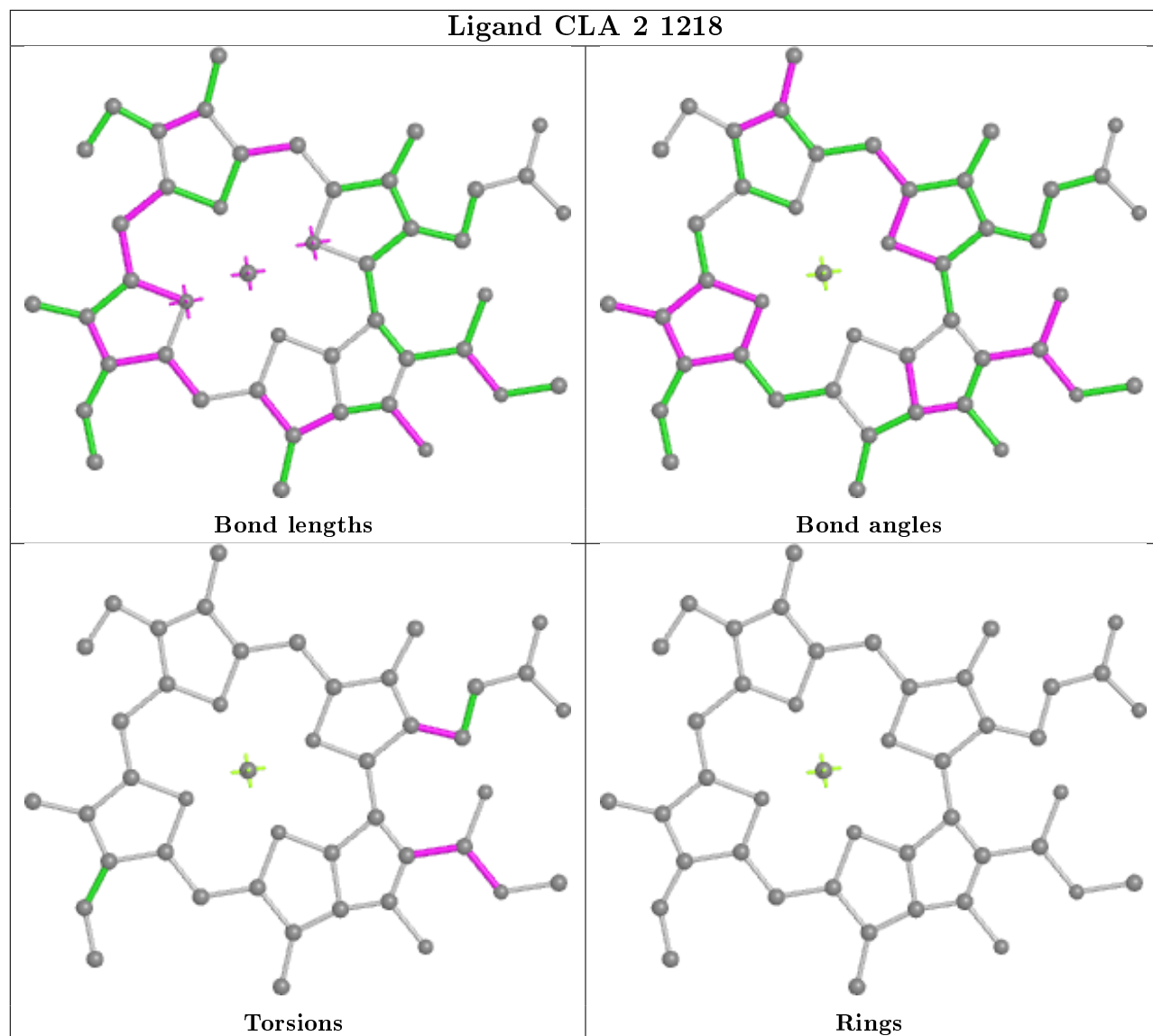
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1112	CLA	7	0
11	1	1118	CLA	2	0
11	2	1235	CLA	2	0
11	A	1124	CLA	3	0
11	2	1211	CLA	2	0
11	B	1214	CLA	2	0
11	B	1220	CLA	3	0
11	A	1136	CLA	4	0
11	1	1110	CLA	2	0
14	F	4013	BCR	6	0
11	A	1118	CLA	5	0
14	8	4022	BCR	8	0
11	1	1112	CLA	3	0
11	2	1202	CLA	3	0
11	B	1208	CLA	3	0
11	B	1227	CLA	4	0
11	1	1011	CLA	1	0
11	B	1228	CLA	2	0
11	B	1240	CLA	1	0
11	A	1135	CLA	1	0
11	1	1134	CLA	3	0
11	B	1219	CLA	2	0
11	1	1012	CLA	5	0
11	1	1104	CLA	1	0
11	2	1206	CLA	6	0
11	2	1240	CLA	2	0
11	2	1220	CLA	1	0
11	2	1239	CLA	4	0
11	A	1105	CLA	1	0
11	A	1121	CLA	4	0
11	A	1107	CLA	5	0
16	B	5002	LMG	1	0
11	B	1013	CLA	9	0
11	B	1225	CLA	3	0
14	2	4010	BCR	6	0
14	1	4003	BCR	2	0
11	2	1021	CLA	6	0
11	2	1223	CLA	2	0
11	B	1201	CLA	4	0
11	B	1211	CLA	5	0
12	2	2002	PQN	3	0
11	B	1230	CLA	5	0

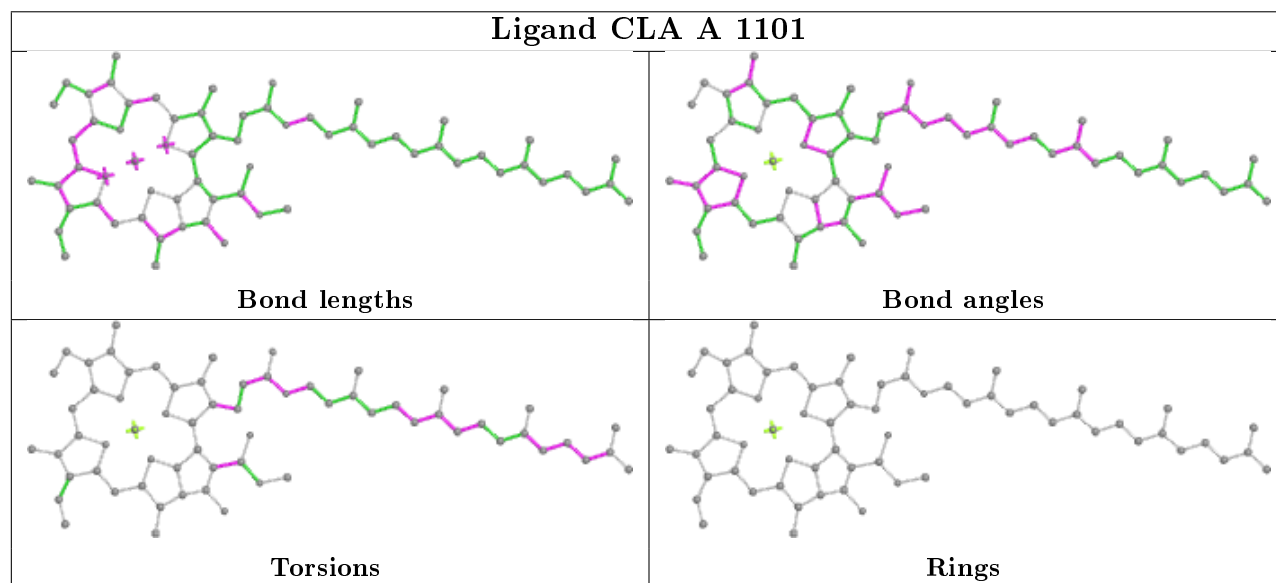
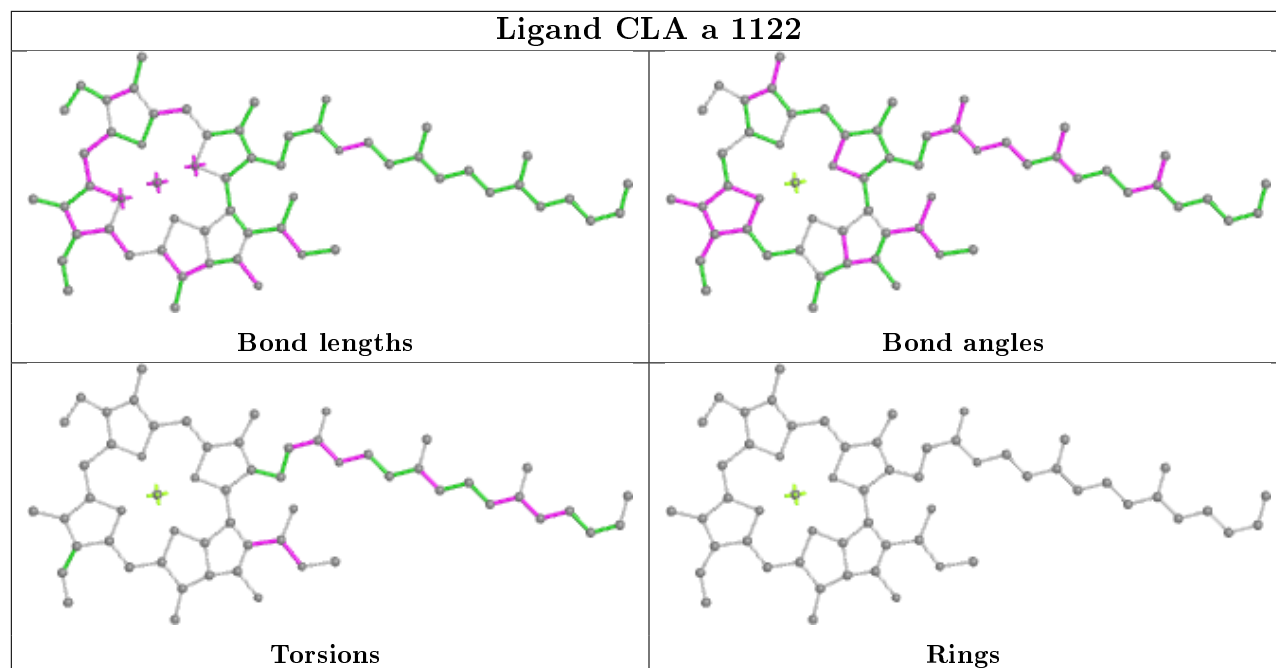
Continued on next page...

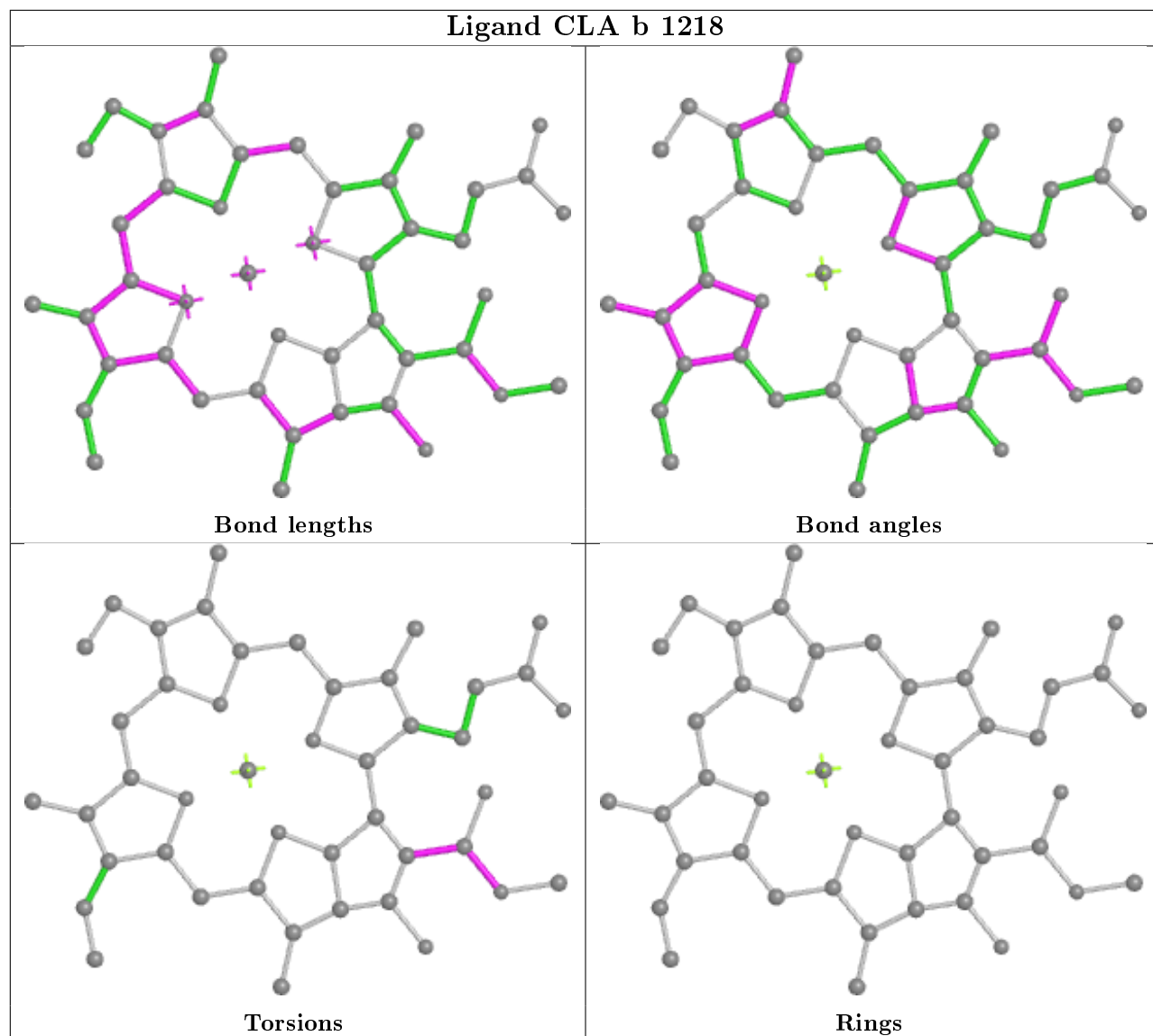
Continued from previous page...

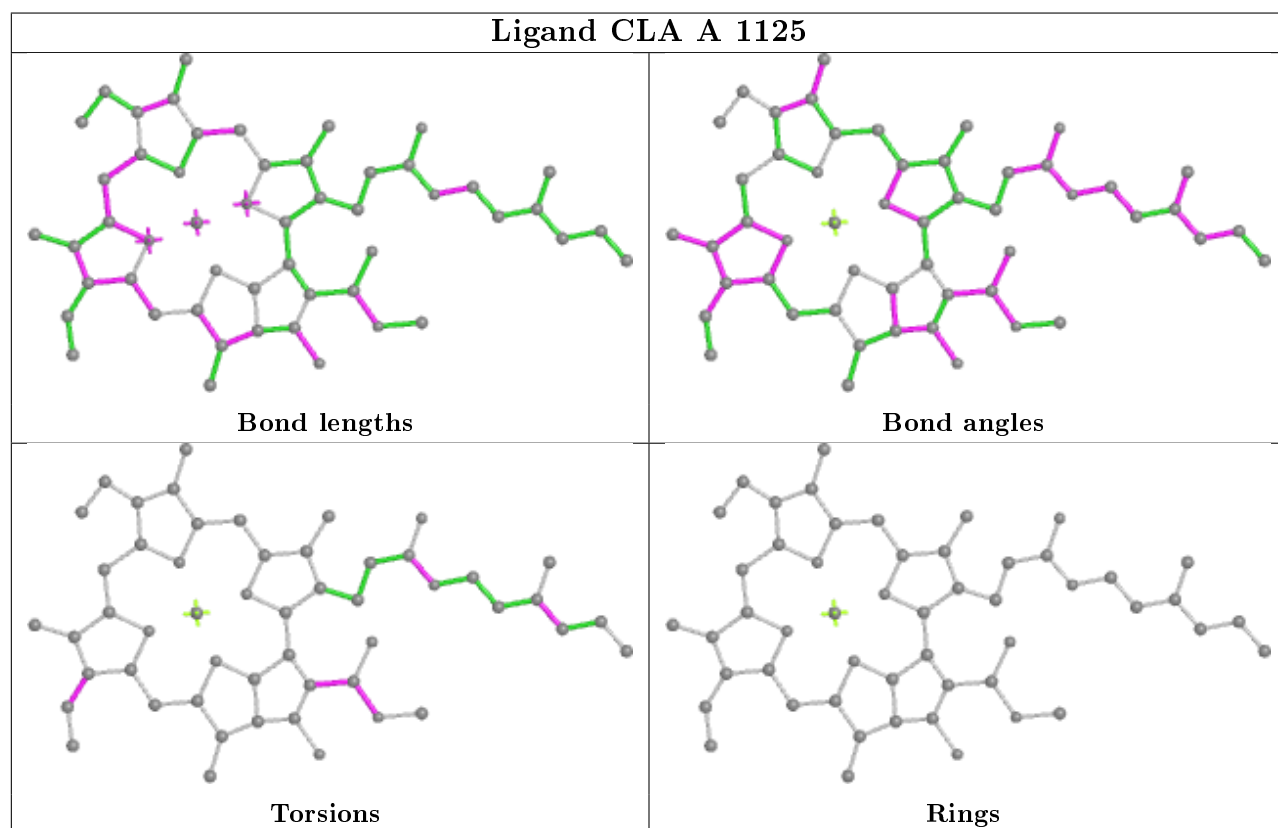
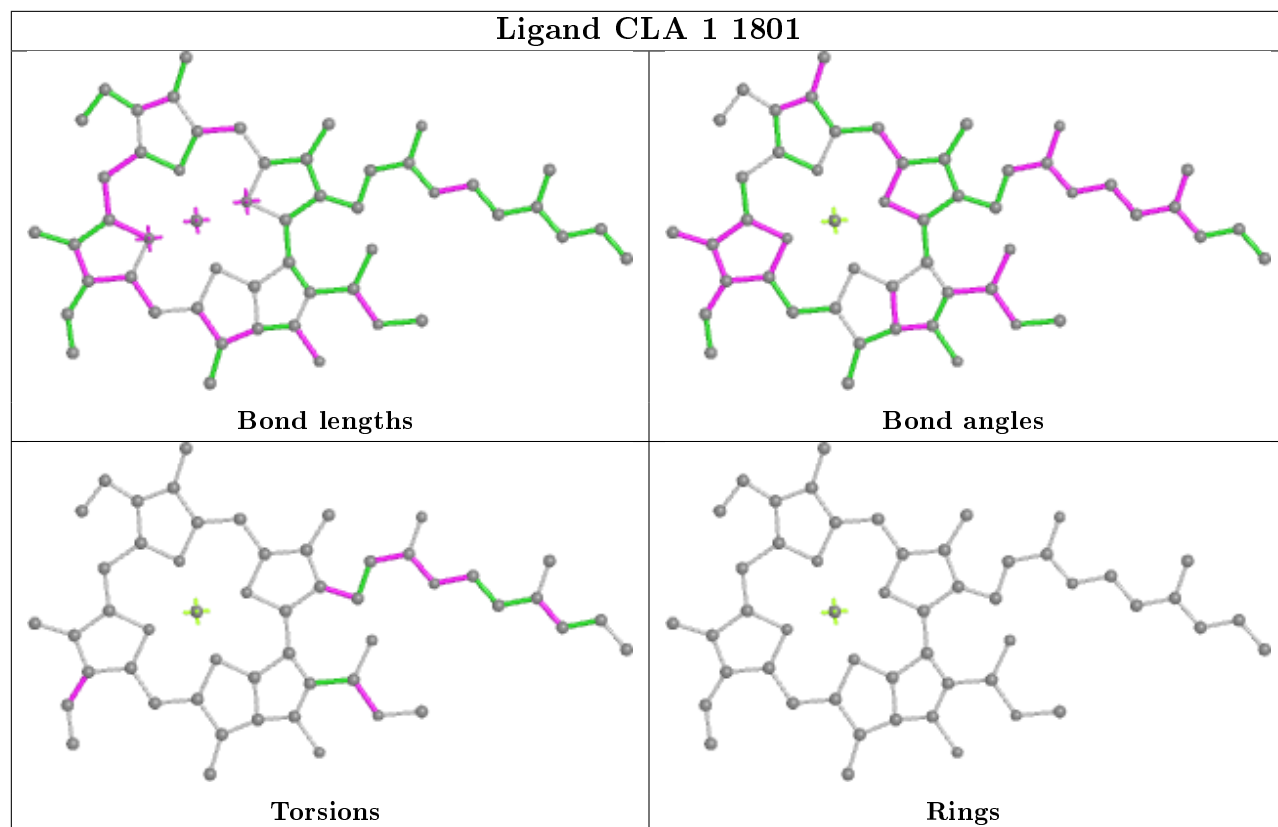
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	5002	LMG	1	0
11	2	1205	CLA	4	0
14	2	4004	BCR	2	0
11	A	1108	CLA	2	0
14	1	4007	BCR	7	0
14	F	4018	BCR	11	0
11	1	1113	CLA	3	0
11	2	1210	CLA	2	0
11	1	1107	CLA	3	0
14	6	4013	BCR	7	0
14	B	4014	BCR	6	0
14	2	4017	BCR	9	0
14	B	4005	BCR	7	0
11	1	1105	CLA	1	0
11	1	1102	CLA	1	0
11	1	1117	CLA	2	0
11	A	1102	CLA	4	0
11	2	1013	CLA	5	0
11	2	1207	CLA	4	0
11	B	1229	CLA	6	0
11	2	1222	CLA	3	0
11	A	1110	CLA	2	0
11	1	1128	CLA	9	0

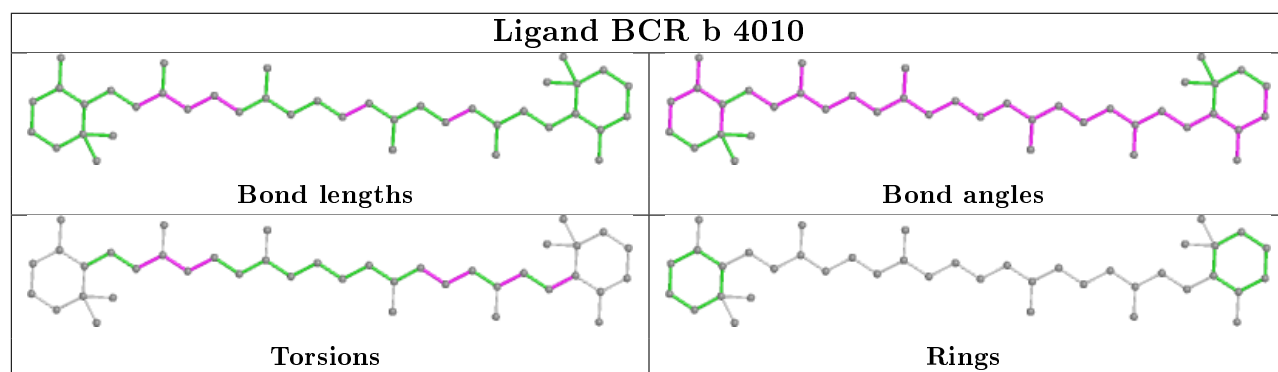
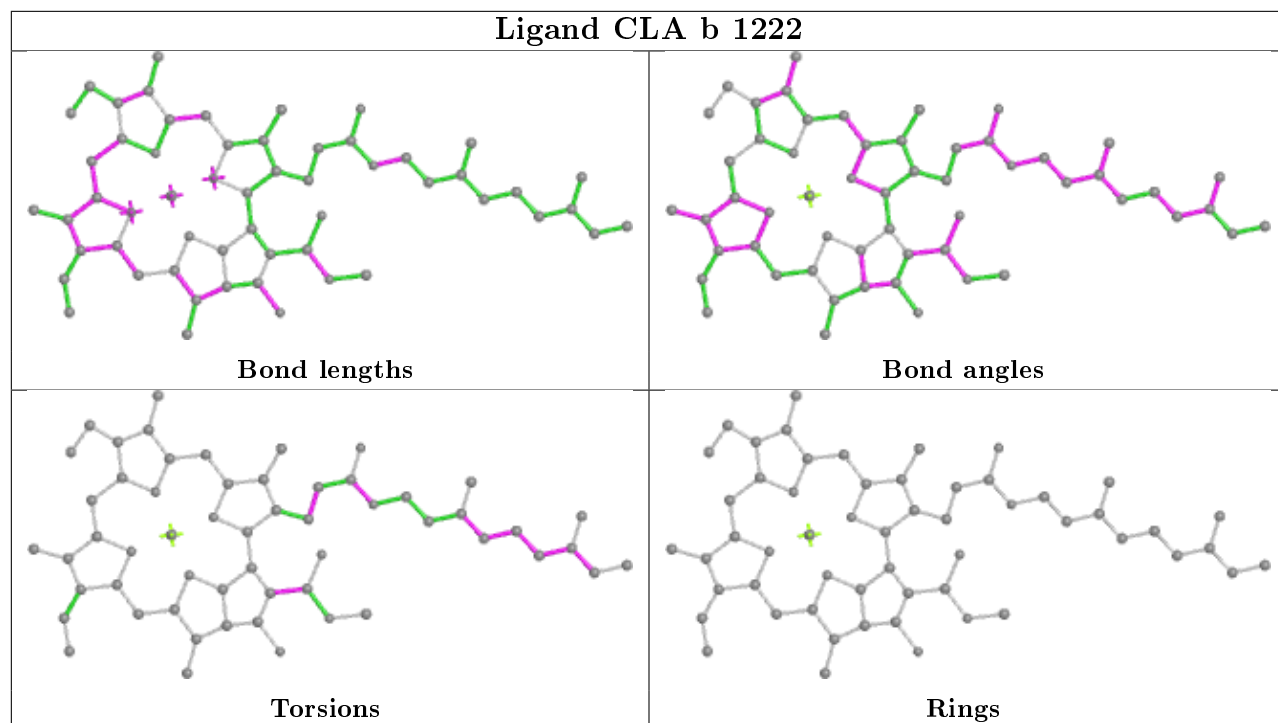
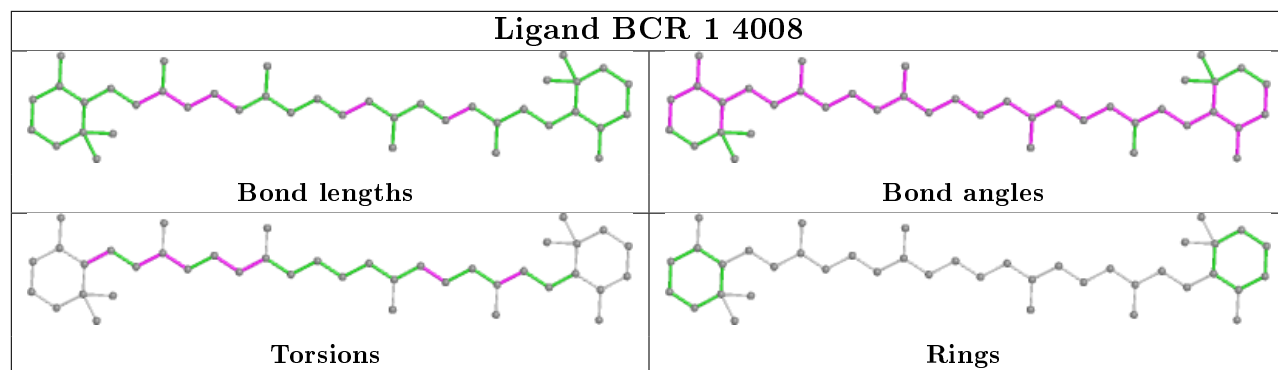
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

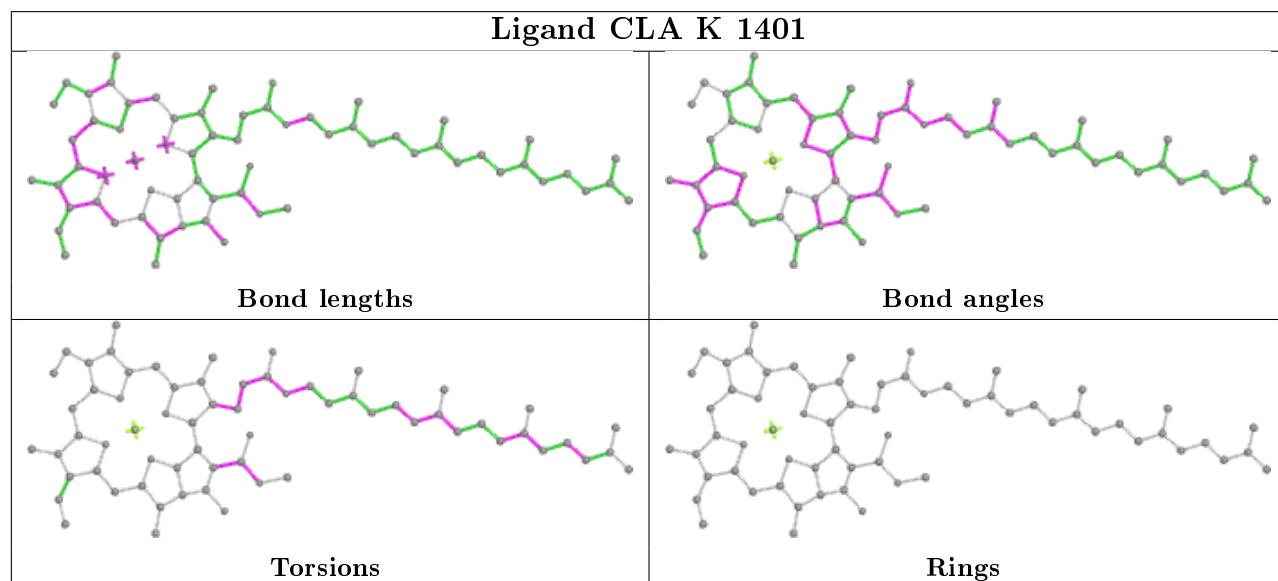
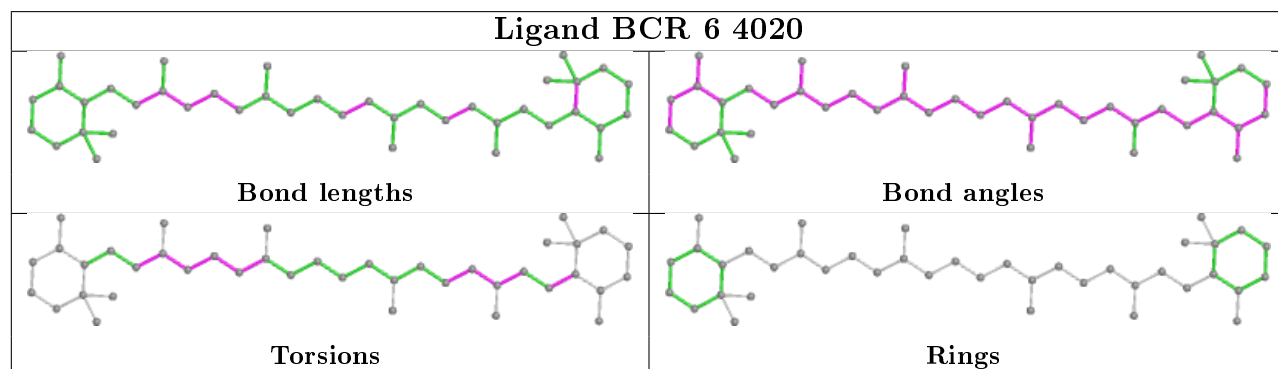
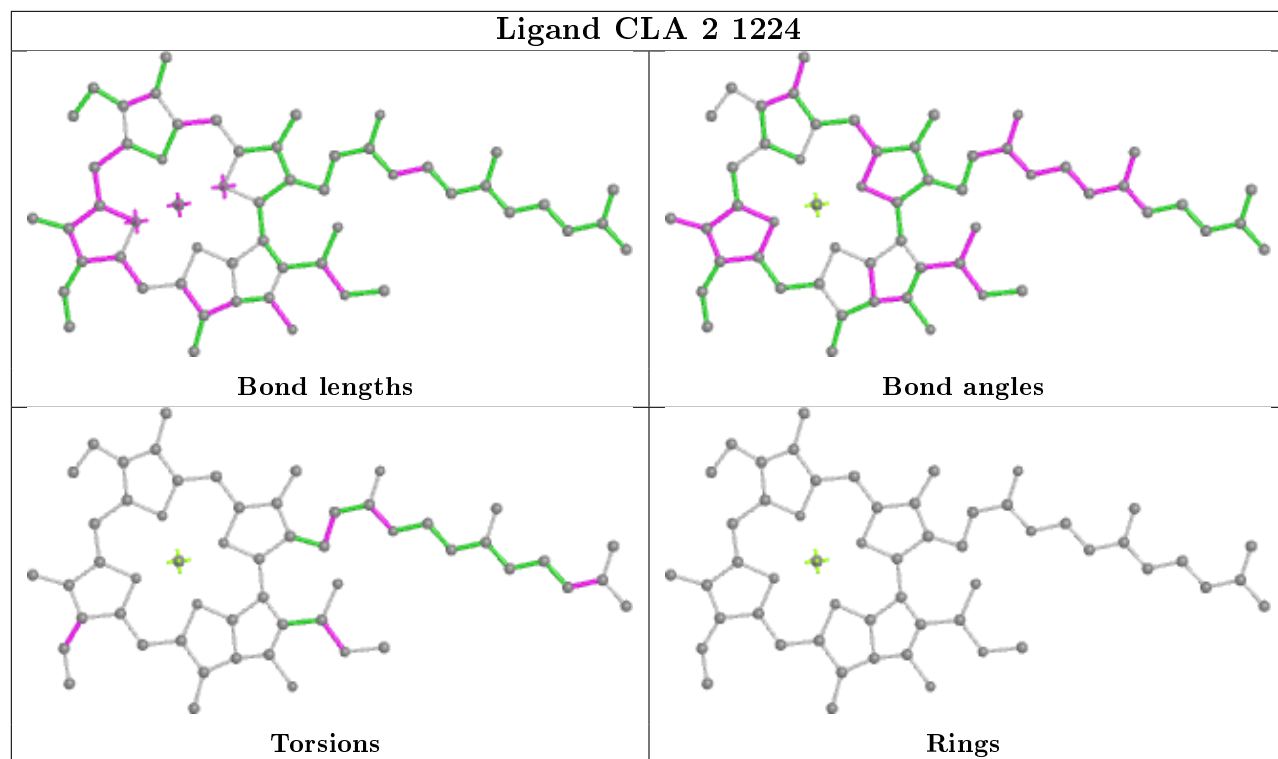


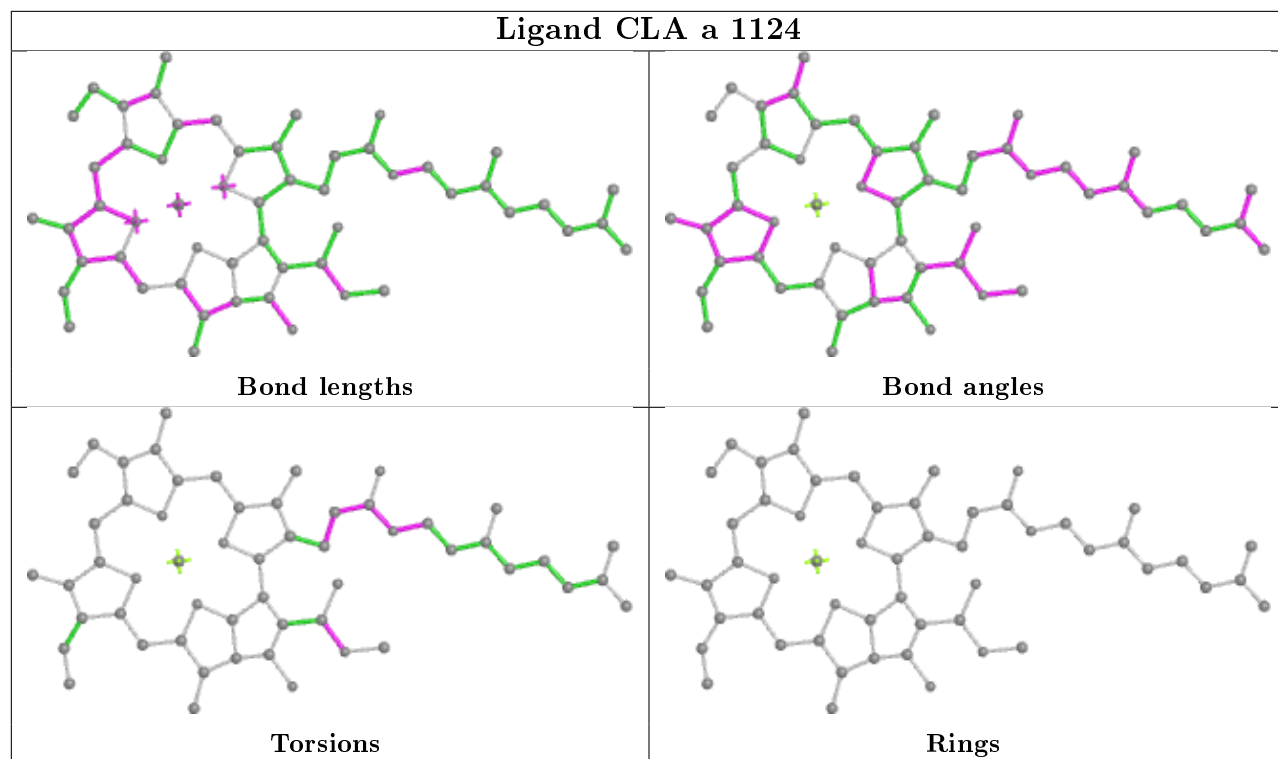


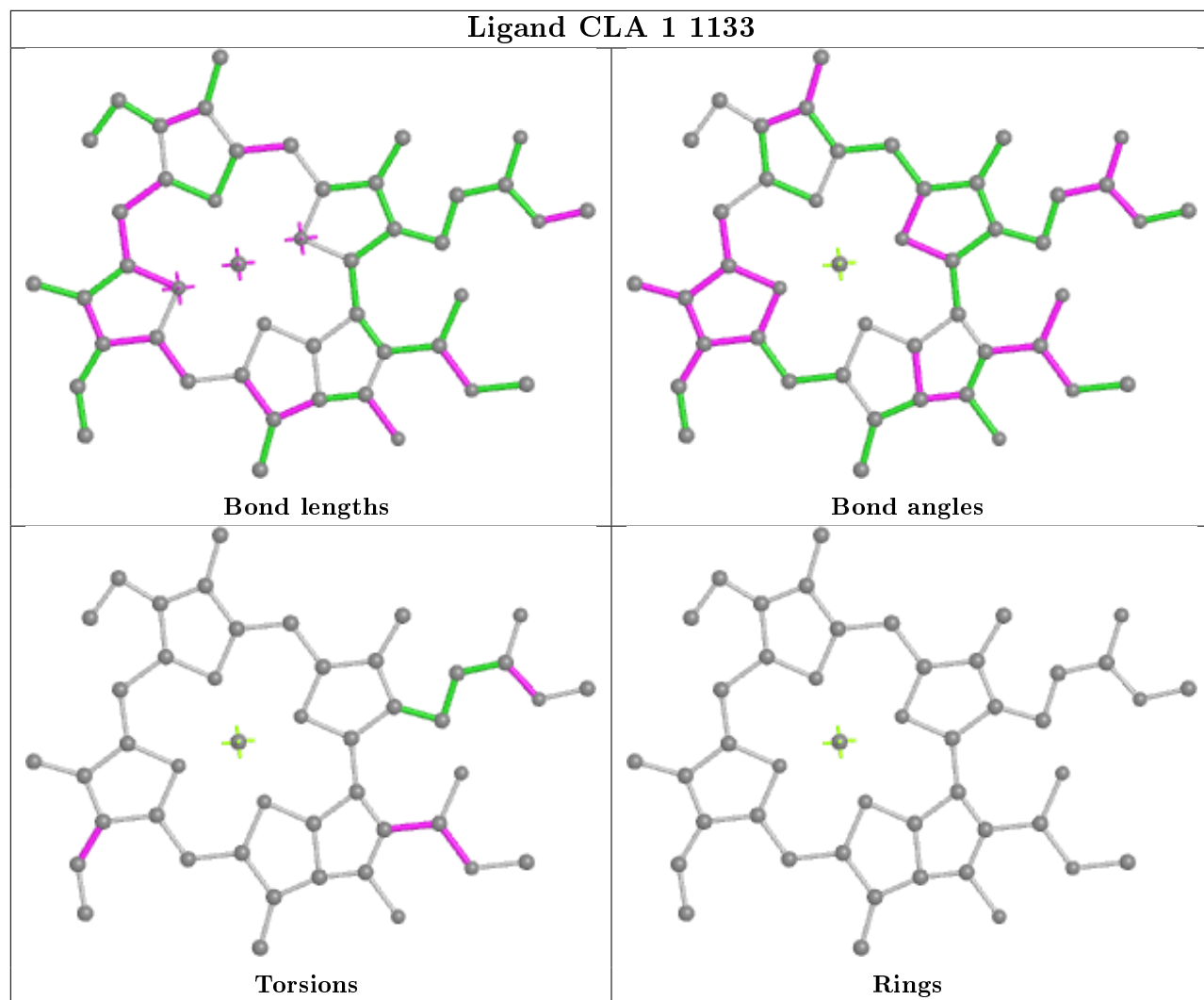


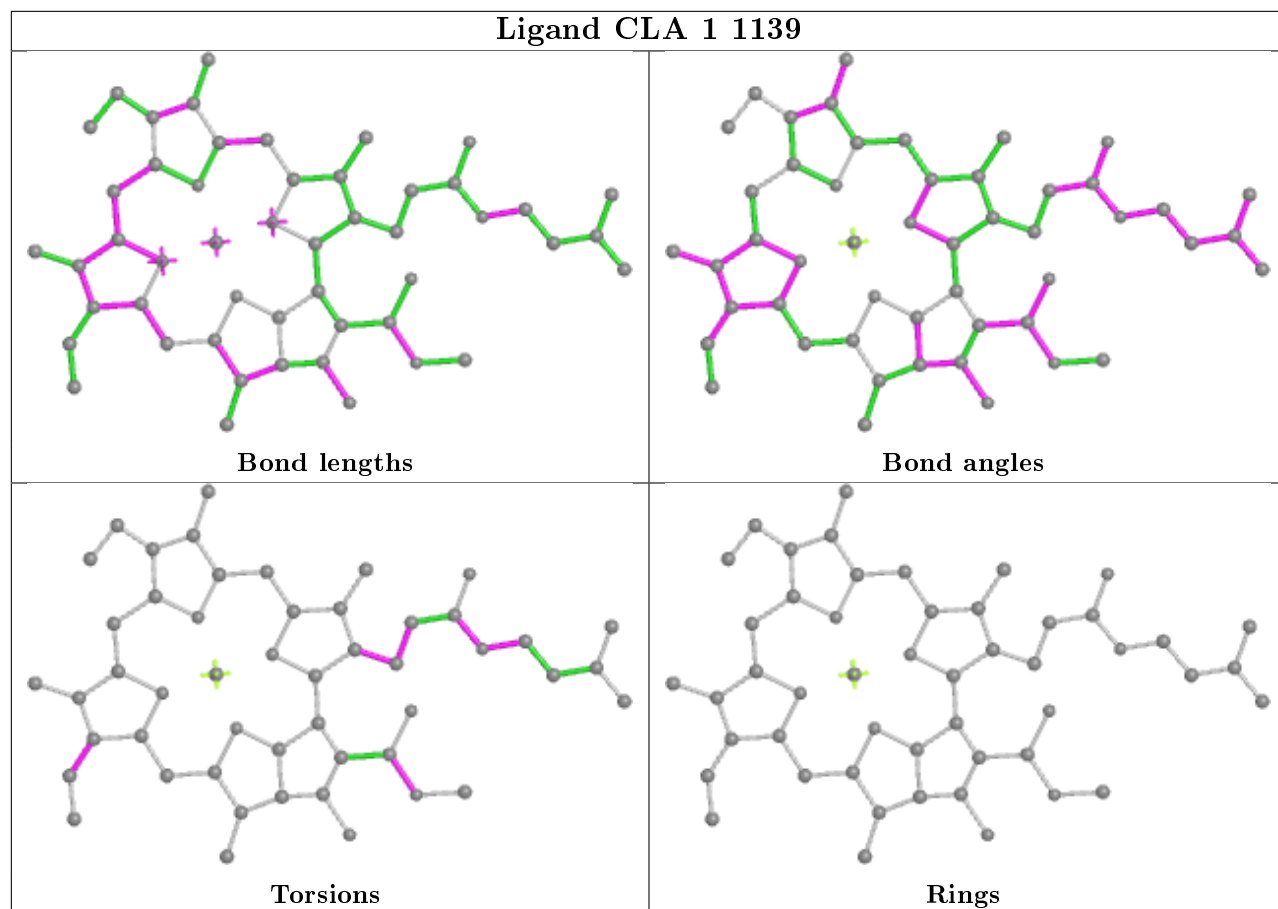


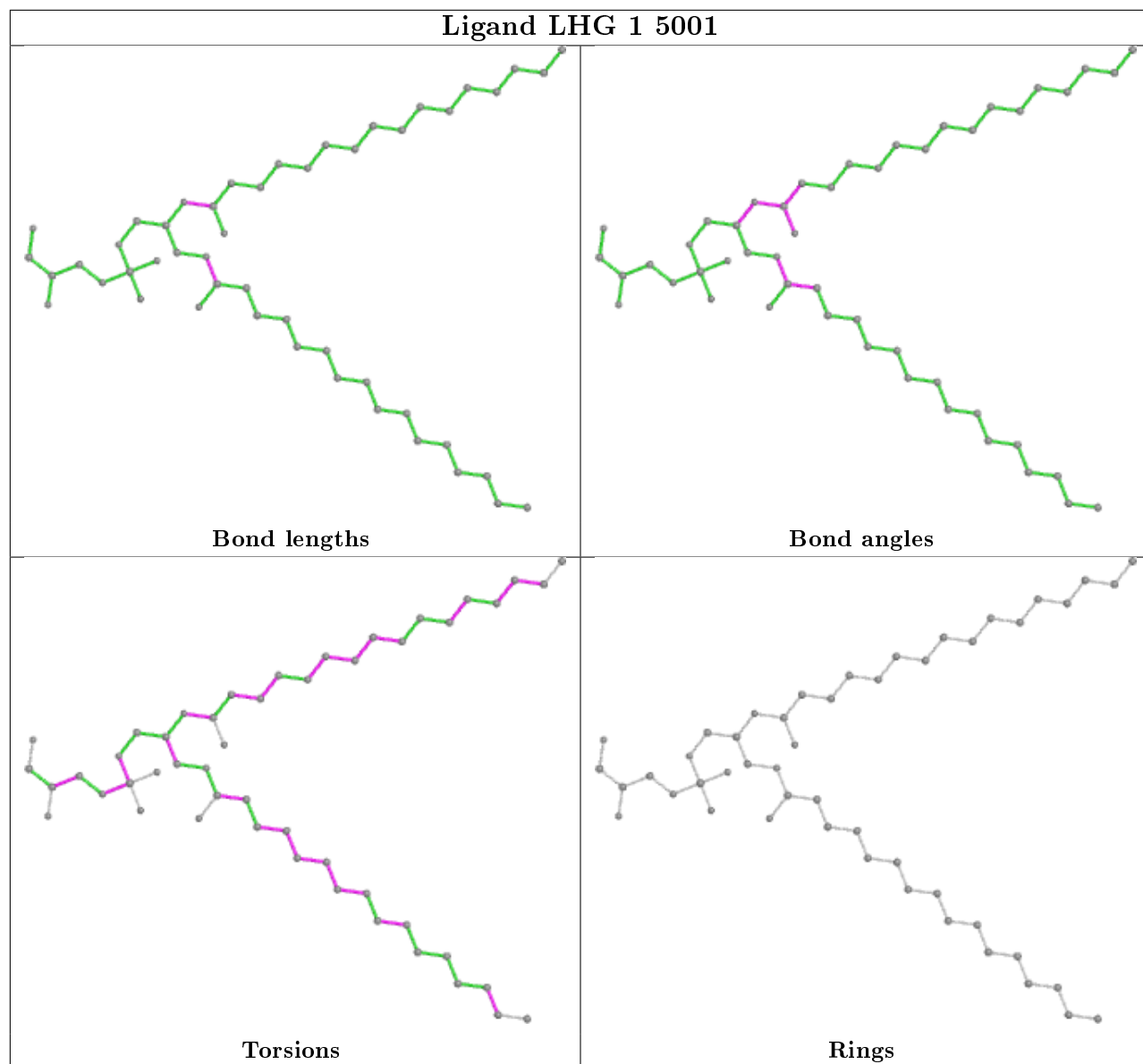


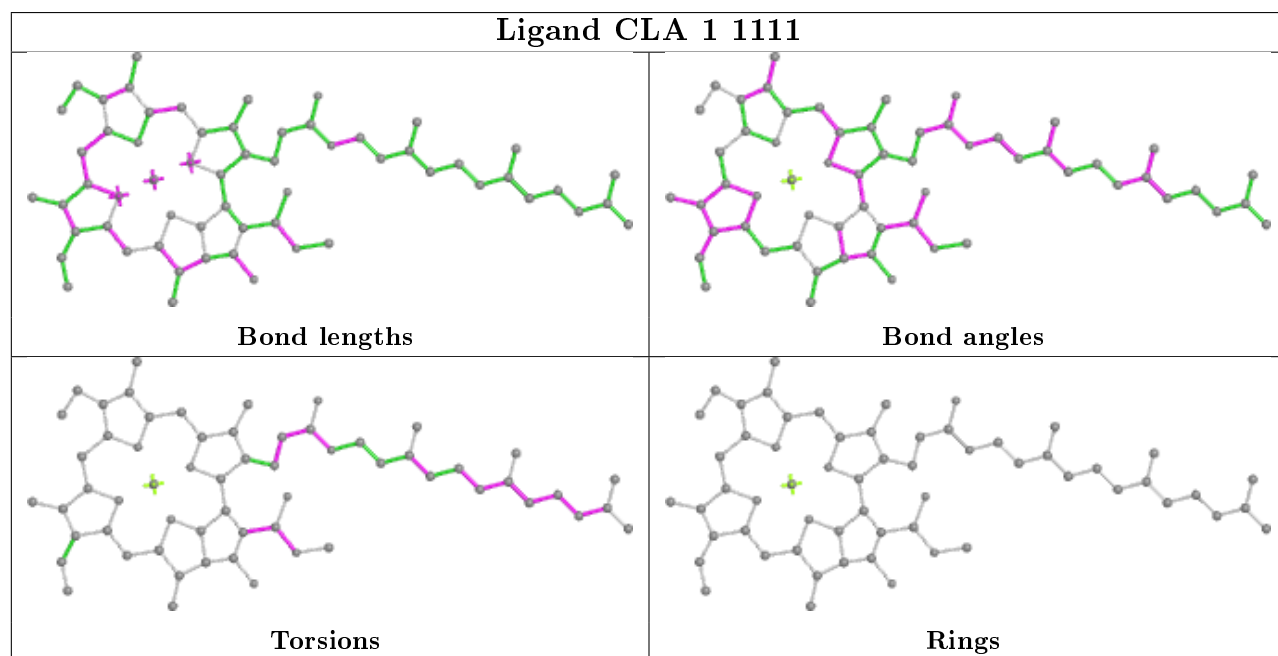
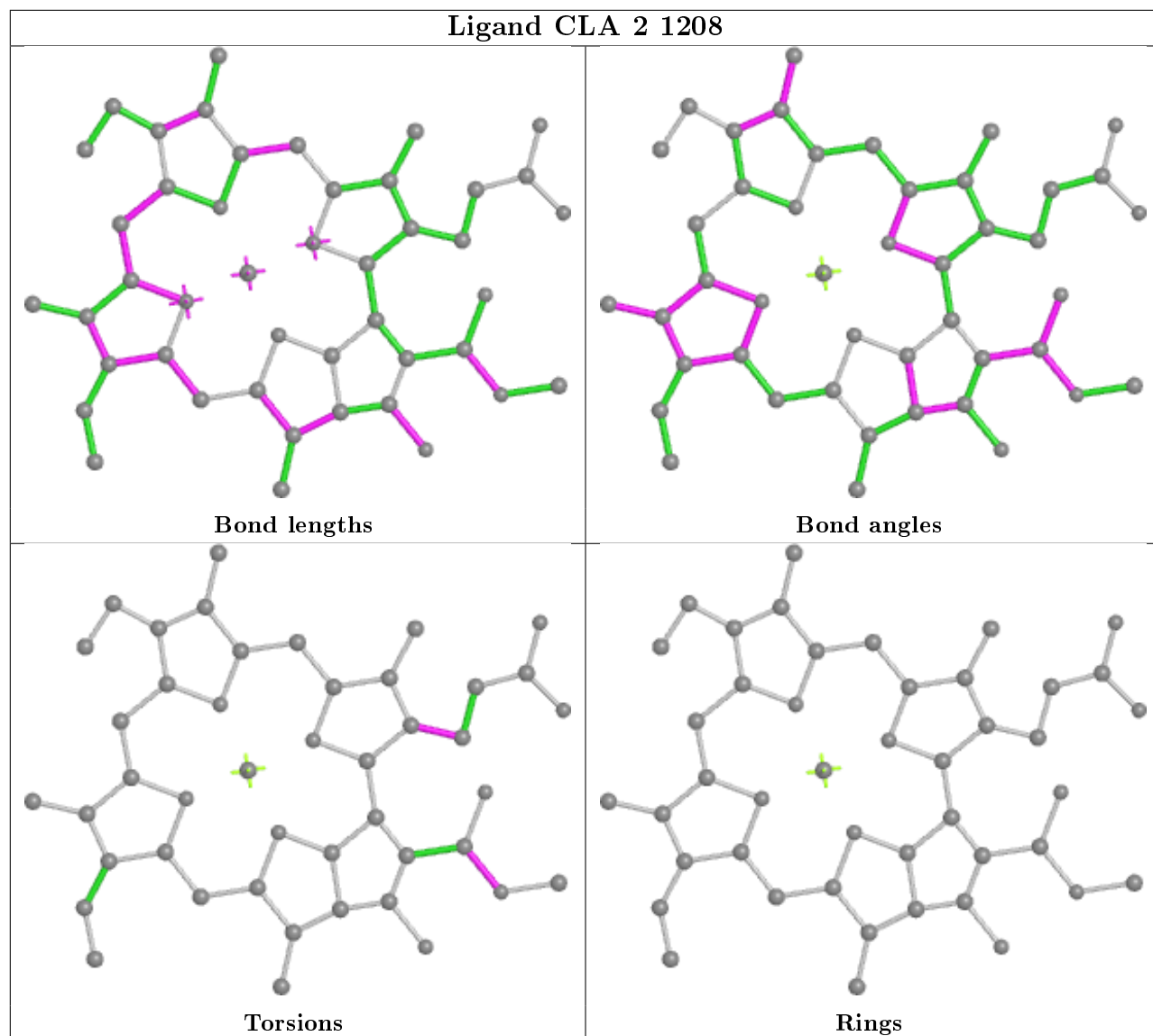


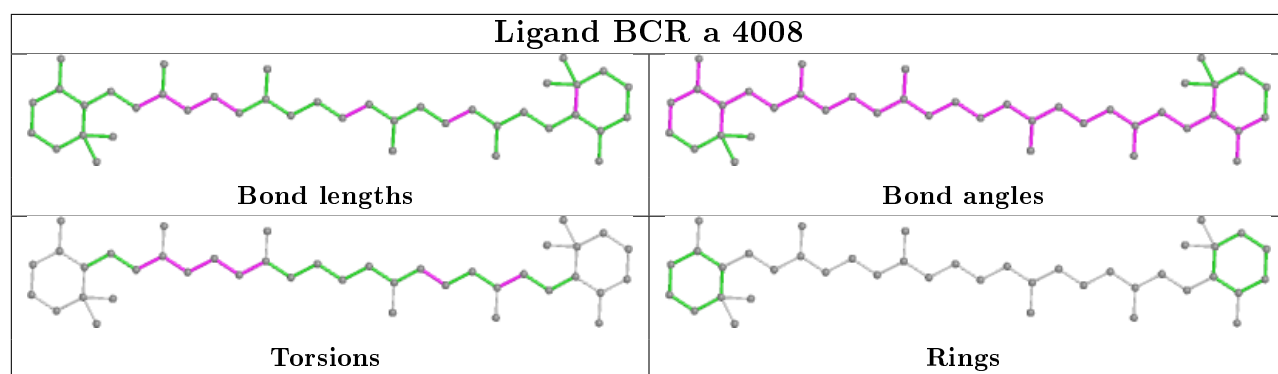
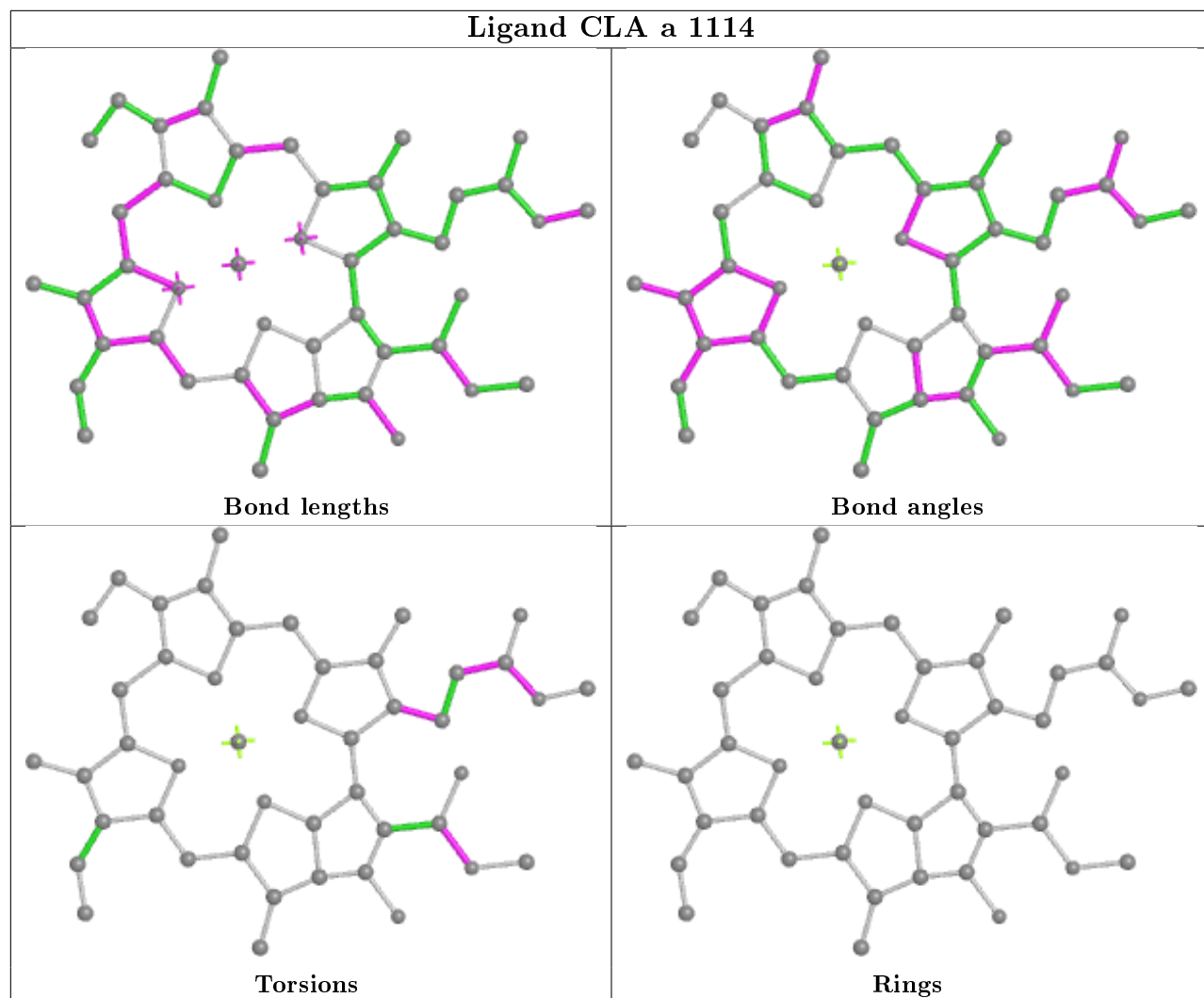


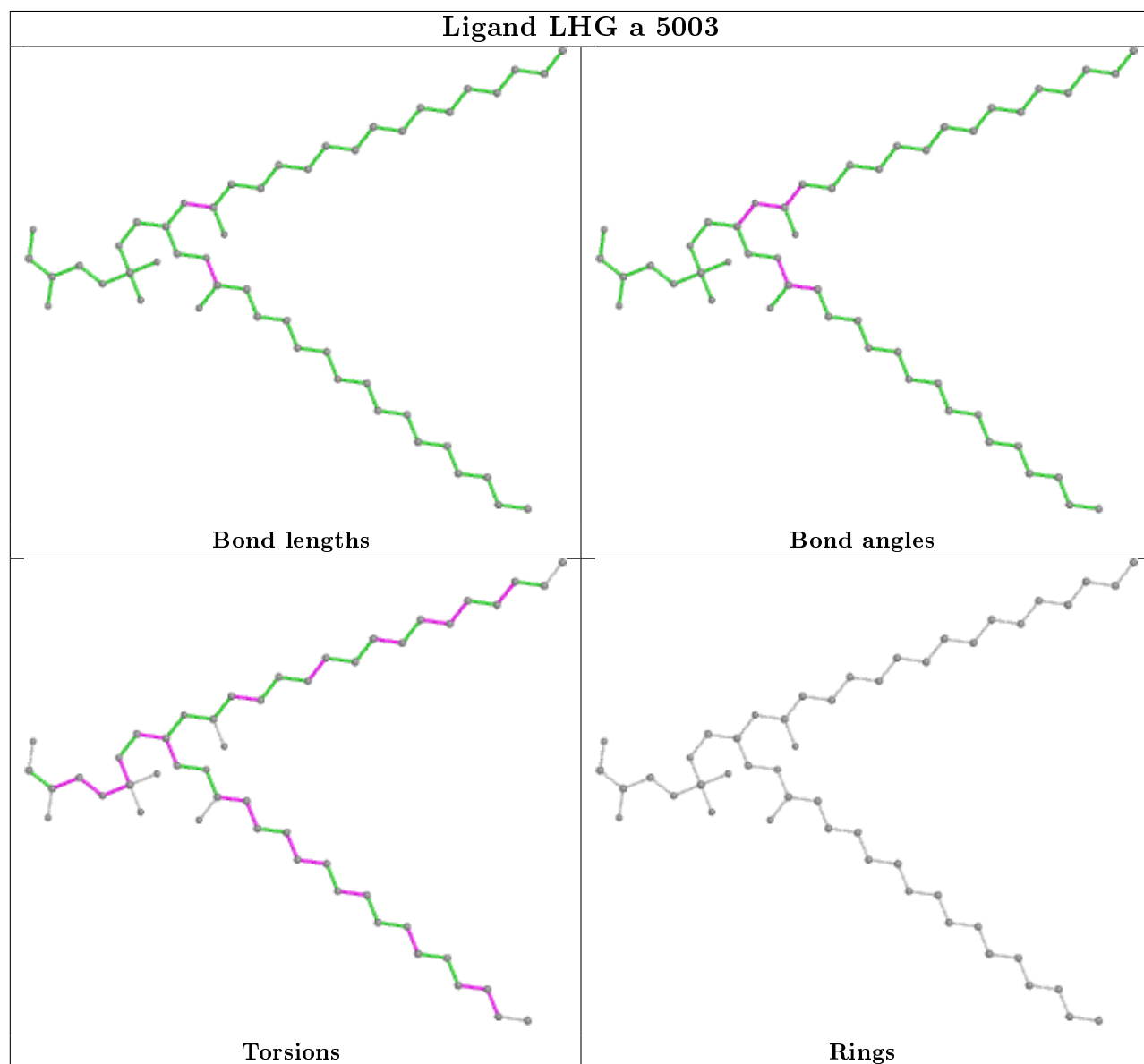
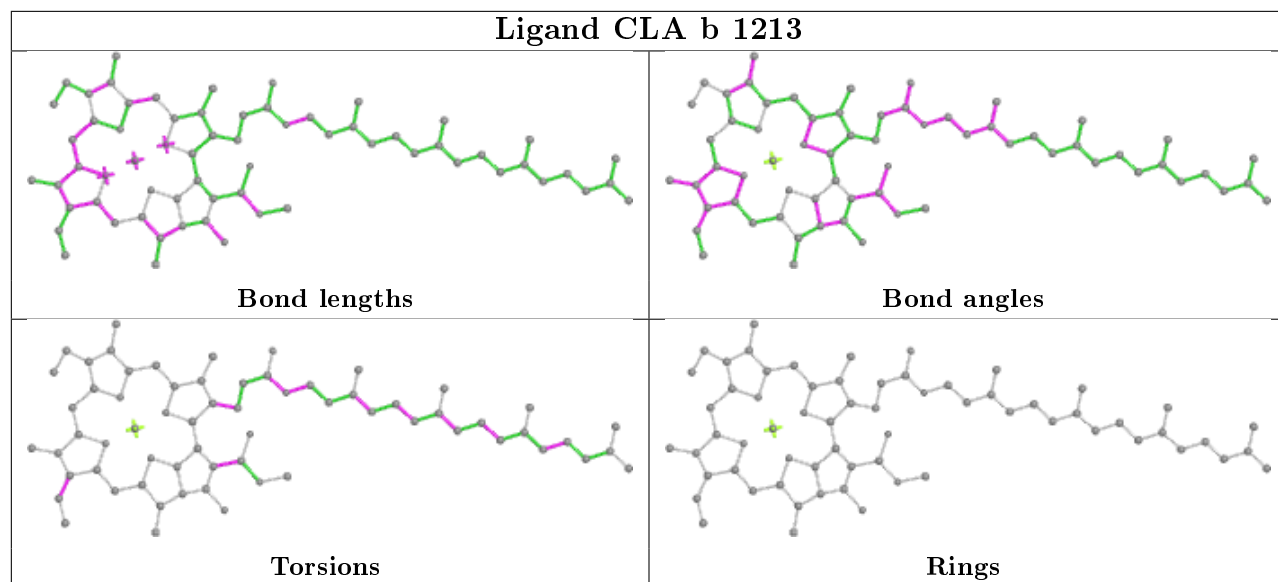


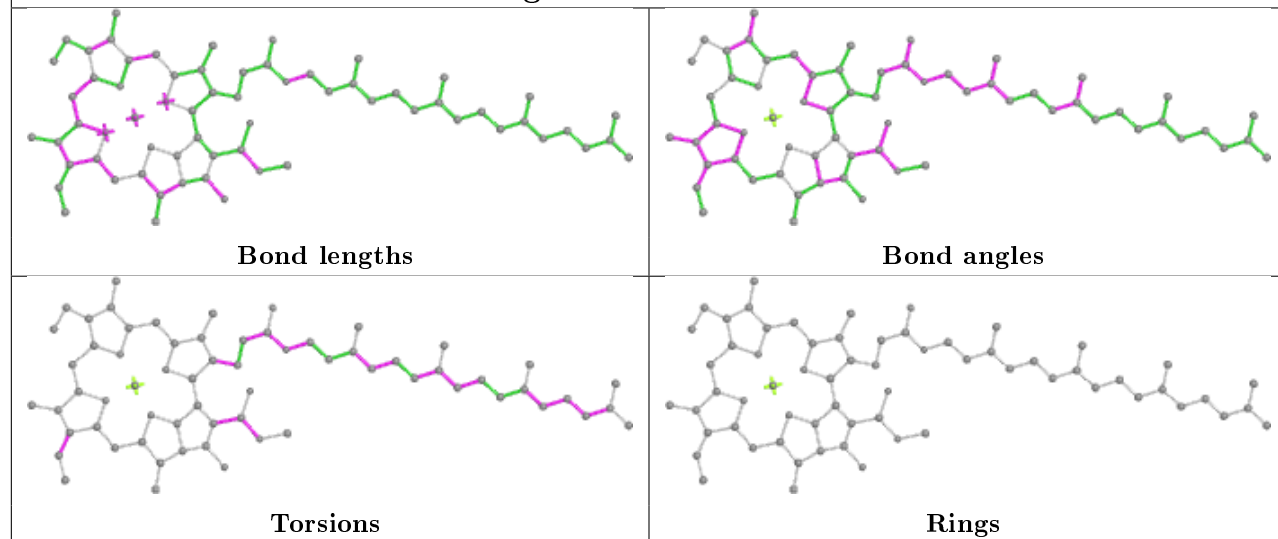
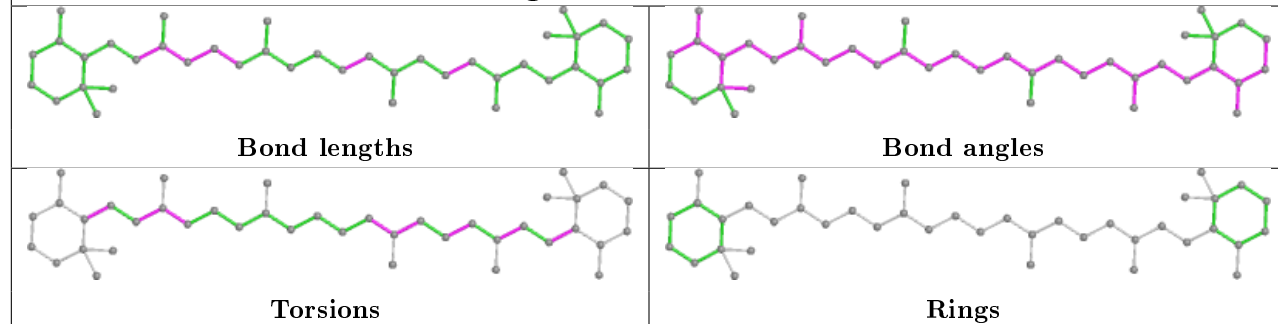


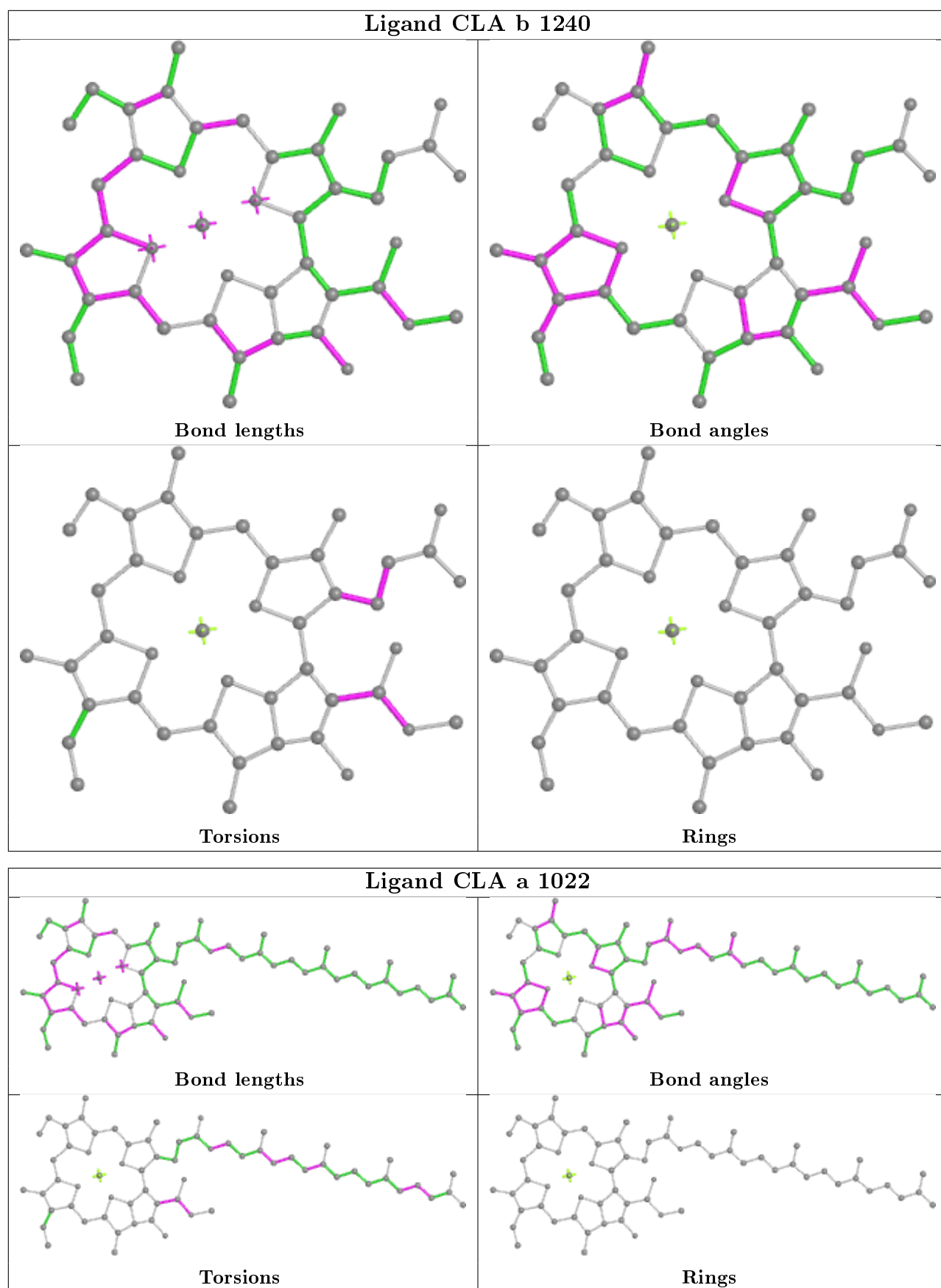




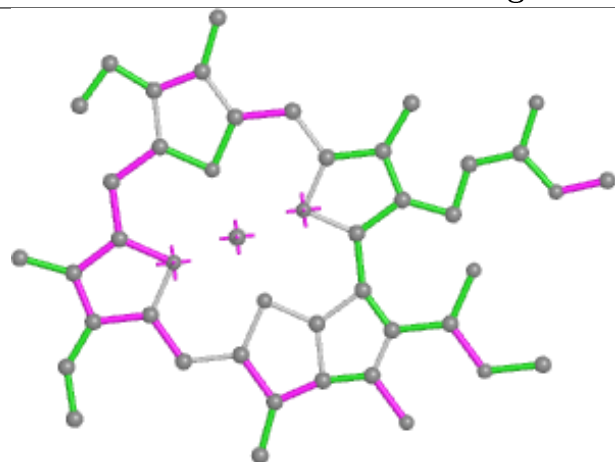




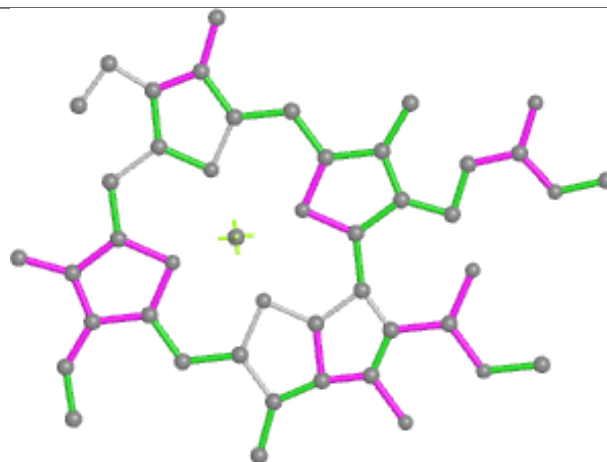
Ligand CLA B 1210**Ligand BCR b 4011**



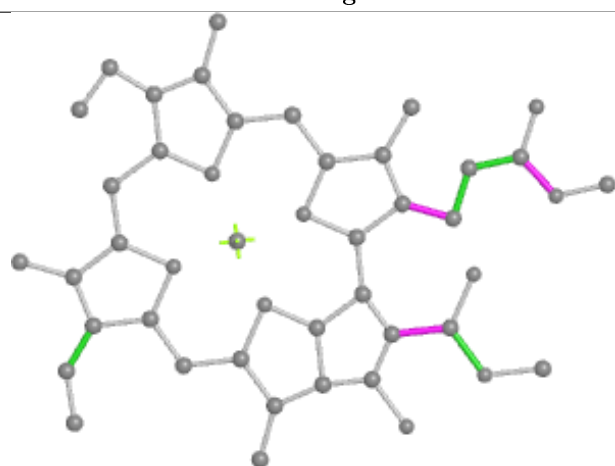
Ligand CLA A 1120



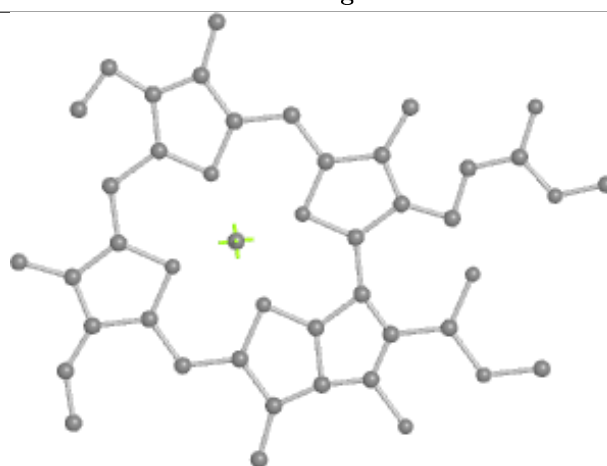
Bond lengths



Bond angles

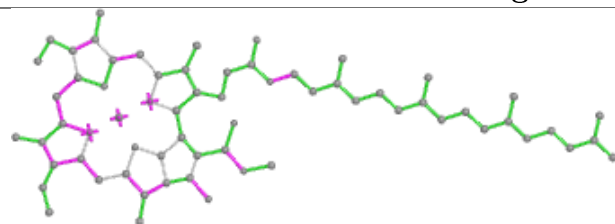


Torsions

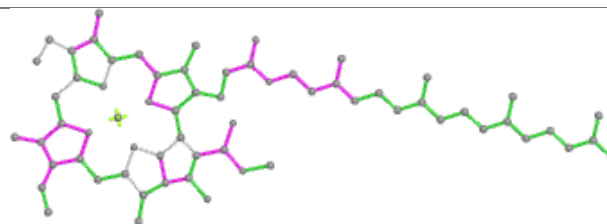


Rings

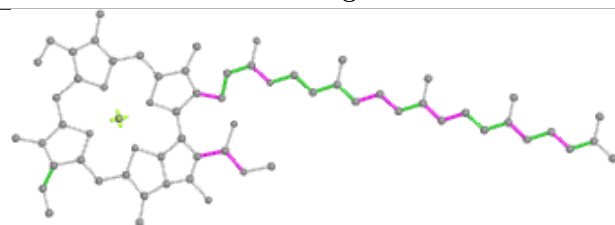
Ligand CLA 8 1501



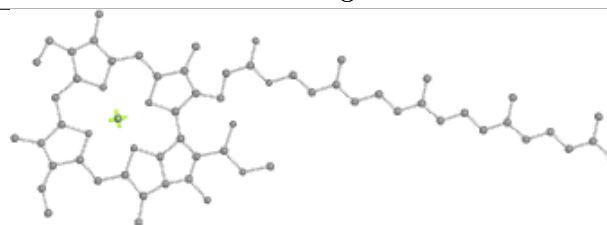
Bond lengths



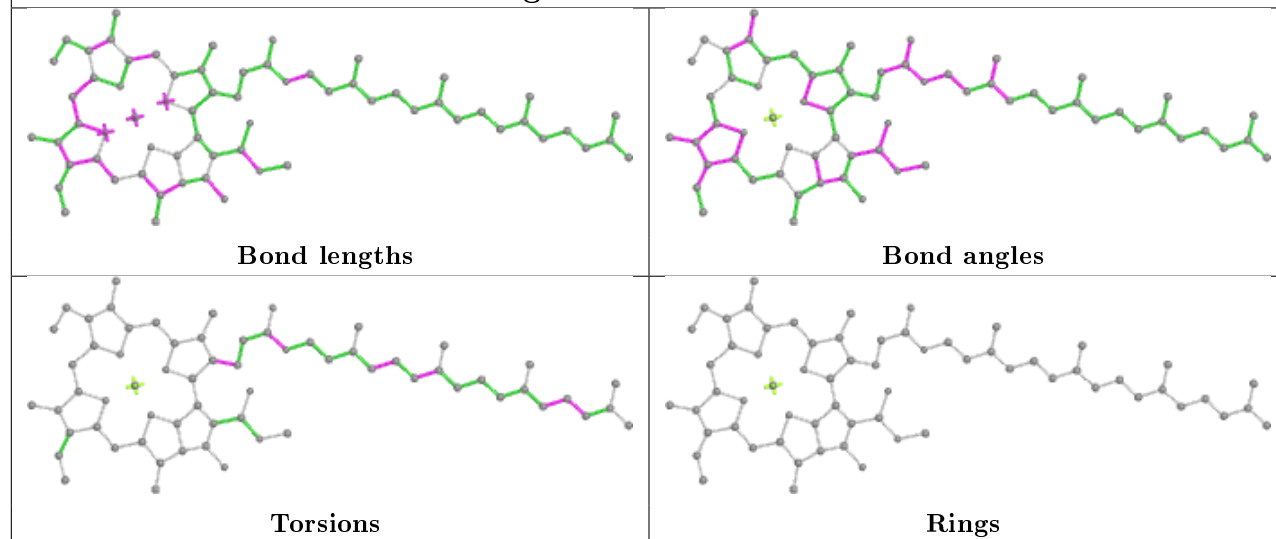
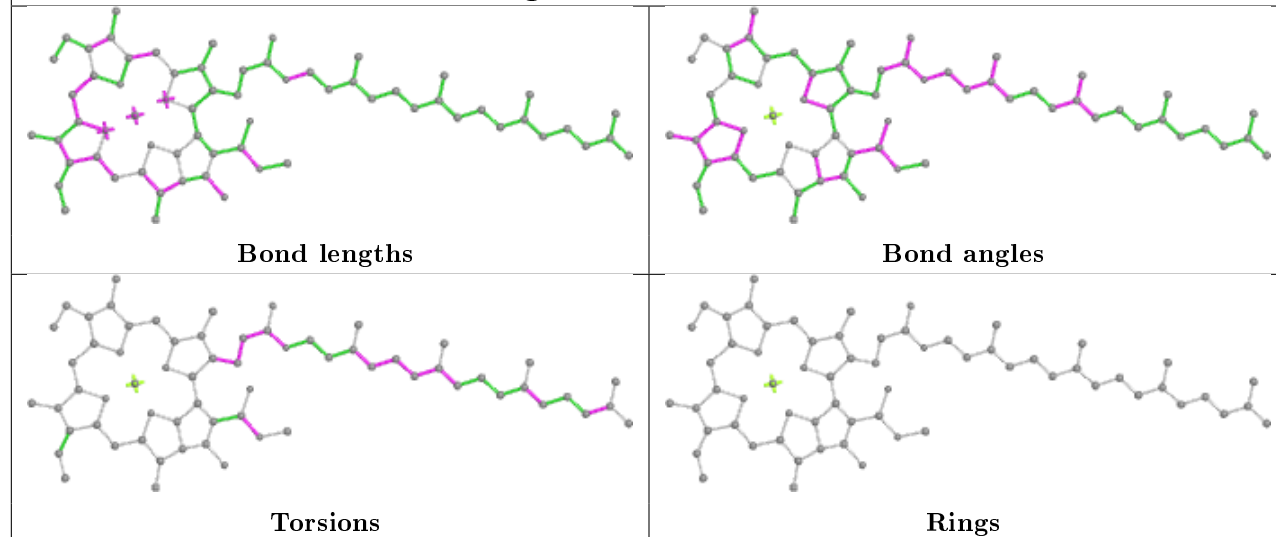
Bond angles

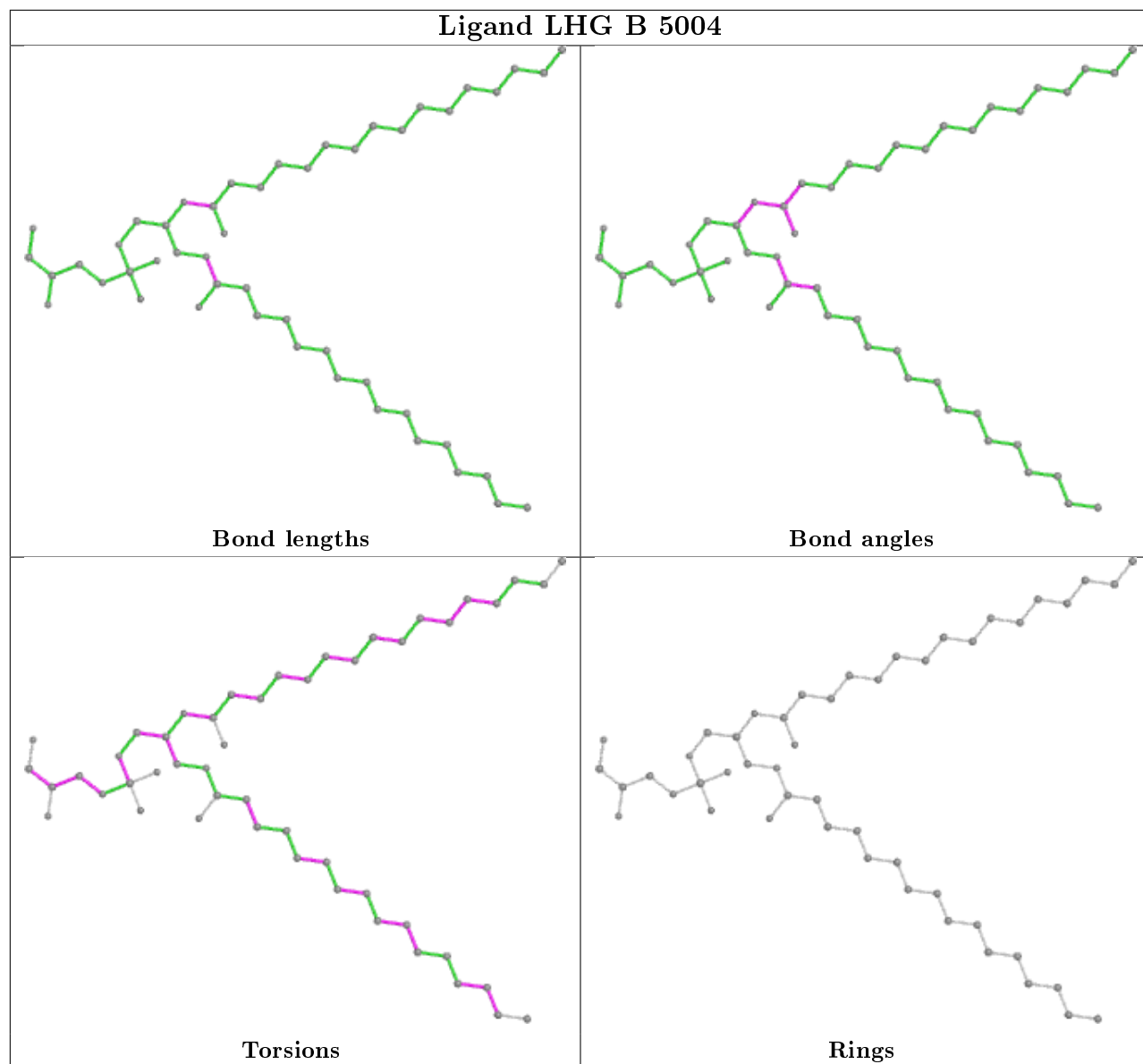


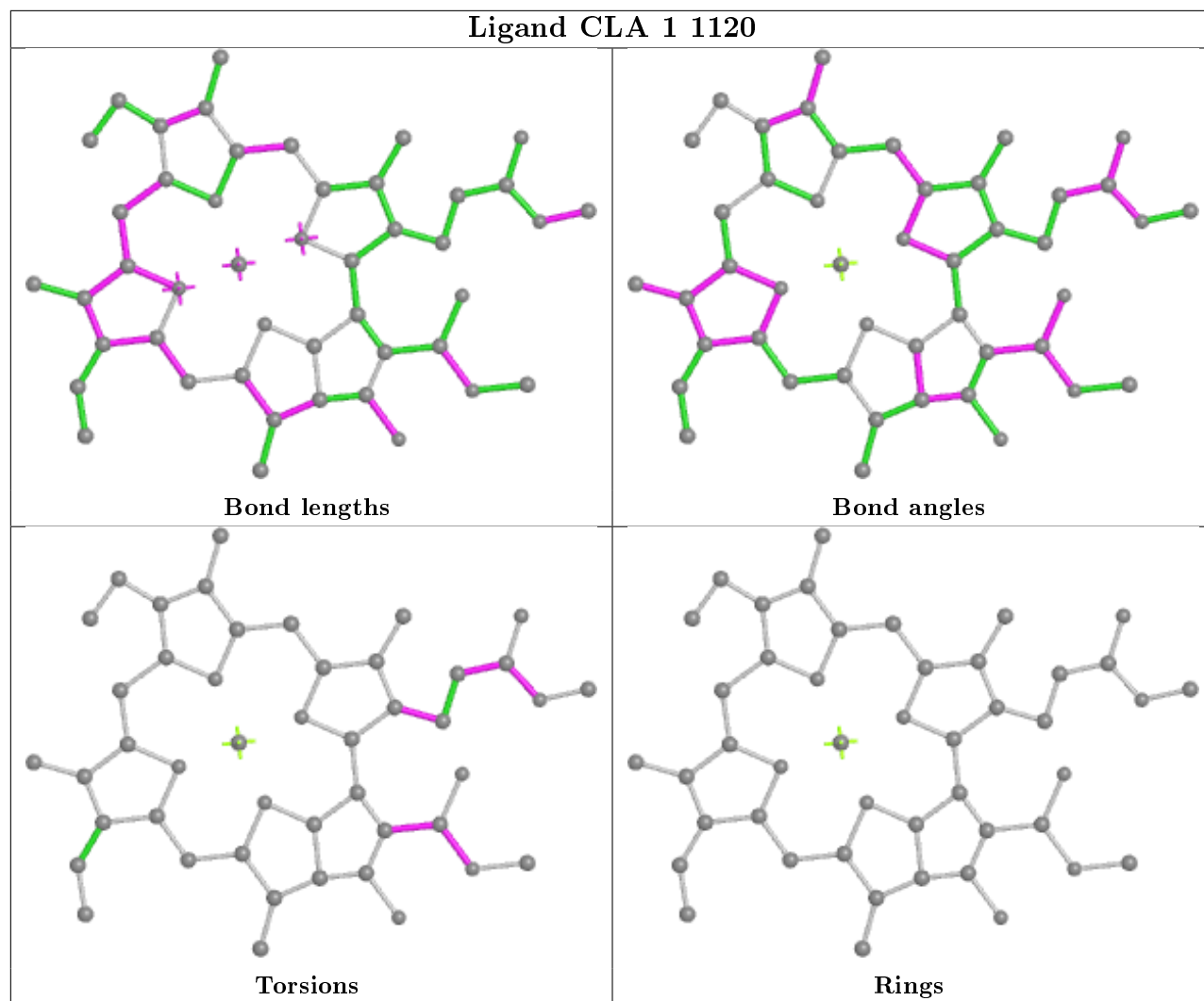
Torsions

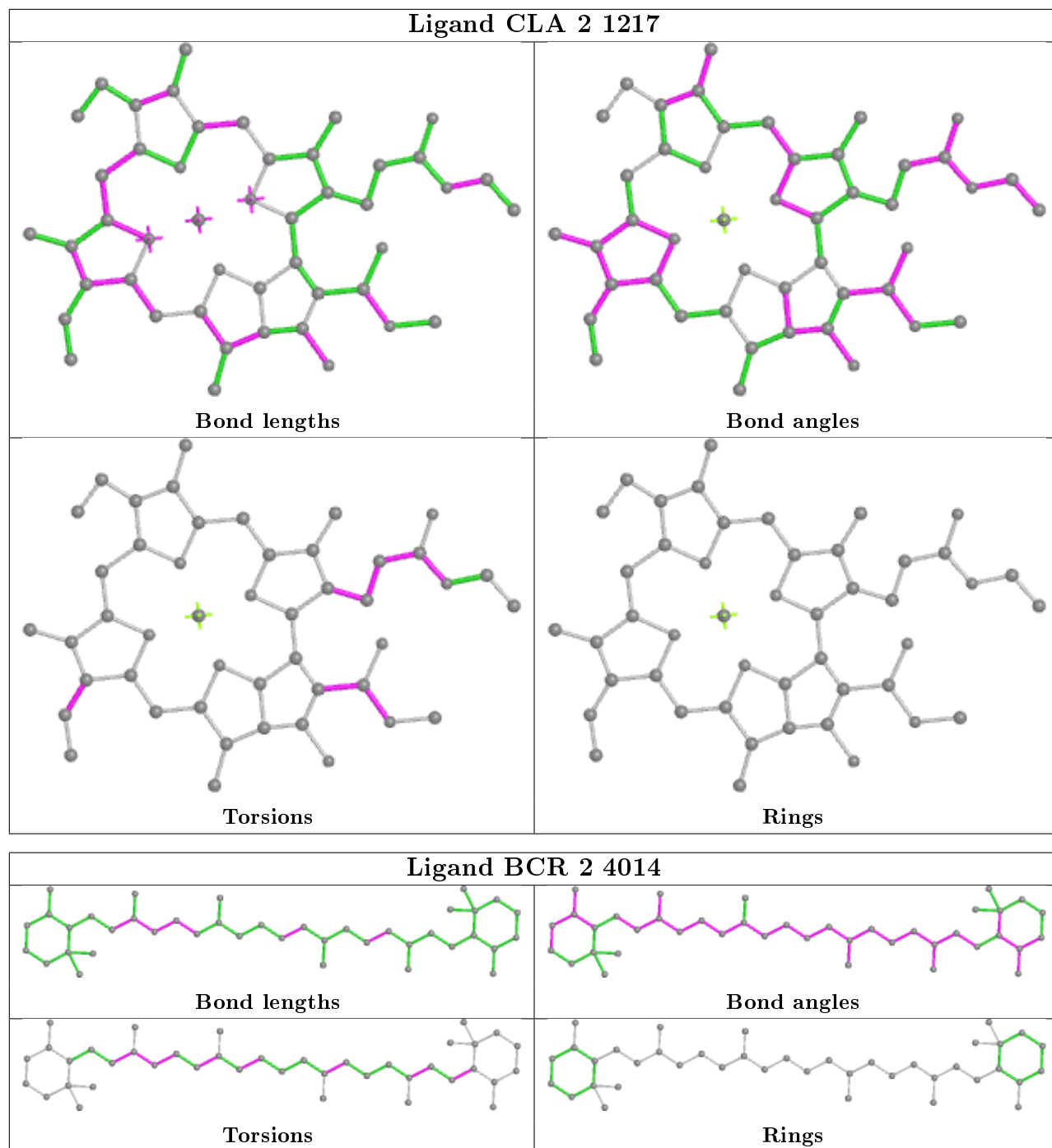


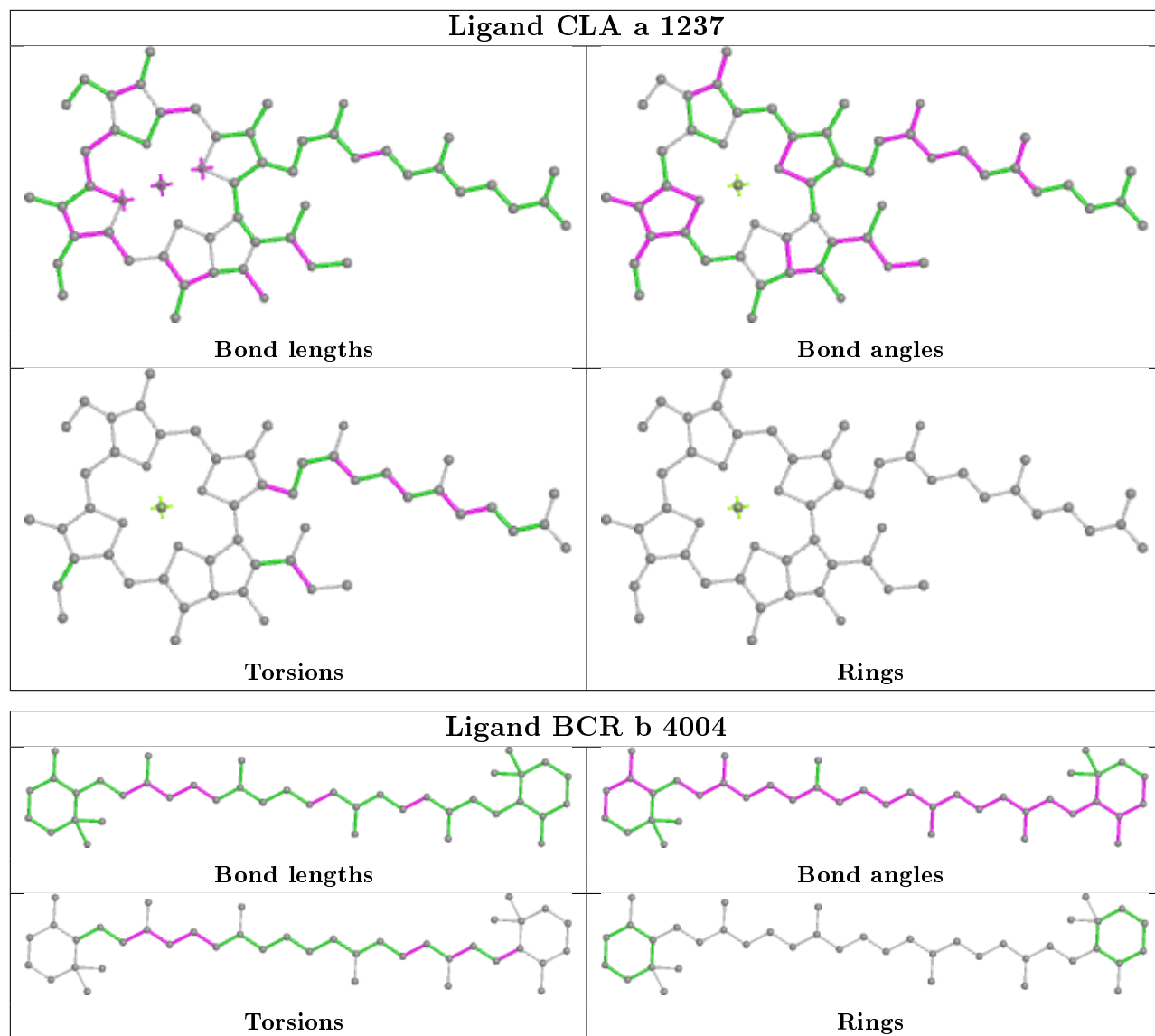
Rings

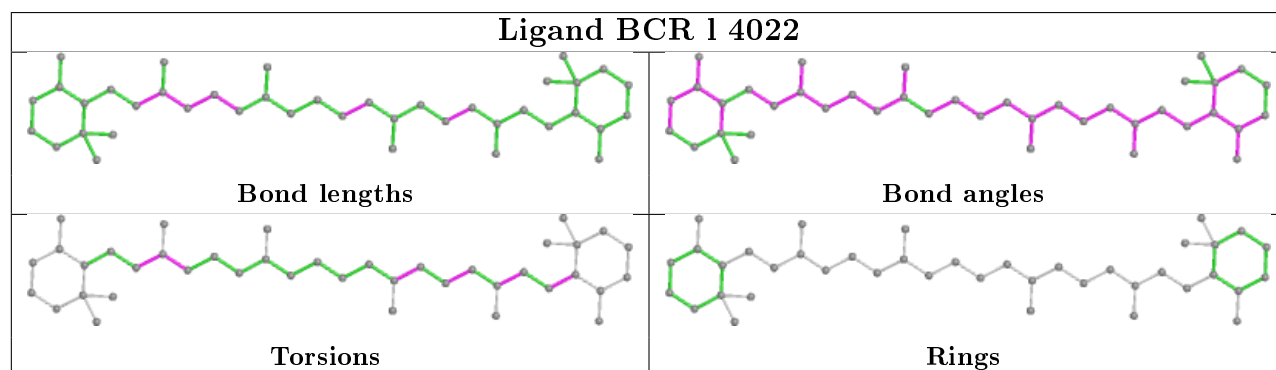
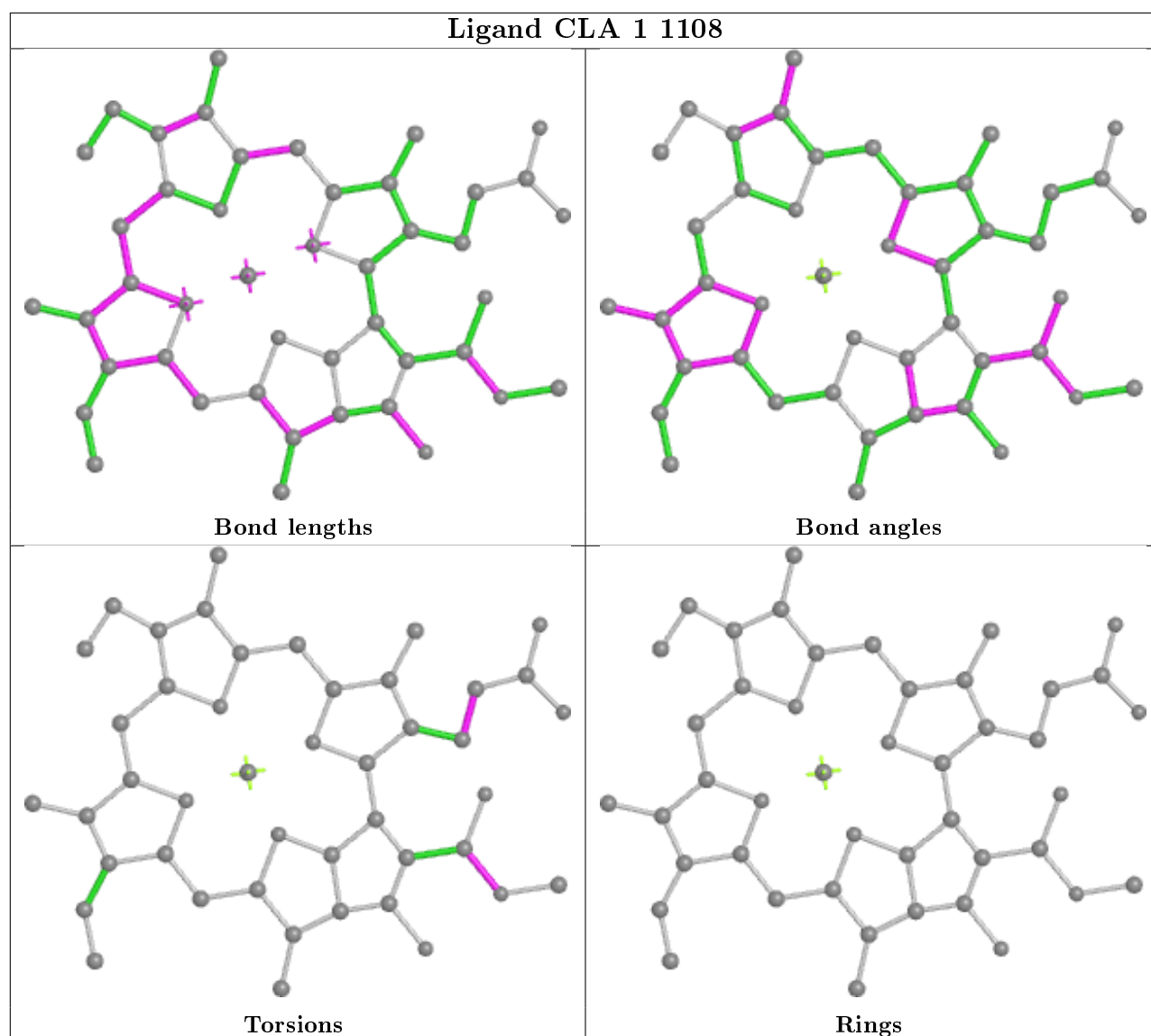
Ligand CLA B 1216**Ligand CLA B 1213**

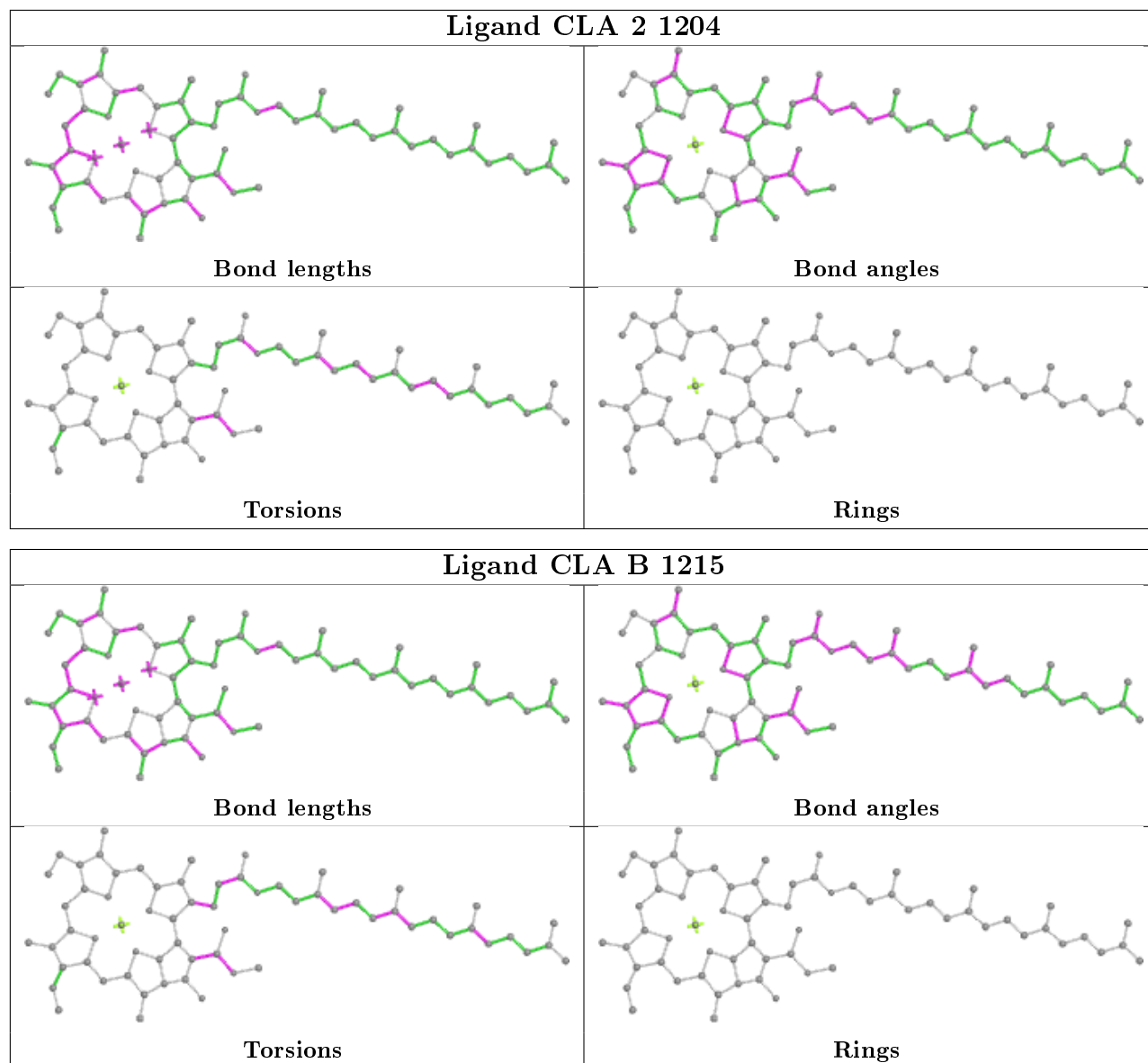




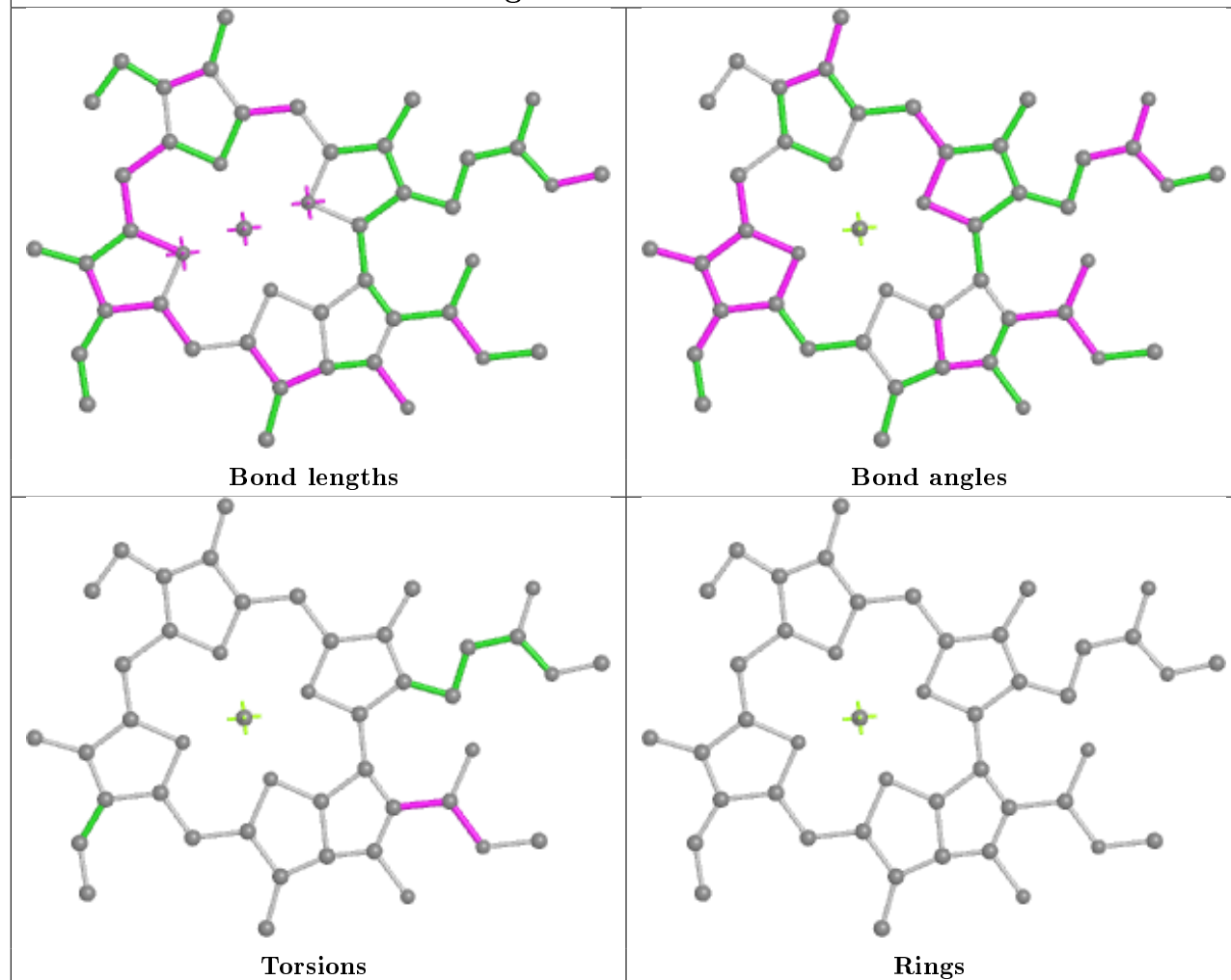




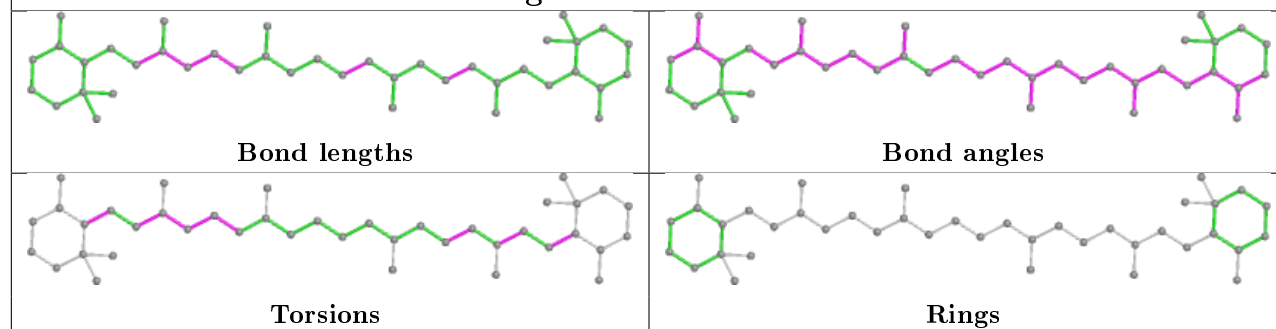




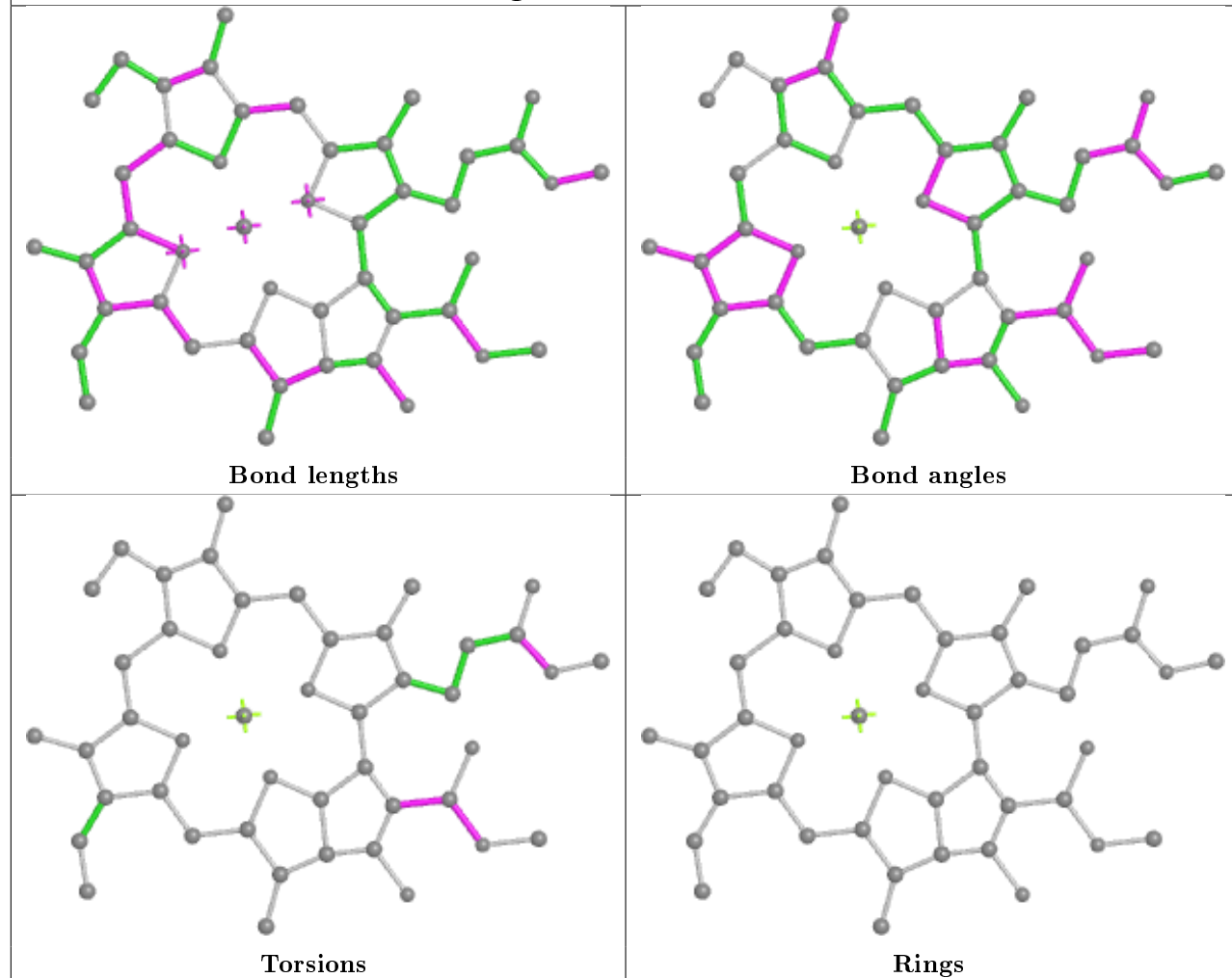
Ligand CLA A 1133



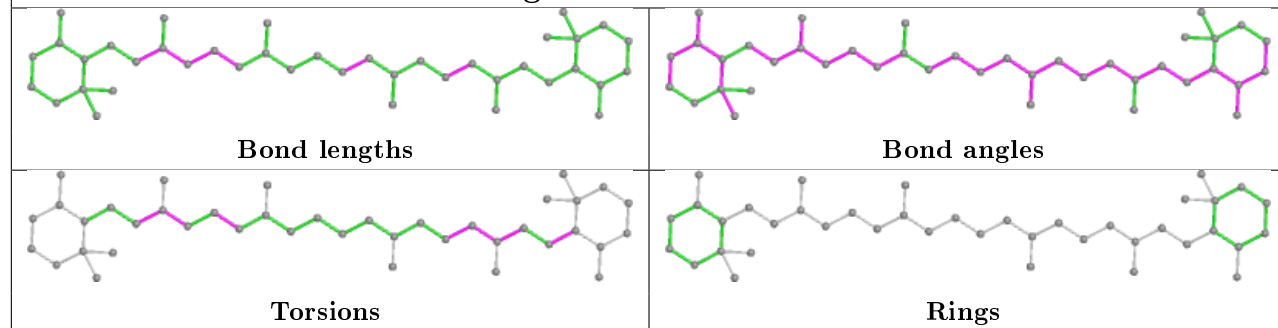
Ligand BCR 7 4021

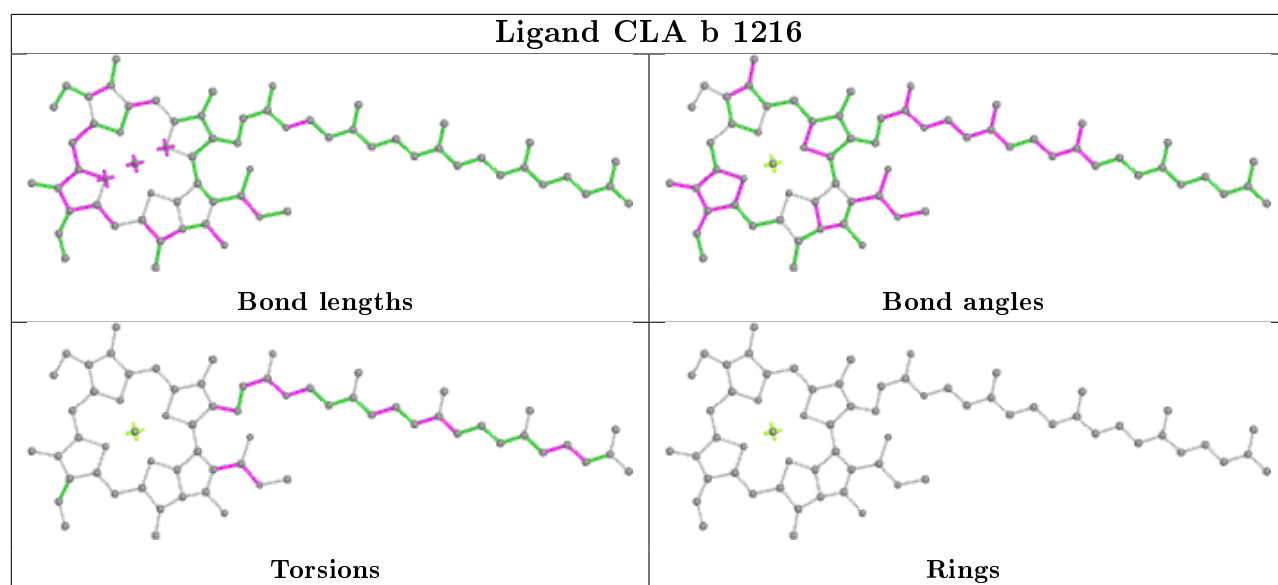
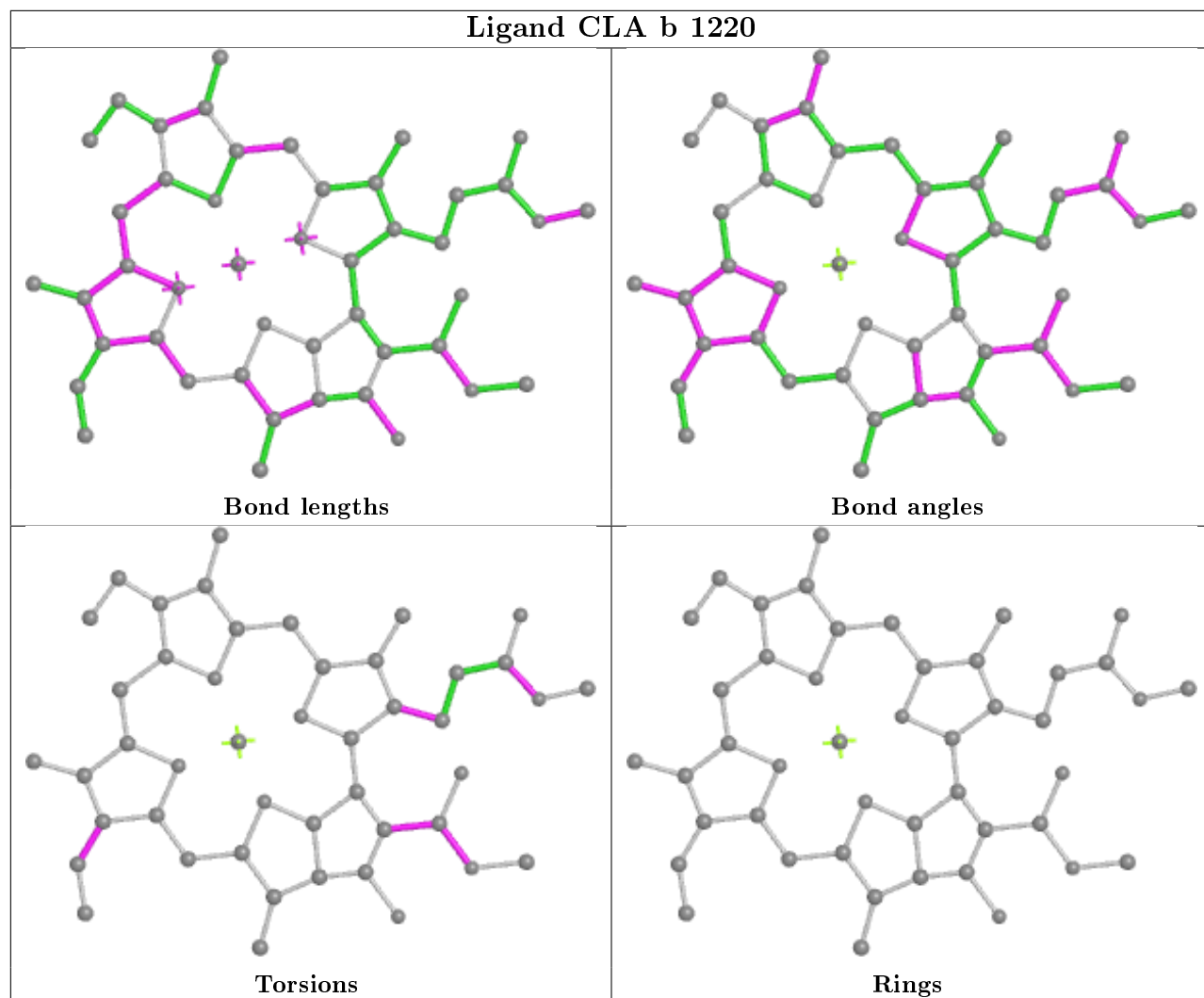


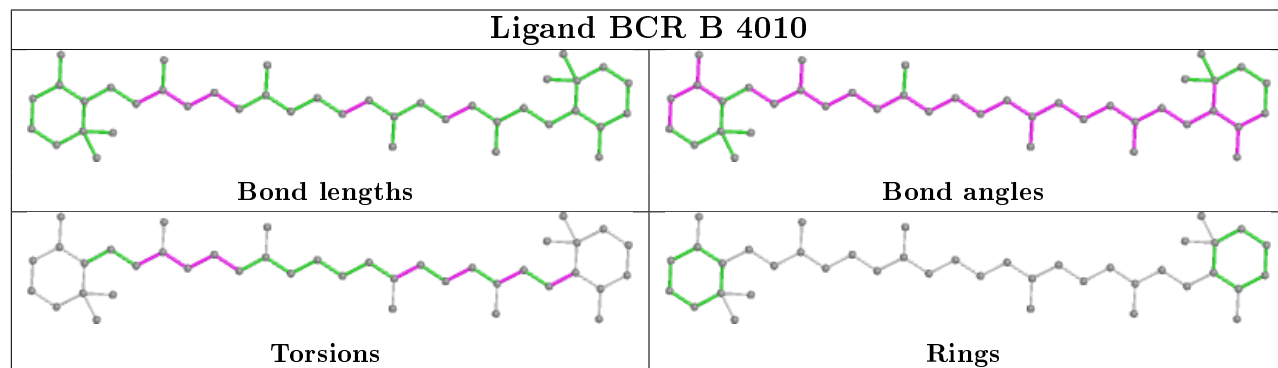
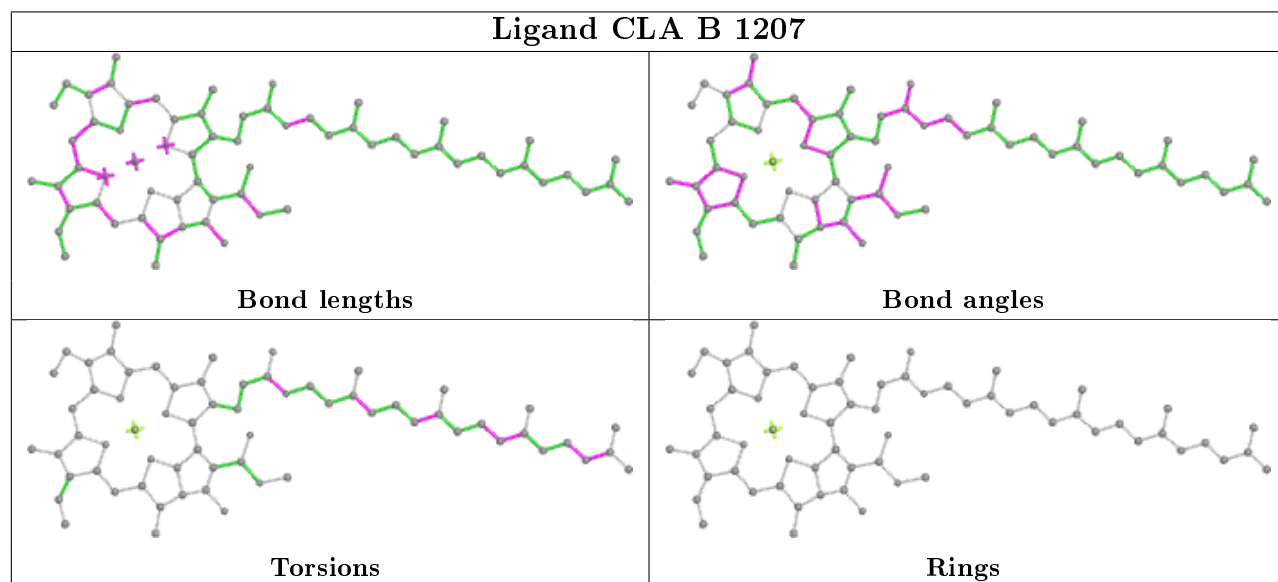
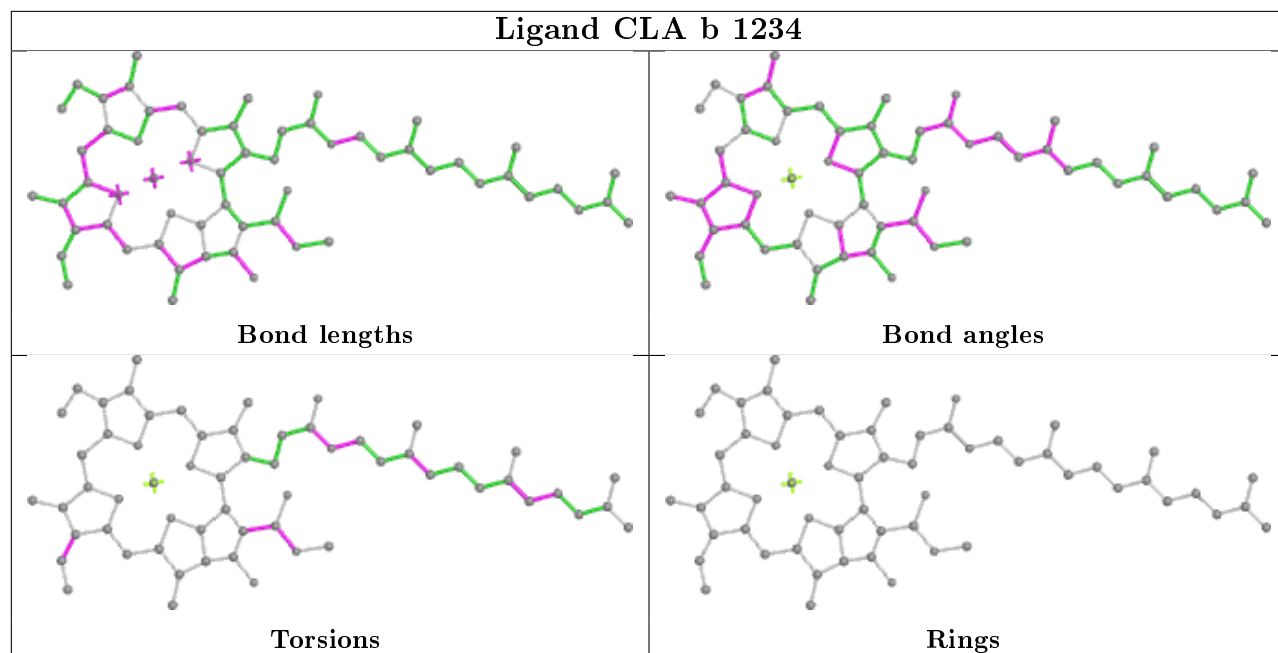
Ligand CLA 1 1138



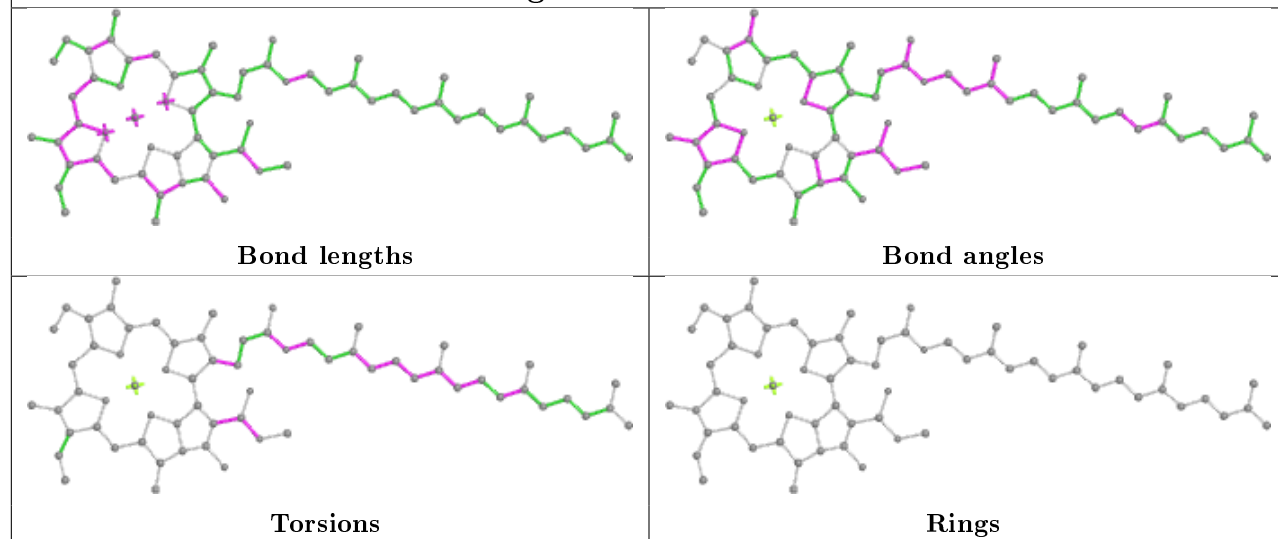
Ligand BCR F 4020



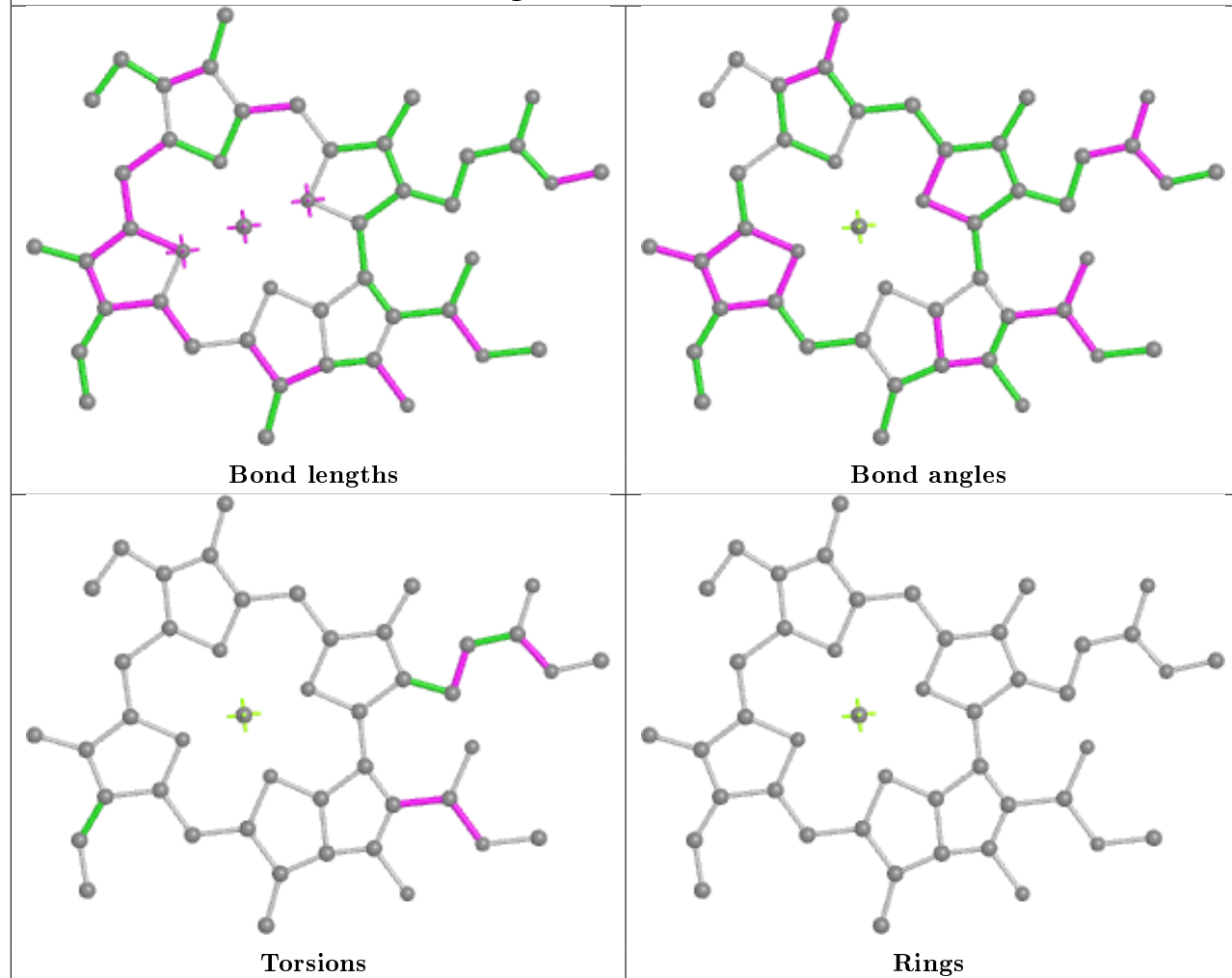


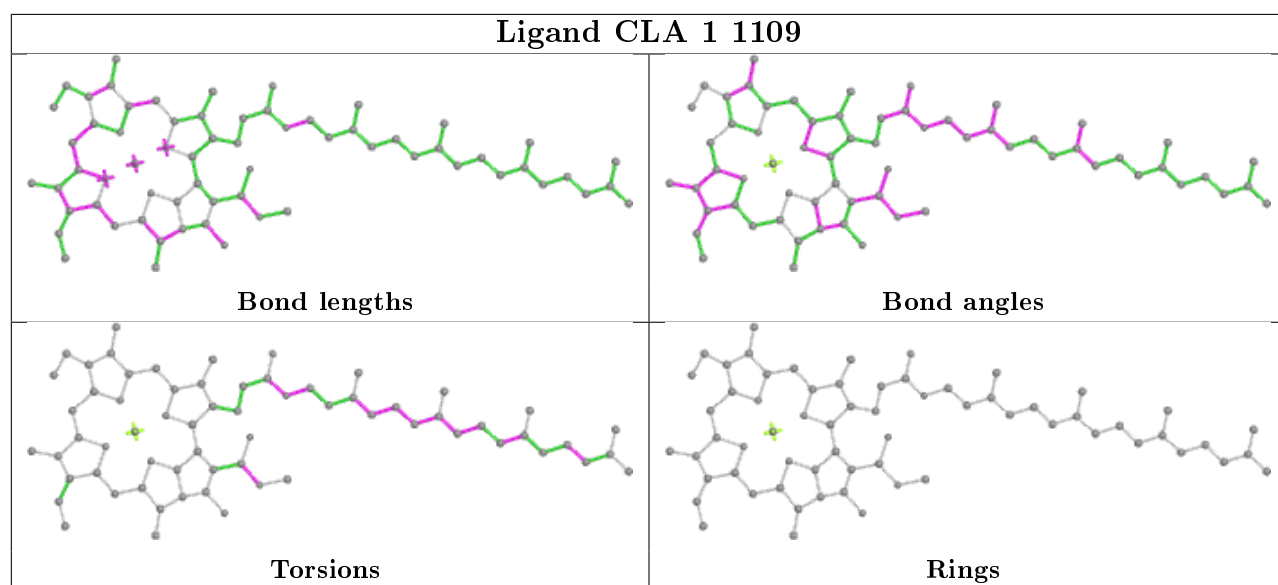
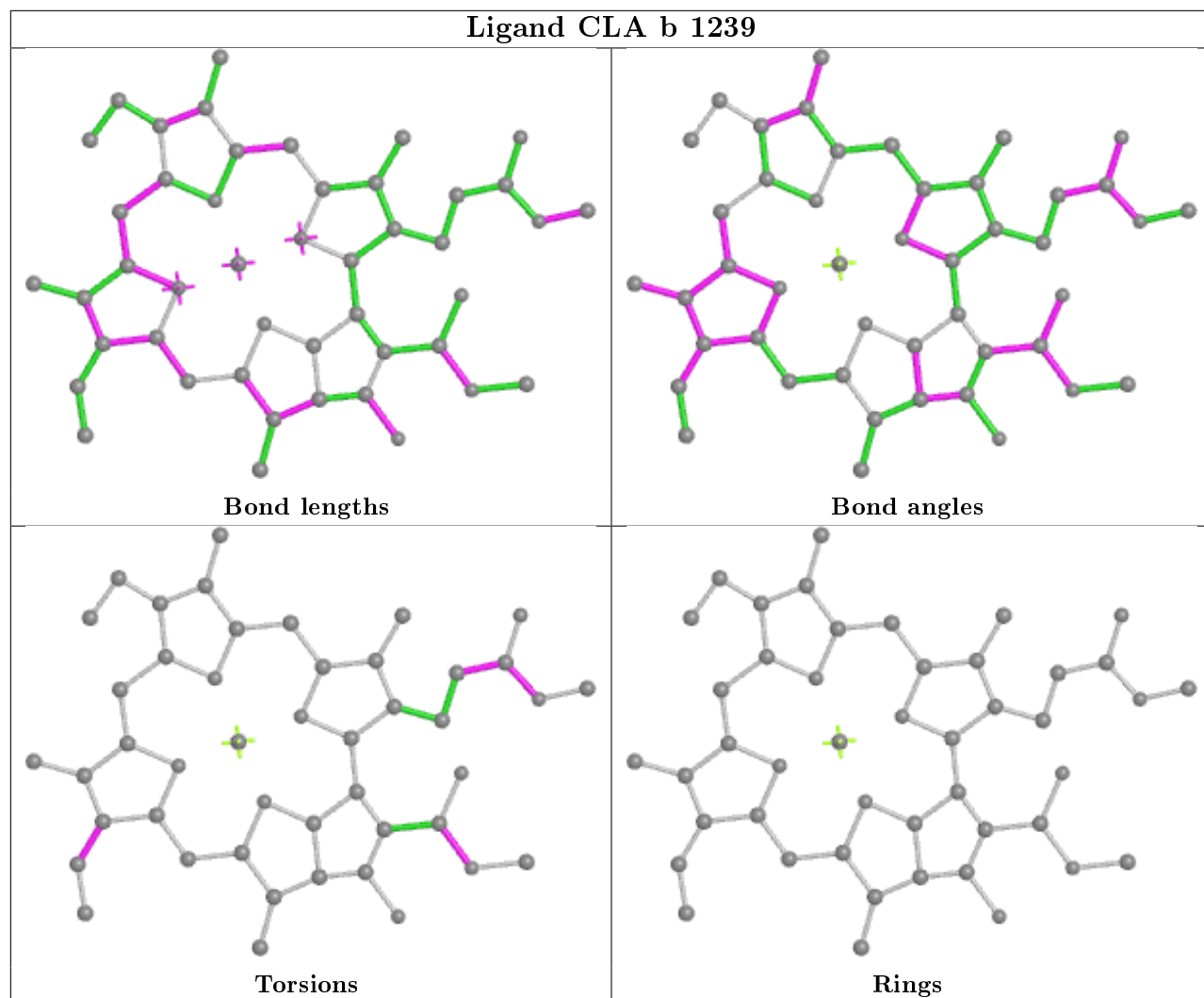


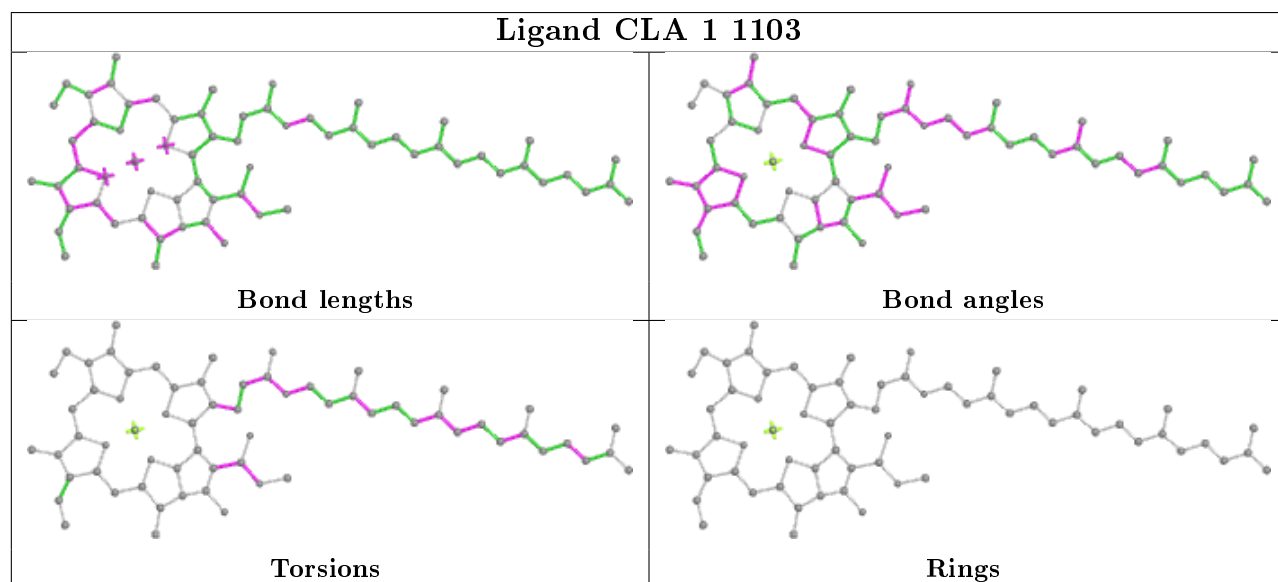
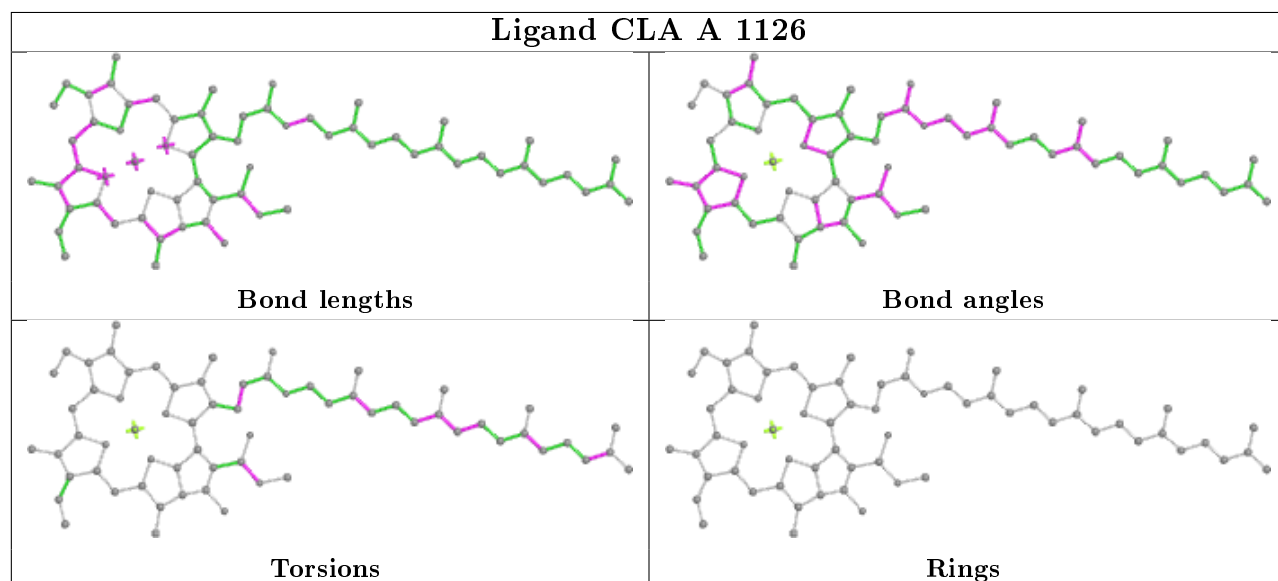
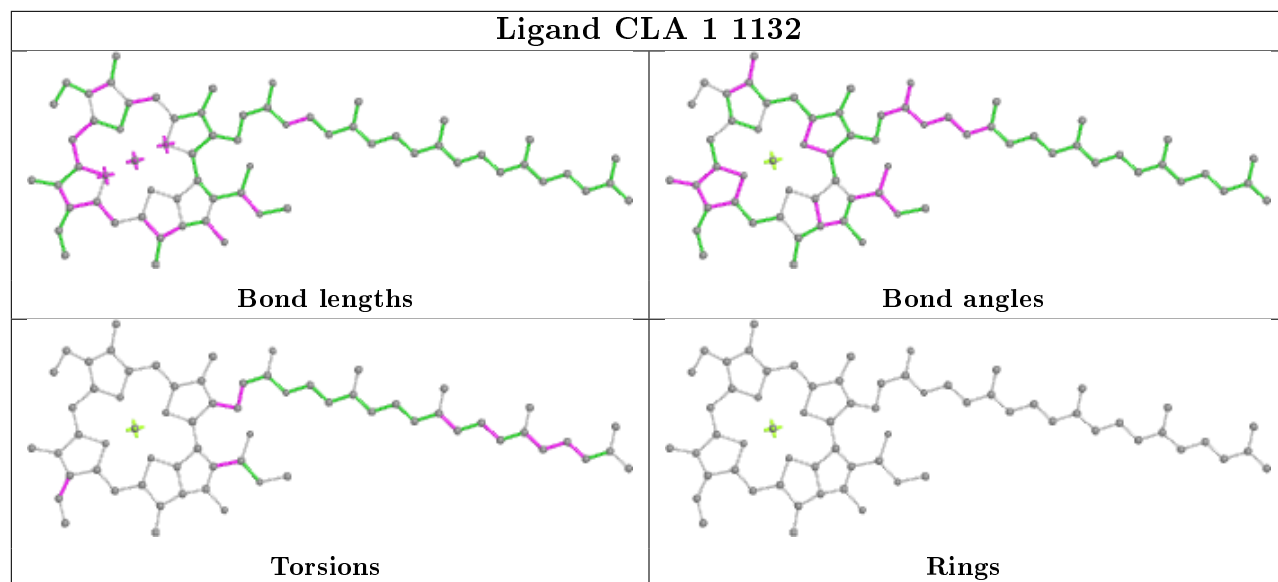
Ligand CLA a 1103

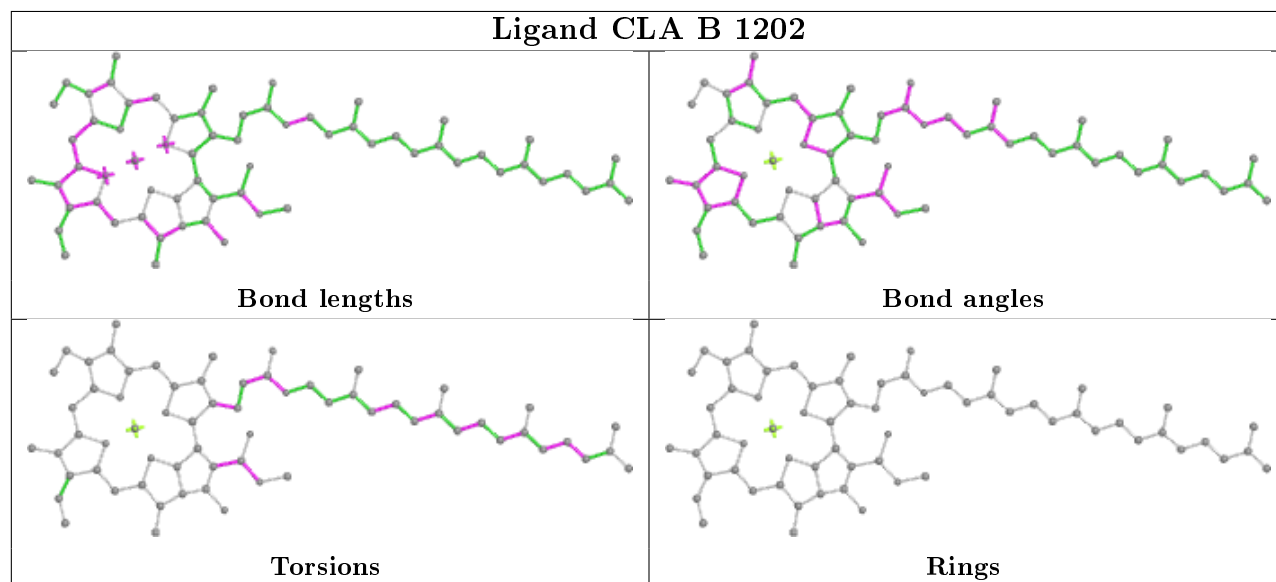
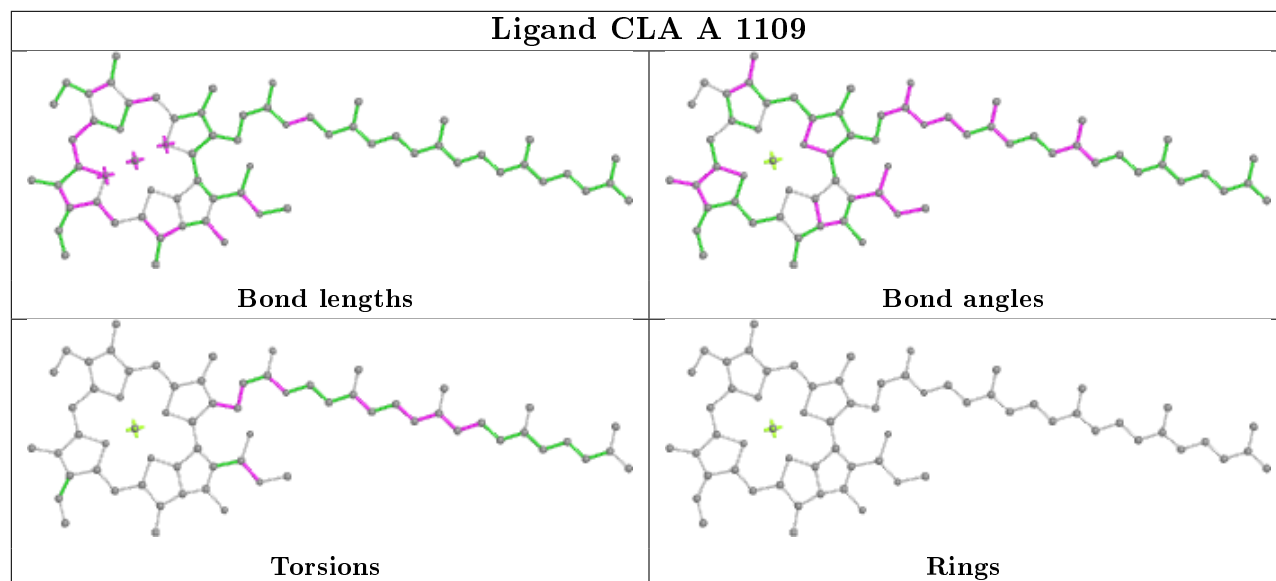
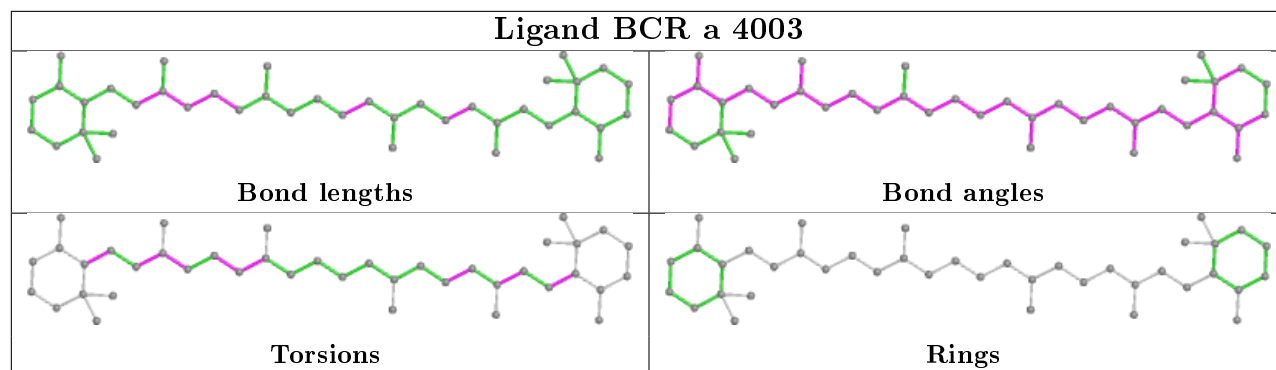


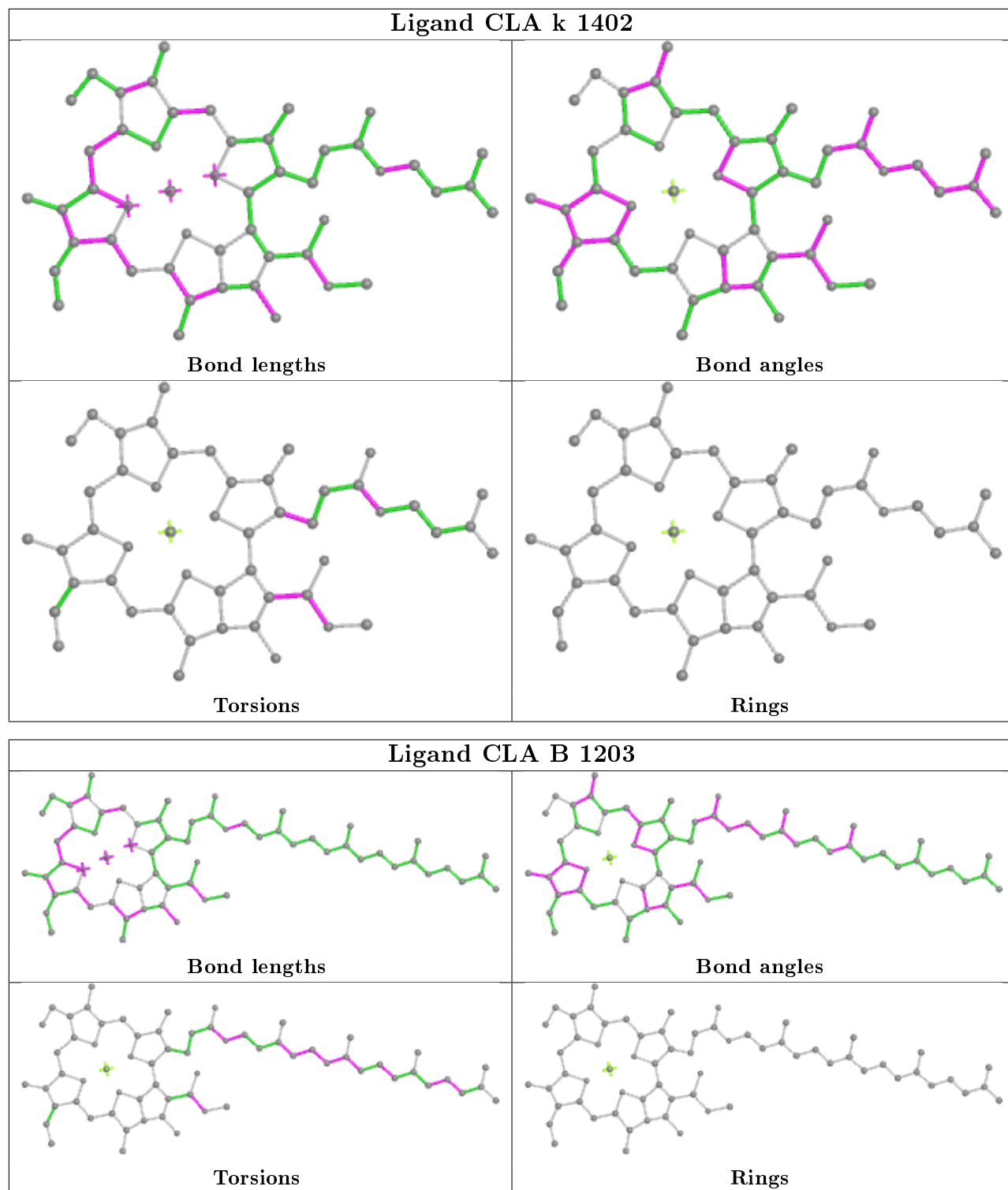
Ligand CLA 1 1129

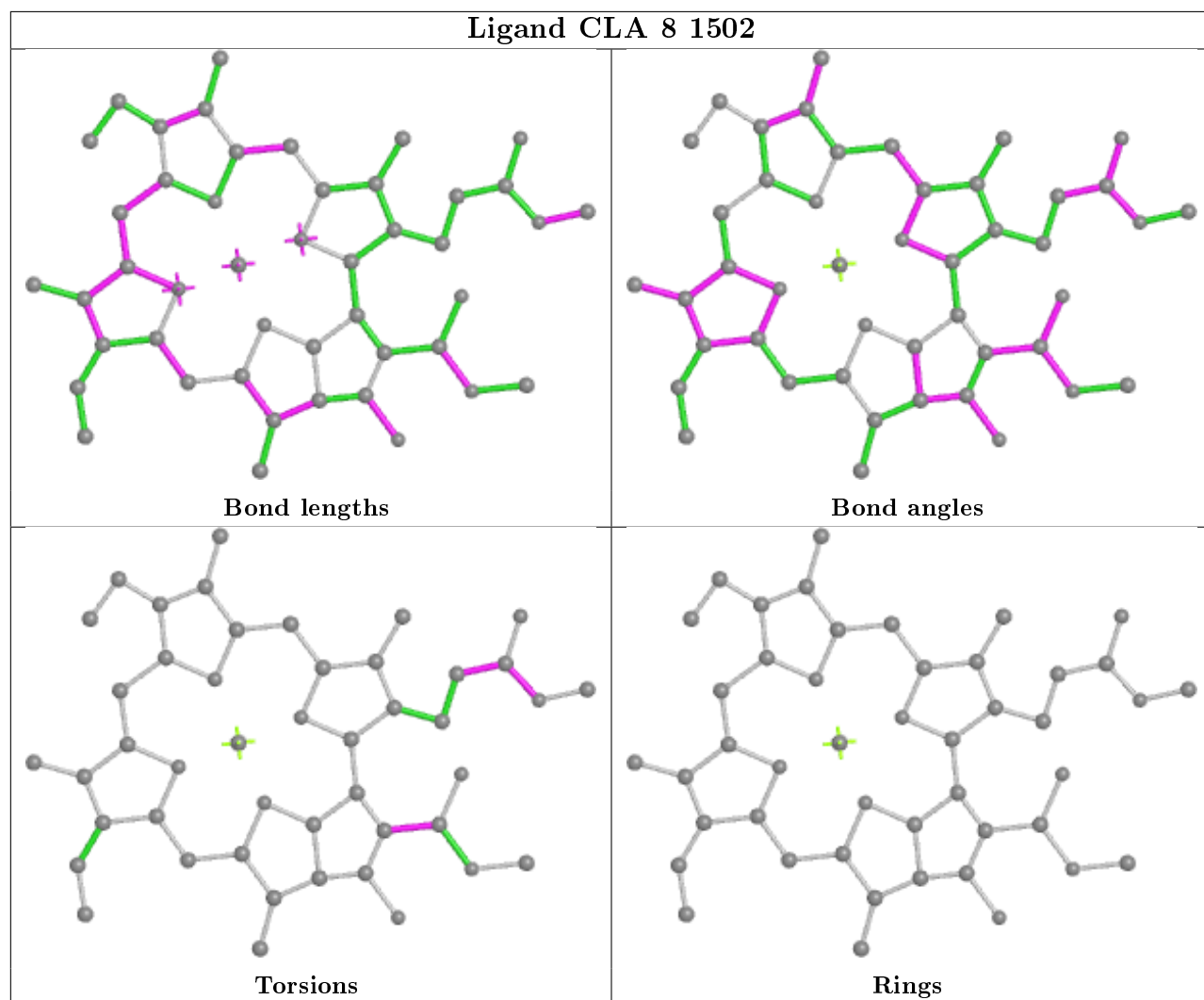
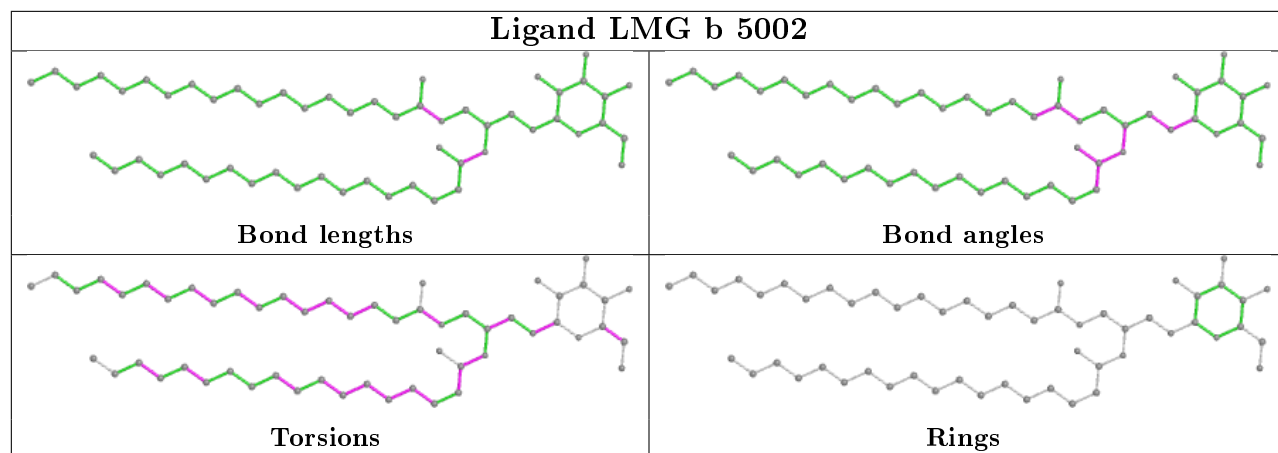




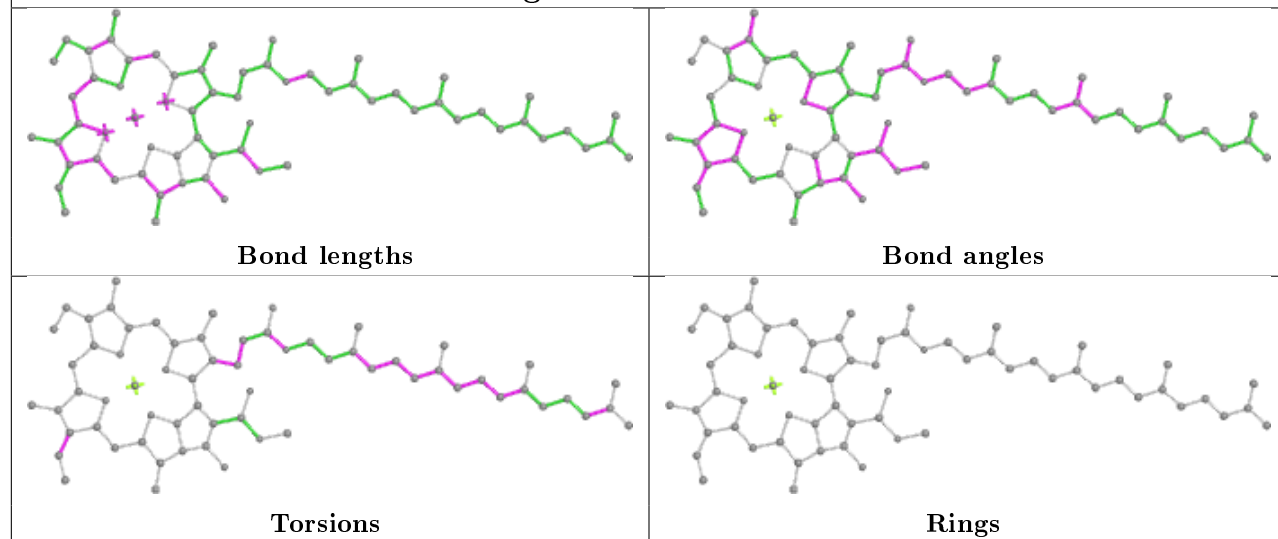




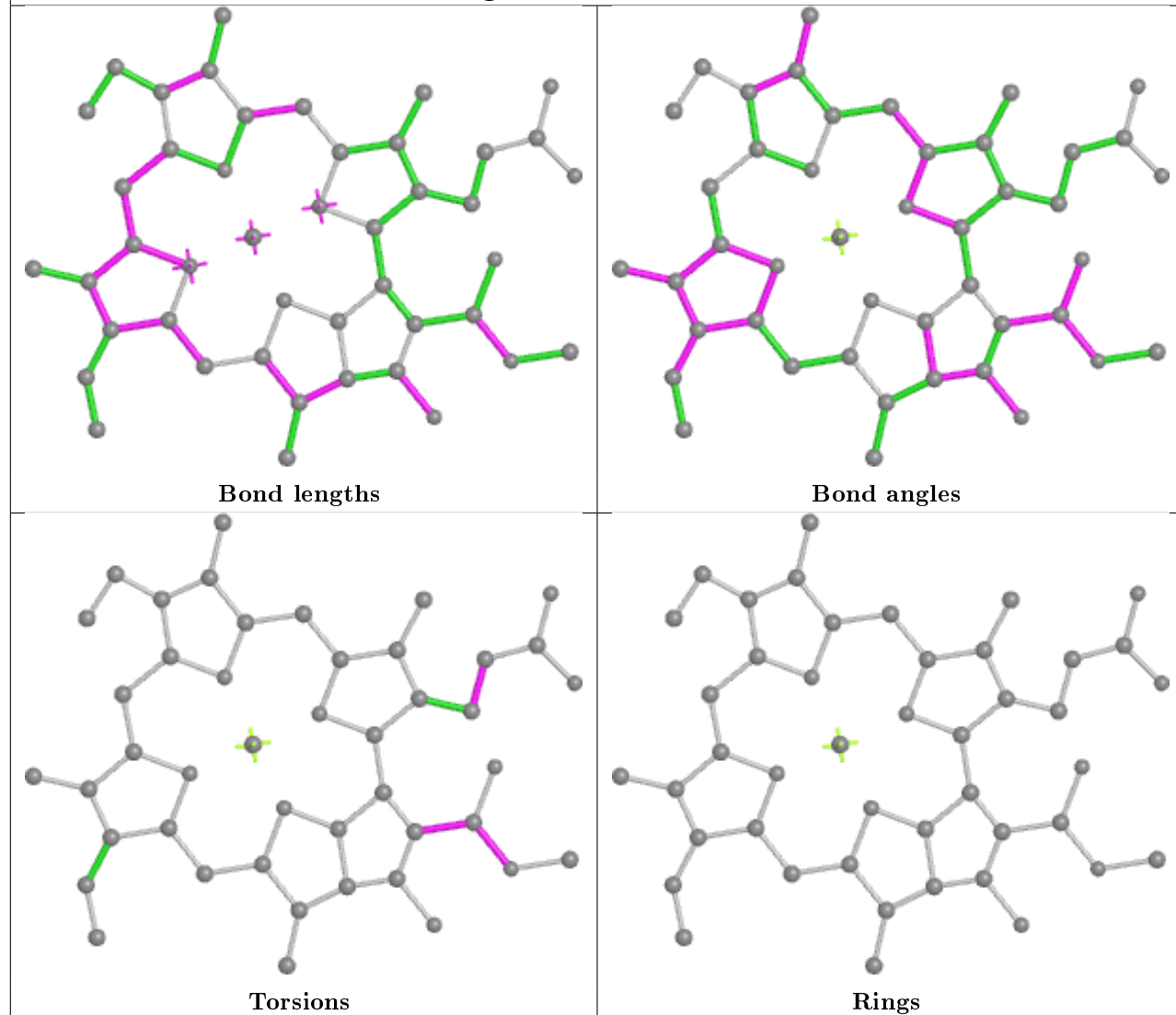


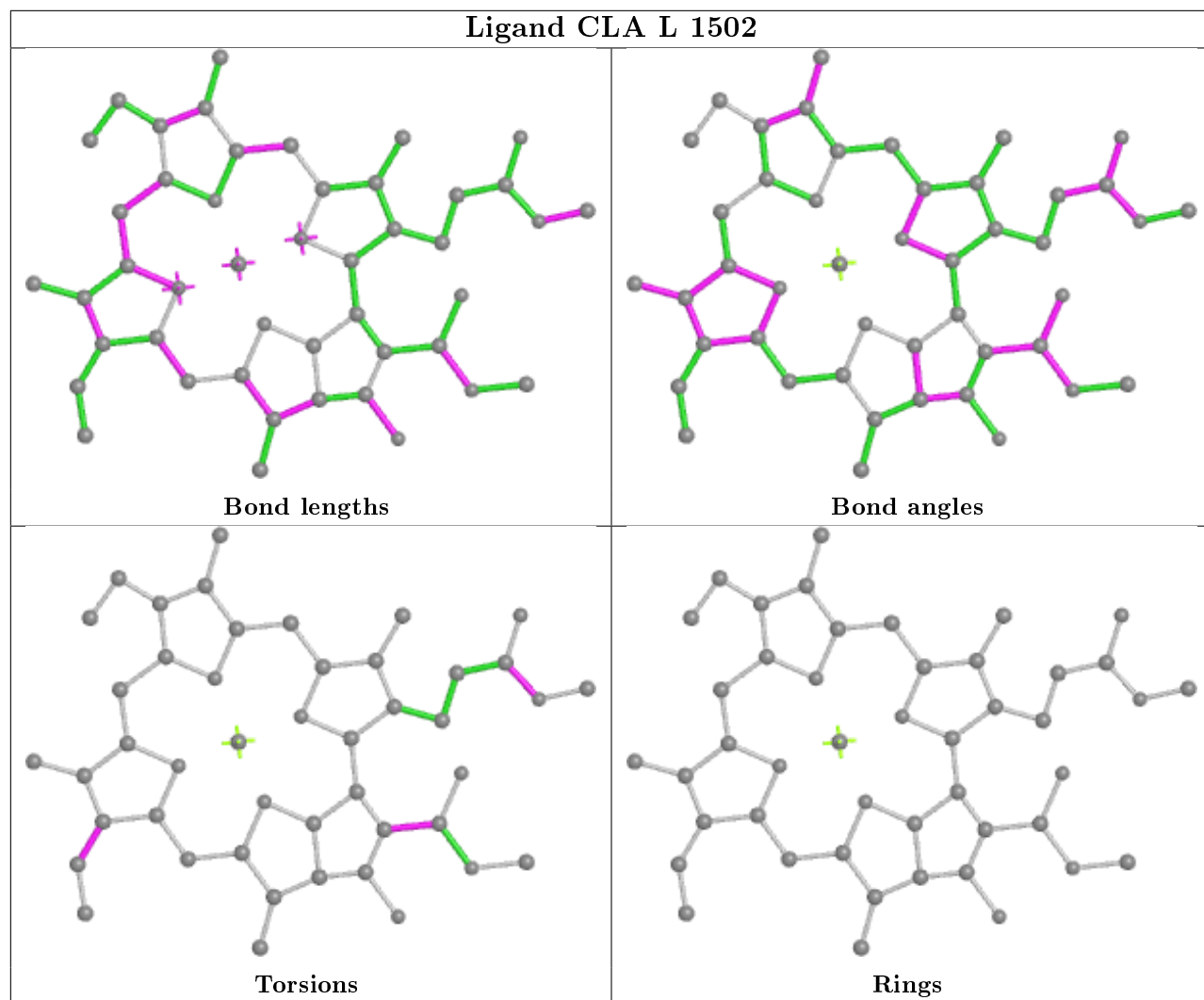
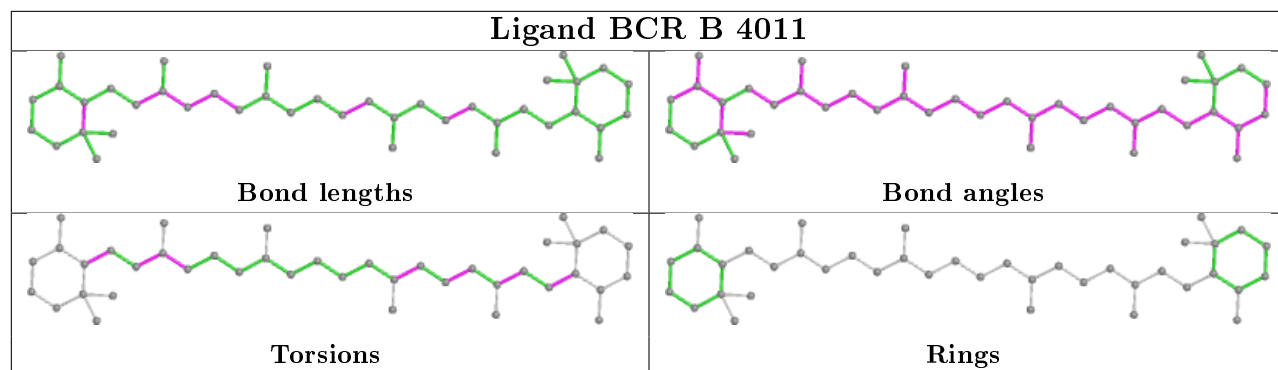


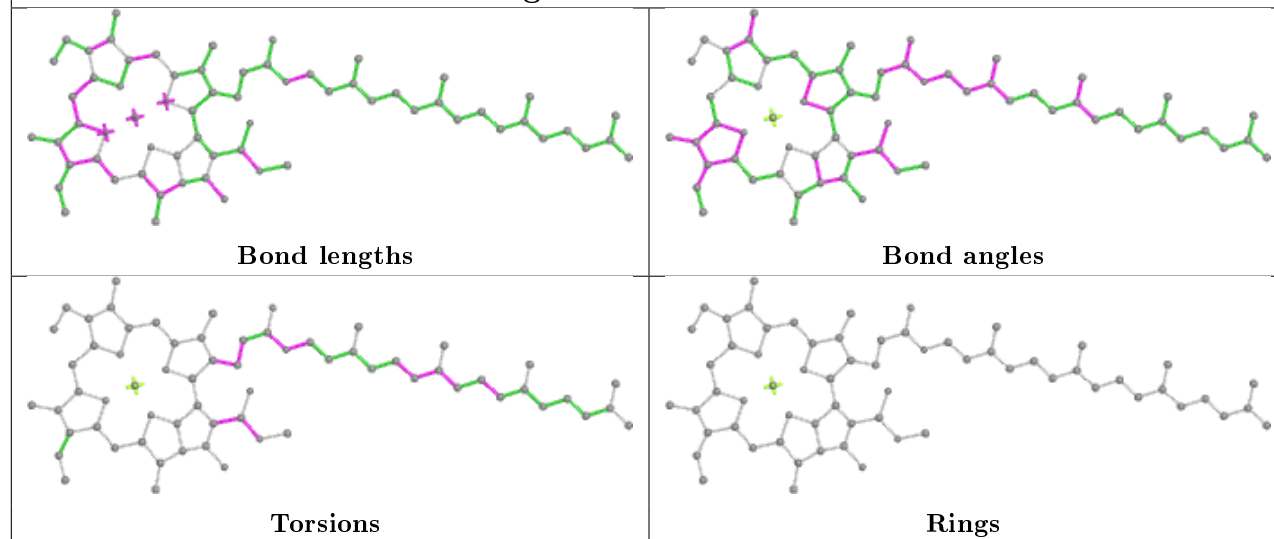
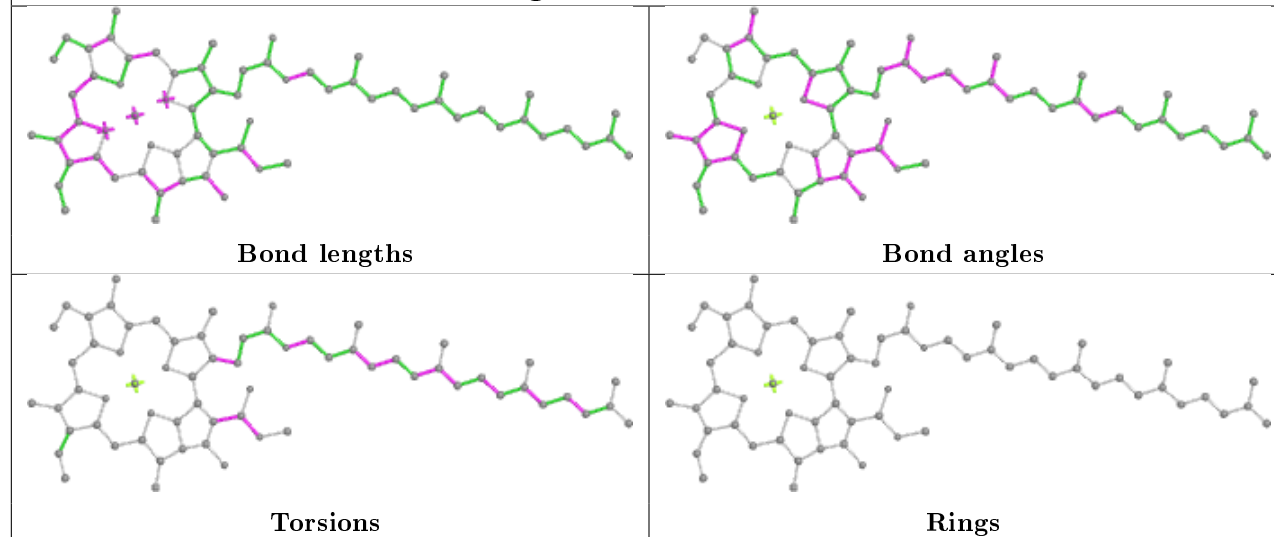
Ligand CLA A 1119

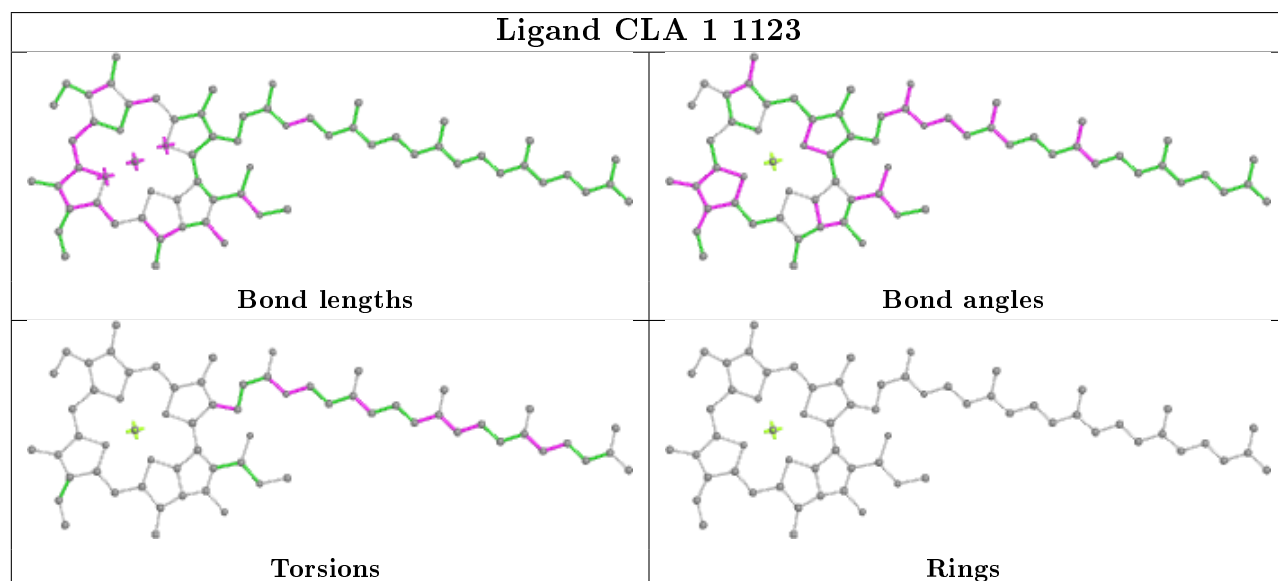
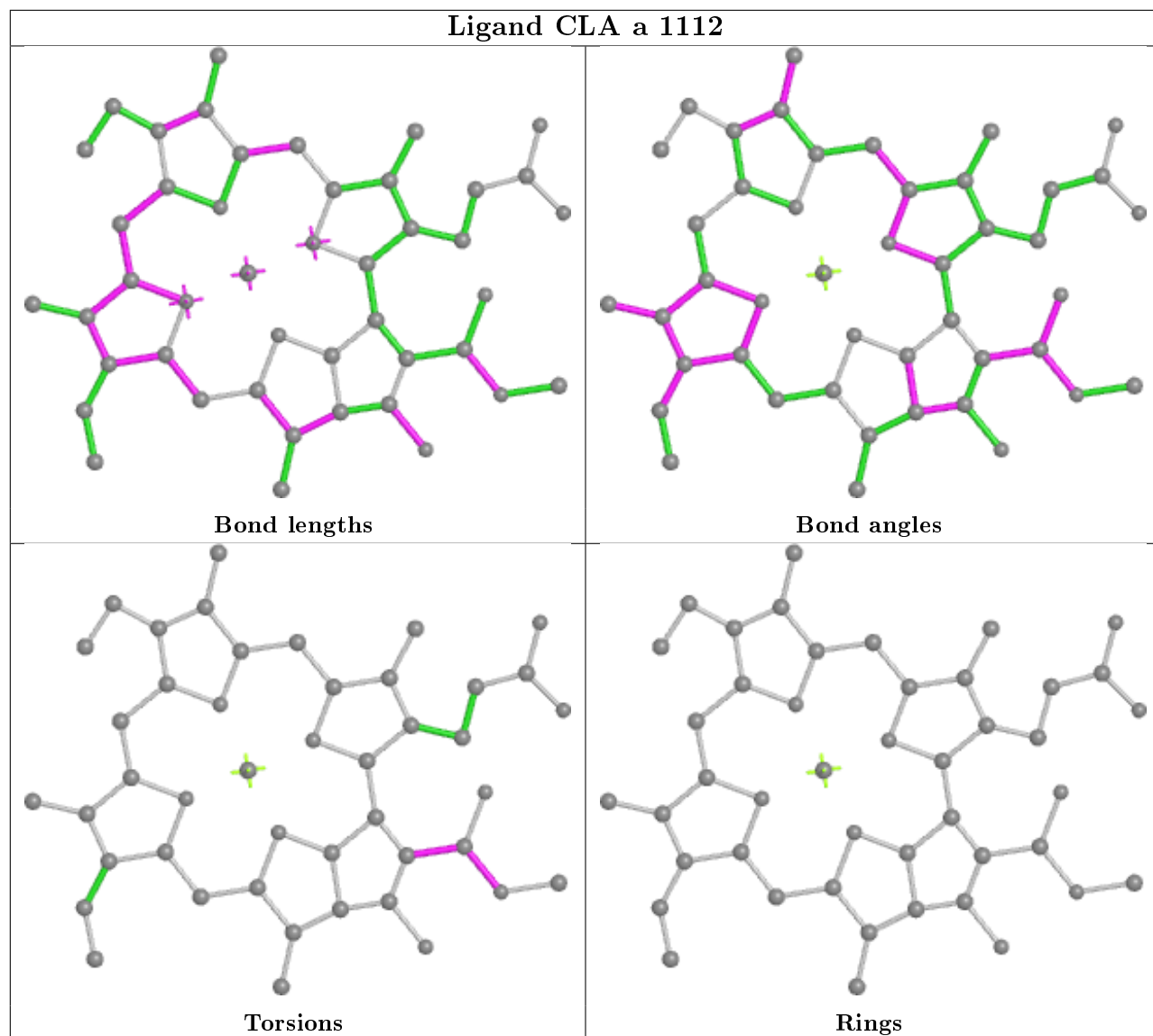


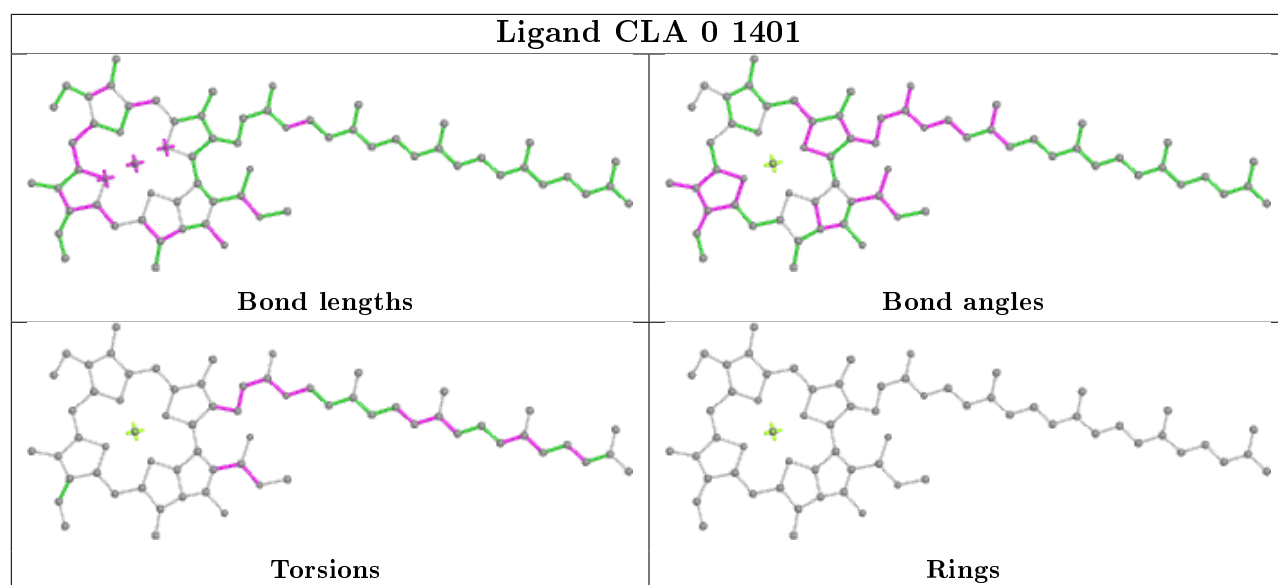
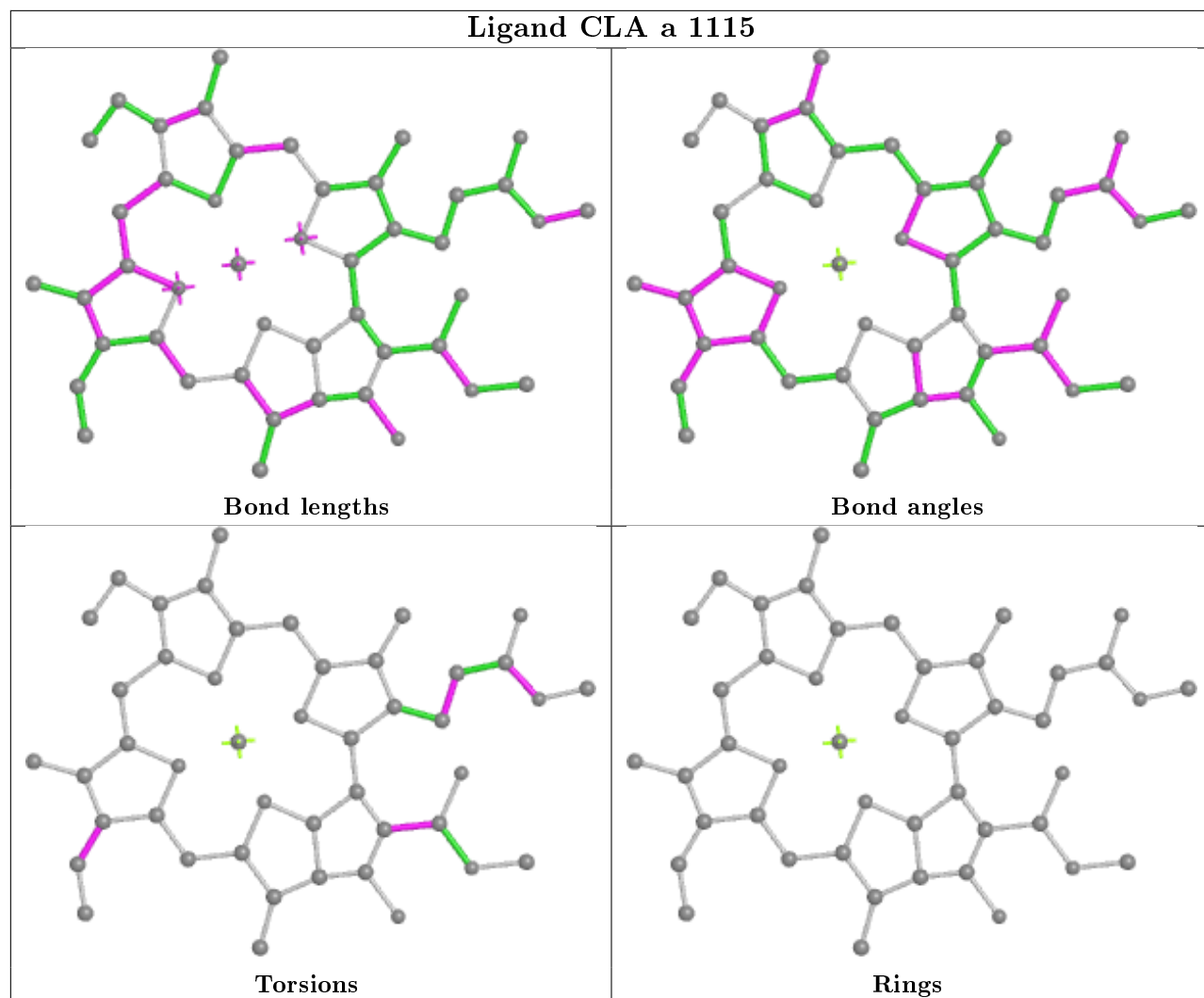
Ligand CLA A 1113

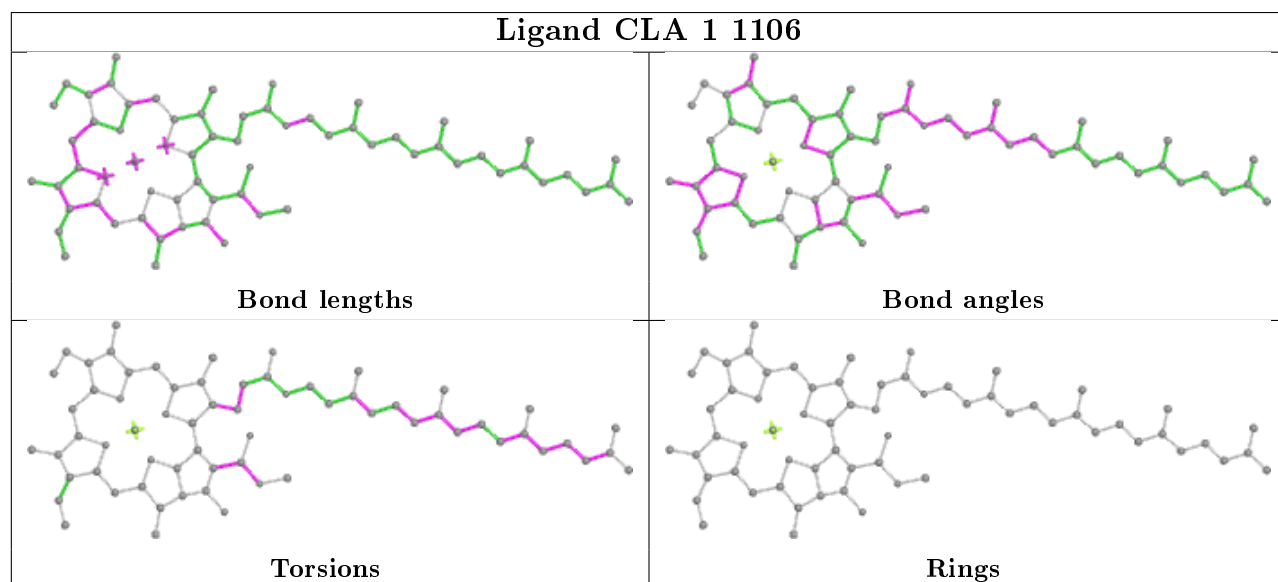
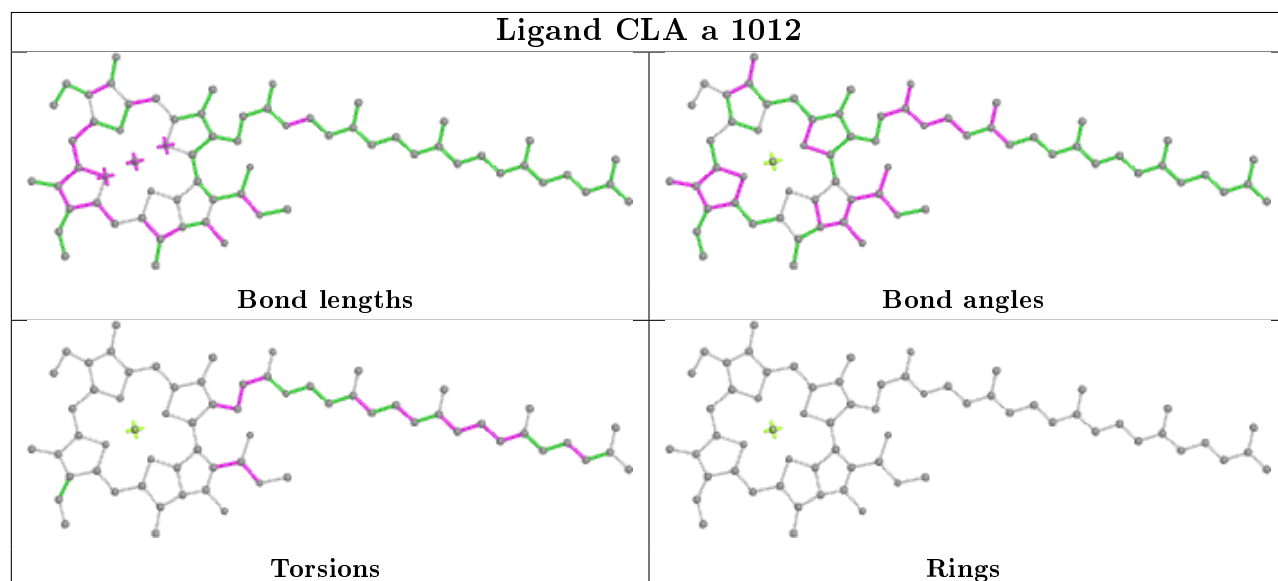
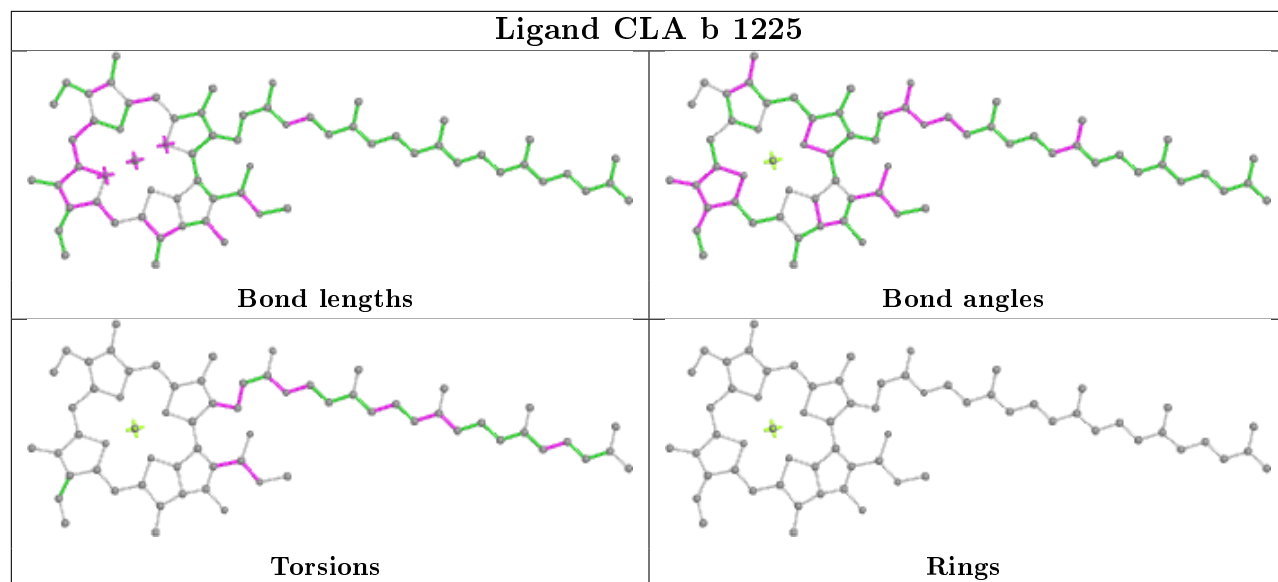


