



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 10:31 PM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 2.13.1
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) : 2.13.1

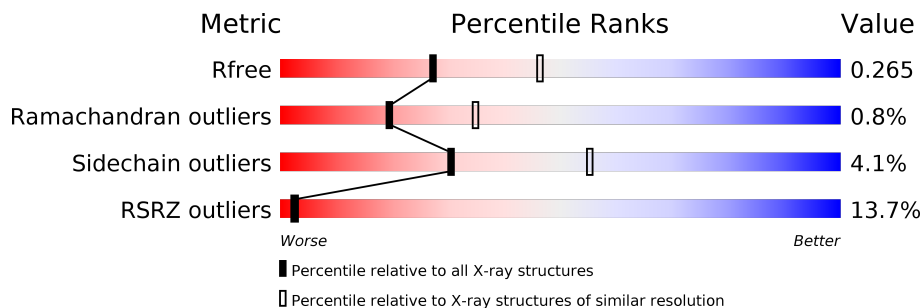
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
1	a	751	
2	2	731	
2	B	731	
3	3	80	
3	C	80	
4	D	141	

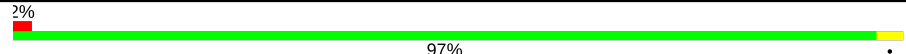
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Mol	Chain	Length	Quality of chain
4	d	141	19% 95% • •
5	5	69	23% 91% 9%
5	E	69	14% 90% 10%
6	6	143	43% 97% •
6	F	143	5% 98% •
6	f	143	19% 99% •
7	I	40	93% 8%
7	i	40	8% 95% 5%
8	7	40	33% 98% •
8	J	40	5% 95% 5%
8	j	40	20% 98% •
9	K	80	34% 78% 19% • •
10	L	157	4% 95% 5%
10	l	157	9% 94% 6%
11	9	31	10% 94% • •
11	M	31	3% 100%
11	m	31	100%
12	b	729	2% 96% •
13	c	81	5% 96% •
14	e	68	49% 91% 9%
15	k	78	78% 77% 21% •
16	1	744	20% 97% •
17	4	140	19% 98% •
18	h	38	18% 89% 11%
19	8	79	54% 86% 14%

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Mol	Chain	Length	Quality of chain
20	0	154	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	0	1501	X	-	-	-
21	CLA	0	1502	X	-	-	-
21	CLA	0	1503	X	-	-	-
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	-	-
21	CLA	1	1013	X	-	-	-
21	CLA	1	1101	X	-	-	-
21	CLA	1	1102	X	-	-	-
21	CLA	1	1103	X	-	-	-
21	CLA	1	1104	X	-	-	-
21	CLA	1	1105	X	-	-	-
21	CLA	1	1106	X	-	-	-
21	CLA	1	1107	X	-	-	-
21	CLA	1	1108	X	-	-	-
21	CLA	1	1109	X	-	-	-
21	CLA	1	1110	X	-	-	-
21	CLA	1	1111	X	-	-	-
21	CLA	1	1112	X	-	-	-
21	CLA	1	1113	X	-	-	-
21	CLA	1	1114	X	-	-	-
21	CLA	1	1115	X	-	-	-
21	CLA	1	1116	X	-	-	-
21	CLA	1	1117	X	-	-	-
21	CLA	1	1118	X	-	-	-
21	CLA	1	1119	X	-	-	-
21	CLA	1	1120	X	-	-	-
21	CLA	1	1121	X	-	-	-
21	CLA	1	1122	X	-	-	-
21	CLA	1	1123	X	-	-	-
21	CLA	1	1124	X	-	-	-
21	CLA	1	1125	X	-	-	-
21	CLA	1	1126	X	-	-	-
21	CLA	1	1127	X	-	-	-
21	CLA	1	1128	X	-	-	-
21	CLA	1	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	1130	X	-	-	-
21	CLA	1	1131	X	-	-	-
21	CLA	1	1132	X	-	-	-
21	CLA	1	1133	X	-	-	-
21	CLA	1	1134	X	-	-	-
21	CLA	1	1135	X	-	-	-
21	CLA	1	1136	X	-	-	-
21	CLA	1	1137	X	-	-	-
21	CLA	1	1138	X	-	-	-
21	CLA	1	1139	X	-	-	-
21	CLA	1	1140	X	-	-	-
21	CLA	1	1801	X	-	-	-
21	CLA	2	1021	X	-	-	-
21	CLA	2	1022	X	-	-	-
21	CLA	2	1023	X	-	-	-
21	CLA	2	1201	X	-	-	-
21	CLA	2	1202	X	-	-	-
21	CLA	2	1203	X	-	-	-
21	CLA	2	1204	X	-	-	-
21	CLA	2	1205	X	-	-	-
21	CLA	2	1206	X	-	-	-
21	CLA	2	1207	X	-	-	-
21	CLA	2	1208	X	-	-	-
21	CLA	2	1209	X	-	-	-
21	CLA	2	1210	X	-	-	-
21	CLA	2	1211	X	-	-	-
21	CLA	2	1212	X	-	-	-
21	CLA	2	1213	X	-	-	-
21	CLA	2	1214	X	-	-	-
21	CLA	2	1215	X	-	-	-
21	CLA	2	1216	X	-	-	-
21	CLA	2	1217	X	-	-	-
21	CLA	2	1218	X	-	-	-
21	CLA	2	1219	X	-	-	-
21	CLA	2	1220	X	-	-	-
21	CLA	2	1221	X	-	-	-
21	CLA	2	1222	X	-	-	-
21	CLA	2	1223	X	-	-	-
21	CLA	2	1224	X	-	-	-
21	CLA	2	1225	X	-	-	-
21	CLA	2	1226	X	-	-	-
21	CLA	2	1227	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	1228	X	-	-	-
21	CLA	2	1229	X	-	-	-
21	CLA	2	1230	X	-	-	-
21	CLA	2	1231	X	-	-	-
21	CLA	2	1232	X	-	-	-
21	CLA	2	1234	X	-	-	-
21	CLA	2	1235	X	-	-	-
21	CLA	2	1236	X	-	-	-
21	CLA	2	1237	X	-	-	-
21	CLA	2	1238	X	-	-	-
21	CLA	2	1239	X	-	-	-
21	CLA	2	1240	X	-	-	X
21	CLA	6	1301	X	-	-	-
21	CLA	6	1302	X	-	-	X
21	CLA	7	1302	X	-	-	-
21	CLA	7	1303	X	-	-	-
21	CLA	8	1401	X	-	-	-
21	CLA	8	1402	X	-	-	-
21	CLA	A	1011	X	-	-	-
21	CLA	A	1012	X	-	-	-
21	CLA	A	1013	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	-	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1801	X	-	-	-
21	CLA	B	1021	X	-	-	-
21	CLA	B	1022	X	-	-	-
21	CLA	B	1023	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	-	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	-	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1232	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	J	1302	X	-	-	-
21	CLA	J	1303	X	-	-	-
21	CLA	K	1401	X	-	-	-
21	CLA	K	1402	X	-	-	-
21	CLA	L	1501	X	-	-	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
21	CLA	a	1011	X	-	-	-
21	CLA	a	1012	X	-	-	-
21	CLA	a	1013	X	-	-	-
21	CLA	a	1101	X	-	-	-
21	CLA	a	1102	X	-	-	-
21	CLA	a	1103	X	-	-	-
21	CLA	a	1104	X	-	-	-
21	CLA	a	1105	X	-	-	-
21	CLA	a	1106	X	-	-	-
21	CLA	a	1107	X	-	-	-
21	CLA	a	1108	X	-	-	-
21	CLA	a	1109	X	-	-	-
21	CLA	a	1110	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	a	1111	X	-	-	-
21	CLA	a	1112	X	-	-	-
21	CLA	a	1113	X	-	-	X
21	CLA	a	1114	X	-	-	-
21	CLA	a	1115	X	-	-	-
21	CLA	a	1116	X	-	-	-
21	CLA	a	1117	X	-	-	-
21	CLA	a	1118	X	-	-	-
21	CLA	a	1119	X	-	-	-
21	CLA	a	1120	X	-	-	-
21	CLA	a	1121	X	-	-	-
21	CLA	a	1122	X	-	-	-
21	CLA	a	1123	X	-	-	-
21	CLA	a	1124	X	-	-	-
21	CLA	a	1125	X	-	-	-
21	CLA	a	1126	X	-	-	-
21	CLA	a	1127	X	-	-	-
21	CLA	a	1128	X	-	-	-
21	CLA	a	1129	X	-	-	-
21	CLA	a	1130	X	-	-	-
21	CLA	a	1131	X	-	-	-
21	CLA	a	1132	X	-	-	-
21	CLA	a	1133	X	-	-	-
21	CLA	a	1134	X	-	-	-
21	CLA	a	1135	X	-	-	-
21	CLA	a	1136	X	-	-	-
21	CLA	a	1137	X	-	-	-
21	CLA	a	1138	X	-	-	-
21	CLA	a	1139	X	-	-	-
21	CLA	a	1140	X	-	-	-
21	CLA	a	1801	X	-	-	-
21	CLA	b	1021	X	-	-	-
21	CLA	b	1022	X	-	-	-
21	CLA	b	1023	X	-	-	-
21	CLA	b	1201	X	-	-	-
21	CLA	b	1202	X	-	-	-
21	CLA	b	1203	X	-	-	-
21	CLA	b	1204	X	-	-	-
21	CLA	b	1205	X	-	-	-
21	CLA	b	1206	X	-	-	-
21	CLA	b	1207	X	-	-	-
21	CLA	b	1208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	b	1209	X	-	-	-
21	CLA	b	1210	X	-	-	-
21	CLA	b	1211	X	-	-	-
21	CLA	b	1212	X	-	-	-
21	CLA	b	1213	X	-	-	-
21	CLA	b	1214	X	-	-	-
21	CLA	b	1215	X	-	-	-
21	CLA	b	1216	X	-	-	-
21	CLA	b	1217	X	-	-	-
21	CLA	b	1218	X	-	-	-
21	CLA	b	1219	X	-	-	-
21	CLA	b	1220	X	-	-	-
21	CLA	b	1221	X	-	-	-
21	CLA	b	1222	X	-	-	-
21	CLA	b	1223	X	-	-	-
21	CLA	b	1224	X	-	-	-
21	CLA	b	1225	X	-	-	-
21	CLA	b	1226	X	-	-	-
21	CLA	b	1227	X	-	-	-
21	CLA	b	1228	X	-	-	-
21	CLA	b	1229	X	-	-	-
21	CLA	b	1230	X	-	-	-
21	CLA	b	1231	X	-	-	-
21	CLA	b	1232	X	-	-	-
21	CLA	b	1234	X	-	-	-
21	CLA	b	1235	X	-	-	-
21	CLA	b	1236	X	-	-	-
21	CLA	b	1237	X	-	-	-
21	CLA	b	1238	X	-	-	-
21	CLA	b	1239	X	-	-	-
21	CLA	b	1240	X	-	-	-
21	CLA	f	1301	X	-	-	-
21	CLA	f	1302	X	-	-	-
21	CLA	j	1302	X	-	-	-
21	CLA	j	1303	X	-	-	-
21	CLA	k	1401	X	-	-	-
21	CLA	k	1402	X	-	-	-
21	CLA	l	1501	X	-	-	-
21	CLA	l	1502	X	-	-	-
21	CLA	l	1503	X	-	-	-
24	BCR	1	4001	-	-	-	X
24	BCR	1	4019	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	2	4004	-	-	-	X
24	BCR	2	4018	-	-	-	X
24	BCR	6	4016	-	-	-	X
24	BCR	8	4001	-	-	-	X
24	BCR	A	4019	-	-	-	X
24	BCR	B	4018	-	-	-	X
24	BCR	a	4019	-	-	-	X
24	BCR	b	4018	-	-	-	X
24	BCR	k	4001	-	-	-	X
25	LHG	1	5007	-	-	-	X
25	LHG	2	5004	-	-	-	X
25	LHG	B	5006	-	-	-	X
25	LHG	F	5002	-	-	-	X
25	LHG	a	5007	-	-	-	X
26	LMG	2	5005	-	-	-	X
26	LMG	A	5008	-	-	-	X
26	LMG	b	5007	-	-	-	X
31	SQD	F	5001	-	-	-	X
34	ZEX	7	4015	-	-	-	X
34	ZEX	F	4016	X	-	-	-
35	LMT	1	6001	-	-	-	X

2 Entry composition [i](#)

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	751	5878	3847	1000	1003	28	0	0	0
1	a	751	5878	3847	1000	1003	28	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

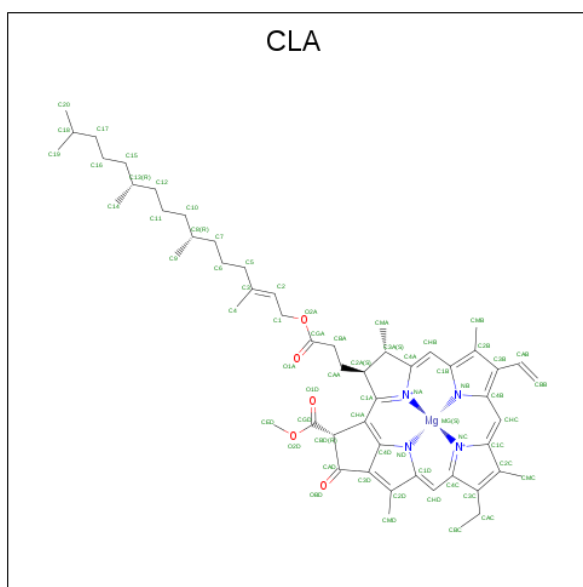
- Molecule 19 is a protein called Photosystem I reaction center subunit PsaK 2.

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

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

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

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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

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

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

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

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

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

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

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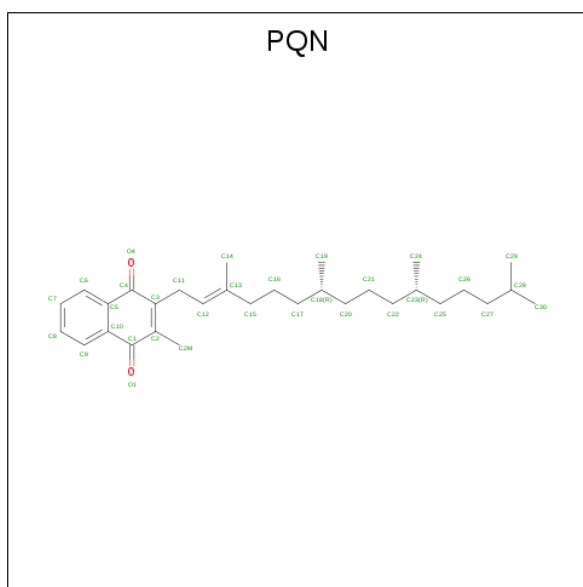
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
21	2	1	60	50	1	4	5	0	0
21	2	1	45	35	1	4	5	0	0
21	2	1	65	55	1	4	5	0	0
21	2	1	50	40	1	4	5	0	0
21	2	1	41	33	1	4	3	0	0
21	2	1	50	40	1	4	5	0	0
21	2	1	59	49	1	4	5	0	0
21	2	1	60	50	1	4	5	0	0
21	2	1	50	40	1	4	5	0	0
21	2	1	52	42	1	4	5	0	0
21	2	1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

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

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



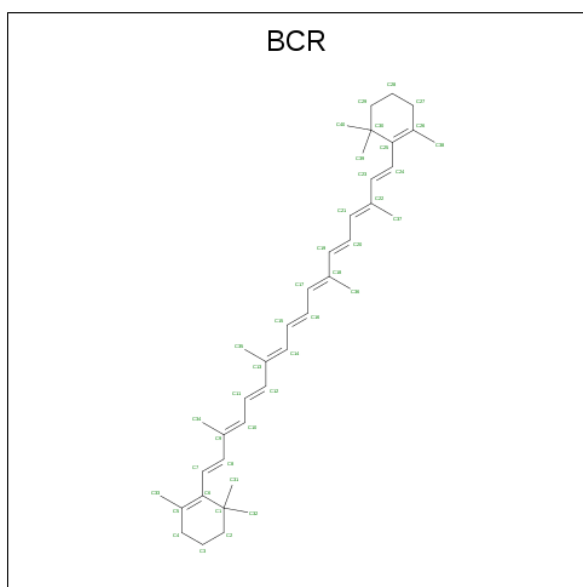
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		
22	a	1	Total	C	O	0	0
			33	31	2		
22	b	1	Total	C	O	0	0
			33	31	2		
22	1	1	Total	C	O	0	0
			33	31	2		
22	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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

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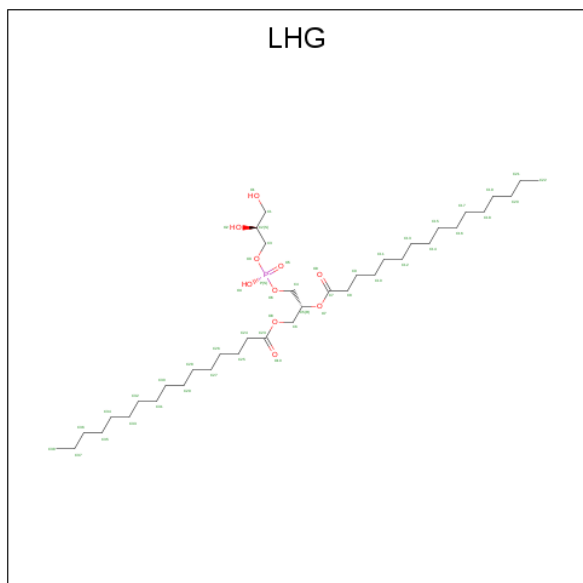
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total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

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

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



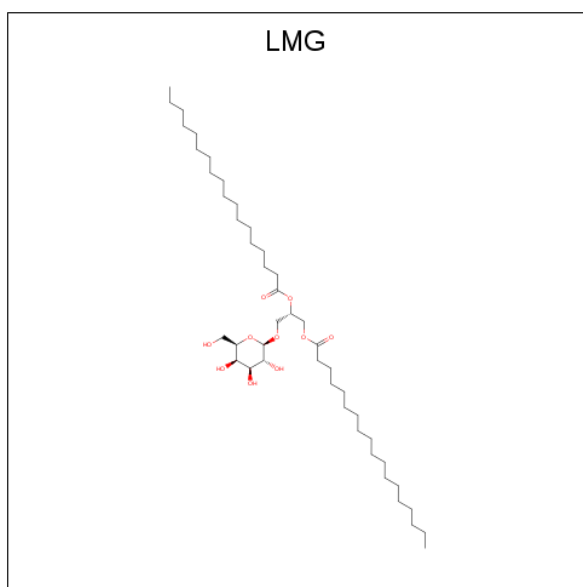
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	F	1	Total C O P 49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

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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



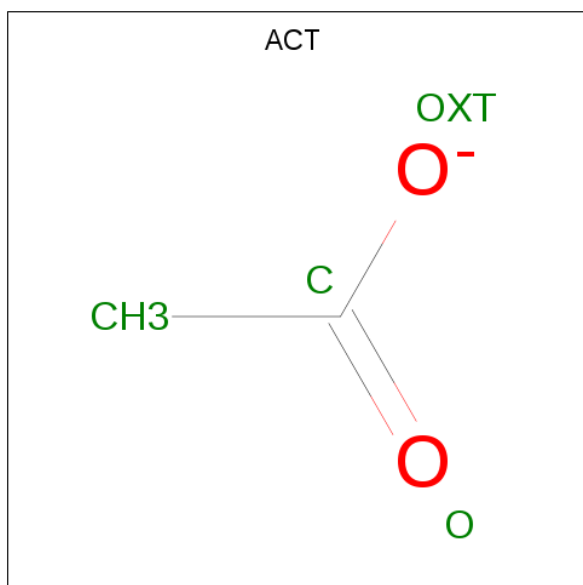
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			50	40	10		
26	A	1	Total	C	O	0	0
			48	38	10		
26	A	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	a	1	Total	C	O	0	0
			50	40	10		
26	a	1	Total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

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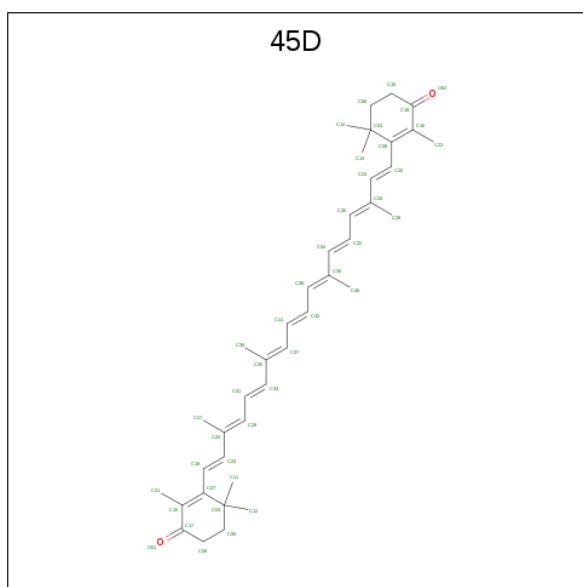
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	2	1	Total	C	O	0	0
			55	45	10		
26	0	1	Total	C	O	0	0
			55	45	10		

- Molecule 27 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

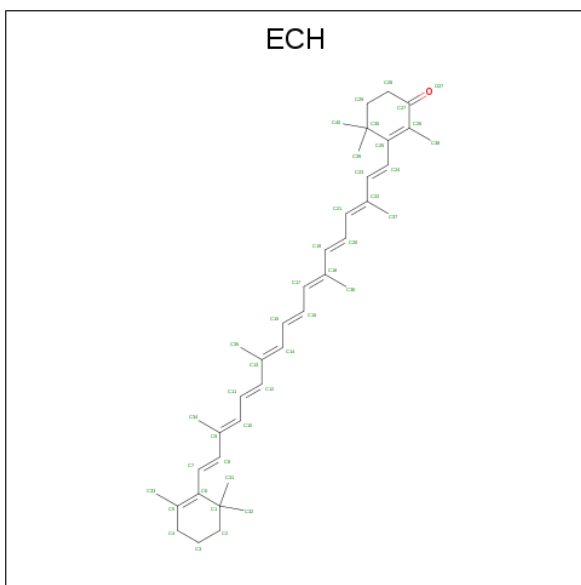


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	B	1	Total	C O	0	0
			42	40 2		
28	h	1	Total	C O	0	0
			42	40 2		

- Molecule 29 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

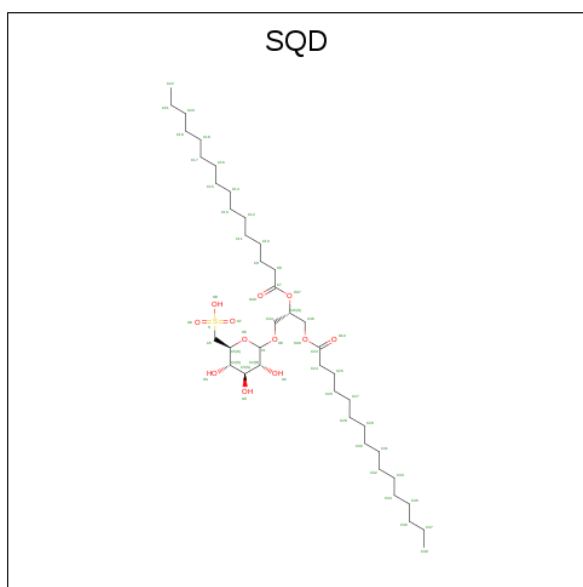
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	B	1	Total	Cl	0	0
			1	1		
29	b	1	Total	Cl	0	0
			1	1		
29	2	1	Total	Cl	0	0
			1	1		

- Molecule 30 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



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

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



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

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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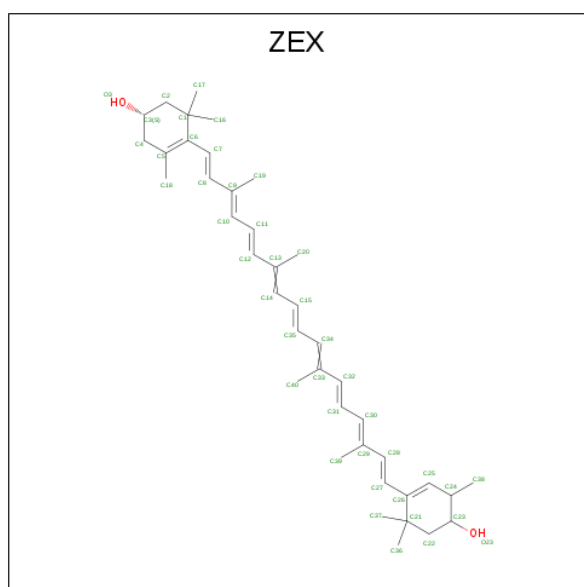
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total Ca 1 1	0	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

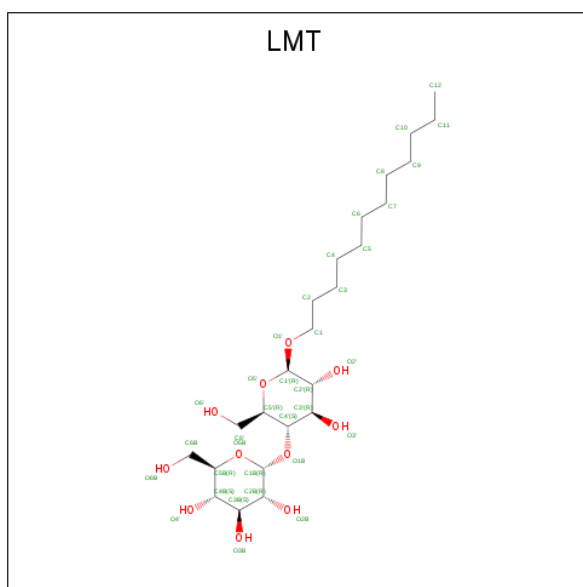
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Mg 1 1	0	0
33	b	1	Total Mg 1 1	0	0

- Molecule 34 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



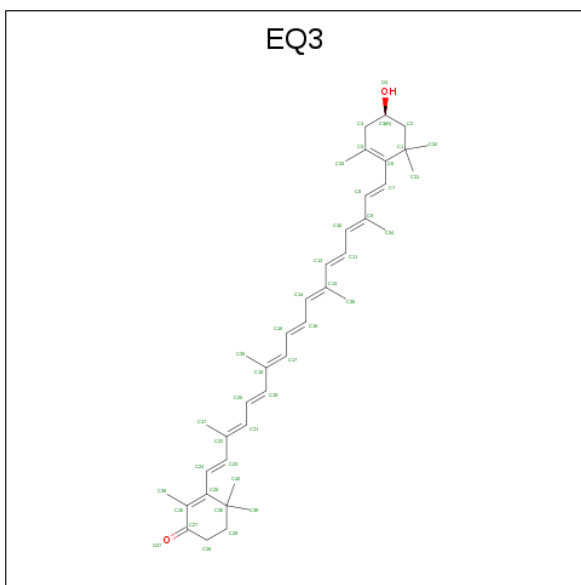
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total C O 42 40 2	0	0
34	J	1	Total C O 42 40 2	0	0
34	j	1	Total C O 42 40 2	0	0
34	7	1	Total C O 42 40 2	0	0

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



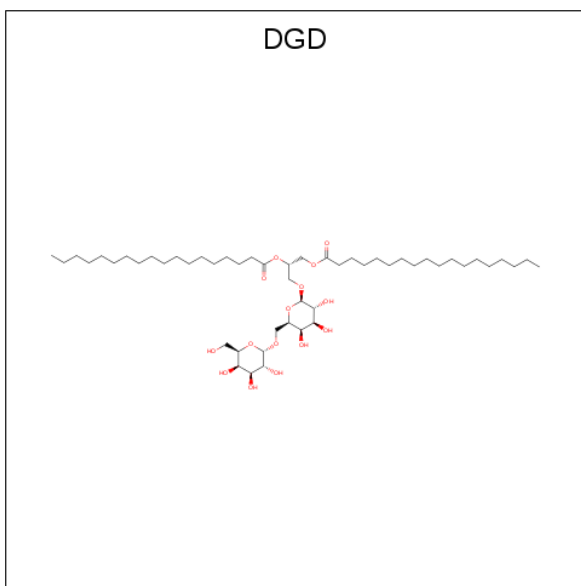
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	F	1	Total	C	O	0	0
			35	24	11		
35	L	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	0	1	Total	C	O	0	0
			35	24	11		

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



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

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



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

- Molecule 38 is water.

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

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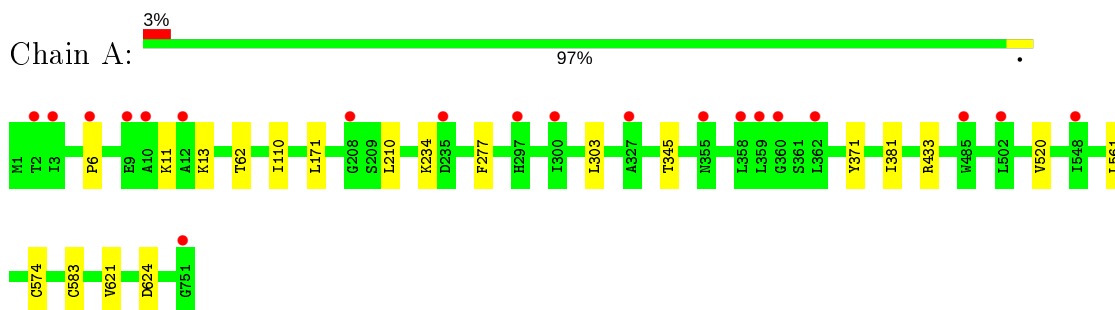
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	2	24	Total 24	O 24	0	0
38	3	11	Total 11	O 11	0	0
38	4	13	Total 13	O 13	0	0
38	5	4	Total 4	O 4	0	0
38	6	1	Total 1	O 1	0	0
38	h	3	Total 3	O 3	0	0
38	7	1	Total 1	O 1	0	0
38	8	2	Total 2	O 2	0	0
38	0	33	Total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

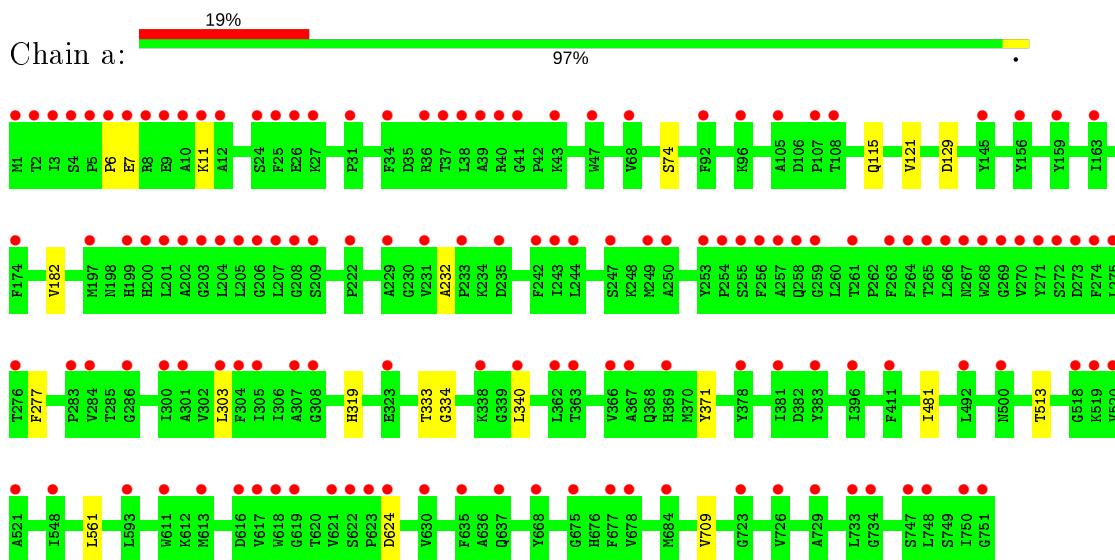
3 Residue-property plots [i](#)

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

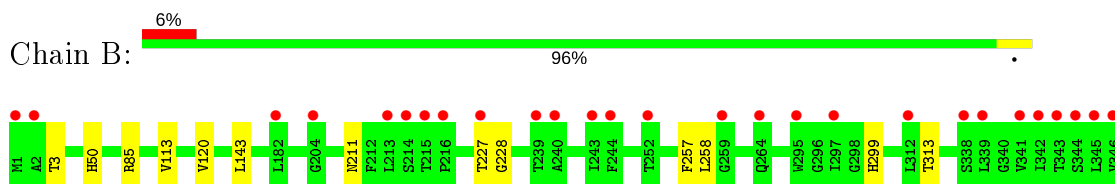
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

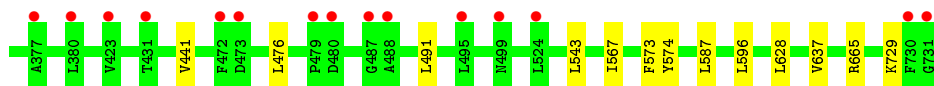


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

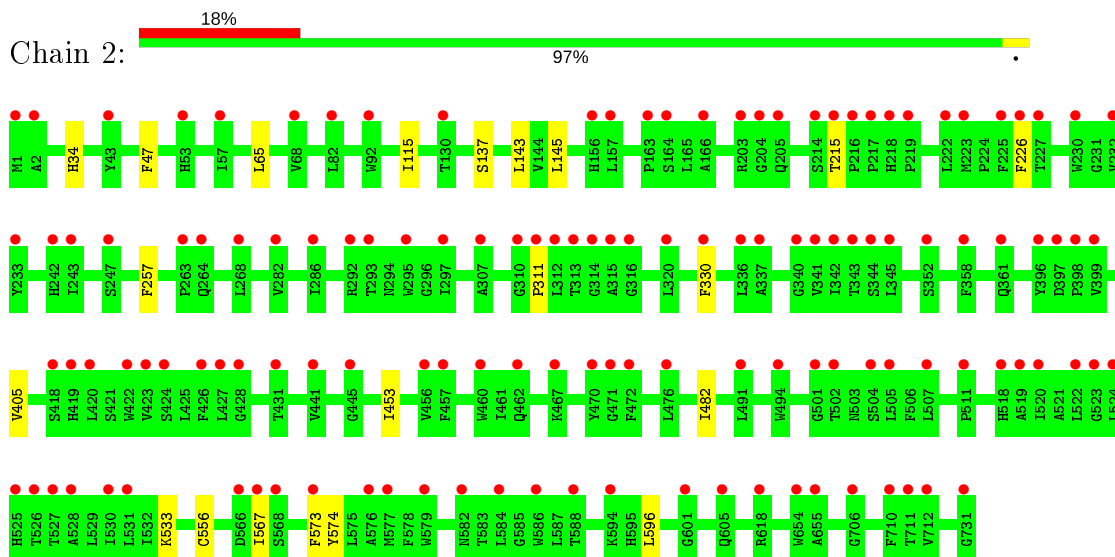


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

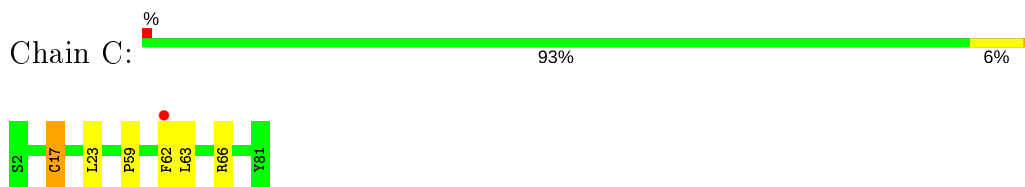




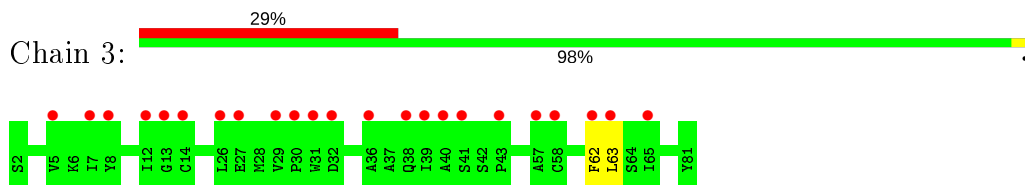
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



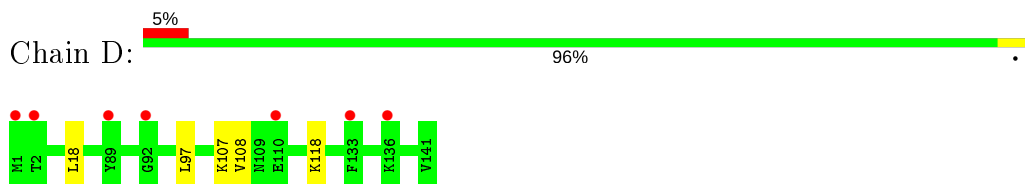
- Molecule 3: Photosystem I iron-sulfur center



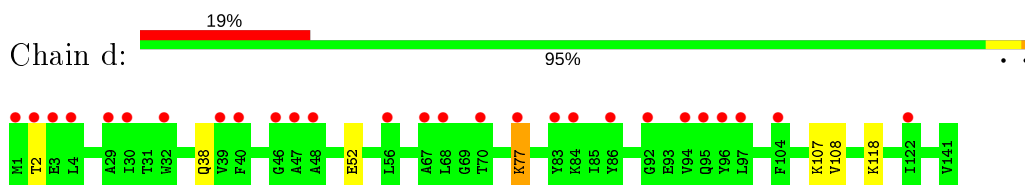
- Molecule 3: Photosystem I iron-sulfur center



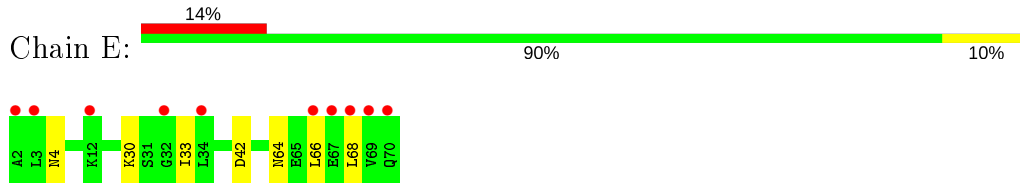
- Molecule 4: Photosystem I reaction center subunit II



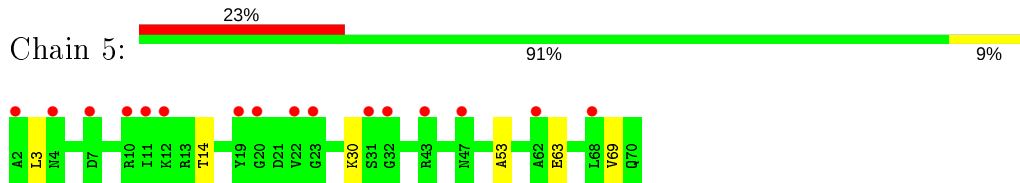
- Molecule 4: Photosystem I reaction center subunit II



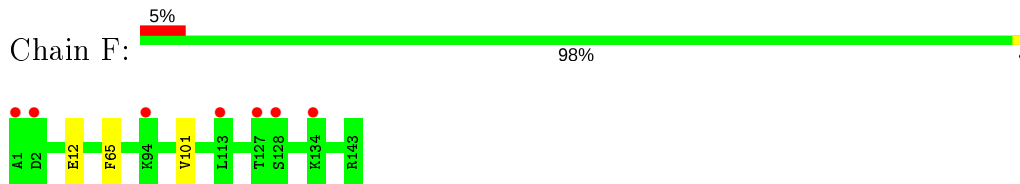
- Molecule 5: Photosystem I reaction center subunit IV



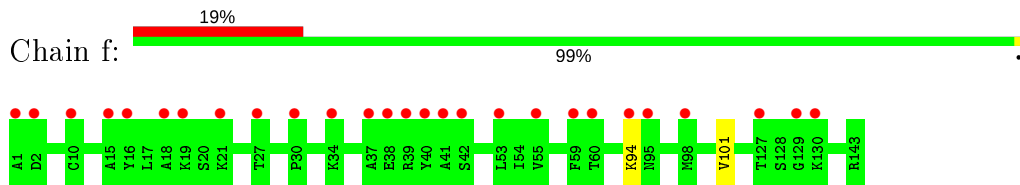
- Molecule 5: Photosystem I reaction center subunit IV



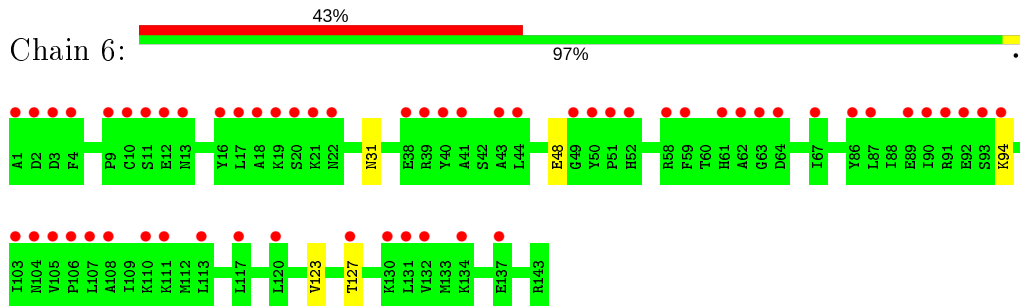
- Molecule 6: Photosystem I reaction center subunit III



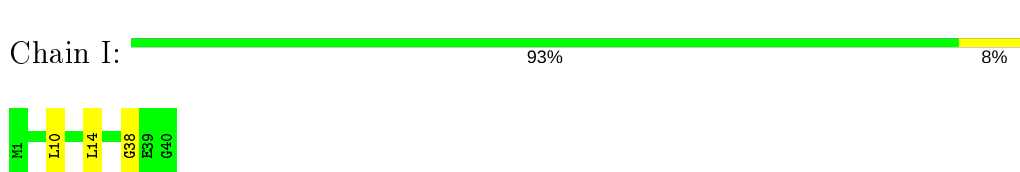
- Molecule 6: Photosystem I reaction center subunit III



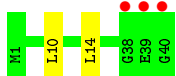
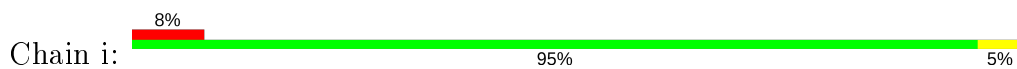
- Molecule 6: Photosystem I reaction center subunit III



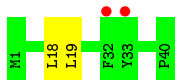
- Molecule 7: Photosystem I reaction center subunit VIII



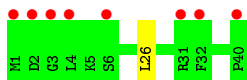
- Molecule 7: Photosystem I reaction center subunit VIII



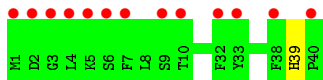
- Molecule 8: Photosystem I reaction center subunit IX



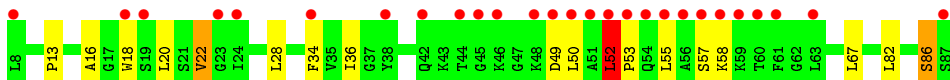
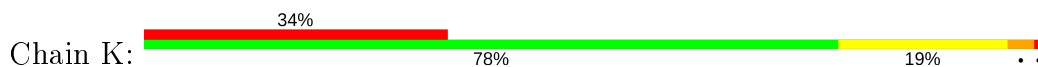
- Molecule 8: Photosystem I reaction center subunit IX



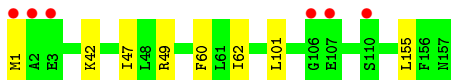
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit PsaK 2



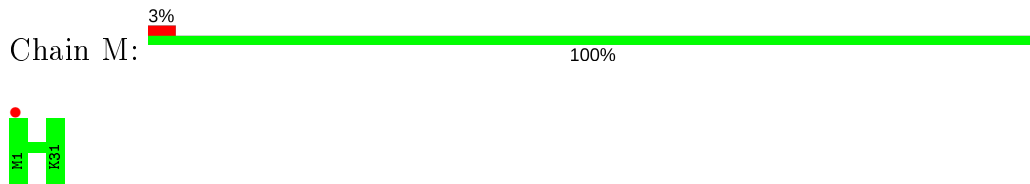
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII

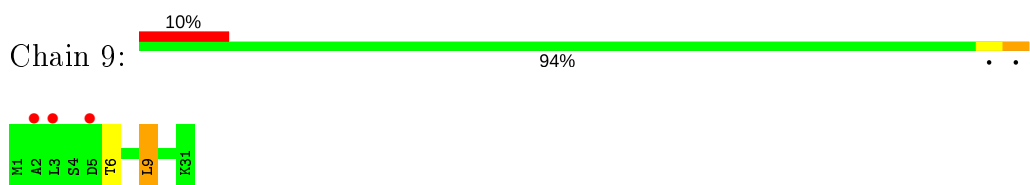


- Molecule 11: Photosystem I reaction center subunit XII

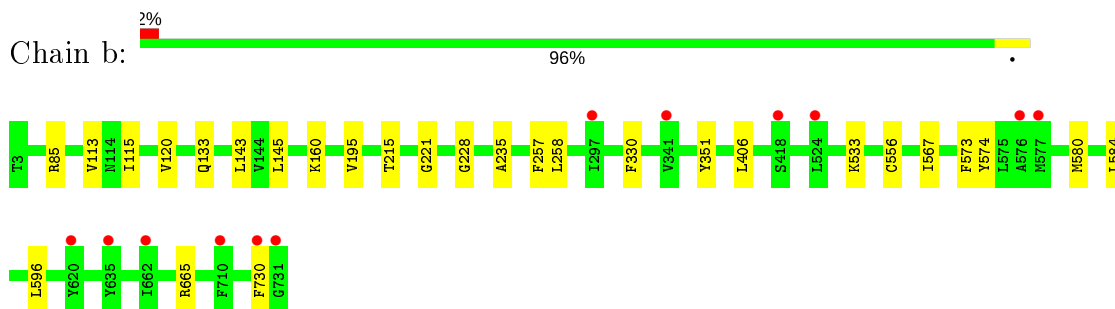


There are no outlier residues recorded for this chain.

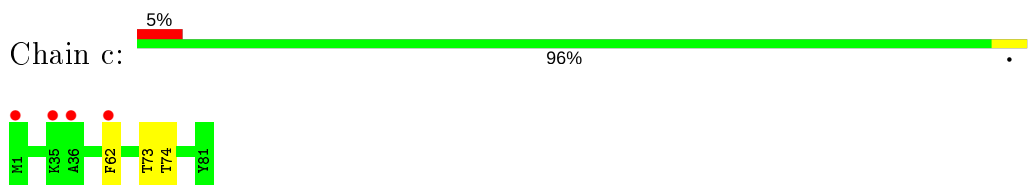
- Molecule 11: Photosystem I reaction center subunit XII



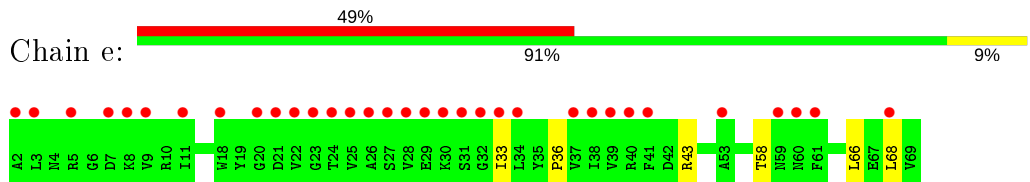
- Molecule 12: Photosystem I P700 chlorophyll a apoprotein A2



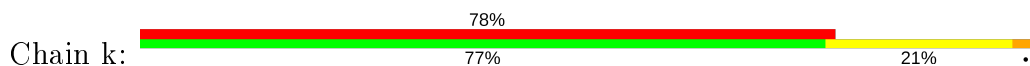
- Molecule 13: Photosystem I iron-sulfur center

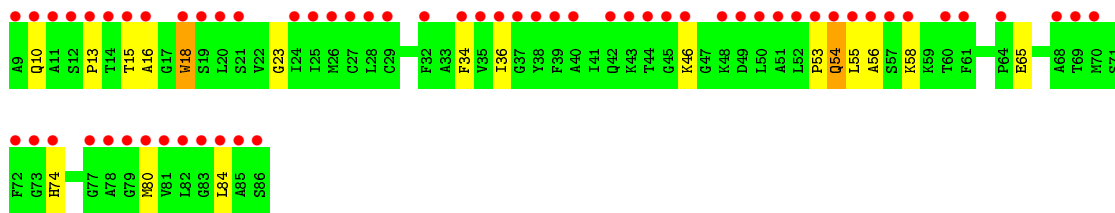


- Molecule 14: Photosystem I reaction center subunit IV



- Molecule 15: Photosystem I reaction center subunit PsaK 2

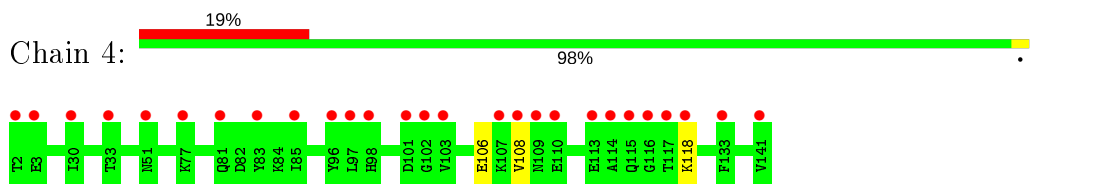




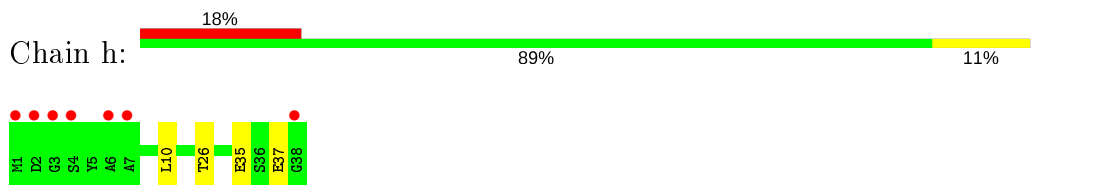
• Molecule 16: Photosystem I P700 chlorophyll a apoprotein A1



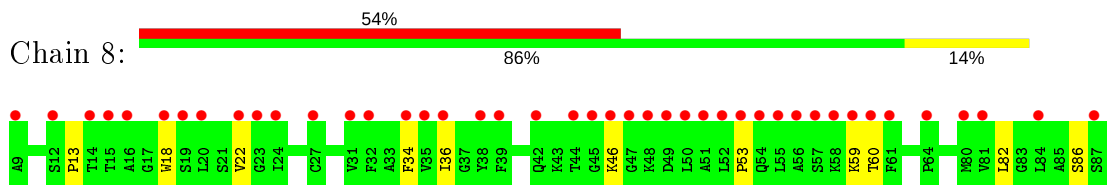
• Molecule 17: Photosystem I reaction center subunit II



• Molecule 18: Photosystem I reaction center subunit VIII

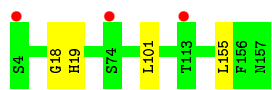


• Molecule 19: Photosystem I reaction center subunit PsaK 2



- Molecule 20: Photosystem I reaction center subunit XI

Chain 0:  2%
97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	212.17Å 137.62Å 225.09Å 90.00° 116.74° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.48-2.50) 99.4 (49.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.265	Depositor DCC
R_{free} test set	7881 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	77117	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

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

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, MG, DGD, CL, SF4, LMT, CLA, PQN, ECH, BCR, ACT, ZEX, LMG, 45D, EQ3, CA, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/6078	0.46	0/8284
1	a	0.27	0/6078	0.42	0/8284
2	2	0.26	0/5994	0.41	0/8195
2	B	0.33	0/5994	0.45	2/8195 (0.0%)
3	3	0.24	0/610	0.45	0/826
3	C	0.37	1/610 (0.2%)	0.56	1/826 (0.1%)
4	D	0.29	0/1126	0.49	0/1517
4	d	0.26	0/1126	0.48	0/1517
5	5	0.25	0/552	0.39	0/745
5	E	0.26	0/552	0.44	0/745
6	6	0.25	0/1143	0.40	0/1553
6	F	0.26	0/1143	0.43	0/1553
6	f	0.25	0/1143	0.40	0/1553
7	I	0.26	0/322	0.43	0/438
7	i	0.26	0/322	0.44	0/438
8	7	0.27	0/328	0.42	0/443
8	J	0.28	0/328	0.46	0/443
8	j	0.26	0/328	0.42	0/443
9	K	0.29	0/590	0.53	0/797
10	L	0.28	0/1208	0.47	0/1640
10	l	0.27	0/1208	0.43	0/1640
11	9	0.25	0/241	0.55	1/326 (0.3%)
11	M	0.27	0/241	0.41	0/326
11	m	0.27	0/241	0.39	0/326
12	b	0.31	0/5981	0.46	1/8178 (0.0%)
13	c	0.26	0/618	0.49	0/836
14	e	0.26	0/542	0.42	0/733
15	k	0.28	0/570	0.45	0/770
16	1	0.26	0/6024	0.41	0/8209
17	4	0.26	0/1118	0.45	0/1507
18	h	0.26	0/309	0.43	0/421
19	8	0.27	0/576	0.46	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	0	0.28	0/1186	0.43	0/1611
All	All	0.29	1/54430 (0.0%)	0.44	5/74096 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	17	CYS	CB-SG	5.38	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	665	ARG	N-CA-C	7.42	131.03	111.00
2	B	587	LEU	CA-CB-CG	6.99	131.38	115.30
2	B	665	ARG	N-CA-C	6.41	128.31	111.00
11	9	9	LEU	CA-CB-CG	6.23	129.62	115.30
3	C	17	CYS	CA-CB-SG	5.76	124.37	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	52	LEU	Peptide