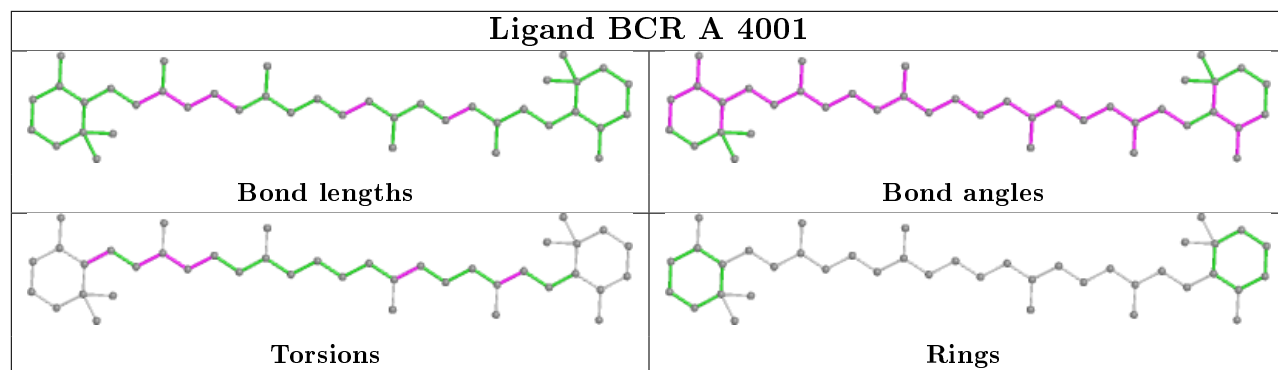
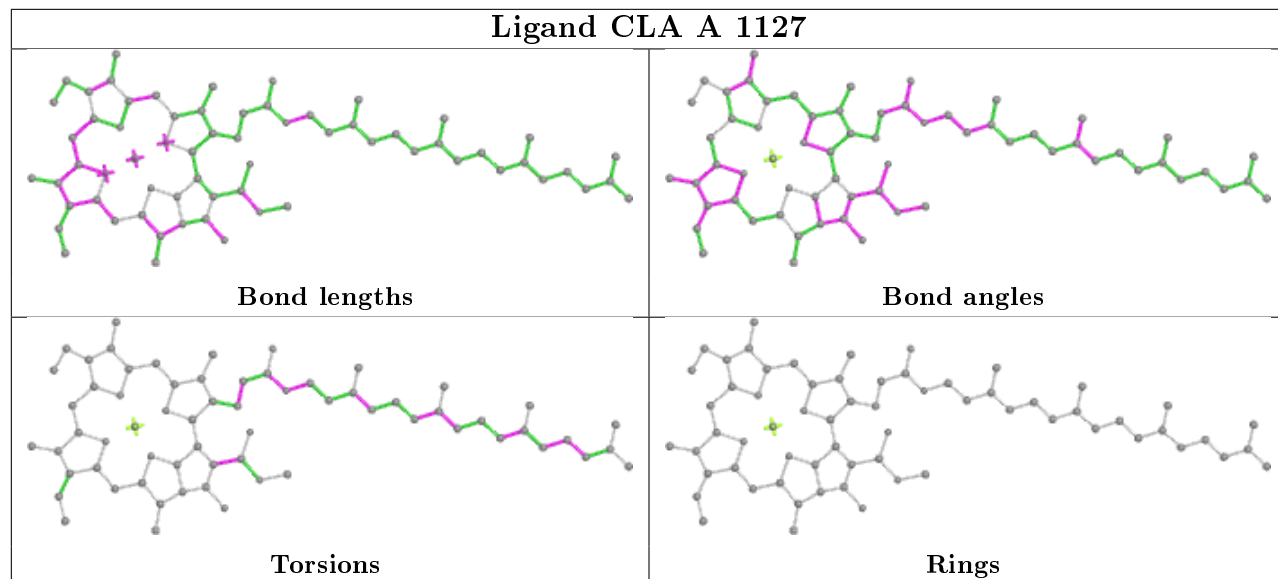
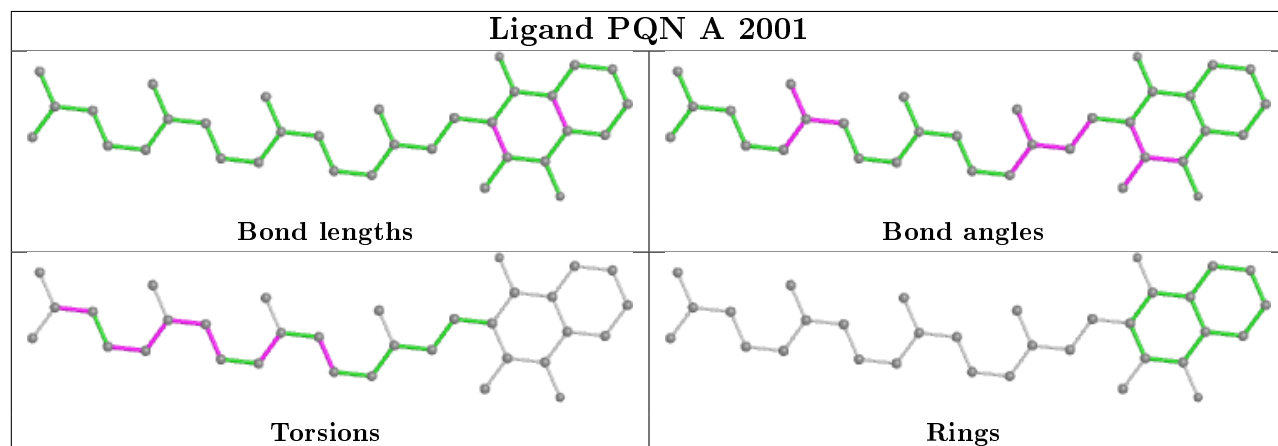


Ligand CLA A 1131**Ligand CLA 1 1022**

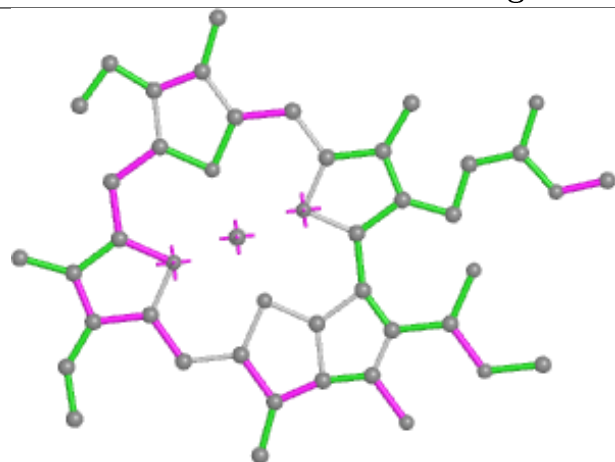




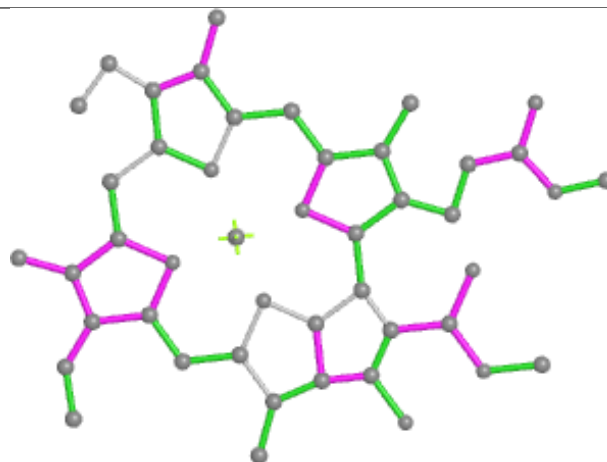


Ligand BCR A 4001**Ligand CLA A 1127****Ligand PQN A 2001**

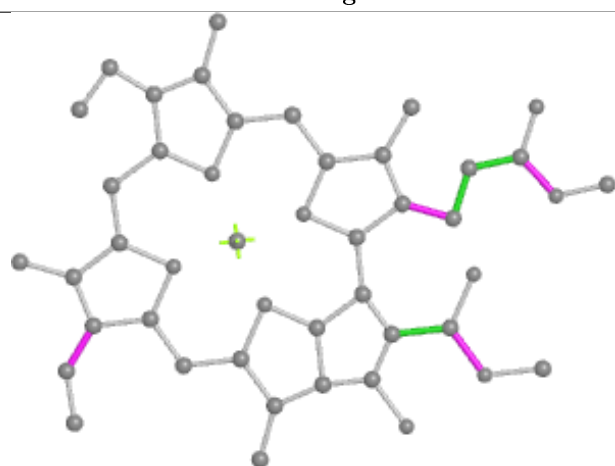
Ligand CLA A 1114



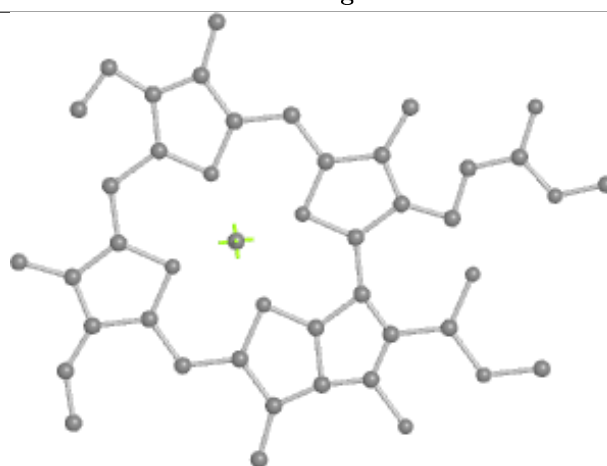
Bond lengths



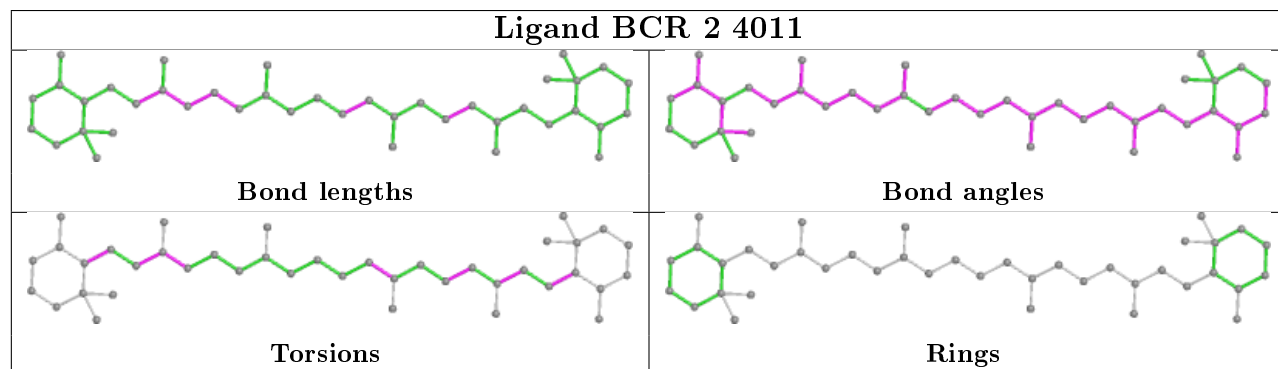
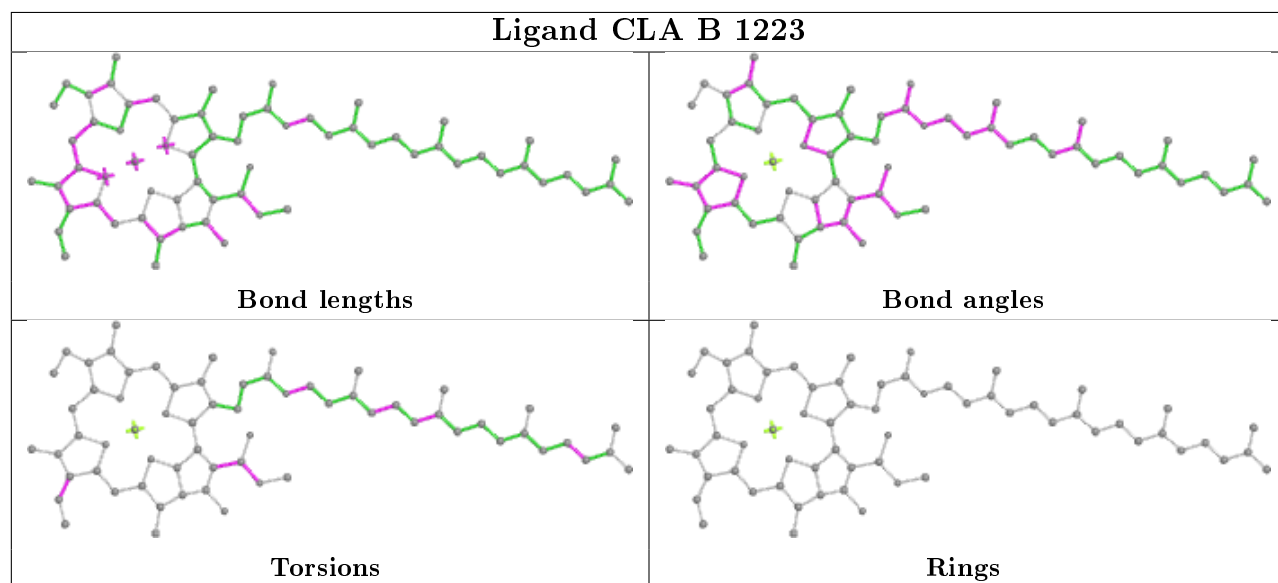
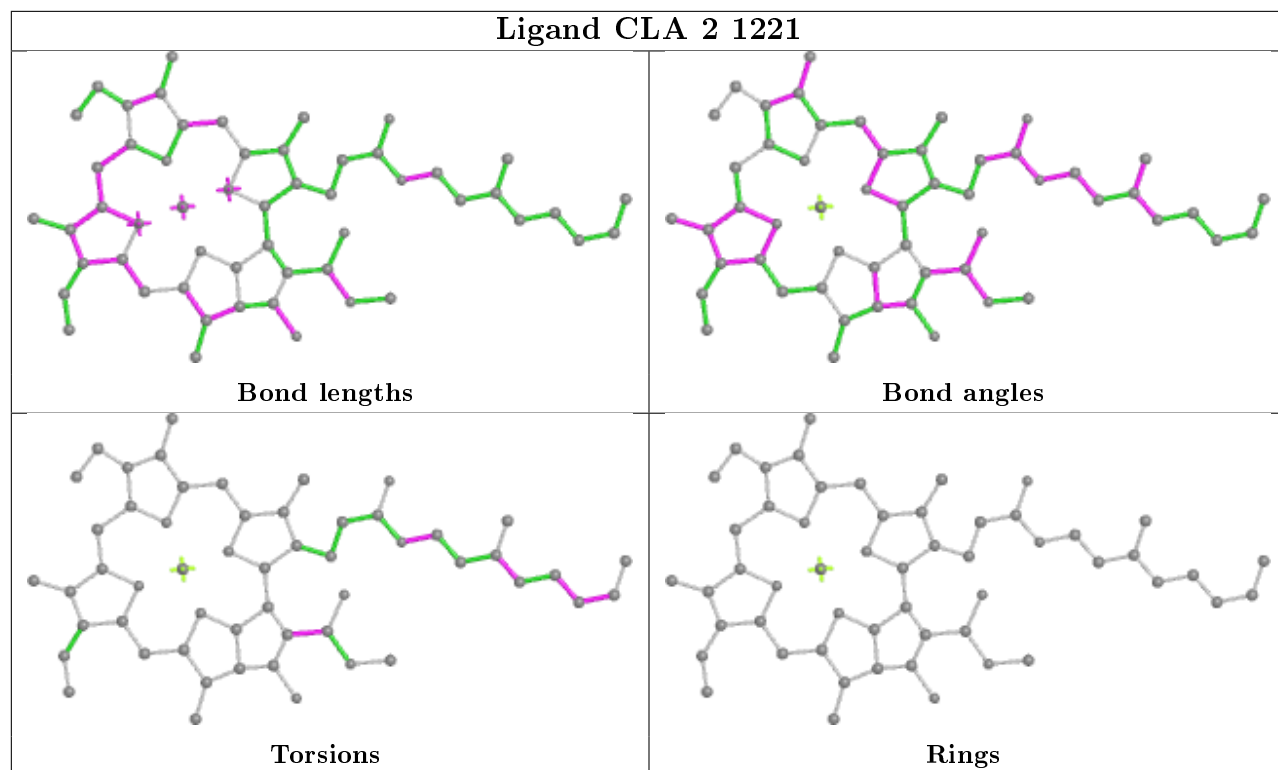
Bond angles

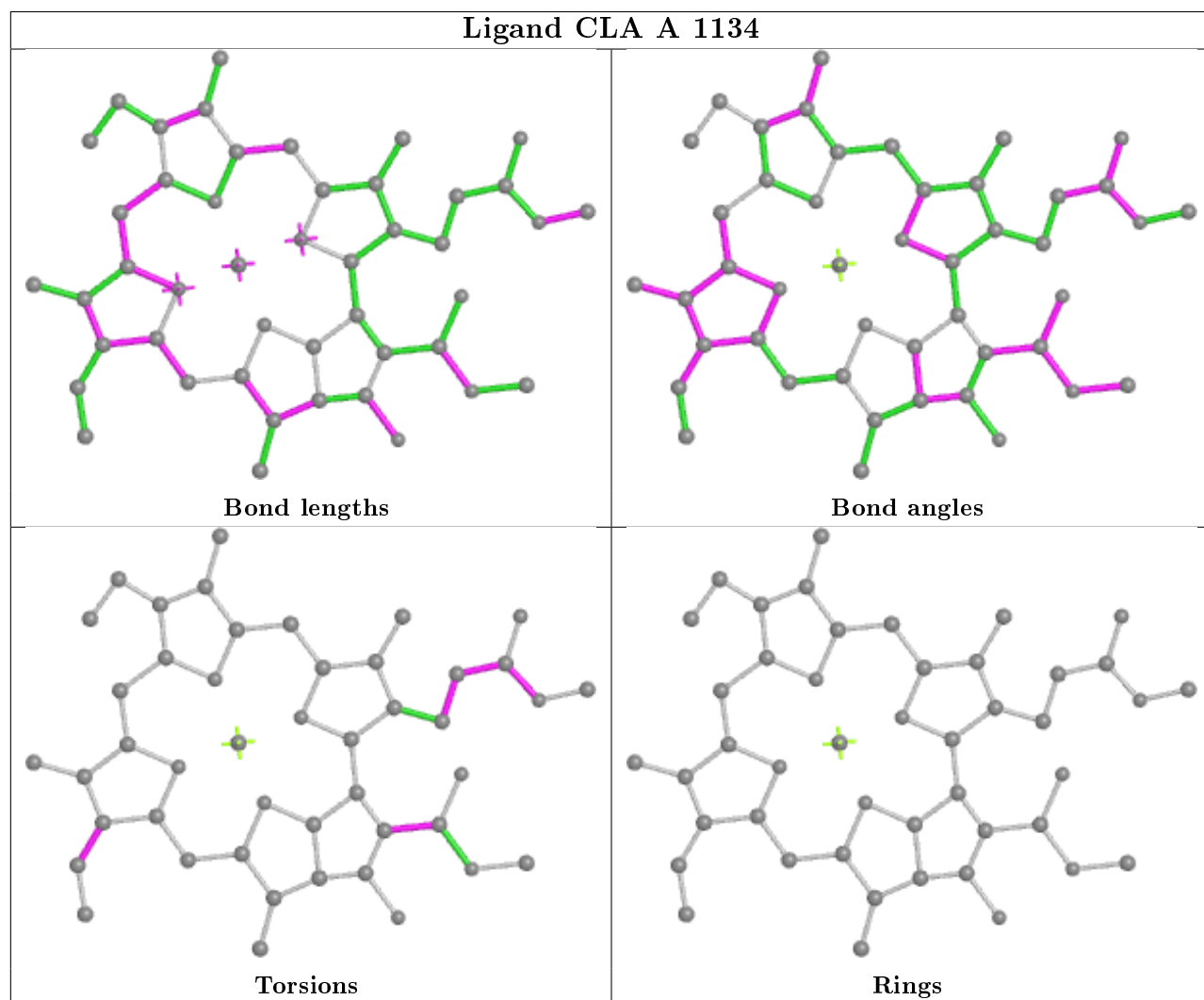
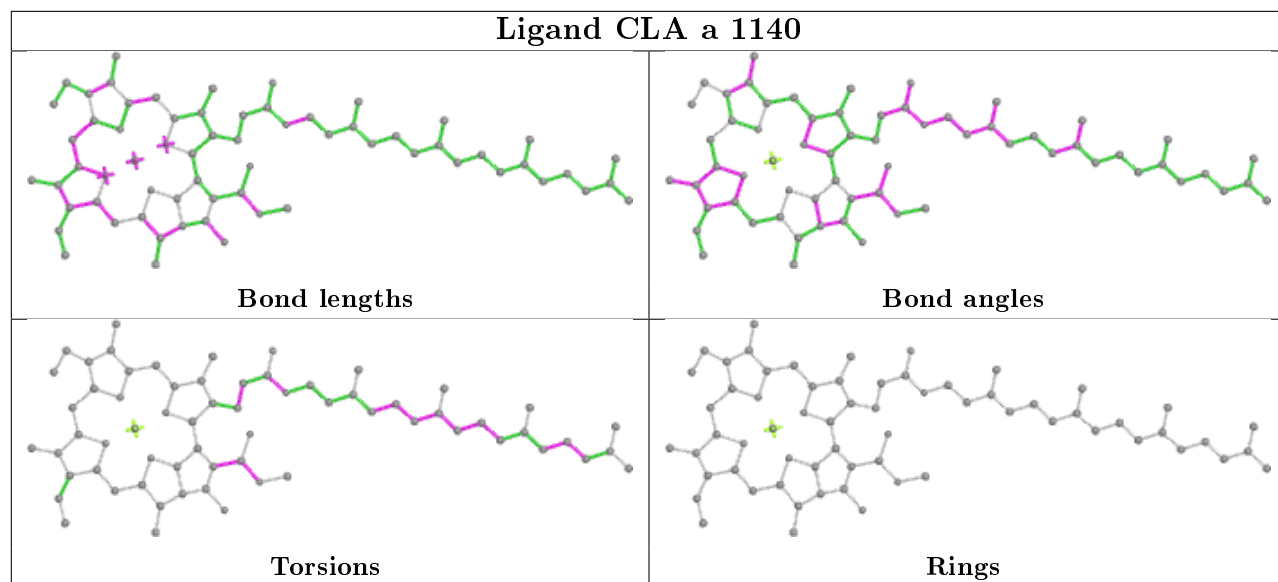


Torsions

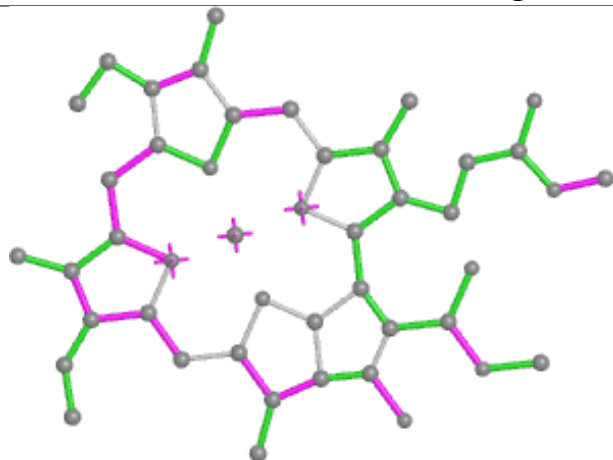


Rings

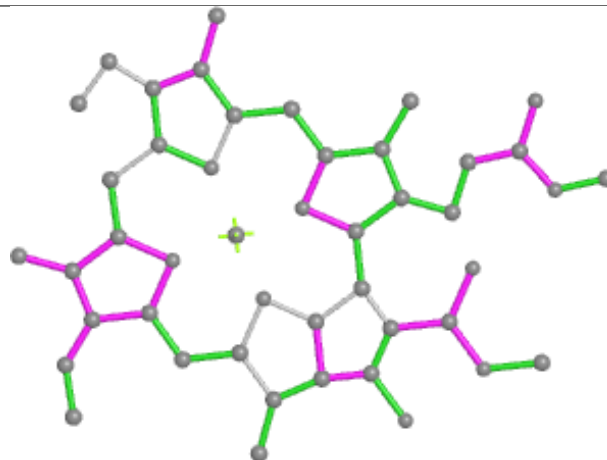




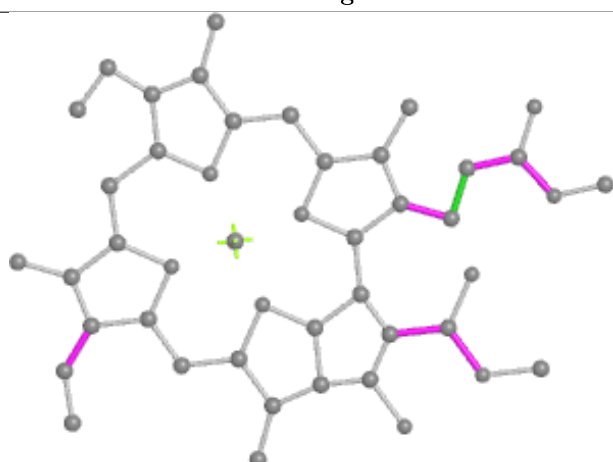
Ligand CLA 1 1114



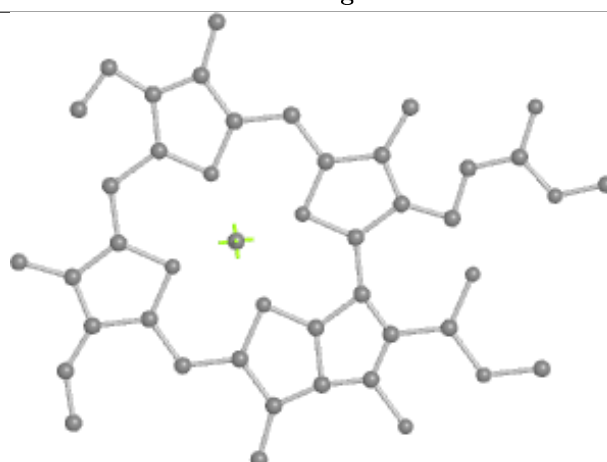
Bond lengths



Bond angles

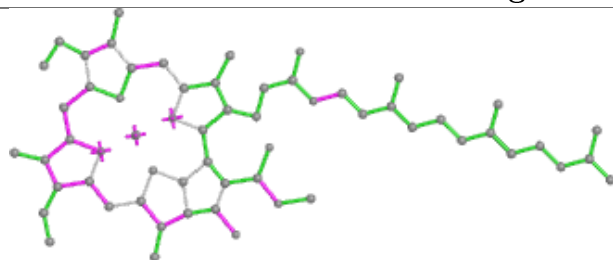


Torsions

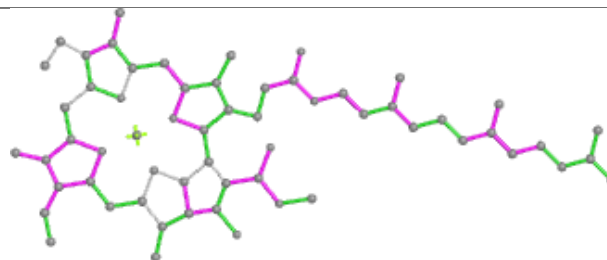


Rings

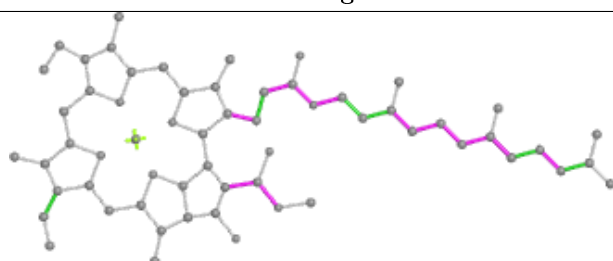
Ligand CLA b 1235



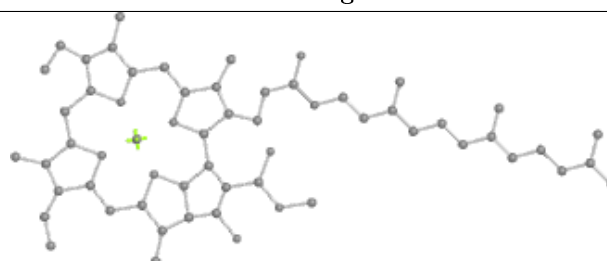
Bond lengths



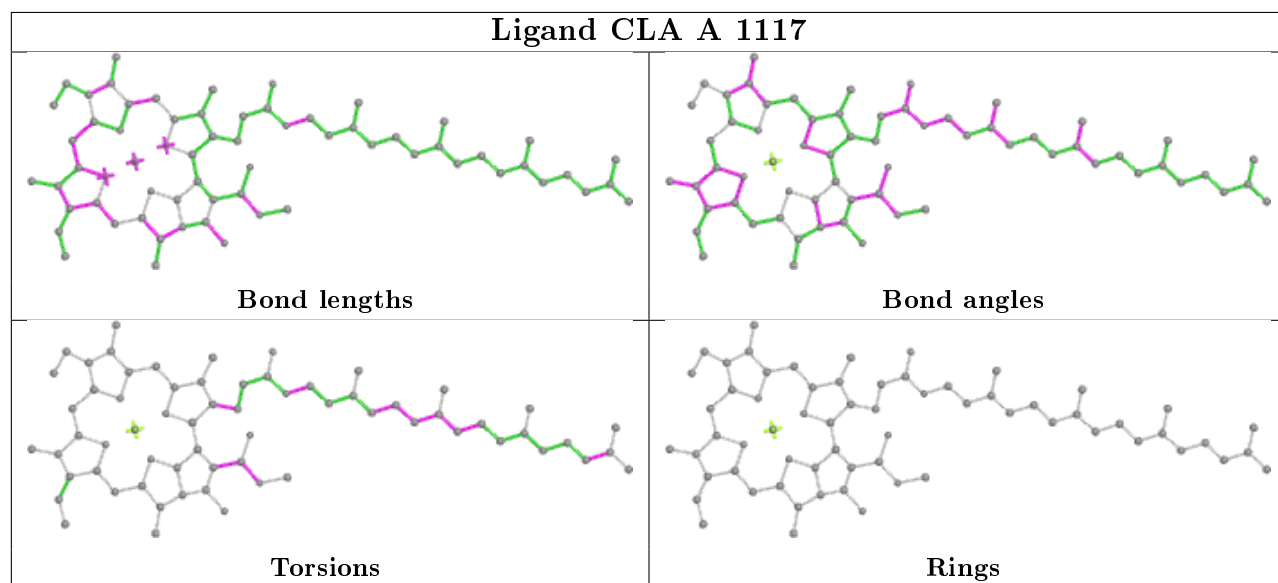
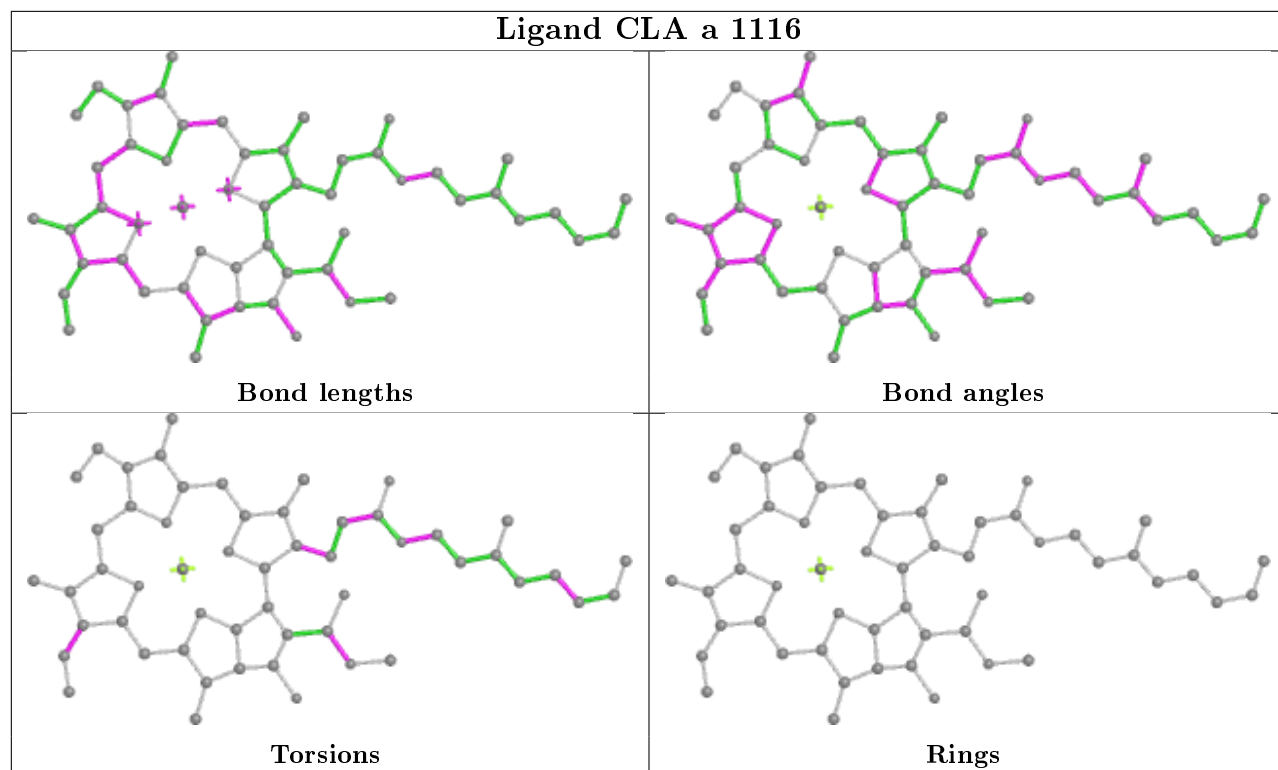
Bond angles

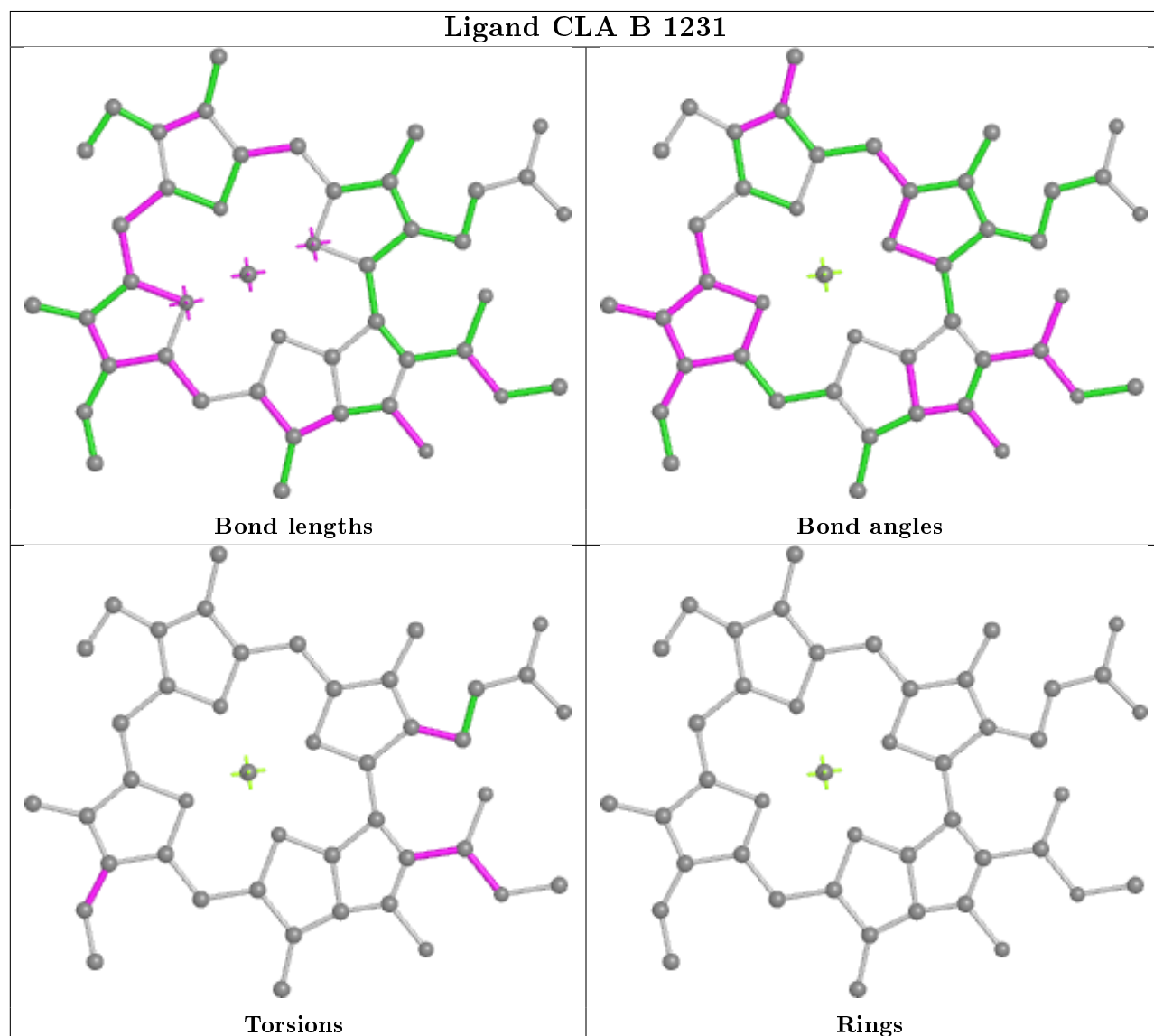
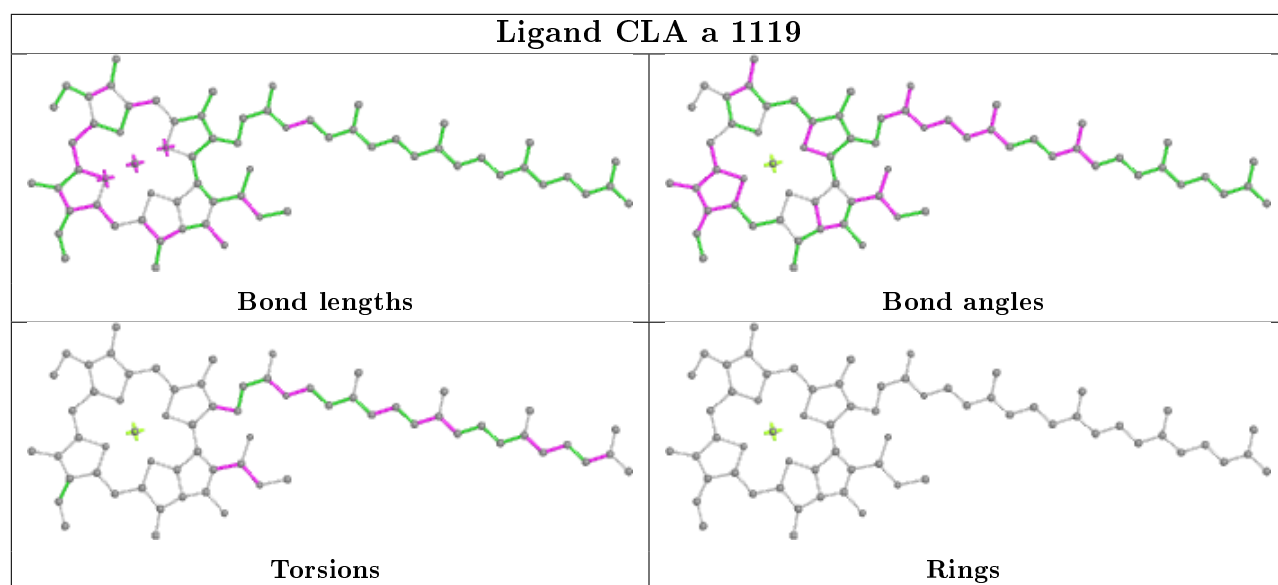


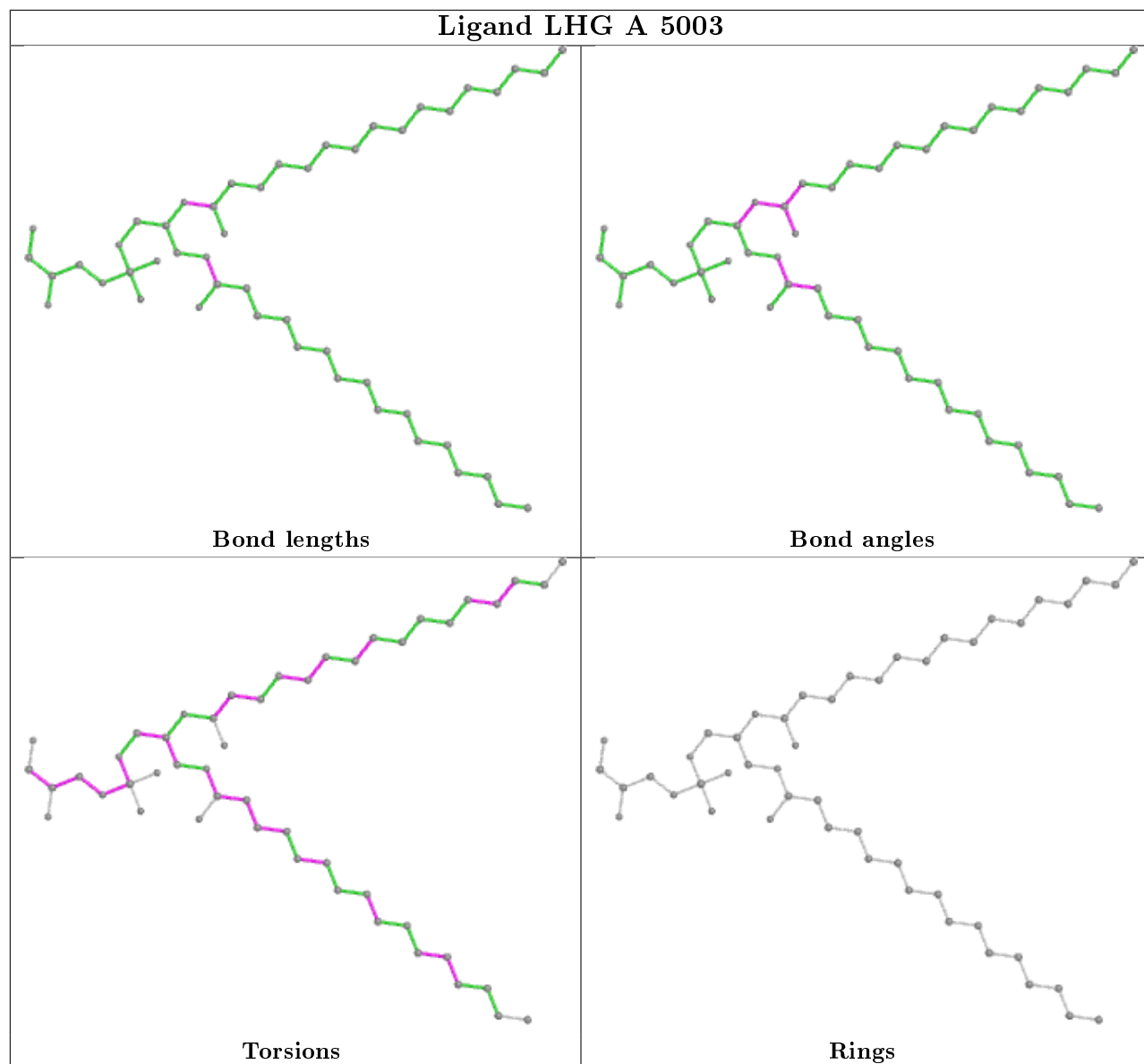
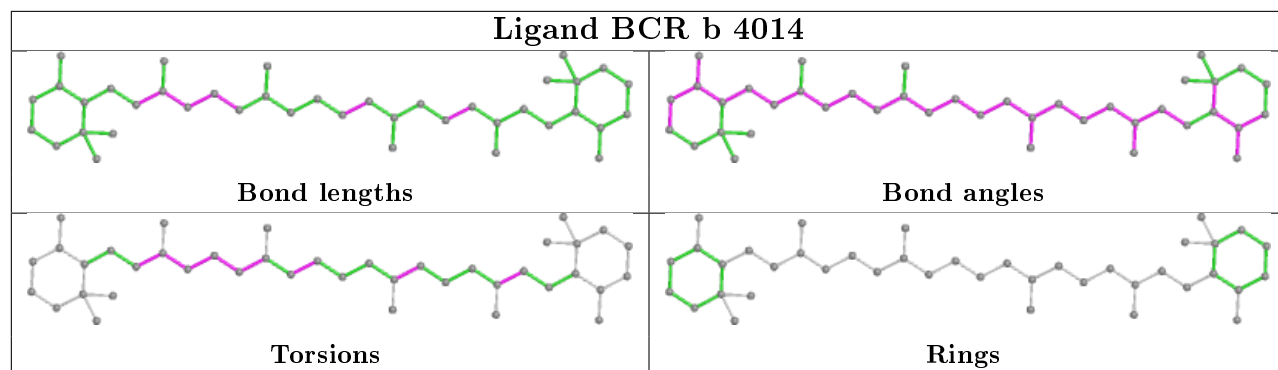
Torsions

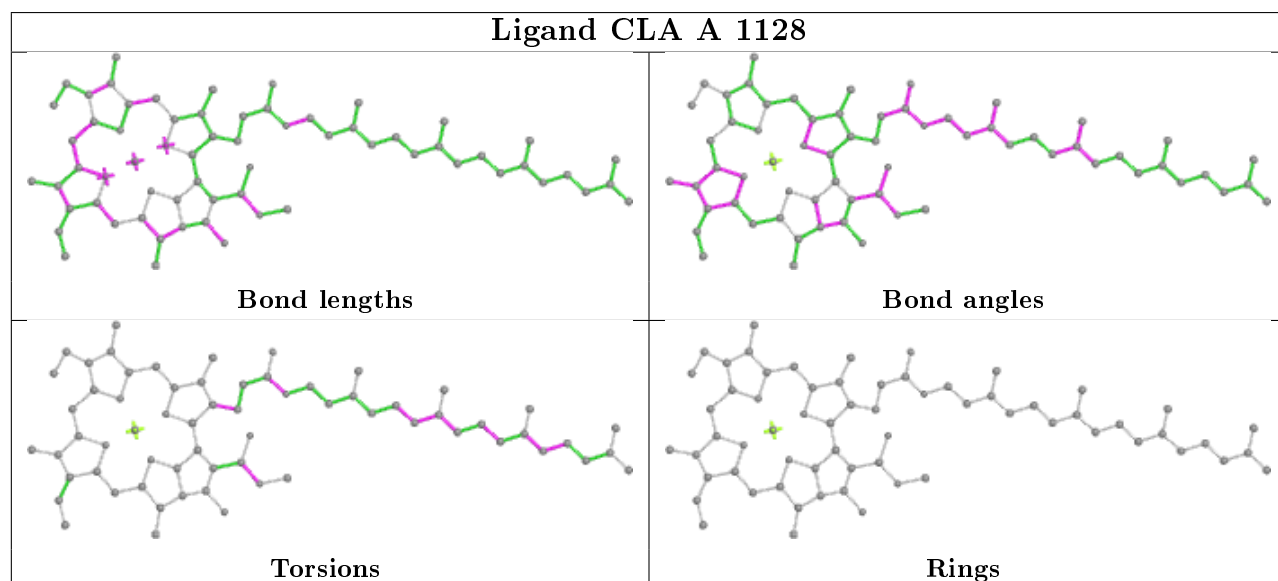
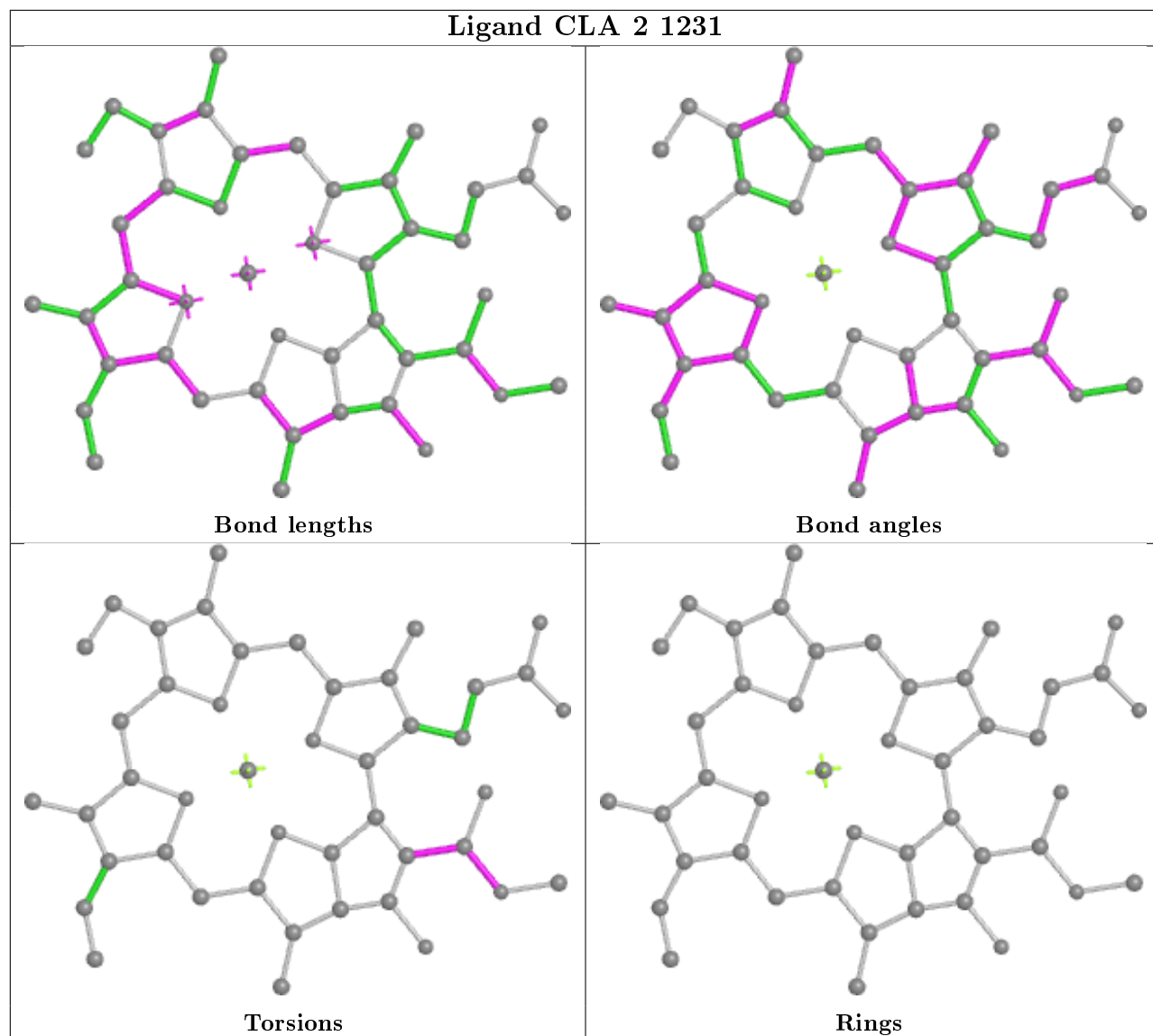


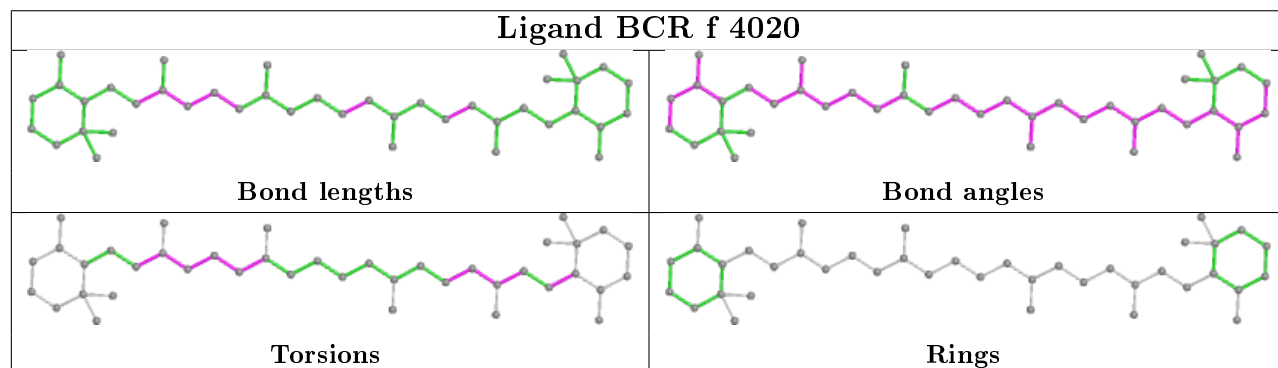
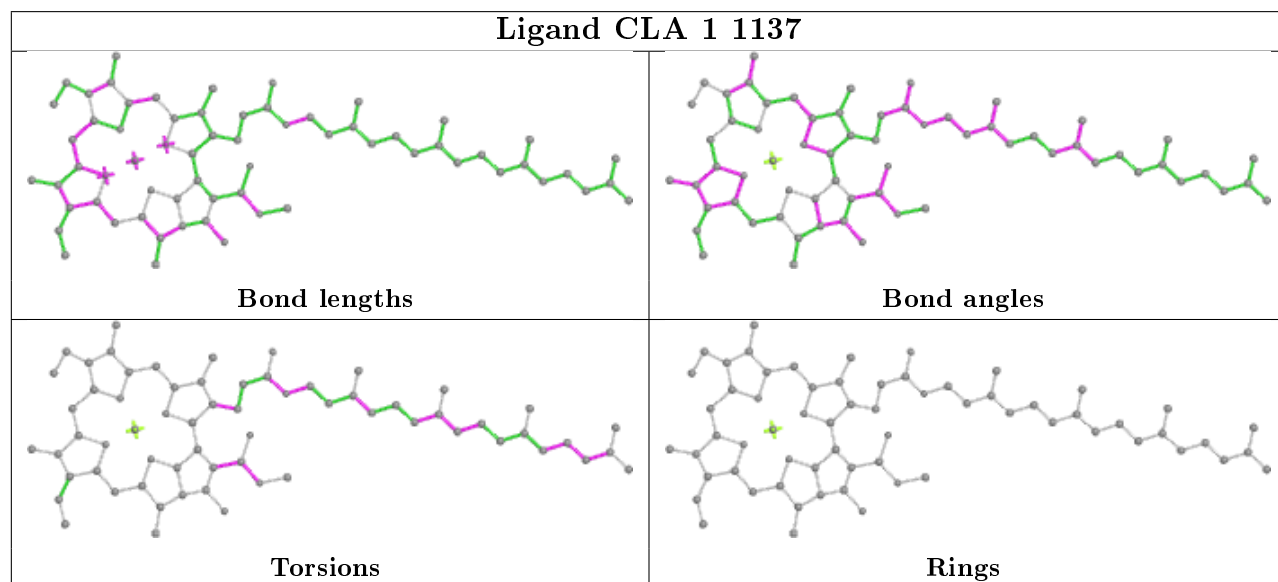
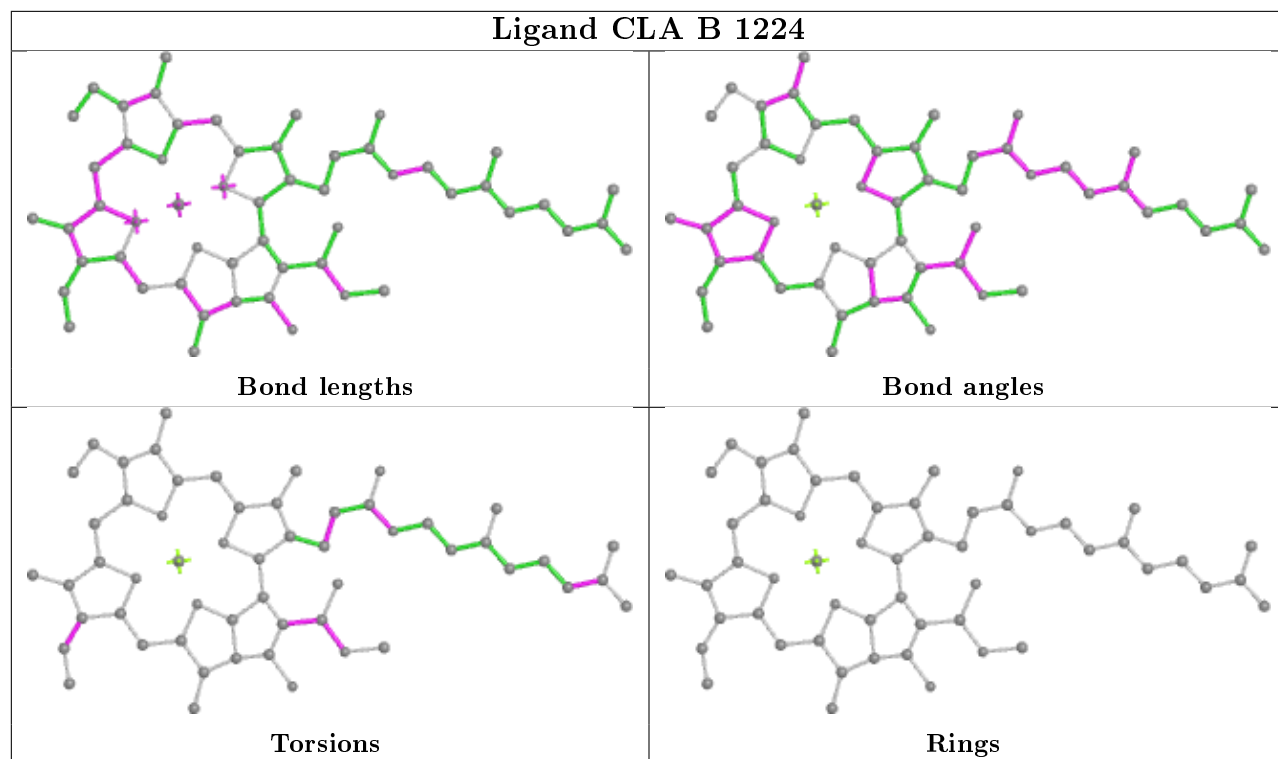
Rings



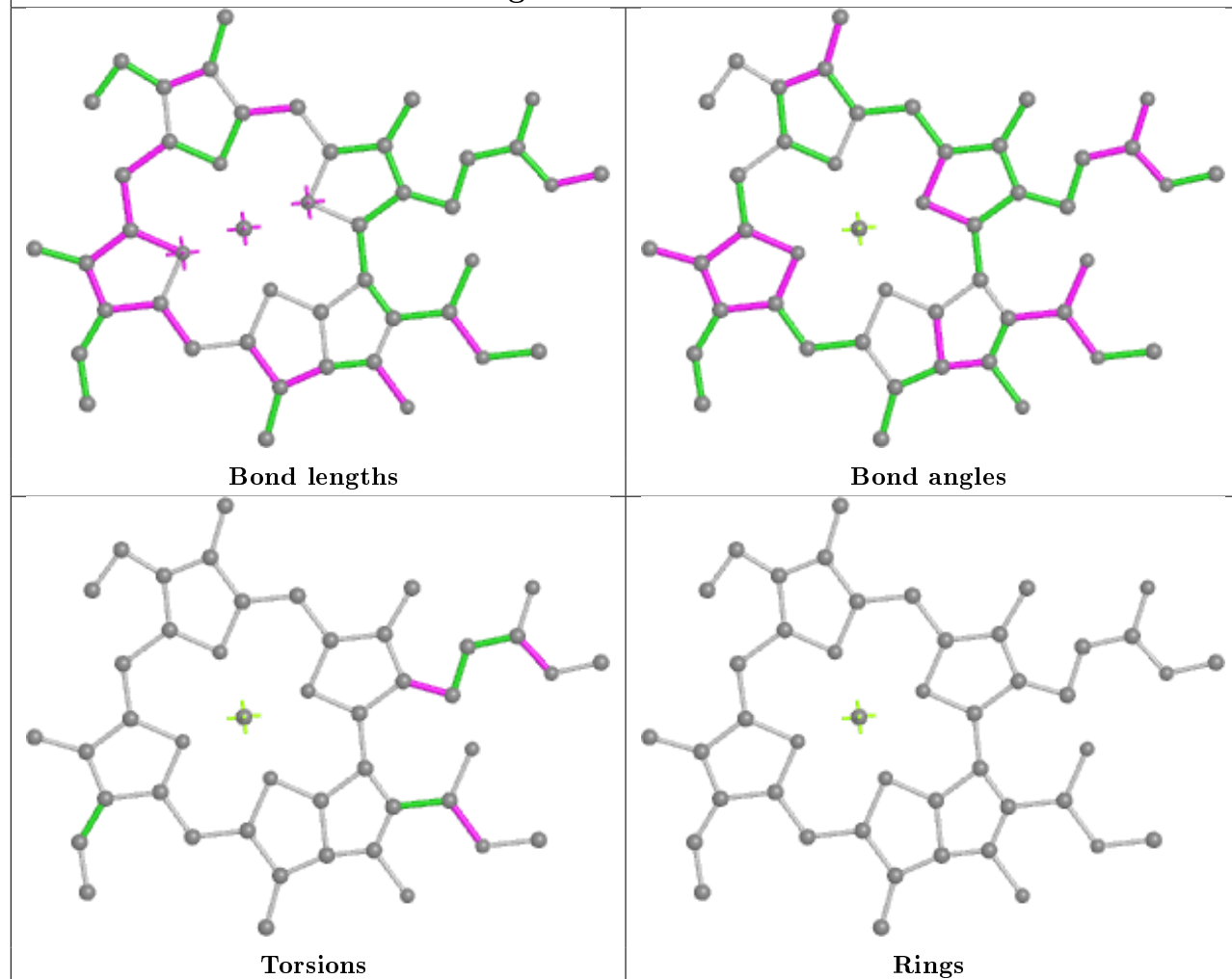




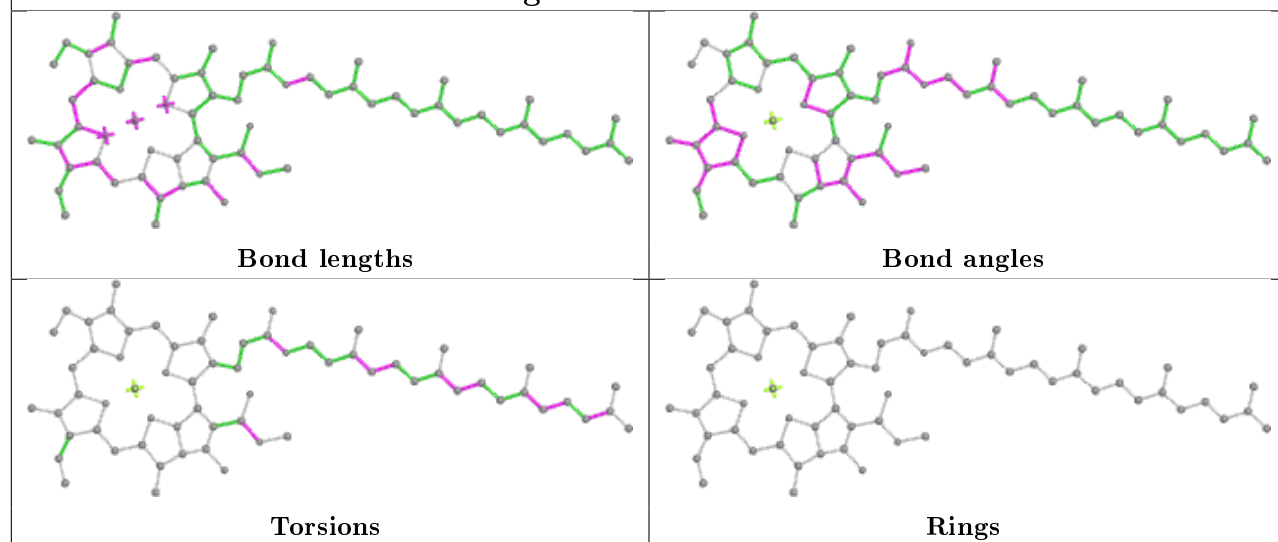


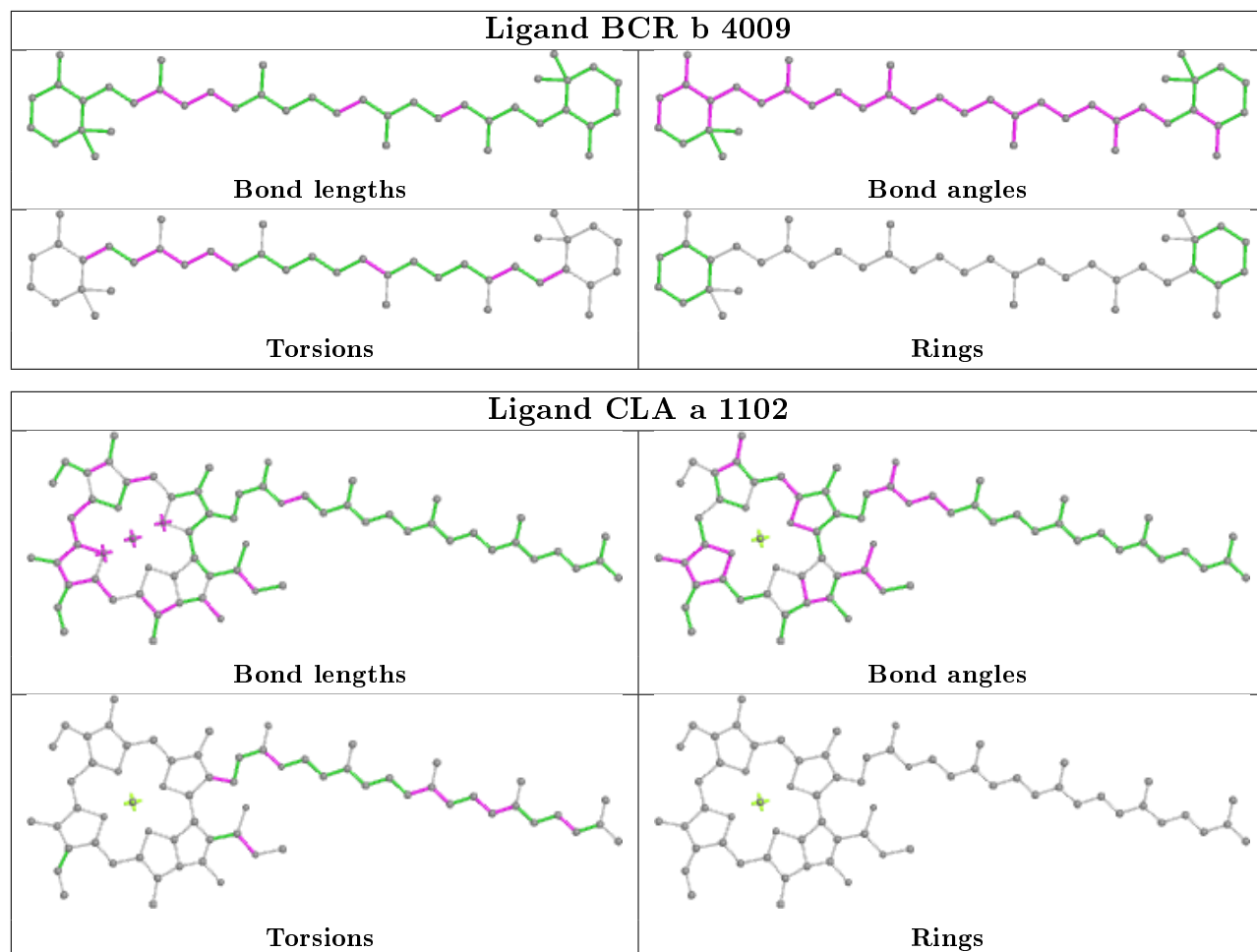


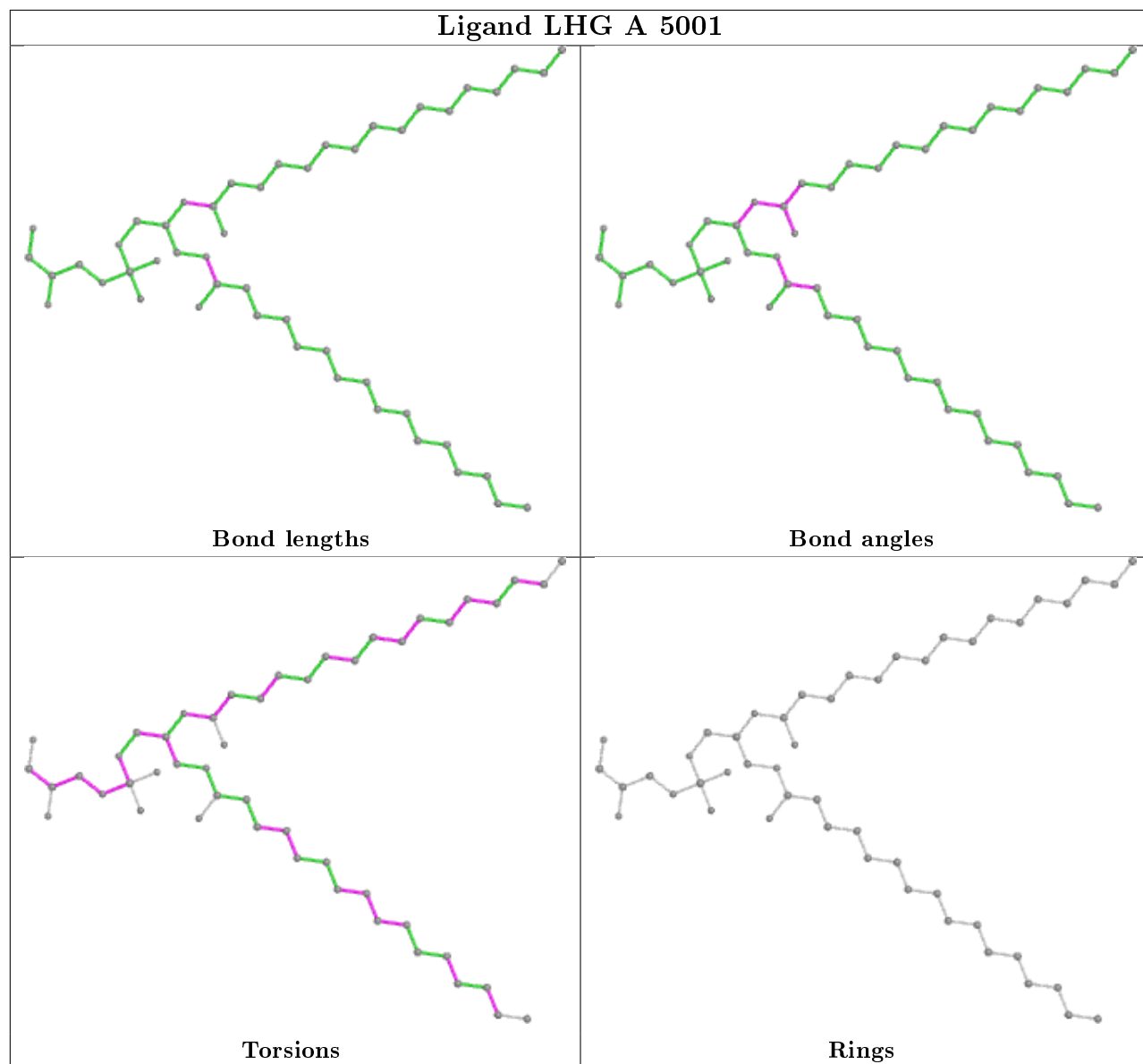
Ligand CLA 1 1130

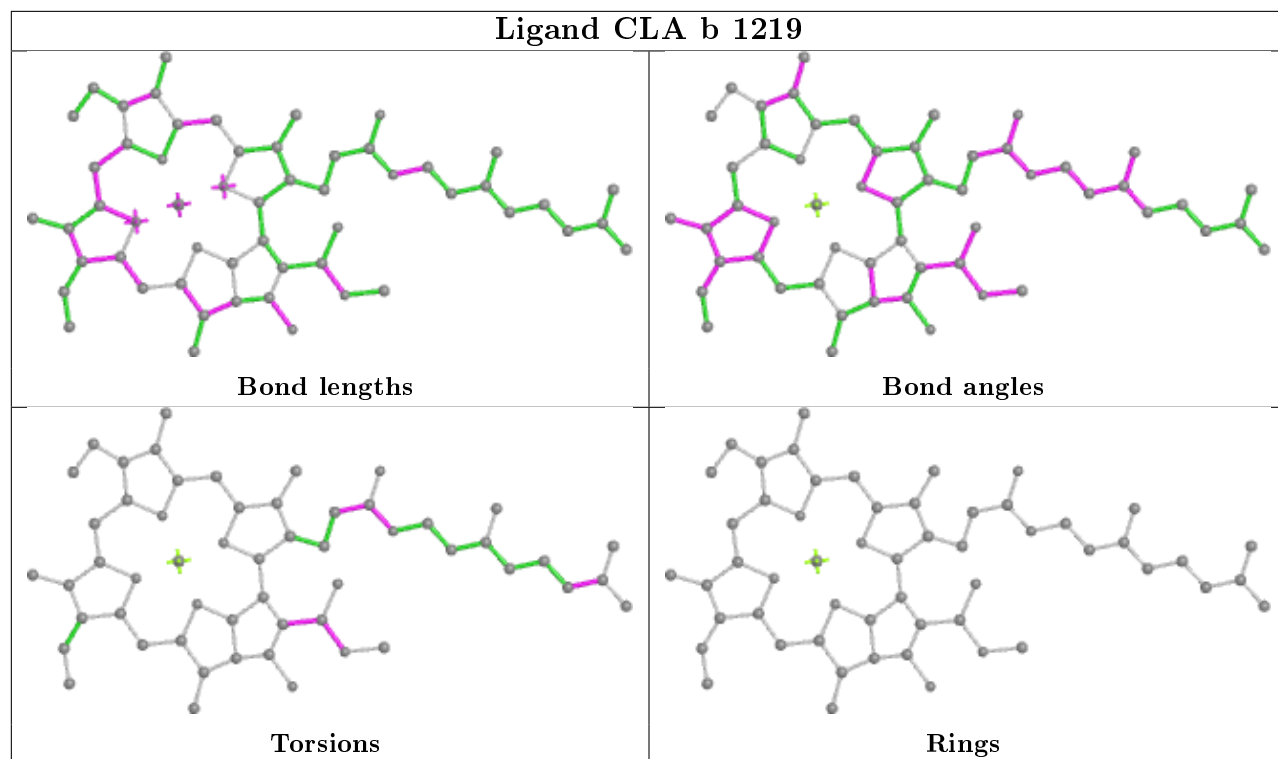


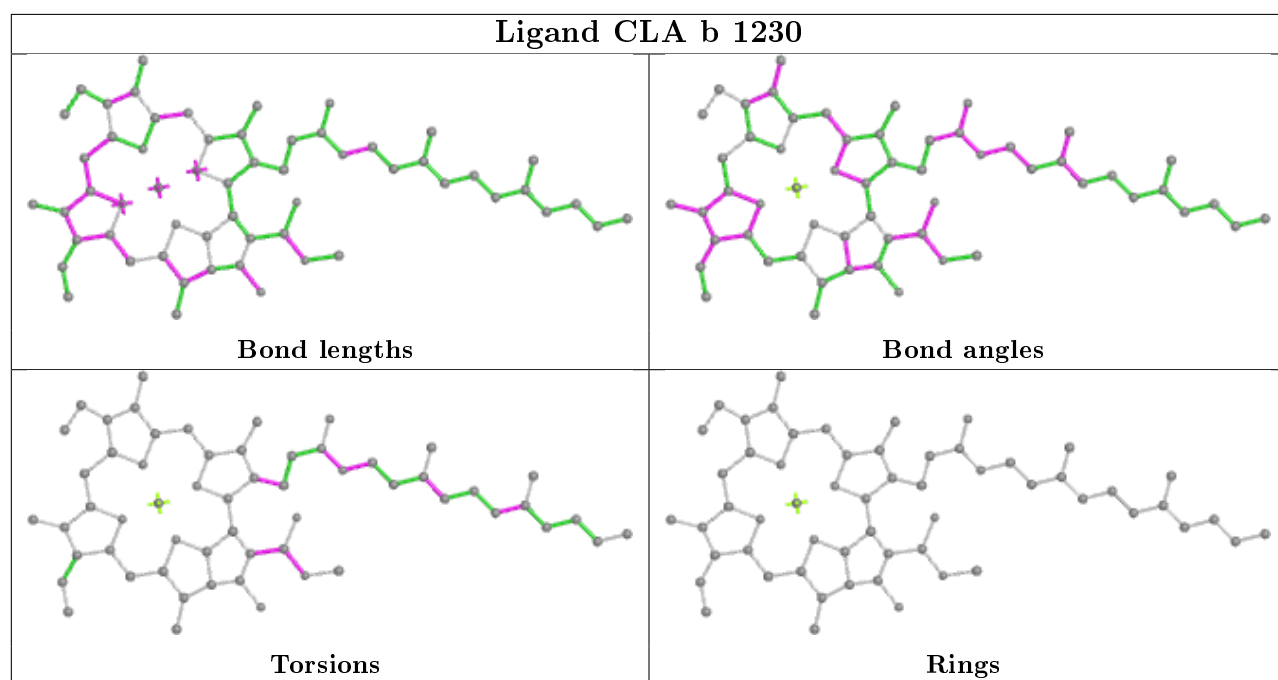
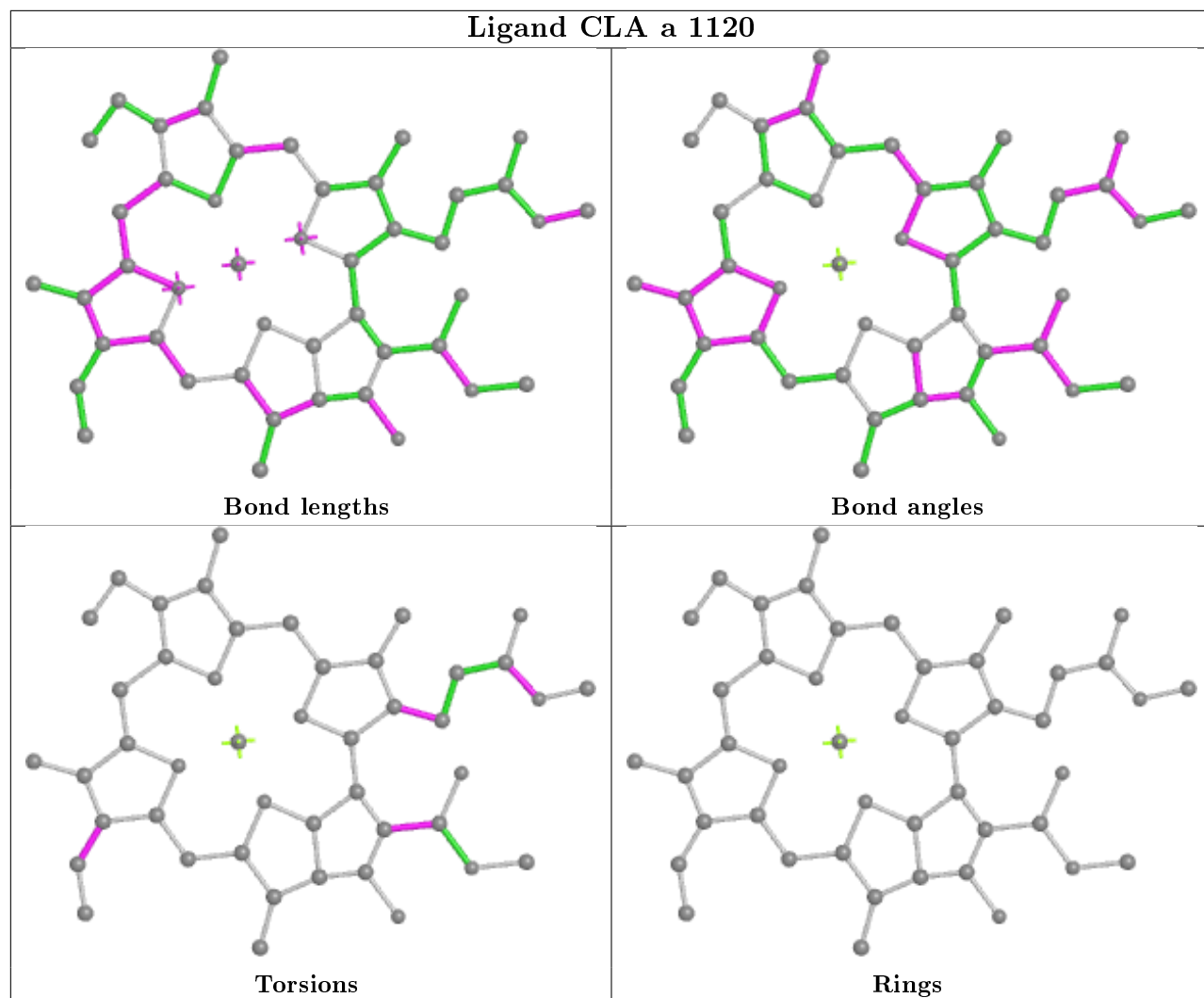
Ligand CLA B 1206

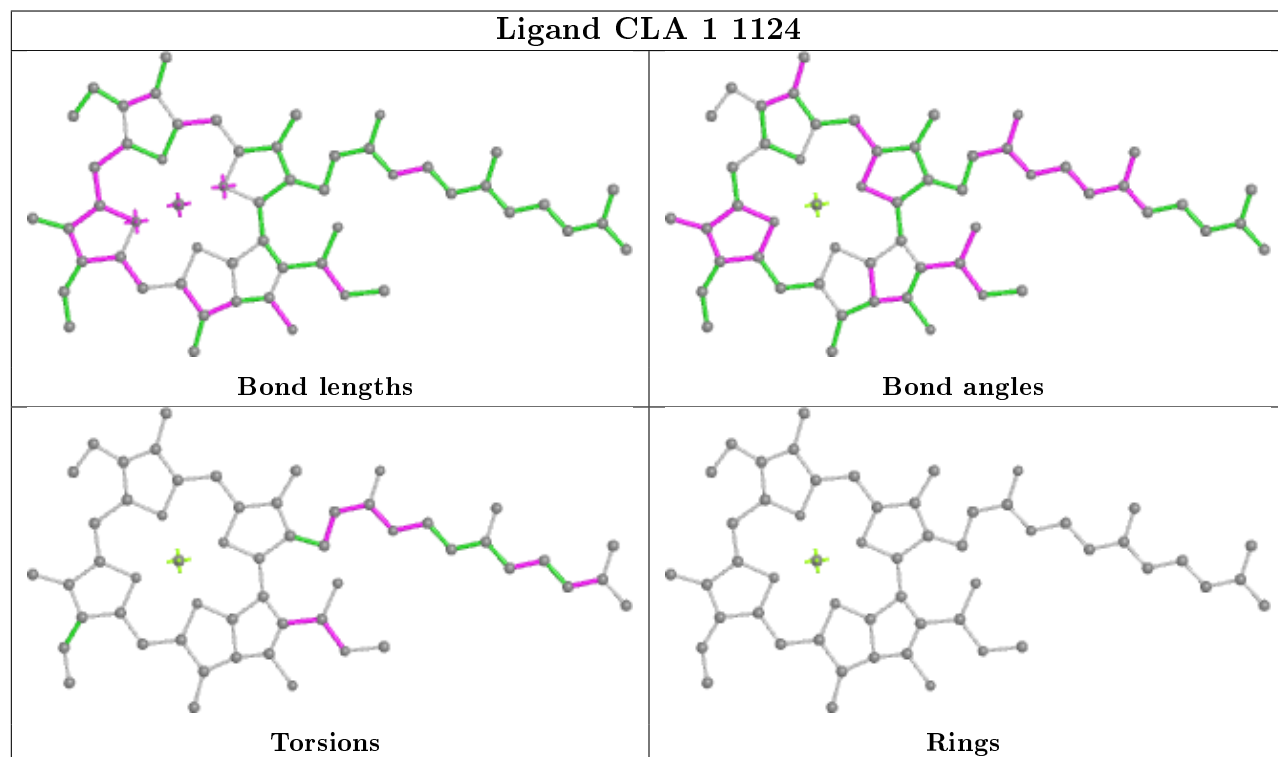
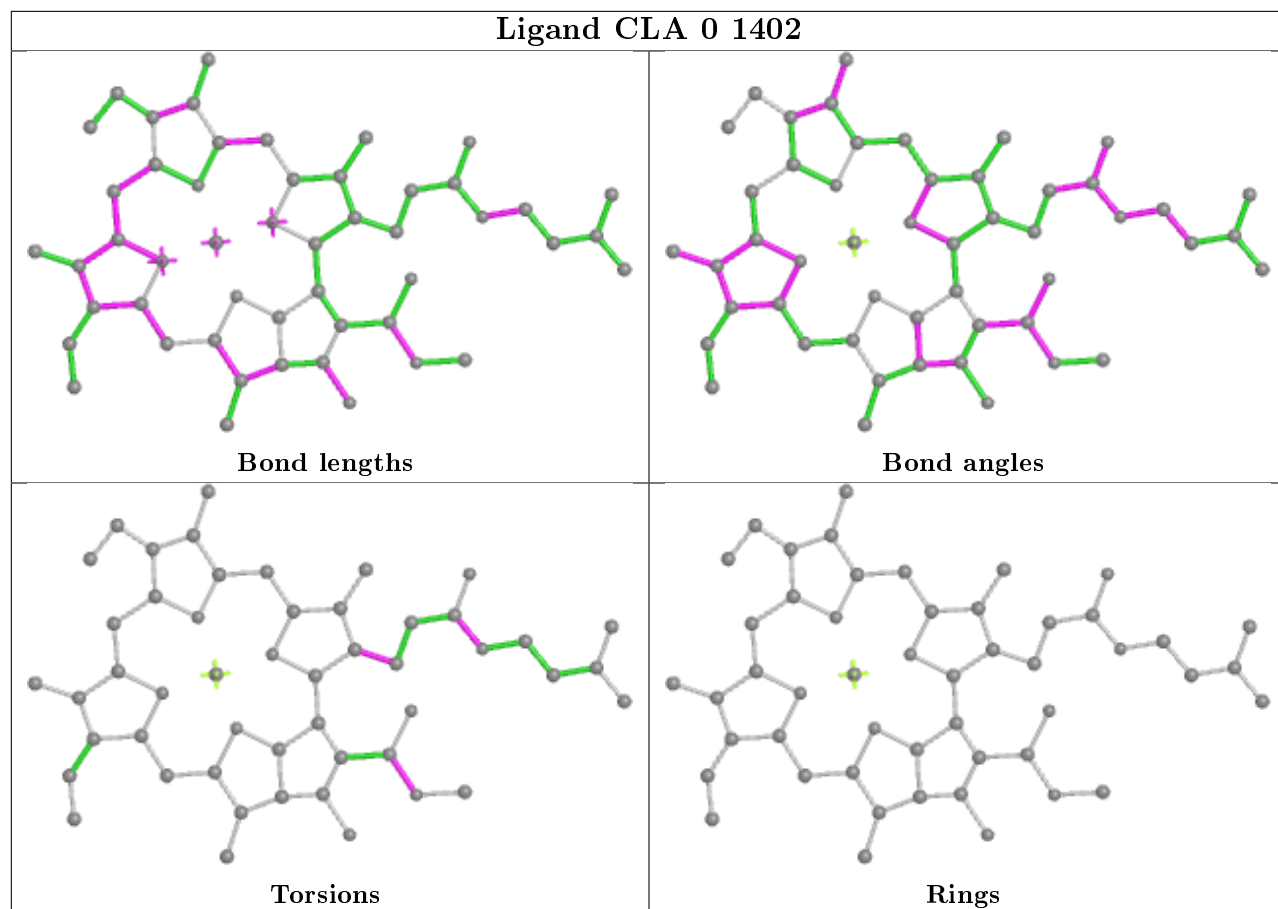


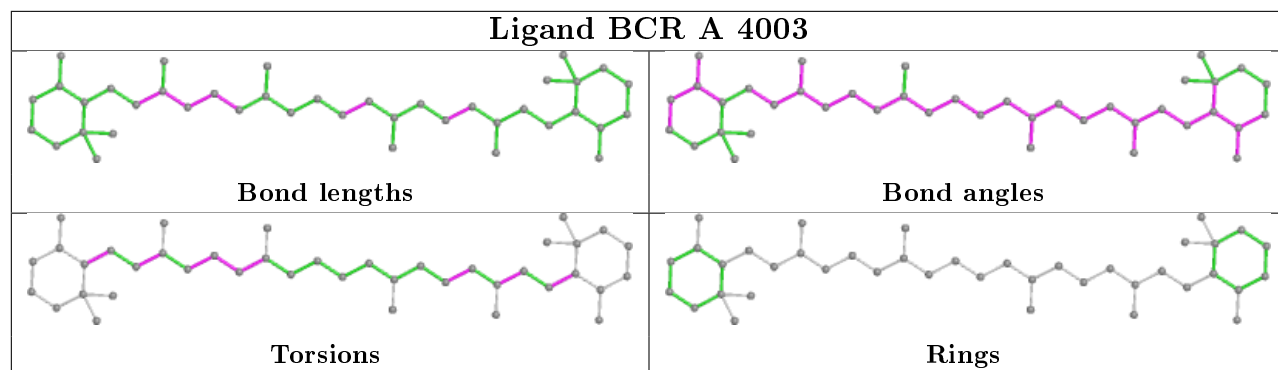
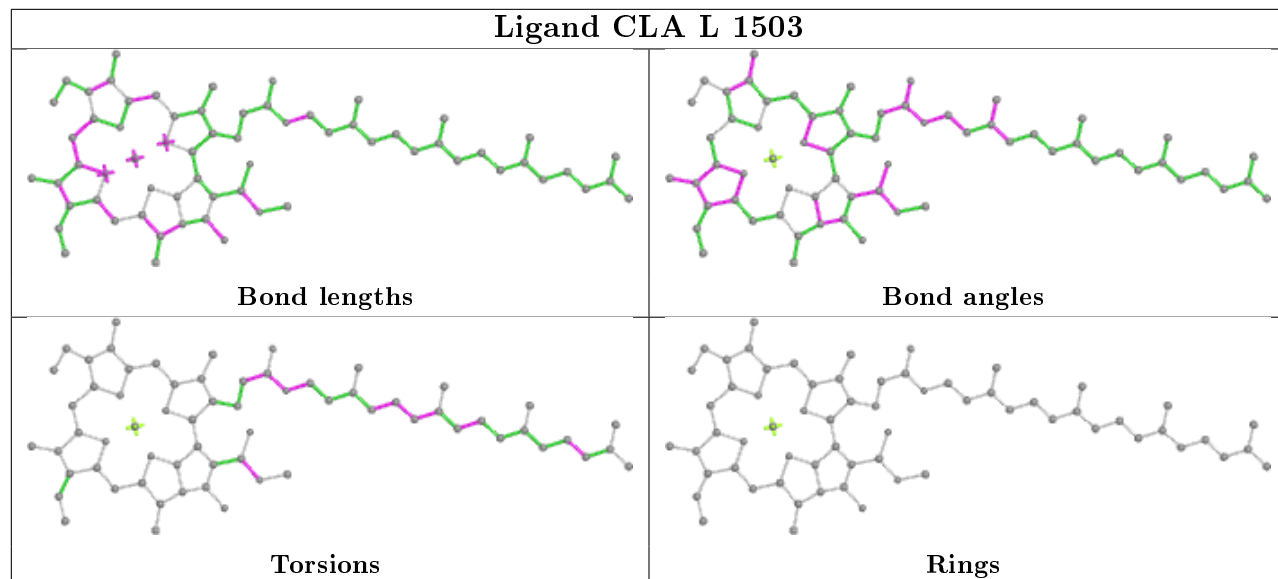
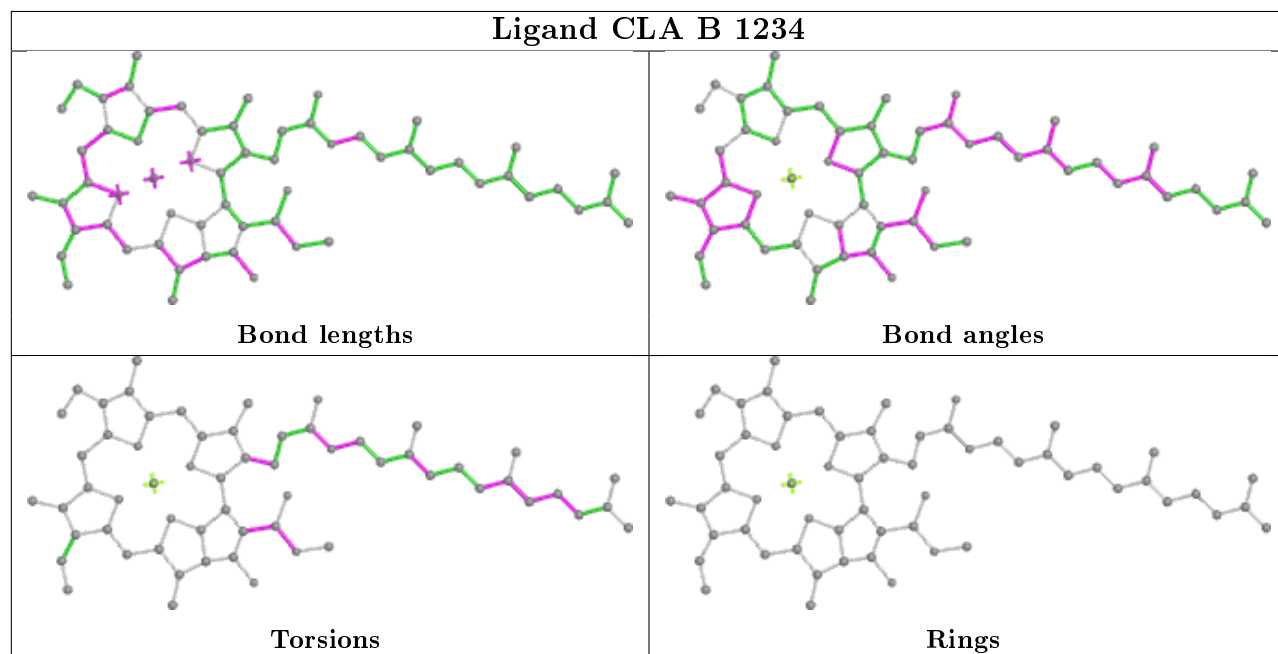


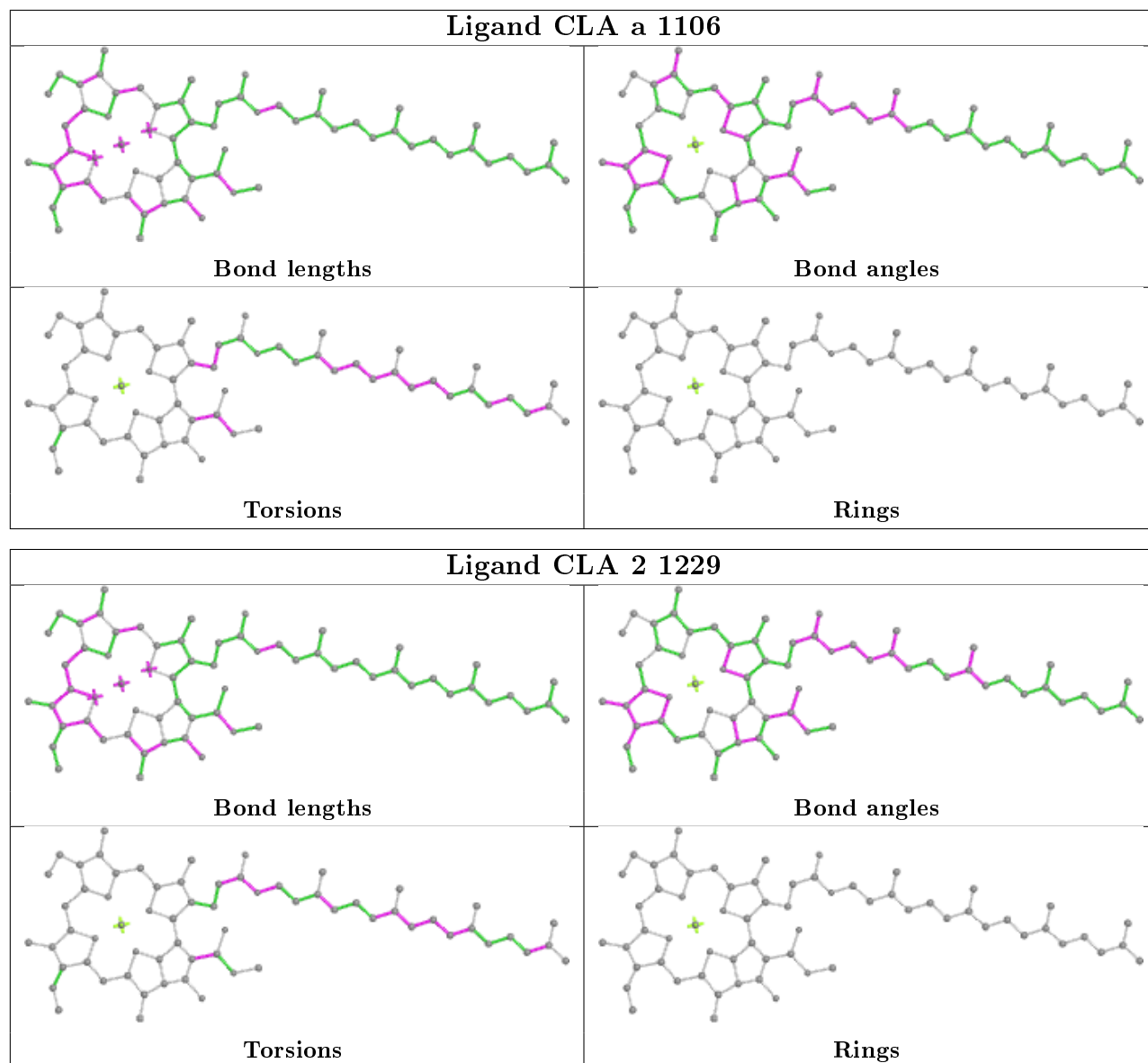


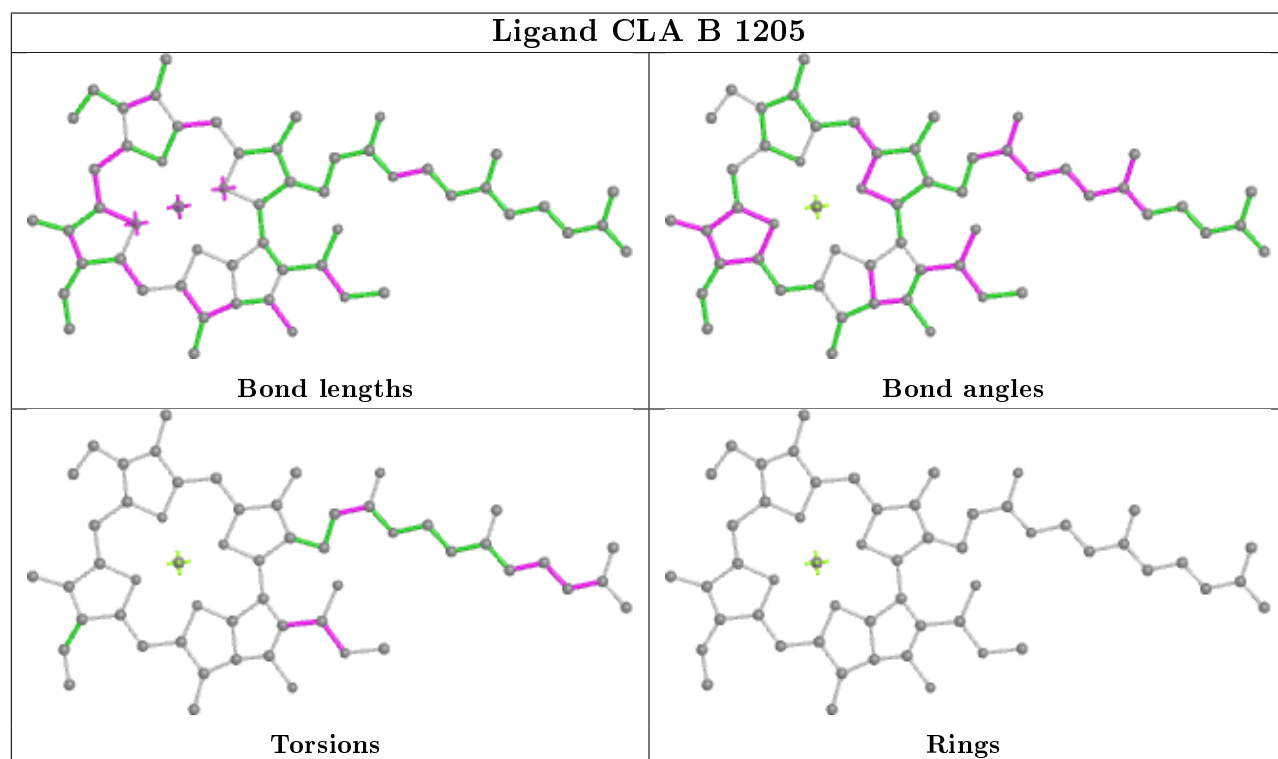
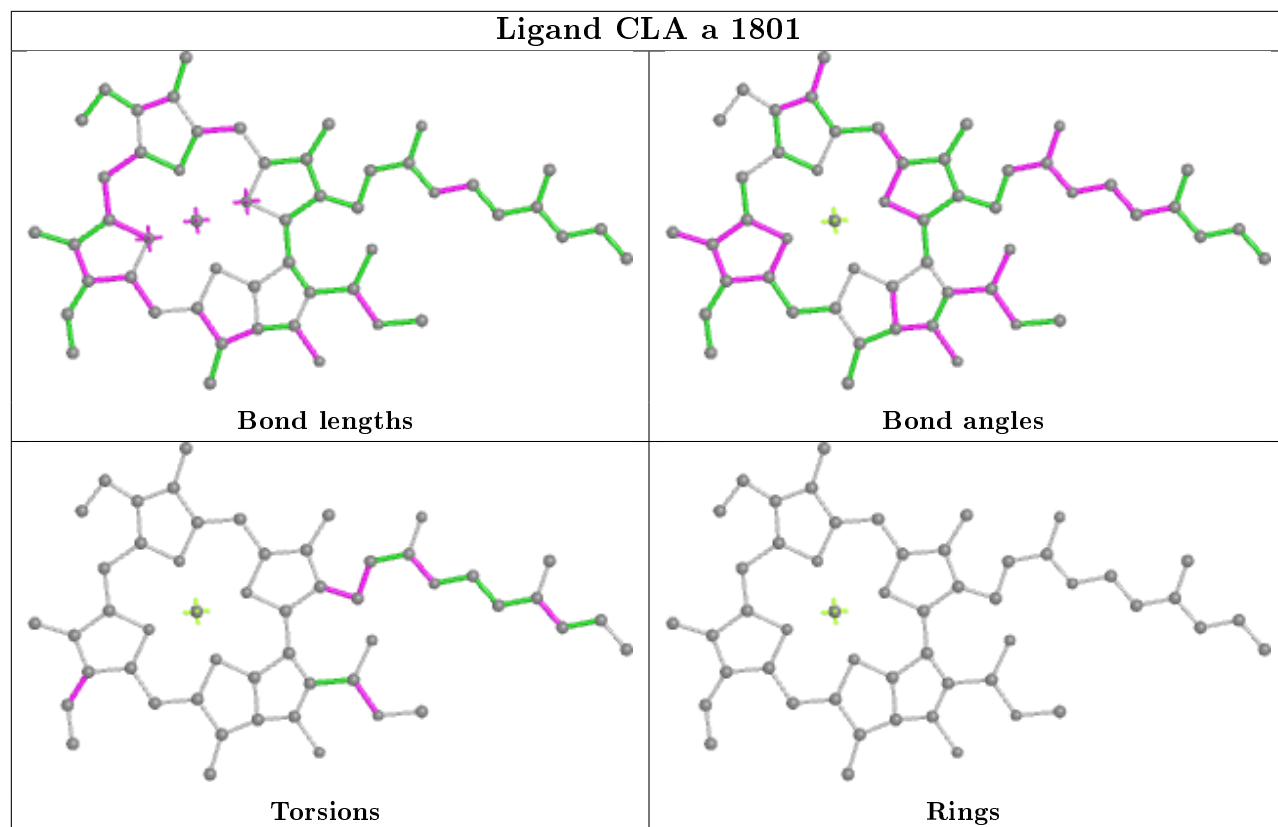


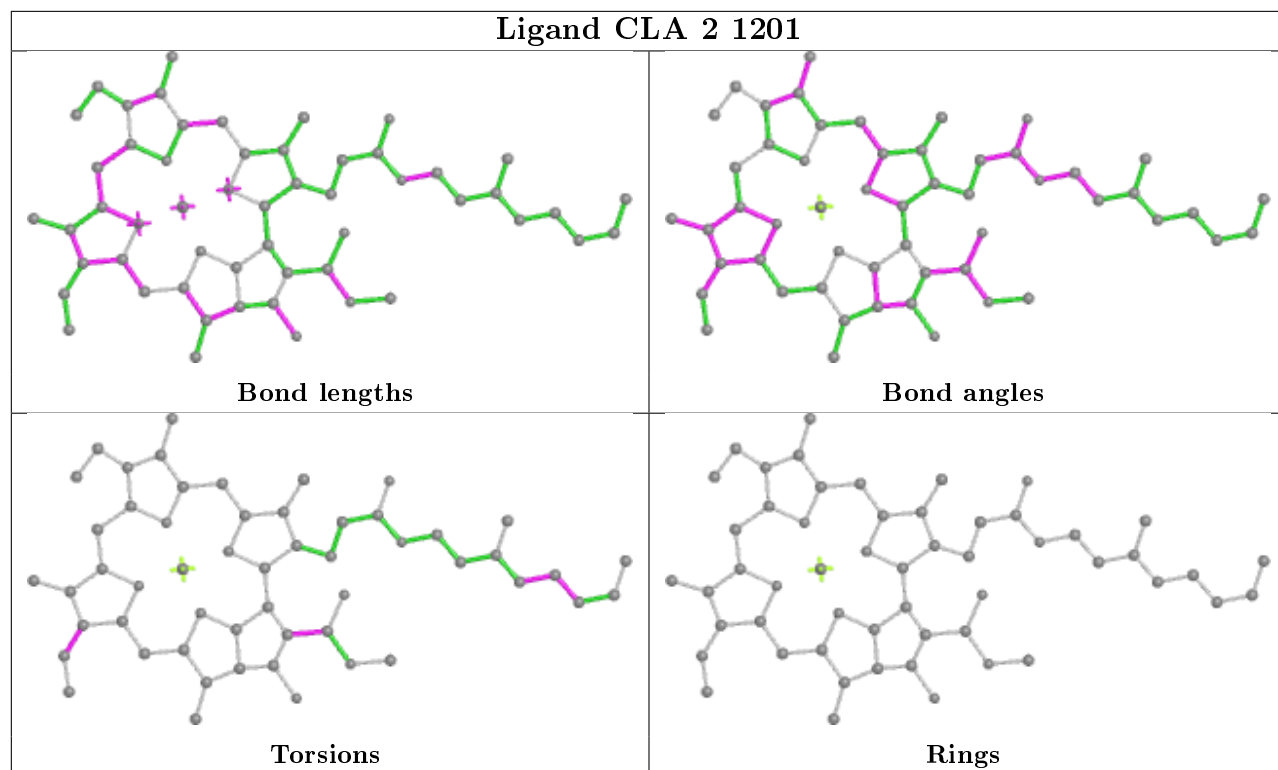


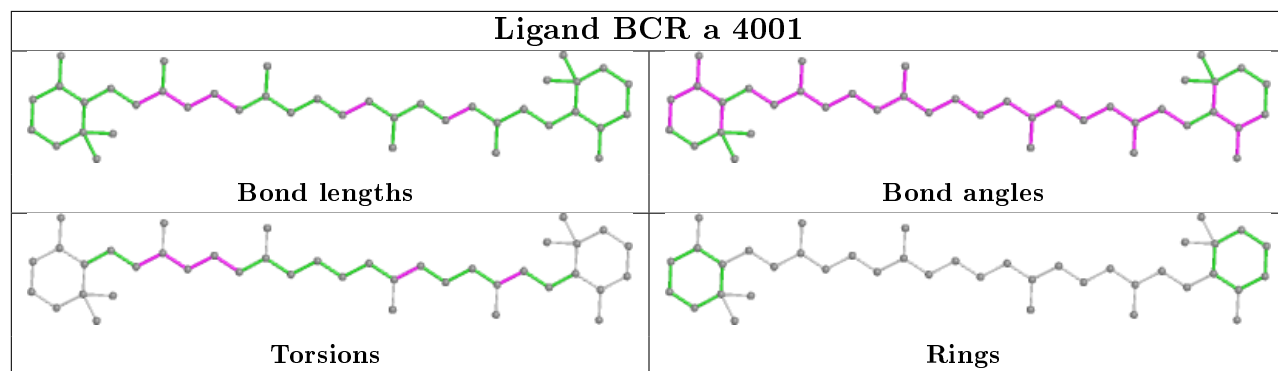
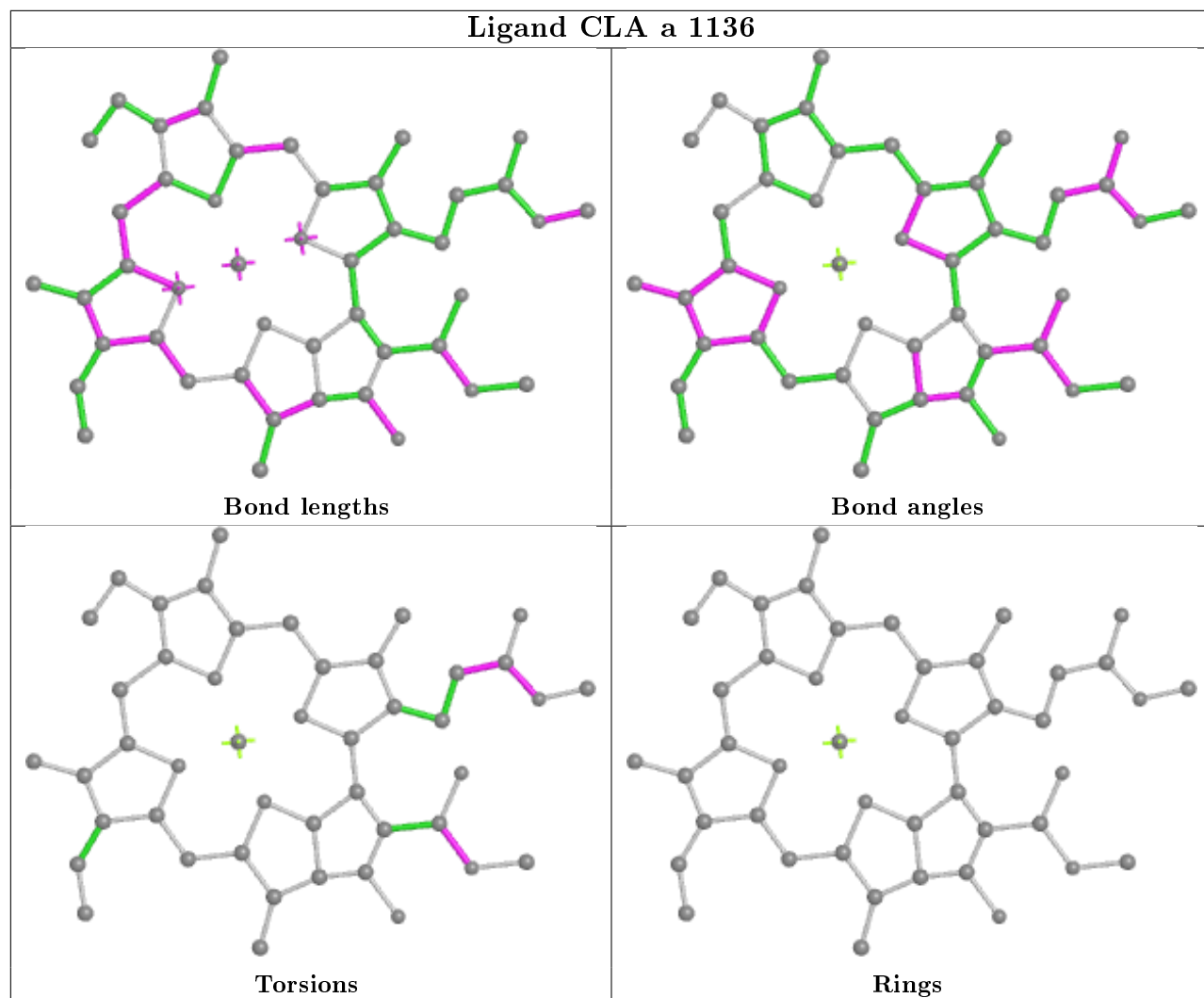


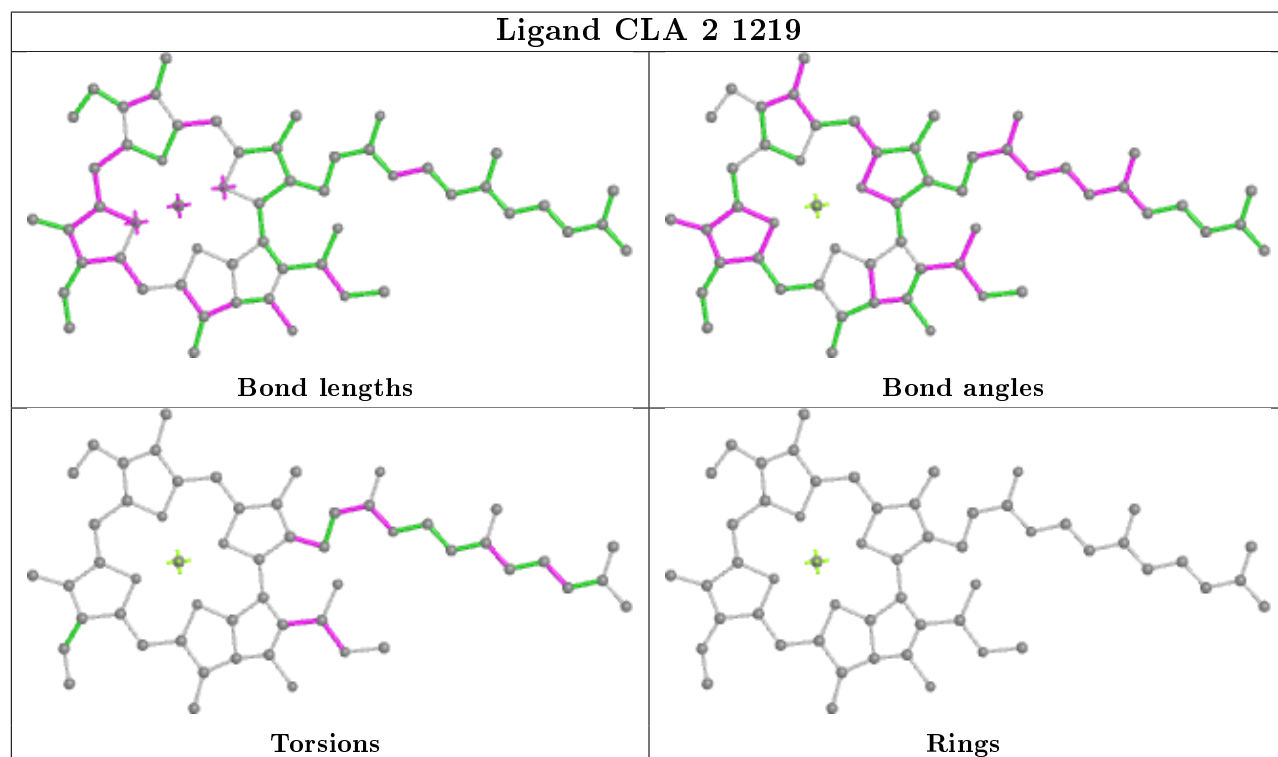
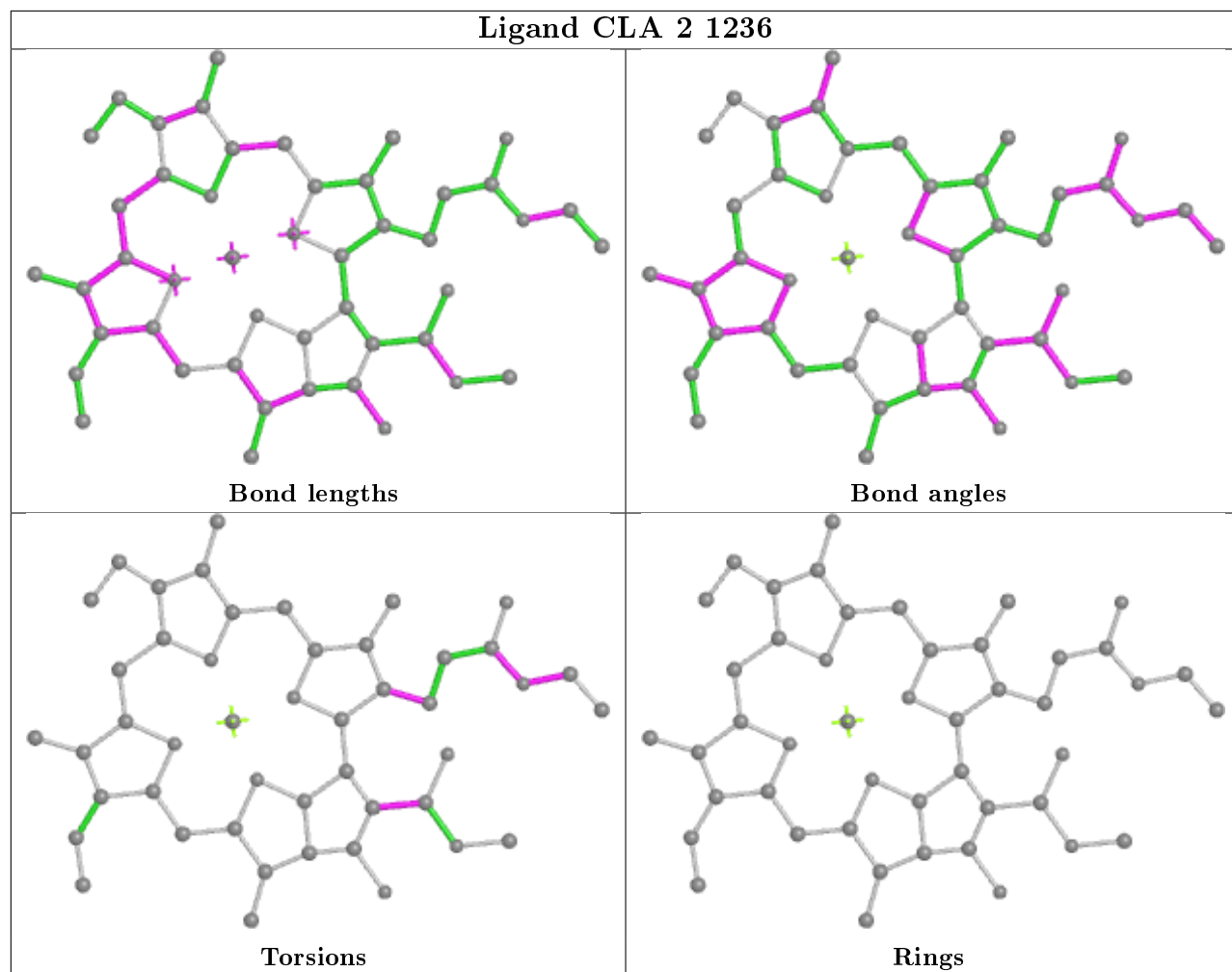
Ligand BCR A 4003**Ligand CLA L 1503****Ligand CLA B 1234**

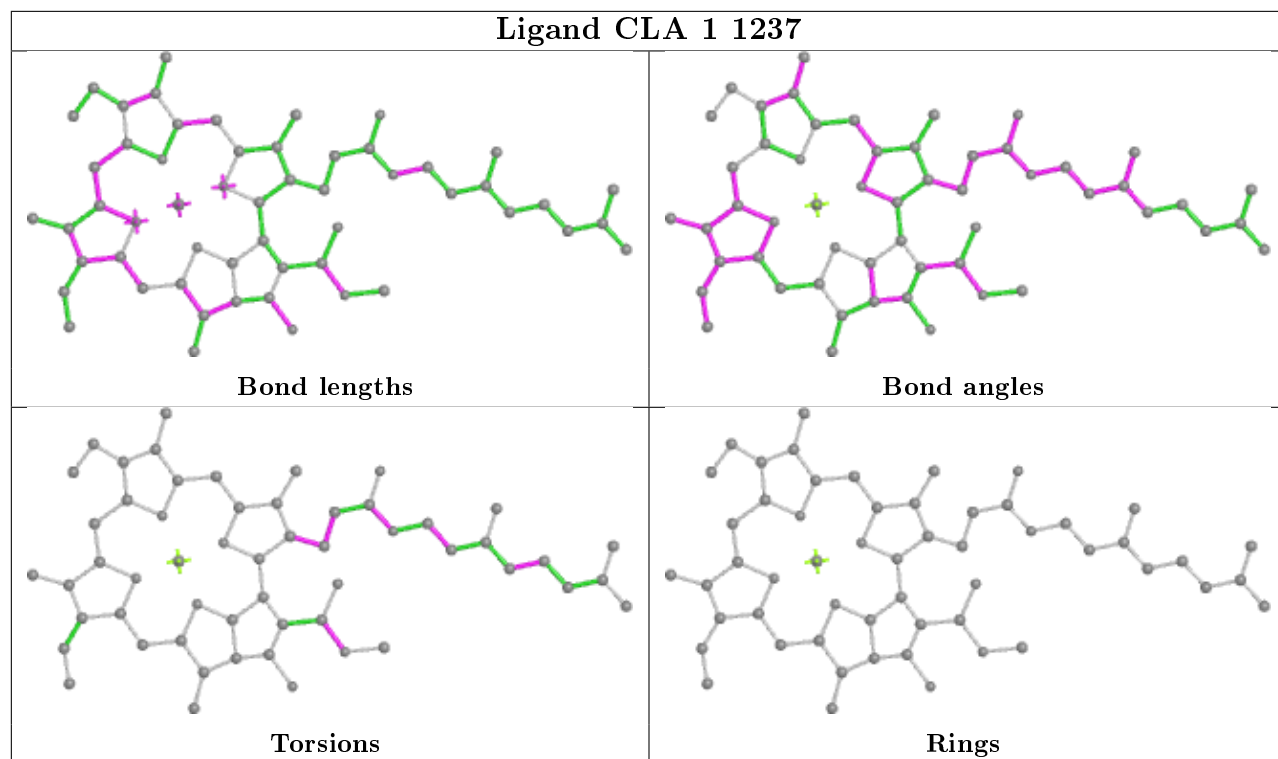


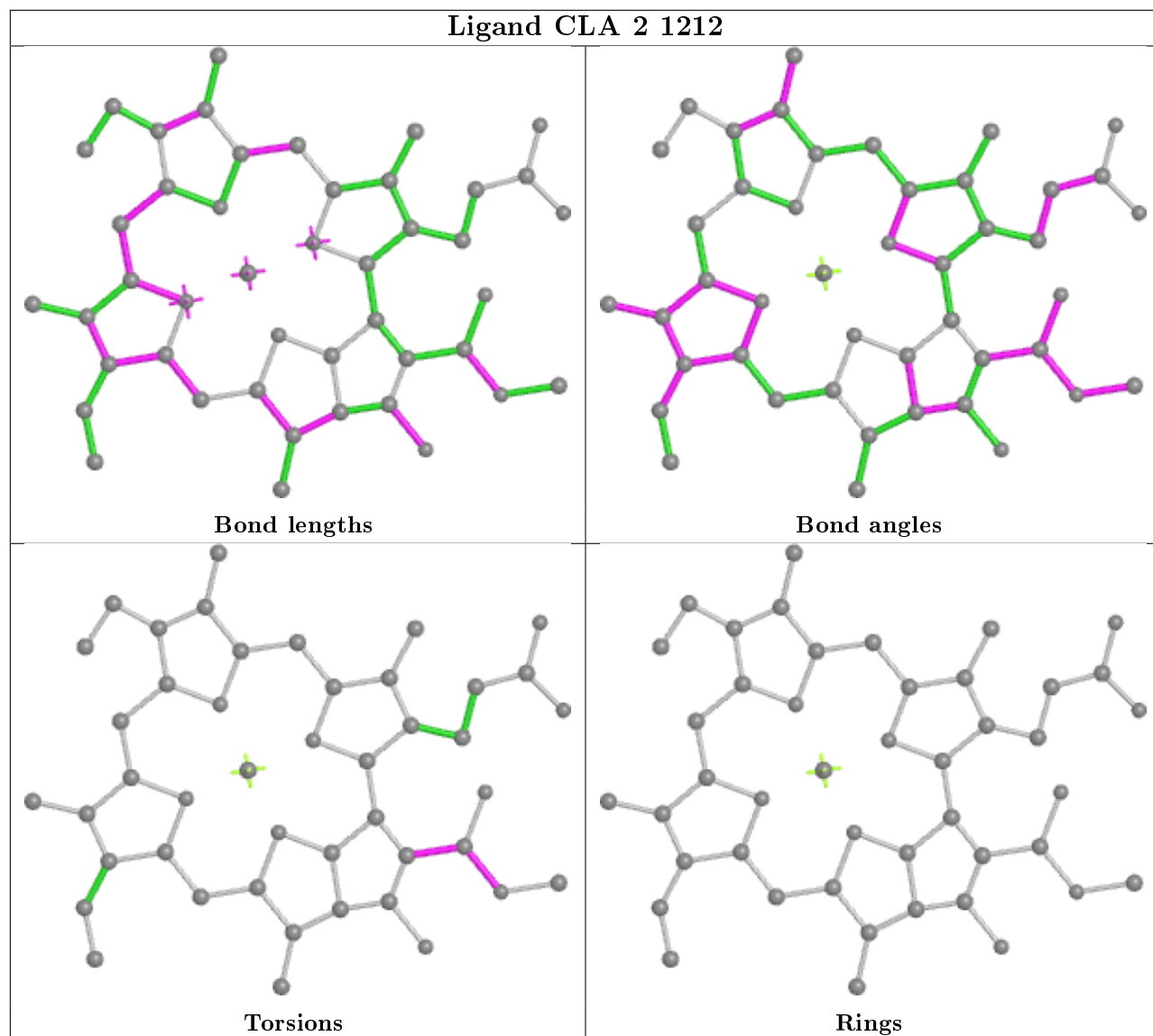


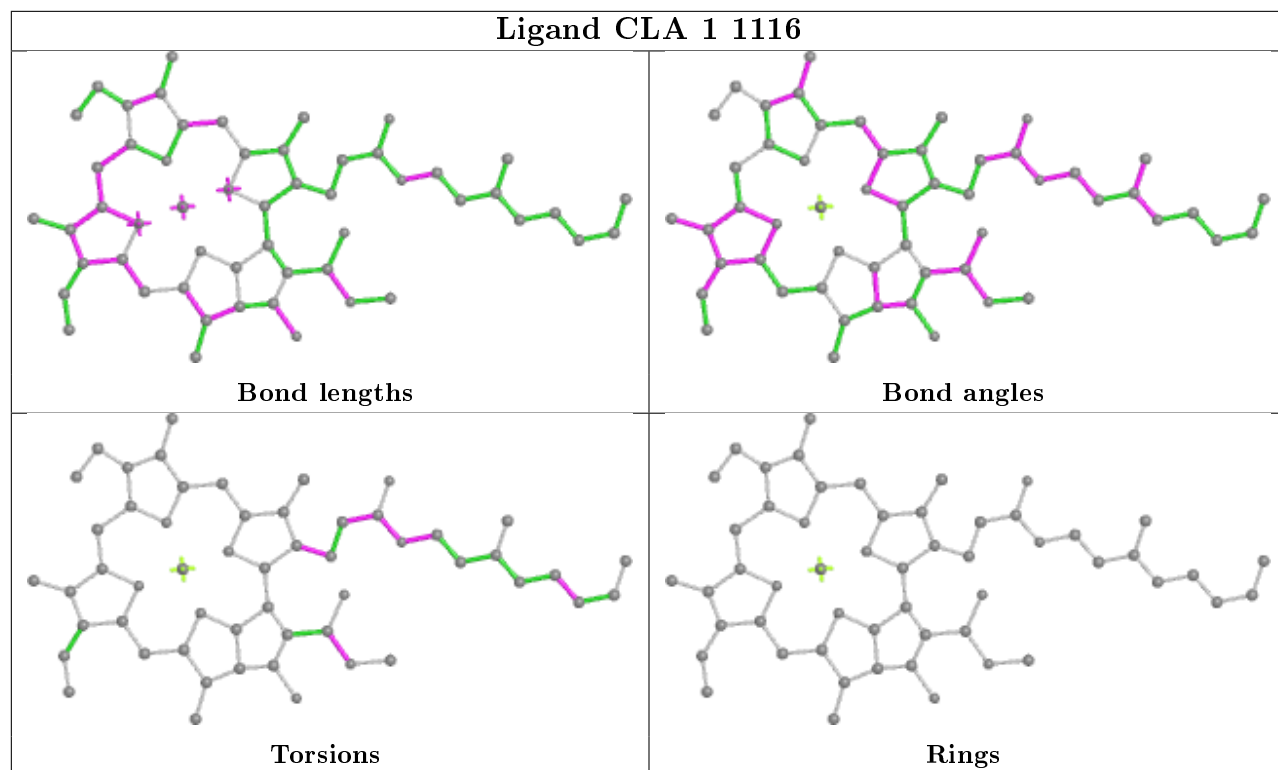
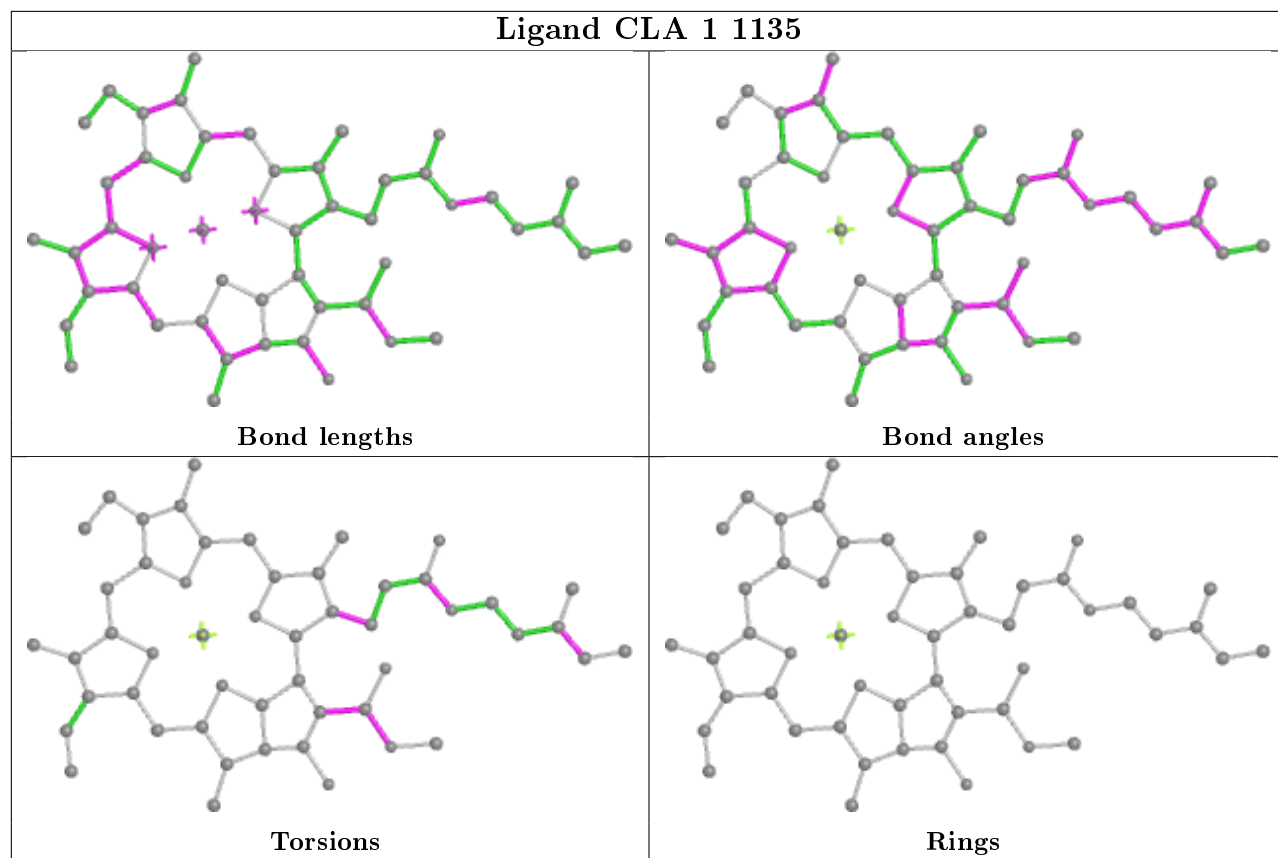


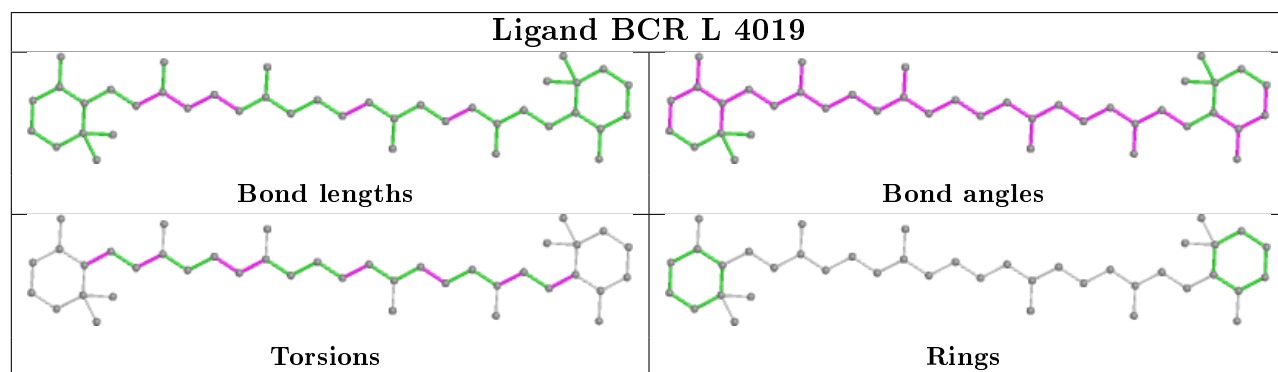
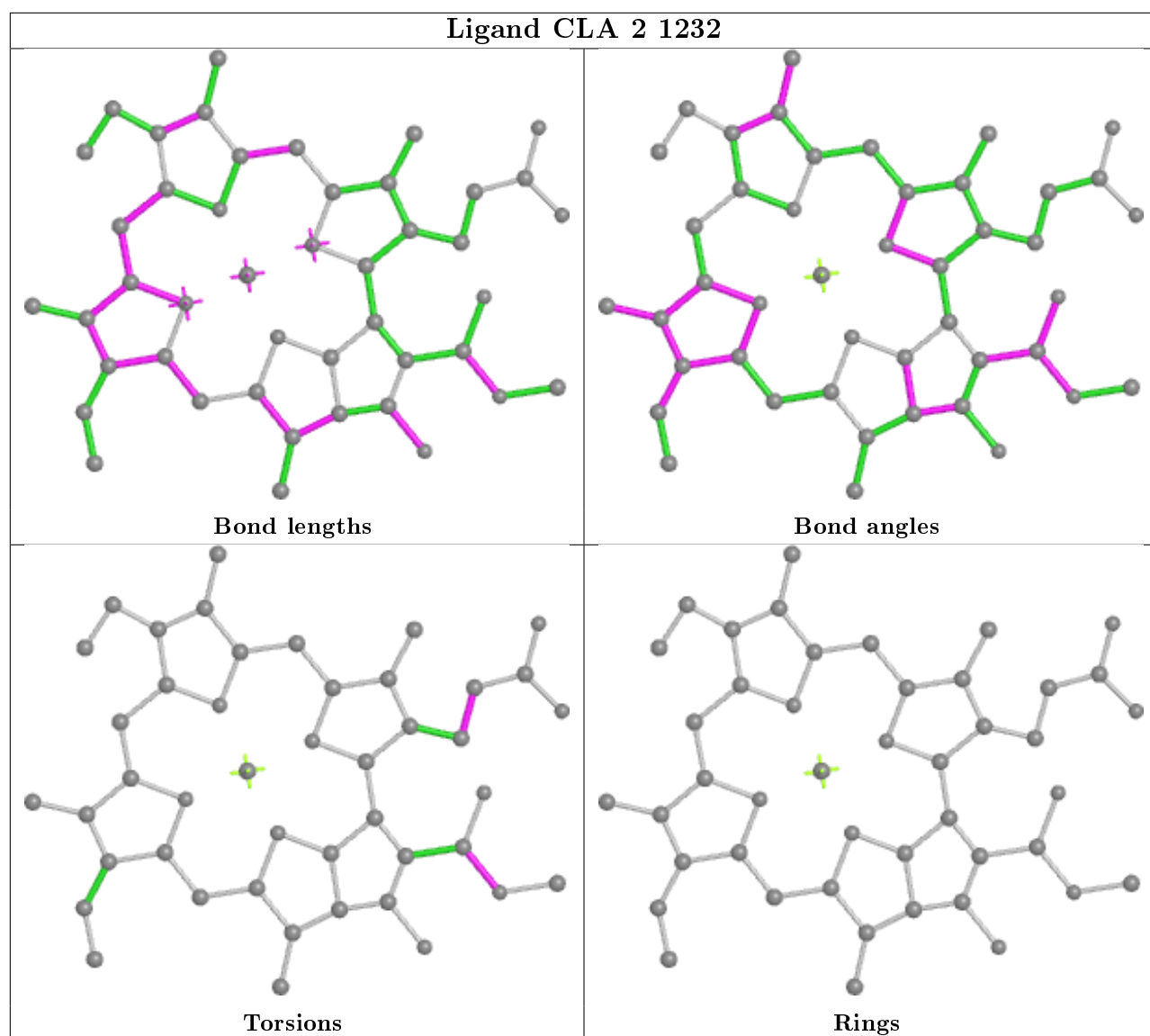


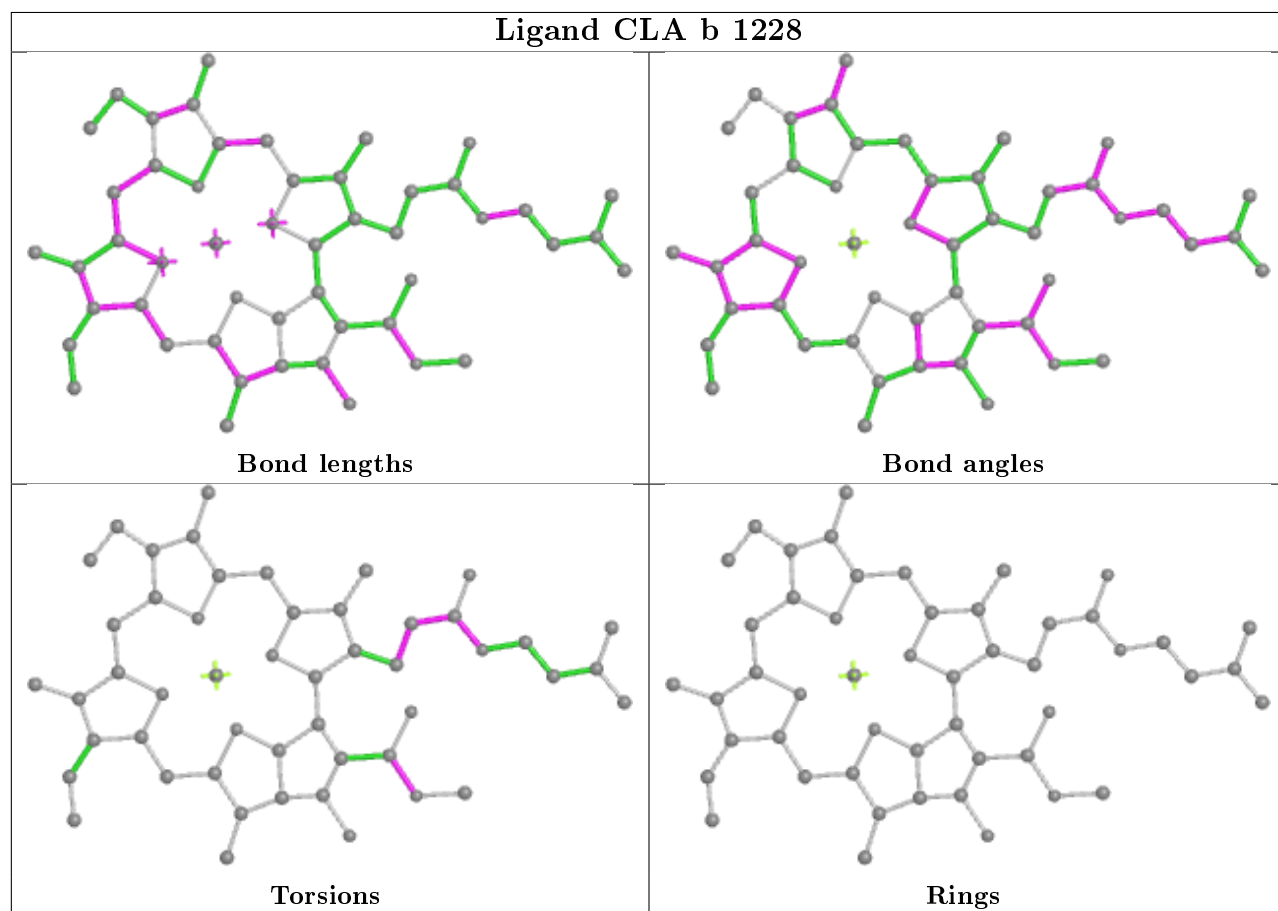
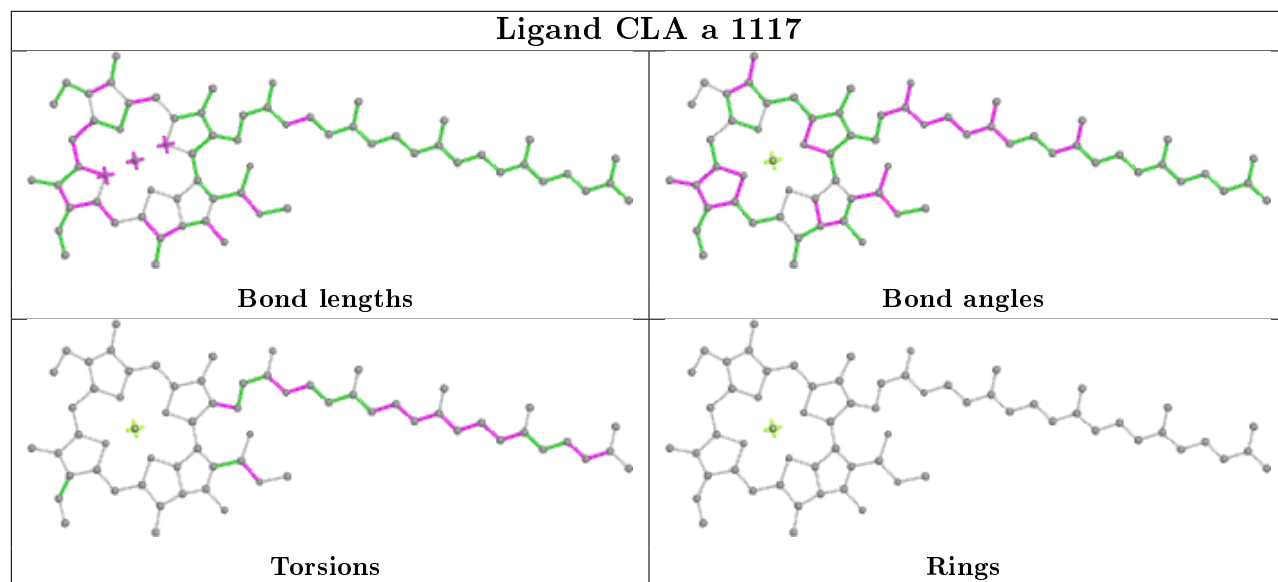


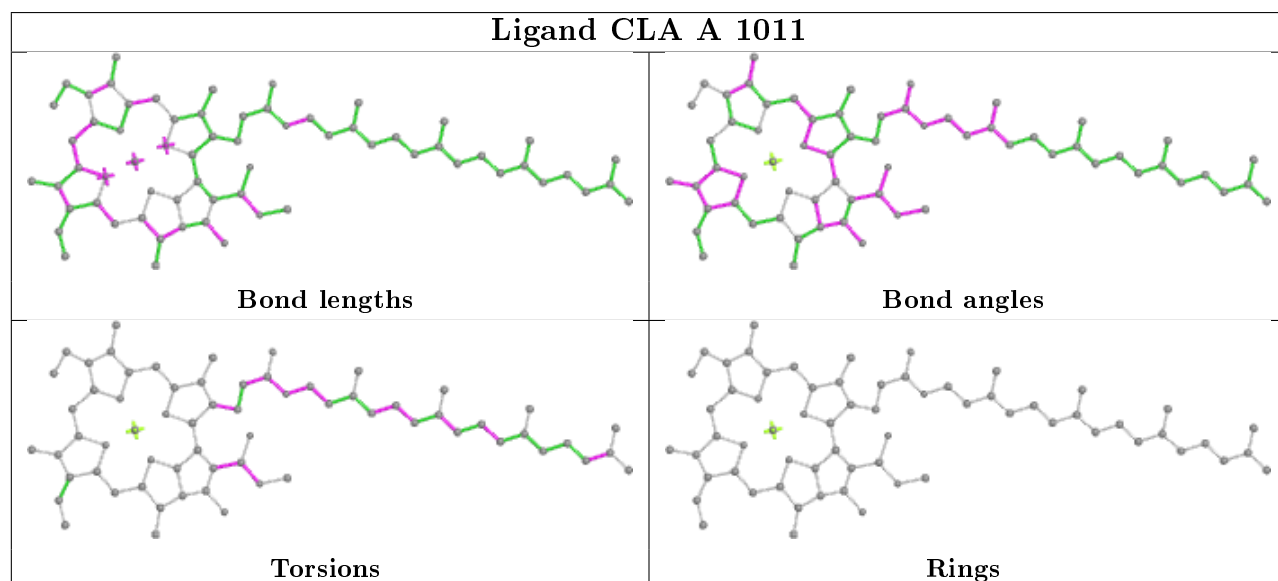
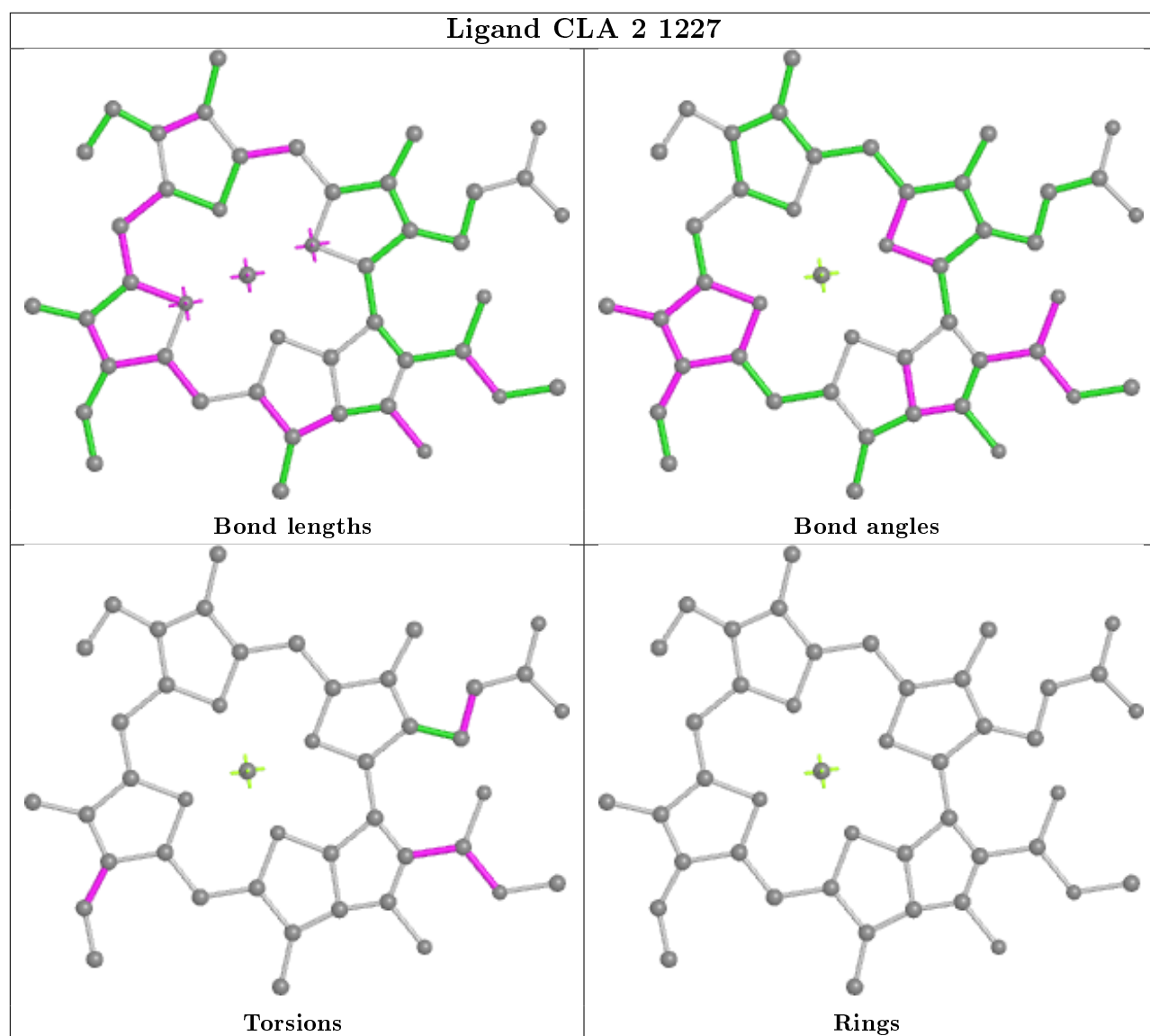




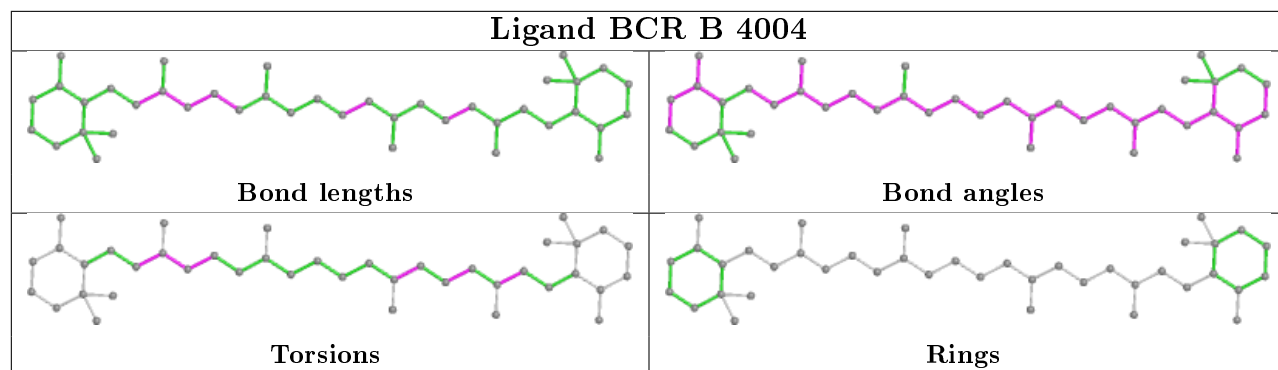




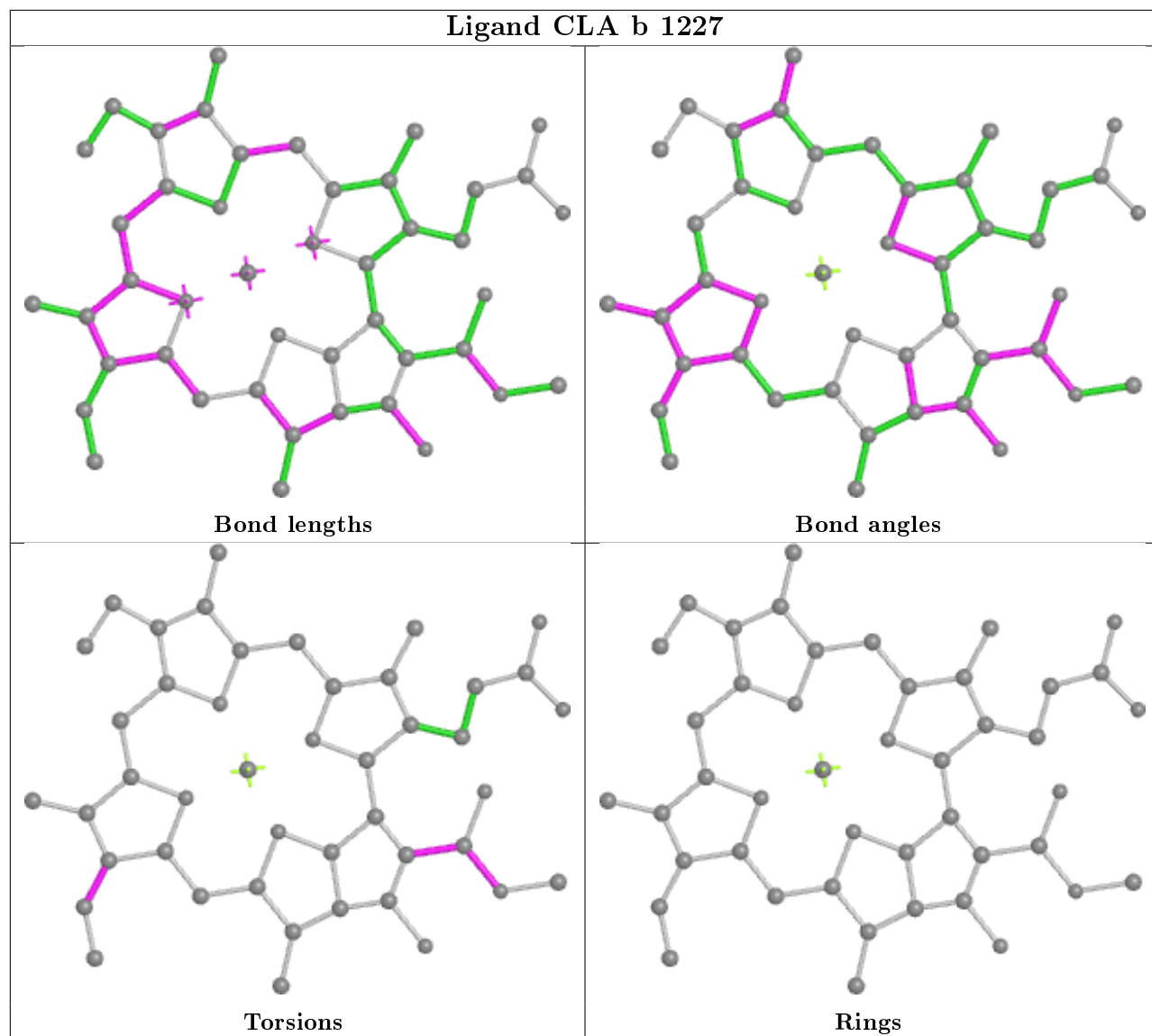




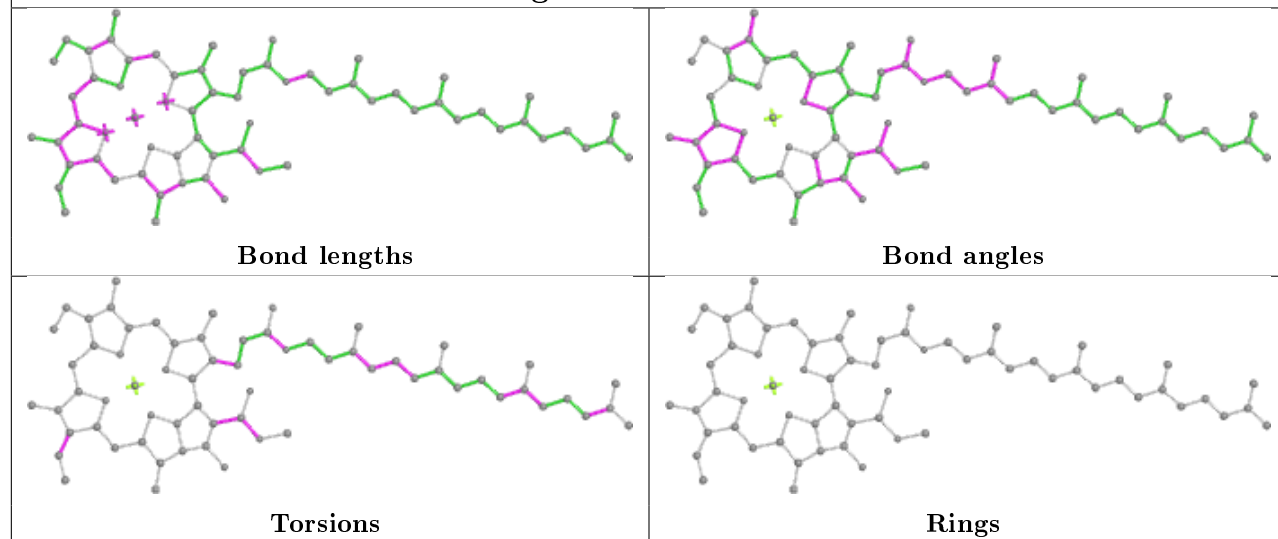
Ligand BCR B 4004



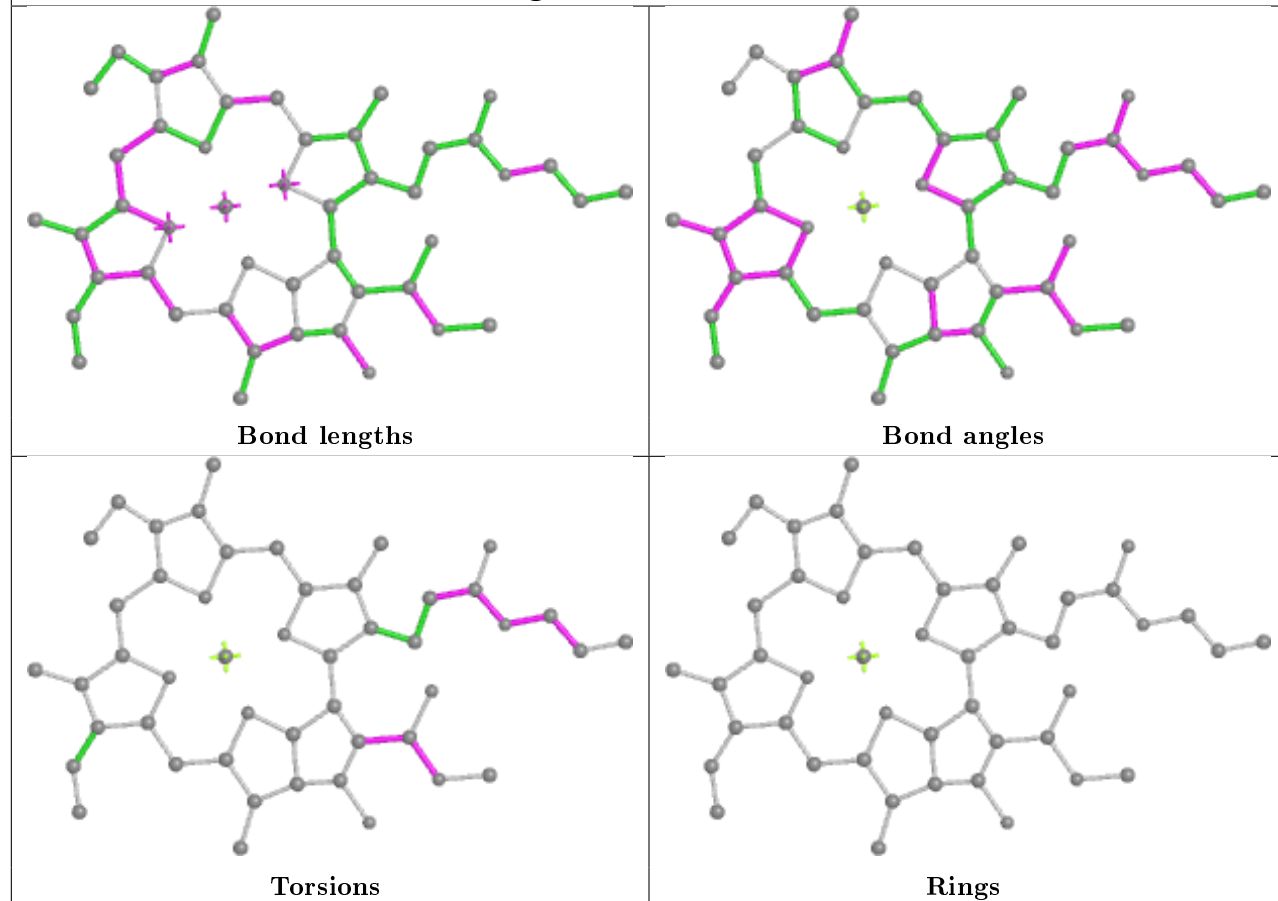
Ligand CLA b 1227

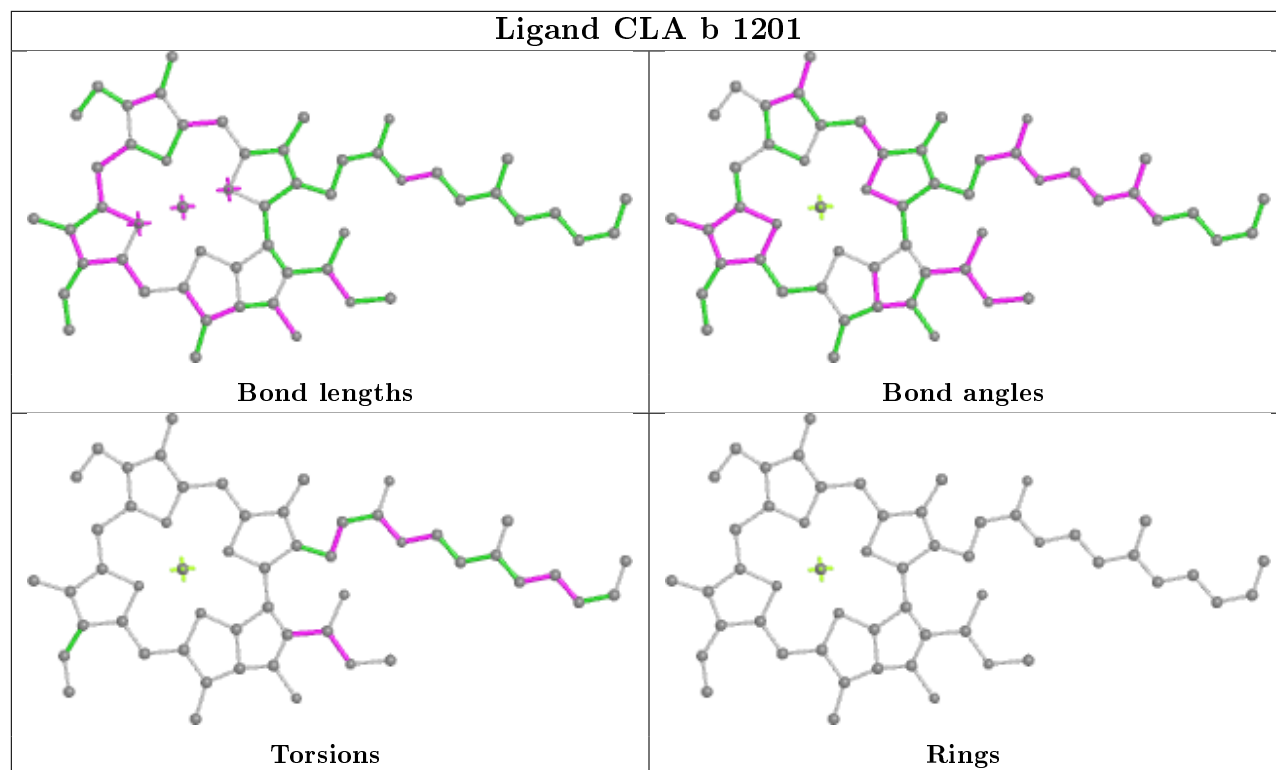


Ligand CLA 1 1501

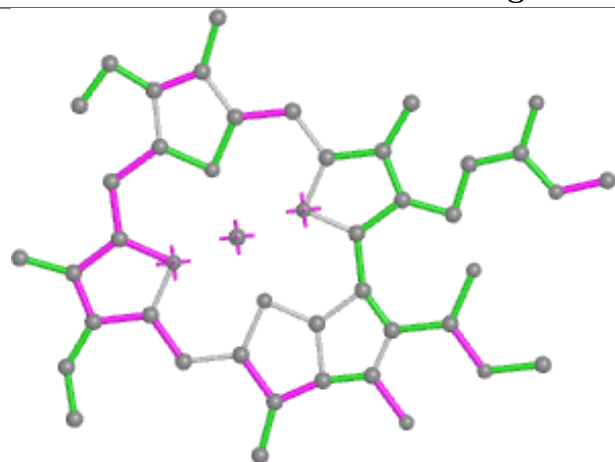


Ligand CLA a 1105

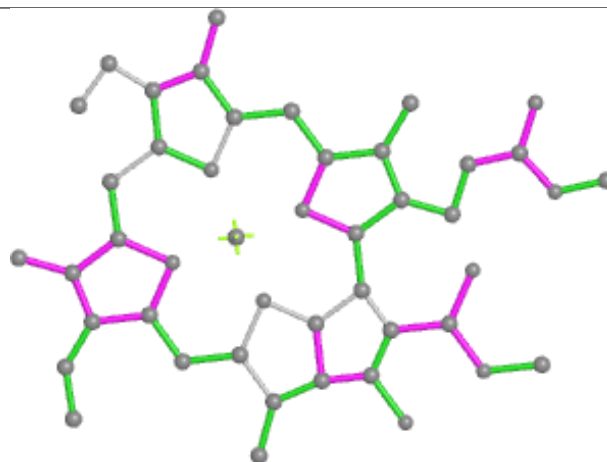




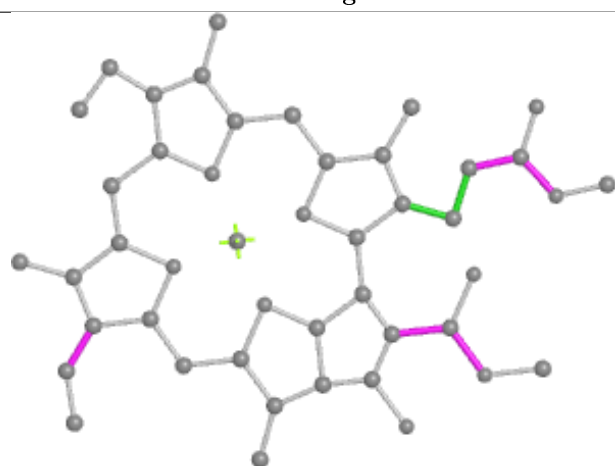
Ligand CLA B 1239



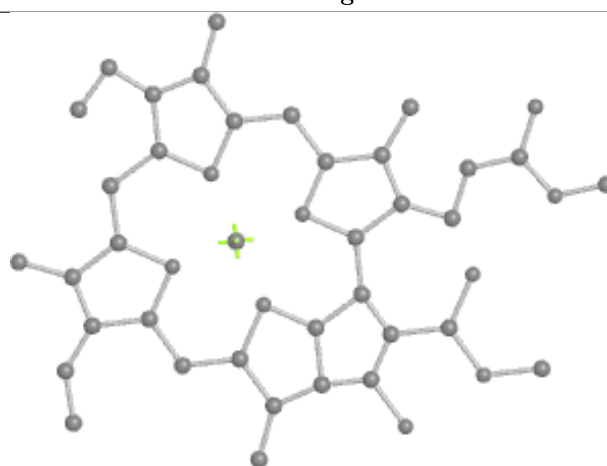
Bond lengths



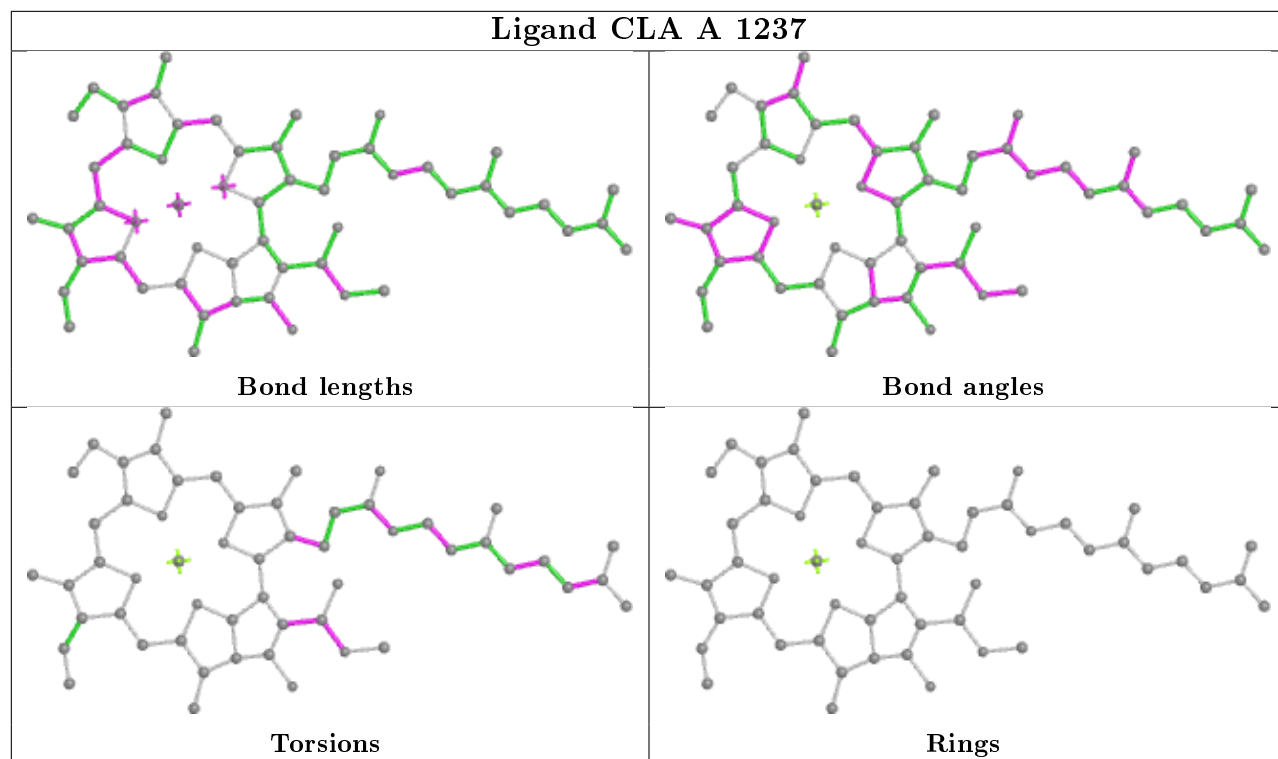
Bond angles



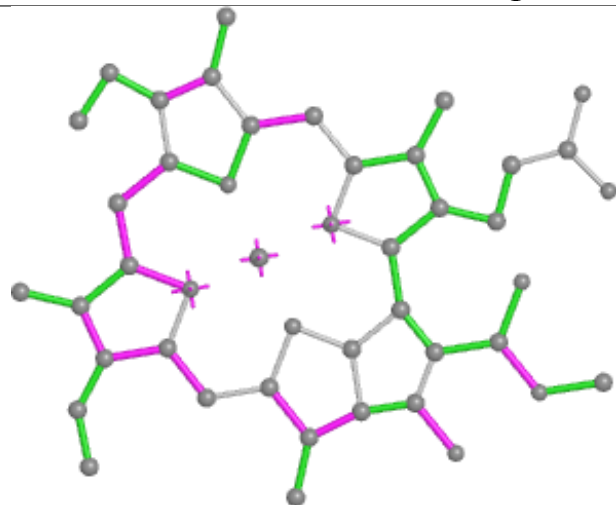
Torsions



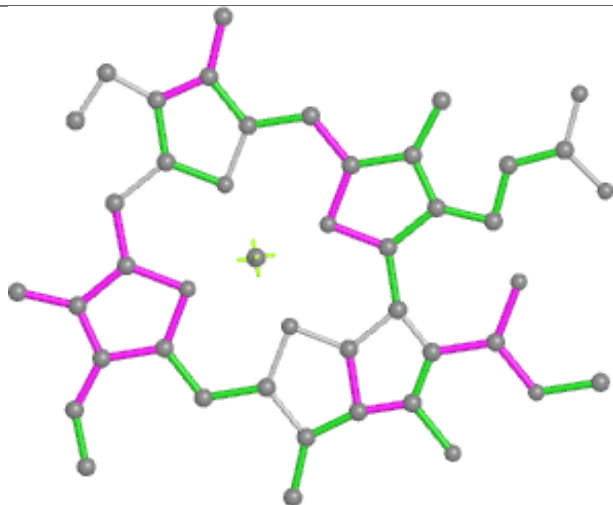
Rings



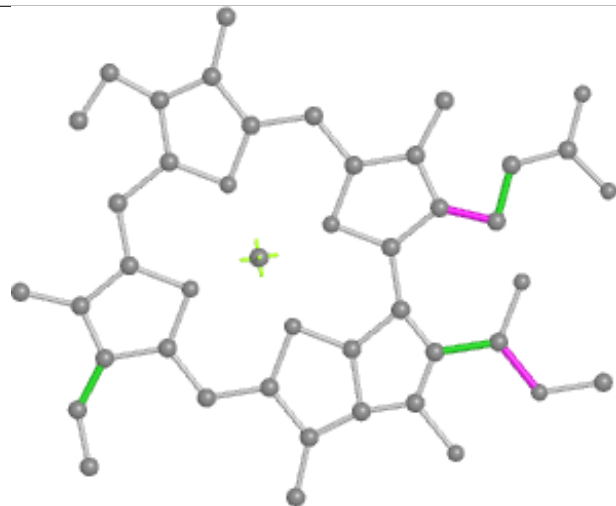
Ligand CLA B 1209



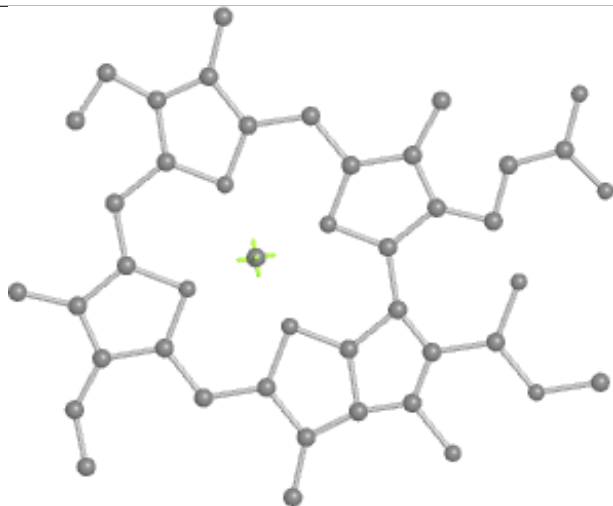
Bond lengths



Bond angles

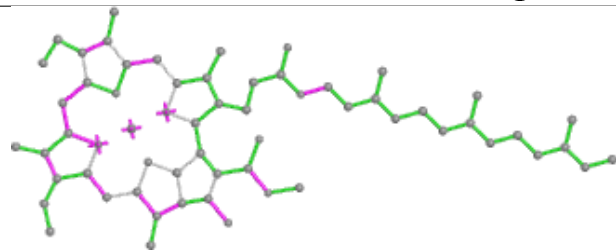


Torsions

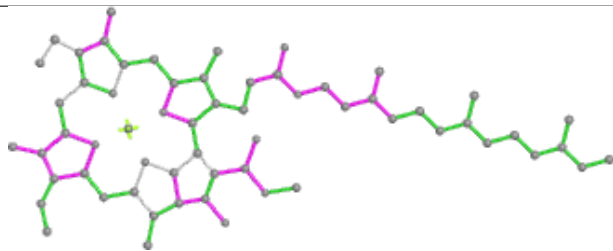


Rings

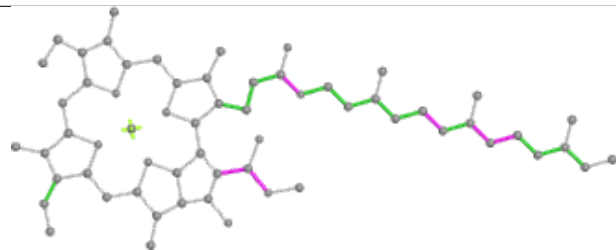
Ligand CLA a 1118



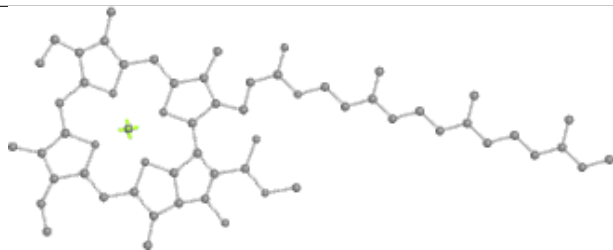
Bond lengths



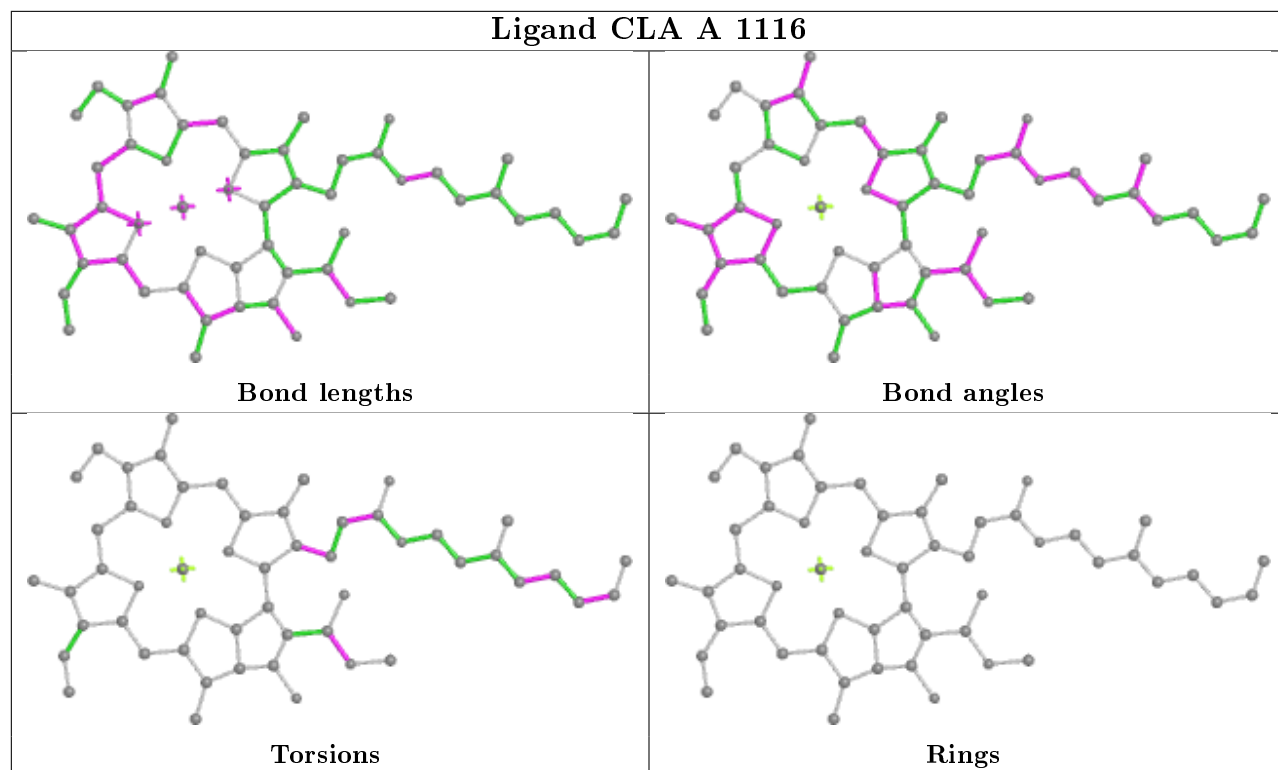
Bond angles



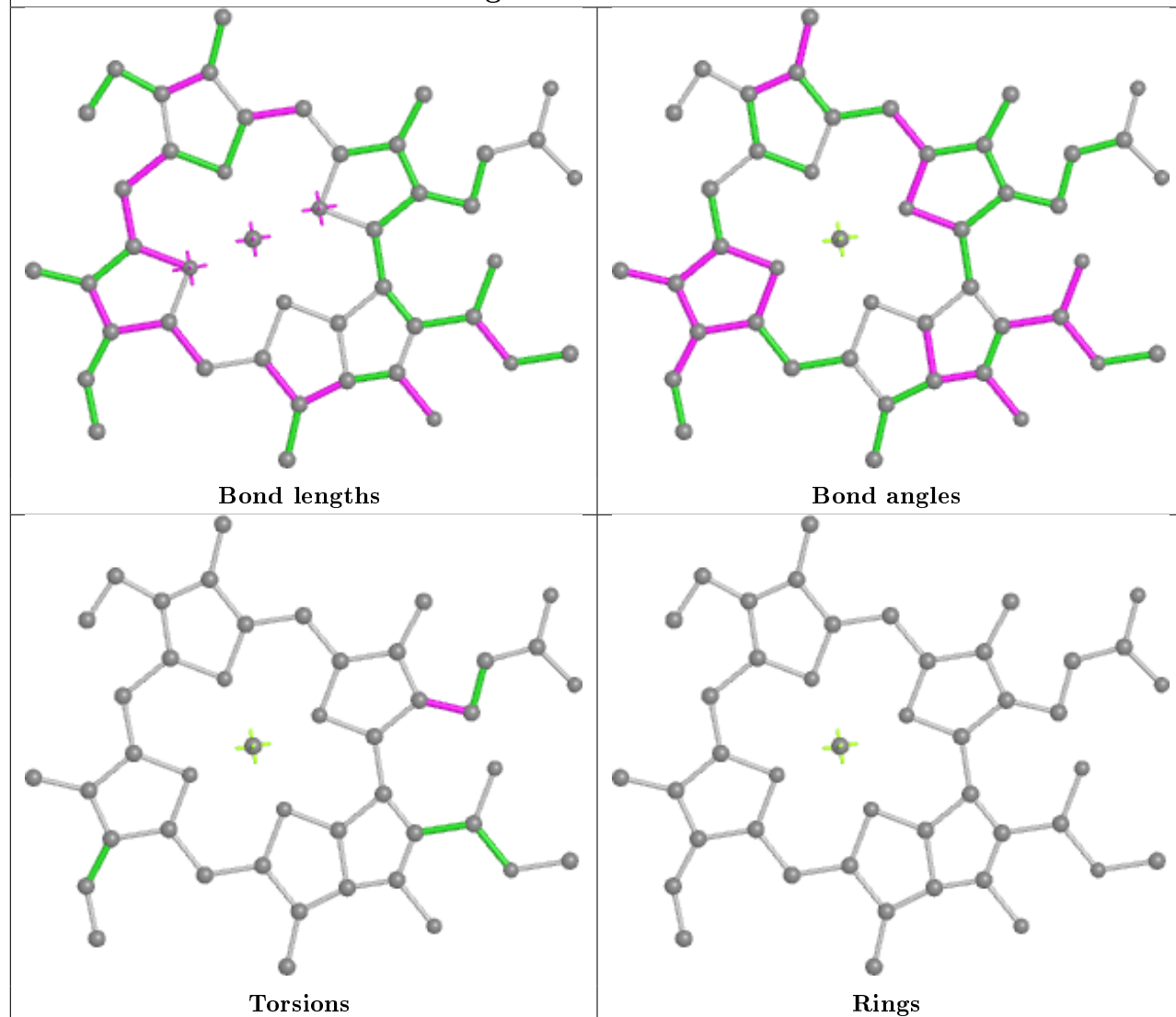
Torsions



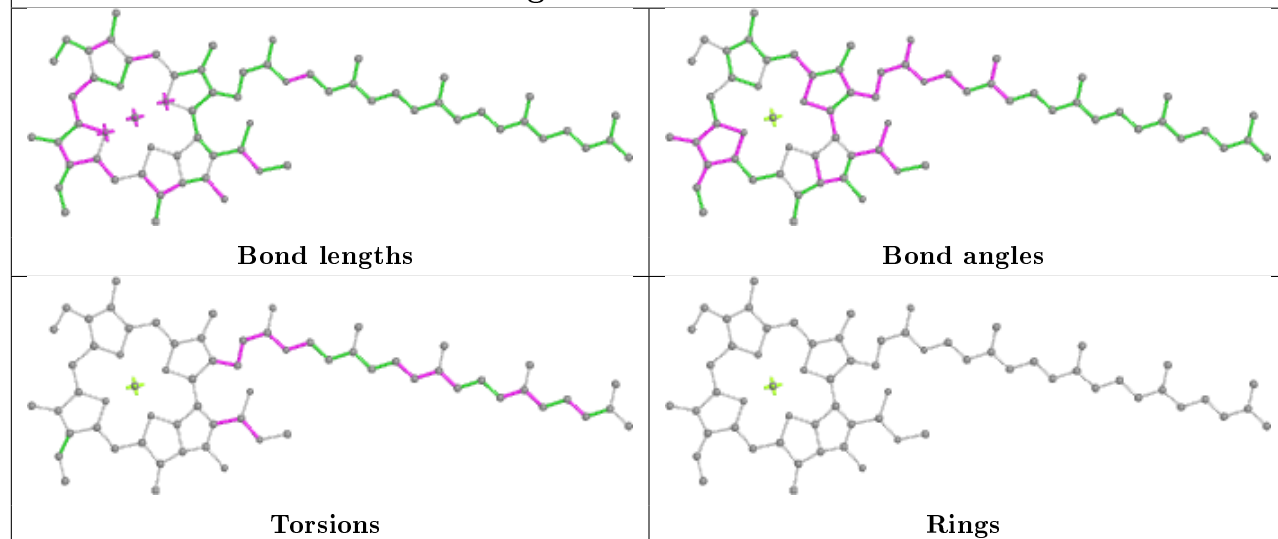
Rings



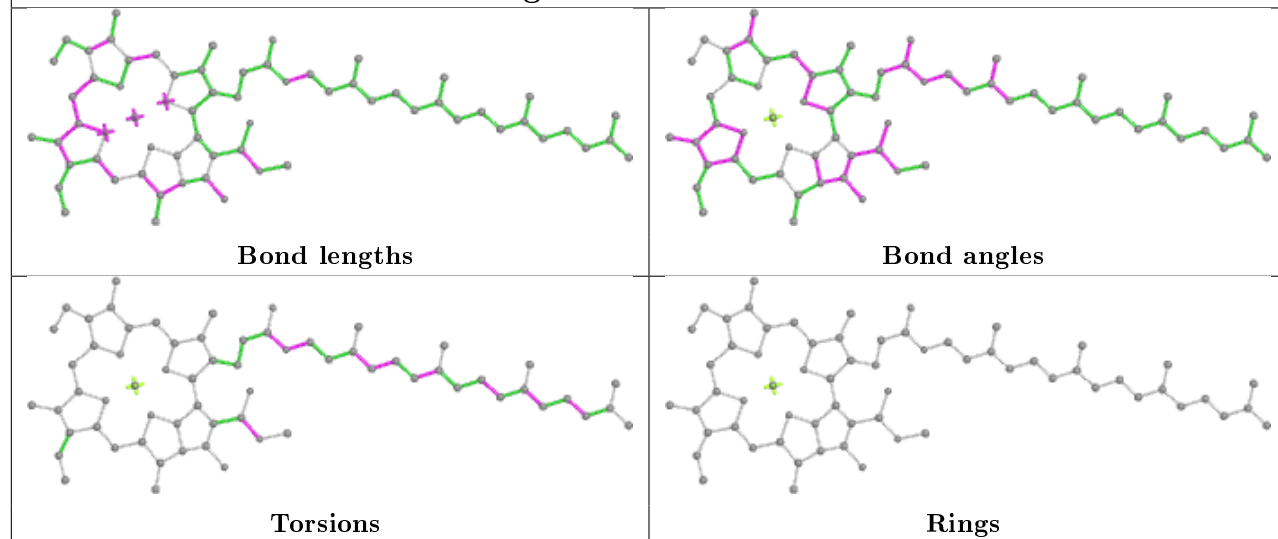
Ligand CLA 2 1209



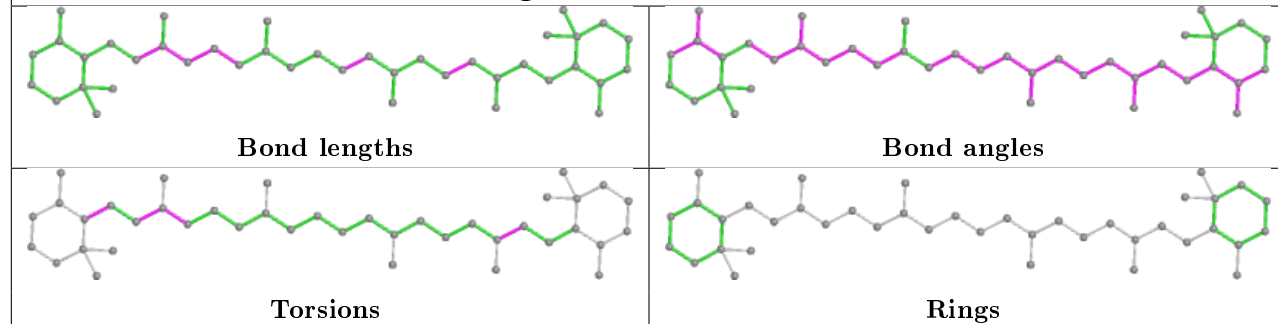
Ligand CLA k 1401

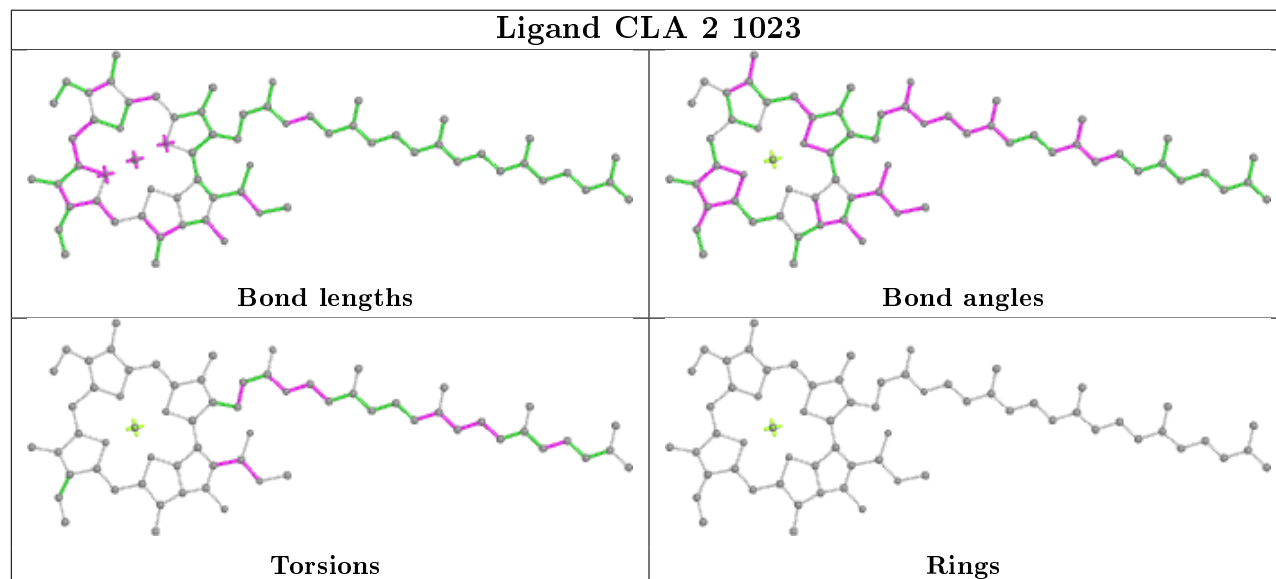
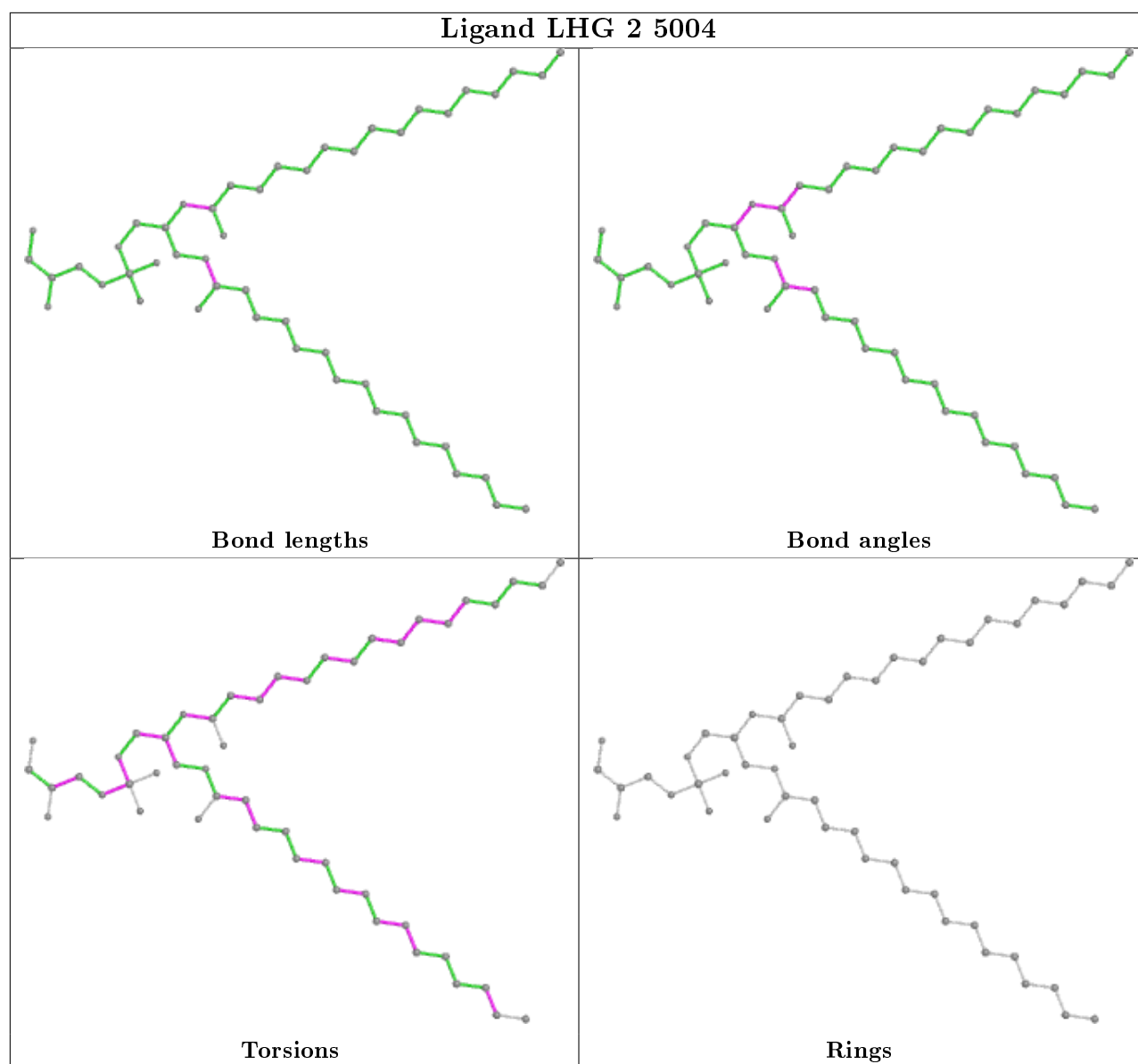