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/751 (100%)	719 (96%)	28 (4%)	2 (0%)	41	61
1	a	749/751 (100%)	712 (95%)	31 (4%)	6 (1%)	19	35
2	2	729/731 (100%)	694 (95%)	33 (4%)	2 (0%)	41	61
2	B	729/731 (100%)	697 (96%)	28 (4%)	4 (0%)	29	48
3	3	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	12	21
3	C	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	5	8
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	39
5	5	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	4	6
5	E	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
6	6	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	22	39
6	F	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	22	39
6	f	141/143 (99%)	134 (95%)	7 (5%)	0	100	100
7	I	38/40 (95%)	36 (95%)	1 (3%)	1 (3%)	5	8
7	i	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	7	38/40 (95%)	38 (100%)	0	0	100	100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	K	79/80 (99%)	66 (84%)	6 (8%)	7 (9%)	1	0
10	L	155/157 (99%)	148 (96%)	7 (4%)	0	100	100
10	l	155/157 (99%)	150 (97%)	3 (2%)	2 (1%)	12	21
11	9	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	b	727/729 (100%)	701 (96%)	22 (3%)	4 (1%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	c	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12	21
14	e	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	10	18
15	k	76/78 (97%)	60 (79%)	7 (9%)	9 (12%)	0	0
16	1	742/744 (100%)	706 (95%)	34 (5%)	2 (0%)	41	61
17	4	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
18	h	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	7
19	8	77/79 (98%)	64 (83%)	9 (12%)	4 (5%)	2	2
20	0	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22	39
All	All	6706/6771 (99%)	6374 (95%)	277 (4%)	55 (1%)	19	35

All (55) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/603 (100%)	585 (97%)	18 (3%)	41 68
1	a	603/603 (100%)	588 (98%)	15 (2%)	47 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	583/583 (100%)	564 (97%)	19 (3%)	38	64
2	B	583/583 (100%)	563 (97%)	20 (3%)	37	63
3	3	68/68 (100%)	67 (98%)	1 (2%)	65	85
3	C	68/68 (100%)	64 (94%)	4 (6%)	19	37
4	D	116/116 (100%)	111 (96%)	5 (4%)	29	53
4	d	116/116 (100%)	109 (94%)	7 (6%)	19	37
5	5	58/58 (100%)	54 (93%)	4 (7%)	15	30
5	E	58/58 (100%)	51 (88%)	7 (12%)	5	9
6	6	119/119 (100%)	115 (97%)	4 (3%)	37	63
6	F	119/119 (100%)	117 (98%)	2 (2%)	60	82
6	f	119/119 (100%)	117 (98%)	2 (2%)	60	82
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	34
7	i	32/32 (100%)	30 (94%)	2 (6%)	18	34
8	7	35/35 (100%)	34 (97%)	1 (3%)	42	69
8	J	35/35 (100%)	33 (94%)	2 (6%)	20	39
8	j	35/35 (100%)	34 (97%)	1 (3%)	42	69
9	K	60/60 (100%)	46 (77%)	14 (23%)	1	1
10	L	118/118 (100%)	110 (93%)	8 (7%)	16	30
10	l	118/118 (100%)	111 (94%)	7 (6%)	19	37
11	9	25/25 (100%)	23 (92%)	2 (8%)	12	23
11	M	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	b	582/582 (100%)	559 (96%)	23 (4%)	31	56
13	c	69/69 (100%)	67 (97%)	2 (3%)	42	69
14	e	57/57 (100%)	52 (91%)	5 (9%)	10	19
15	k	57/58 (98%)	46 (81%)	11 (19%)	1	2
16	1	596/596 (100%)	577 (97%)	19 (3%)	39	65
17	4	115/115 (100%)	112 (97%)	3 (3%)	46	72
18	h	31/31 (100%)	28 (90%)	3 (10%)	8	16
19	8	58/59 (98%)	51 (88%)	7 (12%)	5	9
20	0	116/116 (100%)	113 (97%)	3 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5434/5436 (100%)	5211 (96%)	223 (4%)	30 55

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	13	LYS
1	A	62	THR
1	A	110	ILE
1	A	171	LEU
1	A	210	LEU
1	A	234	LYS
1	A	277	PHE
1	A	303	LEU
1	A	345	THR
1	A	371	TYR
1	A	381	ILE
1	A	433	ARG
1	A	520	VAL
1	A	561	LEU
1	A	583	CYS
1	A	621	VAL
1	A	624	ASP
2	B	50	HIS
2	B	85	ARG
2	B	113	VAL
2	B	120	VAL
2	B	143	LEU
2	B	257	PHE
2	B	258	LEU
2	B	299	HIS
2	B	313	THR
2	B	441	VAL
2	B	476	LEU
2	B	491	LEU
2	B	543	LEU
2	B	567	ILE
2	B	573	PHE
2	B	574	TYR
2	B	596	LEU
2	B	628	LEU
2	B	637	VAL

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Mol	Chain	Res	Type
2	B	729	LYS
3	C	17	CYS
3	C	23	LEU
3	C	63	LEU
3	C	66	ARG
4	D	18	LEU
4	D	97	LEU
4	D	107	LYS
4	D	108	VAL
4	D	118	LYS
5	E	4	ASN
5	E	30	LYS
5	E	33	ILE
5	E	42	ASP
5	E	64	ASN
5	E	66	LEU
5	E	68	LEU
6	F	12	GLU
6	F	101	VAL
7	I	10	LEU
7	I	14	LEU
8	J	18	LEU
8	J	19	LEU
9	K	18	TRP
9	K	20	LEU
9	K	22	VAL
9	K	28	LEU
9	K	34	PHE
9	K	36	ILE
9	K	49	ASP
9	K	50	LEU
9	K	52	LEU
9	K	55	LEU
9	K	58	LYS
9	K	67	LEU
9	K	82	LEU
9	K	86	SER
10	L	1	MET
10	L	42	LYS
10	L	47	ILE
10	L	49	ARG
10	L	60	PHE

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Mol	Chain	Res	Type
10	L	62	ILE
10	L	101	LEU
10	L	155	LEU
1	a	7	GLU
1	a	11	LYS
1	a	74	SER
1	a	129	ASP
1	a	277	PHE
1	a	303	LEU
1	a	319	HIS
1	a	333	THR
1	a	340	LEU
1	a	371	TYR
1	a	481	ILE
1	a	513	THR
1	a	561	LEU
1	a	624	ASP
1	a	709	VAL
12	b	85	ARG
12	b	113	VAL
12	b	115	ILE
12	b	120	VAL
12	b	133	GLN
12	b	143	LEU
12	b	145	LEU
12	b	160	LYS
12	b	195	VAL
12	b	215	THR
12	b	257	PHE
12	b	258	LEU
12	b	330	PHE
12	b	351	TYR
12	b	406	LEU
12	b	533	LYS
12	b	567	ILE
12	b	573	PHE
12	b	574	TYR
12	b	580	MET
12	b	584	LEU
12	b	596	LEU
12	b	730	PHE
13	c	73	THR

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Mol	Chain	Res	Type
13	c	74	THR
4	d	2	THR
4	d	38	GLN
4	d	52	GLU
4	d	77	LYS
4	d	107	LYS
4	d	108	VAL
4	d	118	LYS
14	e	33	ILE
14	e	43	ARG
14	e	58	THR
14	e	66	LEU
14	e	68	LEU
6	f	94	LYS
6	f	101	VAL
7	i	10	LEU
7	i	14	LEU
8	j	26	LEU
15	k	10	GLN
15	k	18	TRP
15	k	34	PHE
15	k	36	ILE
15	k	46	LYS
15	k	54	GLN
15	k	58	LYS
15	k	65	GLU
15	k	74	HIS
15	k	80	MET
15	k	84	LEU
10	l	19	HIS
10	l	42	LYS
10	l	44	LEU
10	l	101	LEU
10	l	136	PHE
10	l	143	GLU
10	l	155	LEU
16	1	11	LYS
16	1	73	PHE
16	1	153	THR
16	1	251	GLU
16	1	252	LEU
16	1	260	LEU

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Mol	Chain	Res	Type
16	1	273	ASP
16	1	277	PHE
16	1	303	LEU
16	1	319	HIS
16	1	340	LEU
16	1	371	TYR
16	1	459	ASP
16	1	513	THR
16	1	561	LEU
16	1	583	CYS
16	1	585	VAL
16	1	709	VAL
16	1	714	GLN
2	2	34	HIS
2	2	47	PHE
2	2	65	LEU
2	2	115	ILE
2	2	137	SER
2	2	143	LEU
2	2	145	LEU
2	2	215	THR
2	2	226	PHE
2	2	257	PHE
2	2	330	PHE
2	2	405	VAL
2	2	453	ILE
2	2	482	ILE
2	2	533	LYS
2	2	567	ILE
2	2	573	PHE
2	2	574	TYR
2	2	596	LEU
3	3	63	LEU
17	4	106	GLU
17	4	108	VAL
17	4	118	LYS
5	5	3	LEU
5	5	30	LYS
5	5	63	GLU
5	5	69	VAL
6	6	31	ASN
6	6	48	GLU

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Mol	Chain	Res	Type
6	6	123	VAL
6	6	127	THR
18	h	10	LEU
18	h	26	THR
18	h	35	GLU
8	7	39	HIS
19	8	22	VAL
19	8	34	PHE
19	8	36	ILE
19	8	46	LYS
19	8	59	LYS
19	8	60	THR
19	8	82	LEU
20	0	19	HIS
20	0	101	LEU
20	0	155	LEU
11	9	6	THR
11	9	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	276	HIS
2	2	277	HIS
2	2	518	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
21	CLA	A	1012	38	59,73,73	1.27	7 (11%)	67,113,113	1.85	8 (11%)
21	CLA	2	1220	-	36,53,73	1.62	9 (25%)	39,89,113	2.04	6 (15%)
26	LMG	0	5001	-	55,55,55	1.14	6 (10%)	63,63,63	1.28	6 (9%)
21	CLA	B	1214	-	59,73,73	1.27	9 (15%)	67,113,113	1.63	6 (8%)
21	CLA	1	1112	-	44,58,73	1.47	9 (20%)	49,95,113	2.10	7 (14%)
21	CLA	1	1139	-	59,73,73	1.27	9 (15%)	67,113,113	1.78	6 (8%)
21	CLA	1	1122	-	54,68,73	1.32	9 (16%)	61,107,113	1.80	5 (8%)
21	CLA	1	1011	-	59,73,73	1.26	7 (11%)	67,113,113	1.84	8 (11%)
24	BCR	a	4001	-	41,41,41	0.70	0	56,56,56	3.44	14 (25%)
37	DGD	L	5004	-	67,67,67	1.07	6 (8%)	81,81,81	1.02	2 (2%)
21	CLA	2	1231	38	40,54,73	1.50	8 (20%)	44,90,113	1.91	5 (11%)
21	CLA	b	1220	-	59,73,73	1.26	8 (13%)	67,113,113	1.77	7 (10%)
21	CLA	2	1213	-	44,58,73	1.45	8 (18%)	49,95,113	2.09	5 (10%)
21	CLA	B	1204	-	59,73,73	1.27	8 (13%)	67,113,113	1.64	6 (8%)
21	CLA	2	1229	-	59,73,73	1.28	8 (13%)	67,113,113	1.67	6 (8%)
21	CLA	2	1214	-	53,67,73	1.34	9 (16%)	59,105,113	1.75	9 (15%)
21	CLA	a	1102	-	59,73,73	1.25	8 (13%)	67,113,113	1.85	7 (10%)
27	ACT	a	7001	-	1,3,3	6.51	1 (100%)	0,3,3	0.00	-
21	CLA	B	1220	-	51,65,73	1.36	7 (13%)	57,103,113	1.87	7 (12%)
35	LMT	F	6001	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	1 (2%)
21	CLA	1	1131	-	59,73,73	1.26	8 (13%)	67,113,113	1.64	5 (7%)
21	CLA	A	1801	25	59,73,73	1.24	7 (11%)	67,113,113	1.80	7 (10%)
21	CLA	j	1302	-	59,73,73	1.27	8 (13%)	67,113,113	1.79	5 (7%)
25	LHG	l	5002	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
24	BCR	1	4001	-	41,41,41	0.70	0	56,56,56	3.27	10 (17%)
23	SF4	C	3003	3	0,12,12	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	6	4016	-	41,41,41	0.70	0	56,56,56	3.42	13 (23%)
21	CLA	b	1225	-	59,73,73	1.24	7 (11%)	67,113,113	1.65	7 (10%)
21	CLA	2	1023	-	59,73,73	1.25	8 (13%)	67,113,113	1.91	7 (10%)
26	LMG	A	5004	-	48,48,55	0.98	4 (8%)	56,56,63	1.09	3 (5%)
25	LHG	2	5004	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
21	CLA	b	1202	-	59,73,73	1.23	7 (11%)	67,113,113	1.83	7 (10%)
21	CLA	A	1114	38	59,73,73	1.29	8 (13%)	67,113,113	1.64	6 (8%)
24	BCR	B	4010	-	41,41,41	0.65	0	56,56,56	3.18	11 (19%)
21	CLA	a	1116	-	54,68,73	1.33	8 (14%)	61,107,113	1.82	7 (11%)
34	ZEX	7	4015	-	42,43,43	5.79	4 (9%)	55,60,60	6.95	12 (21%)
34	ZEX	j	4015	-	42,43,43	5.77	3 (7%)	55,60,60	7.02	13 (23%)
21	CLA	b	1216	38	59,73,73	1.27	9 (15%)	67,113,113	1.71	5 (7%)
21	CLA	b	1211	-	59,73,73	1.25	9 (15%)	67,113,113	1.69	3 (4%)
28	45D	B	4011	-	43,43,43	3.44	15 (34%)	54,60,60	2.24	18 (33%)
21	CLA	A	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.77	9 (13%)
21	CLA	B	1213	-	59,73,73	1.28	9 (15%)	67,113,113	1.81	9 (13%)
21	CLA	2	1236	-	44,58,73	1.48	8 (18%)	49,95,113	1.86	7 (14%)
21	CLA	B	1216	38	59,73,73	1.30	9 (15%)	67,113,113	1.71	6 (8%)
21	CLA	B	1237	38	59,73,73	1.23	7 (11%)	67,113,113	1.71	8 (11%)
25	LHG	B	5004	-	48,48,48	0.37	0	51,54,54	1.12	3 (5%)
21	CLA	1	1013	-	59,73,73	1.26	7 (11%)	67,113,113	1.89	9 (13%)
21	CLA	2	1206	2	59,73,73	1.26	8 (13%)	67,113,113	1.84	7 (10%)
24	BCR	1	4007	-	41,41,41	0.64	0	56,56,56	3.27	10 (17%)
21	CLA	2	1022	38	59,73,73	1.26	7 (11%)	67,113,113	1.82	8 (11%)
21	CLA	a	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.83	9 (13%)
24	BCR	A	4008	-	41,41,41	0.64	0	56,56,56	2.91	9 (16%)
21	CLA	a	1121	-	59,73,73	1.27	9 (15%)	67,113,113	1.72	8 (11%)
21	CLA	B	1219	-	59,73,73	1.28	7 (11%)	67,113,113	1.71	6 (8%)
21	CLA	A	1126	-	59,73,73	1.25	6 (10%)	67,113,113	1.75	5 (7%)
21	CLA	B	1240	-	59,73,73	1.29	9 (15%)	67,113,113	1.73	8 (11%)
21	CLA	b	1214	-	59,73,73	1.27	8 (13%)	67,113,113	1.67	7 (10%)
21	CLA	b	1235	-	59,73,73	1.25	8 (13%)	67,113,113	1.73	6 (8%)
21	CLA	2	1230	-	41,55,73	1.52	8 (19%)	45,91,113	2.02	7 (15%)
21	CLA	B	1217	-	59,73,73	1.28	9 (15%)	67,113,113	1.82	9 (13%)
21	CLA	A	1116	-	59,73,73	1.28	9 (15%)	67,113,113	1.67	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	f	1301	38	44,58,73	1.47	7 (15%)	49,95,113	1.87	7 (14%)
21	CLA	a	1115	-	59,73,73	1.27	7 (11%)	67,113,113	1.74	6 (8%)
21	CLA	b	1227	-	59,73,73	1.24	8 (13%)	67,113,113	1.69	7 (10%)
21	CLA	2	1234	-	44,58,73	1.49	8 (18%)	49,95,113	1.99	8 (16%)
21	CLA	b	1208	-	54,68,73	1.30	7 (12%)	61,107,113	1.66	5 (8%)
24	BCR	A	4012	-	41,41,41	0.71	0	56,56,56	3.11	10 (17%)
24	BCR	1	4003	-	41,41,41	0.69	0	56,56,56	3.25	11 (19%)
21	CLA	b	1230	-	59,73,73	1.25	8 (13%)	67,113,113	1.80	7 (10%)
21	CLA	b	1203	-	59,73,73	1.25	8 (13%)	67,113,113	1.70	6 (8%)
21	CLA	B	1207	-	59,73,73	1.31	8 (13%)	67,113,113	1.86	9 (13%)
21	CLA	a	1011	-	59,73,73	1.26	7 (11%)	67,113,113	1.88	9 (13%)
21	CLA	2	1237	38	59,73,73	1.24	8 (13%)	67,113,113	1.72	7 (10%)
24	BCR	f	4016	-	41,41,41	0.73	0	56,56,56	3.28	12 (21%)
21	CLA	2	1210	-	59,73,73	1.28	9 (15%)	67,113,113	1.71	7 (10%)
21	CLA	k	1401	-	44,58,73	1.47	8 (18%)	49,95,113	2.03	7 (14%)
22	PQN	A	2001	-	34,34,34	0.41	0	42,45,45	1.21	4 (9%)
24	BCR	l	4022	-	41,41,41	0.69	0	56,56,56	3.22	12 (21%)
21	CLA	1	1134	16	59,73,73	1.27	9 (15%)	67,113,113	1.72	6 (8%)
24	BCR	k	4001	-	41,41,41	0.67	0	56,56,56	3.16	10 (17%)
24	BCR	2	4018	-	41,41,41	0.76	0	56,56,56	3.24	19 (33%)
21	CLA	A	1110	-	59,73,73	1.28	8 (13%)	67,113,113	1.65	4 (5%)
21	CLA	1	1124	-	50,64,73	1.38	9 (18%)	56,102,113	1.79	7 (12%)
21	CLA	2	1201	-	59,73,73	1.25	8 (13%)	67,113,113	1.85	7 (10%)
25	LHG	a	5007	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
21	CLA	2	1216	-	44,58,73	1.44	8 (18%)	49,95,113	2.02	5 (10%)
21	CLA	A	1113	-	59,73,73	1.28	8 (13%)	67,113,113	1.72	8 (11%)
21	CLA	B	1231	38	59,73,73	1.25	9 (15%)	67,113,113	1.78	8 (11%)
21	CLA	A	1011	-	59,73,73	1.26	8 (13%)	67,113,113	2.26	14 (20%)
25	LHG	1	5001	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
27	ACT	B	7001	-	1,3,3	6.52	1 (100%)	0,3,3	0.00	-
21	CLA	b	1240	-	59,73,73	1.28	8 (13%)	67,113,113	1.77	7 (10%)
24	BCR	0	4022	-	41,41,41	0.71	0	56,56,56	3.25	14 (25%)
21	CLA	b	1222	38	59,73,73	1.24	8 (13%)	67,113,113	1.75	9 (13%)
21	CLA	a	1133	-	59,73,73	1.29	9 (15%)	67,113,113	1.67	6 (8%)
21	CLA	b	1229	-	59,73,73	1.28	8 (13%)	67,113,113	1.66	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	1235	-	47,61,73	1.42	9 (19%)	52,98,113	1.92	5 (9%)
21	CLA	1	1115	-	59,73,73	1.27	8 (13%)	67,113,113	1.68	6 (8%)
23	SF4	3	3003	-	0,12,12	0.00	-	-		
21	CLA	1	1106	16	59,73,73	1.24	7 (11%)	67,113,113	1.75	5 (7%)
21	CLA	2	1211	-	44,58,73	1.47	9 (20%)	49,95,113	1.99	7 (14%)
21	CLA	1	1113	-	38,52,73	1.57	8 (21%)	40,87,113	2.05	5 (12%)
21	CLA	A	1123	38	59,73,73	1.27	8 (13%)	67,113,113	1.82	7 (10%)
21	CLA	a	1013	-	59,73,73	1.22	8 (13%)	67,113,113	1.79	6 (8%)
27	ACT	A	7001	-	1,3,3	7.80	1 (100%)	0,3,3	0.00	-
24	BCR	B	4014	-	41,41,41	0.71	0	56,56,56	3.12	12 (21%)
21	CLA	2	1226	-	49,63,73	1.40	8 (16%)	55,101,113	1.88	8 (14%)
21	CLA	B	1023	-	59,73,73	1.26	8 (13%)	67,113,113	1.83	8 (11%)
21	CLA	b	1224	-	59,73,73	1.25	9 (15%)	67,113,113	1.72	7 (10%)
24	BCR	h	4018	-	41,41,41	0.69	0	56,56,56	3.34	10 (17%)
21	CLA	1	1111	-	59,73,73	1.27	8 (13%)	67,113,113	1.72	9 (13%)
25	LHG	6	5001	-	11,11,48	0.48	0	12,14,54	0.52	0
22	PQN	B	2002	-	34,34,34	0.88	2 (5%)	42,45,45	1.27	3 (7%)
25	LHG	F	5002	-	48,48,48	0.37	0	51,54,54	0.96	2 (3%)
21	CLA	2	1225	-	59,73,73	1.28	8 (13%)	67,113,113	1.66	6 (8%)
21	CLA	b	1022	-	59,73,73	1.25	7 (11%)	67,113,113	1.74	8 (11%)
21	CLA	1	1116	-	59,73,73	1.27	9 (15%)	67,113,113	1.76	7 (10%)
21	CLA	a	1131	-	59,73,73	1.27	9 (15%)	67,113,113	1.62	5 (7%)
21	CLA	1	1119	38	59,73,73	1.24	7 (11%)	67,113,113	1.85	7 (10%)
31	SQD	F	5001	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
21	CLA	F	1302	6	59,73,73	1.28	8 (13%)	67,113,113	1.73	6 (8%)
21	CLA	2	1223	-	49,63,73	1.40	8 (16%)	55,101,113	1.89	6 (10%)
21	CLA	a	1123	1	59,73,73	1.28	9 (15%)	67,113,113	1.73	6 (8%)
24	BCR	J	4013	-	41,41,41	0.69	0	56,56,56	3.22	12 (21%)
21	CLA	A	1112	-	59,73,73	1.26	8 (13%)	67,113,113	1.82	7 (10%)
21	CLA	A	1103	-	59,73,73	1.22	8 (13%)	67,113,113	1.73	5 (7%)
21	CLA	a	1107	1	44,58,73	1.47	8 (18%)	49,95,113	2.02	9 (18%)
23	SF4	3	3002	-	0,12,12	0.00	-	-		
21	CLA	a	1122	-	59,73,73	1.26	9 (15%)	67,113,113	1.80	7 (10%)
21	CLA	B	1211	-	59,73,73	1.27	7 (11%)	67,113,113	1.75	7 (10%)
21	CLA	B	1239	-	59,73,73	1.29	8 (13%)	67,113,113	1.80	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1236	-	44,58,73	1.48	8 (18%)	49,95,113	1.85	6 (12%)
24	BCR	A	4001	-	41,41,41	0.68	0	56,56,56	3.06	12 (21%)
21	CLA	8	1402	-	40,54,73	1.53	7 (17%)	44,90,113	1.89	5 (11%)
21	CLA	7	1302	8	35,49,73	1.65	9 (25%)	38,84,113	2.08	5 (13%)
21	CLA	L	1503	38	59,73,73	1.26	9 (15%)	67,113,113	1.75	9 (13%)
24	BCR	1	4002	-	41,41,41	0.64	0	56,56,56	3.26	11 (19%)
21	CLA	B	1224	-	59,73,73	1.25	8 (13%)	67,113,113	1.71	6 (8%)
21	CLA	a	1127	-	59,73,73	1.28	9 (15%)	67,113,113	1.72	6 (8%)
23	SF4	1	3001	2,16	0,12,12	0.00	-	-		
21	CLA	a	1105	-	52,66,73	1.36	8 (15%)	58,104,113	1.83	7 (12%)
21	CLA	a	1132	-	59,73,73	1.25	7 (11%)	67,113,113	1.71	8 (11%)
21	CLA	K	1401	38	59,73,73	1.26	6 (10%)	67,113,113	1.81	10 (14%)
25	LHG	A	5007	-	48,48,48	0.40	0	51,54,54	1.11	3 (5%)
21	CLA	1	1137	-	45,59,73	1.47	9 (20%)	50,96,113	1.94	7 (14%)
21	CLA	2	1238	38	59,73,73	1.27	7 (11%)	67,113,113	1.66	7 (10%)
24	BCR	b	4010	-	41,41,41	0.64	0	56,56,56	3.06	7 (12%)
24	BCR	b	4017	-	41,41,41	0.63	0	56,56,56	3.28	10 (17%)
24	BCR	2	4011	-	41,41,41	0.68	0	56,56,56	2.94	9 (16%)
21	CLA	a	1128	-	59,73,73	1.25	7 (11%)	67,113,113	1.86	9 (13%)
21	CLA	B	1208	-	59,73,73	1.25	7 (11%)	67,113,113	1.71	7 (10%)
21	CLA	1	1107	-	45,59,73	1.45	7 (15%)	50,96,113	1.99	8 (16%)
21	CLA	a	1106	-	59,73,73	1.24	9 (15%)	67,113,113	1.79	6 (8%)
21	CLA	b	1212	-	59,73,73	1.30	9 (15%)	67,113,113	1.61	6 (8%)
21	CLA	1	1101	-	59,73,73	1.29	9 (15%)	67,113,113	1.78	7 (10%)
34	ZEX	J	4015	-	42,43,43	5.80	3 (7%)	55,60,60	6.94	10 (18%)
25	LHG	l	5001	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
26	LMG	1	5004	-	55,55,55	1.14	6 (10%)	63,63,63	1.04	2 (3%)
21	CLA	a	1103	-	59,73,73	1.22	8 (13%)	67,113,113	1.73	7 (10%)
26	LMG	b	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.30	4 (6%)
21	CLA	1	1132	-	59,73,73	1.26	8 (13%)	67,113,113	1.78	8 (11%)
21	CLA	B	1226	-	59,73,73	1.24	7 (11%)	67,113,113	1.76	9 (13%)
26	LMG	B	5002	-	55,55,55	1.14	6 (10%)	63,63,63	1.07	5 (7%)
21	CLA	A	1105	-	59,73,73	1.30	8 (13%)	67,113,113	1.62	6 (8%)
21	CLA	b	1228	-	59,73,73	1.28	9 (15%)	67,113,113	1.68	6 (8%)
21	CLA	b	1206	12	59,73,73	1.25	8 (13%)	67,113,113	1.80	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1215	-	59,73,73	1.24	8 (13%)	67,113,113	1.76	8 (11%)
21	CLA	0	1502	28	59,73,73	1.27	7 (11%)	67,113,113	1.77	6 (8%)
25	LHG	A	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1102	21	59,73,73	1.25	8 (13%)	67,113,113	1.79	8 (11%)
21	CLA	1	1103	-	59,73,73	1.22	9 (15%)	67,113,113	1.78	3 (4%)
24	BCR	I	4018	-	41,41,41	0.60	0	56,56,56	3.10	14 (25%)
23	SF4	a	3001	1,12	0,12,12	0.00	-	-		
21	CLA	k	1402	-	43,57,73	1.48	9 (20%)	46,93,113	2.13	7 (15%)
21	CLA	1	1118	-	59,73,73	1.25	7 (11%)	67,113,113	1.74	8 (11%)
21	CLA	B	1202	-	59,73,73	1.25	8 (13%)	67,113,113	1.75	7 (10%)
21	CLA	L	1502	-	59,73,73	1.23	6 (10%)	67,113,113	1.75	8 (11%)
26	LMG	1	5002	-	50,50,55	1.03	5 (10%)	58,58,63	1.06	2 (3%)
25	LHG	b	5004	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
21	CLA	B	1222	38	49,63,73	1.34	7 (14%)	55,101,113	1.93	8 (14%)
24	BCR	B	4005	-	41,41,41	0.67	0	56,56,56	3.22	10 (17%)
21	CLA	B	1230	-	59,73,73	1.26	9 (15%)	67,113,113	1.68	4 (5%)
21	CLA	b	1234	-	47,61,73	1.42	6 (12%)	52,98,113	1.93	9 (17%)
21	CLA	1	1129	-	44,58,73	1.46	7 (15%)	49,95,113	2.00	8 (16%)
24	BCR	2	4005	-	41,41,41	0.73	0	56,56,56	3.34	10 (17%)
23	SF4	c	3003	13	0,12,12	0.00	-	-		
24	BCR	0	4019	-	41,41,41	0.67	0	56,56,56	3.10	11 (19%)
26	LMG	2	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.07	2 (3%)
21	CLA	B	1212	-	49,63,73	1.41	8 (16%)	55,101,113	1.83	6 (10%)
21	CLA	A	1122	-	54,68,73	1.32	8 (14%)	61,107,113	1.75	8 (13%)
25	LHG	a	5005	-	48,48,48	0.38	0	51,54,54	1.10	3 (5%)
21	CLA	B	1238	38	59,73,73	1.30	8 (13%)	67,113,113	1.50	6 (8%)
24	BCR	a	4008	-	41,41,41	0.65	0	56,56,56	3.28	12 (21%)
21	CLA	A	1121	-	59,73,73	1.25	8 (13%)	67,113,113	1.74	6 (8%)
21	CLA	B	1209	-	59,73,73	1.29	8 (13%)	67,113,113	1.79	7 (10%)
21	CLA	a	1111	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	6 (8%)
21	CLA	1	1130	-	49,63,73	1.37	8 (16%)	55,101,113	1.83	7 (12%)
21	CLA	l	1501	10	59,73,73	1.25	8 (13%)	67,113,113	1.78	10 (14%)
21	CLA	a	1113	-	44,58,73	1.47	9 (20%)	49,95,113	1.99	8 (16%)
21	CLA	F	1301	38	59,73,73	1.27	8 (13%)	67,113,113	1.69	7 (10%)
21	CLA	B	1228	-	59,73,73	1.24	7 (11%)	67,113,113	1.71	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	1106	1	59,73,73	1.23	6 (10%)	67,113,113	1.74	7 (10%)
21	CLA	A	1138	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	7 (10%)
21	CLA	b	1239	-	59,73,73	1.29	9 (15%)	67,113,113	1.77	6 (8%)
21	CLA	a	1129	-	46,60,73	1.44	8 (17%)	51,97,113	1.91	8 (15%)
23	SF4	C	3002	3	0,12,12	0.00	-	-		
21	CLA	A	1136	-	59,73,73	1.30	8 (13%)	67,113,113	1.66	7 (10%)
21	CLA	b	1021	-	59,73,73	1.25	8 (13%)	67,113,113	1.71	6 (8%)
24	BCR	K	4001	-	41,41,41	0.58	0	56,56,56	3.17	16 (28%)
30	ECH	M	4021	-	42,42,42	0.65	0	55,58,58	1.68	11 (20%)
21	CLA	1	1105	-	44,58,73	1.50	9 (20%)	49,95,113	1.92	6 (12%)
21	CLA	B	1210	-	59,73,73	1.28	8 (13%)	67,113,113	1.73	8 (11%)
24	BCR	9	4021	-	41,41,41	0.67	0	56,56,56	3.27	17 (30%)
21	CLA	2	1207	-	50,64,73	1.38	8 (16%)	56,102,113	1.85	8 (14%)
30	ECH	b	4011	-	42,42,42	0.82	1 (2%)	55,58,58	2.42	15 (27%)
21	CLA	b	1226	-	59,73,73	1.29	8 (13%)	67,113,113	1.60	8 (11%)
21	CLA	b	1205	-	59,73,73	1.24	7 (11%)	67,113,113	1.73	6 (8%)
21	CLA	B	1234	-	59,73,73	1.27	7 (11%)	67,113,113	1.74	7 (10%)
21	CLA	2	1208	-	54,68,73	1.34	8 (14%)	61,107,113	1.72	6 (9%)
21	CLA	1	1123	-	59,73,73	1.27	9 (15%)	67,113,113	1.75	7 (10%)
35	LMT	1	6001	-	36,36,36	1.15	4 (11%)	47,47,47	0.98	3 (6%)
26	LMG	K	5009	-	55,55,55	1.17	7 (12%)	63,63,63	1.26	5 (7%)
21	CLA	a	1130	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	5 (7%)
21	CLA	B	1223	-	59,73,73	1.29	8 (13%)	67,113,113	1.71	6 (8%)
21	CLA	a	1140	-	59,73,73	1.26	8 (13%)	67,113,113	1.76	7 (10%)
24	BCR	b	4014	-	41,41,41	0.71	0	56,56,56	3.19	12 (21%)
21	CLA	2	1021	-	59,73,73	1.23	7 (11%)	67,113,113	1.77	6 (8%)
21	CLA	1	1135	-	46,60,73	1.45	8 (17%)	51,97,113	1.93	8 (15%)
21	CLA	b	1201	-	59,73,73	1.26	9 (15%)	67,113,113	1.66	6 (8%)
26	LMG	b	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.18	6 (9%)
21	CLA	a	1109	-	59,73,73	1.23	7 (11%)	67,113,113	1.87	7 (10%)
21	CLA	2	1204	-	59,73,73	1.26	8 (13%)	67,113,113	1.74	6 (8%)
21	CLA	A	1135	-	59,73,73	1.26	9 (15%)	67,113,113	1.76	7 (10%)
35	LMT	L	6001	-	36,36,36	1.15	5 (13%)	47,47,47	1.16	4 (8%)
21	CLA	A	1104	-	59,73,73	1.26	7 (11%)	67,113,113	1.73	9 (13%)
24	BCR	A	4002	-	41,41,41	0.66	0	56,56,56	3.14	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	A	4003	-	41,41,41	0.69	0	56,56,56	3.15	13 (23%)
22	PQN	1	2001	-	34,34,34	0.44	0	42,45,45	1.09	3 (7%)
21	CLA	2	1227	-	36,53,73	1.63	9 (25%)	39,89,113	1.94	4 (10%)
21	CLA	b	1217	-	45,59,73	1.47	9 (20%)	50,96,113	1.87	7 (14%)
21	CLA	a	1112	-	59,73,73	1.26	9 (15%)	67,113,113	1.83	7 (10%)
21	CLA	J	1303	-	59,73,73	1.27	9 (15%)	67,113,113	1.77	7 (10%)
21	CLA	b	1236	-	59,73,73	1.28	8 (13%)	67,113,113	1.68	6 (8%)
21	CLA	1	1133	-	59,73,73	1.28	8 (13%)	67,113,113	1.75	6 (8%)
21	CLA	2	1205	-	59,73,73	1.25	9 (15%)	67,113,113	1.82	6 (8%)
26	LMG	A	5008	-	55,55,55	1.14	6 (10%)	63,63,63	1.04	2 (3%)
21	CLA	a	1801	25	49,63,73	1.40	9 (18%)	55,101,113	1.89	5 (9%)
21	CLA	0	1501	20	59,73,73	1.25	9 (15%)	67,113,113	1.70	6 (8%)
21	CLA	1	1801	25	50,64,73	1.39	9 (18%)	56,102,113	1.91	8 (14%)
21	CLA	2	1219	-	47,61,73	1.43	8 (17%)	52,98,113	1.97	9 (17%)
21	CLA	a	1012	38	59,73,73	1.25	7 (11%)	67,113,113	1.80	10 (14%)
24	BCR	2	4010	-	41,41,41	0.74	0	56,56,56	3.62	14 (25%)
31	SQD	B	5008	-	53,54,54	0.80	0	62,65,65	0.91	3 (4%)
21	CLA	2	1217	-	46,60,73	1.45	8 (17%)	51,97,113	1.91	7 (13%)
34	ZEX	F	4016	-	42,43,43	5.85	2 (4%)	55,60,60	7.03	13 (23%)
24	BCR	1	4008	-	41,41,41	0.62	0	56,56,56	3.19	10 (17%)
21	CLA	1	1121	-	49,63,73	1.39	9 (18%)	55,101,113	1.90	7 (12%)
25	LHG	1	5003	21	48,48,48	0.40	0	51,54,54	1.09	3 (5%)
24	BCR	8	4001	-	41,41,41	0.66	0	56,56,56	3.23	10 (17%)
21	CLA	A	1137	-	59,73,73	1.28	9 (15%)	67,113,113	1.64	6 (8%)
21	CLA	B	1201	-	59,73,73	1.24	8 (13%)	67,113,113	1.67	7 (10%)
21	CLA	A	1132	-	59,73,73	1.27	7 (11%)	67,113,113	1.66	6 (8%)
21	CLA	B	1229	-	59,73,73	1.27	8 (13%)	67,113,113	1.72	5 (7%)
21	CLA	b	1218	-	59,73,73	1.26	7 (11%)	67,113,113	1.72	8 (11%)
21	CLA	a	1104	-	59,73,73	1.24	7 (11%)	67,113,113	1.70	7 (10%)
21	CLA	1	1125	-	59,73,73	1.28	8 (13%)	67,113,113	1.81	7 (10%)
30	ECH	B	4006	-	42,42,42	0.91	2 (4%)	55,58,58	2.52	15 (27%)
21	CLA	b	1231	38	59,73,73	1.25	9 (15%)	67,113,113	1.85	6 (8%)
21	CLA	A	1129	-	52,66,73	1.32	8 (15%)	58,104,113	1.83	9 (15%)
24	BCR	j	4013	-	41,41,41	0.74	0	56,56,56	3.24	13 (23%)
25	LHG	a	5003	21	48,48,48	0.39	0	51,54,54	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PQN	a	2001	-	34,34,34	0.47	0	42,45,45	1.01	2 (4%)
21	CLA	A	1111	-	59,73,73	1.26	8 (13%)	67,113,113	1.78	8 (11%)
21	CLA	b	1215	-	59,73,73	1.25	8 (13%)	67,113,113	1.82	8 (11%)
21	CLA	L	1501	10	59,73,73	1.26	7 (11%)	67,113,113	1.73	6 (8%)
21	CLA	A	1134	1	59,73,73	1.27	9 (15%)	67,113,113	1.74	7 (10%)
21	CLA	1	1110	-	44,58,73	1.48	9 (20%)	49,95,113	1.96	5 (10%)
21	CLA	0	1503	38	59,73,73	1.26	8 (13%)	67,113,113	1.69	5 (7%)
24	BCR	B	4017	-	41,41,41	0.65	0	56,56,56	3.27	12 (21%)
21	CLA	f	1302	-	59,73,73	1.27	9 (15%)	67,113,113	1.69	7 (10%)
21	CLA	2	1202	-	59,73,73	1.25	7 (11%)	67,113,113	1.78	8 (11%)
21	CLA	b	1204	-	59,73,73	1.27	8 (13%)	67,113,113	1.62	7 (10%)
21	CLA	A	1130	-	54,68,73	1.31	8 (14%)	61,107,113	1.91	10 (16%)
31	SQD	b	5006	-	53,54,54	0.79	0	62,65,65	0.90	3 (4%)
21	CLA	6	1302	6	37,51,73	1.59	8 (21%)	40,86,113	2.36	7 (17%)
21	CLA	A	1107	1	59,73,73	1.26	7 (11%)	67,113,113	1.80	8 (11%)
21	CLA	b	1237	38	59,73,73	1.23	6 (10%)	67,113,113	1.76	10 (14%)
21	CLA	2	1215	-	54,68,73	1.32	9 (16%)	61,107,113	1.86	8 (13%)
21	CLA	B	1235	-	59,73,73	1.23	7 (11%)	67,113,113	1.85	5 (7%)
21	CLA	A	1133	-	59,73,73	1.26	8 (13%)	67,113,113	1.60	4 (5%)
21	CLA	2	1232	-	36,53,73	1.60	9 (25%)	39,89,113	2.05	5 (12%)
21	CLA	a	1139	38	59,73,73	1.28	9 (15%)	67,113,113	1.75	6 (8%)
22	PQN	2	2002	-	34,34,34	0.38	0	42,45,45	1.27	3 (7%)
21	CLA	B	1221	-	59,73,73	1.24	9 (15%)	67,113,113	1.73	7 (10%)
21	CLA	1	1126	-	59,73,73	1.25	7 (11%)	67,113,113	1.80	7 (10%)
21	CLA	a	1124	-	49,63,73	1.36	8 (16%)	55,101,113	1.90	8 (14%)
24	BCR	b	4005	-	41,41,41	0.64	0	56,56,56	3.15	12 (21%)
25	LHG	M	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1115	-	59,73,73	1.25	7 (11%)	67,113,113	1.68	7 (10%)
21	CLA	2	1222	-	44,58,73	1.46	7 (15%)	49,95,113	2.04	8 (16%)
21	CLA	B	1218	-	59,73,73	1.27	9 (15%)	67,113,113	1.75	9 (13%)
24	BCR	a	4003	-	41,41,41	0.73	0	56,56,56	3.31	11 (19%)
21	CLA	a	1117	-	59,73,73	1.27	8 (13%)	67,113,113	1.70	5 (7%)
21	CLA	7	1303	-	35,49,73	1.62	8 (22%)	38,84,113	2.10	6 (15%)
26	LMG	b	5007	-	55,55,55	1.14	6 (10%)	63,63,63	1.14	3 (4%)
25	LHG	A	5003	21	48,48,48	0.40	0	51,54,54	1.02	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	1104	-	59,73,73	1.25	9 (15%)	67,113,113	1.72	7 (10%)
36	EQ3	I	4020	-	43,43,43	4.12	25 (58%)	56,60,60	2.21	22 (39%)
21	CLA	b	1207	-	59,73,73	1.27	8 (13%)	67,113,113	1.70	7 (10%)
21	CLA	1	1109	16	59,73,73	1.26	9 (15%)	67,113,113	1.77	7 (10%)
21	CLA	2	1212	-	35,49,73	1.62	8 (22%)	38,84,113	2.16	6 (15%)
21	CLA	2	1218	-	59,73,73	1.27	8 (13%)	67,113,113	1.74	9 (13%)
21	CLA	B	1021	-	59,73,73	1.24	8 (13%)	67,113,113	1.80	6 (8%)
21	CLA	B	1227	-	49,63,73	1.41	8 (16%)	55,101,113	1.80	5 (9%)
21	CLA	A	1131	-	59,73,73	1.28	8 (13%)	67,113,113	1.64	5 (7%)
24	BCR	a	4019	-	41,41,41	0.71	0	56,56,56	3.49	12 (21%)
30	ECH	b	4006	-	42,42,42	0.72	1 (2%)	55,58,58	2.25	15 (27%)
21	CLA	j	1303	-	49,63,73	1.41	9 (18%)	55,101,113	1.86	7 (12%)
31	SQD	f	5001	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
21	CLA	A	1117	-	59,73,73	1.28	8 (13%)	67,113,113	1.68	6 (8%)
24	BCR	B	4018	-	41,41,41	0.72	0	56,56,56	3.45	14 (25%)
21	CLA	A	1128	-	59,73,73	1.25	7 (11%)	67,113,113	1.88	9 (13%)
25	LHG	1	5007	-	48,48,48	0.40	0	51,54,54	1.02	2 (3%)
21	CLA	b	1238	38	59,73,73	1.27	7 (11%)	67,113,113	1.69	7 (10%)
24	BCR	l	4019	-	41,41,41	0.63	0	56,56,56	2.88	12 (21%)
21	CLA	l	1502	-	59,73,73	1.26	7 (11%)	67,113,113	1.70	6 (8%)
21	CLA	B	1022	38	59,73,73	1.29	7 (11%)	67,113,113	1.68	7 (10%)
21	CLA	2	1240	-	35,49,73	1.65	9 (25%)	38,84,113	2.07	5 (13%)
21	CLA	K	1402	-	59,73,73	1.27	9 (15%)	67,113,113	1.68	6 (8%)
25	LHG	L	5005	-	48,48,48	0.40	0	51,54,54	0.95	2 (3%)
24	BCR	2	4017	-	41,41,41	0.65	0	56,56,56	3.23	12 (21%)
21	CLA	a	1110	-	53,67,73	1.36	9 (16%)	59,105,113	1.83	6 (10%)
28	45D	h	4020	21	43,43,43	3.51	17 (39%)	54,60,60	3.40	23 (42%)
24	BCR	2	4014	-	41,41,41	0.72	0	56,56,56	3.32	13 (23%)
24	BCR	1	4012	-	41,41,41	0.68	0	56,56,56	3.22	9 (16%)
21	CLA	b	1221	38	59,73,73	1.25	8 (13%)	67,113,113	1.89	8 (11%)
31	SQD	L	5002	-	53,54,54	0.80	0	62,65,65	0.89	3 (4%)
21	CLA	b	1210	-	59,73,73	1.26	9 (15%)	67,113,113	1.70	7 (10%)
26	LMG	a	5002	-	50,50,55	1.04	4 (8%)	58,58,63	1.09	2 (3%)
24	BCR	L	4019	-	41,41,41	0.69	0	56,56,56	2.85	14 (25%)
21	CLA	B	1203	-	59,73,73	1.25	8 (13%)	67,113,113	1.69	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	ECH	2	4006	-	42,42,42	0.80	1 (2%)	55,58,58	2.53	16 (29%)
21	CLA	A	1119	38	59,73,73	1.22	6 (10%)	67,113,113	1.65	6 (8%)
21	CLA	1	1140	-	59,73,73	1.27	8 (13%)	67,113,113	1.74	7 (10%)
21	CLA	1	1114	-	36,53,73	1.62	9 (25%)	39,89,113	1.93	5 (12%)
25	LHG	B	5006	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
35	LMT	l	6001	-	36,36,36	1.11	4 (11%)	47,47,47	1.20	3 (6%)
21	CLA	b	1209	-	59,73,73	1.27	8 (13%)	67,113,113	1.84	9 (13%)
21	CLA	A	1139	38	59,73,73	1.25	9 (15%)	67,113,113	1.74	4 (5%)
24	BCR	a	4007	-	41,41,41	0.65	0	56,56,56	3.09	12 (21%)
24	BCR	b	4004	-	41,41,41	0.67	0	56,56,56	3.29	14 (25%)
21	CLA	a	1118	-	59,73,73	1.26	8 (13%)	67,113,113	1.63	7 (10%)
21	CLA	1	1102	-	49,63,73	1.36	8 (16%)	55,101,113	2.03	10 (18%)
24	BCR	7	4013	-	41,41,41	0.71	0	56,56,56	3.29	15 (26%)
21	CLA	A	1125	-	59,73,73	1.26	6 (10%)	67,113,113	1.80	10 (14%)
21	CLA	6	1301	38	41,55,73	1.51	9 (21%)	45,91,113	1.92	8 (17%)
21	CLA	B	1232	-	44,58,73	1.49	9 (20%)	49,95,113	1.99	6 (12%)
24	BCR	A	4019	-	41,41,41	0.71	0	56,56,56	3.60	14 (25%)
21	CLA	2	1228	-	36,53,73	1.59	9 (25%)	39,89,113	2.12	5 (12%)
23	SF4	c	3002	-	0,12,12	0.00	-	-	-	-
21	CLA	a	1136	-	59,73,73	1.28	9 (15%)	67,113,113	1.89	10 (14%)