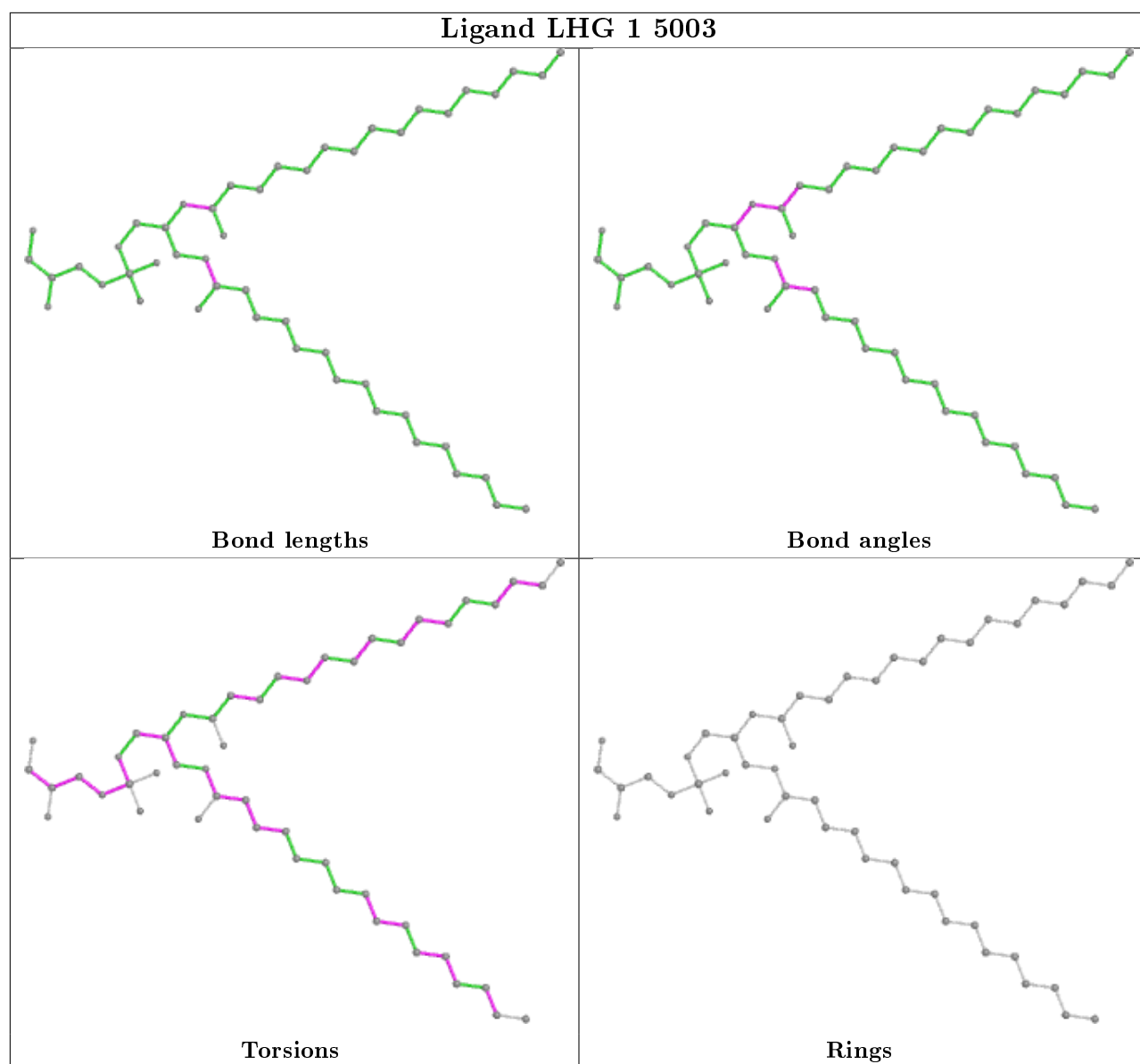
Ligand CLA A 1022

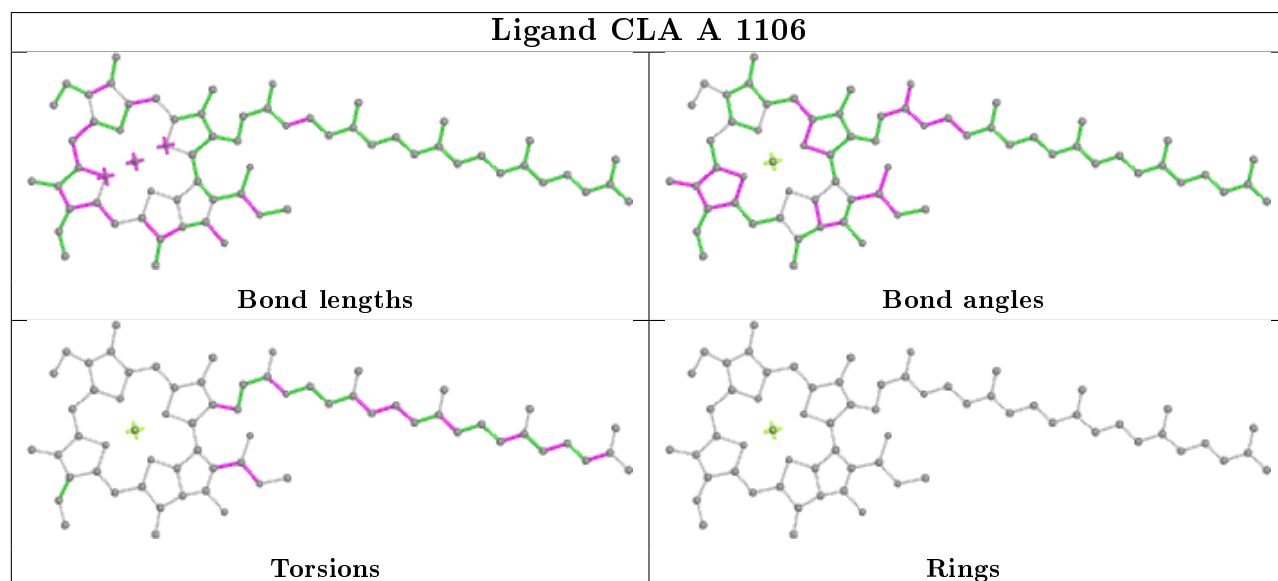
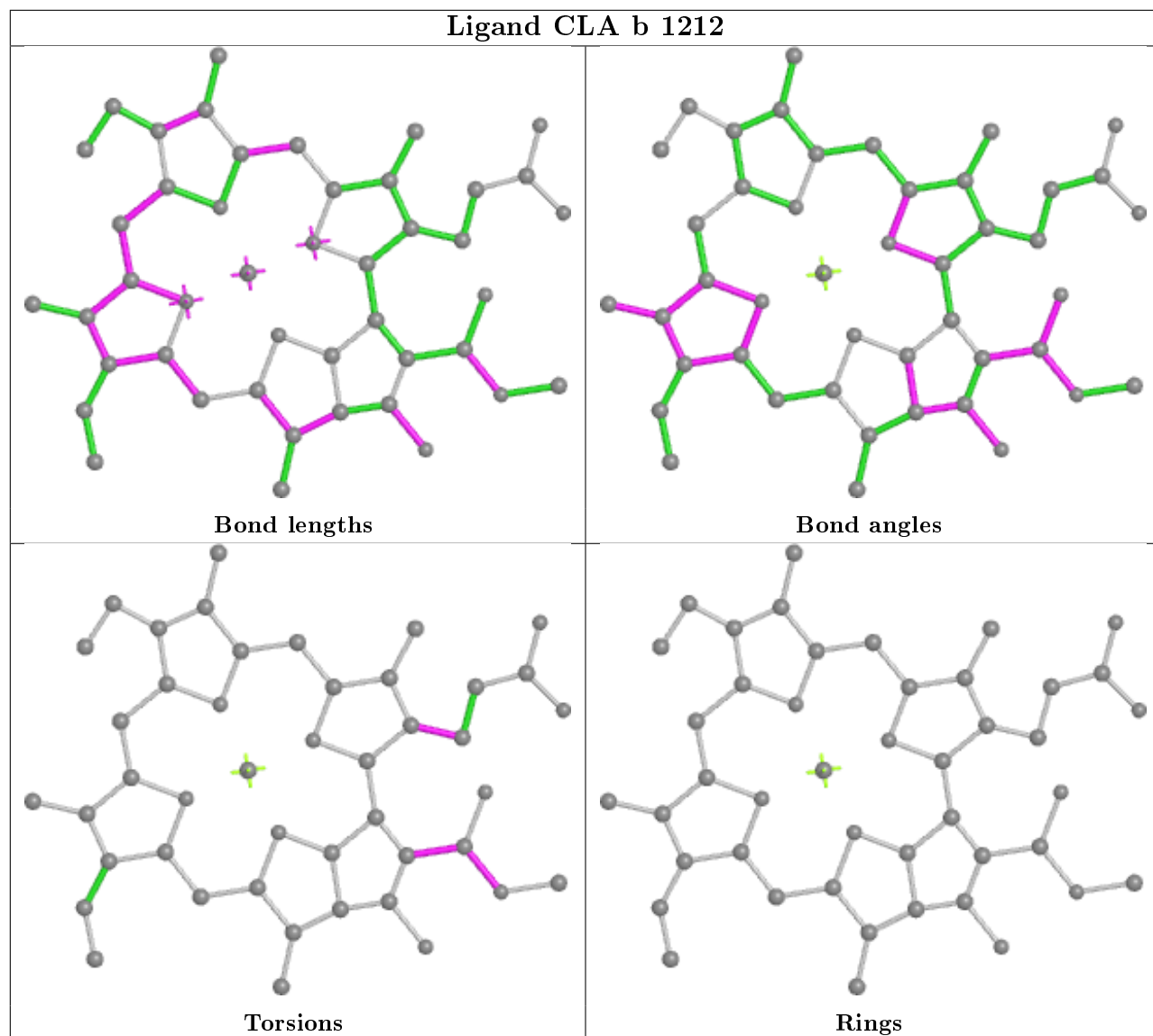


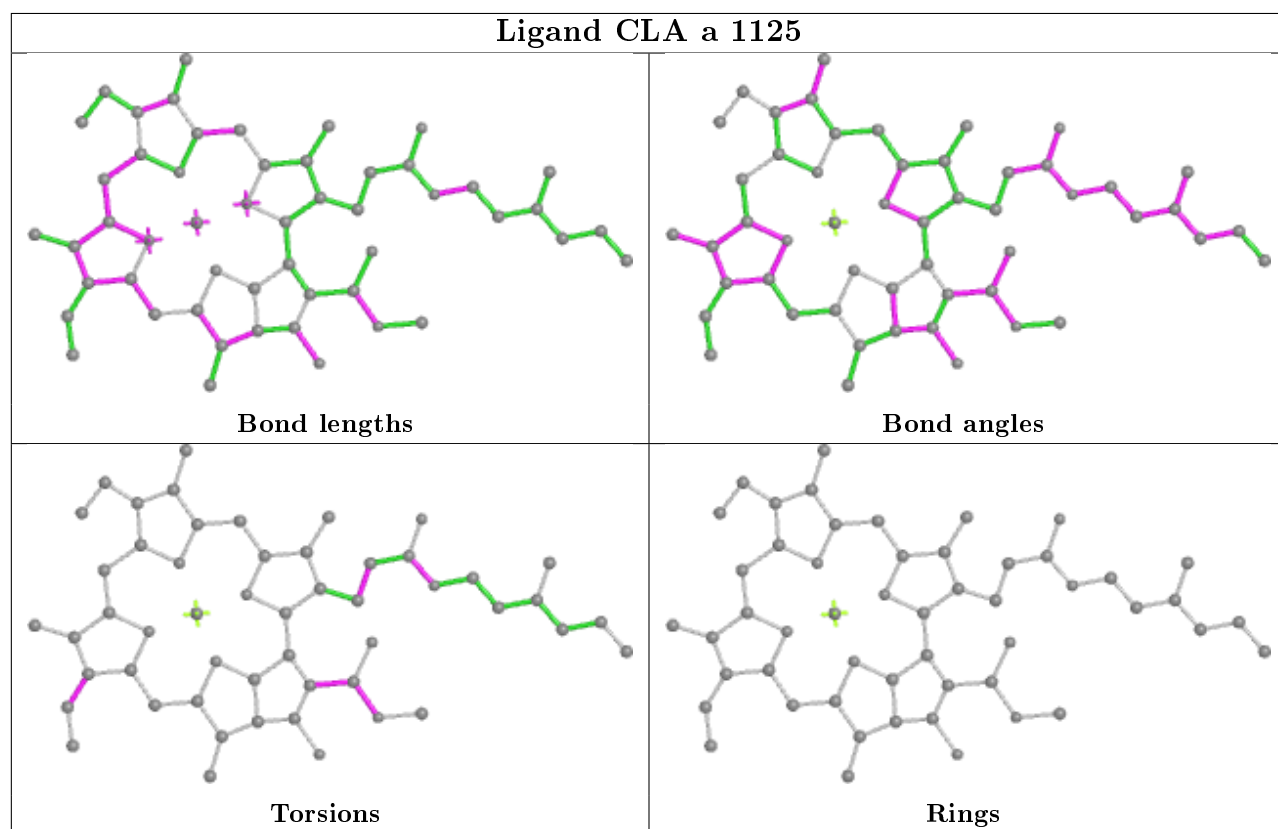
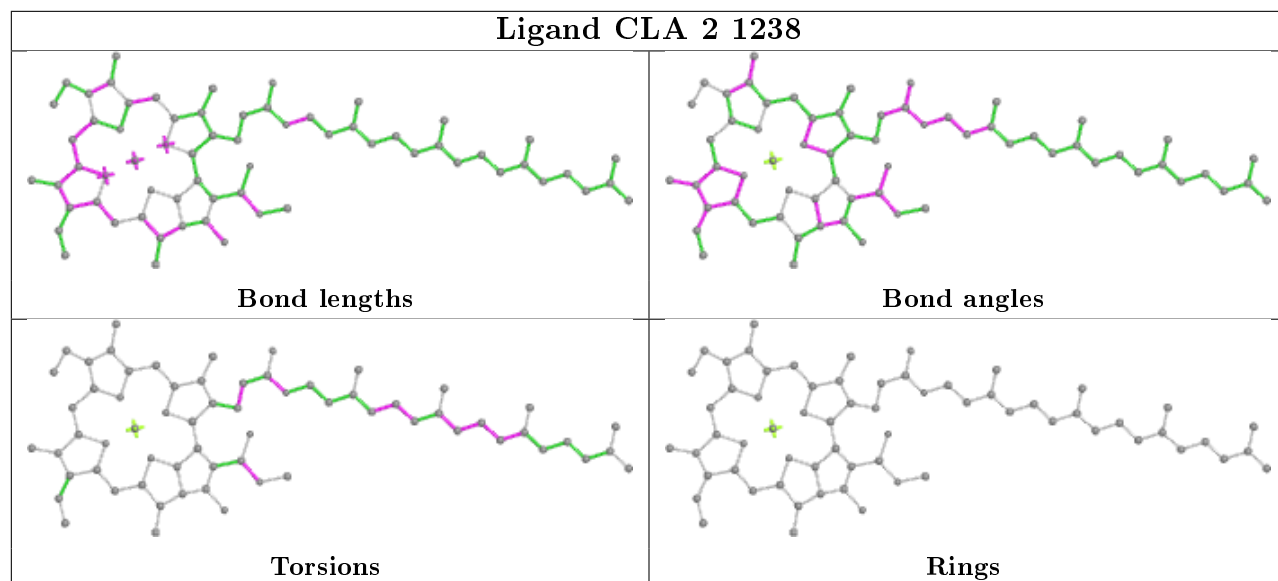
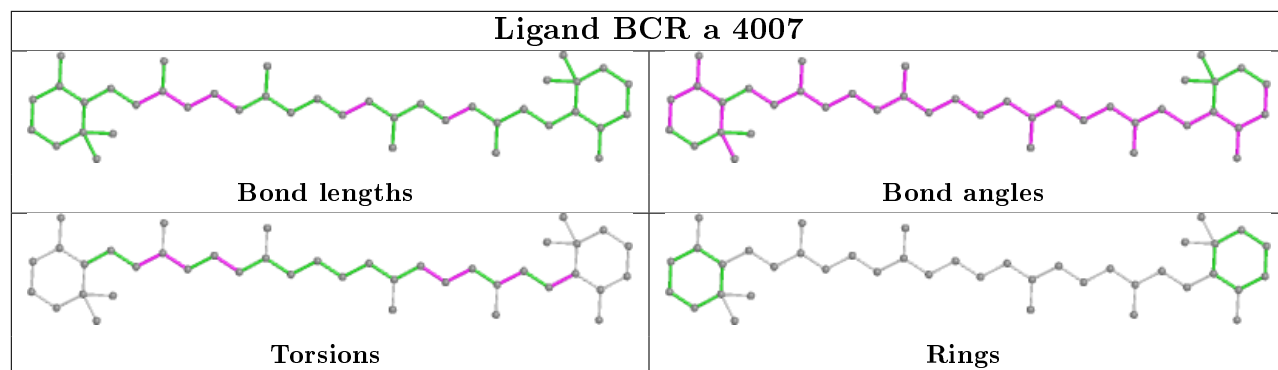
Ligand BCR M 4021



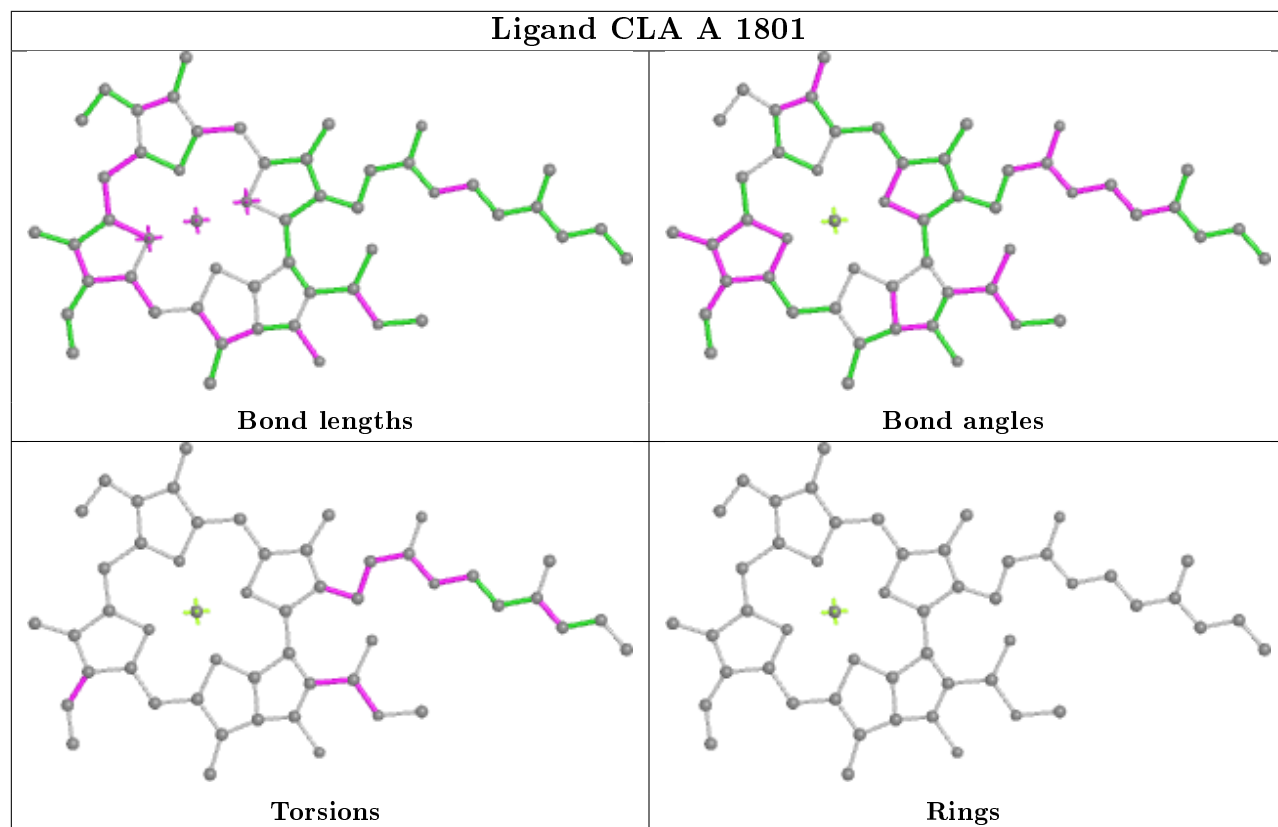




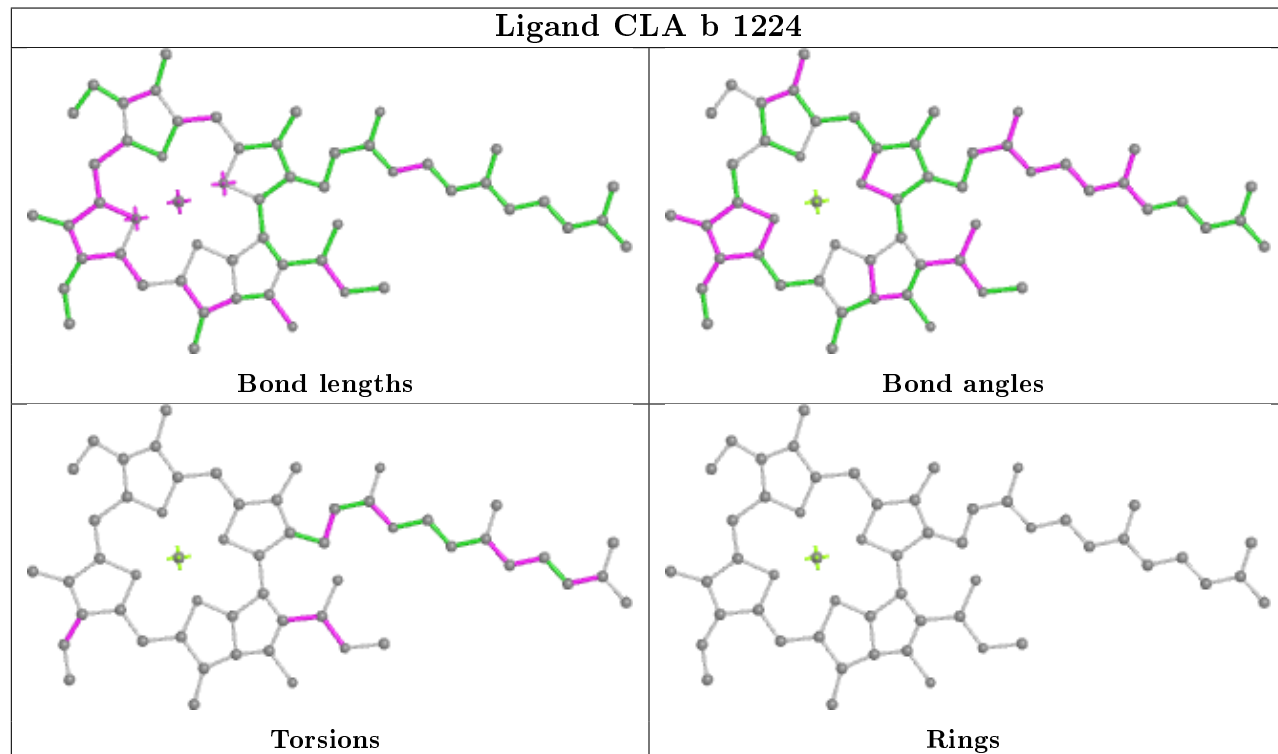


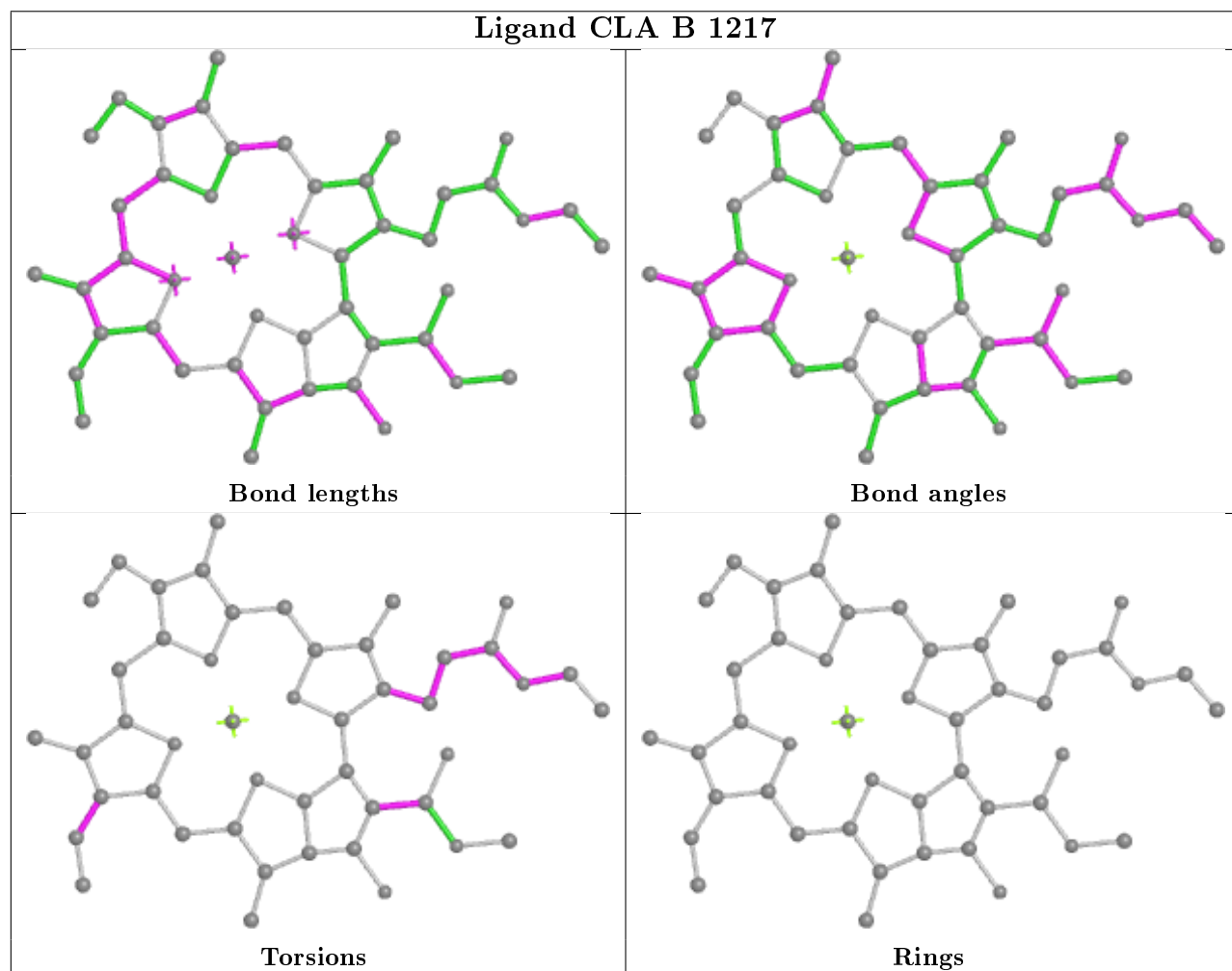
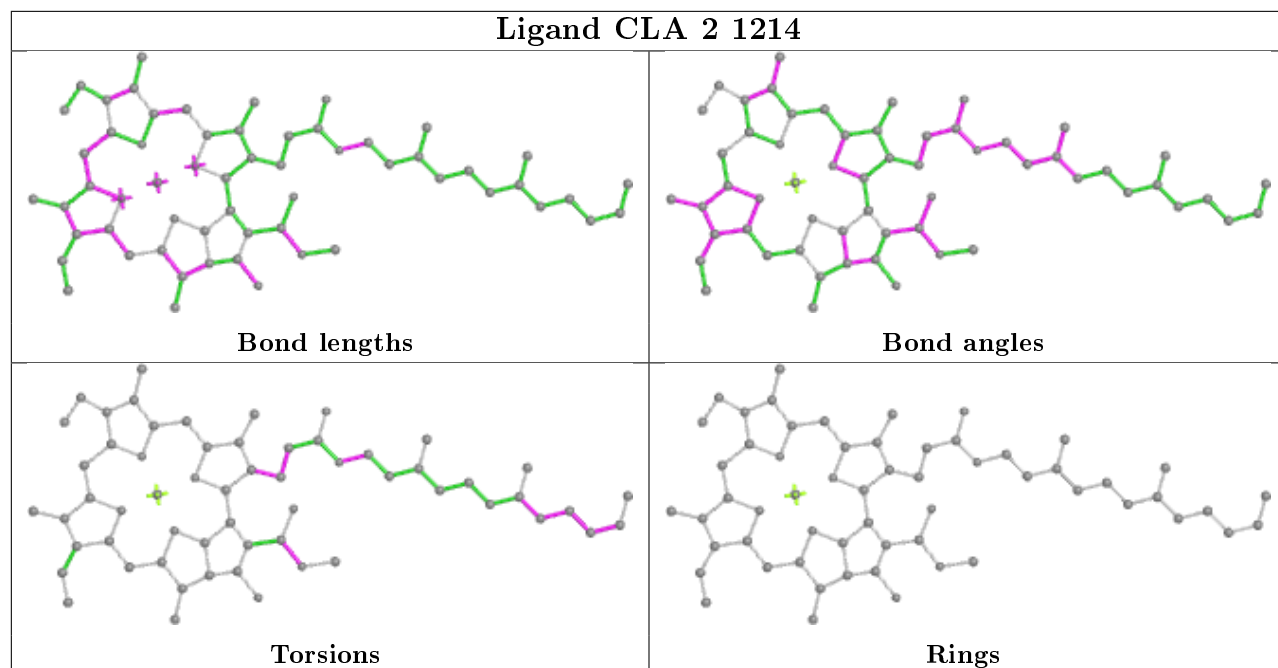


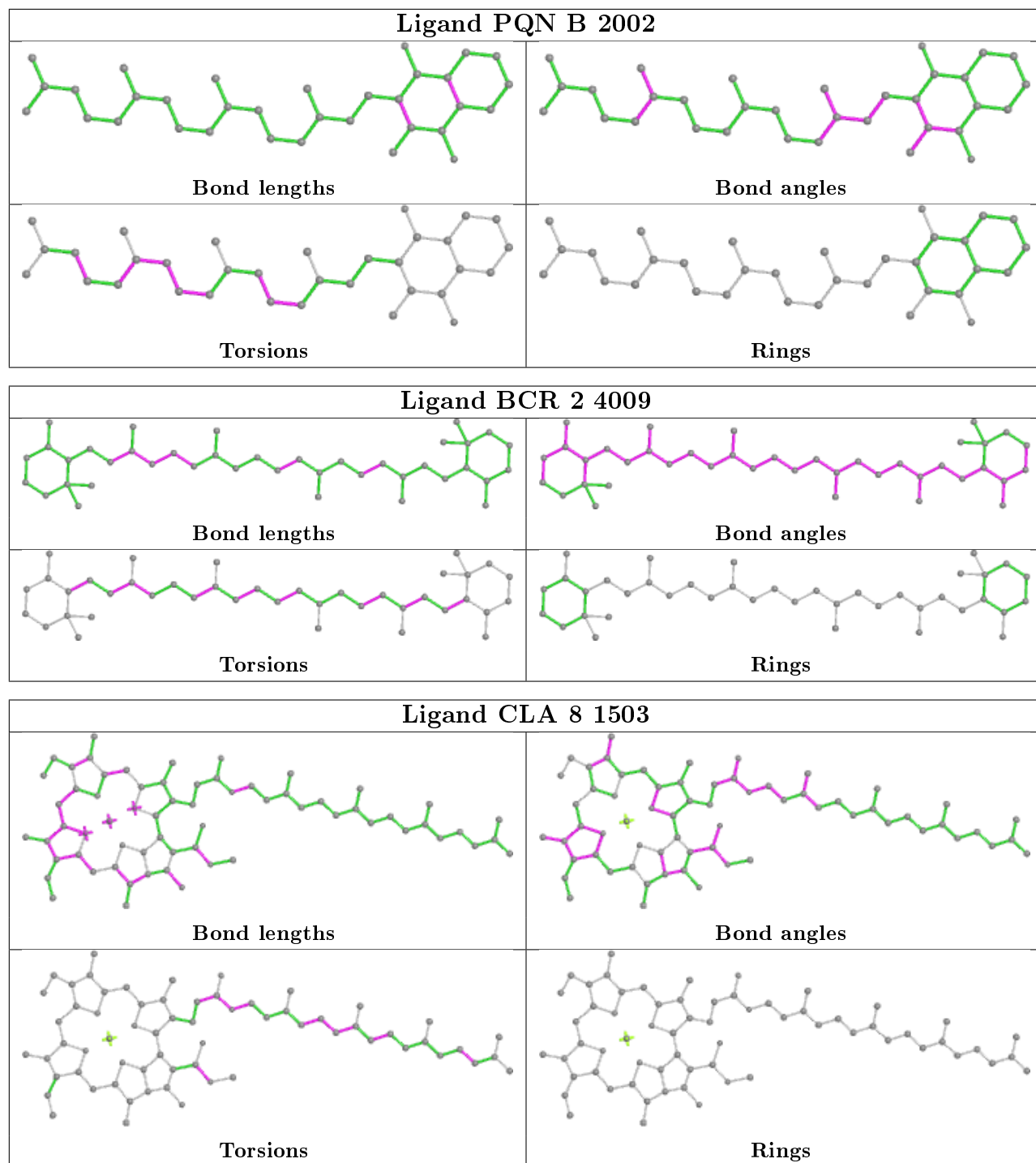
Ligand CLA A 1801

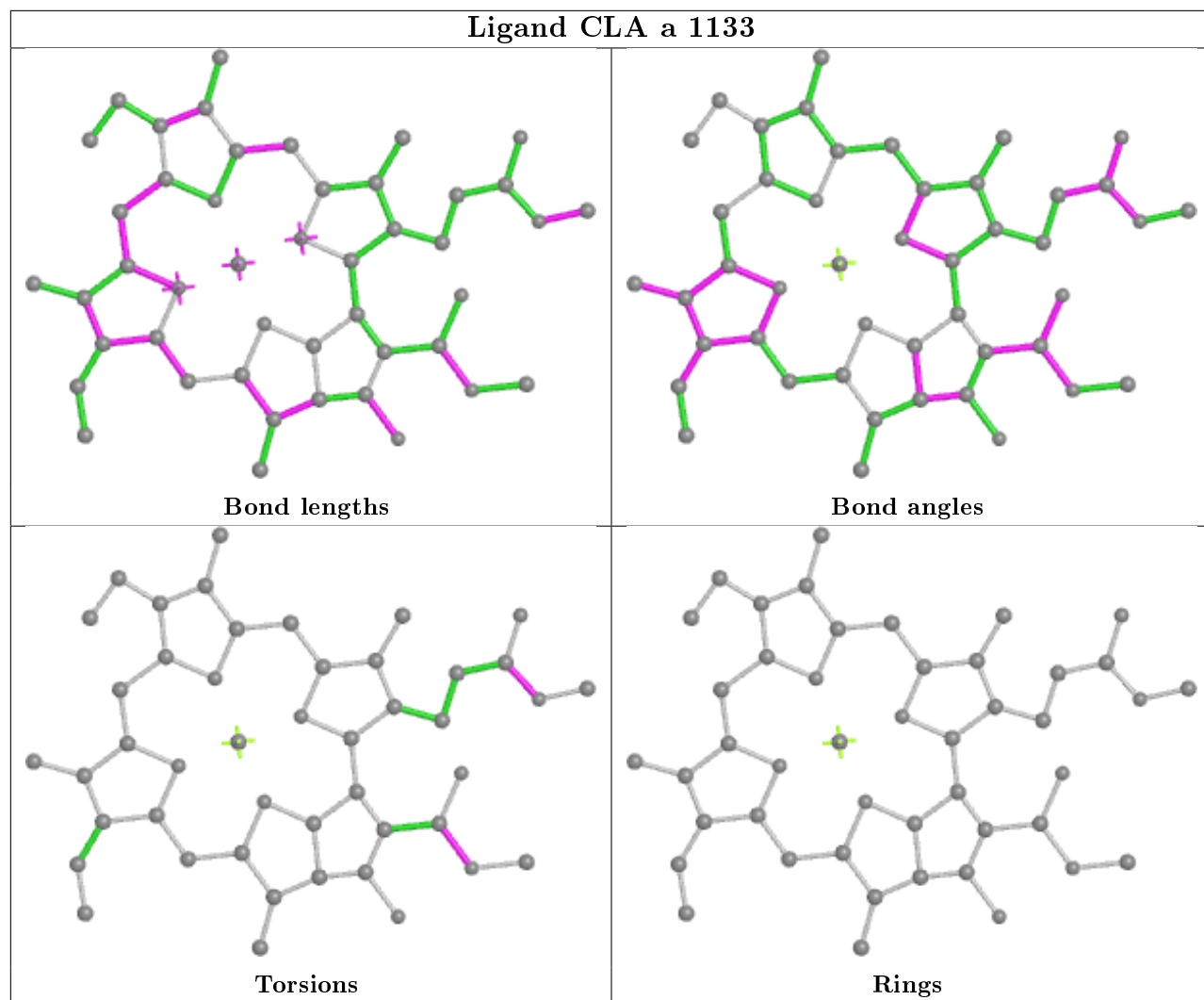


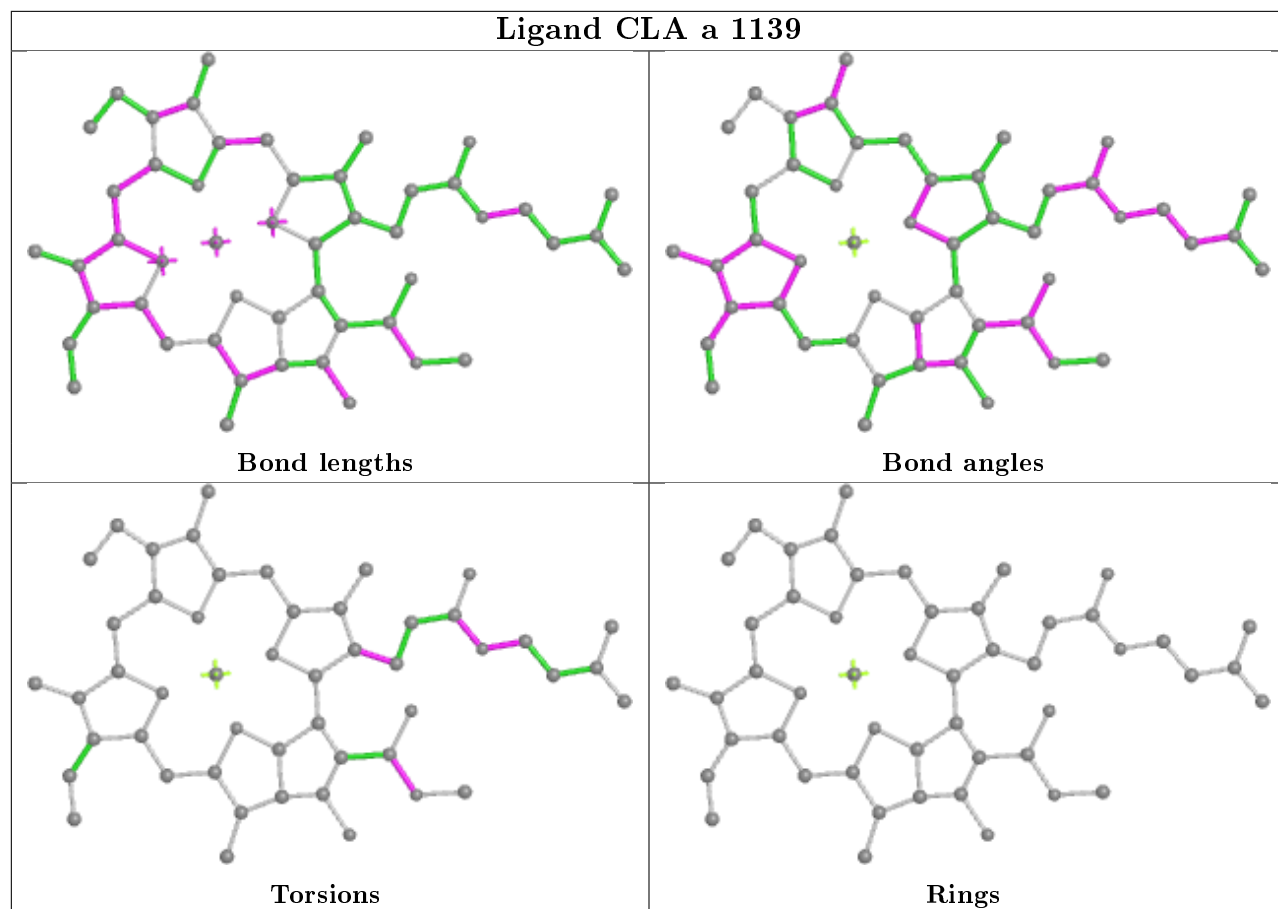
Ligand CLA b 1224

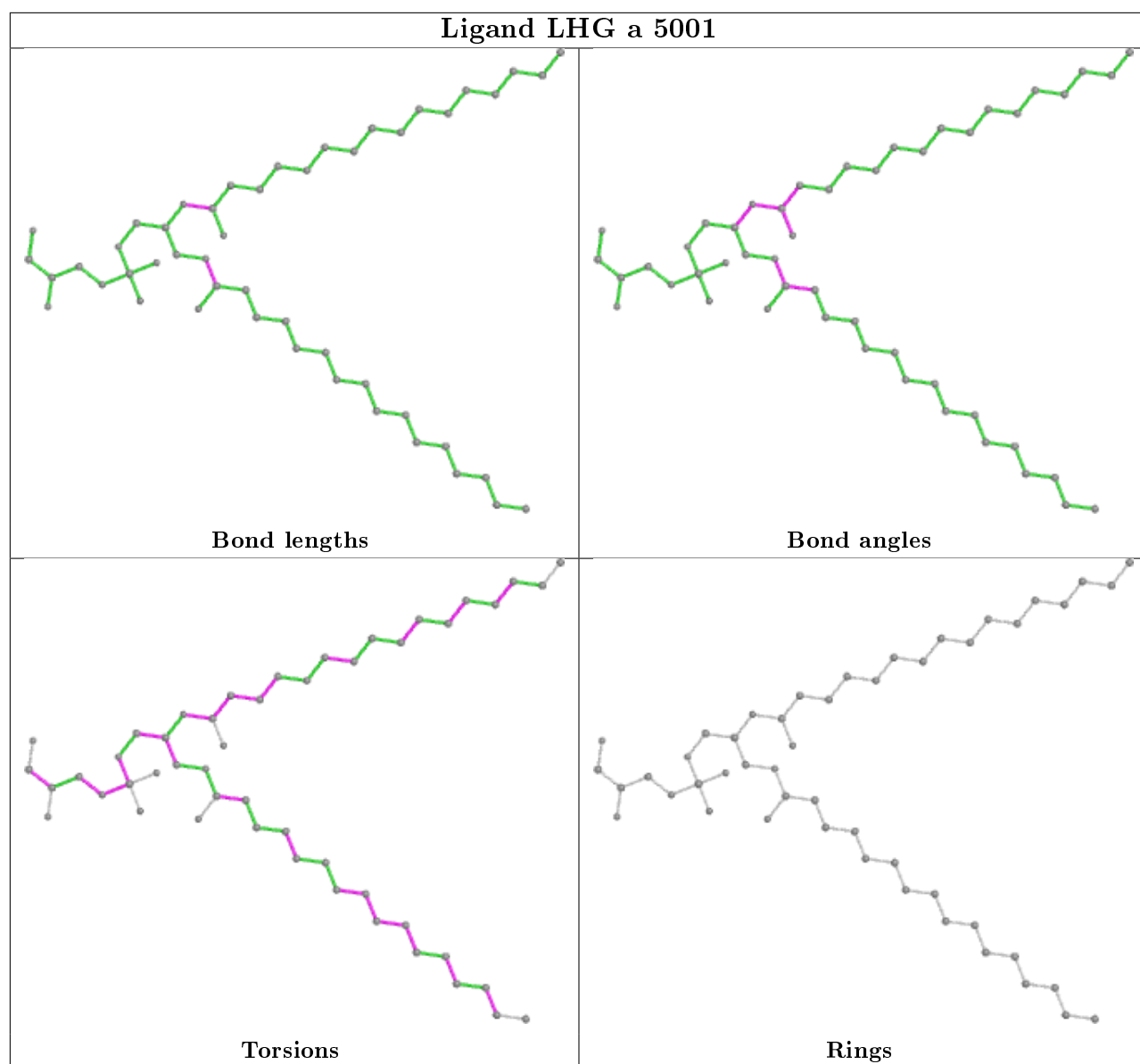


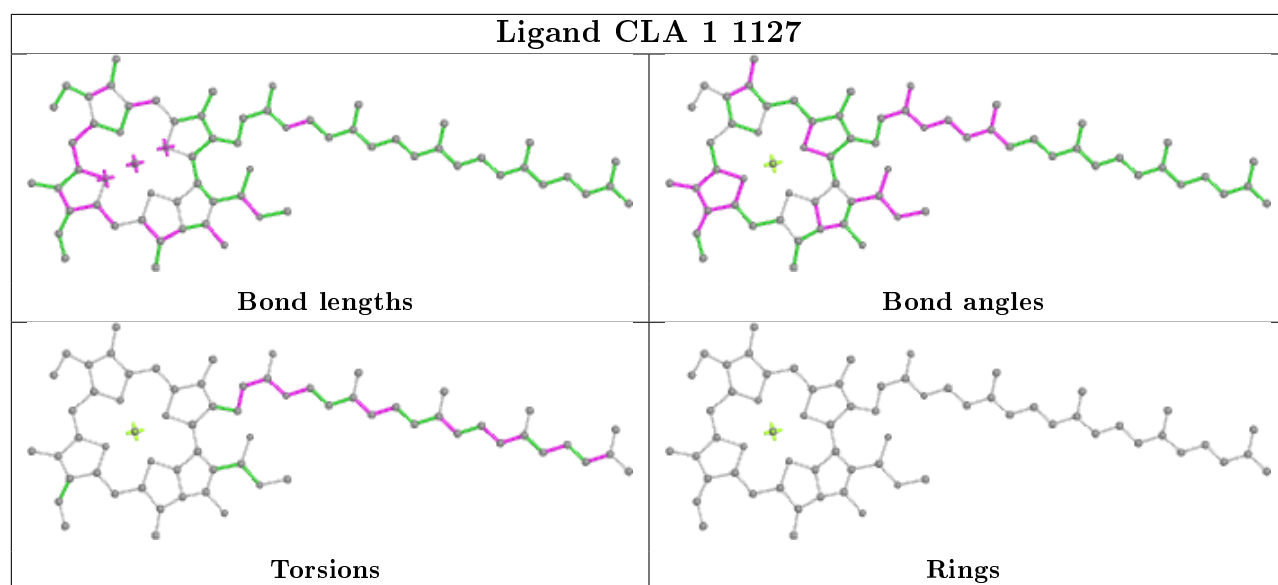
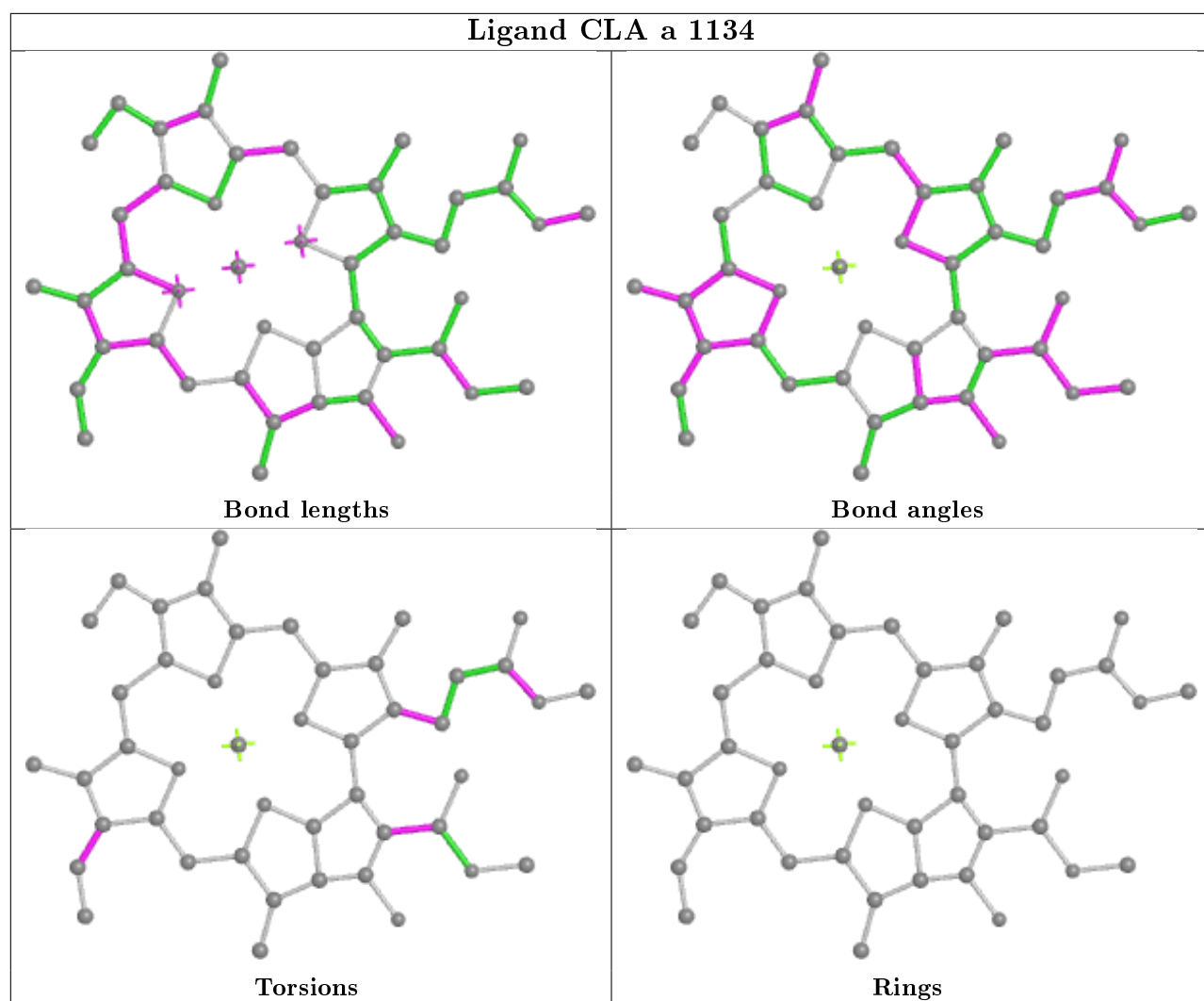




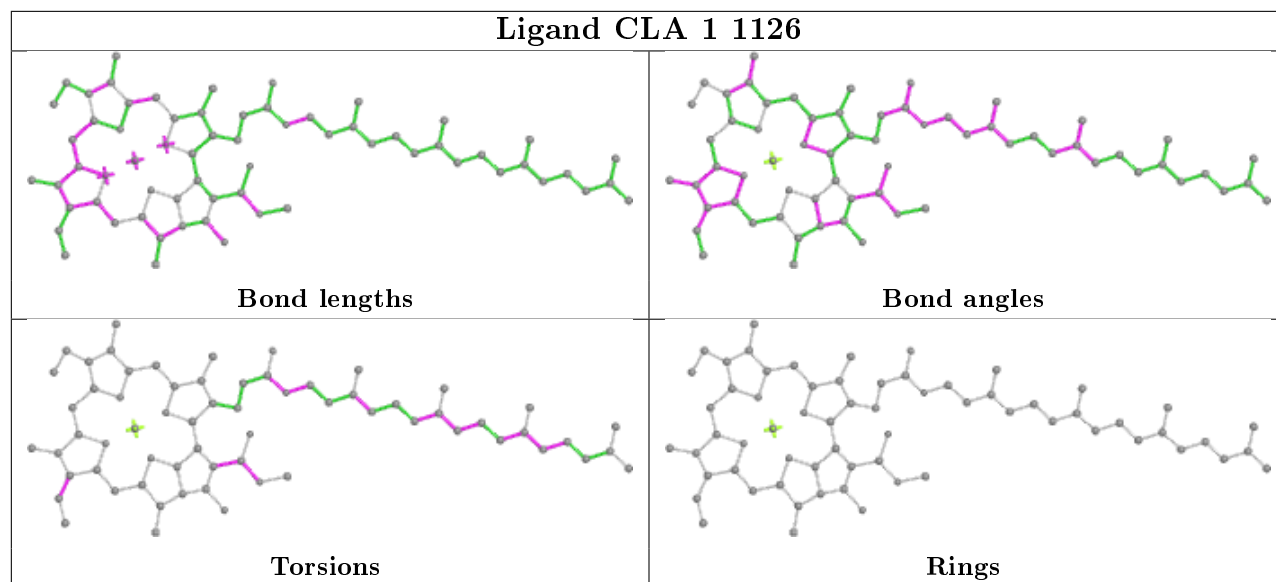




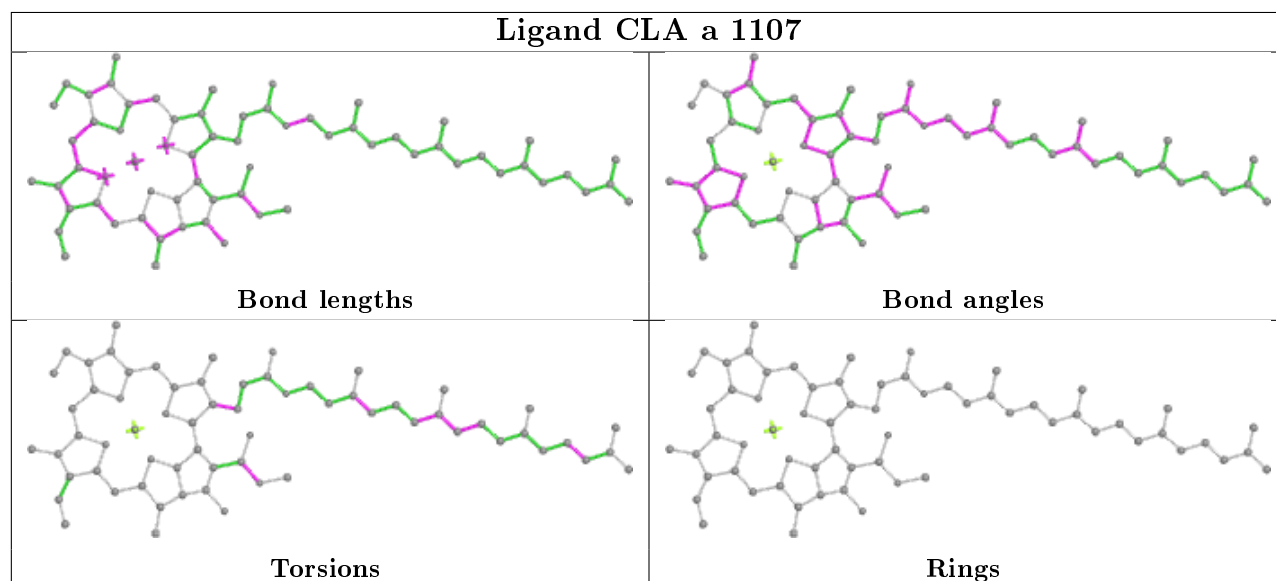




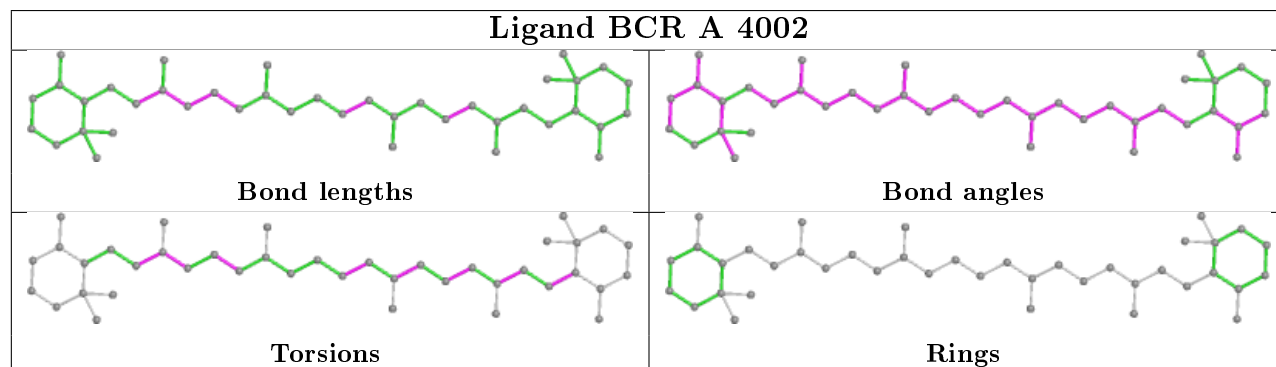
Ligand CLA 1 1126



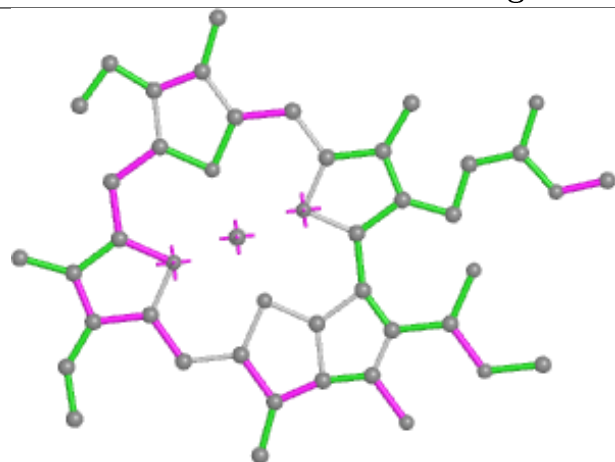
Ligand CLA a 1107



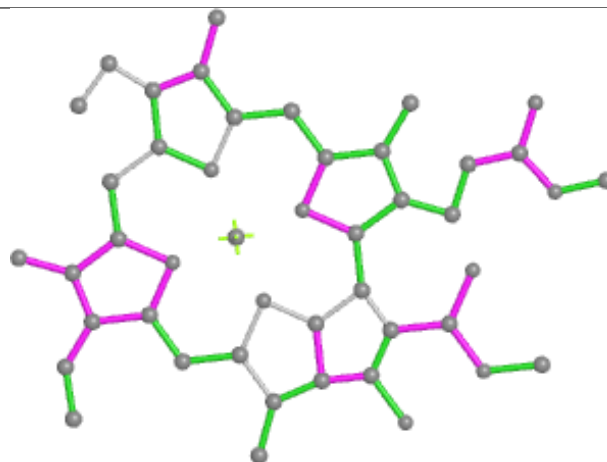
Ligand BCR A 4002



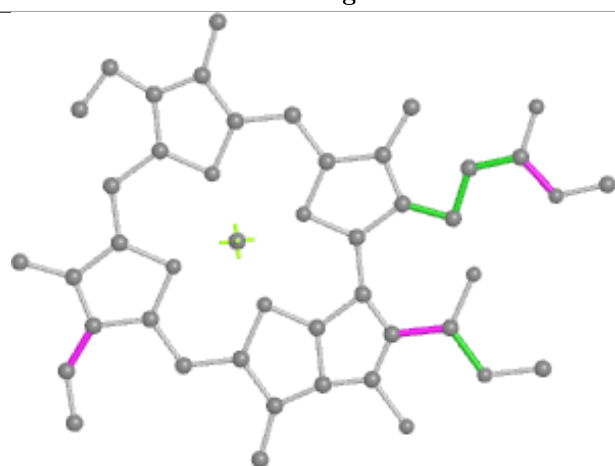
Ligand CLA A 1129



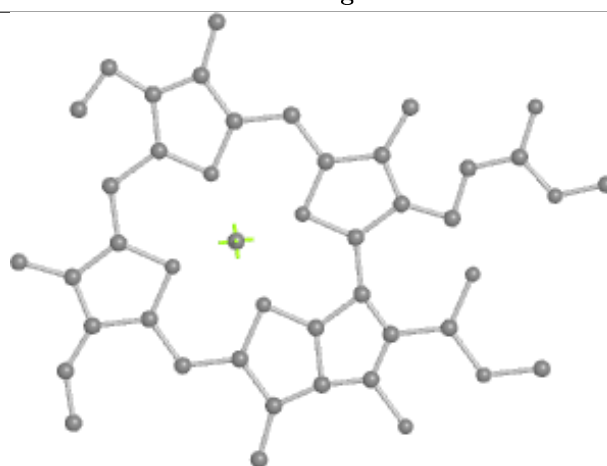
Bond lengths



Bond angles

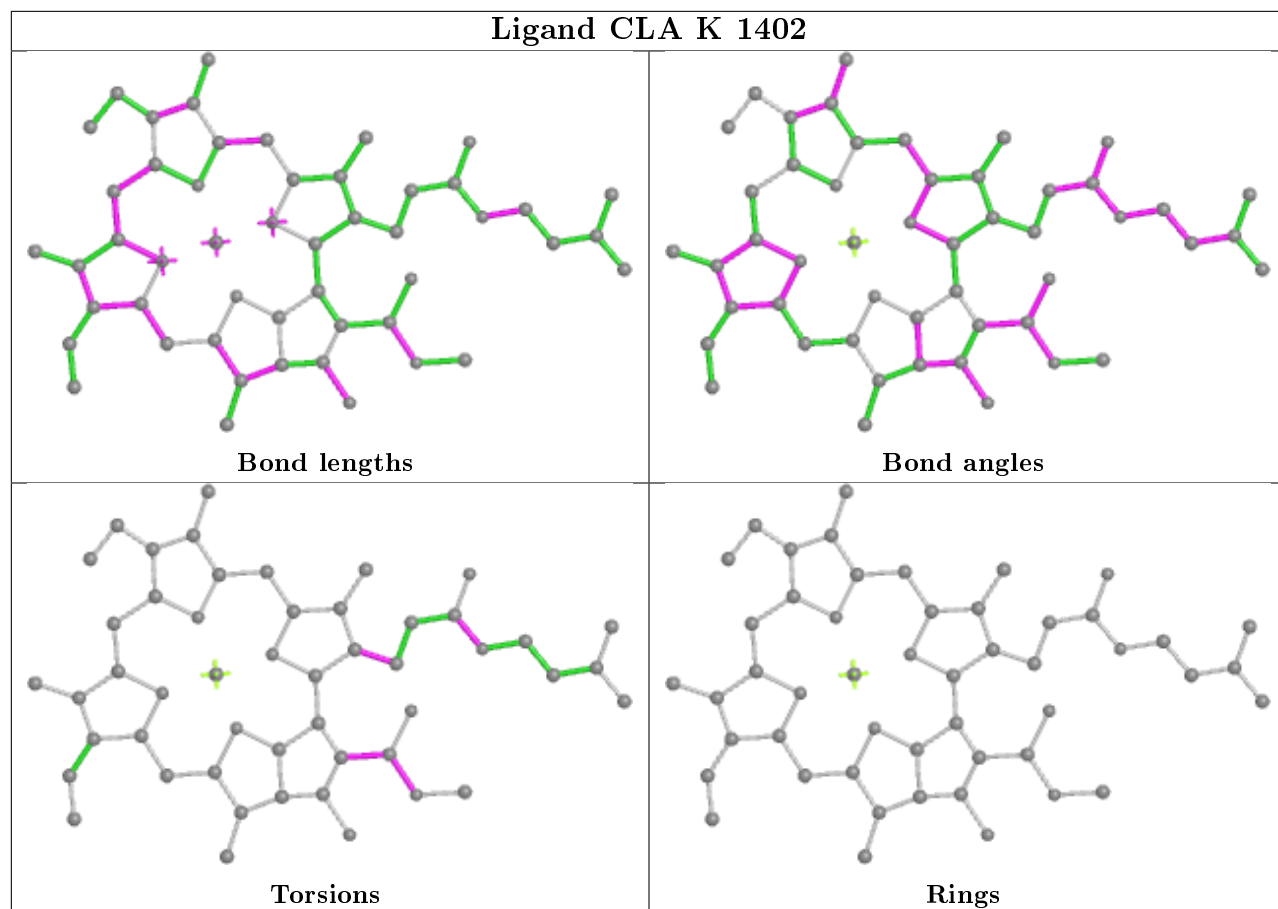


Torsions

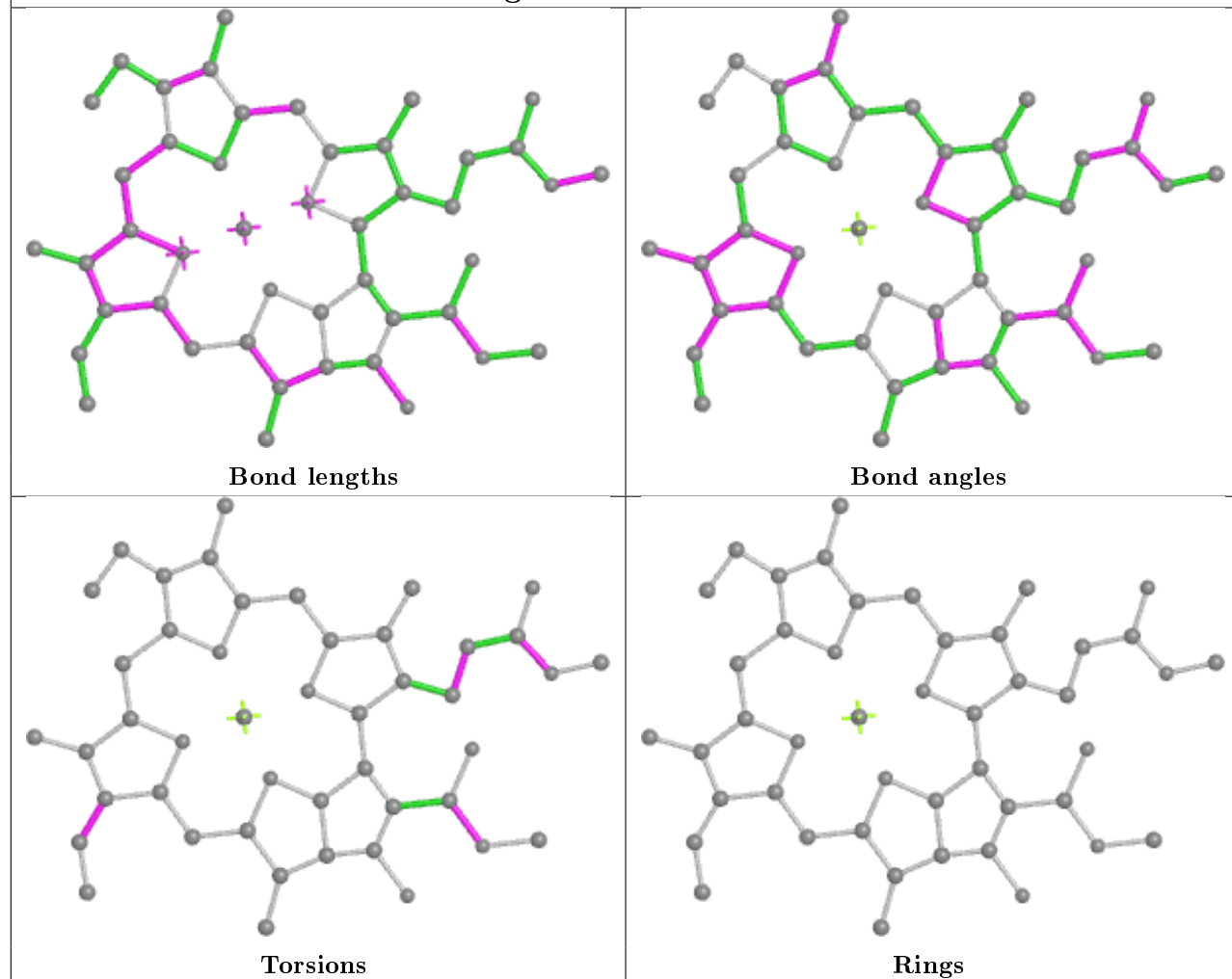


Rings

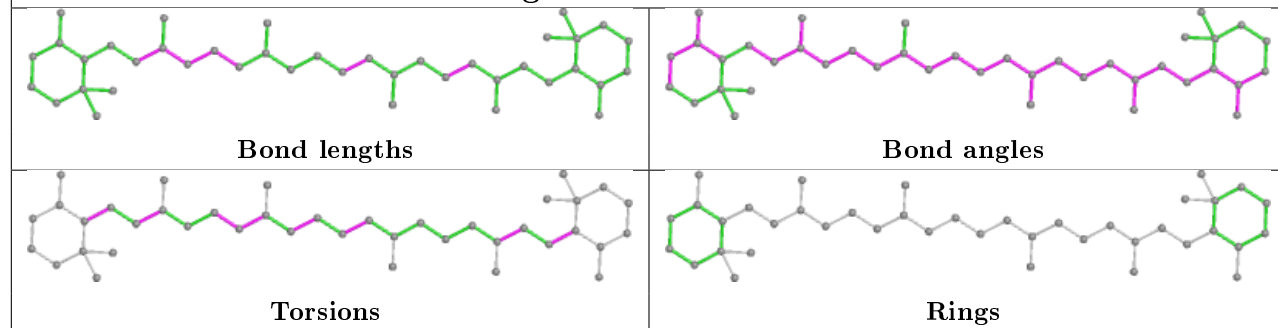
Ligand CLA K 1402

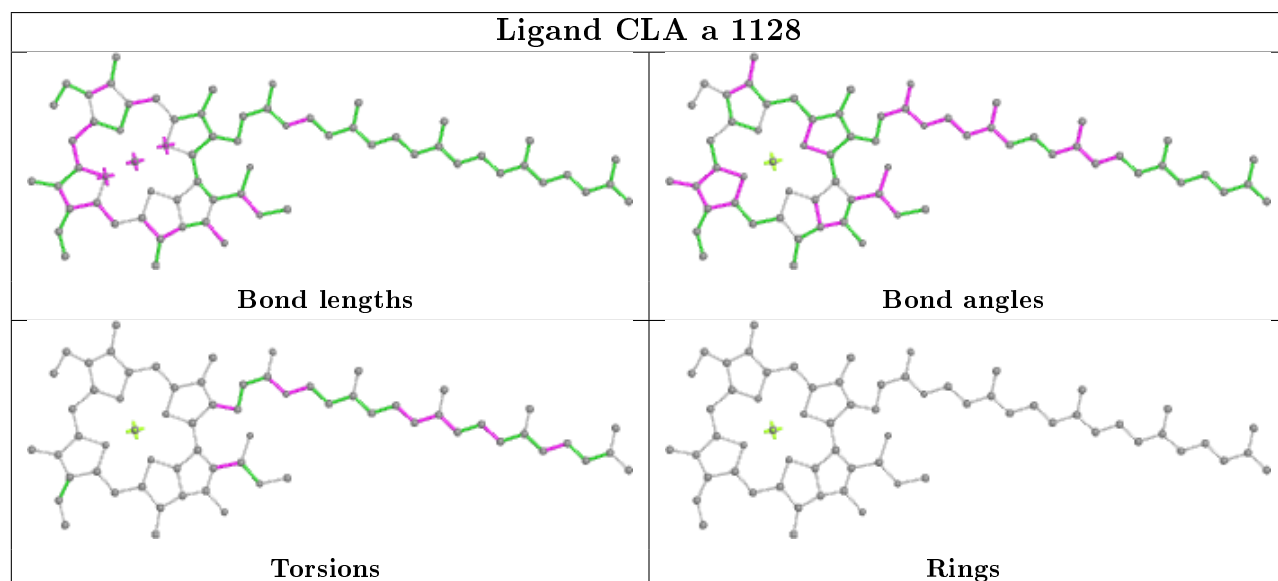
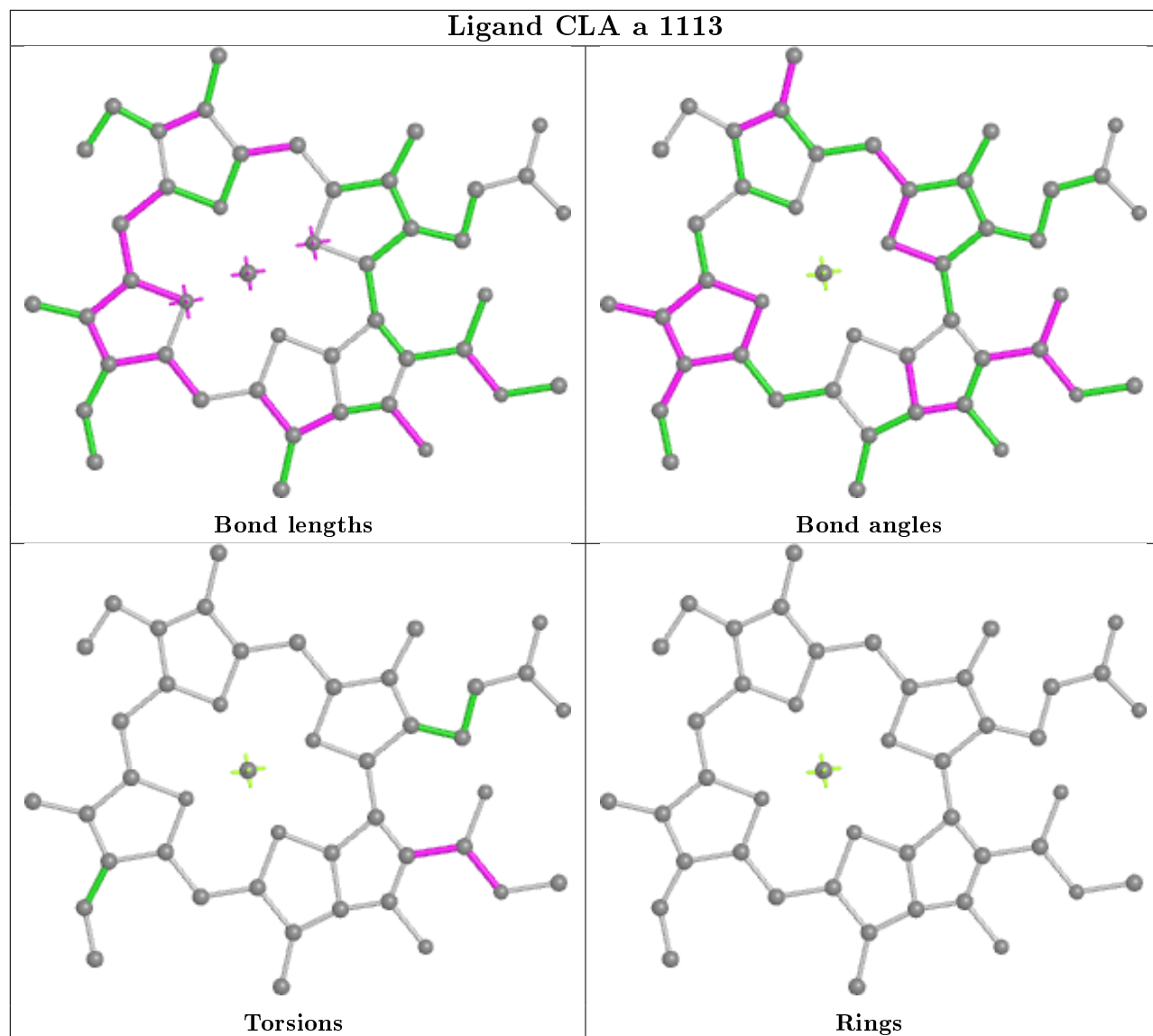


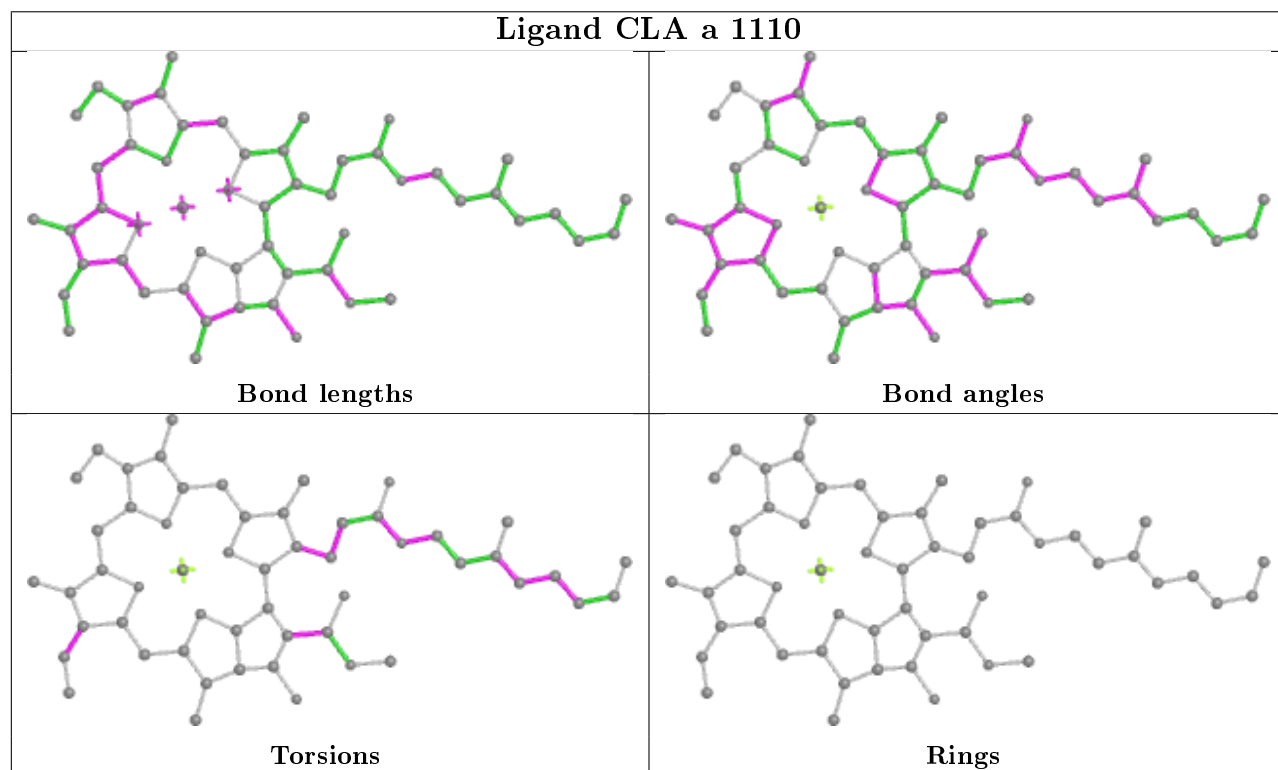
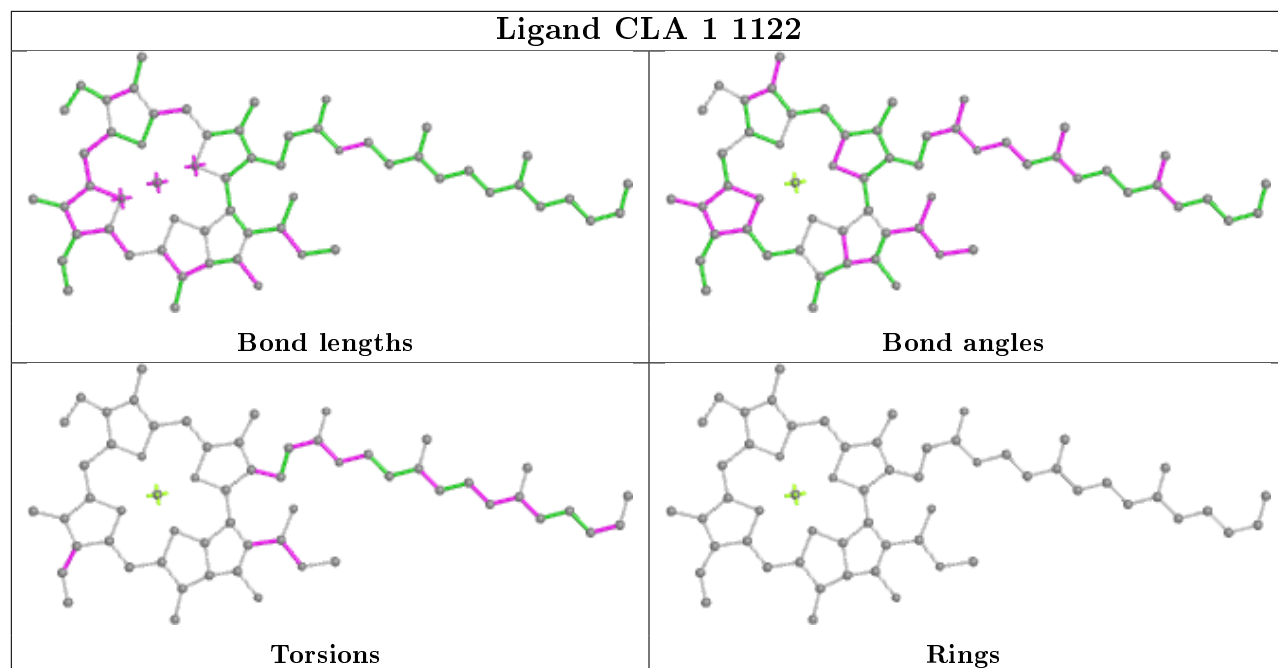
Ligand CLA A 1115



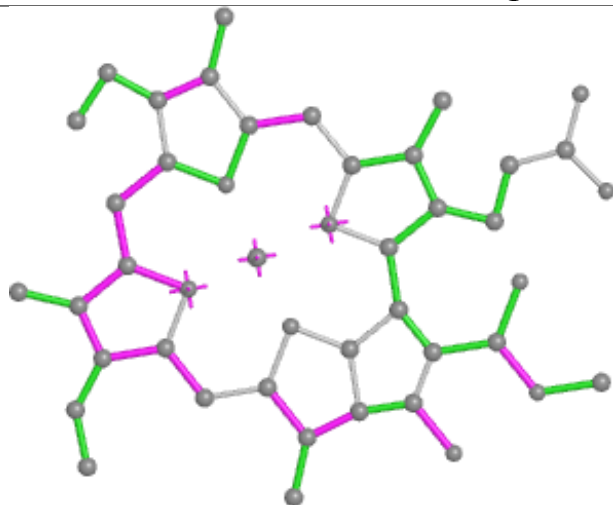
Ligand BCR B 4009



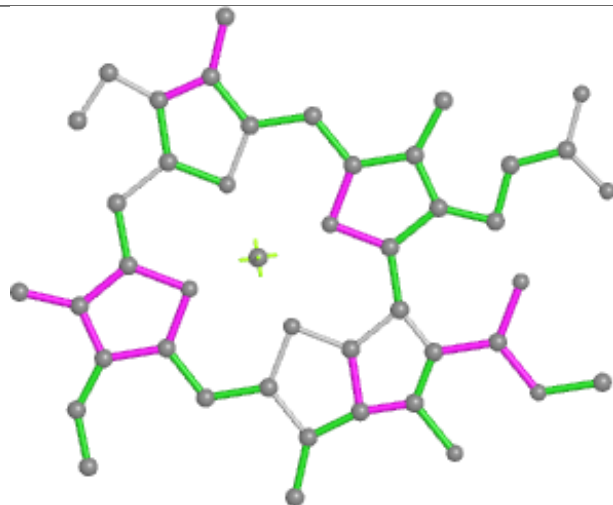




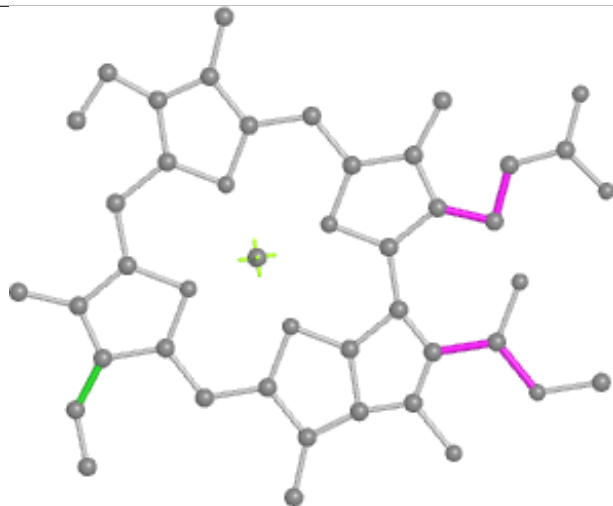
Ligand CLA B 1212



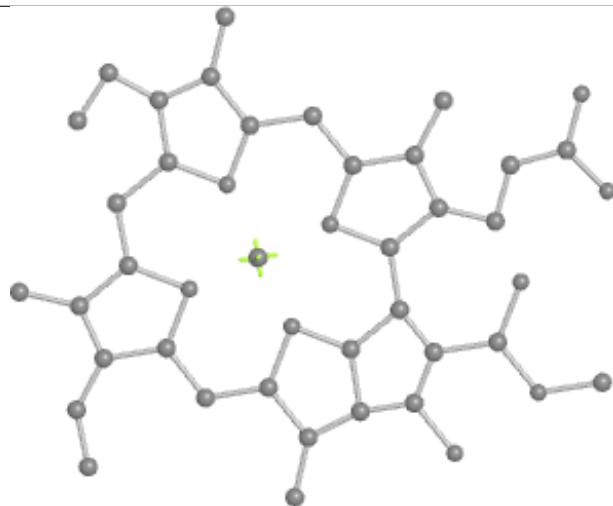
Bond lengths



Bond angles

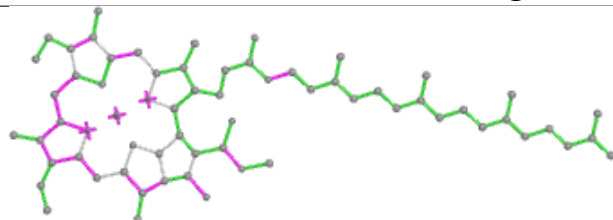


Torsions

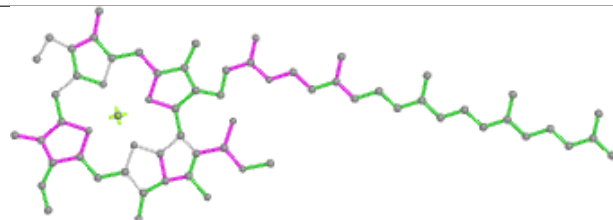


Rings

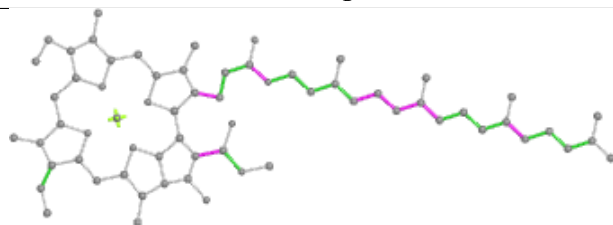
Ligand CLA L 1501



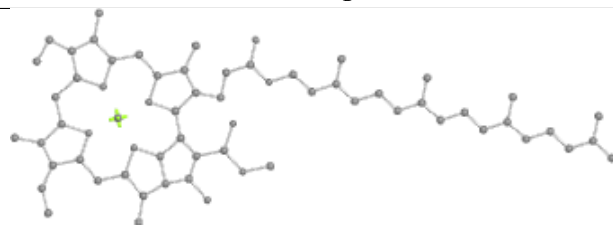
Bond lengths



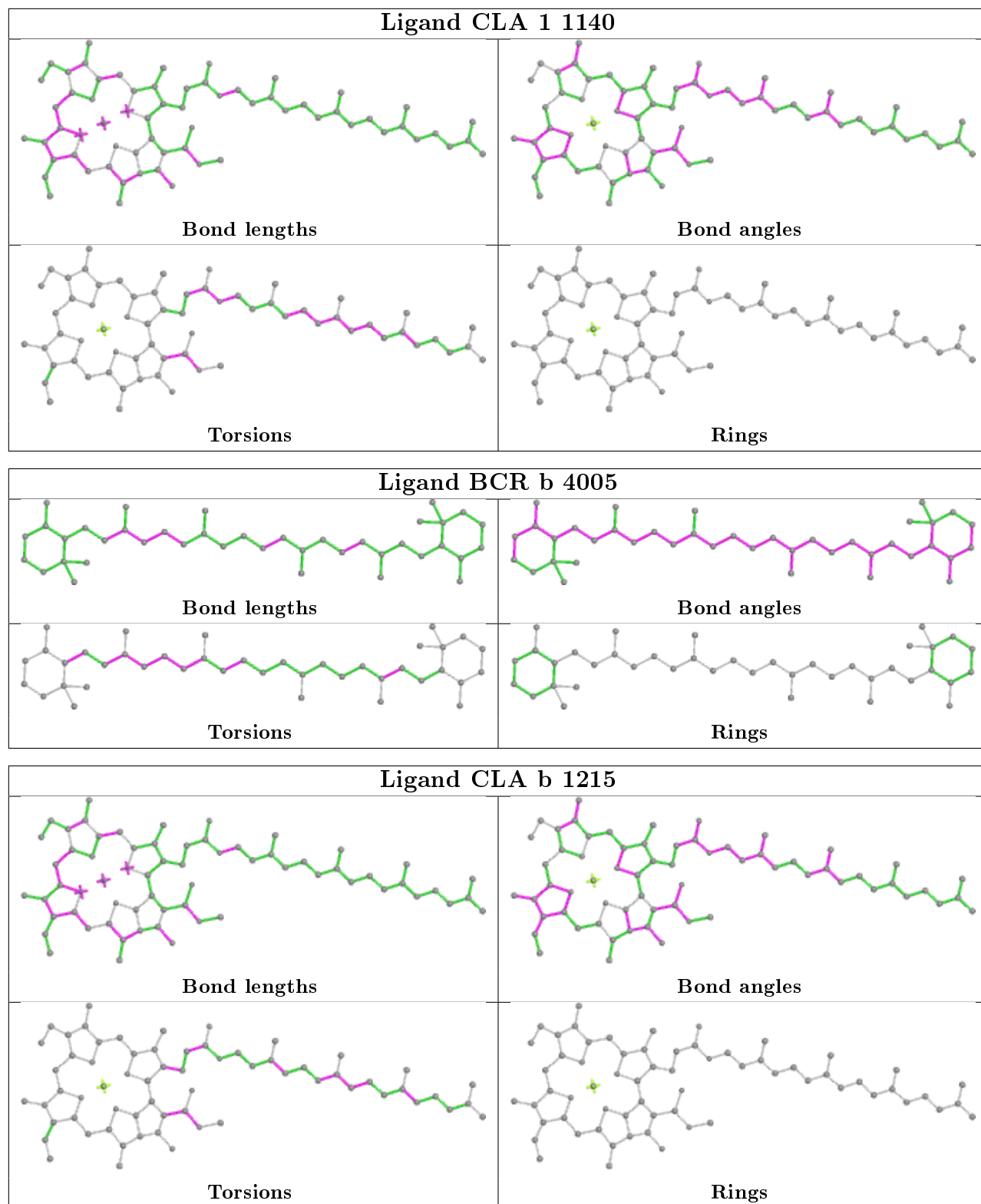
Bond angles

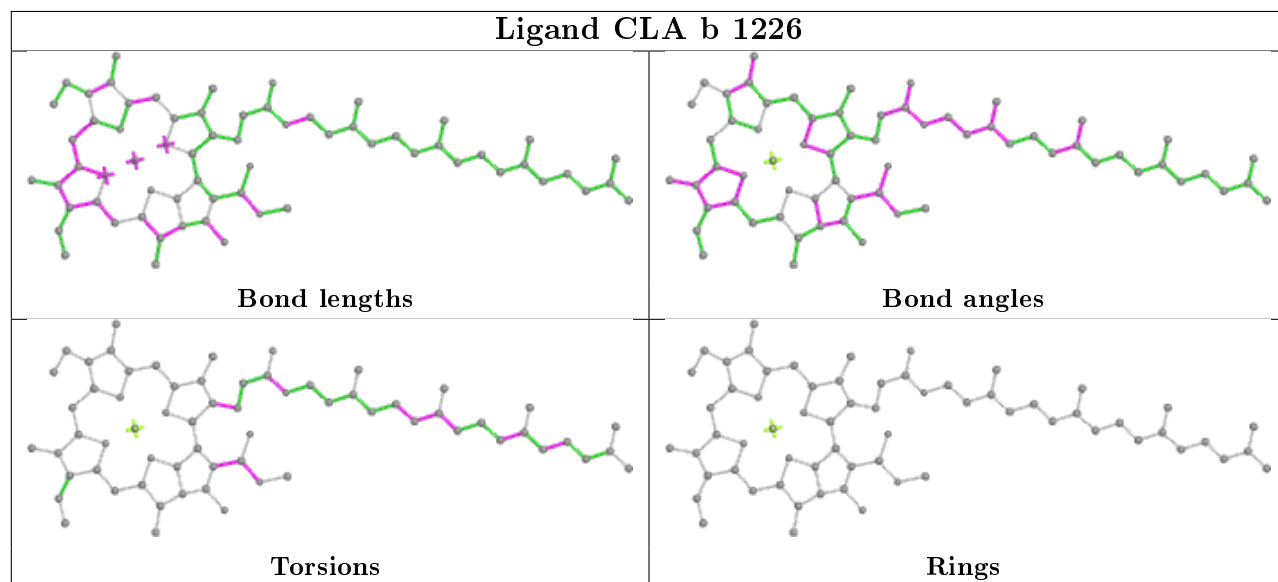
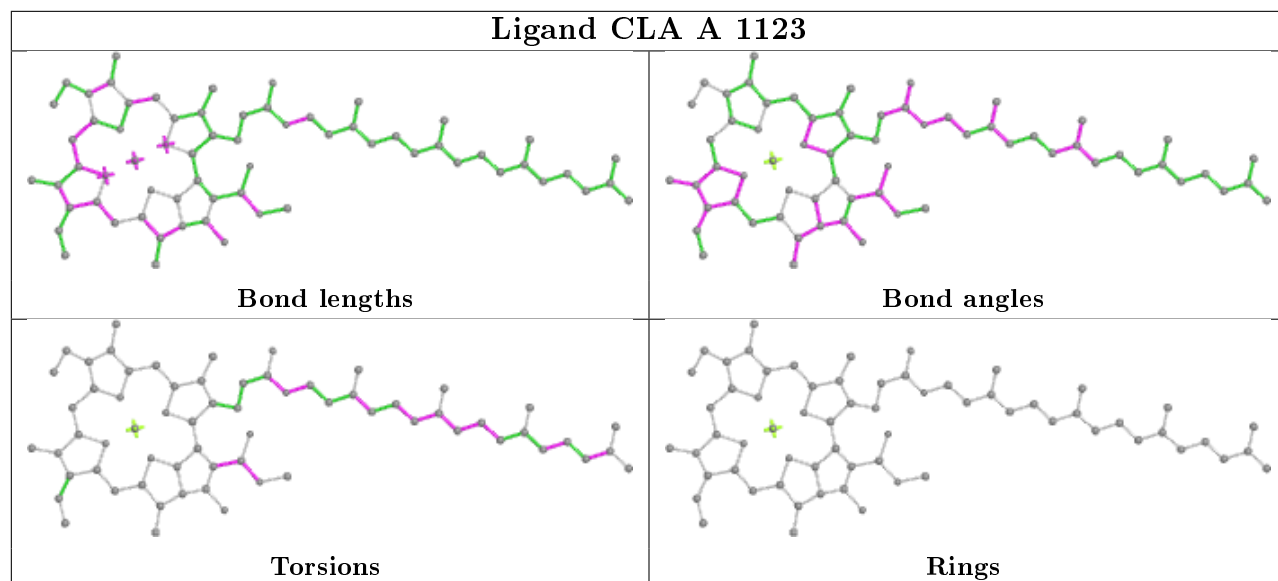
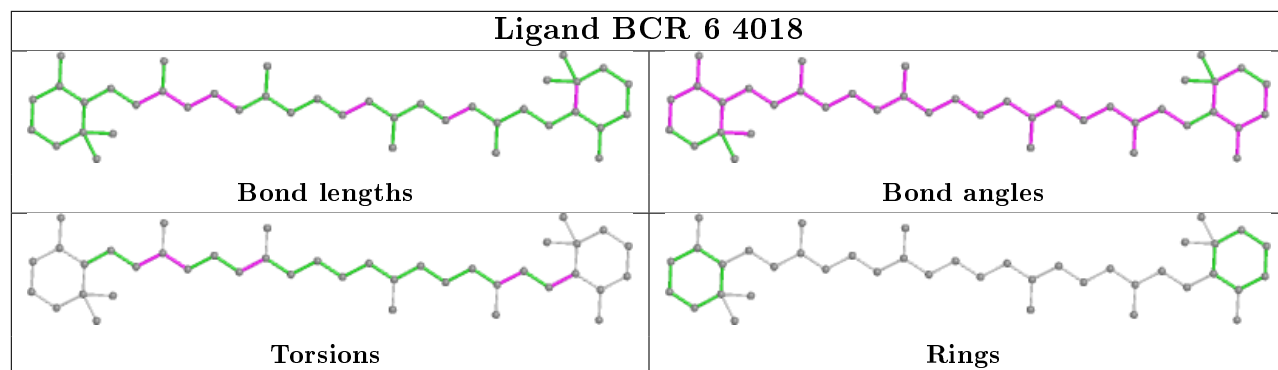


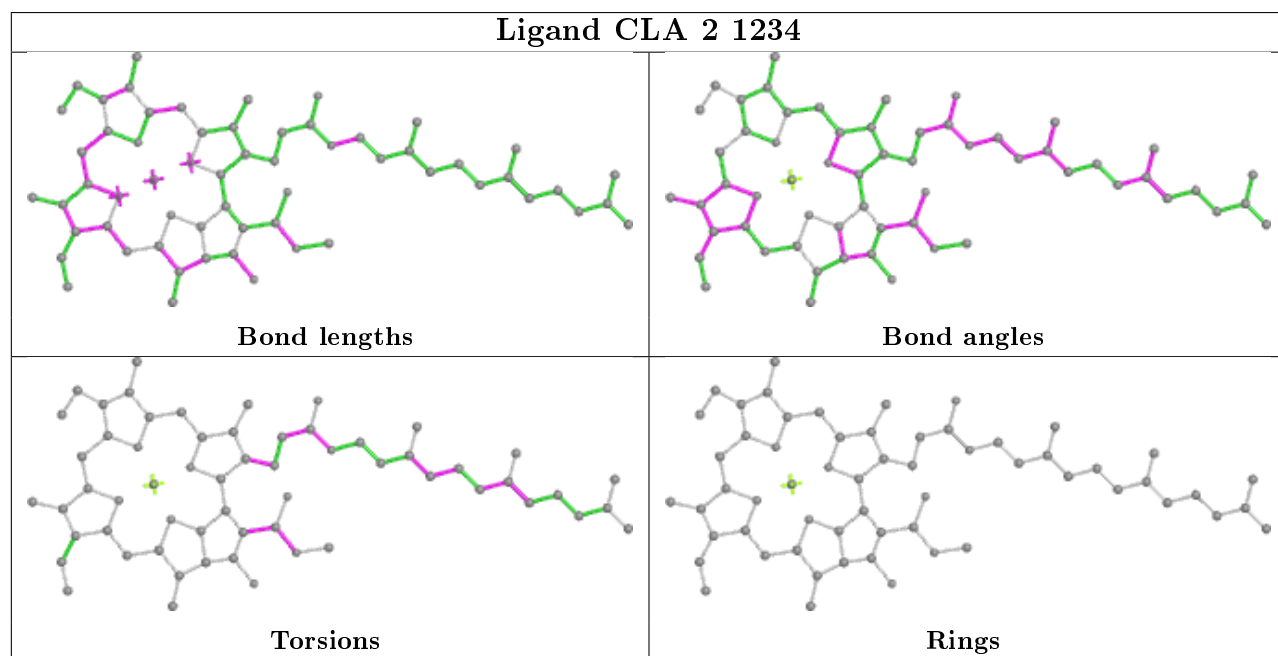
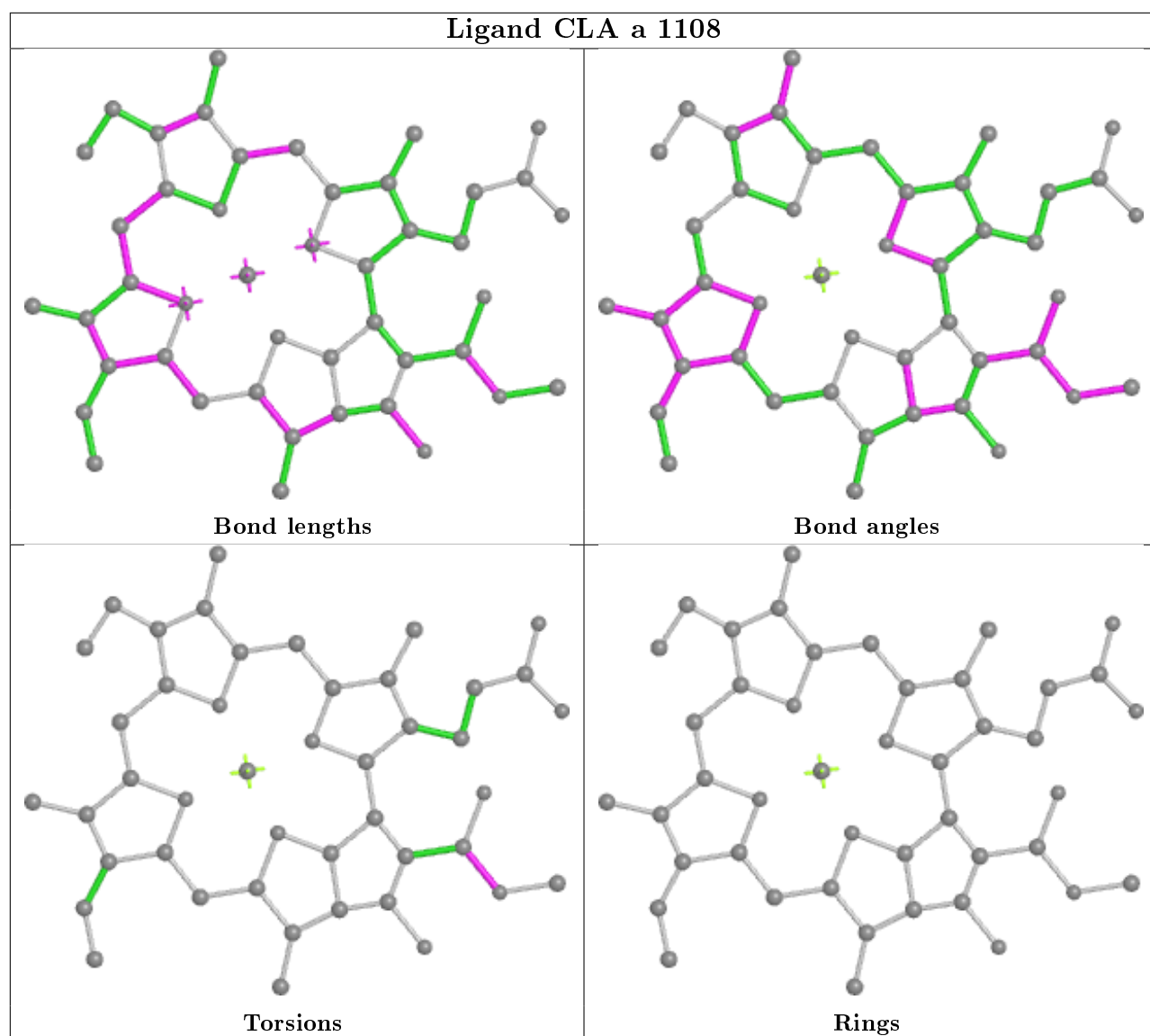
Torsions

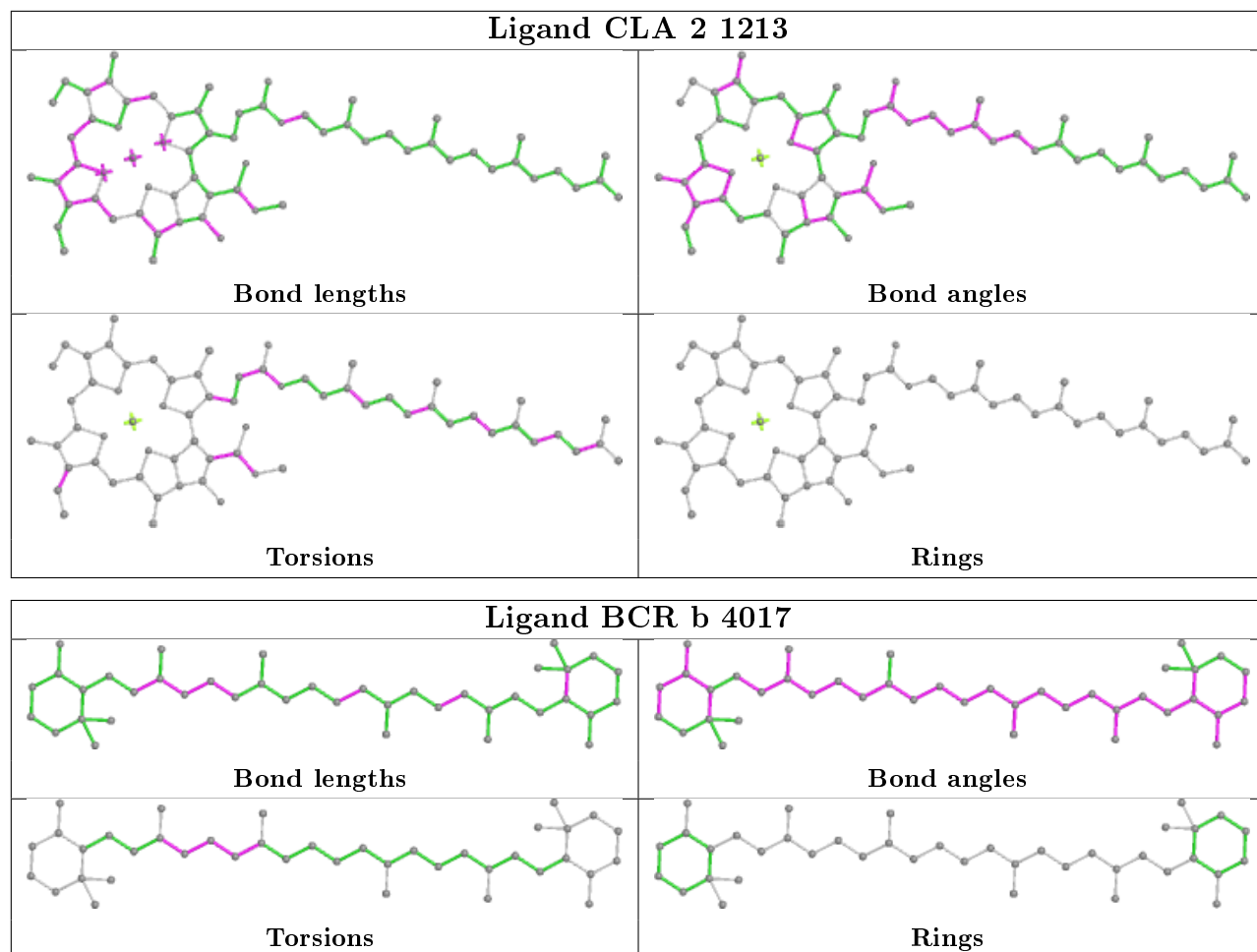


Rings

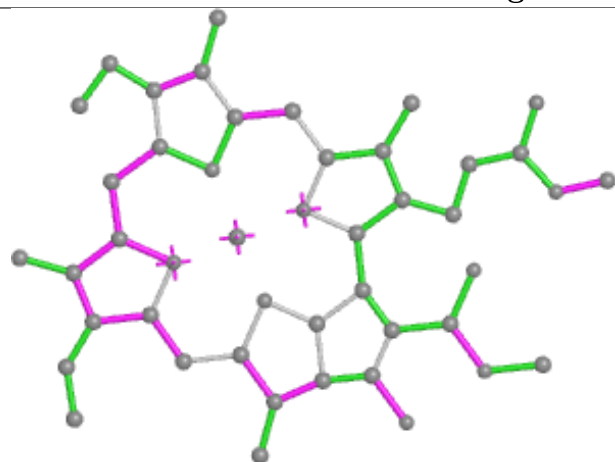




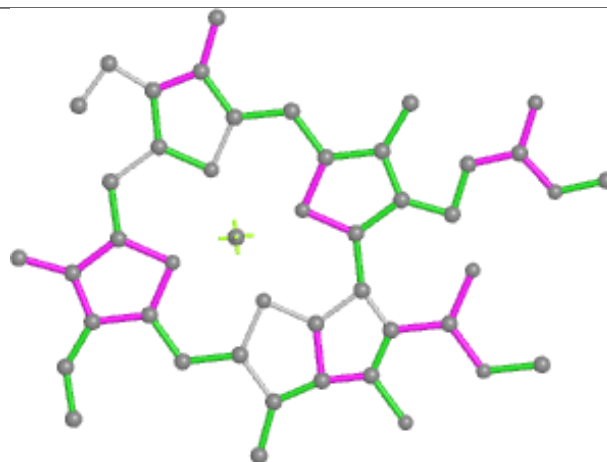




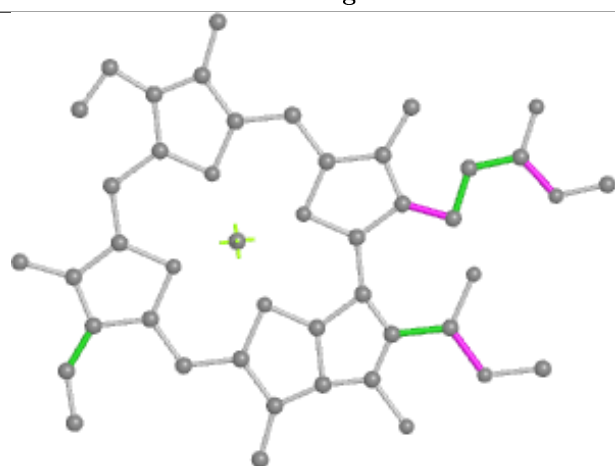
Ligand CLA A 1130



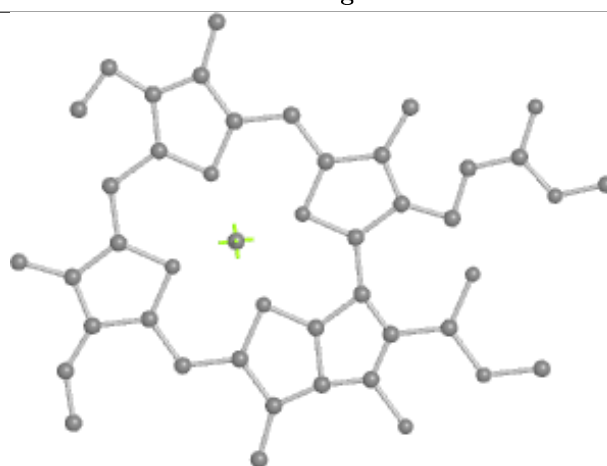
Bond lengths



Bond angles

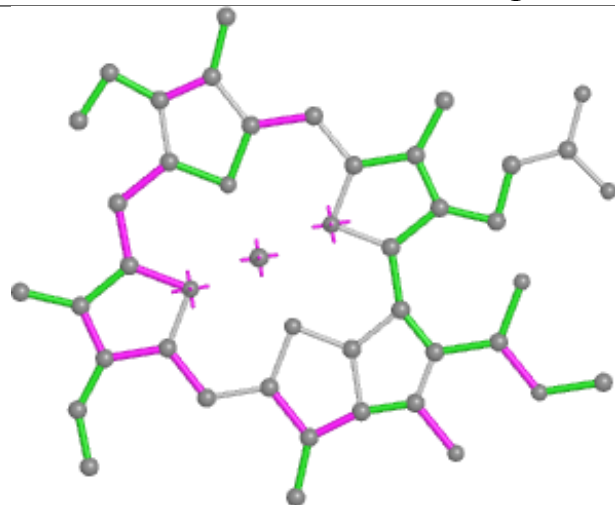


Torsions

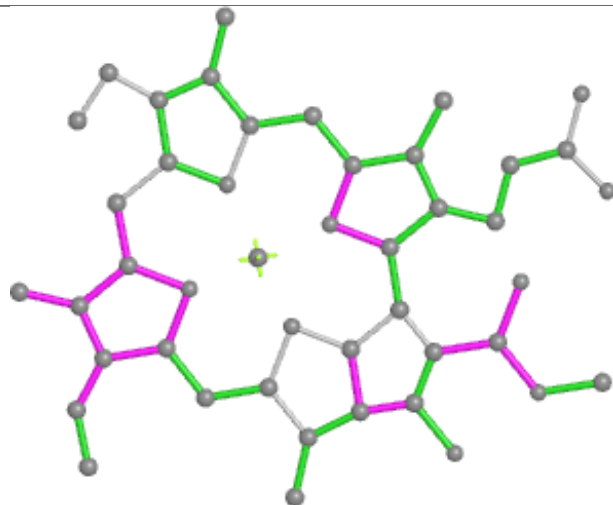


Rings

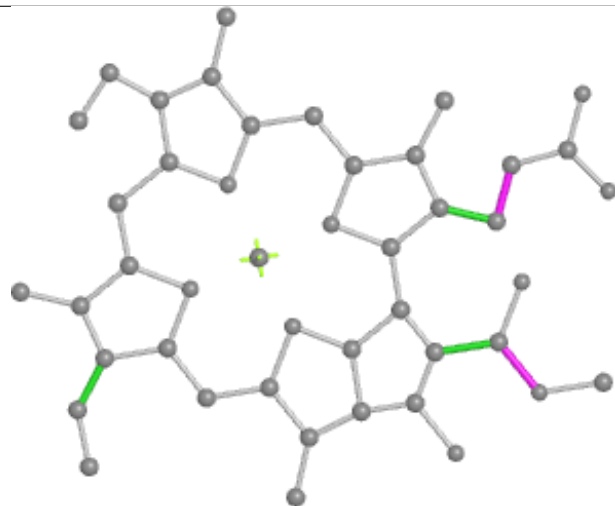
Ligand CLA B 1232



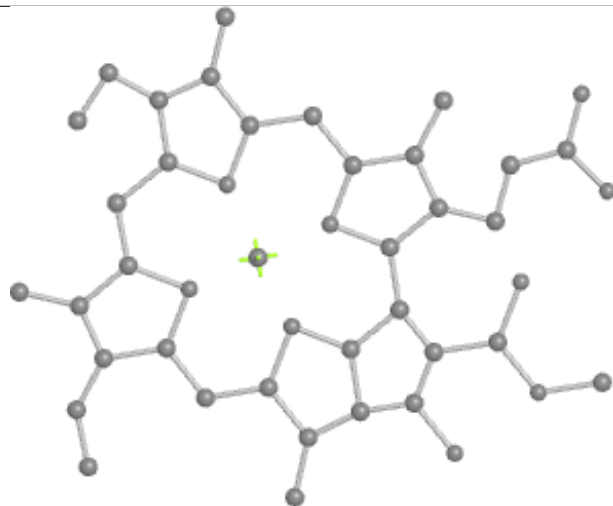
Bond lengths



Bond angles

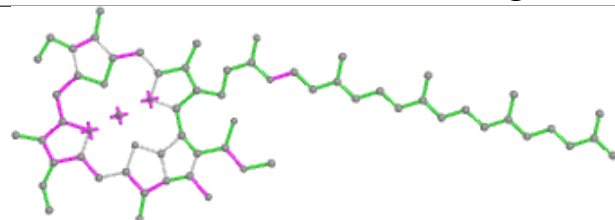


Torsions

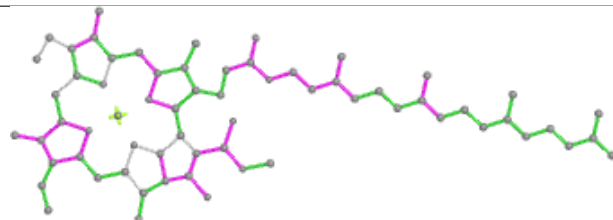


Rings

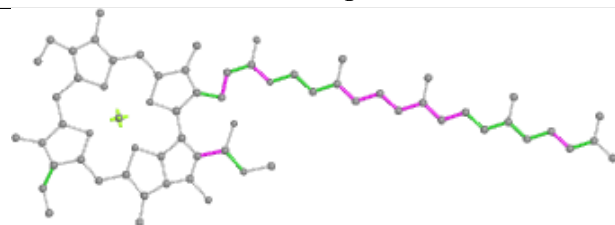
Ligand CLA A 1012



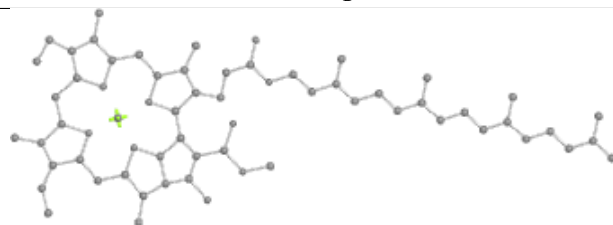
Bond lengths



Bond angles

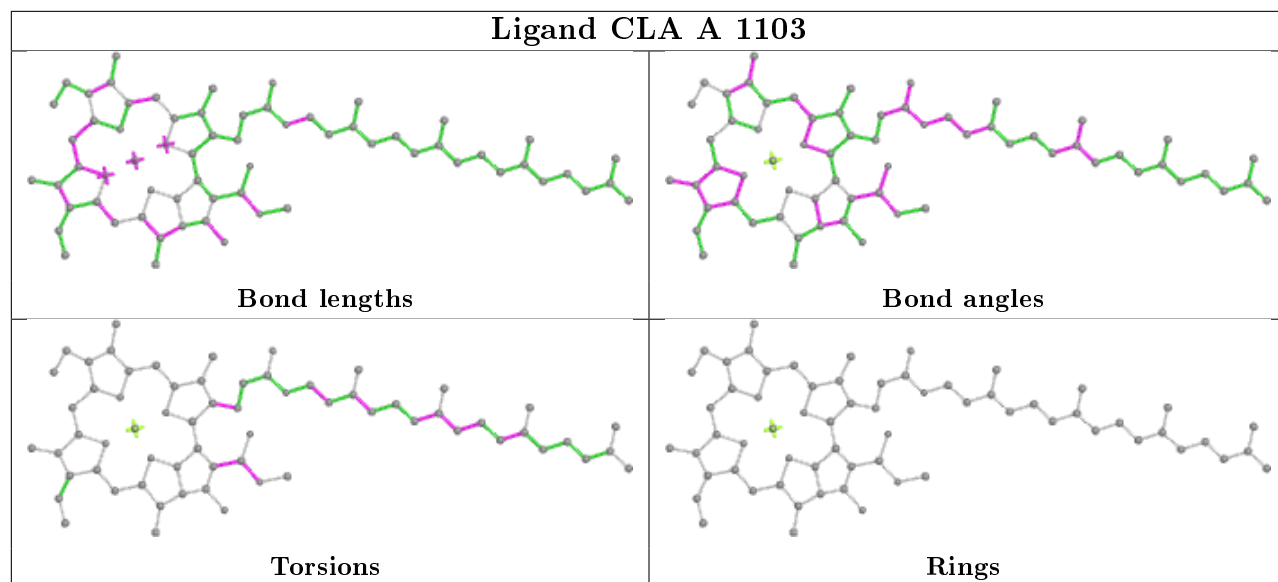


Torsions

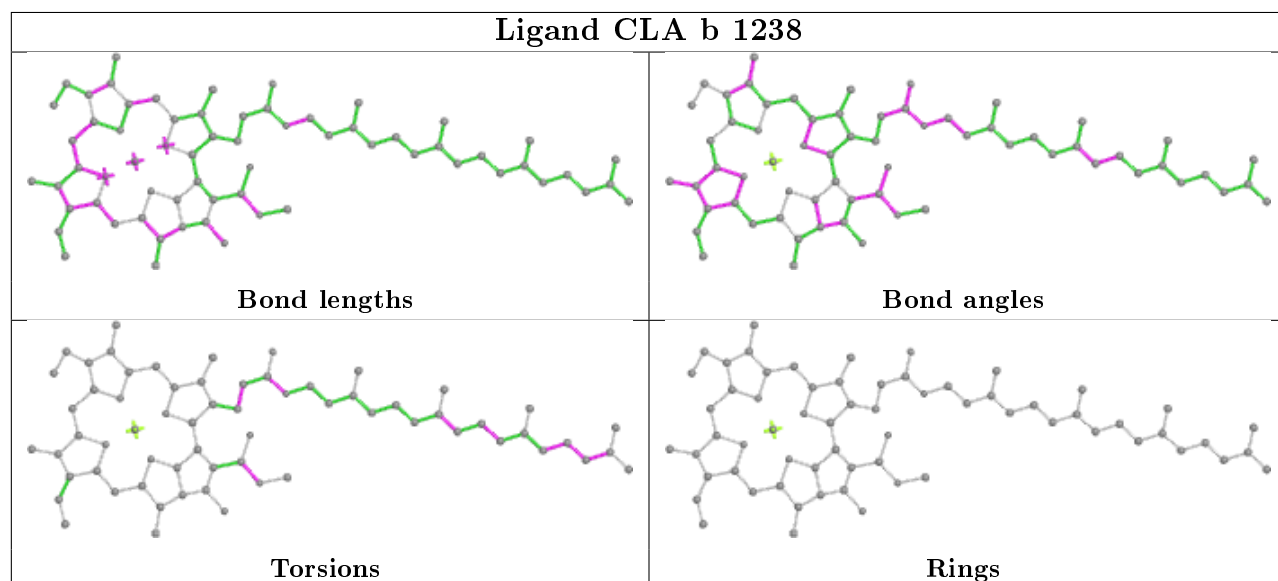


Rings

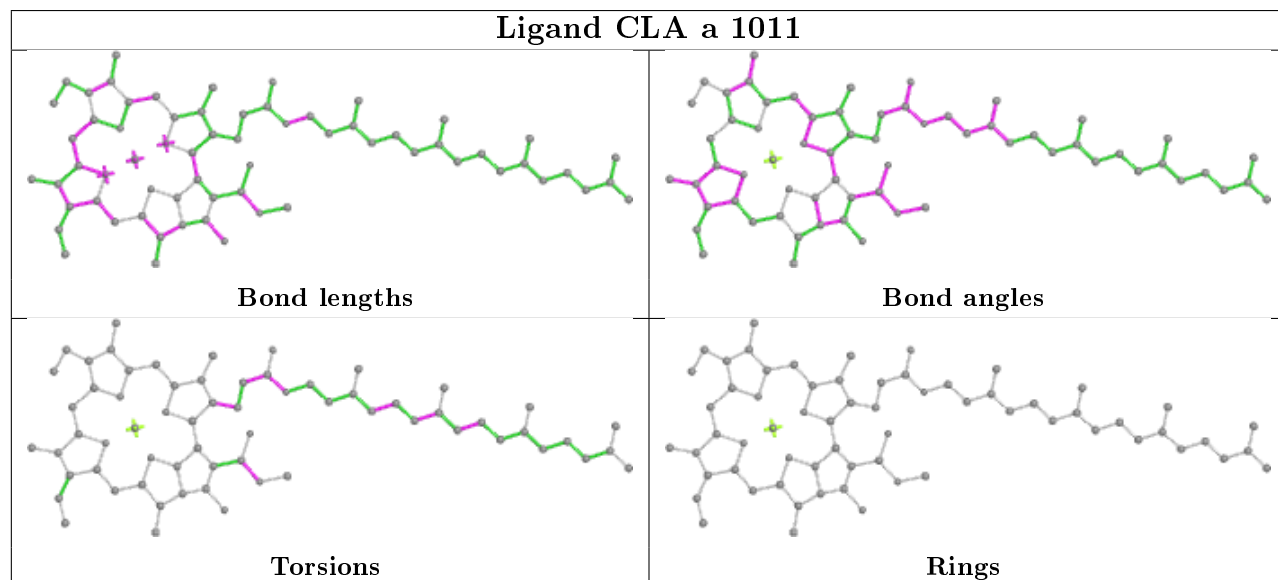
Ligand CLA A 1103

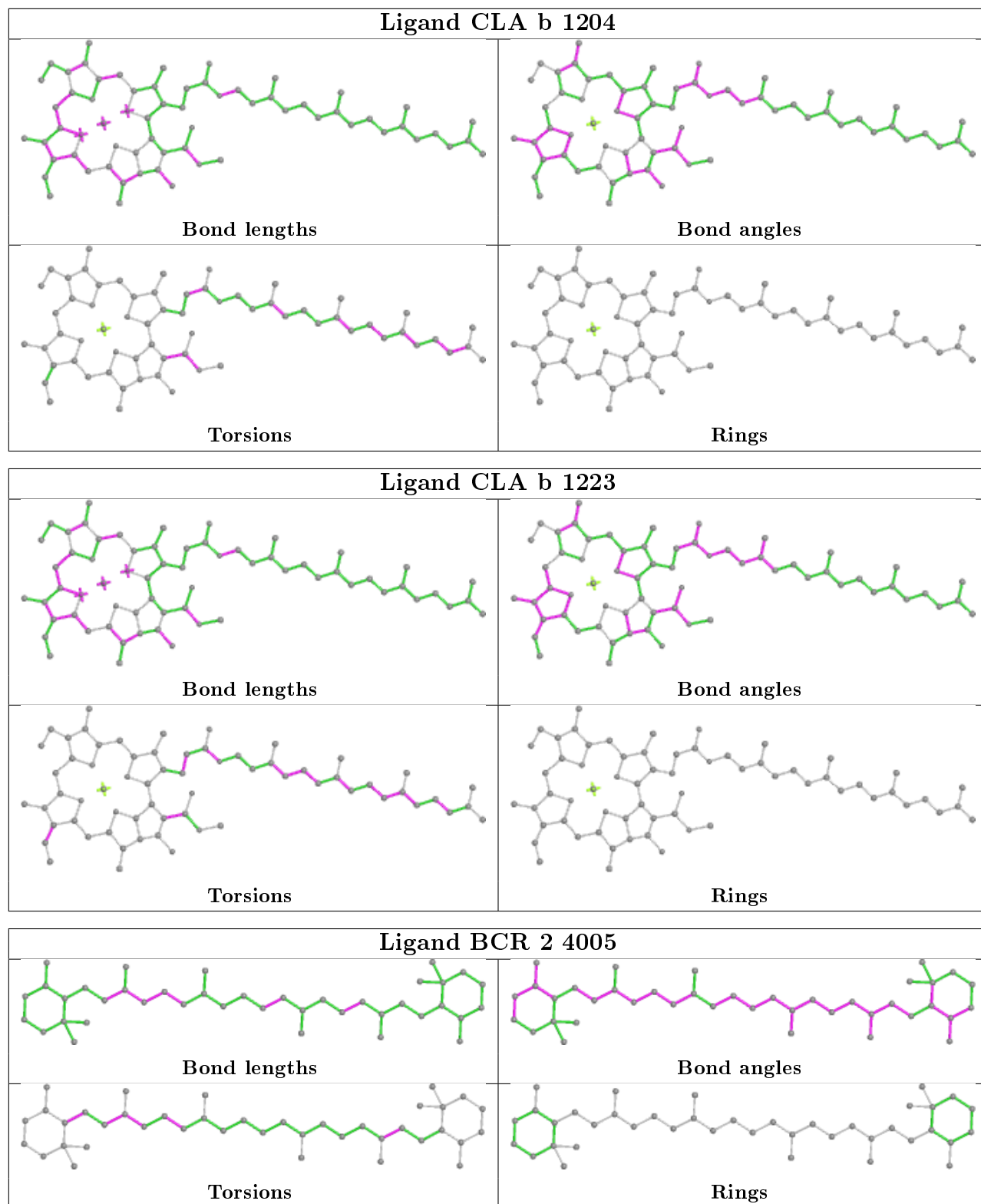


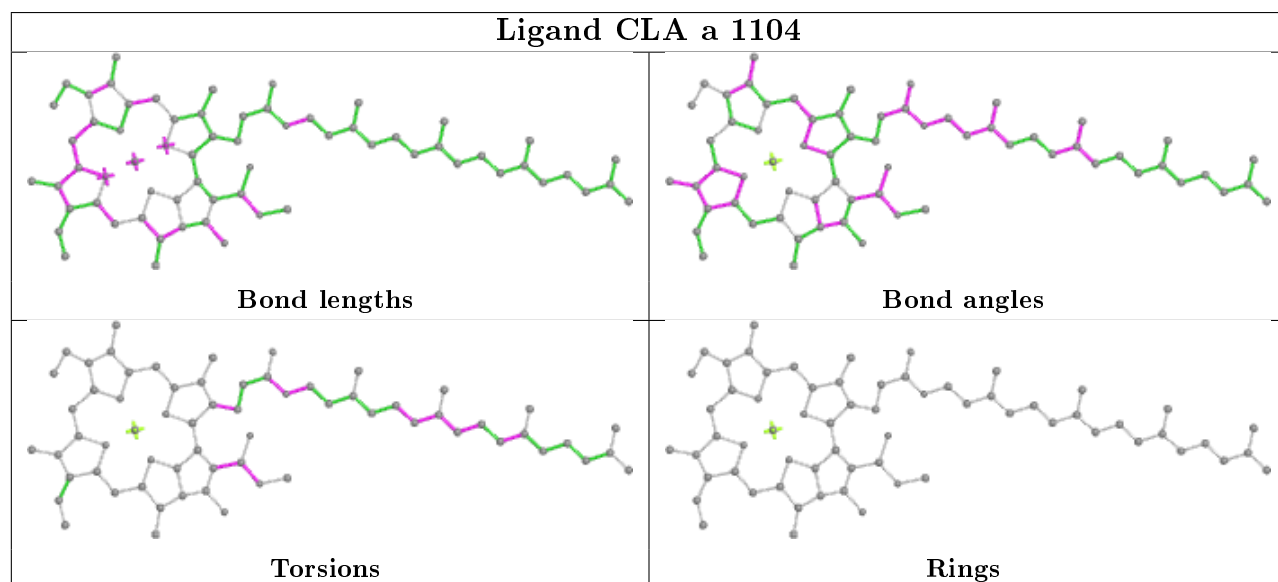
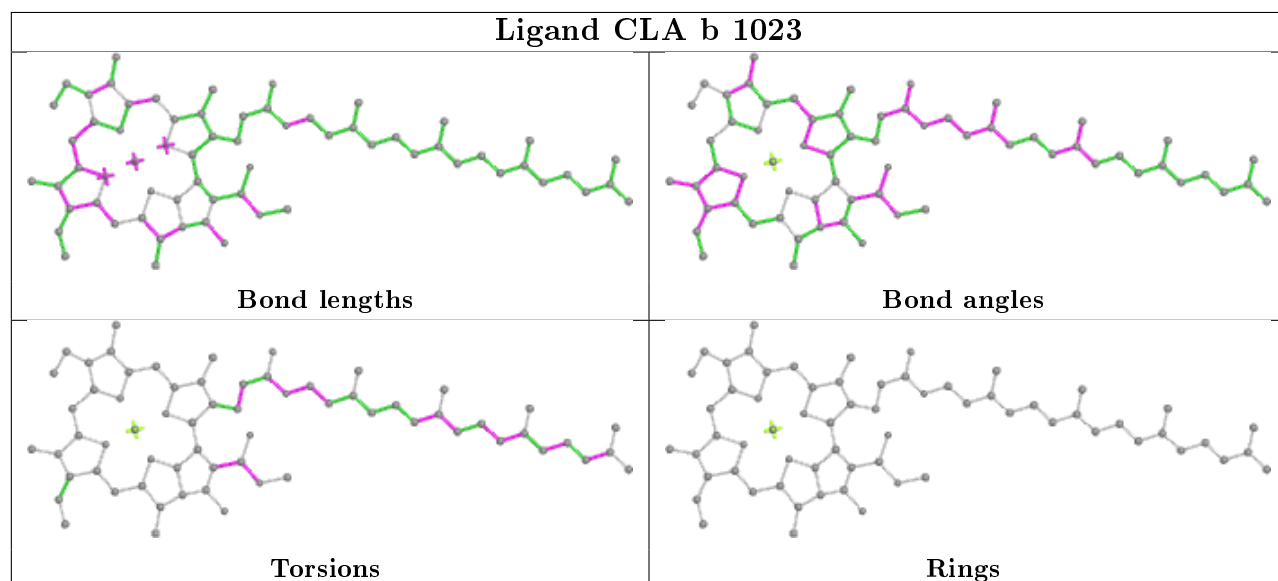
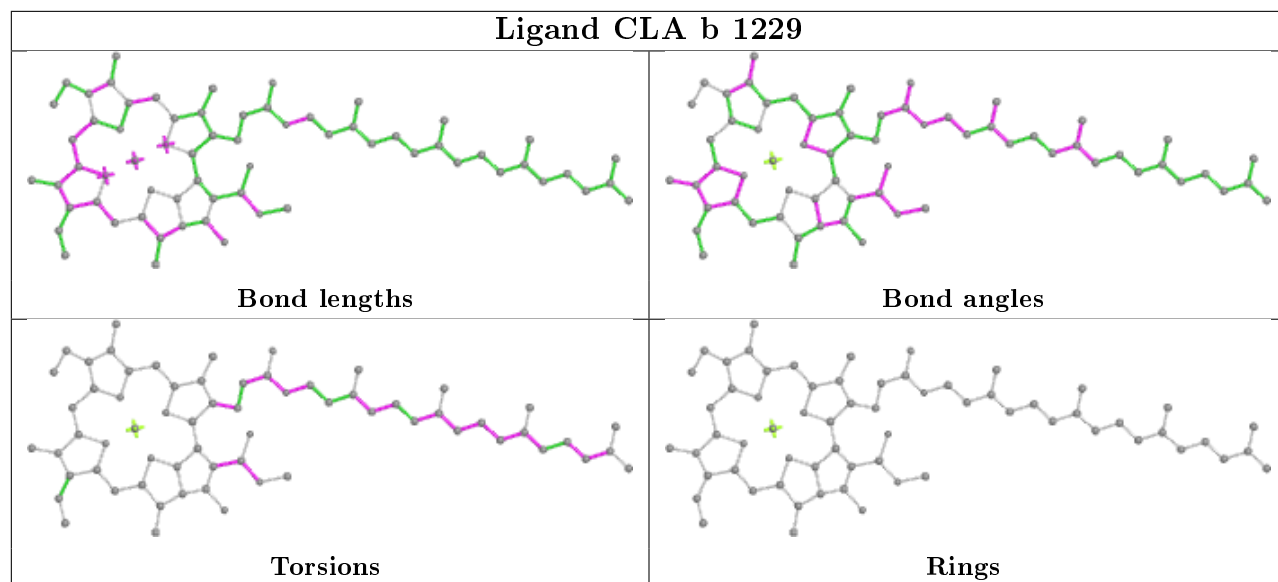
Ligand CLA b 1238

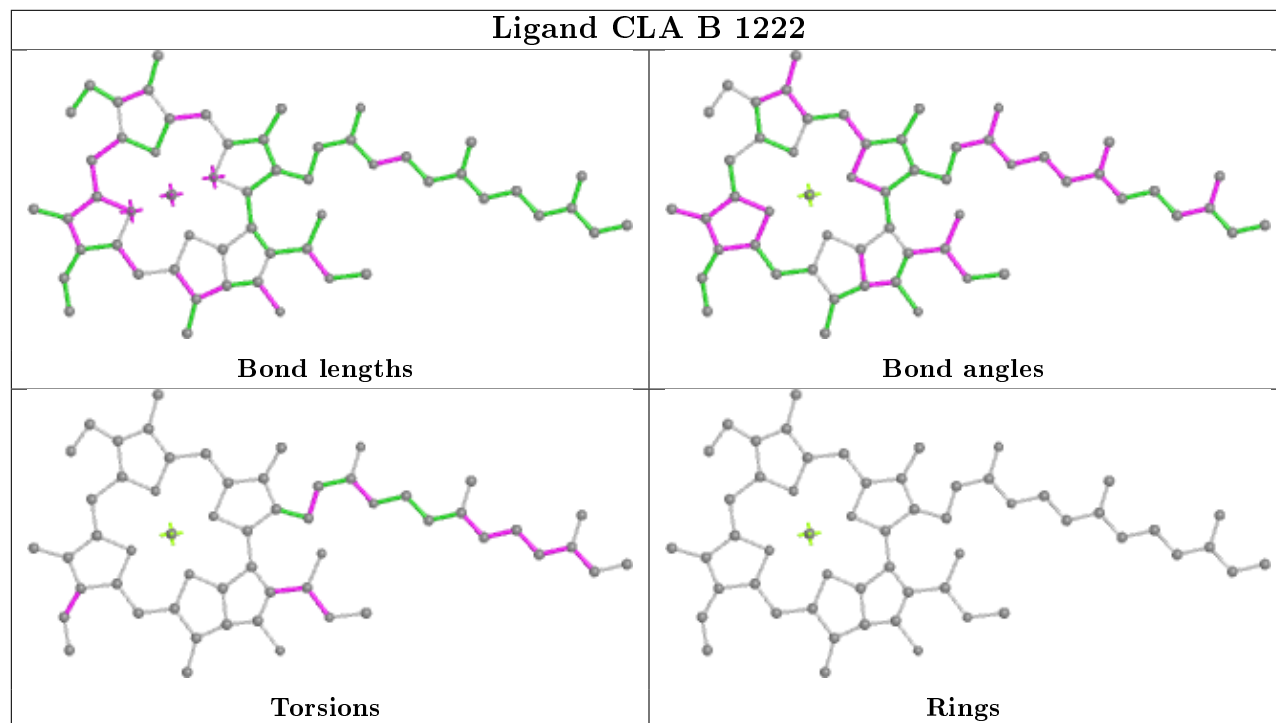
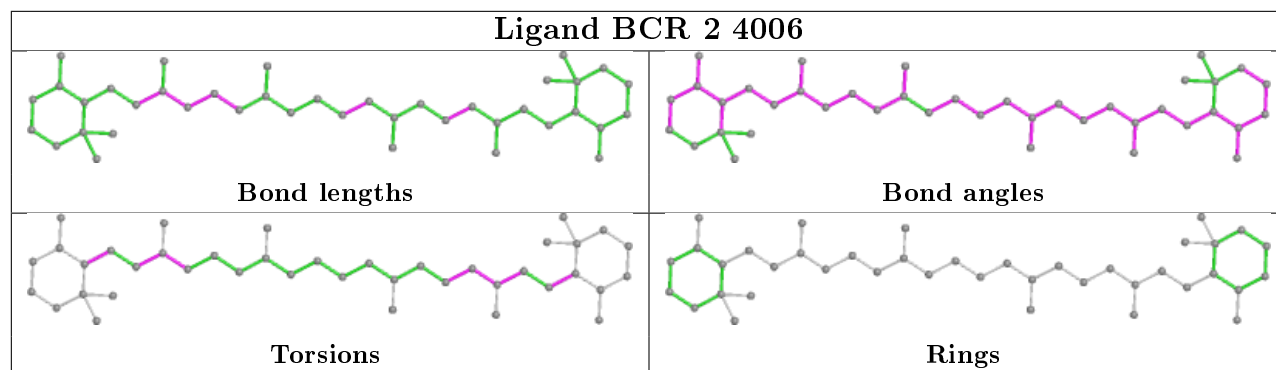
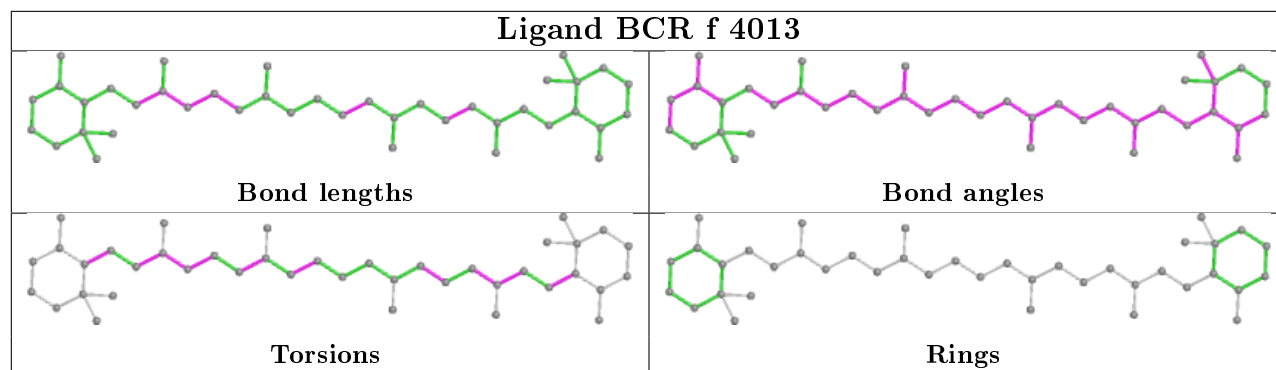


Ligand CLA a 1011

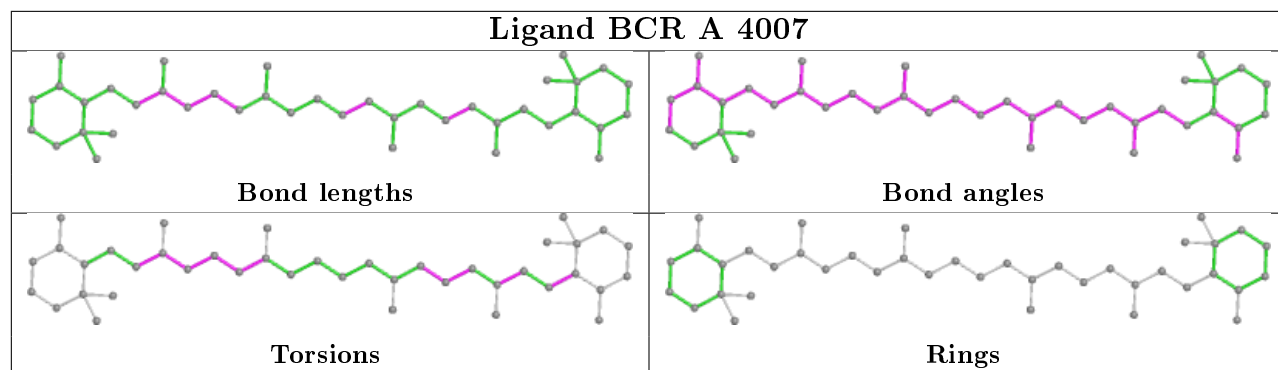




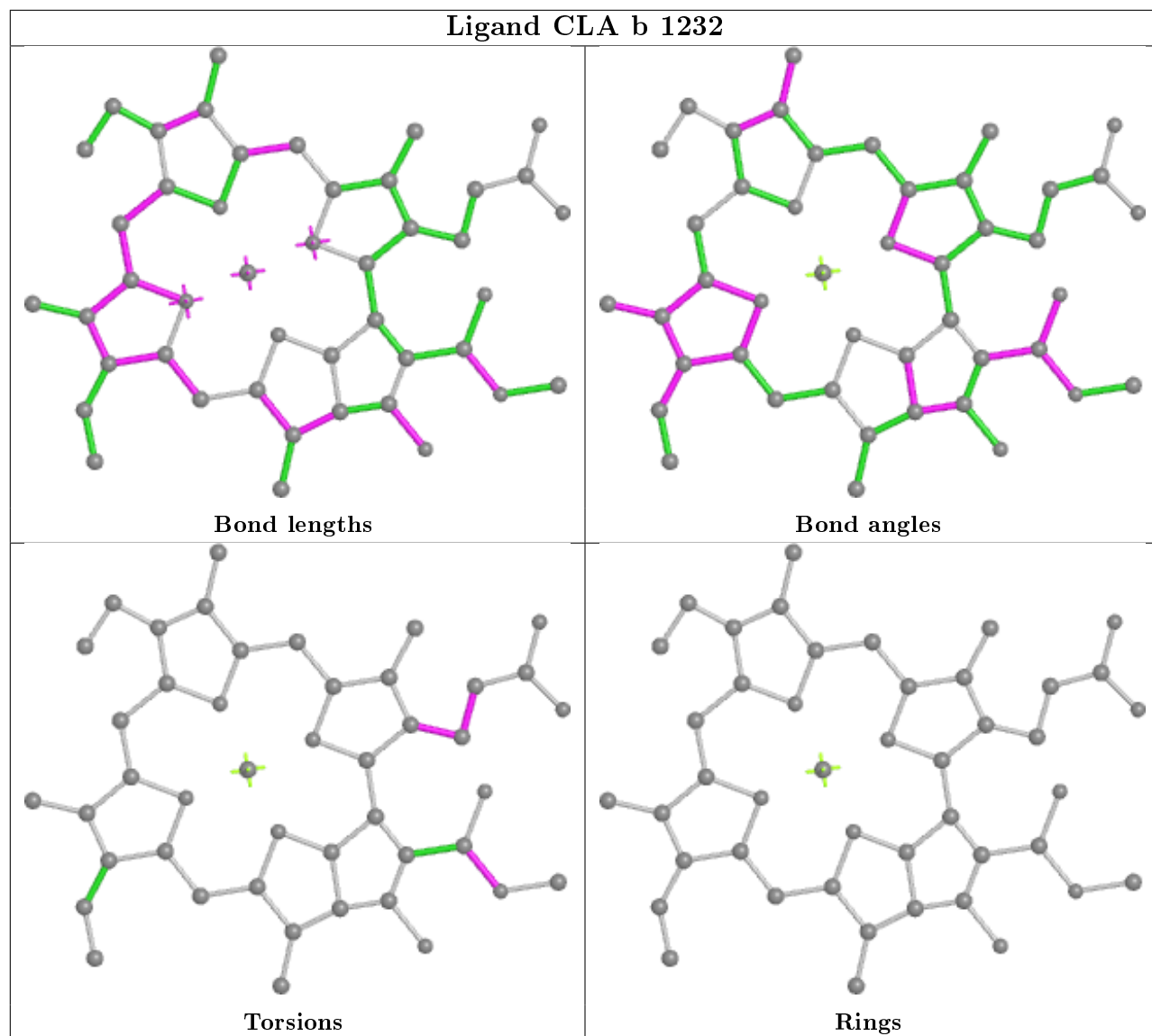




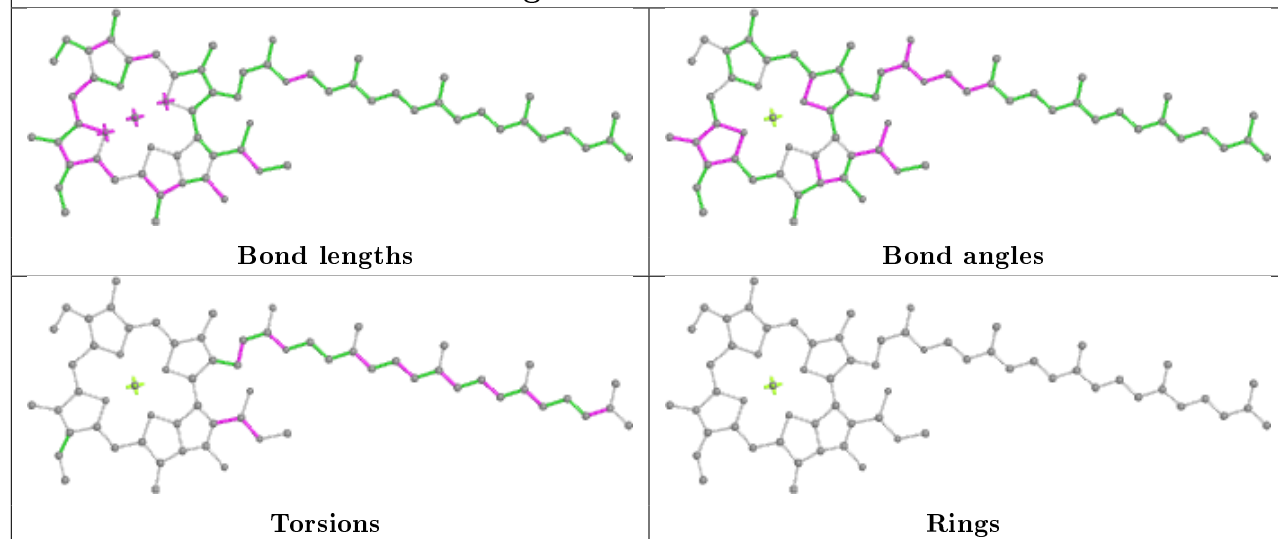
Ligand BCR A 4007



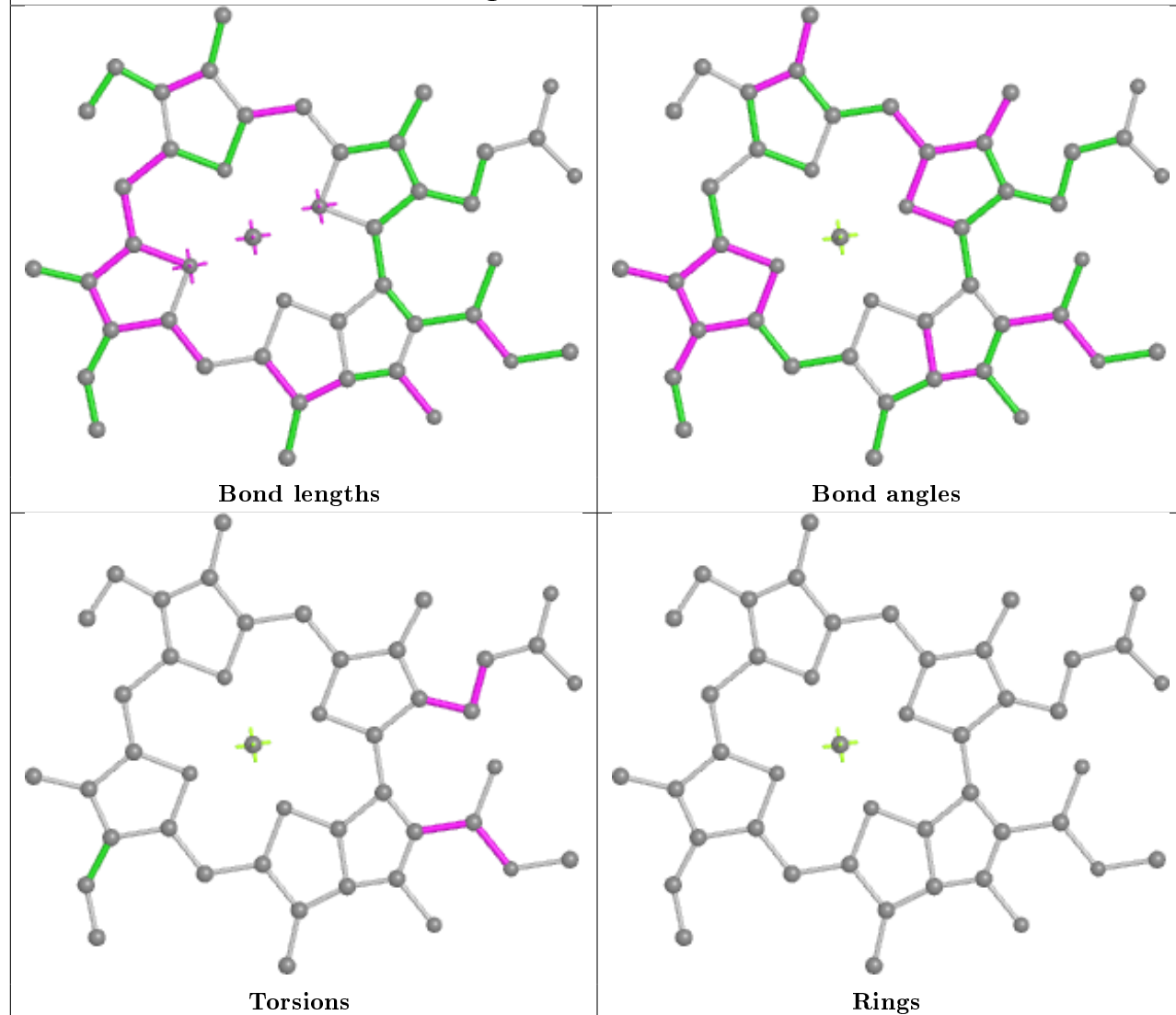
Ligand CLA b 1232



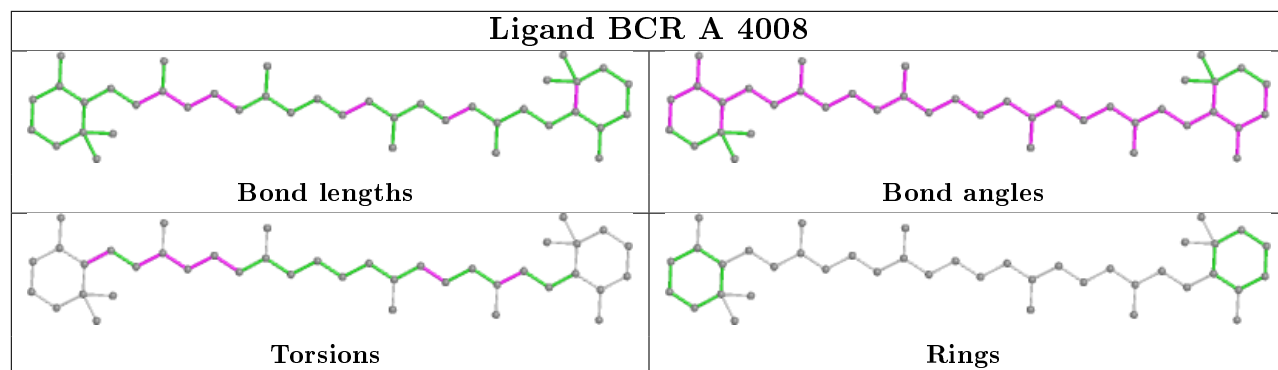
Ligand CLA A 1132



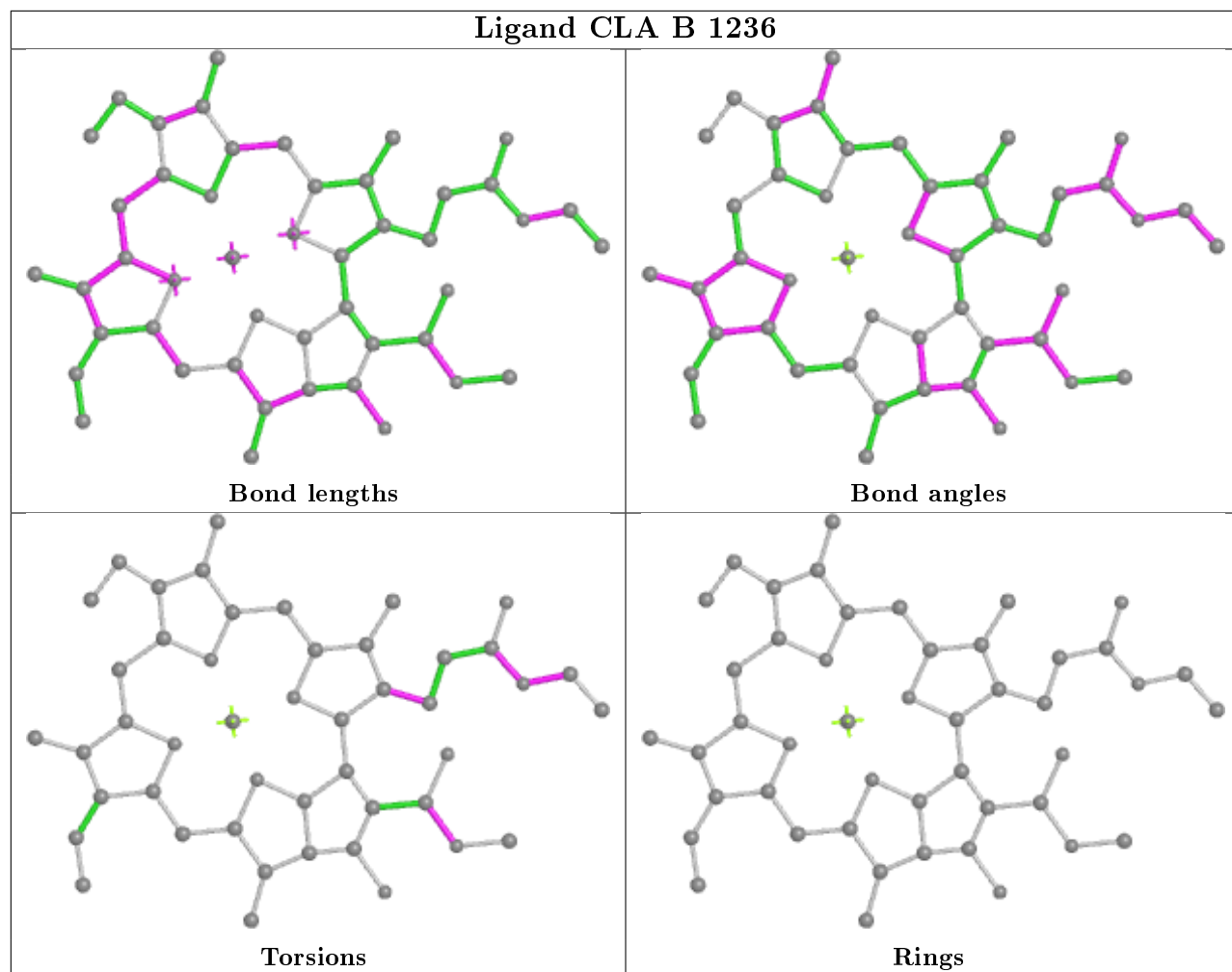
Ligand CLA b 1231



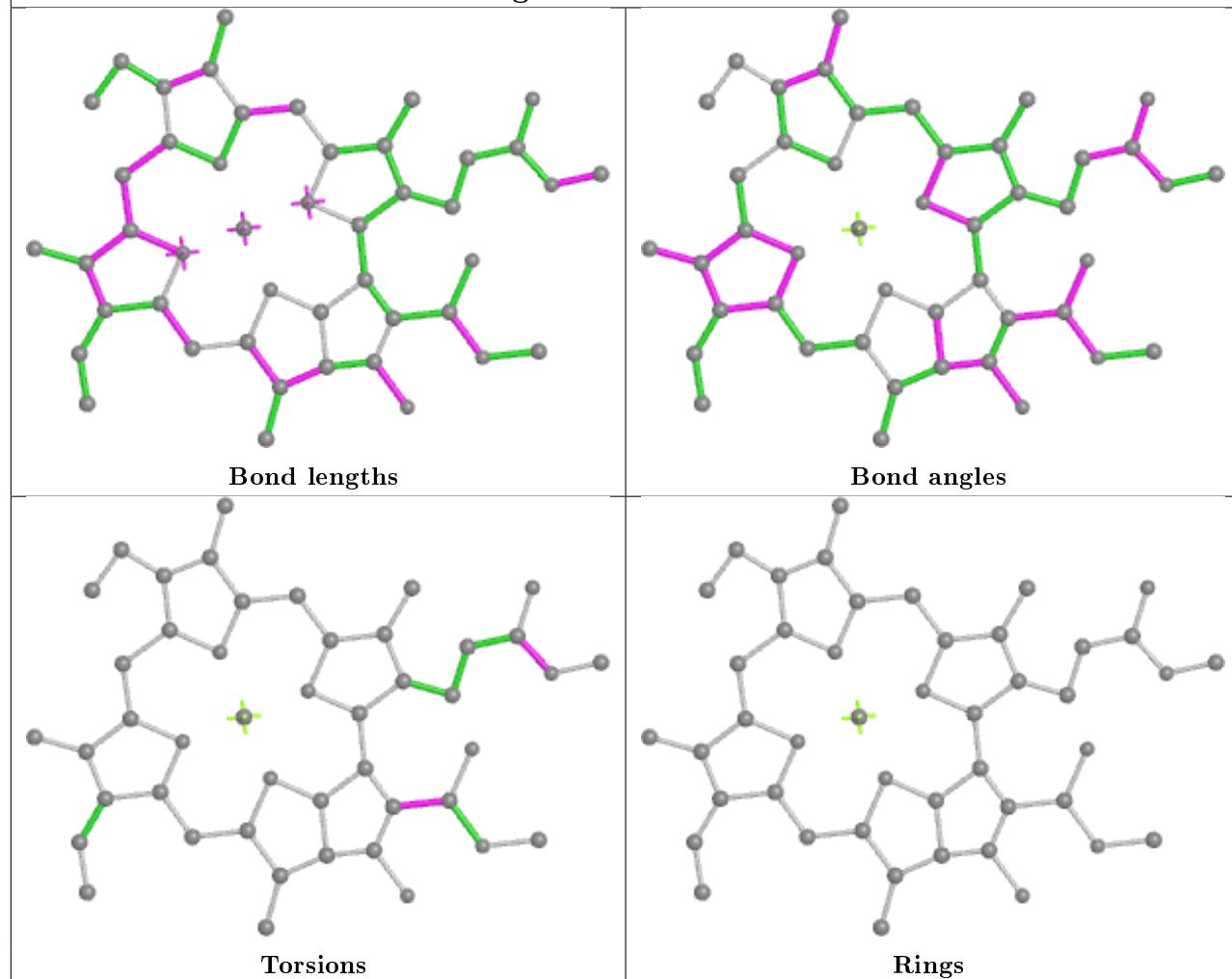
Ligand BCR A 4008



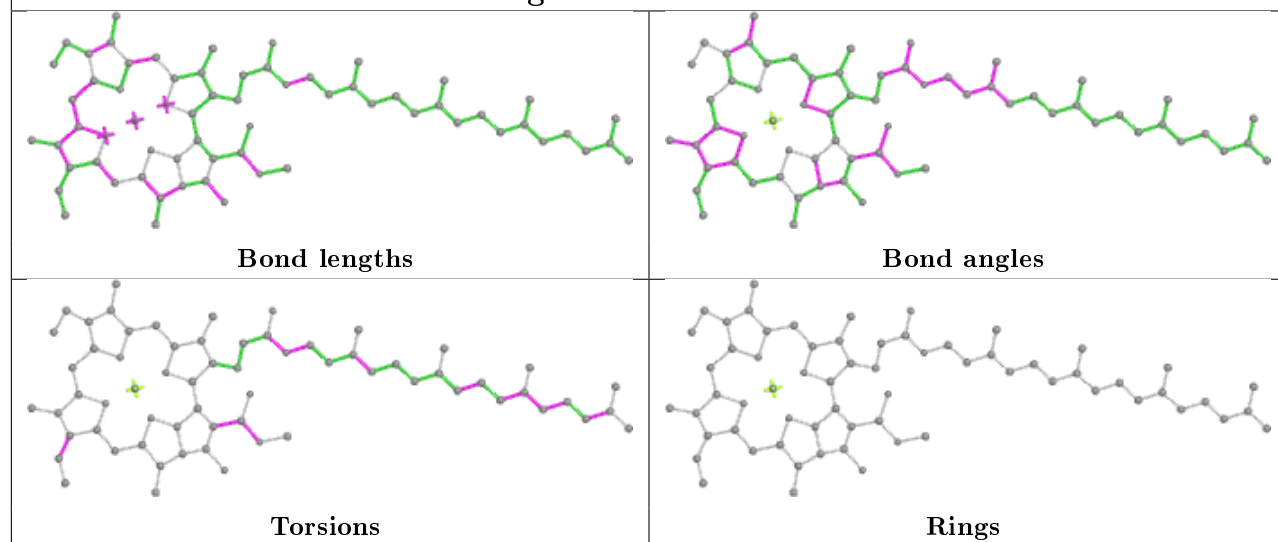
Ligand CLA B 1236

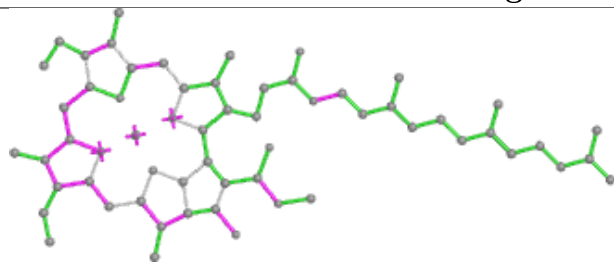
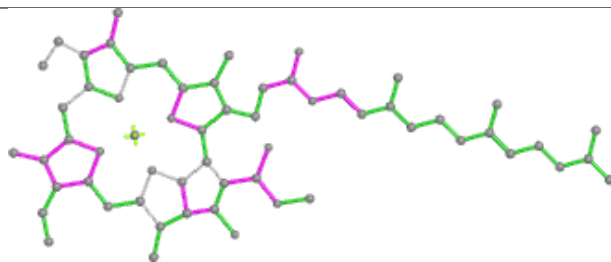
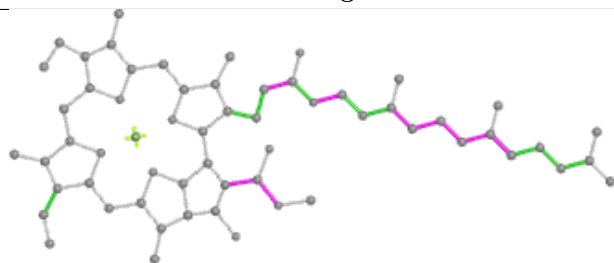
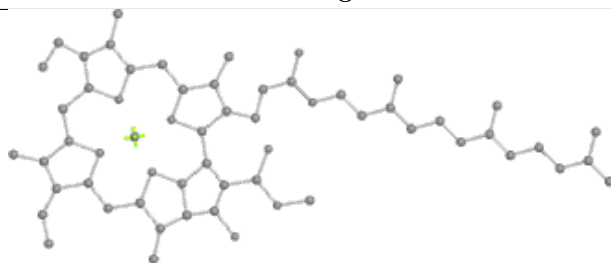
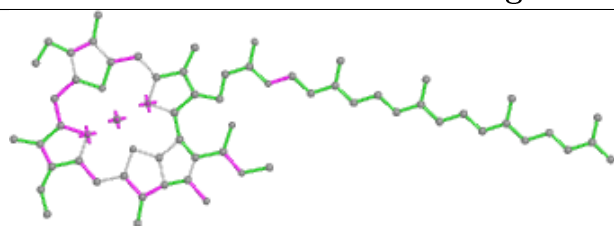
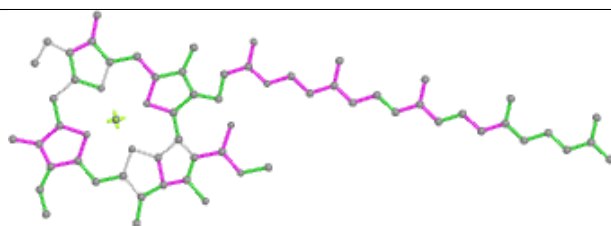
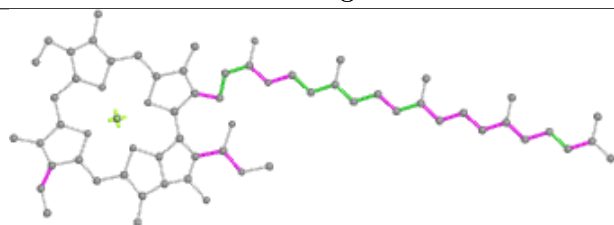
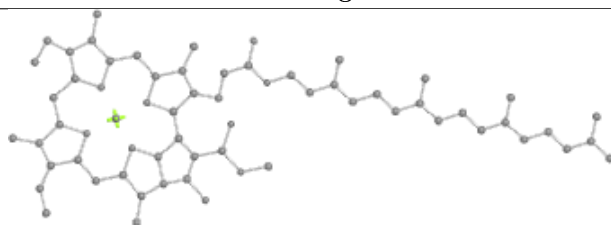


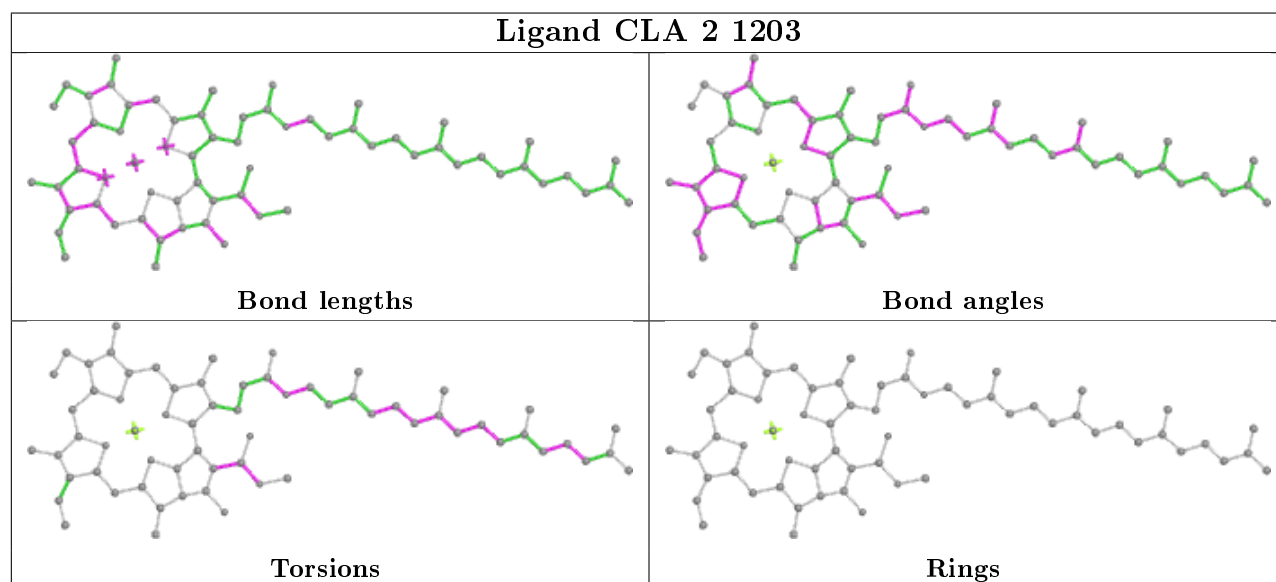
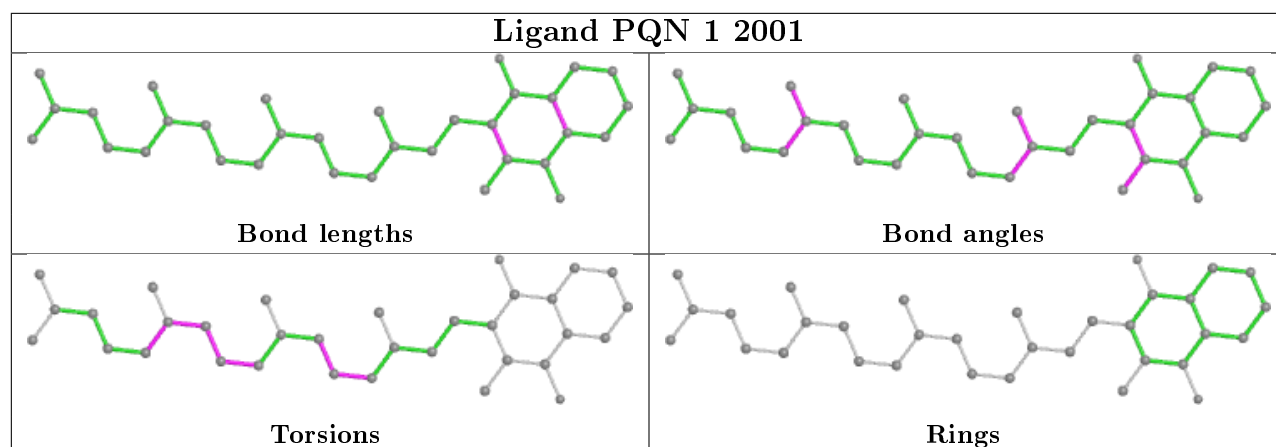
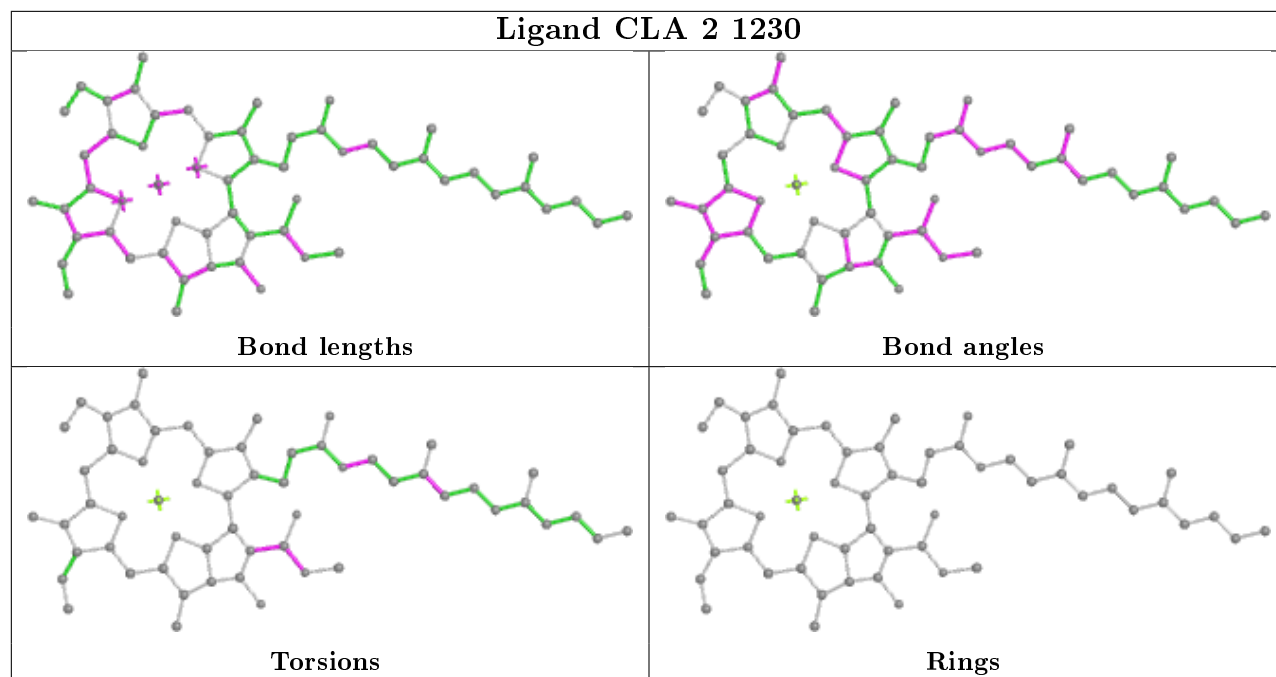
Ligand CLA 1 1502



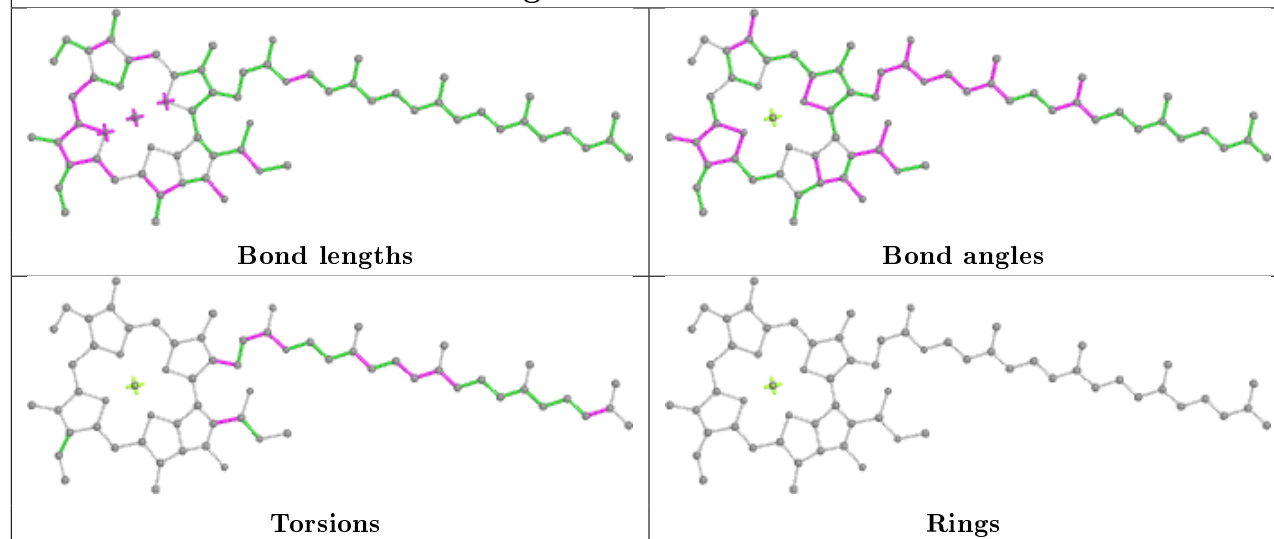
Ligand CLA a 1126



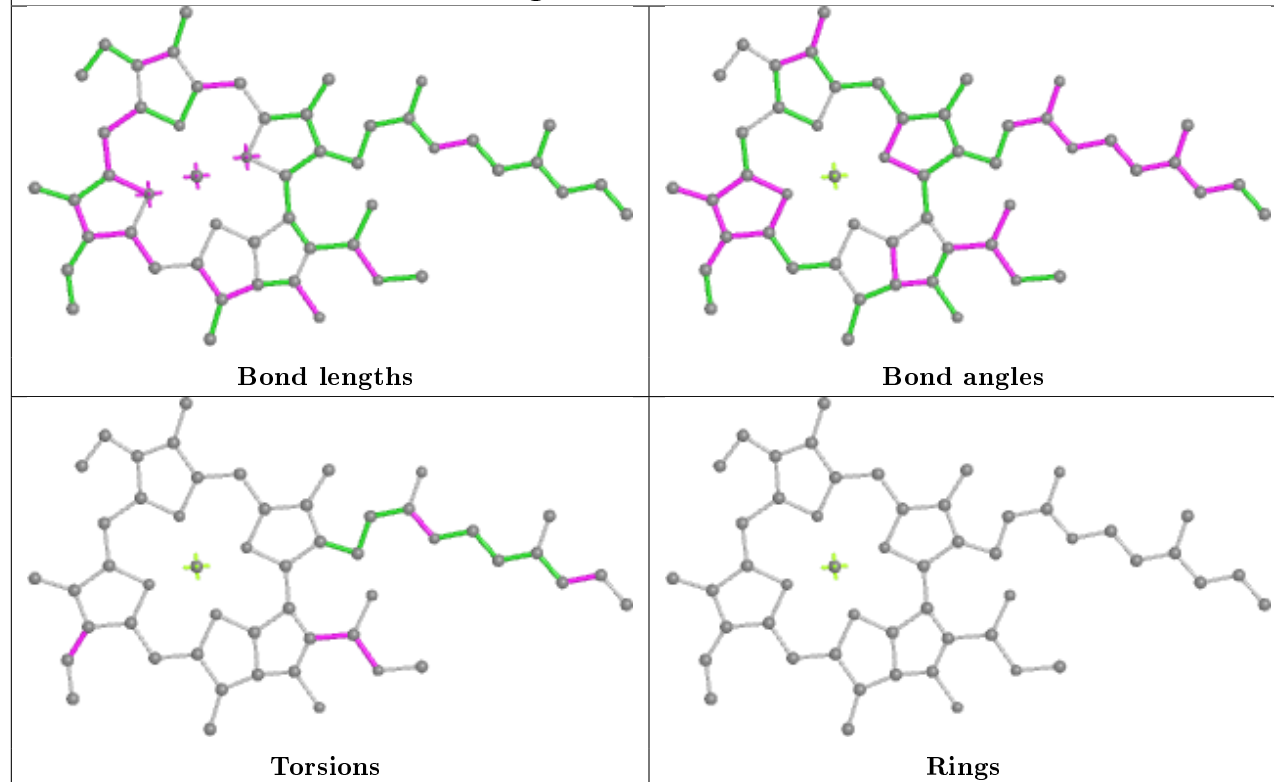
Ligand CLA B 1235**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1104****Bond lengths****Bond angles****Torsions****Rings**

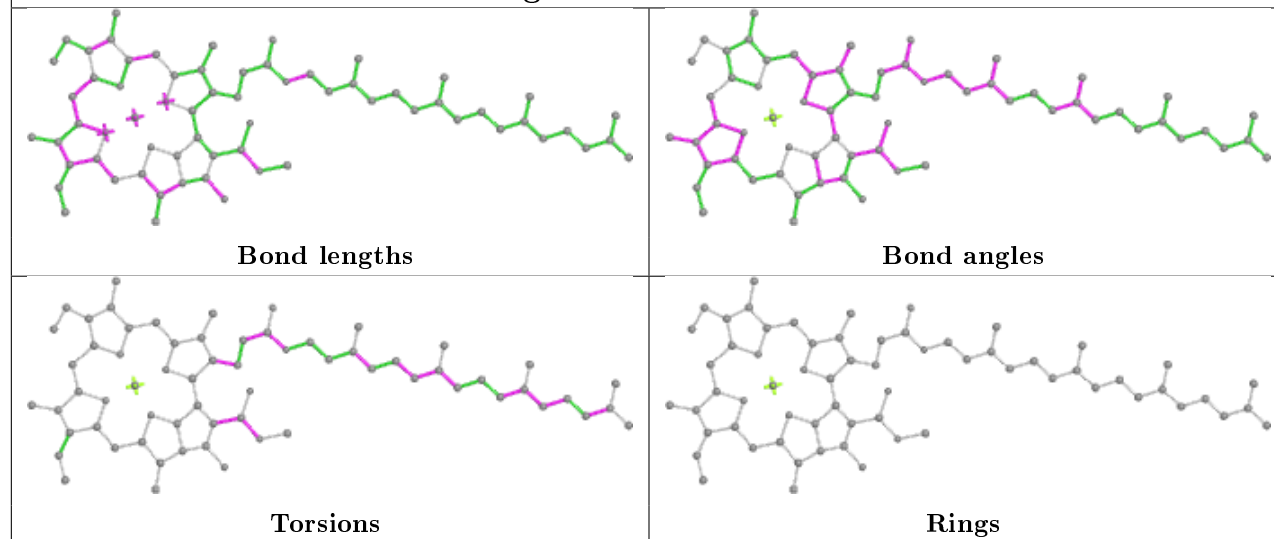
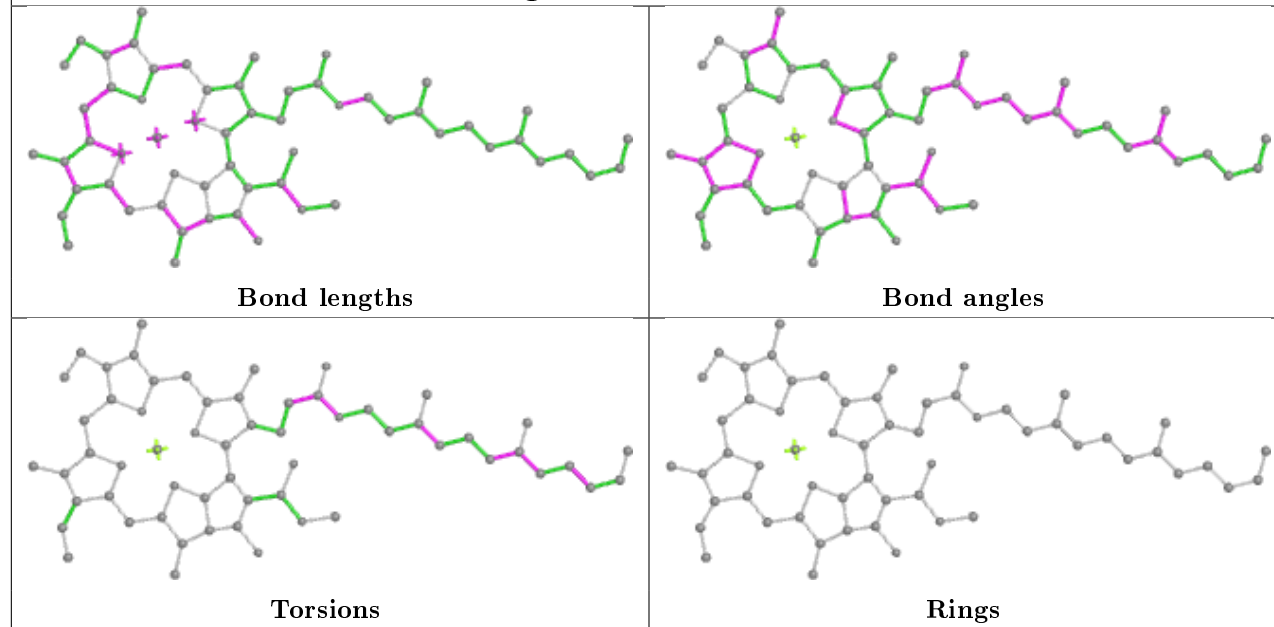


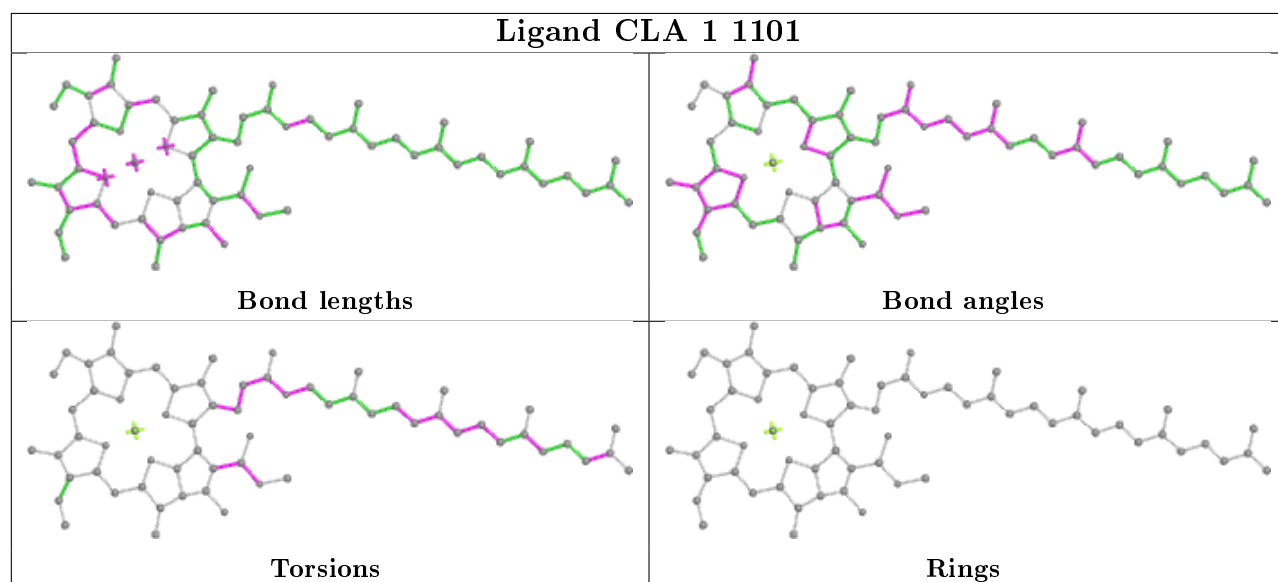
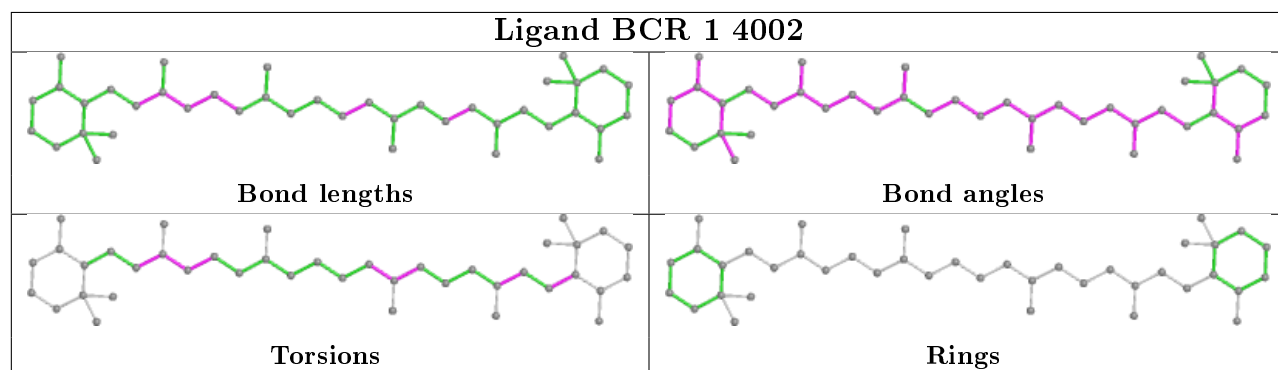
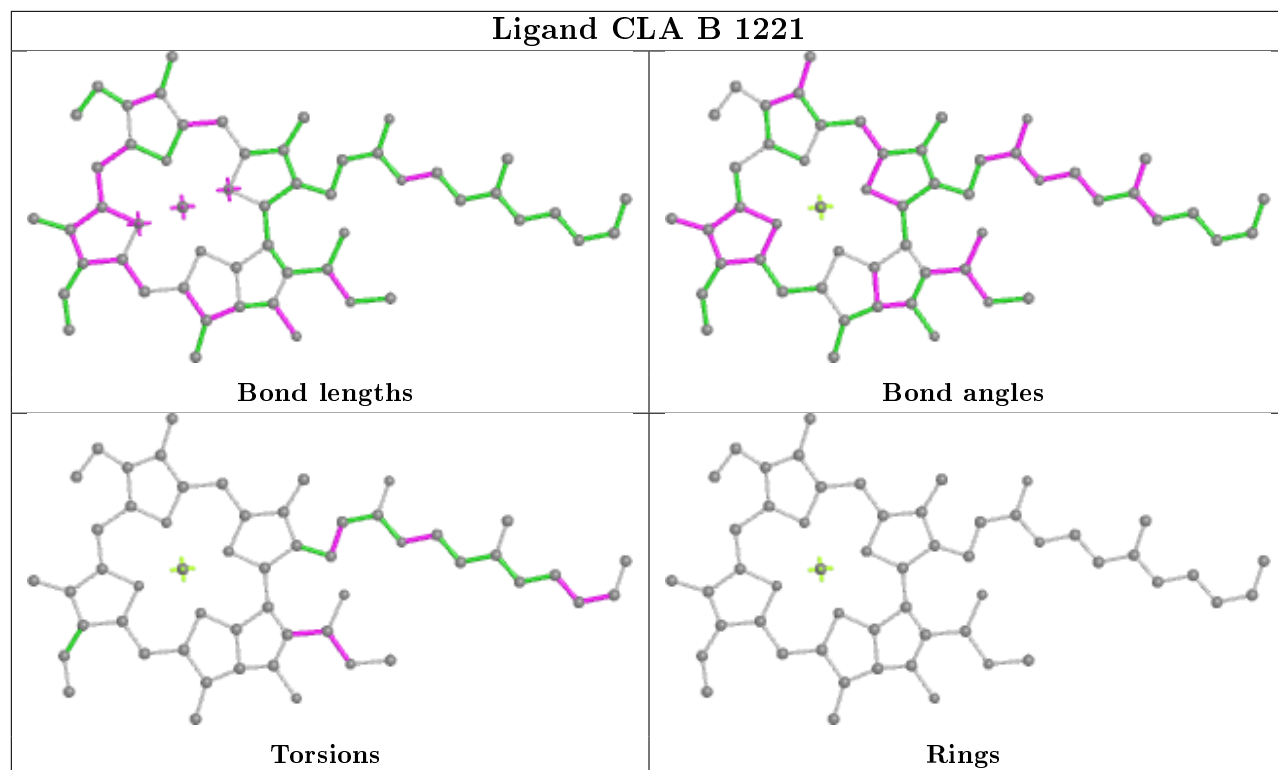
Ligand CLA A 1137

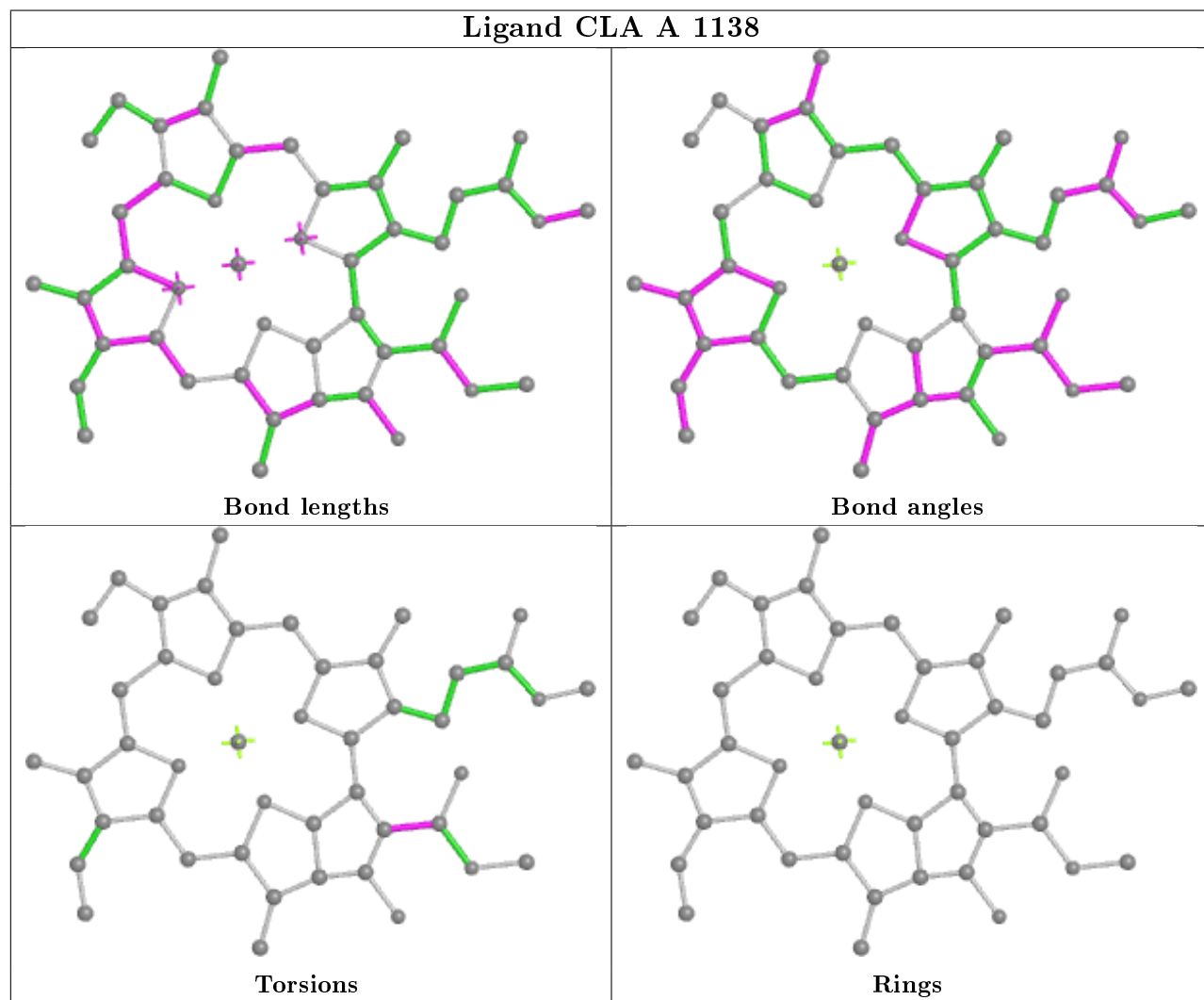
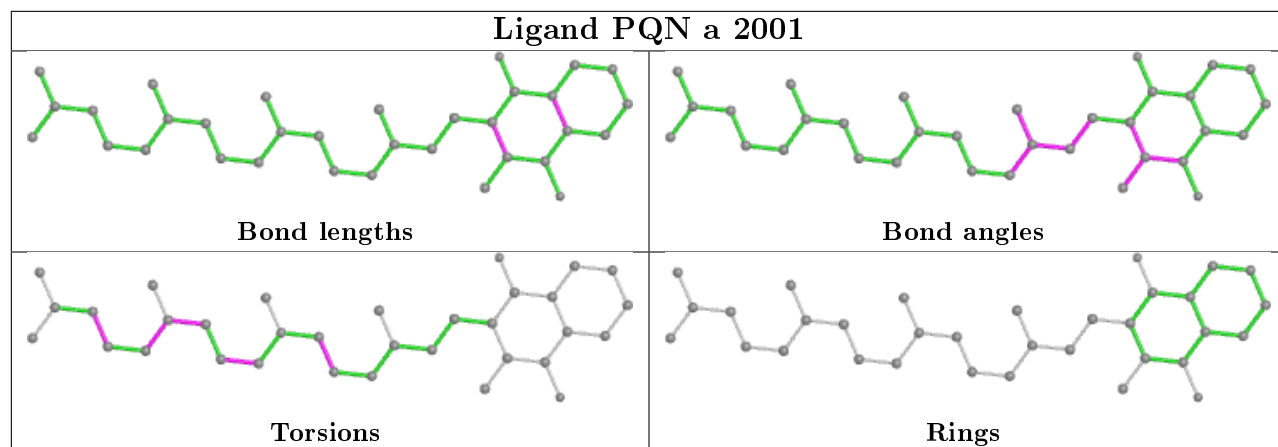