25	LHG	A	5006	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
21	CLA	A	1140	-	59,73,73	1.27	9 (15%)	67,113,113	1.71	7 (10%)
26	LMG	a	5004	-	55,55,55	1.14	7 (12%)	63,63,63	1.21	4 (6%)
21	CLA	1	1136	-	59,73,73	1.29	8 (13%)	67,113,113	1.71	7 (10%)
21	CLA	2	1209	-	36,53,73	1.64	9 (25%)	39,89,113	2.08	5 (12%)
21	CLA	2	1203	-	59,73,73	1.27	9 (15%)	67,113,113	1.67	7 (10%)
21	CLA	8	1401	-	36,53,73	1.61	8 (22%)	39,89,113	2.08	7 (17%)
21	CLA	A	1108	-	47,61,73	1.41	9 (19%)	52,98,113	1.91	5 (9%)
21	CLA	2	1239	-	59,73,73	1.29	9 (15%)	67,113,113	1.79	9 (13%)
21	CLA	1	1108	-	40,54,73	1.54	9 (22%)	44,90,113	1.89	4 (9%)
21	CLA	A	1013	-	59,73,73	1.25	9 (15%)	67,113,113	1.79	9 (13%)
21	CLA	1	1138	-	54,68,73	1.35	9 (16%)	61,107,113	1.78	6 (9%)
21	CLA	b	1223	-	59,73,73	1.25	7 (11%)	67,113,113	1.72	8 (11%)
30	ECH	m	4021	-	42,42,42	0.65	0	55,58,58	1.68	10 (18%)
25	LHG	0	5002	-	48,48,48	0.39	0	51,54,54	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	4018	-	41,41,41	0.70	0	56,56,56	3.35	8 (14%)
21	CLA	2	1221	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	8 (11%)
21	CLA	A	1120	-	59,73,73	1.26	7 (11%)	67,113,113	1.74	10 (14%)
21	CLA	B	1205	-	59,73,73	1.23	6 (10%)	67,113,113	1.77	6 (8%)
24	BCR	L	4022	-	41,41,41	0.61	0	56,56,56	3.06	10 (17%)
21	CLA	1	1012	38	59,73,73	1.25	7 (11%)	67,113,113	1.90	9 (13%)
21	CLA	b	1023	-	59,73,73	1.24	8 (13%)	67,113,113	1.89	8 (11%)
21	CLA	B	1225	-	59,73,73	1.30	8 (13%)	67,113,113	1.67	5 (7%)
25	LHG	A	5005	-	48,48,48	0.40	0	51,54,54	1.09	4 (7%)
21	CLA	1	1127	-	59,73,73	1.30	8 (13%)	67,113,113	1.64	6 (8%)
21	CLA	a	1137	-	44,58,73	1.49	9 (20%)	49,95,113	1.94	6 (12%)
26	LMG	A	5002	-	50,50,55	1.06	5 (10%)	58,58,63	1.17	4 (6%)
26	LMG	B	5005	-	55,55,55	1.13	6 (10%)	63,63,63	1.09	3 (4%)
21	CLA	l	1503	-	59,73,73	1.23	7 (11%)	67,113,113	1.69	8 (11%)
25	LHG	l	5004	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
30	ECH	i	4020	-	42,42,42	0.81	1 (2%)	55,58,58	2.40	17 (30%)
25	LHG	1	5005	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
21	CLA	b	1219	-	54,68,73	1.34	8 (14%)	61,107,113	1.80	7 (11%)
24	BCR	A	4007	-	41,41,41	0.63	0	56,56,56	2.90	13 (23%)
24	BCR	a	4002	-	41,41,41	0.65	0	56,56,56	3.53	12 (21%)
21	CLA	a	1134	1	43,57,73	1.50	9 (20%)	46,93,113	2.07	7 (15%)
21	CLA	1	1120	-	59,73,73	1.28	8 (13%)	67,113,113	1.76	6 (8%)
25	LHG	l	5003	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
21	CLA	b	1232	-	59,73,73	1.27	9 (15%)	67,113,113	1.71	7 (10%)
25	LHG	a	5001	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
21	CLA	A	1124	38	59,73,73	1.25	7 (11%)	67,113,113	1.72	9 (13%)
25	LHG	0	5004	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
21	CLA	2	1224	-	49,63,73	1.36	8 (16%)	55,101,113	1.89	7 (12%)
35	LMT	0	6001	-	36,36,36	1.13	4 (11%)	47,47,47	1.17	3 (6%)
21	CLA	A	1109	21	59,73,73	1.25	7 (11%)	67,113,113	1.77	7 (10%)
21	CLA	J	1302	8	59,73,73	1.27	8 (13%)	67,113,113	1.86	7 (10%)
21	CLA	a	1135	-	59,73,73	1.29	8 (13%)	67,113,113	1.63	6 (8%)
21	CLA	a	1138	-	59,73,73	1.27	8 (13%)	67,113,113	1.80	5 (7%)
26	LMG	2	5002	-	55,55,55	1.14	6 (10%)	63,63,63	1.08	2 (3%)
21	CLA	b	1213	-	59,73,73	1.26	9 (15%)	67,113,113	1.79	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	1	4019	-	41,41,41	0.67	0	56,56,56	3.36	8 (14%)
21	CLA	1	1117	-	59,73,73	1.26	7 (11%)	67,113,113	1.69	6 (8%)
24	BCR	a	4012	-	41,41,41	0.69	0	56,56,56	3.12	14 (25%)
21	CLA	a	1114	-	46,60,73	1.44	9 (19%)	51,97,113	1.98	8 (15%)
21	CLA	B	1206	2	59,73,73	1.26	8 (13%)	67,113,113	1.84	8 (11%)
31	SQD	L	5001	-	50,51,54	0.80	0	59,62,65	0.93	4 (6%)
27	ACT	B	7002	-	1,3,3	6.86	1 (100%)	0,3,3	0.00	-
21	CLA	A	1127	-	59,73,73	1.28	7 (11%)	67,113,113	1.63	8 (11%)
24	BCR	i	4018	-	41,41,41	0.70	0	56,56,56	3.39	12 (21%)
23	SF4	A	3001	1,2	0,12,12	0.00	-	-	-	-
21	CLA	1	1128	-	59,73,73	1.26	8 (13%)	67,113,113	1.83	8 (11%)
21	CLA	a	1126	-	59,73,73	1.25	7 (11%)	67,113,113	1.88	6 (8%)
31	SQD	0	5005	-	53,54,54	0.80	0	62,65,65	0.89	3 (4%)
24	BCR	B	4004	-	41,41,41	0.68	0	56,56,56	3.19	12 (21%)
21	CLA	A	1118	-	59,73,73	1.27	8 (13%)	67,113,113	1.66	6 (8%)
21	CLA	a	1108	-	51,65,73	1.38	9 (17%)	57,103,113	1.88	7 (12%)
22	PQN	b	2002	-	34,34,34	0.77	2 (5%)	42,45,45	1.27	5 (11%)
21	CLA	a	1125	-	59,73,73	1.27	8 (13%)	67,113,113	1.84	9 (13%)
21	CLA	a	1120	-	49,63,73	1.40	9 (18%)	55,101,113	1.90	7 (12%)
24	BCR	2	4004	-	41,41,41	0.68	0	56,56,56	3.26	9 (16%)
21	CLA	a	1119	-	59,73,73	1.25	8 (13%)	67,113,113	1.68	8 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1012	38	2/2/20/25	22/37/135/135	-
21	CLA	2	1220	-	3/3/16/25	5/11/111/135	-
26	LMG	0	5001	-	-	24/50/70/70	0/1/1/1
21	CLA	B	1214	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1112	-	3/3/17/25	8/19/117/135	-
21	CLA	1	1139	-	3/3/20/25	14/37/135/135	-
21	CLA	b	1235	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1011	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	a	4001	-	-	16/29/63/63	0/2/2/2
37	DGD	L	5004	-	-	23/55/95/95	0/2/2/2
21	CLA	2	1231	38	3/3/16/25	4/15/113/135	-
21	CLA	b	1220	-	3/3/20/25	12/37/135/135	-
21	CLA	2	1213	-	3/3/17/25	8/19/117/135	-
21	CLA	B	1204	-	2/2/20/25	17/37/135/135	-
21	CLA	2	1229	-	3/3/20/25	21/37/135/135	-
21	CLA	2	1214	-	3/3/18/25	16/30/128/135	-
23	SF4	A	3001	1,2	-	-	0/6/5/5
21	CLA	a	1102	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1220	-	3/3/18/25	15/28/126/135	-
35	LMT	F	6001	-	-	8/21/61/61	0/2/2/2
21	CLA	1	1131	-	3/3/20/25	12/37/135/135	-
21	CLA	A	1801	25	3/3/20/25	20/37/135/135	-
21	CLA	j	1302	-	3/3/20/25	19/37/135/135	-
25	LHG	l	5002	-	-	32/53/53/53	-
24	BCR	1	4001	-	-	10/29/63/63	0/2/2/2
23	SF4	C	3003	3	-	-	0/6/5/5
24	BCR	6	4016	-	-	13/29/63/63	0/2/2/2
21	CLA	b	1225	-	3/3/20/25	13/37/135/135	-
25	LHG	M	5001	-	-	31/53/53/53	-
26	LMG	A	5004	-	-	18/43/63/70	0/1/1/1
25	LHG	2	5004	-	-	25/53/53/53	-
21	CLA	b	1202	-	2/2/20/25	18/37/135/135	-
21	CLA	A	1114	38	3/3/20/25	21/37/135/135	-
24	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
21	CLA	a	1116	-	2/2/19/25	10/31/129/135	-
34	ZEX	7	4015	-	-	7/29/67/67	0/2/2/2
34	ZEX	j	4015	-	-	7/29/67/67	0/2/2/2
21	CLA	b	1216	38	3/3/20/25	21/37/135/135	-
21	CLA	b	1211	-	3/3/20/25	17/37/135/135	-
28	45D	B	4011	-	-	11/29/69/69	0/2/2/2
21	CLA	A	1101	-	1/1/20/25	8/37/135/135	-
21	CLA	B	1213	-	3/3/20/25	14/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	1236	-	3/3/17/25	9/19/117/135	-
21	CLA	B	1216	38	3/3/20/25	23/37/135/135	-
21	CLA	B	1237	38	3/3/20/25	12/37/135/135	-
25	LHG	B	5004	-	-	28/53/53/53	-
21	CLA	1	1013	-	3/3/20/25	17/37/135/135	-
21	CLA	2	1206	2	3/3/20/25	14/37/135/135	-
24	BCR	1	4007	-	-	16/29/63/63	0/2/2/2
21	CLA	2	1022	38	3/3/20/25	7/37/135/135	-
21	CLA	a	1101	-	2/2/20/25	11/37/135/135	-
24	BCR	A	4008	-	-	5/29/63/63	0/2/2/2
21	CLA	a	1121	-	3/3/20/25	24/37/135/135	-
21	CLA	B	1219	-	2/2/20/25	17/37/135/135	-
21	CLA	A	1126	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1240	-	3/3/20/25	17/37/135/135	-
21	CLA	b	1214	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1122	-	3/3/19/25	14/31/129/135	-
21	CLA	2	1230	-	3/3/16/25	11/16/114/135	-
21	CLA	B	1217	-	3/3/20/25	16/37/135/135	-
21	CLA	A	1116	-	3/3/20/25	21/37/135/135	-
21	CLA	f	1301	38	3/3/17/25	5/19/117/135	-
21	CLA	a	1115	-	2/2/20/25	8/37/135/135	-
21	CLA	b	1227	-	3/3/20/25	13/37/135/135	-
21	CLA	2	1234	-	3/3/17/25	9/19/117/135	-
21	CLA	b	1208	-	3/3/19/25	15/31/129/135	-
24	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
24	BCR	1	4003	-	-	13/29/63/63	0/2/2/2
21	CLA	1	1127	-	3/3/20/25	21/37/135/135	-
21	CLA	b	1203	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1207	-	2/2/20/25	11/37/135/135	-
21	CLA	a	1011	-	3/3/20/25	20/37/135/135	-
21	CLA	2	1237	38	3/3/20/25	14/37/135/135	-
24	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
21	CLA	2	1210	-	2/2/20/25	22/37/135/135	-
21	CLA	k	1401	-	3/3/17/25	5/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1104	-	3/3/20/25	15/37/135/135	-
24	BCR	l	4022	-	-	14/29/63/63	0/2/2/2
21	CLA	1	1134	16	3/3/20/25	22/37/135/135	-
24	BCR	k	4001	-	-	10/29/63/63	0/2/2/2
24	BCR	2	4018	-	-	14/29/63/63	0/2/2/2
21	CLA	A	1110	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1124	-	3/3/18/25	11/27/125/135	-
21	CLA	2	1201	-	3/3/20/25	12/37/135/135	-
25	LHG	a	5007	-	-	34/53/53/53	-
21	CLA	2	1216	-	3/3/17/25	6/19/117/135	-
21	CLA	A	1113	-	3/3/20/25	22/37/135/135	-
21	CLA	B	1231	38	1/1/20/25	20/37/135/135	-
25	LHG	1	5001	-	-	27/53/53/53	-
21	CLA	b	1240	-	3/3/20/25	20/37/135/135	-
24	BCR	0	4022	-	-	9/29/63/63	0/2/2/2
21	CLA	b	1222	38	3/3/20/25	15/37/135/135	-
21	CLA	a	1133	-	2/2/20/25	18/37/135/135	-
21	CLA	b	1229	-	3/3/20/25	14/37/135/135	-
21	CLA	2	1235	-	3/3/17/25	9/23/121/135	-
21	CLA	1	1115	-	3/3/20/25	9/37/135/135	-
23	SF4	3	3003	-	-	-	0/6/5/5
21	CLA	1	1106	16	3/3/20/25	17/37/135/135	-
21	CLA	2	1211	-	3/3/17/25	10/19/117/135	-
21	CLA	1	1113	-	3/3/15/25	7/11/110/135	-
21	CLA	A	1123	38	2/2/20/25	12/37/135/135	-
21	CLA	a	1013	-	3/3/20/25	12/37/135/135	-
24	BCR	B	4014	-	-	8/29/63/63	0/2/2/2
21	CLA	2	1226	-	3/3/18/25	15/25/123/135	-
21	CLA	B	1023	-	3/3/20/25	5/37/135/135	-
21	CLA	b	1224	-	3/3/20/25	12/37/135/135	-
24	BCR	h	4018	-	-	13/29/63/63	0/2/2/2
21	CLA	1	1111	-	3/3/20/25	15/37/135/135	-
25	LHG	6	5001	-	-	6/12/12/53	-
22	PQN	B	2002	-	-	10/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	F	5002	-	-	40/53/53/53	-
21	CLA	2	1225	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1022	-	2/2/20/25	10/37/135/135	-
21	CLA	1	1116	-	3/3/20/25	17/37/135/135	-
21	CLA	a	1131	-	3/3/20/25	14/37/135/135	-
21	CLA	1	1119	38	3/3/20/25	15/37/135/135	-
31	SQD	F	5001	-	-	23/49/69/69	0/1/1/1
21	CLA	F	1302	6	3/3/20/25	19/37/135/135	-
21	CLA	2	1223	-	2/2/18/25	8/25/123/135	-
21	CLA	a	1123	1	2/2/20/25	16/37/135/135	-
24	BCR	J	4013	-	-	14/29/63/63	0/2/2/2
21	CLA	A	1112	-	3/3/20/25	19/37/135/135	-
21	CLA	A	1103	-	3/3/20/25	19/37/135/135	-
21	CLA	a	1107	1	3/3/17/25	7/19/117/135	-
25	LHG	L	5005	-	-	24/53/53/53	-
21	CLA	a	1122	-	3/3/20/25	24/37/135/135	-
21	CLA	B	1211	-	3/3/20/25	19/37/135/135	-
21	CLA	B	1239	-	3/3/20/25	17/37/135/135	-
21	CLA	B	1236	-	3/3/17/25	5/19/117/135	-
24	BCR	A	4001	-	-	5/29/63/63	0/2/2/2
21	CLA	8	1402	-	3/3/16/25	11/15/113/135	-
21	CLA	7	1302	8	2/2/15/25	3/8/106/135	-
21	CLA	L	1503	38	2/2/20/25	20/37/135/135	-
24	BCR	1	4002	-	-	14/29/63/63	0/2/2/2
21	CLA	B	1224	-	3/3/20/25	21/37/135/135	-
21	CLA	a	1127	-	3/3/20/25	23/37/135/135	-
21	CLA	b	1023	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1105	-	3/3/18/25	8/29/127/135	-
21	CLA	a	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	K	1401	38	3/3/20/25	15/37/135/135	-
25	LHG	A	5007	-	-	29/53/53/53	-
21	CLA	1	1137	-	3/3/17/25	9/21/119/135	-
21	CLA	2	1238	38	3/3/20/25	11/37/135/135	-
24	BCR	b	4010	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	4017	-	-	11/29/63/63	0/2/2/2
24	BCR	2	4011	-	-	15/29/63/63	0/2/2/2
21	CLA	a	1128	-	3/3/20/25	23/37/135/135	-
21	CLA	B	1208	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1107	-	3/3/17/25	9/21/119/135	-
21	CLA	a	1106	-	3/3/20/25	17/37/135/135	-
21	CLA	b	1212	-	2/2/20/25	16/37/135/135	-
21	CLA	1	1101	-	1/1/20/25	15/37/135/135	-
21	CLA	j	1303	-	3/3/18/25	11/25/123/135	-
25	LHG	l	5001	-	-	31/53/53/53	-
26	LMG	1	5004	-	-	20/50/70/70	0/1/1/1
21	CLA	a	1103	-	2/2/20/25	22/37/135/135	-
26	LMG	b	5005	-	-	17/50/70/70	0/1/1/1
21	CLA	1	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	B	1226	-	3/3/20/25	22/37/135/135	-
26	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
21	CLA	A	1105	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1228	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1206	12	3/3/20/25	18/37/135/135	-
21	CLA	B	1215	-	3/3/20/25	17/37/135/135	-
21	CLA	0	1502	28	3/3/20/25	12/37/135/135	-
25	LHG	A	5001	-	-	35/53/53/53	-
21	CLA	A	1102	21	3/3/20/25	18/37/135/135	-
21	CLA	1	1103	-	2/2/20/25	26/37/135/135	-
24	BCR	I	4018	-	-	10/29/63/63	0/2/2/2
23	SF4	a	3001	1,12	-	-	0/6/5/5
21	CLA	k	1402	-	3/3/16/25	13/18/116/135	-
21	CLA	1	1118	-	3/3/20/25	16/37/135/135	-
21	CLA	B	1202	-	2/2/20/25	19/37/135/135	-
21	CLA	L	1502	-	3/3/20/25	13/37/135/135	-
26	LMG	1	5002	-	-	20/45/65/70	0/1/1/1
25	LHG	b	5004	-	-	25/53/53/53	-
21	CLA	B	1222	38	3/3/18/25	8/25/123/135	-
24	BCR	B	4005	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1230	-	3/3/20/25	20/37/135/135	-
21	CLA	b	1234	-	3/3/17/25	4/23/121/135	-
21	CLA	1	1129	-	3/3/17/25	7/19/117/135	-
24	BCR	2	4005	-	-	11/29/63/63	0/2/2/2
23	SF4	c	3003	13	-	-	0/6/5/5
24	BCR	0	4019	-	-	10/29/63/63	0/2/2/2
26	LMG	2	5005	-	-	17/50/70/70	0/1/1/1
21	CLA	B	1212	-	3/3/18/25	12/25/123/135	-
21	CLA	A	1122	-	3/3/19/25	13/31/129/135	-
25	LHG	a	5005	-	-	30/53/53/53	-
21	CLA	B	1238	38	3/3/20/25	8/37/135/135	-
24	BCR	a	4008	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1121	-	3/3/20/25	19/37/135/135	-
21	CLA	B	1209	-	2/2/20/25	19/37/135/135	-
21	CLA	a	1111	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1130	-	3/3/18/25	9/25/123/135	-
21	CLA	l	1501	10	3/3/20/25	21/37/135/135	-
21	CLA	a	1113	-	3/3/17/25	9/19/117/135	-
21	CLA	F	1301	38	3/3/20/25	15/37/135/135	-
21	CLA	B	1228	-	3/3/20/25	17/37/135/135	-
21	CLA	A	1106	1	3/3/20/25	19/37/135/135	-
21	CLA	A	1138	-	3/3/20/25	14/37/135/135	-
21	CLA	b	1239	-	3/3/20/25	12/37/135/135	-
21	CLA	a	1129	-	3/3/17/25	10/22/120/135	-
23	SF4	C	3002	3	-	-	0/6/5/5
21	CLA	A	1136	-	3/3/20/25	19/37/135/135	-
21	CLA	b	1021	-	3/3/20/25	22/37/135/135	-
24	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
30	ECH	M	4021	-	-	8/29/66/66	0/2/2/2
21	CLA	1	1105	-	3/3/17/25	4/19/117/135	-
21	CLA	B	1210	-	2/2/20/25	17/37/135/135	-
24	BCR	9	4021	-	-	13/29/63/63	0/2/2/2
21	CLA	2	1207	-	2/2/18/25	14/27/125/135	-
30	ECH	b	4011	-	-	11/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	1226	-	3/3/20/25	15/37/135/135	-
21	CLA	b	1205	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1234	-	1/1/20/25	11/37/135/135	-
21	CLA	2	1208	-	3/3/19/25	13/31/129/135	-
21	CLA	1	1123	-	1/1/20/25	15/37/135/135	-
35	LMT	1	6001	-	-	8/21/61/61	0/2/2/2
26	LMG	K	5009	-	-	17/50/70/70	0/1/1/1
21	CLA	a	1130	-	3/3/20/25	15/37/135/135	-
21	CLA	B	1223	-	3/3/20/25	10/37/135/135	-
21	CLA	a	1140	-	3/3/20/25	12/37/135/135	-
24	BCR	b	4014	-	-	10/29/63/63	0/2/2/2
21	CLA	2	1021	-	3/3/20/25	14/37/135/135	-
21	CLA	1	1135	-	1/1/17/25	12/22/120/135	-
21	CLA	b	1201	-	3/3/20/25	13/37/135/135	-
26	LMG	b	5002	-	-	12/50/70/70	0/1/1/1
21	CLA	a	1109	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1204	-	3/3/20/25	15/37/135/135	-
21	CLA	A	1135	-	1/1/20/25	17/37/135/135	-
35	LMT	L	6001	-	-	9/21/61/61	0/2/2/2
21	CLA	A	1104	-	2/2/20/25	16/37/135/135	-
24	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
24	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
22	PQN	1	2001	-	-	3/23/43/43	0/2/2/2
21	CLA	2	1227	-	3/3/16/25	2/11/111/135	-
21	CLA	b	1217	-	3/3/17/25	10/21/119/135	-
21	CLA	a	1112	-	3/3/20/25	17/37/135/135	-
21	CLA	J	1303	-	3/3/20/25	22/37/135/135	-
21	CLA	1	1121	-	3/3/18/25	12/25/123/135	-
21	CLA	1	1133	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1205	-	3/3/20/25	19/37/135/135	-
26	LMG	A	5008	-	-	24/50/70/70	0/1/1/1
21	CLA	a	1801	25	3/3/18/25	13/25/123/135	-
21	CLA	0	1501	20	3/3/20/25	16/37/135/135	-
21	CLA	1	1801	25	3/3/18/25	11/27/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	1219	-	2/2/17/25	9/23/121/135	-
21	CLA	a	1012	38	3/3/20/25	19/37/135/135	-
24	BCR	2	4010	-	-	12/29/63/63	0/2/2/2
31	SQD	B	5008	-	-	23/49/69/69	0/1/1/1
21	CLA	2	1217	-	3/3/17/25	12/22/120/135	-
34	ZEX	F	4016	-	1/1/12/27	7/29/67/67	0/2/2/2
24	BCR	1	4008	-	-	9/29/63/63	0/2/2/2
21	CLA	b	1236	-	3/3/20/25	13/37/135/135	-
25	LHG	1	5003	21	-	32/53/53/53	-
24	BCR	8	4001	-	-	10/29/63/63	0/2/2/2
21	CLA	A	1137	-	3/3/20/25	16/37/135/135	-
21	CLA	B	1201	-	3/3/20/25	15/37/135/135	-
21	CLA	A	1132	-	3/3/20/25	13/37/135/135	-
21	CLA	B	1229	-	3/3/20/25	16/37/135/135	-
21	CLA	b	1218	-	3/3/20/25	18/37/135/135	-
21	CLA	a	1104	-	3/3/20/25	25/37/135/135	-
21	CLA	b	1232	-	3/3/20/25	18/37/135/135	-
30	ECH	B	4006	-	-	7/29/66/66	0/2/2/2
21	CLA	b	1231	38	3/3/20/25	22/37/135/135	-
21	CLA	A	1129	-	2/2/18/25	11/29/127/135	-
24	BCR	j	4013	-	-	9/29/63/63	0/2/2/2
25	LHG	a	5003	21	-	39/53/53/53	-
22	PQN	a	2001	-	-	7/23/43/43	0/2/2/2
21	CLA	A	1111	-	3/3/20/25	16/37/135/135	-
21	CLA	b	1215	-	3/3/20/25	17/37/135/135	-
21	CLA	L	1501	10	3/3/20/25	17/37/135/135	-
21	CLA	A	1134	1	3/3/20/25	19/37/135/135	-
21	CLA	1	1110	-	3/3/17/25	8/19/117/135	-
21	CLA	0	1503	38	3/3/20/25	20/37/135/135	-
24	BCR	B	4017	-	-	9/29/63/63	0/2/2/2
21	CLA	f	1302	-	3/3/20/25	23/37/135/135	-
21	CLA	2	1202	-	2/2/20/25	21/37/135/135	-
21	CLA	b	1204	-	3/3/20/25	12/37/135/135	-
21	CLA	A	1130	-	3/3/19/25	6/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	b	5006	-	-	27/49/69/69	0/1/1/1
21	CLA	6	1302	6	3/3/15/25	5/11/109/135	-
21	CLA	A	1107	1	3/3/20/25	19/37/135/135	-
21	CLA	b	1237	38	3/3/20/25	14/37/135/135	-
21	CLA	2	1215	-	3/3/19/25	16/31/129/135	-
21	CLA	B	1235	-	3/3/20/25	14/37/135/135	-
21	CLA	A	1133	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1139	38	3/3/20/25	13/37/135/135	-
22	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
21	CLA	B	1221	-	3/3/20/25	12/37/135/135	-
21	CLA	1	1126	-	3/3/20/25	20/37/135/135	-
21	CLA	a	1124	-	3/3/18/25	9/25/123/135	-
24	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
21	CLA	2	1023	-	3/3/20/25	16/37/135/135	-
21	CLA	A	1115	-	3/3/20/25	7/37/135/135	-
21	CLA	2	1222	-	3/3/17/25	6/19/117/135	-
21	CLA	B	1218	-	3/3/20/25	21/37/135/135	-
24	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1117	-	3/3/20/25	20/37/135/135	-
21	CLA	7	1303	-	3/3/15/25	3/8/106/135	-
26	LMG	b	5007	-	-	18/50/70/70	0/1/1/1
25	LHG	A	5003	21	-	27/53/53/53	-
22	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
36	EQ3	I	4020	-	-	8/29/68/68	0/2/2/2
21	CLA	b	1207	-	2/2/20/25	13/37/135/135	-
21	CLA	1	1109	16	3/3/20/25	17/37/135/135	-
21	CLA	2	1212	-	3/3/15/25	5/8/106/135	-
21	CLA	2	1218	-	3/3/20/25	18/37/135/135	-
21	CLA	B	1021	-	3/3/20/25	10/37/135/135	-
21	CLA	B	1227	-	2/2/18/25	13/25/123/135	-
21	CLA	A	1131	-	3/3/20/25	17/37/135/135	-
24	BCR	a	4019	-	-	9/29/63/63	0/2/2/2
30	ECH	b	4006	-	-	7/29/66/66	0/2/2/2
34	ZEX	J	4015	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	f	5001	-	-	19/49/69/69	0/1/1/1
21	CLA	A	1117	-	3/3/20/25	16/37/135/135	-
24	BCR	B	4018	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1128	-	3/3/20/25	16/37/135/135	-
25	LHG	1	5007	-	-	30/53/53/53	-
21	CLA	b	1238	38	3/3/20/25	7/37/135/135	-
24	BCR	l	4019	-	-	7/29/63/63	0/2/2/2
21	CLA	l	1502	-	3/3/20/25	15/37/135/135	-
21	CLA	B	1022	38	3/3/20/25	6/37/135/135	-
23	SF4	1	3001	2,16	-	-	0/6/5/5
21	CLA	2	1240	-	2/2/15/25	4/8/106/135	-
21	CLA	K	1402	-	1/1/20/25	17/37/135/135	-
23	SF4	3	3002	-	-	-	0/6/5/5
24	BCR	2	4017	-	-	12/29/63/63	0/2/2/2
21	CLA	a	1110	-	3/3/18/25	17/30/128/135	-
28	45D	h	4020	21	-	15/29/69/69	0/2/2/2
24	BCR	2	4014	-	-	7/29/63/63	0/2/2/2
24	BCR	1	4012	-	-	14/29/63/63	0/2/2/2
21	CLA	b	1221	38	3/3/20/25	13/37/135/135	-
31	SQD	L	5002	-	-	18/49/69/69	0/1/1/1
21	CLA	b	1210	-	2/2/20/25	20/37/135/135	-
26	LMG	a	5002	-	-	18/45/65/70	0/1/1/1
24	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
21	CLA	B	1203	-	2/2/20/25	15/37/135/135	-
30	ECH	2	4006	-	-	11/29/66/66	0/2/2/2
21	CLA	A	1119	38	3/3/20/25	18/37/135/135	-
21	CLA	1	1140	-	3/3/20/25	14/37/135/135	-
21	CLA	1	1114	-	3/3/16/25	5/11/111/135	-
25	LHG	B	5006	-	-	34/53/53/53	-
35	LMT	l	6001	-	-	6/21/61/61	0/2/2/2
21	CLA	b	1209	-	2/2/20/25	18/37/135/135	-
21	CLA	A	1139	38	3/3/20/25	15/37/135/135	-
24	BCR	a	4007	-	-	9/29/63/63	0/2/2/2
24	BCR	b	4004	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	1118	-	3/3/20/25	19/37/135/135	-
21	CLA	1	1102	-	3/3/18/25	11/25/123/135	-
24	BCR	7	4013	-	-	12/29/63/63	0/2/2/2
21	CLA	A	1125	-	2/2/20/25	21/37/135/135	-
21	CLA	6	1301	38	3/3/16/25	6/16/114/135	-
21	CLA	B	1232	-	3/3/17/25	4/19/117/135	-
24	BCR	A	4019	-	-	11/29/63/63	0/2/2/2
21	CLA	2	1228	-	3/3/16/25	7/11/111/135	-
23	SF4	c	3002	-	-	-	0/6/5/5
21	CLA	a	1136	-	3/3/20/25	17/37/135/135	-
25	LHG	A	5006	-	-	29/53/53/53	-
21	CLA	A	1140	-	3/3/20/25	17/37/135/135	-
26	LMG	a	5004	-	-	15/50/70/70	0/1/1/1
21	CLA	1	1136	-	3/3/20/25	18/37/135/135	-
21	CLA	2	1209	-	1/1/16/25	6/11/111/135	-
21	CLA	2	1203	-	3/3/20/25	20/37/135/135	-
21	CLA	8	1401	-	3/3/16/25	4/11/111/135	-
21	CLA	A	1108	-	3/3/17/25	11/23/121/135	-
21	CLA	2	1239	-	3/3/20/25	17/37/135/135	-
21	CLA	1	1108	-	3/3/16/25	10/15/113/135	-
21	CLA	A	1013	-	3/3/20/25	15/37/135/135	-
21	CLA	1	1138	-	3/3/19/25	13/31/129/135	-
21	CLA	b	1223	-	2/2/20/25	13/37/135/135	-
30	ECH	m	4021	-	-	7/29/66/66	0/2/2/2
25	LHG	0	5002	-	-	24/53/53/53	-
24	BCR	b	4018	-	-	10/29/63/63	0/2/2/2
21	CLA	2	1221	-	3/3/20/25	15/37/135/135	-
21	CLA	A	1120	-	3/3/20/25	17/37/135/135	-
21	CLA	B	1205	-	3/3/20/25	16/37/135/135	-
24	BCR	L	4022	-	-	10/29/63/63	0/2/2/2
21	CLA	1	1012	38	2/2/20/25	21/37/135/135	-
21	CLA	A	1011	-	3/3/20/25	11/37/135/135	-
21	CLA	B	1225	-	3/3/20/25	13/37/135/135	-
25	LHG	A	5005	-	-	36/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	1230	-	3/3/20/25	21/37/135/135	-
21	CLA	a	1137	-	3/3/17/25	7/19/117/135	-
26	LMG	A	5002	-	-	21/45/65/70	0/1/1/1
26	LMG	B	5005	-	-	11/50/70/70	0/1/1/1
21	CLA	l	1503	-	3/3/20/25	23/37/135/135	-
25	LHG	l	5004	-	-	28/53/53/53	-
30	ECH	i	4020	-	-	10/29/66/66	0/2/2/2
25	LHG	l	5005	-	-	36/53/53/53	-
21	CLA	b	1219	-	3/3/19/25	18/31/129/135	-
24	BCR	A	4007	-	-	9/29/63/63	0/2/2/2
24	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
21	CLA	a	1134	1	3/3/16/25	10/18/116/135	-
21	CLA	l	1120	-	3/3/20/25	19/37/135/135	-
25	LHG	l	5003	-	-	33/53/53/53	-
21	CLA	l	1125	-	3/3/20/25	15/37/135/135	-
25	LHG	a	5001	-	-	27/53/53/53	-
21	CLA	A	1124	38	3/3/20/25	10/37/135/135	-
25	LHG	0	5004	-	-	32/53/53/53	-
21	CLA	2	1224	-	3/3/18/25	17/25/123/135	-
35	LMT	0	6001	-	-	14/21/61/61	0/2/2/2
21	CLA	A	1109	21	3/3/20/25	15/37/135/135	-
21	CLA	J	1302	8	3/3/20/25	13/37/135/135	-
21	CLA	a	1135	-	2/2/20/25	23/37/135/135	-
21	CLA	a	1138	-	3/3/20/25	13/37/135/135	-
26	LMG	2	5002	-	-	11/50/70/70	0/1/1/1
21	CLA	b	1213	-	3/3/20/25	17/37/135/135	-
24	BCR	l	4019	-	-	14/29/63/63	0/2/2/2
21	CLA	l	1117	-	3/3/20/25	16/37/135/135	-
24	BCR	a	4012	-	-	7/29/63/63	0/2/2/2
21	CLA	a	1114	-	3/3/17/25	8/22/120/135	-
21	CLA	B	1206	2	3/3/20/25	17/37/135/135	-
31	SQD	L	5001	-	-	21/46/66/69	0/1/1/1
21	CLA	A	1127	-	3/3/20/25	17/37/135/135	-
24	BCR	i	4018	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	1232	-	2/2/16/25	5/11/111/135	-
21	CLA	1	1128	-	3/3/20/25	18/37/135/135	-
21	CLA	a	1126	-	3/3/20/25	21/37/135/135	-
31	SQD	0	5005	-	-	27/49/69/69	0/1/1/1
24	BCR	B	4004	-	-	15/29/63/63	0/2/2/2
21	CLA	A	1118	-	3/3/20/25	17/37/135/135	-
21	CLA	a	1108	-	3/3/18/25	13/28/126/135	-
22	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
21	CLA	a	1125	-	3/3/20/25	11/37/135/135	-
21	CLA	a	1120	-	2/2/18/25	10/25/123/135	-
24	BCR	2	4004	-	-	13/29/63/63	0/2/2/2
21	CLA	a	1119	-	3/3/20/25	17/37/135/135	-