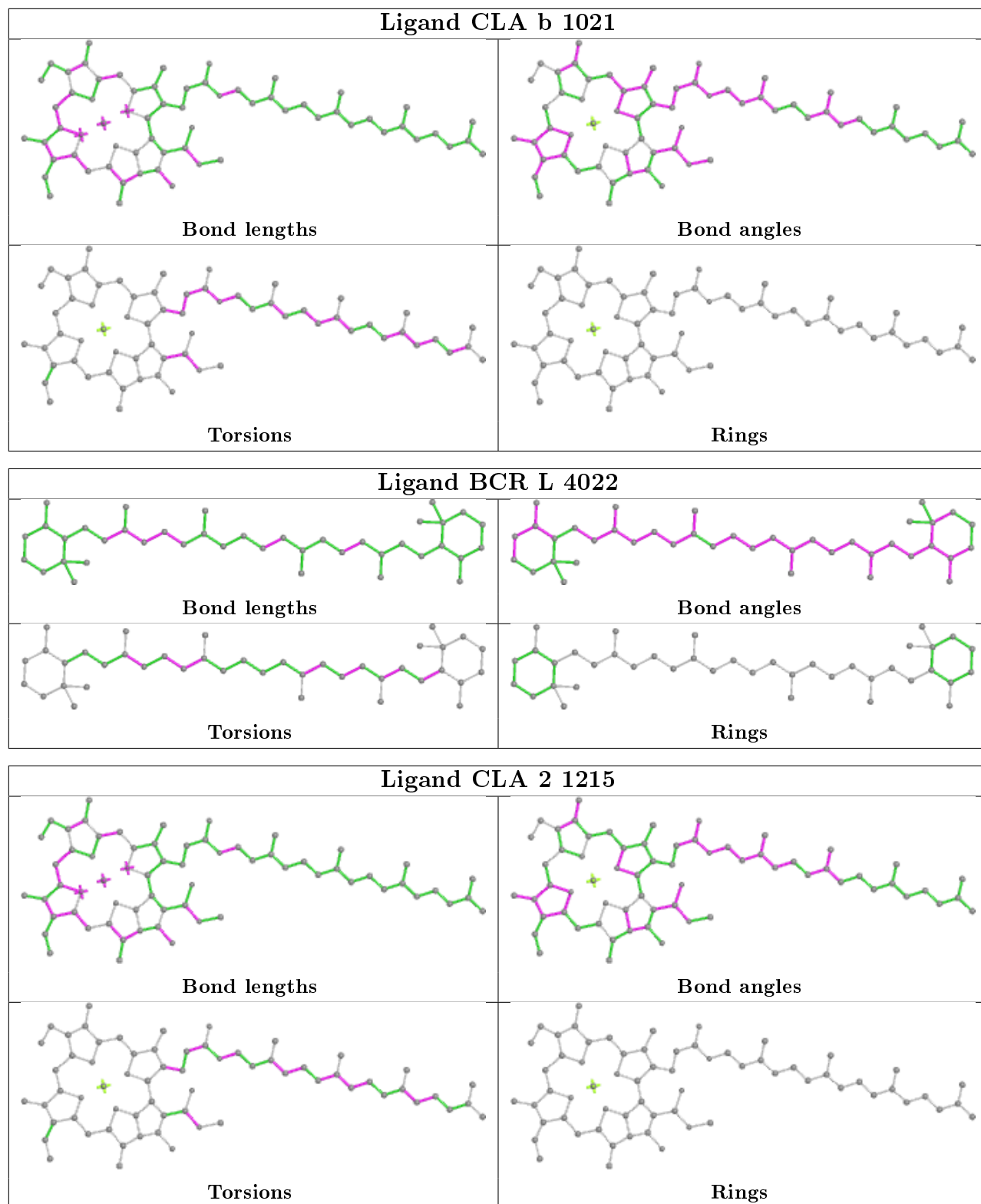
Ligand CLA 1 1125

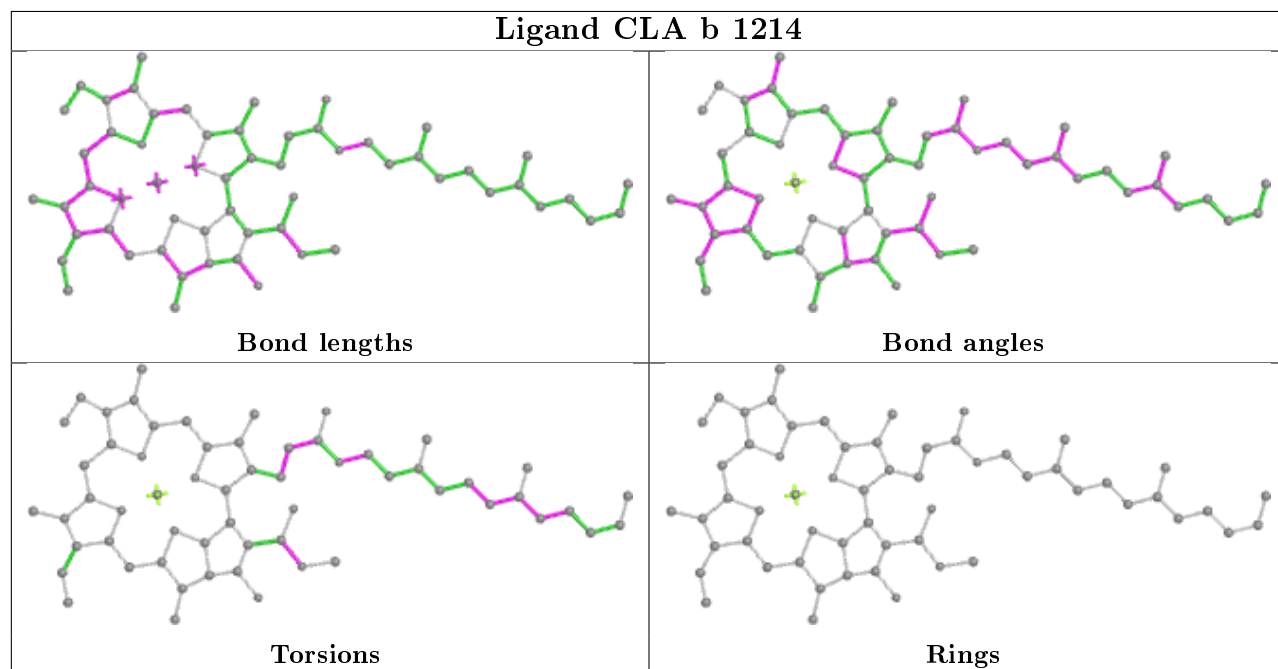
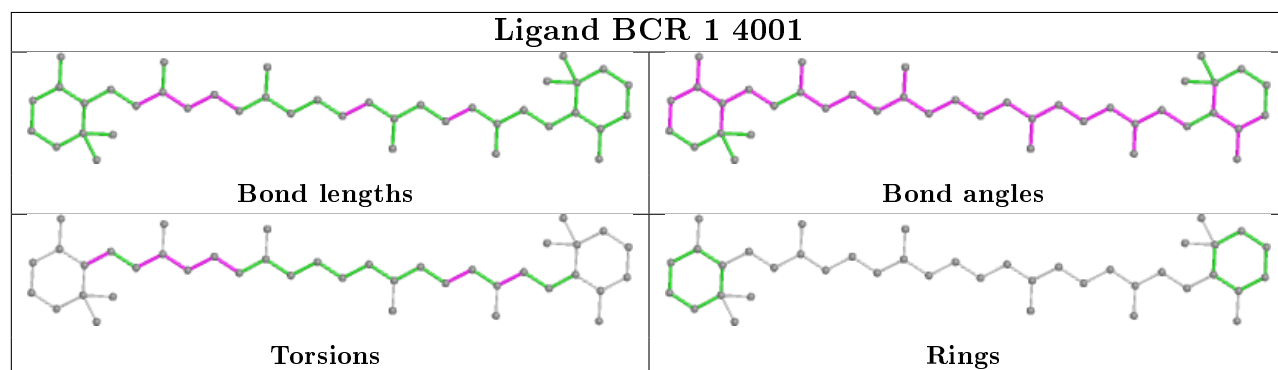
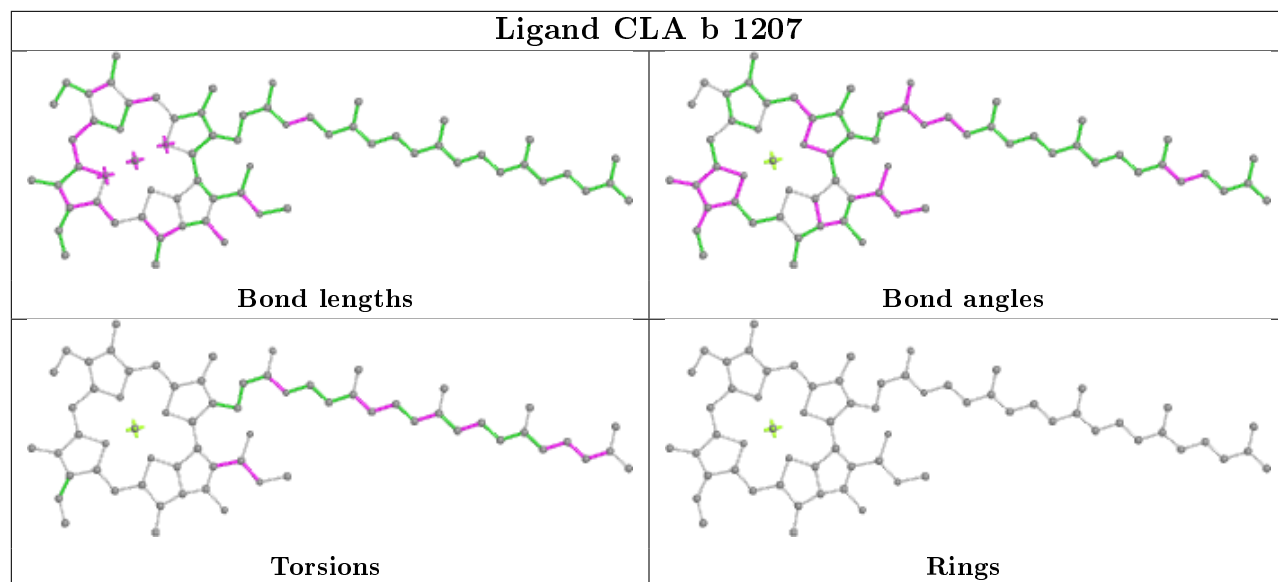


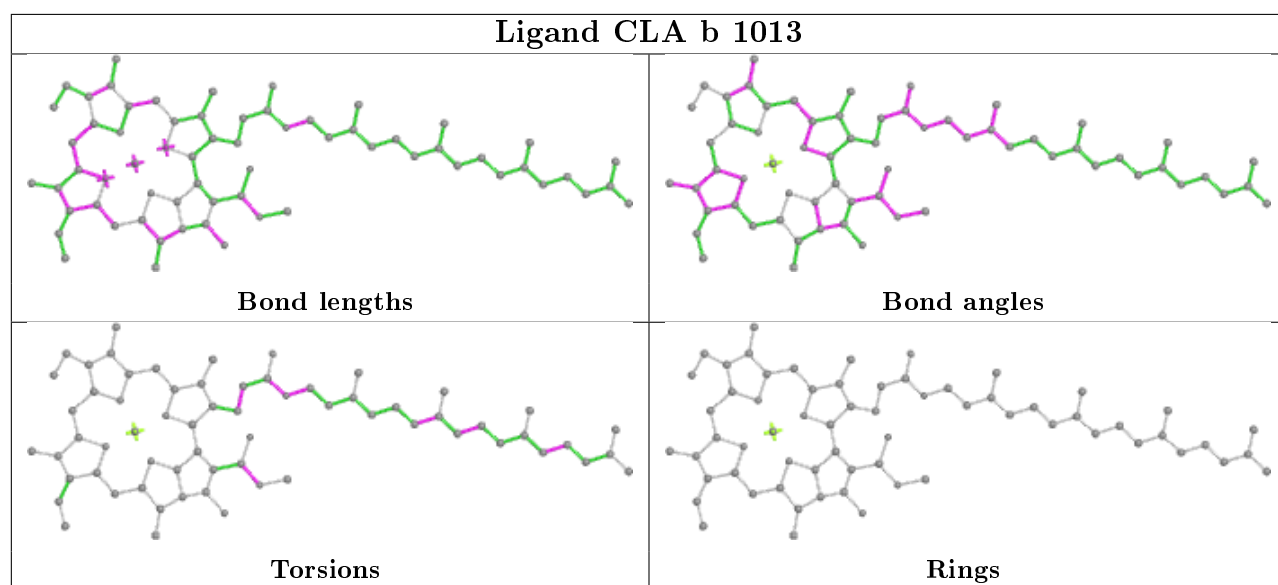
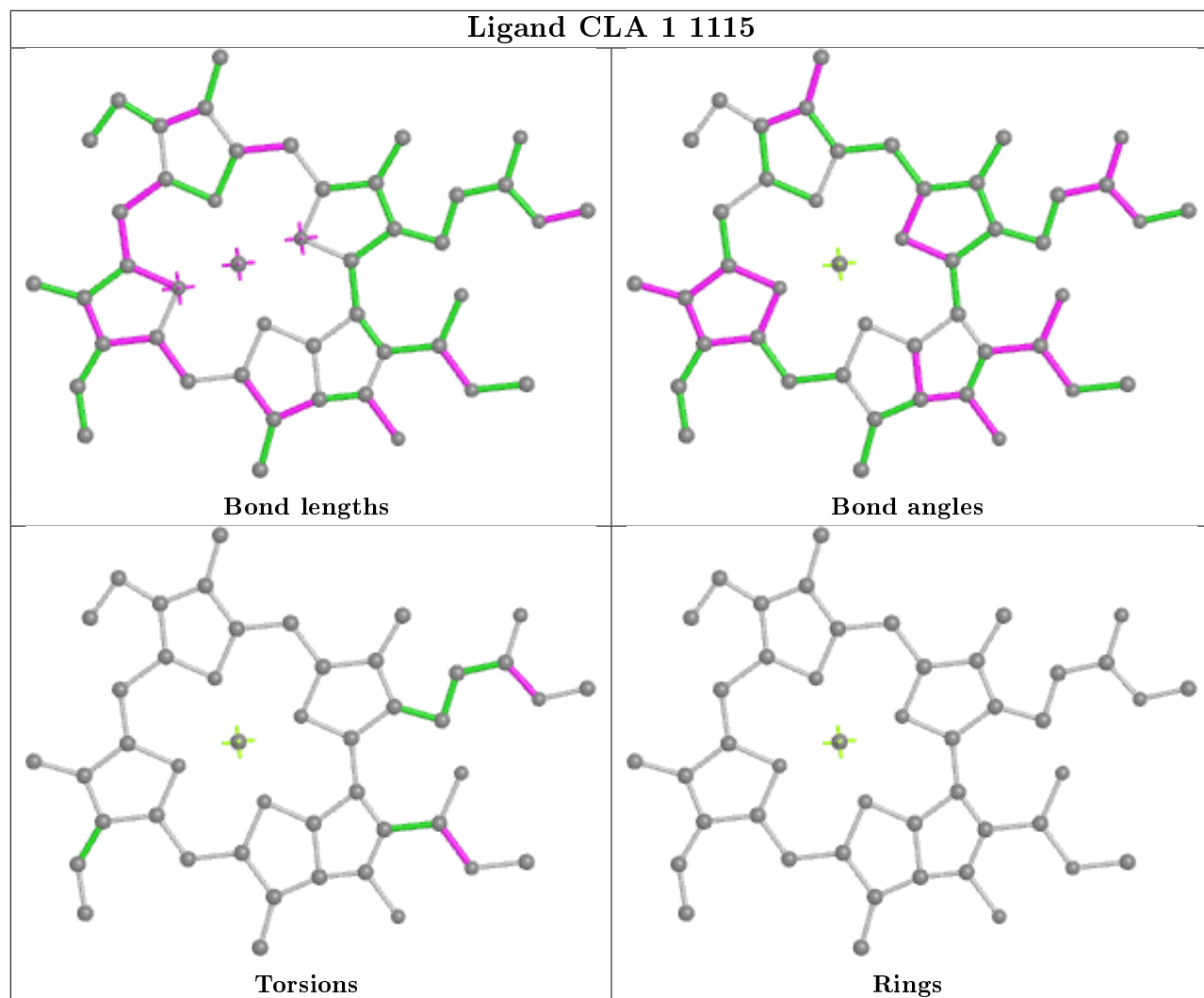
Ligand CLA B 1021**Ligand CLA A 1122**

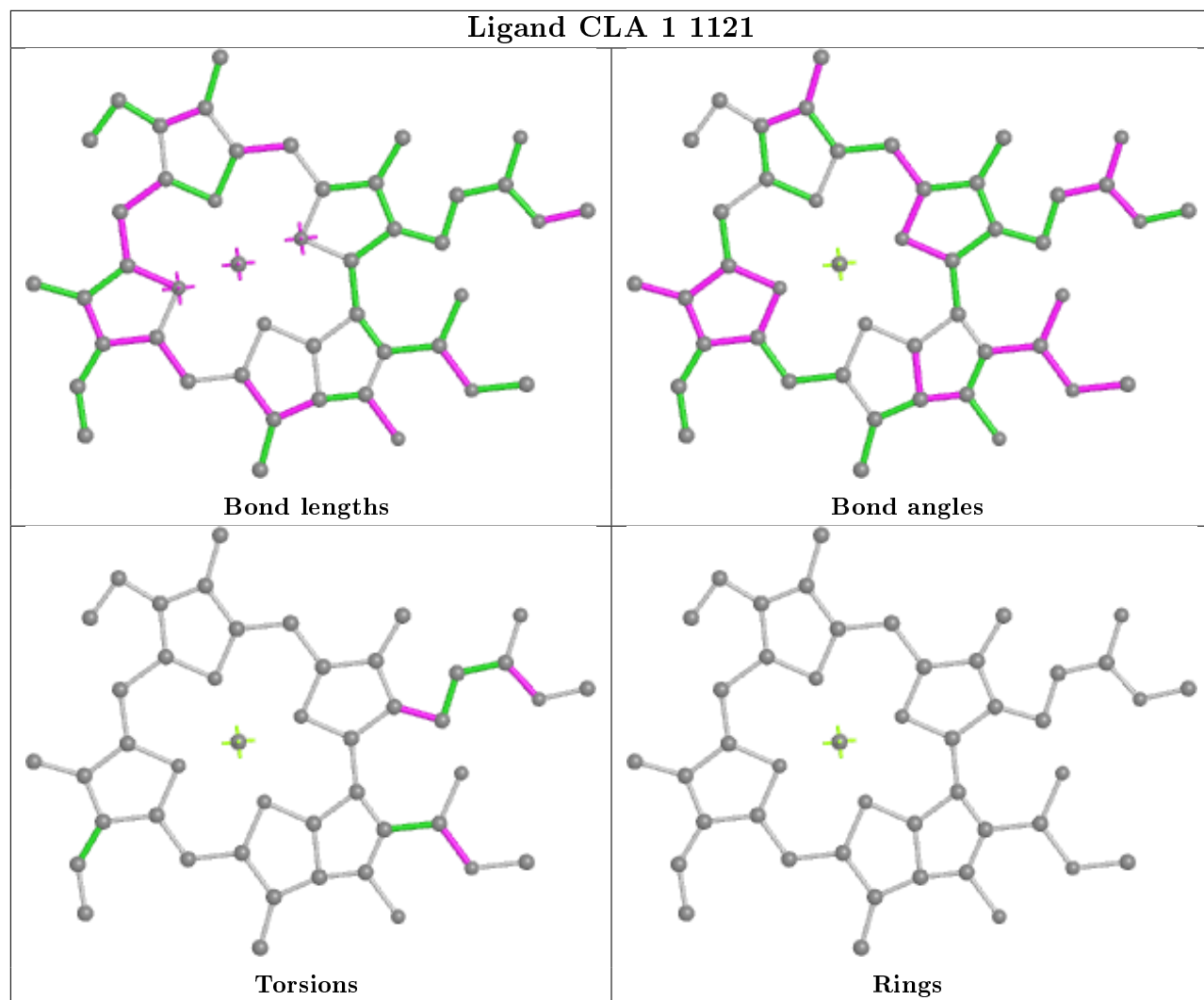


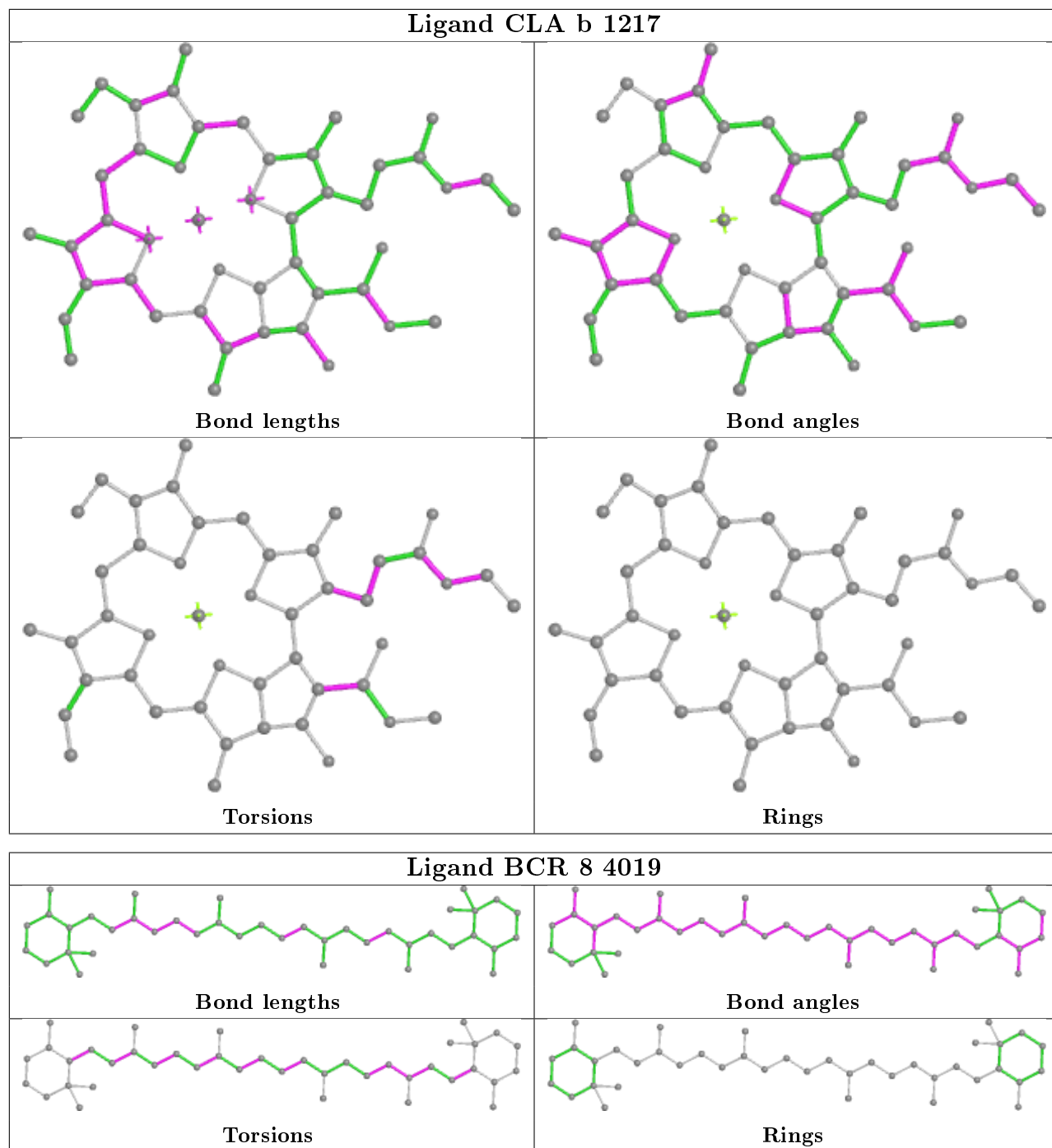


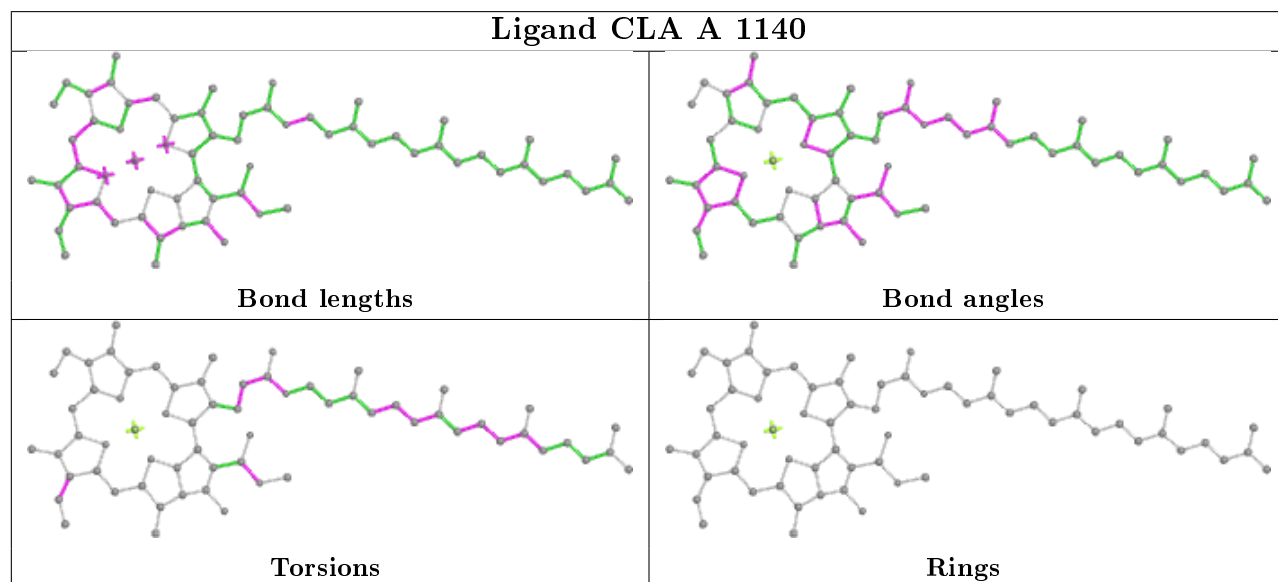
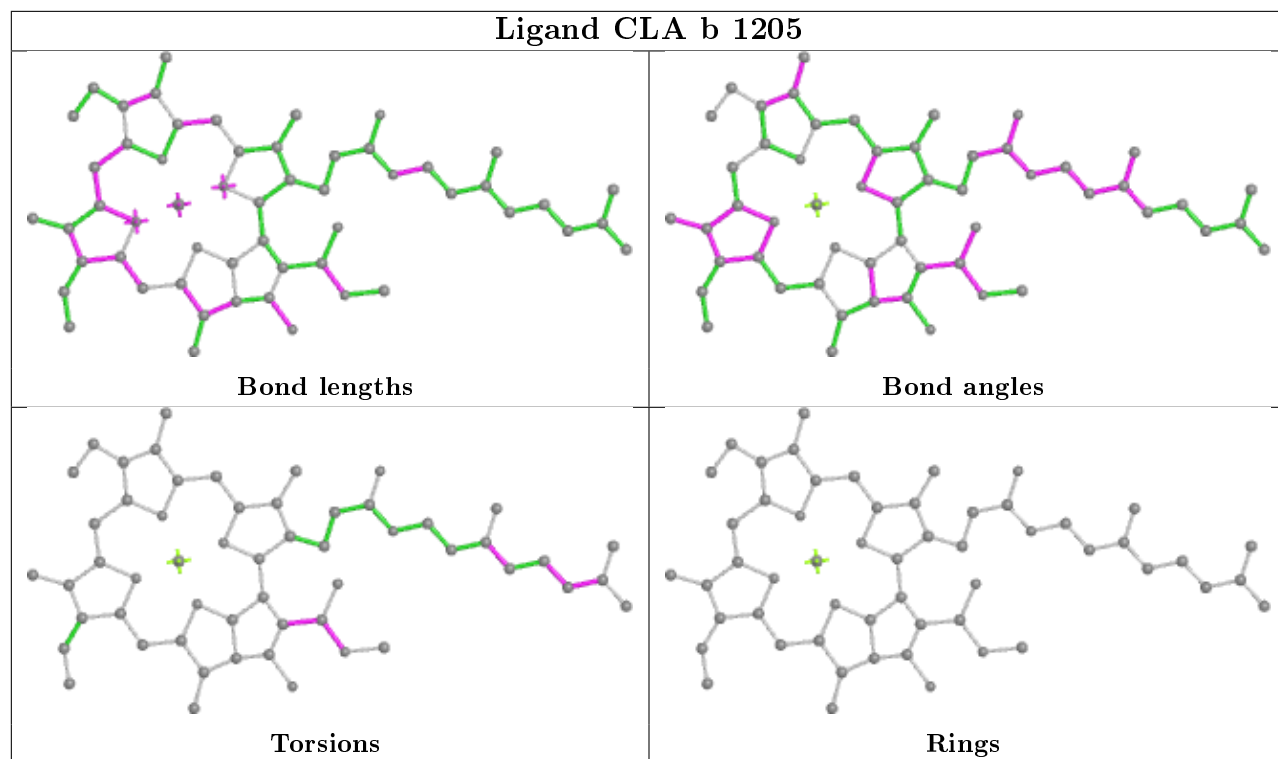


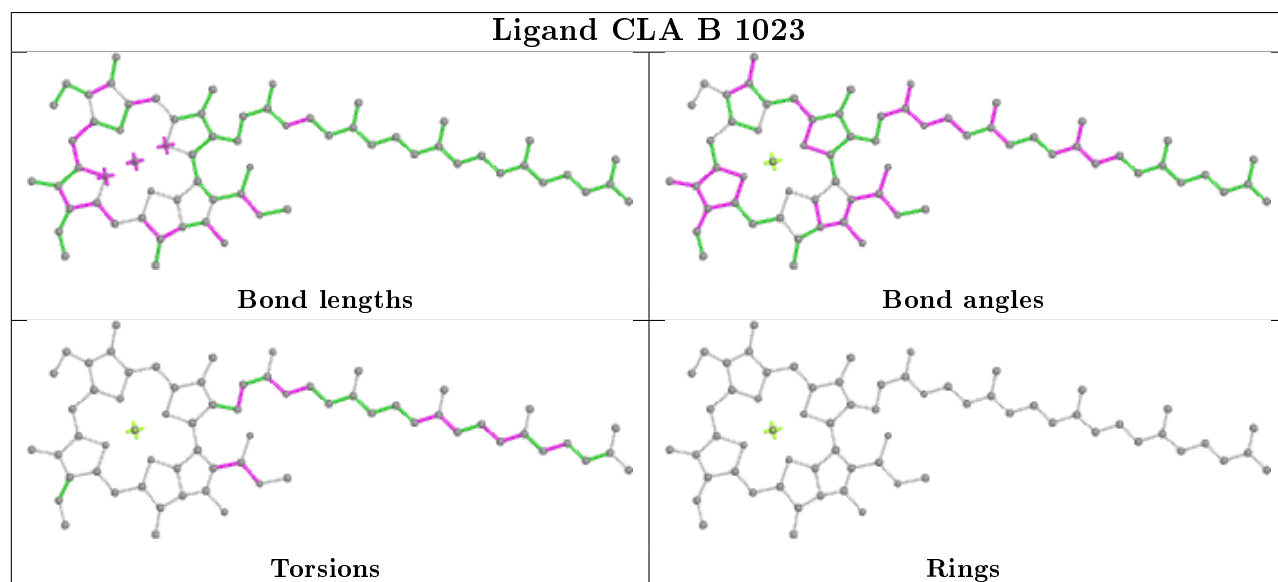
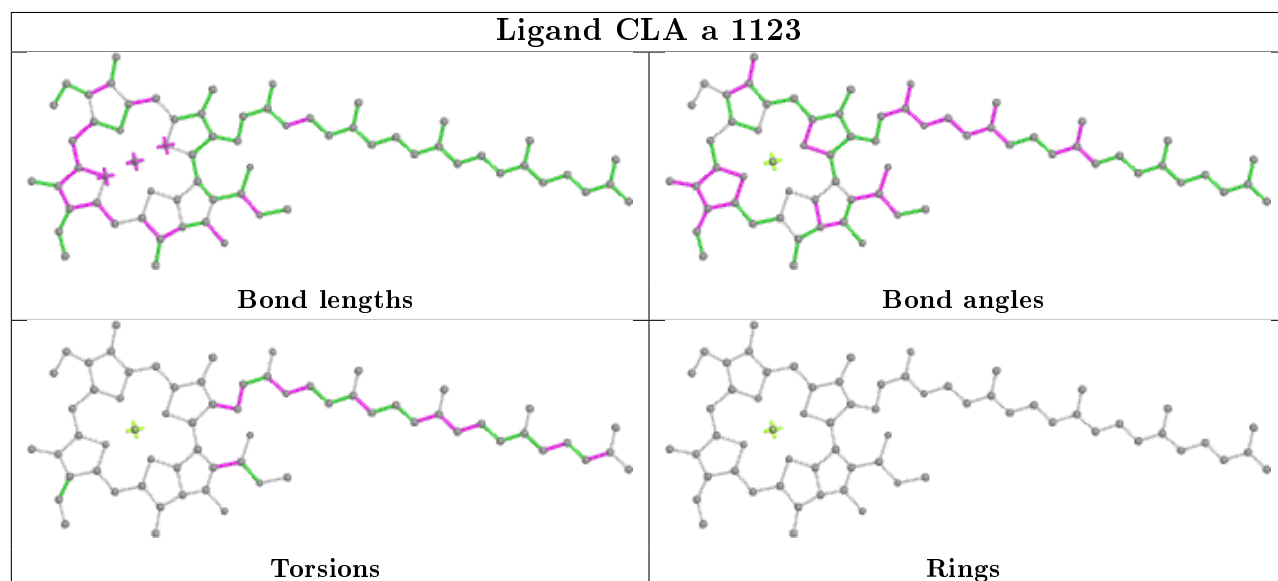
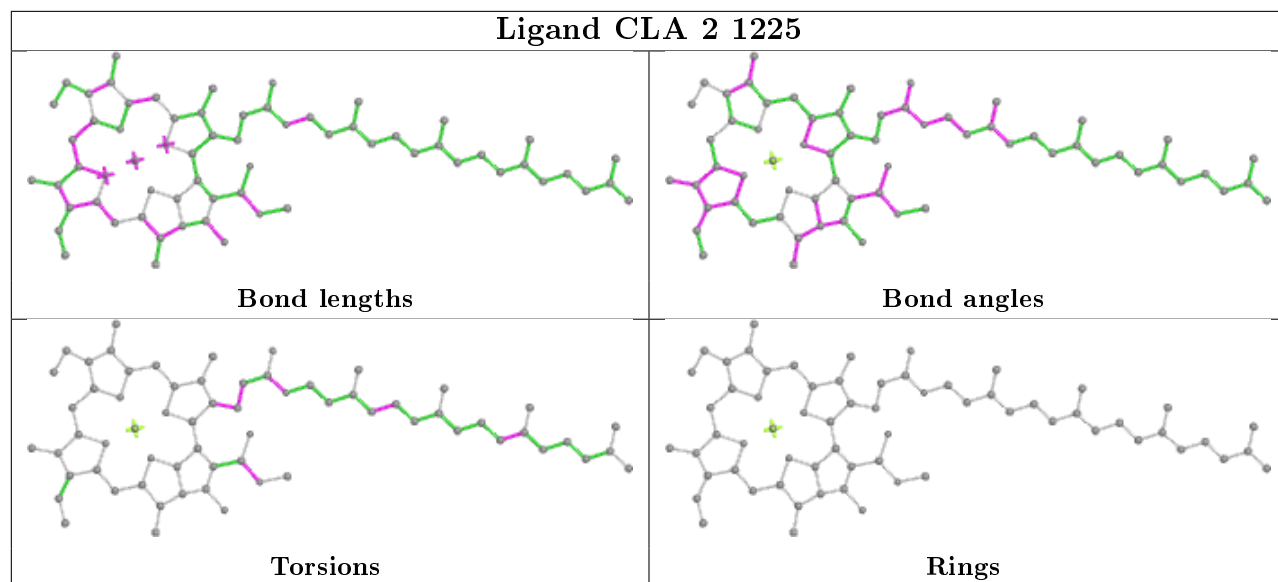


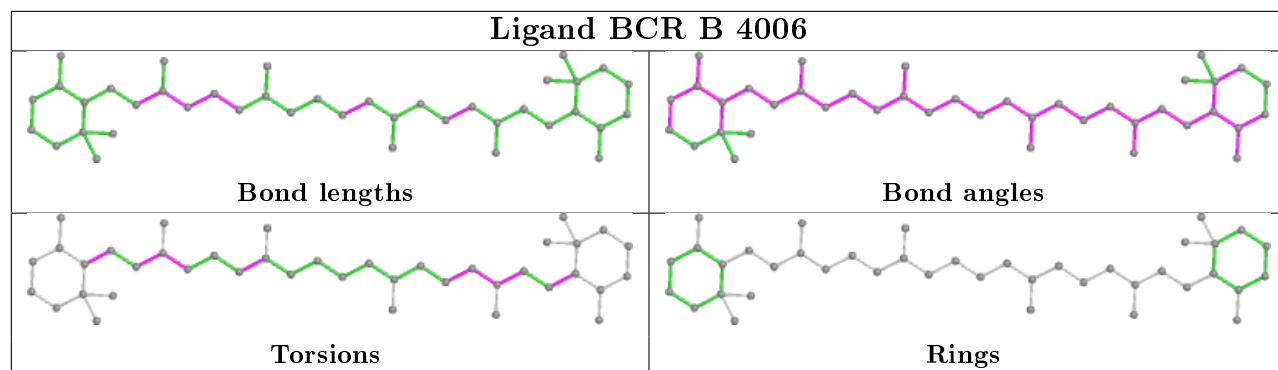
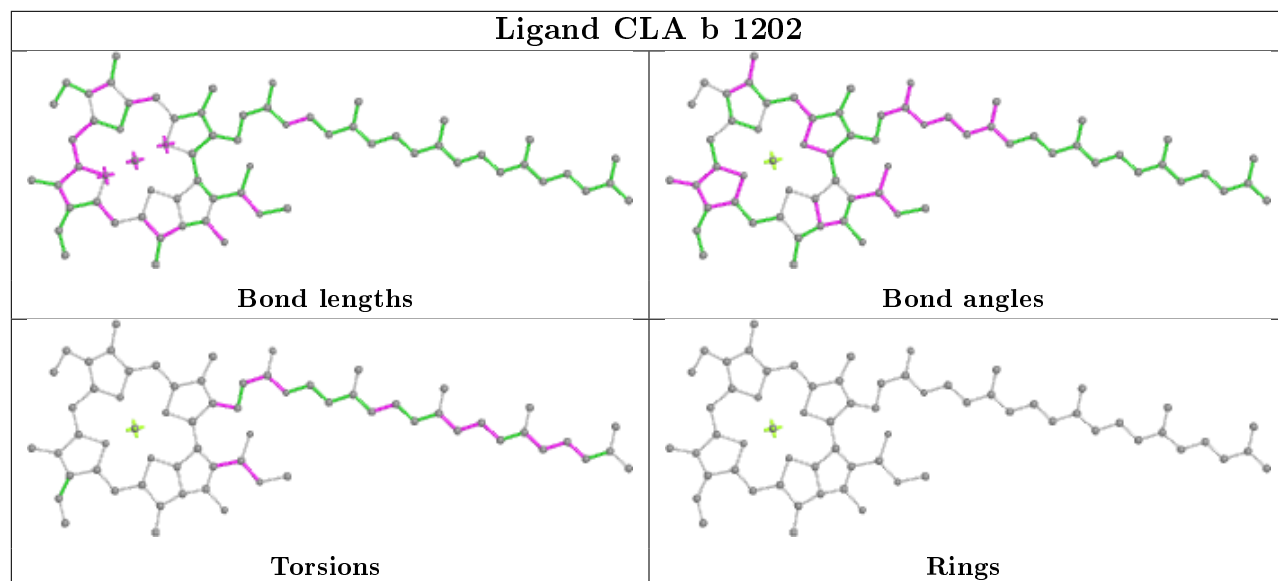
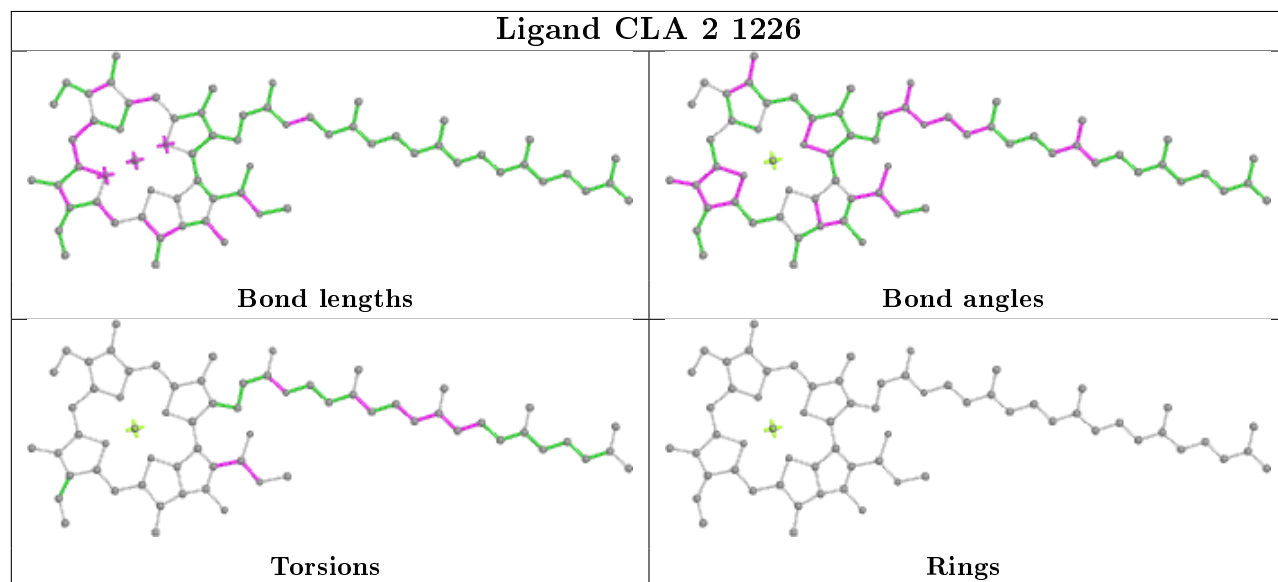


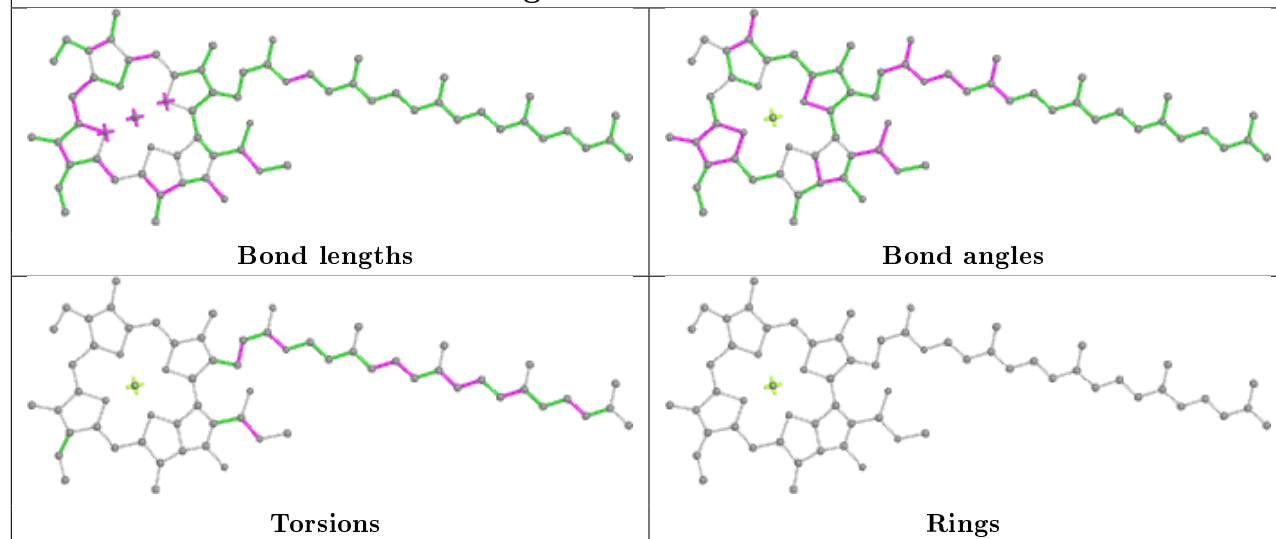
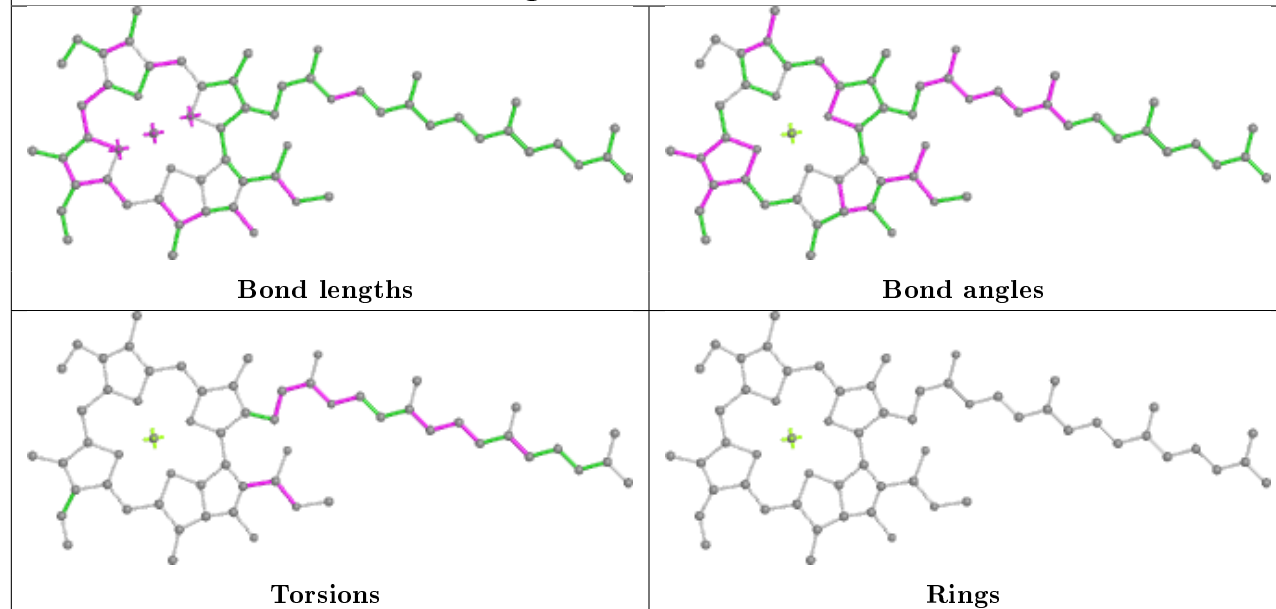




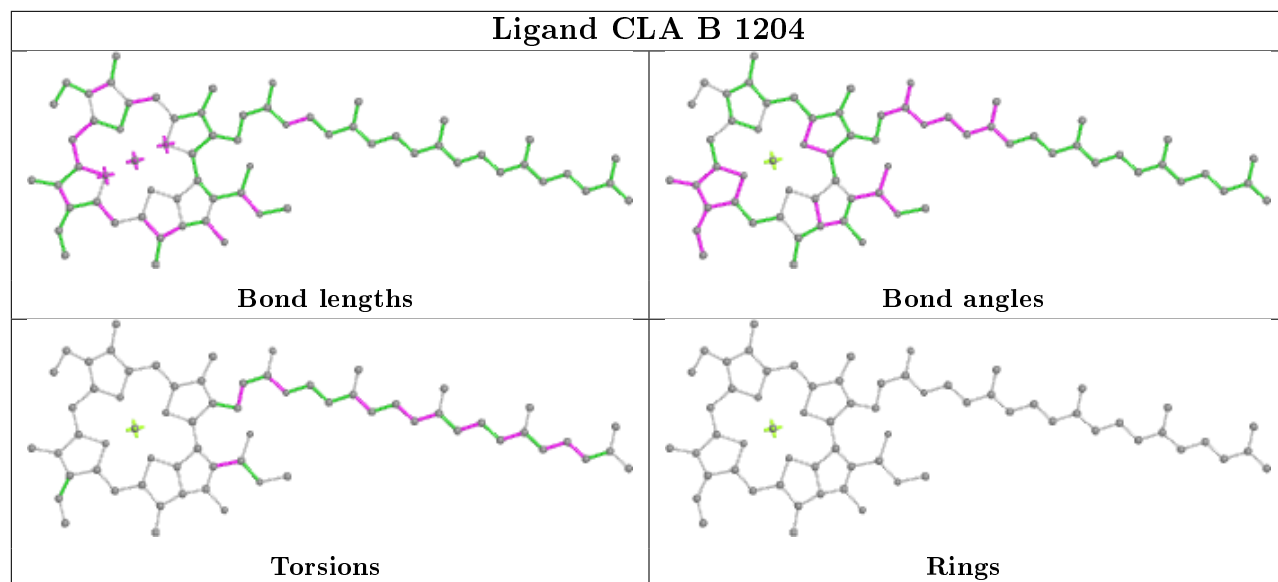




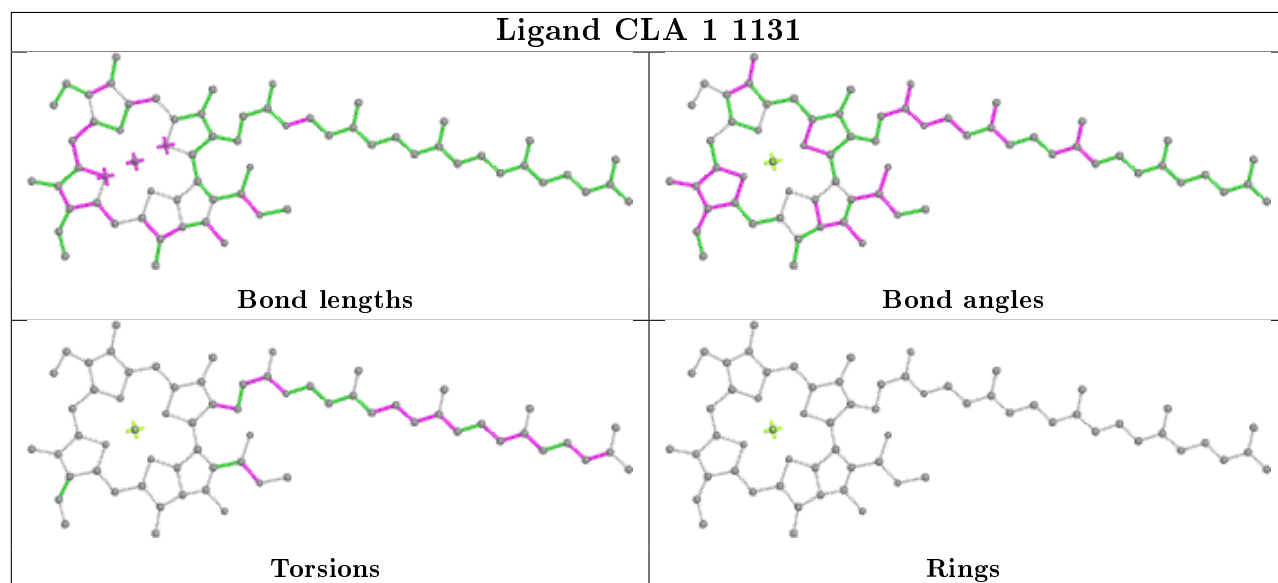
Ligand BCR B 4006**Ligand CLA b 1202****Ligand CLA 2 1226**

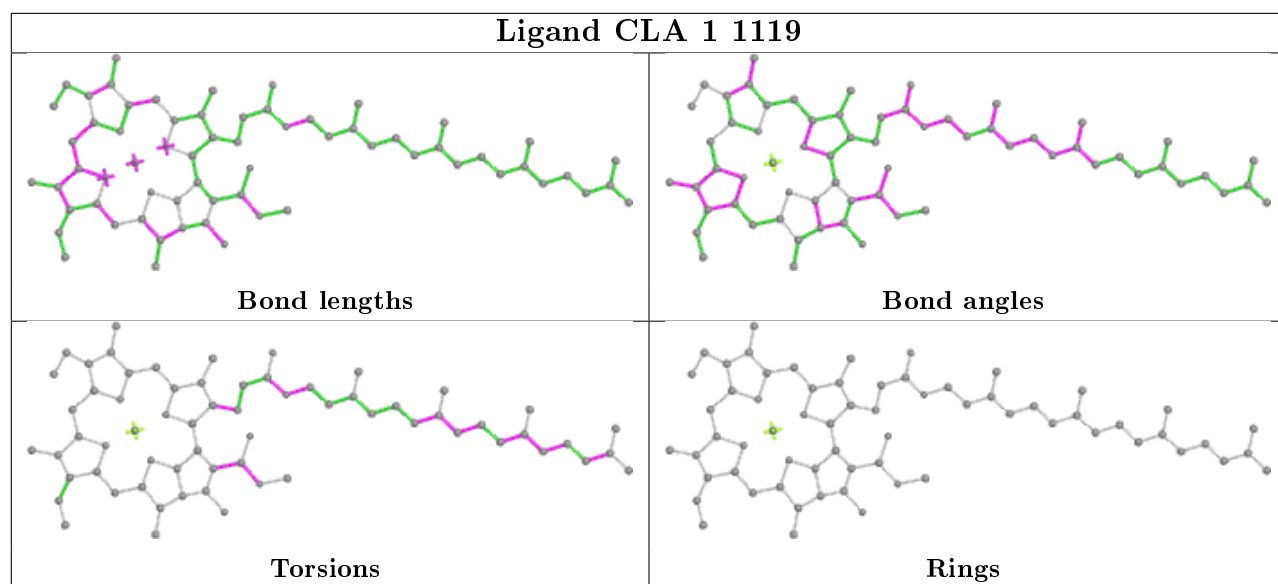
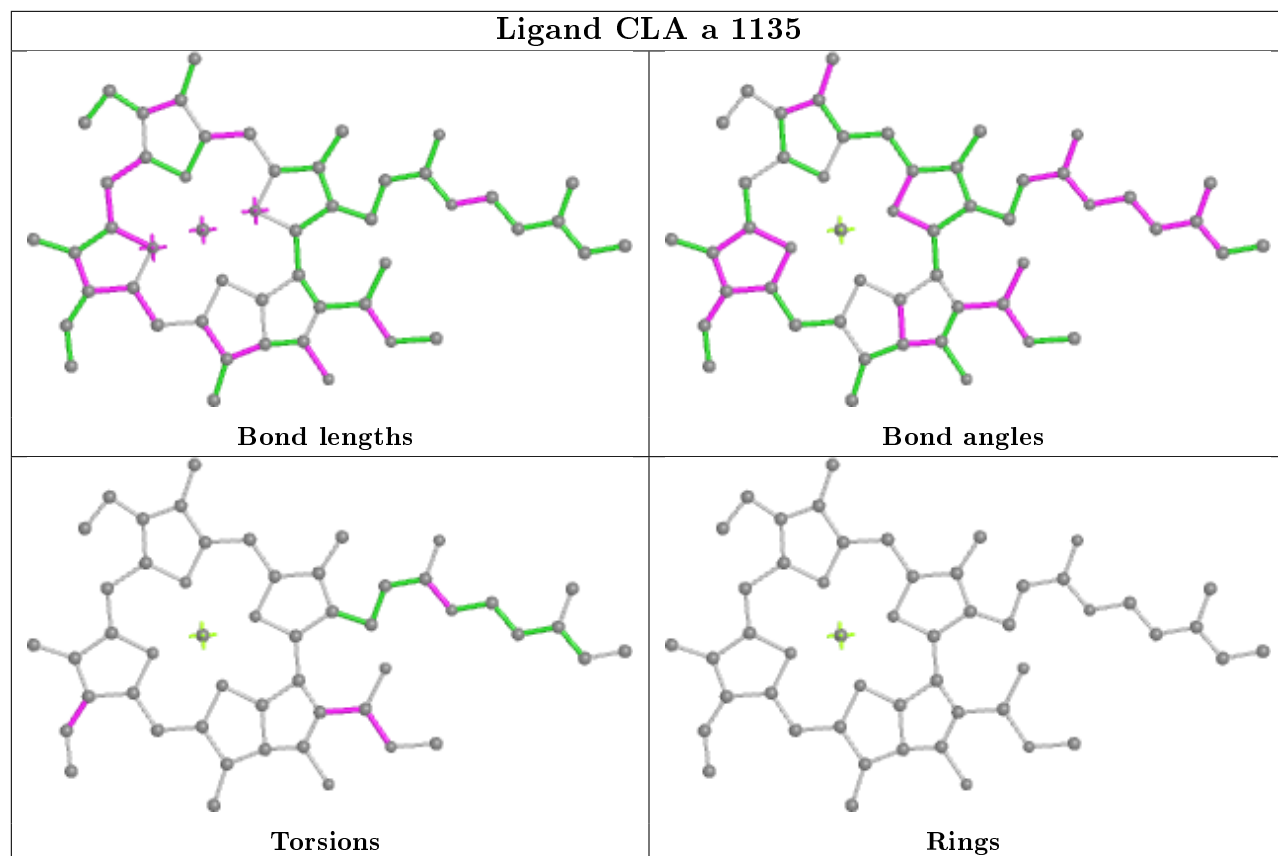
Ligand CLA B 1238**Ligand CLA A 1111**

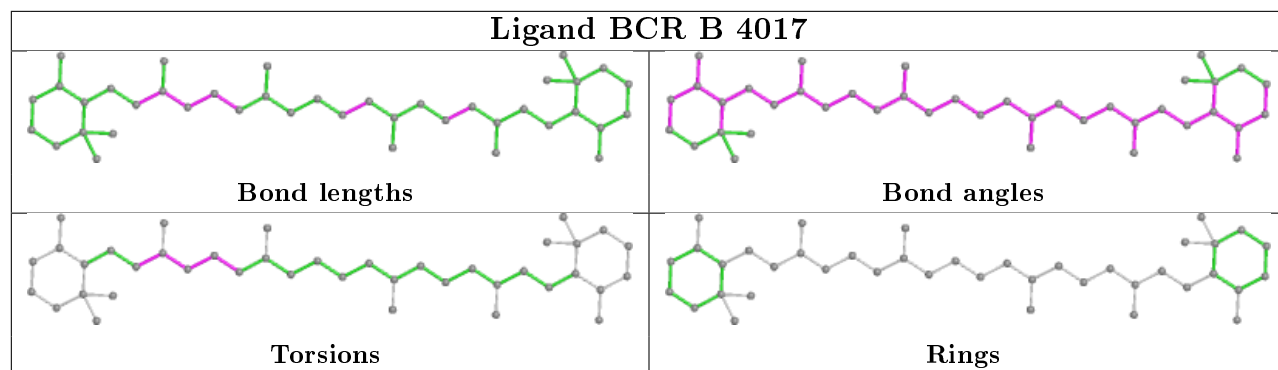
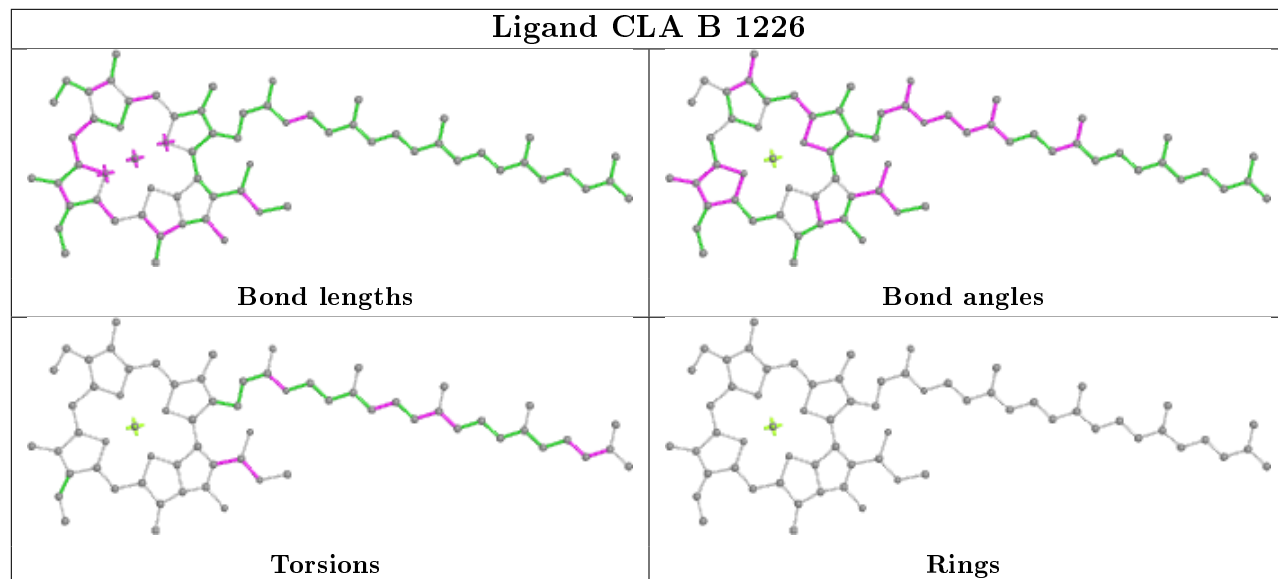
Ligand CLA B 1204



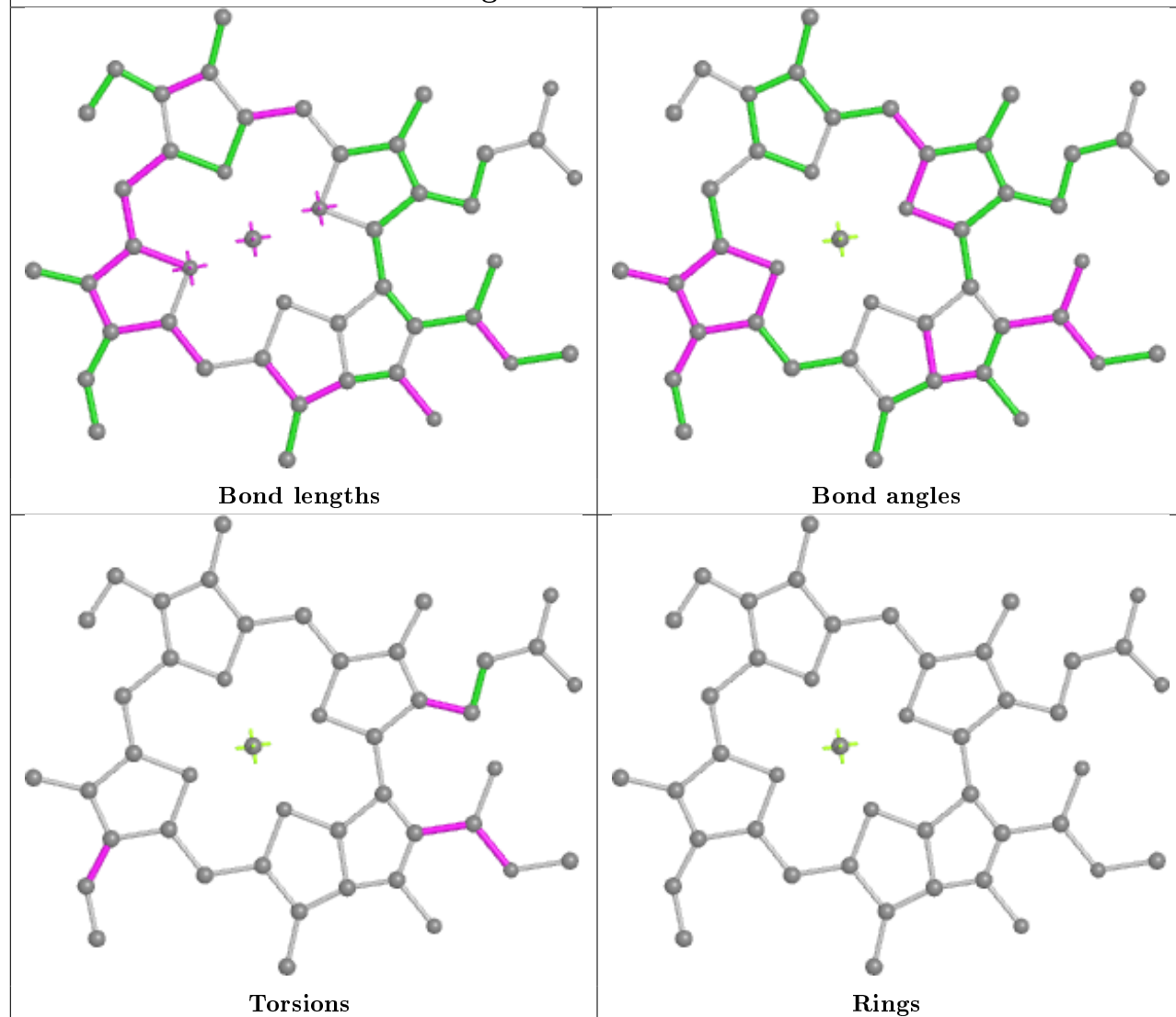
Ligand CLA 1 1131



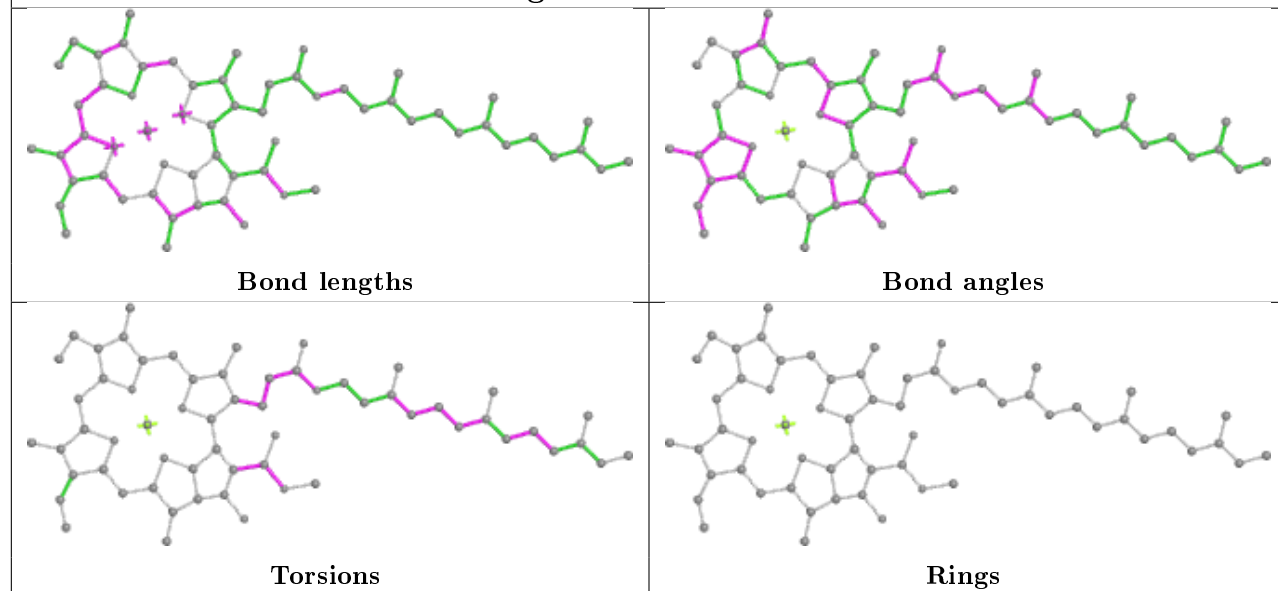


Ligand BCR B 4017**Ligand CLA B 1226**

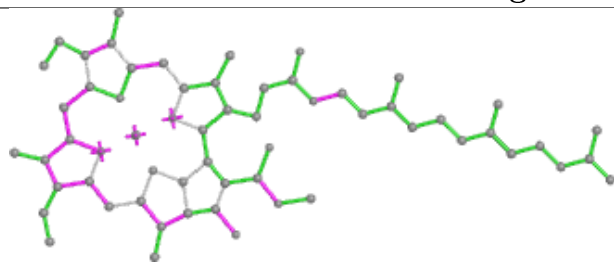
Ligand CLA A 1112



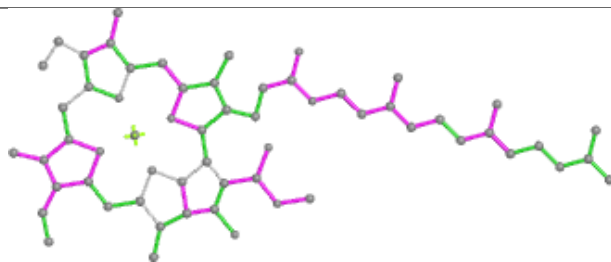
Ligand CLA 1 1118



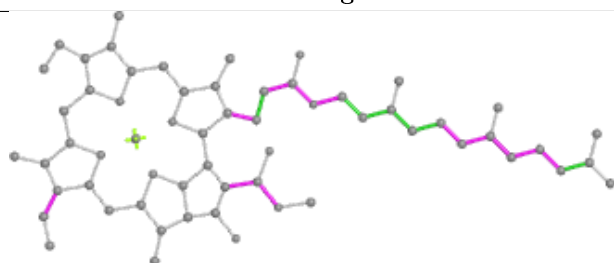
Ligand CLA 2 1235



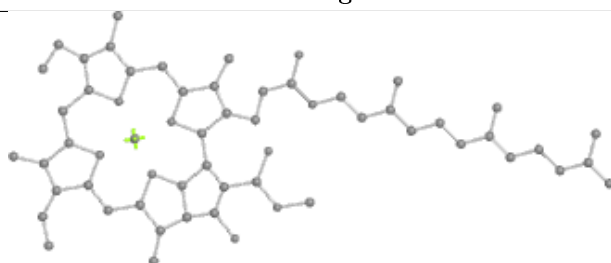
Bond lengths



Bond angles

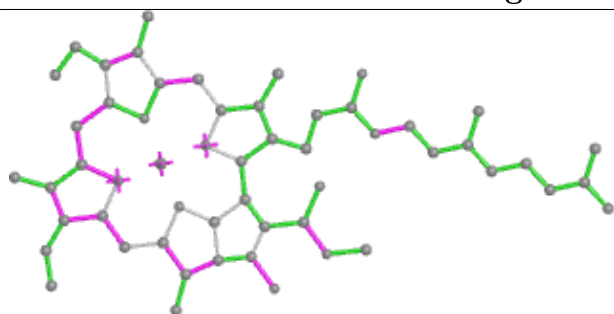


Torsions

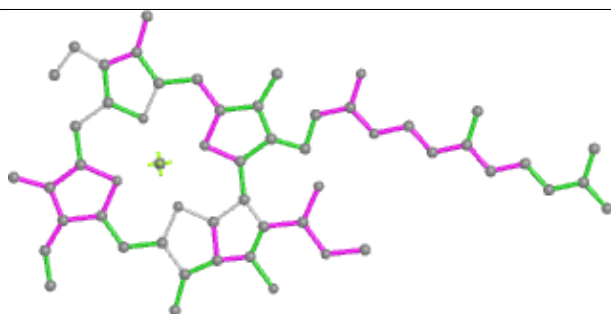


Rings

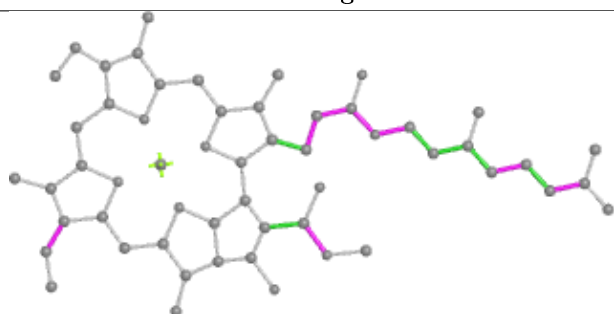
Ligand CLA A 1124



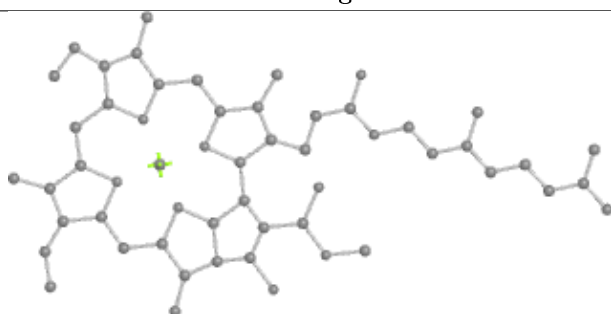
Bond lengths



Bond angles

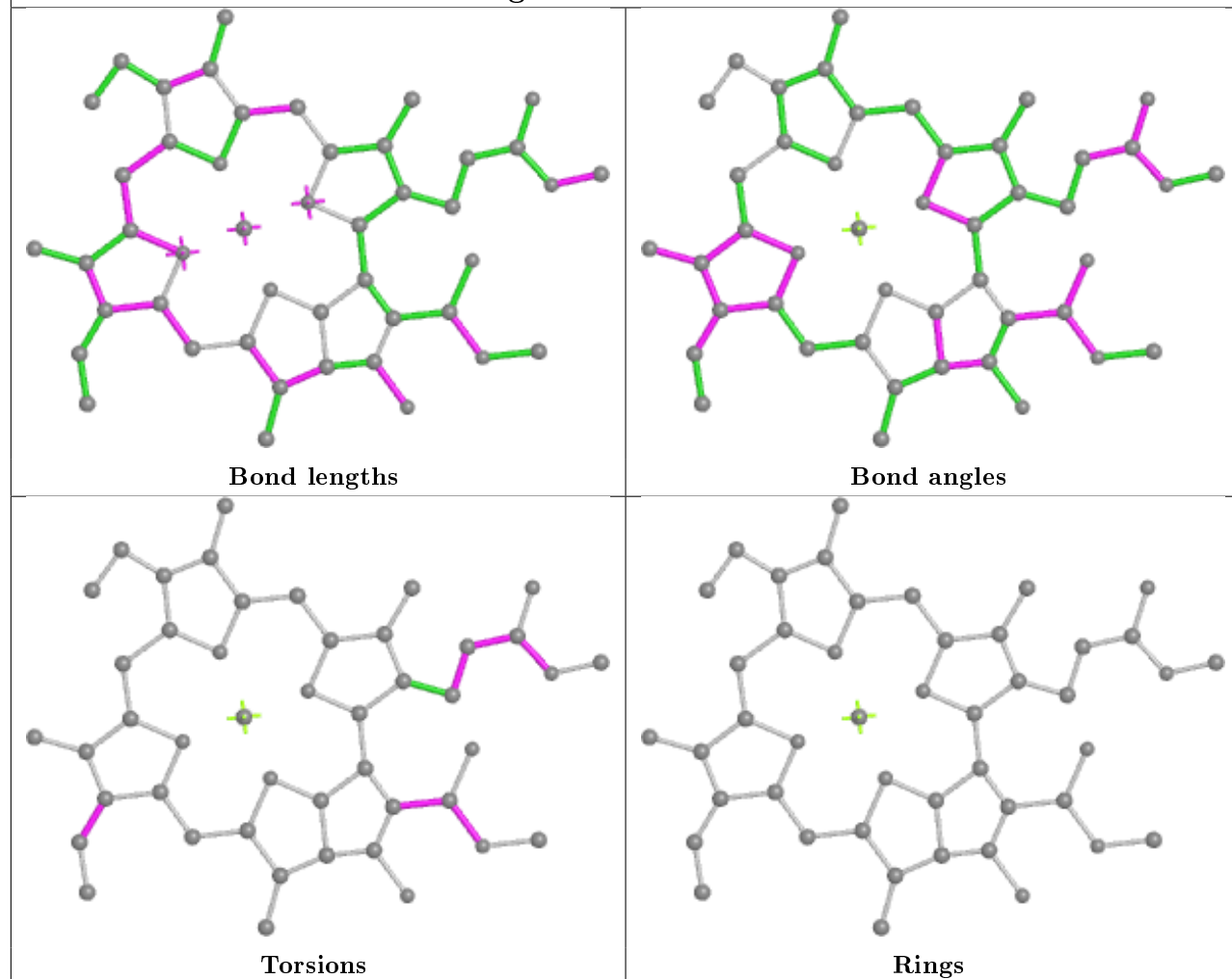


Torsions

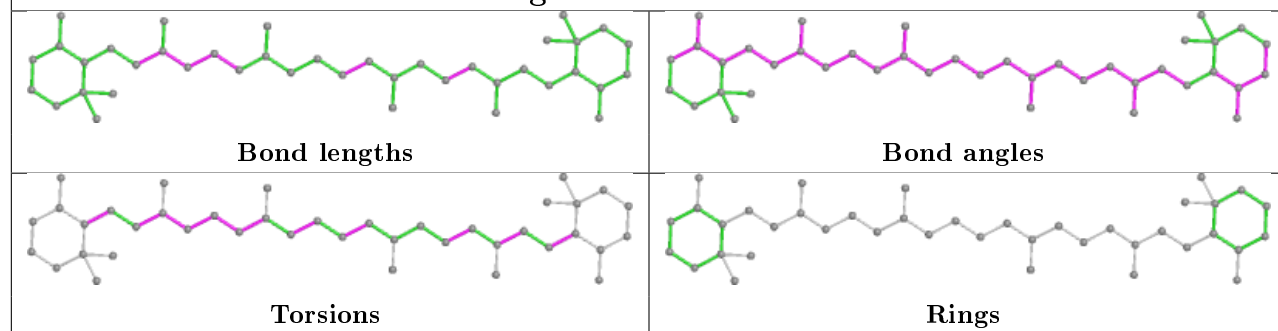


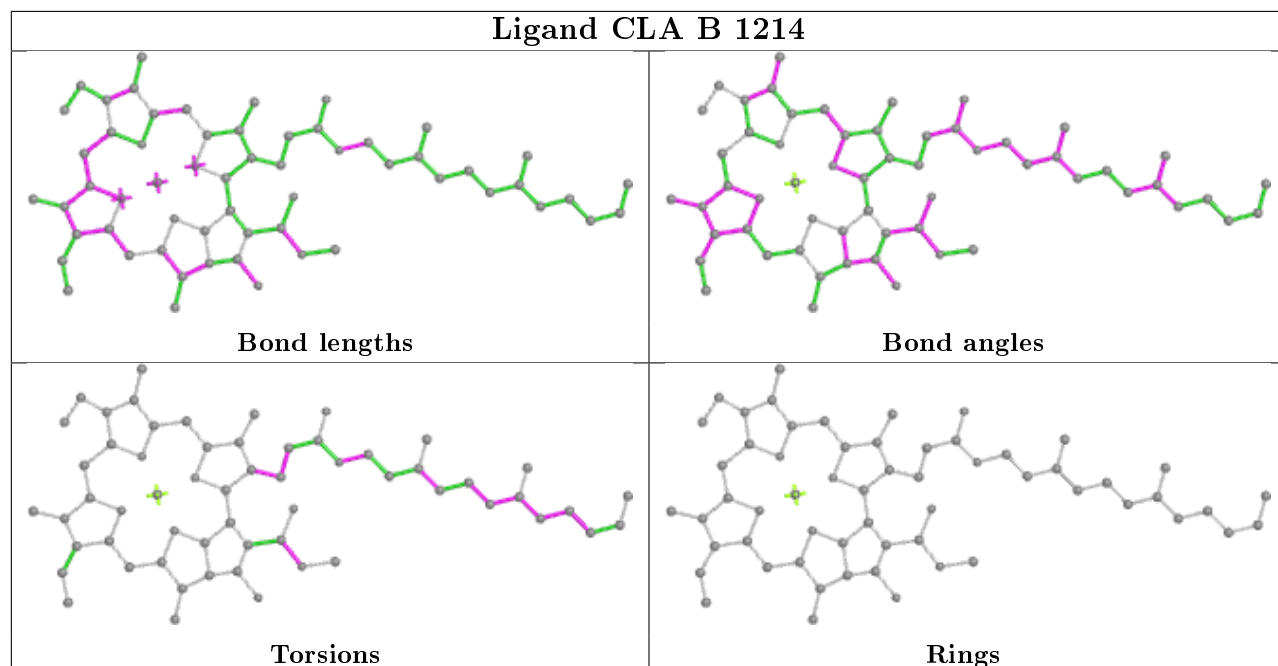
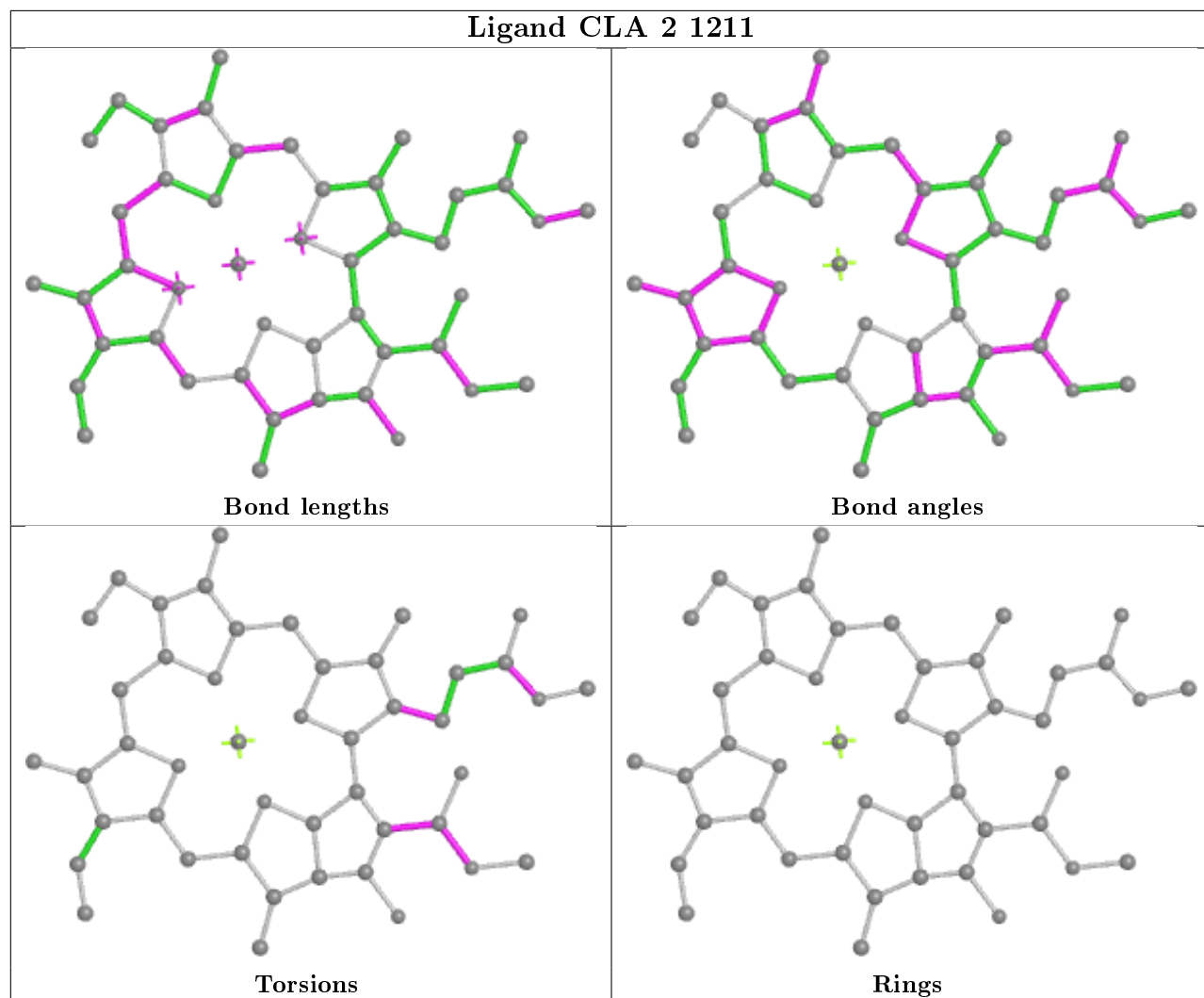
Rings

Ligand CLA 1 1136

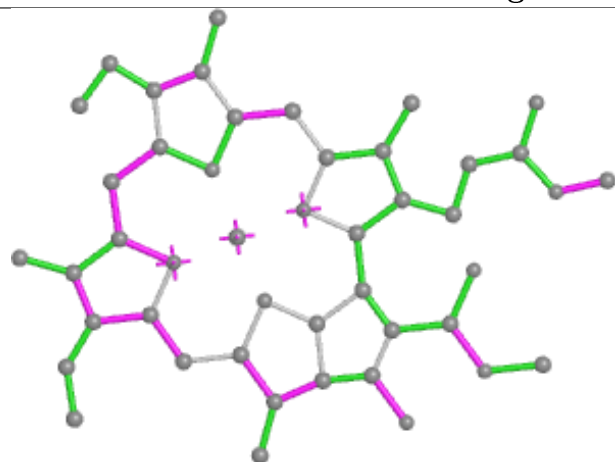


Ligand BCR 1 4019

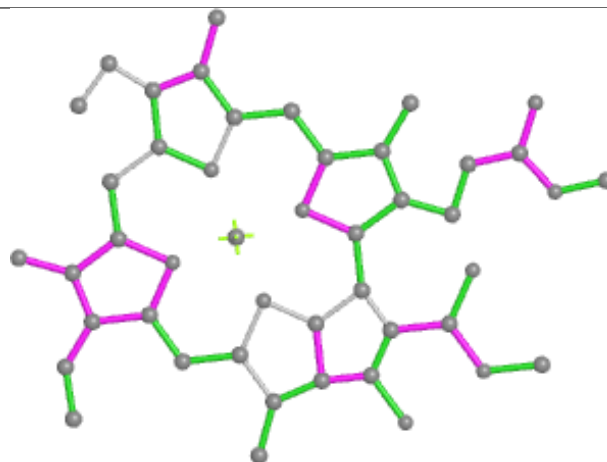




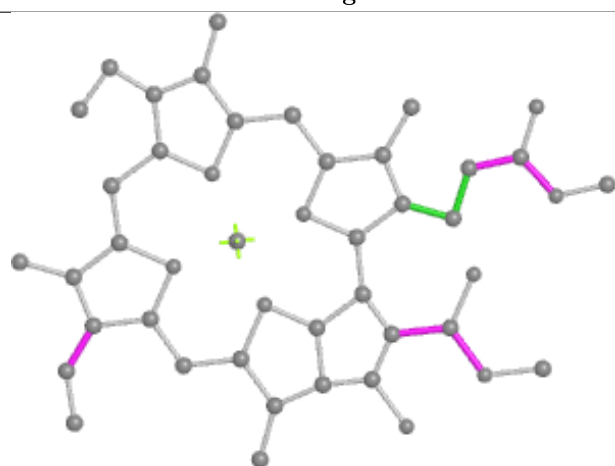
Ligand CLA B 1220



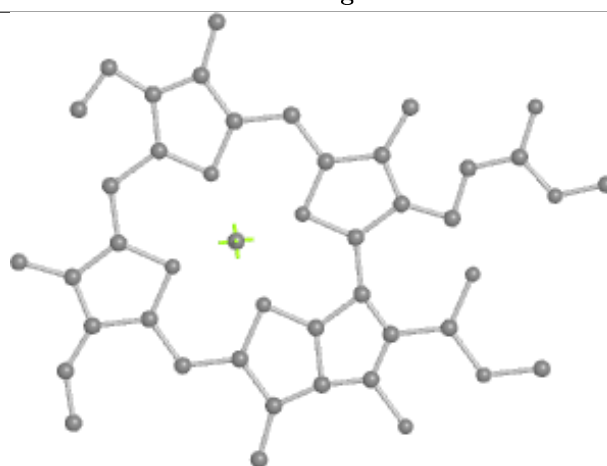
Bond lengths



Bond angles

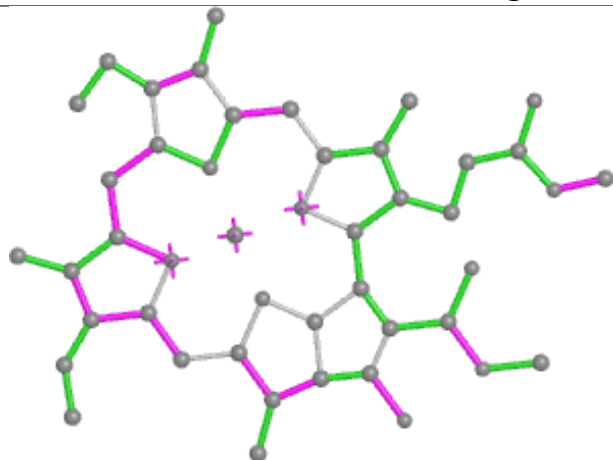


Torsions

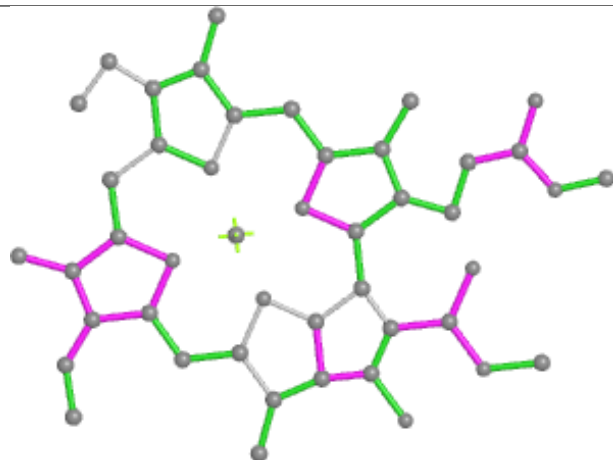


Rings

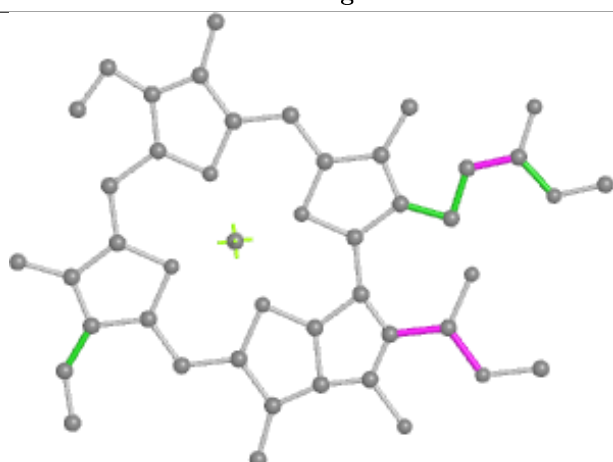
Ligand CLA A 1136



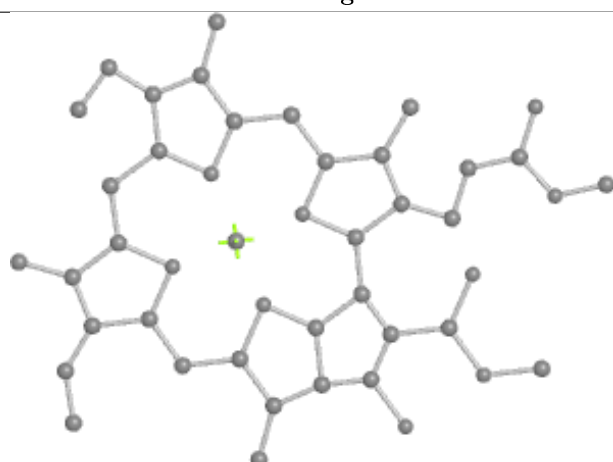
Bond lengths



Bond angles

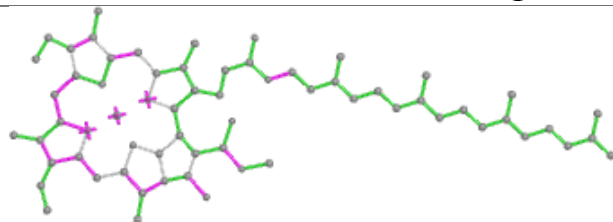


Torsions

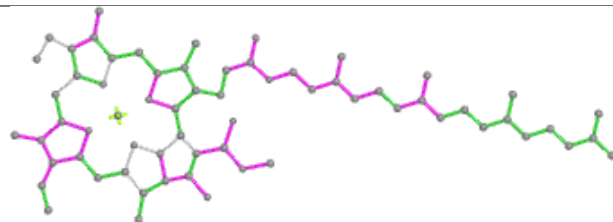


Rings

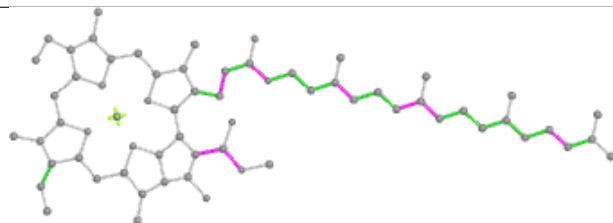
Ligand CLA a 1127



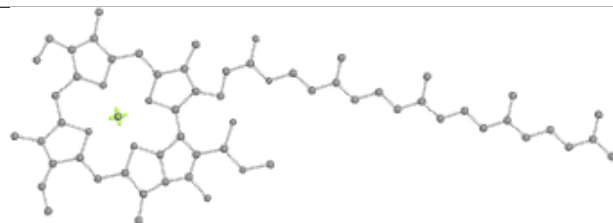
Bond lengths



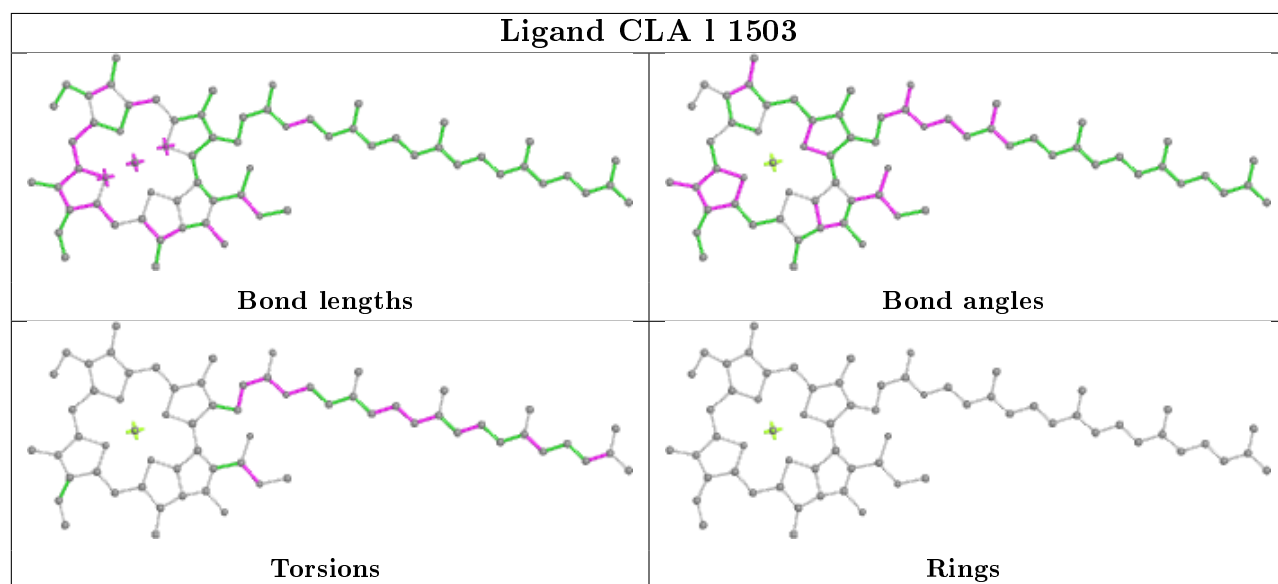
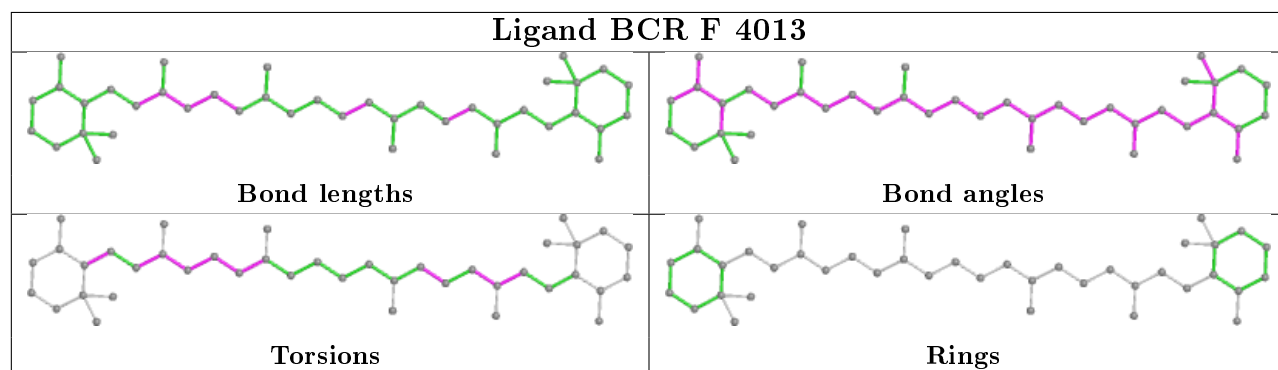
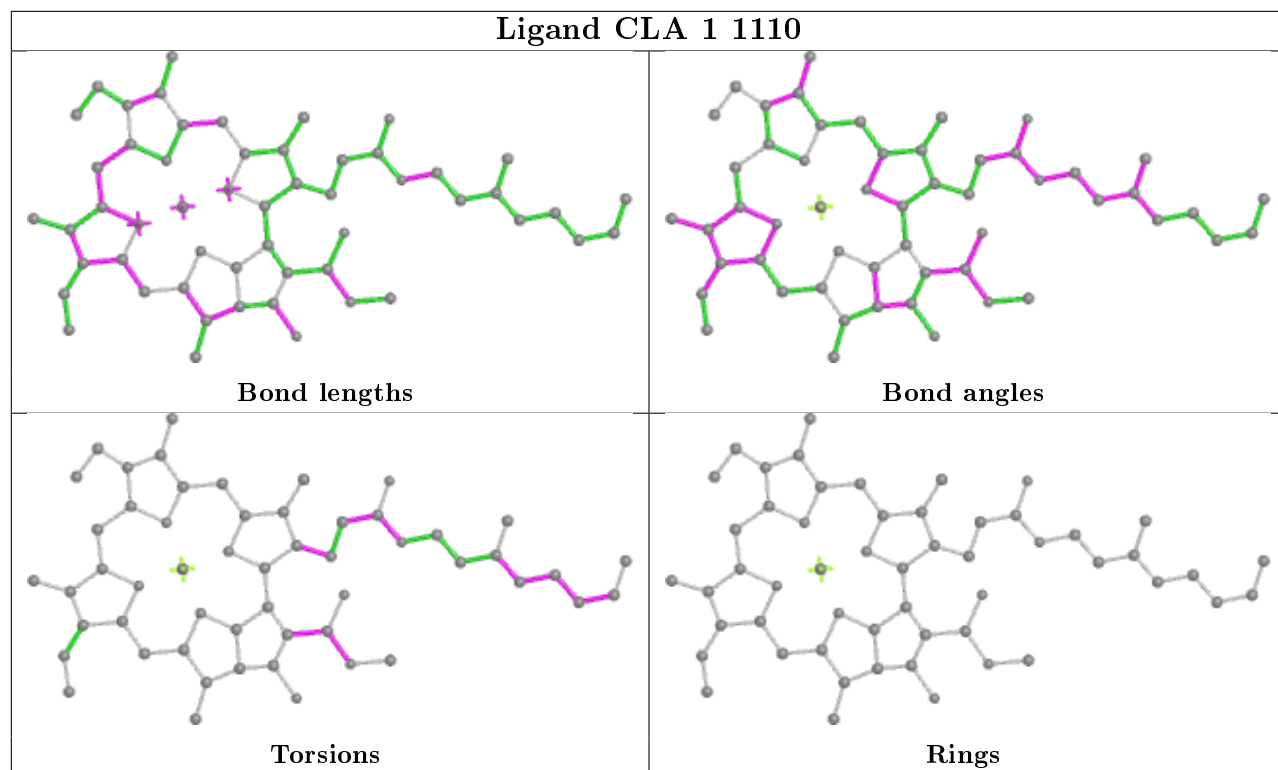
Bond angles



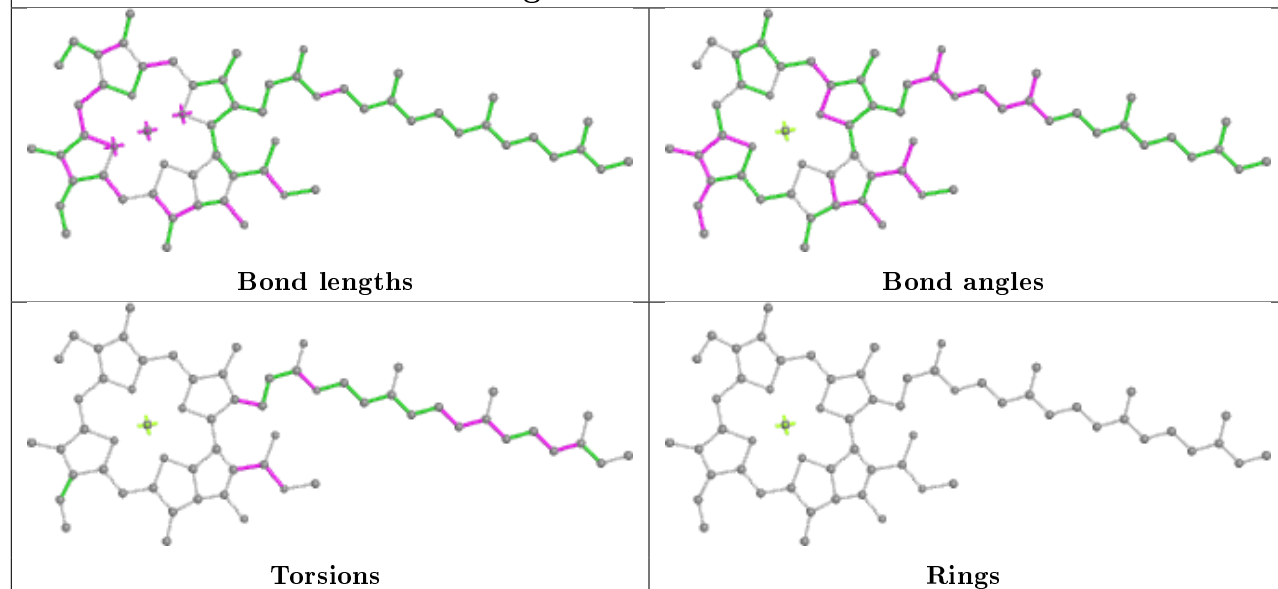
Torsions



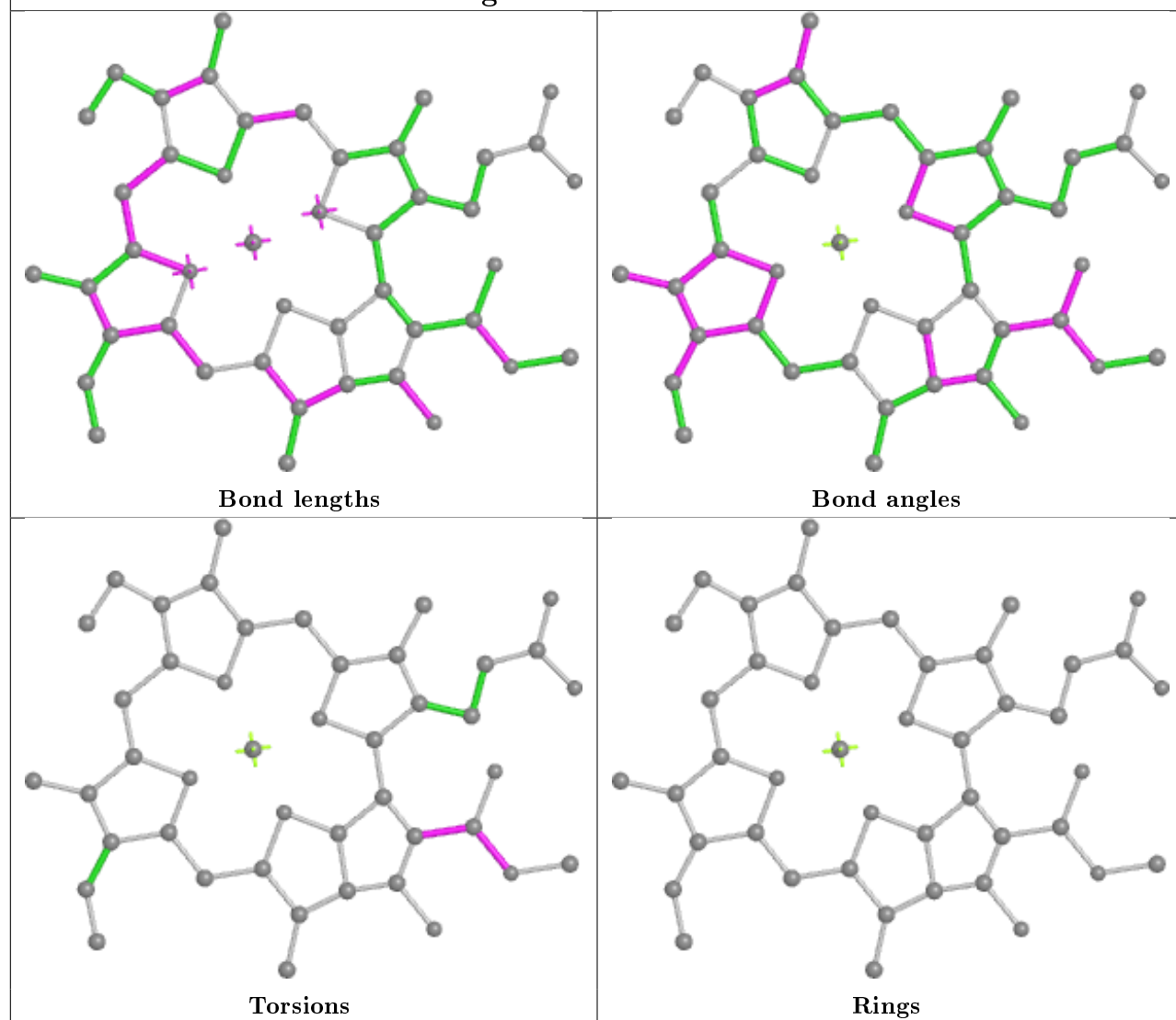
Rings

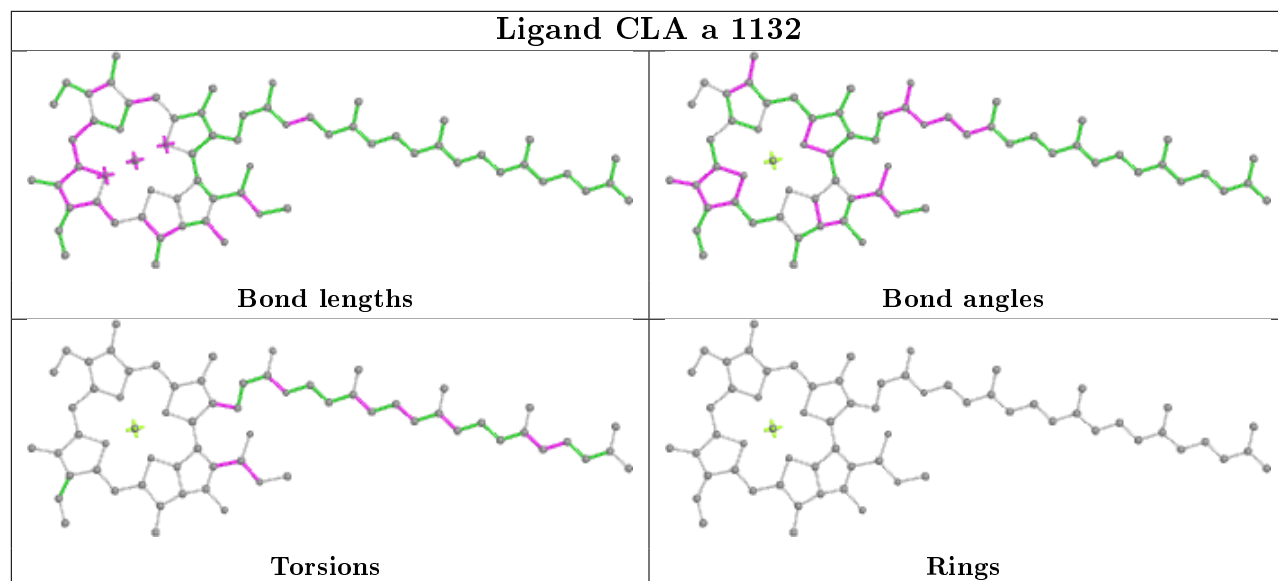
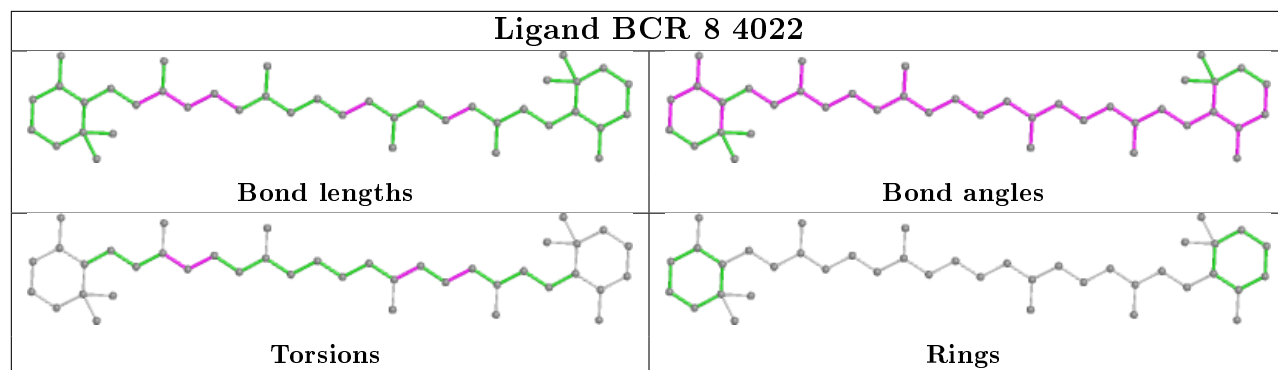


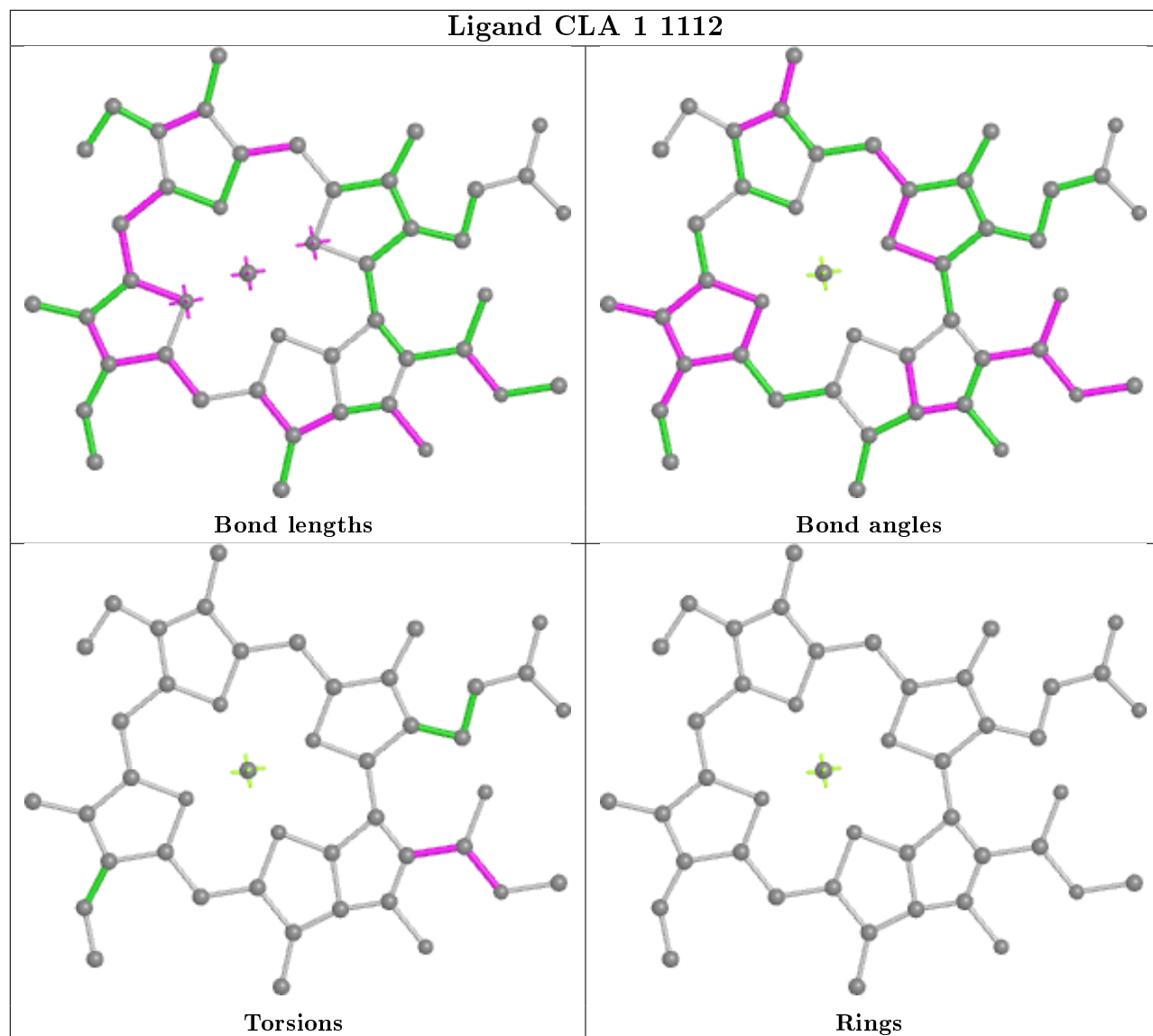
Ligand CLA A 1118



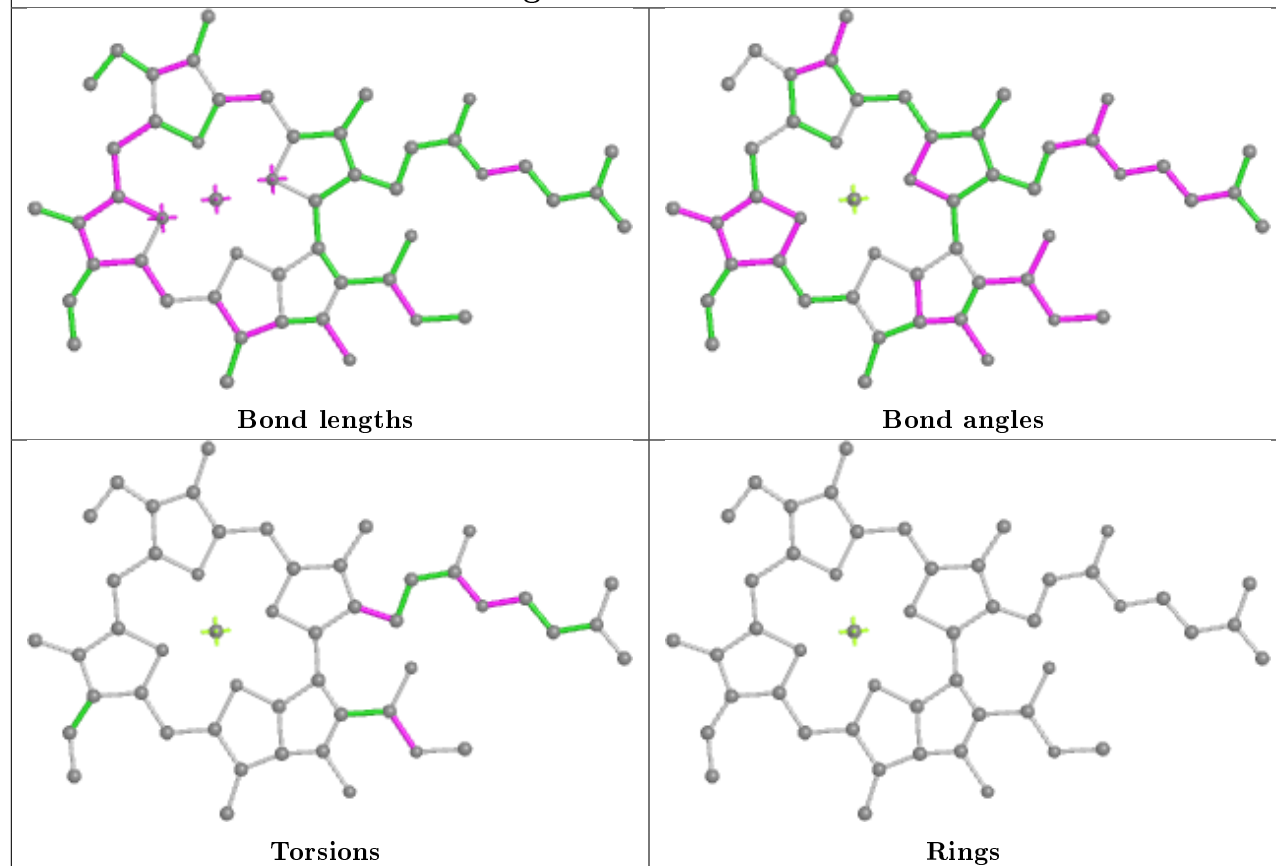
Ligand CLA B 1218



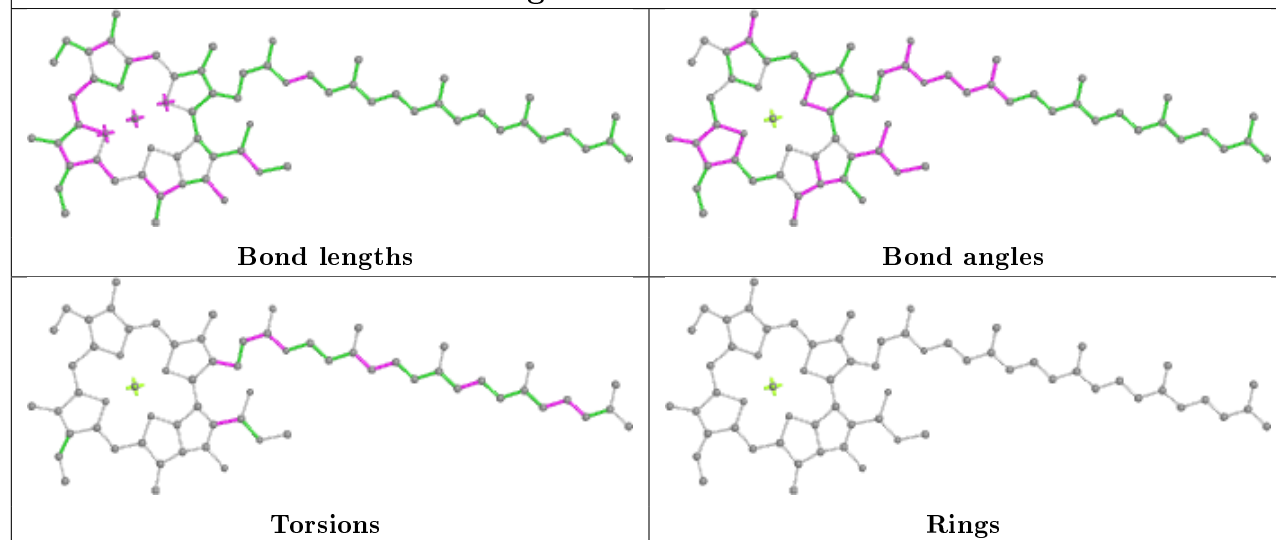




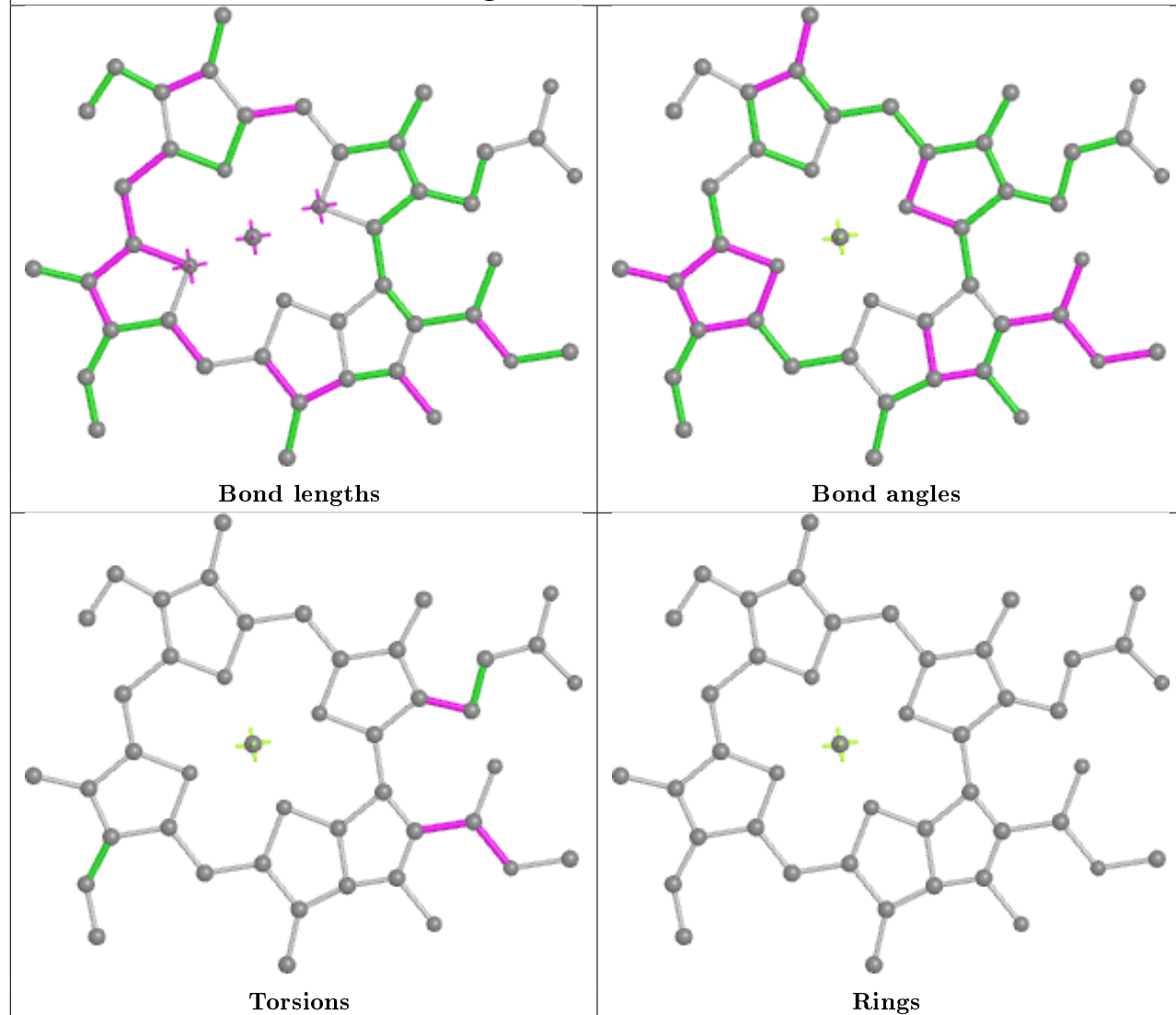
Ligand CLA A 1139



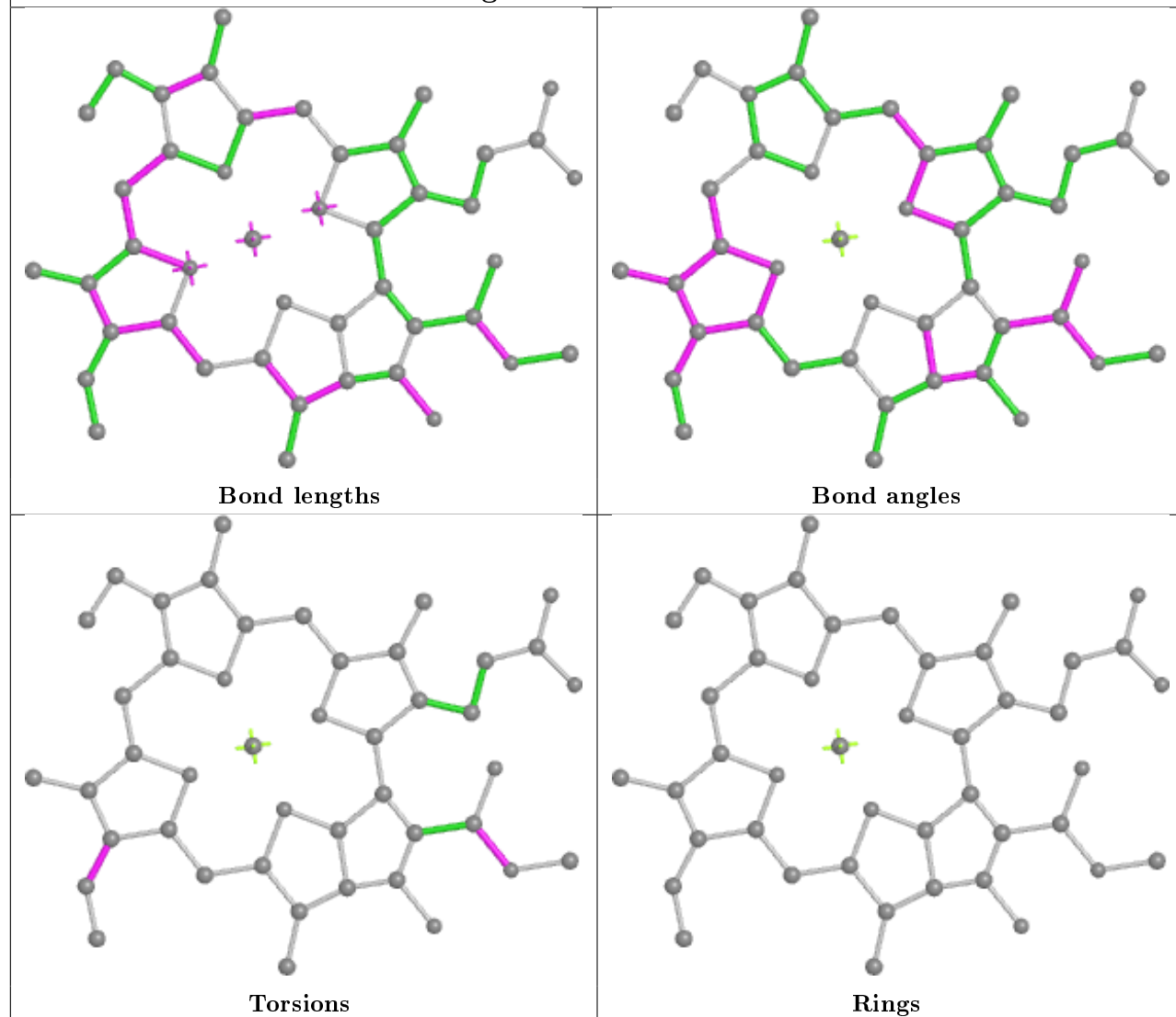
Ligand CLA 2 1202



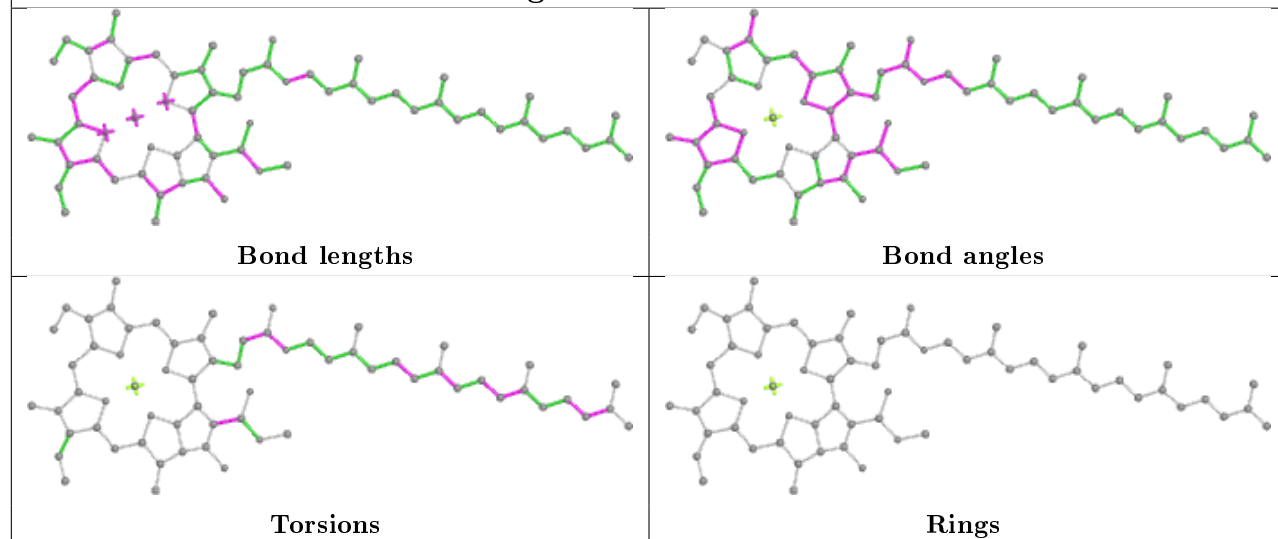
Ligand CLA B 1208



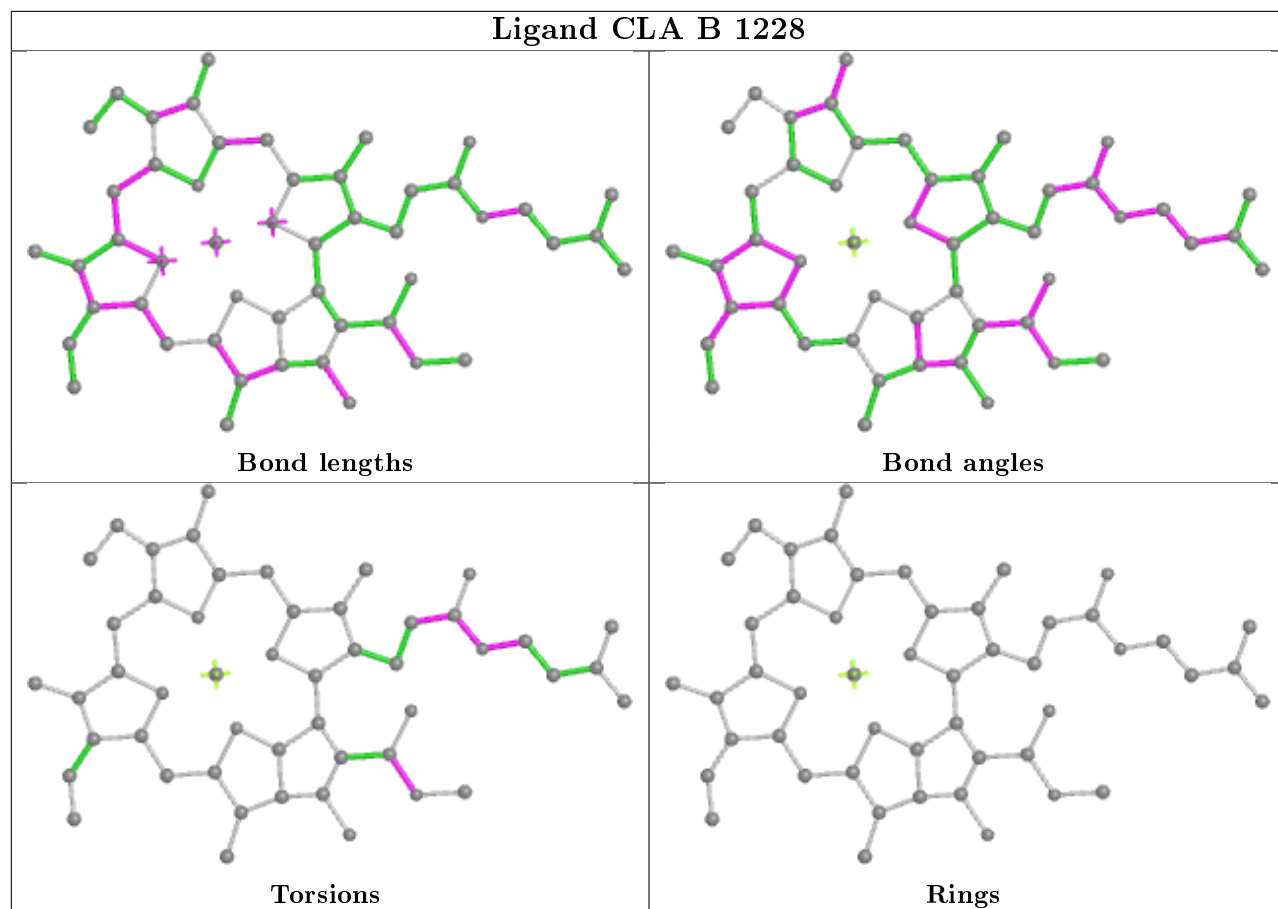
Ligand CLA B 1227



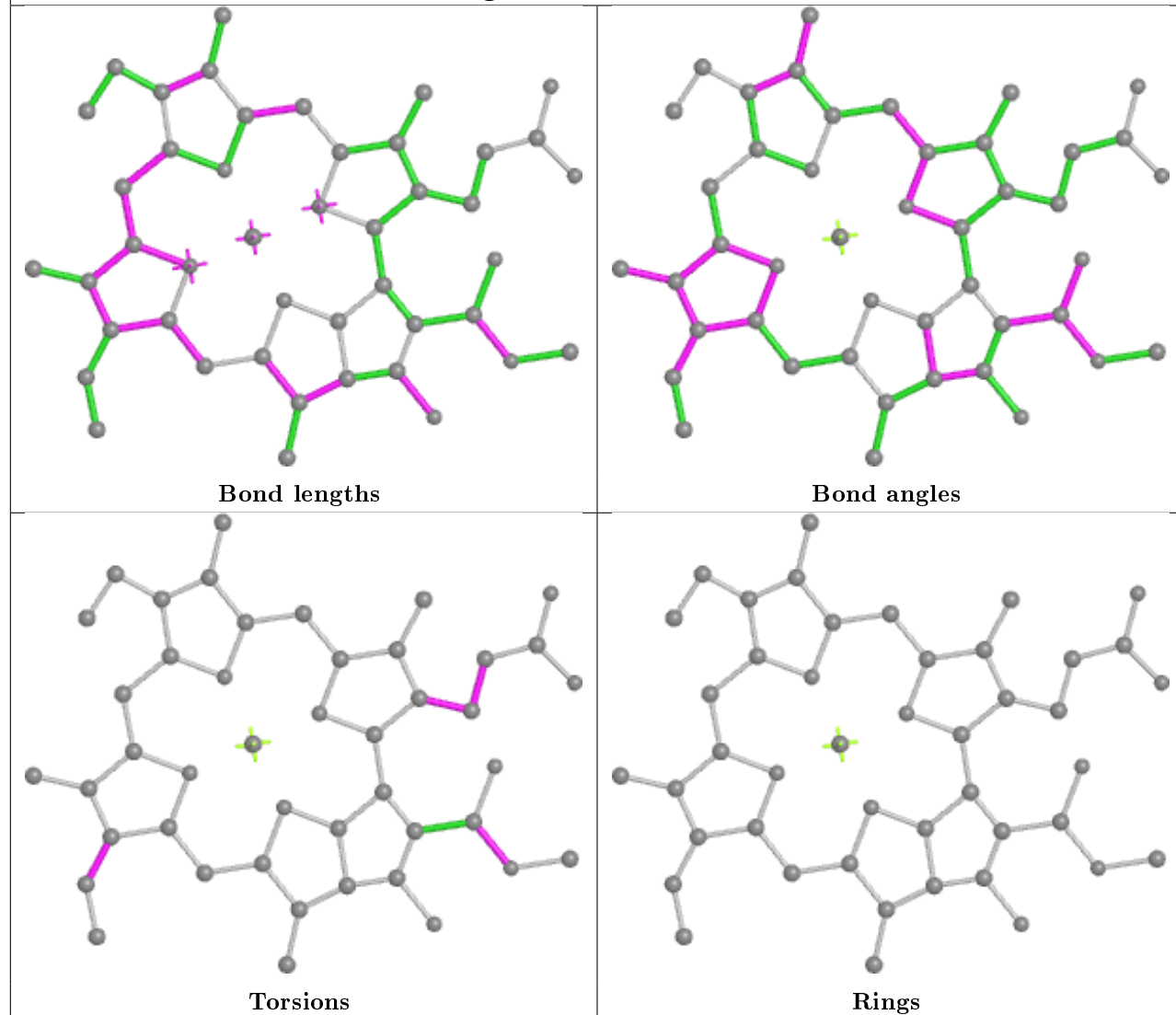
Ligand CLA 1 1011

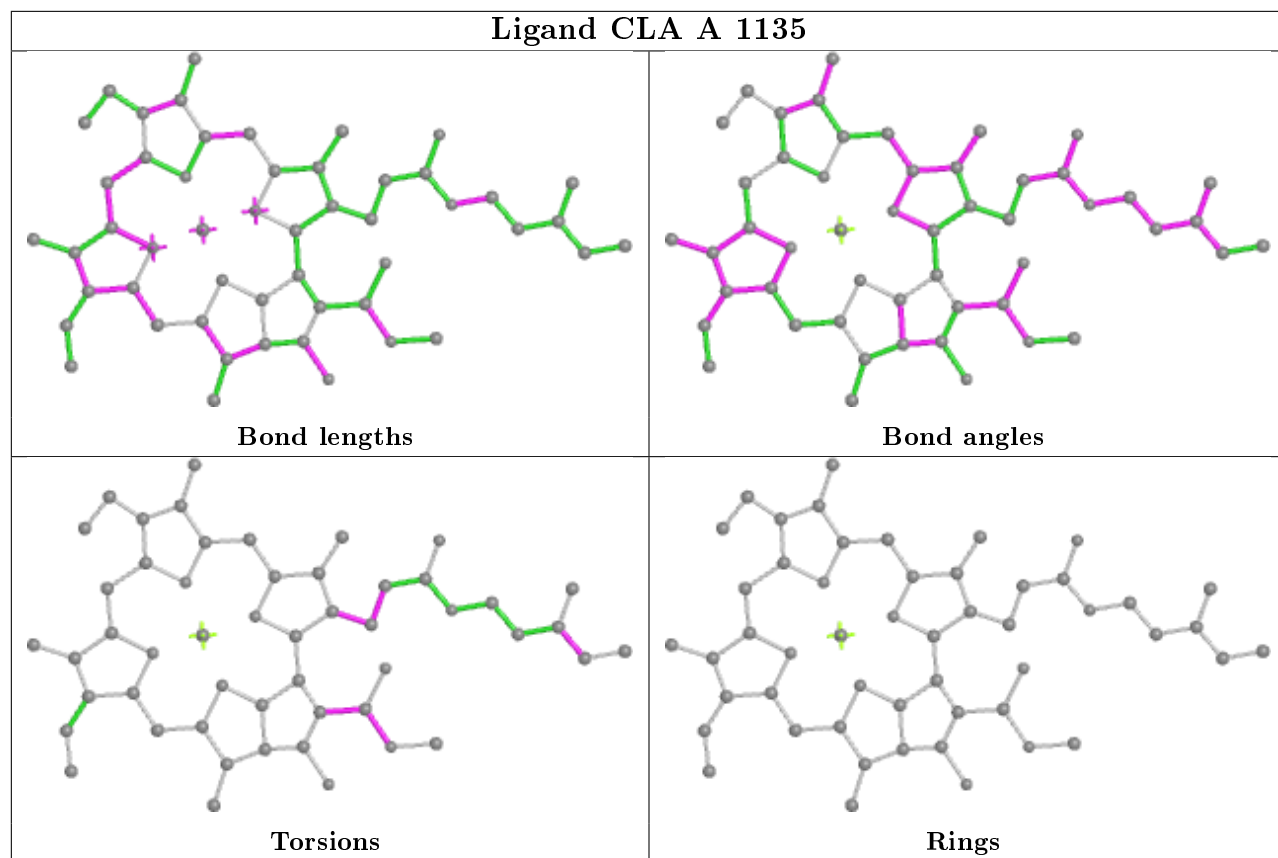


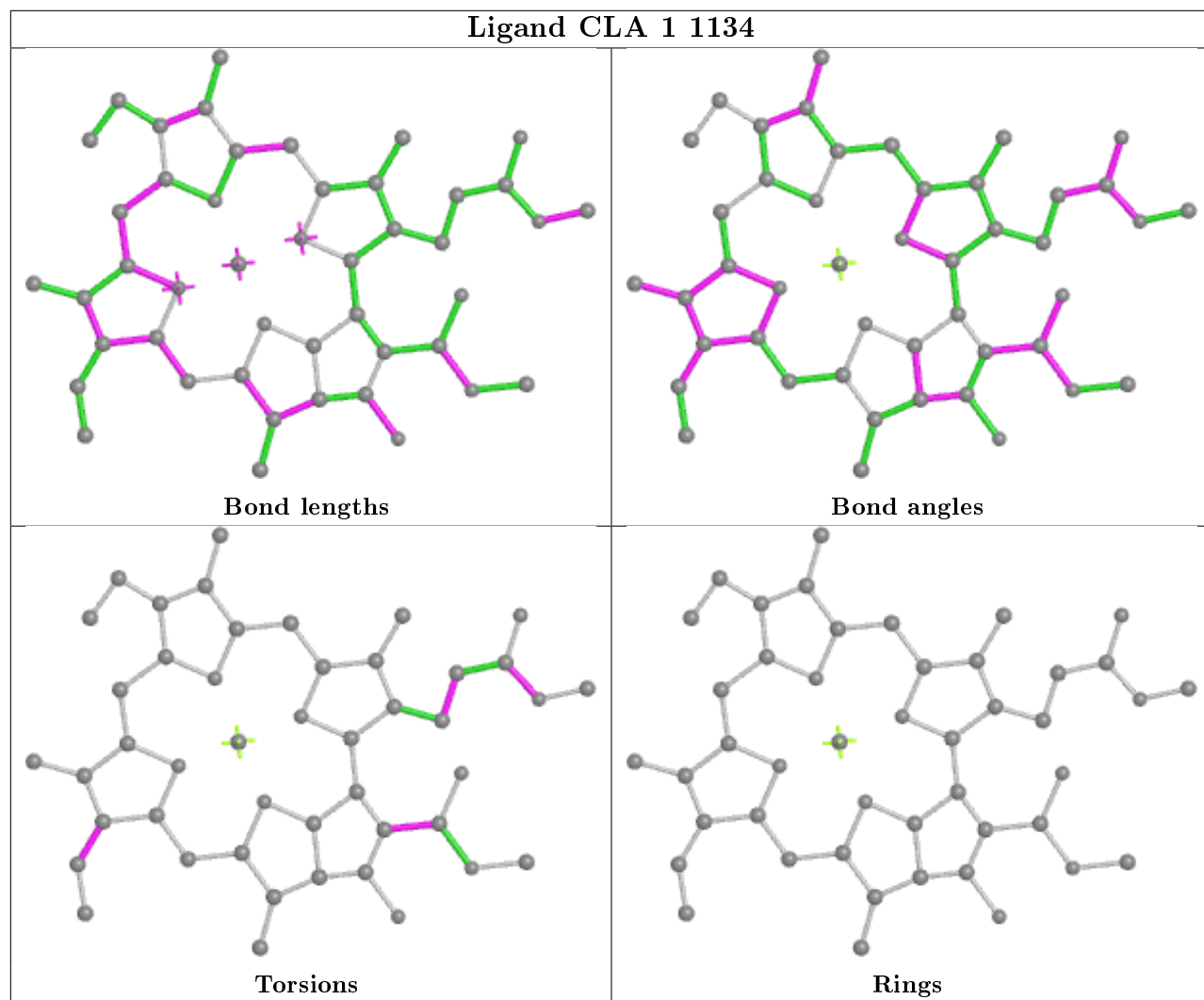
Ligand CLA B 1228



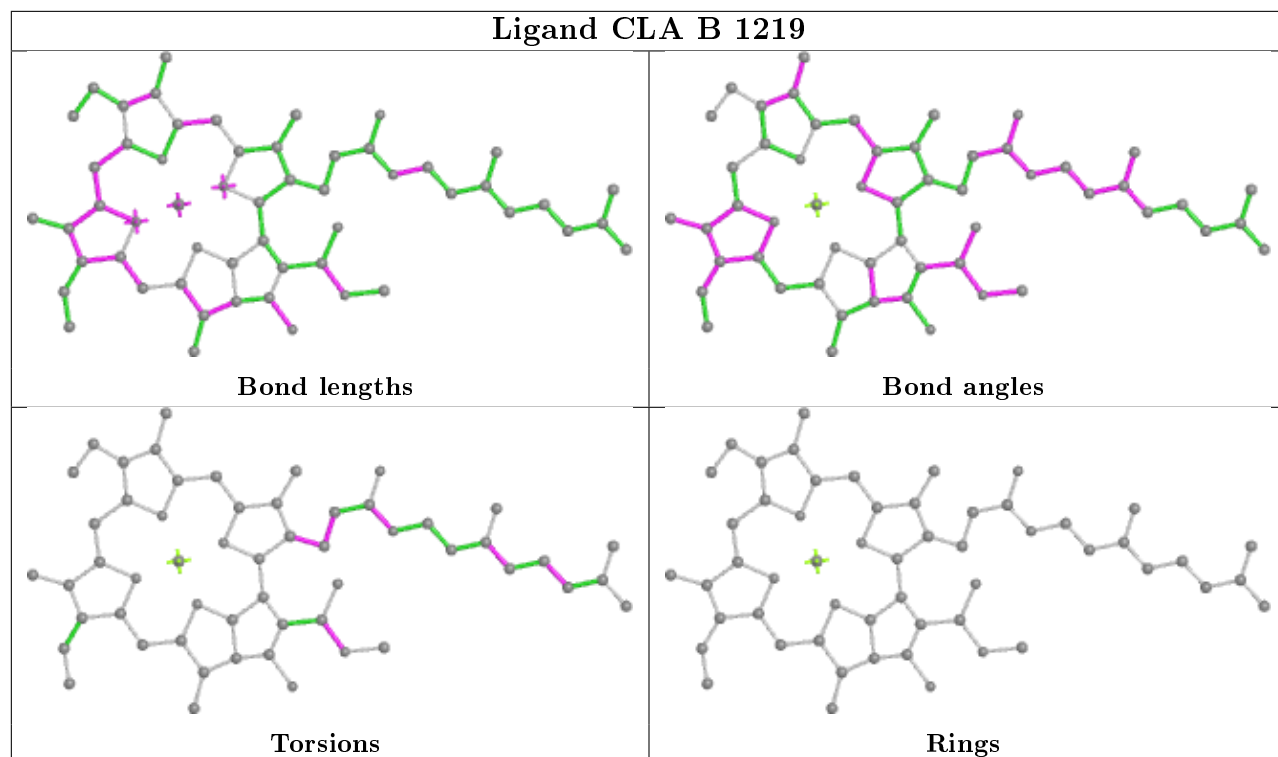
Ligand CLA B 1240



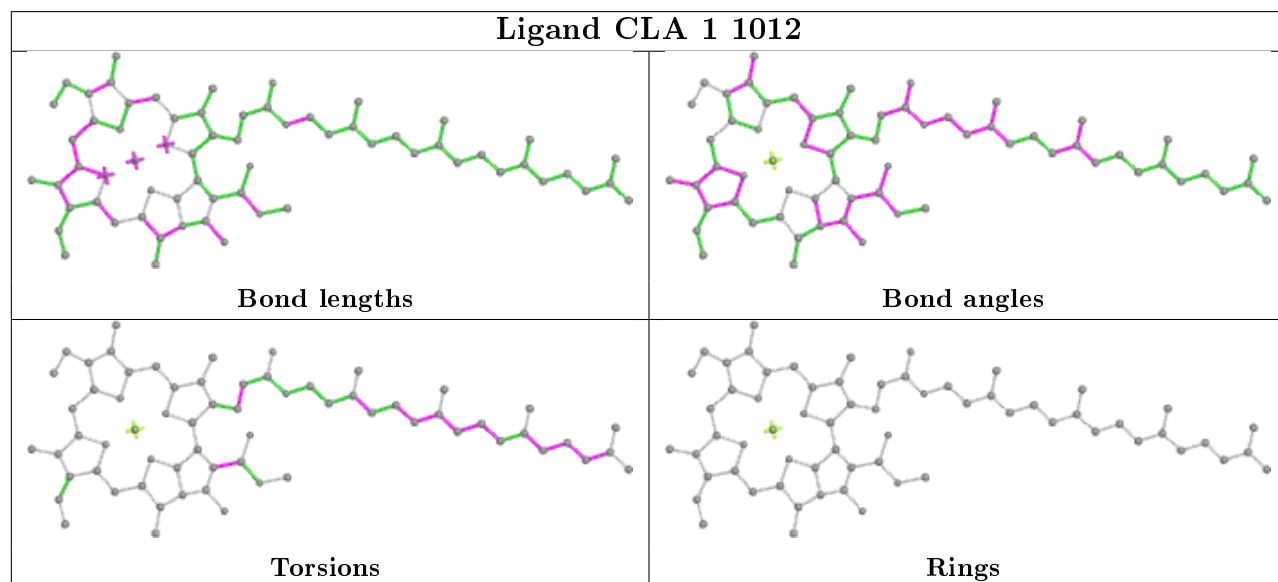


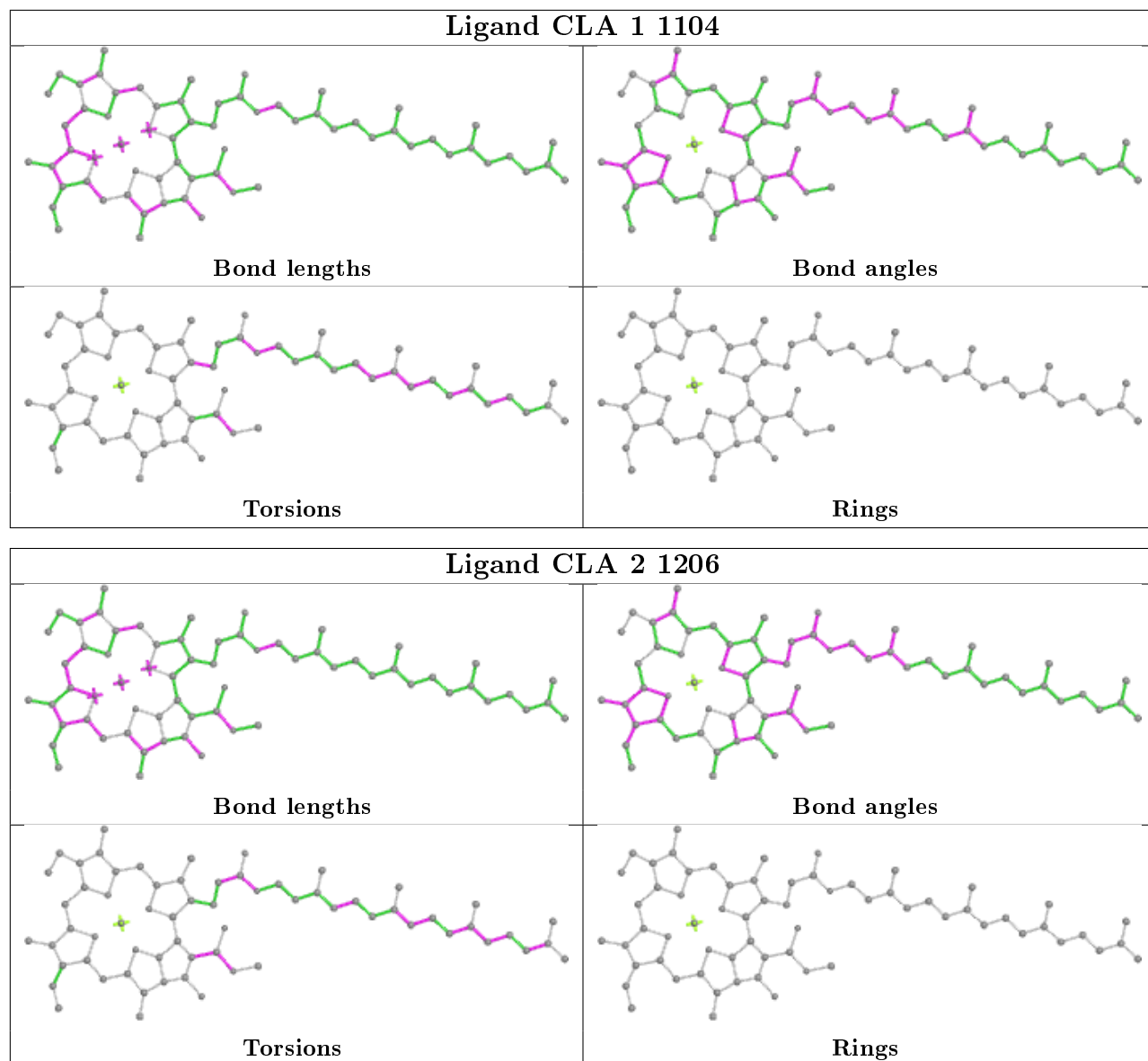


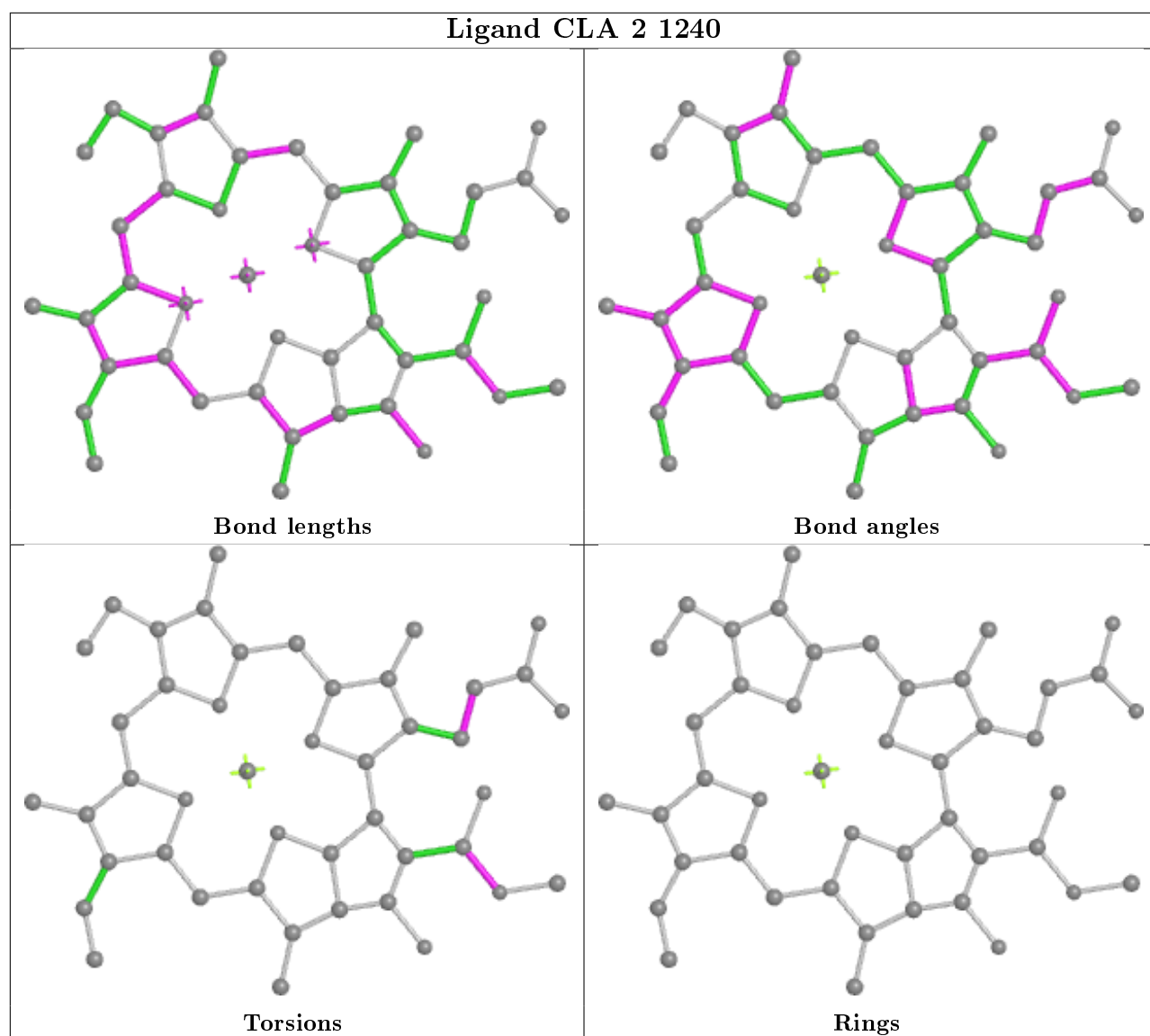
Ligand CLA B 1219

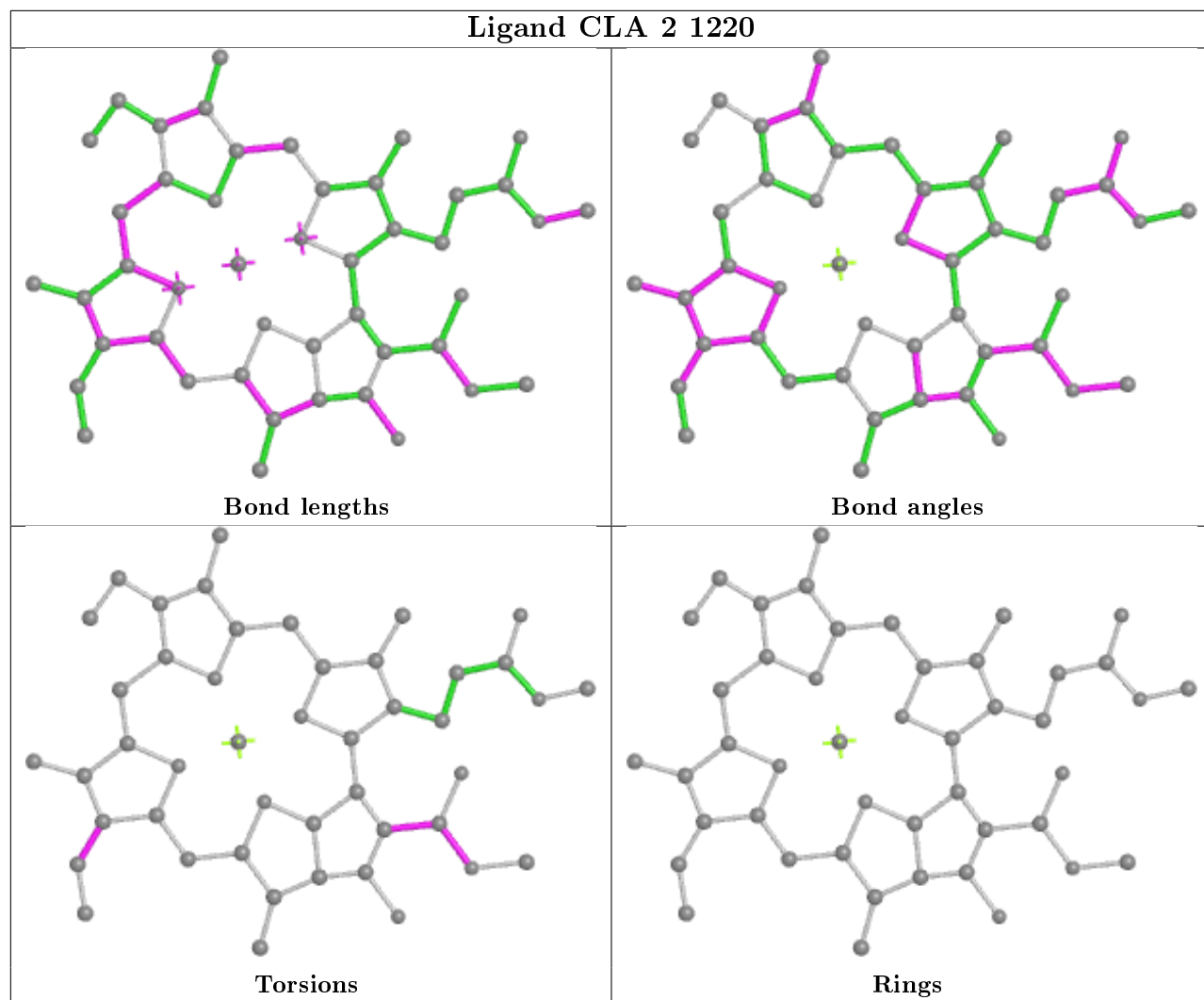


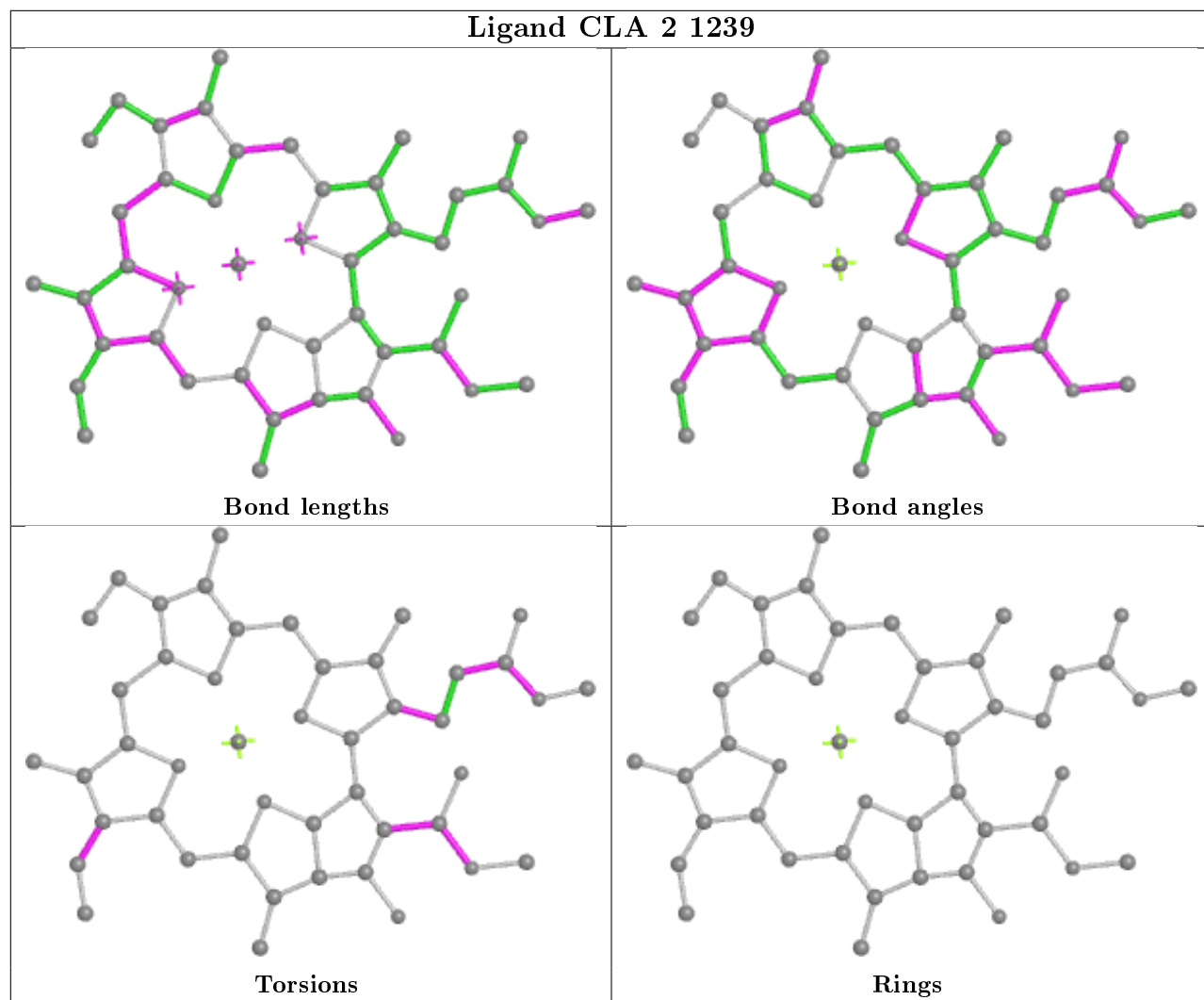
Ligand CLA 1 1012

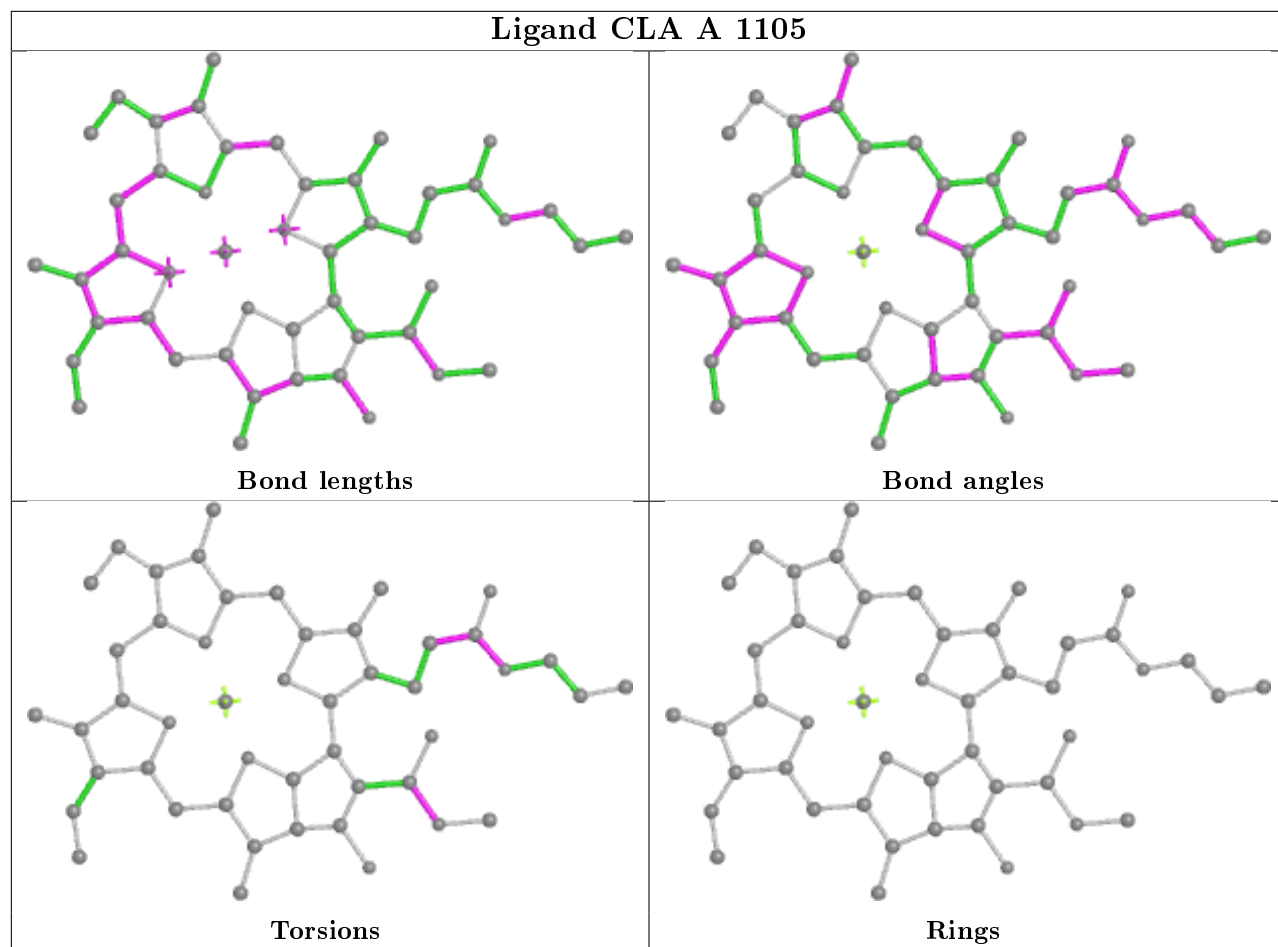




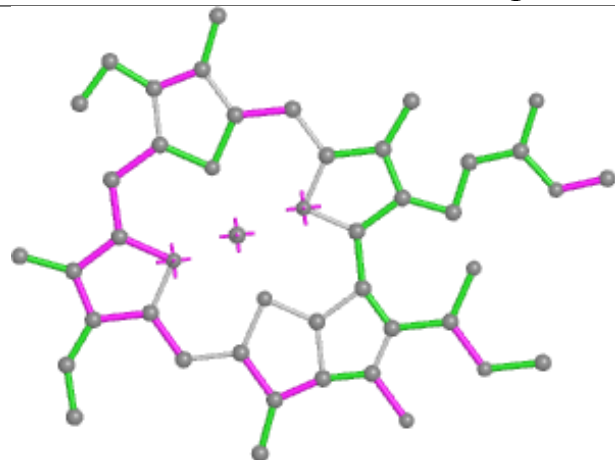




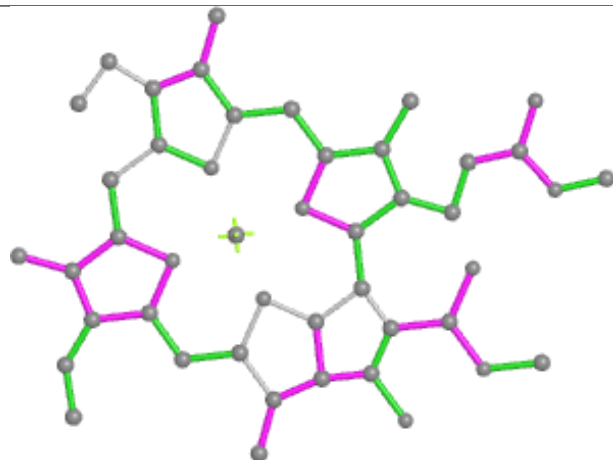




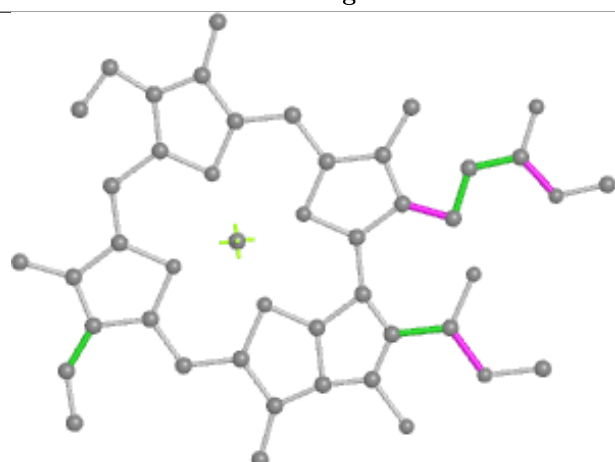
Ligand CLA A 1121



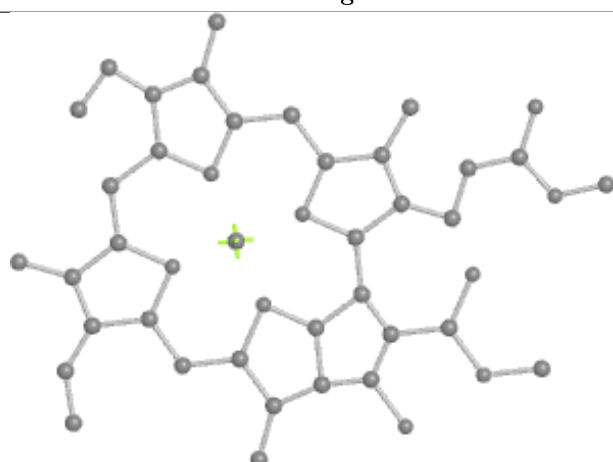
Bond lengths



Bond angles

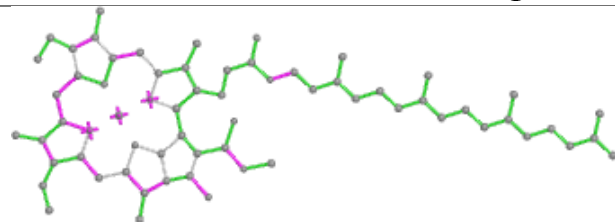


Torsions

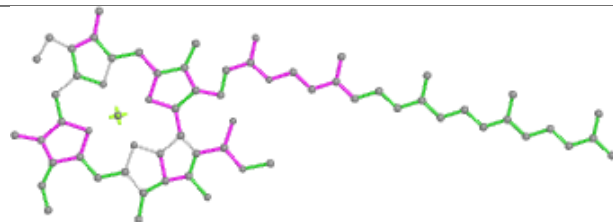


Rings

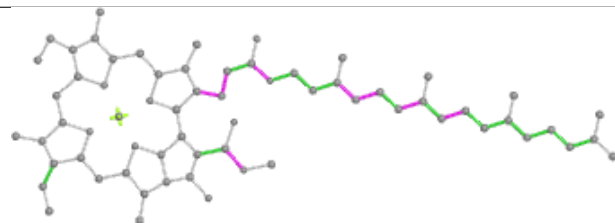
Ligand CLA A 1107



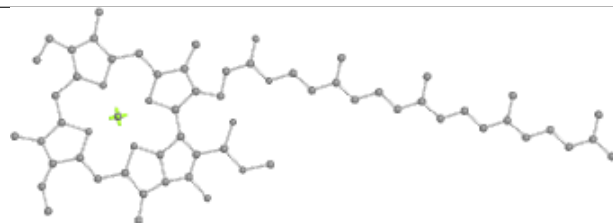
Bond lengths



Bond angles

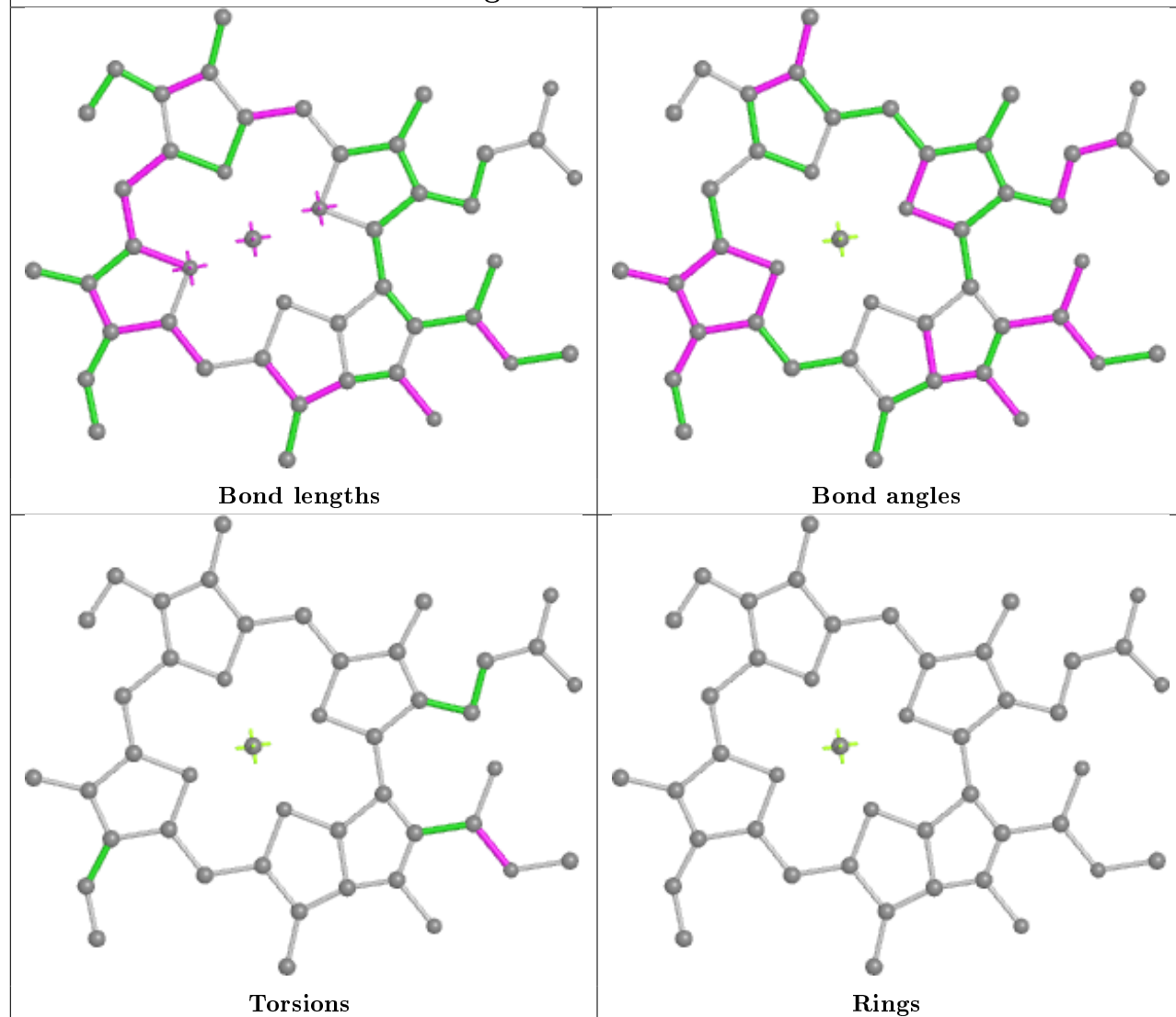


Torsions

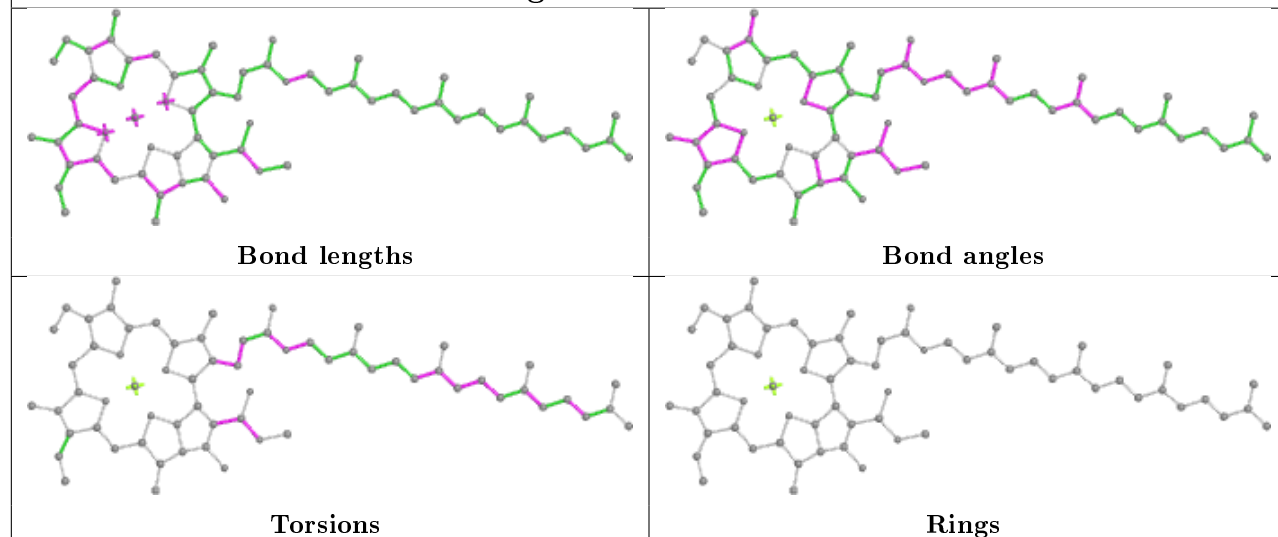


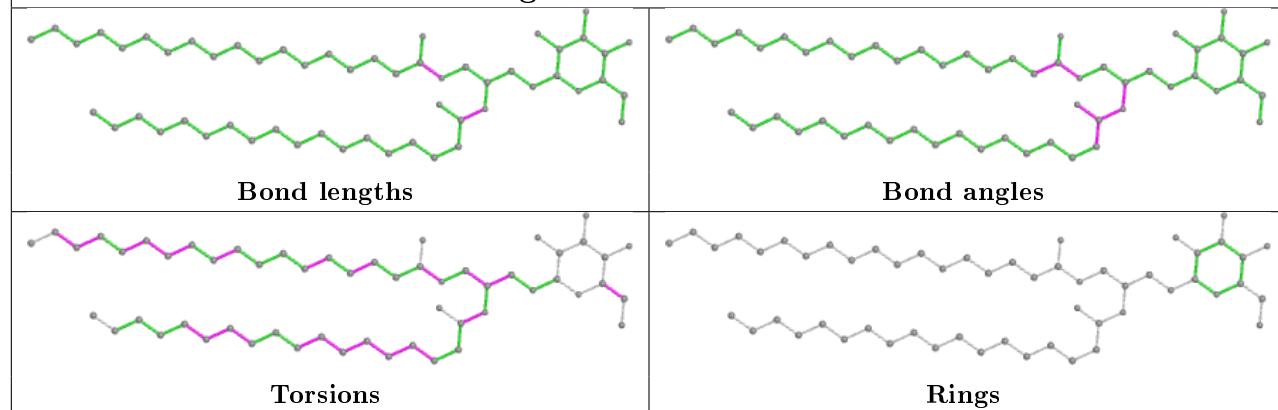
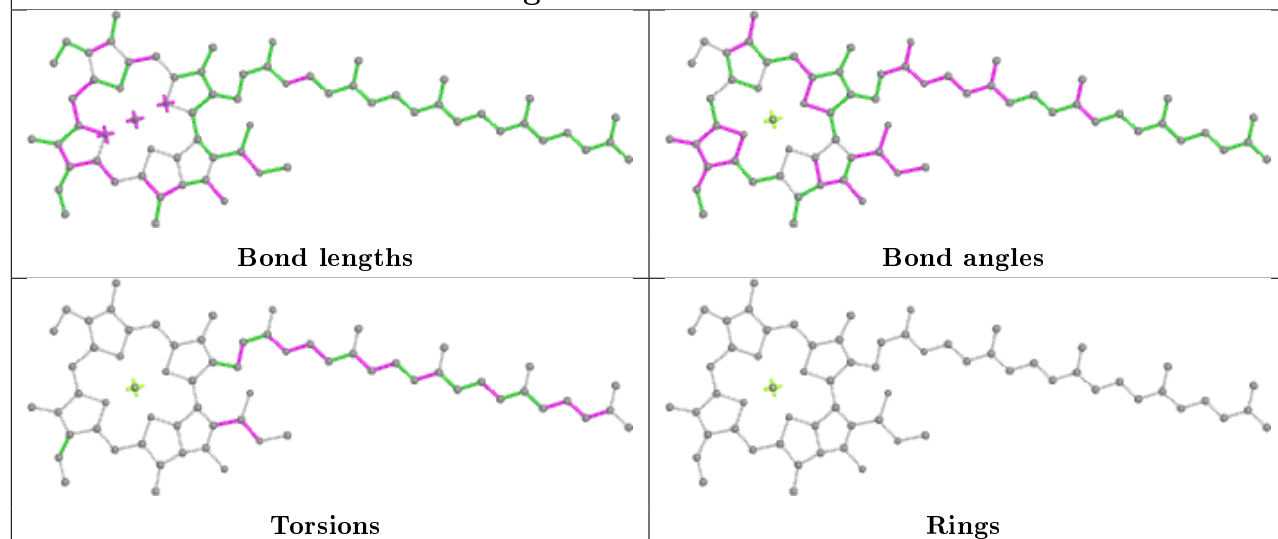
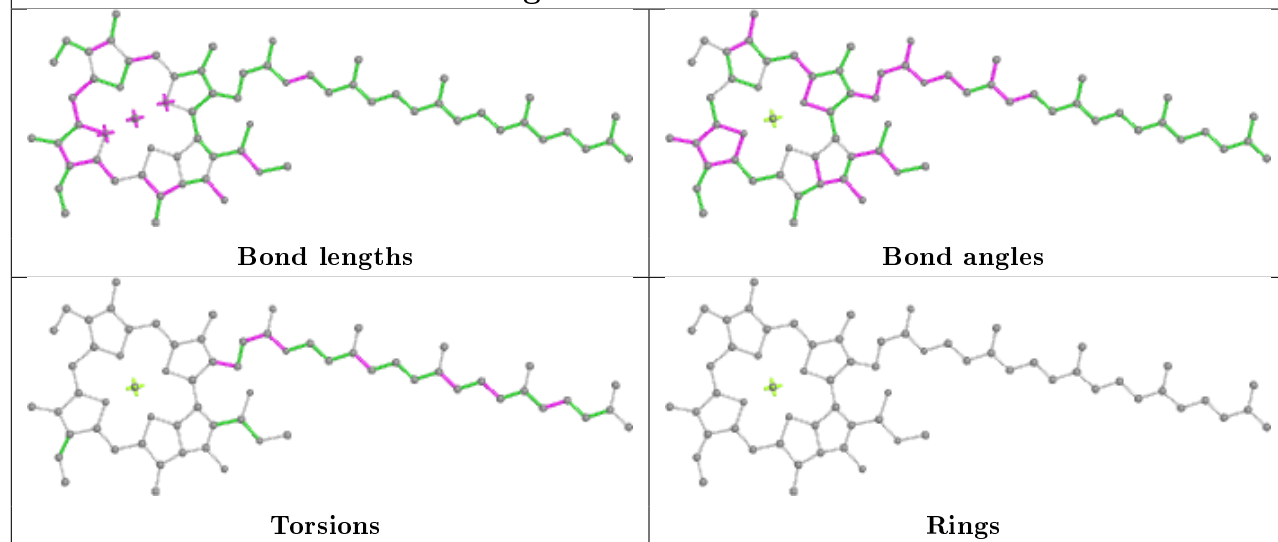
Rings

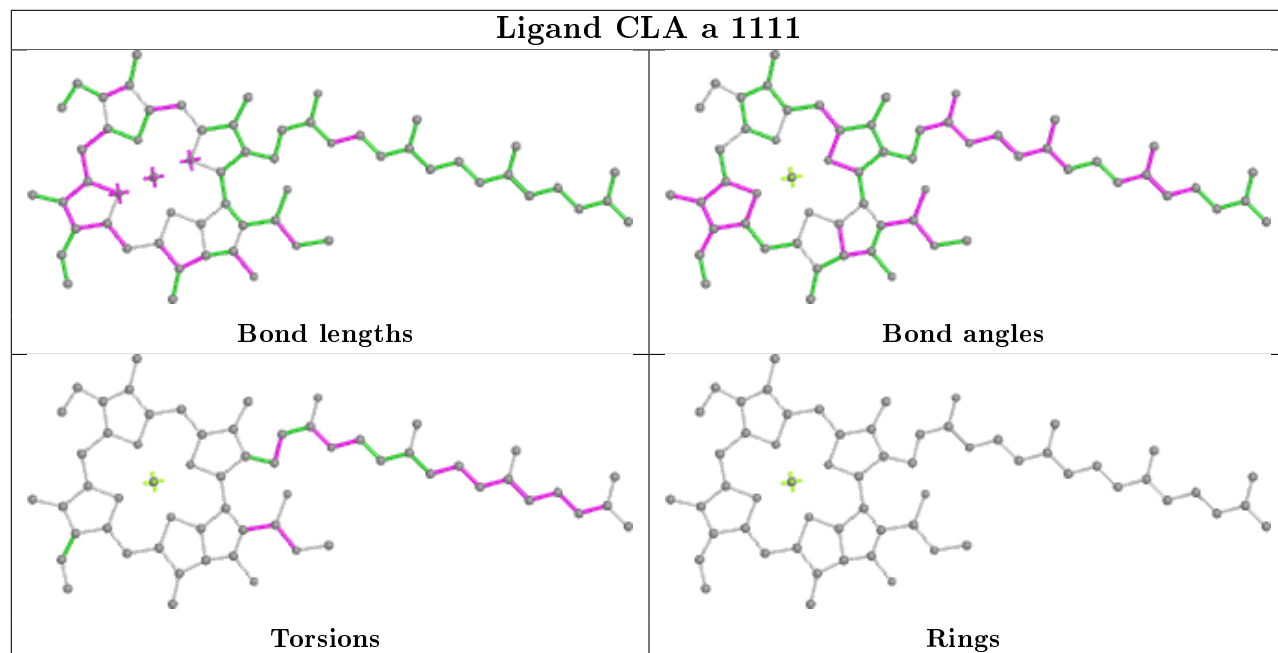
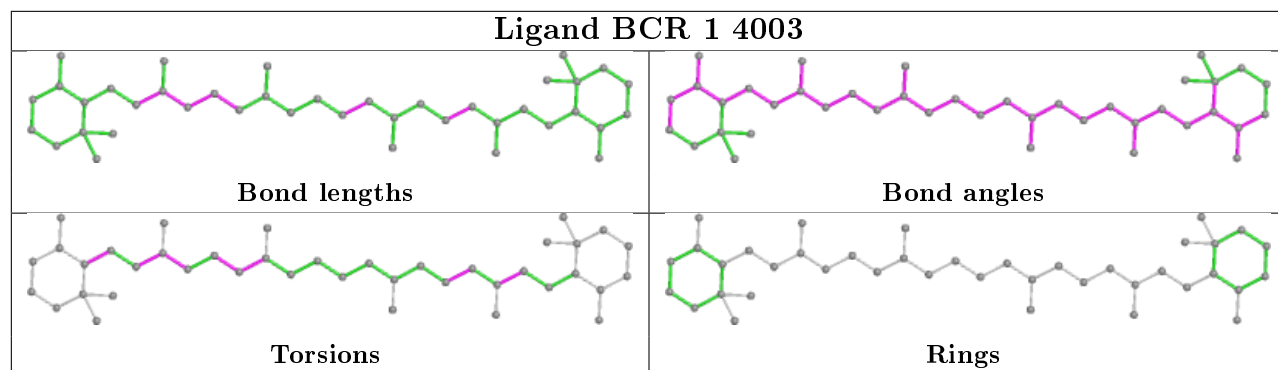
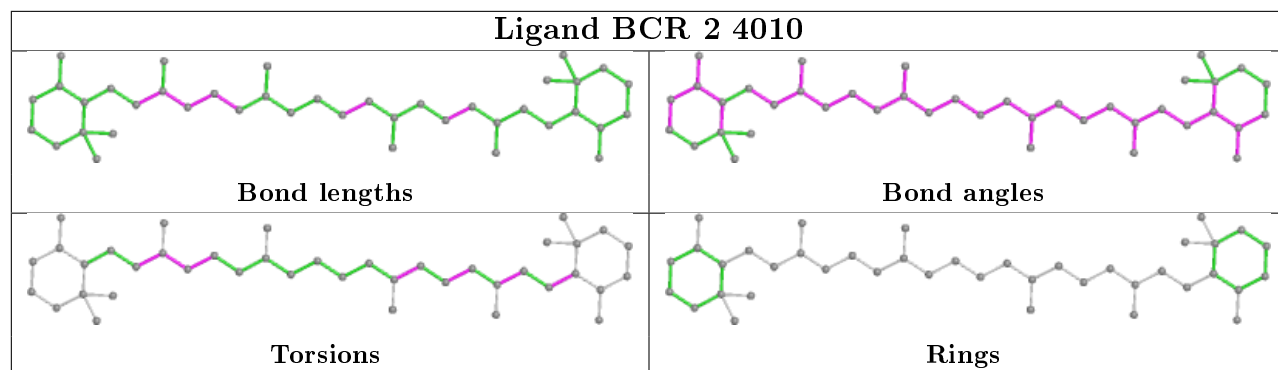
Ligand CLA b 1208

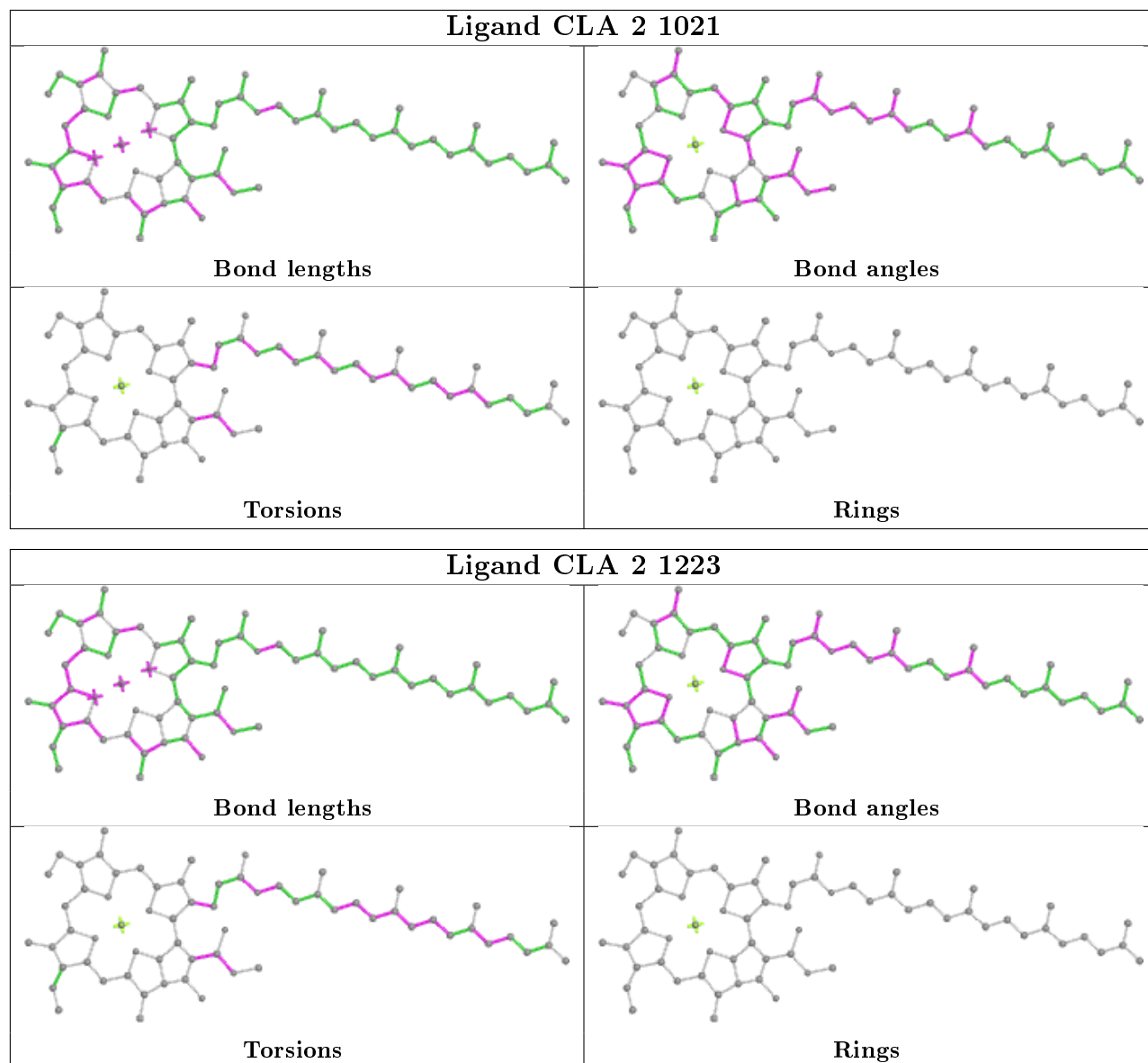


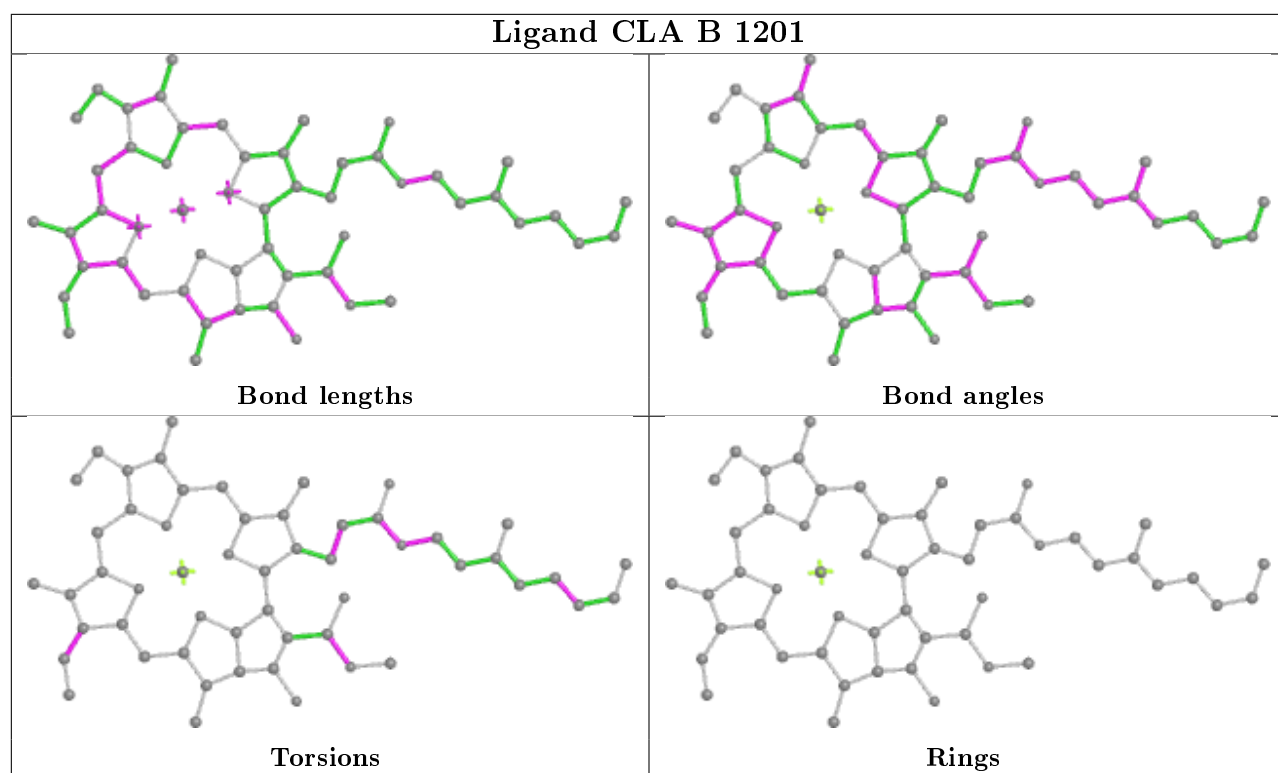
Ligand CLA a 1101



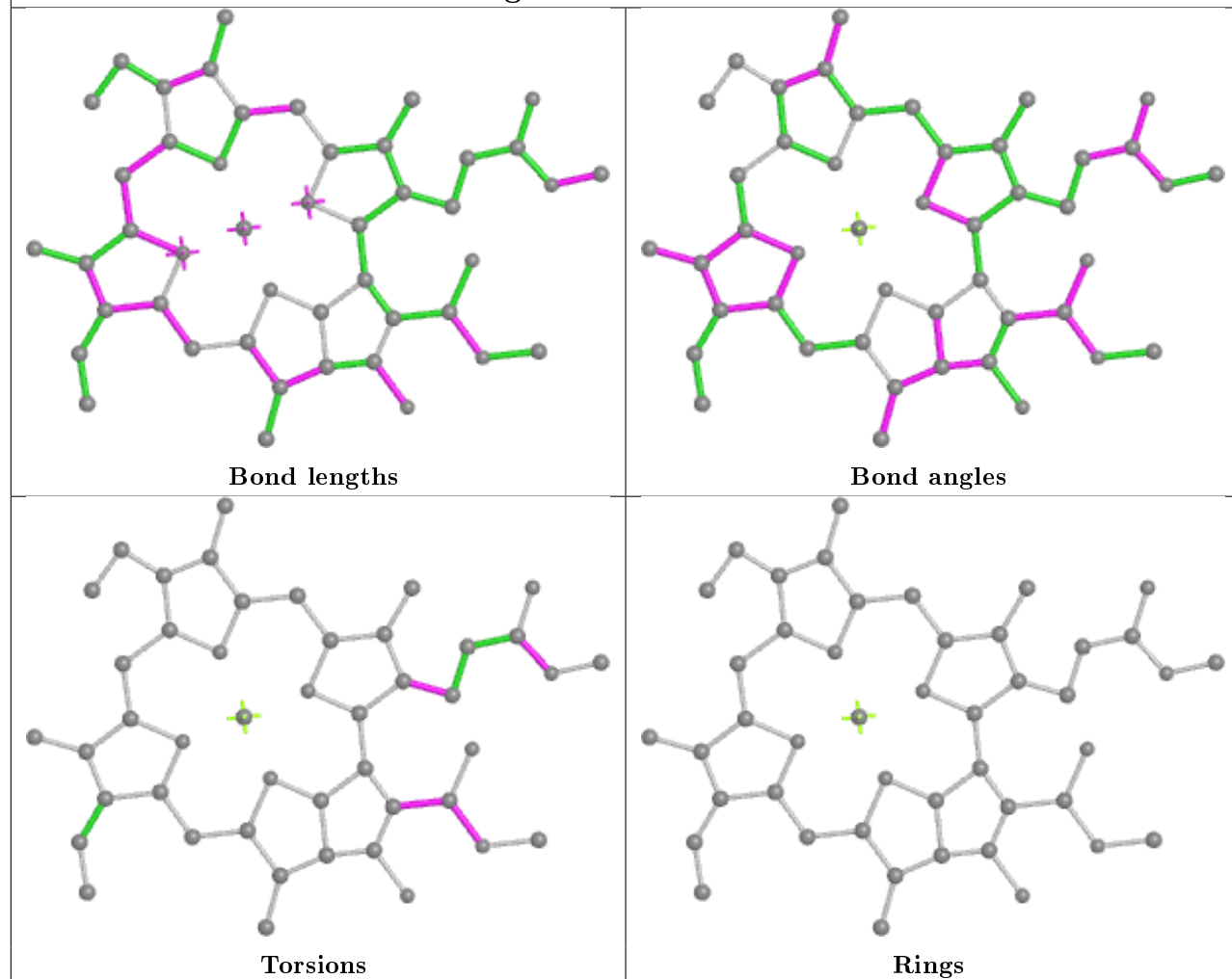
Ligand LMG B 5002**Ligand CLA B 1013****Ligand CLA B 1225**



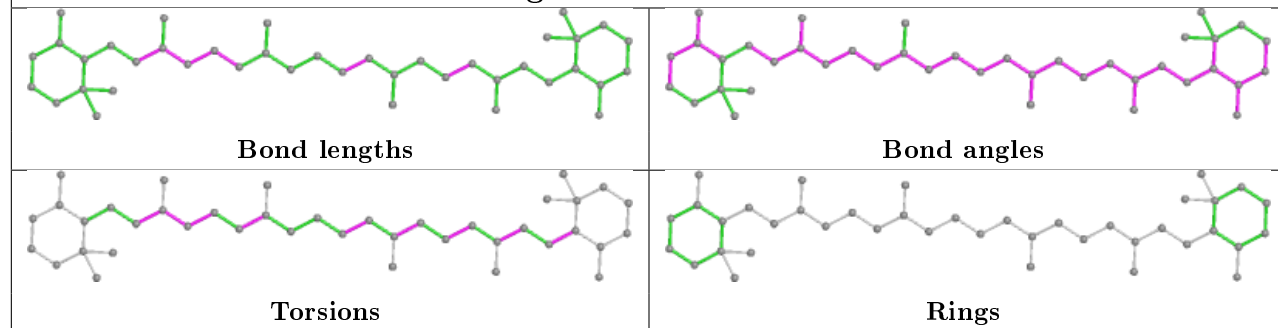


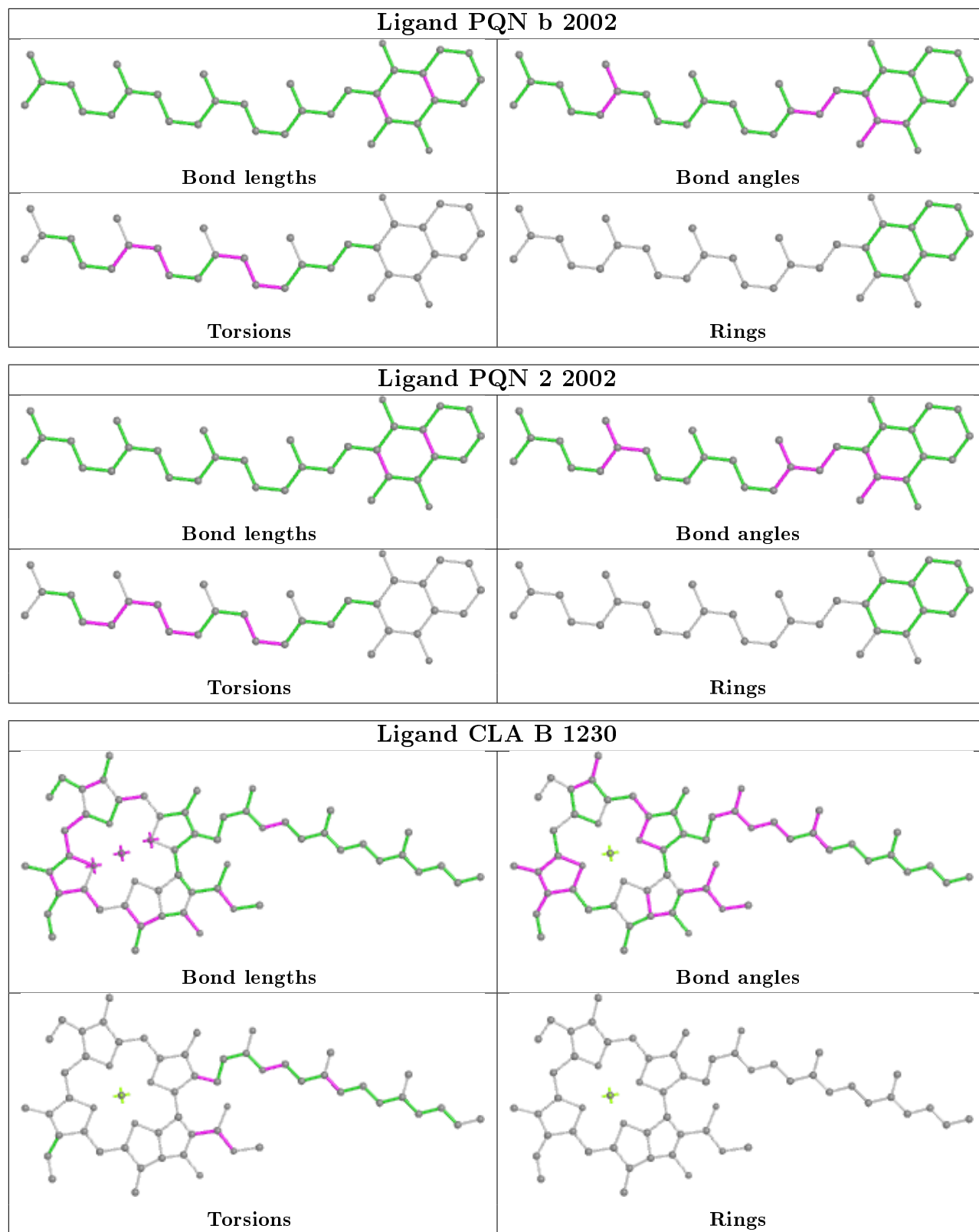


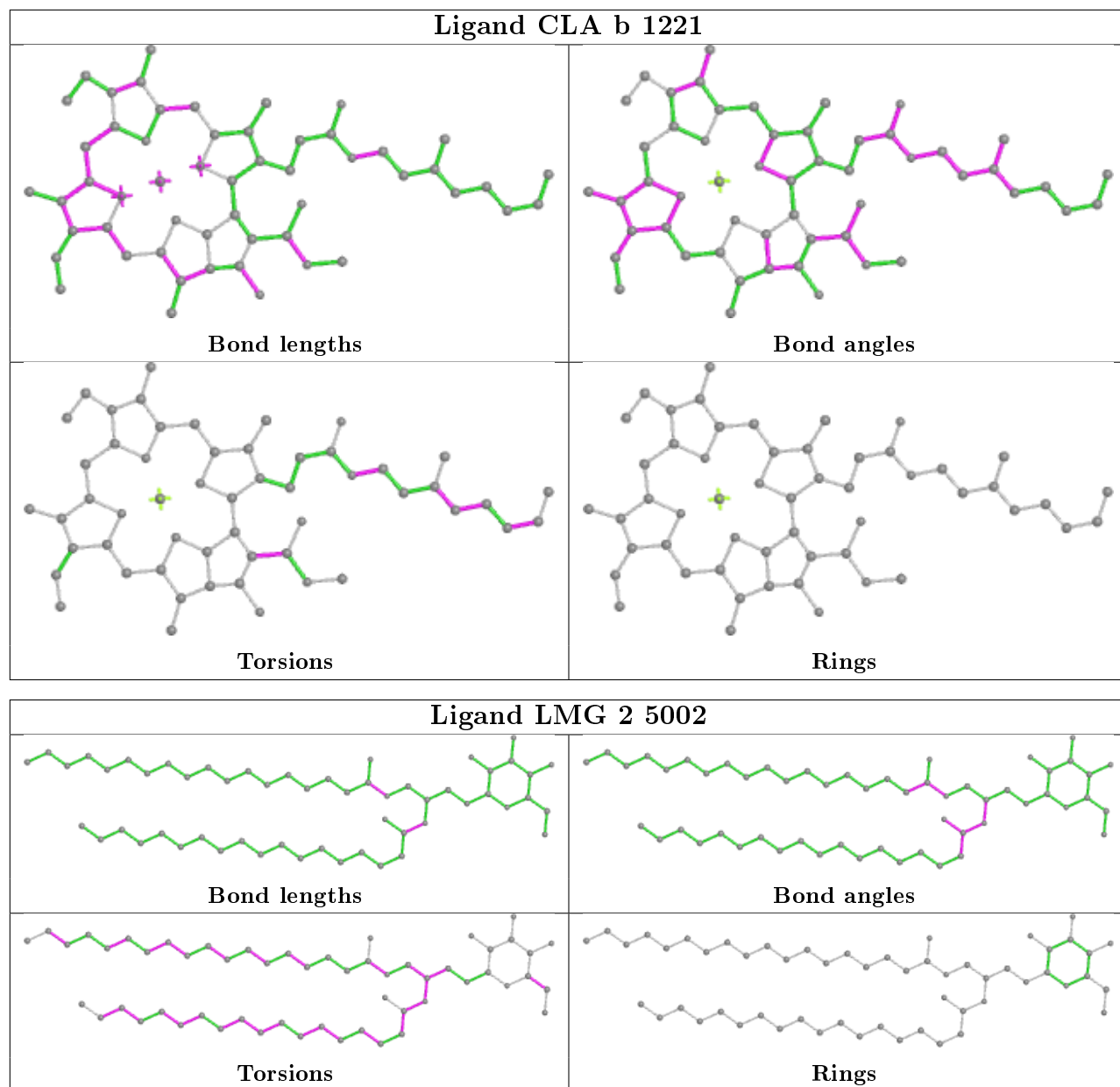
Ligand CLA B 1211



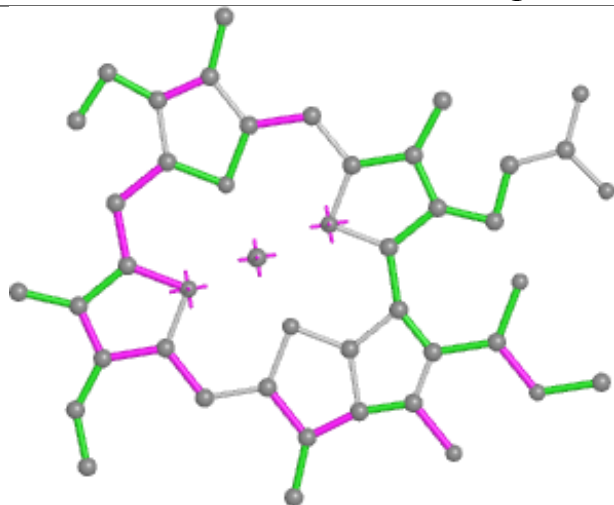
Ligand BCR a 4002



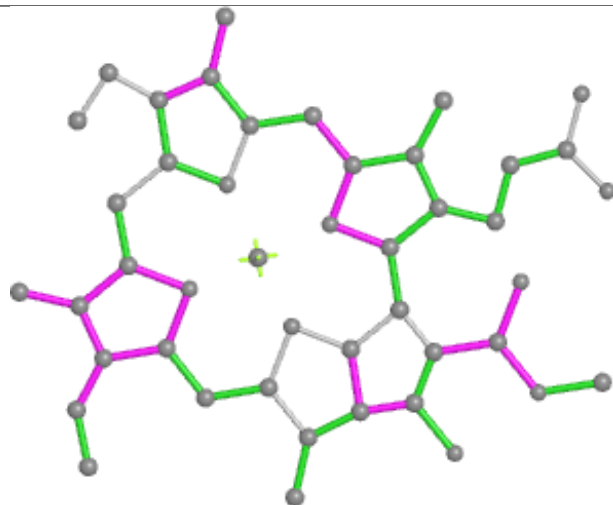




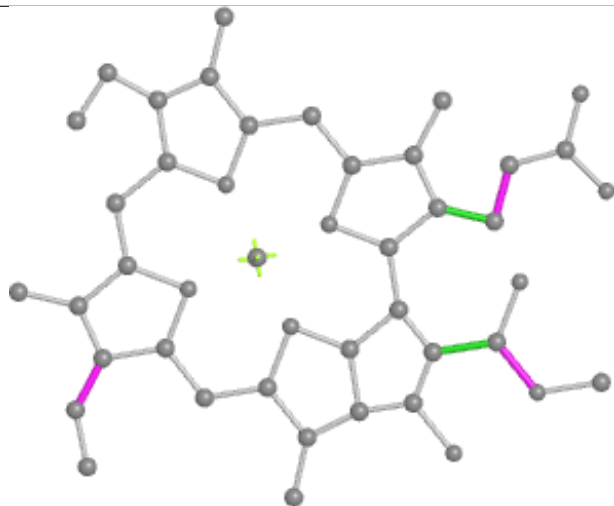
Ligand CLA b 1209



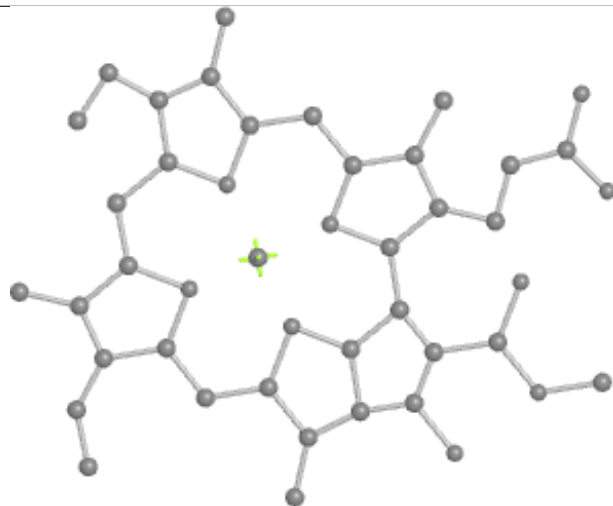
Bond lengths



Bond angles

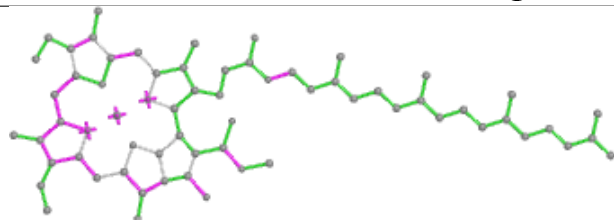


Torsions

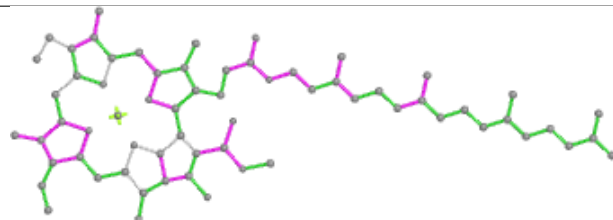


Rings

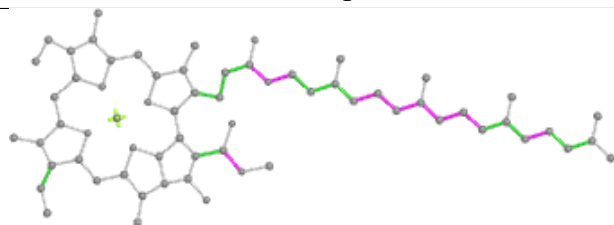
Ligand CLA b 1203



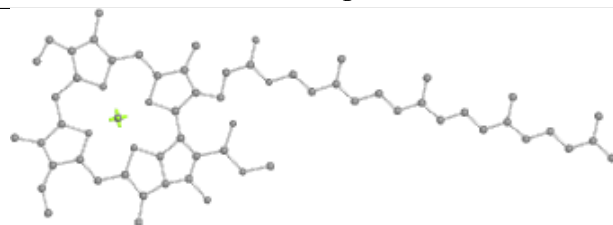
Bond lengths



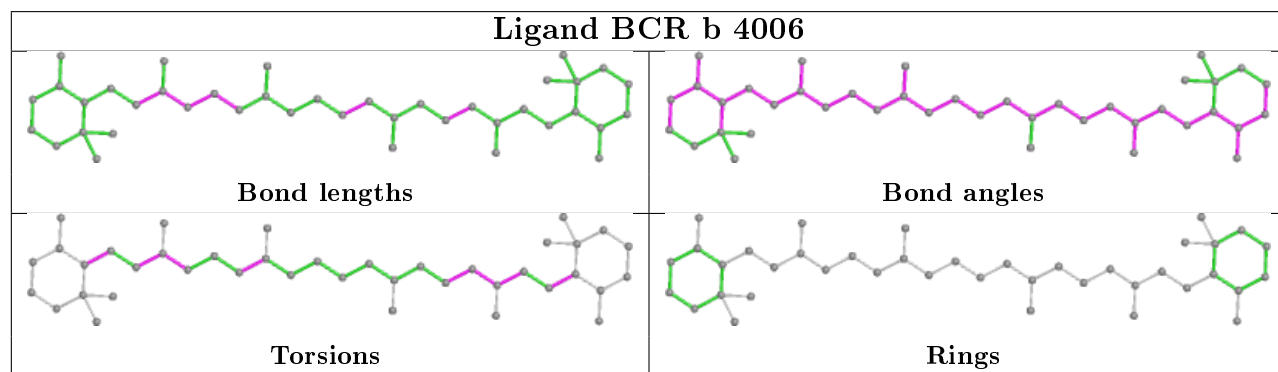
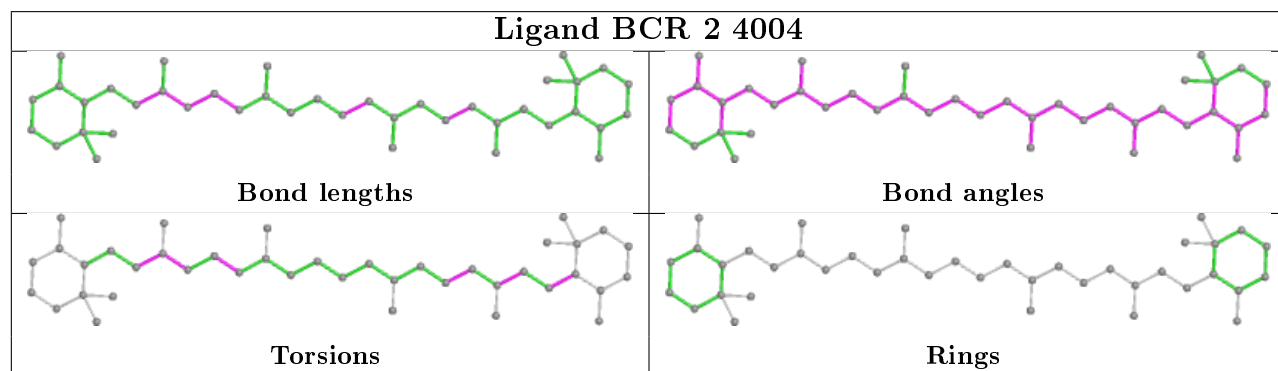
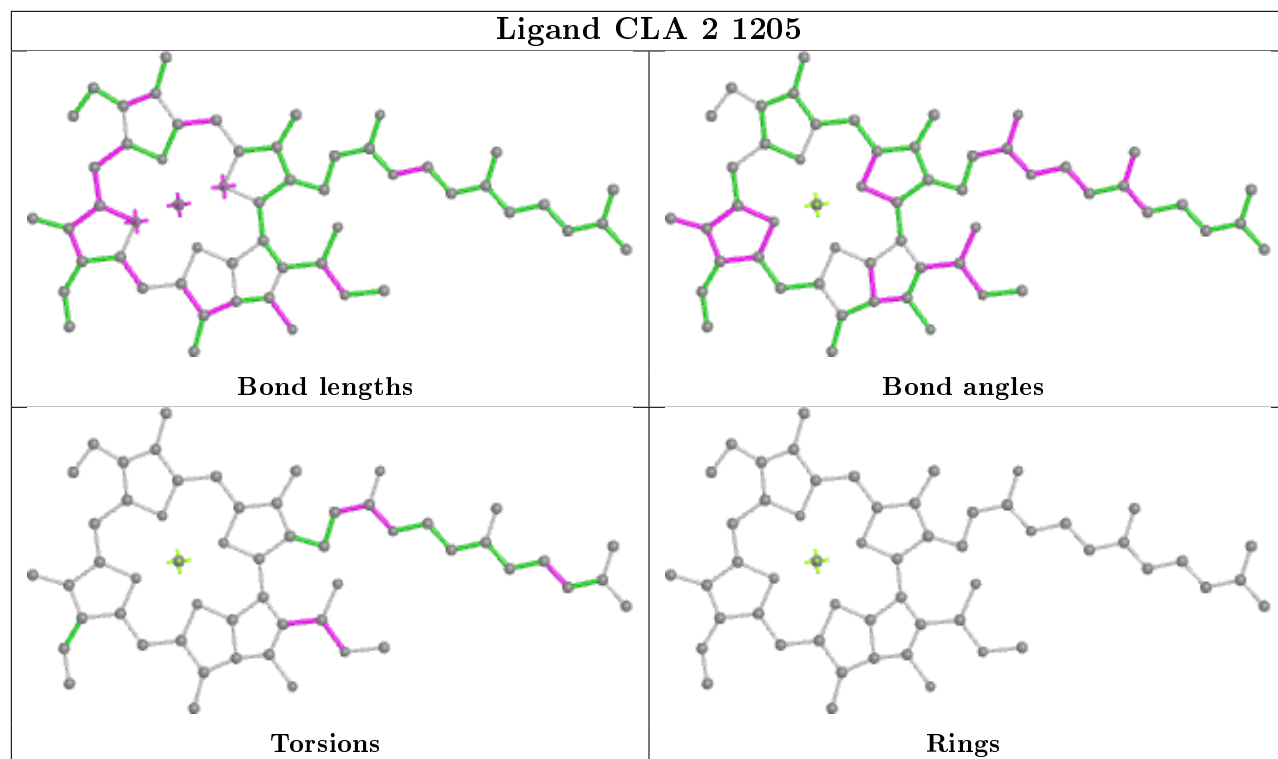
Bond angles



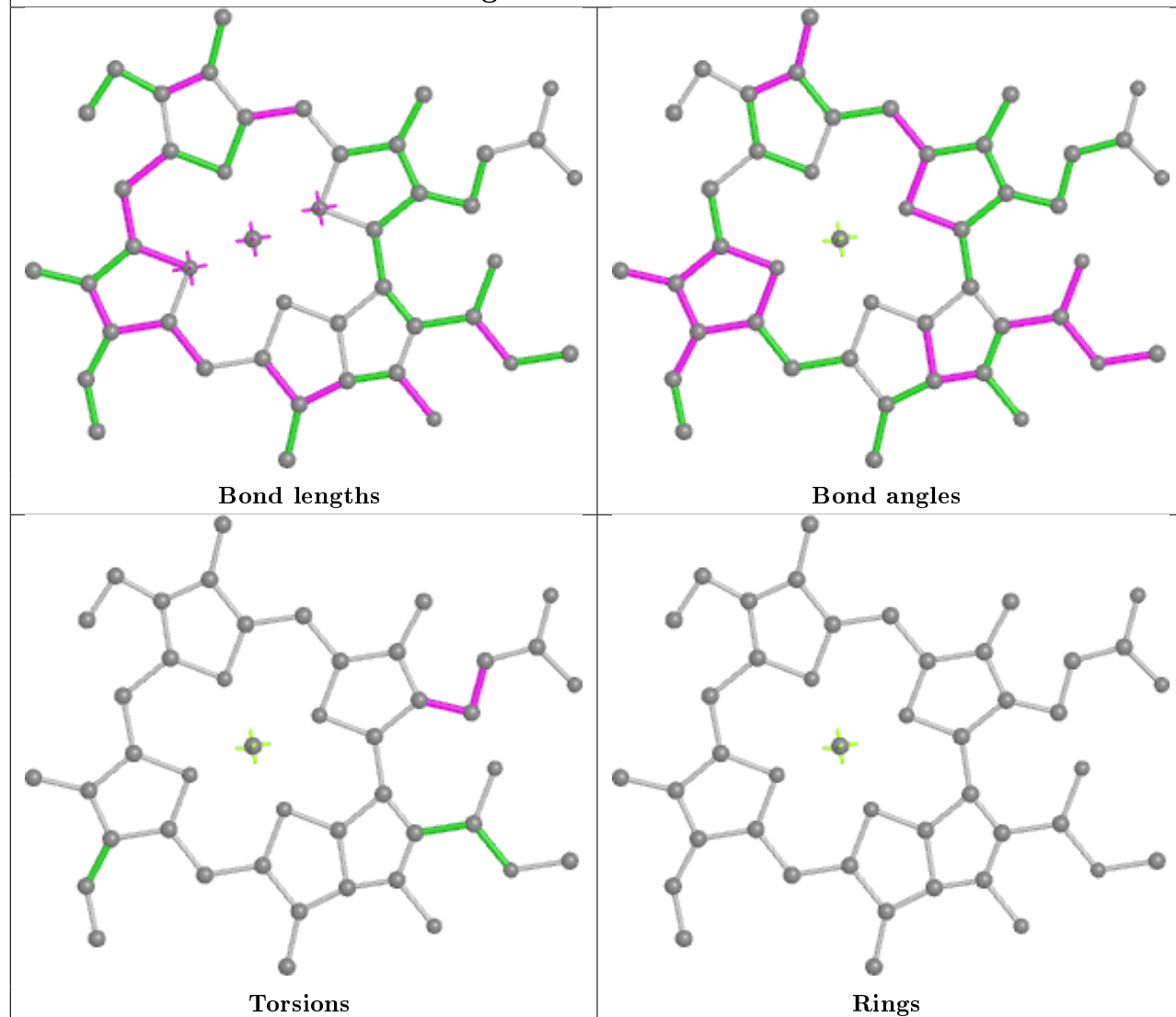
Torsions



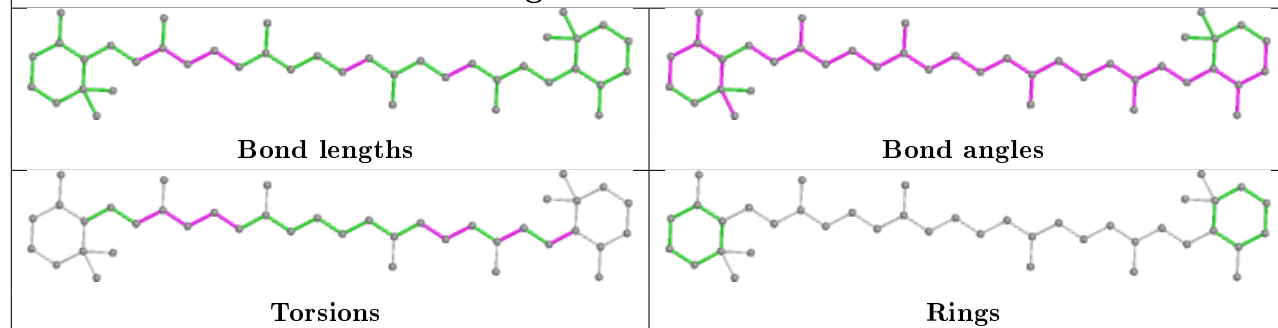
Rings

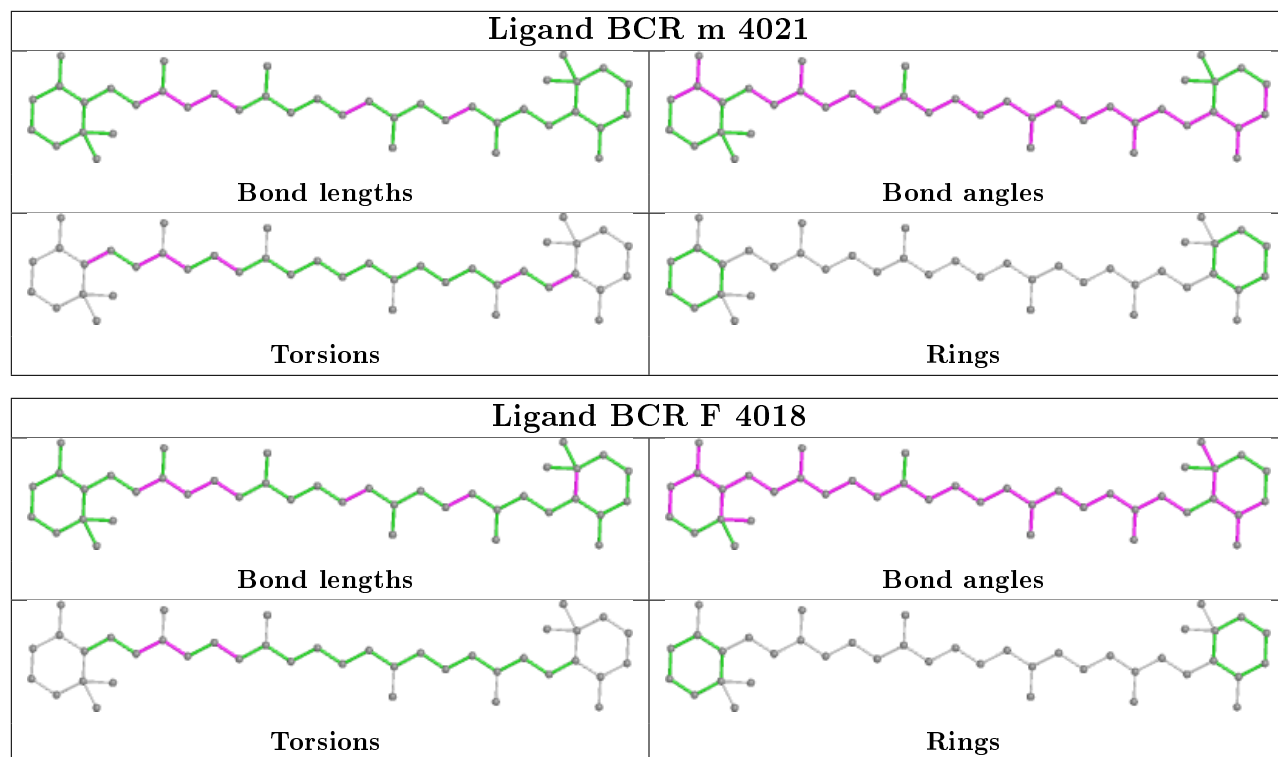


Ligand CLA A 1108

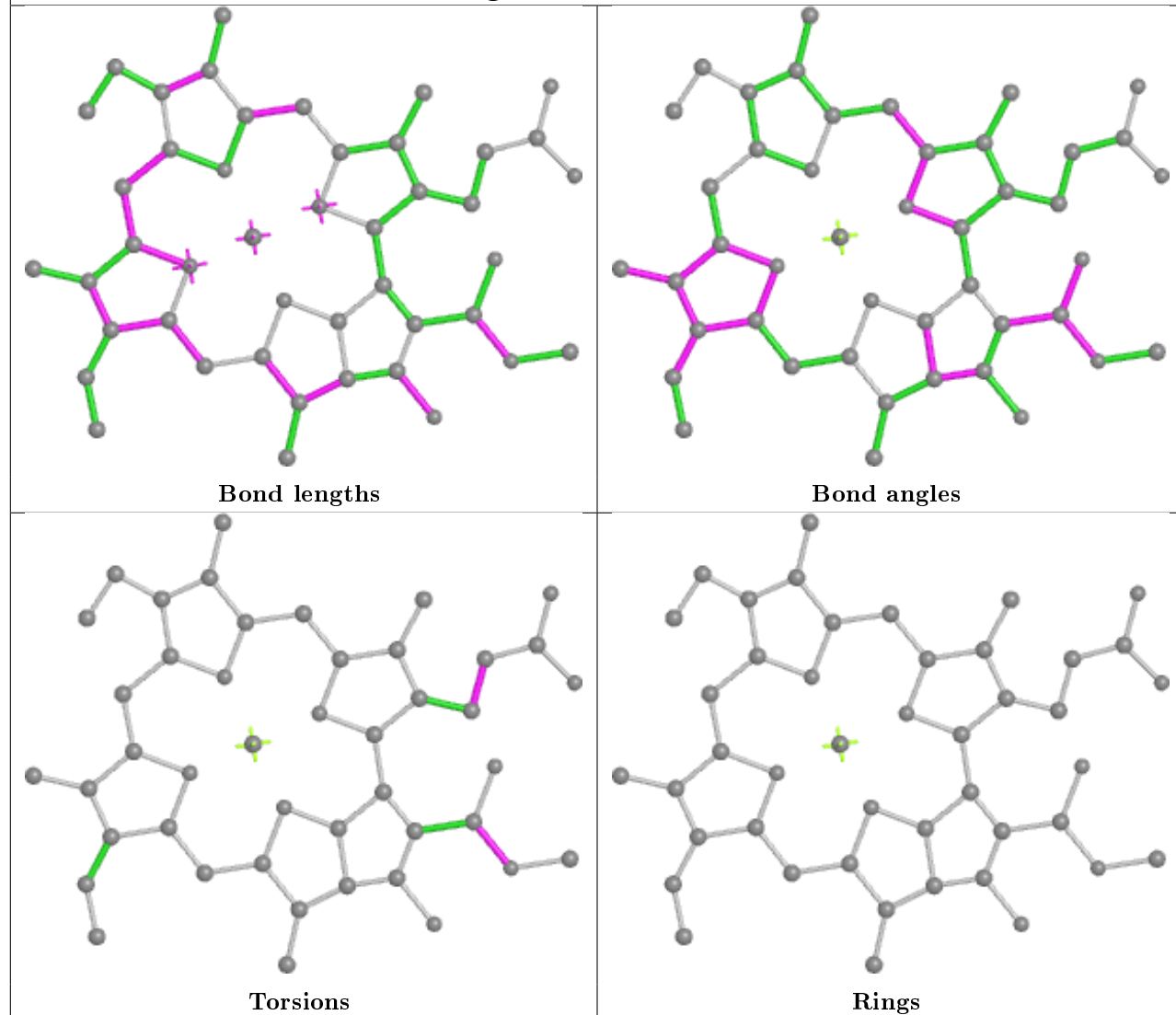


Ligand BCR 1 4007

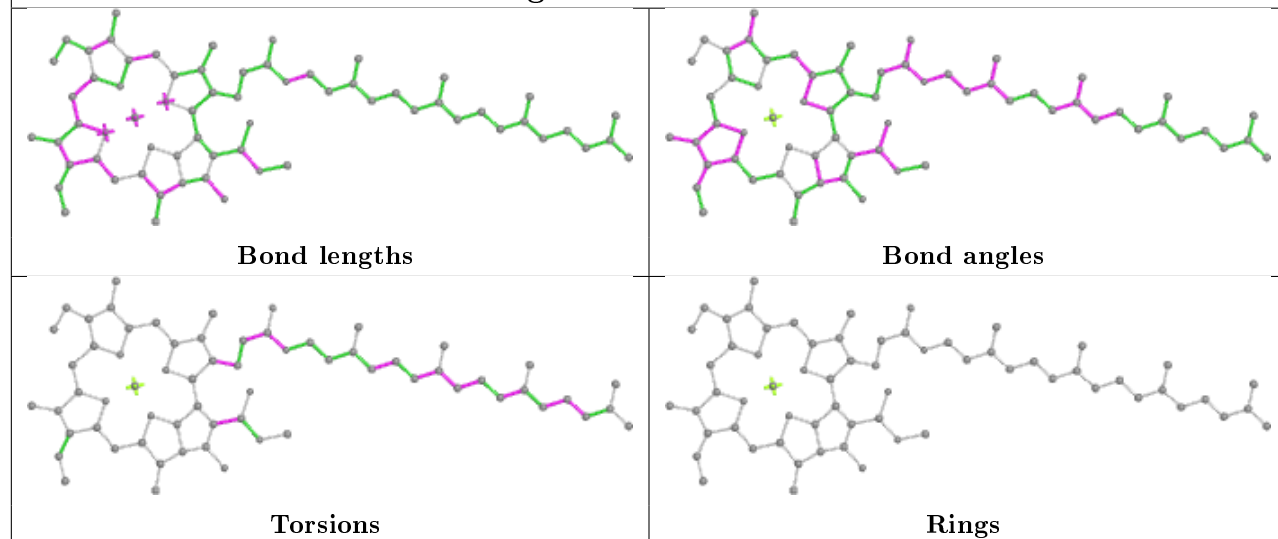


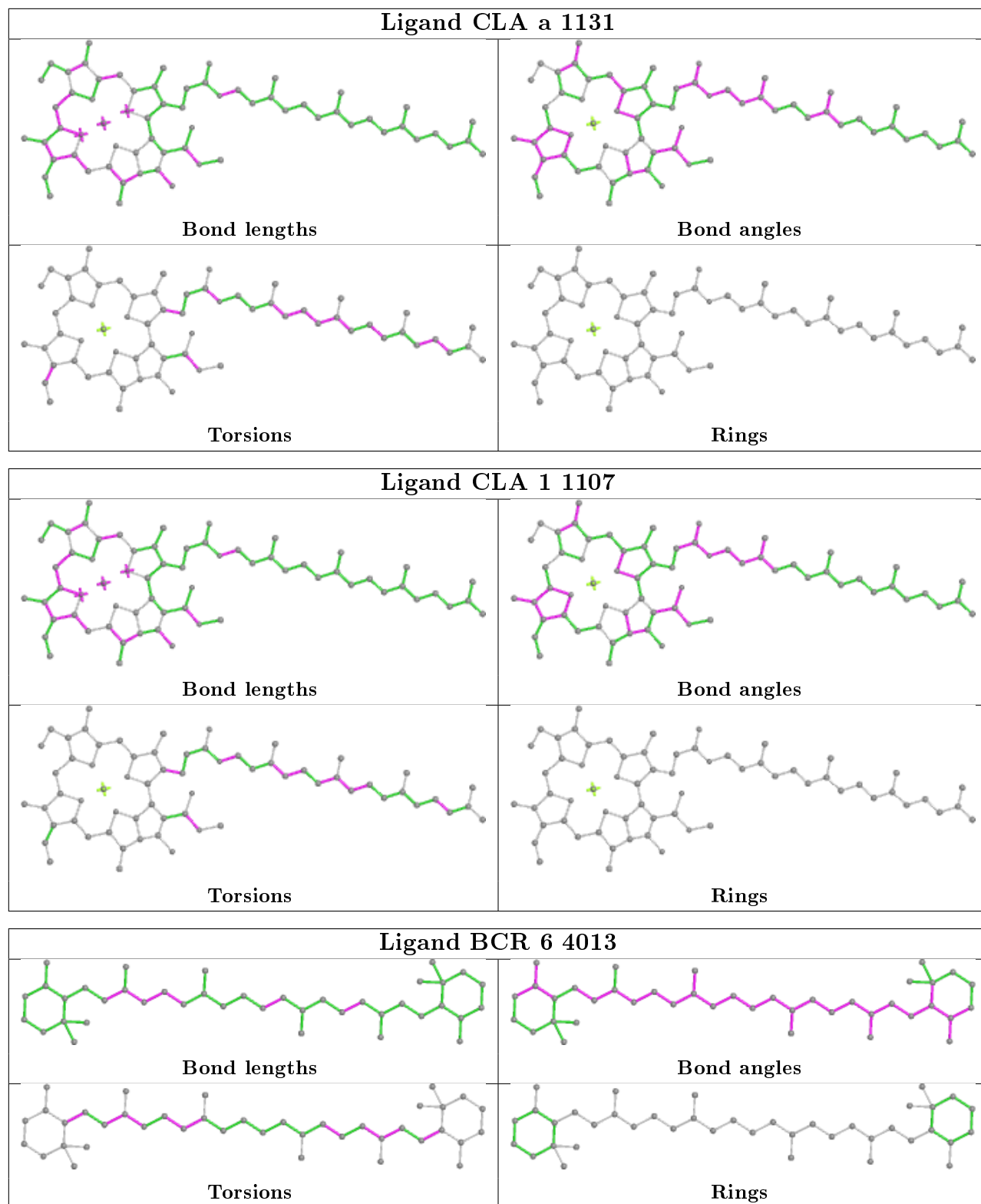


Ligand CLA 1 1113

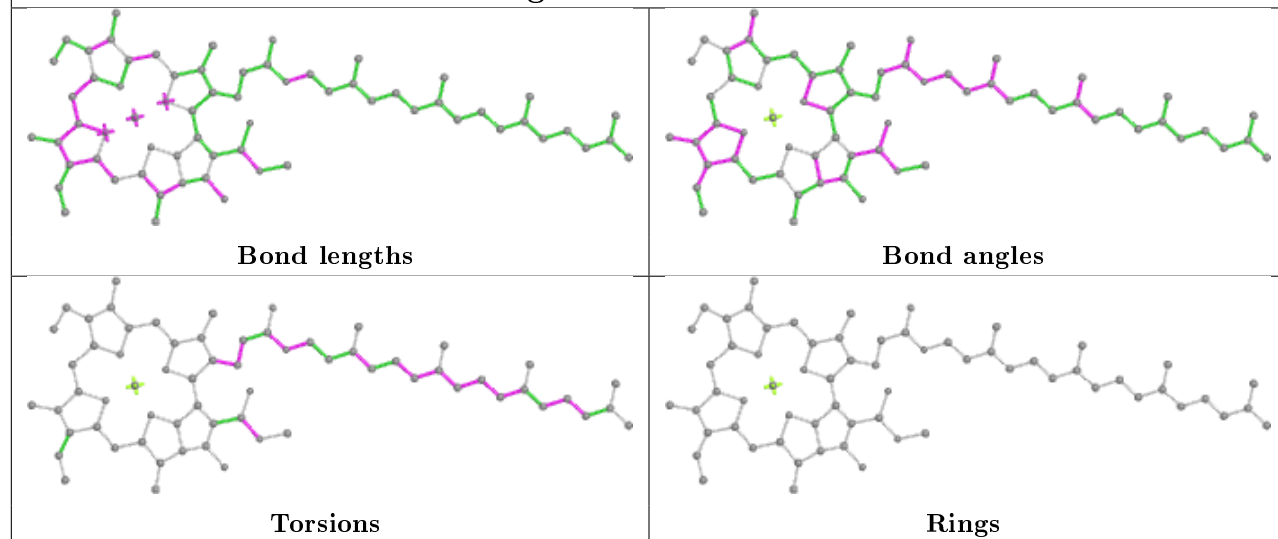


Ligand CLA 2 1210

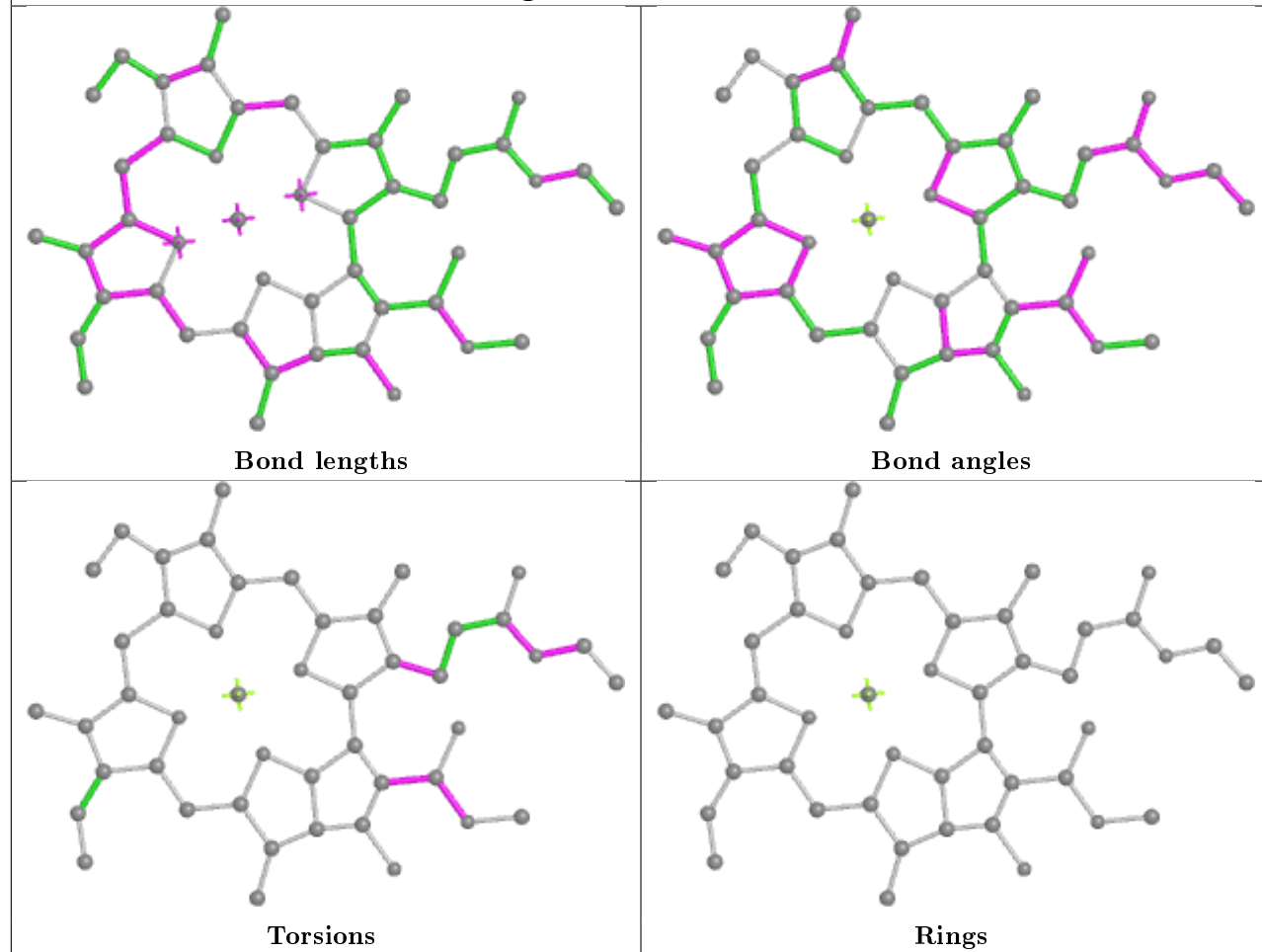


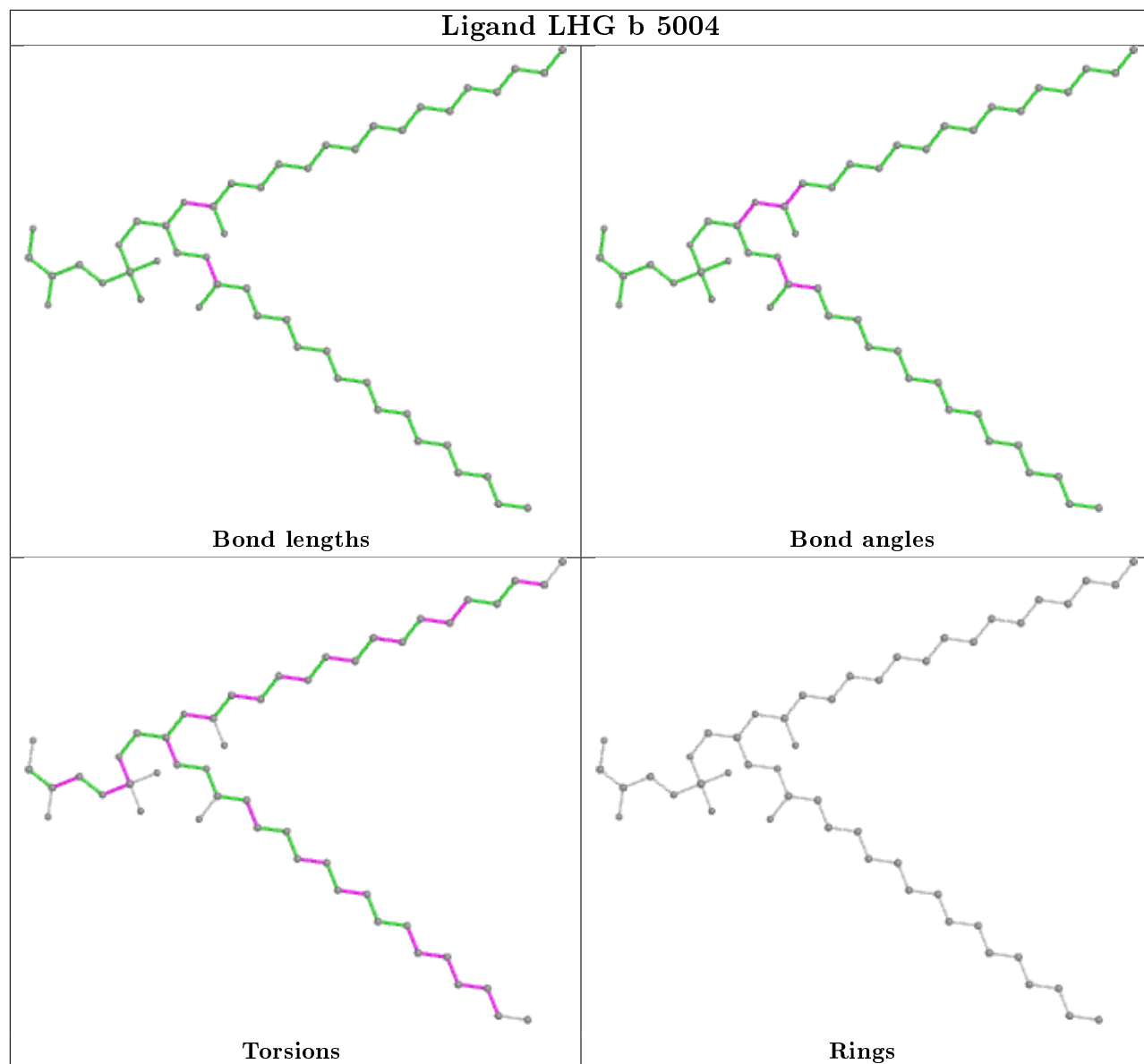
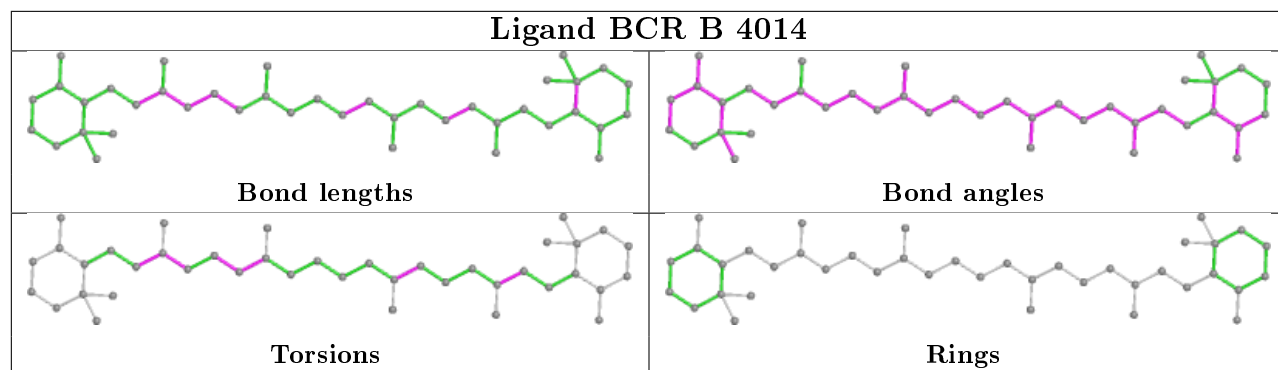


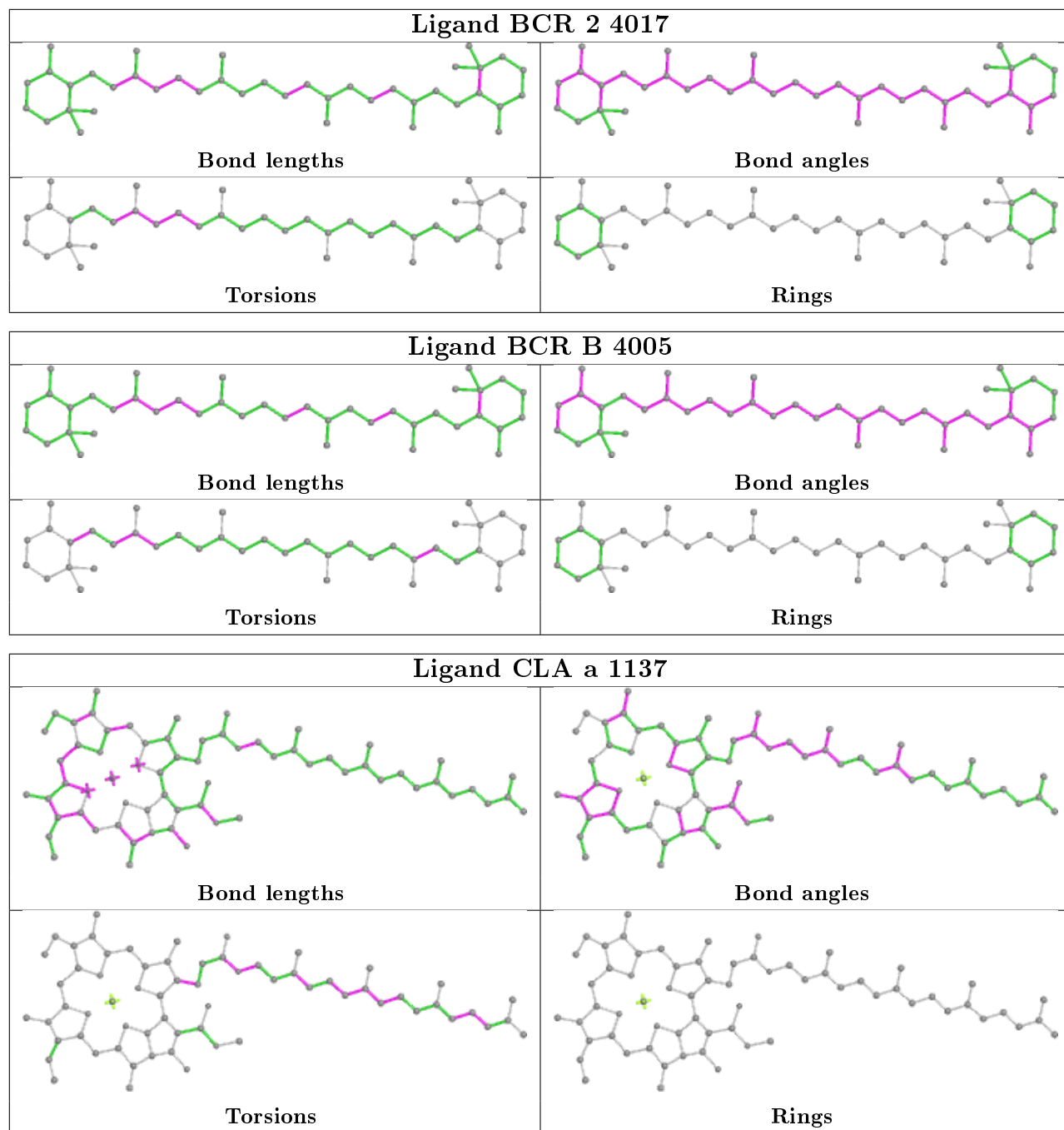
Ligand CLA a 1109

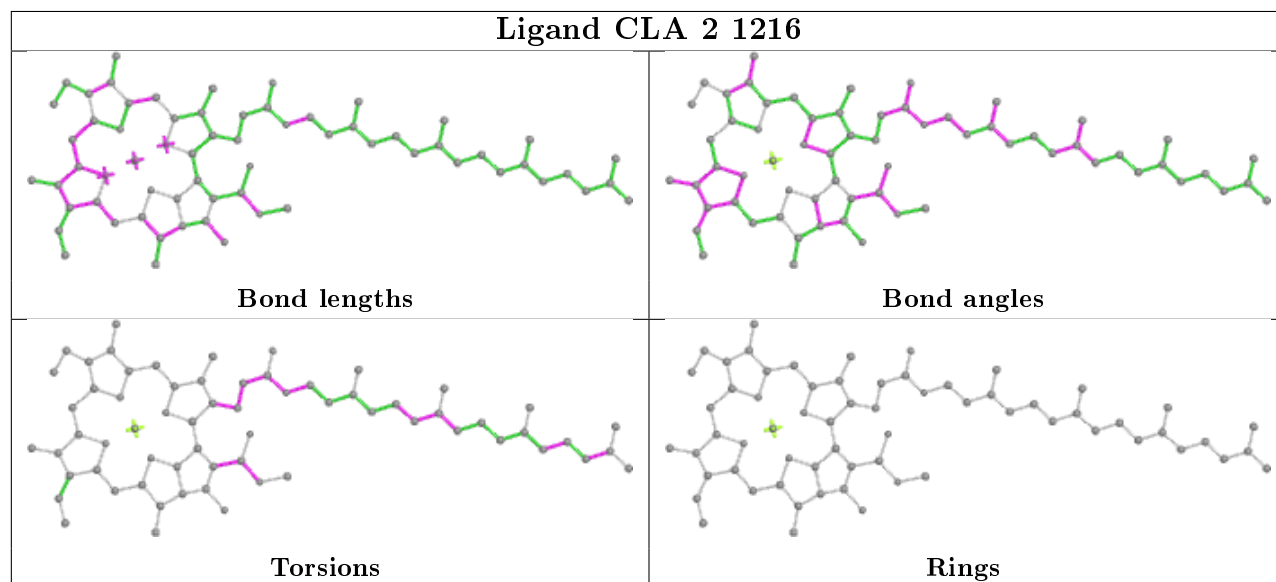
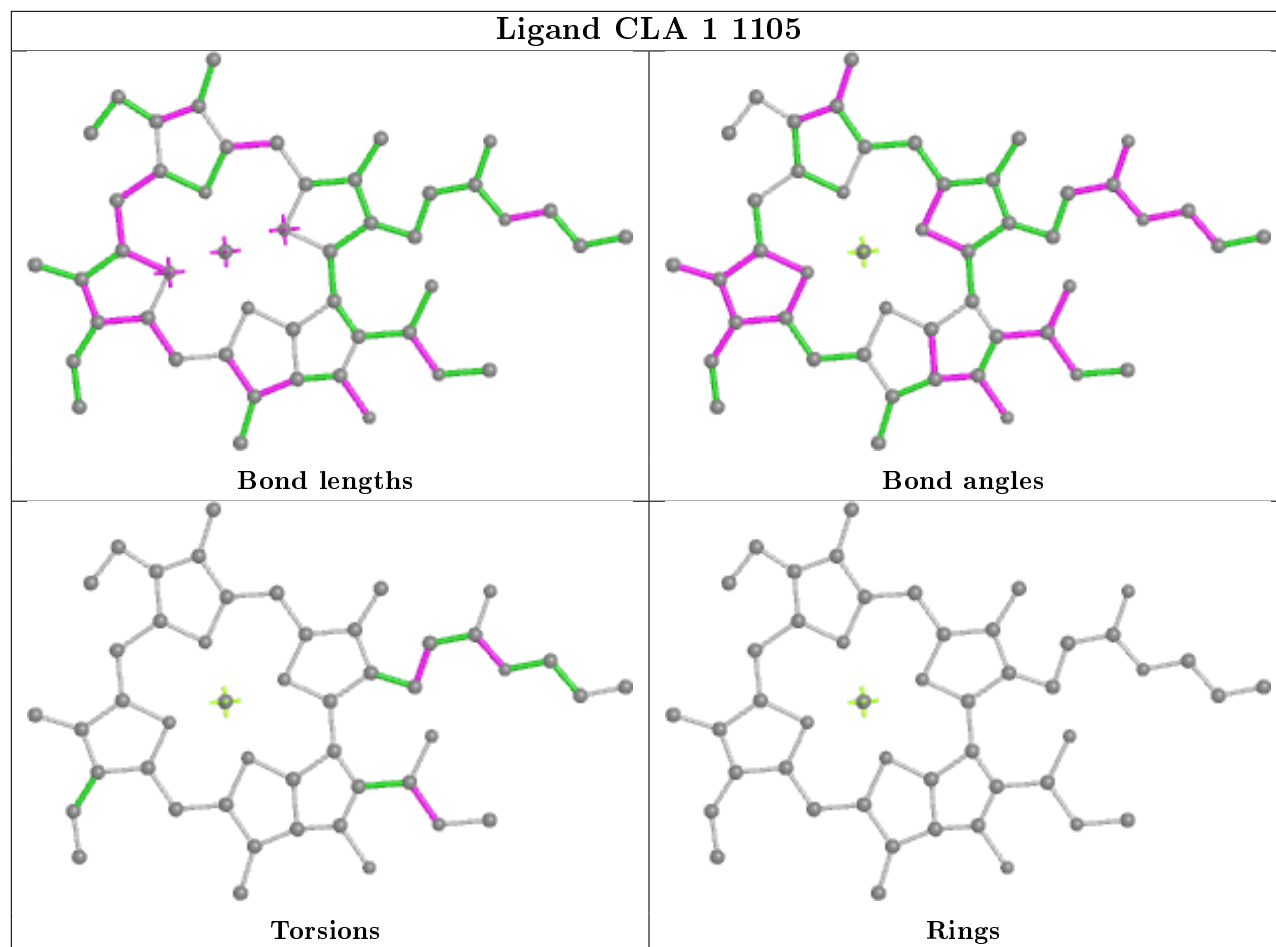


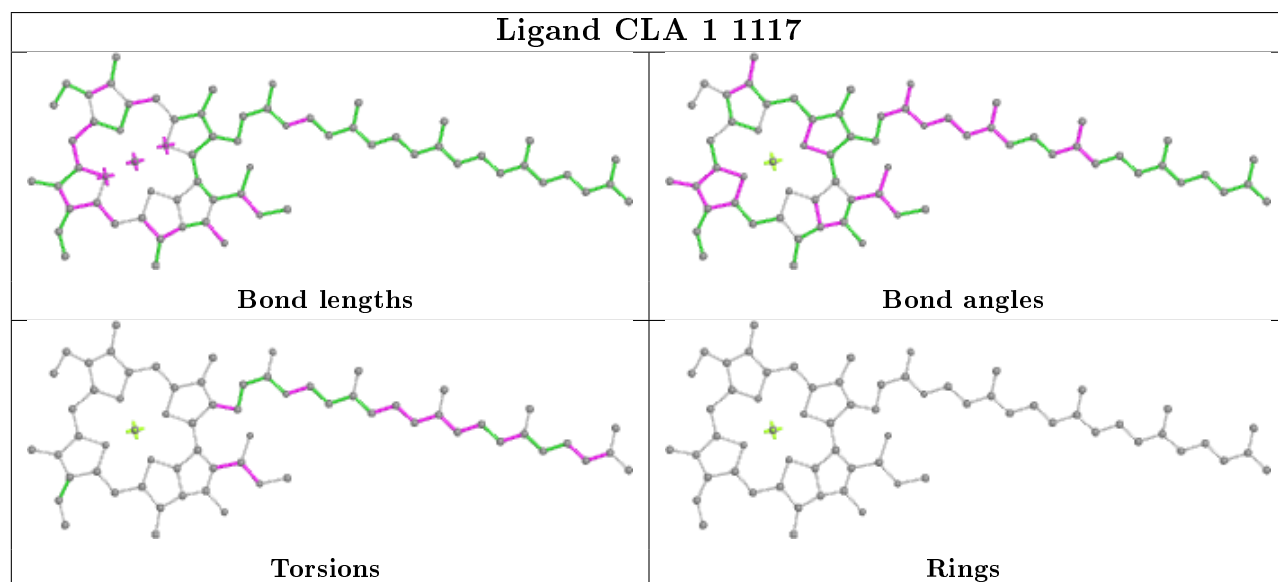
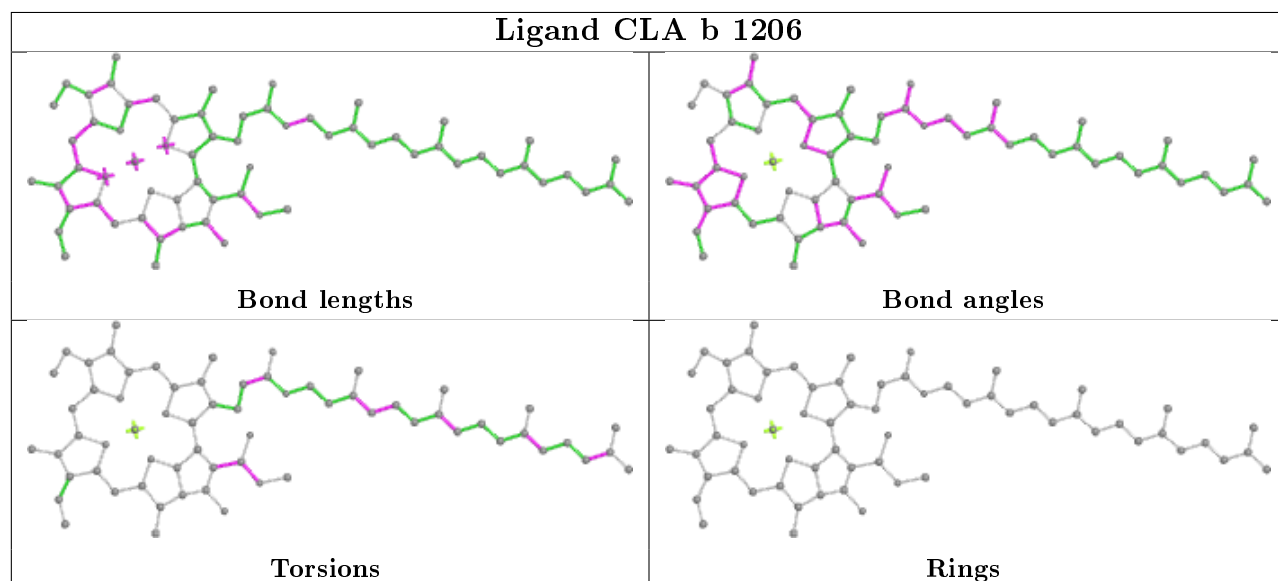
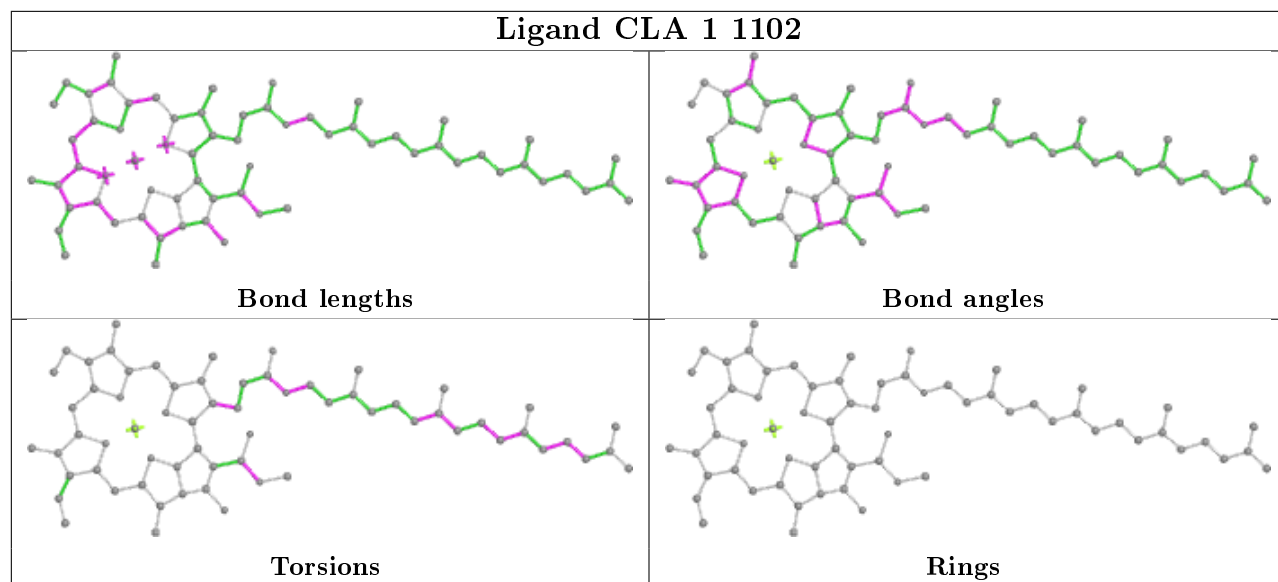
Ligand CLA b 1236



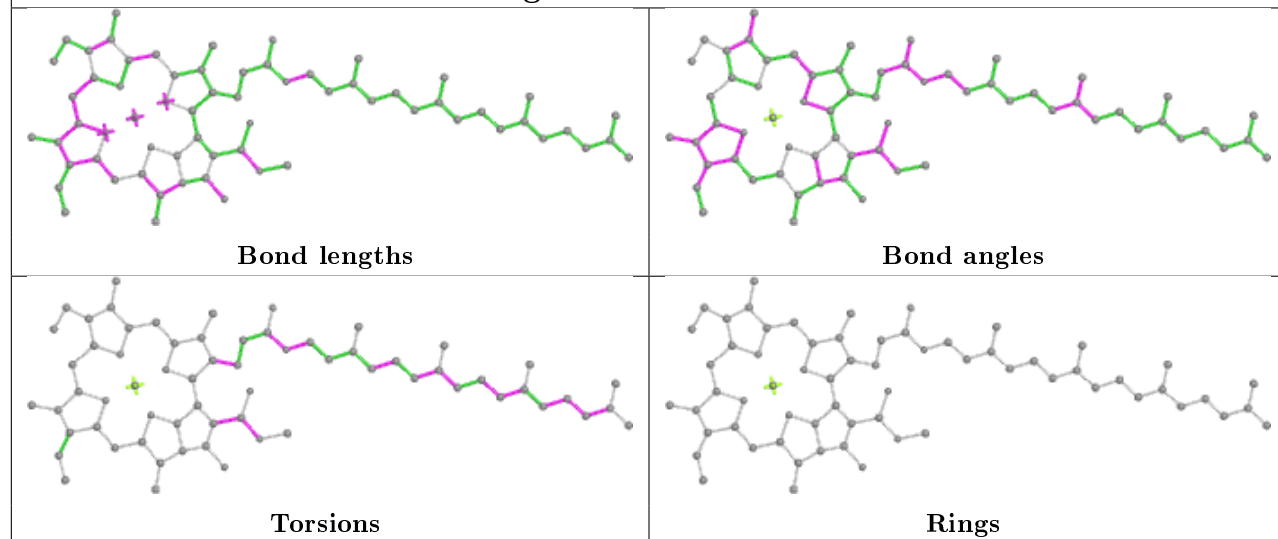




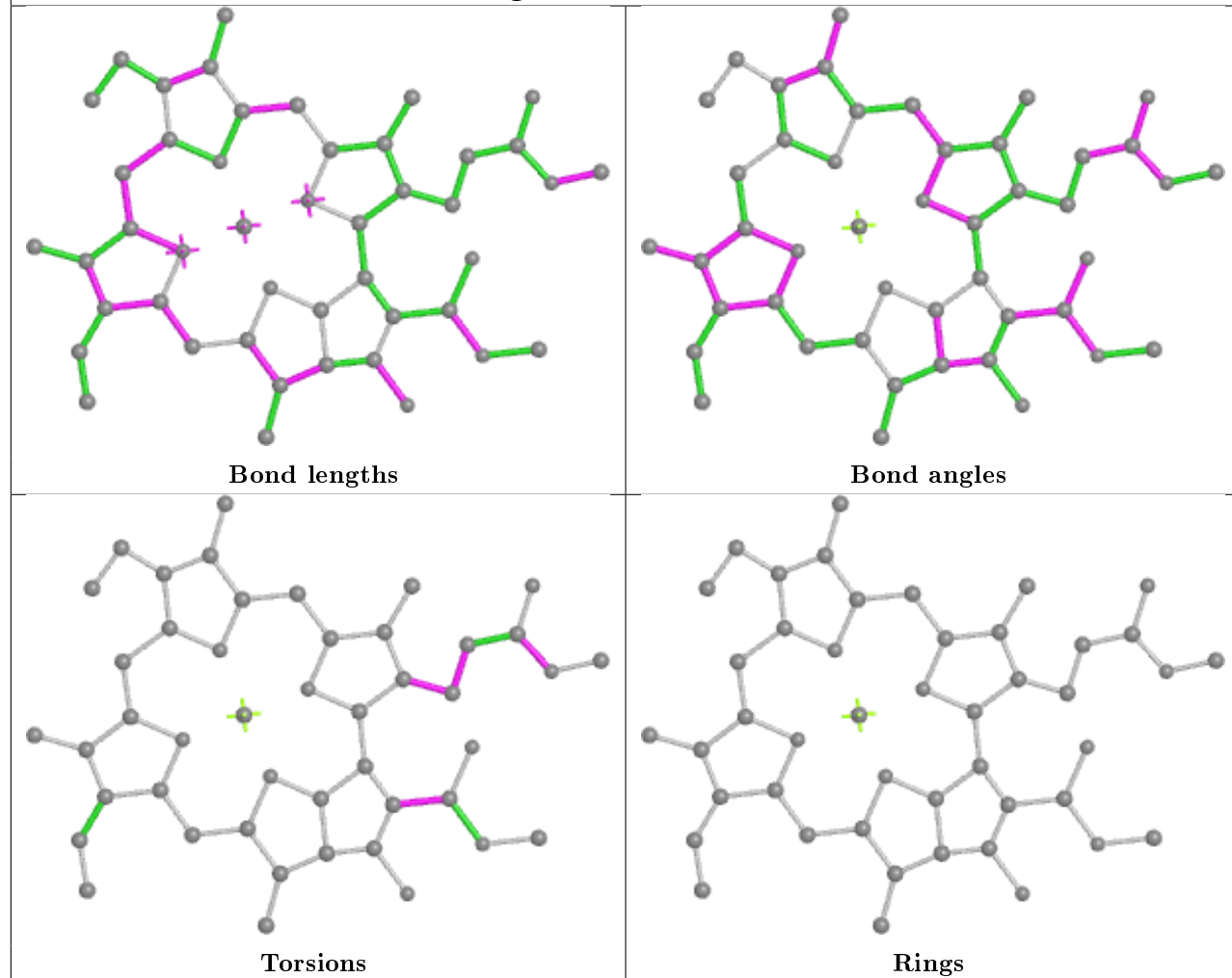


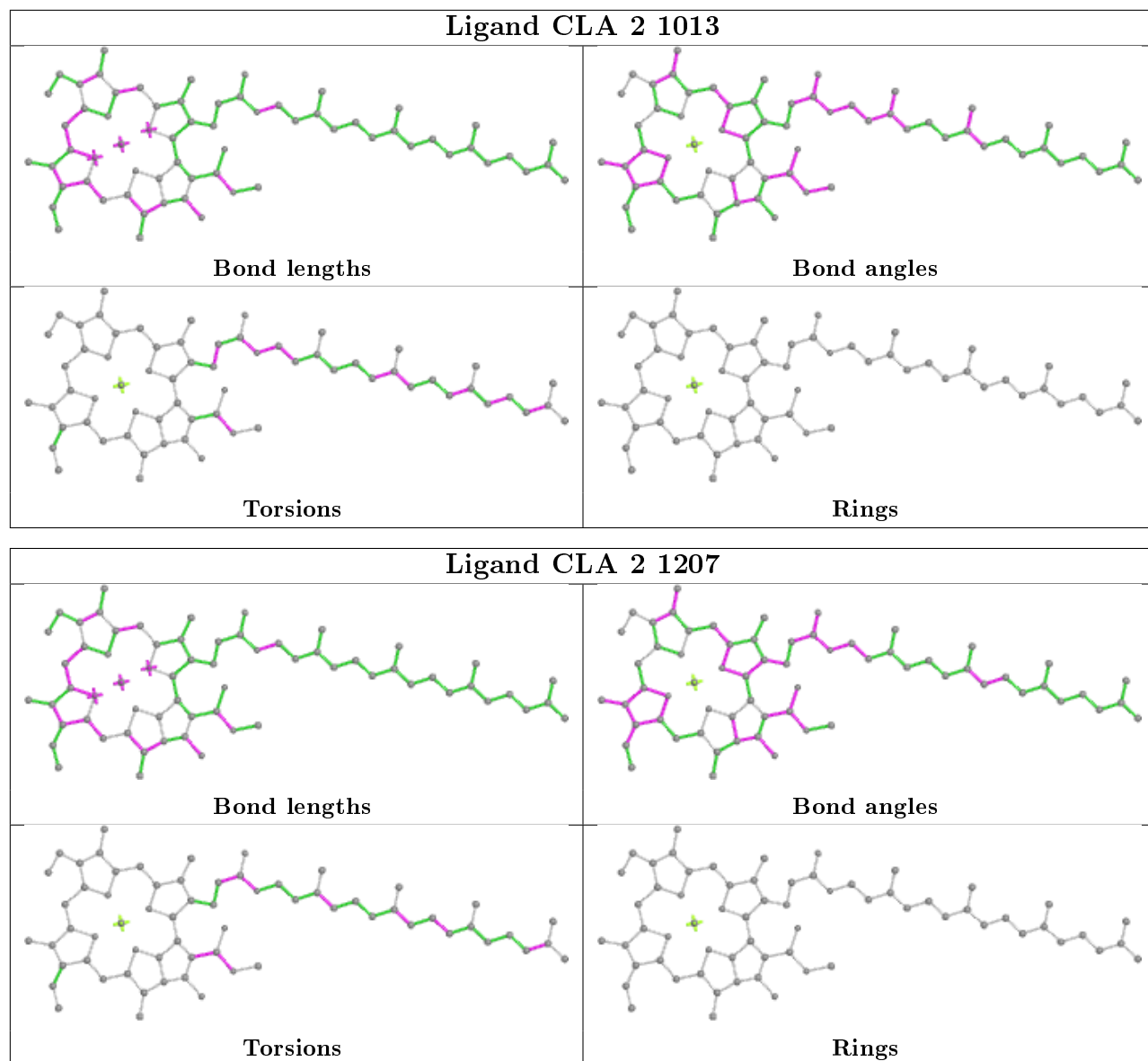


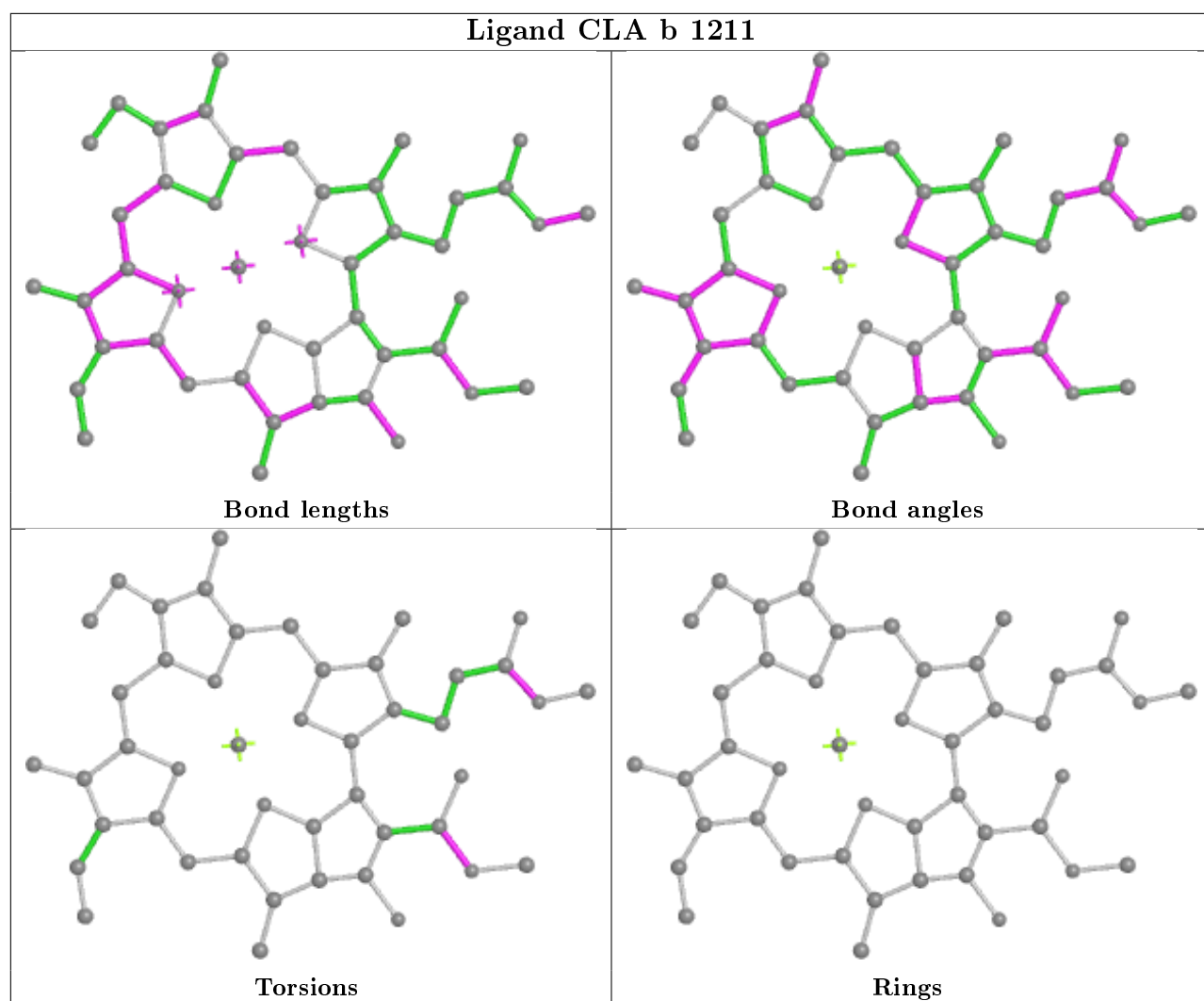
Ligand CLA A 1102

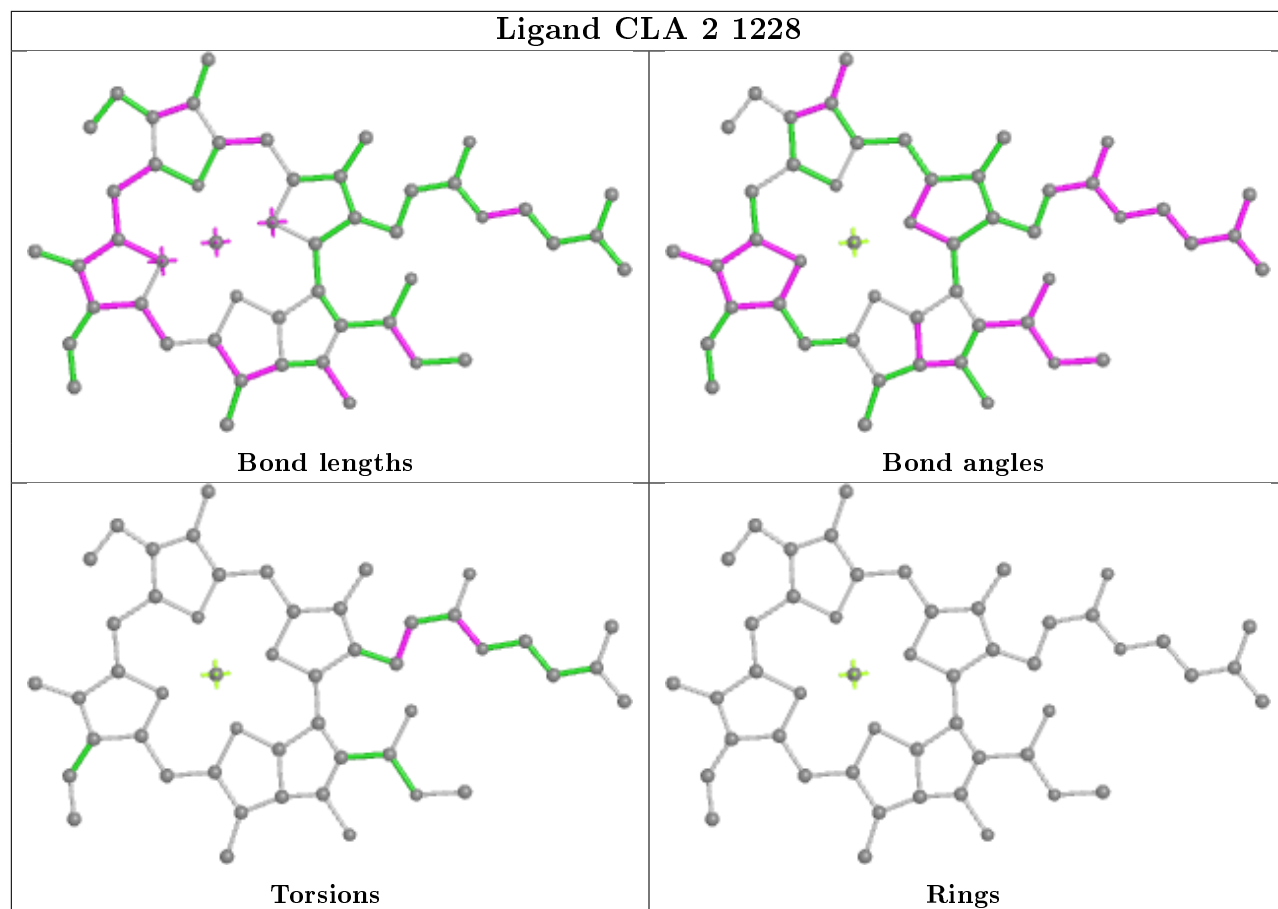


Ligand CLA a 1129

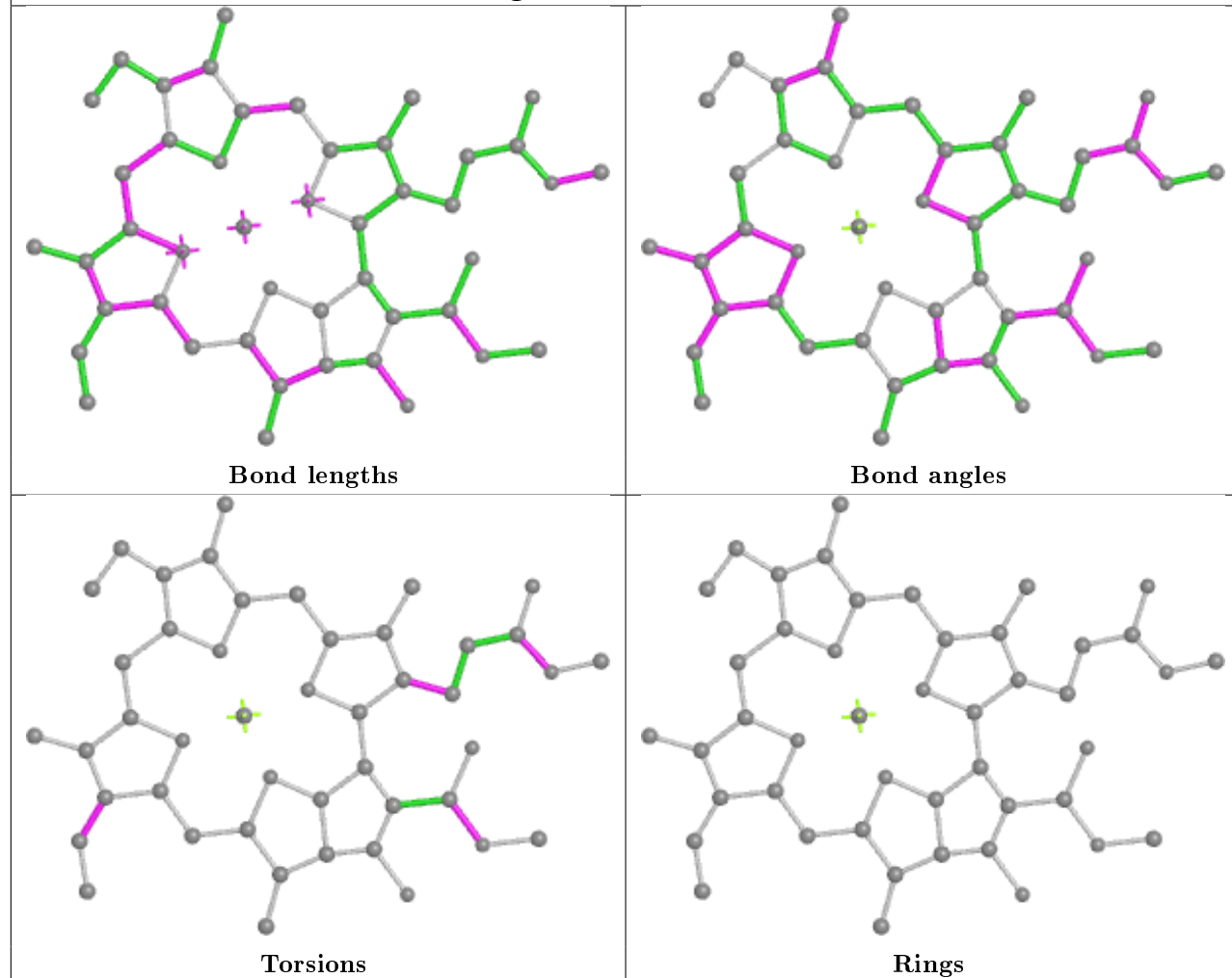




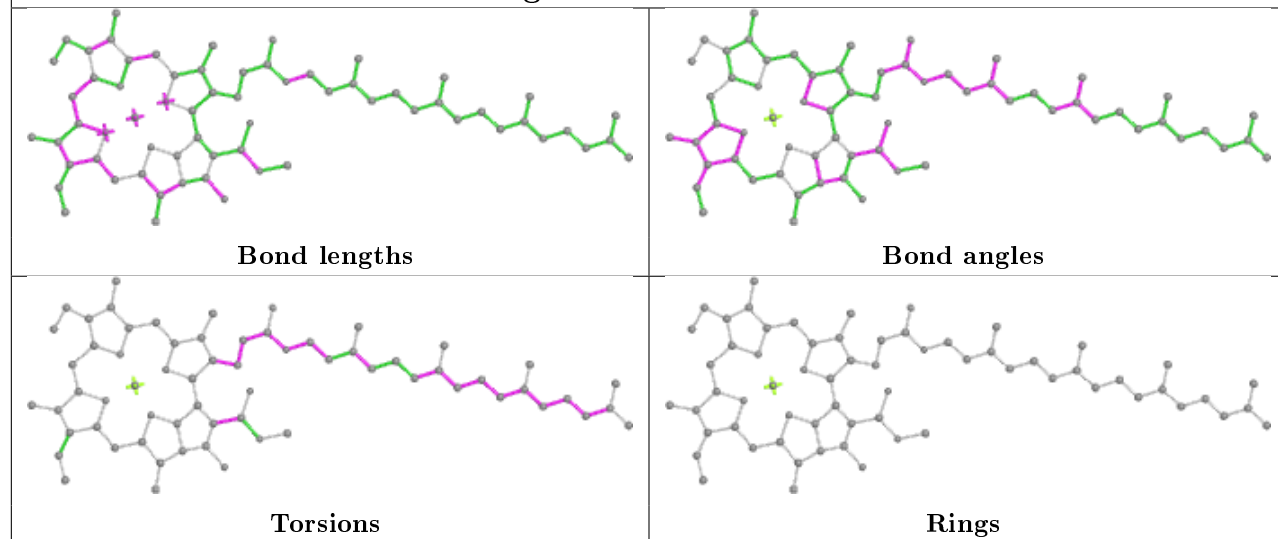


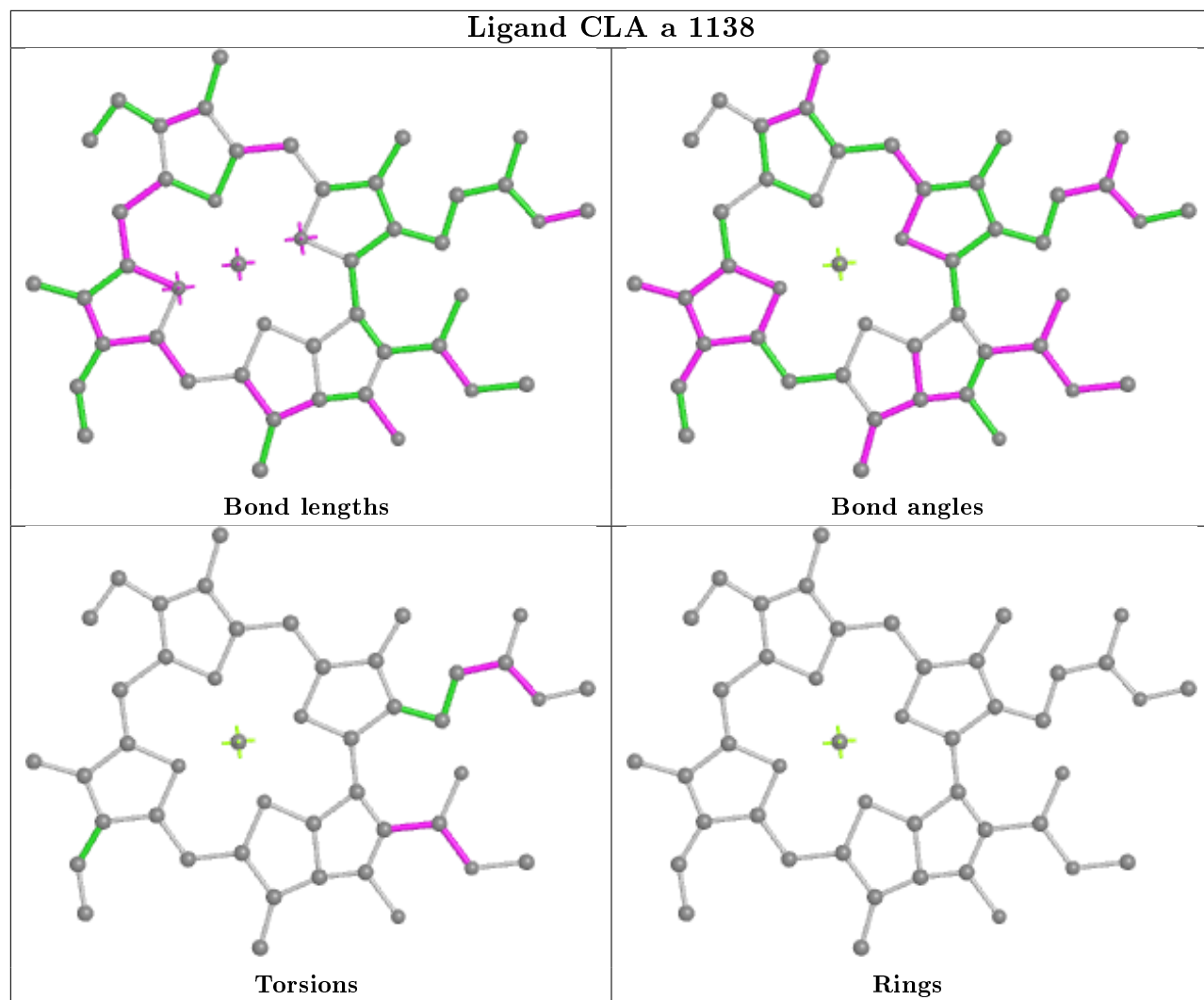
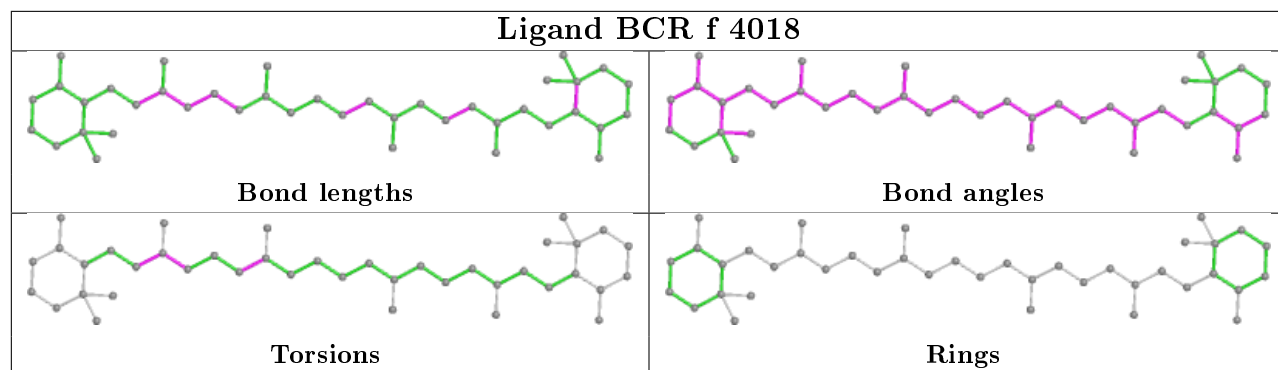


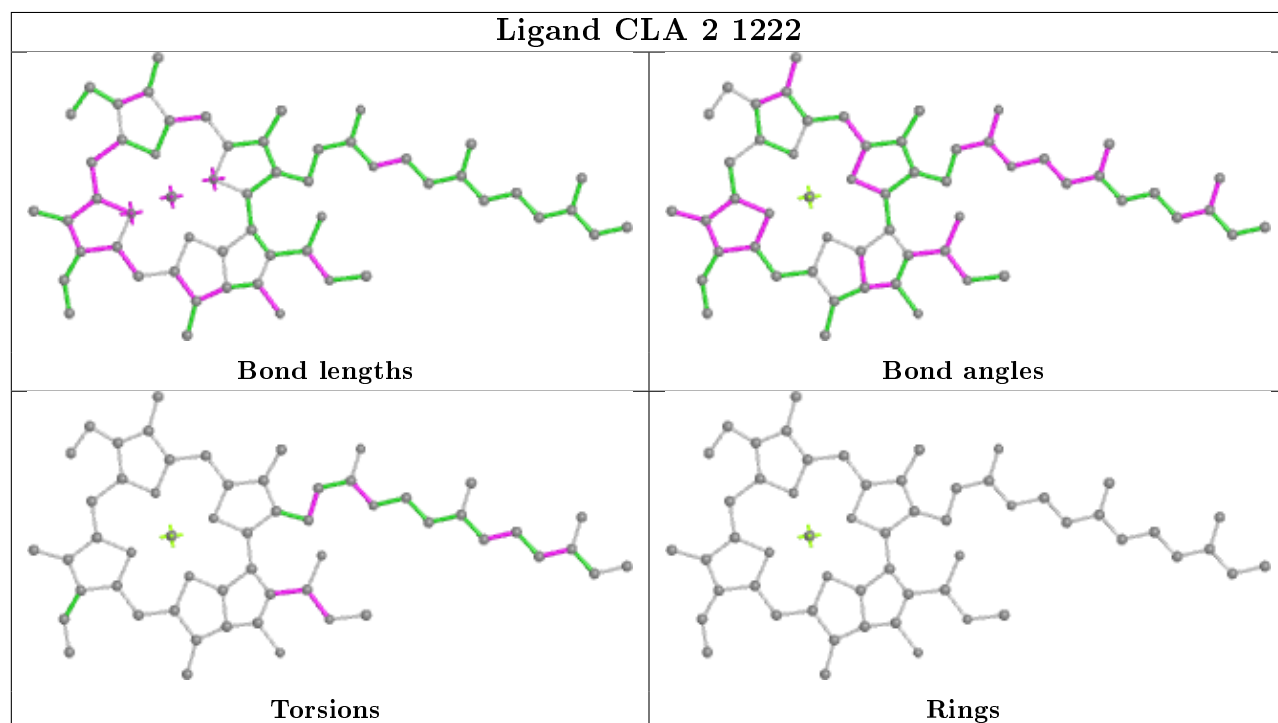
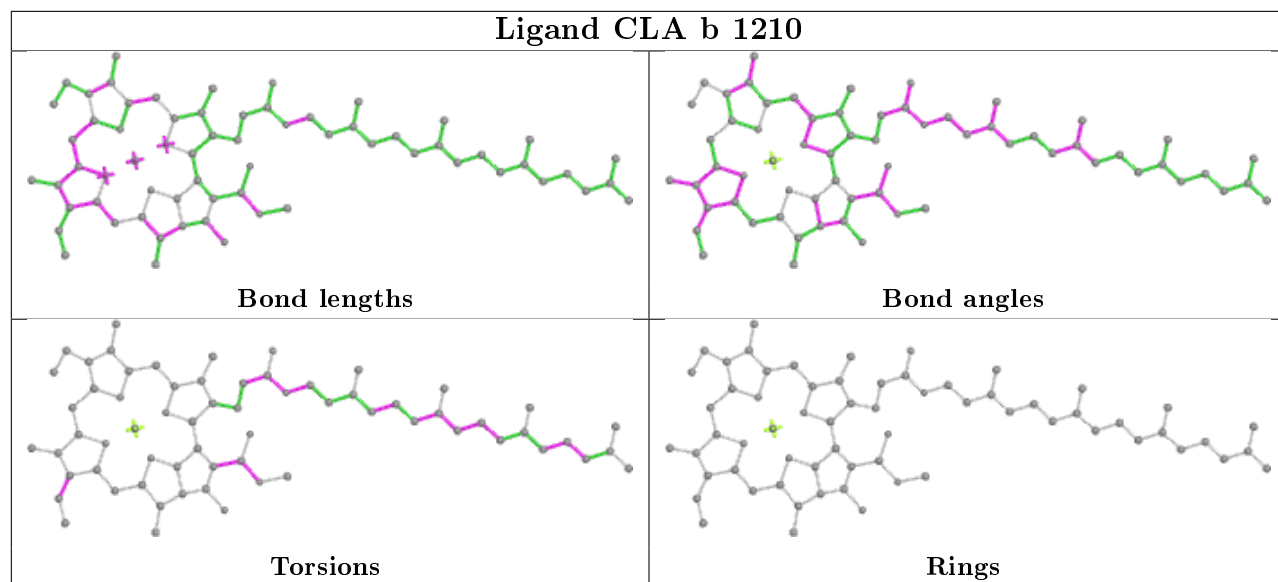
Ligand CLA a 1130



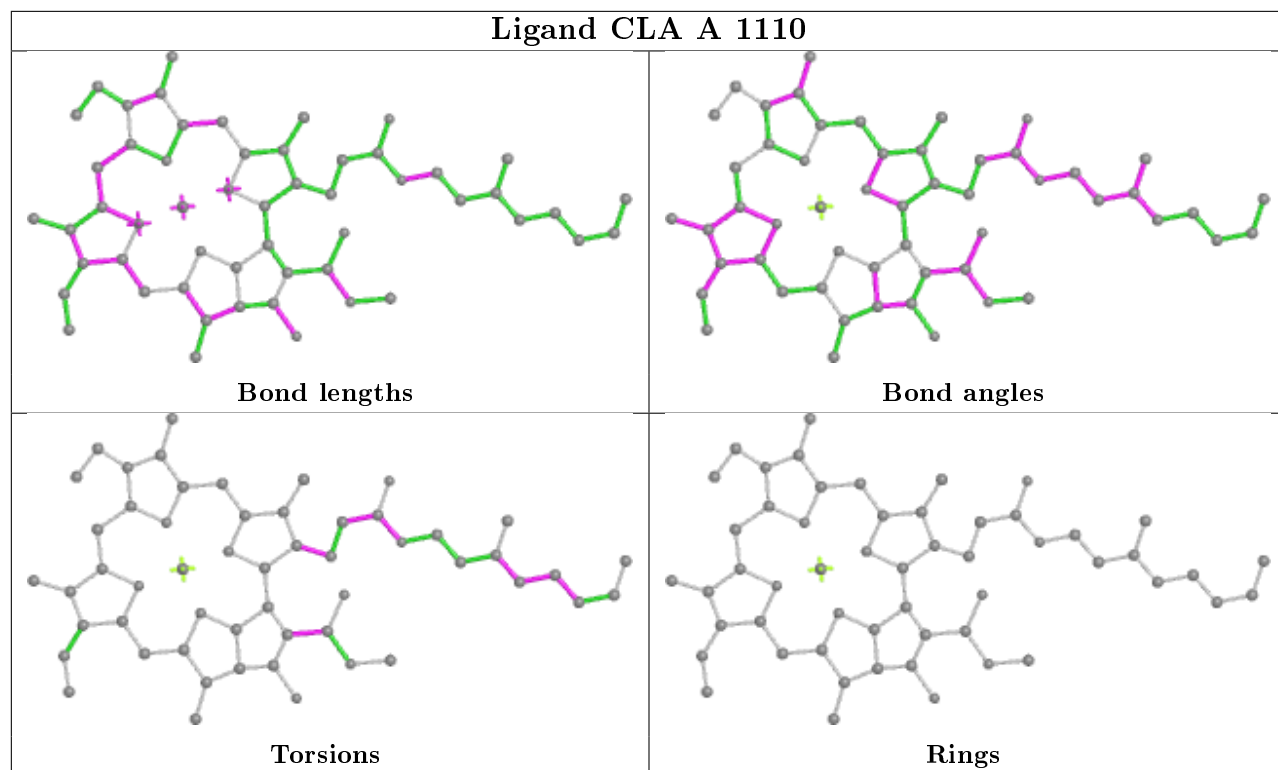
Ligand CLA B 1229



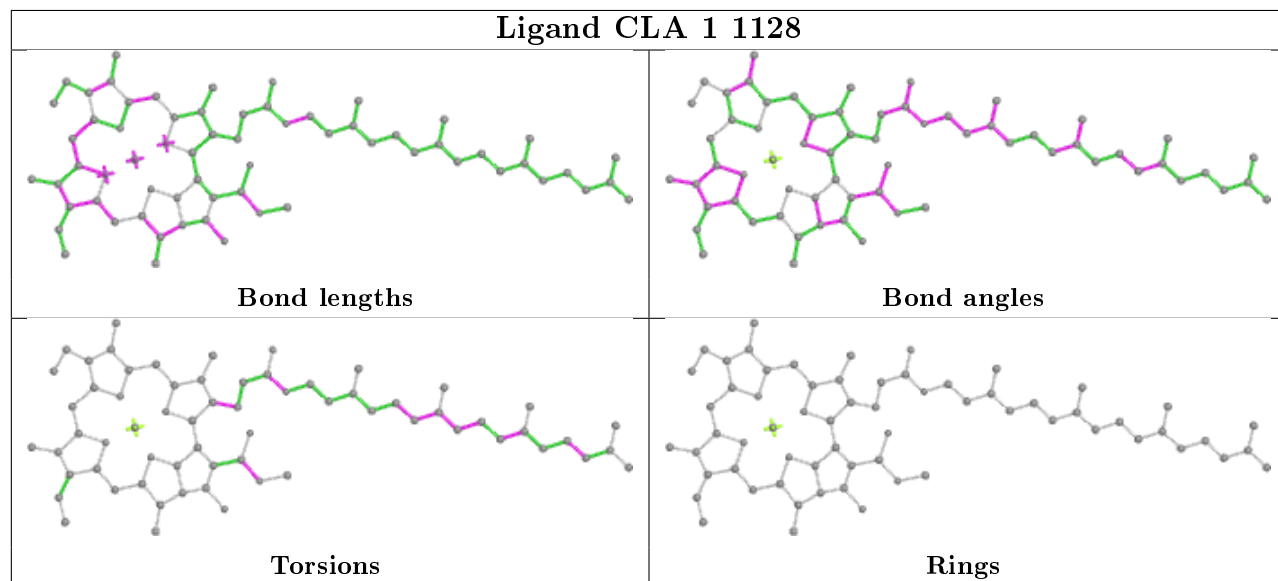


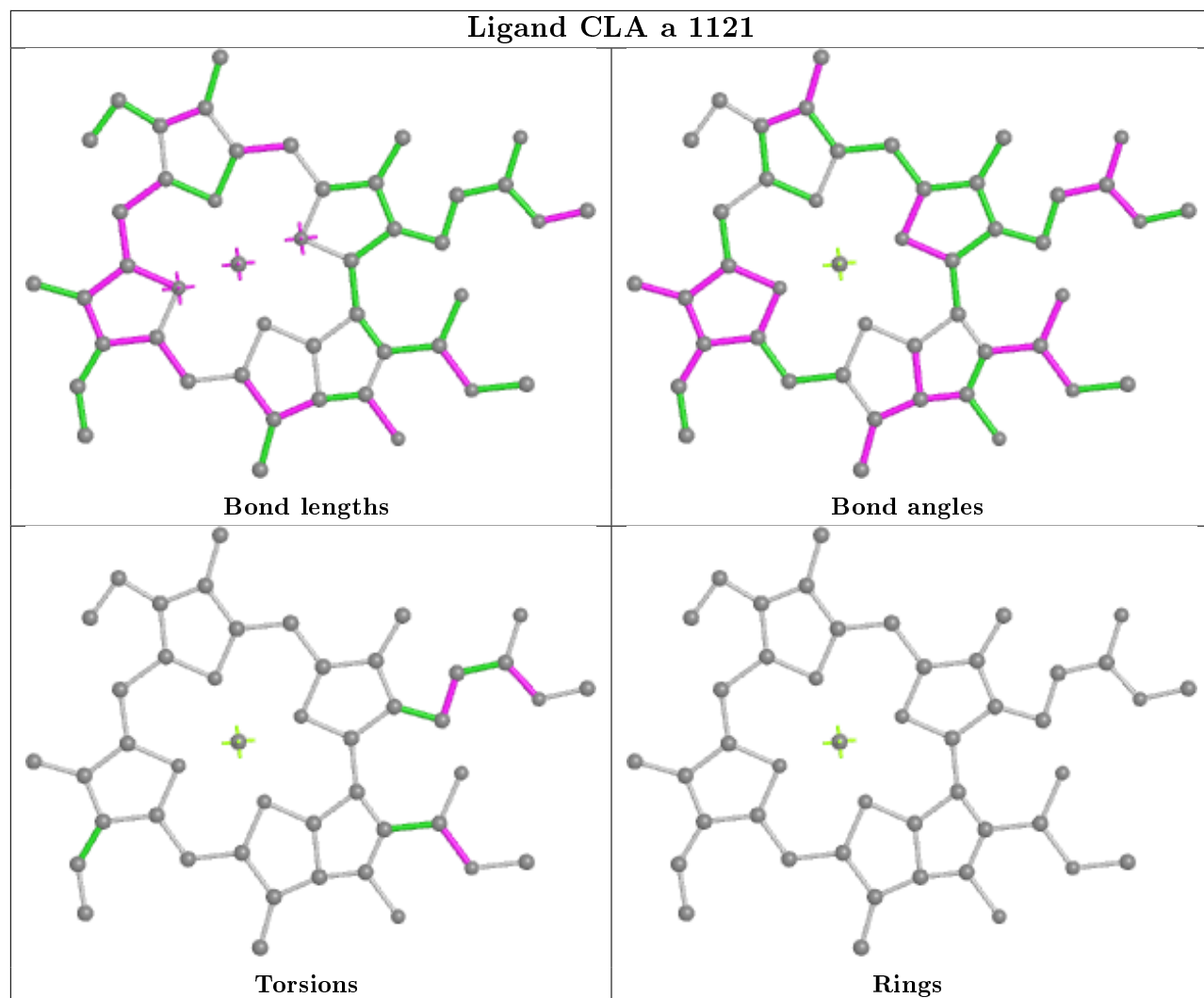


Ligand CLA A 1110



Ligand CLA 1 1128





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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

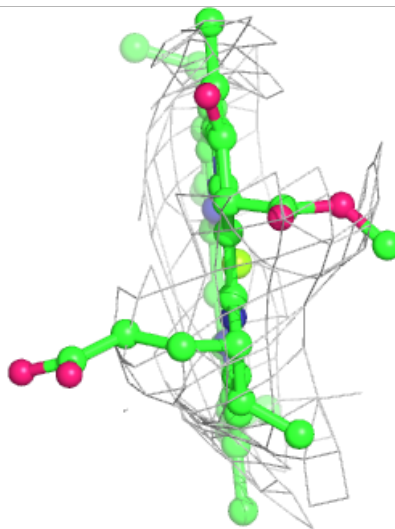
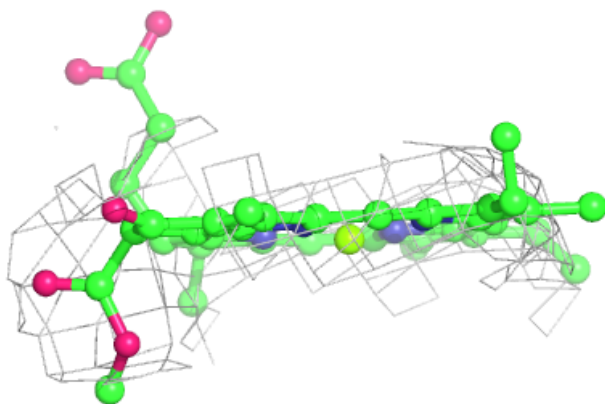
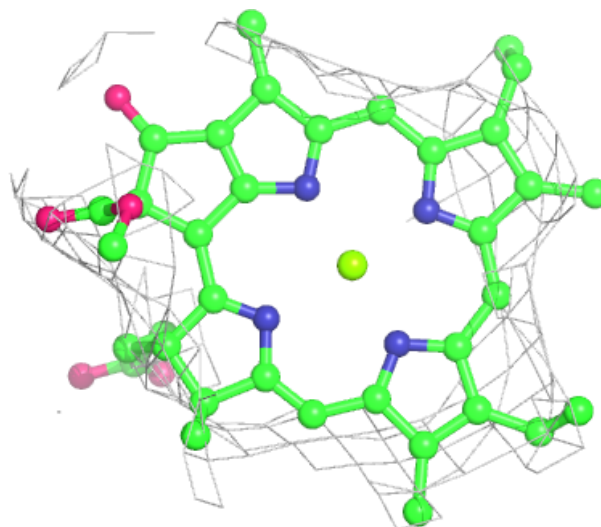
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

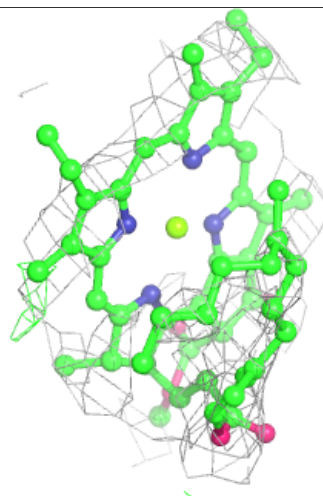
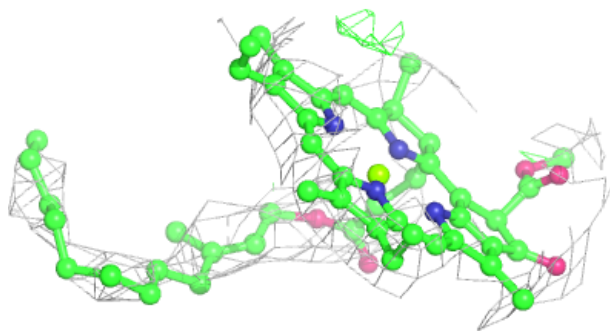
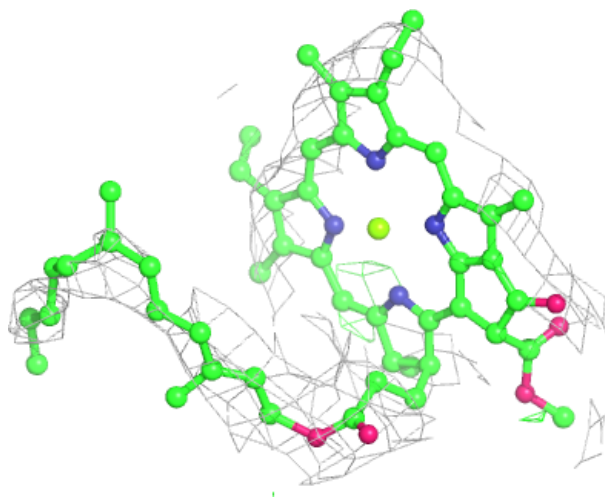
Electron density around CLA 2 1218:

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



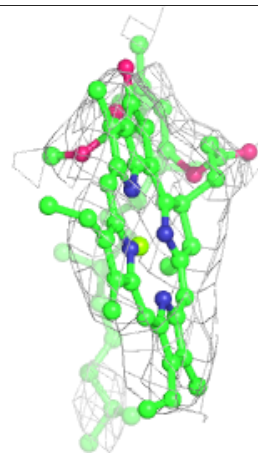
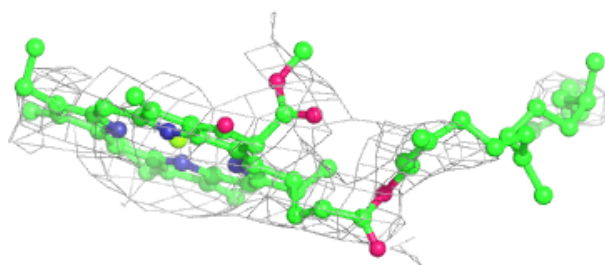
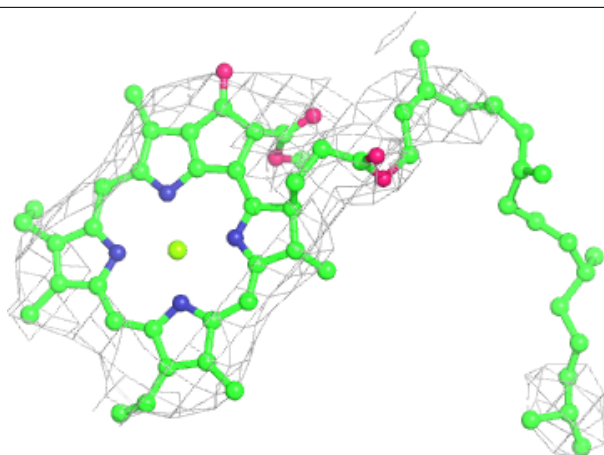
Electron density around CLA a 1122:

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



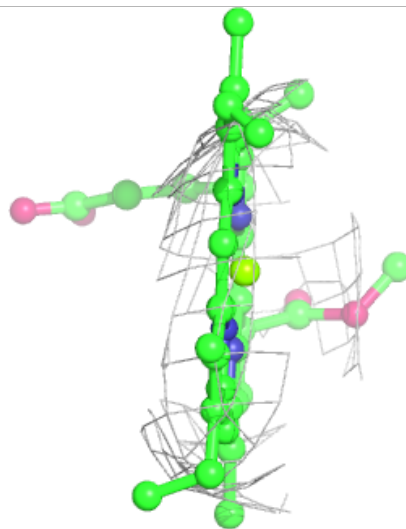
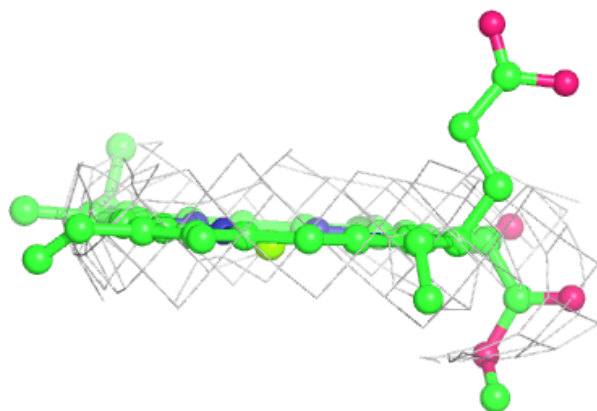
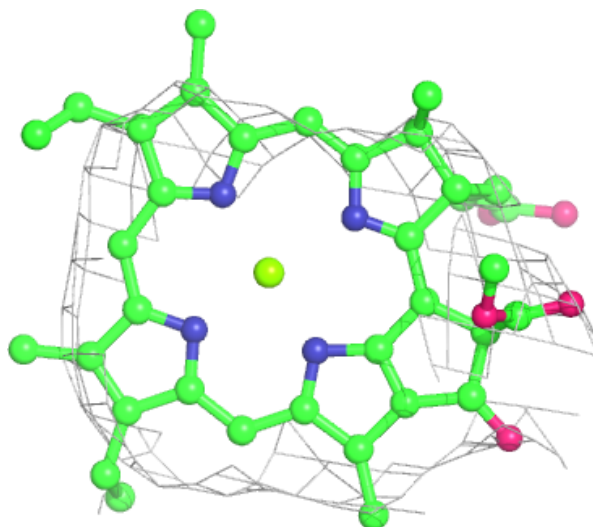
Electron density around CLA A 1101:

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



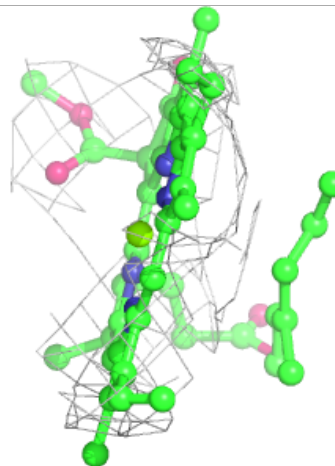
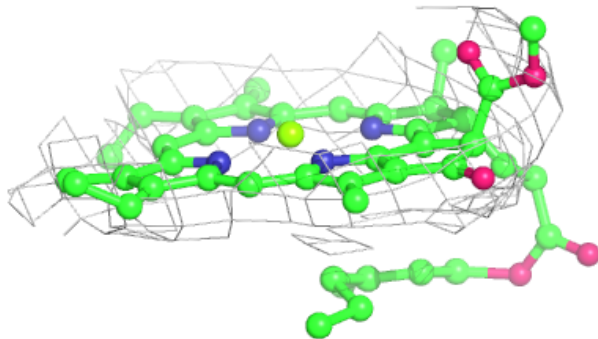
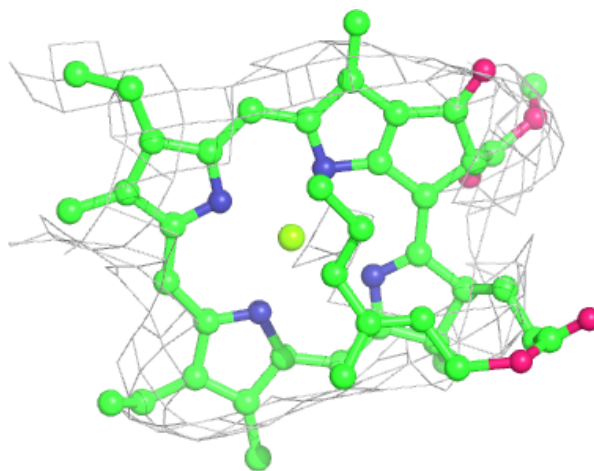
Electron density around CLA b 1218:

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



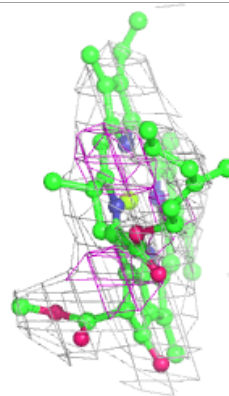
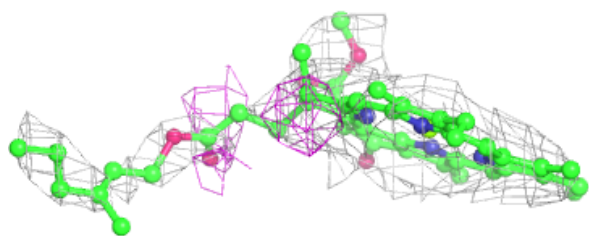
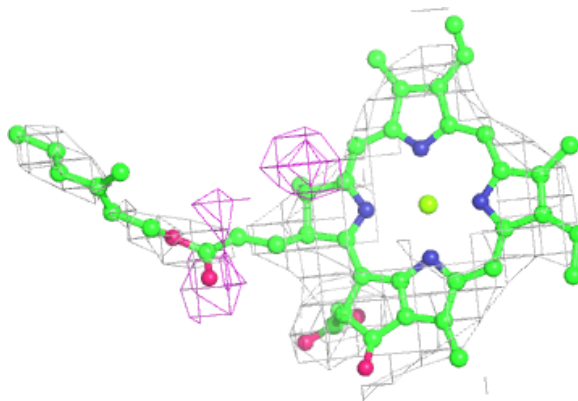
Electron density around CLA 1 1801:

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

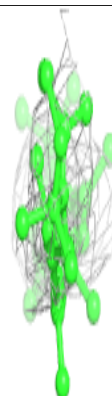
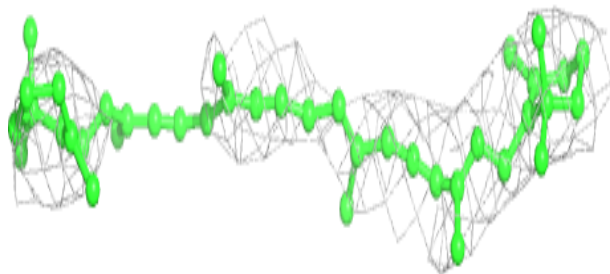
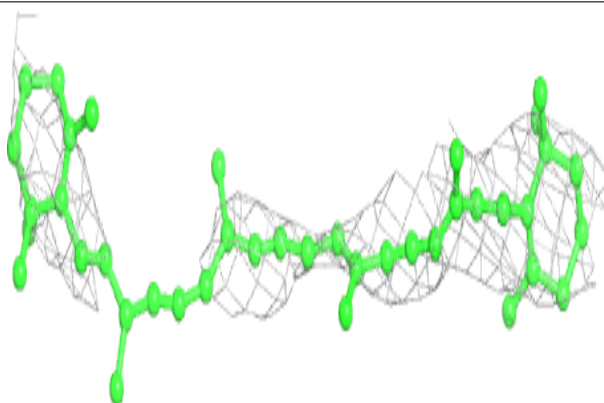


Electron density around CLA A 1125:

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

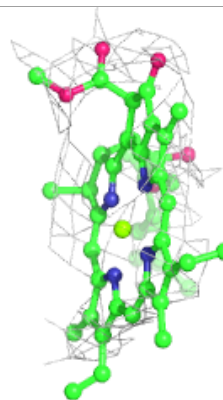
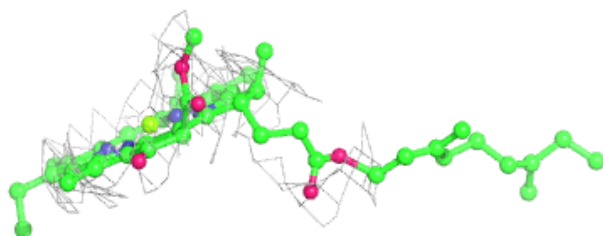
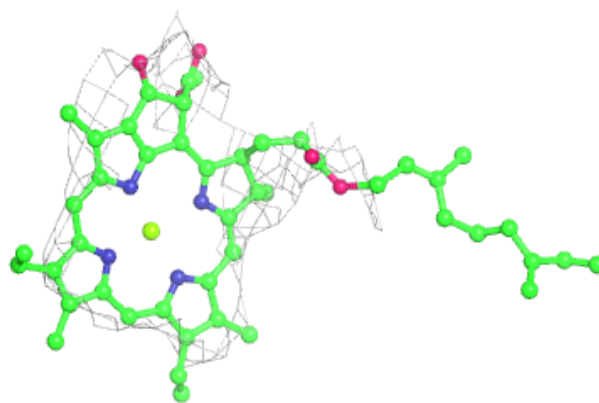
**Electron density around BCR 1 4008:**

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

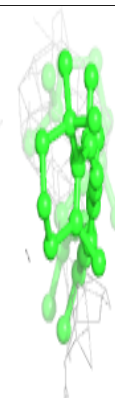
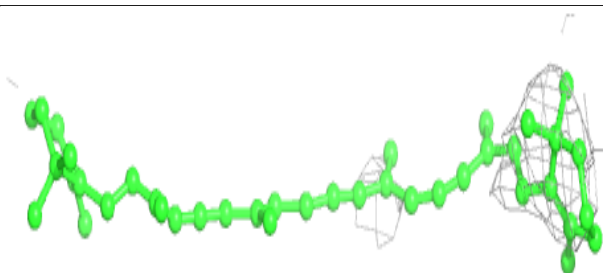
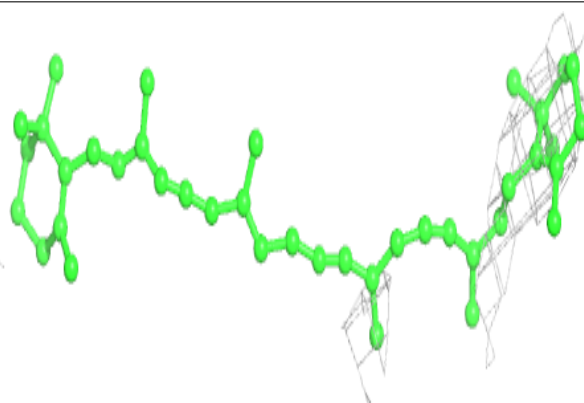


Electron density around CLA b 1222:

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

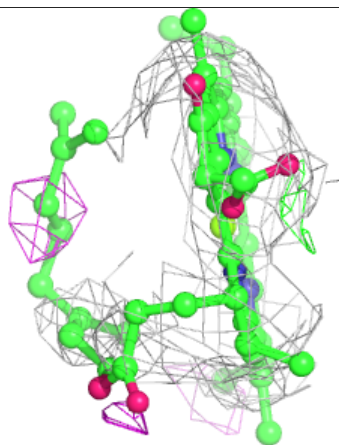
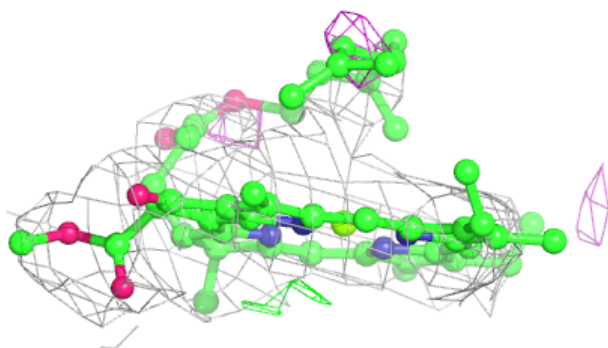
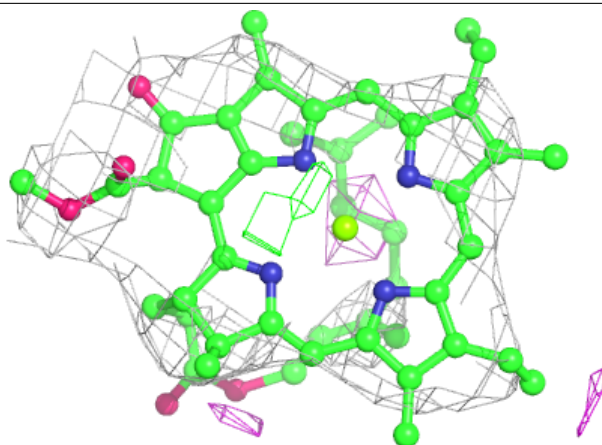
**Electron density around BCR b 4010:**

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



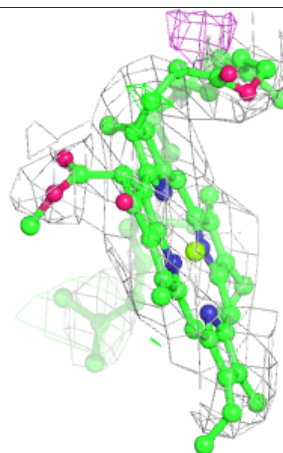
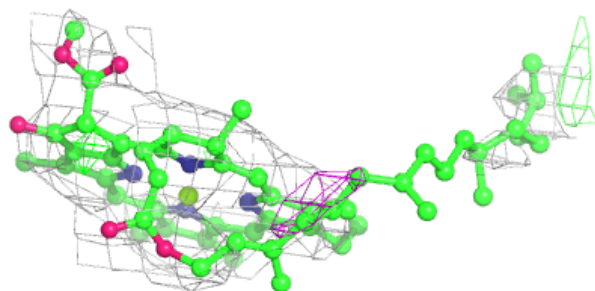
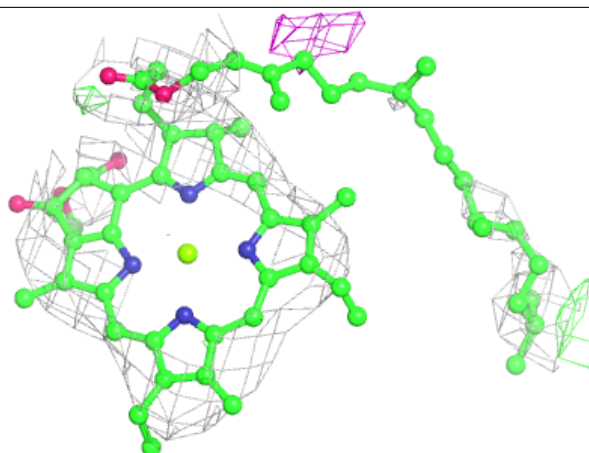
Electron density around CLA 2 1224:

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

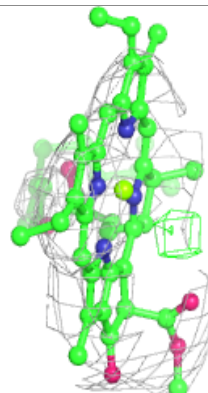
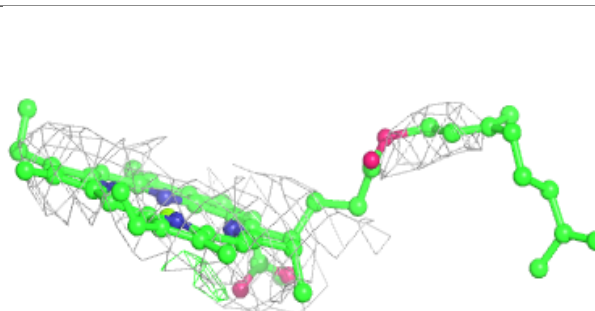
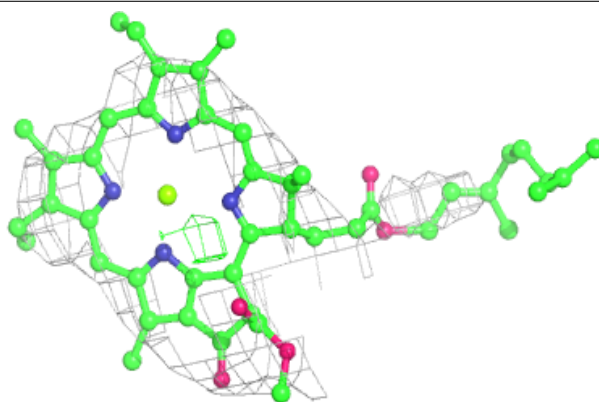


Electron density around CLA K 1401:

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

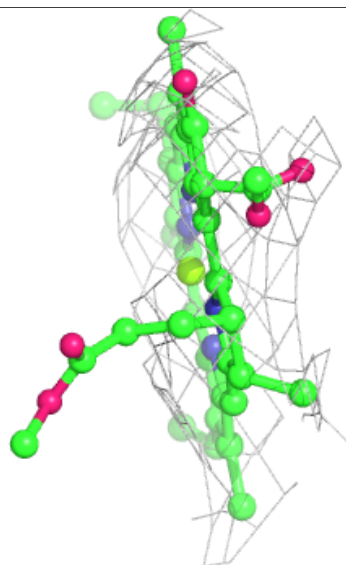
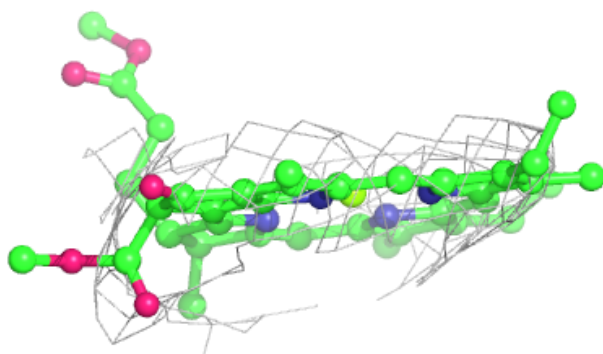
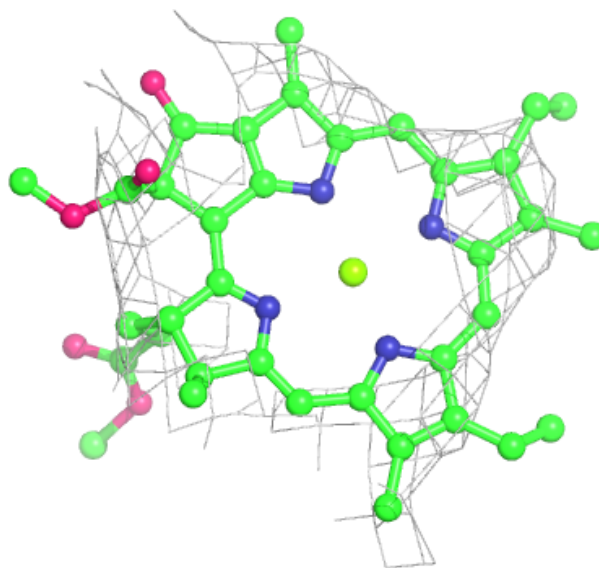
**Electron density around CLA a 1124:**

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



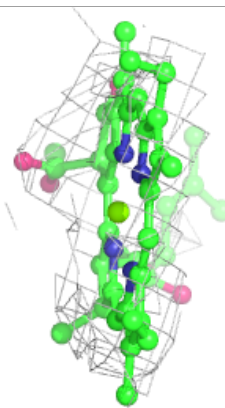
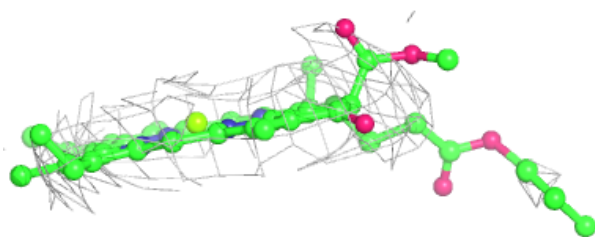
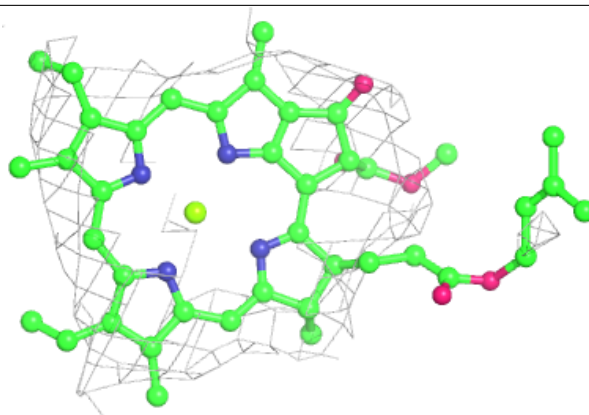
Electron density around CLA 1 1133:

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

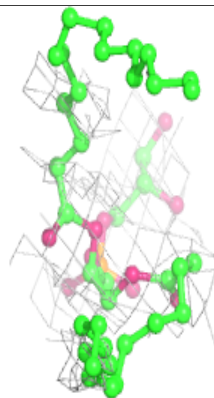
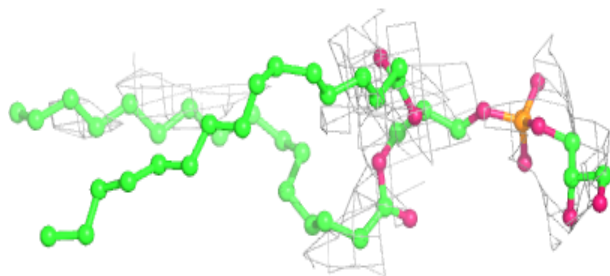
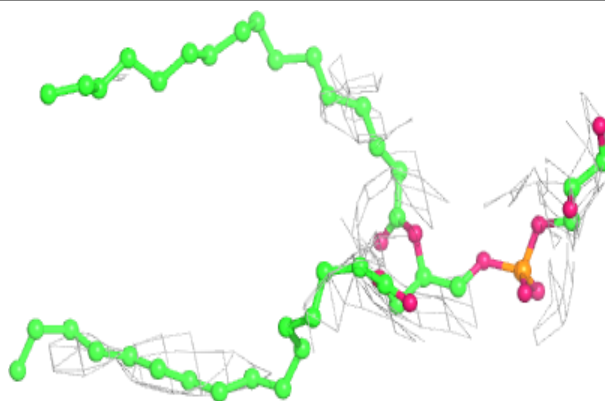


Electron density around CLA 1 1139:

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

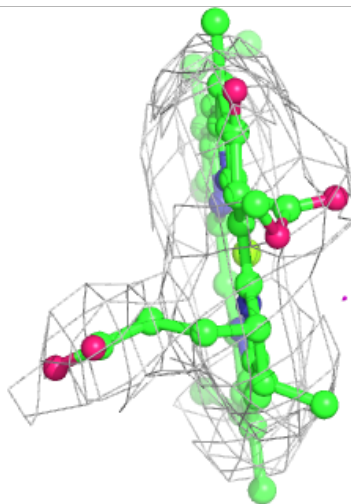
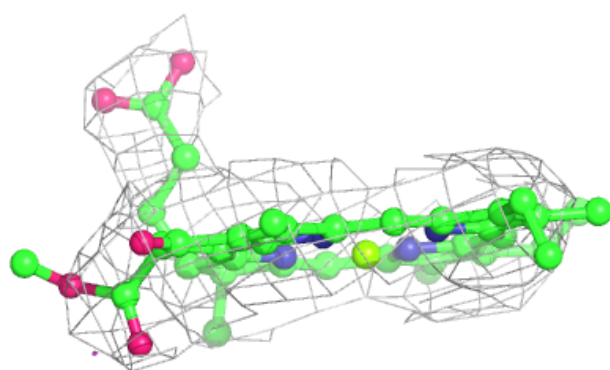
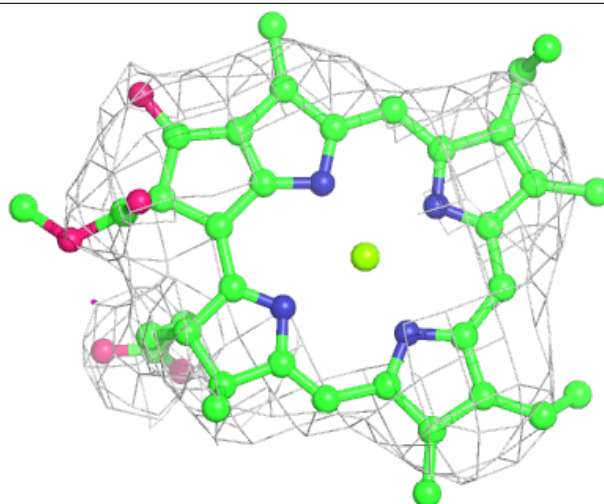
**Electron density around LHG 1 5001:**

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



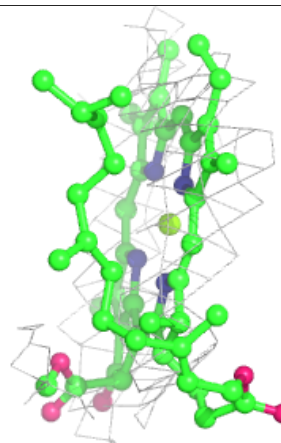
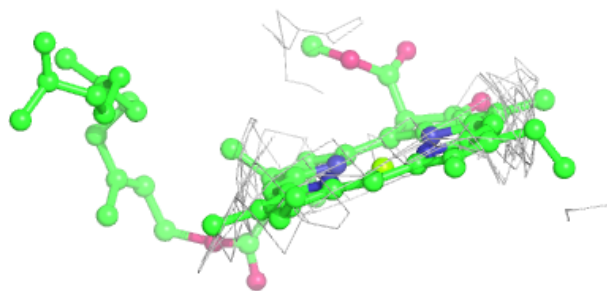
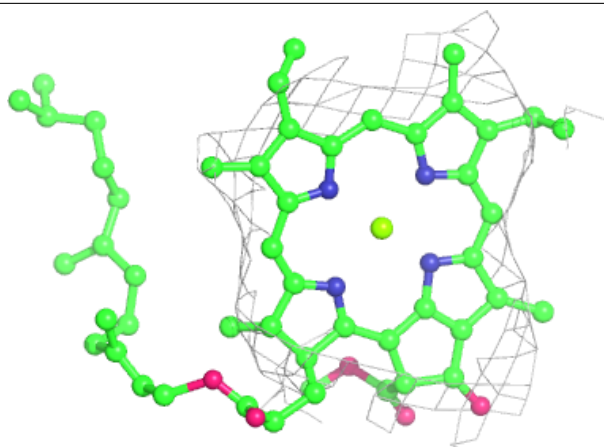
Electron density around CLA 2 1208:

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



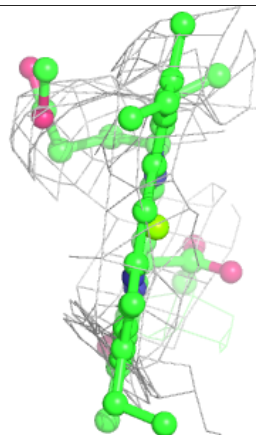
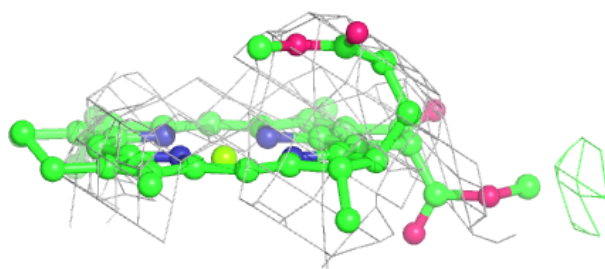
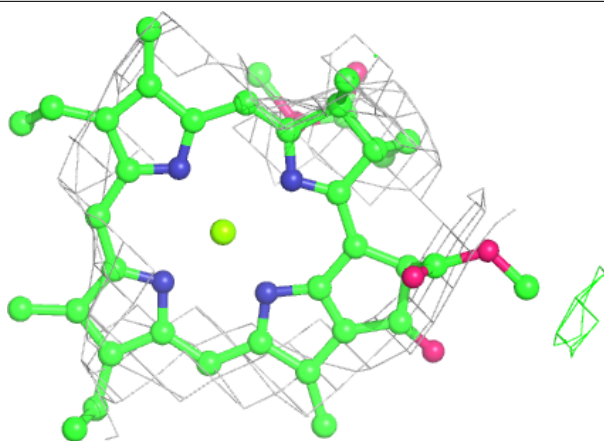
Electron density around CLA 1 1111:

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

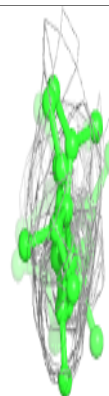
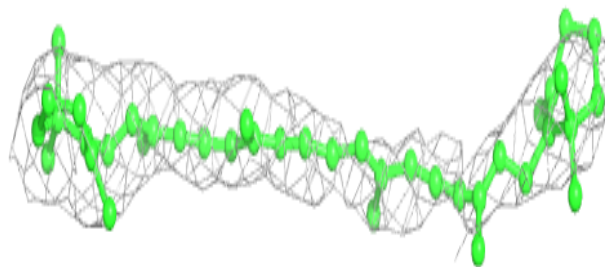
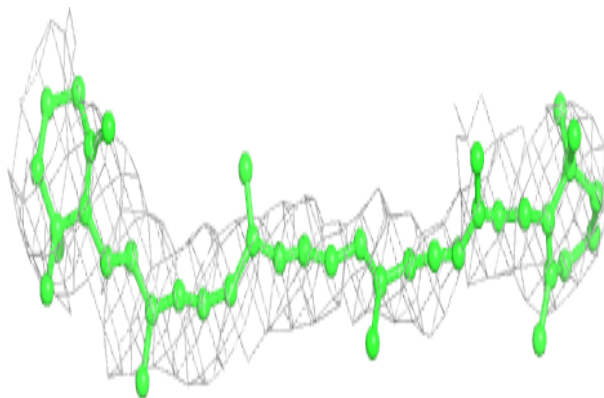


Electron density around CLA a 1114:

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

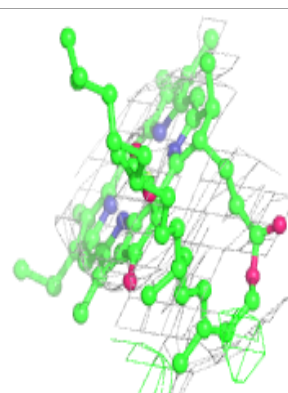
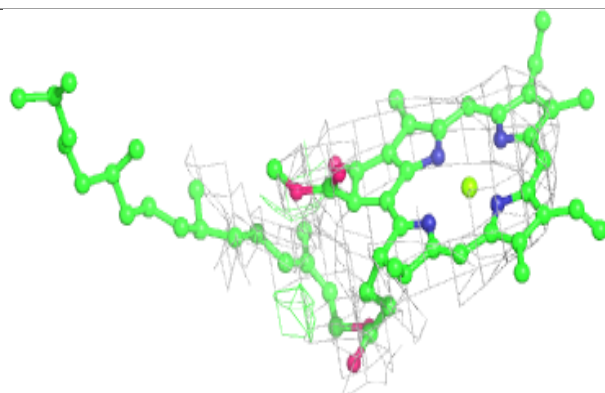
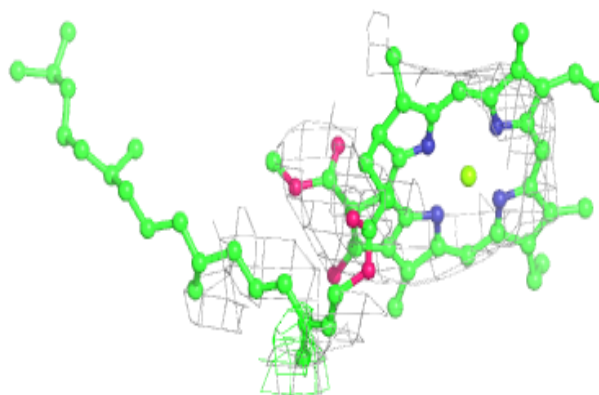
**Electron density around BCR a 4008:**

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

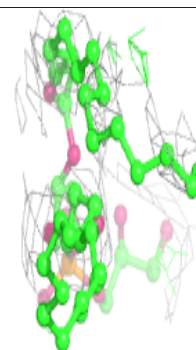
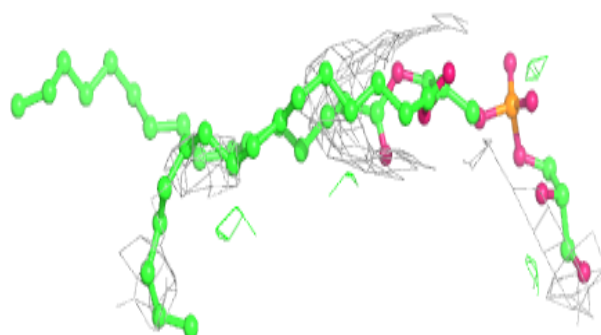
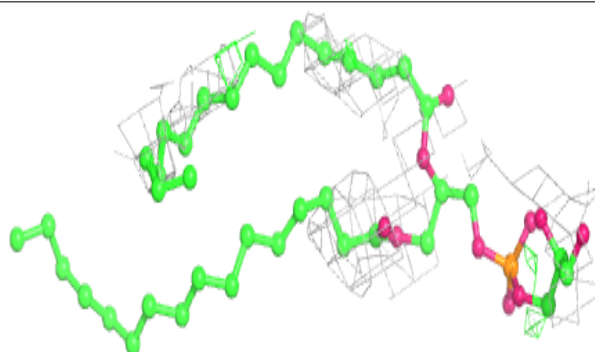


Electron density around CLA b 1213:

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

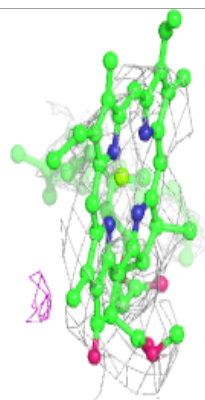
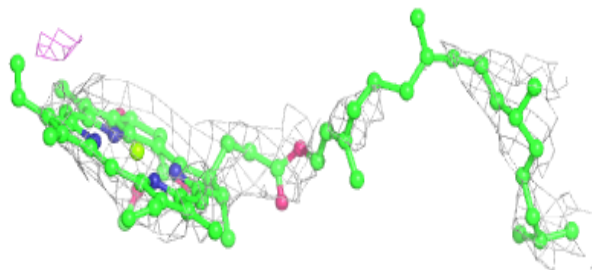
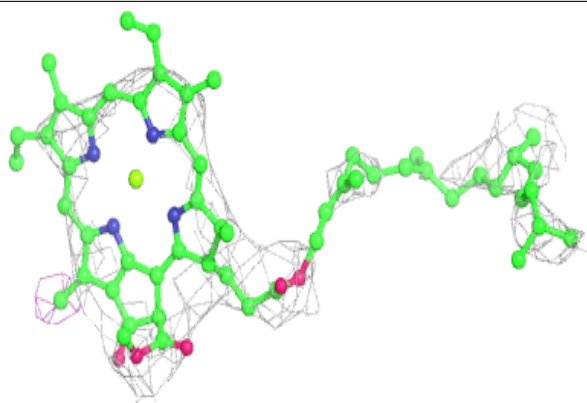
**Electron density around LHG a 5003:**

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

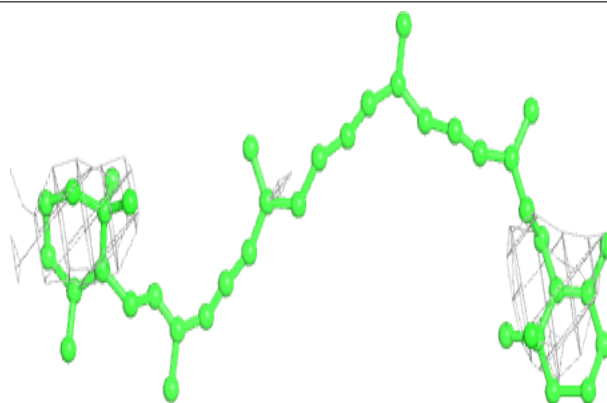


Electron density around CLA B 1210:

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

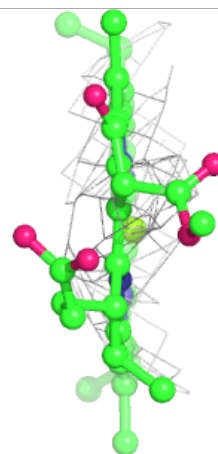
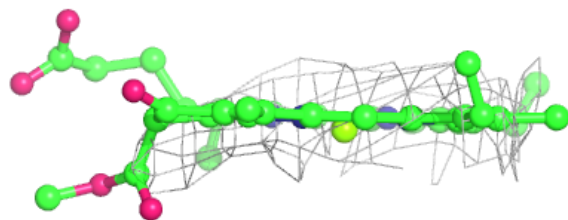
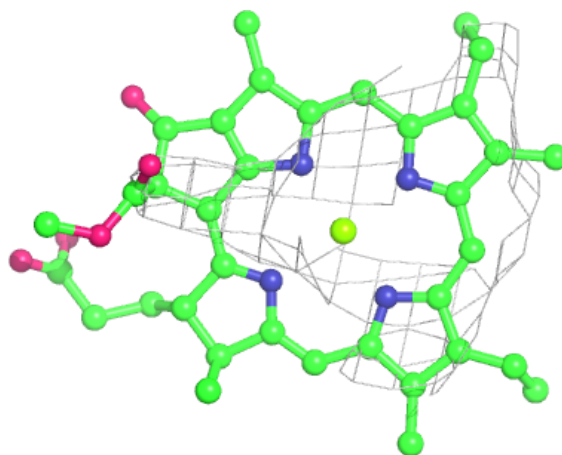
**Electron density around BCR b 4011:**

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



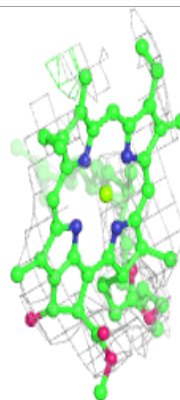
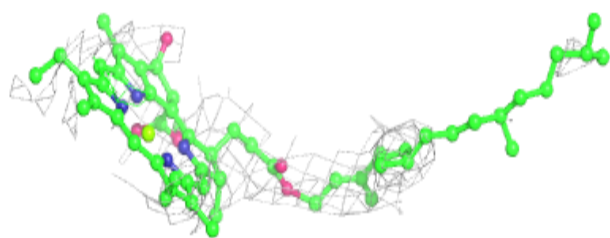
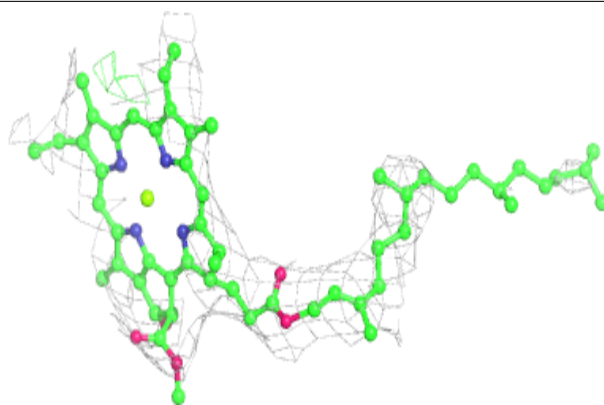
Electron density around CLA b 1240:

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



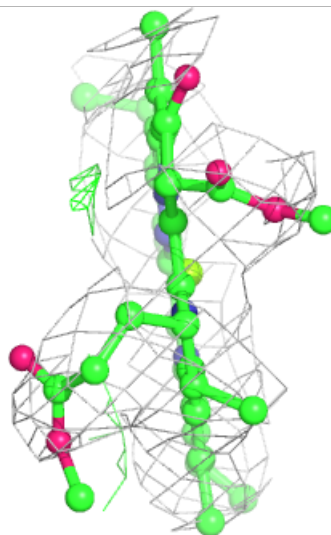
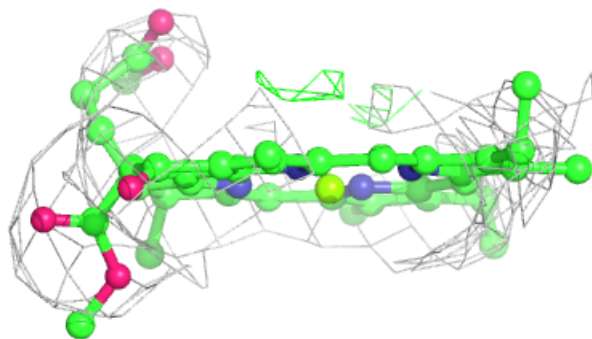
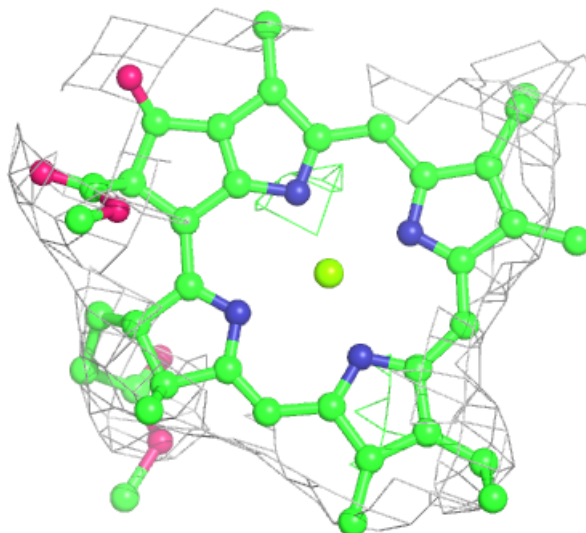
Electron density around CLA a 1022:

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



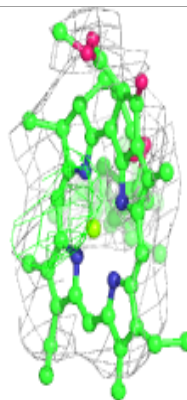
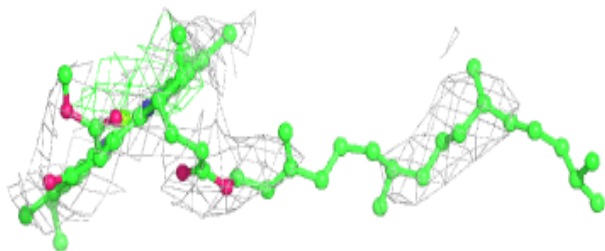
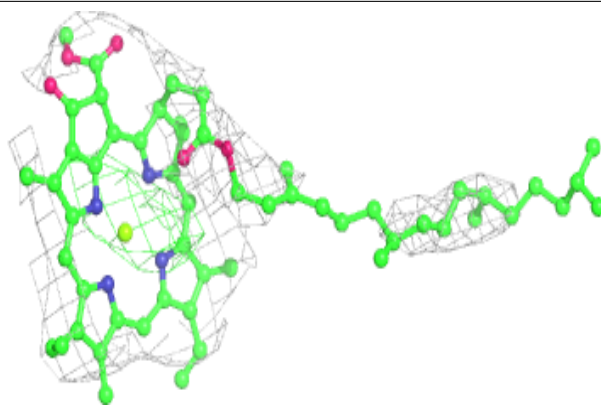
Electron density around CLA A 1120:

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

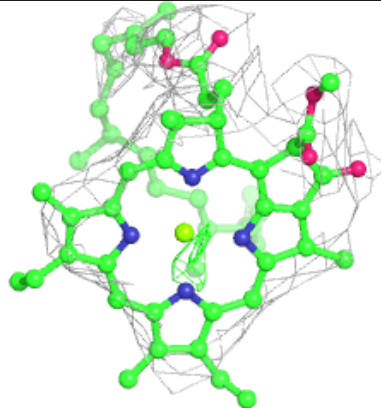
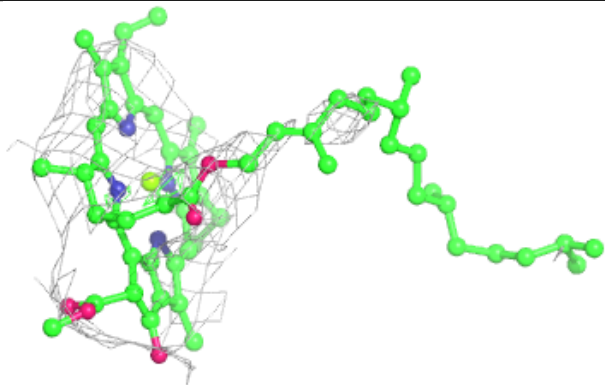
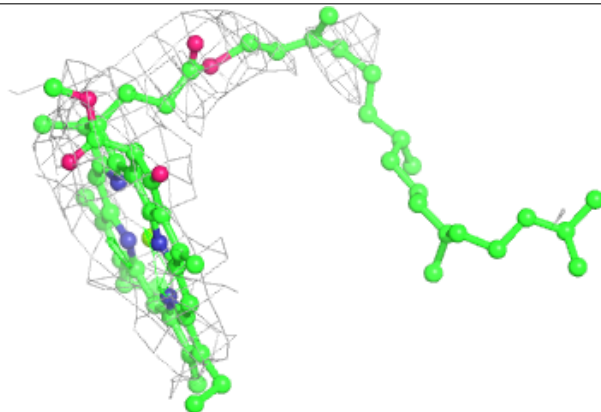


Electron density around CLA 8 1501:

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

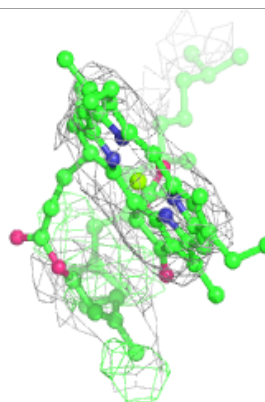
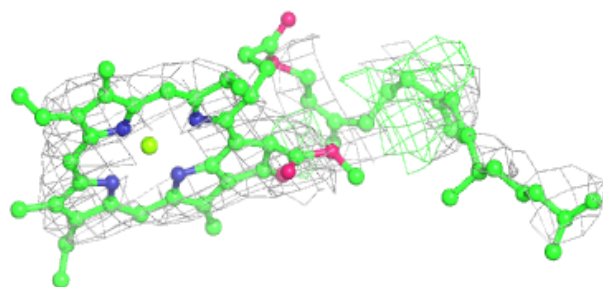
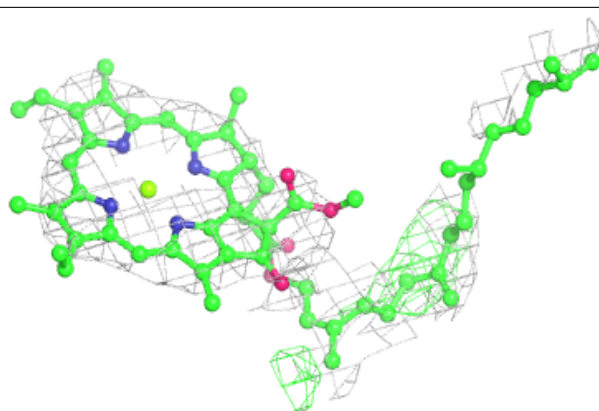
**Electron density around CLA B 1216:**

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



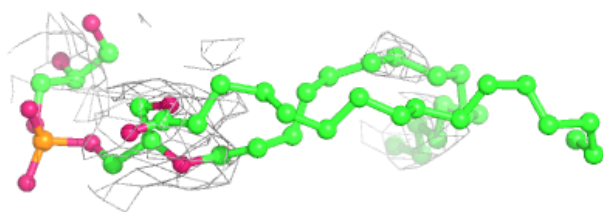
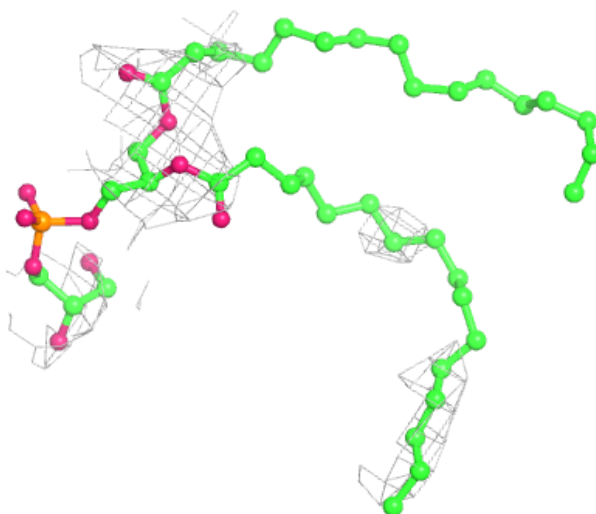
Electron density around CLA B 1213:

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



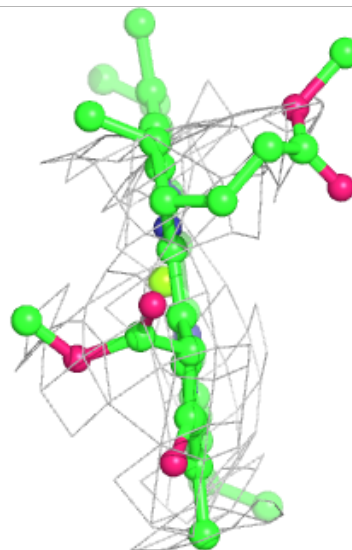
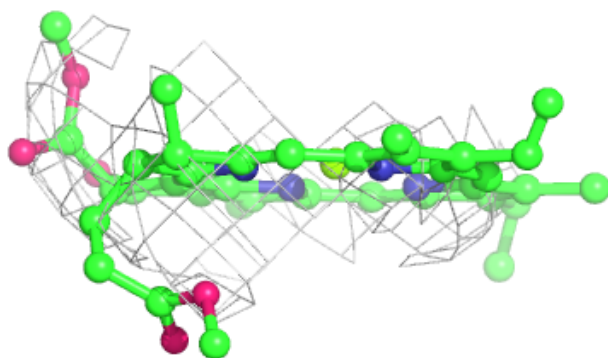
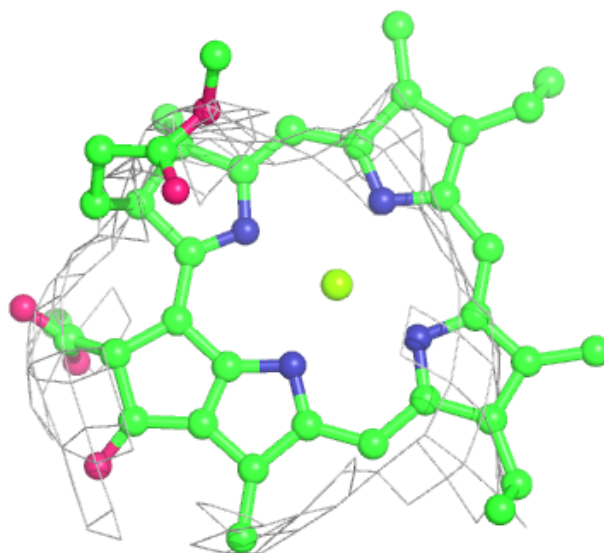
Electron density around LHG B 5004:

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



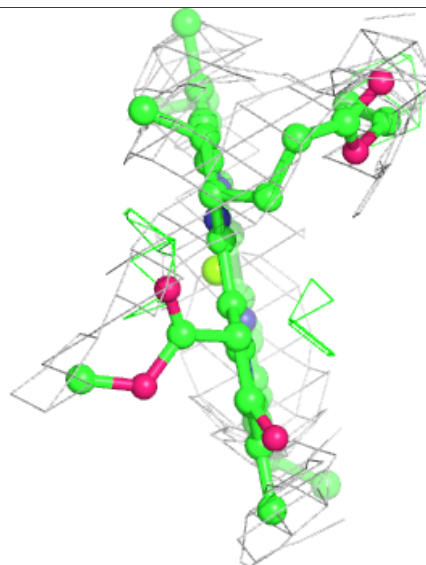
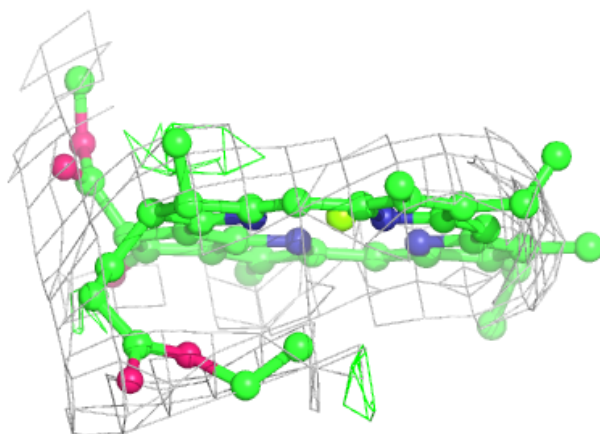
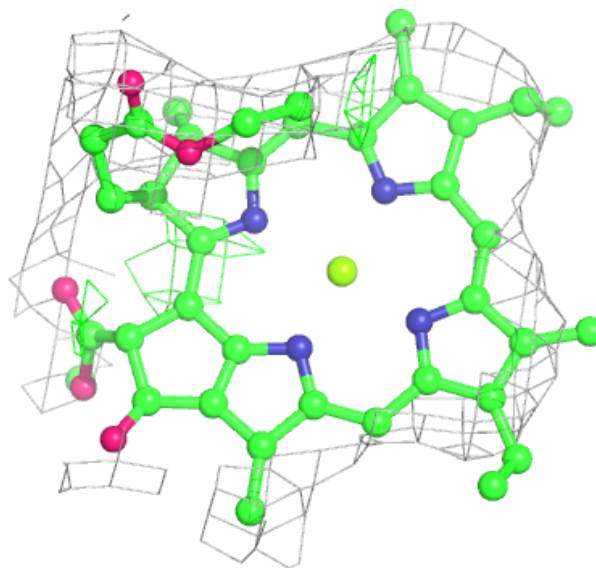
Electron density around CLA 1 1120:

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



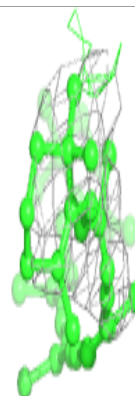
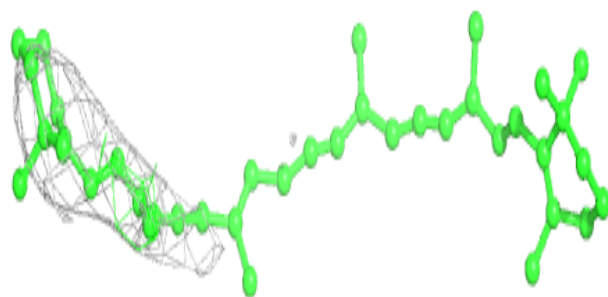
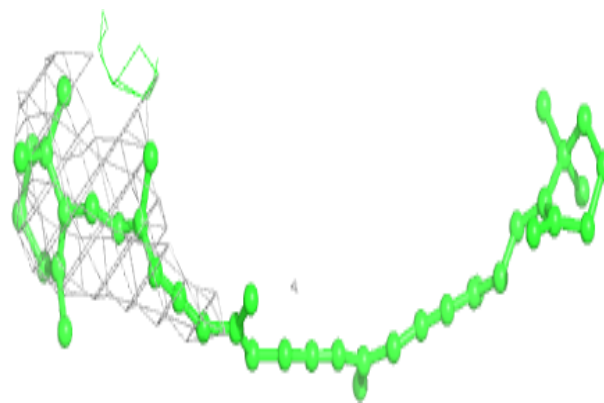
Electron density around CLA 2 1217:

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



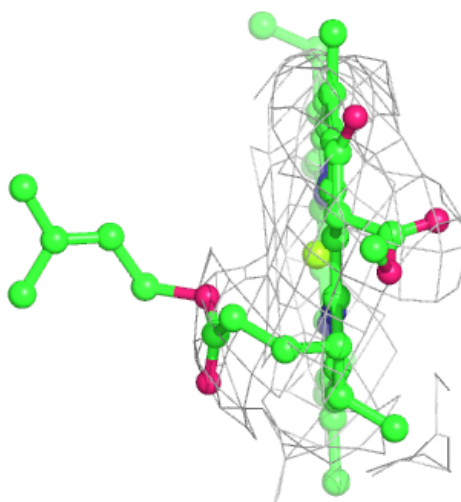
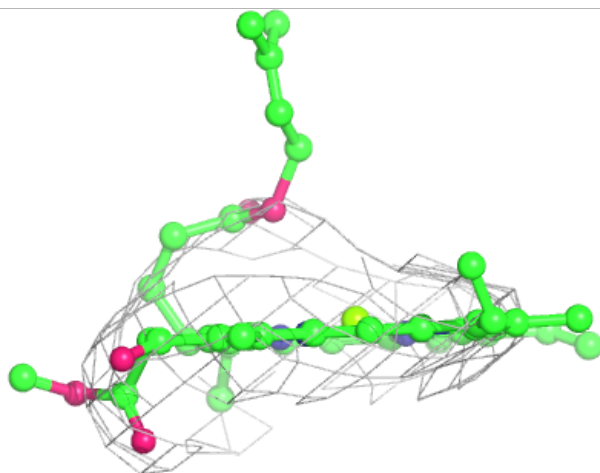
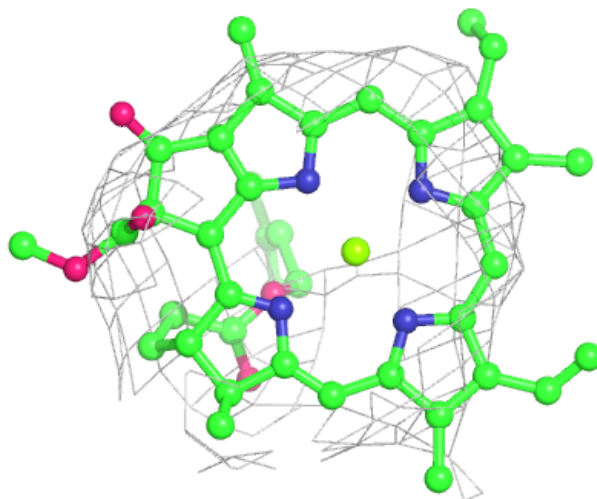
Electron density around BCR 2 4014:

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



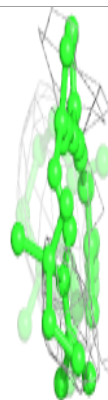
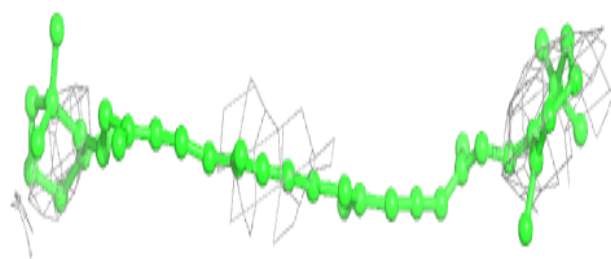
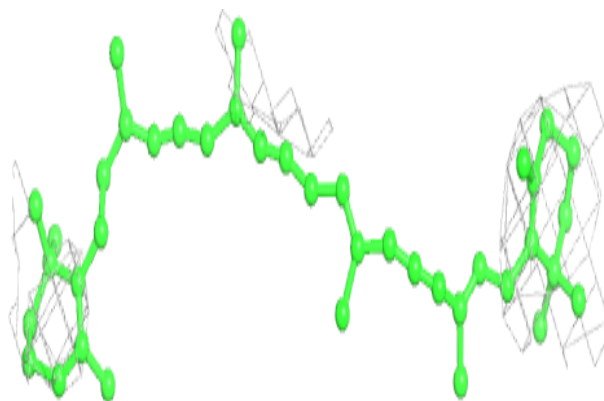
Electron density around CLA K 1402:

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



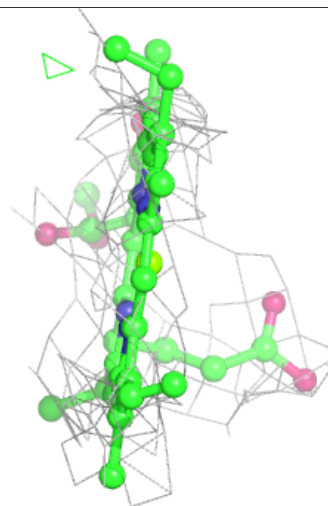
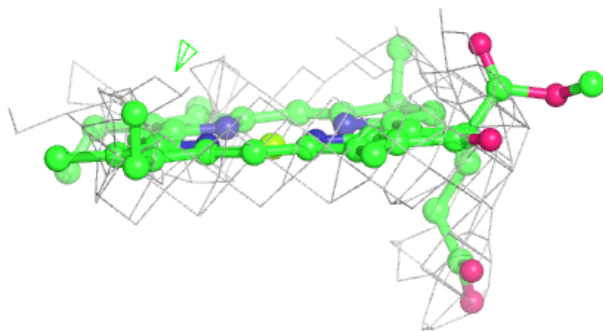
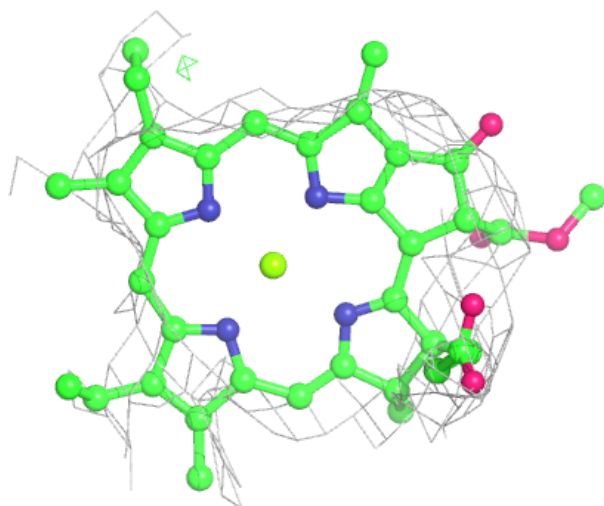
Electron density around BCR b 4004:

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



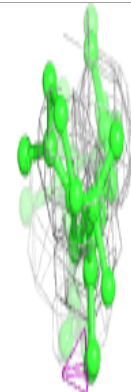
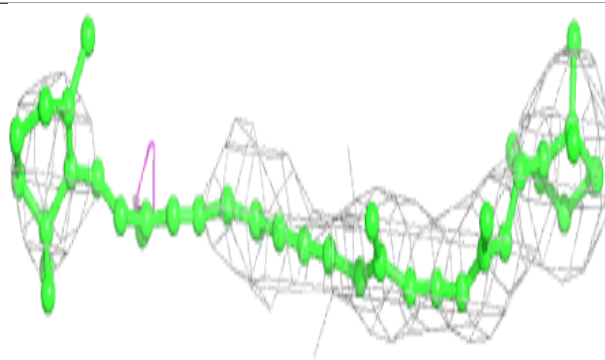
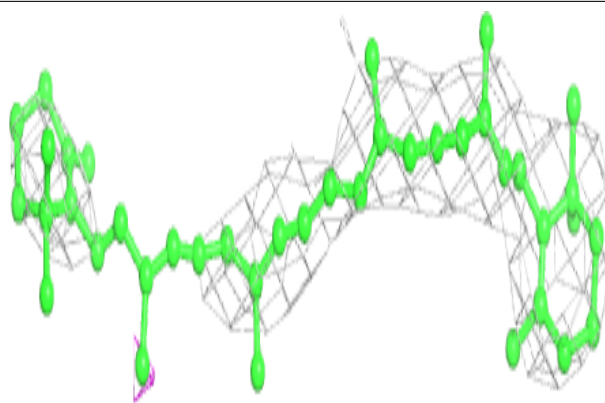
Electron density around CLA 1 1108:

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

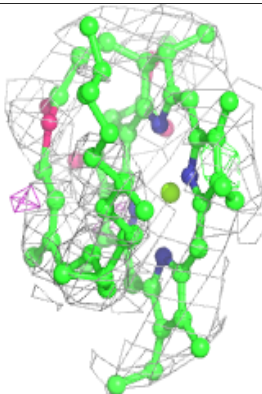
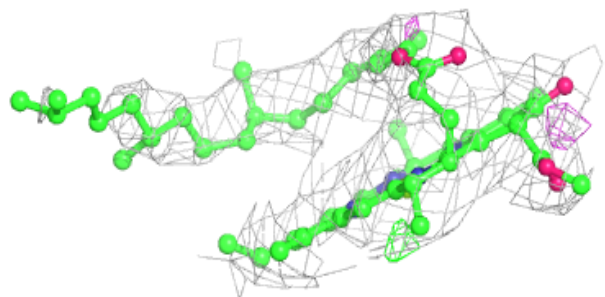
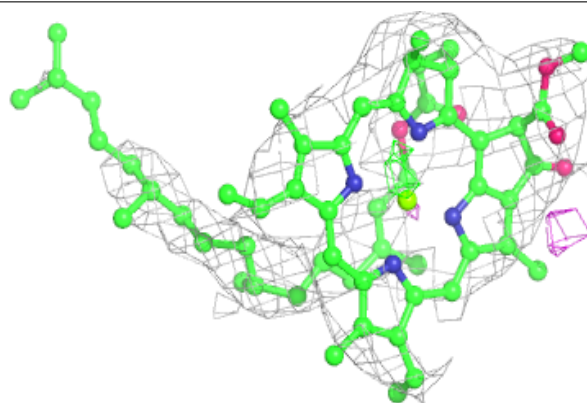


Electron density around BCR 1 4022:

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

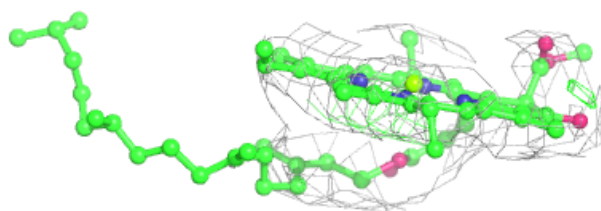
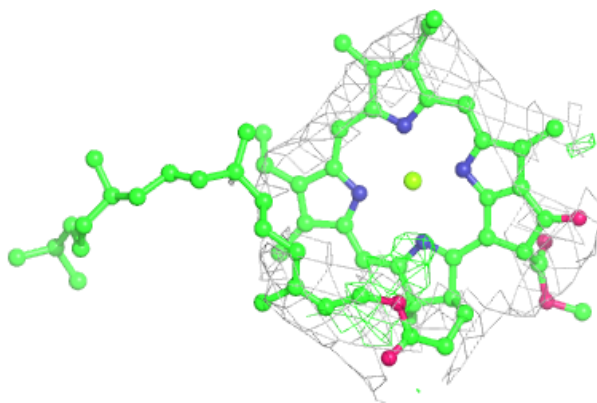
**Electron density around CLA 2 1204:**

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



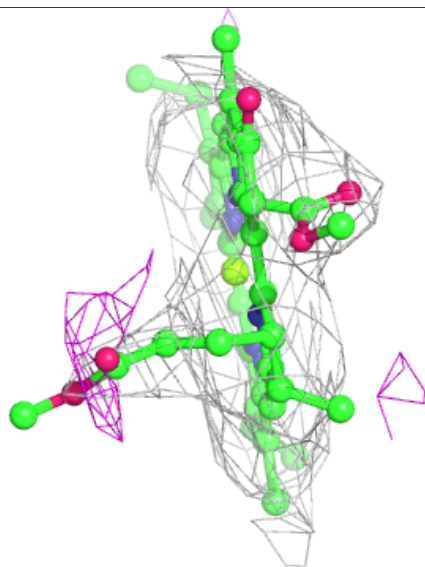
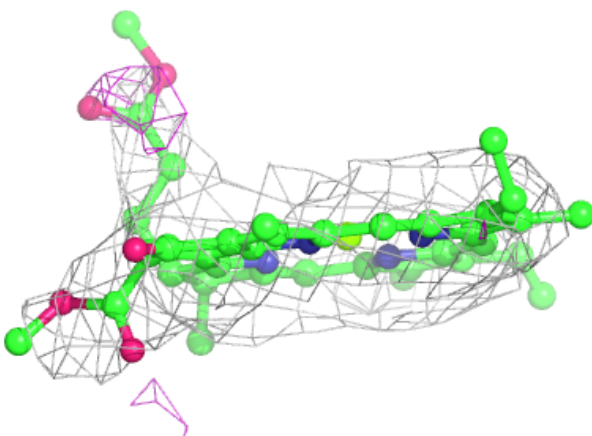
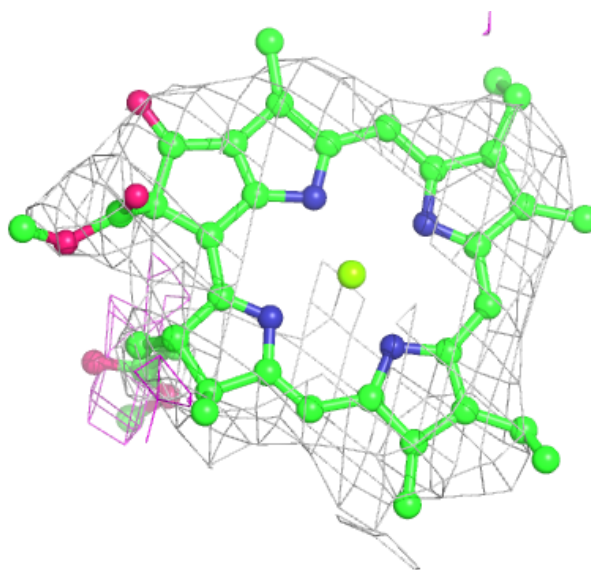
Electron density around CLA B 1215:

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



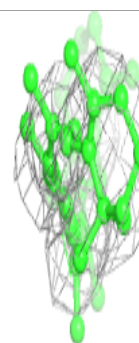
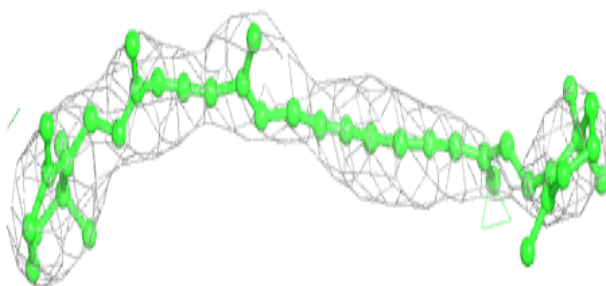
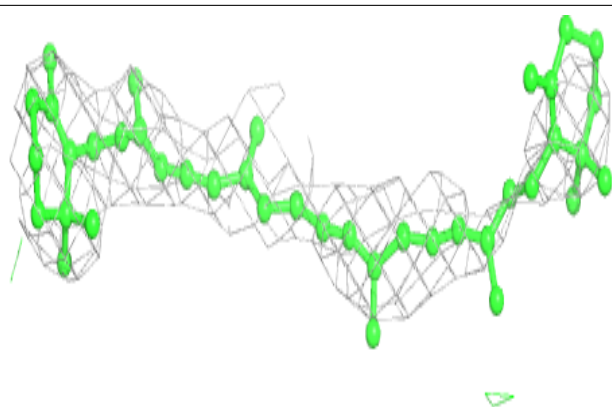
Electron density around CLA A 1133:

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

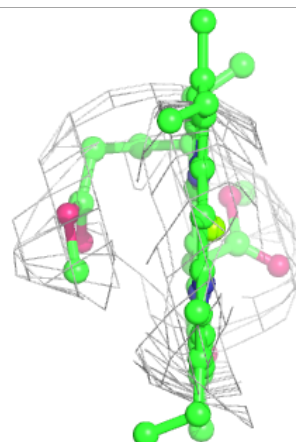
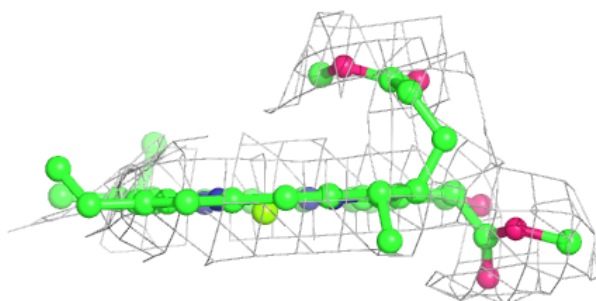
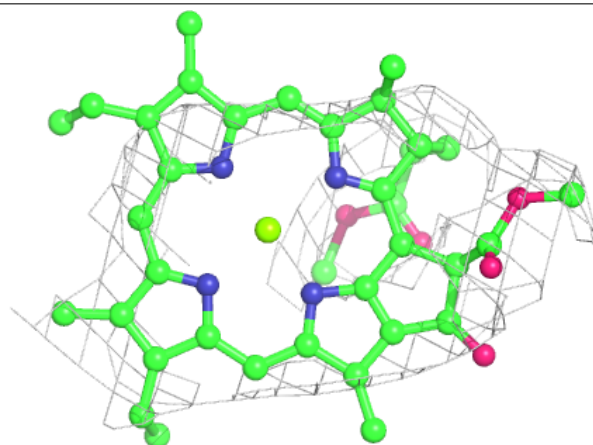


Electron density around BCR 7 4021:

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

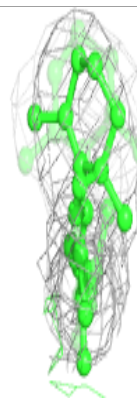
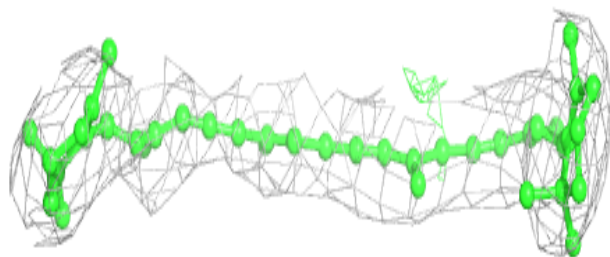
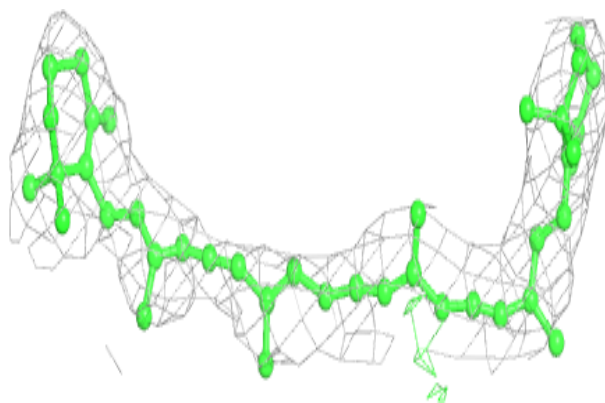
**Electron density around CLA 1 1138:**

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



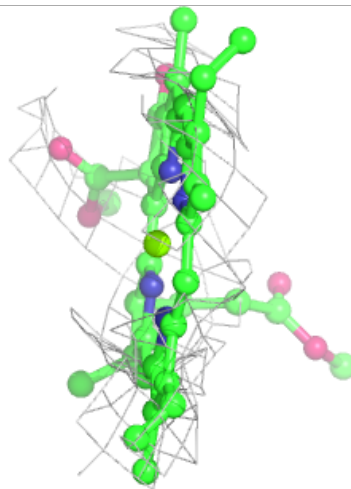
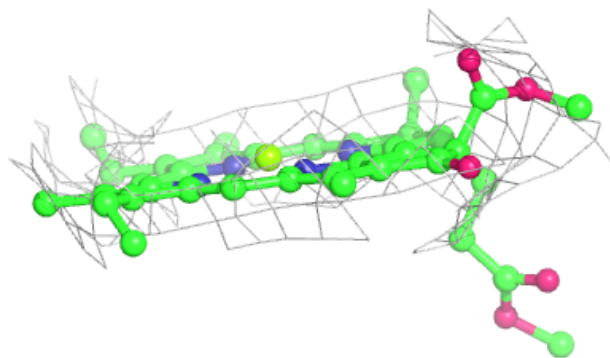
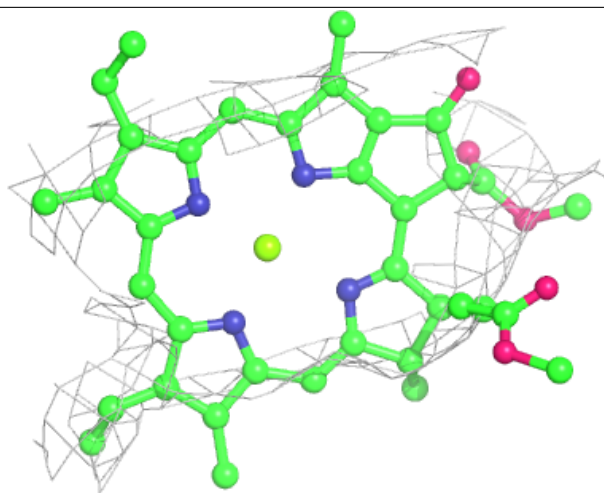
Electron density around BCR F 4020:

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



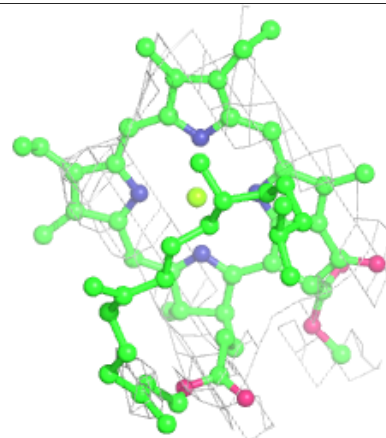
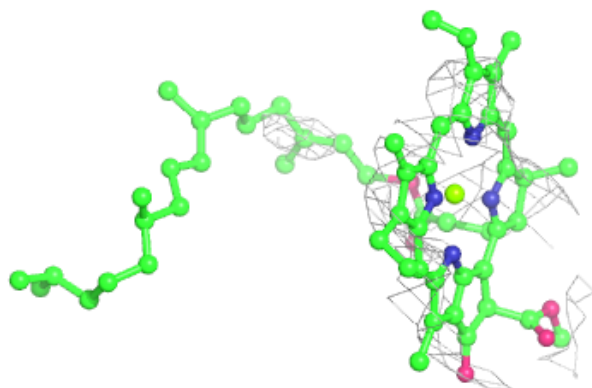
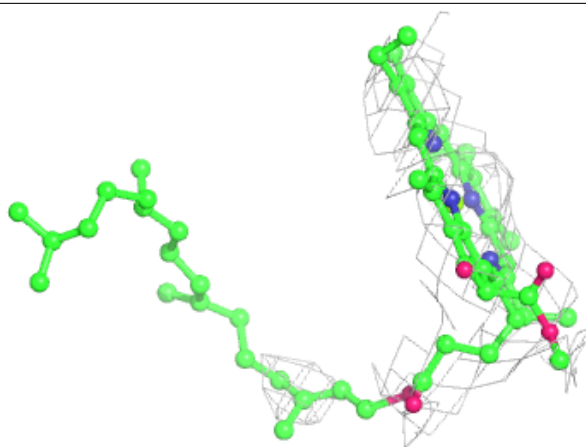
Electron density around CLA b 1220:

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

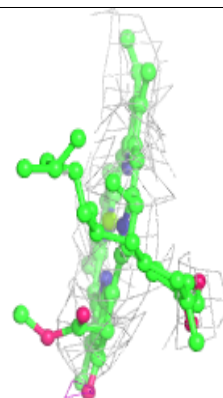
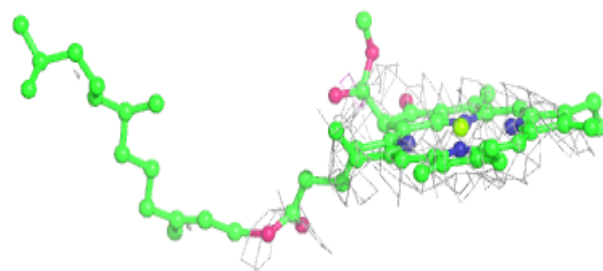
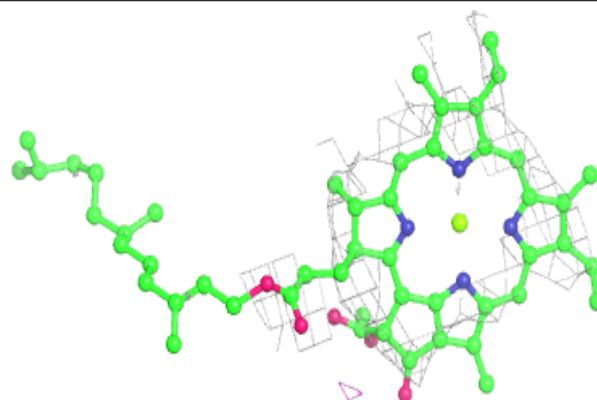


Electron density around CLA b 1216:

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

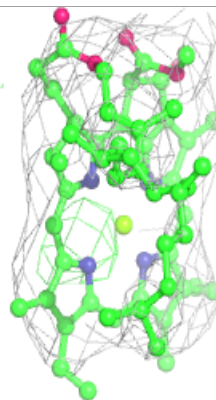
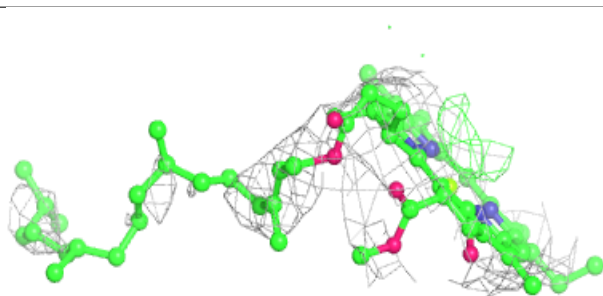
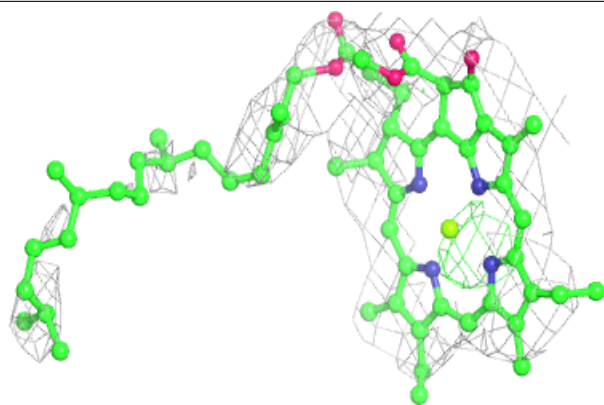
**Electron density around CLA b 1234:**