All (2502) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	4016	ZEX	C38-C24	37.43	2.55	1.53
34	J	4015	ZEX	C38-C24	37.01	2.54	1.53
34	j	4015	ZEX	C38-C24	36.94	2.54	1.53
34	7	4015	ZEX	C38-C24	36.93	2.54	1.53
28	h	4020	45D	C08-C16	13.47	1.54	1.35
36	I	4020	EQ3	C25-C26	13.39	1.54	1.35
28	B	4011	45D	C08-C16	12.95	1.53	1.35
28	h	4020	45D	C07-C15	12.67	1.53	1.35
28	B	4011	45D	C07-C15	11.93	1.52	1.35
36	I	4020	EQ3	C4-C3	11.27	1.71	1.52
36	I	4020	EQ3	C5-C6	10.88	1.53	1.34
27	A	7001	ACT	CH3-C	7.80	1.58	1.48
27	B	7002	ACT	CH3-C	6.86	1.57	1.48
27	B	7001	ACT	CH3-C	6.52	1.57	1.48
27	a	7001	ACT	CH3-C	6.51	1.57	1.48
21	B	1238	CLA	MG-NA	6.49	2.21	2.06
21	B	1210	CLA	MG-NA	6.47	2.21	2.06
21	a	1101	CLA	MG-NA	6.47	2.21	2.06
21	B	1213	CLA	MG-NA	6.46	2.21	2.06
21	1	1127	CLA	MG-NA	6.46	2.21	2.06
21	b	1238	CLA	MG-NA	6.45	2.21	2.06
21	a	1120	CLA	MG-NA	6.45	2.21	2.06
21	B	1240	CLA	MG-NA	6.44	2.21	2.06
21	1	1121	CLA	MG-NA	6.44	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1123	CLA	MG-NA	6.43	2.21	2.06
21	1	1124	CLA	MG-NA	6.43	2.21	2.06
21	2	1218	CLA	MG-NA	6.43	2.21	2.06
21	1	1123	CLA	MG-NA	6.43	2.21	2.06
21	A	1113	CLA	MG-NA	6.43	2.21	2.06
36	I	4020	EQ3	C2-C3	-6.42	1.43	1.52
21	a	1108	CLA	MG-NA	6.42	2.21	2.06
21	A	1127	CLA	MG-NA	6.42	2.21	2.06
21	a	1123	CLA	MG-NA	6.42	2.21	2.06
21	2	1209	CLA	MG-NA	6.42	2.21	2.06
21	A	1105	CLA	MG-NA	6.41	2.21	2.06
21	2	1219	CLA	MG-NA	6.41	2.21	2.06
21	a	1121	CLA	MG-NA	6.41	2.21	2.06
21	B	1209	CLA	MG-NA	6.41	2.21	2.06
21	A	1136	CLA	MG-NA	6.41	2.21	2.06
21	j	1303	CLA	MG-NA	6.41	2.21	2.06
21	B	1239	CLA	MG-NA	6.41	2.21	2.06
21	A	1122	CLA	MG-NA	6.40	2.21	2.06
21	b	1226	CLA	MG-NA	6.40	2.21	2.06
21	1	1128	CLA	MG-NA	6.40	2.21	2.06
21	1	1101	CLA	MG-NA	6.39	2.21	2.06
21	B	1207	CLA	MG-NA	6.39	2.21	2.06
21	1	1114	CLA	MG-NA	6.39	2.21	2.06
21	1	1125	CLA	MG-NA	6.39	2.21	2.06
21	b	1240	CLA	MG-NA	6.39	2.21	2.06
21	A	1012	CLA	MG-NA	6.39	2.21	2.06
21	a	1136	CLA	MG-NA	6.38	2.21	2.06
21	1	1105	CLA	MG-NA	6.38	2.21	2.06
21	8	1401	CLA	MG-NA	6.38	2.21	2.06
21	2	1234	CLA	MG-NA	6.38	2.21	2.06
21	A	1114	CLA	MG-NA	6.38	2.21	2.06
21	b	1218	CLA	MG-NA	6.38	2.21	2.06
21	1	1111	CLA	MG-NA	6.37	2.21	2.06
21	B	1022	CLA	MG-NA	6.37	2.21	2.06
21	1	1120	CLA	MG-NA	6.37	2.21	2.06
21	A	1118	CLA	MG-NA	6.37	2.21	2.06
21	a	1114	CLA	MG-NA	6.37	2.21	2.06
21	a	1137	CLA	MG-NA	6.36	2.21	2.06
21	a	1133	CLA	MG-NA	6.36	2.21	2.06
21	b	1217	CLA	MG-NA	6.36	2.21	2.06
21	f	1301	CLA	MG-NA	6.35	2.21	2.06
21	2	1214	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1212	CLA	MG-NA	6.35	2.21	2.06
21	2	1211	CLA	MG-NA	6.35	2.21	2.06
21	F	1302	CLA	MG-NA	6.35	2.21	2.06
21	k	1401	CLA	MG-NA	6.35	2.21	2.06
21	2	1240	CLA	MG-NA	6.35	2.21	2.06
21	1	1135	CLA	MG-NA	6.34	2.21	2.06
21	B	1234	CLA	MG-NA	6.34	2.21	2.06
21	A	1117	CLA	MG-NA	6.34	2.21	2.06
21	b	1239	CLA	MG-NA	6.34	2.21	2.06
21	a	1117	CLA	MG-NA	6.34	2.21	2.06
21	1	1113	CLA	MG-NA	6.34	2.21	2.06
21	B	1218	CLA	MG-NA	6.34	2.21	2.06
21	2	1238	CLA	MG-NA	6.33	2.21	2.06
21	B	1216	CLA	MG-NA	6.33	2.21	2.06
21	a	1105	CLA	MG-NA	6.33	2.21	2.06
21	6	1301	CLA	MG-NA	6.33	2.21	2.06
21	F	1301	CLA	MG-NA	6.33	2.21	2.06
21	B	1204	CLA	MG-NA	6.32	2.21	2.06
21	a	1113	CLA	MG-NA	6.32	2.21	2.06
21	8	1402	CLA	MG-NA	6.32	2.21	2.06
21	A	1131	CLA	MG-NA	6.32	2.21	2.06
21	a	1134	CLA	MG-NA	6.32	2.21	2.06
21	2	1220	CLA	MG-NA	6.32	2.21	2.06
21	1	1139	CLA	MG-NA	6.32	2.21	2.06
21	2	1239	CLA	MG-NA	6.31	2.21	2.06
21	b	1228	CLA	MG-NA	6.31	2.21	2.06
21	B	1220	CLA	MG-NA	6.31	2.21	2.06
21	A	1134	CLA	MG-NA	6.31	2.21	2.06
21	f	1302	CLA	MG-NA	6.31	2.21	2.06
21	1	1129	CLA	MG-NA	6.31	2.21	2.06
21	a	1140	CLA	MG-NA	6.31	2.21	2.06
21	B	1232	CLA	MG-NA	6.31	2.21	2.06
21	A	1101	CLA	MG-NA	6.31	2.21	2.06
21	6	1302	CLA	MG-NA	6.31	2.21	2.06
21	7	1303	CLA	MG-NA	6.31	2.21	2.06
21	b	1221	CLA	MG-NA	6.30	2.21	2.06
21	a	1135	CLA	MG-NA	6.30	2.21	2.06
21	a	1139	CLA	MG-NA	6.30	2.21	2.06
21	2	1236	CLA	MG-NA	6.30	2.21	2.06
21	B	1223	CLA	MG-NA	6.30	2.21	2.06
21	A	1130	CLA	MG-NA	6.30	2.21	2.06
21	2	1230	CLA	MG-NA	6.29	2.21	2.06