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

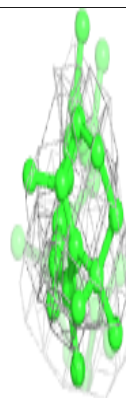
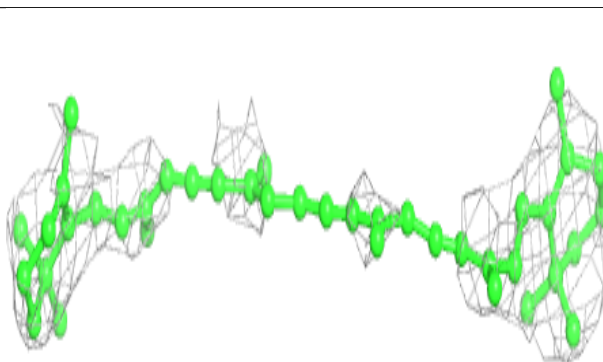
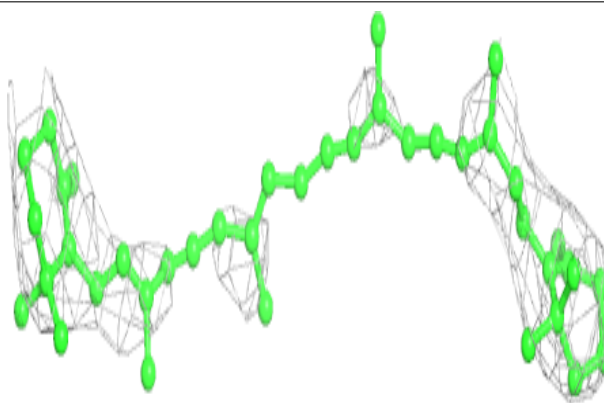


Electron density around CLA B 1207:

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

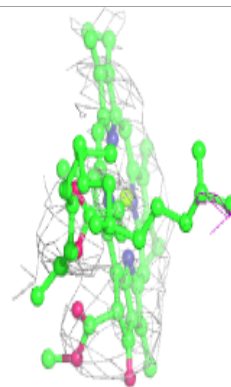
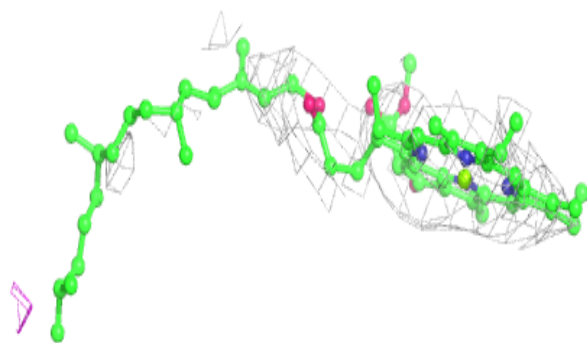
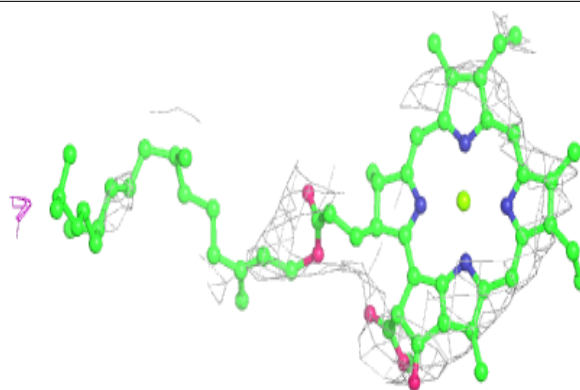
**Electron density around BCR B 4010:**

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



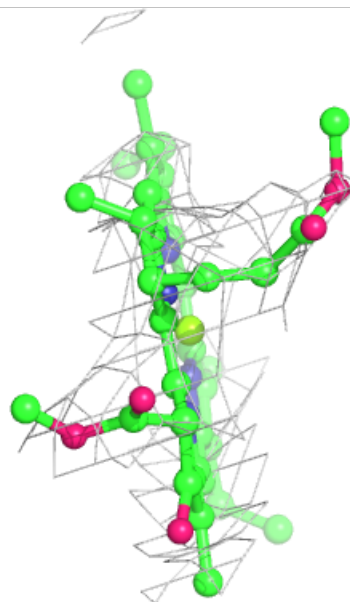
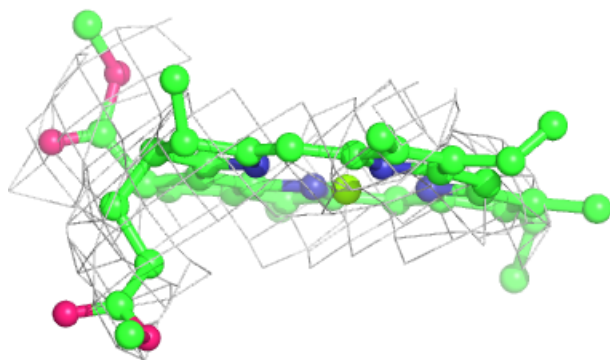
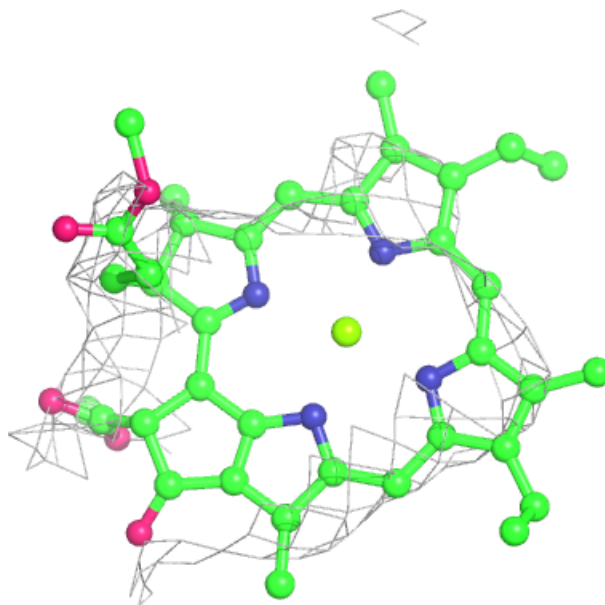
Electron density around CLA a 1103:

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



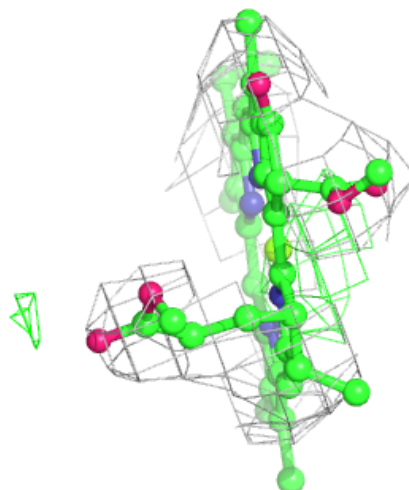
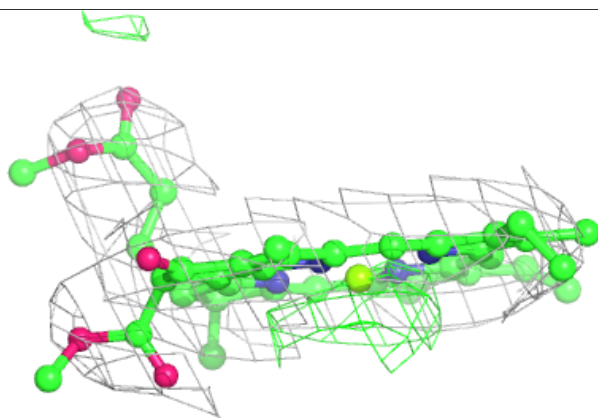
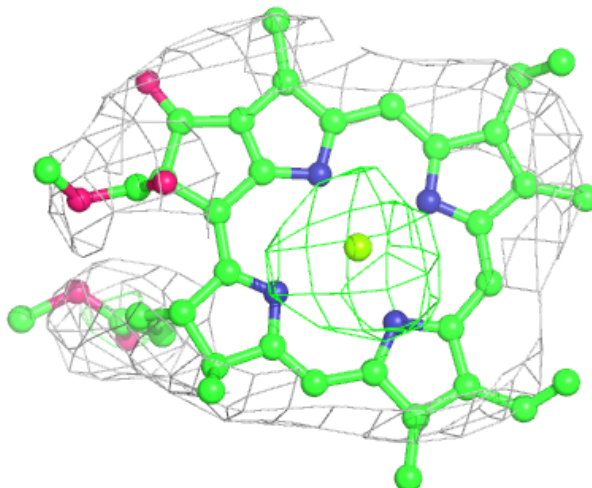
Electron density around CLA 1 1129:

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



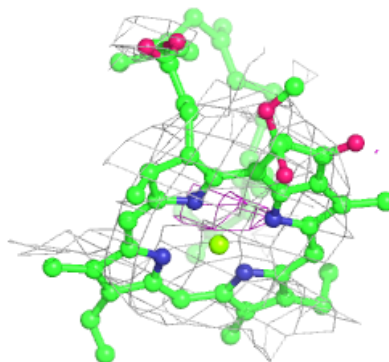
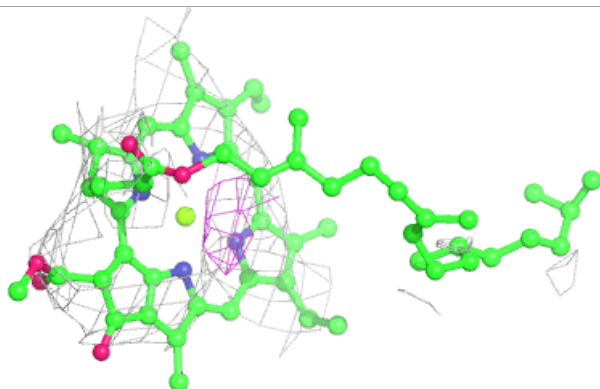
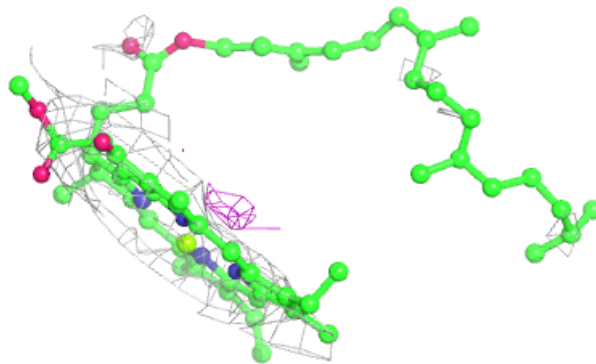
Electron density around CLA b 1239:

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

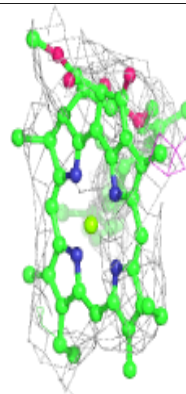
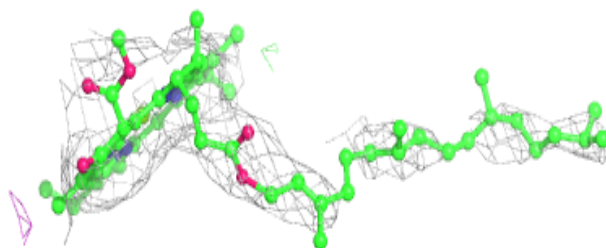
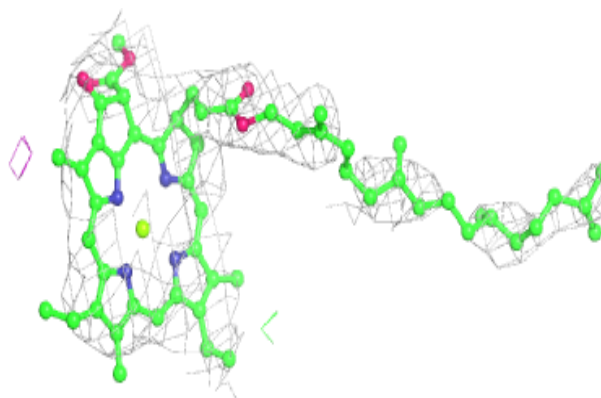


Electron density around CLA 1 1109:

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

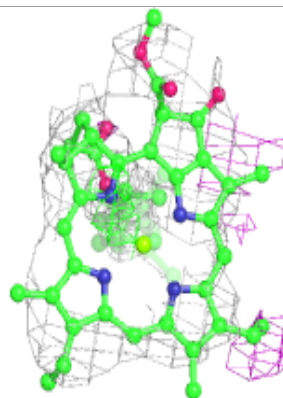
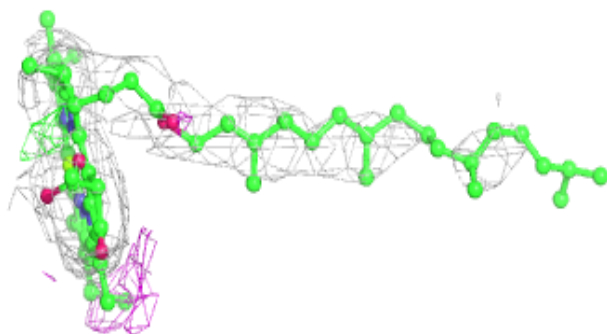
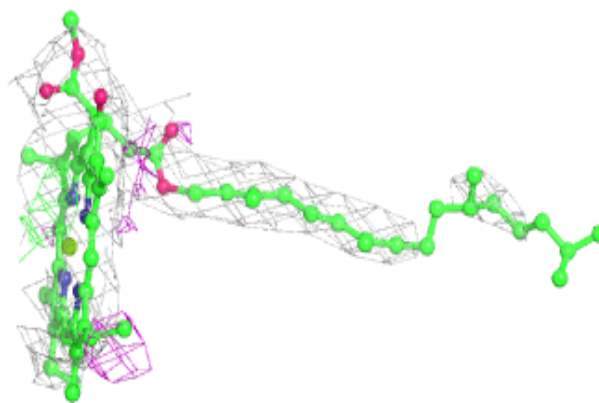
**Electron density around CLA 1 1132:**

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

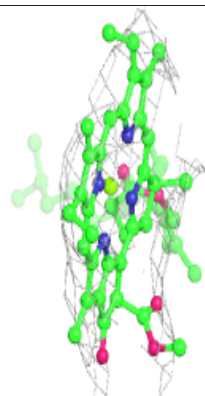
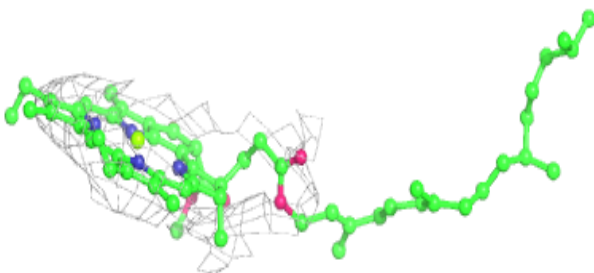
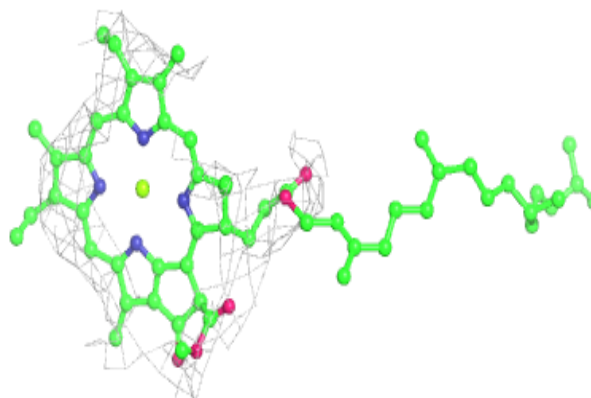


Electron density around CLA A 1126:

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

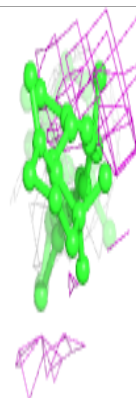
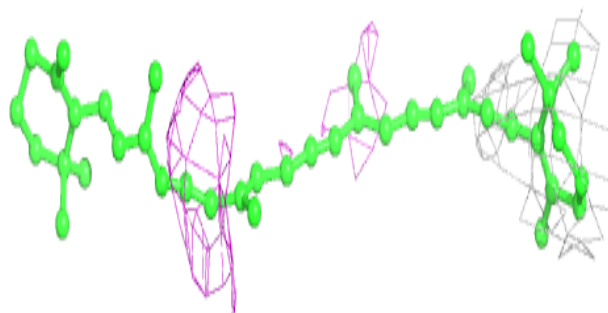
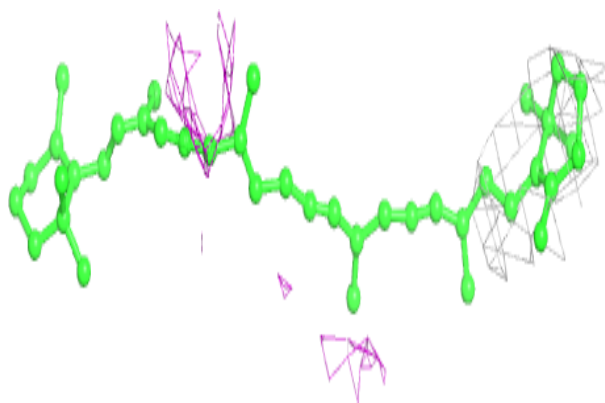
**Electron density around CLA 1 1103:**

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

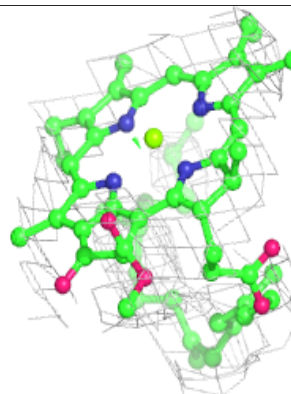
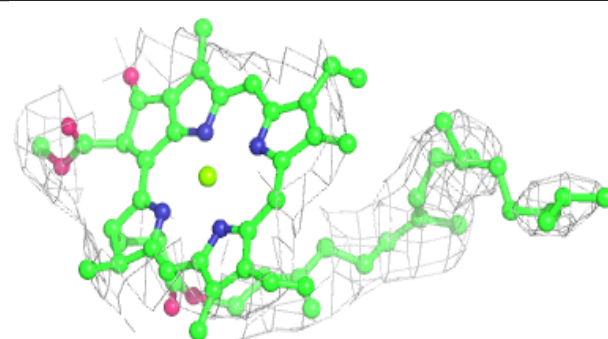
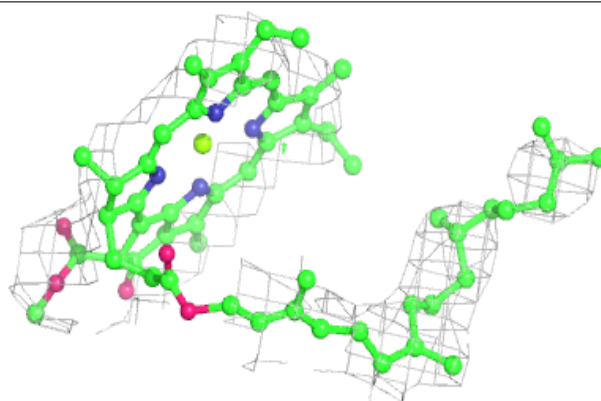


Electron density around BCR a 4003:

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

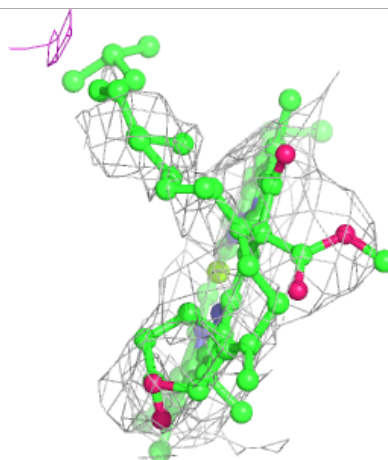
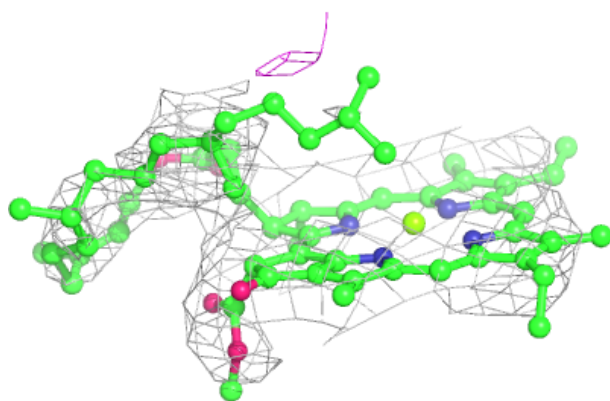
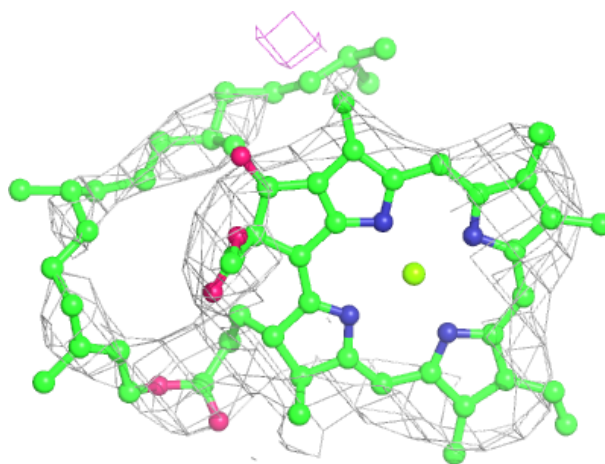
**Electron density around CLA A 1109:**

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



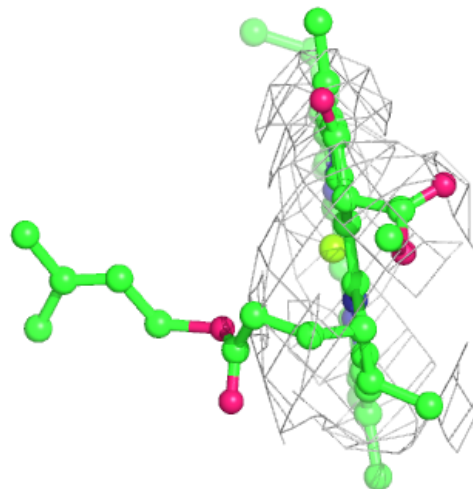
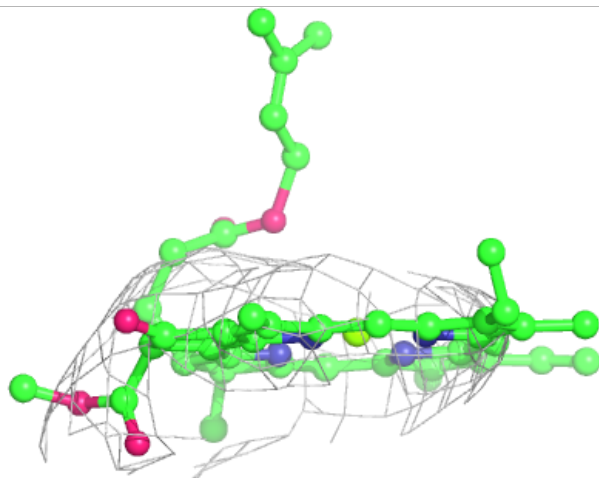
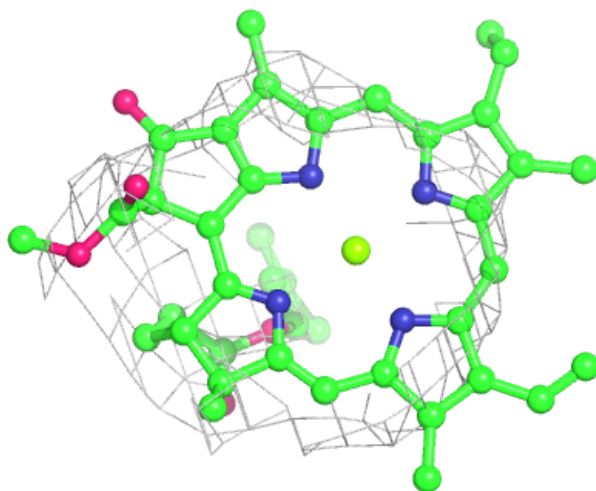
Electron density around CLA B 1202:

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



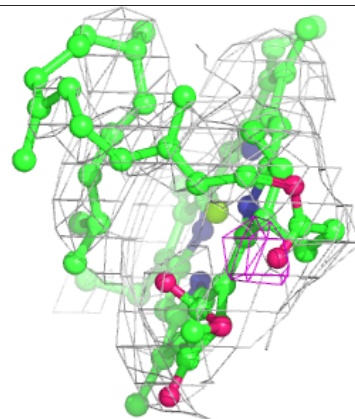
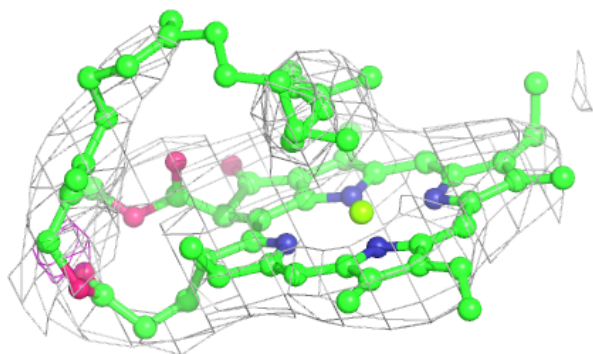
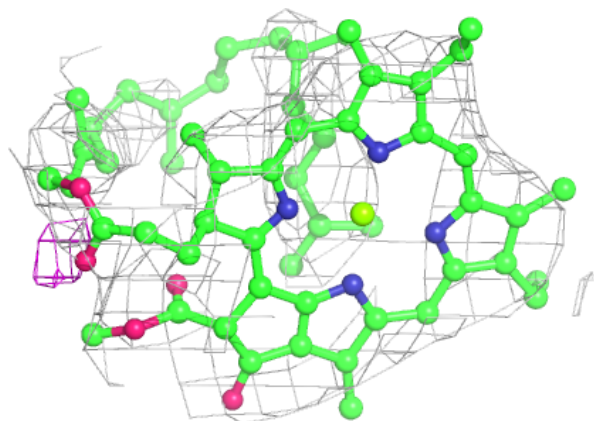
Electron density around CLA k 1402:

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

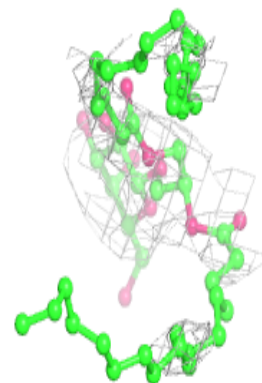
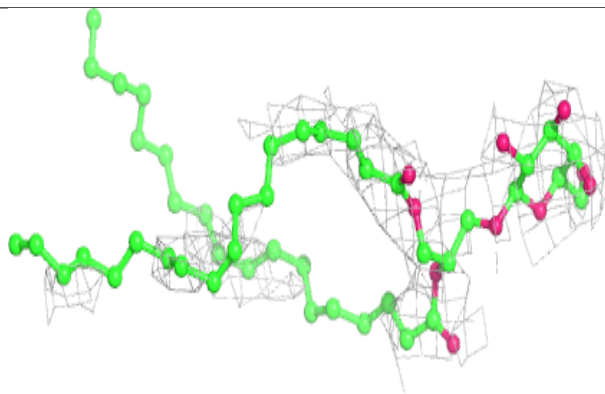
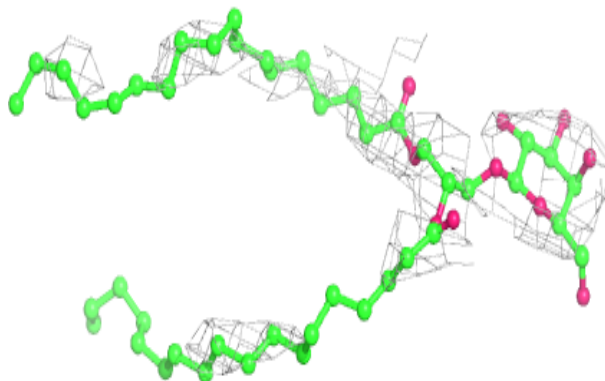


Electron density around CLA B 1203:

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

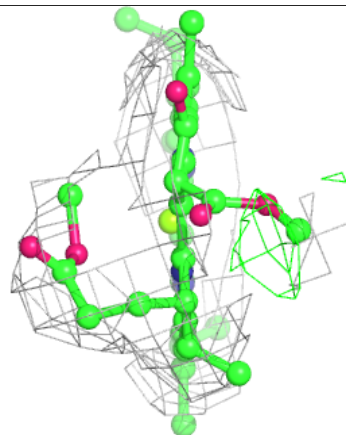
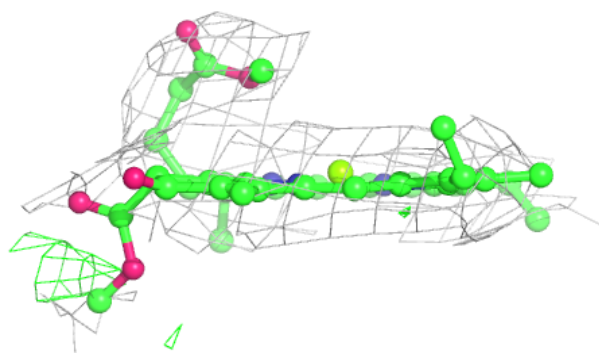
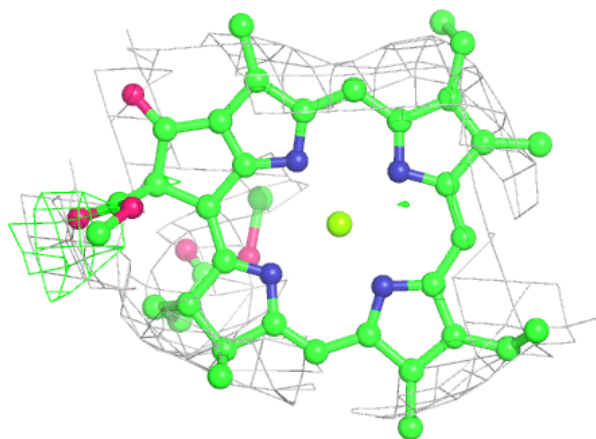
**Electron density around LMG b 5002:**

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

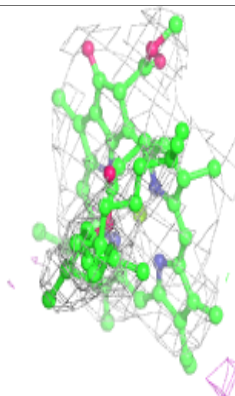
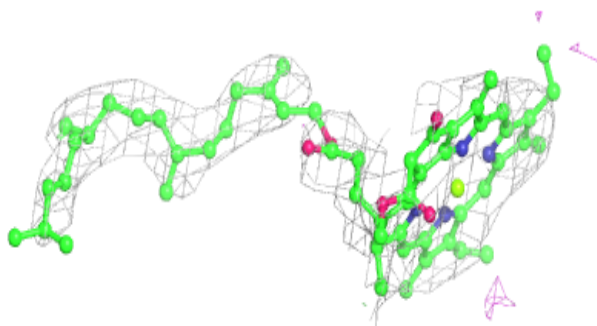
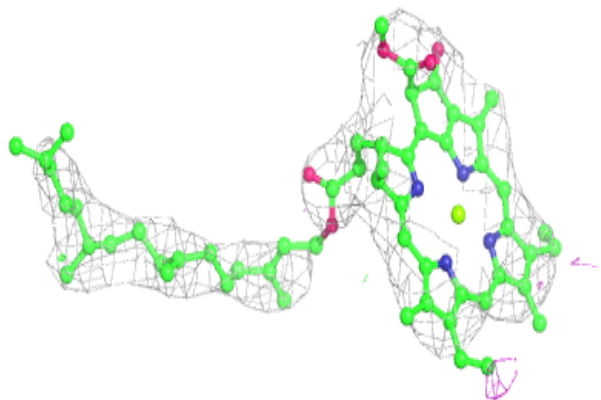


Electron density around CLA 8 1502:

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

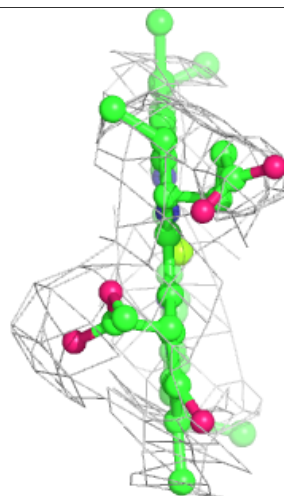
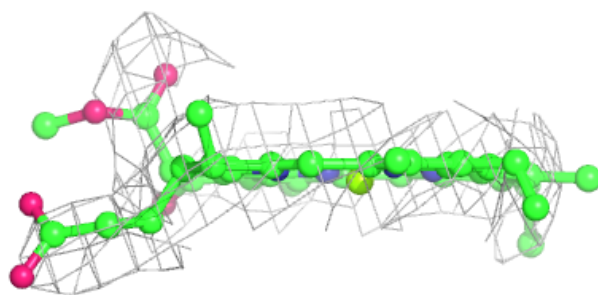
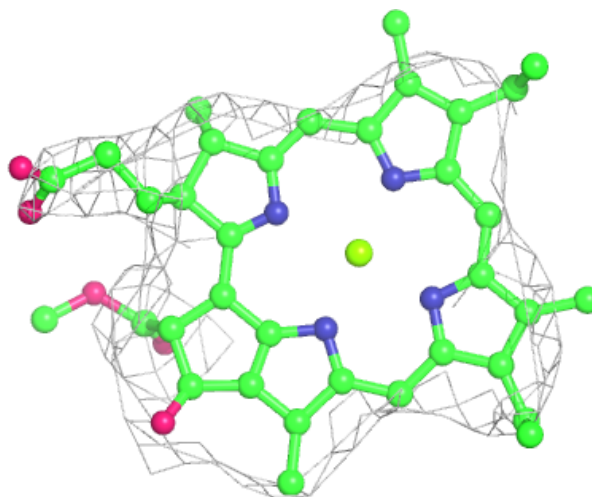
**Electron density around CLA A 1119:**

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



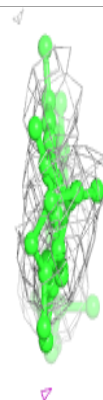
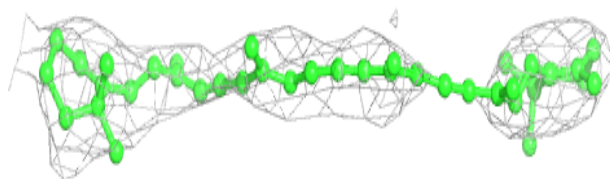
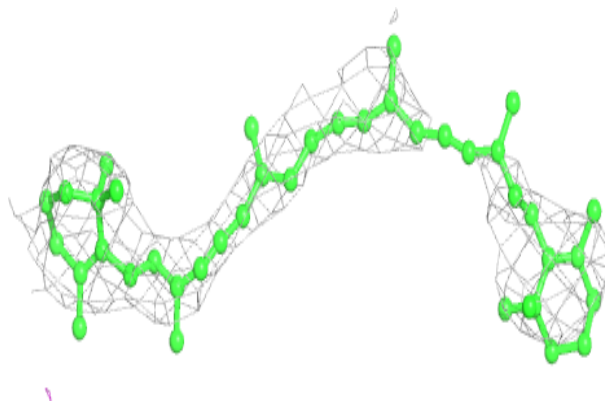
Electron density around CLA A 1113:

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



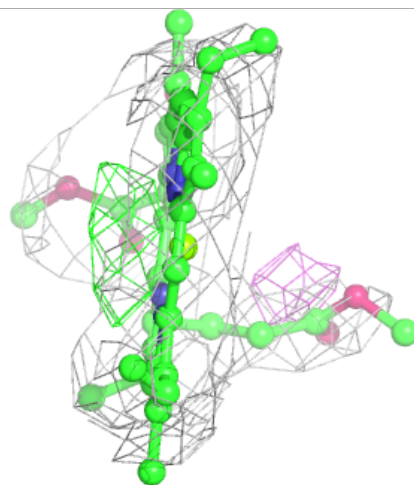
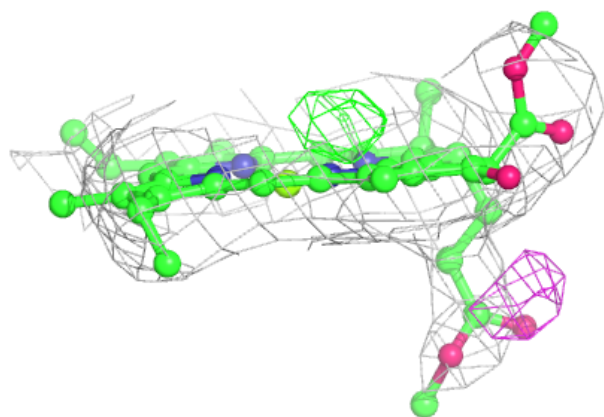
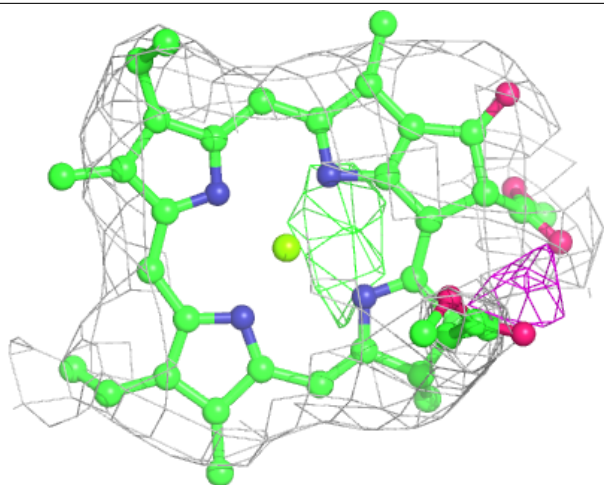
Electron density around BCR B 4011:

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



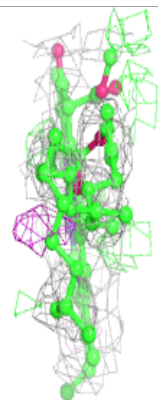
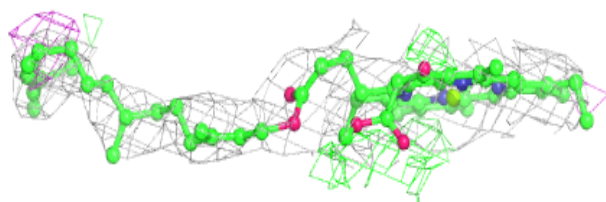
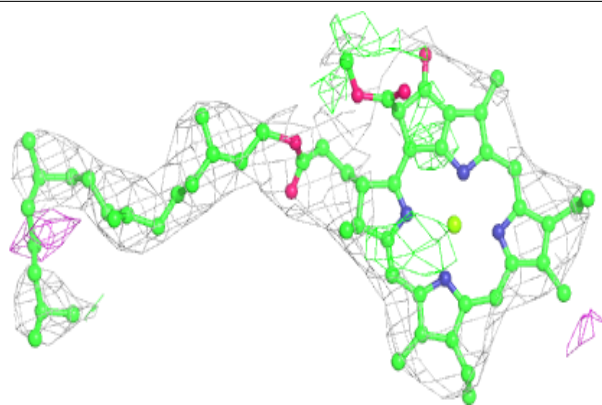
Electron density around CLA L 1502:

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

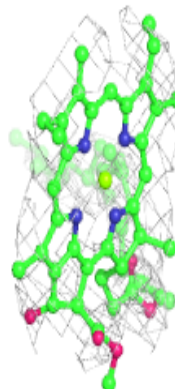
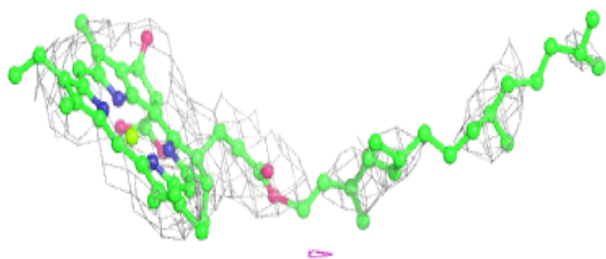
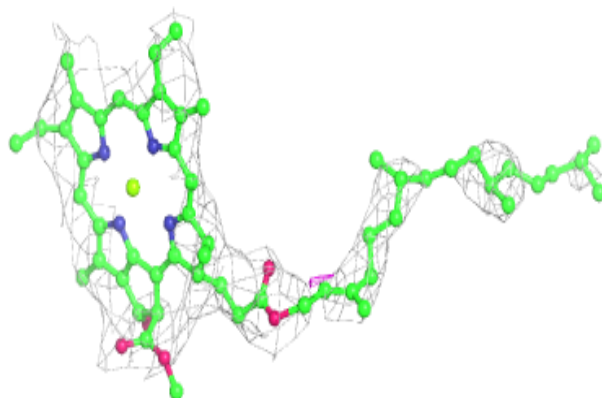


Electron density around CLA A 1131:

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

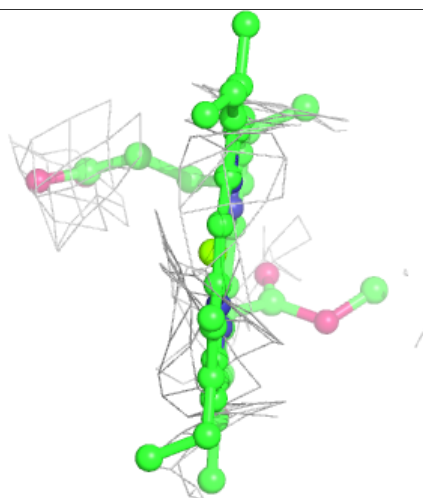
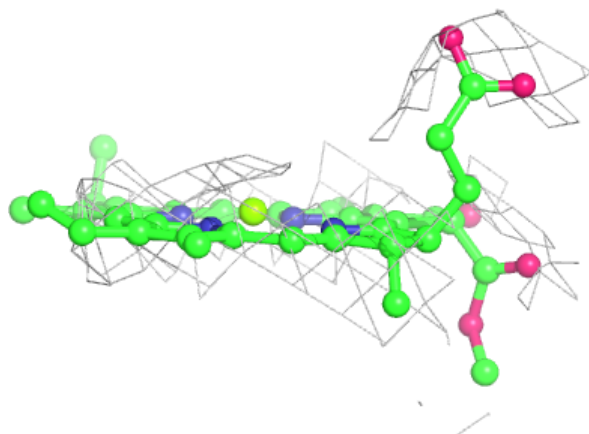
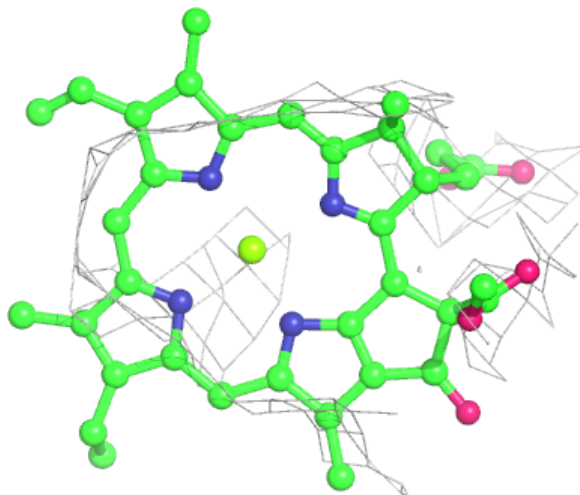
**Electron density around CLA 1 1022:**

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



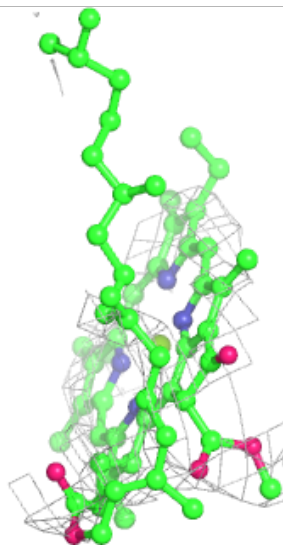
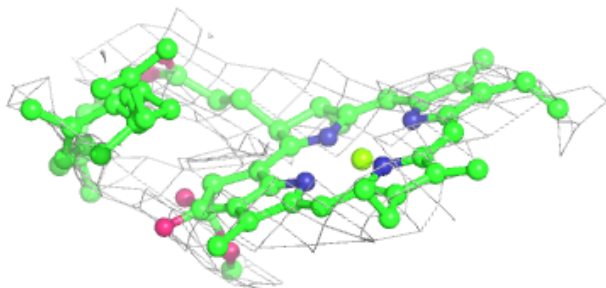
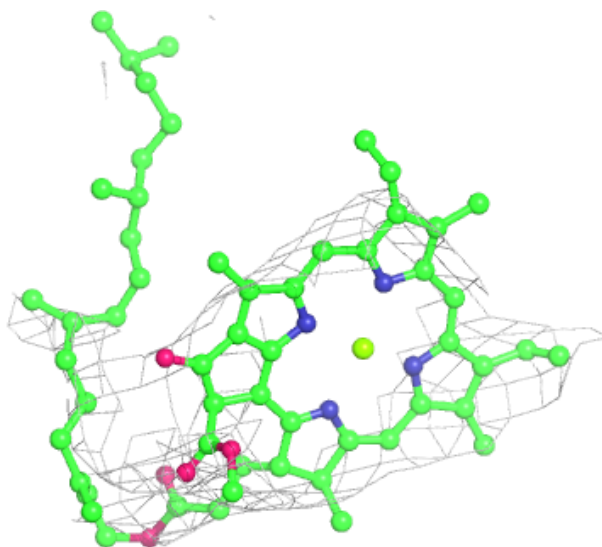
Electron density around CLA a 1112:

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



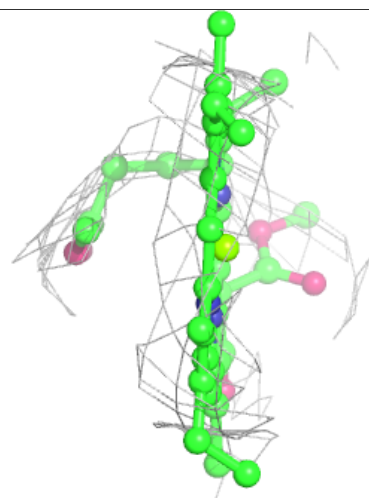
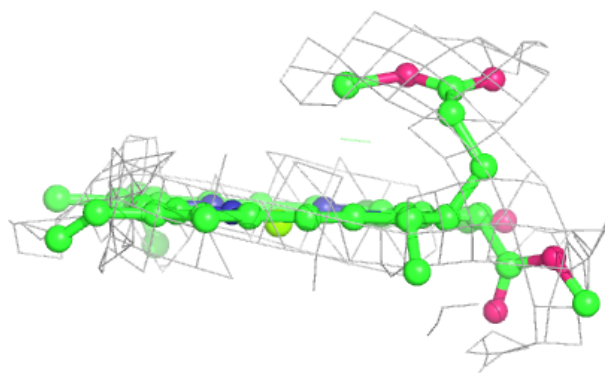
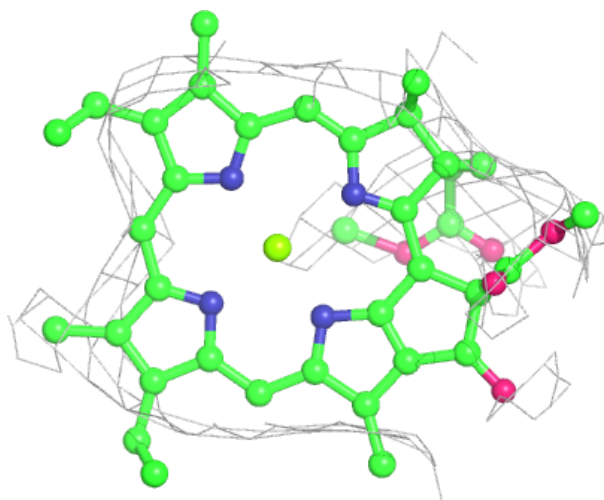
Electron density around CLA 1 1123:

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



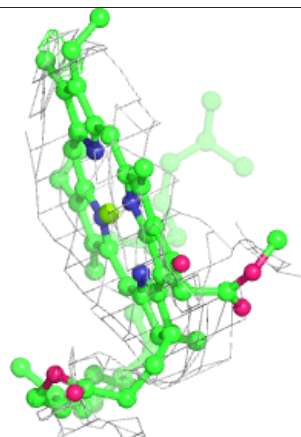
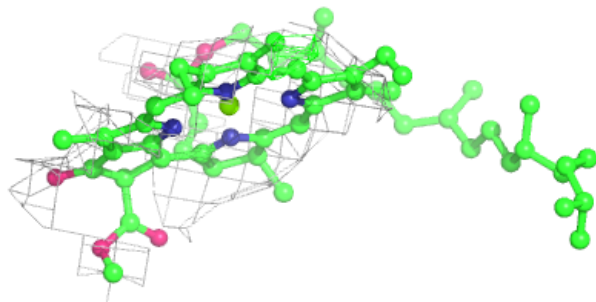
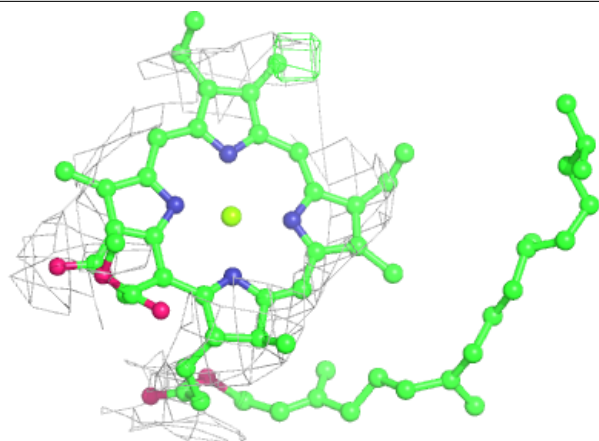
Electron density around CLA a 1115:

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

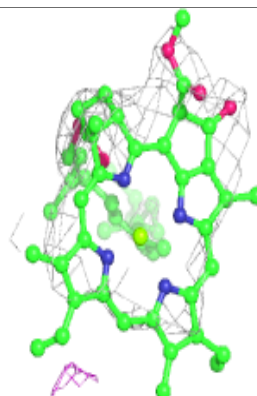
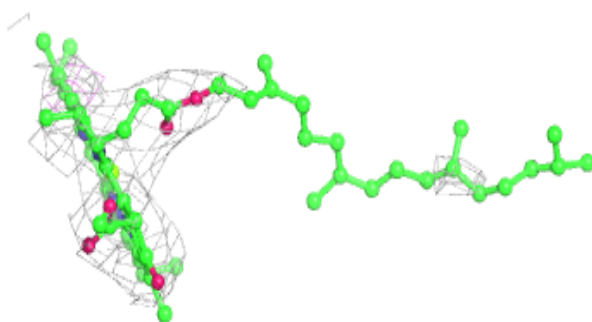
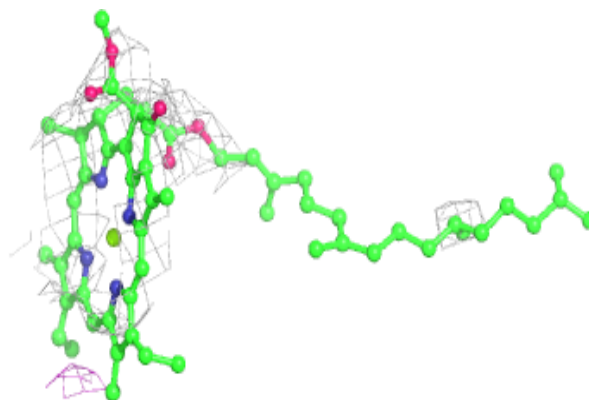


Electron density around CLA 0 1401:

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

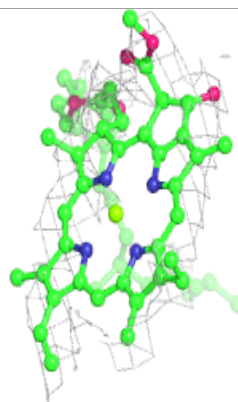
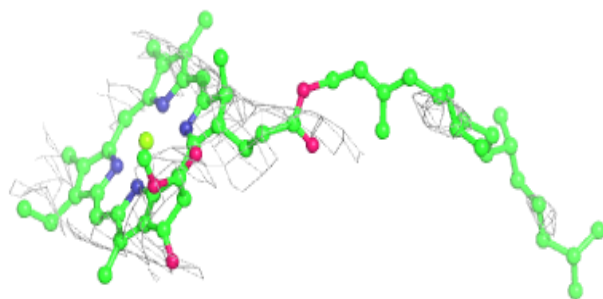
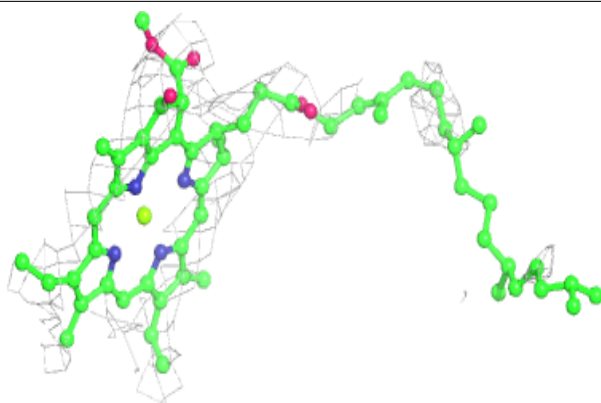
**Electron density around CLA b 1225:**

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

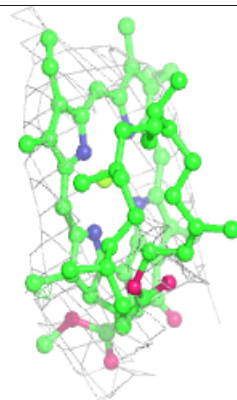
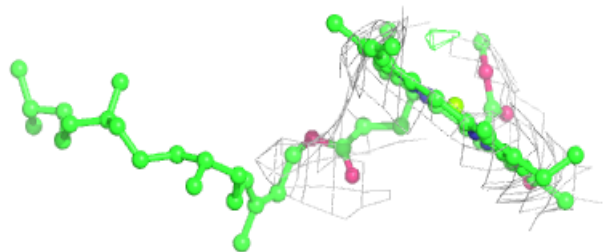
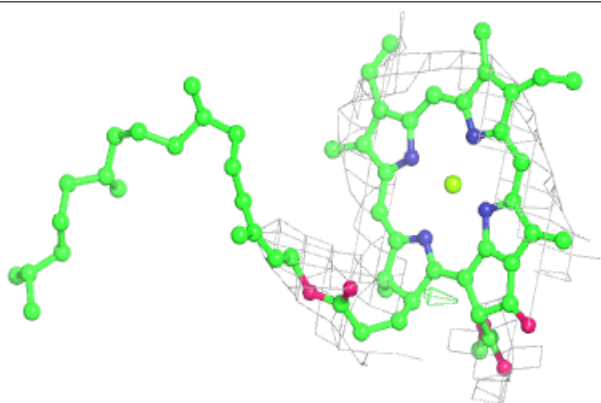


Electron density around CLA a 1012:

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

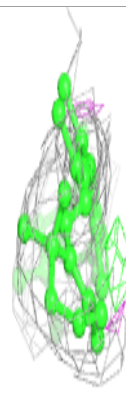
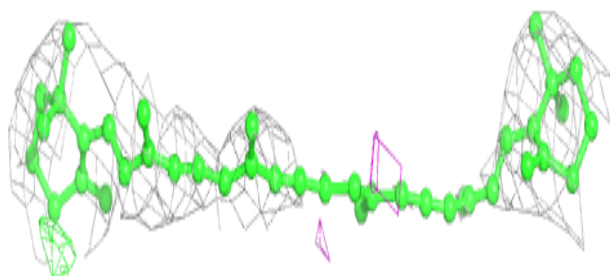
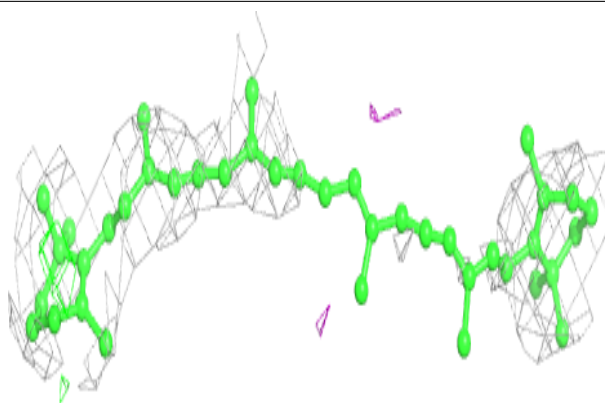
**Electron density around CLA 1 1106:**

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



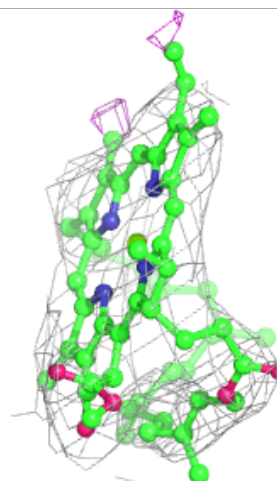
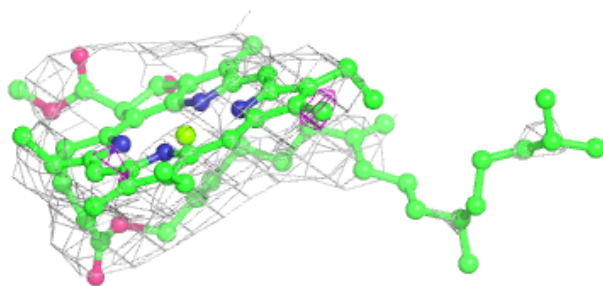
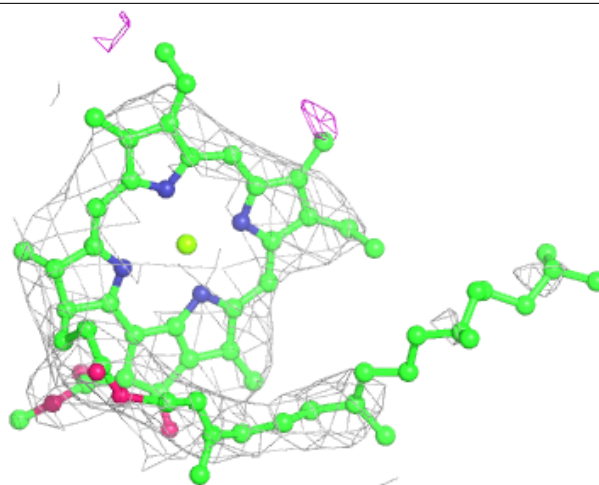
Electron density around BCR A 4001:

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



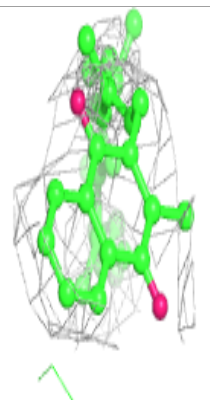
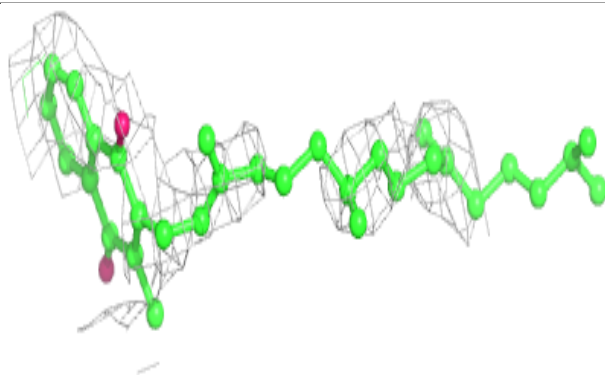
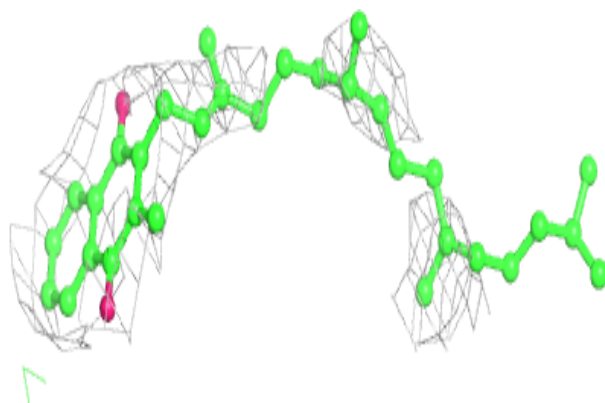
Electron density around CLA A 1127:

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



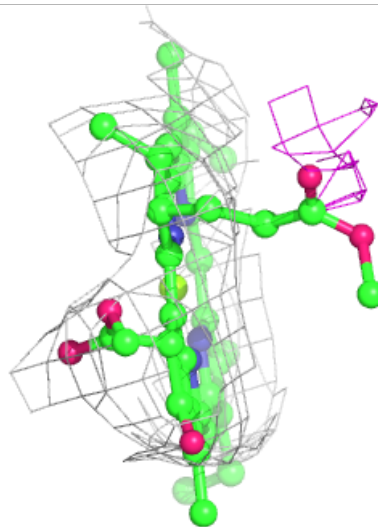
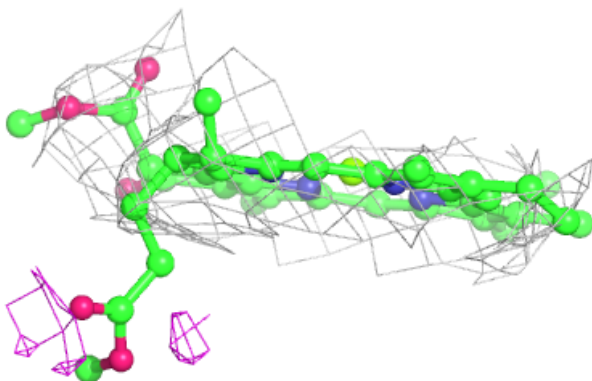
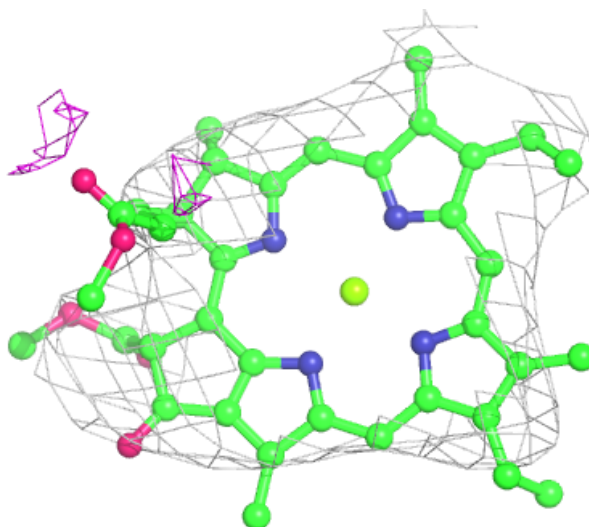
Electron density around PQN A 2001:

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



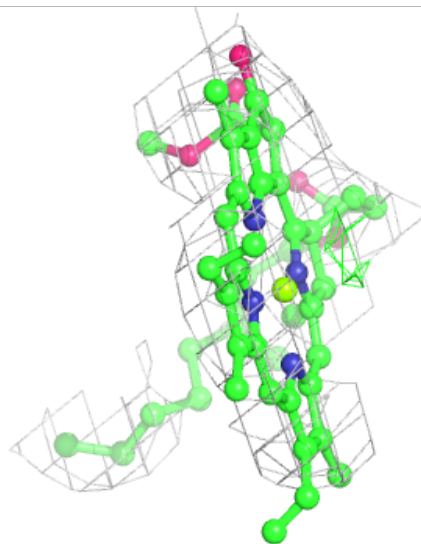
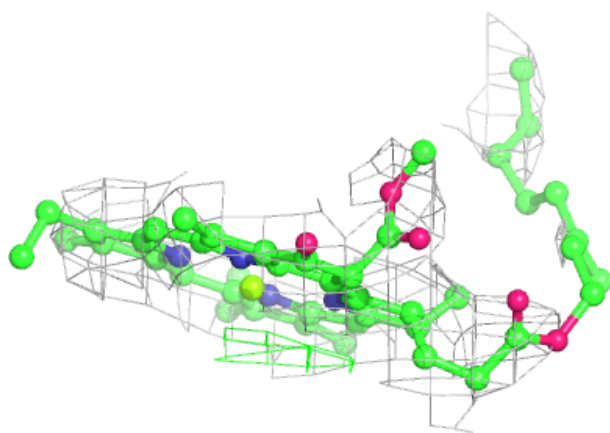
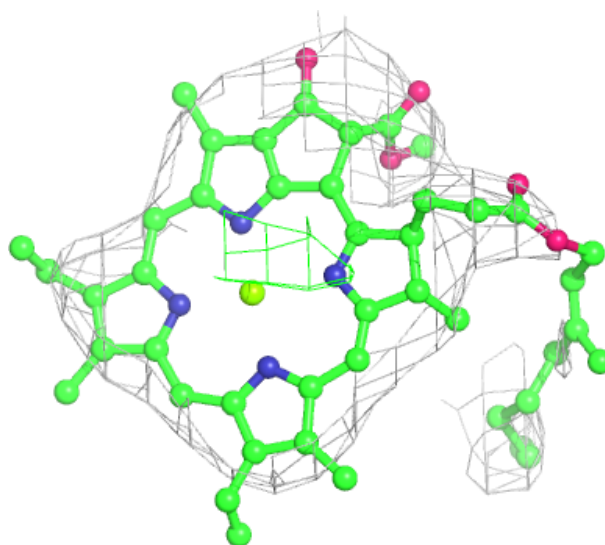
Electron density around CLA A 1114:

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



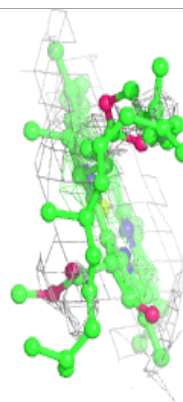
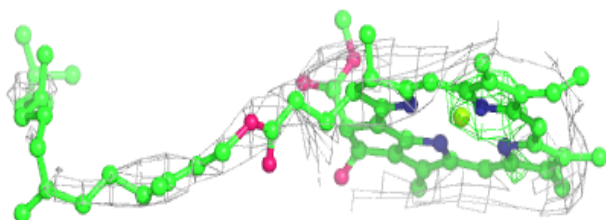
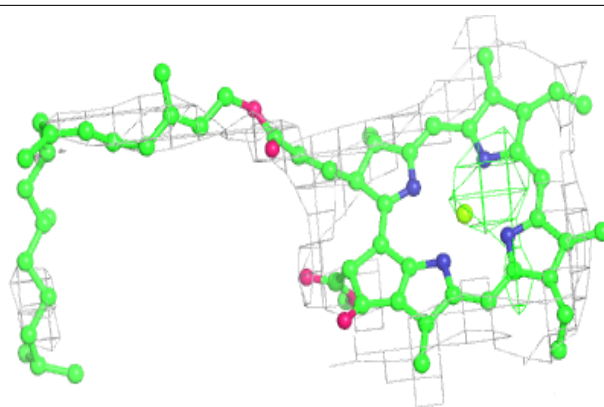
Electron density around CLA 2 1221:

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

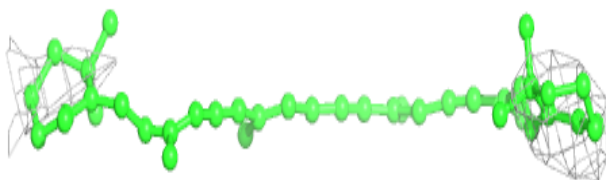
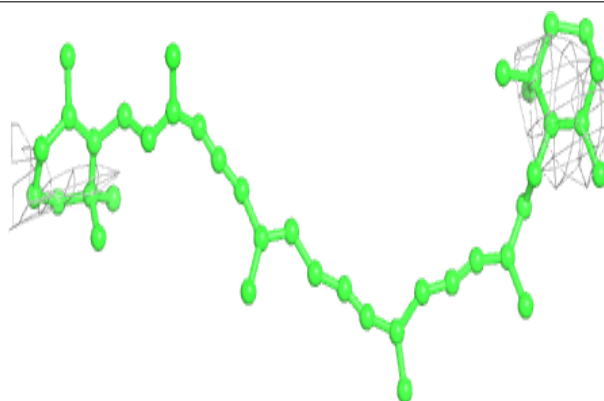


Electron density around CLA B 1223:

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

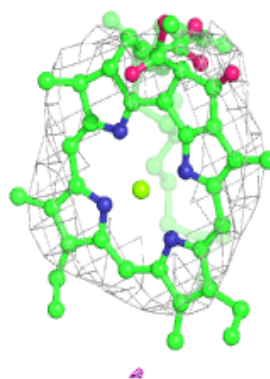
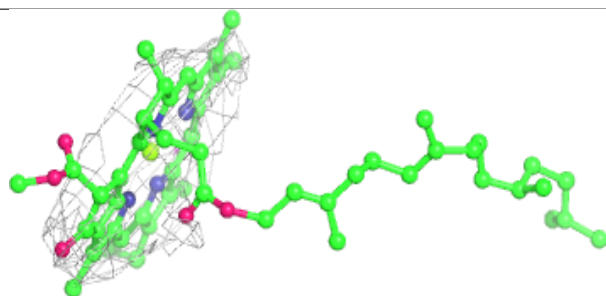
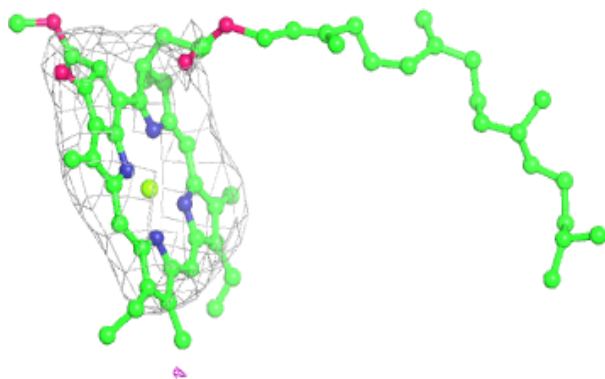
**Electron density around BCR 2 4011:**

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



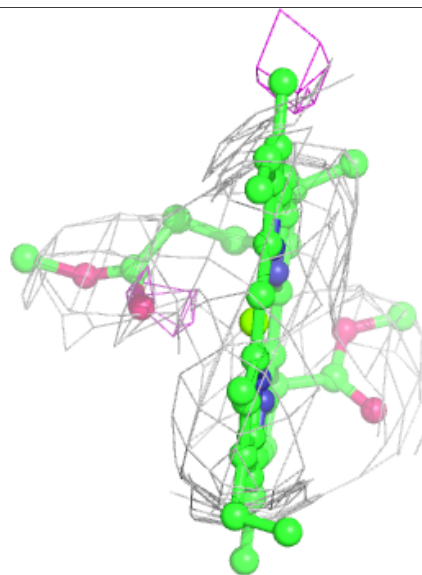
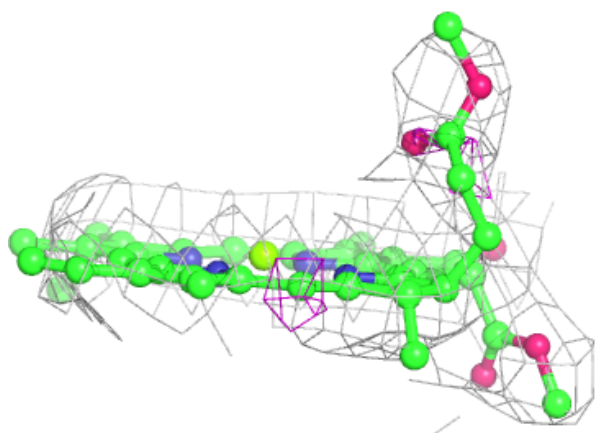
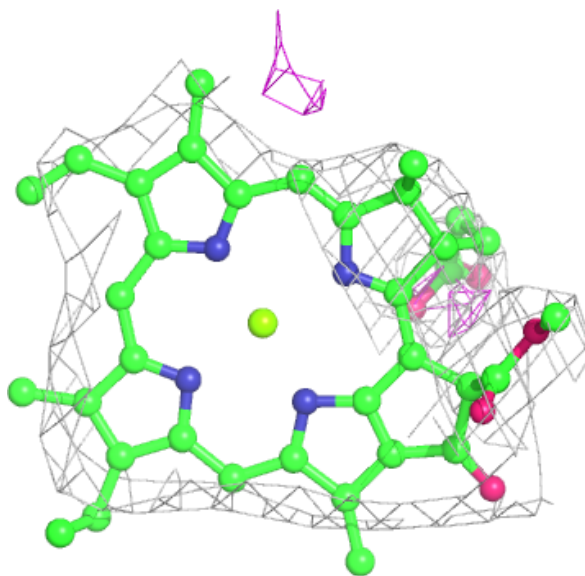
Electron density around CLA a 1140:

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



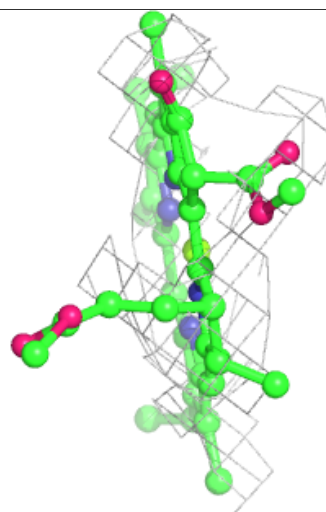
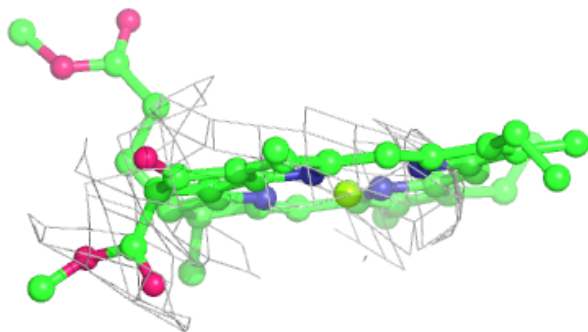
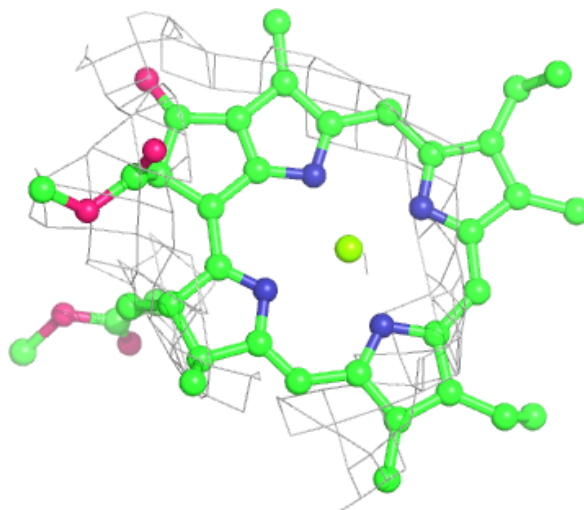
Electron density around CLA A 1134:

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



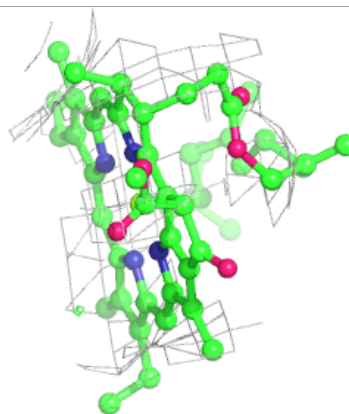
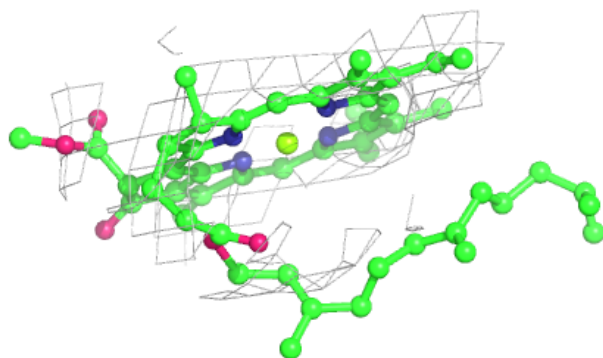
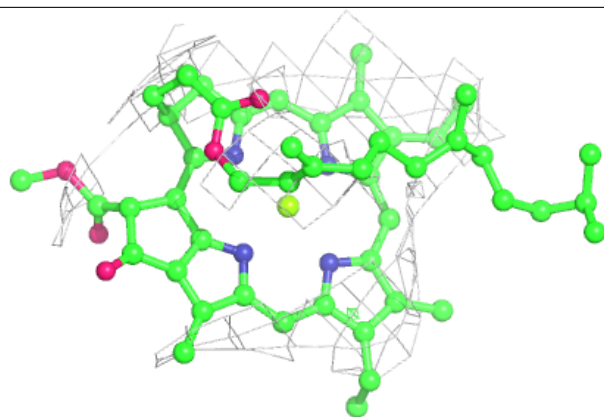
Electron density around CLA 1 1114:

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



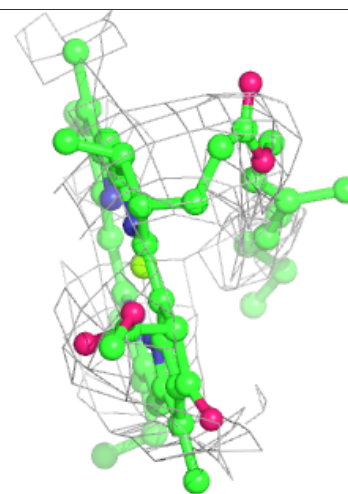
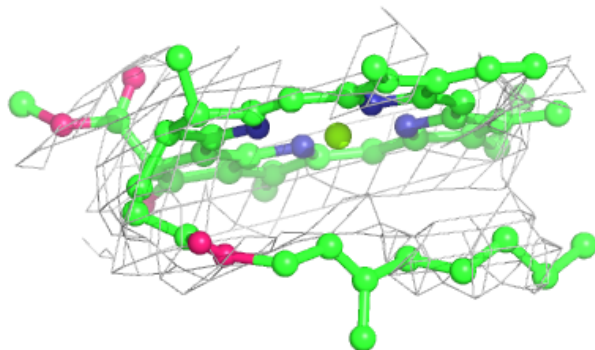
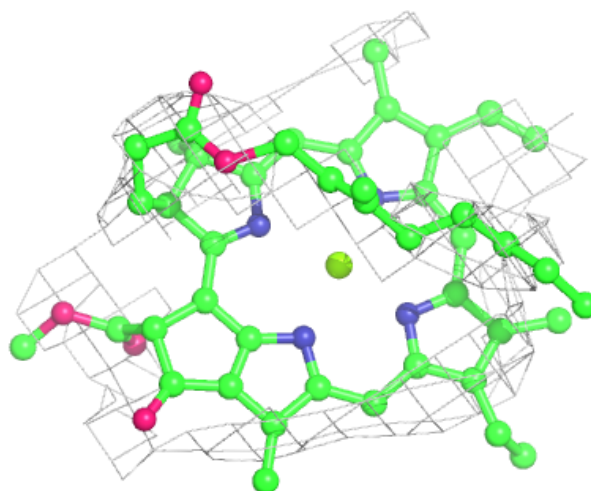
Electron density around CLA b 1235:

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



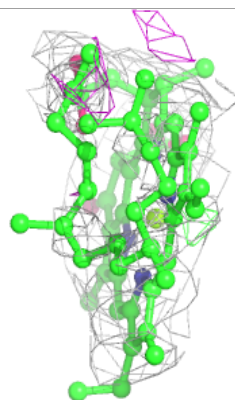
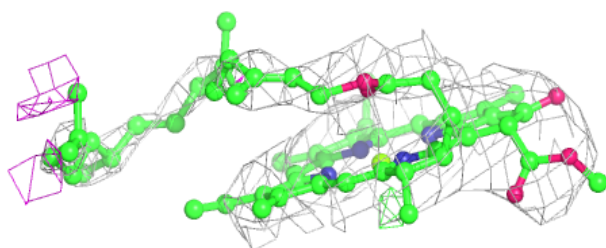
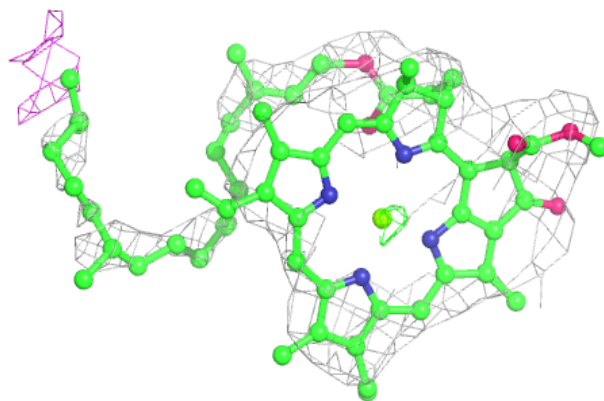
Electron density around CLA a 1116:

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

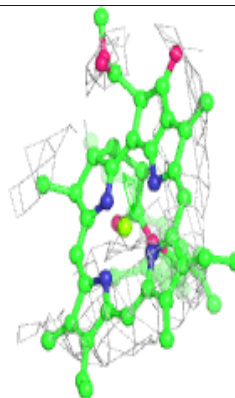
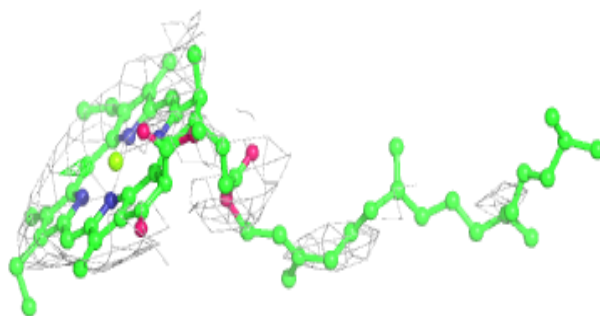
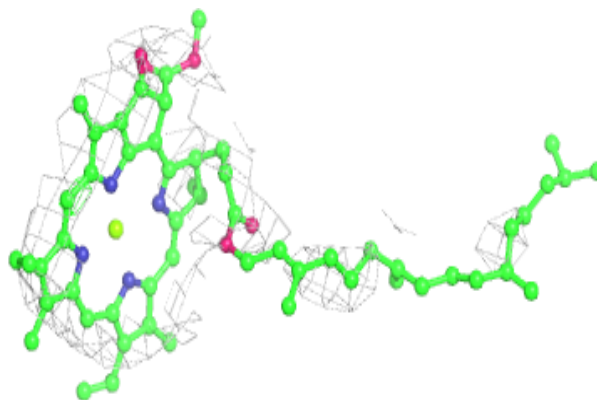


Electron density around CLA A 1117:

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

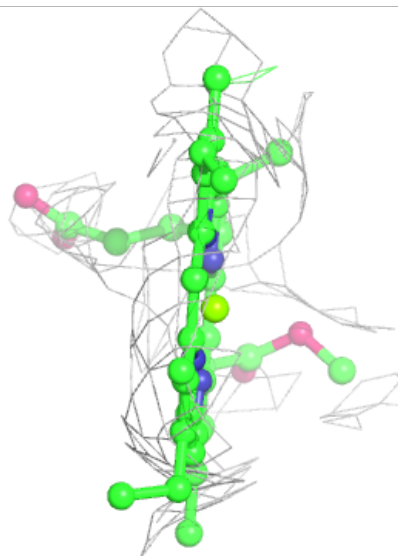
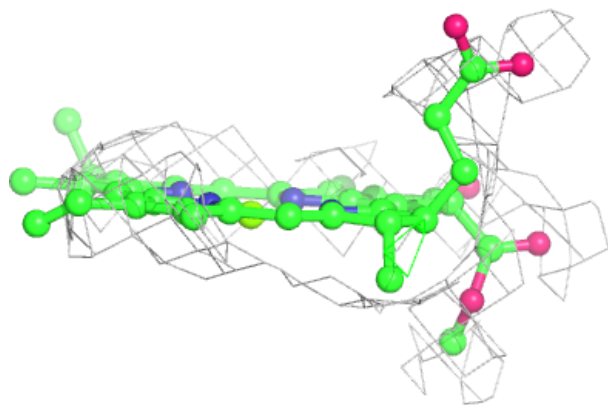
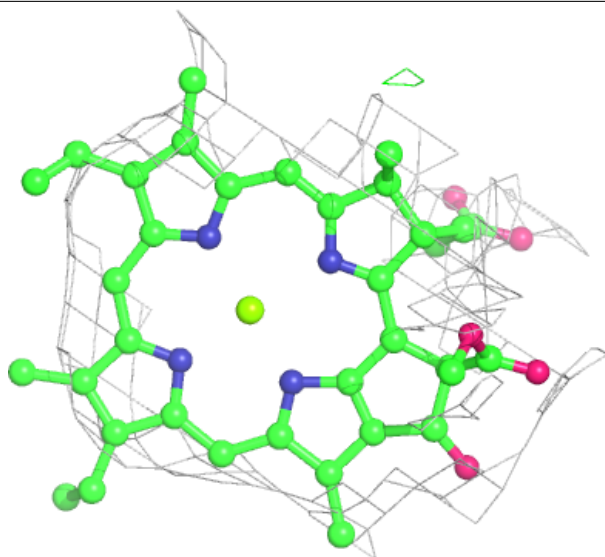
**Electron density around CLA a 1119:**

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



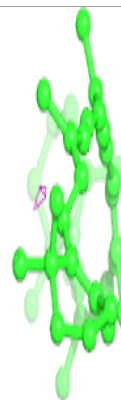
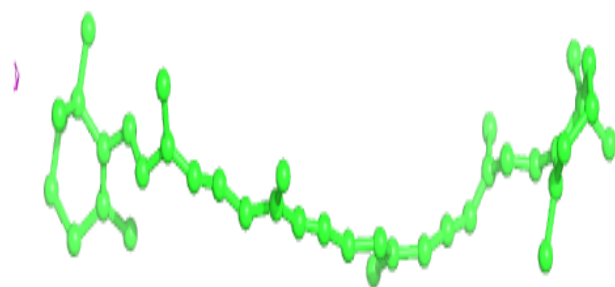
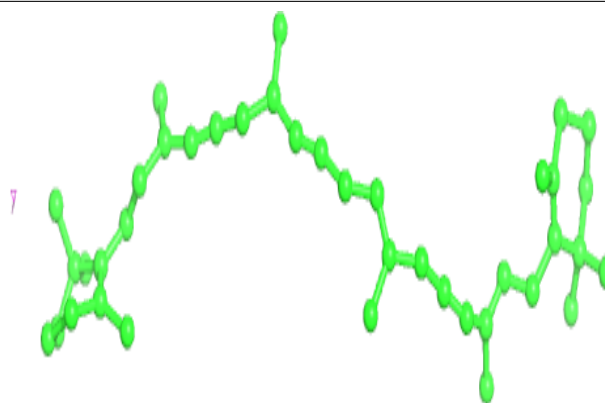
Electron density around CLA B 1231:

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

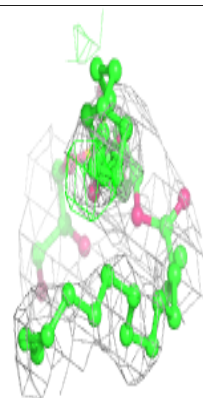
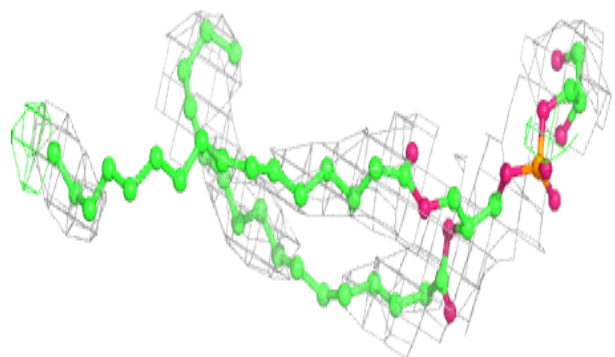
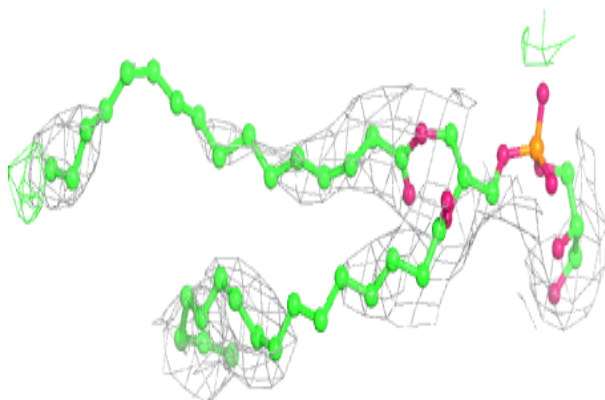


Electron density around BCR b 4014:

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

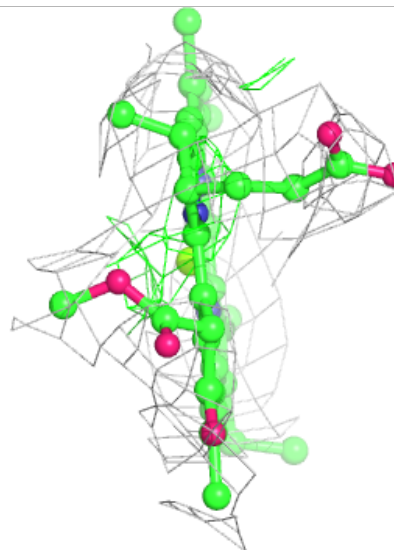
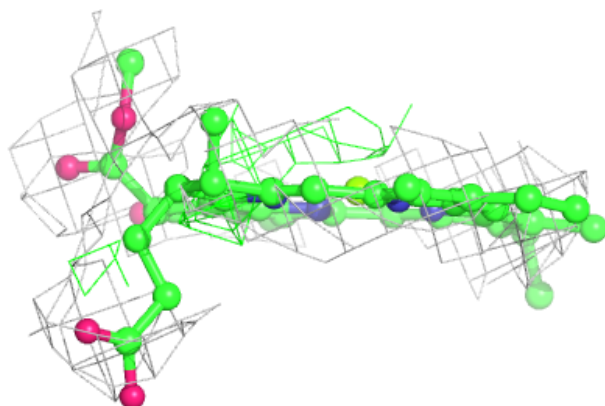
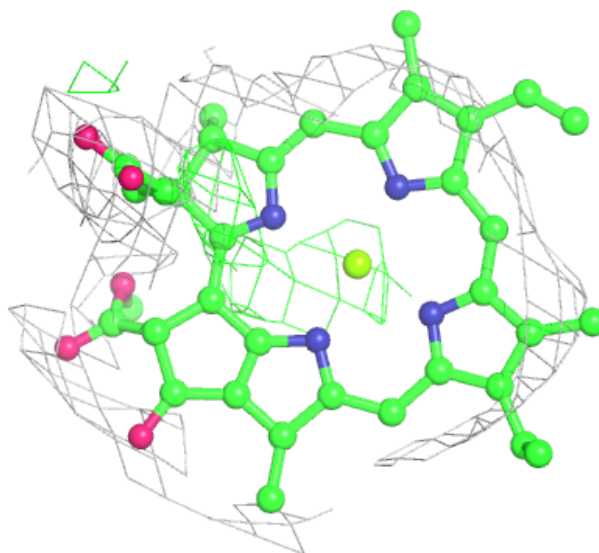
**Electron density around LHG A 5003:**

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



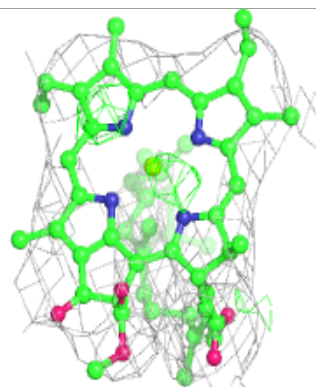
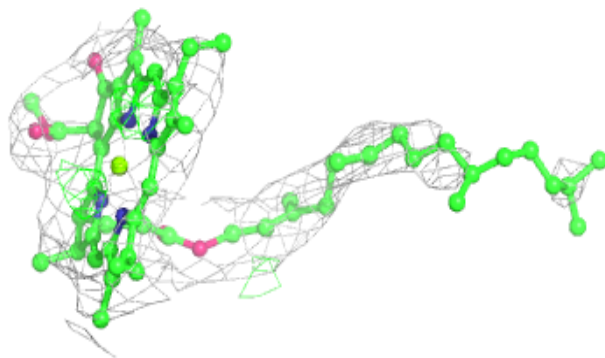
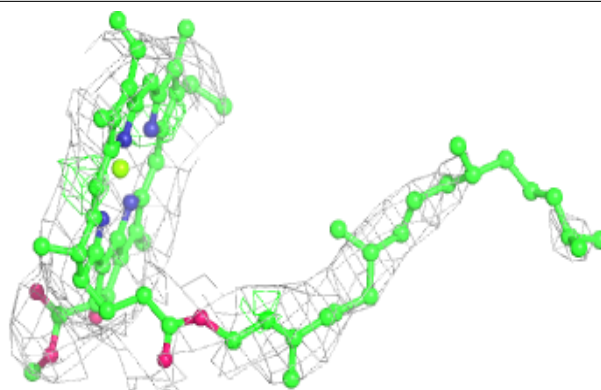
Electron density around CLA 2 1231:

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



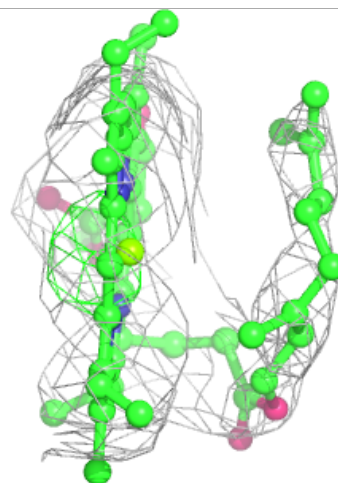
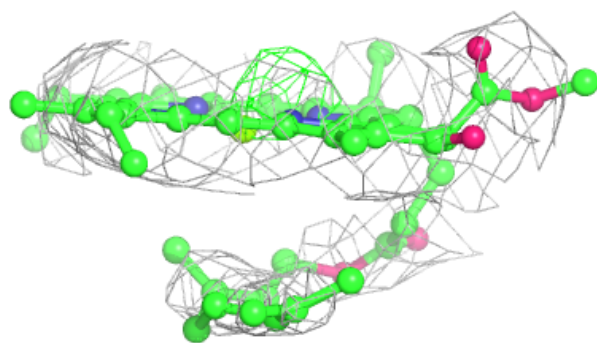
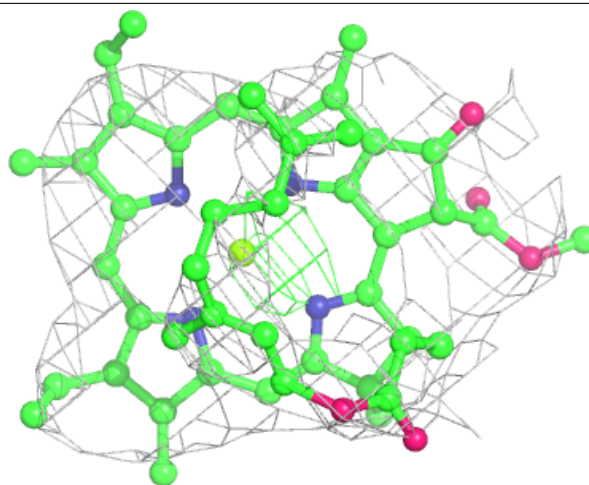
Electron density around CLA A 1128:

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



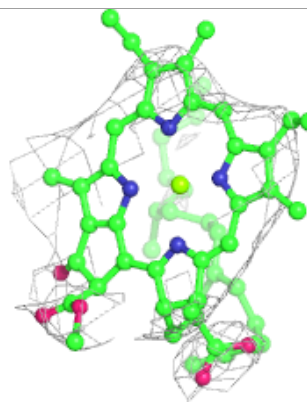
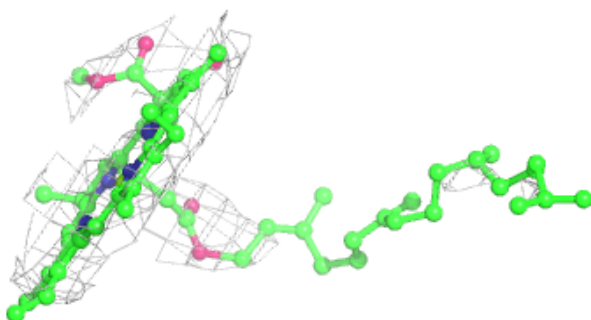
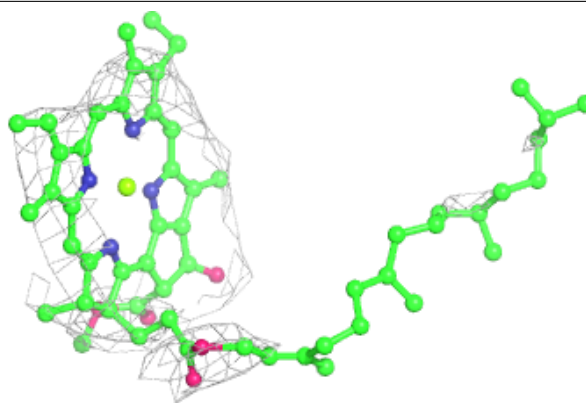
Electron density around CLA B 1224:

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

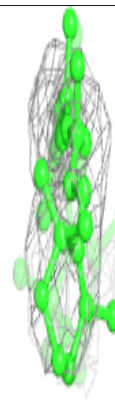
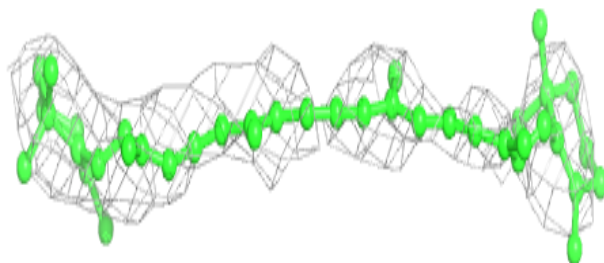
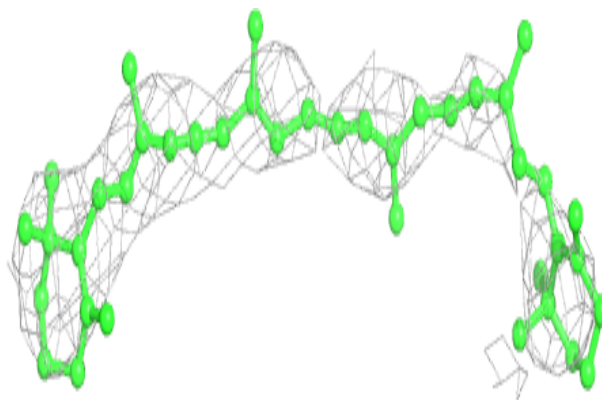


Electron density around CLA 1 1137:

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

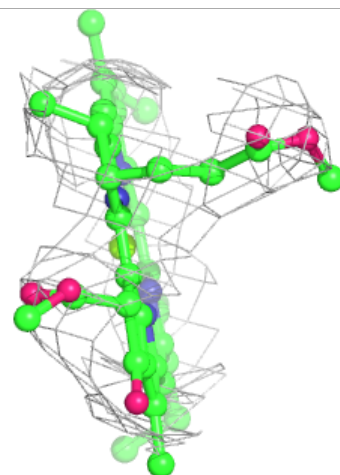
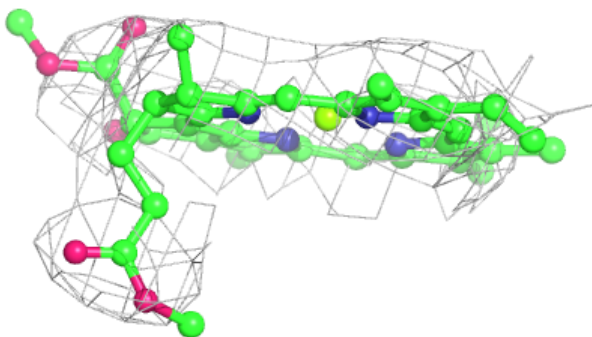
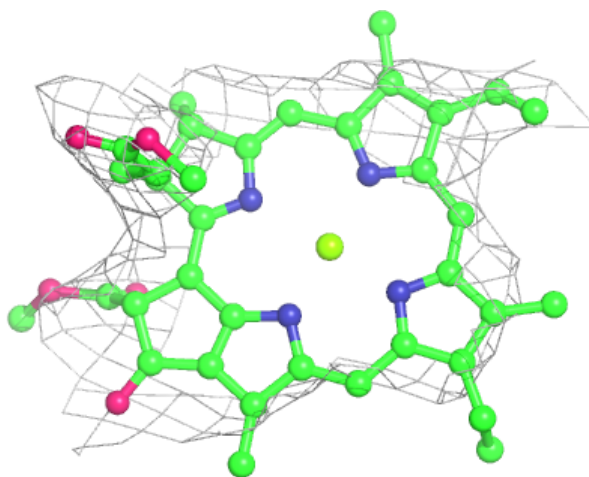
**Electron density around BCR f 4020:**

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



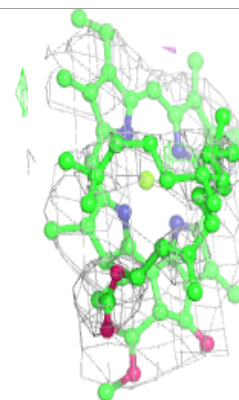
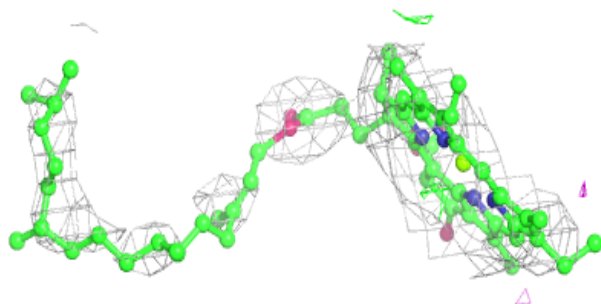
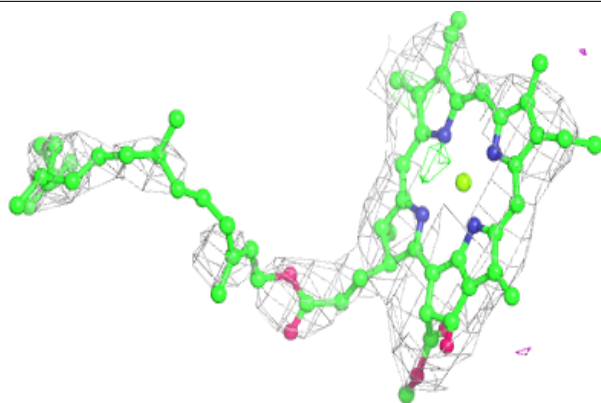
Electron density around CLA 1 1130:

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

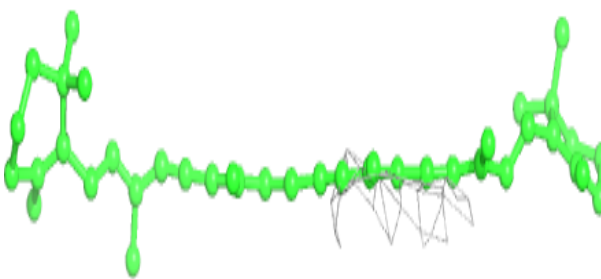
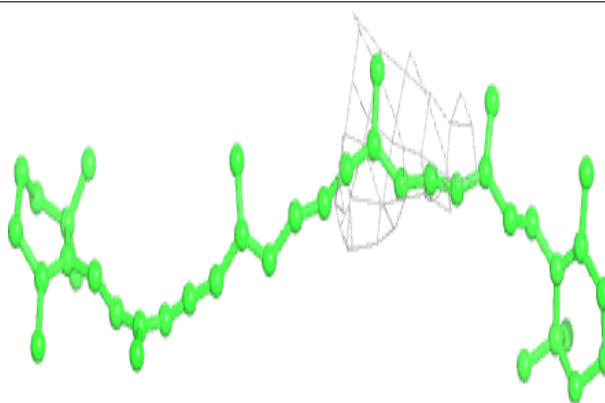


Electron density around CLA B 1206:

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

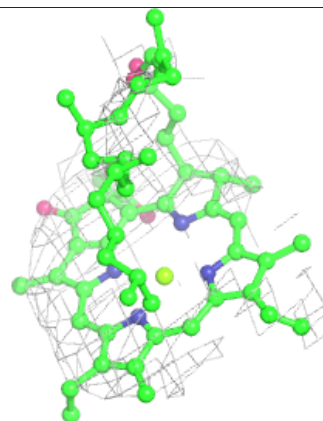
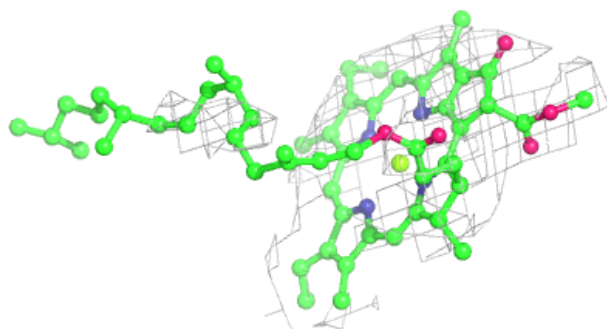
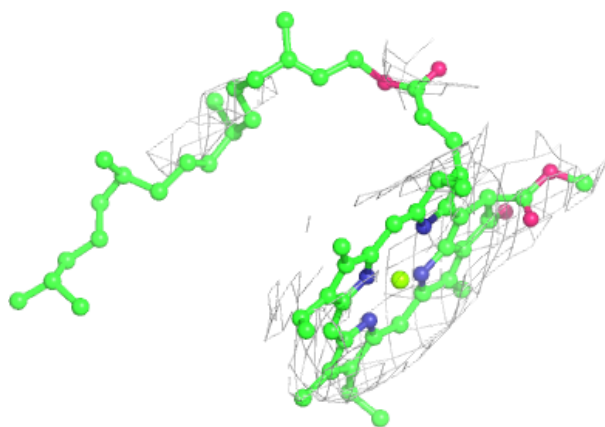
**Electron density around BCR b 4009:**

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

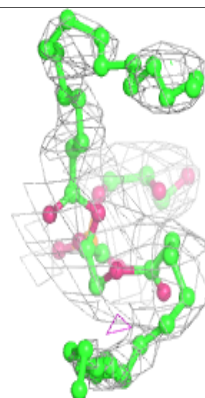
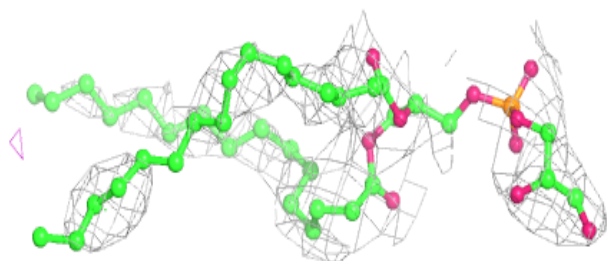
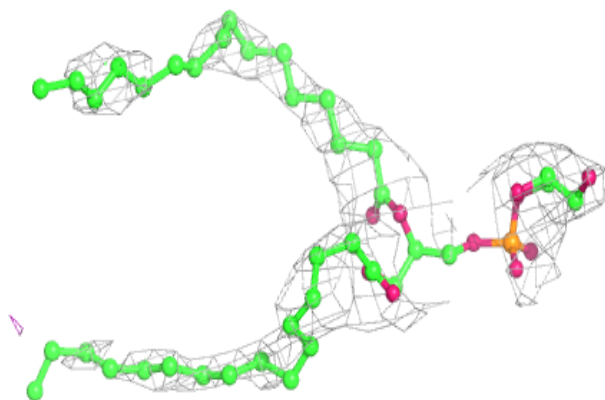


Electron density around CLA a 1102:

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

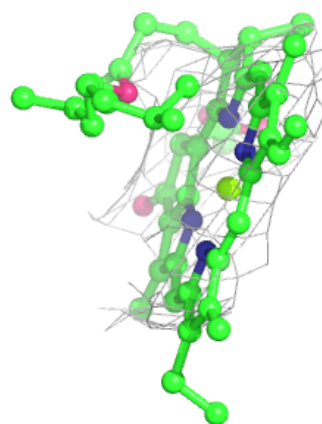
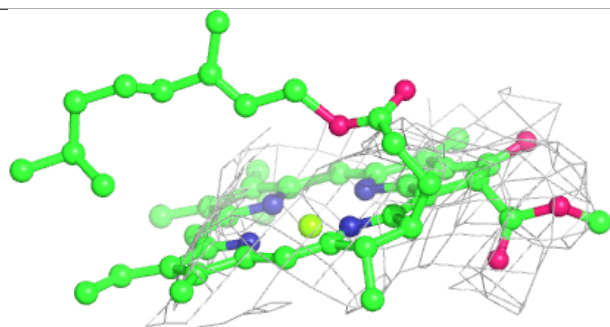
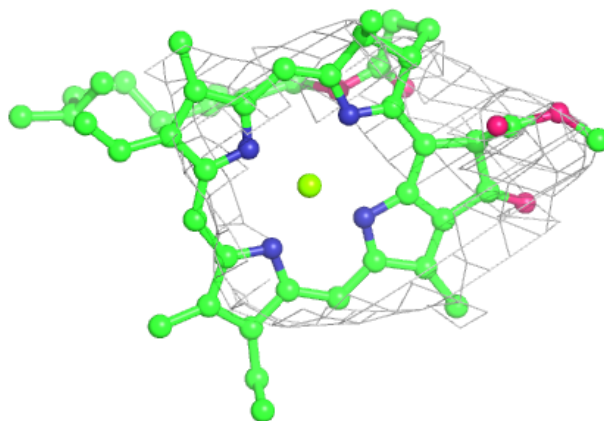
**Electron density around LHG A 5001:**

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



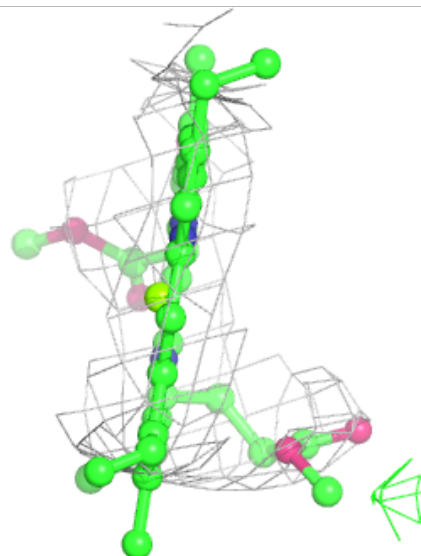
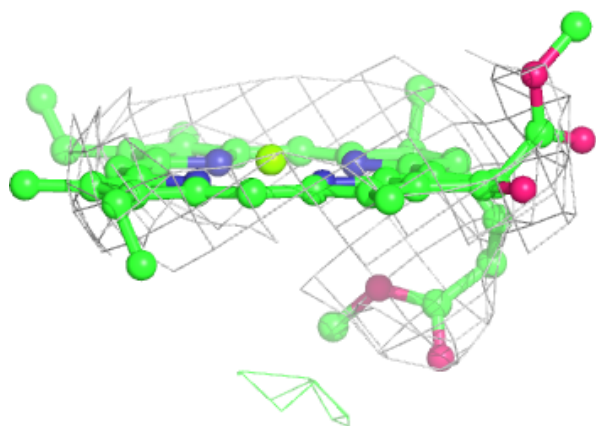
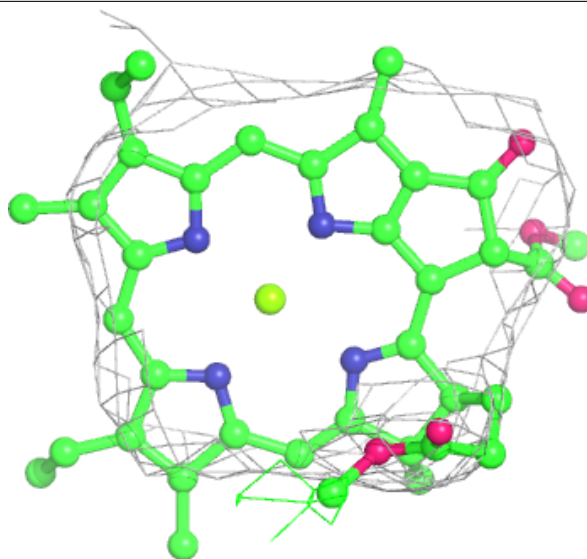
Electron density around CLA b 1219:

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



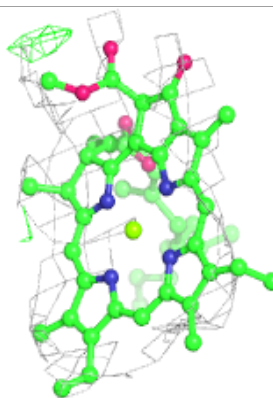
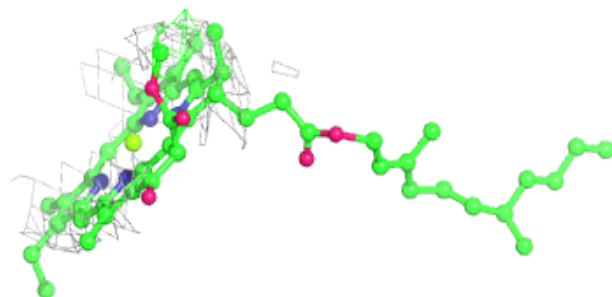
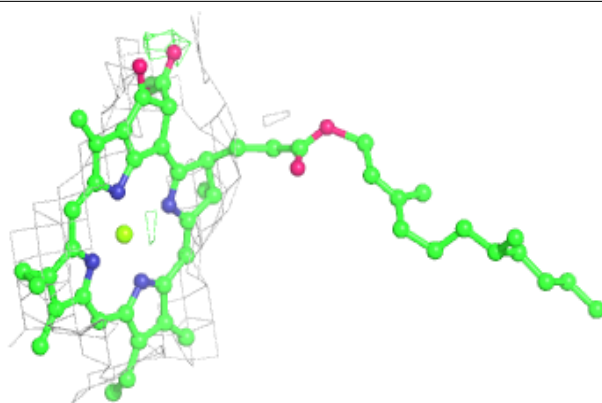
Electron density around CLA a 1120:

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



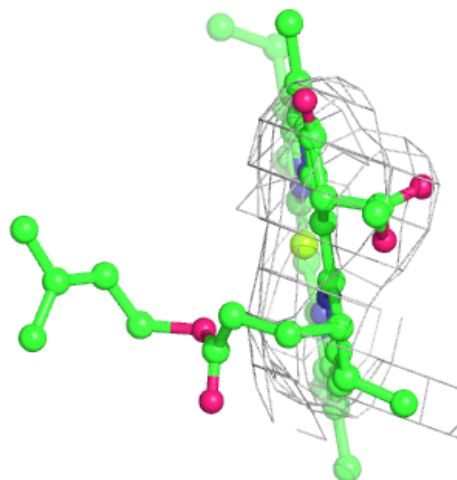
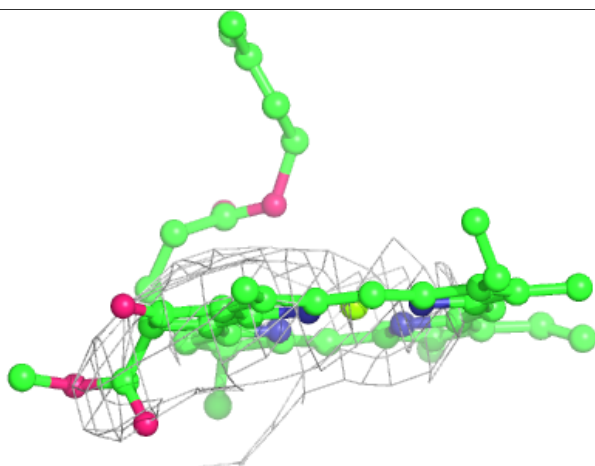
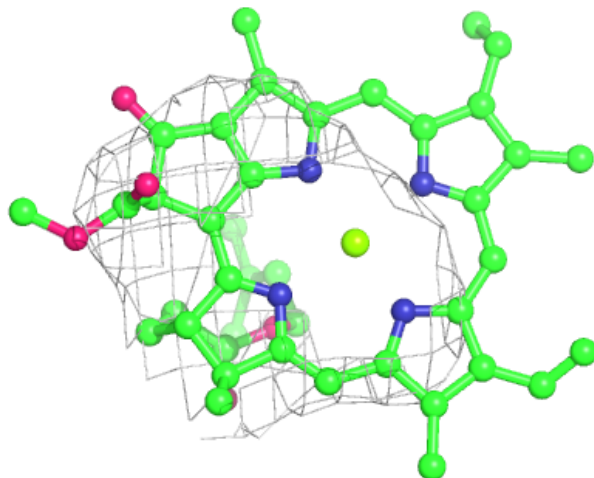
Electron density around CLA b 1230:

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



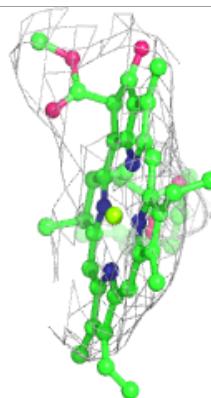
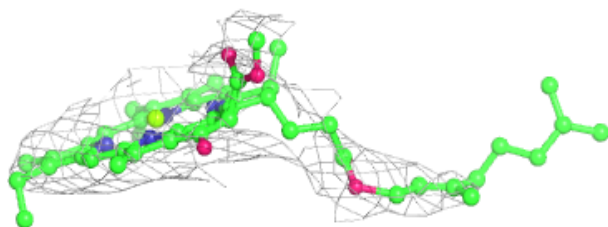
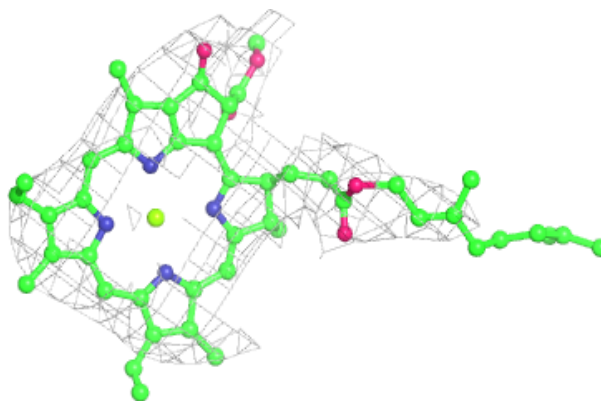
Electron density around CLA 0 1402:

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

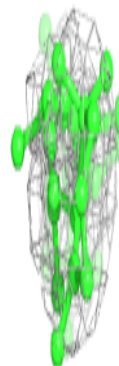
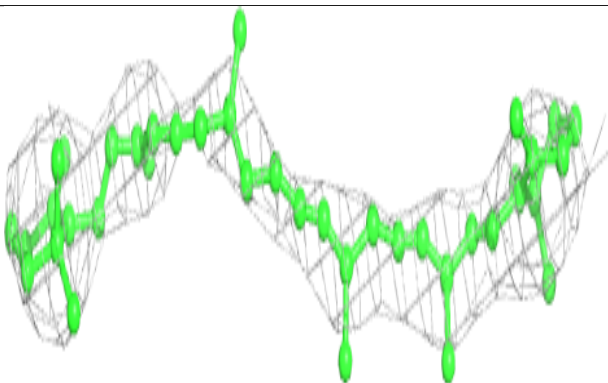
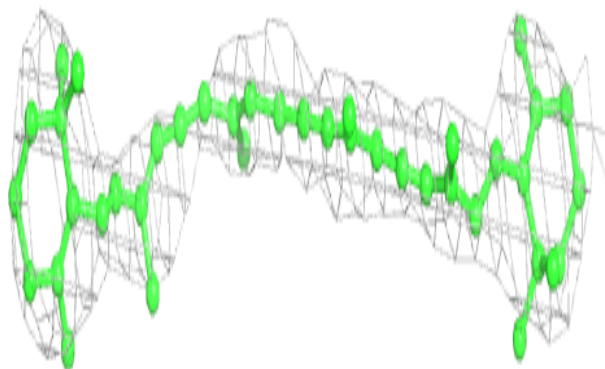


Electron density around CLA 1 1124:

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

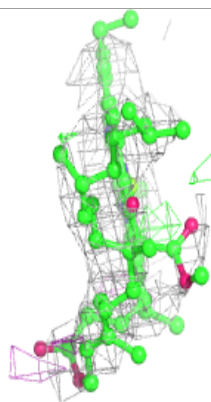
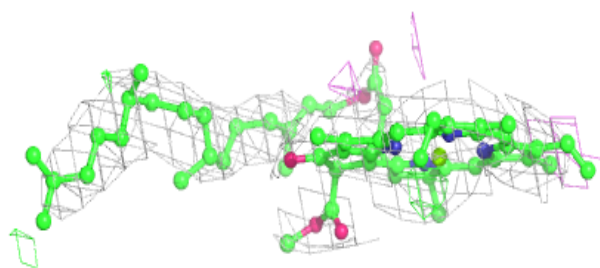
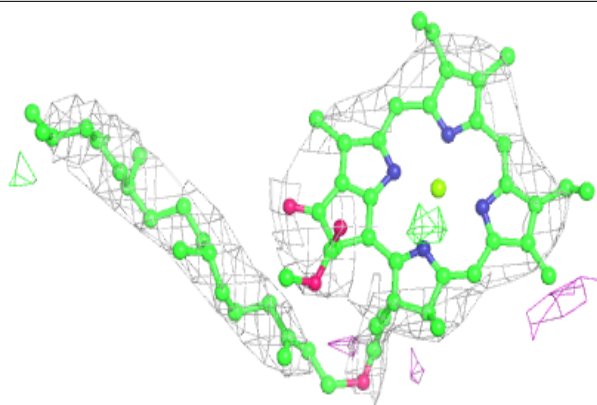
**Electron density around BCR A 4003:**

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

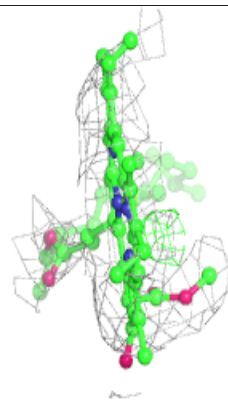
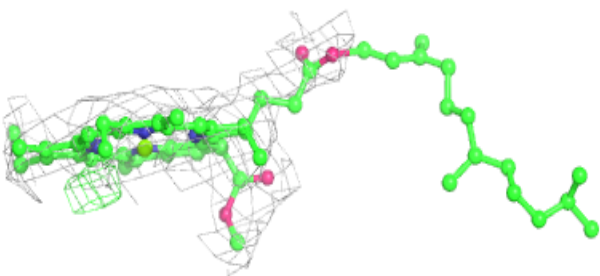
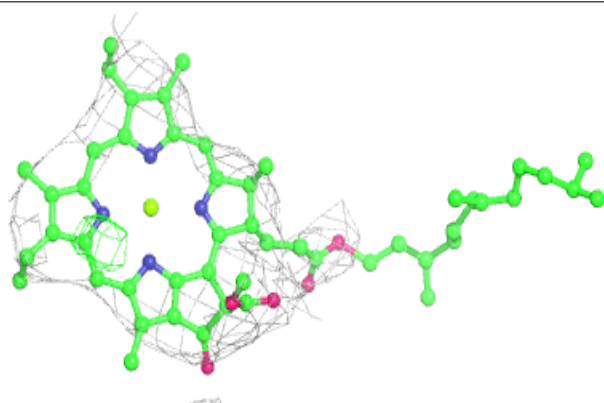


Electron density around CLA L 1503:

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

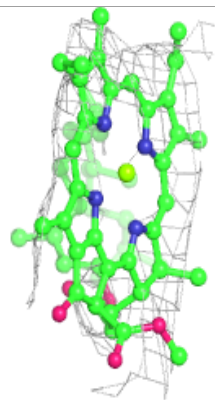
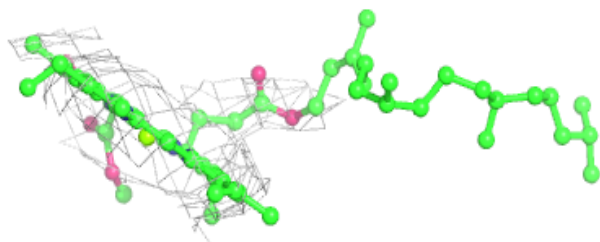
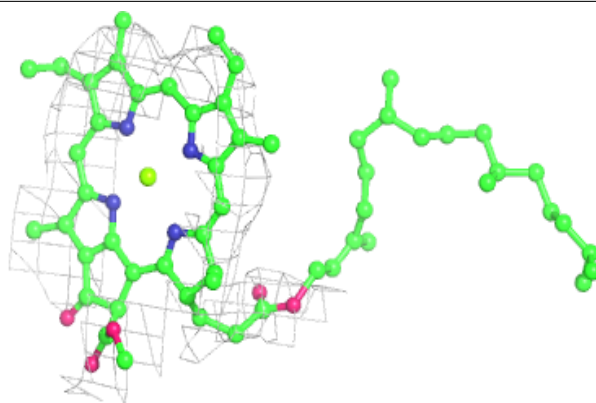
**Electron density around CLA B 1234:**

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



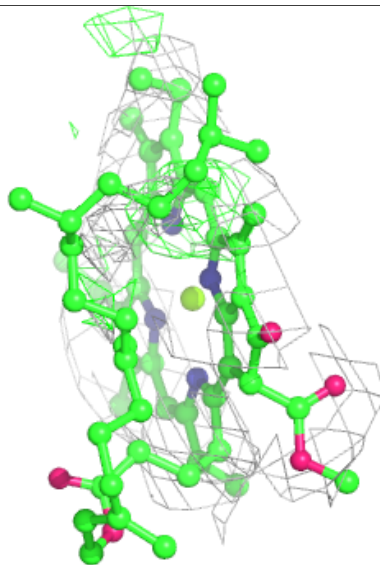
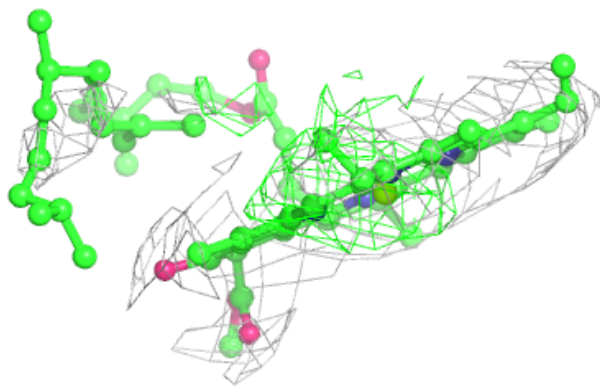
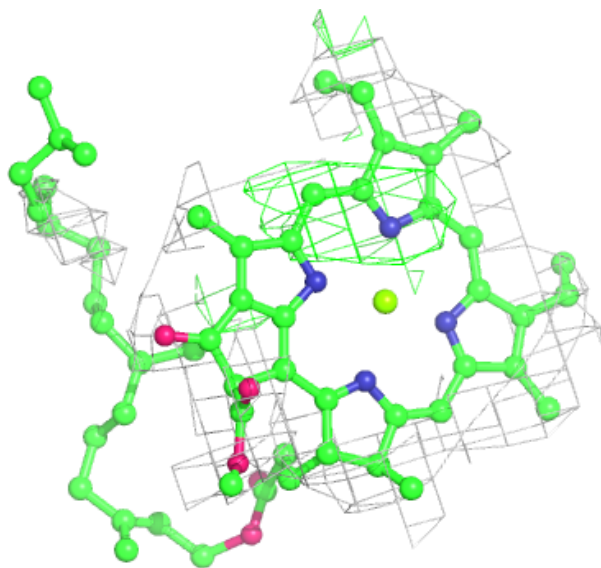
Electron density around CLA a 1106:

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



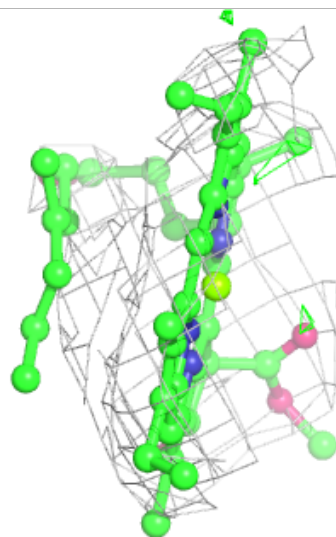
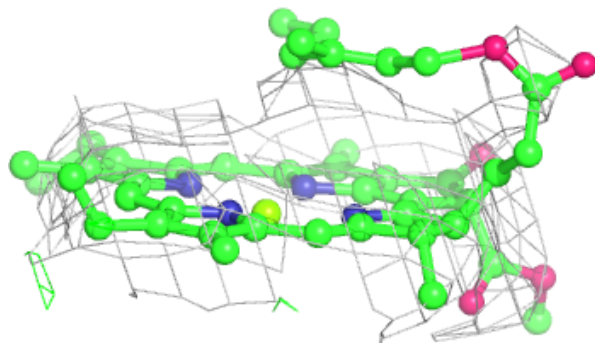
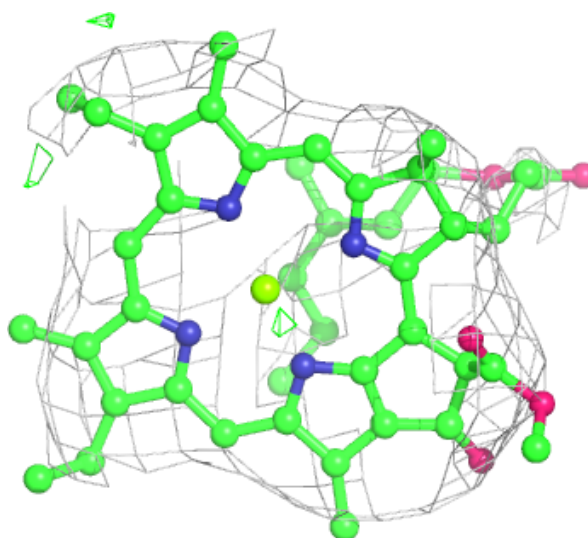
Electron density around CLA 2 1229:

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



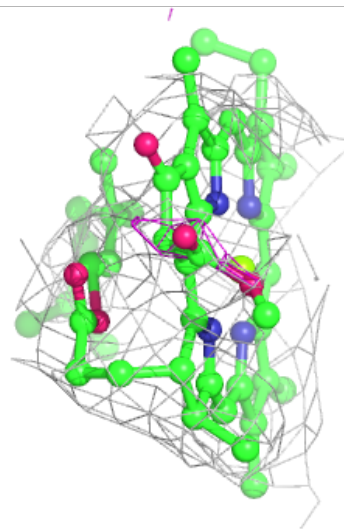
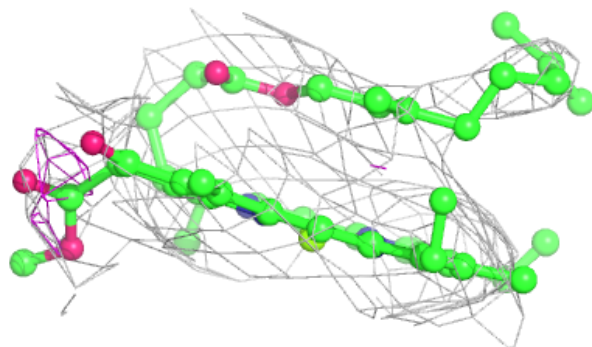
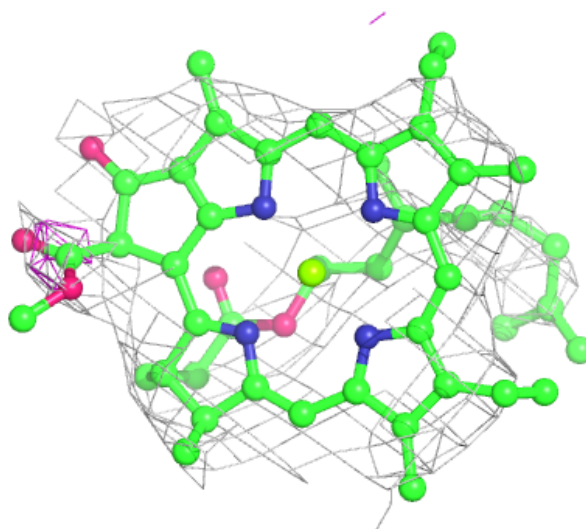
Electron density around CLA a 1801:

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



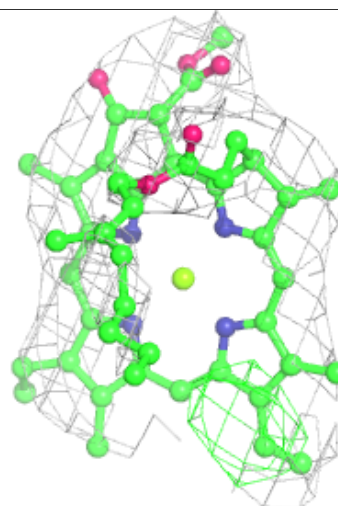
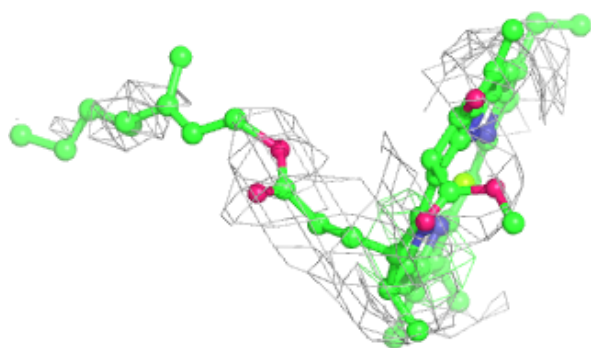
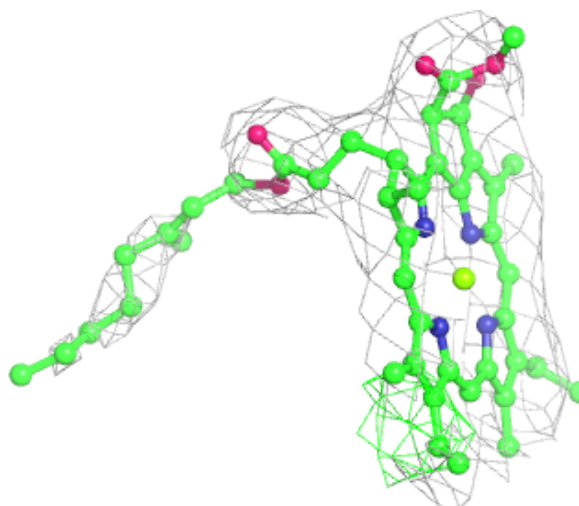
Electron density around CLA B 1205:

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



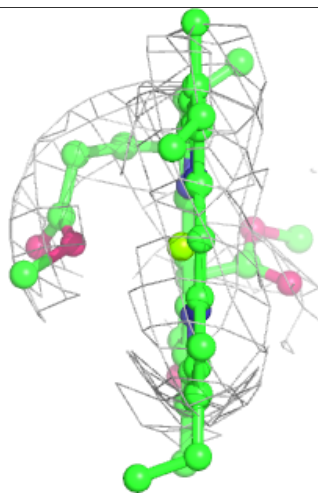
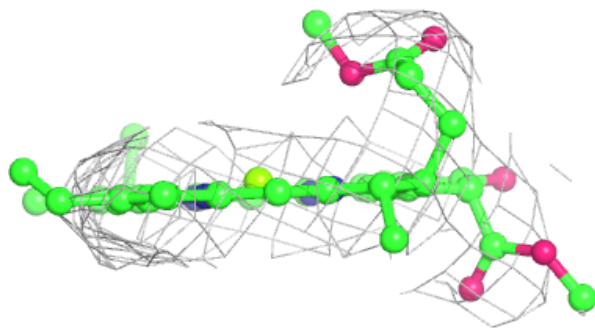
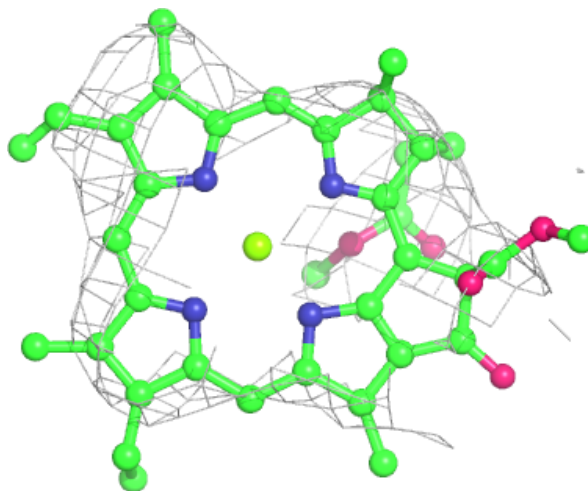
Electron density around CLA 2 1201:

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



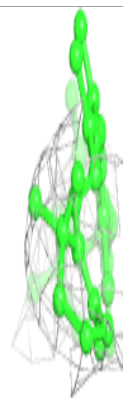
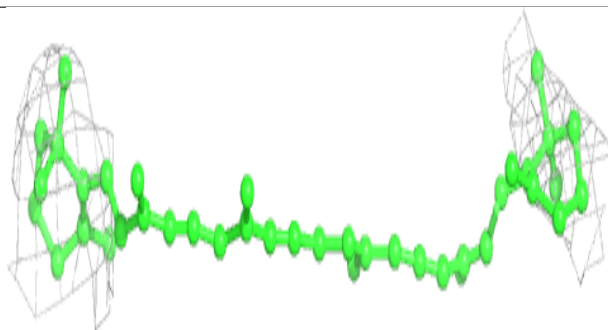
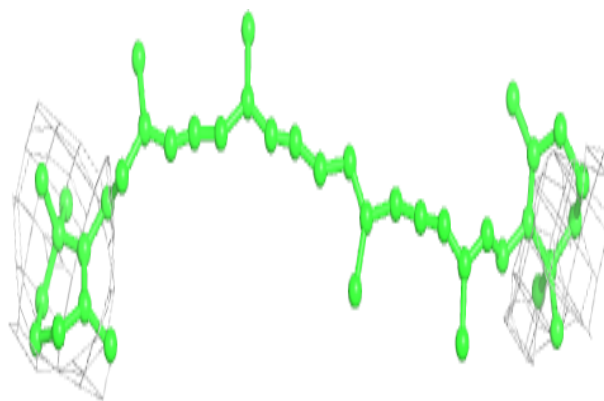
Electron density around CLA a 1136:

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



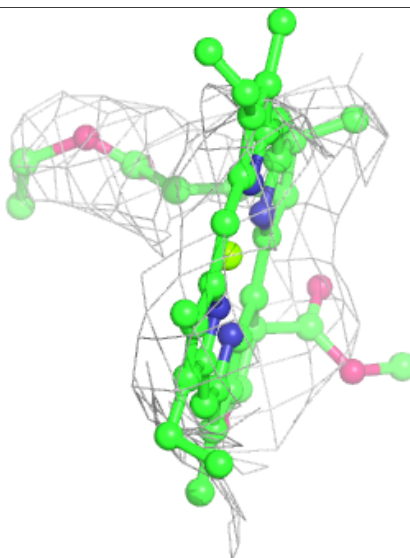
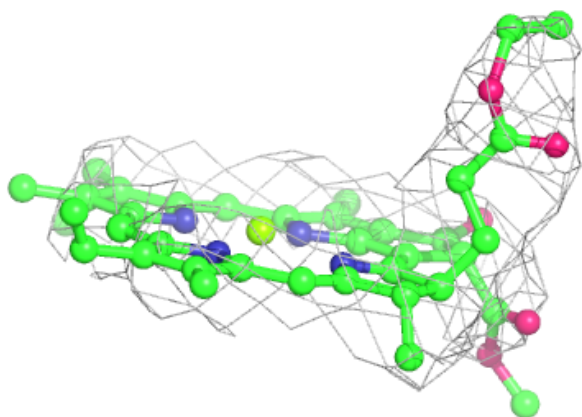
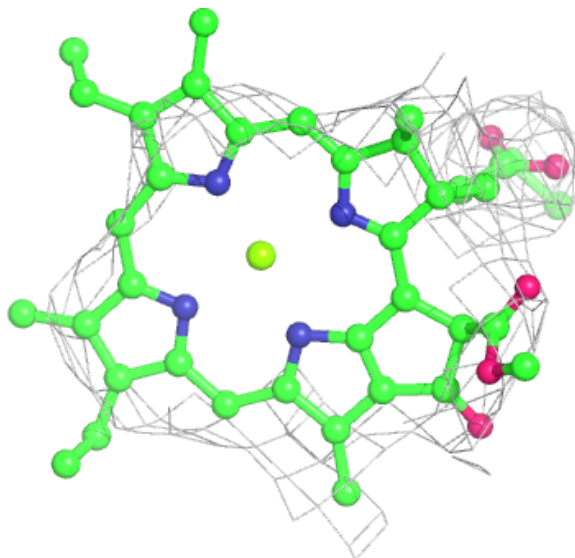
Electron density around BCR a 4001:

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



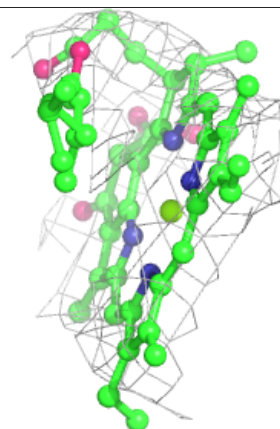
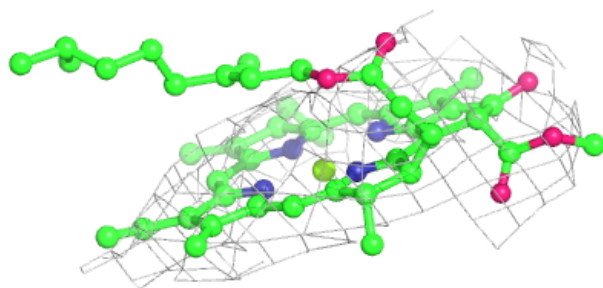
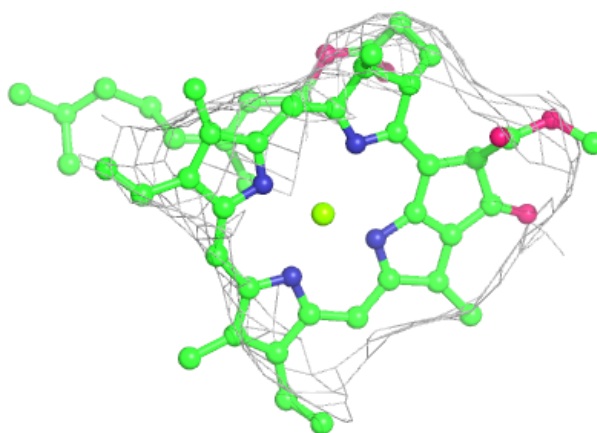
Electron density around CLA 2 1236:

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



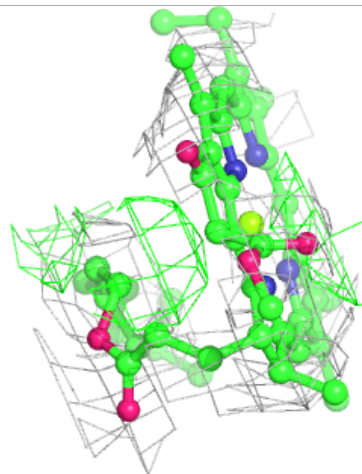
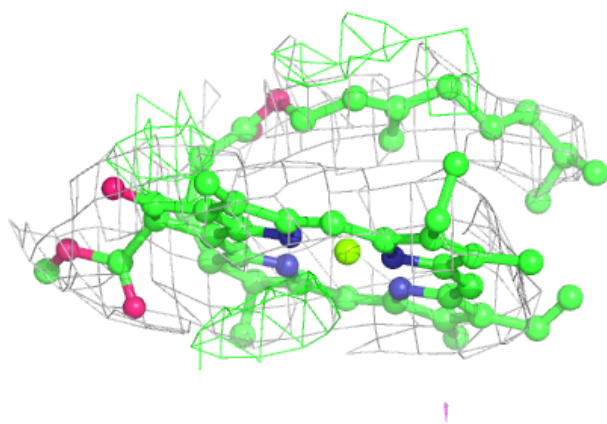
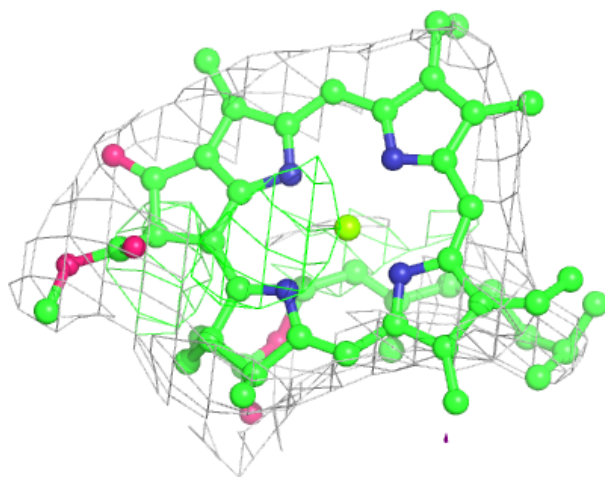
Electron density around CLA 2 1219:

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



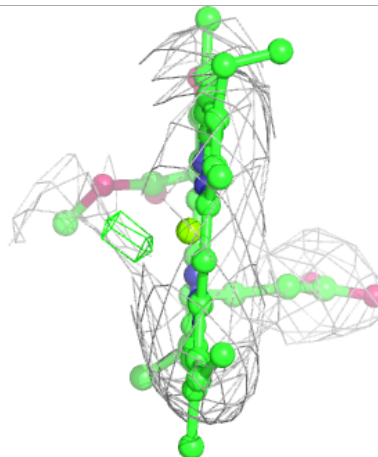
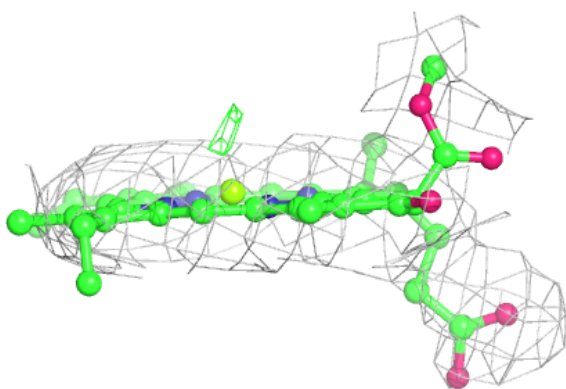
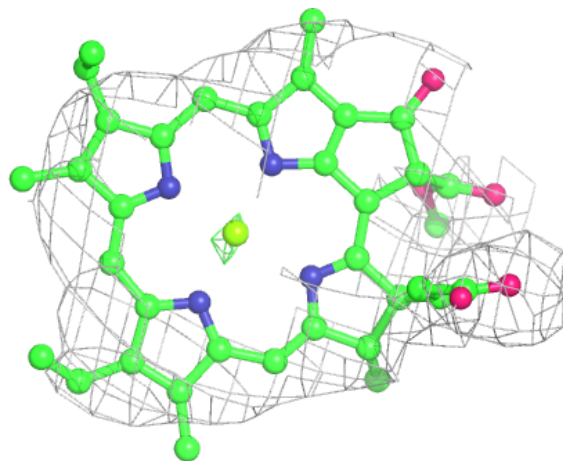
Electron density around CLA 1 1237:

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



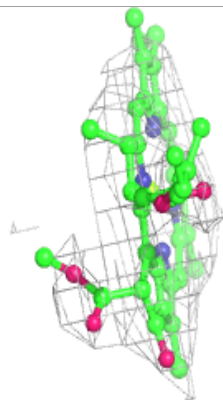
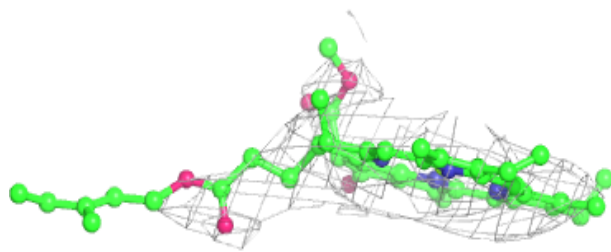
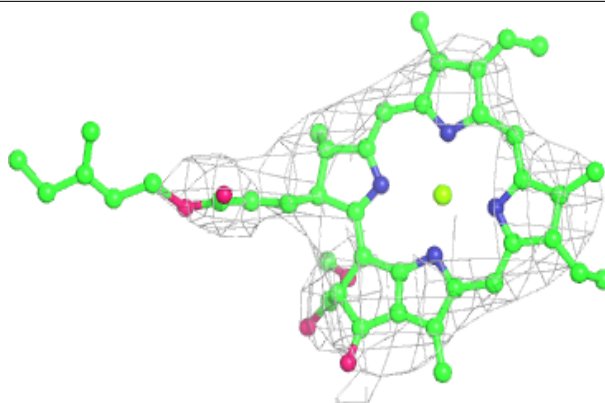
Electron density around CLA 2 1212:

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



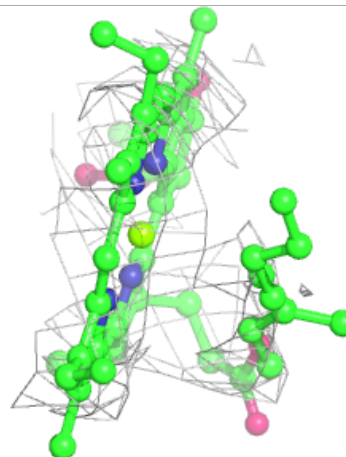
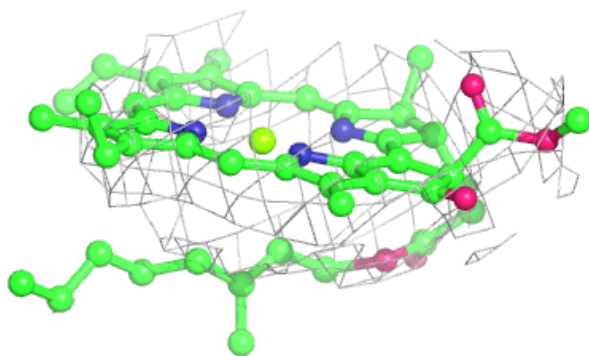
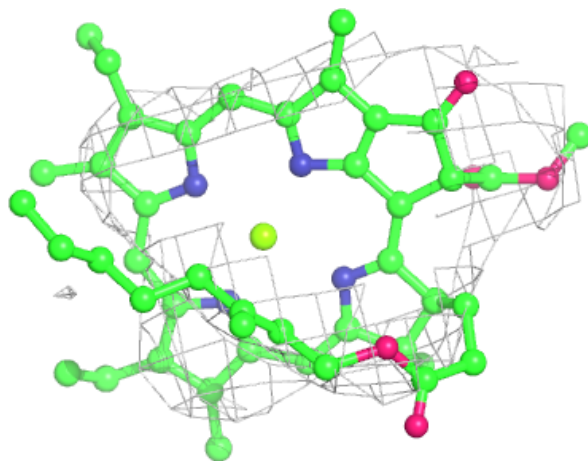
Electron density around CLA 1 1135:

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



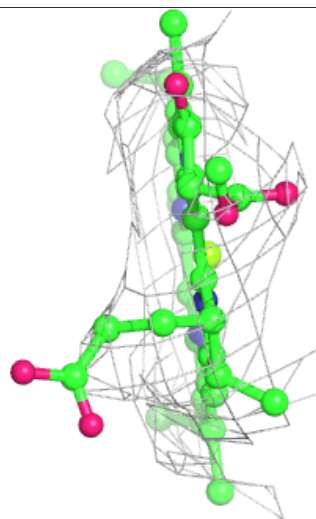
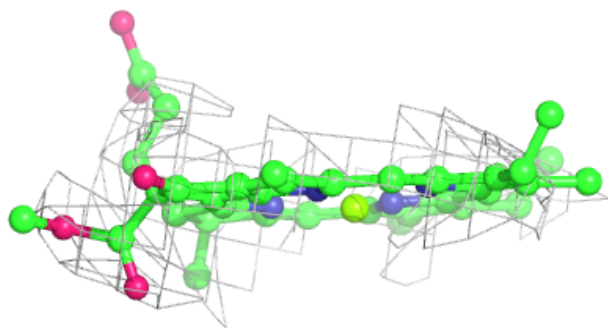
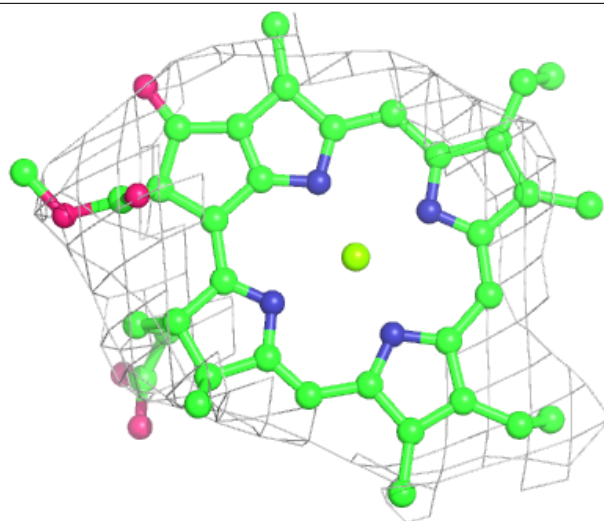
Electron density around CLA 1 1116:

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



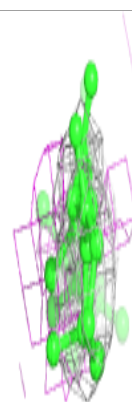
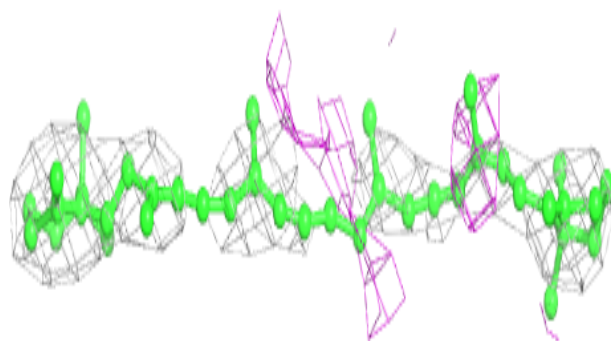
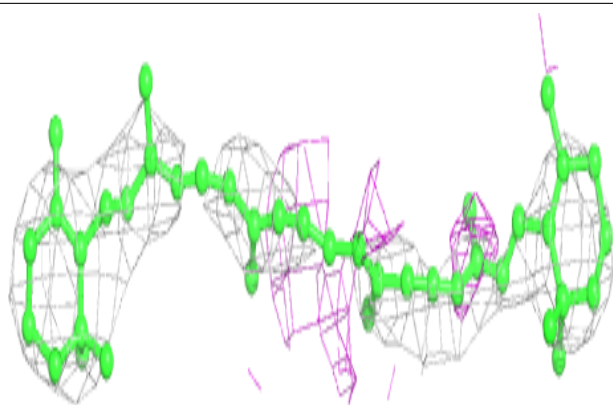
Electron density around CLA 2 1232:

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

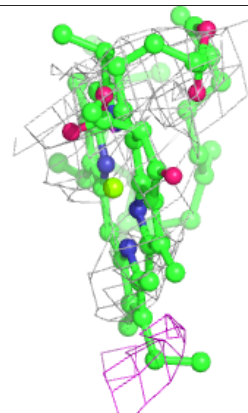
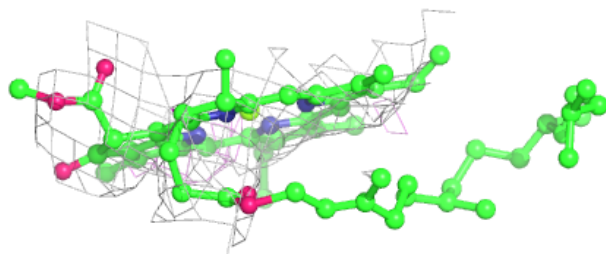
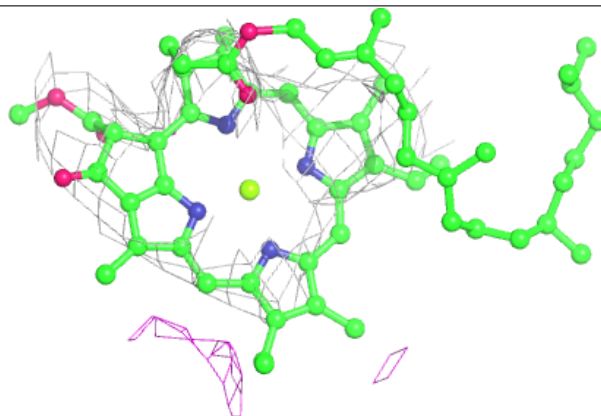


Electron density around BCR L 4019:

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

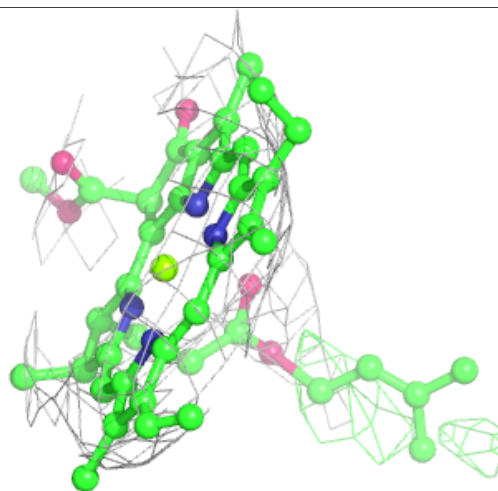
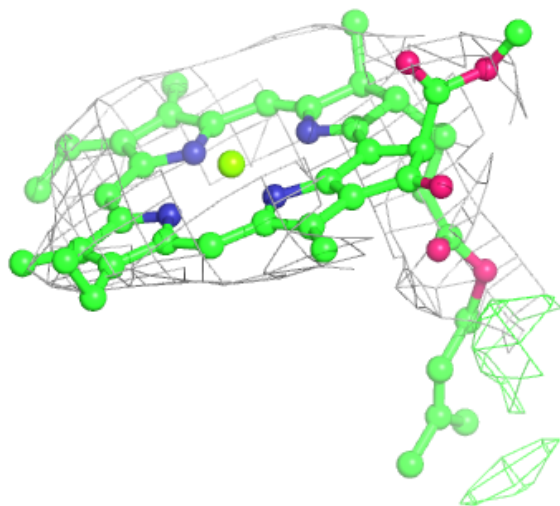
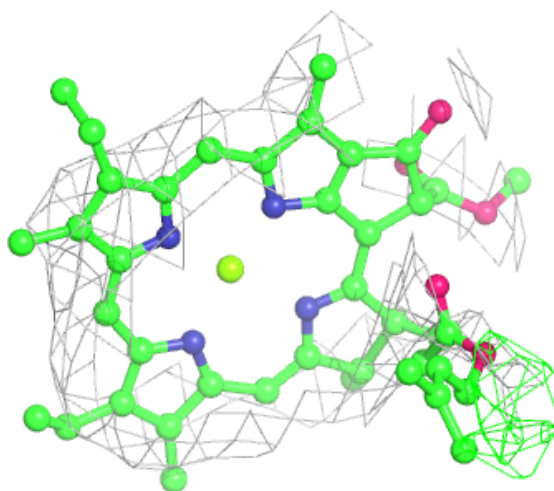
**Electron density around CLA a 1117:**

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



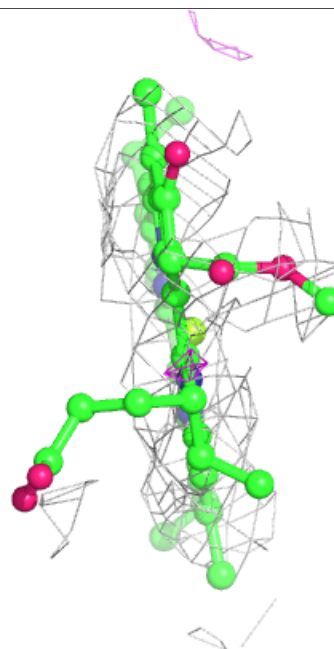
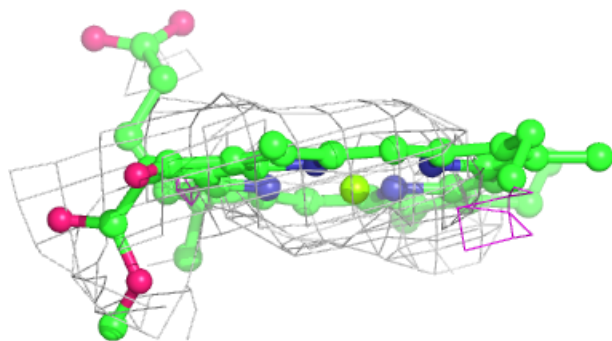
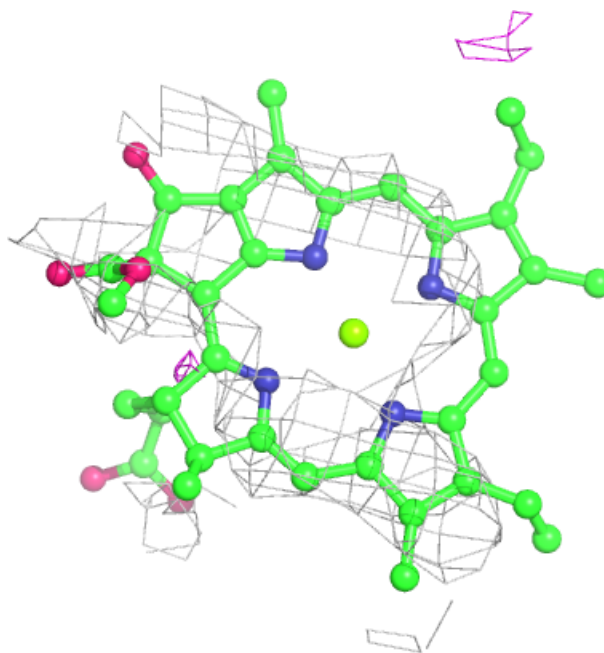
Electron density around CLA b 1228:

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



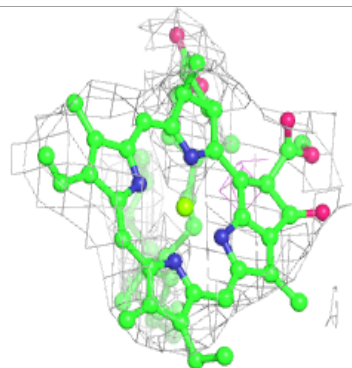
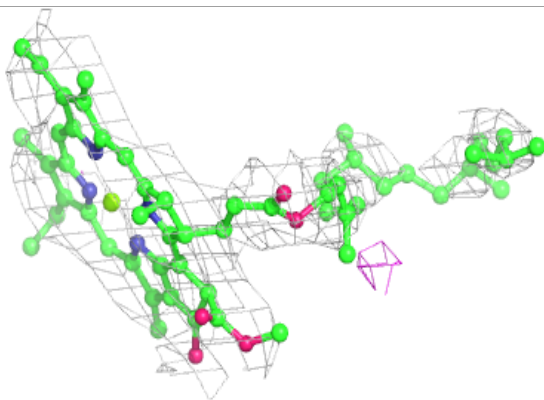
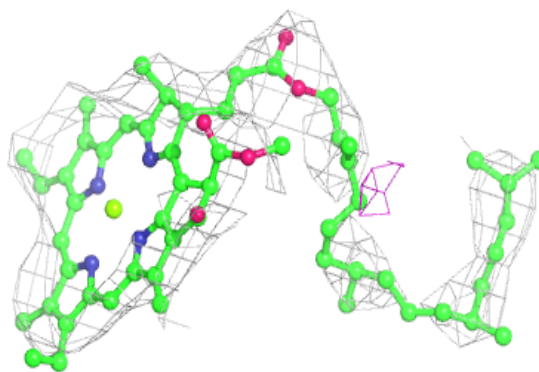
Electron density around CLA 2 1227:

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

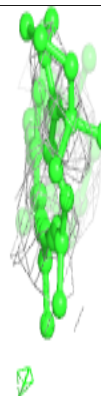
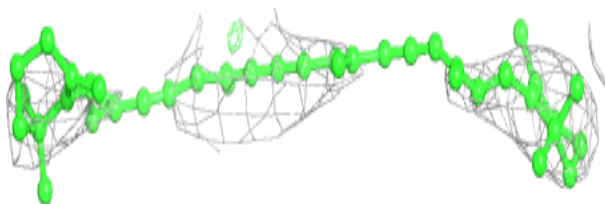
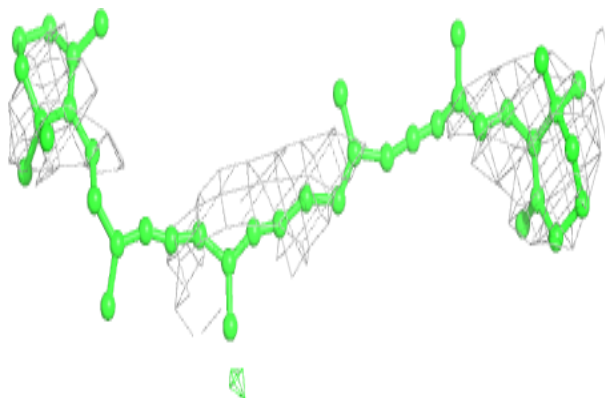


Electron density around CLA A 1011:

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

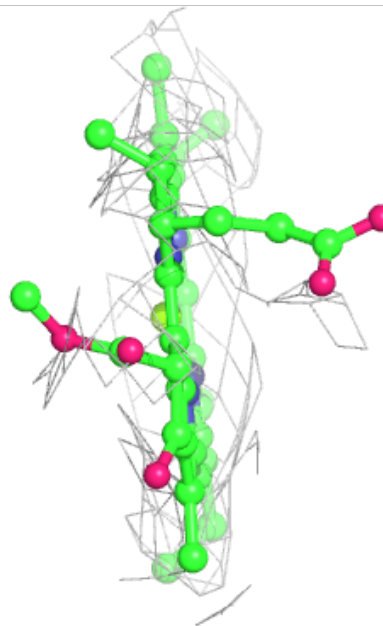
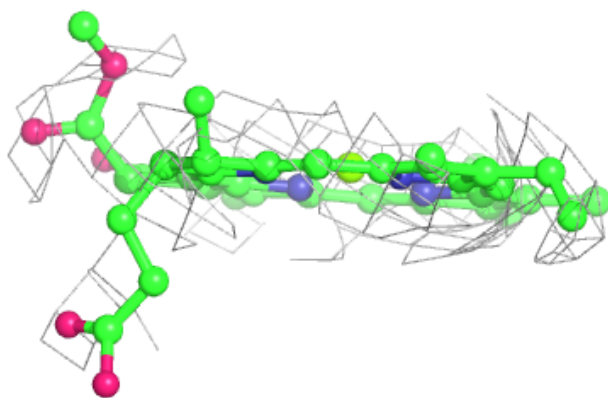
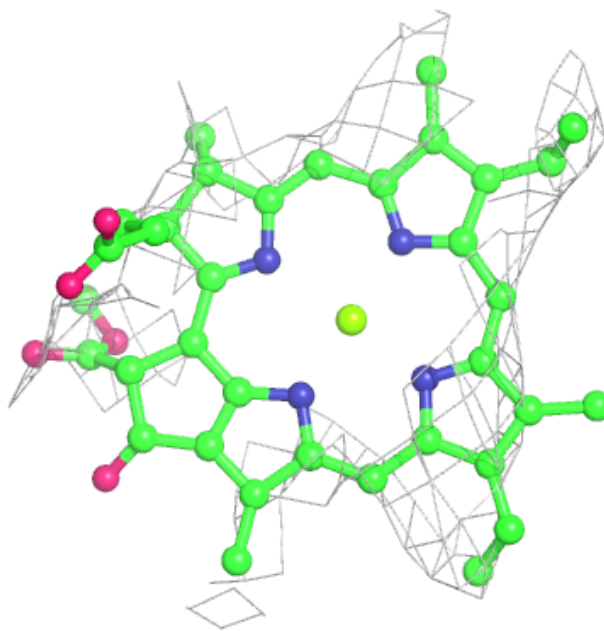
**Electron density around BCR B 4004:**

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



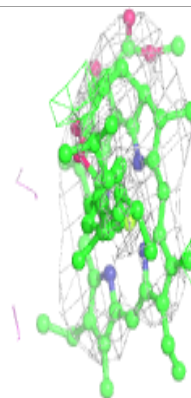
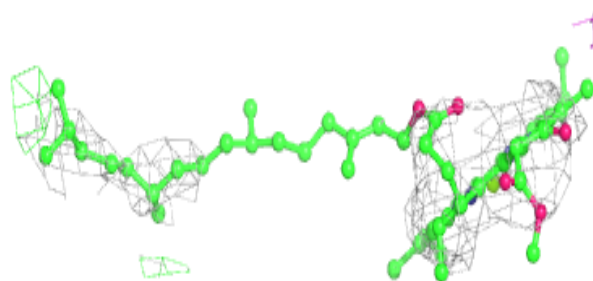
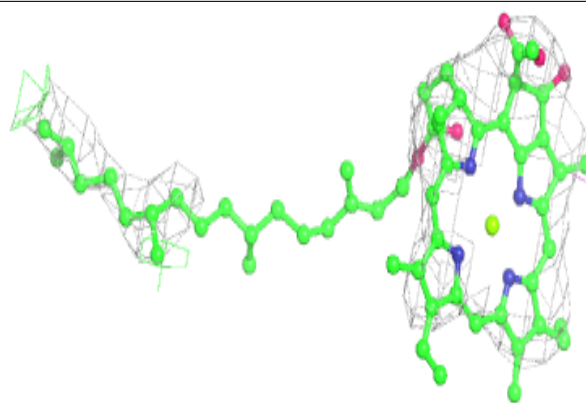
Electron density around CLA b 1227:

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



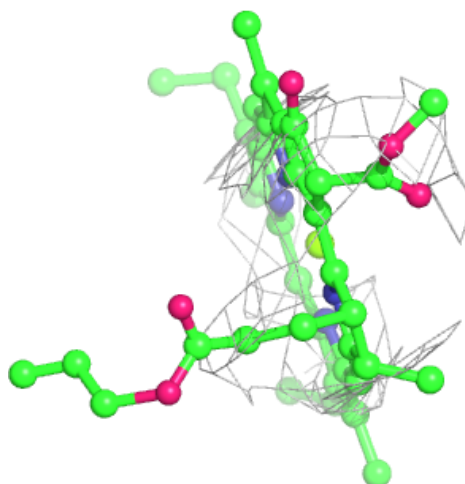
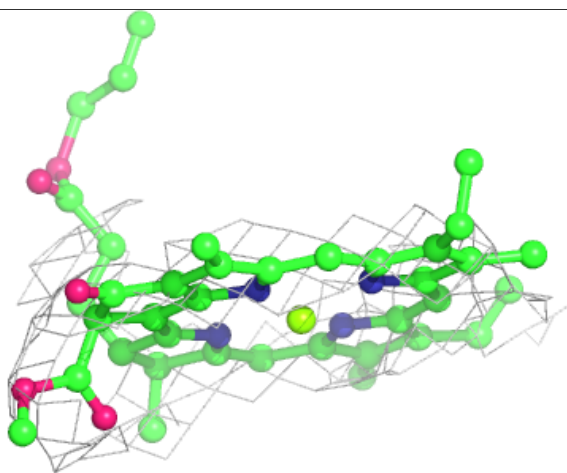
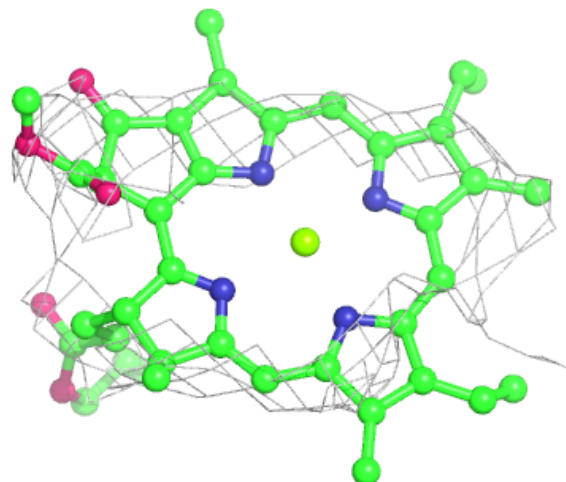
Electron density around CLA 11501:

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



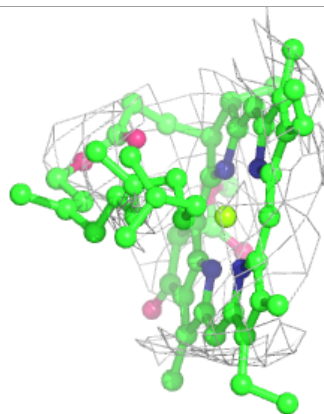
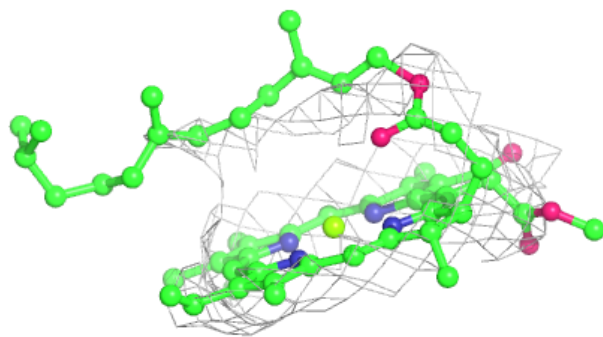
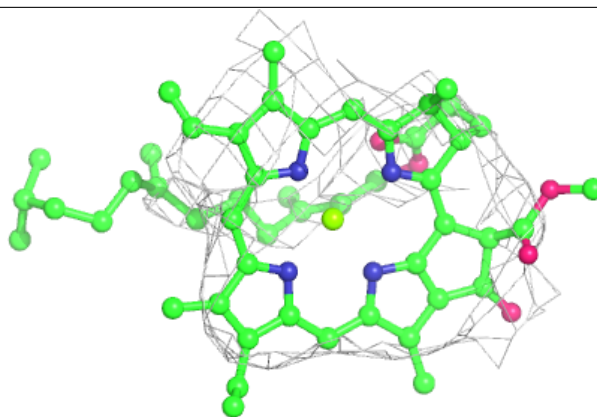
Electron density around CLA a 1105:

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



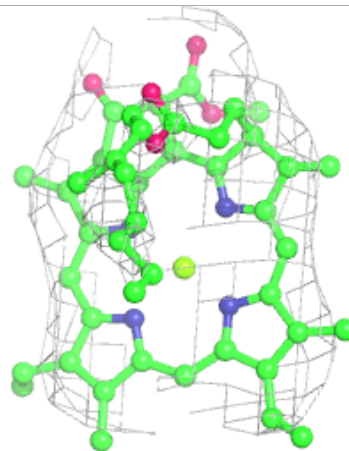
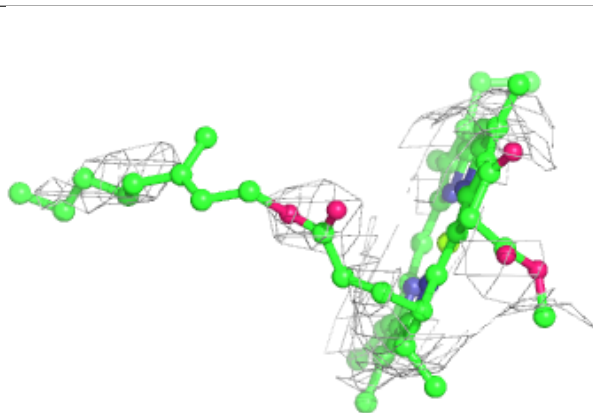
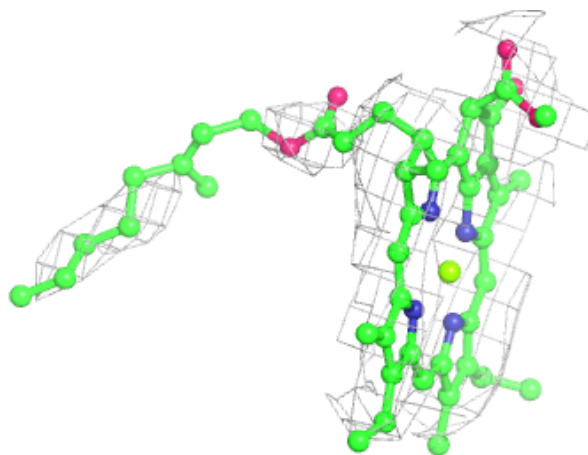
Electron density around CLA 2 1235:

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



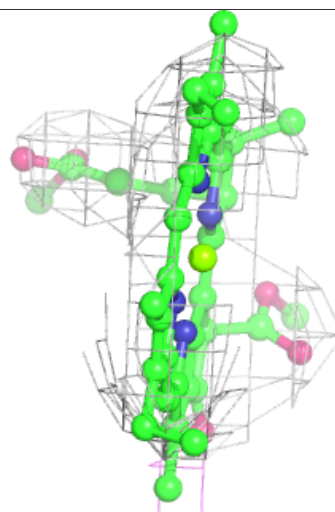
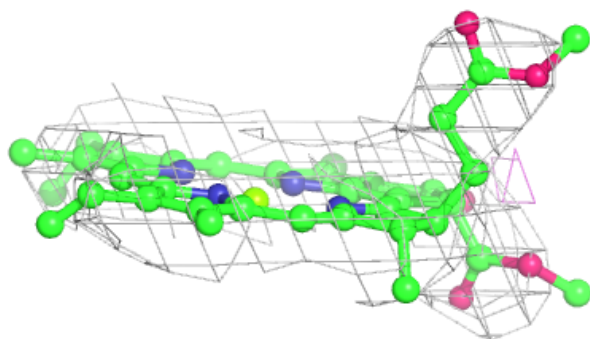
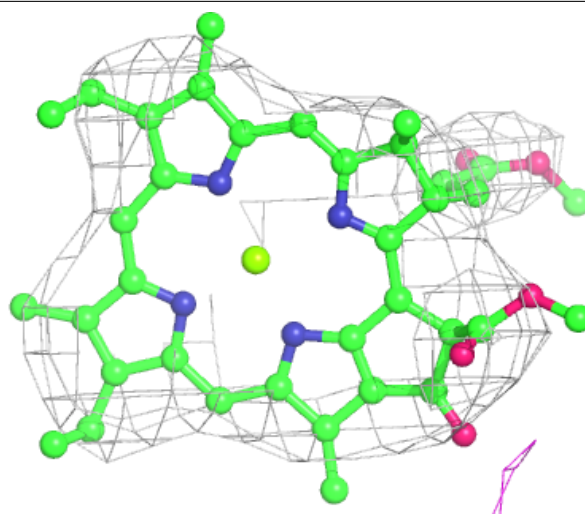
Electron density around CLA b 1201:

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



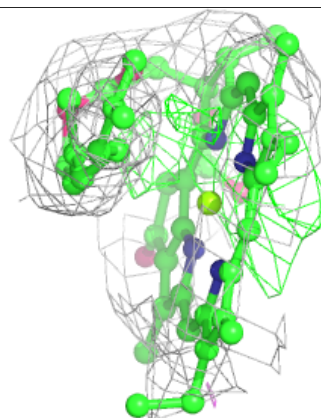
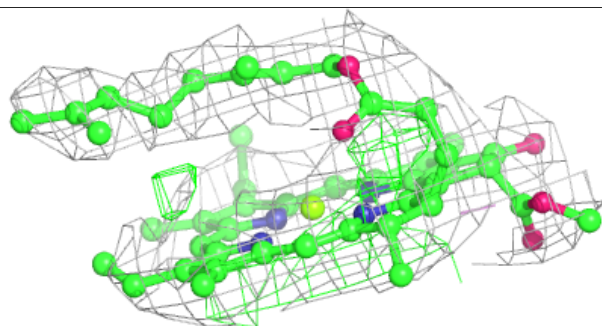
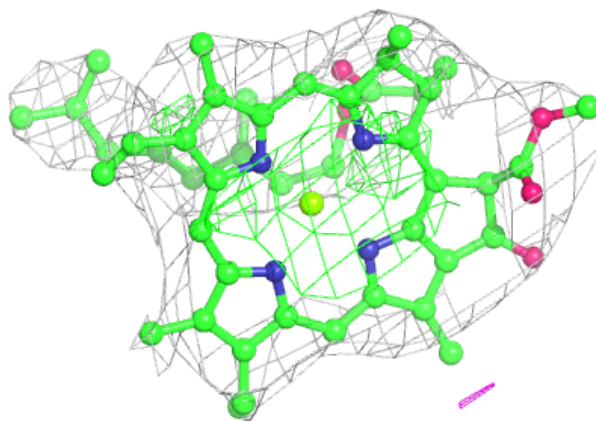
Electron density around CLA B 1239:

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



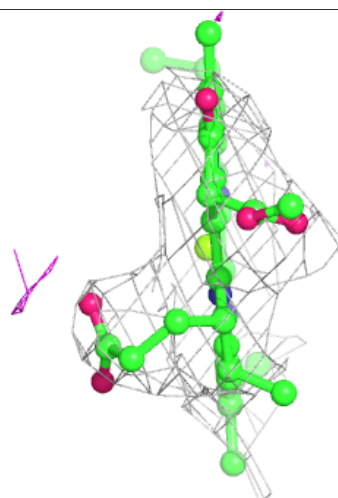
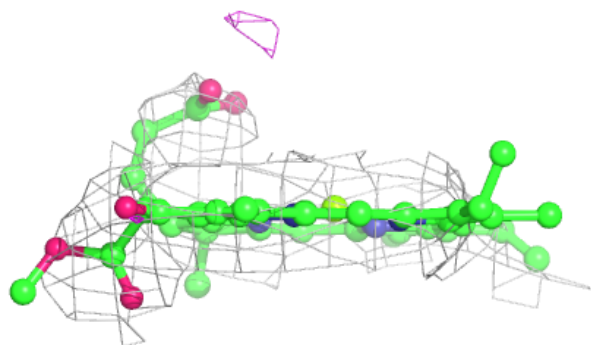
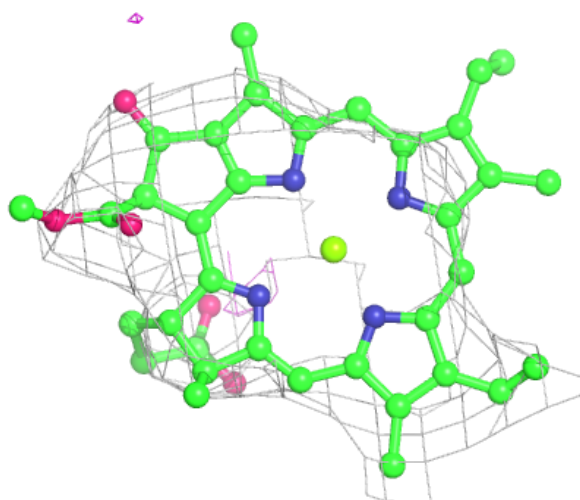
Electron density around CLA A 1237:

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



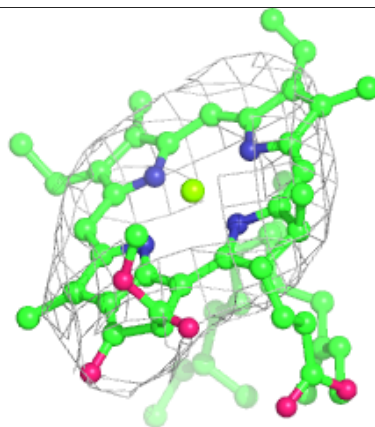
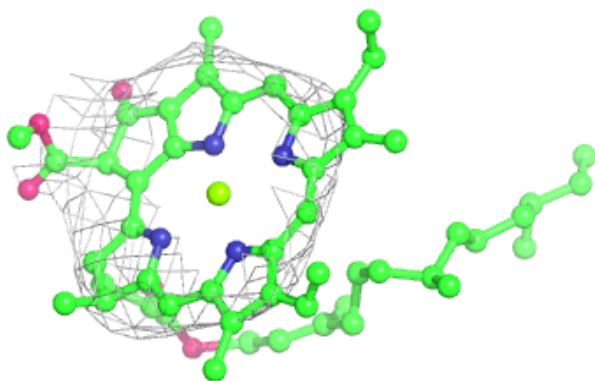
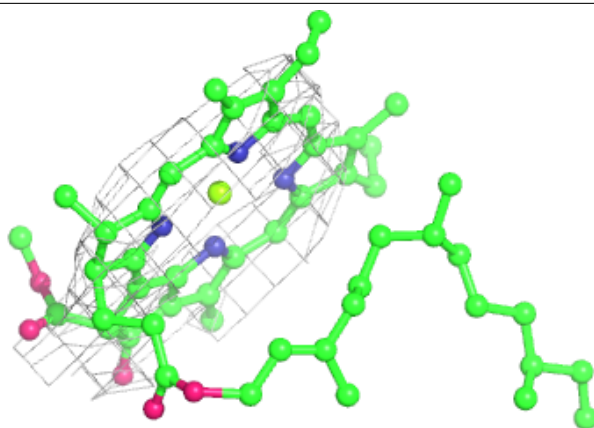
Electron density around CLA B 1209:

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



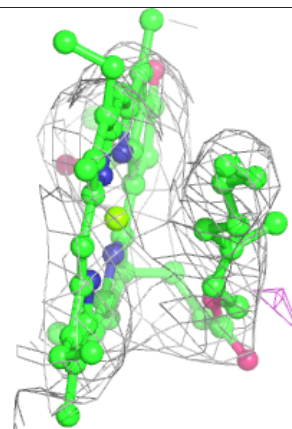
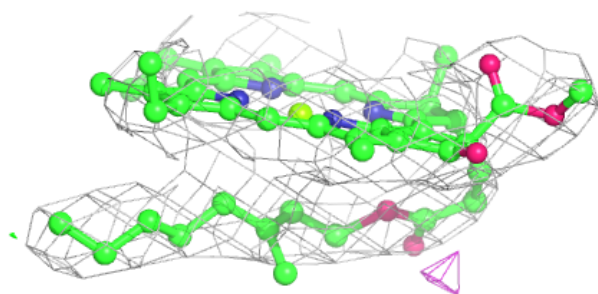
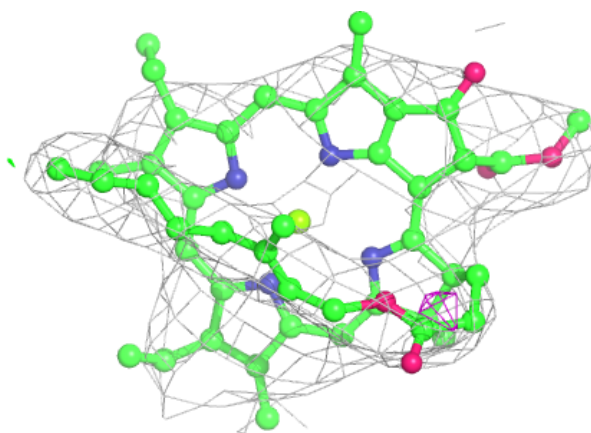
Electron density around CLA a 1118:

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



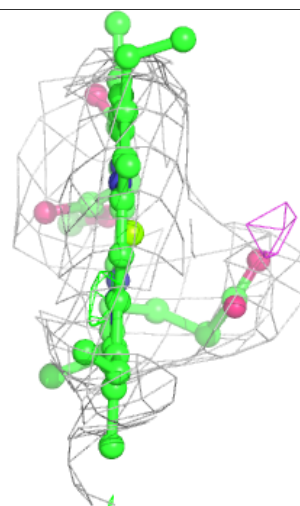
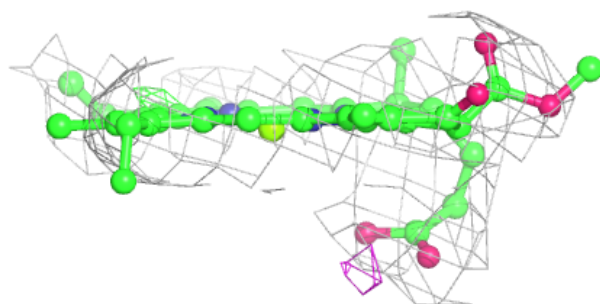
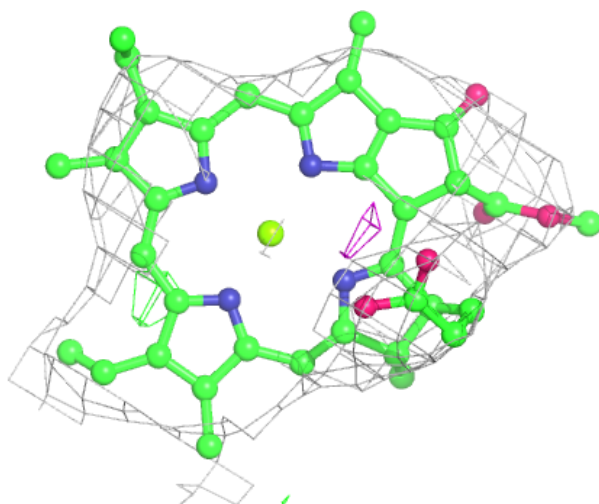
Electron density around CLA A 1116:

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



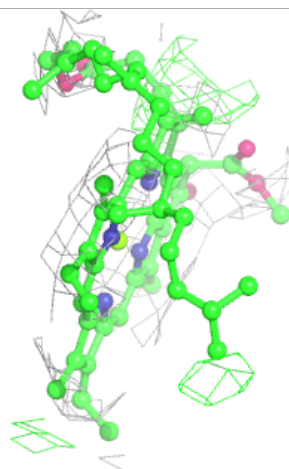
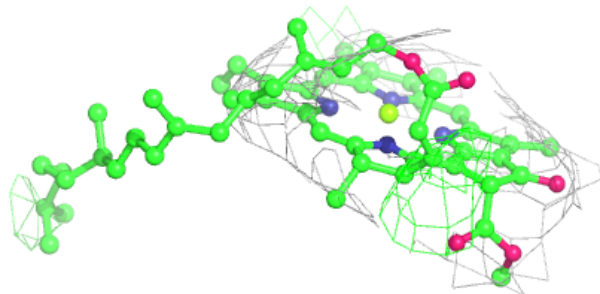
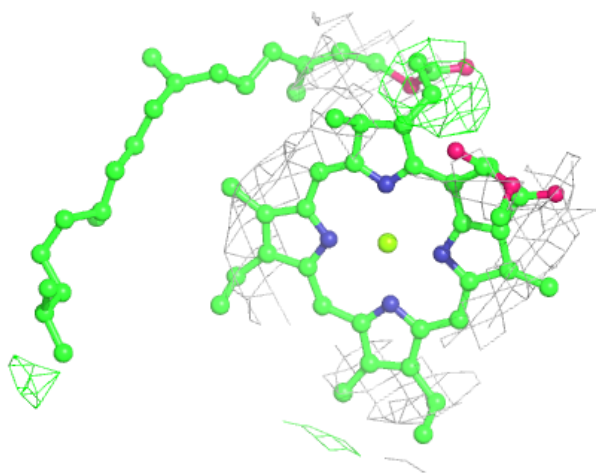
Electron density around CLA 2 1209:

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



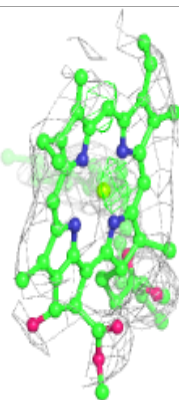
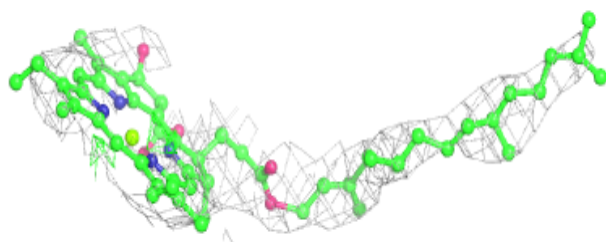
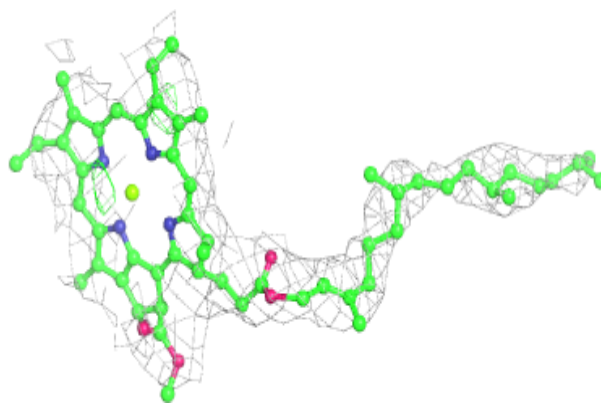
Electron density around CLA k 1401:

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

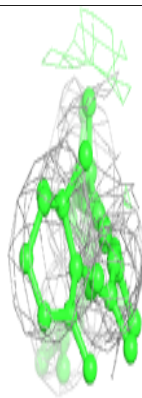
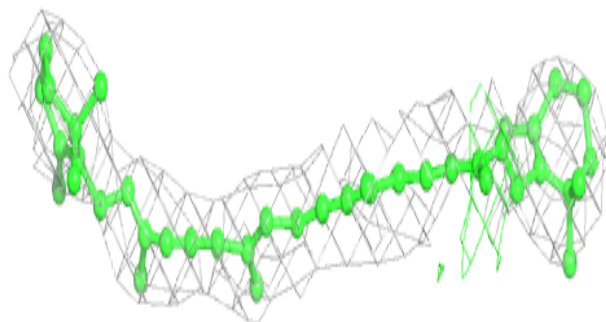
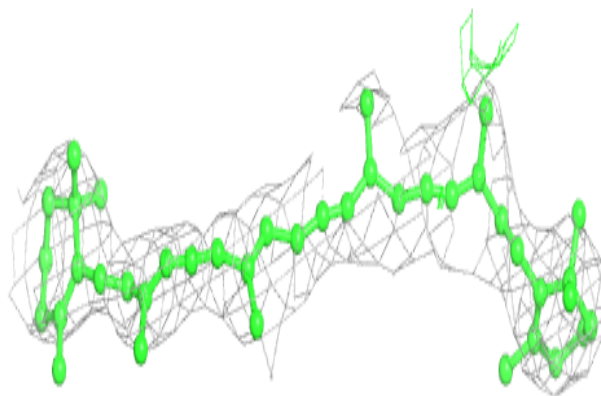


Electron density around CLA A 1022:

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

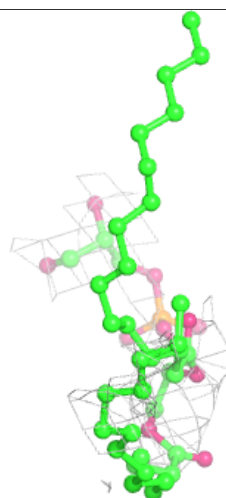
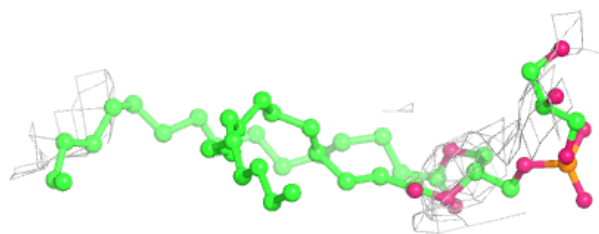
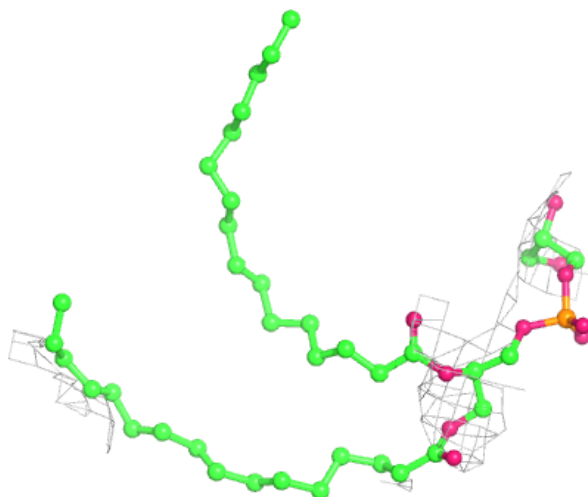
**Electron density around BCR M 4021:**

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



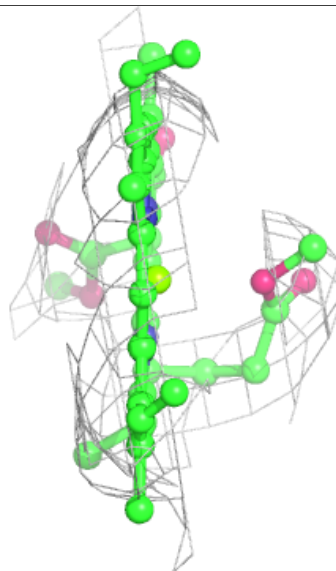
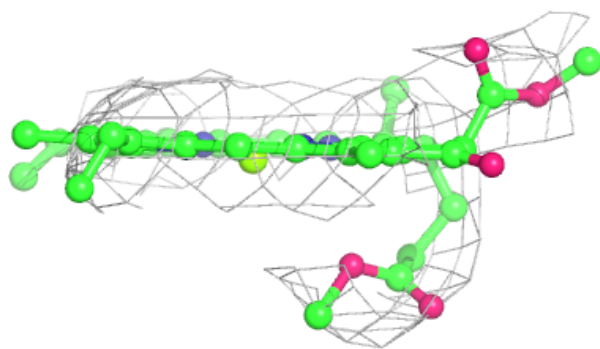
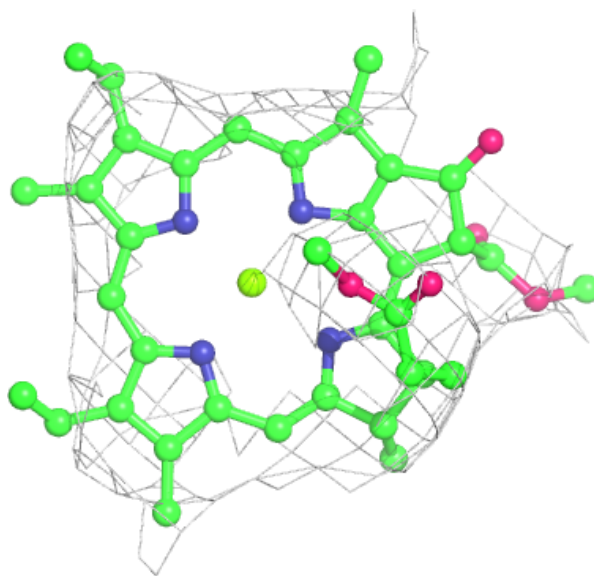
Electron density around LHG 2 5004:

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



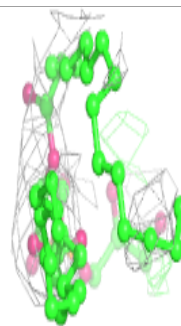
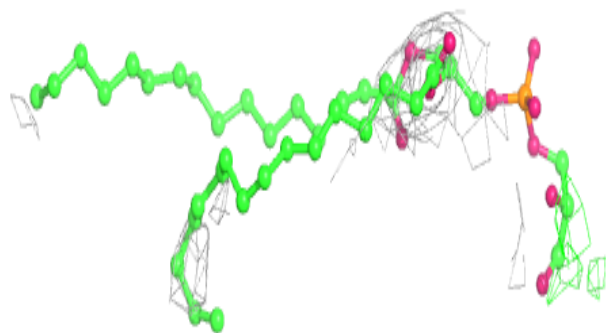
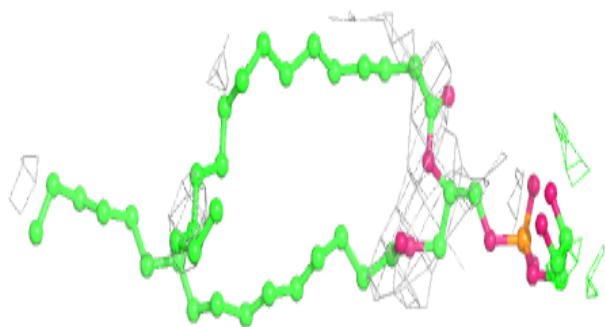
Electron density around CLA 1 1136:

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



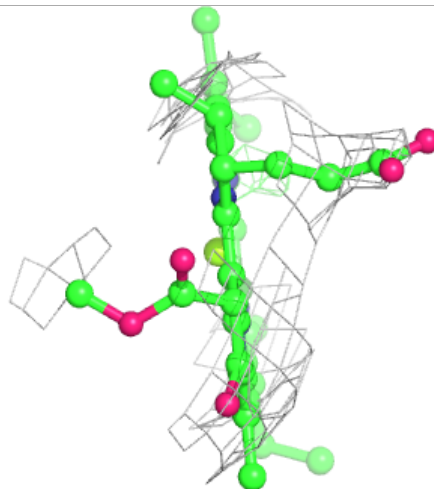
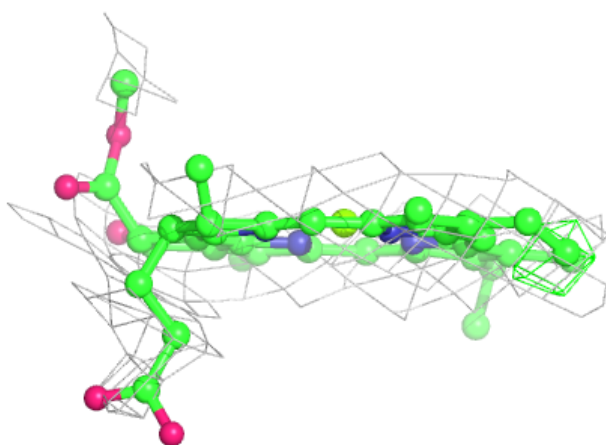
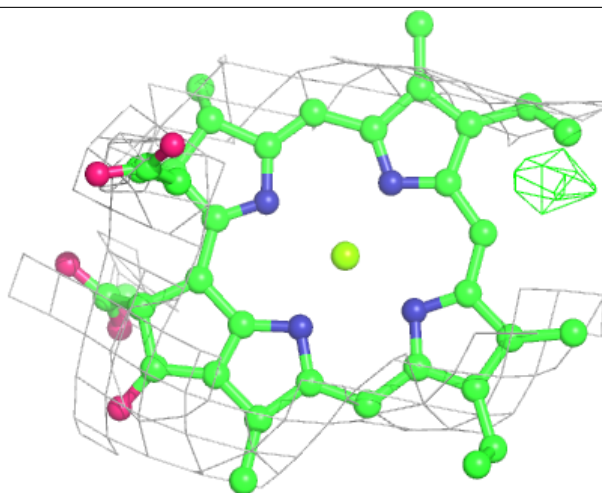
Electron density around LHG 1 5003:

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



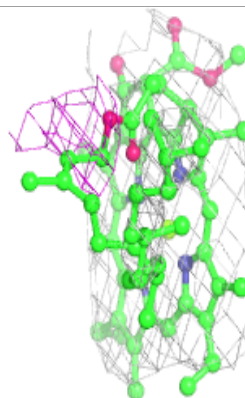
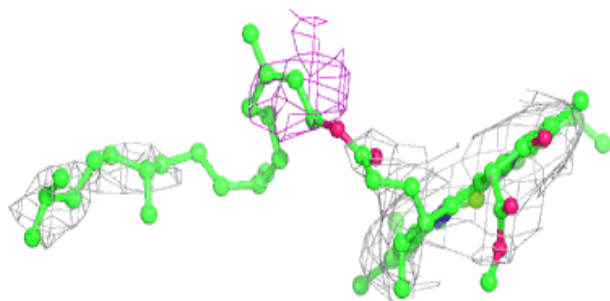
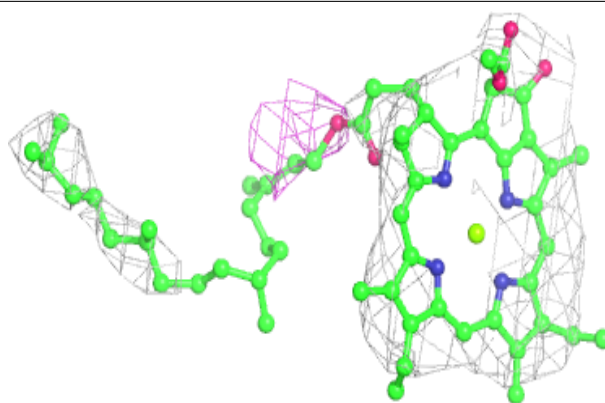
Electron density around CLA b 1212:

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

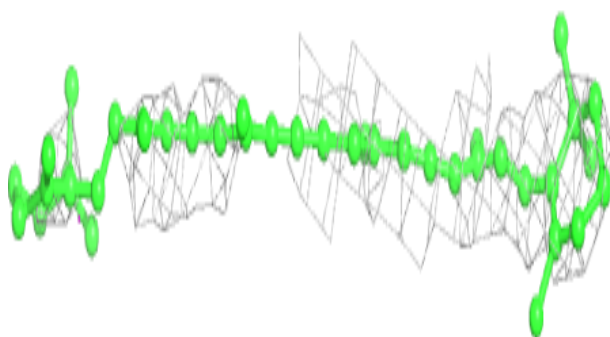
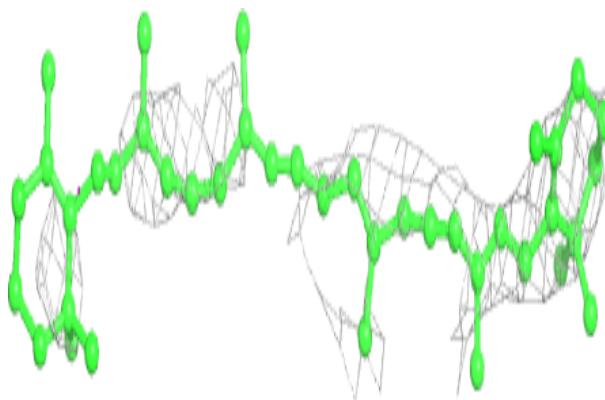


Electron density around CLA A 1106:

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

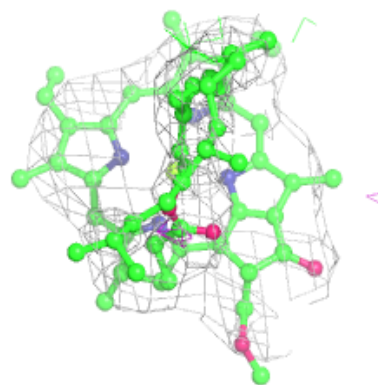
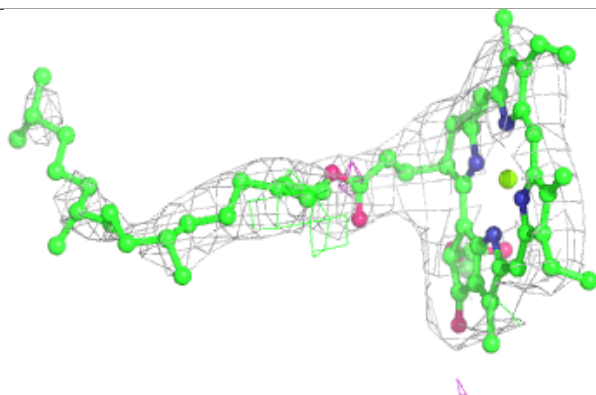
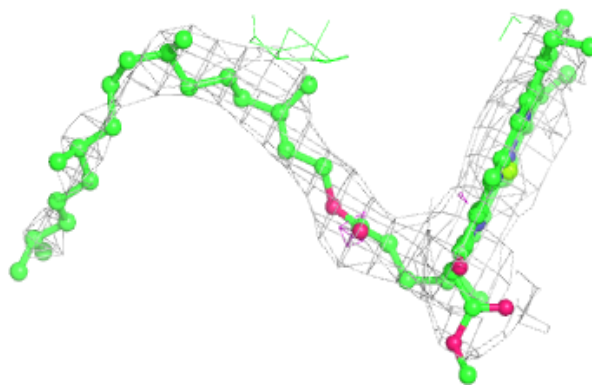
**Electron density around BCR a 4007:**

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

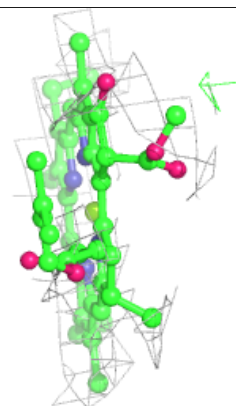
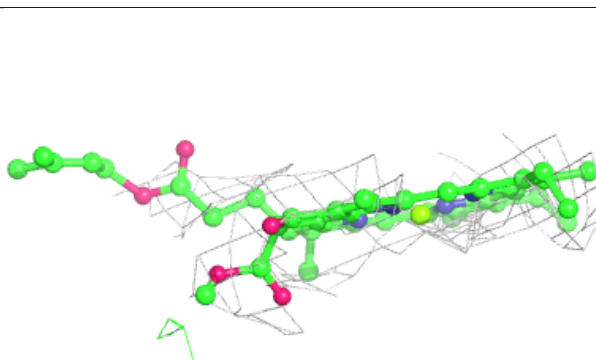
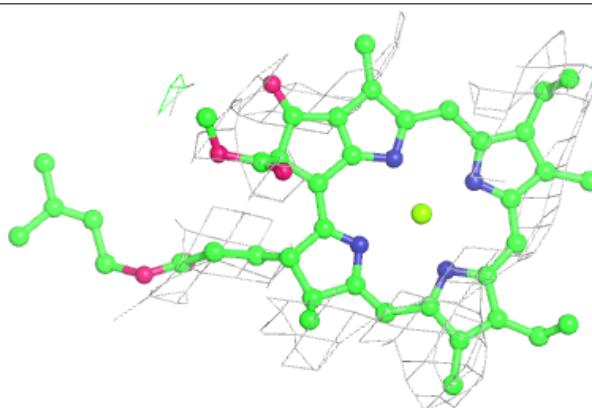


Electron density around CLA 2 1238:

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

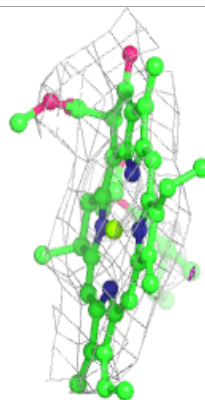
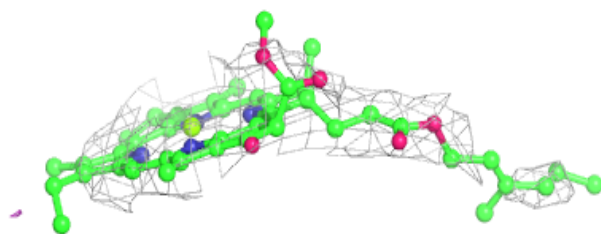
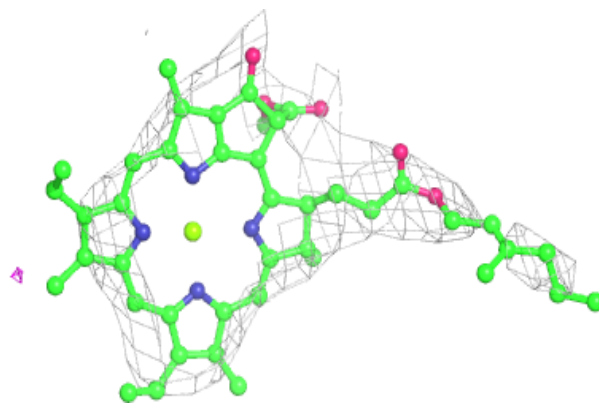
**Electron density around CLA a 1139:**

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



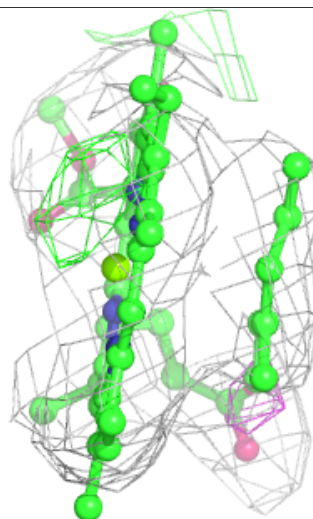
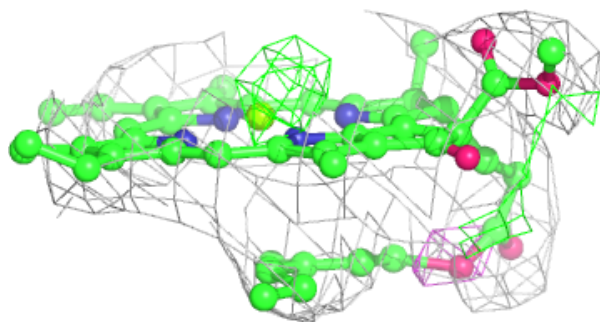
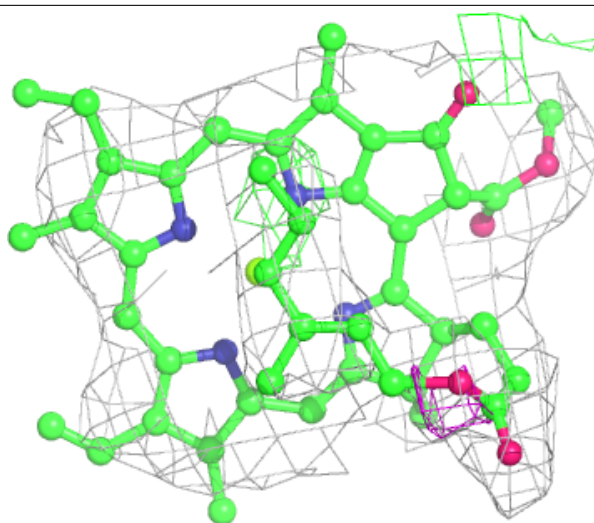
Electron density around CLA a 1125:

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



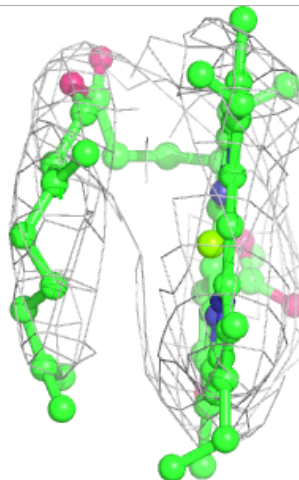
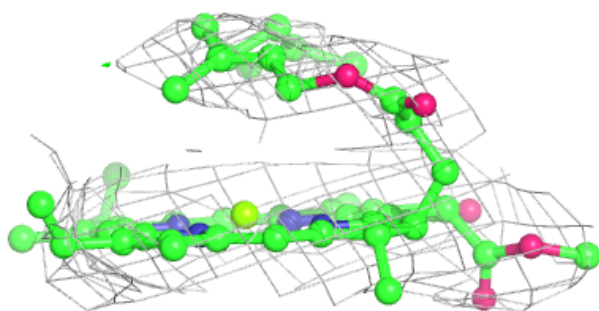
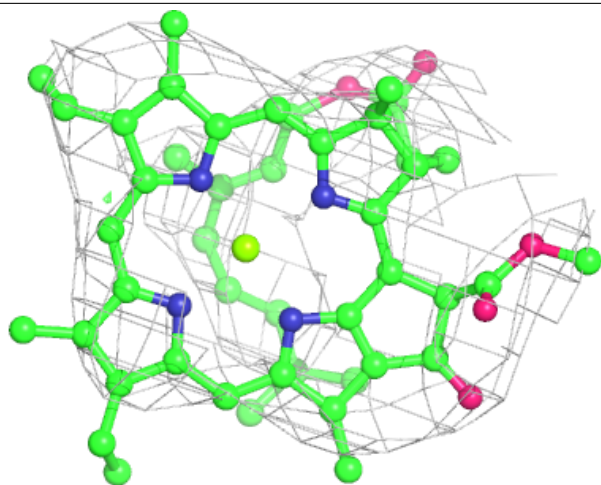
Electron density around CLA A 1801:

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



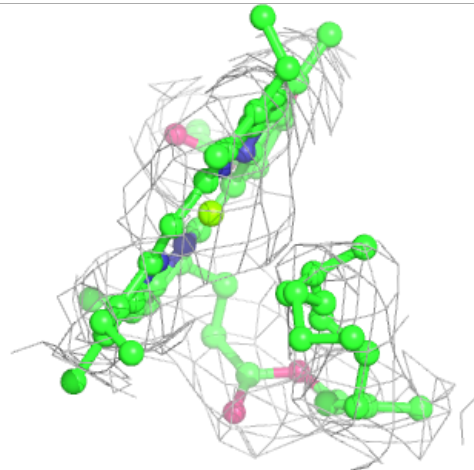
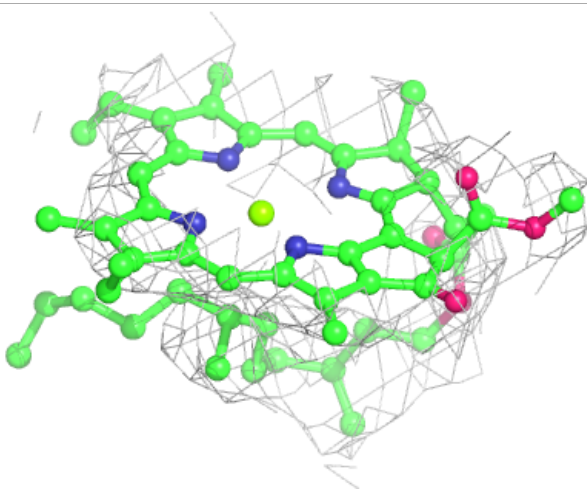
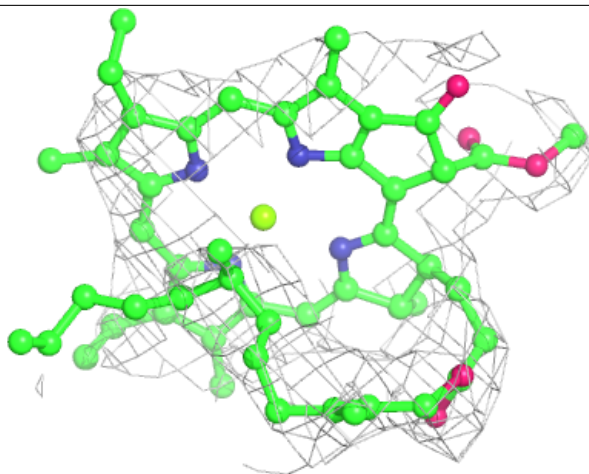
Electron density around CLA b 1224:

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



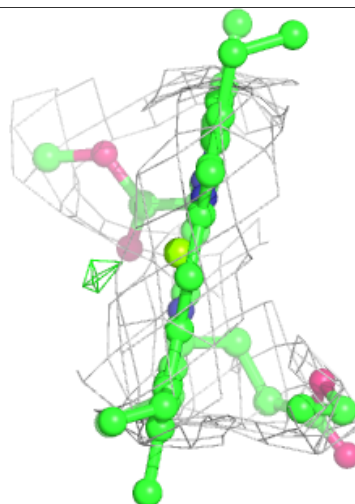
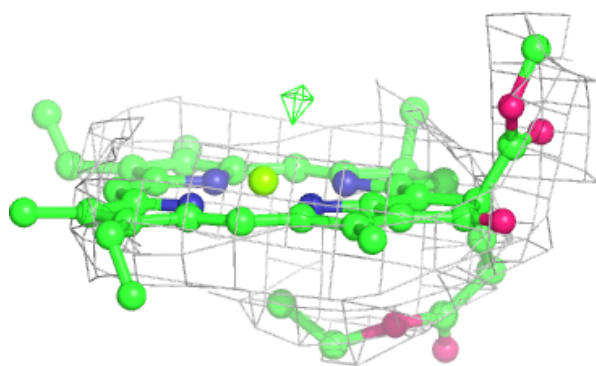
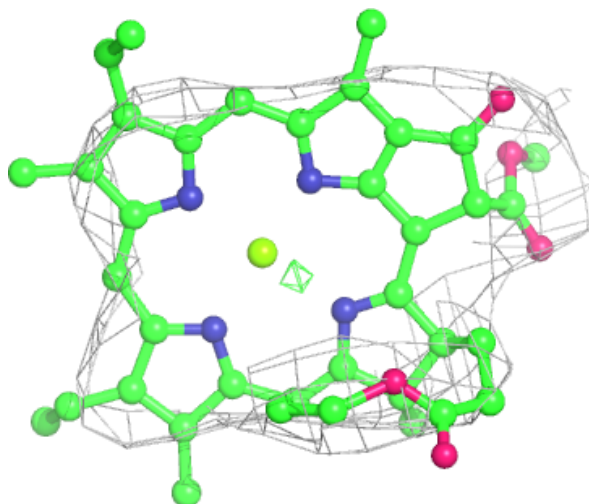
Electron density around CLA 2 1214:

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



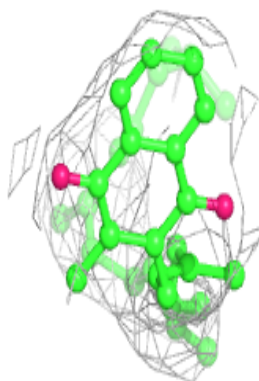
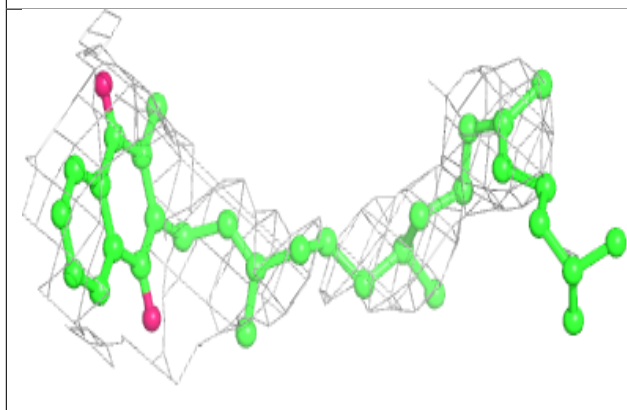
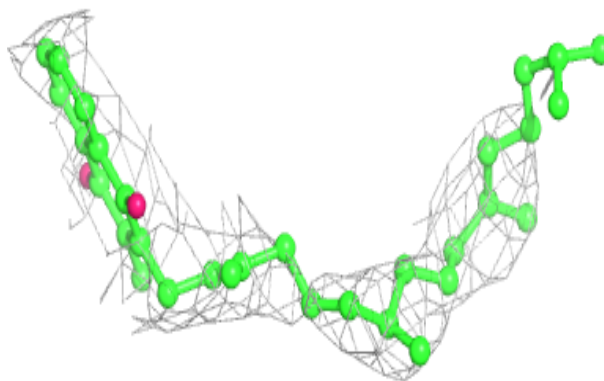
Electron density around CLA B 1217:

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

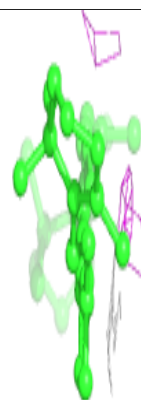
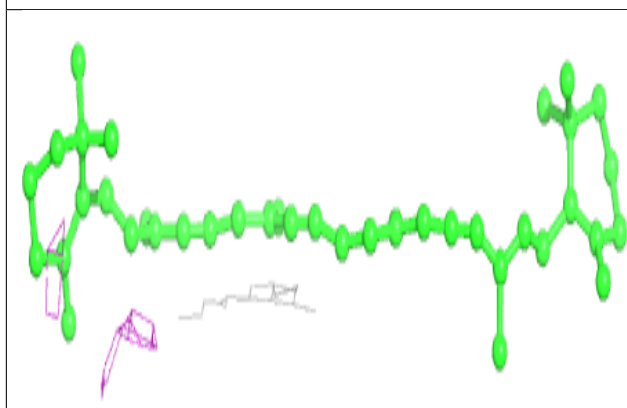
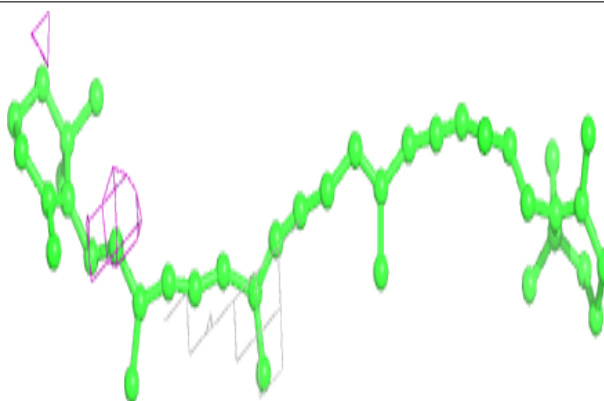


Electron density around PQN B 2002:

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

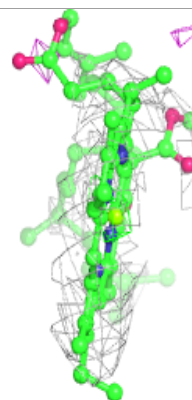
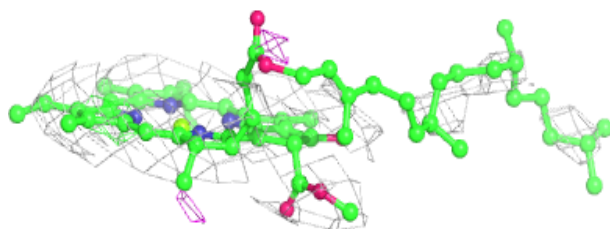
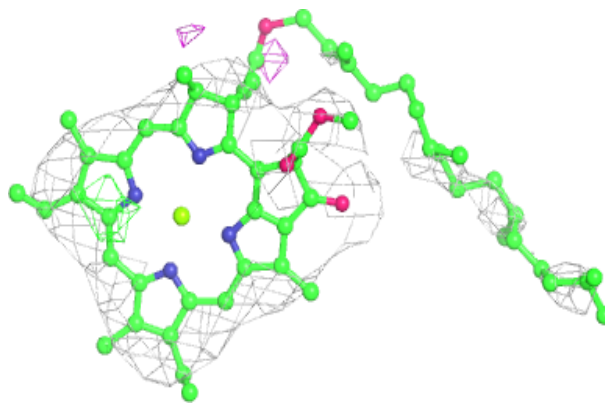
**Electron density around BCR 2 4009:**

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

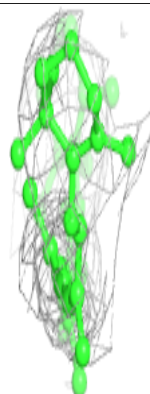
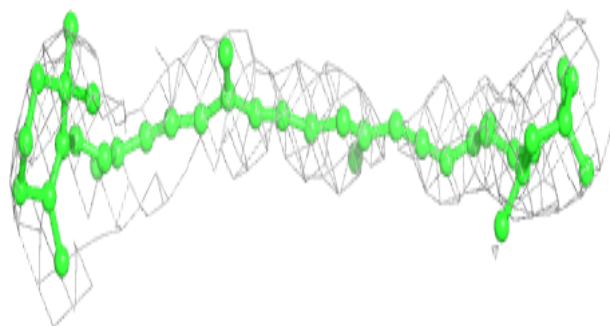
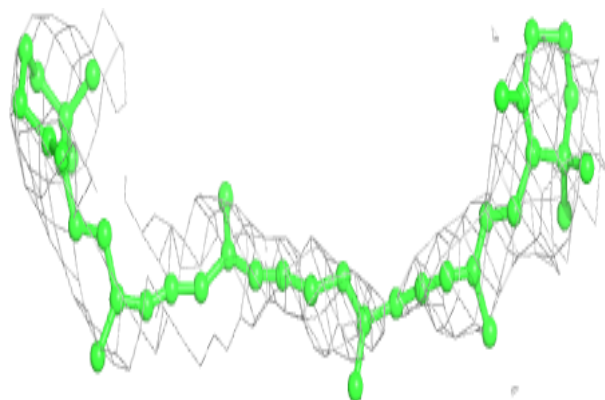


Electron density around CLA 8 1503:

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

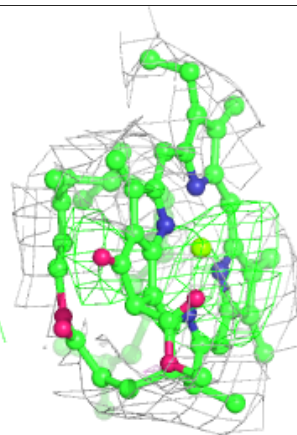
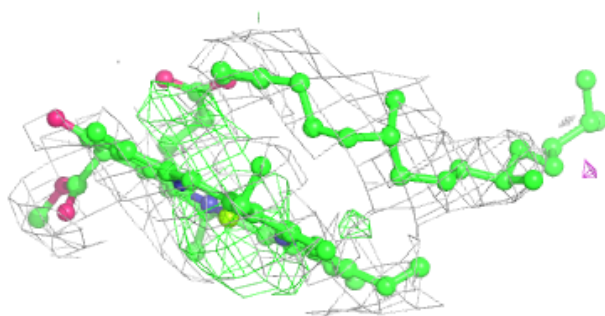
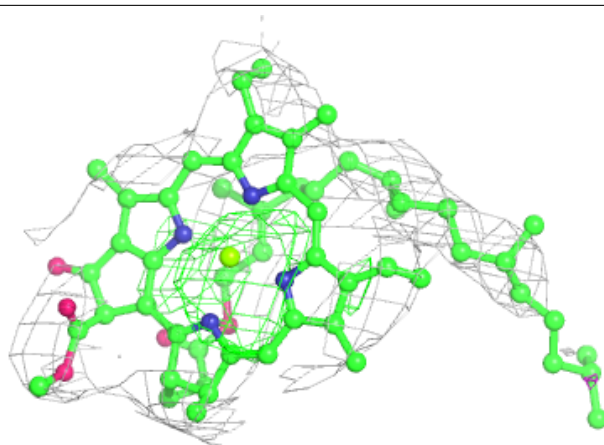
**Electron density around BCR 6 4020:**

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

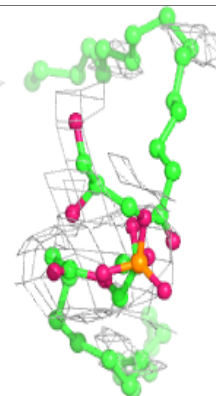
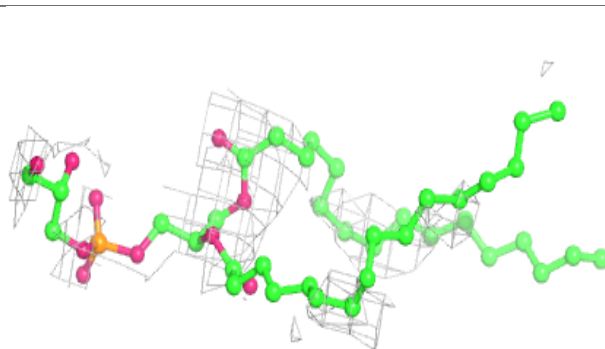
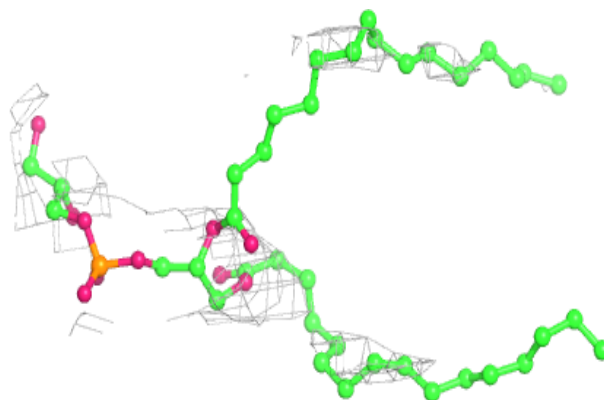


Electron density around CLA B 1204:

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

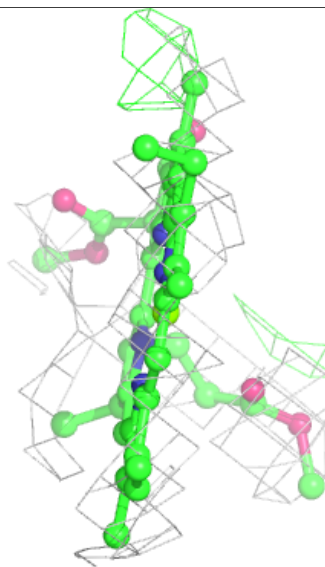
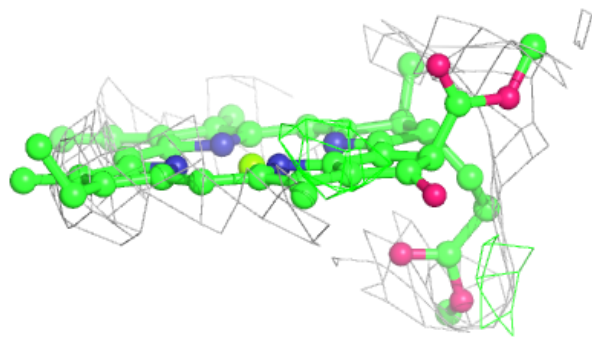
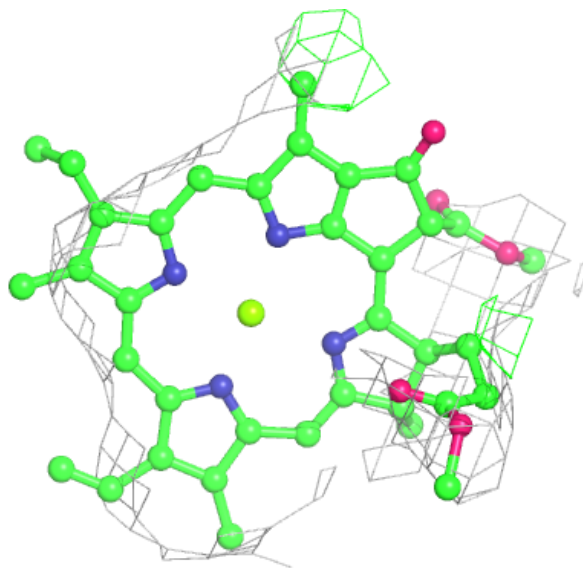
**Electron density around LHG a 5001:**

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



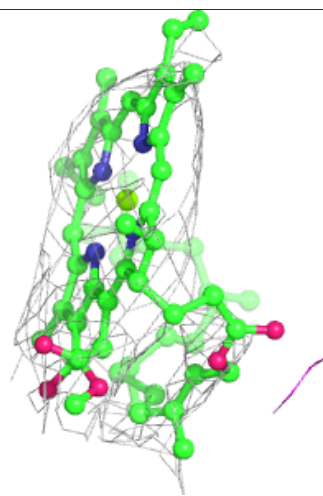
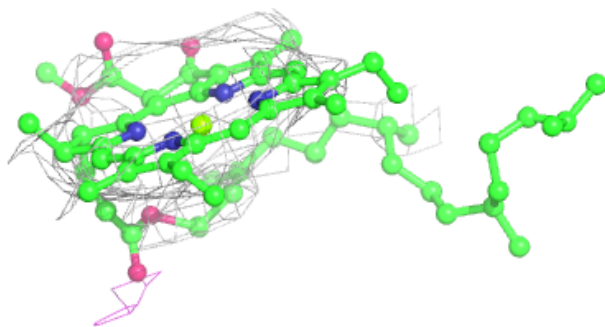
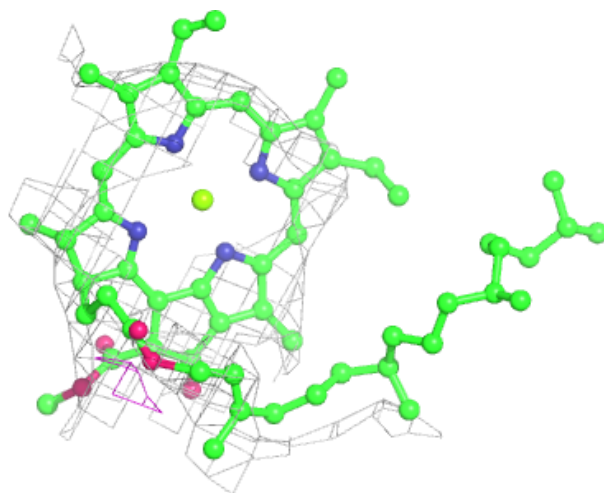
Electron density around CLA a 1134:

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



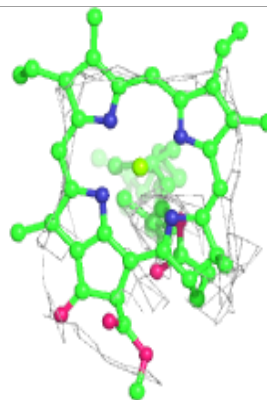
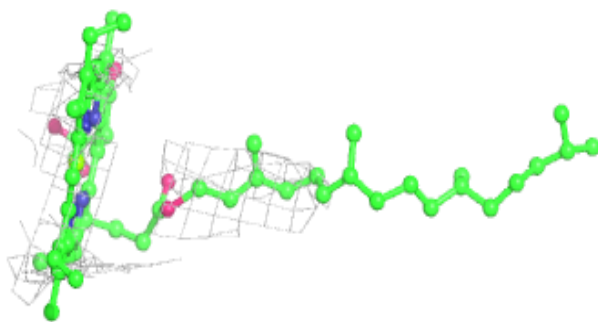
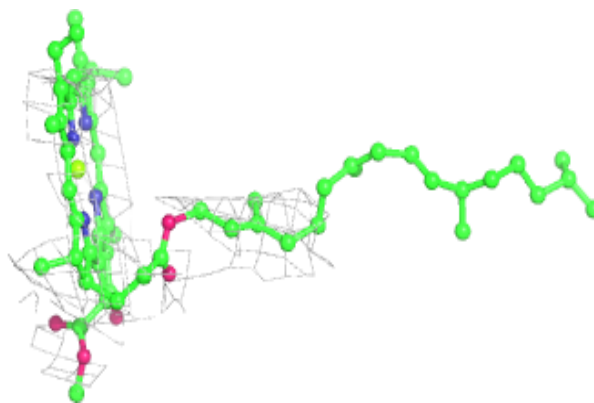
Electron density around CLA 1 1127:

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

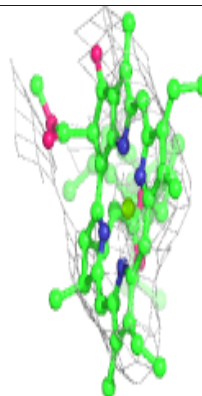
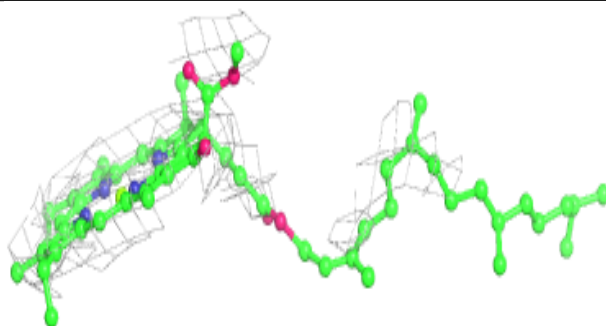
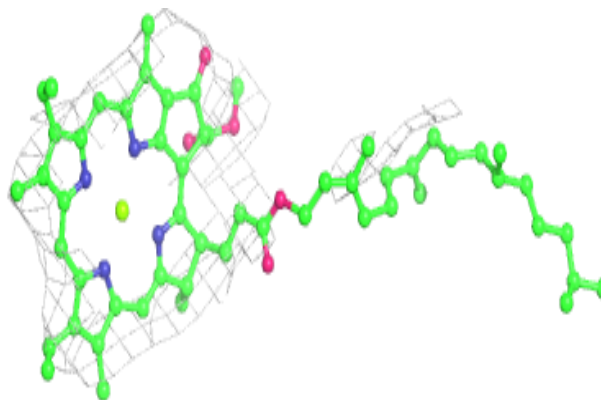


Electron density around CLA 1 1126:

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

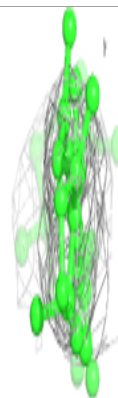
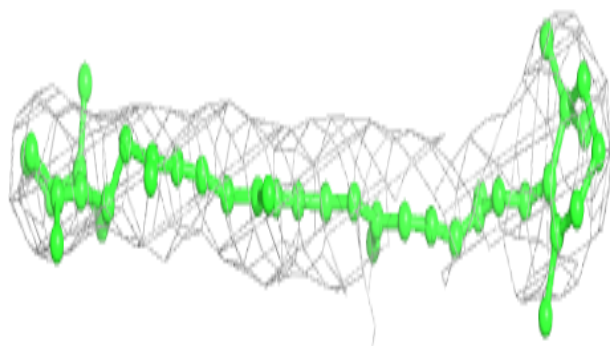
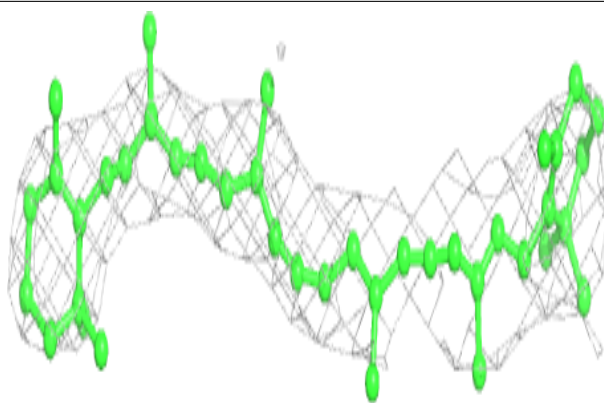
**Electron density around CLA a 1107:**

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



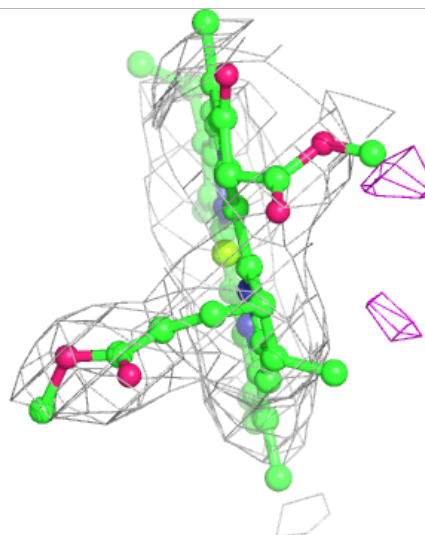
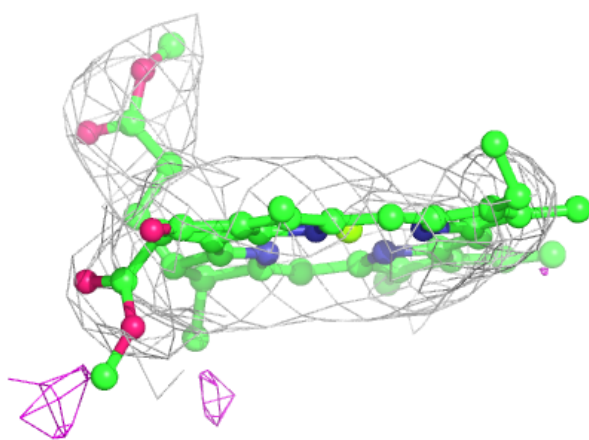
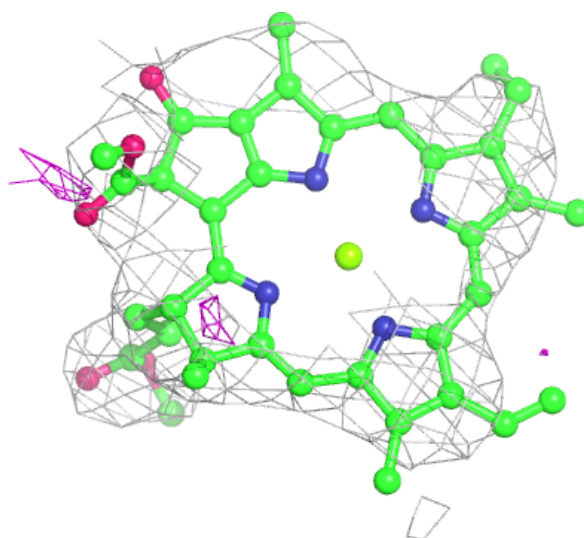
Electron density around BCR A 4002:

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



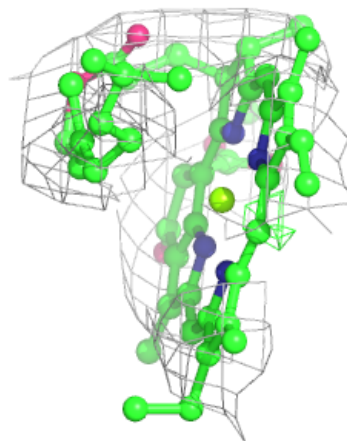
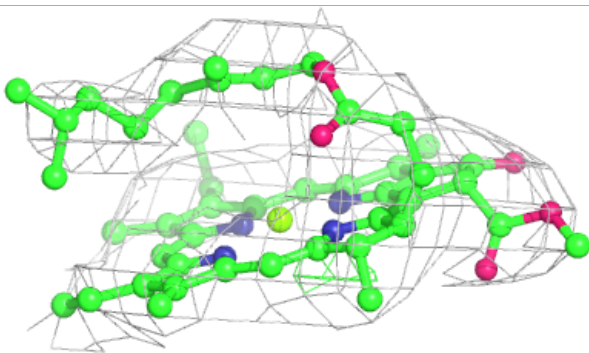
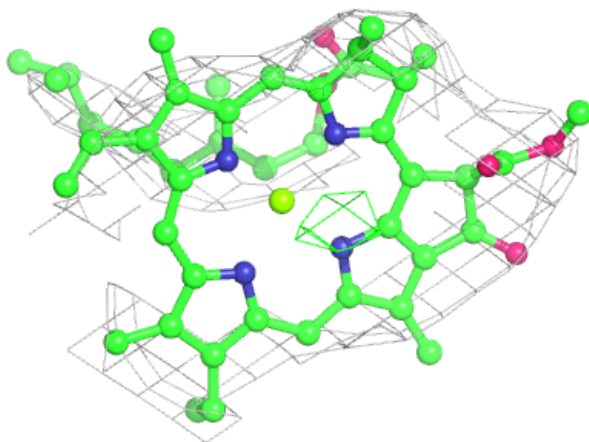
Electron density around CLA A 1129:

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



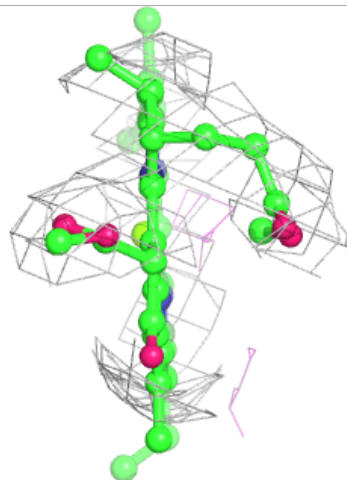
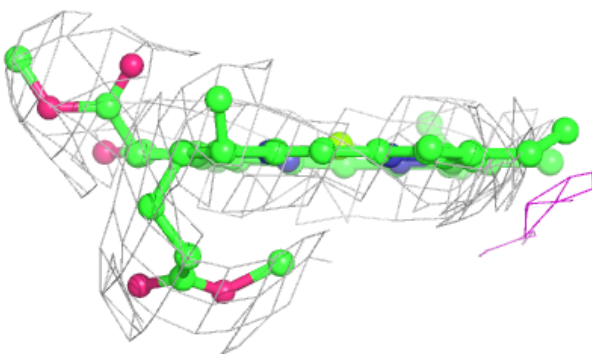
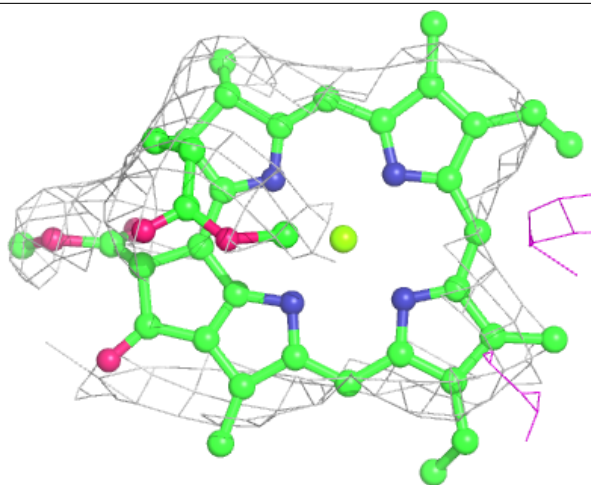
Electron density around CLA a 1237:

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



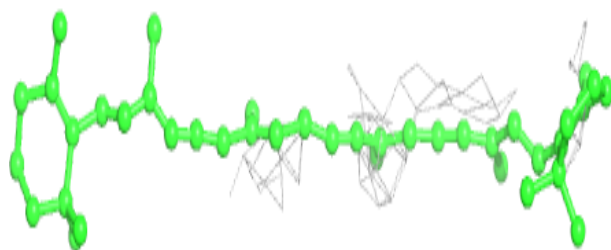
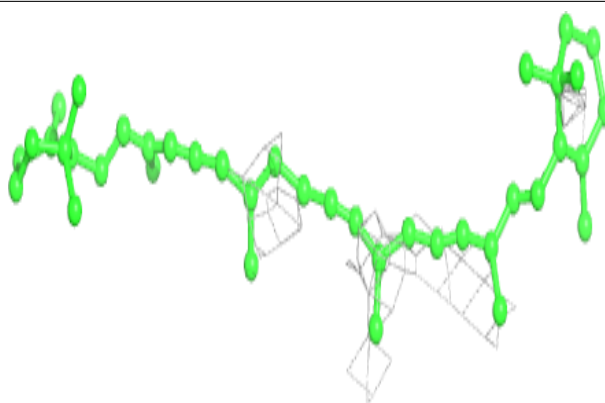
Electron density around CLA A 1115:

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



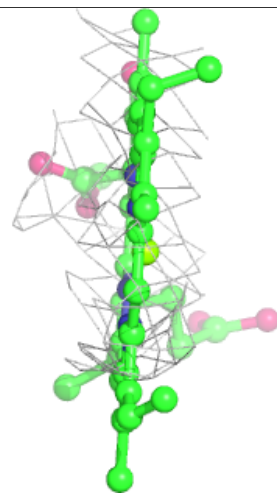
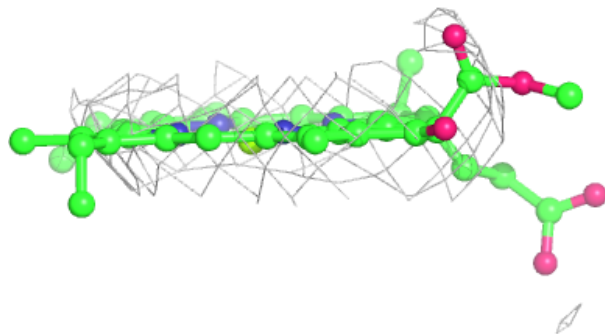
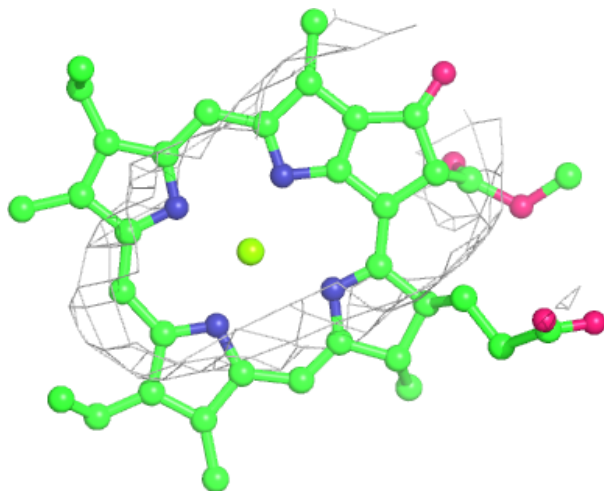
Electron density around BCR B 4009:

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



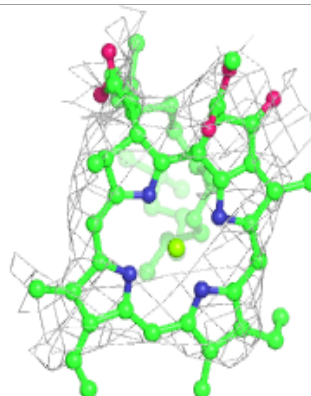
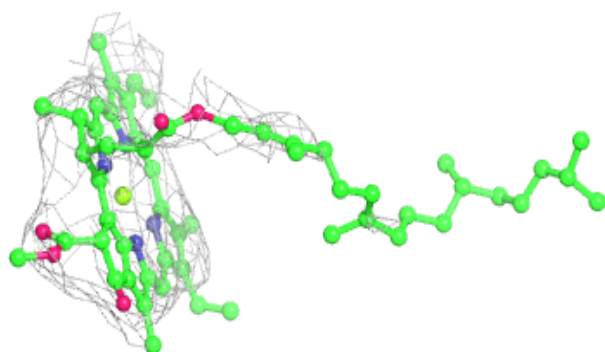
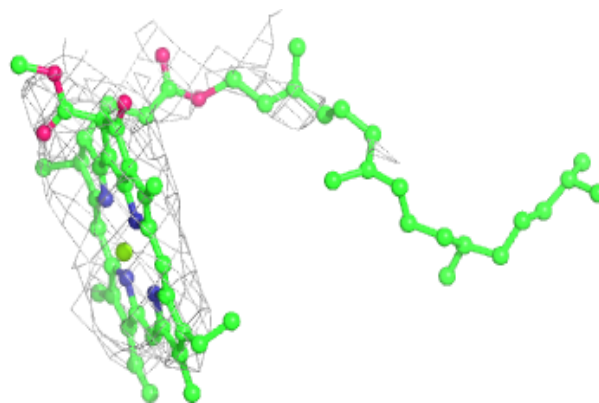
Electron density around CLA a 1113:

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



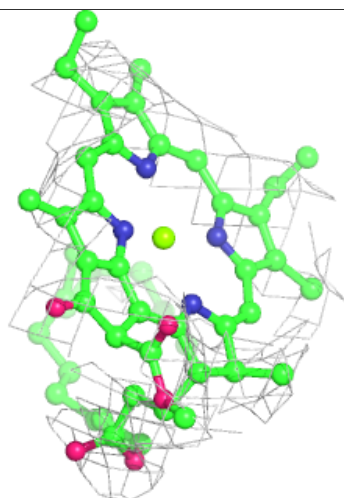
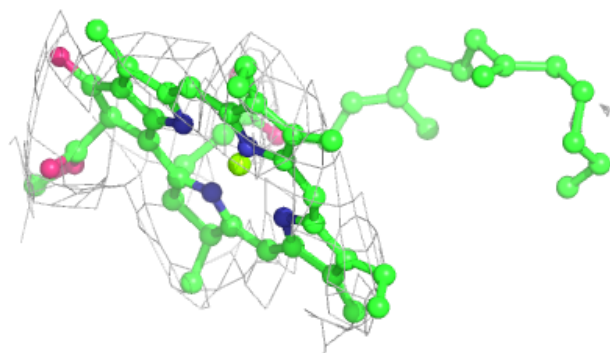
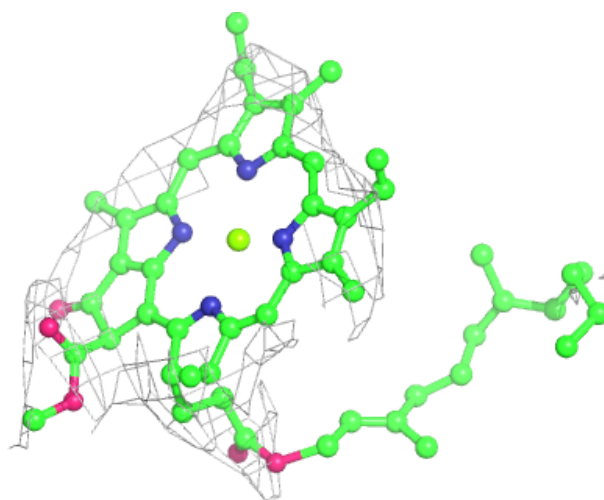
Electron density around CLA a 1128:

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



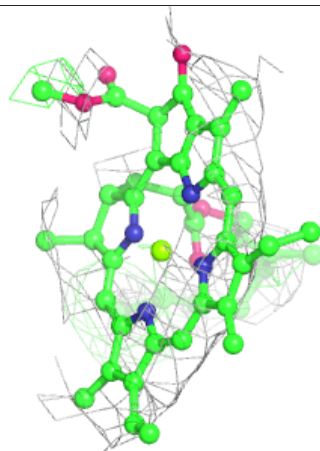
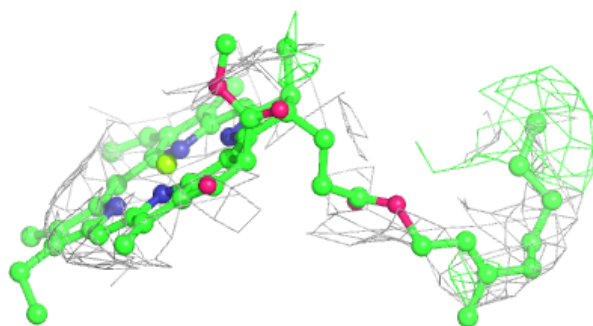
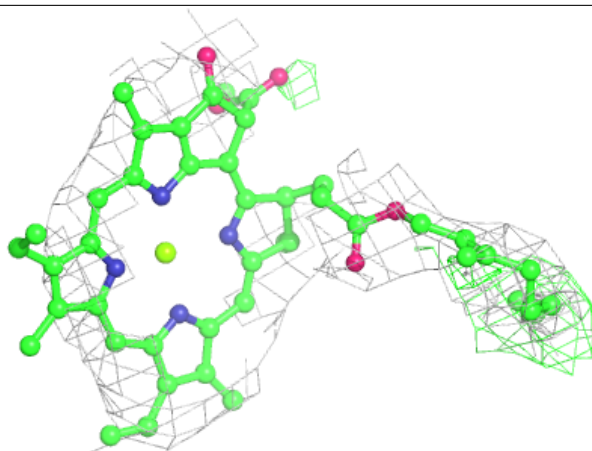
Electron density around CLA 1 1122:

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



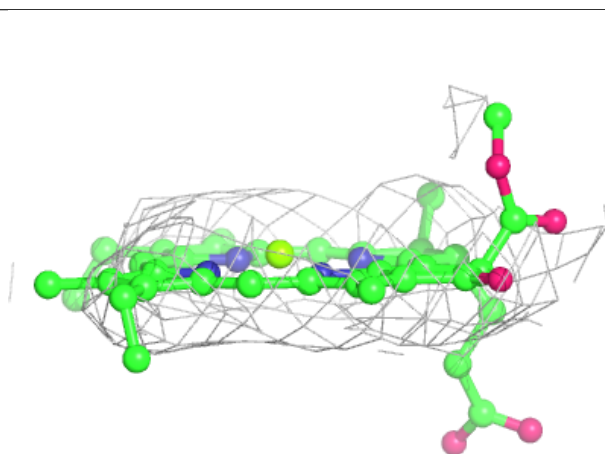
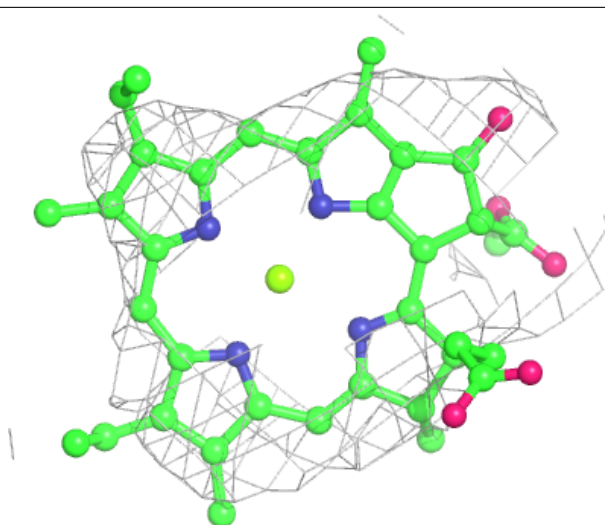
Electron density around CLA a 1110:

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



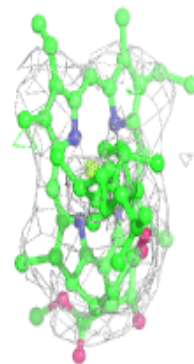
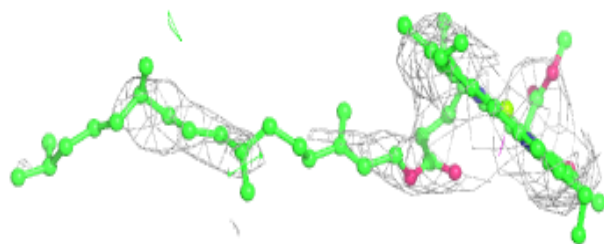
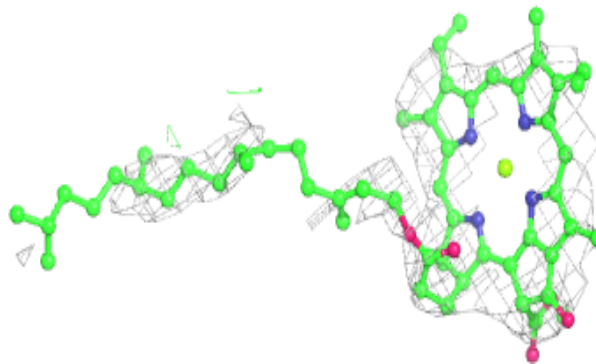
Electron density around CLA B 1212:

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

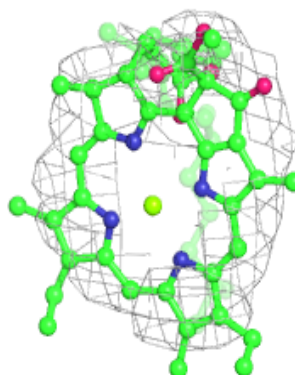
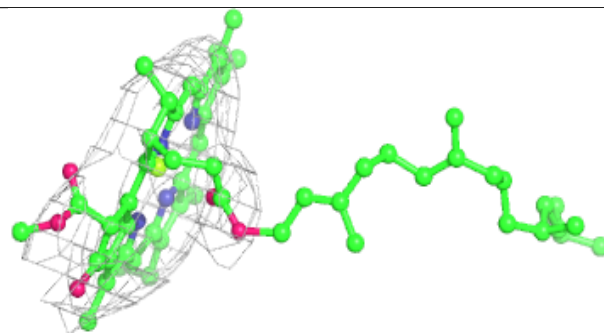
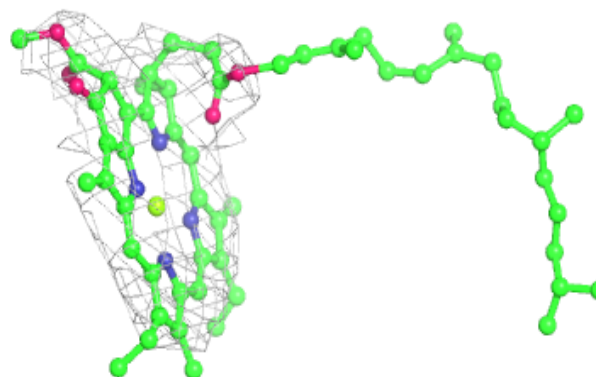


Electron density around CLA L 1501:

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

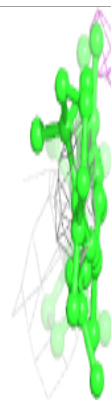
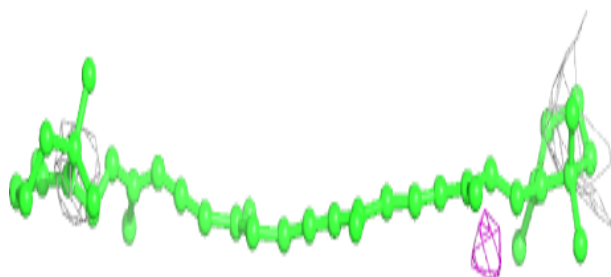
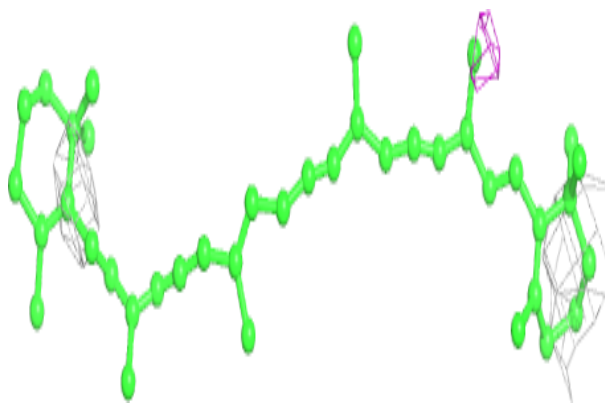
**Electron density around CLA 1 1140:**

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

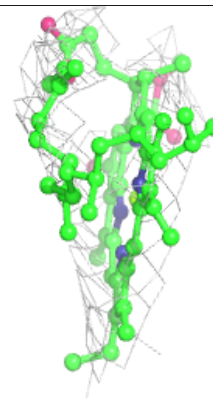
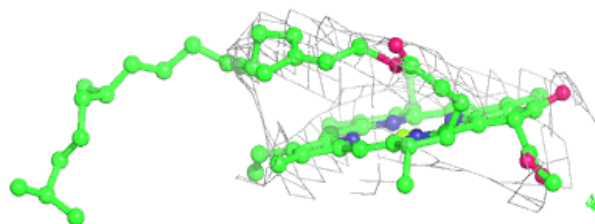
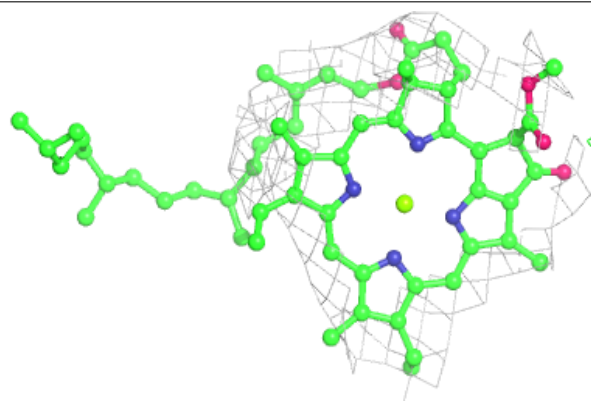


Electron density around BCR b 4005:

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

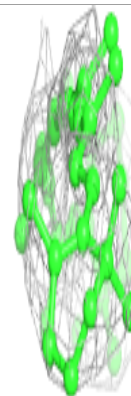
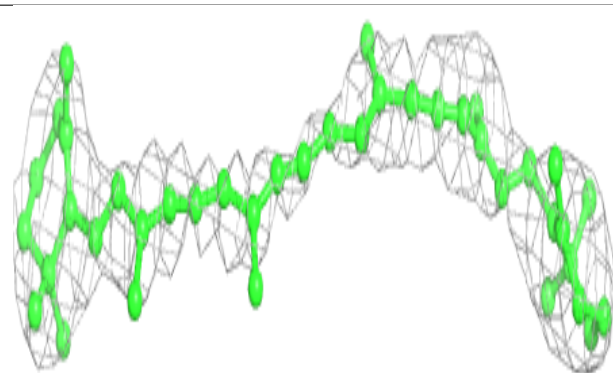
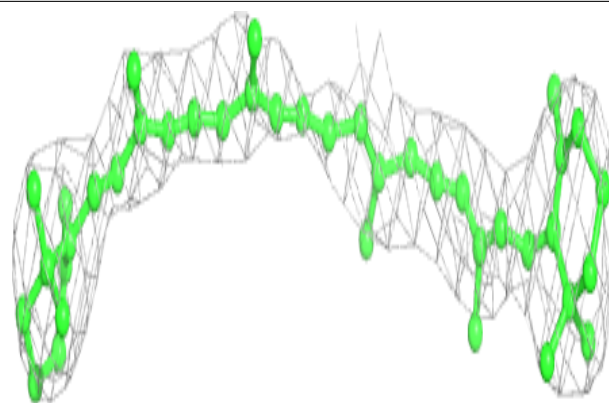
**Electron density around CLA b 1215:**

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



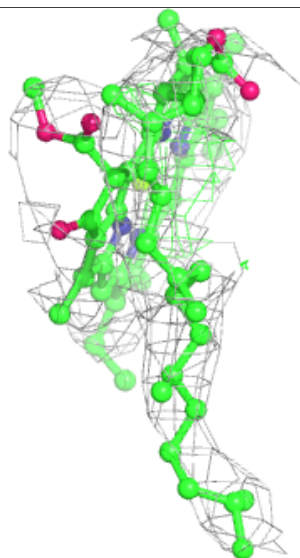
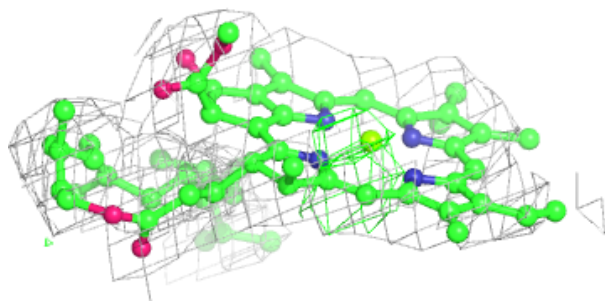
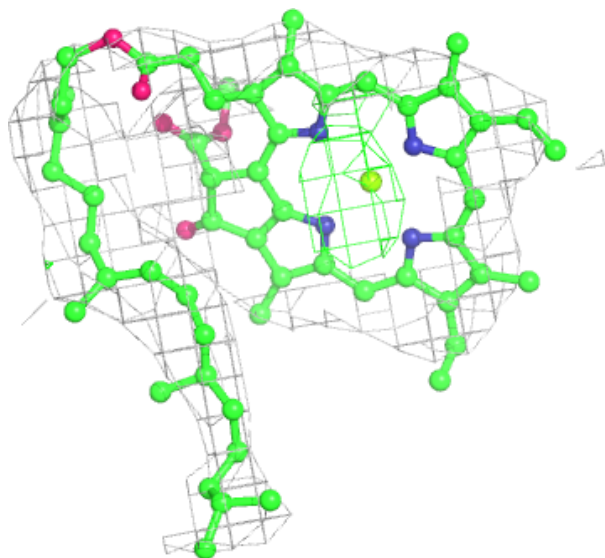
Electron density around BCR 6 4018:

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



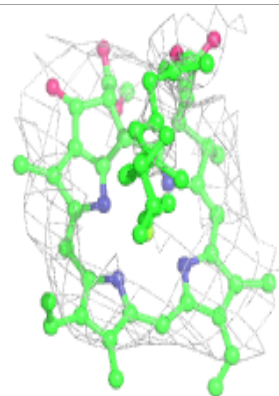
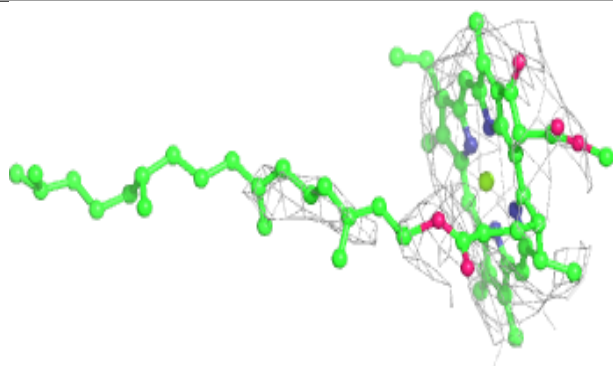
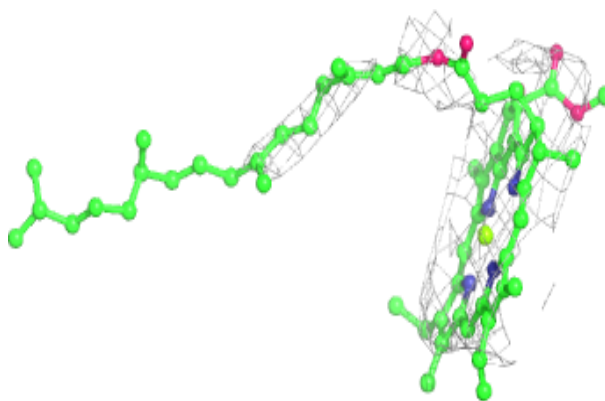
Electron density around CLA A 1123:

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

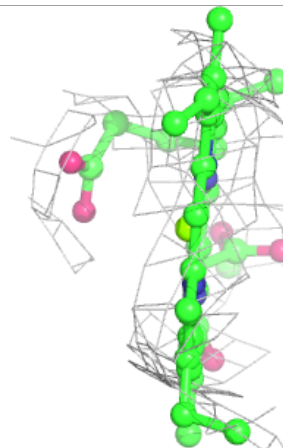
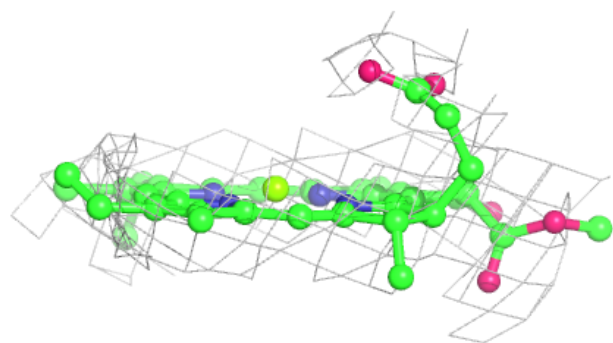
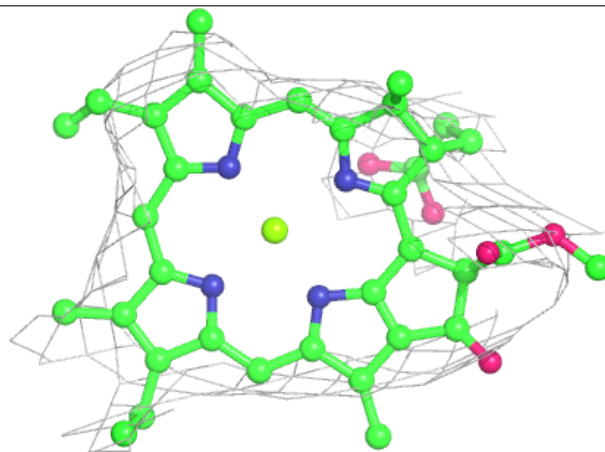


Electron density around CLA b 1226:

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

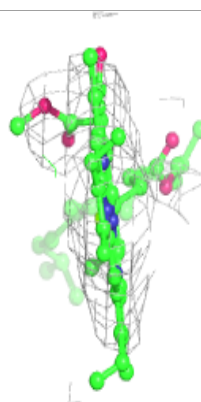
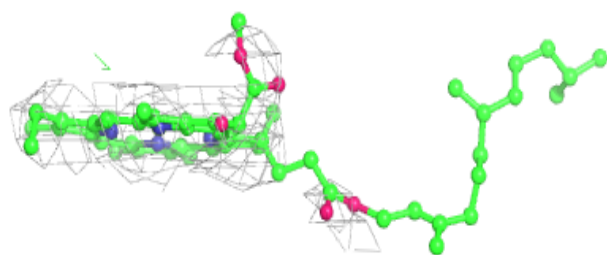
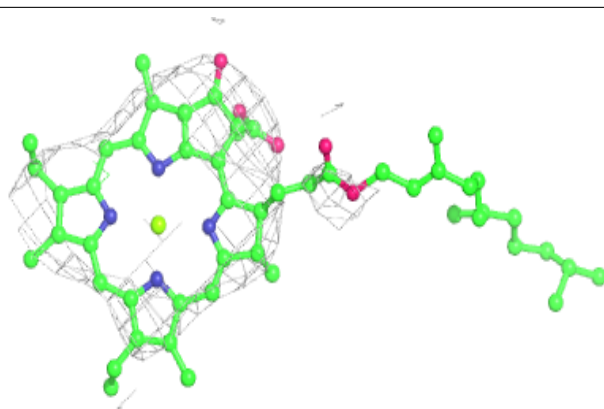
**Electron density around CLA a 1108:**

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

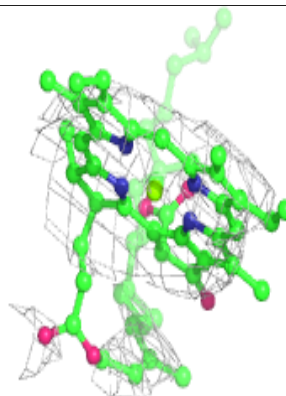
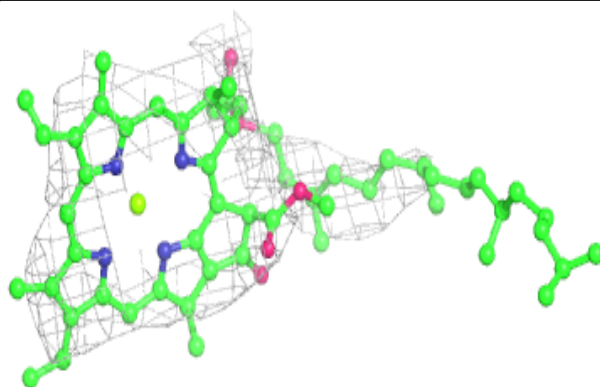
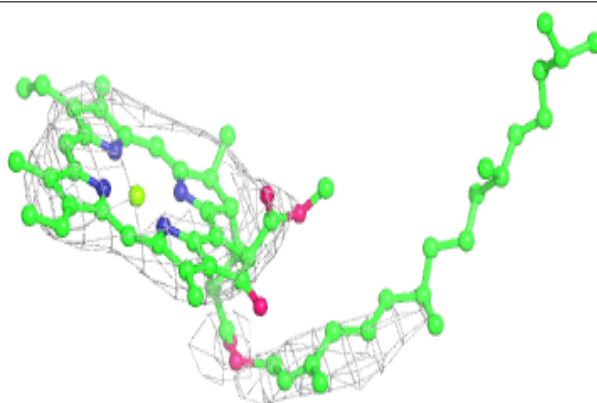


Electron density around CLA 2 1234:

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

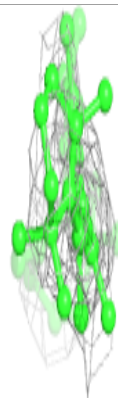
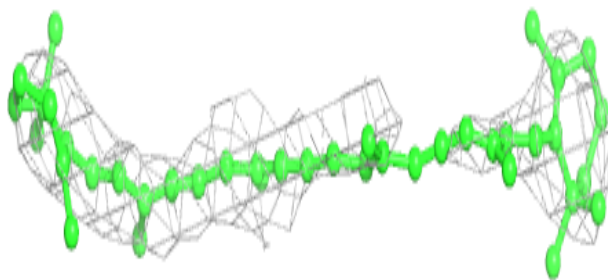
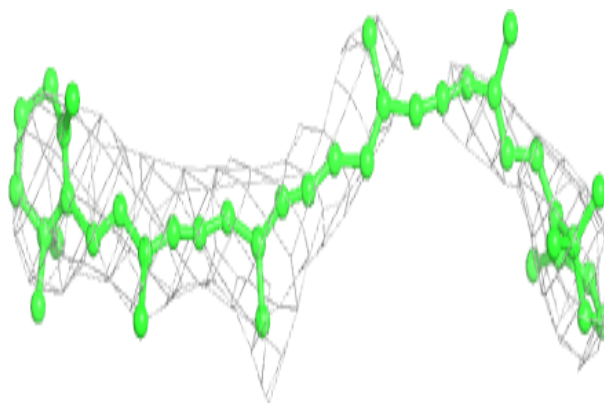
**Electron density around CLA 2 1213:**

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



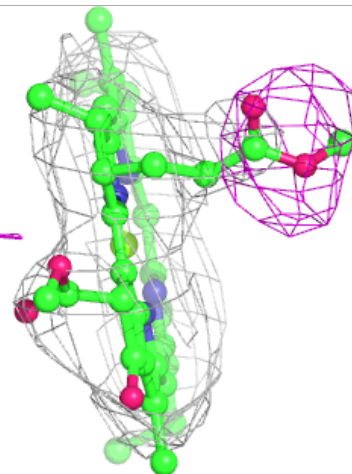
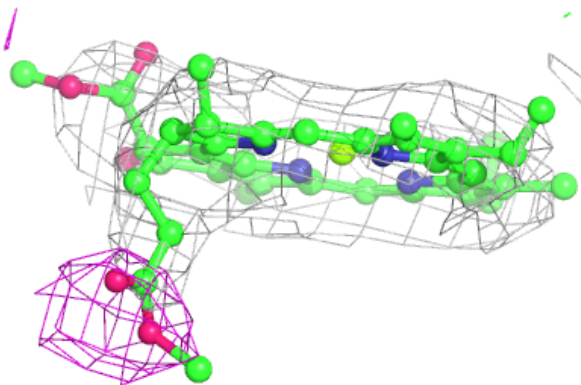
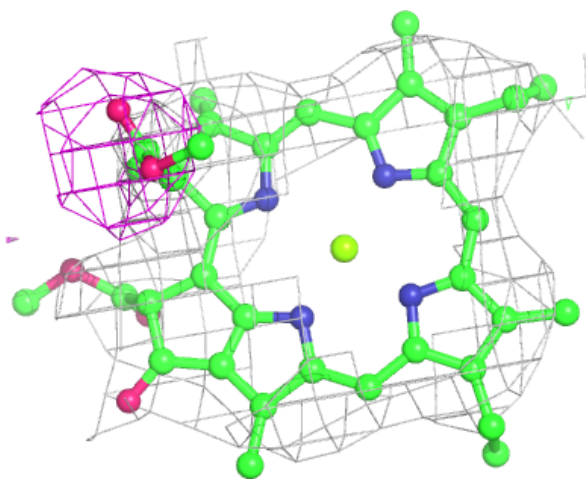
Electron density around BCR b 4017:

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



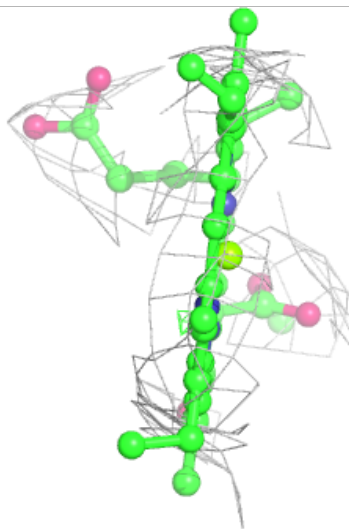
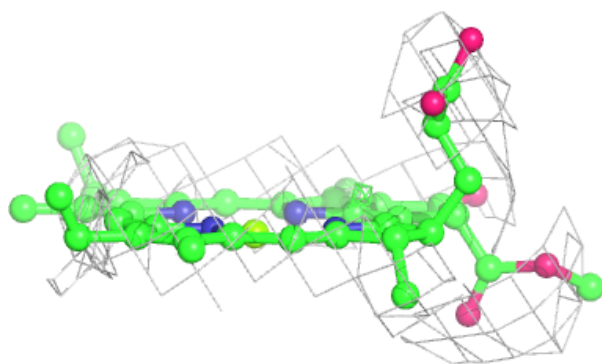
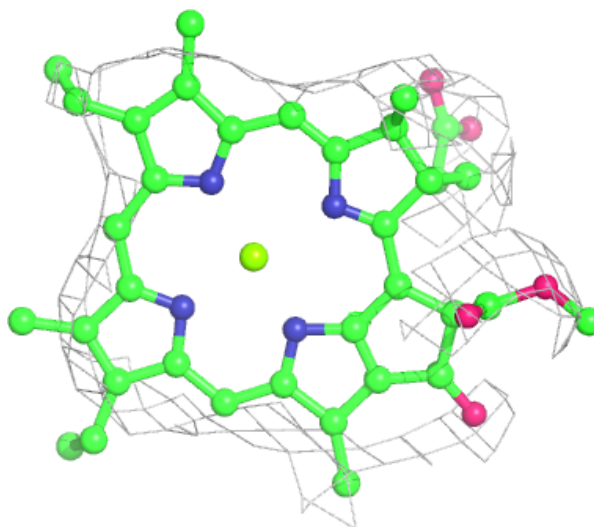
Electron density around CLA A 1130:

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



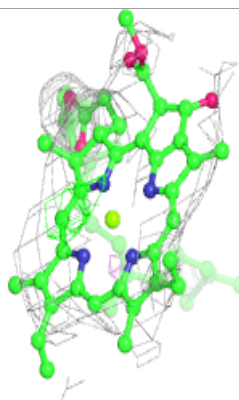
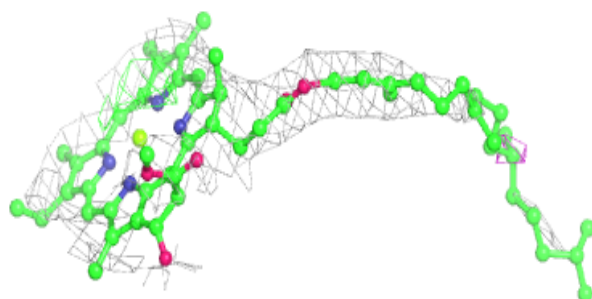
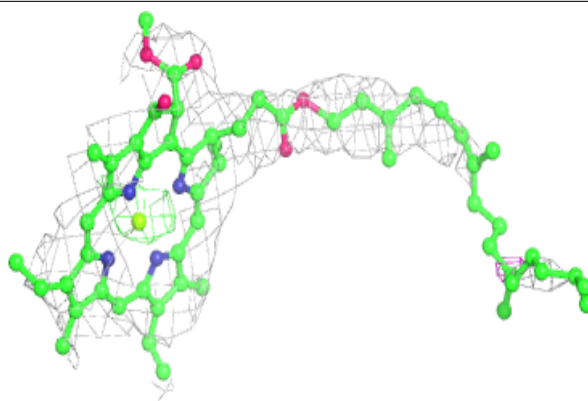
Electron density around CLA B 1232:

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

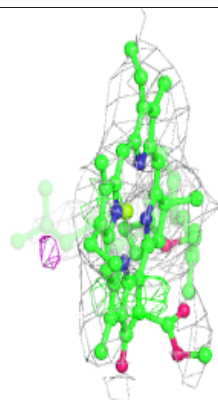
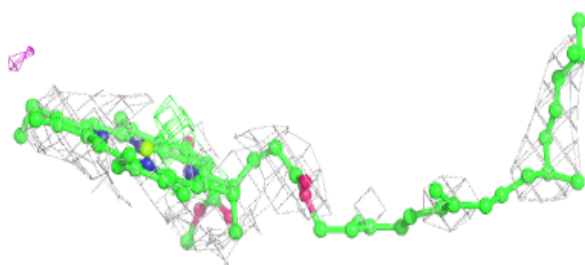
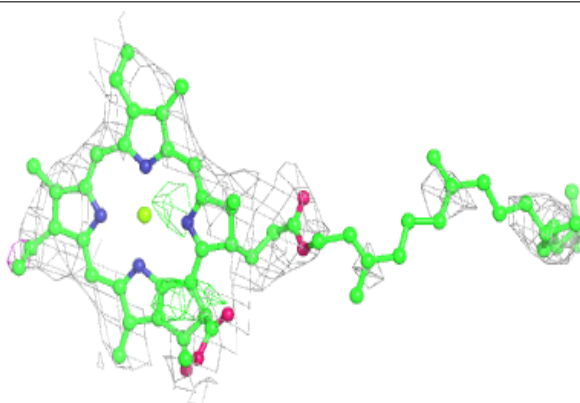


Electron density around CLA A 1012:

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

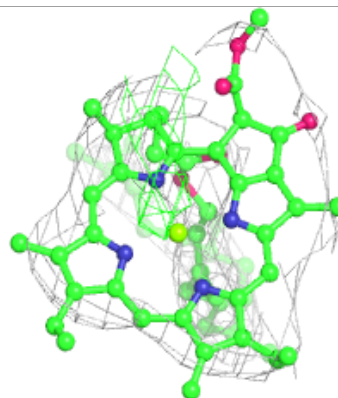
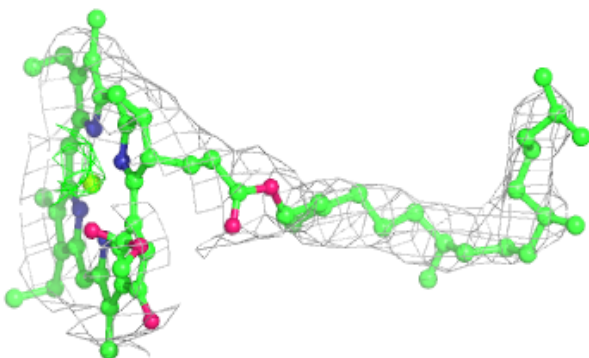
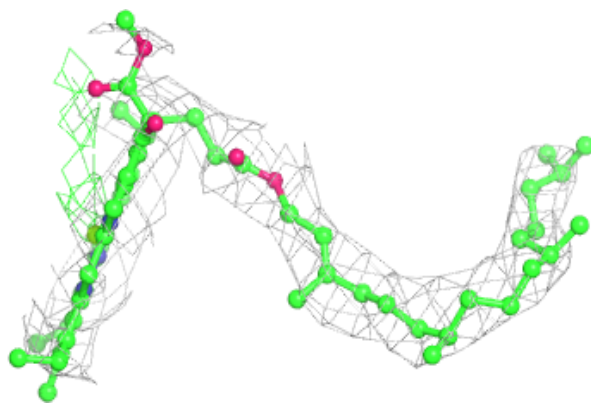
**Electron density around CLA A 1103:**

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

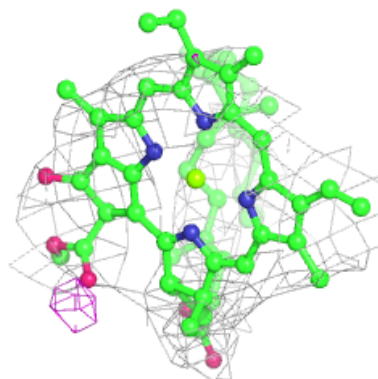
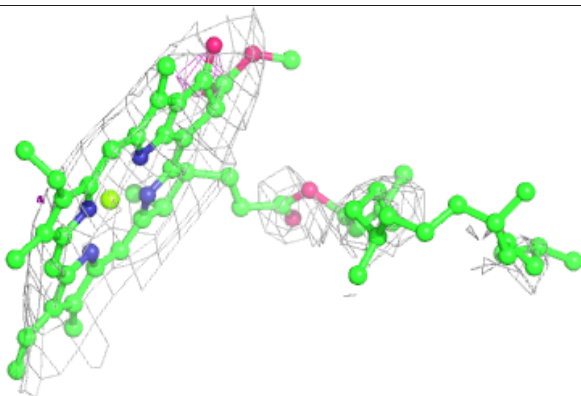
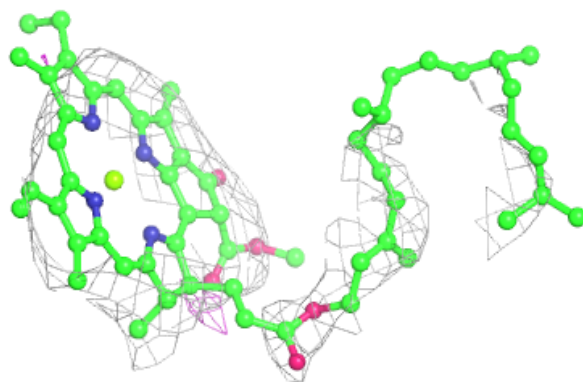


Electron density around CLA b 1238:

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

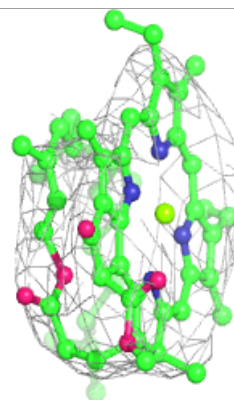
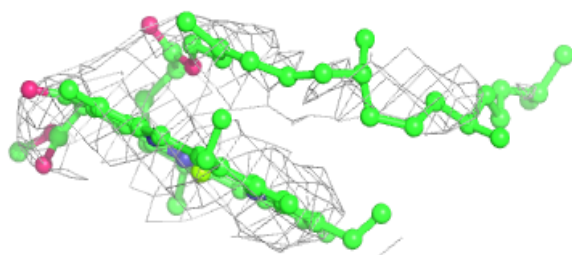
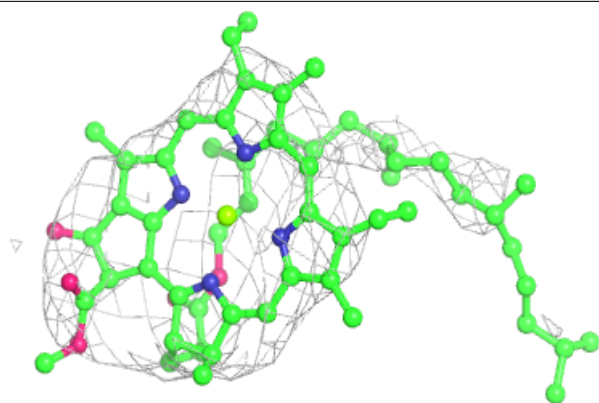
**Electron density around CLA a 1011:**

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

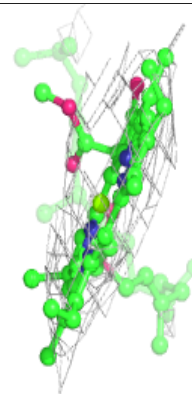
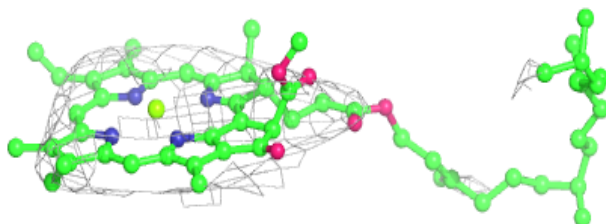
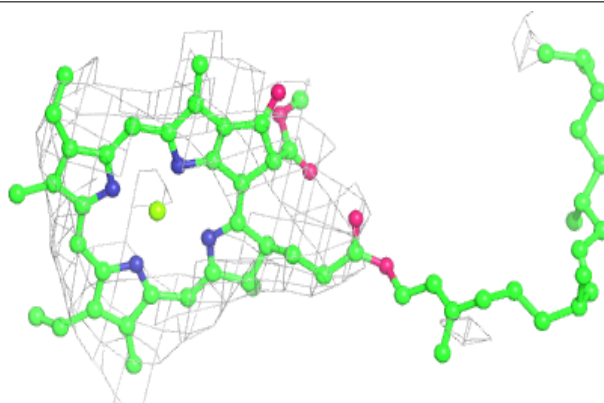


Electron density around CLA b 1204:

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

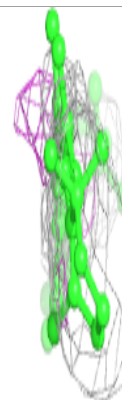
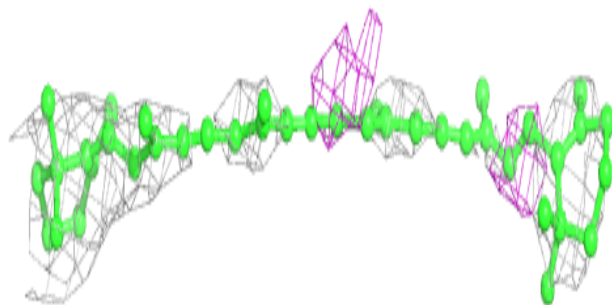
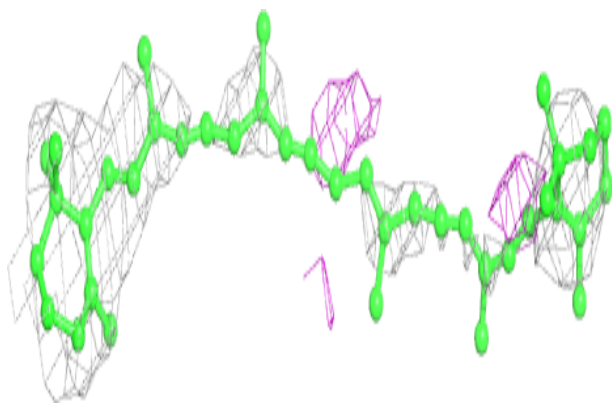
**Electron density around CLA b 1223:**

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



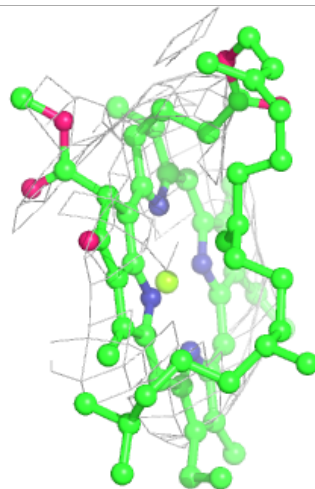
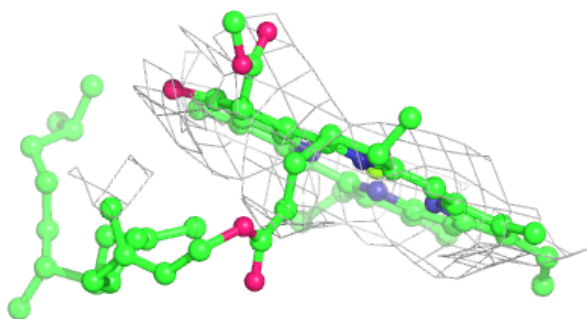
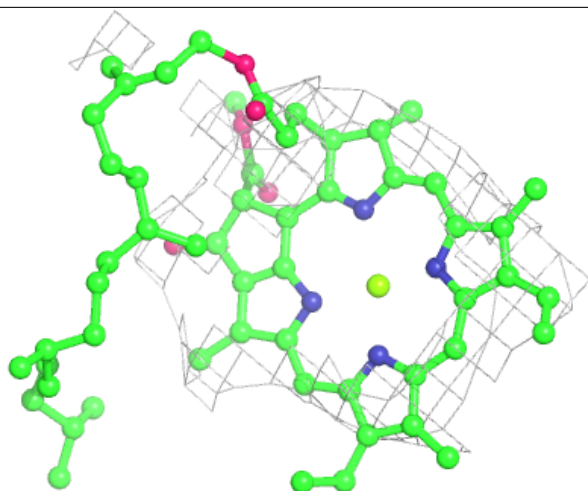
Electron density around BCR 2 4005:

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



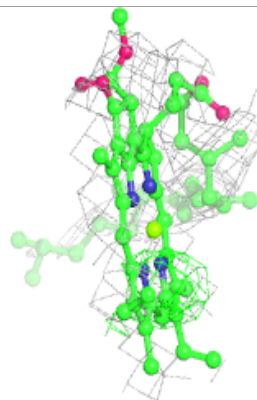
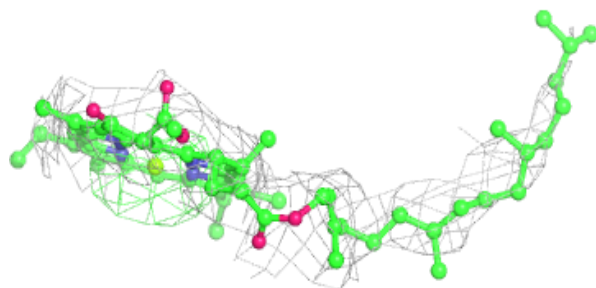
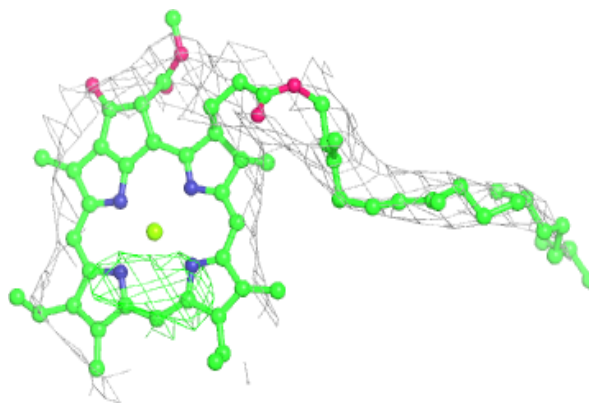
Electron density around CLA b 1229:

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



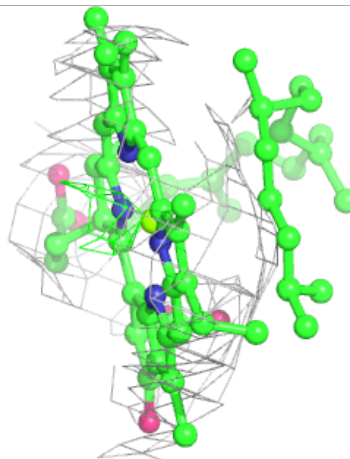
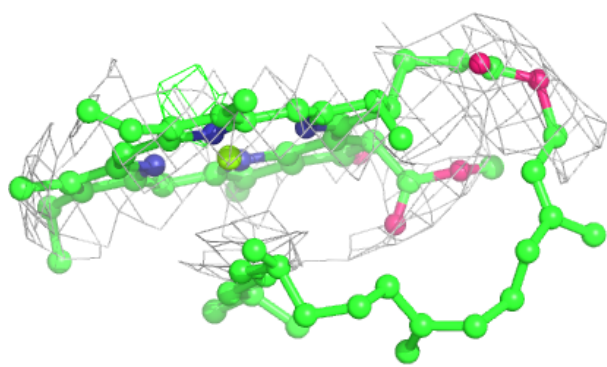
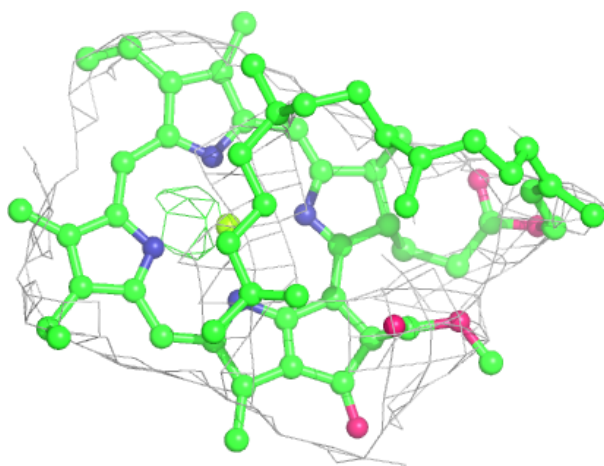
Electron density around CLA b 1023:

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



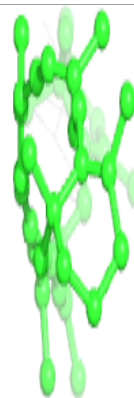
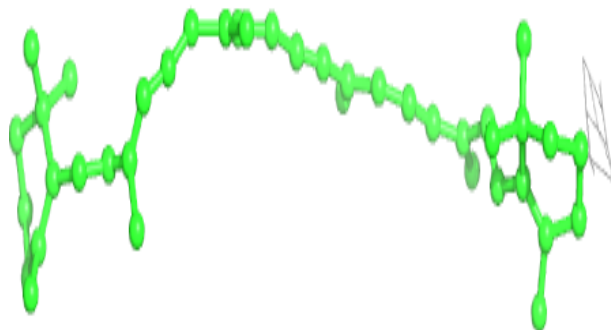
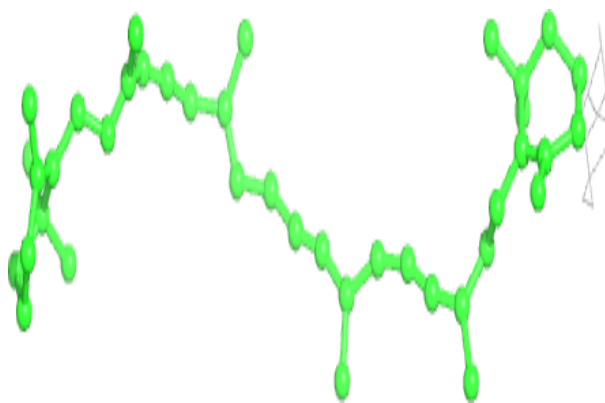
Electron density around CLA a 1104:

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

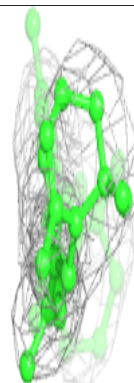
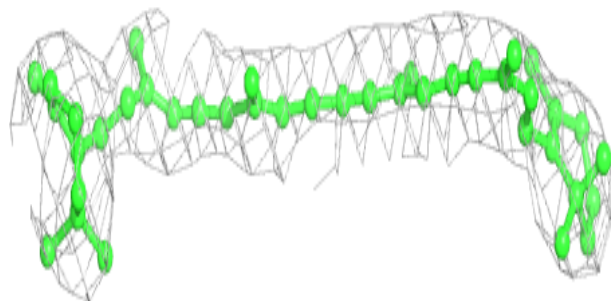
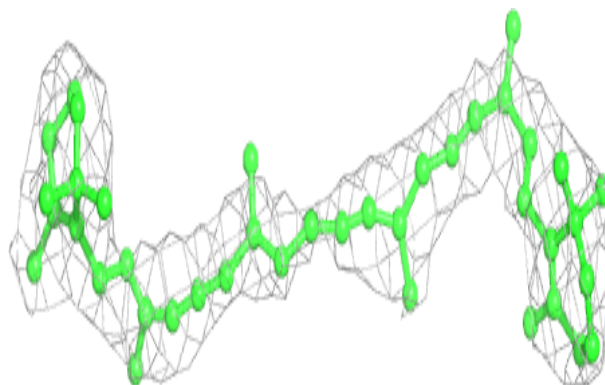


Electron density around BCR f 4013:

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

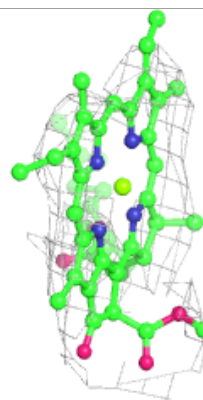
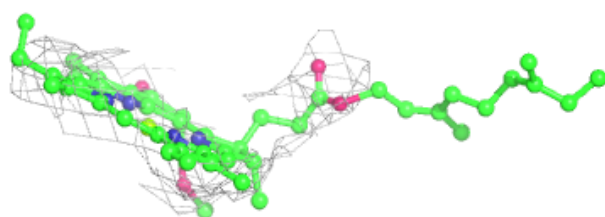
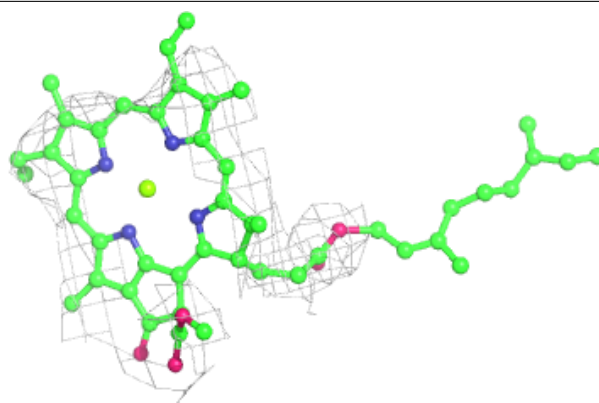
**Electron density around BCR 2 4006:**

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

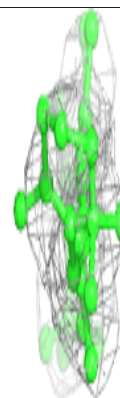
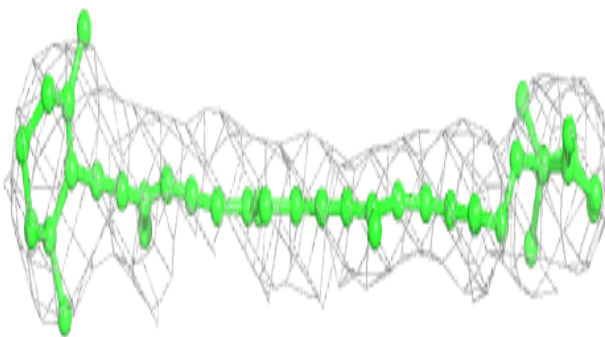
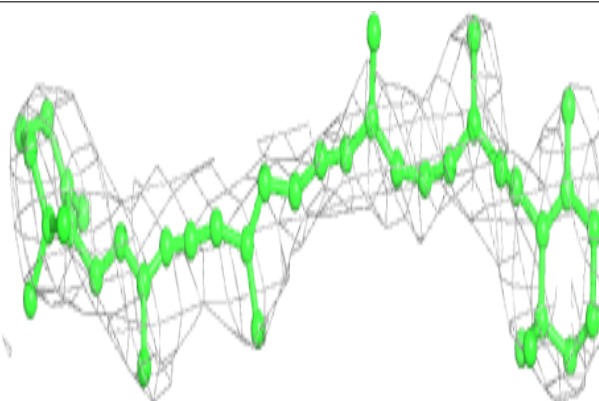


Electron density around CLA B 1222:

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

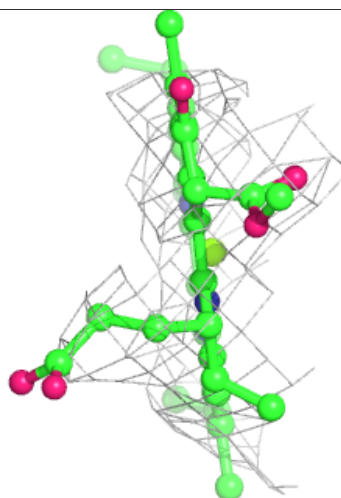
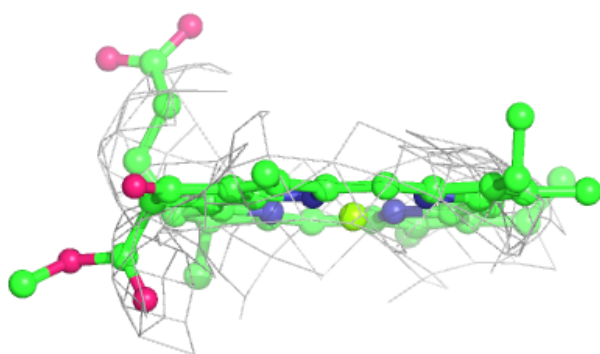
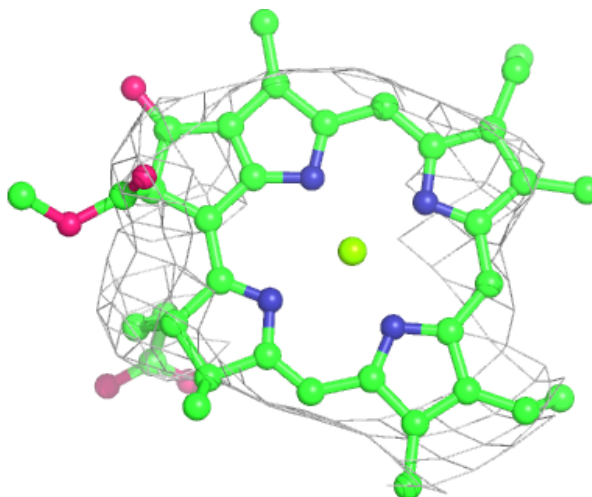
**Electron density around BCR A 4007:**

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



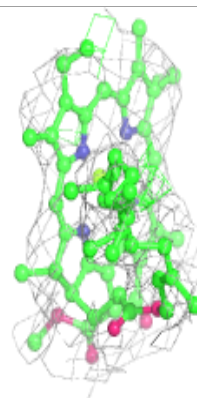
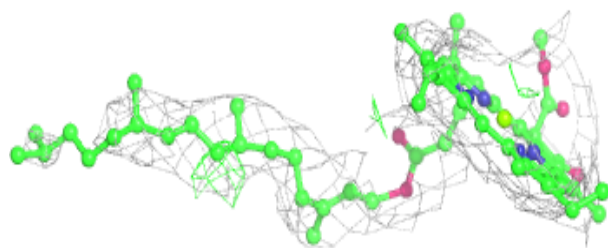
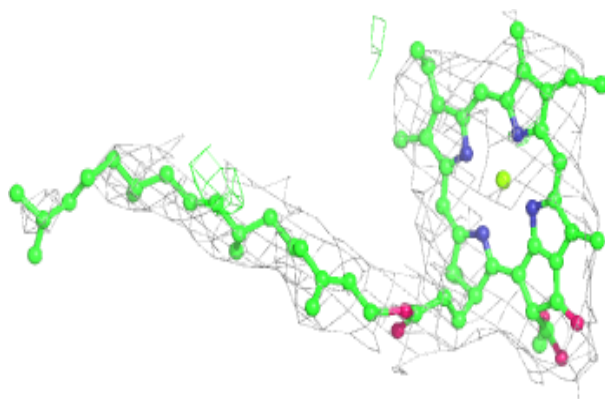
Electron density around CLA b 1232:

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



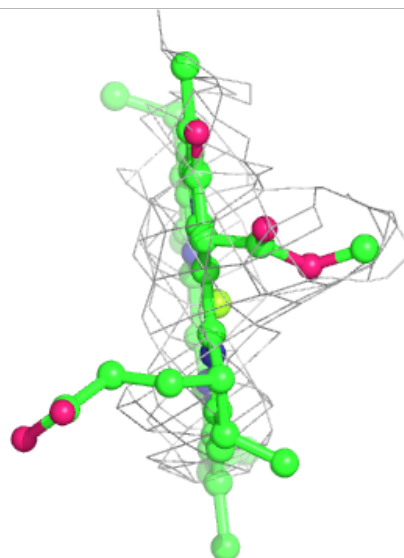
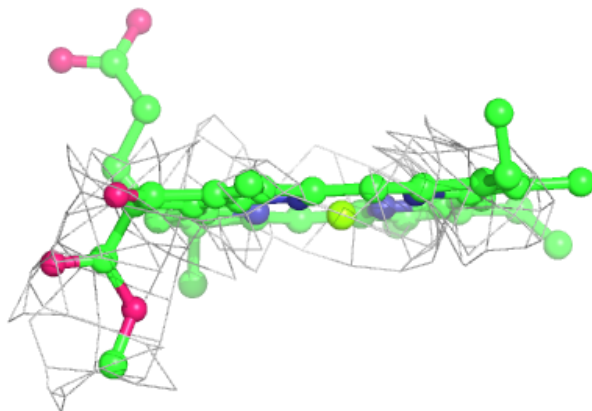
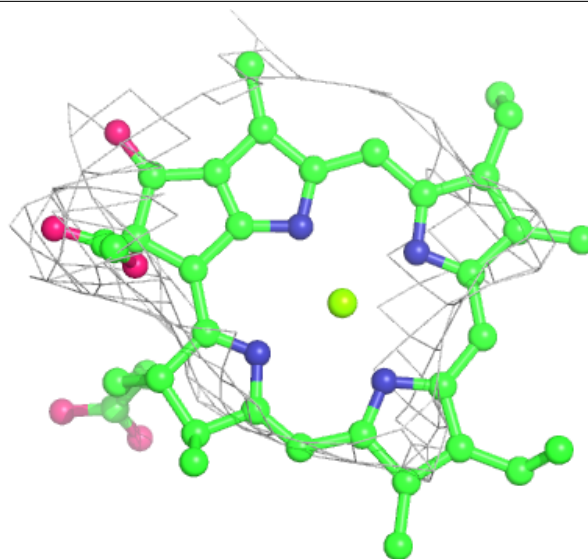
Electron density around CLA A 1132:

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



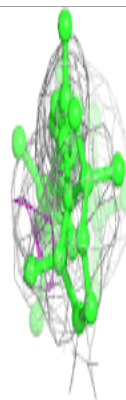
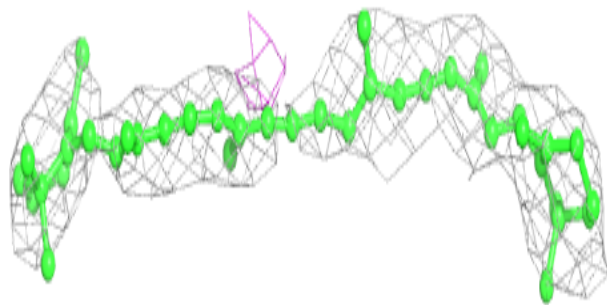
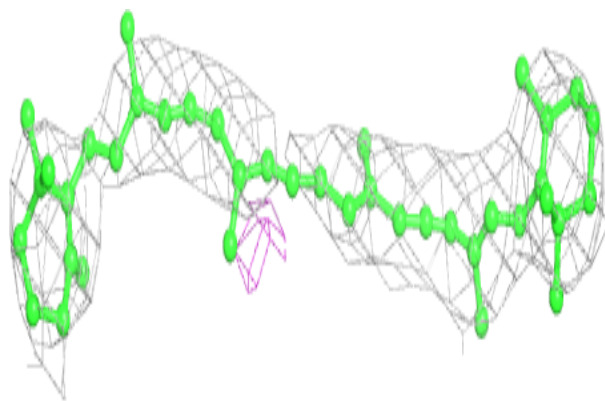
Electron density around CLA b 1231:

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



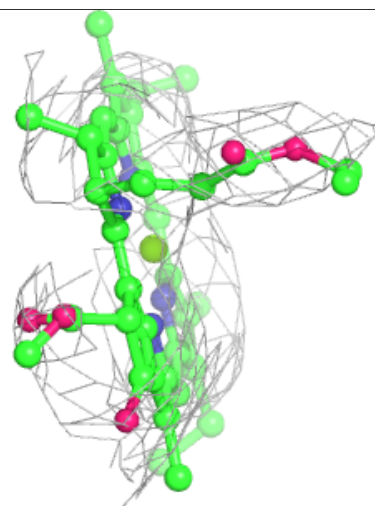
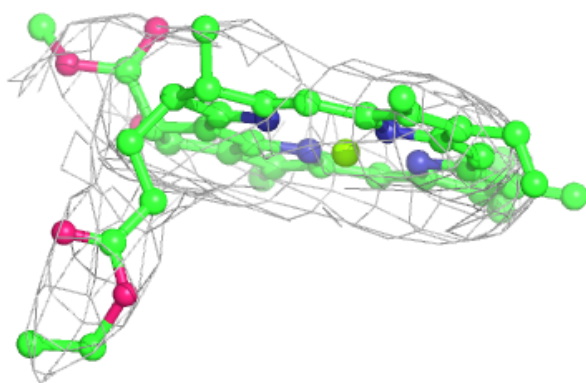
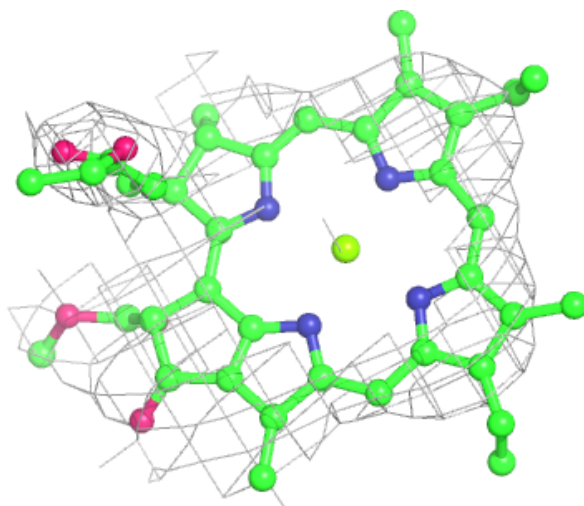
Electron density around BCR A 4008:

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



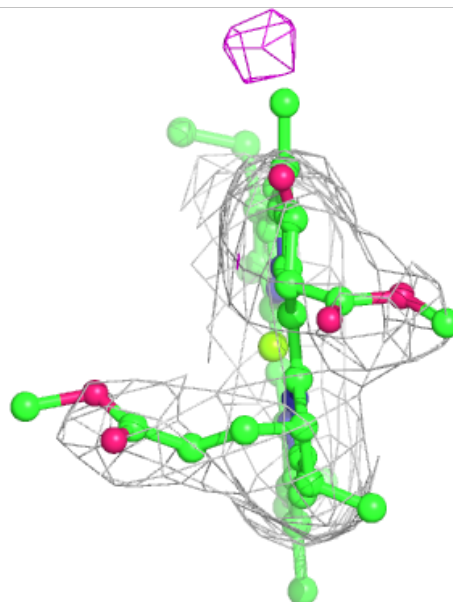
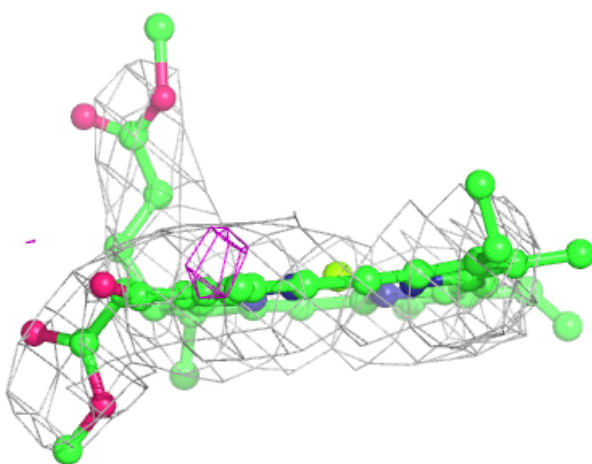
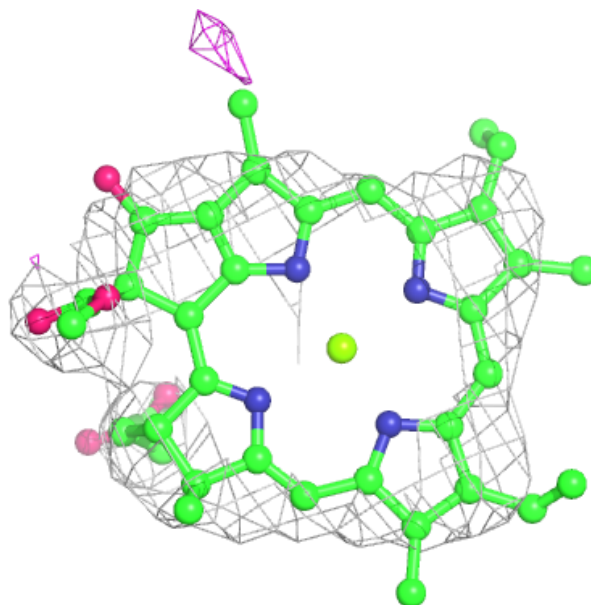
Electron density around CLA B 1236:

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



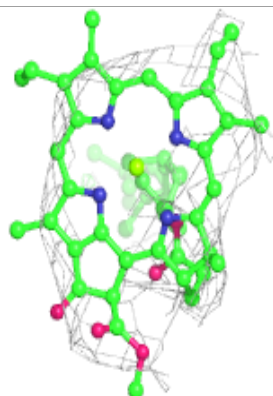
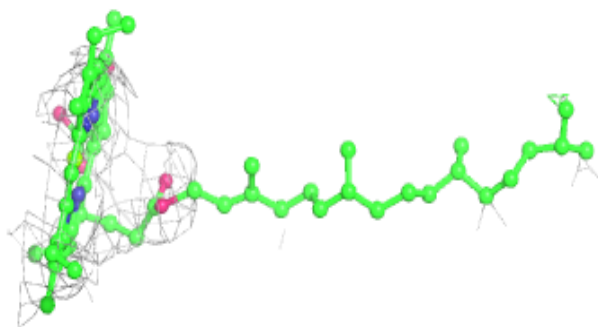
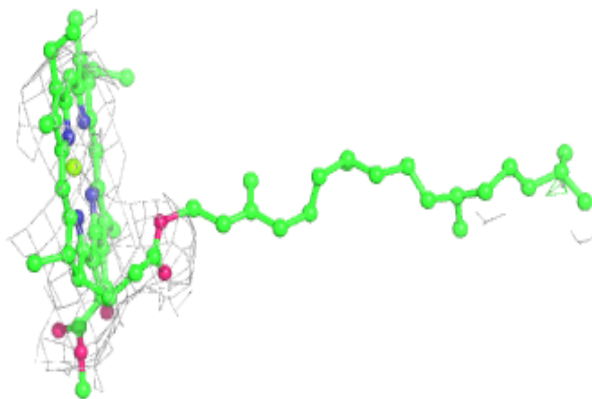
Electron density around CLA 1 1502:

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

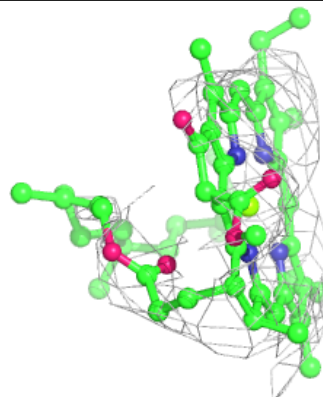
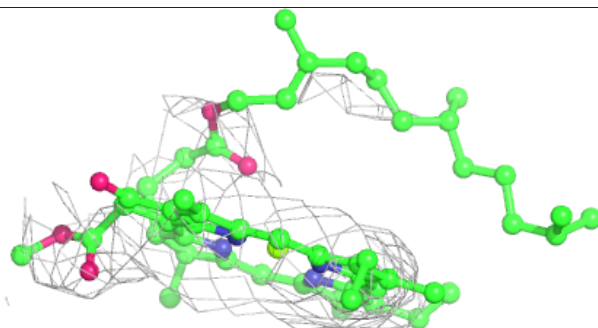
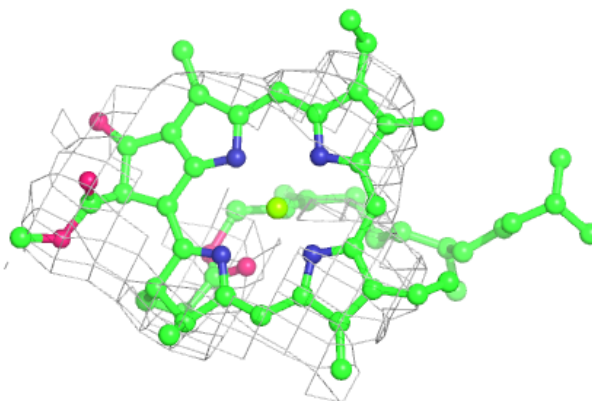


Electron density around CLA a 1126:

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

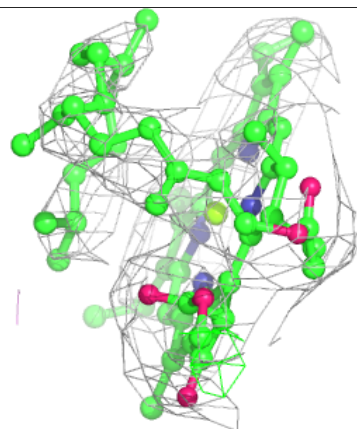
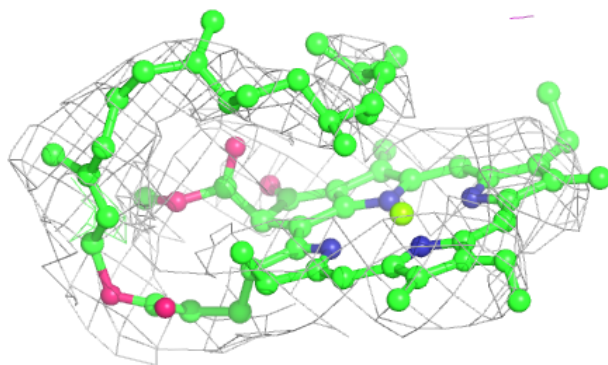
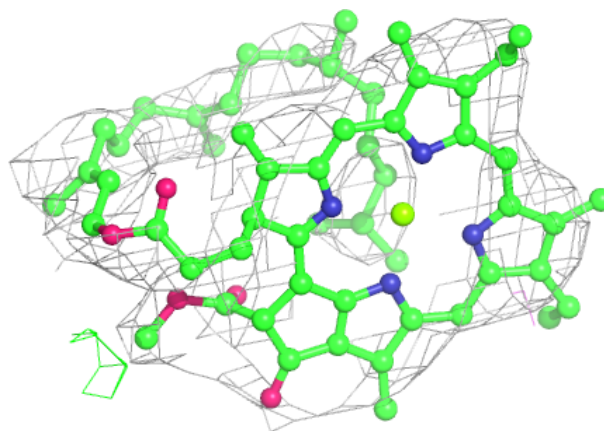
**Electron density around CLA B 1235:**

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

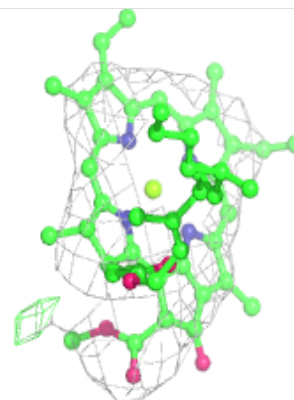
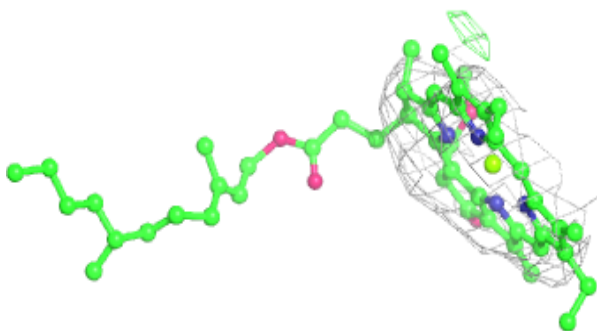
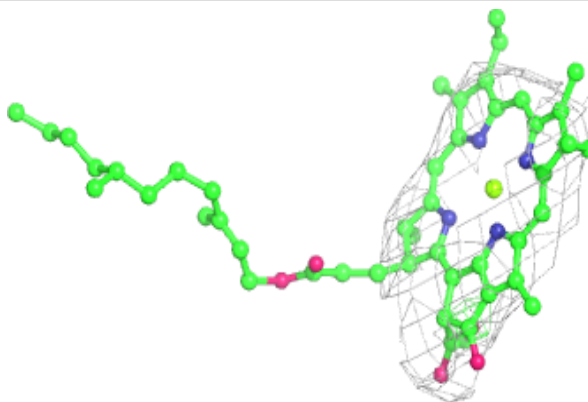


Electron density around CLA A 1104:

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

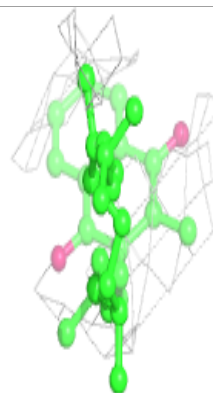
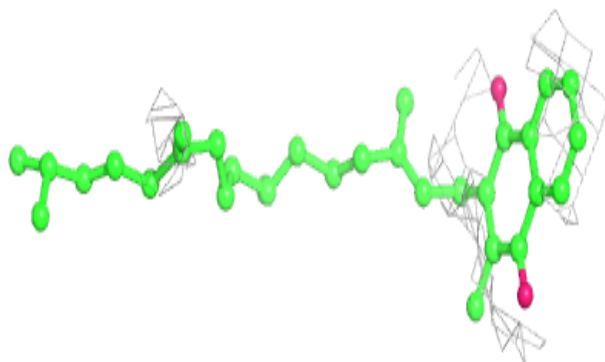
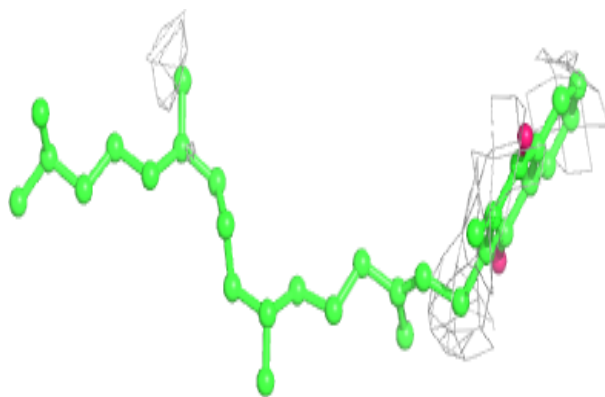
**Electron density around CLA 2 1230:**

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

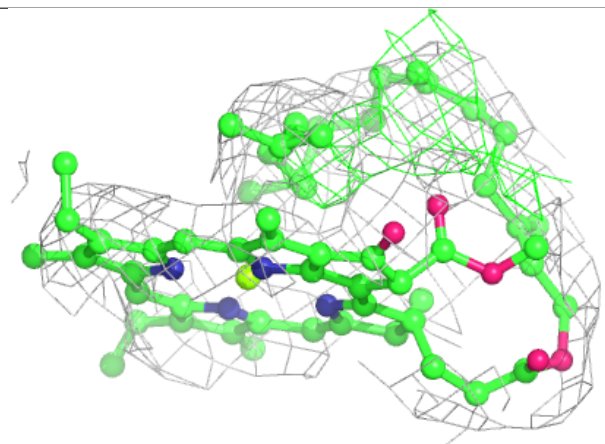
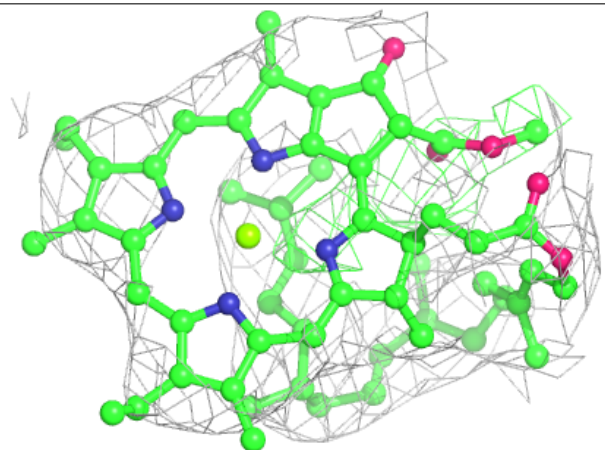


Electron density around PQN 1 2001:

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

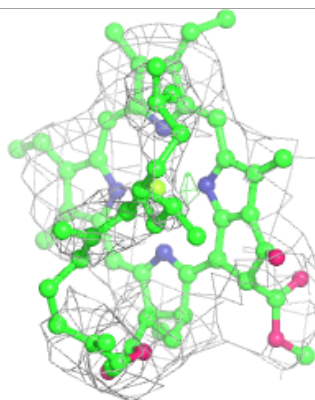
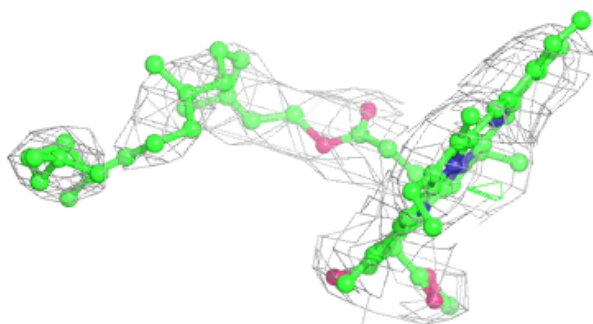
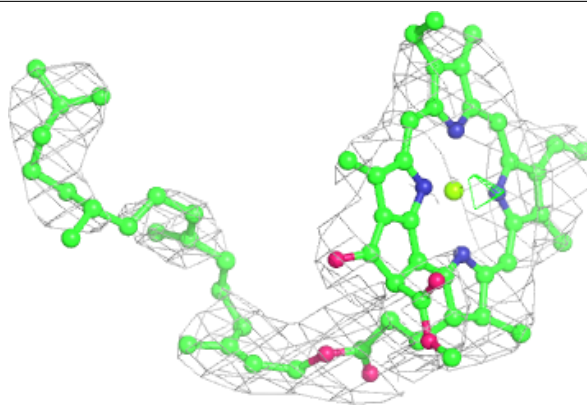
**Electron density around CLA 2 1203:**

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

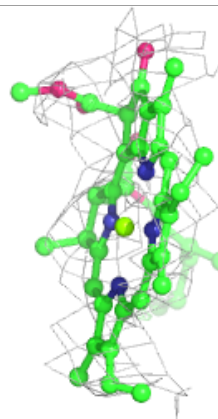
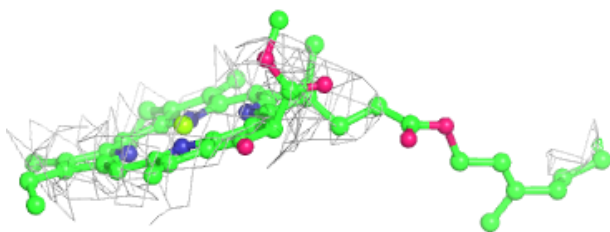
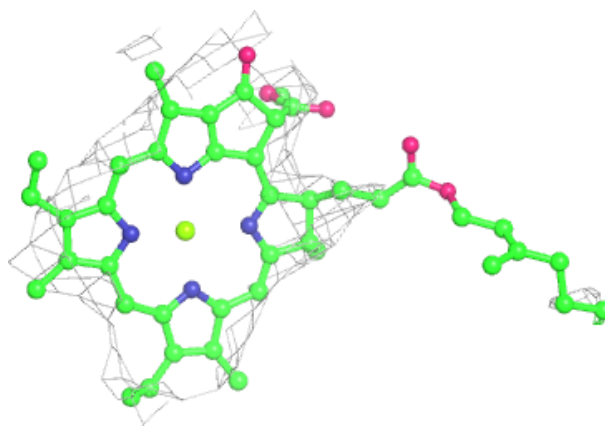


Electron density around CLA A 1137:

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

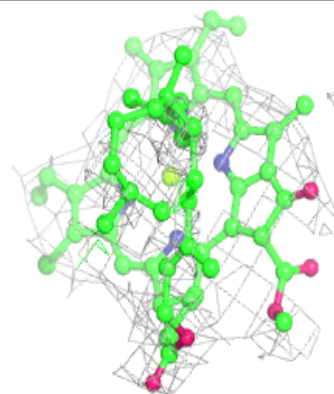
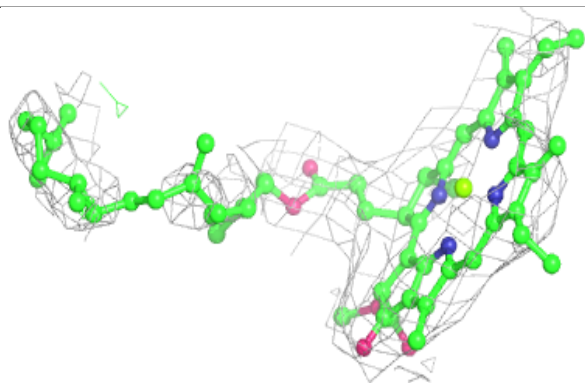
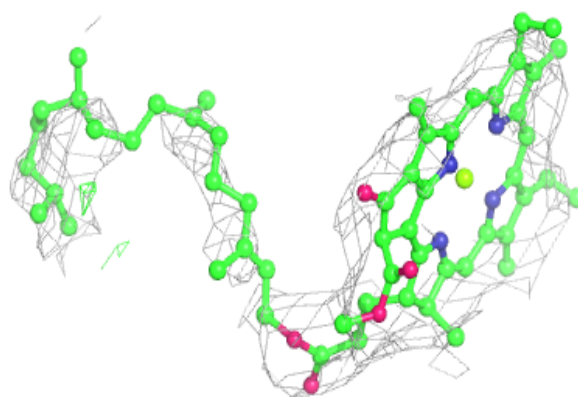
**Electron density around CLA 1 1125:**

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



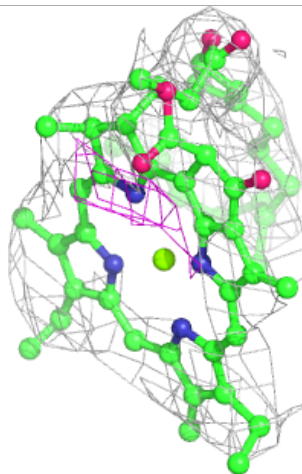
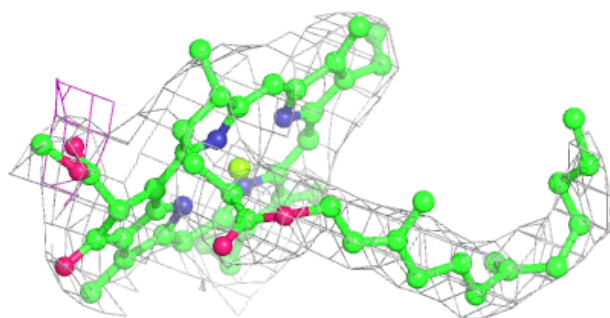
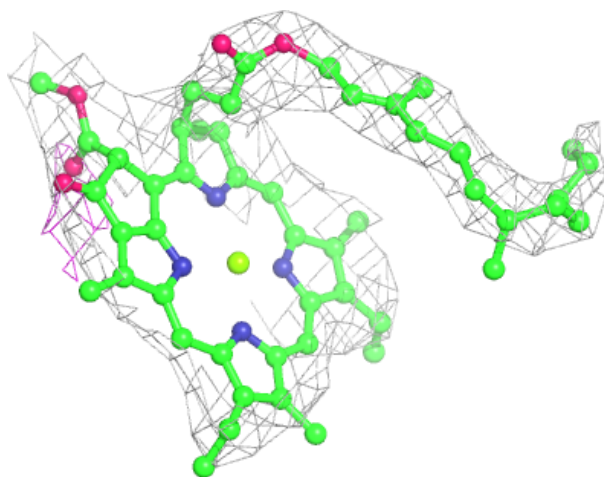
Electron density around CLA B 1021:

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



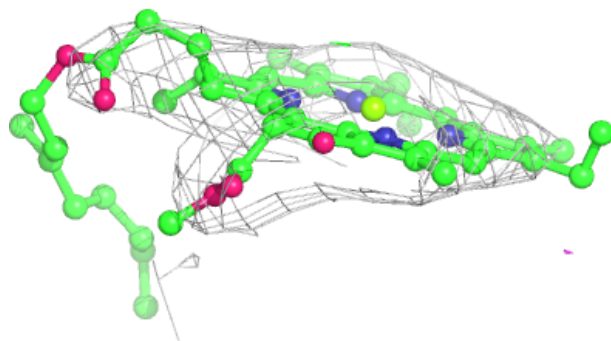
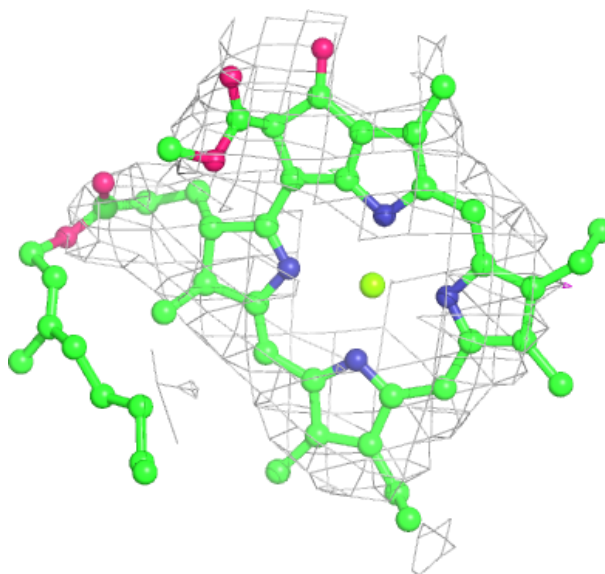
Electron density around CLA A 1122:

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



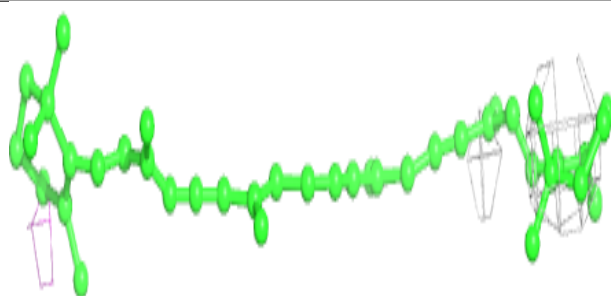
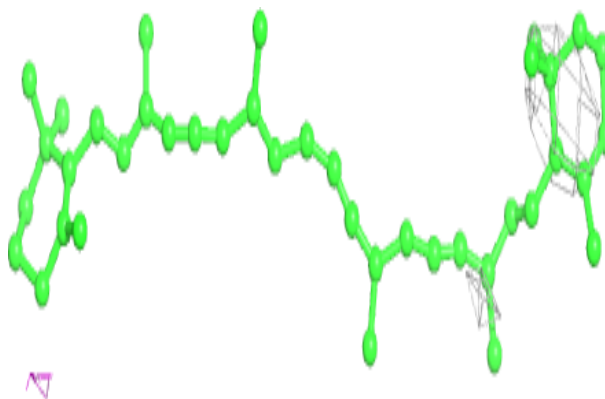
Electron density around CLA B 1221:

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

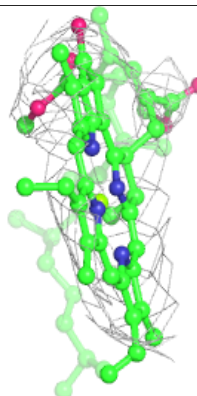
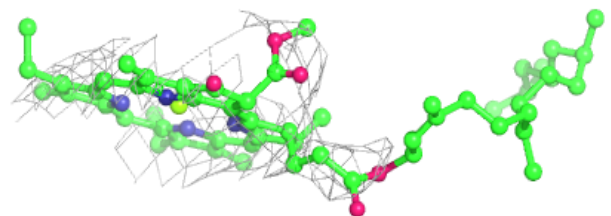
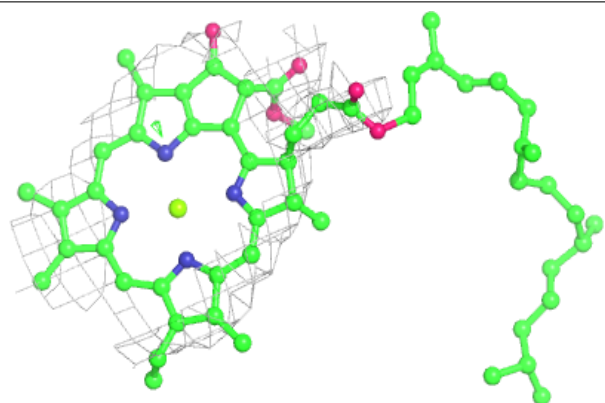


Electron density around BCR 1 4002:

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

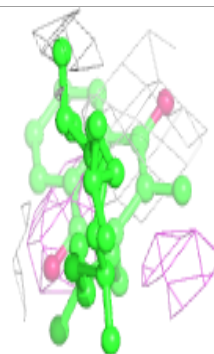
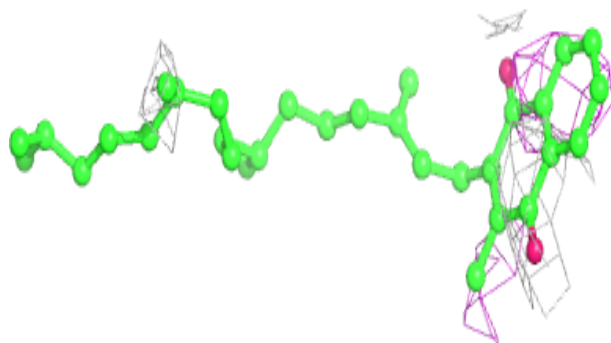
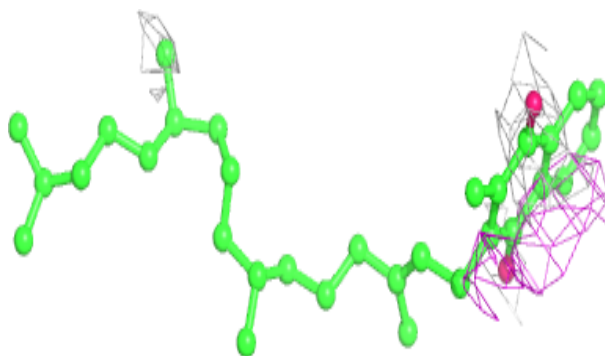
**Electron density around CLA 1 1101:**

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



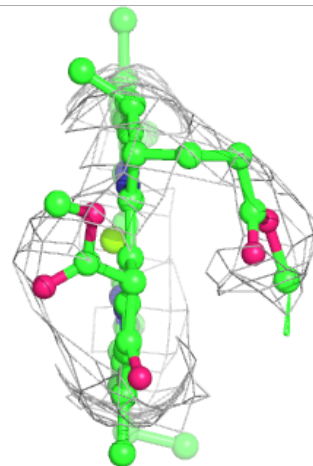
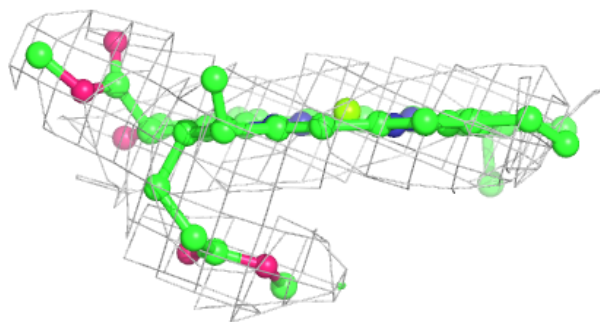
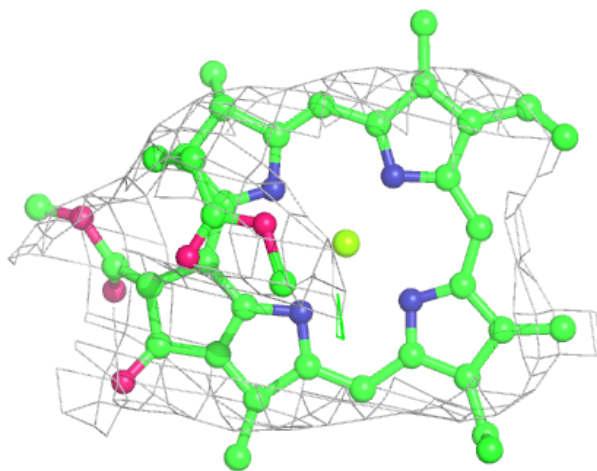
Electron density around PQN a 2001:

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



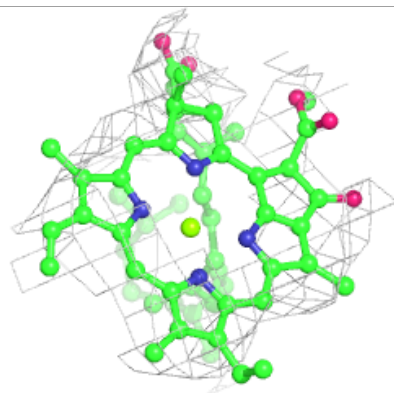
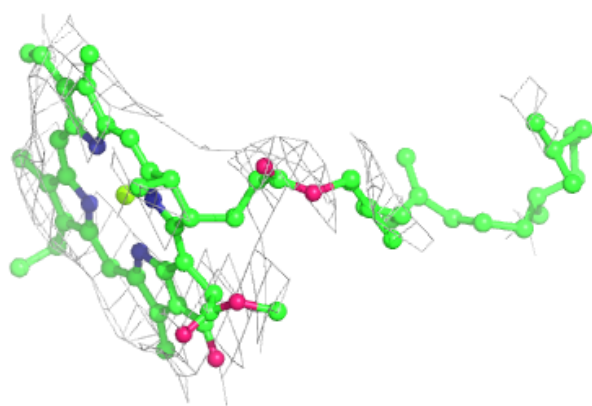
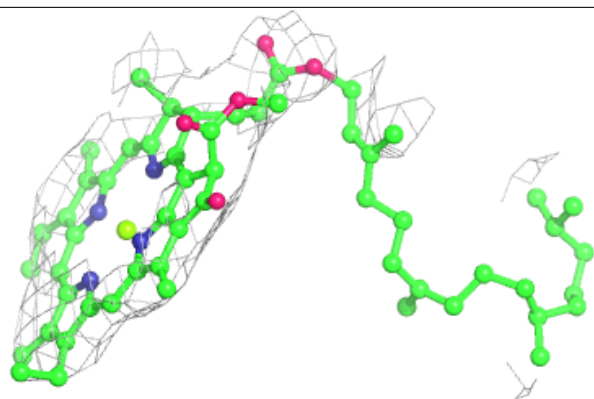
Electron density around CLA A 1138:

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

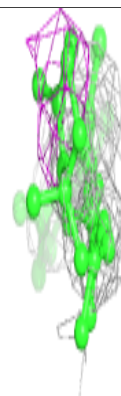
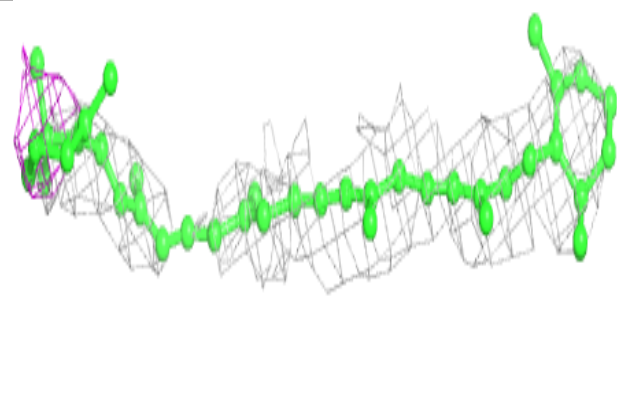
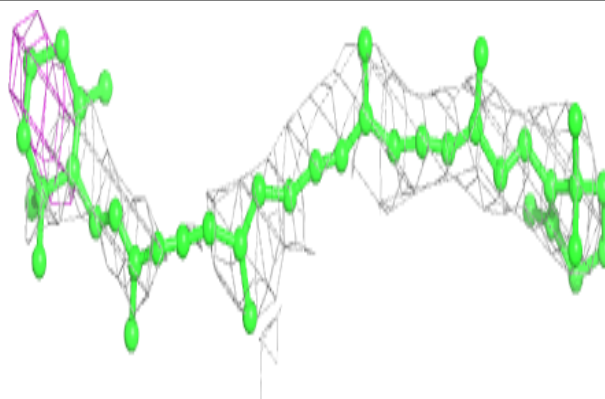


Electron density around CLA b 1021:

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

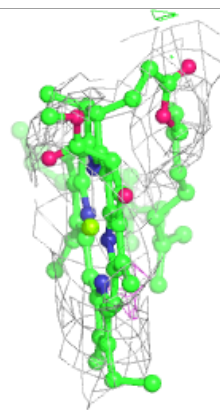
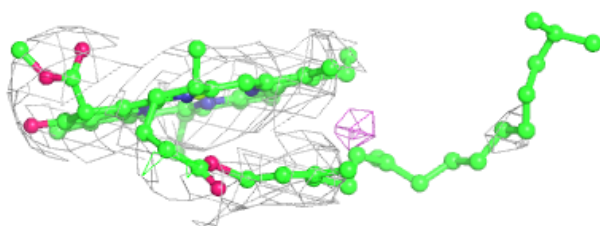
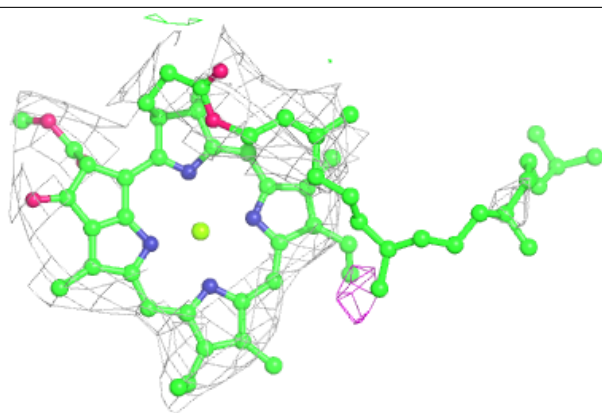
**Electron density around BCR L 4022:**

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

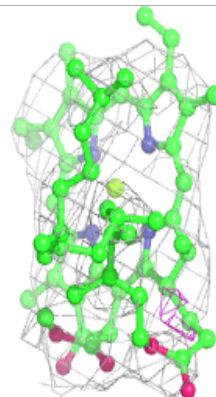
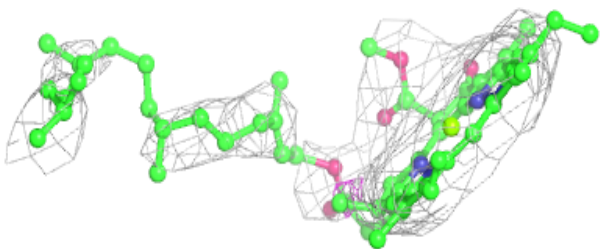
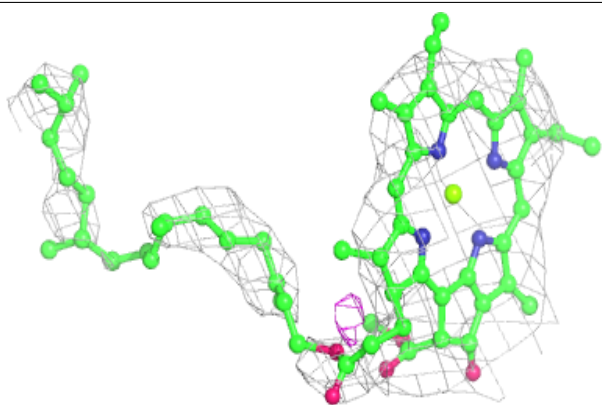


Electron density around CLA 2 1215:

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

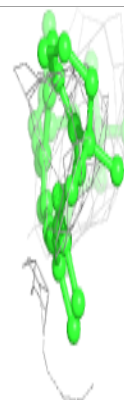
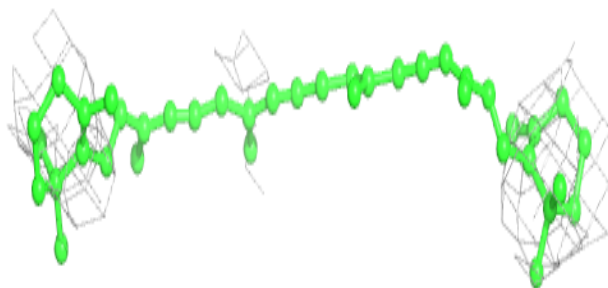
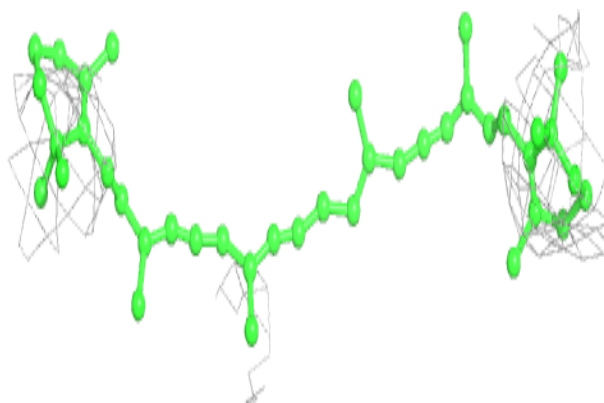
**Electron density around CLA b 1207:**

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

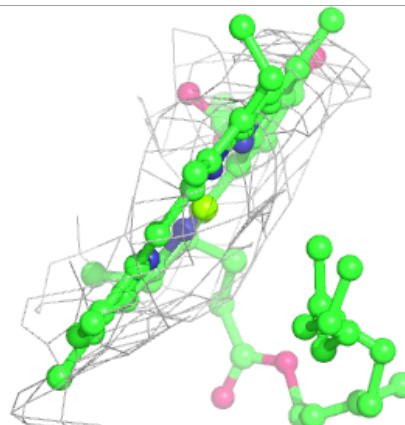
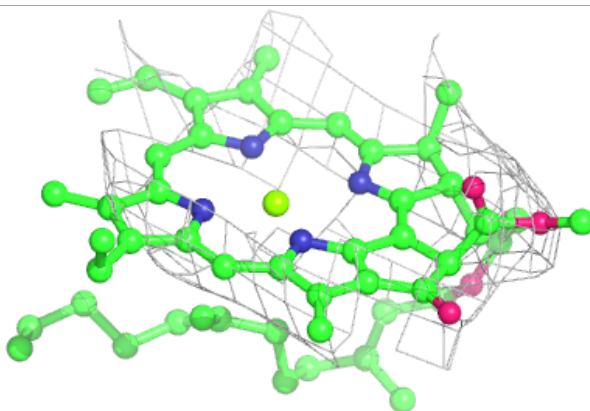
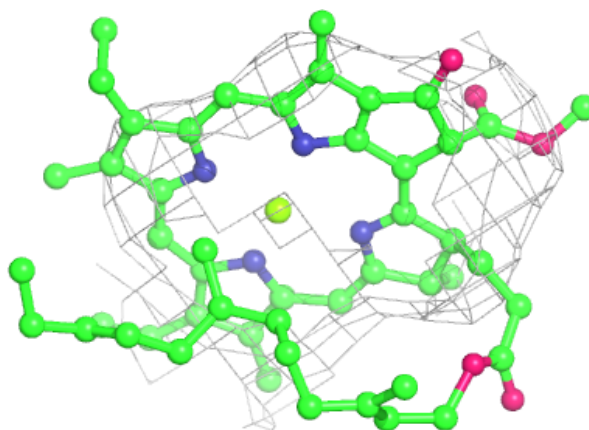


Electron density around BCR 1 4001:

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

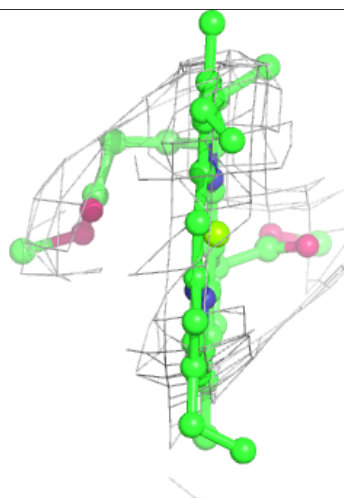
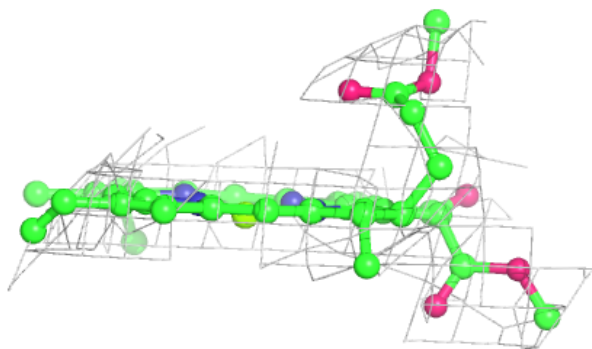
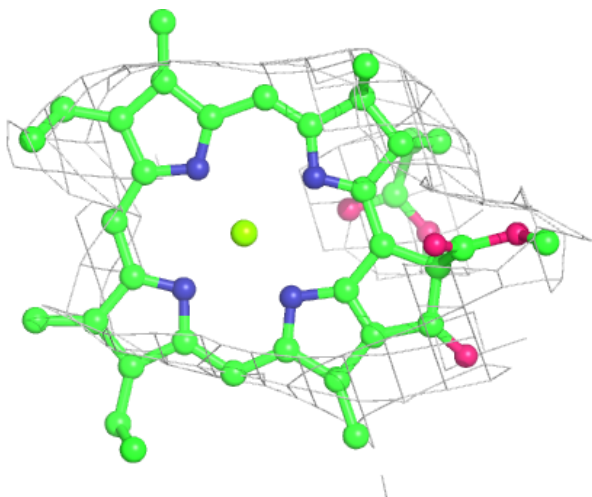
**Electron density around CLA b 1214:**

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



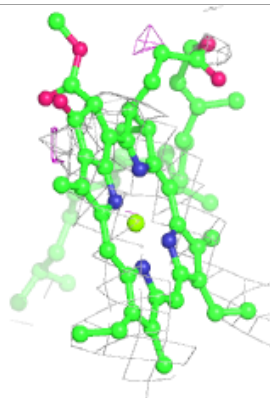
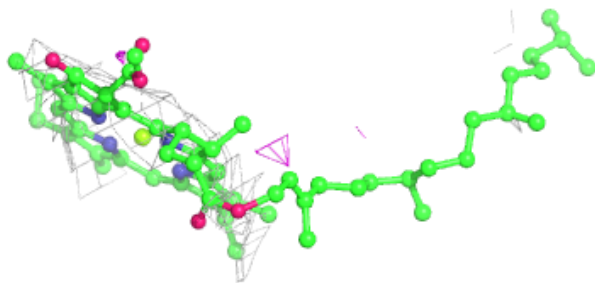
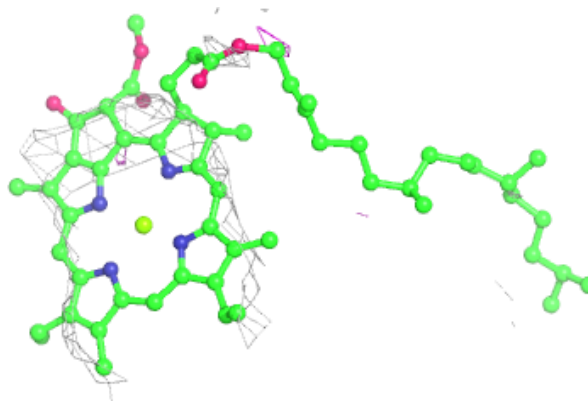
Electron density around CLA 1 1115:

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



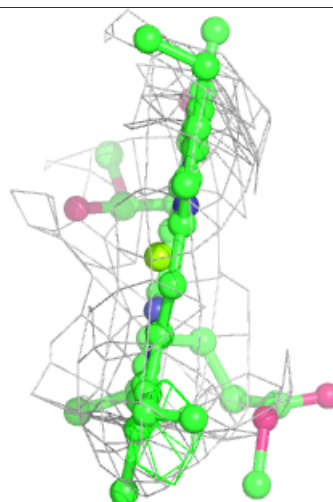
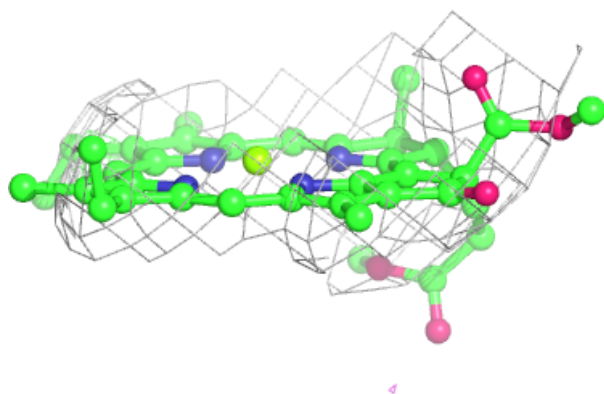
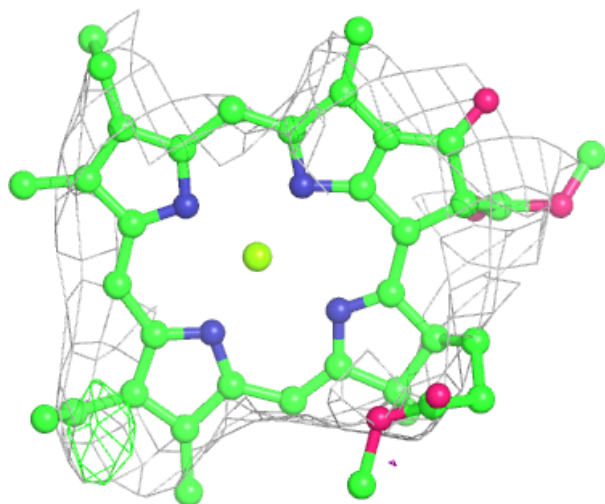
Electron density around CLA b 1013:

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



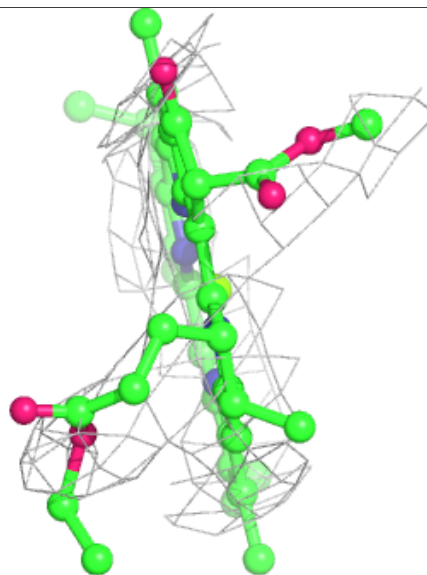
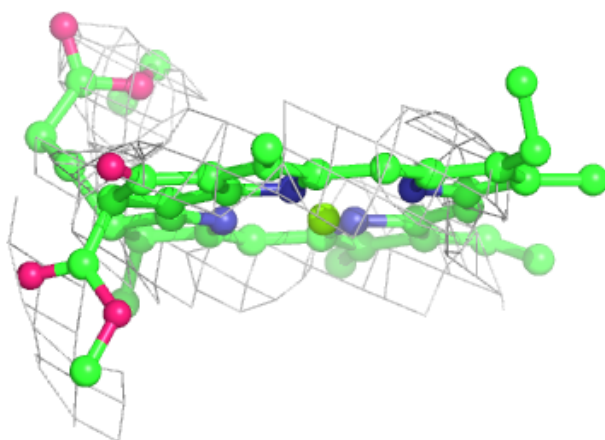
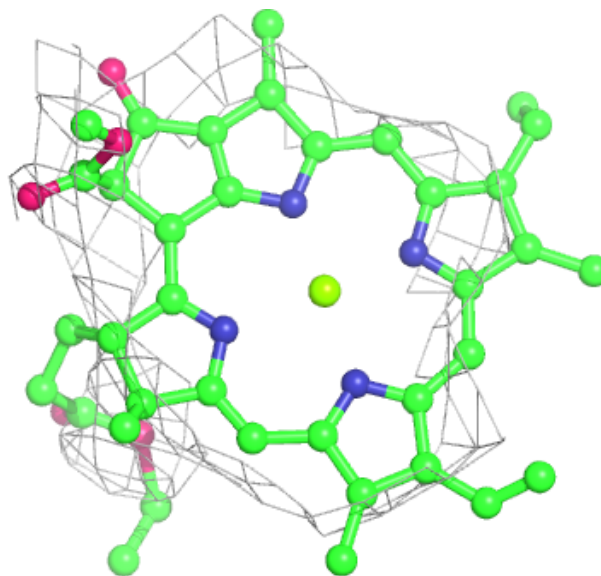
Electron density around CLA 1 1121:

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



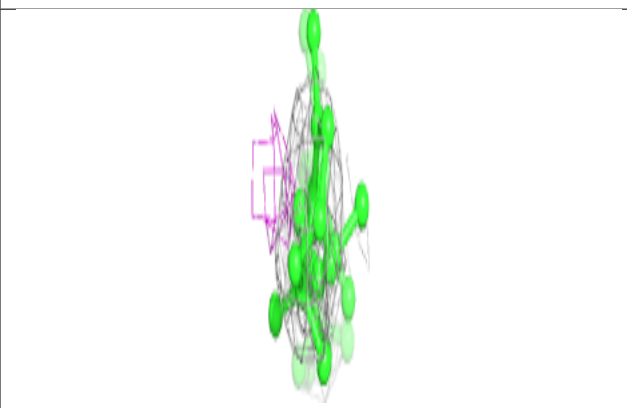
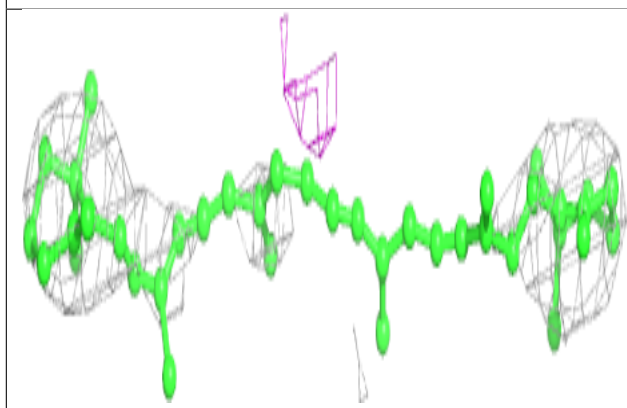
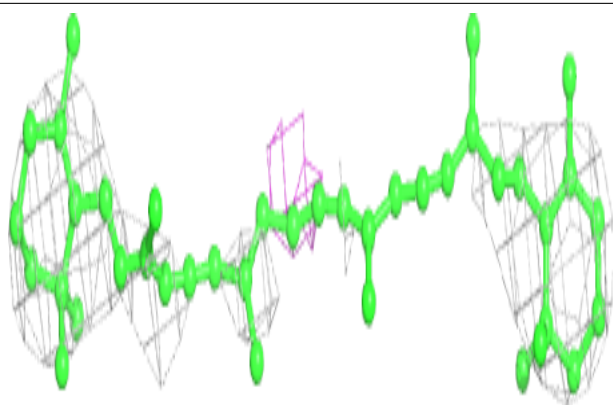
Electron density around CLA b 1217:

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



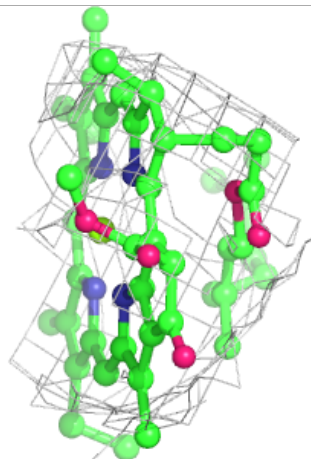
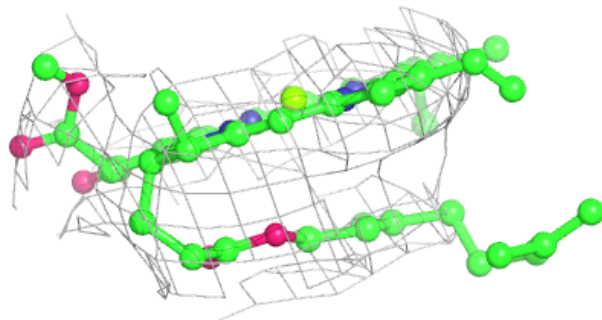
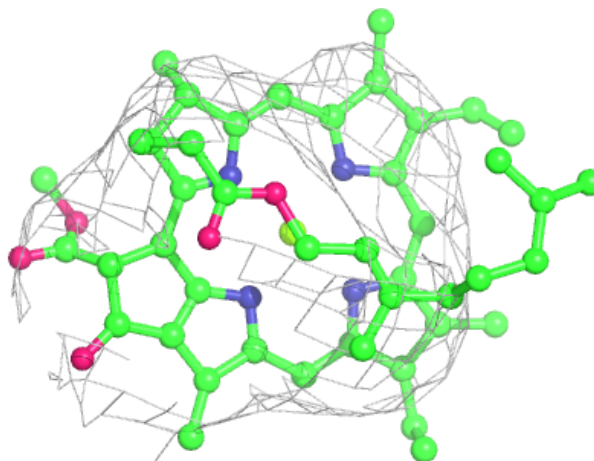
Electron density around BCR 8 4019:

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



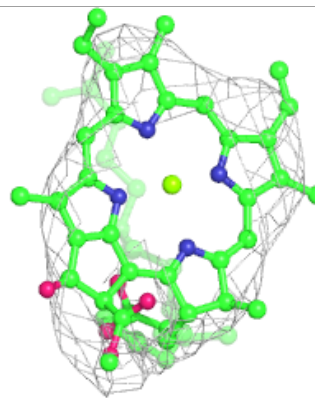
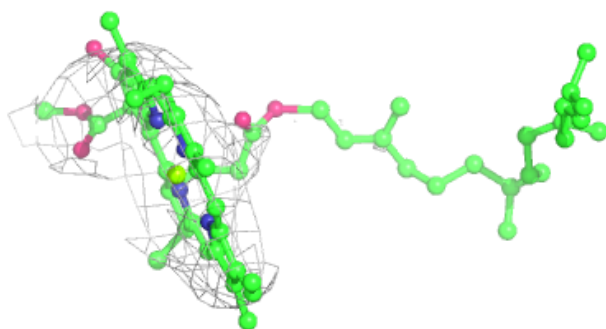
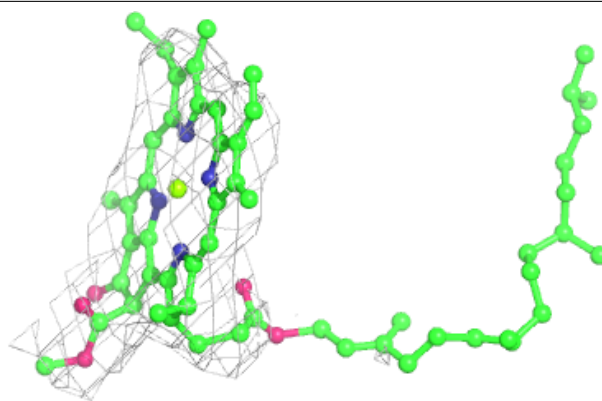
Electron density around CLA b 1205:

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

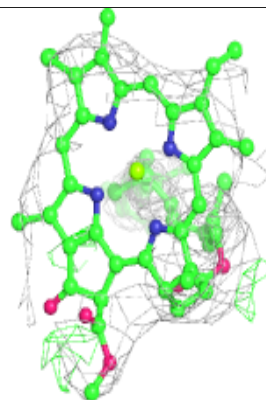
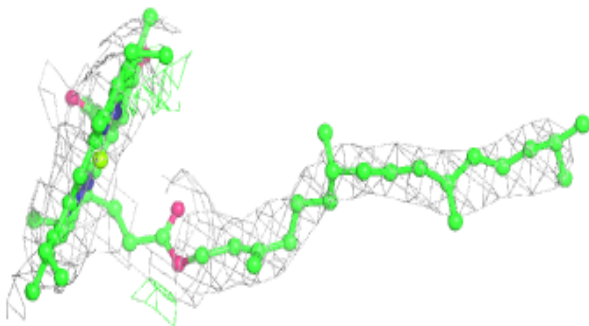
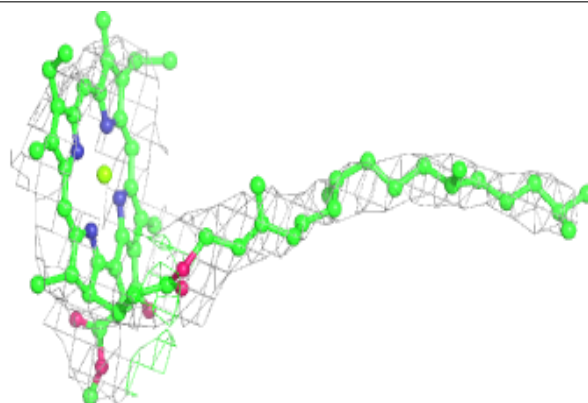


Electron density around CLA A 1140:

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

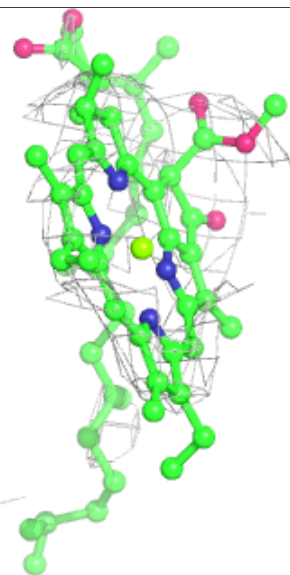
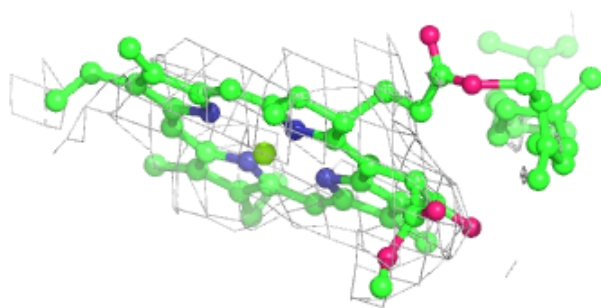
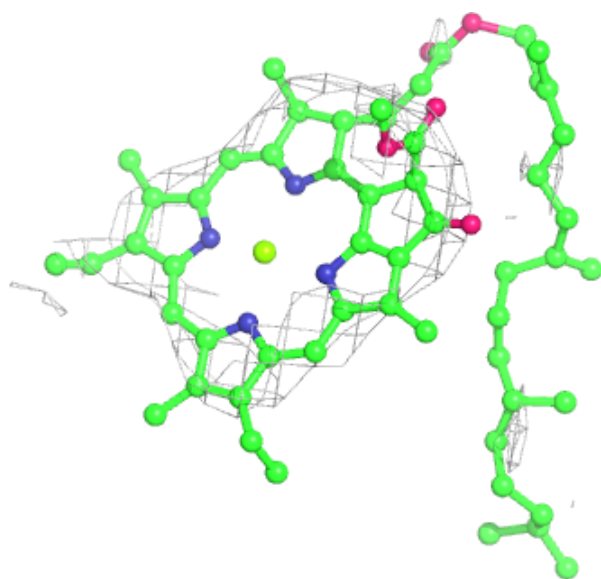
**Electron density around CLA 2 1225:**

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



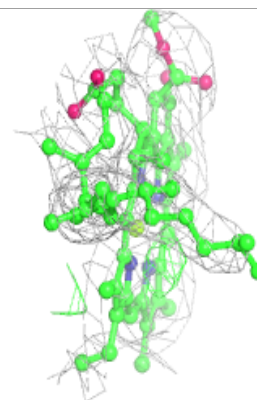
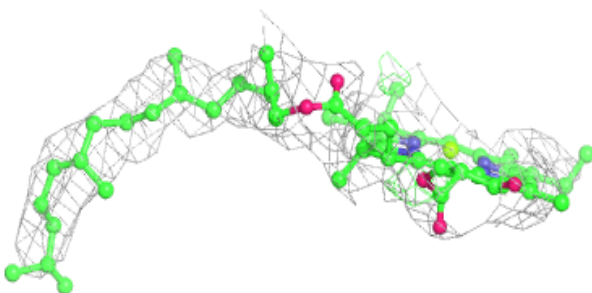
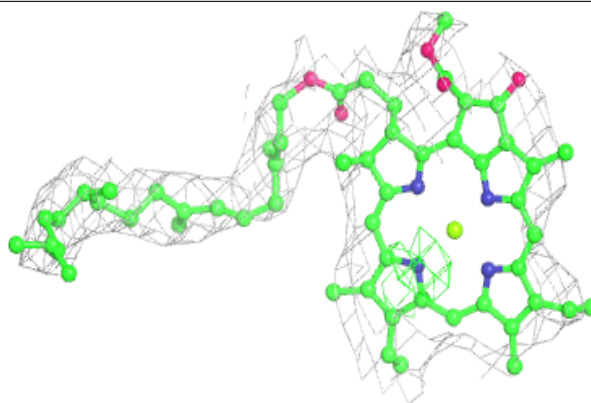
Electron density around CLA a 1123:

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

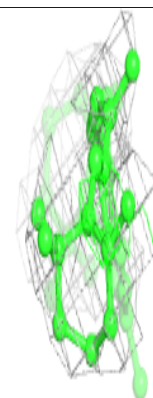
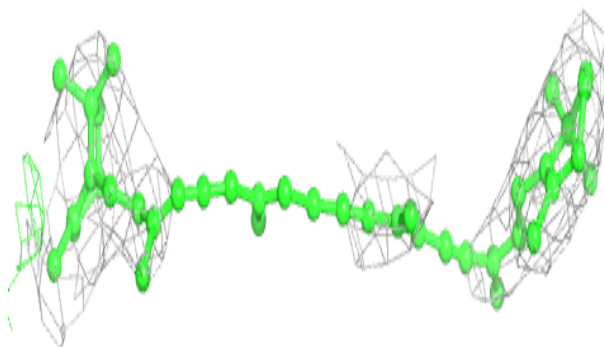
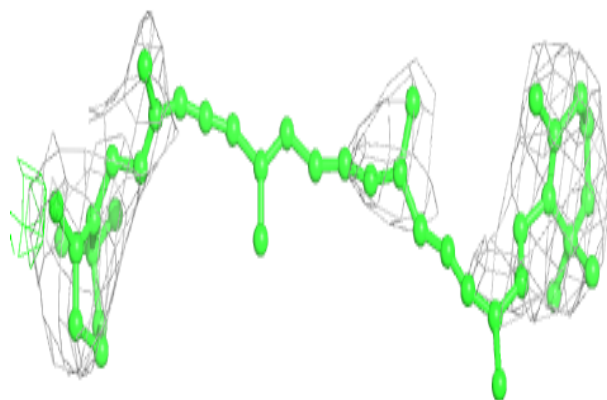


Electron density around CLA B 1023:

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

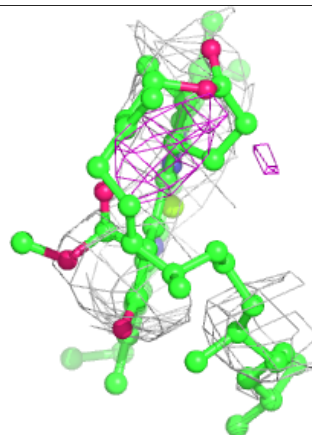
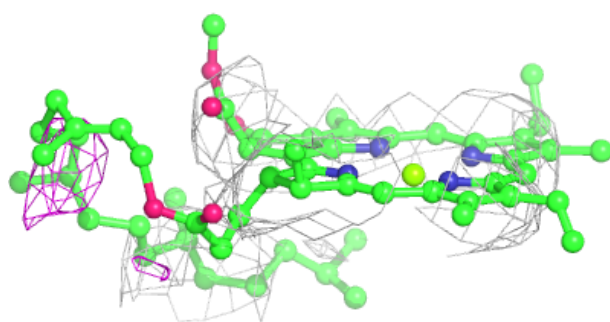
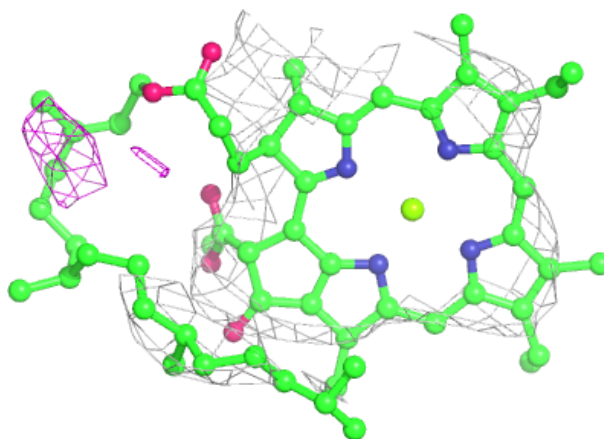
**Electron density around BCR B 4006:**

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

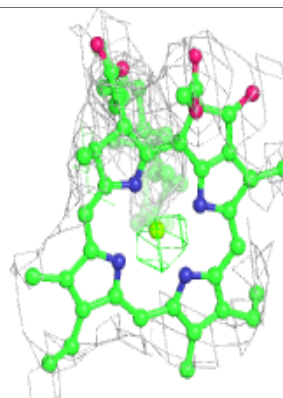
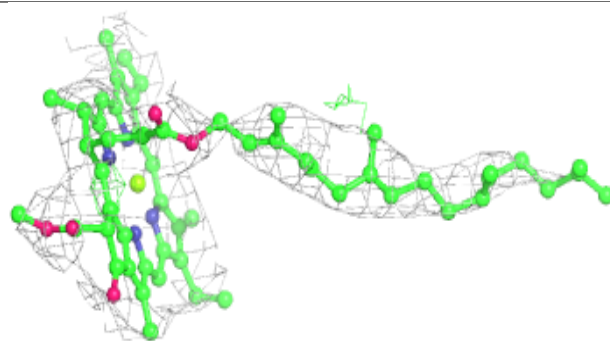
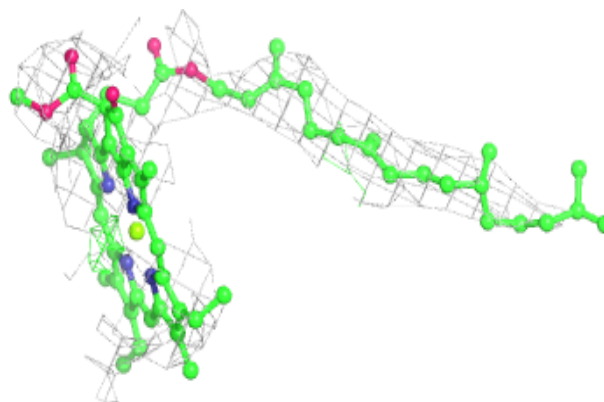


Electron density around CLA b 1202:

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

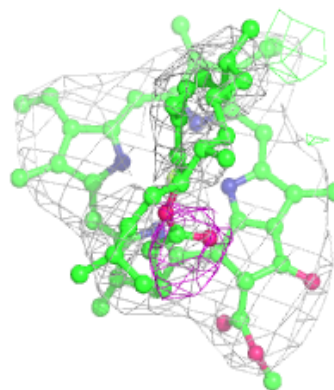
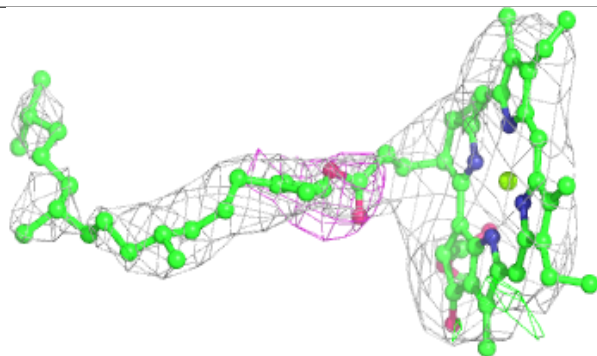
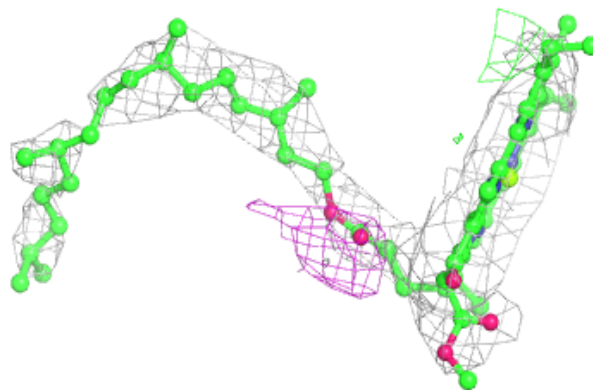
**Electron density around CLA 2 1226:**

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



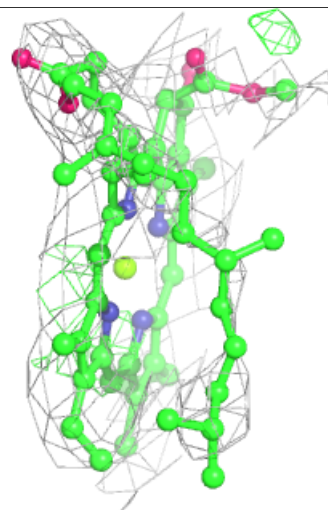
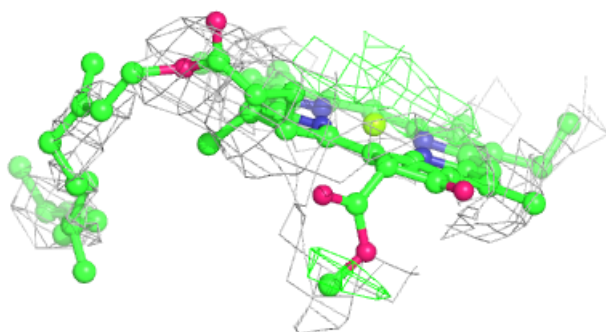
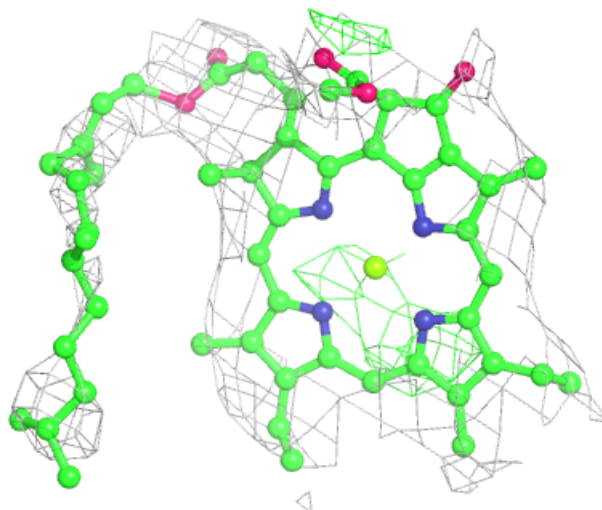
Electron density around CLA B 1238:

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



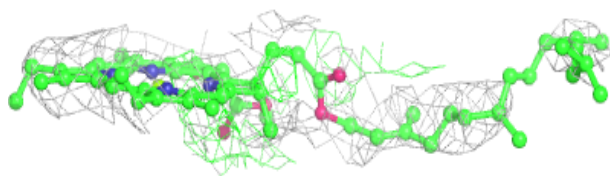
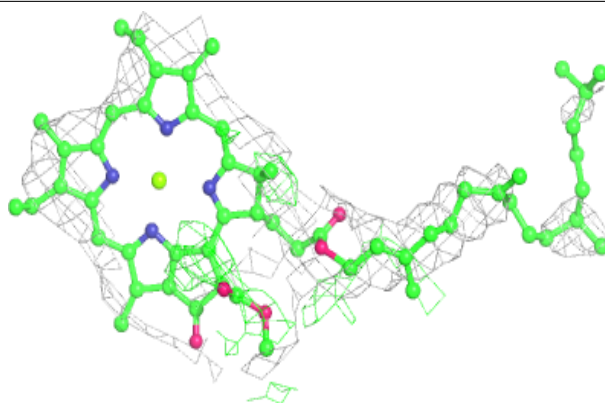
Electron density around CLA A 1111:

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

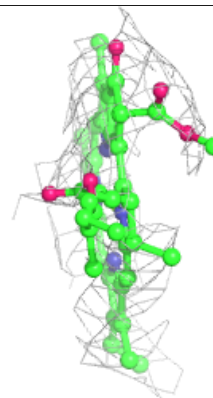
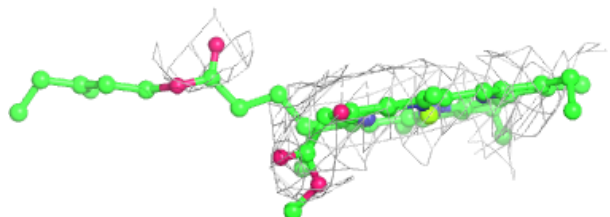
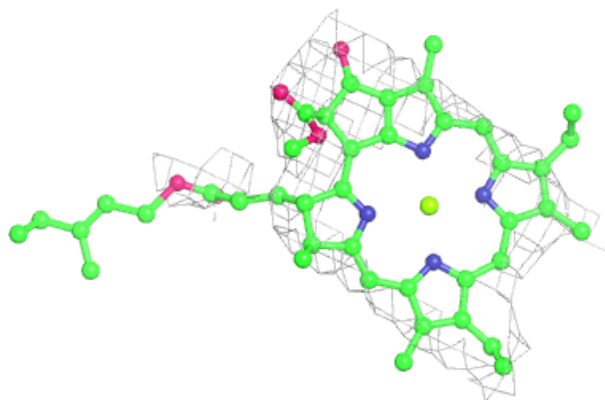


Electron density around CLA 1 1131:

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

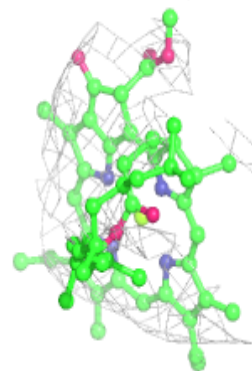
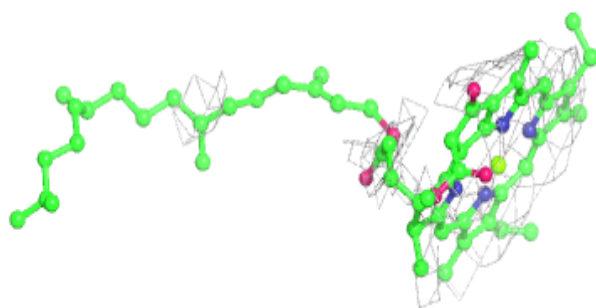
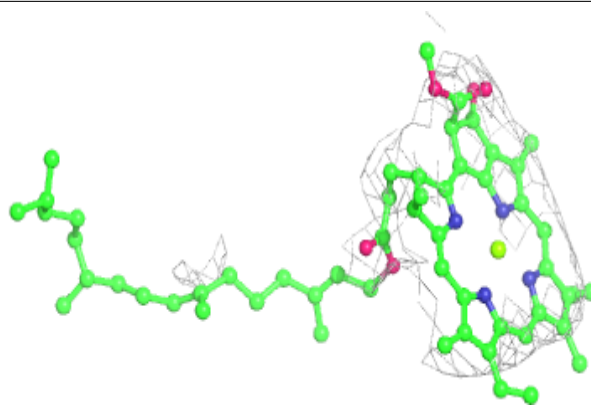
**Electron density around CLA a 1135:**