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1227	CLA	MG-NA	6.26	2.21	2.06
21	b	1232	CLA	MG-NA	6.26	2.21	2.06
21	1	1109	CLA	MG-NA	6.26	2.21	2.06
21	a	1125	CLA	MG-NA	6.26	2.21	2.06
21	1	1122	CLA	MG-NA	6.26	2.21	2.06
21	a	1129	CLA	MG-NA	6.26	2.21	2.06
21	2	1203	CLA	MG-NA	6.26	2.21	2.06
21	2	1221	CLA	MG-NA	6.25	2.21	2.06
21	2	1222	CLA	MG-NA	6.25	2.21	2.06
21	0	1503	CLA	MG-NA	6.25	2.21	2.06
21	j	1302	CLA	MG-NA	6.25	2.21	2.06
21	B	1237	CLA	MG-NA	6.25	2.21	2.06
21	B	1208	CLA	MG-NA	6.25	2.21	2.06
21	J	1303	CLA	MG-NA	6.24	2.21	2.06
21	B	1203	CLA	MG-NA	6.24	2.21	2.06
21	2	1223	CLA	MG-NA	6.24	2.21	2.06
21	A	1116	CLA	MG-NA	6.24	2.21	2.06
21	B	1217	CLA	MG-NA	6.24	2.21	2.06
21	1	1115	CLA	MG-NA	6.24	2.21	2.06
21	b	1223	CLA	MG-NA	6.24	2.21	2.06
21	a	1012	CLA	MG-NA	6.24	2.21	2.06
21	a	1122	CLA	MG-NA	6.23	2.21	2.06
21	a	1116	CLA	MG-NA	6.23	2.21	2.06
21	1	1134	CLA	MG-NA	6.23	2.21	2.06
21	2	1232	CLA	MG-NA	6.23	2.21	2.06
21	2	1215	CLA	MG-NA	6.23	2.21	2.06
21	A	1140	CLA	MG-NA	6.23	2.21	2.06
21	1	1118	CLA	MG-NA	6.23	2.21	2.06
21	1	1140	CLA	MG-NA	6.22	2.21	2.06
21	B	1211	CLA	MG-NA	6.22	2.21	2.06
21	A	1137	CLA	MG-NA	6.22	2.21	2.06
21	b	1210	CLA	MG-NA	6.22	2.21	2.06
21	A	1115	CLA	MG-NA	6.22	2.21	2.06
21	a	1112	CLA	MG-NA	6.22	2.21	2.06
21	1	1126	CLA	MG-NA	6.22	2.21	2.06
21	1	1110	CLA	MG-NA	6.21	2.21	2.06
21	b	1206	CLA	MG-NA	6.21	2.21	2.06
21	1	1116	CLA	MG-NA	6.21	2.21	2.06
21	B	1236	CLA	MG-NA	6.21	2.21	2.06
21	A	1104	CLA	MG-NA	6.21	2.21	2.06
21	B	1227	CLA	MG-NA	6.21	2.21	2.06
21	a	1131	CLA	MG-NA	6.21	2.21	2.06