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

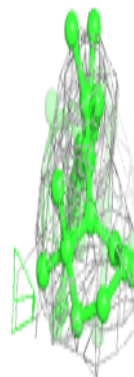
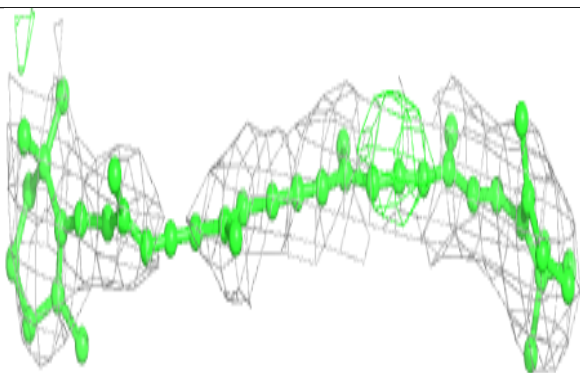
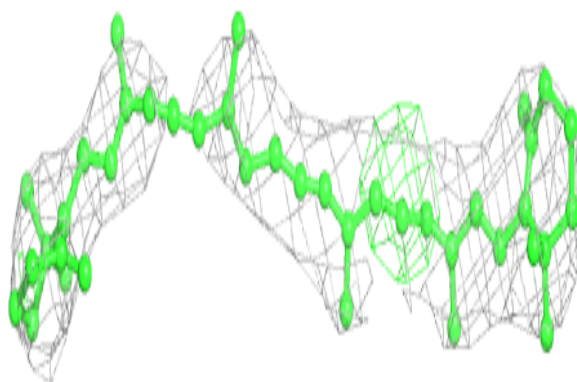


Electron density around CLA 1 1119:

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

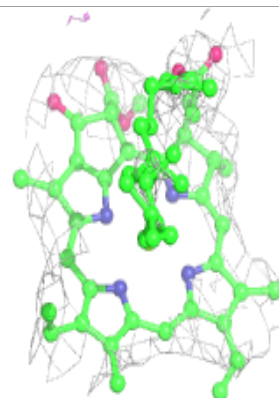
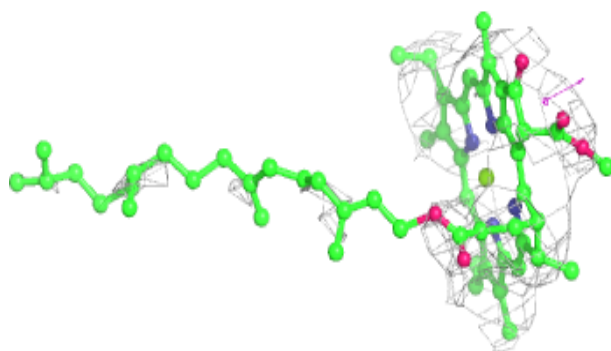
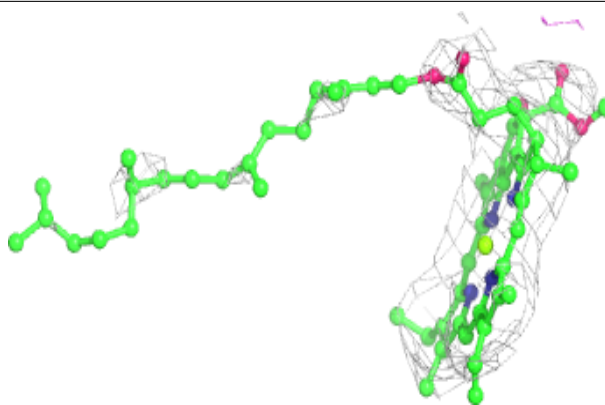
**Electron density around BCR B 4017:**

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



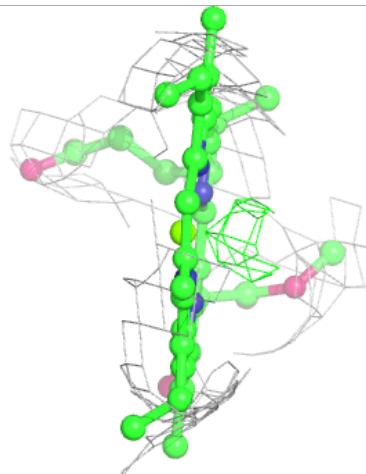
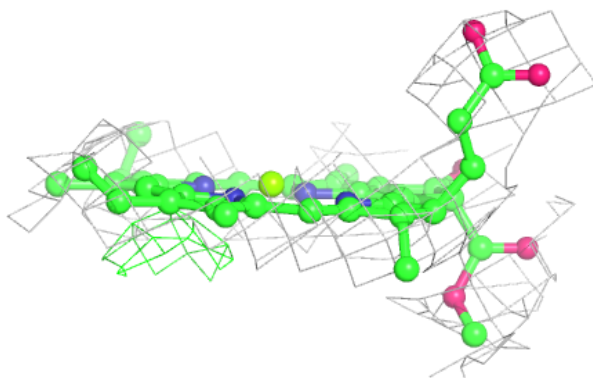
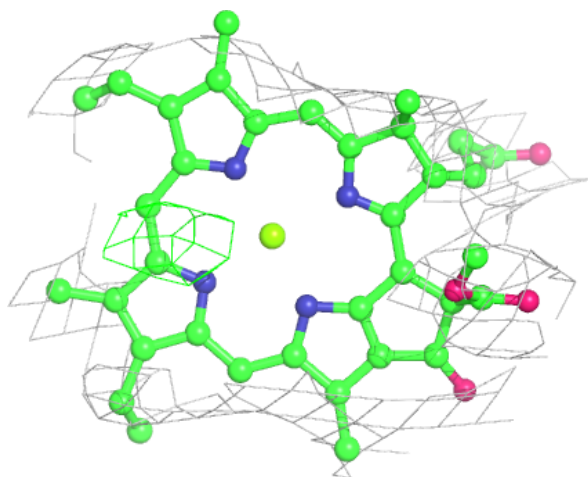
Electron density around CLA B 1226:

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



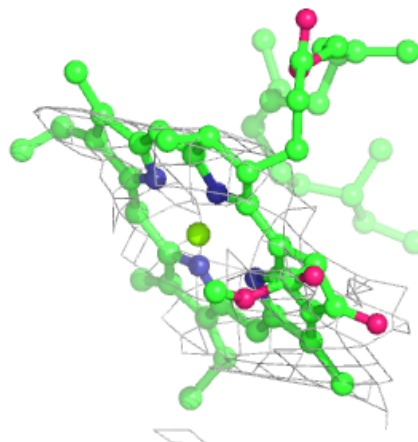
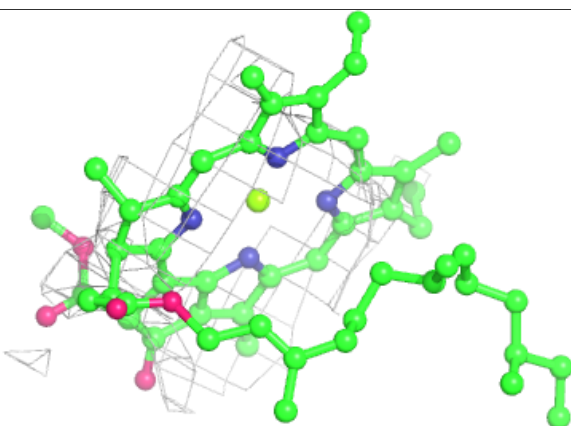
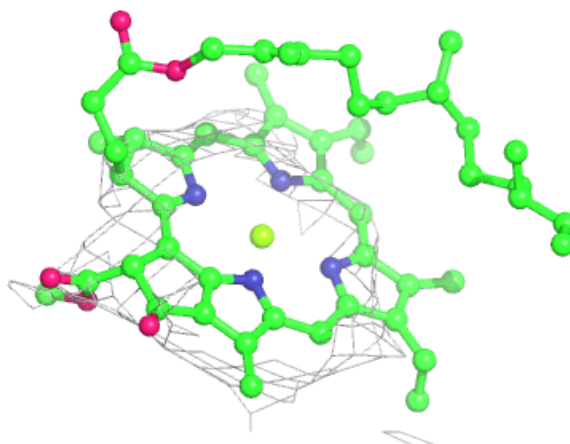
Electron density around CLA A 1112:

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



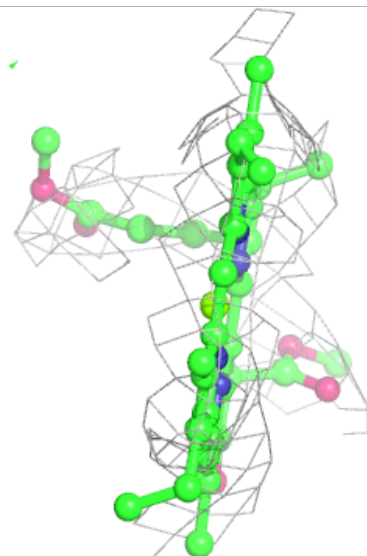
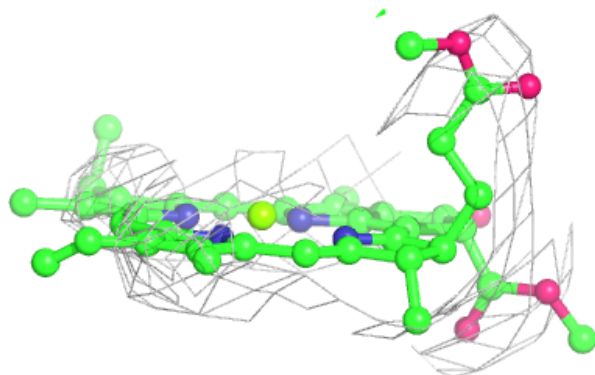
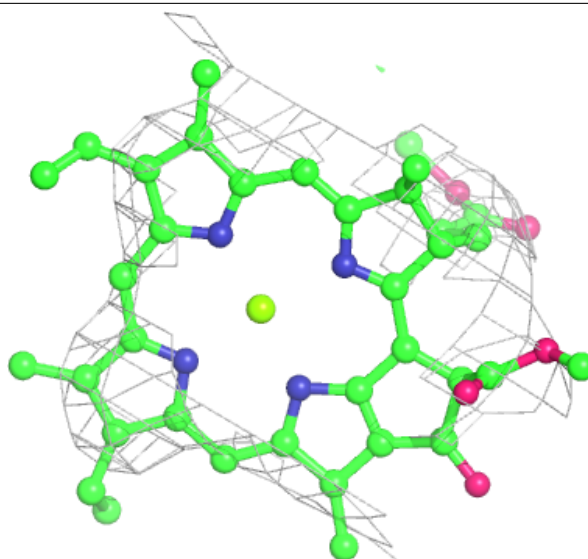
Electron density around CLA 1 1118:

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



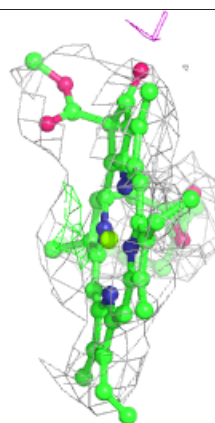
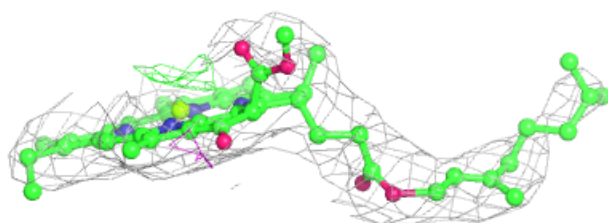
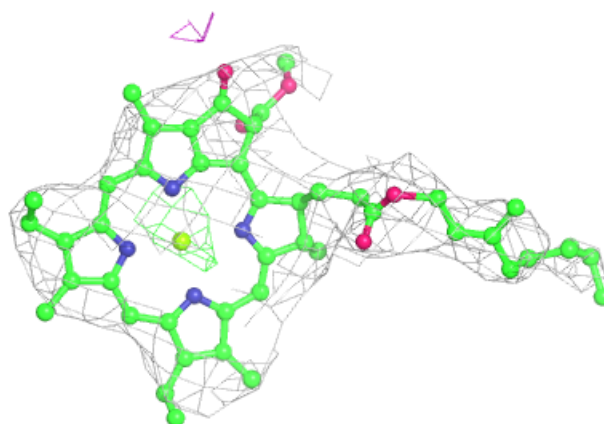
Electron density around CLA a 1133:

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

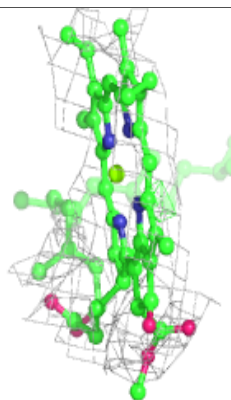
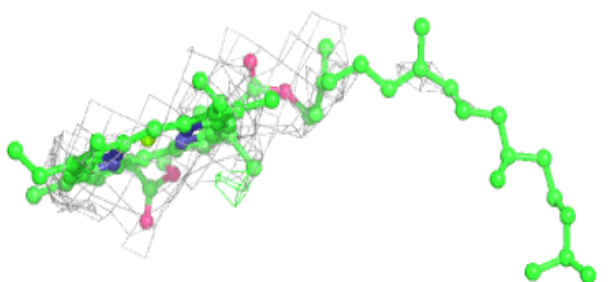
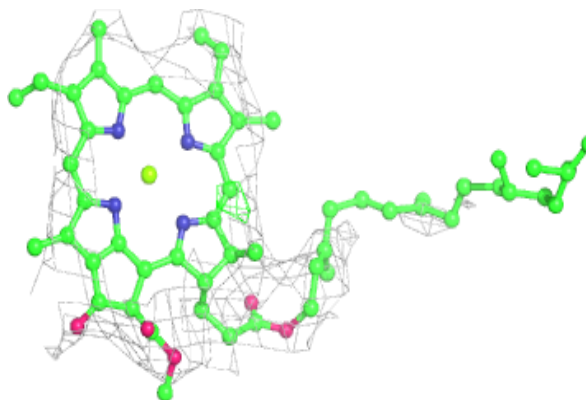


Electron density around CLA A 1124:

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

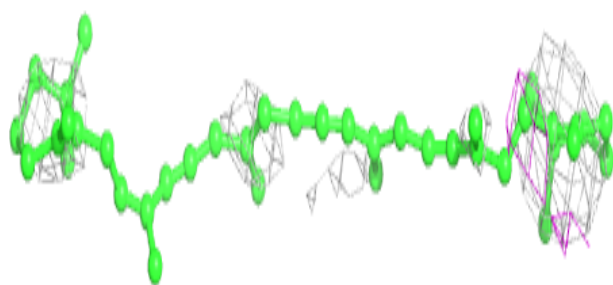
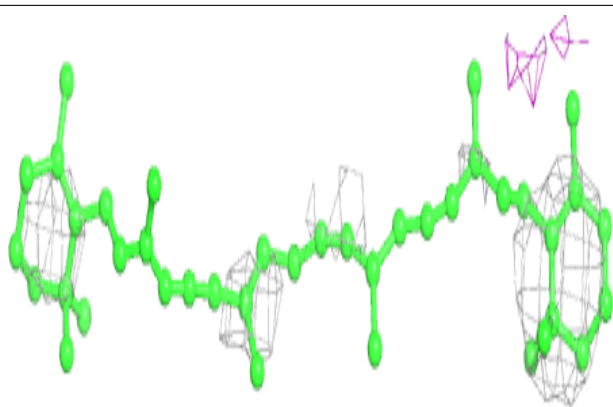
**Electron density around CLA 2 1023:**

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



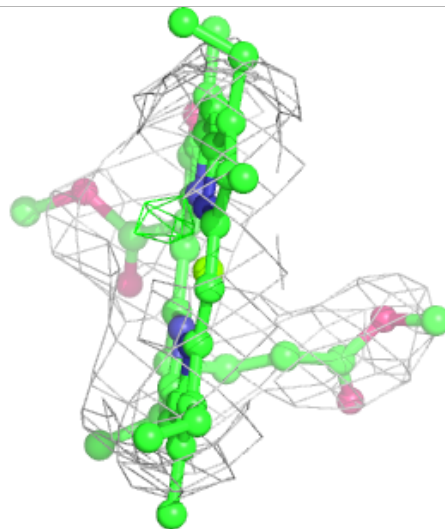
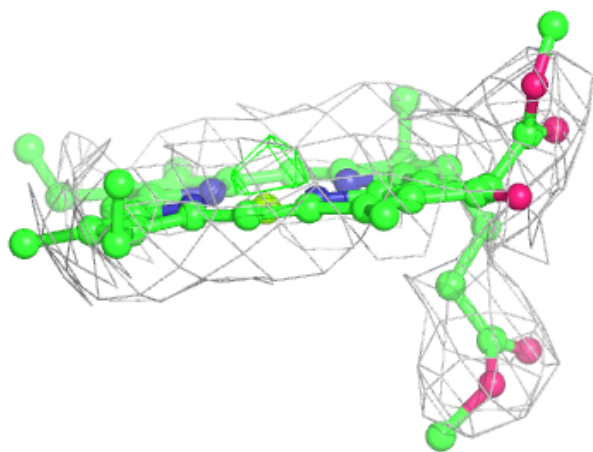
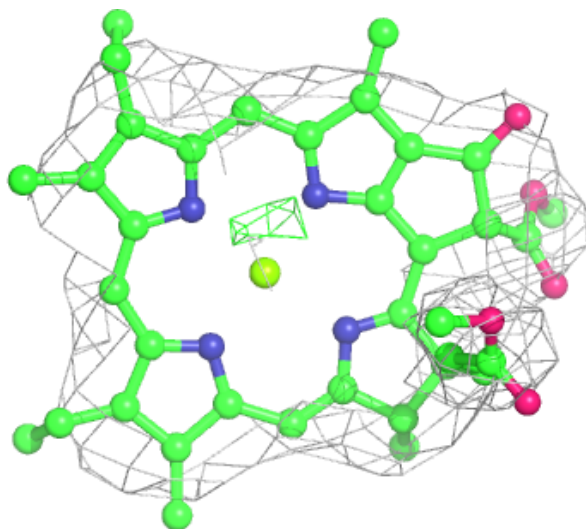
Electron density around BCR 1 4019:

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



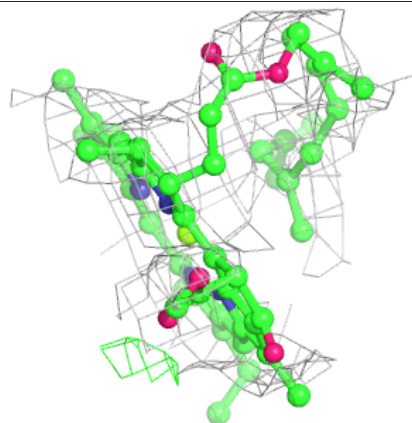
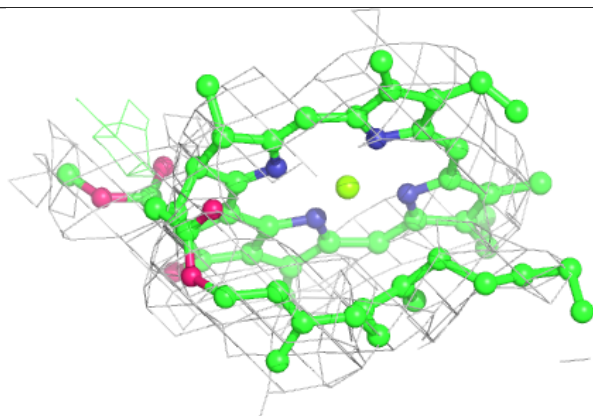
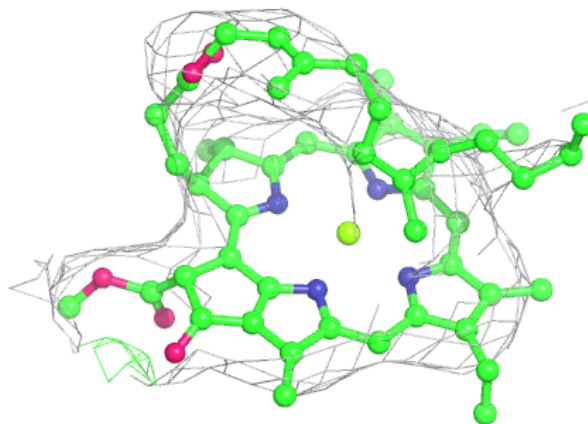
Electron density around CLA 2 1211:

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



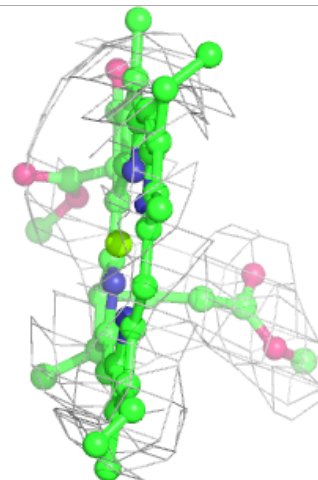
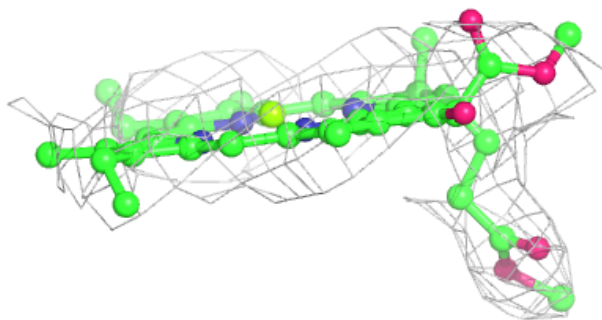
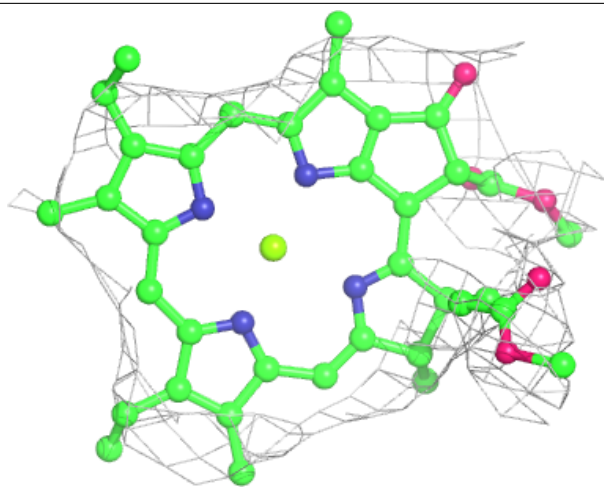
Electron density around CLA B 1214:

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



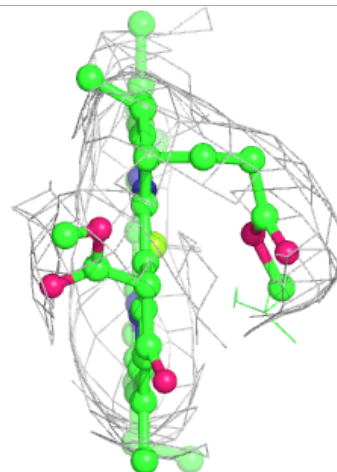
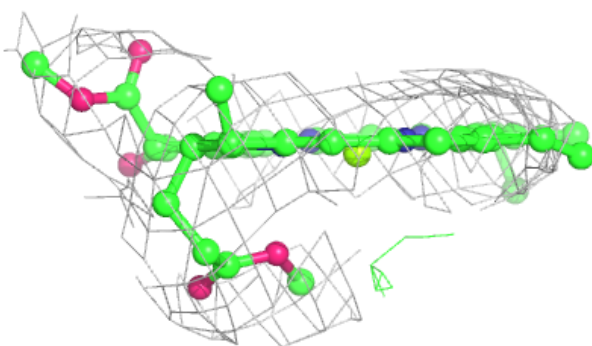
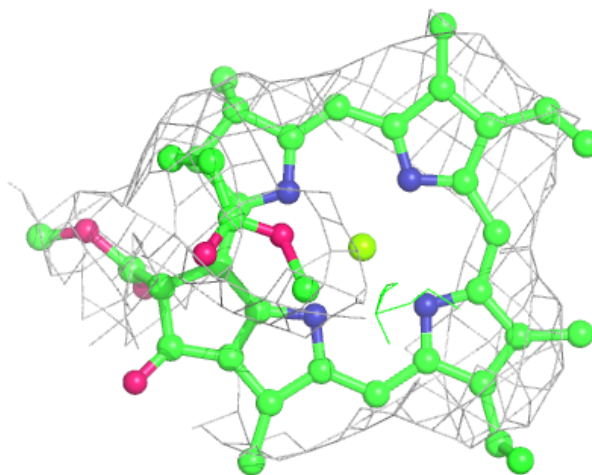
Electron density around CLA B 1220:

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



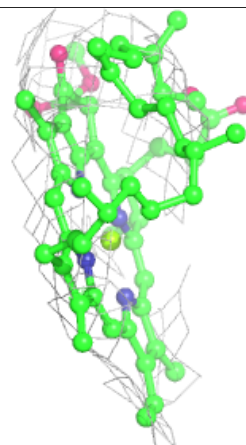
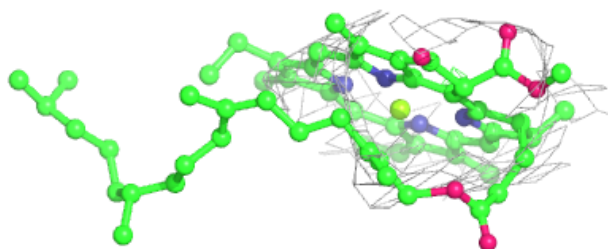
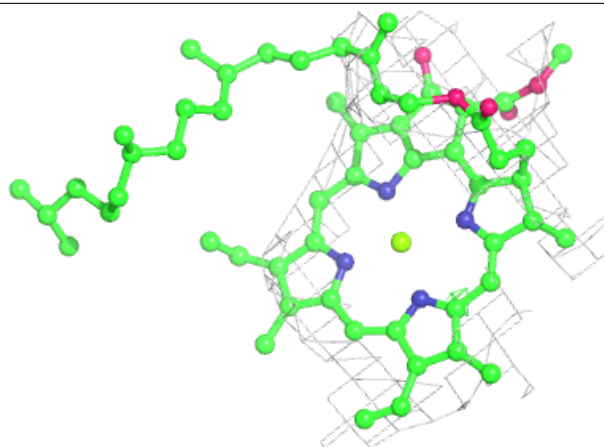
Electron density around CLA A 1136:

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



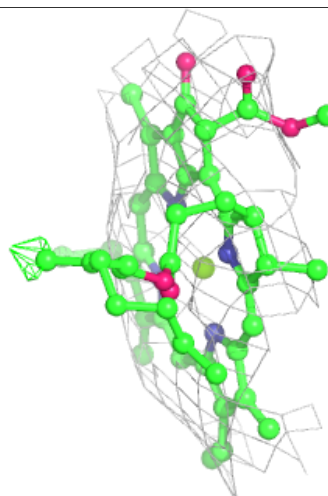
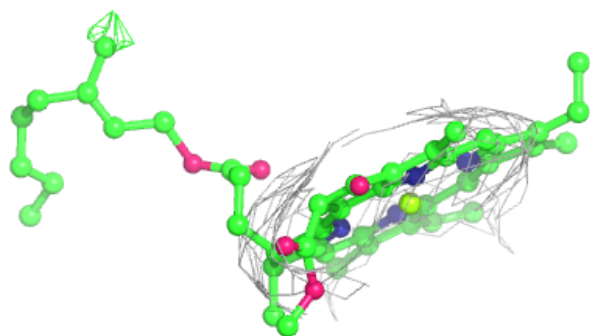
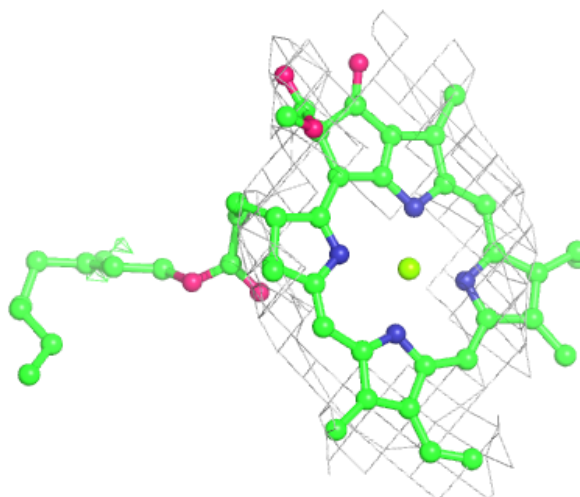
Electron density around CLA a 1127:

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



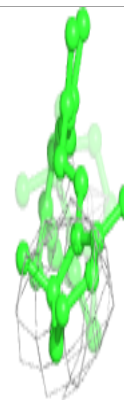
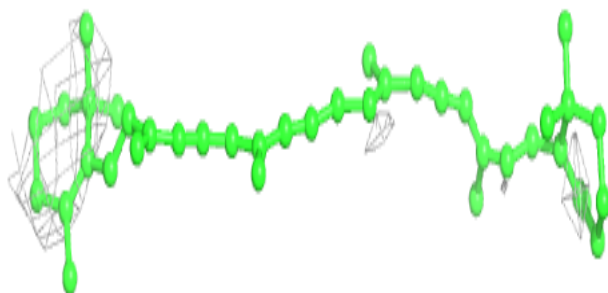
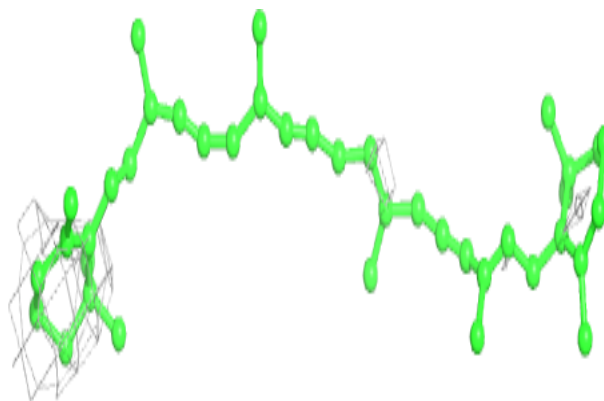
Electron density around CLA 1 1110:

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

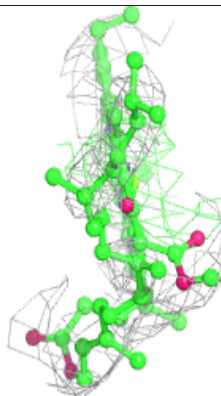
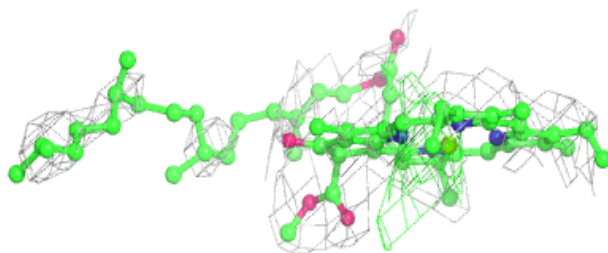
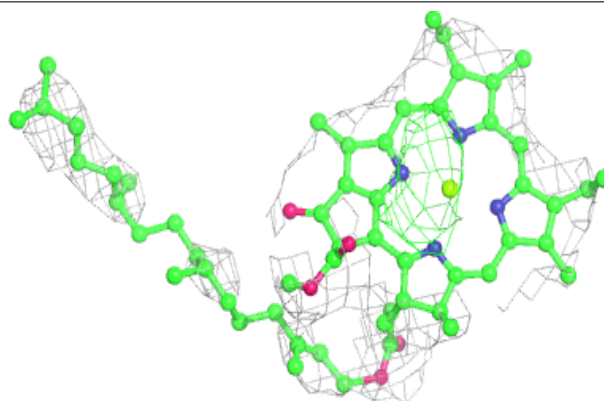


Electron density around BCR F 4013:

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

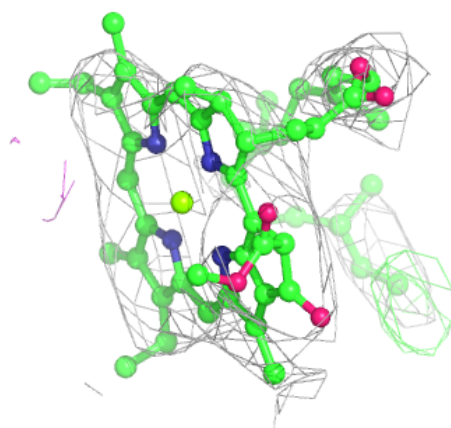
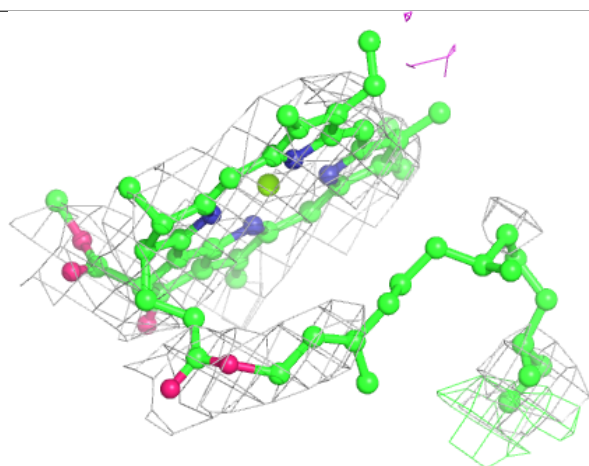
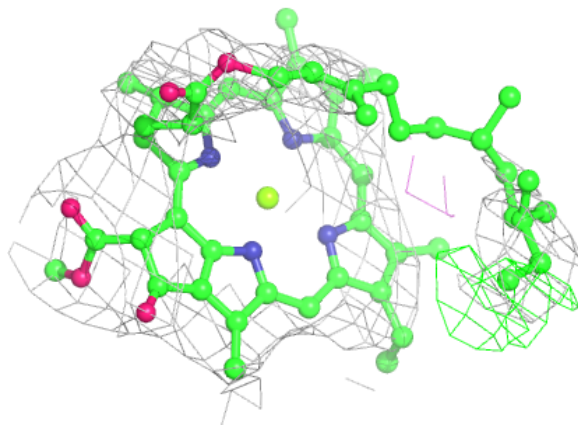
**Electron density around CLA 1 1503:**

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



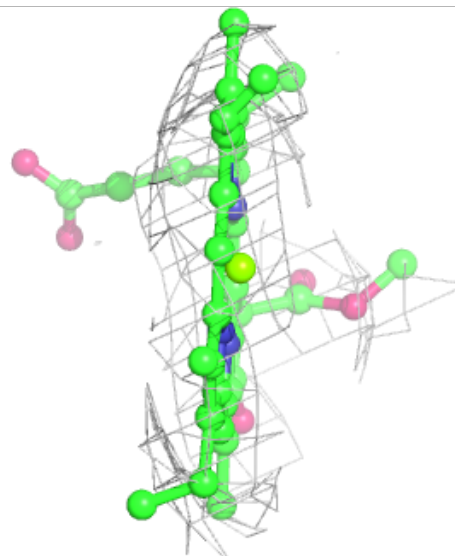
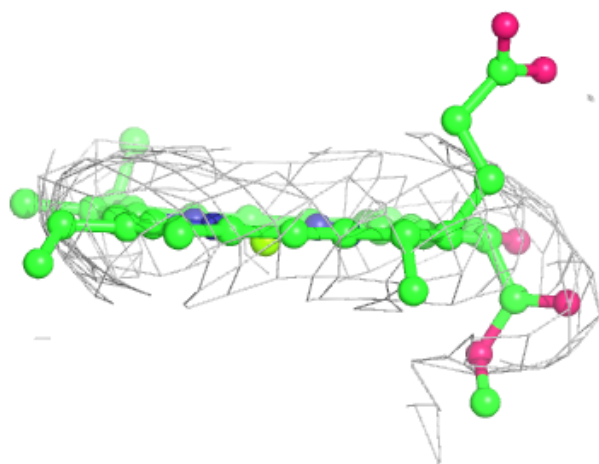
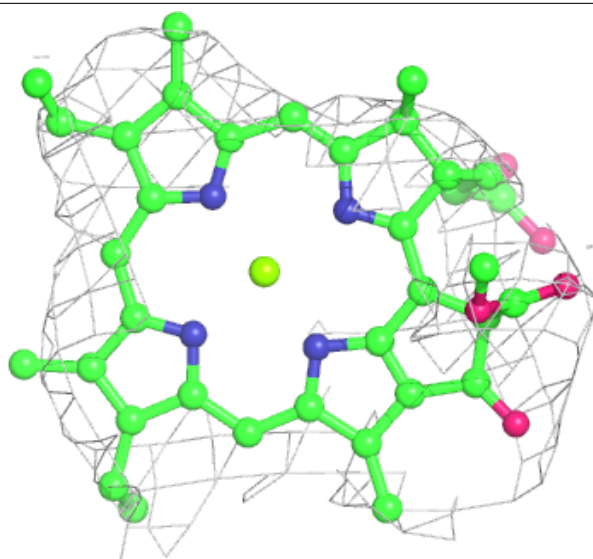
Electron density around CLA A 1118:

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



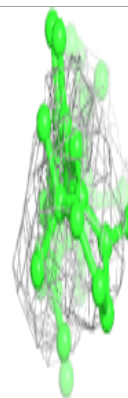
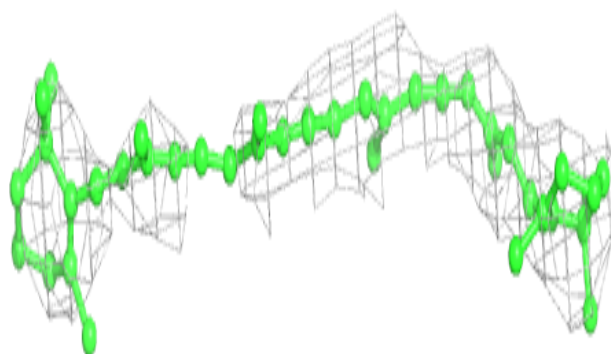
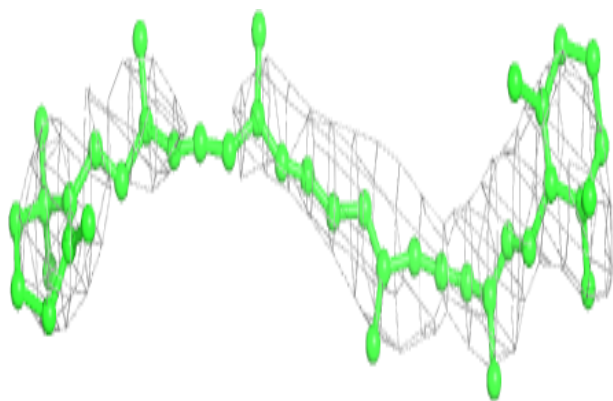
Electron density around CLA B 1218:

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

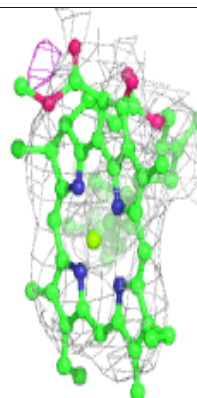
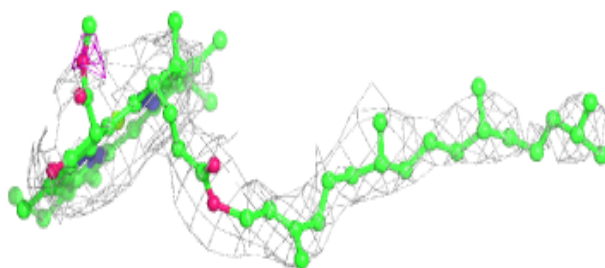
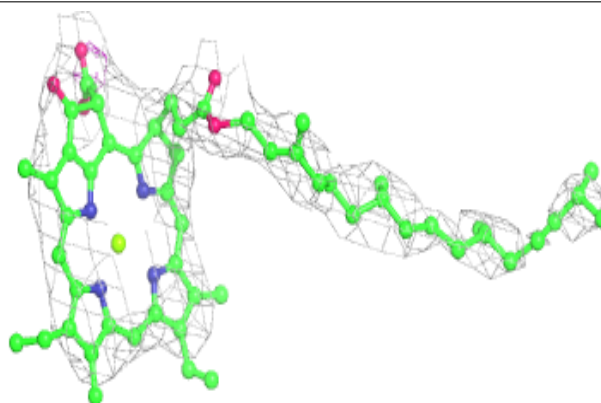


Electron density around BCR 8 4022:

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

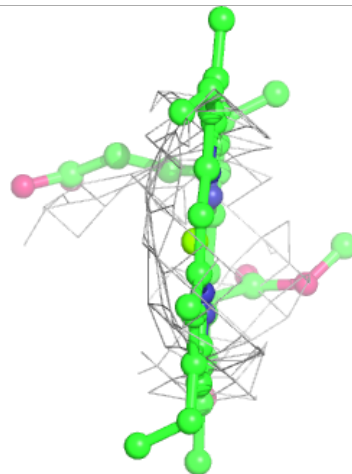
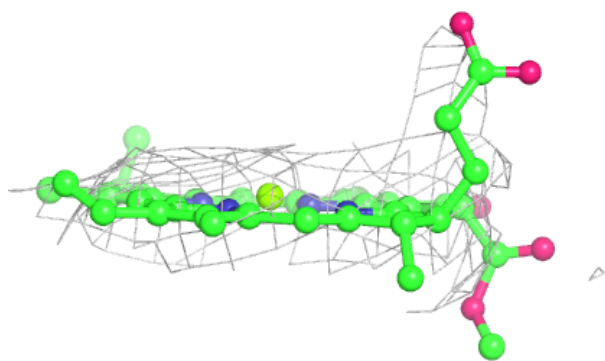
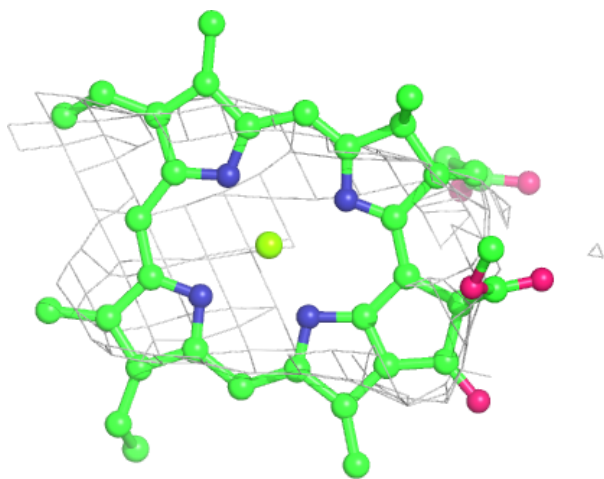
**Electron density around CLA a 1132:**

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



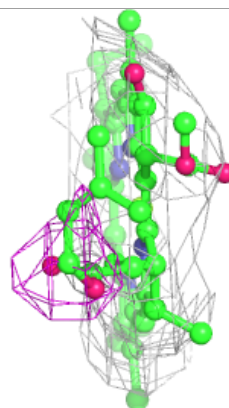
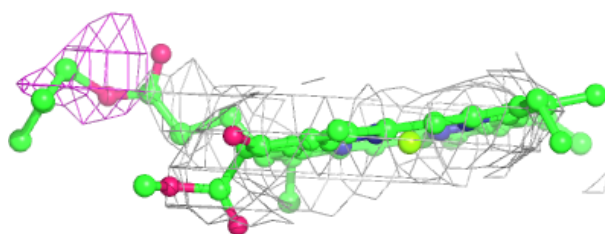
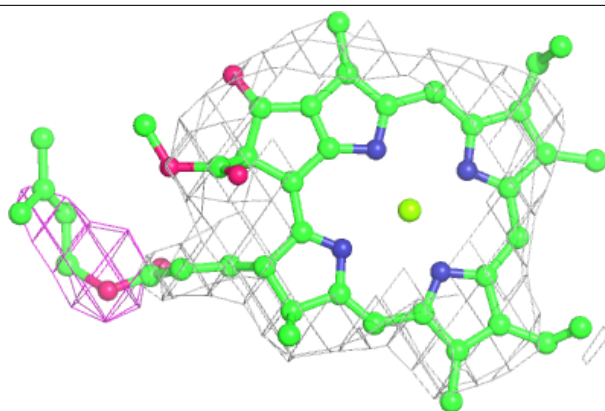
Electron density around CLA 1 1112:

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

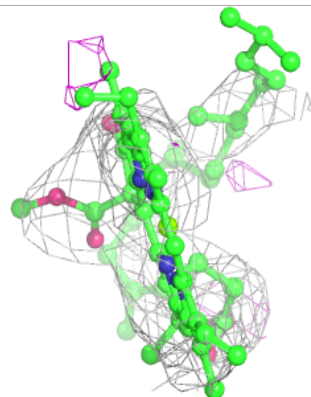
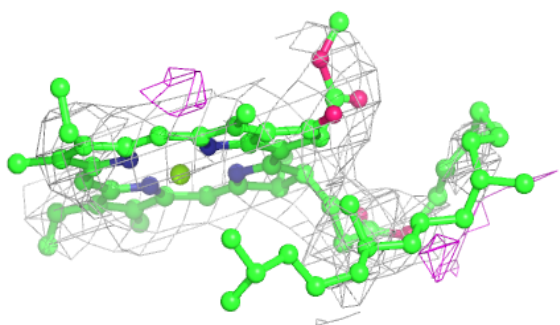
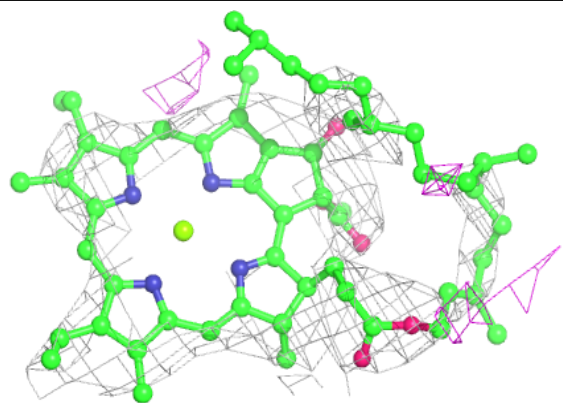


Electron density around CLA A 1139:

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

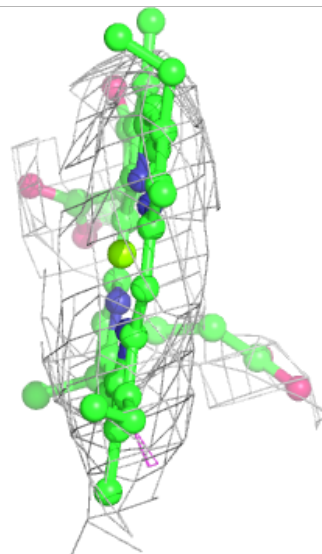
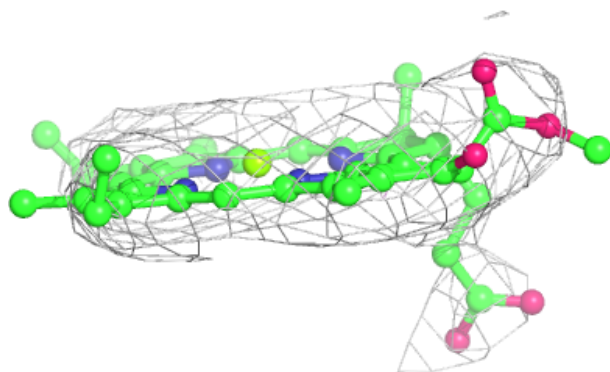
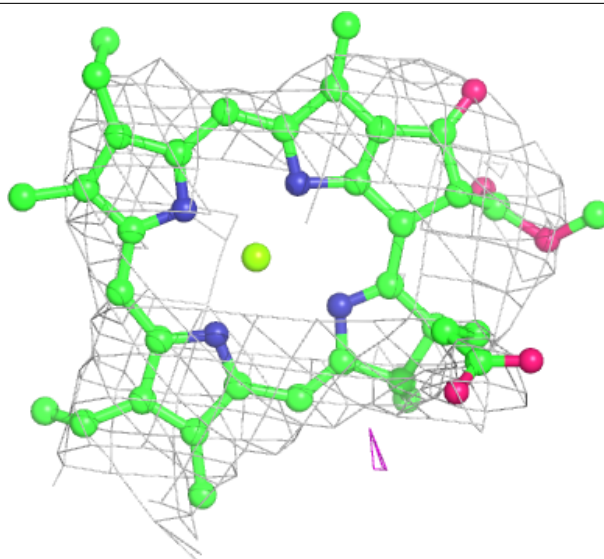
**Electron density around CLA 2 1202:**

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



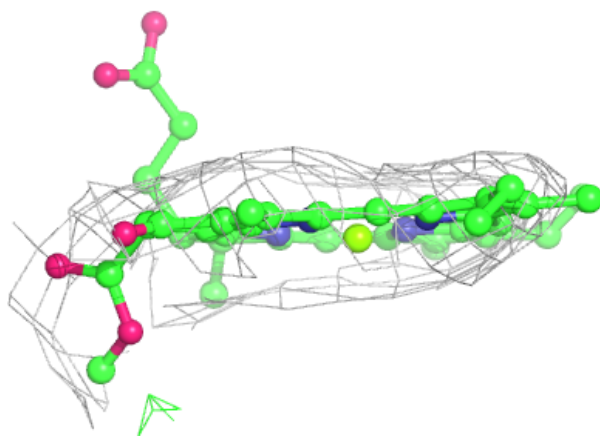
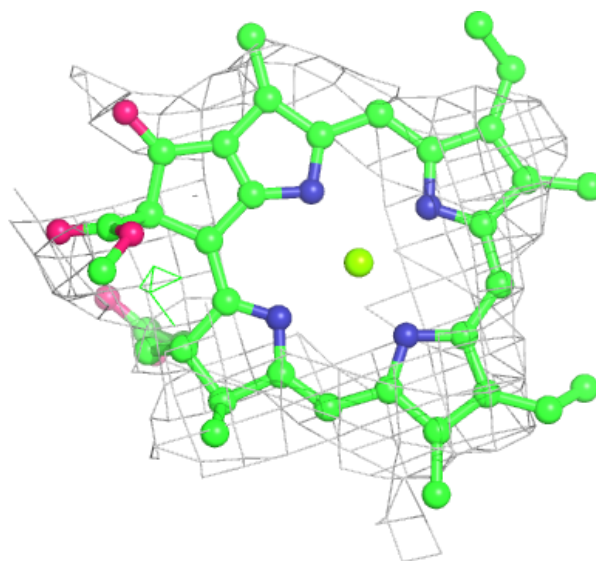
Electron density around CLA B 1208:

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



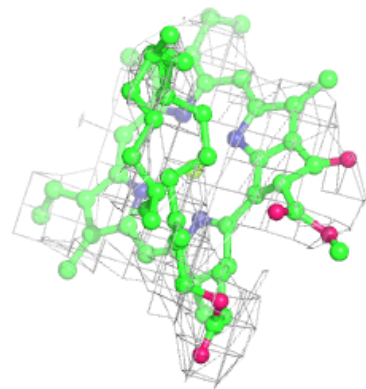
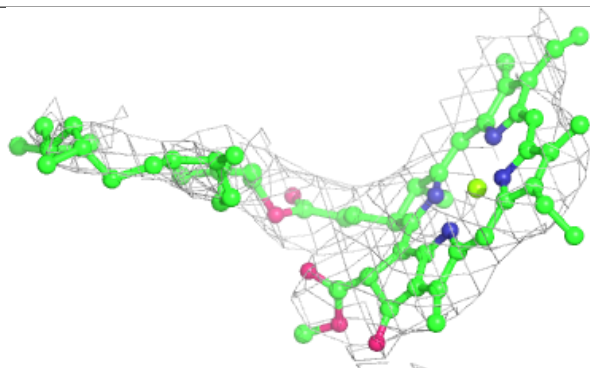
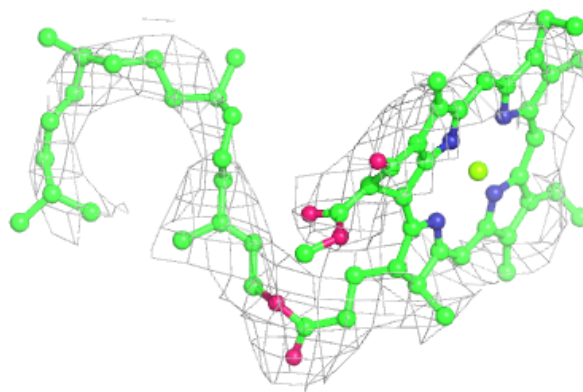
Electron density around CLA B 1227:

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



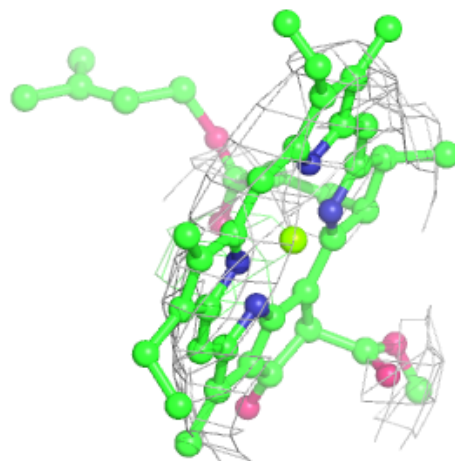
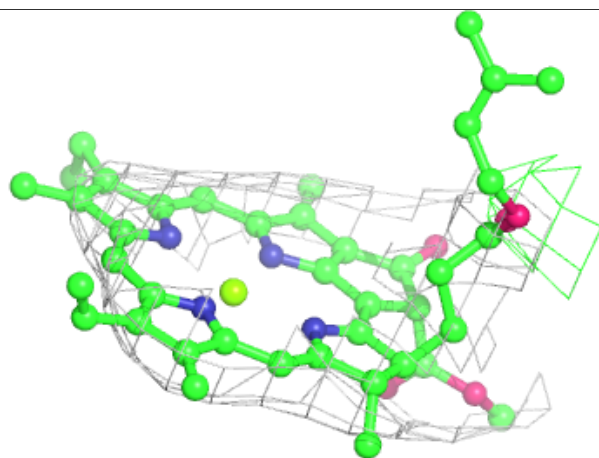
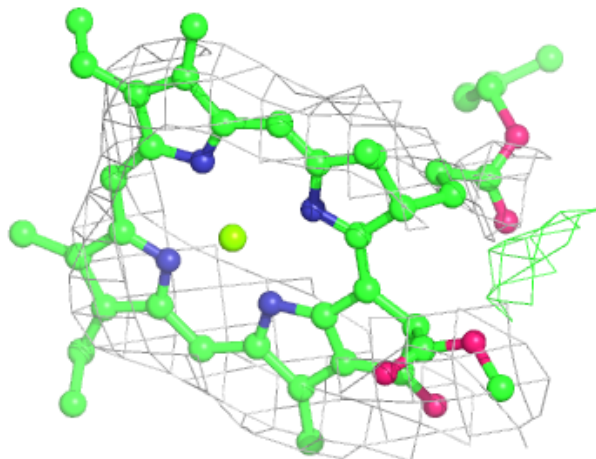
Electron density around CLA 1 1011:

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



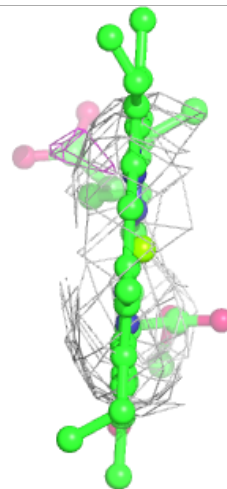
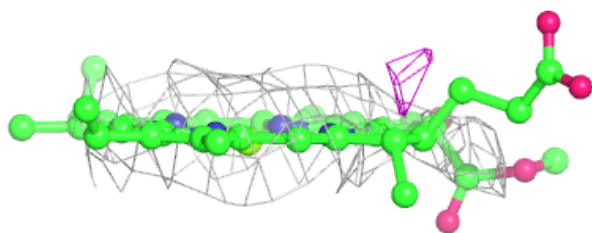
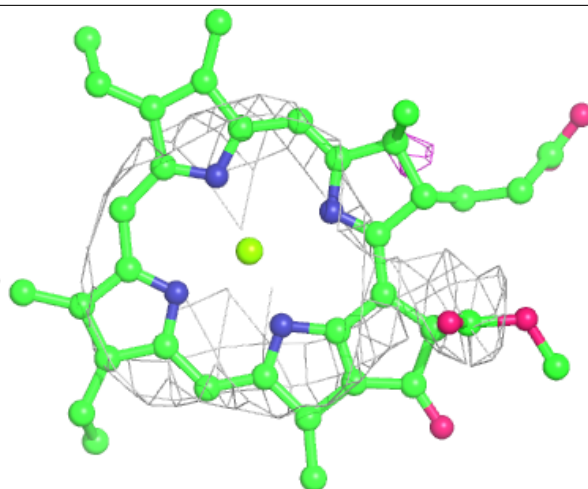
Electron density around CLA B 1228:

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



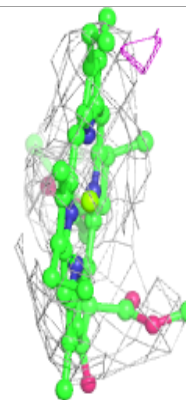
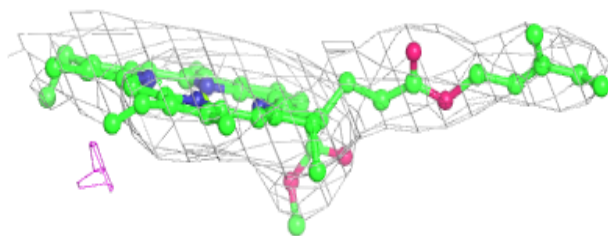
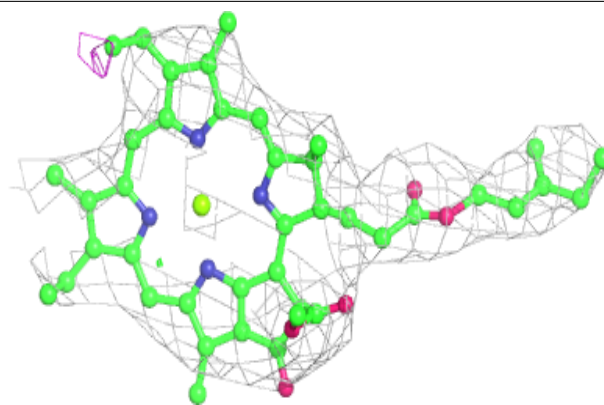
Electron density around CLA B 1240:

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



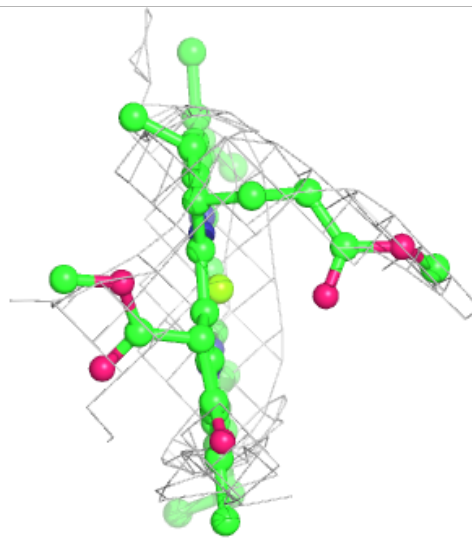
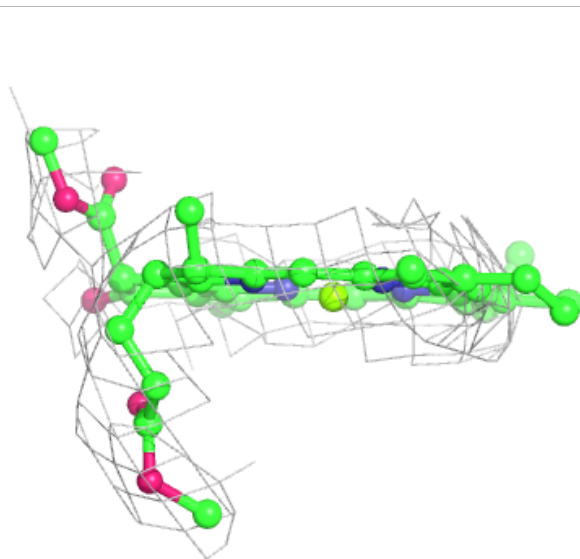
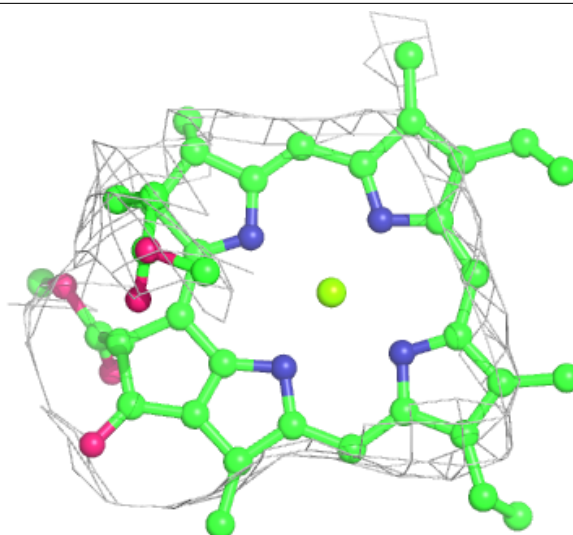
Electron density around CLA A 1135:

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



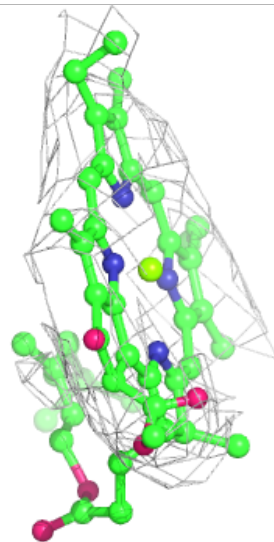
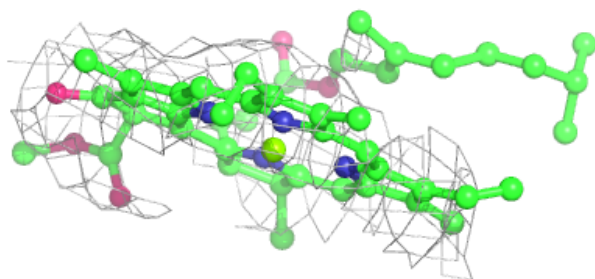
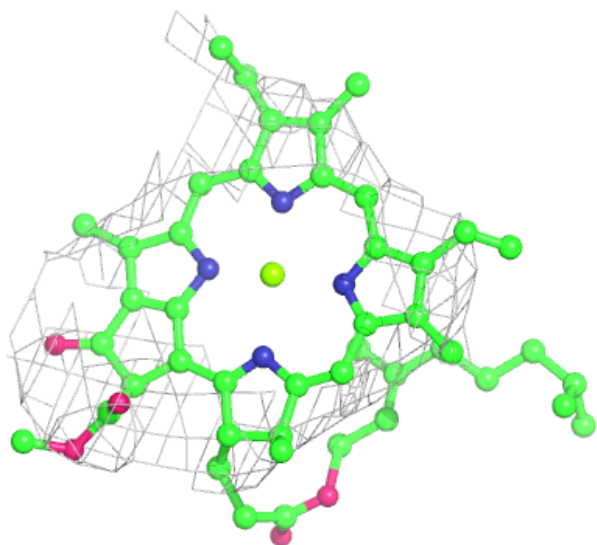
Electron density around CLA 1 1134:

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



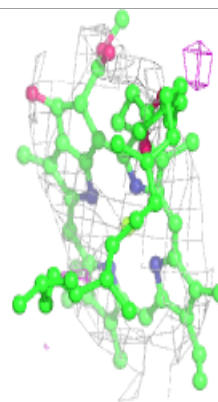
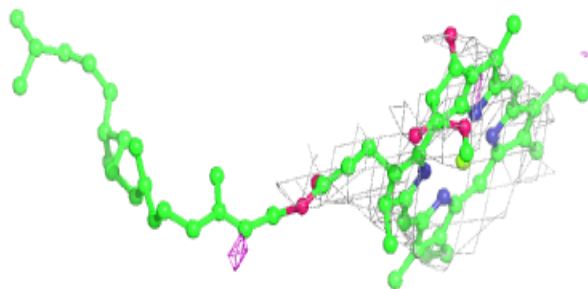
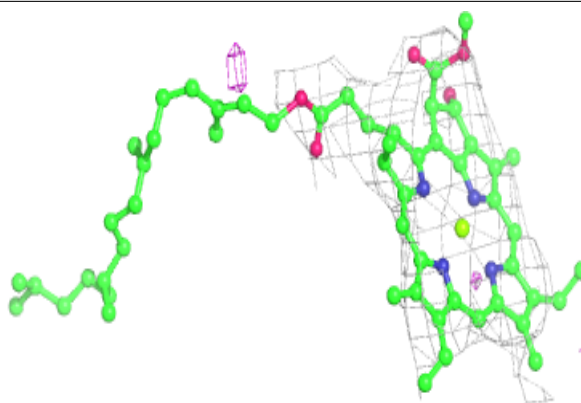
Electron density around CLA B 1219:

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

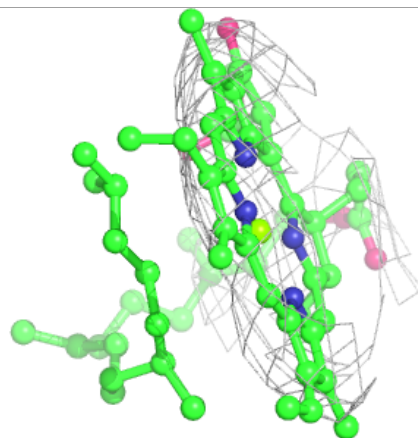
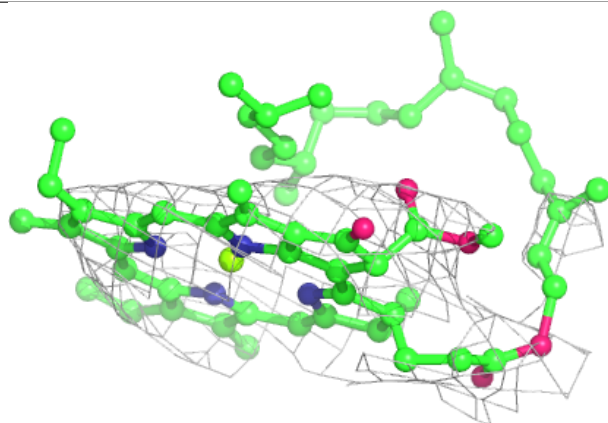
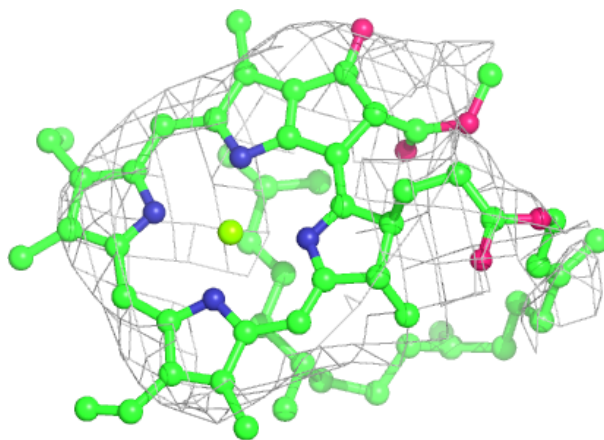


Electron density around CLA 1 1012:

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

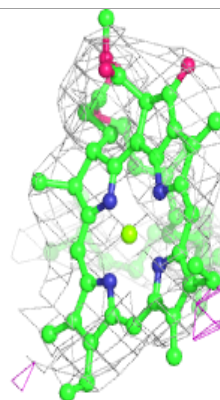
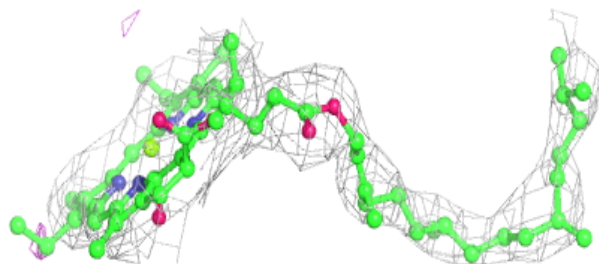
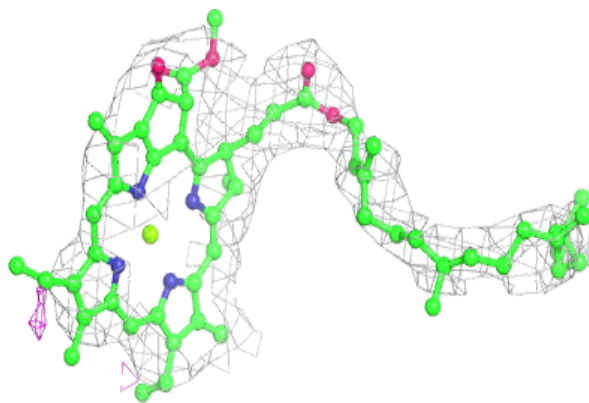
**Electron density around CLA 1 1104:**

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



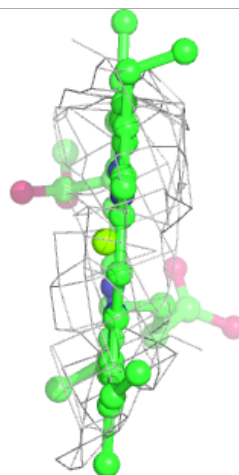
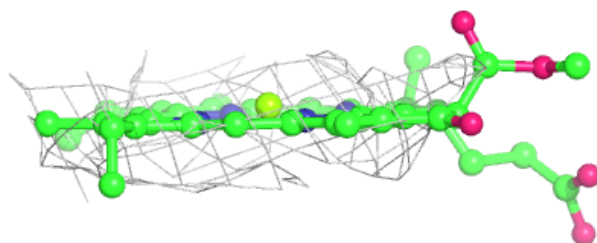
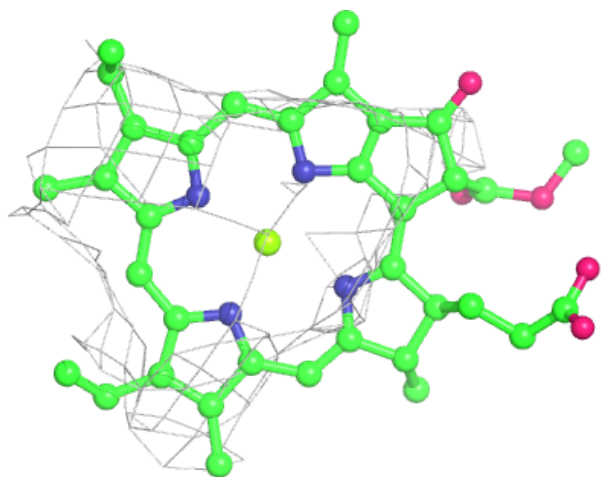
Electron density around CLA 2 1206:

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



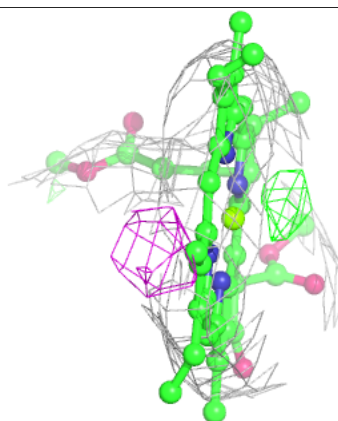
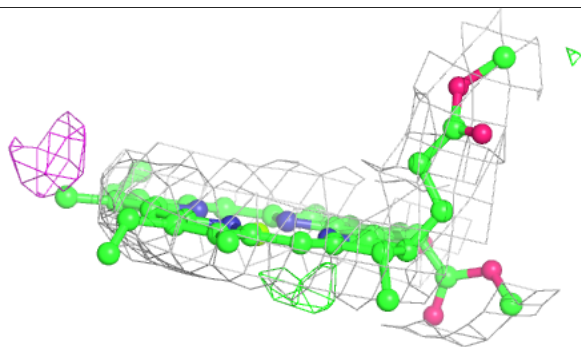
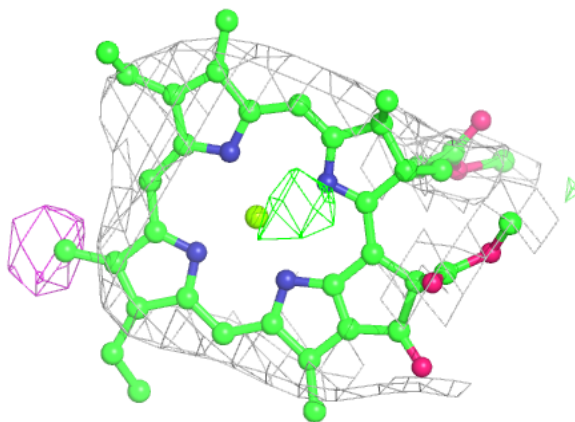
Electron density around CLA 2 1240:

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



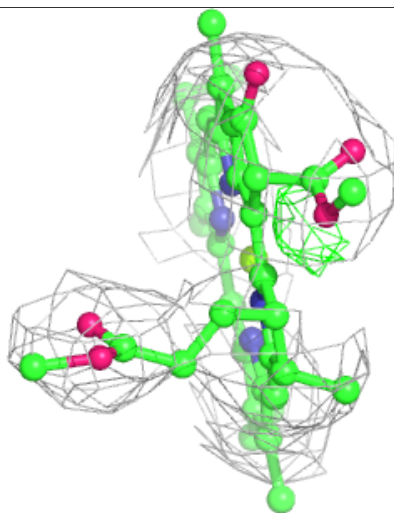
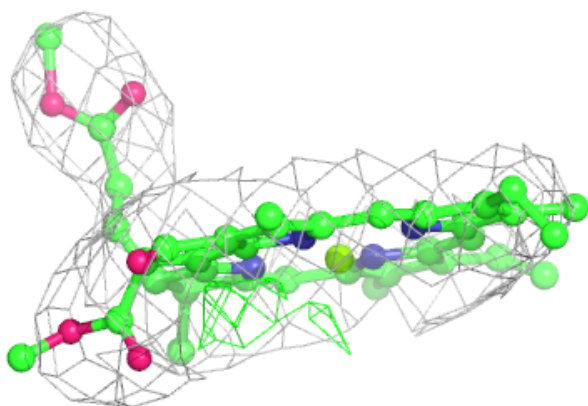
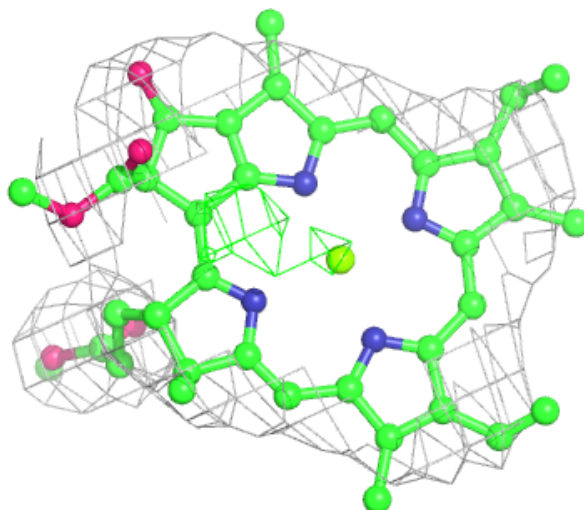
Electron density around CLA 2 1220:

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



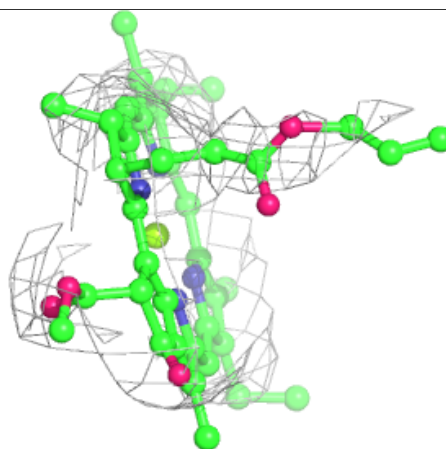
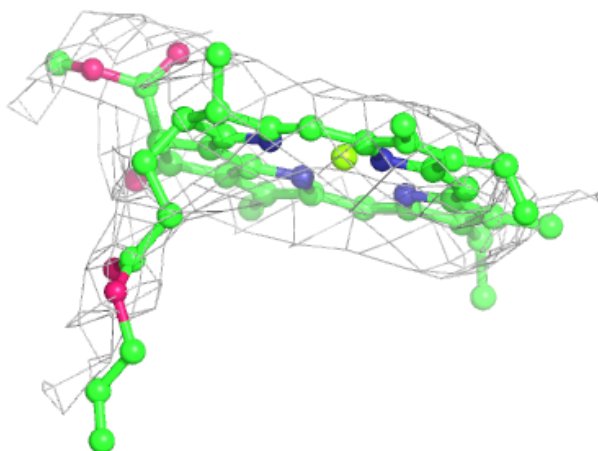
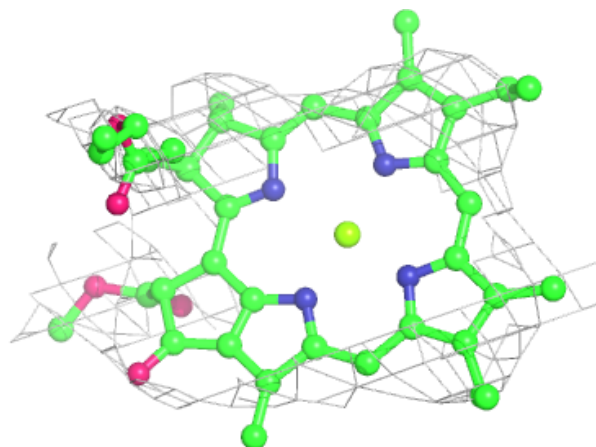
Electron density around CLA 2 1239:

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



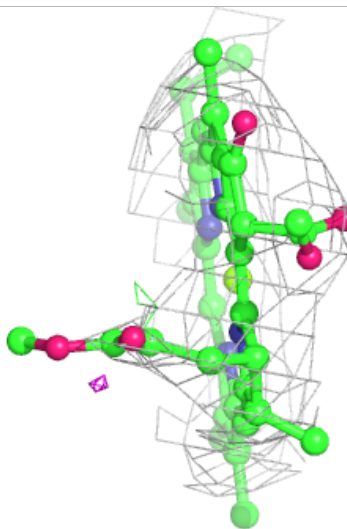
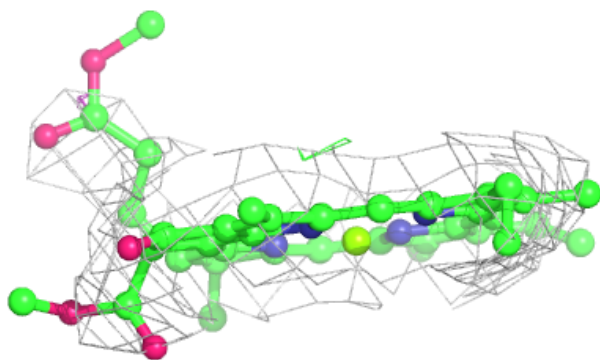
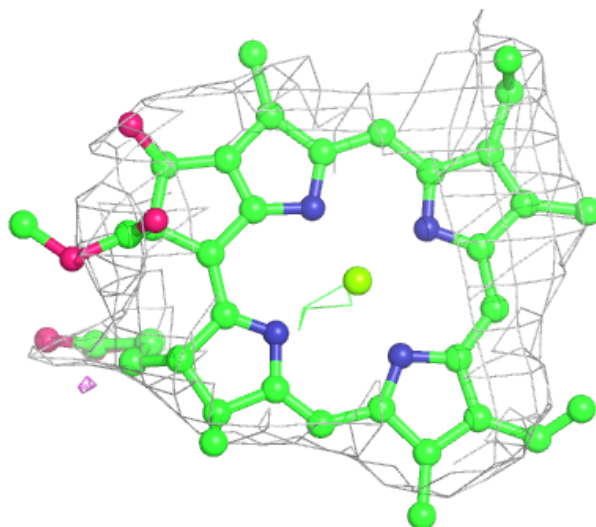
Electron density around CLA A 1105:

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



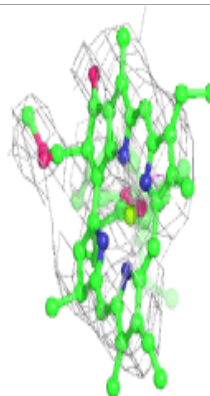
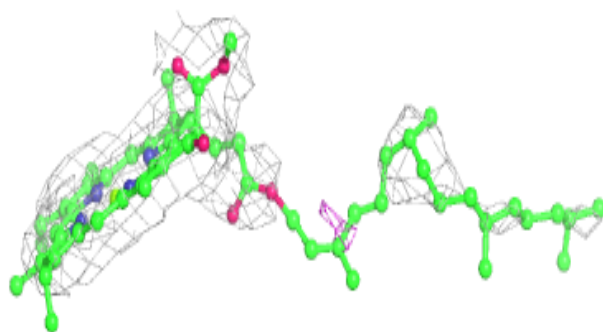
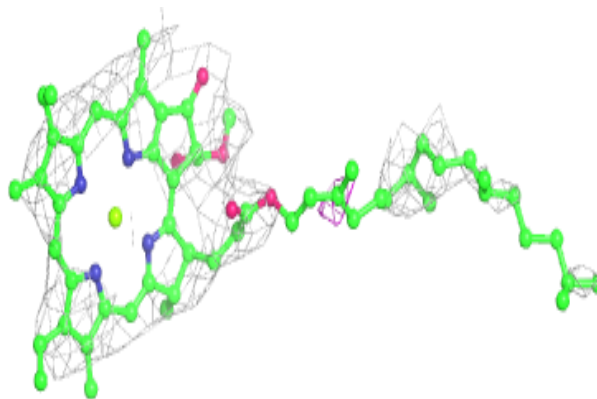
Electron density around CLA A 1121:

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

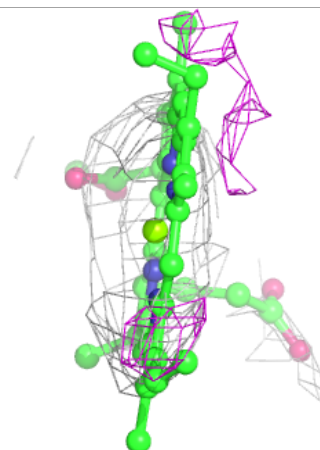
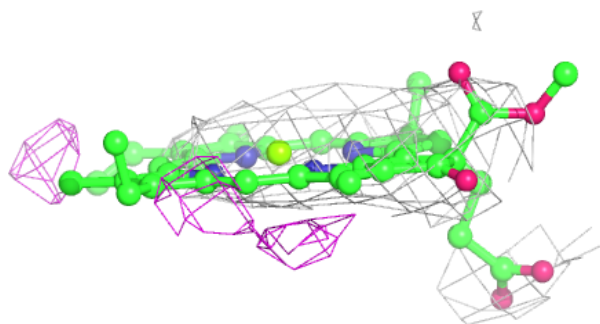
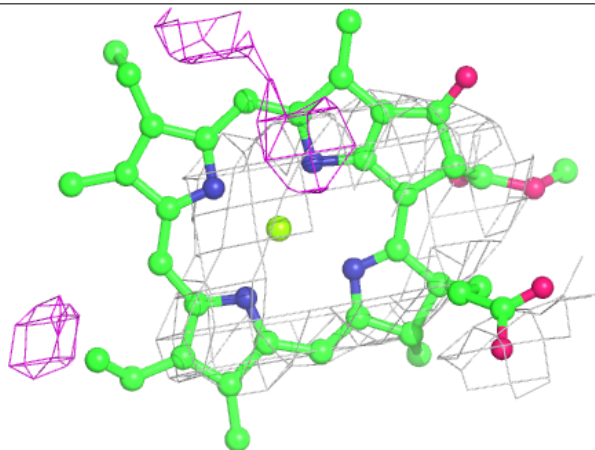


Electron density around CLA A 1107:

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

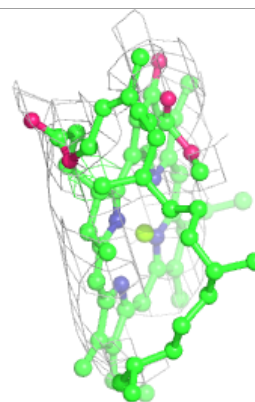
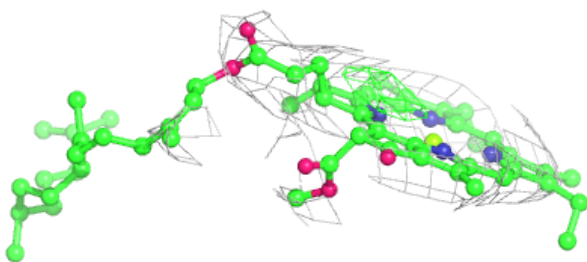
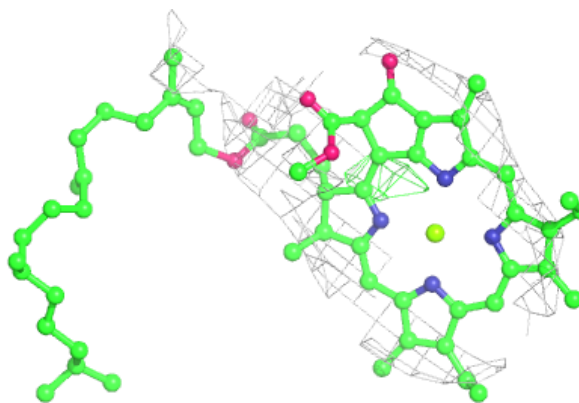
**Electron density around CLA b 1208:**

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

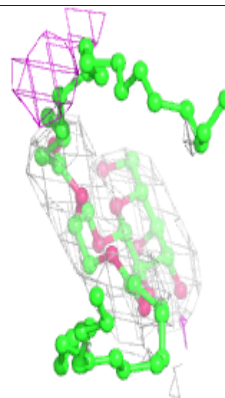
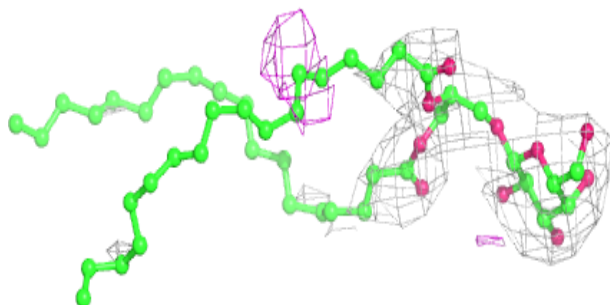
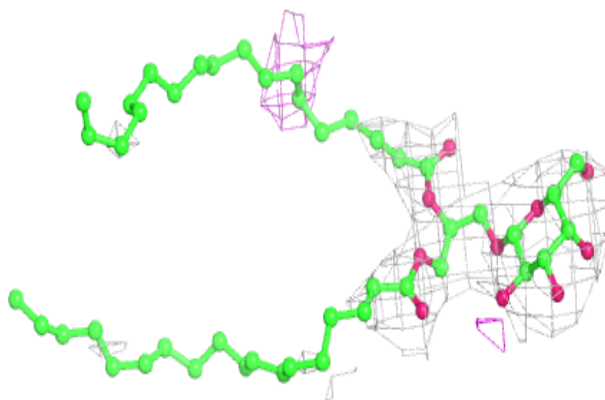


Electron density around CLA a 1101:

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

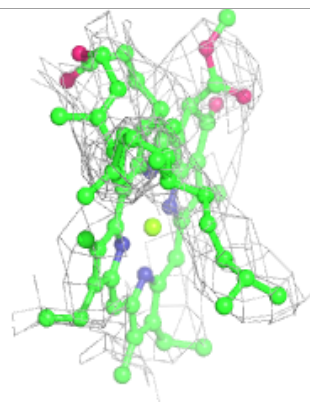
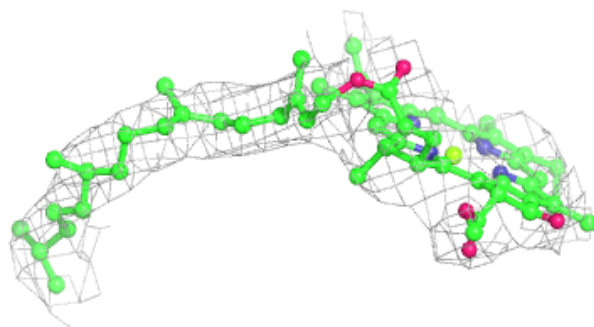
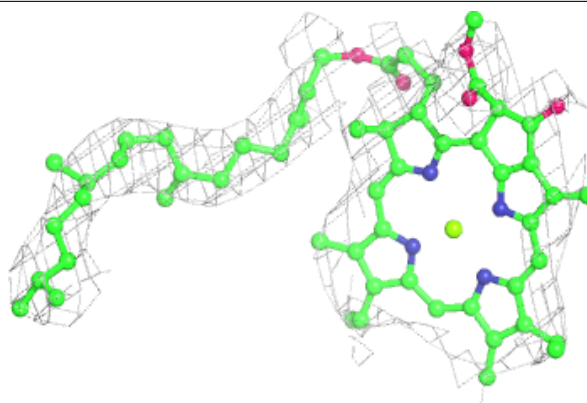
**Electron density around LMG B 5002:**

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

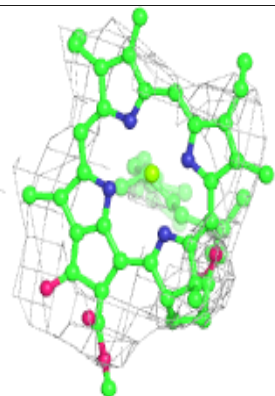
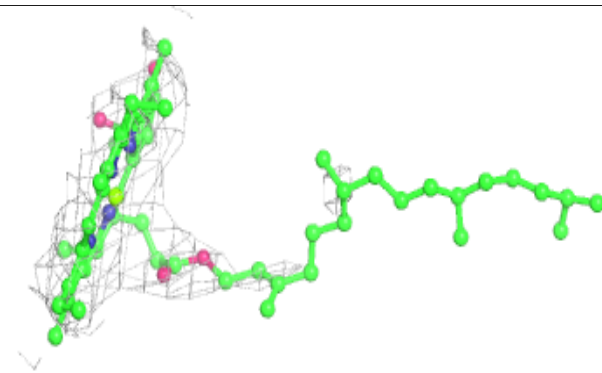
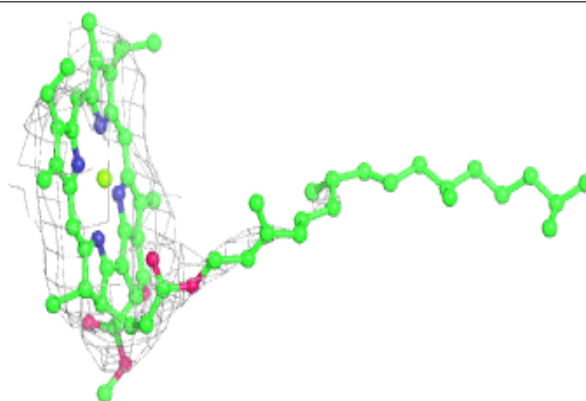


Electron density around CLA B 1013:

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

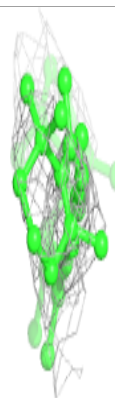
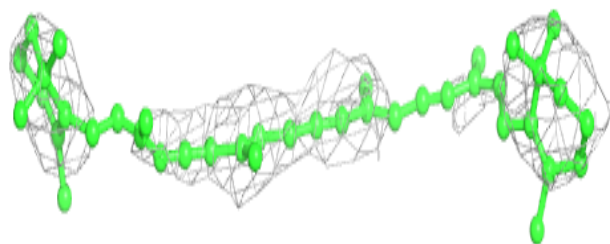
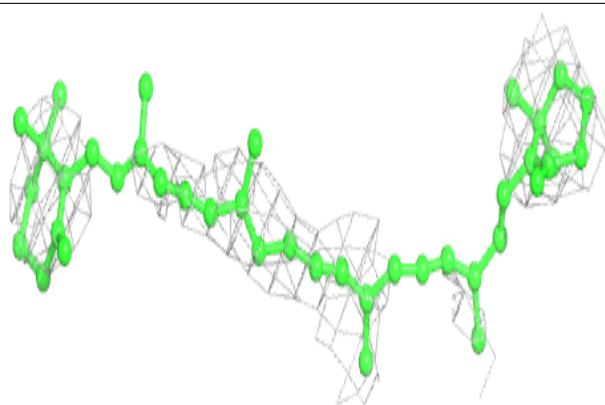
**Electron density around CLA B 1225:**

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

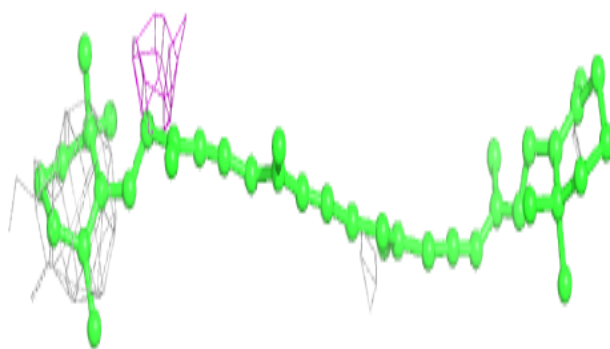
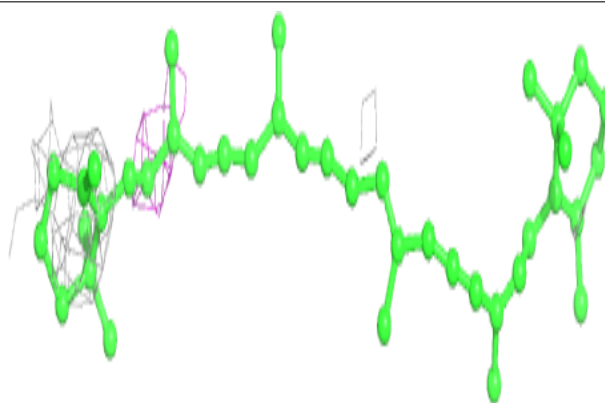


Electron density around BCR 2 4010:

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

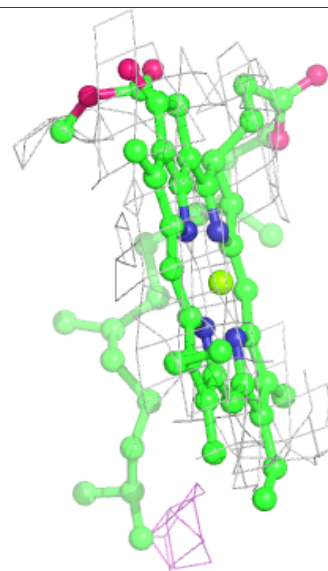
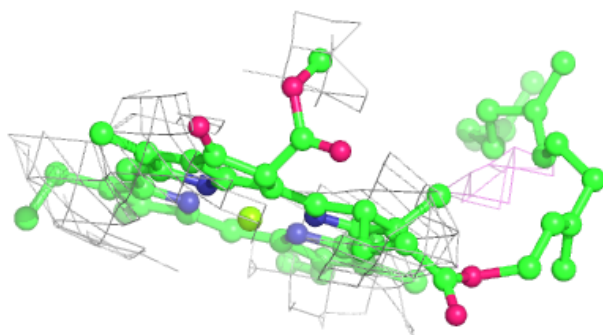
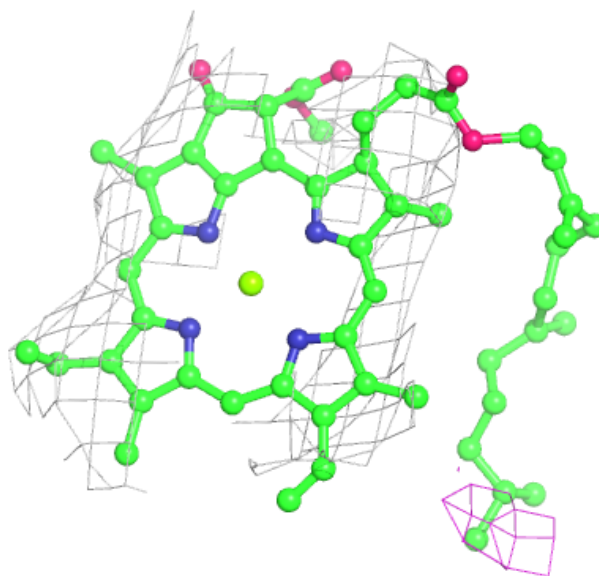
**Electron density around BCR 1 4003:**

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



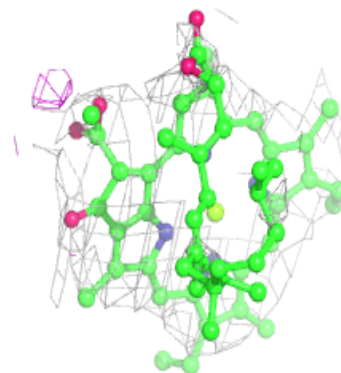
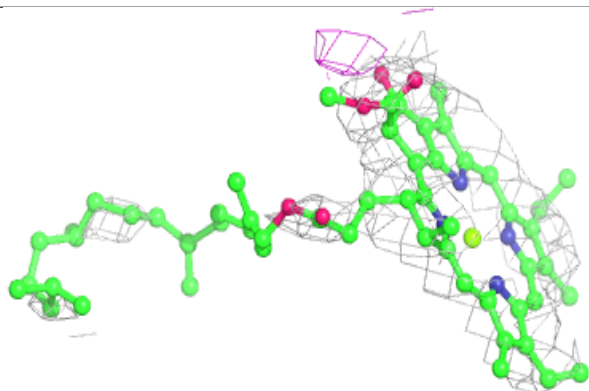
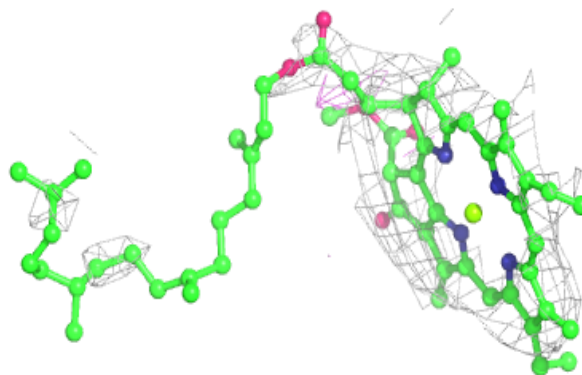
Electron density around CLA a 1111:

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

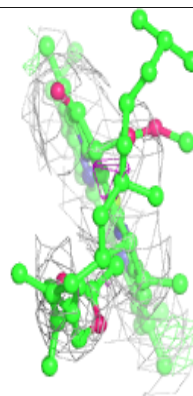
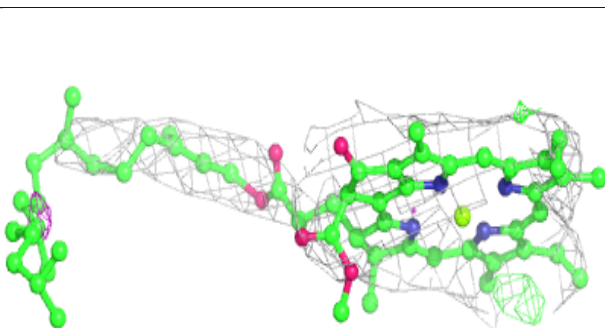
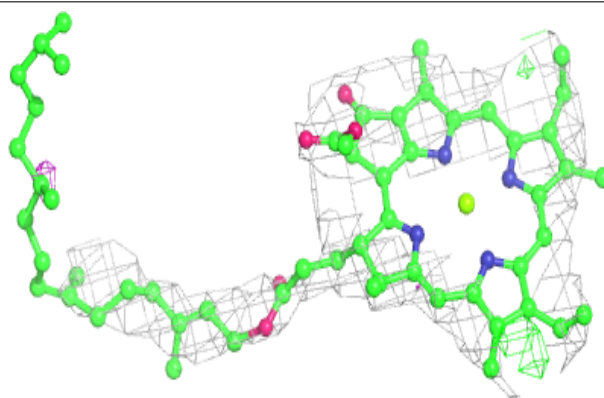


Electron density around CLA 2 1021:

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

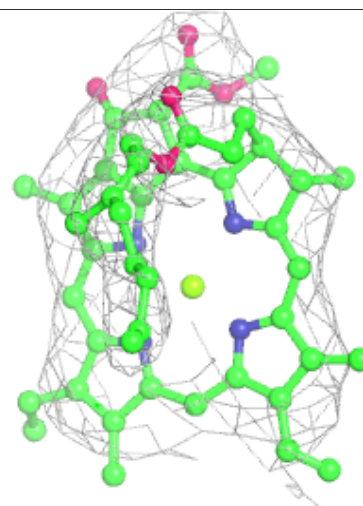
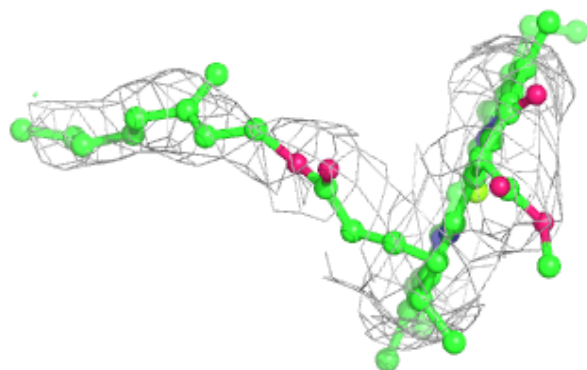
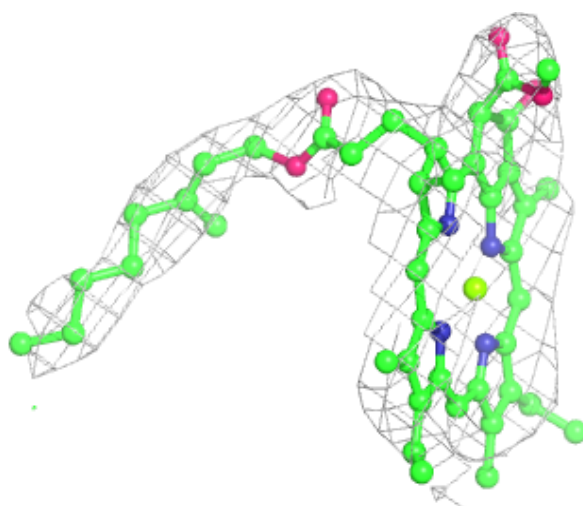
**Electron density around CLA 2 1223:**

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



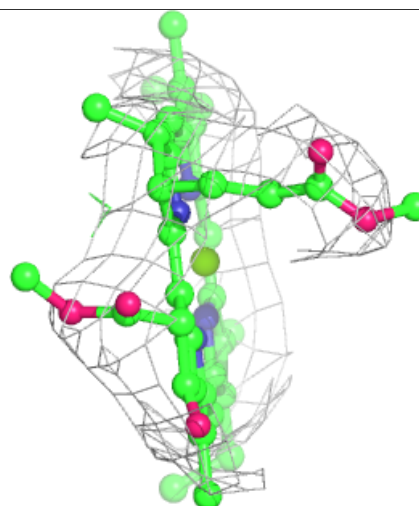
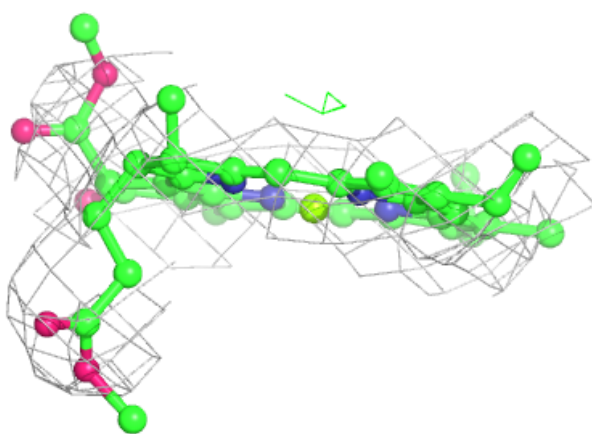
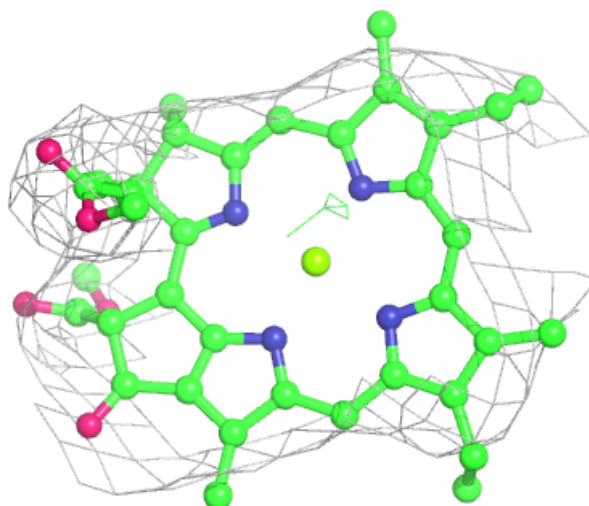
Electron density around CLA B 1201:

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



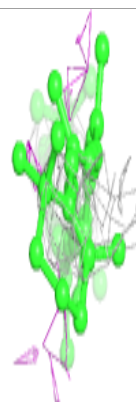
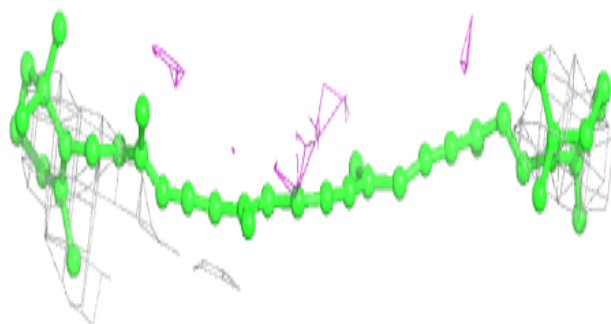
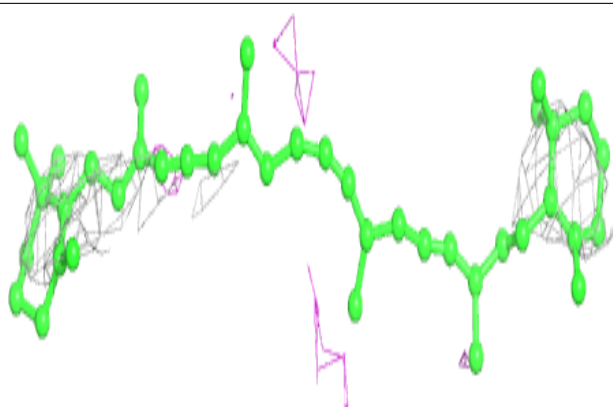
Electron density around CLA B 1211:

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

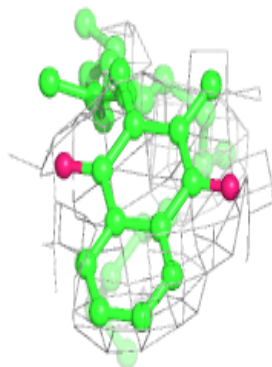
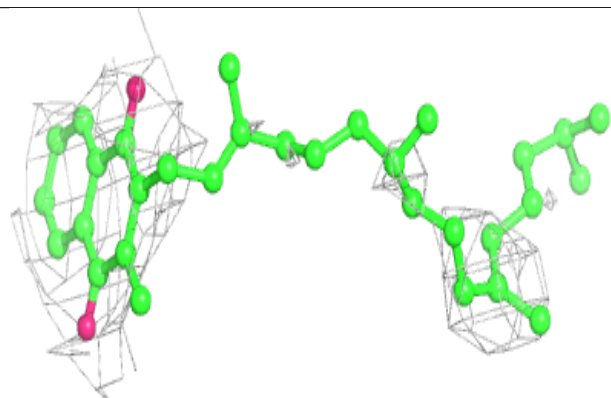
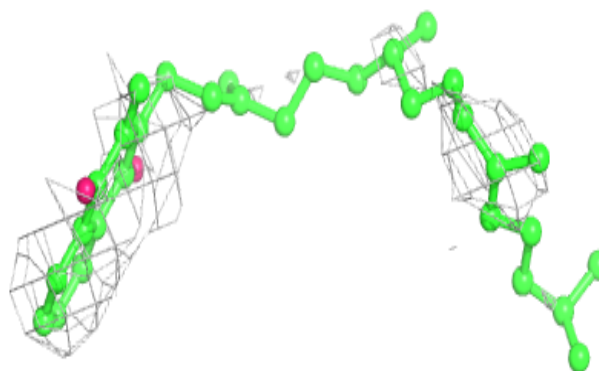


Electron density around BCR a 4002:

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

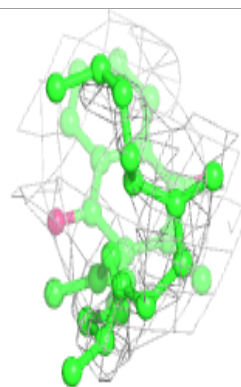
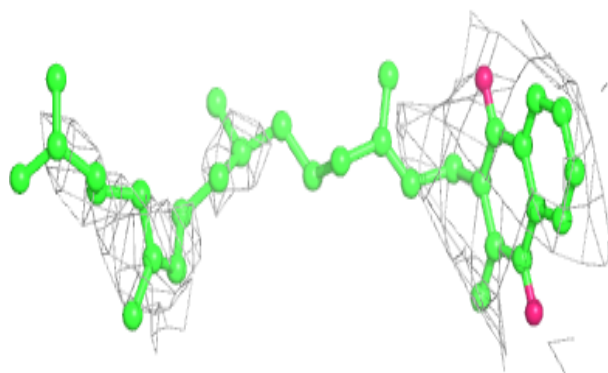
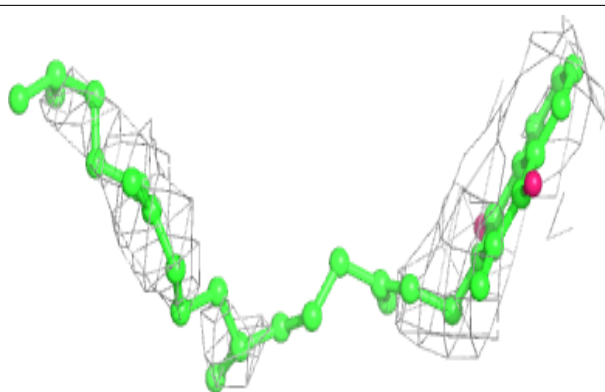
**Electron density around PQN b 2002:**

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

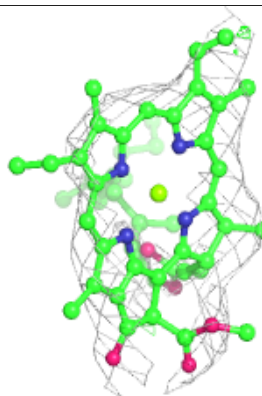
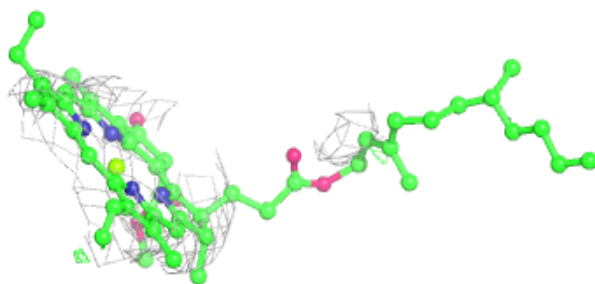
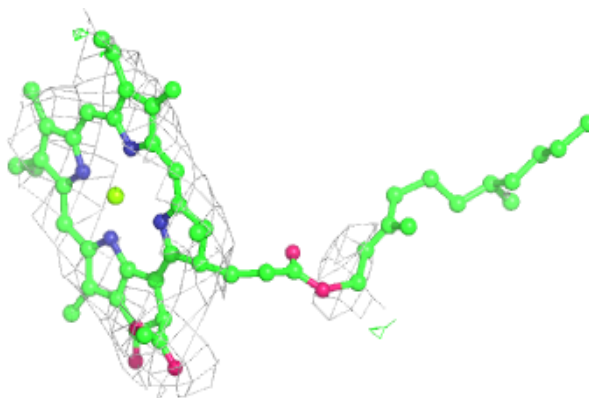


Electron density around PQN 2 2002:

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

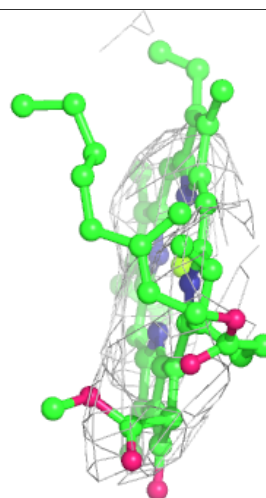
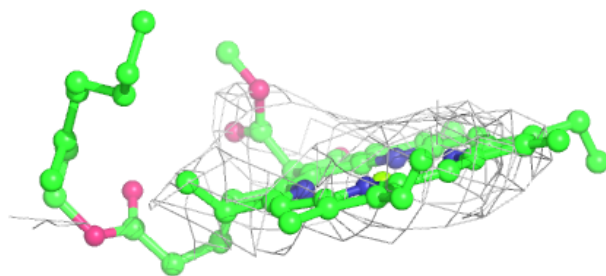
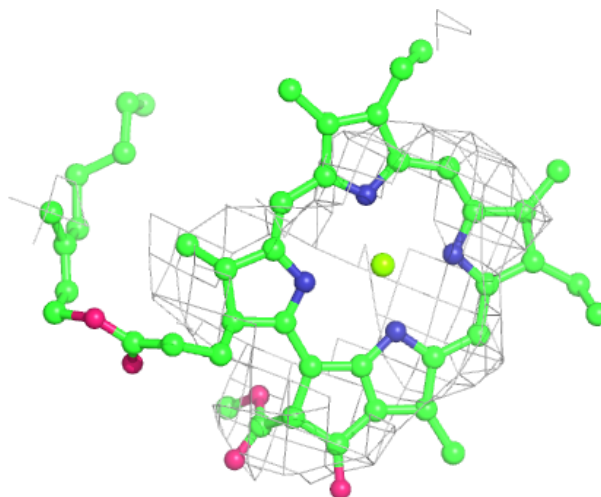
**Electron density around CLA B 1230:**

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



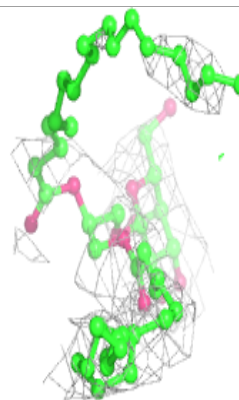
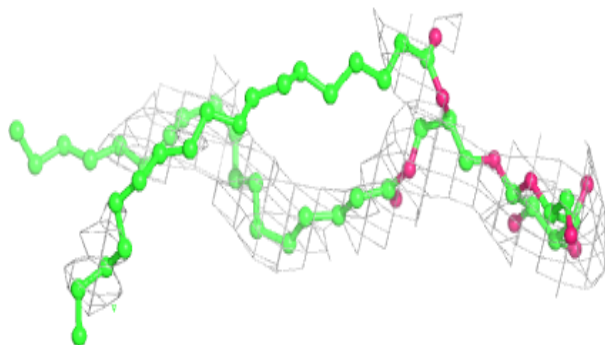
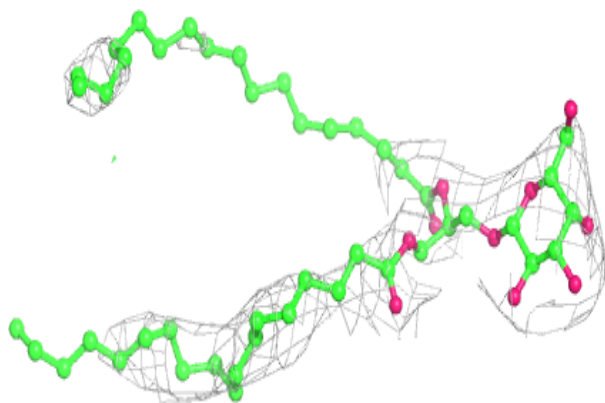
Electron density around CLA b 1221:

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



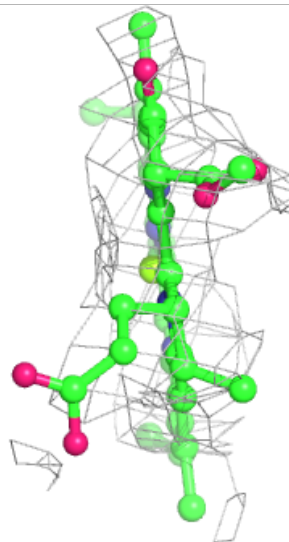
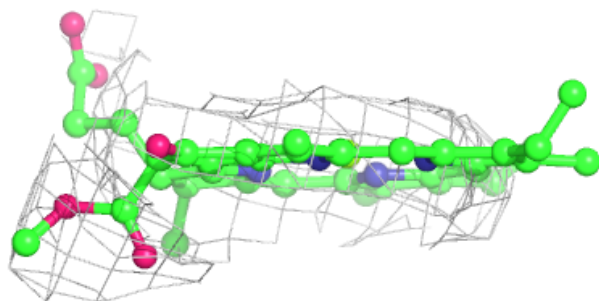
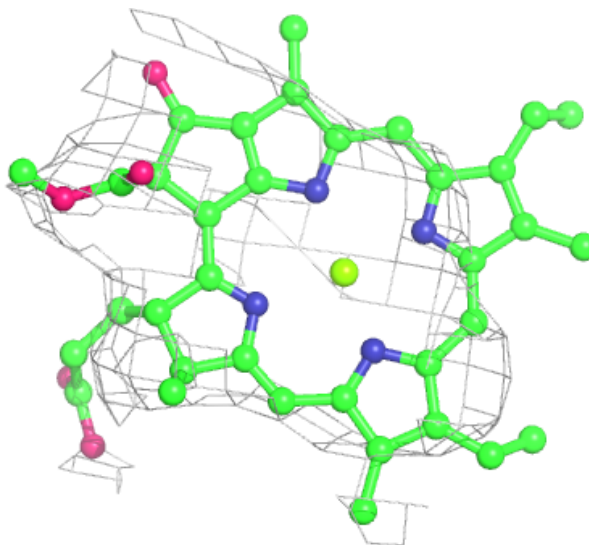
Electron density around LMG 2 5002:

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



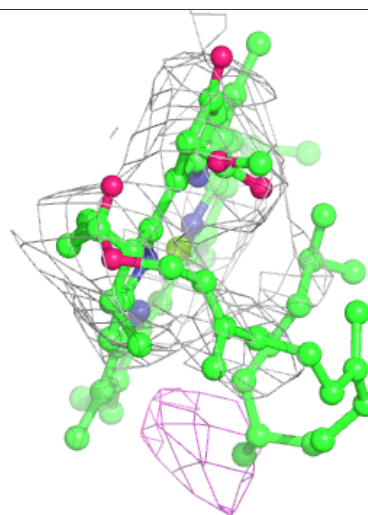
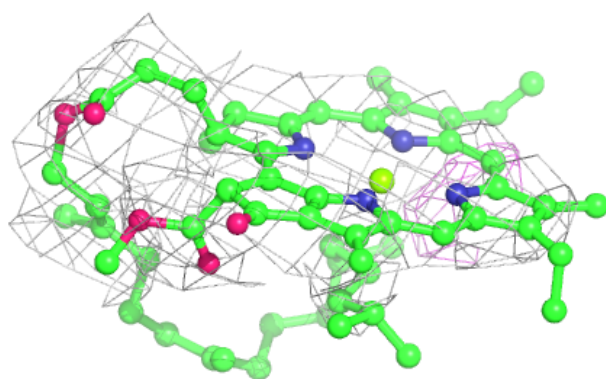
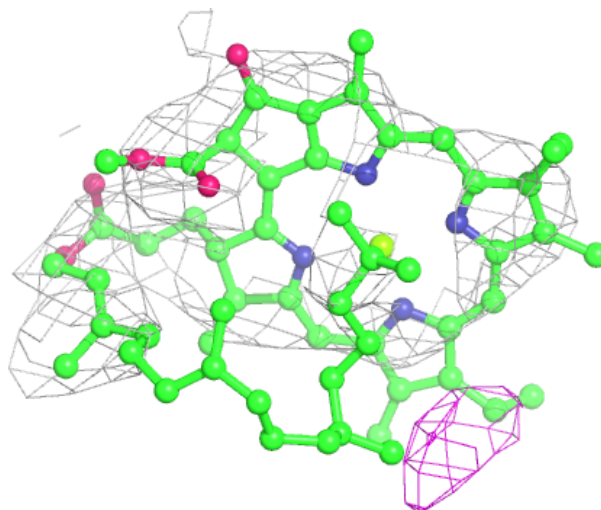
Electron density around CLA b 1209:

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



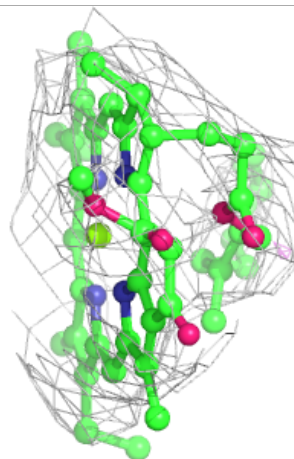
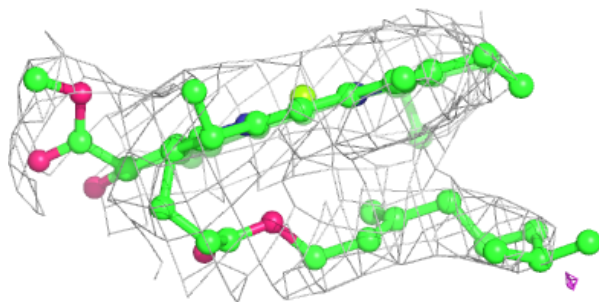
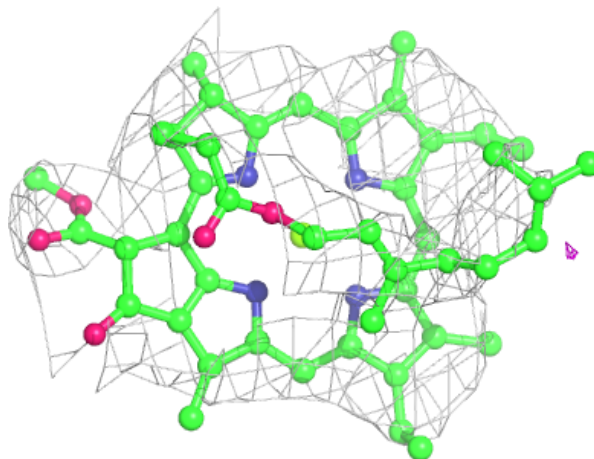
Electron density around CLA b 1203:

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



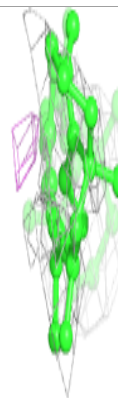
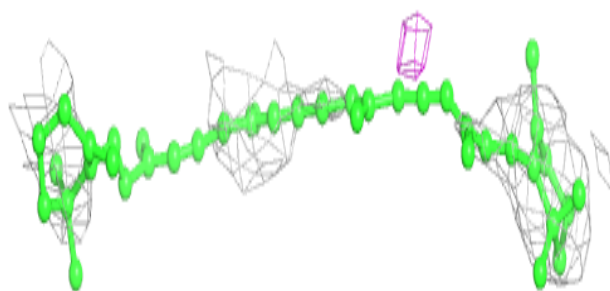
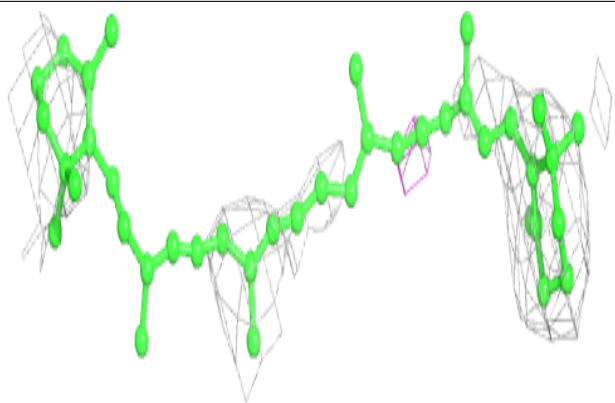
Electron density around CLA 2 1205:

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

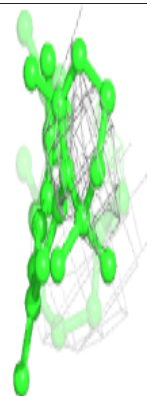
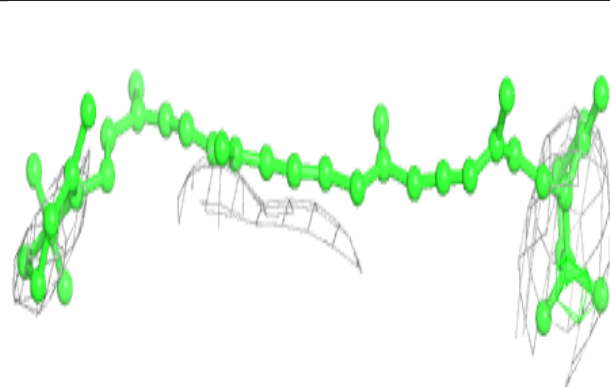
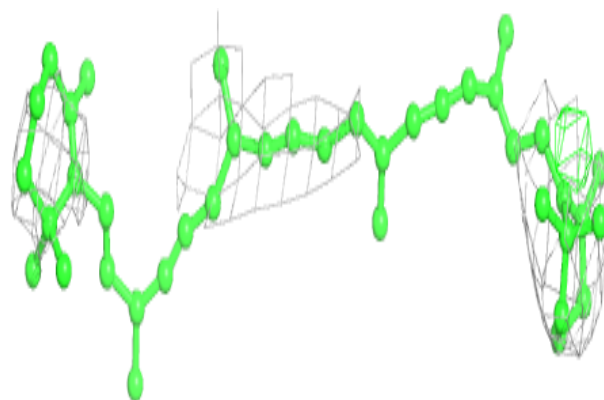


Electron density around BCR 2 4004:

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

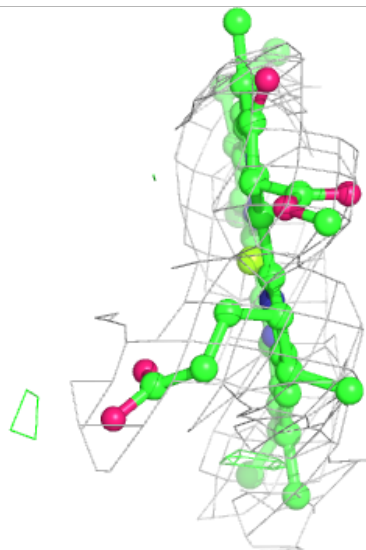
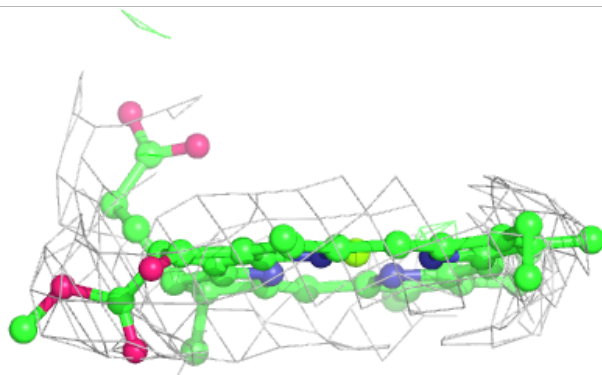
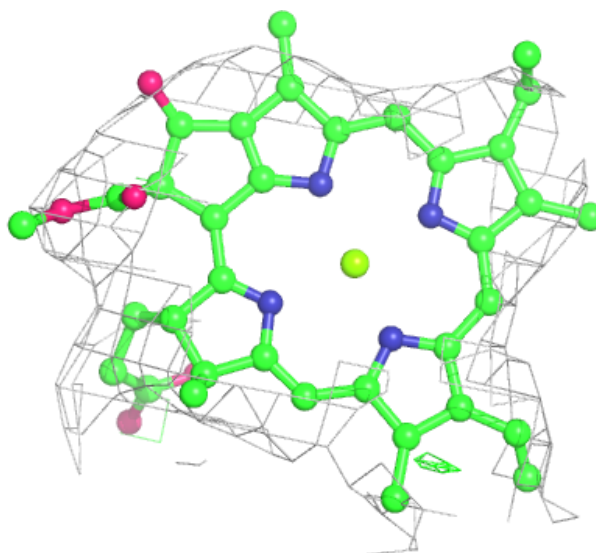
**Electron density around BCR b 4006:**

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



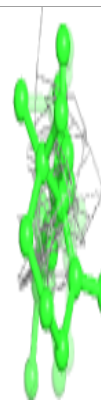
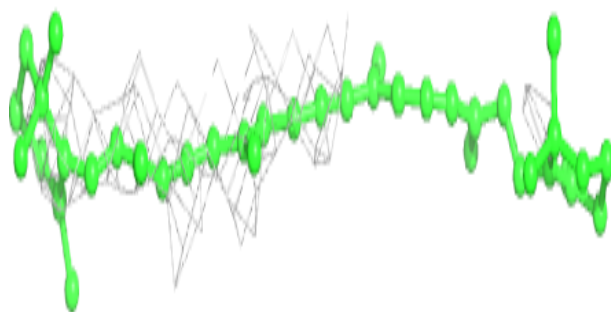
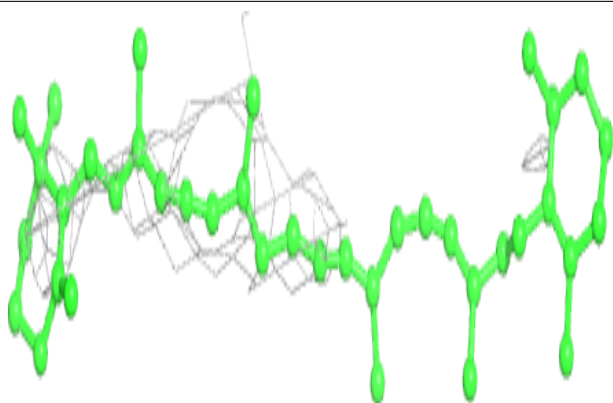
Electron density around CLA A 1108:

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

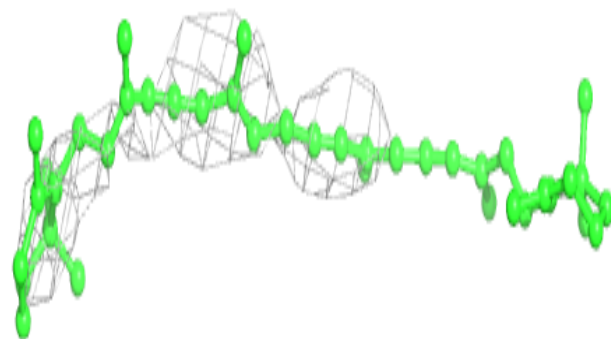
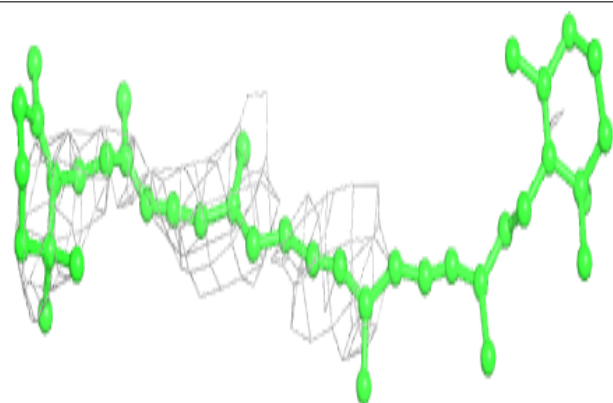


Electron density around BCR 1 4007:

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

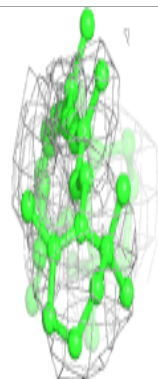
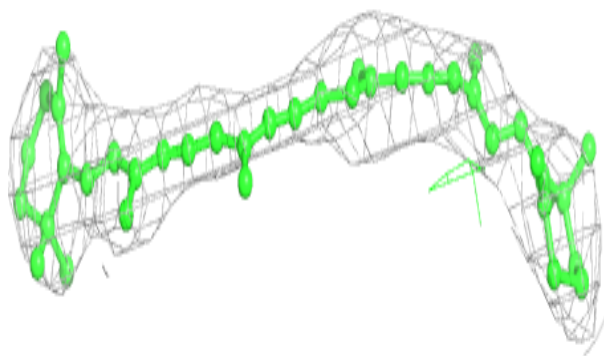
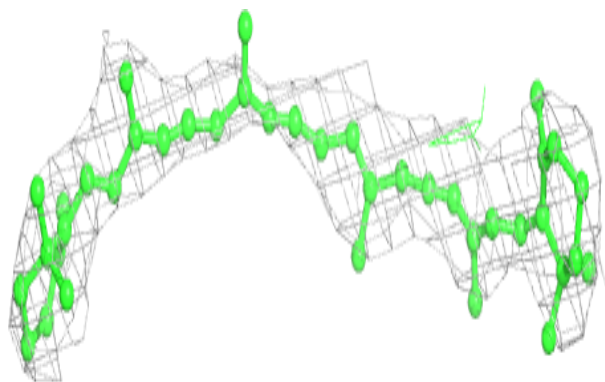
**Electron density around BCR m 4021:**

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



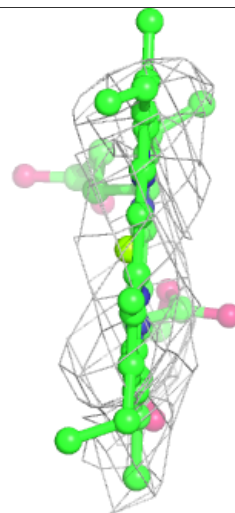
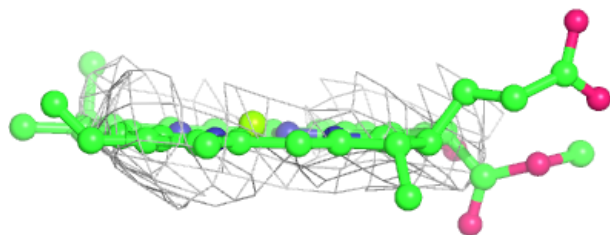
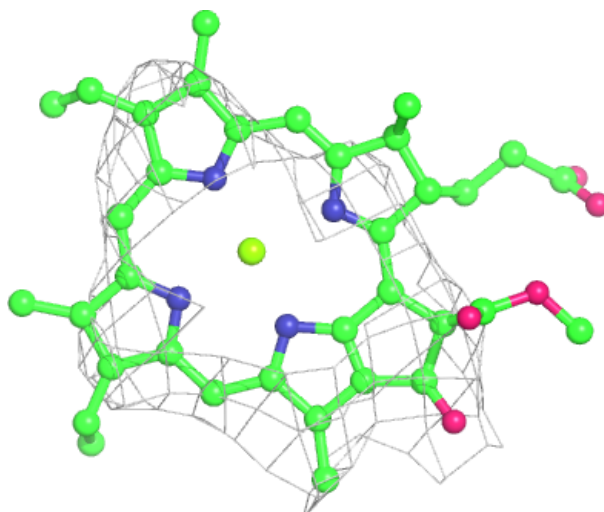
Electron density around BCR F 4018:

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



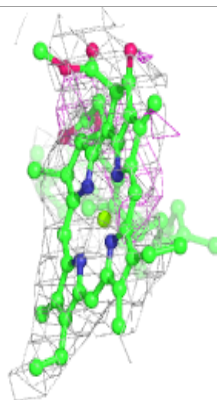
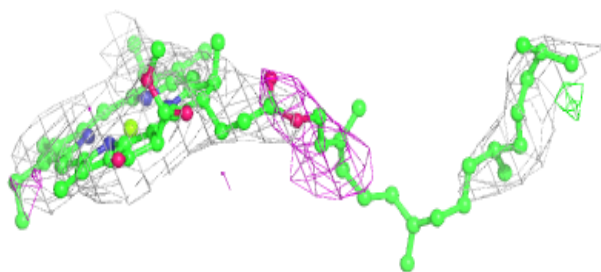
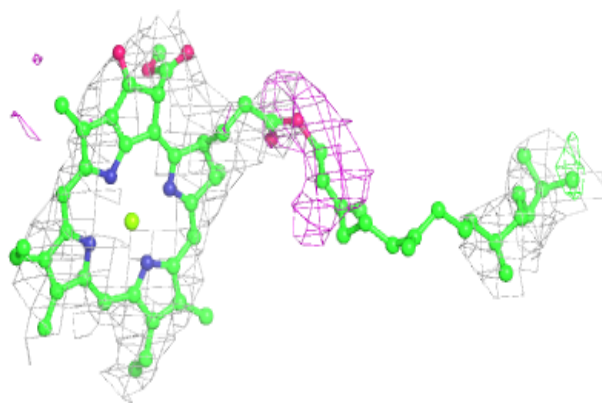
Electron density around CLA 1 1113:

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

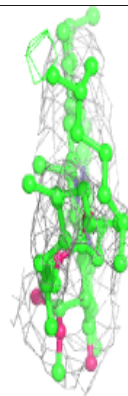
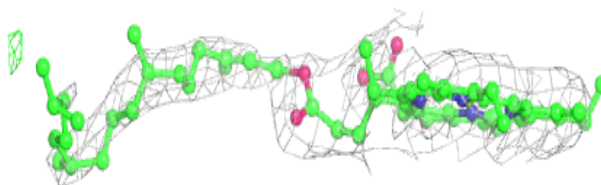
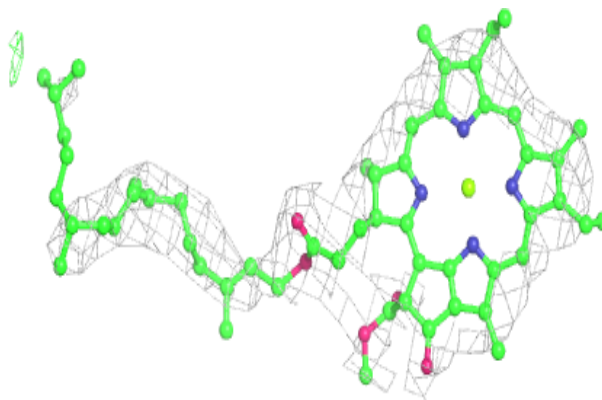


Electron density around CLA 2 1210:

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

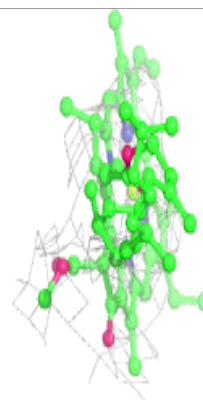
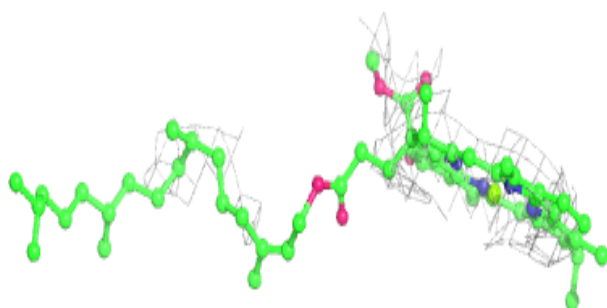
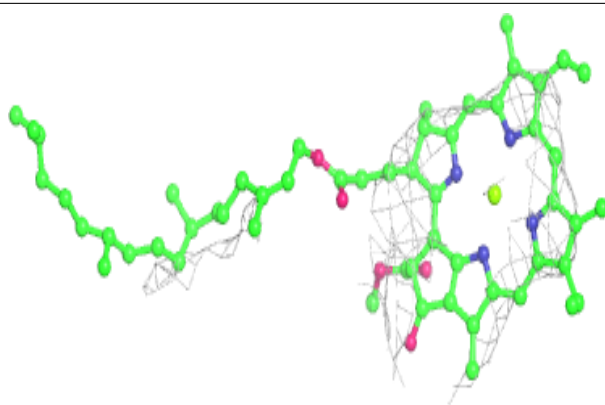
**Electron density around CLA a 1131:**

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

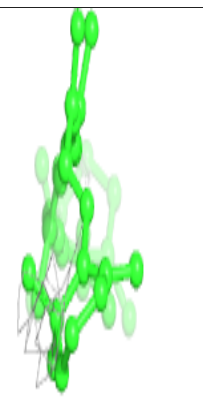
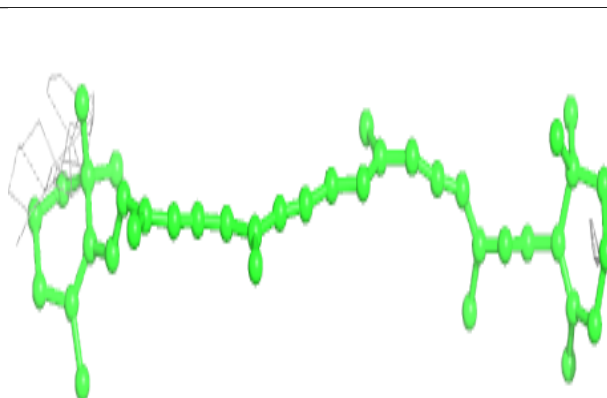
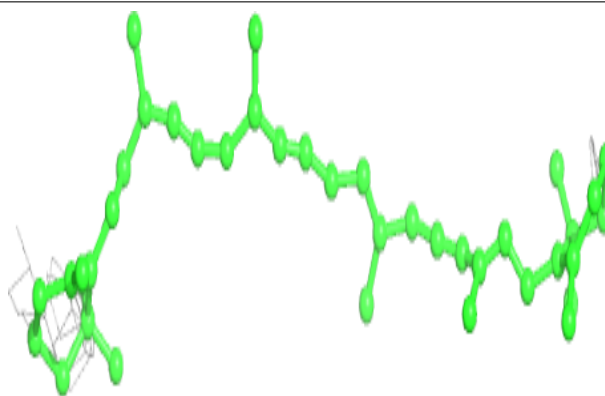


Electron density around CLA 1 1107:

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

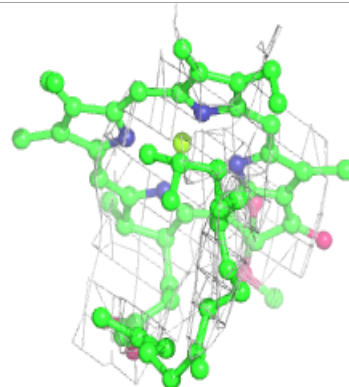
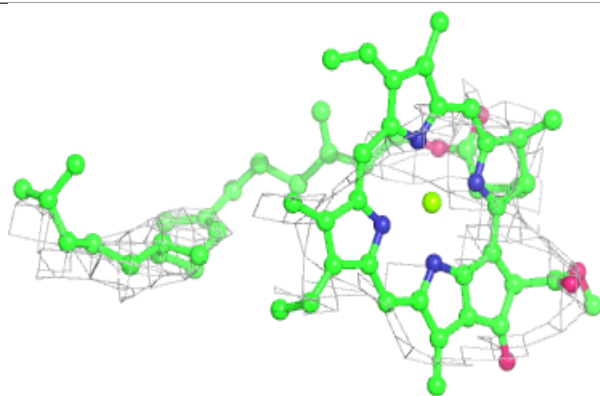
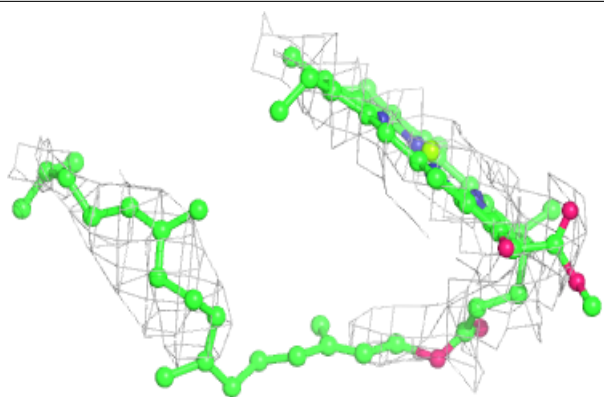
**Electron density around BCR 6 4013:**

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



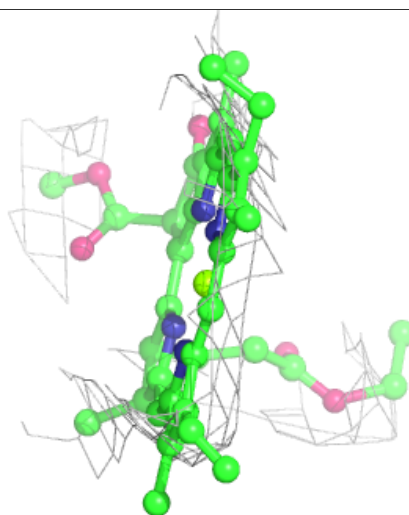
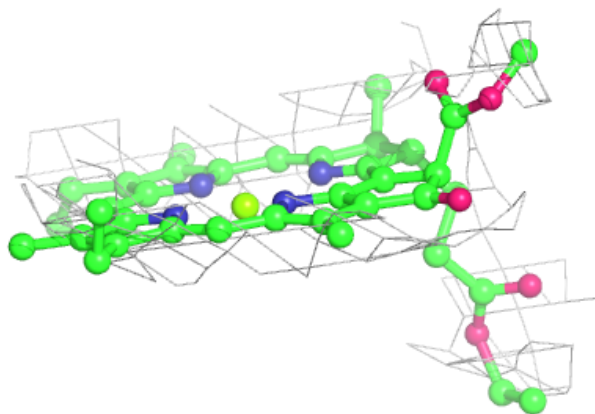
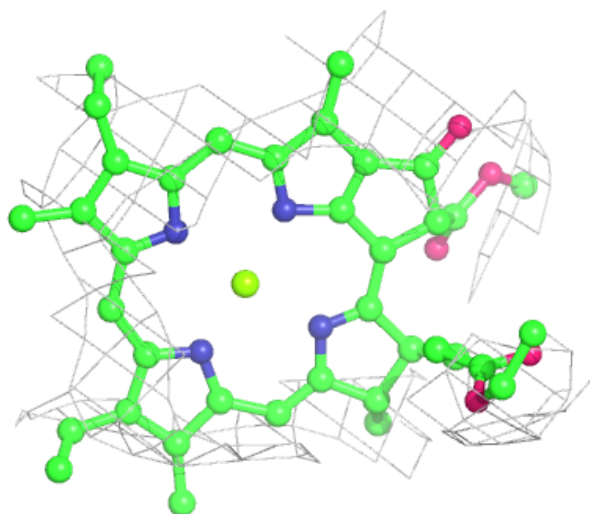
Electron density around CLA a 1109:

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



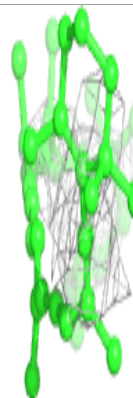
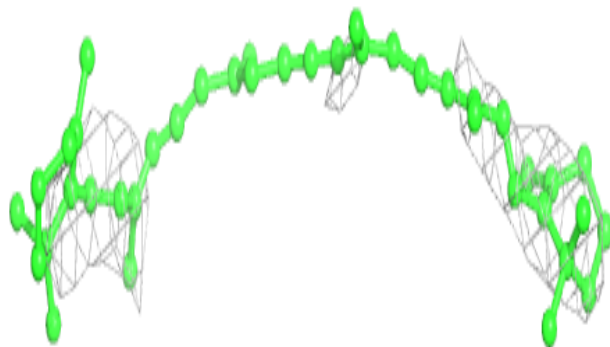
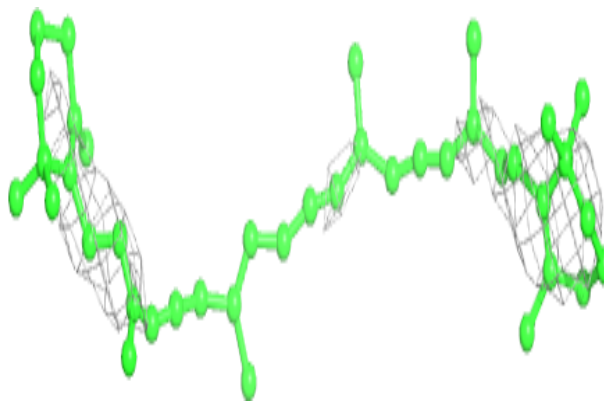
Electron density around CLA b 1236:

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



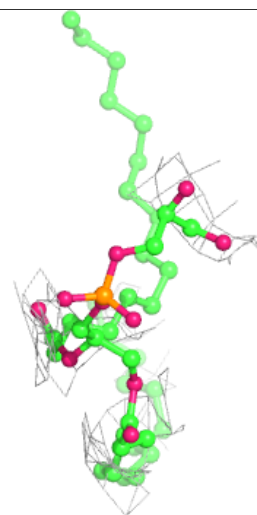
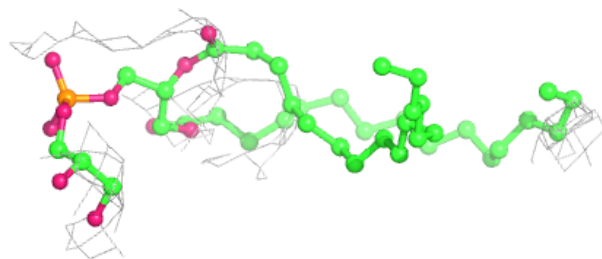
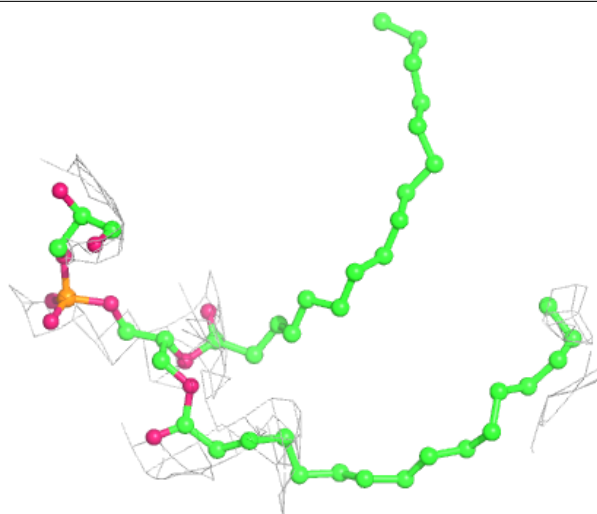
Electron density around BCR B 4014:

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



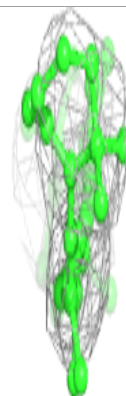
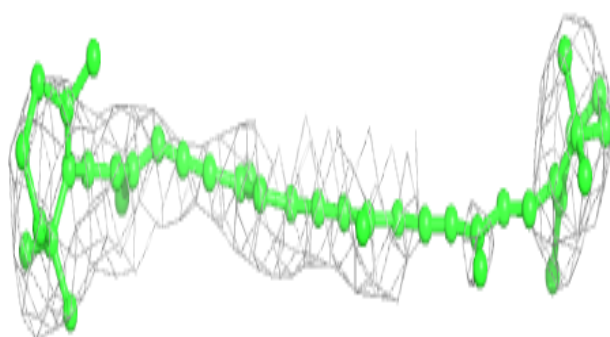
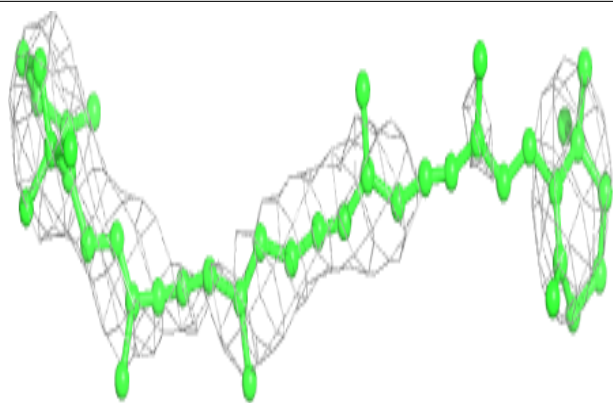
Electron density around LHG b 5004:

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

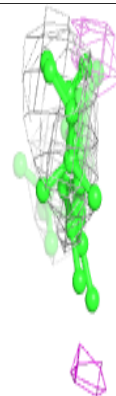
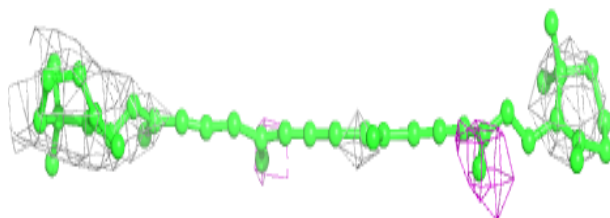
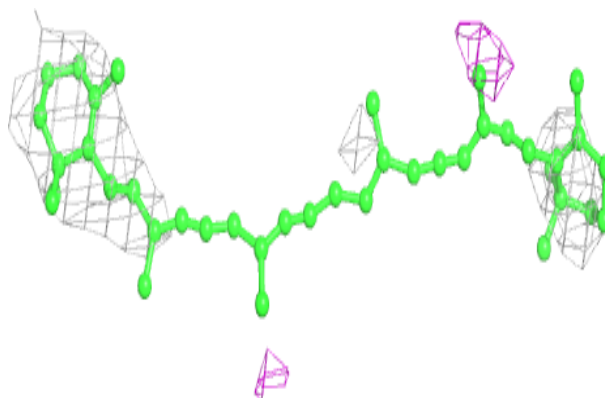


Electron density around BCR 2 4017:

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

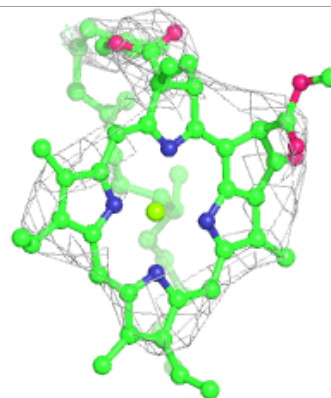
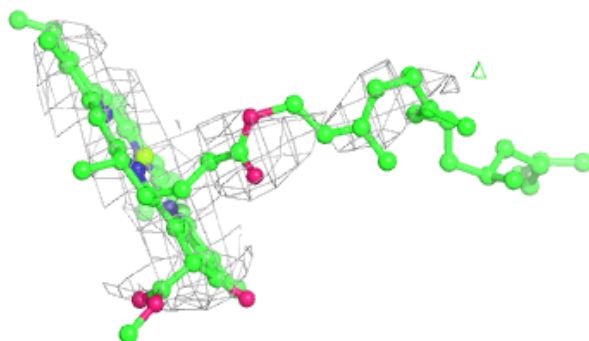
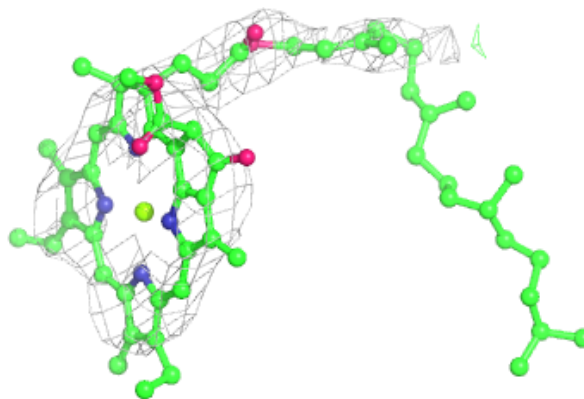
**Electron density around BCR B 4005:**

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



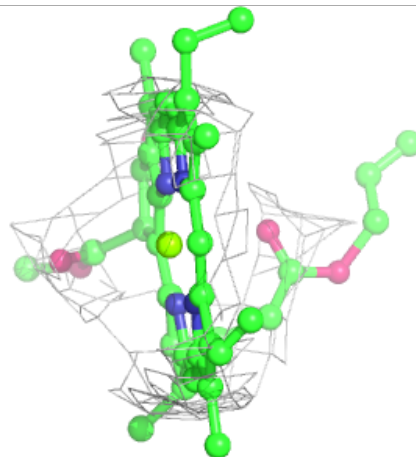
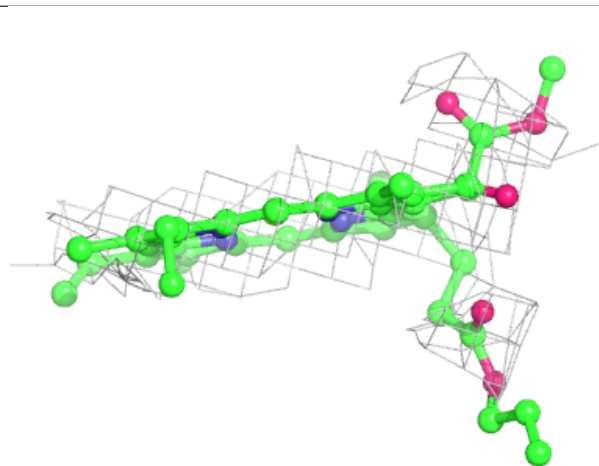
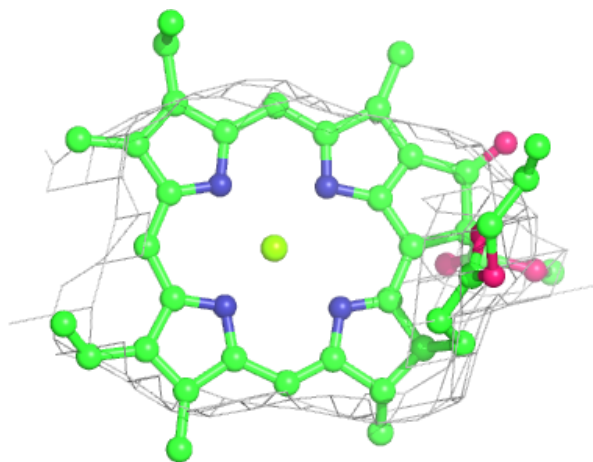
Electron density around CLA a 1137:

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



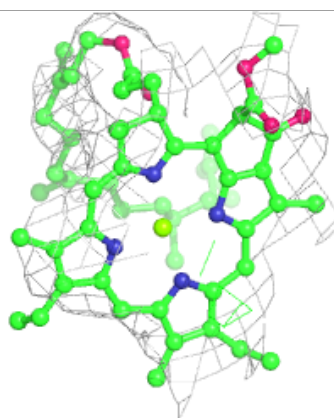
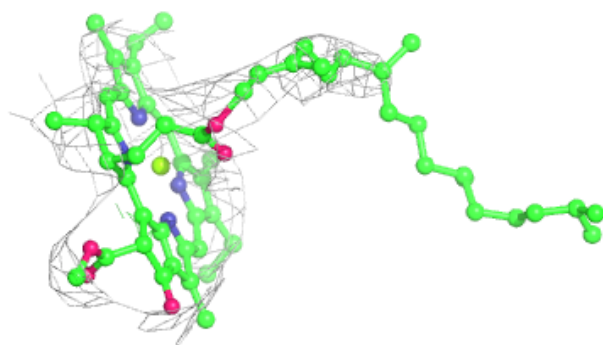
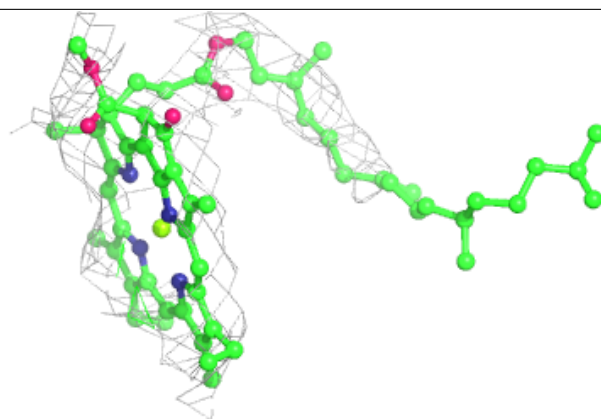
Electron density around CLA 1 1105:

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

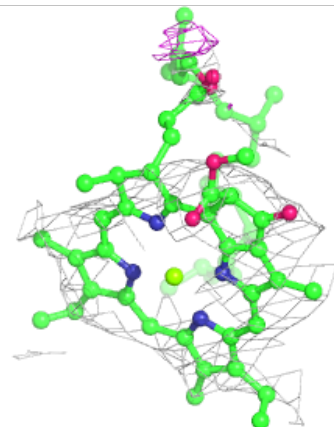
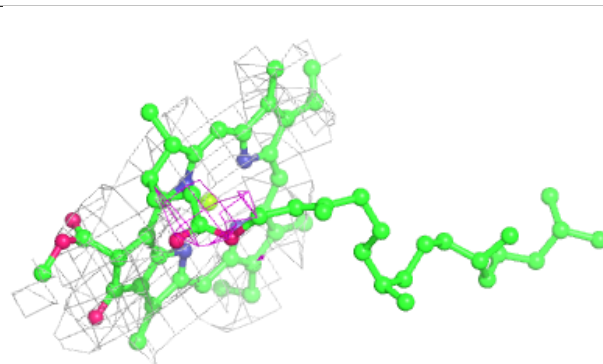
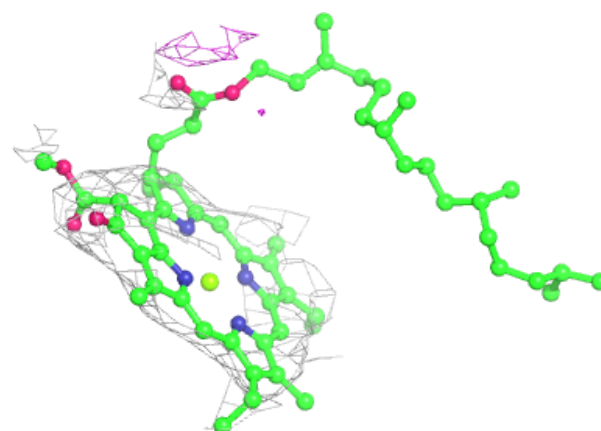


Electron density around CLA 2 1216:

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

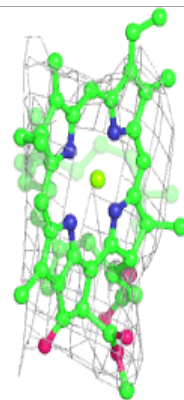
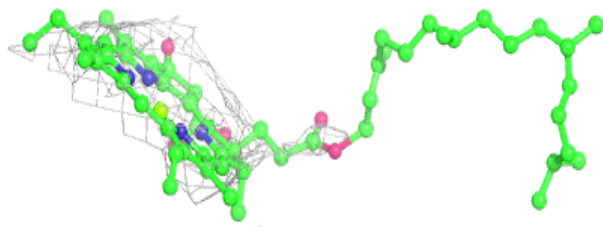
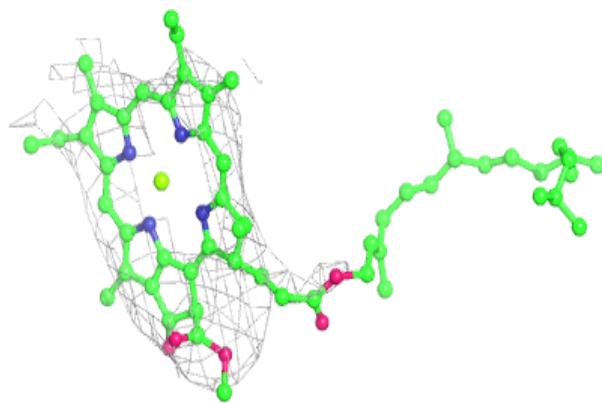
**Electron density around CLA 1 1102:**

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

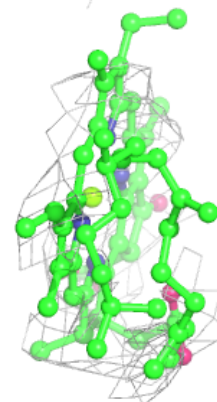
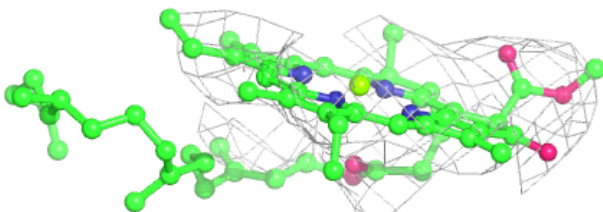
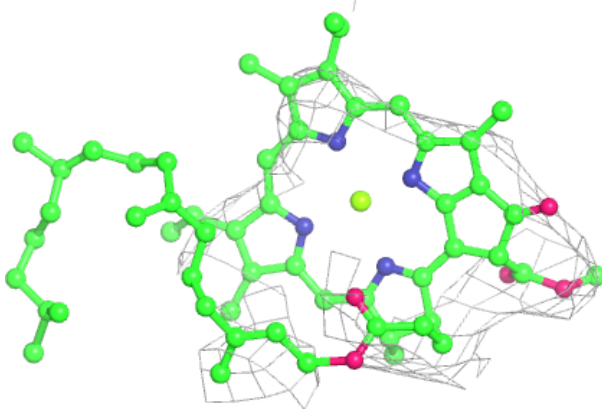


Electron density around CLA b 1206:

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

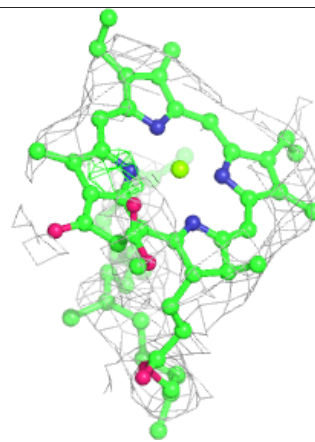
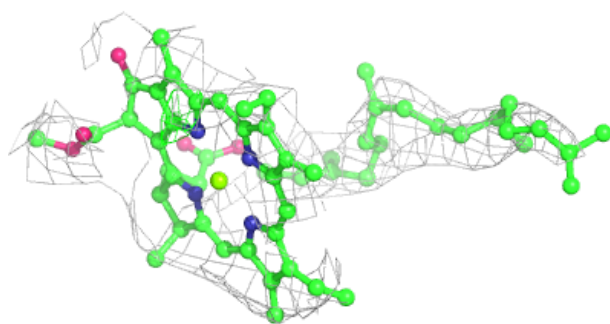
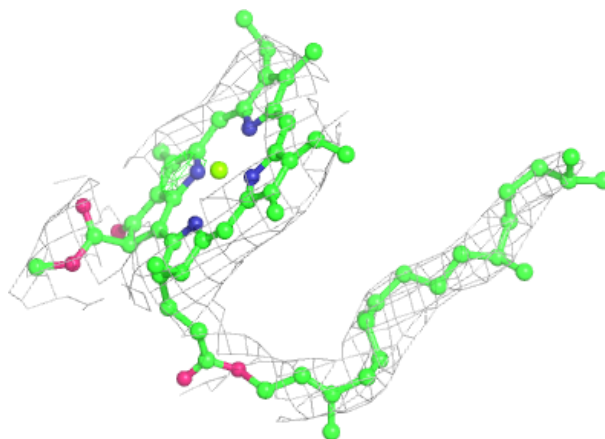
**Electron density around CLA 1 1117:**

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



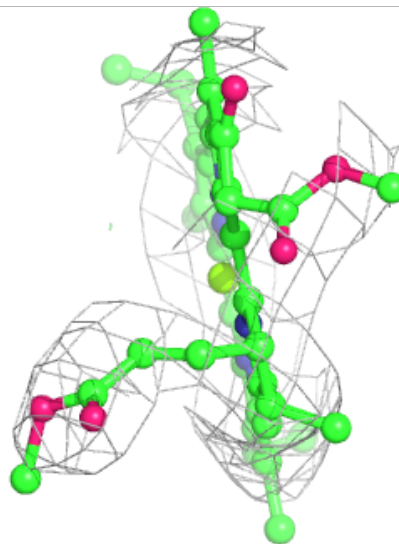
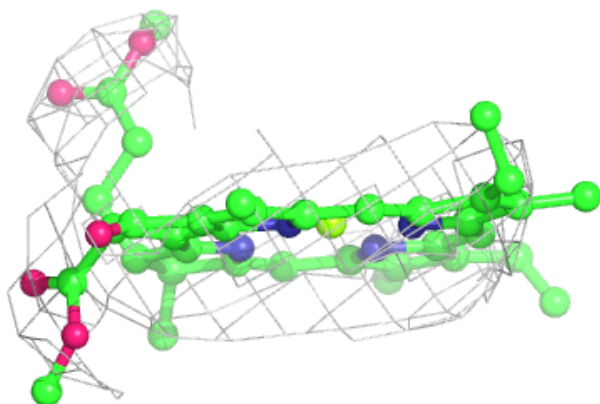
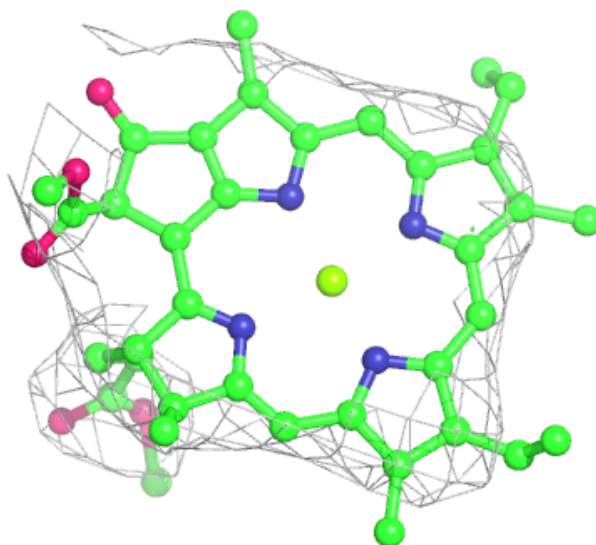
Electron density around CLA A 1102:

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



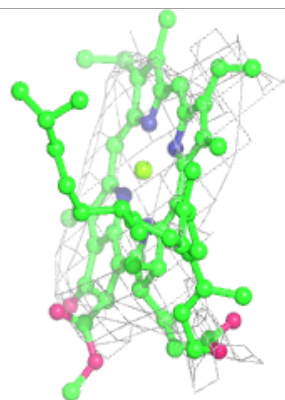
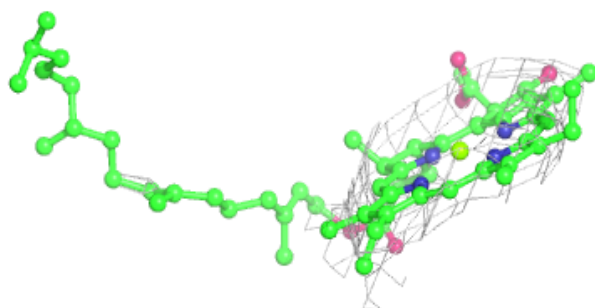
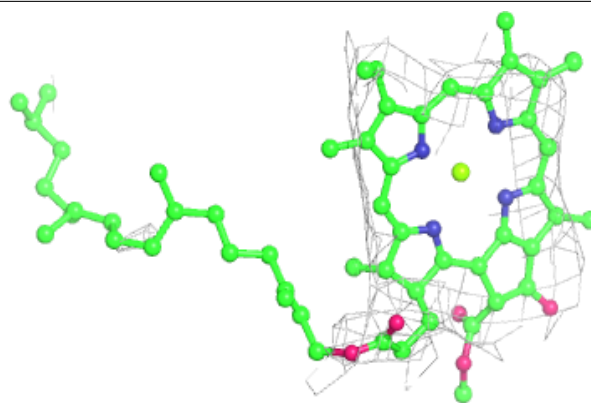
Electron density around CLA a 1129:

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

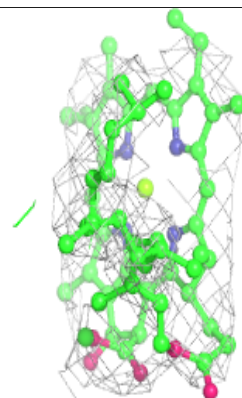
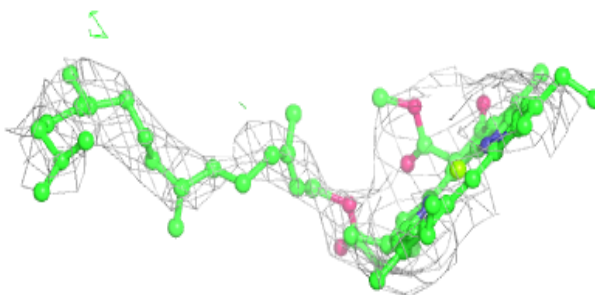
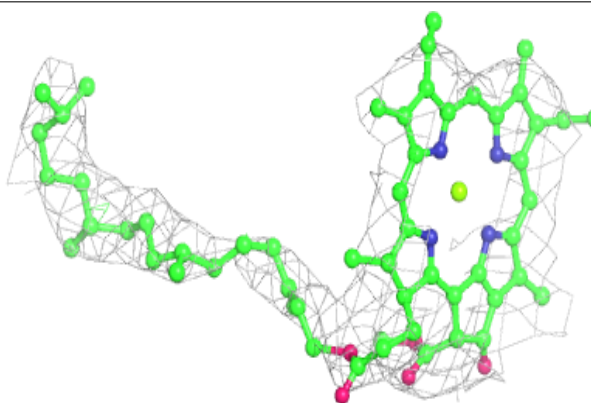


Electron density around CLA 2 1013:

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

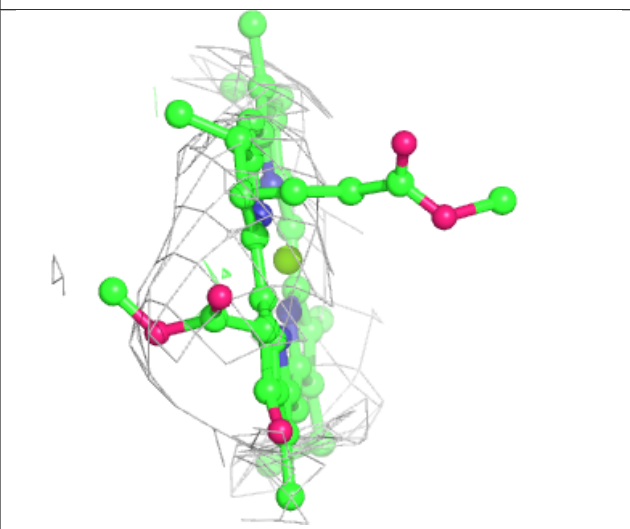
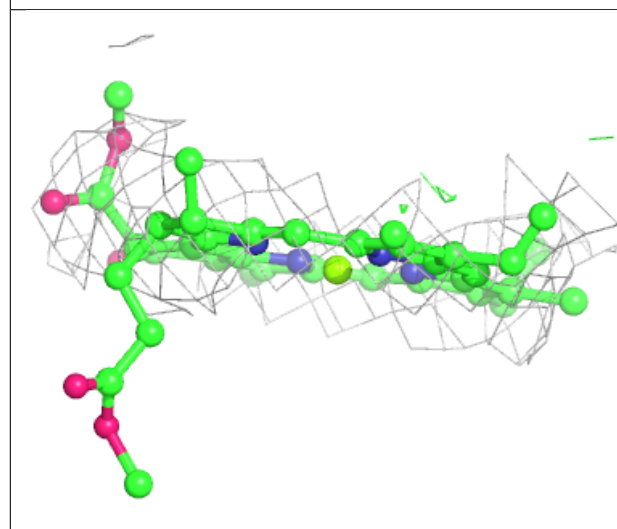
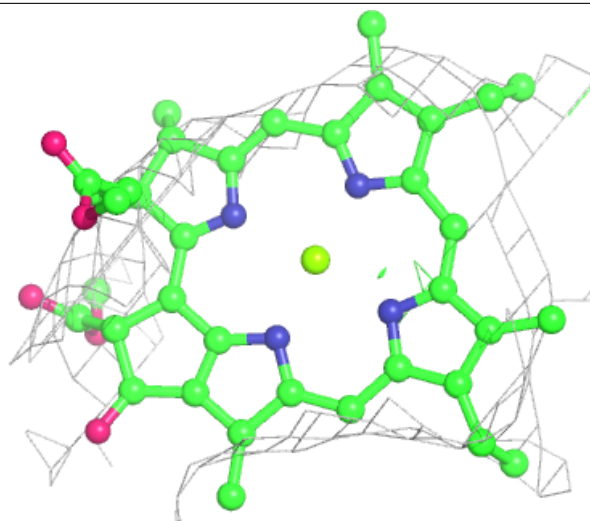
**Electron density around CLA 2 1207:**

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



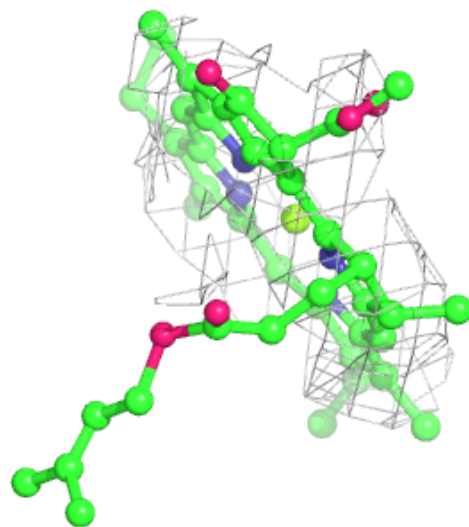
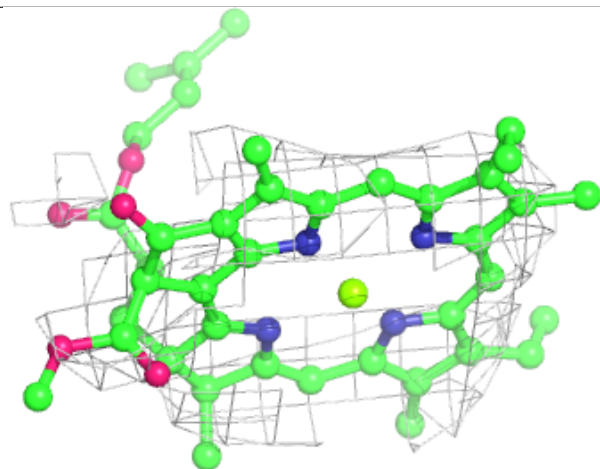
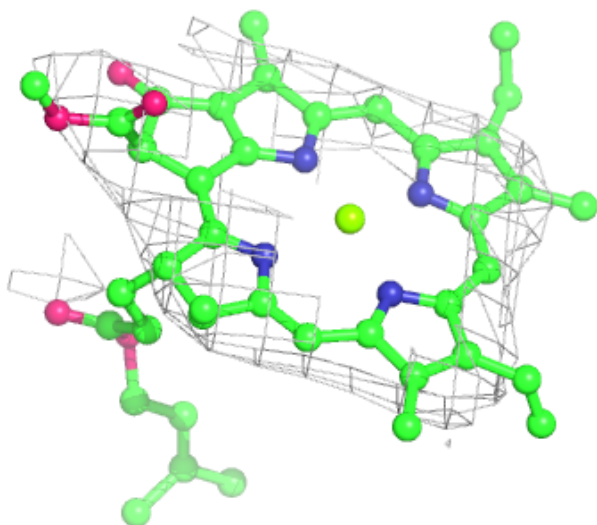
Electron density around CLA b 1211:

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



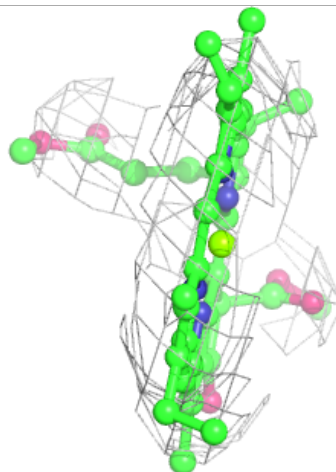
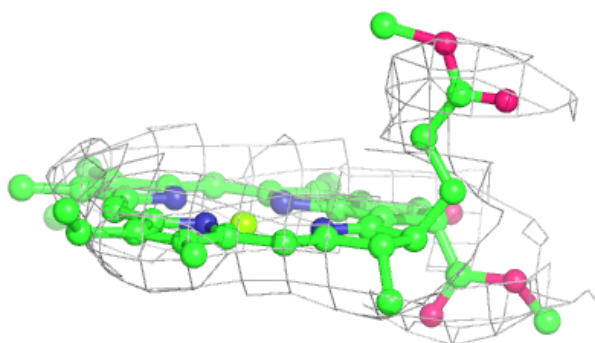
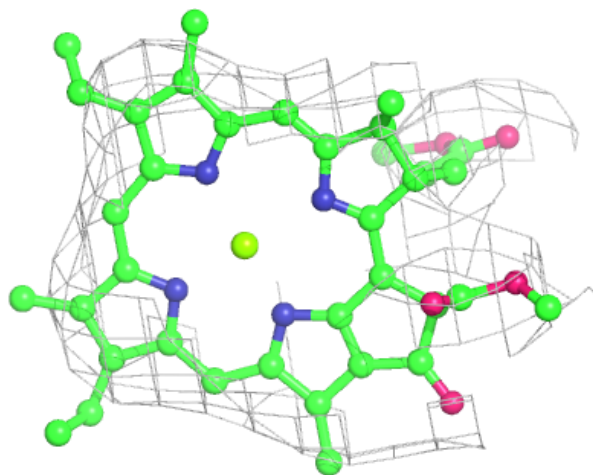
Electron density around CLA 2 1228:

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



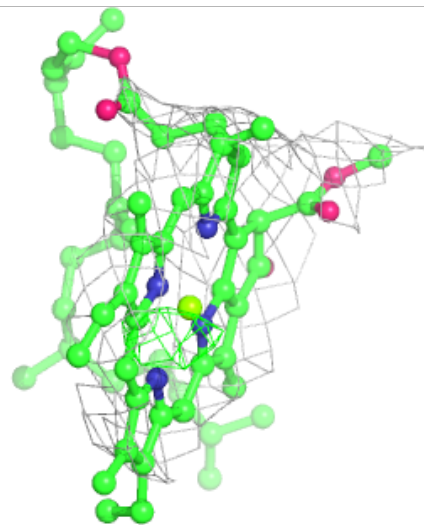
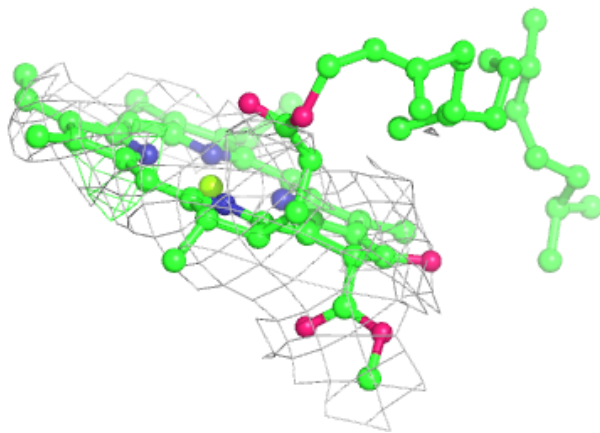
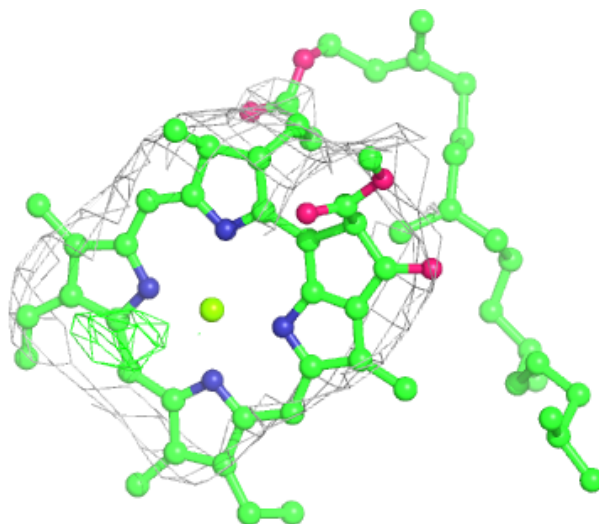
Electron density around CLA a 1130:

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



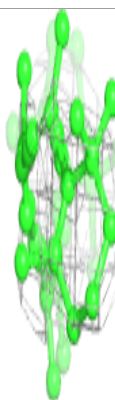
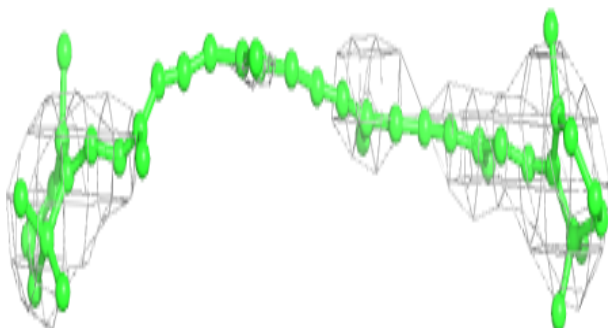
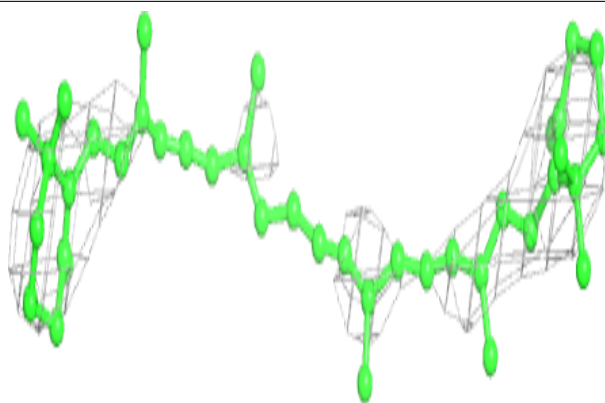
Electron density around CLA B 1229:

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

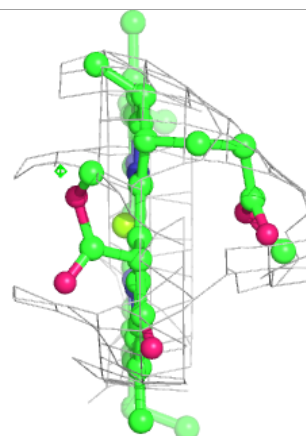
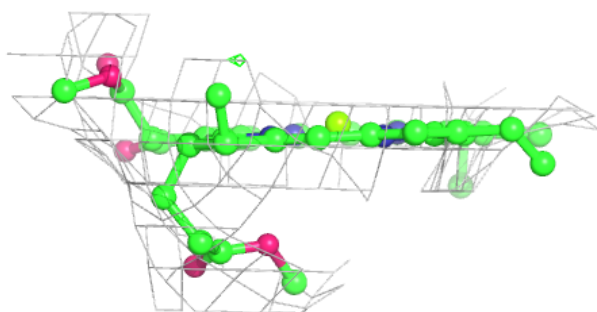
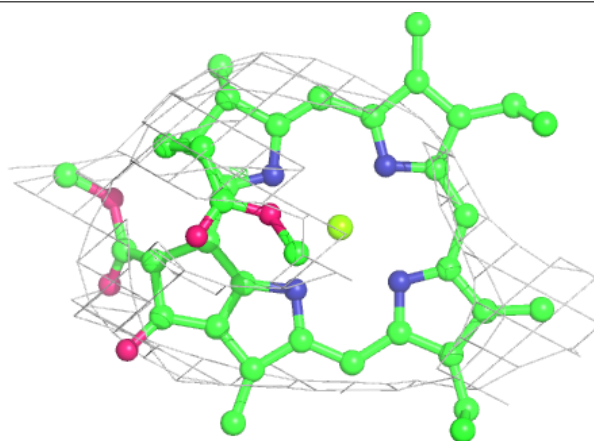


Electron density around BCR f 4018:

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

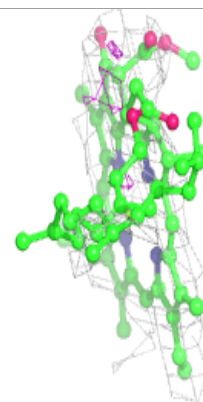
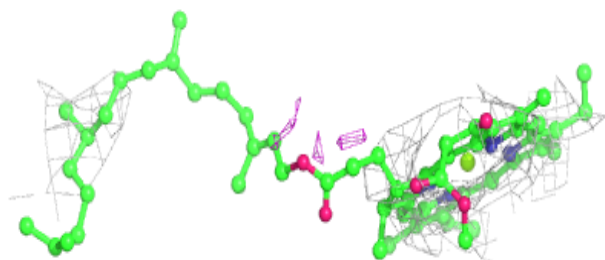
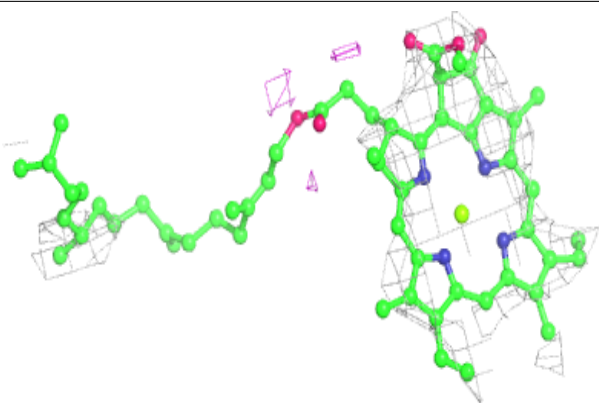
**Electron density around CLA a 1138:**

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

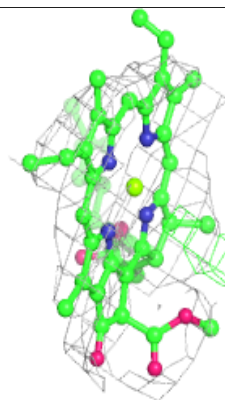
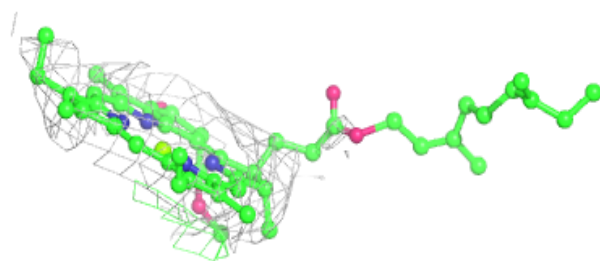
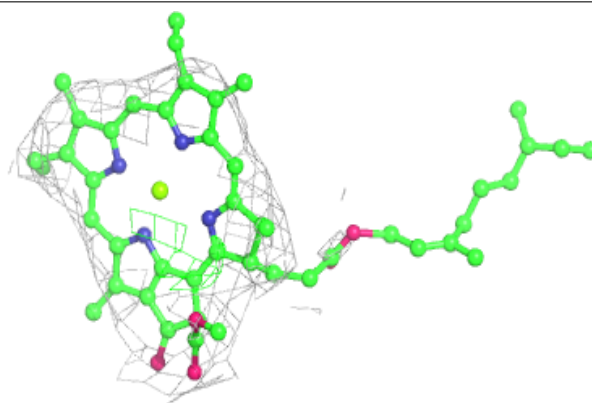


Electron density around CLA b 1210:

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

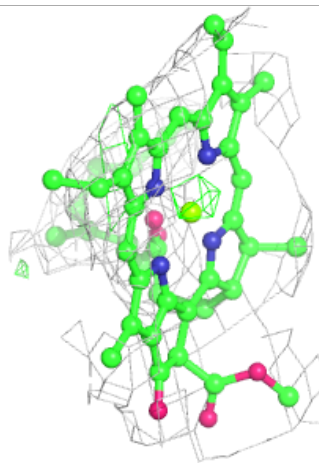
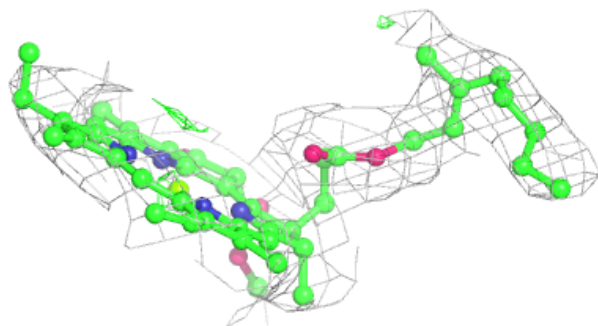
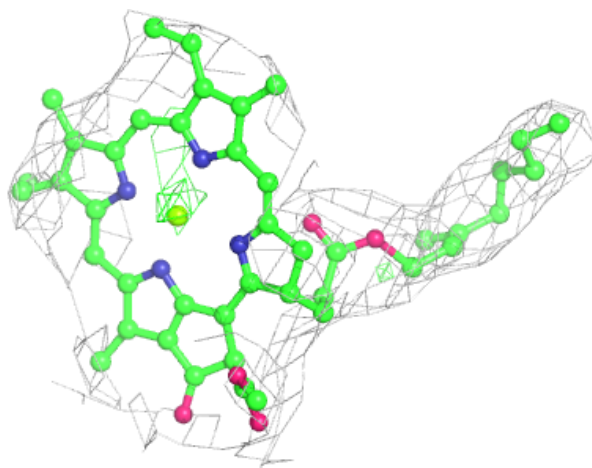
**Electron density around CLA 2 1222:**

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



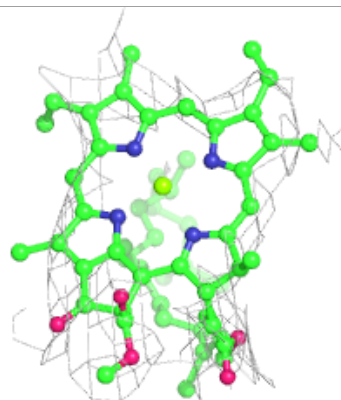
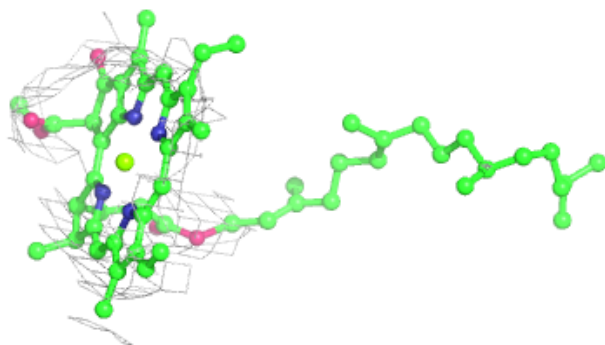
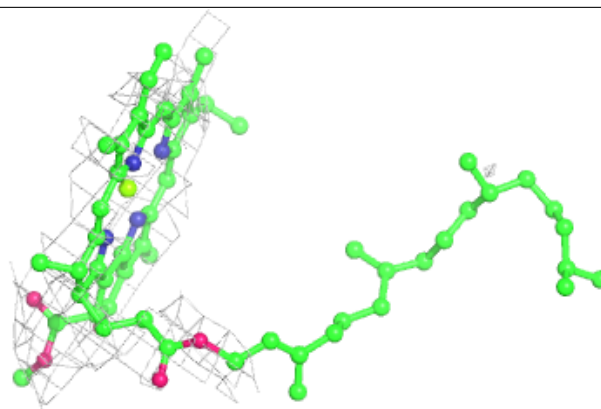
Electron density around CLA A 1110:

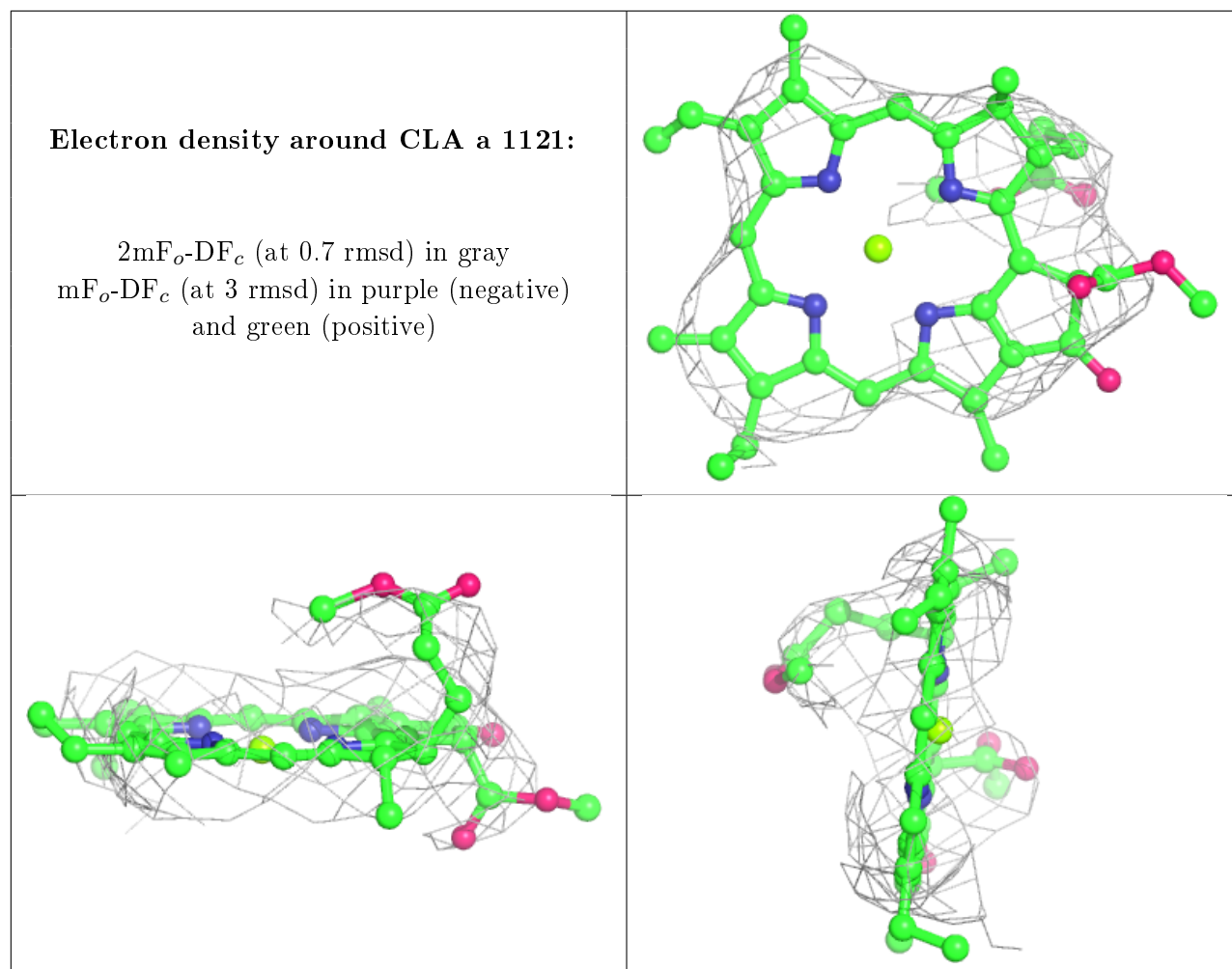
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 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)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.