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1107	CLA	MG-NA	6.16	2.20	2.06
21	b	1204	CLA	MG-NA	6.16	2.20	2.06
21	B	1202	CLA	MG-NA	6.15	2.20	2.06
21	1	1132	CLA	MG-NA	6.15	2.20	2.06
21	a	1102	CLA	MG-NA	6.15	2.20	2.06
21	2	1237	CLA	MG-NA	6.15	2.20	2.06
21	0	1502	CLA	MG-NA	6.15	2.20	2.06
21	A	1121	CLA	MG-NA	6.15	2.20	2.06
21	1	1131	CLA	MG-NA	6.15	2.20	2.06
21	2	1213	CLA	MG-NA	6.14	2.20	2.06
21	b	1215	CLA	MG-NA	6.14	2.20	2.06
21	B	1226	CLA	MG-NA	6.13	2.20	2.06
21	b	1201	CLA	MG-NA	6.13	2.20	2.06
21	1	1013	CLA	MG-NA	6.13	2.20	2.06
21	a	1124	CLA	MG-NA	6.13	2.20	2.06
21	A	1110	CLA	MG-NA	6.12	2.20	2.06
21	b	1211	CLA	MG-NA	6.12	2.20	2.06
21	B	1206	CLA	MG-NA	6.12	2.20	2.06
21	a	1011	CLA	MG-NA	6.12	2.20	2.06
21	b	1227	CLA	MG-NA	6.11	2.20	2.06
21	B	1224	CLA	MG-NA	6.11	2.20	2.06
21	A	1108	CLA	MG-NA	6.11	2.20	2.06
21	B	1205	CLA	MG-NA	6.10	2.20	2.06
21	2	1205	CLA	MG-NA	6.10	2.20	2.06
21	1	1012	CLA	MG-NA	6.10	2.20	2.06
21	A	1139	CLA	MG-NA	6.10	2.20	2.06
21	A	1138	CLA	MG-NA	6.10	2.20	2.06
21	B	1215	CLA	MG-NA	6.10	2.20	2.06
21	2	1201	CLA	MG-NA	6.10	2.20	2.06
21	B	1230	CLA	MG-NA	6.10	2.20	2.06
21	B	1221	CLA	MG-NA	6.10	2.20	2.06
21	2	1021	CLA	MG-NA	6.10	2.20	2.06
21	B	1229	CLA	MG-NA	6.09	2.20	2.06
21	a	1126	CLA	MG-NA	6.09	2.20	2.06
21	a	1106	CLA	MG-NA	6.08	2.20	2.06
21	2	1023	CLA	MG-NA	6.08	2.20	2.06
21	B	1231	CLA	MG-NA	6.08	2.20	2.06
21	2	1224	CLA	MG-NA	6.08	2.20	2.06
21	A	1126	CLA	MG-NA	6.07	2.20	2.06
21	B	1222	CLA	MG-NA	6.06	2.20	2.06
21	2	1228	CLA	MG-NA	6.06	2.20	2.06
21	b	1237	CLA	MG-NA	6.05	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1230	CLA	MG-NA	6.05	2.20	2.06
21	b	1224	CLA	MG-NA	6.05	2.20	2.06
21	b	1235	CLA	MG-NA	6.05	2.20	2.06
21	b	1216	CLA	MG-NA	6.04	2.20	2.06
21	2	1216	CLA	MG-NA	6.04	2.20	2.06
21	B	1021	CLA	MG-NA	6.04	2.20	2.06
21	b	1231	CLA	MG-NA	6.04	2.20	2.06
21	1	1119	CLA	MG-NA	6.04	2.20	2.06
21	A	1124	CLA	MG-NA	6.04	2.20	2.06
21	A	1119	CLA	MG-NA	6.02	2.20	2.06
21	b	1205	CLA	MG-NA	6.02	2.20	2.06
21	A	1011	CLA	MG-NA	6.01	2.20	2.06
21	L	1502	CLA	MG-NA	6.01	2.20	2.06
21	b	1023	CLA	MG-NA	6.00	2.20	2.06
21	b	1222	CLA	MG-NA	5.98	2.20	2.06
21	B	1023	CLA	MG-NA	5.98	2.20	2.06
21	A	1013	CLA	MG-NA	5.98	2.20	2.06
21	a	1103	CLA	MG-NA	5.96	2.20	2.06
21	l	1503	CLA	MG-NA	5.93	2.20	2.06
21	A	1106	CLA	MG-NA	5.93	2.20	2.06
21	B	1235	CLA	MG-NA	5.93	2.20	2.06
21	1	1103	CLA	MG-NA	5.92	2.20	2.06
21	b	1202	CLA	MG-NA	5.91	2.20	2.06
21	A	1103	CLA	MG-NA	5.83	2.20	2.06
21	a	1013	CLA	MG-NA	5.81	2.20	2.06
28	B	4011	45D	C23-C25	4.78	1.56	1.45
36	I	4020	EQ3	C1-C6	-4.71	1.47	1.53
28	h	4020	45D	C23-C25	4.67	1.56	1.45
36	I	4020	EQ3	C4-C5	-4.62	1.43	1.51
36	I	4020	EQ3	C11-C10	4.53	1.57	1.43
36	I	4020	EQ3	C15-C14	4.51	1.57	1.43
28	B	4011	45D	C24-C26	4.50	1.55	1.45
28	B	4011	45D	C33-C35	4.38	1.55	1.45
28	h	4020	45D	C33-C35	4.25	1.55	1.45
28	B	4011	45D	C34-C36	4.24	1.55	1.45
28	h	4020	45D	C24-C26	4.09	1.54	1.45
28	h	4020	45D	C34-C36	4.06	1.54	1.45
36	I	4020	EQ3	C23-C22	3.95	1.54	1.45
36	I	4020	EQ3	C7-C6	3.89	1.58	1.45
36	I	4020	EQ3	C12-C13	3.77	1.54	1.45
28	B	4011	45D	C42-C38	3.73	1.55	1.43
36	I	4020	EQ3	C19-C18	3.73	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	4011	45D	C41-C37	3.69	1.54	1.43
28	h	4020	45D	C42-C38	3.66	1.54	1.43
28	B	4011	45D	C32-C30	3.58	1.54	1.43
28	B	4011	45D	C31-C29	3.49	1.54	1.43
28	h	4020	45D	C41-C37	3.47	1.54	1.43
28	h	4020	45D	C31-C29	3.41	1.54	1.43
21	B	1202	CLA	CBB-CAB	3.41	1.51	1.29
21	A	1117	CLA	CBB-CAB	3.41	1.51	1.29
21	b	1202	CLA	CBB-CAB	3.40	1.51	1.29
21	j	1302	CLA	CBB-CAB	3.39	1.51	1.29
21	2	1234	CLA	CBB-CAB	3.39	1.51	1.29
21	A	1127	CLA	CBB-CAB	3.38	1.51	1.29
21	A	1013	CLA	CBB-CAB	3.38	1.51	1.29
21	1	1132	CLA	CBB-CAB	3.38	1.51	1.29
21	6	1302	CLA	CBB-CAB	3.38	1.51	1.29
21	a	1113	CLA	CBB-CAB	3.38	1.51	1.29
21	a	1117	CLA	CBB-CAB	3.38	1.51	1.29
21	B	1213	CLA	CBB-CAB	3.38	1.51	1.29
21	l	1501	CLA	CBB-CAB	3.38	1.51	1.29
21	B	1234	CLA	CBB-CAB	3.38	1.51	1.29
21	A	1123	CLA	CBB-CAB	3.38	1.51	1.29
21	b	1234	CLA	CBB-CAB	3.38	1.51	1.29
21	B	1228	CLA	CBB-CAB	3.38	1.51	1.29
21	6	1301	CLA	CBB-CAB	3.37	1.51	1.29
21	L	1501	CLA	CBB-CAB	3.37	1.51	1.29
21	2	1230	CLA	CBB-CAB	3.37	1.51	1.29
21	l	1503	CLA	CBB-CAB	3.37	1.51	1.29
21	2	1023	CLA	CBB-CAB	3.37	1.51	1.29
21	A	1109	CLA	CBB-CAB	3.37	1.51	1.29
21	B	1206	CLA	CBB-CAB	3.37	1.51	1.29
21	b	1222	CLA	CBB-CAB	3.37	1.51	1.29
21	8	1402	CLA	CBB-CAB	3.37	1.51	1.29
21	2	1212	CLA	CBB-CAB	3.37	1.51	1.29
21	A	1131	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1128	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1801	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1121	CLA	CBB-CAB	3.37	1.51	1.29
21	k	1401	CLA	CBB-CAB	3.37	1.51	1.29
21	K	1401	CLA	CBB-CAB	3.37	1.51	1.29
21	A	1102	CLA	CBB-CAB	3.37	1.51	1.29
21	B	1224	CLA	CBB-CAB	3.37	1.51	1.29
21	1	1103	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1138	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1118	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1104	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1126	CLA	CBB-CAB	3.37	1.51	1.29
21	a	1102	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1119	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1224	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1134	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1130	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1125	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1209	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1216	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1113	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1118	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1206	CLA	CBB-CAB	3.36	1.51	1.29
21	B	1023	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1114	CLA	CBB-CAB	3.36	1.51	1.29
21	8	1401	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1231	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1104	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1215	CLA	CBB-CAB	3.36	1.51	1.29
21	a	1132	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1101	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1232	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1119	CLA	CBB-CAB	3.36	1.51	1.29
21	B	1210	CLA	CBB-CAB	3.36	1.51	1.29
21	K	1402	CLA	CBB-CAB	3.36	1.51	1.29
21	B	1236	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1204	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1236	CLA	CBB-CAB	3.36	1.51	1.29
21	B	1220	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1222	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1240	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1236	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1106	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1109	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1120	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1128	CLA	CBB-CAB	3.36	1.51	1.29
21	B	1222	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1801	CLA	CBB-CAB	3.36	1.51	1.29
21	j	1303	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1210	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1224	CLA	CBB-CAB	3.36	1.51	1.29
21	a	1012	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1122	CLA	CBB-CAB	3.36	1.51	1.29
21	a	1114	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1103	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1132	CLA	CBB-CAB	3.36	1.51	1.29
21	7	1303	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1013	CLA	CBB-CAB	3.36	1.51	1.29
21	L	1503	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1202	CLA	CBB-CAB	3.36	1.51	1.29
21	J	1302	CLA	CBB-CAB	3.36	1.51	1.29
21	2	1239	CLA	CBB-CAB	3.36	1.51	1.29
21	A	1134	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1104	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1230	CLA	CBB-CAB	3.36	1.51	1.29
21	a	1013	CLA	CBB-CAB	3.36	1.51	1.29
21	b	1201	CLA	CBB-CAB	3.36	1.51	1.29
21	1	1117	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1123	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1111	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1102	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1235	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1130	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1106	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1206	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1203	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1213	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1109	CLA	CBB-CAB	3.35	1.51	1.29
21	F	1301	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1218	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1211	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1130	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1124	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1125	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1226	CLA	CBB-CAB	3.35	1.51	1.29
21	k	1402	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1230	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1120	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1022	CLA	CBB-CAB	3.35	1.51	1.29
21	l	1502	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1221	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1217	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1231	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1021	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1108	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1115	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1125	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1207	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1012	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1012	CLA	CBB-CAB	3.35	1.51	1.29
21	a	1112	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1217	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1123	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1211	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1218	CLA	CBB-CAB	3.35	1.51	1.29
21	J	1303	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1201	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1113	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1238	CLA	CBB-CAB	3.35	1.51	1.29
21	B	1209	CLA	CBB-CAB	3.35	1.51	1.29
21	A	1128	CLA	CBB-CAB	3.35	1.51	1.29
21	b	1223	CLA	CBB-CAB	3.35	1.51	1.29
21	1	1135	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1221	CLA	CBB-CAB	3.35	1.51	1.29
21	2	1231	CLA	CBB-CAB	3.34	1.51	1.29
21	B	1221	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1136	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1108	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1134	CLA	CBB-CAB	3.34	1.51	1.29
21	B	1216	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1107	CLA	CBB-CAB	3.34	1.51	1.29
21	B	1021	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1801	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1011	CLA	CBB-CAB	3.34	1.51	1.29
21	0	1503	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1139	CLA	CBB-CAB	3.34	1.51	1.29
21	b	1239	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1219	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1022	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1208	CLA	CBB-CAB	3.34	1.51	1.29
21	B	1203	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1105	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1215	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1122	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1115	CLA	CBB-CAB	3.34	1.51	1.29
21	f	1301	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1211	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1108	CLA	CBB-CAB	3.34	1.51	1.29
21	b	1023	CLA	CBB-CAB	3.34	1.51	1.29
21	f	1302	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1140	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1118	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1218	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1131	CLA	CBB-CAB	3.34	1.51	1.29
21	b	1227	CLA	CBB-CAB	3.34	1.51	1.29
21	b	1205	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1126	CLA	CBB-CAB	3.34	1.51	1.29
21	2	1240	CLA	CBB-CAB	3.34	1.51	1.29
21	B	1232	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1135	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1124	CLA	CBB-CAB	3.34	1.51	1.29
21	A	1122	CLA	CBB-CAB	3.34	1.51	1.29
21	1	1124	CLA	CBB-CAB	3.34	1.51	1.29
21	b	1203	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1105	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1138	CLA	CBB-CAB	3.34	1.51	1.29
21	a	1140	CLA	CBB-CAB	3.34	1.51	1.29
21	7	1302	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1107	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1137	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1120	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1215	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1201	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1235	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1219	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1208	CLA	CBB-CAB	3.33	1.51	1.29
21	0	1502	CLA	CBB-CAB	3.33	1.51	1.29
21	2	1238	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1103	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1139	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1228	CLA	CBB-CAB	3.33	1.51	1.29
21	2	1223	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1011	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1133	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1223	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1127	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1119	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1216	CLA	CBB-CAB	3.33	1.51	1.29
21	1	1105	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1204	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1204	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1210	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1208	CLA	CBB-CAB	3.33	1.51	1.29
21	b	1213	CLA	CBB-CAB	3.33	1.51	1.29
21	1	1133	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1139	CLA	CBB-CAB	3.33	1.51	1.29
21	B	1239	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1111	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1115	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1126	CLA	CBB-CAB	3.33	1.51	1.29
21	a	1101	CLA	CBB-CAB	3.33	1.51	1.29
21	2	1021	CLA	CBB-CAB	3.33	1.51	1.29
21	A	1114	CLA	CBB-CAB	3.33	1.51	1.29
21	2	1225	CLA	CBB-CAB	3.32	1.51	1.29
21	B	1207	CLA	CBB-CAB	3.32	1.51	1.29
21	a	1106	CLA	CBB-CAB	3.32	1.51	1.29
21	A	1011	CLA	CBB-CAB	3.32	1.51	1.29
21	b	1232	CLA	CBB-CAB	3.32	1.51	1.29
21	L	1502	CLA	CBB-CAB	3.32	1.51	1.29
21	1	1129	CLA	CBB-CAB	3.32	1.51	1.29
21	A	1121	CLA	CBB-CAB	3.32	1.51	1.29
21	a	1129	CLA	CBB-CAB	3.32	1.51	1.29
21	1	1110	CLA	CBB-CAB	3.32	1.51	1.29
21	B	1022	CLA	CBB-CAB	3.32	1.51	1.29
21	1	1111	CLA	CBB-CAB	3.32	1.51	1.29
21	a	1116	CLA	CBB-CAB	3.32	1.51	1.29
21	A	1129	CLA	CBB-CAB	3.31	1.51	1.29
26	K	5009	LMG	C43-C42	-3.31	1.33	1.51
36	I	4020	EQ3	C35-C13	3.31	1.57	1.50
21	1	1137	CLA	CBB-CAB	3.31	1.51	1.29
21	a	1135	CLA	CBB-CAB	3.31	1.51	1.29
21	A	1110	CLA	CBB-CAB	3.31	1.51	1.29
21	2	1214	CLA	CBB-CAB	3.31	1.51	1.29
21	0	1501	CLA	CBB-CAB	3.31	1.51	1.29
21	b	1226	CLA	CBB-CAB	3.31	1.51	1.29
21	b	1220	CLA	CBB-CAB	3.31	1.51	1.29
21	b	1237	CLA	CBB-CAB	3.31	1.51	1.29
21	A	1107	CLA	CBB-CAB	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1131	CLA	CBB-CAB	3.31	1.51	1.29
21	1	1127	CLA	CBB-CAB	3.31	1.51	1.29
21	B	1219	CLA	CBB-CAB	3.31	1.51	1.29
21	2	1227	CLA	CBB-CAB	3.31	1.51	1.29
21	B	1229	CLA	CBB-CAB	3.31	1.51	1.29
21	A	1140	CLA	CBB-CAB	3.31	1.51	1.29
21	1	1121	CLA	CBB-CAB	3.31	1.51	1.29
21	F	1302	CLA	CBB-CAB	3.31	1.51	1.29
21	1	1112	CLA	CBB-CAB	3.31	1.51	1.29
21	B	1225	CLA	CBB-CAB	3.30	1.51	1.29
21	B	1227	CLA	CBB-CAB	3.30	1.51	1.29
21	2	1228	CLA	CBB-CAB	3.30	1.51	1.29
21	A	1136	CLA	CBB-CAB	3.30	1.51	1.29
21	a	1110	CLA	CBB-CAB	3.30	1.51	1.29
21	1	1116	CLA	CBB-CAB	3.30	1.51	1.29
21	a	1137	CLA	CBB-CAB	3.30	1.51	1.29
21	2	1205	CLA	CBB-CAB	3.30	1.51	1.29
21	b	1209	CLA	CBB-CAB	3.30	1.51	1.29
21	b	1229	CLA	CBB-CAB	3.30	1.51	1.29
21	2	1207	CLA	CBB-CAB	3.29	1.51	1.29
21	B	1214	CLA	CBB-CAB	3.29	1.51	1.29
26	b	5002	LMG	C40-C39	-3.29	1.33	1.51
21	A	1112	CLA	CBB-CAB	3.29	1.51	1.29
21	b	1217	CLA	CBB-CAB	3.29	1.51	1.29
21	b	1225	CLA	CBB-CAB	3.29	1.51	1.29
21	2	1220	CLA	CBB-CAB	3.29	1.51	1.29
26	K	5009	LMG	C37-C36	-3.29	1.33	1.51
21	B	1240	CLA	CBB-CAB	3.29	1.51	1.29
21	B	1205	CLA	CBB-CAB	3.29	1.51	1.29
21	2	1229	CLA	CBB-CAB	3.28	1.51	1.29
26	B	5002	LMG	C40-C39	-3.28	1.33	1.51
21	B	1212	CLA	CBB-CAB	3.28	1.51	1.29
21	A	1133	CLA	CBB-CAB	3.28	1.51	1.29
21	b	1235	CLA	CBB-CAB	3.27	1.51	1.29
21	A	1116	CLA	CBB-CAB	3.27	1.51	1.29
21	1	1136	CLA	CBB-CAB	3.27	1.51	1.29
21	b	1238	CLA	CBB-CAB	3.27	1.51	1.29
26	B	5002	LMG	C25-C24	-3.27	1.33	1.51
21	1	1138	CLA	CBB-CAB	3.27	1.51	1.29
26	b	5002	LMG	C43-C42	-3.27	1.33	1.51
26	b	5005	LMG	C40-C39	-3.27	1.33	1.51
36	I	4020	EQ3	C38-C26	3.27	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	5009	LMG	C22-C21	-3.26	1.33	1.51
26	2	5005	LMG	C37-C36	-3.26	1.33	1.51
26	B	5002	LMG	C43-C42	-3.26	1.33	1.51
26	B	5002	LMG	C19-C18	-3.26	1.33	1.51
21	b	1214	CLA	CBB-CAB	3.26	1.50	1.29
21	b	1212	CLA	CBB-CAB	3.26	1.50	1.29
26	2	5002	LMG	C40-C39	-3.26	1.33	1.51
26	b	5005	LMG	C37-C36	-3.26	1.33	1.51
26	K	5009	LMG	C40-C39	-3.25	1.33	1.51
21	2	1226	CLA	CBB-CAB	3.25	1.50	1.29
26	b	5002	LMG	C37-C36	-3.25	1.33	1.51
26	B	5002	LMG	C37-C36	-3.25	1.33	1.51
26	K	5009	LMG	C19-C18	-3.25	1.33	1.51
26	1	5004	LMG	C19-C18	-3.25	1.33	1.51
26	2	5005	LMG	C40-C39	-3.25	1.33	1.51
26	2	5005	LMG	C22-C21	-3.24	1.33	1.51
26	2	5002	LMG	C37-C36	-3.24	1.33	1.51
26	2	5002	LMG	C19-C18	-3.24	1.33	1.51
26	b	5007	LMG	C19-C18	-3.24	1.33	1.51
36	I	4020	EQ3	O3-C3	-3.24	1.33	1.43
26	a	5004	LMG	C40-C39	-3.24	1.33	1.51
26	0	5001	LMG	C19-C18	-3.24	1.33	1.51
26	2	5002	LMG	C43-C42	-3.23	1.33	1.51
26	1	5004	LMG	C22-C21	-3.23	1.33	1.51
26	b	5002	LMG	C19-C18	-3.23	1.33	1.51
26	A	5002	LMG	C37-C36	-3.23	1.33	1.51
26	B	5005	LMG	C37-C36	-3.23	1.33	1.51
21	A	1101	CLA	CBB-CAB	3.22	1.50	1.29
26	b	5005	LMG	C19-C18	-3.22	1.33	1.51
21	B	1237	CLA	CBB-CAB	3.22	1.50	1.29
26	a	5004	LMG	C43-C42	-3.22	1.33	1.51
37	L	5004	DGD	CAB-C9B	-3.22	1.33	1.51
26	B	5005	LMG	C40-C39	-3.22	1.33	1.51
26	0	5001	LMG	C22-C21	-3.22	1.33	1.51
26	A	5008	LMG	C25-C24	-3.22	1.33	1.51
21	2	1237	CLA	CBB-CAB	3.22	1.50	1.29
26	1	5004	LMG	C25-C24	-3.22	1.33	1.51
26	0	5001	LMG	C25-C24	-3.21	1.33	1.51
26	B	5005	LMG	C22-C21	-3.21	1.33	1.51
26	a	5004	LMG	C25-C24	-3.21	1.33	1.51
26	a	5002	LMG	C37-C36	-3.21	1.33	1.51
26	A	5004	LMG	C25-C24	-3.21	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	5002	LMG	C40-C39	-3.21	1.33	1.51
26	a	5004	LMG	C37-C36	-3.21	1.33	1.51
26	2	5005	LMG	C19-C18	-3.21	1.33	1.51
34	F	4016	ZEX	C24-C25	-3.21	1.47	1.50
26	2	5005	LMG	C25-C24	-3.21	1.33	1.51
26	B	5005	LMG	C19-C18	-3.21	1.33	1.51
26	A	5008	LMG	C40-C39	-3.21	1.33	1.51
26	B	5005	LMG	C25-C24	-3.21	1.33	1.51
26	b	5007	LMG	C40-C39	-3.20	1.33	1.51
26	A	5008	LMG	C22-C21	-3.20	1.33	1.51
26	1	5002	LMG	C37-C36	-3.20	1.33	1.51
28	h	4020	45D	C20-C08	3.20	1.56	1.45
26	1	5002	LMG	C40-C39	-3.20	1.33	1.51
26	A	5008	LMG	C19-C18	-3.20	1.33	1.51
26	b	5005	LMG	C22-C21	-3.20	1.33	1.51
26	1	5002	LMG	C19-C18	-3.20	1.33	1.51
26	A	5008	LMG	C43-C42	-3.20	1.33	1.51
26	b	5002	LMG	C25-C24	-3.20	1.33	1.51
37	L	5004	DGD	CDB-CCB	-3.20	1.33	1.51
26	0	5001	LMG	C43-C42	-3.19	1.33	1.51
26	b	5007	LMG	C37-C36	-3.19	1.33	1.51
37	L	5004	DGD	CDA-CCA	-3.19	1.33	1.51
26	2	5002	LMG	C22-C21	-3.19	1.33	1.51
26	B	5002	LMG	C22-C21	-3.19	1.33	1.51
26	a	5004	LMG	C19-C18	-3.19	1.33	1.51
26	1	5004	LMG	C40-C39	-3.19	1.33	1.51
26	1	5004	LMG	C43-C42	-3.19	1.33	1.51
26	K	5009	LMG	C25-C24	-3.19	1.33	1.51
26	b	5007	LMG	C43-C42	-3.19	1.33	1.51
26	a	5002	LMG	C40-C39	-3.19	1.33	1.51
26	A	5008	LMG	C37-C36	-3.19	1.33	1.51
26	b	5002	LMG	C22-C21	-3.18	1.33	1.51
26	b	5005	LMG	C25-C24	-3.18	1.33	1.51
26	1	5002	LMG	C43-C42	-3.18	1.33	1.51
26	A	5004	LMG	C22-C21	-3.18	1.33	1.51
26	b	5007	LMG	C22-C21	-3.18	1.33	1.51
26	a	5002	LMG	C19-C18	-3.18	1.33	1.51
34	j	4015	ZEX	C24-C25	-3.18	1.47	1.50
26	b	5007	LMG	C25-C24	-3.18	1.33	1.51
26	a	5002	LMG	C43-C42	-3.17	1.33	1.51
34	J	4015	ZEX	C24-C25	-3.17	1.47	1.50
26	2	5002	LMG	C25-C24	-3.17	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	5004	LMG	C22-C21	-3.17	1.33	1.51
28	B	4011	45D	C20-C08	3.17	1.56	1.45
37	L	5004	DGD	CGA-CFA	-3.17	1.33	1.51
37	L	5004	DGD	CAA-C9A	-3.17	1.33	1.51
26	0	5001	LMG	C37-C36	-3.17	1.33	1.51
26	2	5005	LMG	C43-C42	-3.16	1.33	1.51
37	L	5004	DGD	CGB-CFB	-3.16	1.33	1.51
26	A	5002	LMG	C19-C18	-3.16	1.33	1.51
26	1	5004	LMG	C37-C36	-3.16	1.33	1.51
26	0	5001	LMG	C40-C39	-3.16	1.33	1.51
26	A	5002	LMG	C43-C42	-3.15	1.33	1.51
26	b	5005	LMG	C43-C42	-3.15	1.33	1.51
26	A	5004	LMG	C19-C18	-3.13	1.34	1.51
26	B	5005	LMG	C43-C42	-3.13	1.34	1.51
36	I	4020	EQ3	C2-C1	3.09	1.64	1.54
34	7	4015	ZEX	C24-C25	-3.09	1.47	1.50
34	J	4015	ZEX	C27-C26	3.05	1.49	1.46
28	h	4020	45D	C19-C07	3.00	1.55	1.45
21	B	1022	CLA	C1C-C2C	3.00	1.50	1.44
30	b	4006	ECH	C1-C6	-2.99	1.49	1.53
21	2	1226	CLA	C3B-C2B	-2.99	1.36	1.40
28	h	4020	45D	C32-C30	2.99	1.52	1.43
21	A	1101	CLA	C1C-C2C	2.99	1.50	1.44
21	1	1125	CLA	C1C-C2C	2.94	1.50	1.44
21	B	1023	CLA	C1C-C2C	2.93	1.50	1.44
28	B	4011	45D	C19-C07	2.93	1.55	1.45
34	7	4015	ZEX	C27-C26	2.93	1.49	1.46
21	A	1136	CLA	C1C-C2C	2.92	1.50	1.44
21	A	1127	CLA	C1C-C2C	2.91	1.50	1.44
21	a	1135	CLA	C3B-C2B	-2.91	1.36	1.40
21	1	1126	CLA	C1C-C2C	2.90	1.50	1.44
21	B	1225	CLA	C1C-C2C	2.89	1.50	1.44
21	1	1136	CLA	C1C-C2C	2.89	1.50	1.44
21	B	1216	CLA	C1C-C2C	2.89	1.50	1.44
21	1	1801	CLA	C1C-C2C	2.88	1.50	1.44
21	B	1229	CLA	C1C-C2C	2.88	1.50	1.44
36	I	4020	EQ3	C24-C25	2.88	1.55	1.45
21	2	1234	CLA	C1C-C2C	2.88	1.50	1.44
21	f	1301	CLA	C1C-C2C	2.87	1.50	1.44
21	B	1227	CLA	C1C-C2C	2.87	1.50	1.44
36	I	4020	EQ3	C16-C17	2.86	1.52	1.43
21	A	1101	CLA	CHC-C1C	2.86	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1127	CLA	C1C-C2C	2.86	1.50	1.44
21	B	1202	CLA	C1C-C2C	2.86	1.50	1.44
21	0	1502	CLA	C1C-C2C	2.85	1.50	1.44
21	a	1118	CLA	C1C-C2C	2.85	1.50	1.44
21	B	1212	CLA	C1C-C2C	2.85	1.50	1.44
21	b	1212	CLA	C3B-C2B	-2.85	1.36	1.40
21	A	1013	CLA	CHC-C1C	2.85	1.42	1.35
21	1	1011	CLA	C1C-C2C	2.85	1.50	1.44
21	A	1132	CLA	C1C-C2C	2.85	1.50	1.44
21	2	1022	CLA	C1C-C2C	2.85	1.50	1.44
21	2	1240	CLA	C1C-C2C	2.85	1.50	1.44
21	b	1234	CLA	C1C-C2C	2.84	1.50	1.44
36	I	4020	EQ3	C33-C5	2.84	1.55	1.50
21	b	1214	CLA	C1C-C2C	2.84	1.50	1.44
21	a	1011	CLA	C1C-C2C	2.83	1.50	1.44
21	2	1236	CLA	C1C-C2C	2.83	1.50	1.44
21	A	1114	CLA	C3B-C2B	-2.83	1.36	1.40
21	A	1117	CLA	C1C-C2C	2.83	1.50	1.44
21	b	1021	CLA	C1C-C2C	2.83	1.50	1.44
21	B	1225	CLA	C3B-C2B	-2.82	1.36	1.40
21	1	1131	CLA	C1C-C2C	2.82	1.50	1.44
21	2	1229	CLA	C1C-C2C	2.82	1.50	1.44
21	2	1207	CLA	C3B-C2B	-2.82	1.36	1.40
21	A	1126	CLA	C1C-C2C	2.82	1.50	1.44
21	A	1102	CLA	C1C-C2C	2.82	1.50	1.44
21	a	1126	CLA	C1C-C2C	2.82	1.50	1.44
21	b	1229	CLA	C1C-C2C	2.82	1.50	1.44
21	2	1216	CLA	C1C-C2C	2.82	1.50	1.44
21	j	1303	CLA	C1C-C2C	2.81	1.50	1.44
21	A	1136	CLA	CHC-C1C	2.81	1.42	1.35
21	1	1012	CLA	C1C-C2C	2.81	1.50	1.44
21	B	1234	CLA	C1C-C2C	2.81	1.50	1.44
21	a	1127	CLA	C1C-C2C	2.81	1.50	1.44
21	B	1236	CLA	C1C-C2C	2.81	1.50	1.44
21	A	1120	CLA	C1C-C2C	2.81	1.50	1.44
21	B	1235	CLA	C1C-C2C	2.81	1.50	1.44
21	a	1101	CLA	C1C-C2C	2.81	1.50	1.44
21	1	1105	CLA	C1C-C2C	2.81	1.50	1.44
21	2	1208	CLA	C1C-C2C	2.81	1.50	1.44
21	B	1239	CLA	C1C-C2C	2.80	1.50	1.44
21	1	1013	CLA	C1C-C2C	2.80	1.50	1.44
21	2	1215	CLA	C1C-C2C	2.80	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1229	CLA	C3B-C2B	-2.79	1.36	1.40
21	1	1132	CLA	C1C-C2C	2.79	1.50	1.44
21	B	1238	CLA	C1C-C2C	2.79	1.50	1.44
21	b	1240	CLA	C1C-C2C	2.79	1.50	1.44
21	2	1023	CLA	C1C-C2C	2.79	1.50	1.44
21	1	1138	CLA	C1C-C2C	2.79	1.50	1.44
21	B	1023	CLA	CHC-C1C	2.79	1.42	1.35
21	a	1012	CLA	C1C-C2C	2.78	1.50	1.44
21	A	1108	CLA	C1C-C2C	2.78	1.50	1.44
21	a	1116	CLA	C1C-C2C	2.78	1.49	1.44
21	2	1235	CLA	C1C-C2C	2.78	1.49	1.44
21	b	1022	CLA	C1C-C2C	2.78	1.49	1.44
21	A	1105	CLA	C3B-C2B	-2.78	1.36	1.40
21	l	1502	CLA	C1C-C2C	2.78	1.49	1.44
21	A	1118	CLA	C1C-C2C	2.78	1.49	1.44
21	2	1239	CLA	C3B-C2B	-2.78	1.36	1.40
21	A	1104	CLA	C1C-C2C	2.78	1.49	1.44
21	b	1218	CLA	C1C-C2C	2.78	1.49	1.44
21	1	1801	CLA	CHC-C1C	2.78	1.42	1.35
21	B	1211	CLA	C1C-C2C	2.77	1.49	1.44
21	a	1110	CLA	C3B-C2B	-2.77	1.36	1.40
21	B	1228	CLA	C1C-C2C	2.77	1.49	1.44
21	6	1302	CLA	C1C-C2C	2.77	1.49	1.44
21	2	1229	CLA	C3B-C2B	-2.77	1.36	1.40
21	A	1113	CLA	C1C-C2C	2.77	1.49	1.44
21	b	1212	CLA	C1C-C2C	2.77	1.49	1.44
21	b	1202	CLA	C1C-C2C	2.77	1.49	1.44
21	a	1108	CLA	C1C-C2C	2.77	1.49	1.44
21	a	1129	CLA	C1C-C2C	2.77	1.49	1.44
21	B	1220	CLA	C1C-C2C	2.76	1.49	1.44
21	A	1110	CLA	C1C-C2C	2.76	1.49	1.44
21	1	1116	CLA	C1C-C2C	2.76	1.49	1.44
21	2	1203	CLA	C1C-C2C	2.76	1.49	1.44
21	1	1136	CLA	CHC-C1C	2.75	1.42	1.35
21	B	1232	CLA	C3B-C2B	-2.75	1.36	1.40
21	1	1107	CLA	C1C-C2C	2.75	1.49	1.44
21	1	1129	CLA	C1C-C2C	2.75	1.49	1.44
21	b	1239	CLA	C3B-C2B	-2.75	1.36	1.40
21	b	1226	CLA	C3B-C2B	-2.75	1.36	1.40
21	A	1110	CLA	C3B-C2B	-2.75	1.36	1.40
21	l	1503	CLA	C1C-C2C	2.75	1.49	1.44
21	a	1110	CLA	C1C-C2C	2.75	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1101	CLA	C3B-C2B	-2.75	1.36	1.40
21	a	1139	CLA	C1C-C2C	2.75	1.49	1.44
21	b	1219	CLA	C1C-C2C	2.75	1.49	1.44
21	B	1223	CLA	C1C-C2C	2.75	1.49	1.44
21	a	1134	CLA	C1C-C2C	2.75	1.49	1.44
21	2	1227	CLA	C3B-C2B	-2.74	1.36	1.40
21	a	1013	CLA	C1C-C2C	2.74	1.49	1.44
21	1	1113	CLA	C1C-C2C	2.74	1.49	1.44
21	b	1229	CLA	C3B-C2B	-2.74	1.36	1.40
21	1	1108	CLA	C1C-C2C	2.74	1.49	1.44
21	b	1023	CLA	CHC-C1C	2.74	1.42	1.35
21	B	1207	CLA	C1C-C2C	2.74	1.49	1.44
21	1	1101	CLA	C1C-C2C	2.74	1.49	1.44
21	J	1302	CLA	C1C-C2C	2.74	1.49	1.44
21	a	1130	CLA	C1C-C2C	2.74	1.49	1.44
21	J	1303	CLA	C1C-C2C	2.73	1.49	1.44
21	A	1116	CLA	C1C-C2C	2.73	1.49	1.44
21	2	1202	CLA	C1C-C2C	2.73	1.49	1.44
21	B	1223	CLA	C3B-C2B	-2.73	1.36	1.40
21	b	1232	CLA	C1C-C2C	2.73	1.49	1.44
21	7	1302	CLA	C1C-C2C	2.73	1.49	1.44
21	a	1113	CLA	C1C-C2C	2.73	1.49	1.44
21	b	1023	CLA	C1C-C2C	2.73	1.49	1.44
21	2	1230	CLA	C1C-C2C	2.73	1.49	1.44
21	B	1230	CLA	C1C-C2C	2.73	1.49	1.44
21	B	1207	CLA	C1C-NC	-2.73	1.33	1.37
21	1	1138	CLA	C3B-C2B	-2.73	1.36	1.40
21	1	1110	CLA	C1C-C2C	2.72	1.49	1.44
21	B	1219	CLA	C3B-C2B	-2.72	1.36	1.40
21	B	1212	CLA	C3B-C2B	-2.72	1.36	1.40
21	a	1131	CLA	C1C-C2C	2.72	1.49	1.44
21	b	1207	CLA	C1C-C2C	2.72	1.49	1.44
21	k	1402	CLA	C1C-C2C	2.72	1.49	1.44
21	2	1201	CLA	C1C-C2C	2.72	1.49	1.44
21	2	1223	CLA	C1C-C2C	2.72	1.49	1.44
21	A	1011	CLA	CHC-C1C	2.72	1.41	1.35
21	1	1120	CLA	C1C-C2C	2.72	1.49	1.44
21	A	1113	CLA	CHC-C1C	2.71	1.41	1.35
21	B	1213	CLA	C1C-C2C	2.71	1.49	1.44
21	B	1240	CLA	C1C-C2C	2.71	1.49	1.44
21	a	1138	CLA	C1C-C2C	2.71	1.49	1.44
21	2	1220	CLA	C1C-C2C	2.71	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1215	CLA	C1C-C2C	2.71	1.49	1.44
21	b	1217	CLA	C1C-C2C	2.71	1.49	1.44
21	a	1121	CLA	C1C-C2C	2.71	1.49	1.44
21	2	1211	CLA	C1C-C2C	2.71	1.49	1.44
21	A	1133	CLA	C3B-C2B	-2.71	1.36	1.40
21	a	1125	CLA	C1C-C2C	2.71	1.49	1.44
21	B	1219	CLA	C1C-C2C	2.71	1.49	1.44
21	A	1105	CLA	C1C-C2C	2.71	1.49	1.44
21	b	1215	CLA	C1C-C2C	2.70	1.49	1.44
21	b	1207	CLA	C3B-C2B	-2.70	1.36	1.40
35	0	6001	LMT	O3'-C3'	-2.70	1.36	1.43
21	a	1119	CLA	C1C-C2C	2.70	1.49	1.44
21	A	1137	CLA	C1C-NC	-2.70	1.33	1.37
21	B	1214	CLA	C3B-C2B	-2.70	1.36	1.40
21	A	1011	CLA	C1C-C2C	2.70	1.49	1.44
21	B	1208	CLA	C1C-C2C	2.70	1.49	1.44
21	1	1109	CLA	C1C-C2C	2.70	1.49	1.44
21	0	1501	CLA	C1C-C2C	2.70	1.49	1.44
21	a	1136	CLA	C1C-C2C	2.70	1.49	1.44
21	A	1140	CLA	CHC-C1C	2.70	1.41	1.35
21	6	1302	CLA	CHC-C1C	2.70	1.41	1.35
21	2	1207	CLA	C1C-C2C	2.69	1.49	1.44
21	a	1140	CLA	C1C-C2C	2.69	1.49	1.44
21	B	1238	CLA	CHC-C1C	2.69	1.41	1.35
21	2	1217	CLA	C1C-C2C	2.69	1.49	1.44
21	a	1117	CLA	C1C-C2C	2.69	1.49	1.44
36	I	4020	EQ3	C20-C21	2.69	1.51	1.43
21	2	1213	CLA	C1C-C2C	2.69	1.49	1.44
21	1	1133	CLA	C3B-C2B	-2.69	1.36	1.40
21	2	1210	CLA	C1C-C2C	2.69	1.49	1.44
21	1	1137	CLA	C1C-C2C	2.69	1.49	1.44
21	b	1239	CLA	C1C-C2C	2.69	1.49	1.44
21	A	1140	CLA	C1C-C2C	2.69	1.49	1.44
21	2	1222	CLA	CHC-C1C	2.68	1.41	1.35
21	a	1011	CLA	CHC-C1C	2.68	1.41	1.35
21	2	1218	CLA	C1C-C2C	2.68	1.49	1.44
21	1	1126	CLA	CHC-C1C	2.68	1.41	1.35
21	A	1126	CLA	CHC-C1C	2.68	1.41	1.35
21	b	1226	CLA	CHC-C1C	2.68	1.41	1.35
21	8	1402	CLA	C1C-C2C	2.68	1.49	1.44
21	2	1228	CLA	C1C-C2C	2.68	1.49	1.44
21	2	1204	CLA	C1C-C2C	2.68	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1222	CLA	C1C-C2C	2.68	1.49	1.44
21	k	1401	CLA	C1C-C2C	2.68	1.49	1.44
35	F	6001	LMT	O3'-C3'	-2.67	1.36	1.43
21	1	1106	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1207	CLA	C3B-C2B	-2.67	1.36	1.40
21	B	1217	CLA	C1C-C2C	2.67	1.49	1.44
21	a	1115	CLA	C1C-C2C	2.67	1.49	1.44
21	A	1125	CLA	C1C-C2C	2.67	1.49	1.44
35	l	6001	LMT	O3'-C3'	-2.67	1.36	1.43
21	a	1137	CLA	C3B-C2B	-2.67	1.36	1.40
21	b	1220	CLA	C1C-C2C	2.67	1.49	1.44
21	2	1227	CLA	C1C-C2C	2.67	1.49	1.44
21	a	1133	CLA	C3B-C2B	-2.67	1.36	1.40
21	b	1231	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1224	CLA	C1C-C2C	2.67	1.49	1.44
21	a	1104	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1021	CLA	C1C-C2C	2.67	1.49	1.44
21	2	1216	CLA	CHC-C1C	2.67	1.41	1.35
21	a	1112	CLA	C1C-C2C	2.67	1.49	1.44
21	B	1209	CLA	C1C-C2C	2.66	1.49	1.44
21	1	1139	CLA	C1C-C2C	2.66	1.49	1.44
30	B	4006	ECH	C1-C6	-2.66	1.50	1.53
21	a	1123	CLA	C1C-C2C	2.66	1.49	1.44
21	1	1140	CLA	C1C-C2C	2.66	1.49	1.44
21	A	1106	CLA	C1C-C2C	2.66	1.49	1.44
21	1	1114	CLA	C1C-C2C	2.66	1.49	1.44
21	A	1138	CLA	CHC-C1C	2.66	1.41	1.35
21	b	1228	CLA	C1C-C2C	2.66	1.49	1.44
21	A	1133	CLA	C1C-C2C	2.66	1.49	1.44
21	L	1503	CLA	C1C-C2C	2.66	1.49	1.44
21	a	1135	CLA	C1C-C2C	2.66	1.49	1.44
21	b	1216	CLA	C1C-C2C	2.66	1.49	1.44
21	a	1129	CLA	CHC-C1C	2.66	1.41	1.35
21	a	1126	CLA	CHC-C1C	2.66	1.41	1.35
21	b	1211	CLA	C1C-C2C	2.66	1.49	1.44
21	1	1135	CLA	C1C-C2C	2.66	1.49	1.44
21	A	1129	CLA	C1C-C2C	2.66	1.49	1.44
21	2	1209	CLA	C1C-C2C	2.66	1.49	1.44
21	8	1401	CLA	C1C-C2C	2.66	1.49	1.44
21	b	1222	CLA	CHC-C1C	2.66	1.41	1.35
21	A	1108	CLA	CHC-C1C	2.66	1.41	1.35
21	L	1501	CLA	C1C-C2C	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1212	CLA	C1C-C2C	2.65	1.49	1.44
21	A	1801	CLA	C1C-C2C	2.65	1.49	1.44
21	b	1229	CLA	CHC-C1C	2.65	1.41	1.35
21	b	1217	CLA	C3B-C2B	-2.65	1.36	1.40
21	1	1118	CLA	C1C-C2C	2.65	1.49	1.44
21	a	1137	CLA	C1C-C2C	2.65	1.49	1.44
21	j	1302	CLA	C1C-C2C	2.65	1.49	1.44
21	2	1232	CLA	C1C-C2C	2.65	1.49	1.44
21	F	1301	CLA	MG-NC	2.65	2.12	2.06
21	2	1206	CLA	C1C-C2C	2.65	1.49	1.44
21	l	1502	CLA	CHC-C1C	2.65	1.41	1.35
21	b	1235	CLA	C1C-C2C	2.65	1.49	1.44
21	a	1127	CLA	C3B-C2B	-2.65	1.36	1.40
21	1	1101	CLA	C3B-C2B	-2.65	1.36	1.40
21	b	1212	CLA	CHC-C1C	2.65	1.41	1.35
21	B	1204	CLA	C1C-C2C	2.65	1.49	1.44
21	b	1224	CLA	C1C-C2C	2.65	1.49	1.44
21	f	1302	CLA	C1C-C2C	2.65	1.49	1.44
21	A	1801	CLA	CHC-C1C	2.65	1.41	1.35
21	B	1022	CLA	CHC-C1C	2.64	1.41	1.35
21	b	1209	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1111	CLA	C1C-C2C	2.64	1.49	1.44
21	b	1228	CLA	C3B-C2B	-2.64	1.36	1.40
21	2	1225	CLA	C1C-C2C	2.64	1.49	1.44
35	L	6001	LMT	O3'-C3'	-2.64	1.36	1.43
21	a	1132	CLA	C1C-C2C	2.64	1.49	1.44
21	b	1211	CLA	CHC-C1C	2.64	1.41	1.35
21	a	1118	CLA	CHC-C1C	2.64	1.41	1.35
21	2	1231	CLA	C1C-C2C	2.64	1.49	1.44
21	A	1134	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1133	CLA	C1C-C2C	2.64	1.49	1.44
21	a	1131	CLA	CHC-C1C	2.64	1.41	1.35
21	b	1230	CLA	C1C-C2C	2.64	1.49	1.44
21	1	1013	CLA	CHC-C1C	2.64	1.41	1.35
21	B	1225	CLA	CHC-C1C	2.64	1.41	1.35
21	2	1209	CLA	C3B-C2B	-2.64	1.36	1.40
21	a	1123	CLA	MG-NC	2.63	2.12	2.06
21	2	1217	CLA	MG-NC	2.63	2.12	2.06
21	a	1106	CLA	C1C-C2C	2.63	1.49	1.44
21	A	1107	CLA	C1C-C2C	2.63	1.49	1.44
21	A	1013	CLA	C1C-C2C	2.63	1.49	1.44
21	A	1114	CLA	C1C-C2C	2.63	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	0	1502	CLA	CHC-C1C	2.63	1.41	1.35
21	1	1125	CLA	CHC-C1C	2.63	1.41	1.35
21	2	1228	CLA	C3B-C2B	-2.63	1.36	1.40
21	b	1223	CLA	C1C-C2C	2.63	1.49	1.44
21	a	1013	CLA	CHC-C1C	2.63	1.41	1.35
21	1	1112	CLA	C1C-C2C	2.63	1.49	1.44
21	B	1210	CLA	MG-NC	2.63	2.12	2.06
21	A	1127	CLA	CHC-C1C	2.63	1.41	1.35
21	B	1232	CLA	C1C-C2C	2.63	1.49	1.44
21	B	1236	CLA	C3B-C2B	-2.63	1.36	1.40
21	1	1105	CLA	CHC-C1C	2.63	1.41	1.35
21	A	1104	CLA	CHC-C1C	2.63	1.41	1.35
21	1	1012	CLA	CHC-C1C	2.63	1.41	1.35
21	2	1238	CLA	C3B-C2B	-2.62	1.36	1.40
21	2	1219	CLA	C1C-C2C	2.62	1.49	1.44
21	B	1221	CLA	C1C-C2C	2.62	1.49	1.44
21	A	1131	CLA	C1C-C2C	2.62	1.49	1.44
21	A	1137	CLA	C3B-C2B	-2.62	1.36	1.40
21	B	1230	CLA	CHC-C1C	2.62	1.41	1.35
21	6	1301	CLA	C1C-C2C	2.62	1.49	1.44
21	2	1023	CLA	CHC-C1C	2.62	1.41	1.35
21	2	1218	CLA	CHC-C1C	2.62	1.41	1.35
21	A	1111	CLA	C1C-C2C	2.62	1.49	1.44
21	A	1119	CLA	C1C-C2C	2.62	1.49	1.44
21	B	1231	CLA	C1C-C2C	2.62	1.49	1.44
21	l	1503	CLA	CHC-C1C	2.62	1.41	1.35
21	b	1208	CLA	C1C-C2C	2.62	1.49	1.44
21	2	1225	CLA	C3B-C2B	-2.62	1.36	1.40
21	F	1301	CLA	C1C-C2C	2.62	1.49	1.44
21	A	1126	CLA	MG-NC	2.61	2.12	2.06
21	F	1302	CLA	C3B-C2B	-2.61	1.36	1.40
21	b	1235	CLA	CHC-C1C	2.61	1.41	1.35
21	2	1201	CLA	CHC-C1C	2.61	1.41	1.35
21	K	1401	CLA	C1C-C2C	2.61	1.49	1.44
21	1	1124	CLA	C1C-C2C	2.61	1.49	1.44
21	B	1228	CLA	CHC-C1C	2.61	1.41	1.35
21	a	1134	CLA	CHC-C1C	2.61	1.41	1.35
21	b	1203	CLA	C1C-C2C	2.61	1.49	1.44
21	A	1110	CLA	CHC-C1C	2.61	1.41	1.35
21	b	1201	CLA	CHC-C1C	2.61	1.41	1.35
21	2	1221	CLA	C1C-C2C	2.61	1.49	1.44
21	b	1213	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1209	CLA	C3B-C2B	-2.61	1.36	1.40
21	b	1232	CLA	CHC-C1C	2.61	1.41	1.35
36	I	4020	EQ3	C40-C30	2.61	1.58	1.53
21	a	1114	CLA	C1C-C2C	2.61	1.49	1.44
21	b	1210	CLA	C1C-C2C	2.61	1.49	1.44
21	B	1211	CLA	CHC-C1C	2.61	1.41	1.35
28	B	4011	45D	O02-C18	-2.61	1.17	1.23
21	2	1223	CLA	C3B-C2B	-2.61	1.36	1.40
21	b	1236	CLA	C3B-C2B	-2.61	1.36	1.40
21	2	1229	CLA	C1C-NC	-2.61	1.33	1.37
21	b	1230	CLA	C3B-C2B	-2.60	1.36	1.40
21	1	1132	CLA	CHC-C1C	2.60	1.41	1.35
21	2	1212	CLA	CHC-C1C	2.60	1.41	1.35
21	b	1225	CLA	C1C-C2C	2.60	1.49	1.44
21	B	1216	CLA	CHC-C1C	2.60	1.41	1.35
21	A	1118	CLA	CHC-C1C	2.60	1.41	1.35
21	B	1220	CLA	CHC-C1C	2.60	1.41	1.35
21	b	1231	CLA	CHC-C1C	2.60	1.41	1.35
21	a	1131	CLA	C3B-C2B	-2.60	1.36	1.40
21	2	1237	CLA	C1C-C2C	2.60	1.49	1.44
21	1	1115	CLA	C1C-C2C	2.60	1.49	1.44
21	1	1011	CLA	CHC-C1C	2.60	1.41	1.35
21	b	1240	CLA	MG-NC	2.60	2.12	2.06
21	1	1135	CLA	MG-NC	2.60	2.12	2.06
21	A	1120	CLA	CHC-C1C	2.60	1.41	1.35
21	2	1234	CLA	CHC-C1C	2.60	1.41	1.35
21	1	1123	CLA	MG-NC	2.60	2.12	2.06
21	1	1121	CLA	C1C-C2C	2.60	1.49	1.44
21	1	1111	CLA	C1C-C2C	2.60	1.49	1.44
21	k	1401	CLA	CHC-C1C	2.60	1.41	1.35
21	a	1801	CLA	C1C-C2C	2.60	1.49	1.44
21	A	1130	CLA	C1C-C2C	2.60	1.49	1.44
21	2	1208	CLA	CHC-C1C	2.60	1.41	1.35
21	1	1130	CLA	C1C-C2C	2.59	1.49	1.44
21	A	1136	CLA	C3B-C2B	-2.59	1.36	1.40
21	b	1021	CLA	CHC-C1C	2.59	1.41	1.35
21	0	1503	CLA	C1C-C2C	2.59	1.49	1.44
21	2	1238	CLA	CHC-C1C	2.59	1.41	1.35
21	A	1012	CLA	C1C-C2C	2.59	1.49	1.44
21	1	1131	CLA	CHC-C1C	2.59	1.41	1.35
21	B	1206	CLA	C1C-C2C	2.59	1.49	1.44
21	a	1105	CLA	C1C-C2C	2.59	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1133	CLA	C1C-C2C	2.59	1.49	1.44
21	A	1133	CLA	CHC-C1C	2.59	1.41	1.35
21	A	1112	CLA	C1C-C2C	2.59	1.49	1.44
21	0	1501	CLA	CHC-C1C	2.59	1.41	1.35
21	F	1302	CLA	C1C-C2C	2.59	1.49	1.44
21	1	1127	CLA	C3B-C2B	-2.59	1.36	1.40
21	a	1120	CLA	C1C-C2C	2.59	1.49	1.44
21	A	1132	CLA	CHC-C1C	2.59	1.41	1.35
21	7	1302	CLA	C3B-C2B	-2.59	1.36	1.40
21	A	1130	CLA	CHC-C1C	2.59	1.41	1.35
21	a	1101	CLA	CHC-C1C	2.59	1.41	1.35
21	b	1214	CLA	CHC-C1C	2.59	1.41	1.35
21	1	1137	CLA	C1C-NC	-2.59	1.33	1.37
21	a	1110	CLA	CHC-C1C	2.59	1.41	1.35
21	B	1212	CLA	CHC-C1C	2.59	1.41	1.35
21	a	1108	CLA	CHC-C1C	2.59	1.41	1.35
21	1	1104	CLA	C1C-C2C	2.59	1.49	1.44
21	b	1227	CLA	C1C-C2C	2.59	1.49	1.44
21	J	1302	CLA	CHC-C1C	2.59	1.41	1.35
21	B	1227	CLA	C3B-C2B	-2.58	1.36	1.40
21	1	1138	CLA	CHC-C1C	2.58	1.41	1.35
21	b	1202	CLA	CHC-C1C	2.58	1.41	1.35
21	1	1134	CLA	CHC-C1C	2.58	1.41	1.35
21	1	1107	CLA	CHC-C1C	2.58	1.41	1.35
21	a	1128	CLA	C1C-C2C	2.58	1.49	1.44
21	2	1213	CLA	CHC-C1C	2.58	1.41	1.35
21	2	1210	CLA	CHC-C1C	2.58	1.41	1.35
21	2	1203	CLA	CHC-C1C	2.58	1.41	1.35
28	h	4020	45D	C17-C15	2.58	1.53	1.47
21	A	1117	CLA	CHC-C1C	2.58	1.41	1.35
21	b	1216	CLA	C3B-C2B	-2.58	1.36	1.40
21	1	1129	CLA	CHC-C1C	2.58	1.41	1.35
21	0	1502	CLA	MG-NC	2.58	2.12	2.06
21	B	1236	CLA	CHC-C1C	2.58	1.41	1.35
21	b	1226	CLA	C1C-C2C	2.58	1.49	1.44
21	b	1216	CLA	CHC-C1C	2.58	1.41	1.35
21	b	1204	CLA	C3B-C2B	-2.58	1.36	1.40
21	A	1131	CLA	C3B-C2B	-2.58	1.36	1.40
21	1	1134	CLA	C1C-C2C	2.58	1.49	1.44
21	2	1021	CLA	C1C-C2C	2.57	1.49	1.44
21	A	1139	CLA	C1C-C2C	2.57	1.49	1.44
21	B	1227	CLA	CHC-C1C	2.57	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1116	CLA	CHC-C1C	2.57	1.41	1.35
21	8	1402	CLA	CHC-C1C	2.57	1.41	1.35
21	A	1124	CLA	CHC-C1C	2.57	1.41	1.35
21	2	1238	CLA	C1C-C2C	2.57	1.49	1.44
21	b	1219	CLA	C3B-C2B	-2.57	1.36	1.40
21	A	1137	CLA	CHC-C1C	2.57	1.41	1.35
21	A	1129	CLA	CHC-C1C	2.57	1.41	1.35
21	A	1137	CLA	C1C-C2C	2.57	1.49	1.44
21	a	1107	CLA	C1C-C2C	2.57	1.49	1.44
21	2	1240	CLA	CHC-C1C	2.57	1.41	1.35
21	2	1224	CLA	C1C-C2C	2.57	1.49	1.44
21	2	1221	CLA	MG-NC	2.57	2.12	2.06
21	b	1219	CLA	CHC-C1C	2.57	1.41	1.35
21	b	1022	CLA	CHC-C1C	2.57	1.41	1.35
21	2	1219	CLA	C3B-C2B	-2.57	1.36	1.40
21	B	1240	CLA	CHC-C1C	2.57	1.41	1.35
21	a	1125	CLA	CHC-C1C	2.56	1.41	1.35
21	2	1217	CLA	C3B-C2B	-2.56	1.36	1.40
21	1	1137	CLA	CHC-C1C	2.56	1.41	1.35
21	a	1122	CLA	C1C-C2C	2.56	1.49	1.44
21	2	1214	CLA	C1C-C2C	2.56	1.49	1.44
21	B	1207	CLA	CHC-C1C	2.56	1.41	1.35
21	A	1125	CLA	C1C-NC	-2.56	1.34	1.37
21	2	1229	CLA	CHC-C1C	2.56	1.41	1.35
21	B	1217	CLA	C3B-C2B	-2.56	1.36	1.40
21	a	1116	CLA	C3B-C2B	-2.56	1.36	1.40
21	2	1215	CLA	CHC-C1C	2.56	1.41	1.35
21	A	1134	CLA	C3B-C2B	-2.56	1.36	1.40
21	B	1218	CLA	C1C-C2C	2.56	1.49	1.44
21	f	1301	CLA	CHC-C1C	2.56	1.41	1.35
21	1	1119	CLA	C1C-C2C	2.56	1.49	1.44
21	B	1234	CLA	CHC-C1C	2.56	1.41	1.35
21	A	1119	CLA	CHC-C1C	2.56	1.41	1.35
21	1	1131	CLA	C3B-C2B	-2.56	1.36	1.40
21	1	1134	CLA	C3B-C2B	-2.56	1.36	1.40
21	A	1109	CLA	CHC-C1C	2.56	1.41	1.35
21	b	1210	CLA	CHC-C1C	2.56	1.41	1.35
21	B	1214	CLA	C1C-C2C	2.56	1.49	1.44
21	a	1116	CLA	CHC-C1C	2.56	1.41	1.35
21	b	1222	CLA	C1C-C2C	2.55	1.49	1.44
21	B	1211	CLA	MG-NC	2.55	2.12	2.06
21	b	1215	CLA	CHC-C1C	2.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1216	CLA	C3B-C2B	-2.55	1.36	1.40
21	L	1502	CLA	C1C-C2C	2.55	1.49	1.44
21	a	1117	CLA	CHC-C1C	2.55	1.41	1.35
21	B	1210	CLA	C1C-C2C	2.55	1.49	1.44
21	a	1121	CLA	CHC-C1C	2.55	1.41	1.35
21	7	1302	CLA	CHC-C1C	2.55	1.41	1.35
21	2	1225	CLA	CHC-C1C	2.55	1.41	1.35
21	7	1303	CLA	MG-NC	2.55	2.12	2.06
21	1	1127	CLA	CHC-C1C	2.55	1.41	1.35
21	l	1501	CLA	C1C-C2C	2.55	1.49	1.44
21	2	1210	CLA	C1C-NC	-2.55	1.34	1.37
21	a	1127	CLA	CHC-C1C	2.55	1.41	1.35
21	K	1402	CLA	C3B-C2B	-2.55	1.36	1.40
21	k	1402	CLA	CHC-C1C	2.55	1.41	1.35
21	K	1402	CLA	C1C-C2C	2.55	1.49	1.44
21	2	1227	CLA	CHC-C1C	2.55	1.41	1.35
35	1	6001	LMT	O3'-C3'	-2.55	1.37	1.43
21	B	1240	CLA	MG-NC	2.55	2.12	2.06
21	b	1201	CLA	C1C-C2C	2.55	1.49	1.44
21	b	1204	CLA	C1C-C2C	2.55	1.49	1.44
26	A	5004	LMG	C37-C36	-2.55	1.33	1.51
21	b	1234	CLA	C1C-NC	-2.54	1.34	1.37
21	a	1124	CLA	C1C-C2C	2.54	1.49	1.44
21	1	1122	CLA	C1C-C2C	2.54	1.49	1.44
21	a	1139	CLA	CHC-C1C	2.54	1.41	1.35
21	1	1136	CLA	C3B-C2B	-2.54	1.36	1.40
21	B	1206	CLA	CHC-C1C	2.54	1.41	1.35
21	2	1236	CLA	CHC-C1C	2.54	1.41	1.35
21	B	1229	CLA	CHC-C1C	2.54	1.41	1.35
21	j	1303	CLA	CHC-C1C	2.54	1.41	1.35
21	a	1114	CLA	CHC-C1C	2.54	1.41	1.35
21	B	1239	CLA	C3B-C2B	-2.54	1.36	1.40
21	1	1110	CLA	C3B-C2B	-2.54	1.36	1.40
21	2	1235	CLA	CHC-C1C	2.54	1.41	1.35
21	1	1140	CLA	CHC-C1C	2.54	1.41	1.35
21	A	1136	CLA	MG-NC	2.54	2.12	2.06
21	a	1102	CLA	C1C-C2C	2.54	1.49	1.44
21	2	1202	CLA	CHC-C1C	2.54	1.41	1.35
21	b	1234	CLA	CHC-C1C	2.54	1.41	1.35
21	A	1115	CLA	C1C-C2C	2.54	1.49	1.44
21	a	1133	CLA	CHC-C1C	2.54	1.41	1.35
21	A	1116	CLA	CHC-C1C	2.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1109	CLA	C1C-C2C	2.54	1.49	1.44
21	j	1303	CLA	MG-NC	2.54	2.12	2.06
36	I	4020	EQ3	C28-C27	2.53	1.54	1.50
21	B	1203	CLA	MG-NC	2.53	2.12	2.06
21	B	1021	CLA	CHC-C1C	2.53	1.41	1.35
21	b	1218	CLA	CHC-C1C	2.53	1.41	1.35
21	2	1214	CLA	CHC-C1C	2.53	1.41	1.35
21	a	1132	CLA	CHC-C1C	2.53	1.41	1.35
21	a	1136	CLA	C3B-C2B	-2.53	1.36	1.40
21	7	1303	CLA	C1C-C2C	2.53	1.49	1.44
21	b	1220	CLA	C1C-NC	-2.53	1.34	1.37
21	A	1102	CLA	CHC-C1C	2.53	1.41	1.35
21	2	1022	CLA	CHC-C1C	2.53	1.41	1.35
21	1	1117	CLA	C1C-C2C	2.53	1.49	1.44
21	b	1213	CLA	CHC-C1C	2.53	1.41	1.35
21	b	1230	CLA	CHC-C1C	2.53	1.41	1.35
21	2	1204	CLA	C1C-NC	-2.53	1.34	1.37
21	J	1302	CLA	C1C-NC	-2.53	1.34	1.37
21	A	1111	CLA	CHC-C1C	2.53	1.41	1.35
21	1	1120	CLA	CHC-C1C	2.53	1.41	1.35
21	a	1119	CLA	CHC-C1C	2.53	1.41	1.35
21	b	1208	CLA	CHC-C1C	2.53	1.41	1.35
21	a	1105	CLA	C3B-C2B	-2.53	1.36	1.40
21	1	1123	CLA	C1C-C2C	2.53	1.49	1.44
21	B	1202	CLA	CHC-C1C	2.52	1.41	1.35
21	a	1113	CLA	CHC-C1C	2.52	1.41	1.35
21	a	1107	CLA	C1C-NC	-2.52	1.34	1.37
21	a	1138	CLA	CHC-C1C	2.52	1.41	1.35
21	8	1401	CLA	MG-NC	2.52	2.12	2.06
21	2	1204	CLA	CHC-C1C	2.52	1.41	1.35
21	a	1125	CLA	C1C-NC	-2.52	1.34	1.37
21	b	1236	CLA	C1C-C2C	2.52	1.49	1.44
21	A	1012	CLA	CHC-C1C	2.52	1.41	1.35
21	A	1138	CLA	C1C-C2C	2.52	1.49	1.44
21	A	1131	CLA	CHC-C1C	2.52	1.41	1.35
21	B	1231	CLA	CHC-C1C	2.52	1.41	1.35
21	1	1119	CLA	CHC-C1C	2.52	1.41	1.35
21	B	1223	CLA	CHC-C1C	2.52	1.41	1.35
21	1	1115	CLA	CHC-C1C	2.52	1.41	1.35
21	1	1105	CLA	C3B-C2B	-2.52	1.36	1.40
21	b	1205	CLA	C1C-C2C	2.52	1.49	1.44
21	a	1140	CLA	CHC-C1C	2.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	1303	CLA	CHC-C1C	2.52	1.41	1.35
21	a	1801	CLA	MG-NC	2.52	2.12	2.06
21	b	1220	CLA	CHC-C1C	2.52	1.41	1.35
21	A	1124	CLA	C1C-C2C	2.52	1.49	1.44
34	j	4015	ZEX	C27-C26	2.51	1.48	1.46
21	1	1113	CLA	CHC-C1C	2.51	1.41	1.35
21	A	1012	CLA	MG-NC	2.51	2.12	2.06
21	2	1239	CLA	C1C-NC	-2.51	1.34	1.37
21	B	1204	CLA	CHC-C1C	2.51	1.41	1.35
21	A	1115	CLA	CHC-C1C	2.51	1.41	1.35
21	2	1214	CLA	MG-NC	2.51	2.12	2.06
21	A	1139	CLA	CHC-C1C	2.51	1.41	1.35
21	1	1103	CLA	C1C-NC	-2.51	1.34	1.37
21	2	1237	CLA	CHC-C1C	2.51	1.41	1.35
21	1	1127	CLA	MG-NC	2.51	2.12	2.06
21	a	1128	CLA	CHC-C1C	2.51	1.41	1.35
21	B	1201	CLA	CHC-C1C	2.51	1.41	1.35
21	B	1213	CLA	CHC-C1C	2.51	1.41	1.35
21	a	1137	CLA	CHC-C1C	2.51	1.41	1.35
21	2	1208	CLA	C3B-C2B	-2.51	1.36	1.40
21	2	1232	CLA	CHC-C1C	2.51	1.41	1.35
21	1	1114	CLA	CHC-C1C	2.51	1.41	1.35
21	A	1103	CLA	C1C-NC	-2.51	1.34	1.37
21	8	1401	CLA	CHC-C1C	2.51	1.41	1.35
21	1	1106	CLA	CHC-C1C	2.51	1.41	1.35
21	a	1114	CLA	MG-NC	2.51	2.12	2.06
21	A	1114	CLA	CHC-C1C	2.51	1.41	1.35
21	B	1235	CLA	CHC-C1C	2.51	1.41	1.35
21	b	1210	CLA	MG-NC	2.51	2.12	2.06
21	2	1211	CLA	CHC-C1C	2.51	1.41	1.35
21	b	1207	CLA	CHC-C1C	2.51	1.41	1.35
21	a	1012	CLA	C1C-NC	-2.51	1.34	1.37
21	a	1130	CLA	CHC-C1C	2.51	1.41	1.35
21	A	1122	CLA	C1C-C2C	2.50	1.49	1.44
21	a	1136	CLA	CHC-C1C	2.50	1.41	1.35
21	1	1116	CLA	C3B-C2B	-2.50	1.36	1.40
21	1	1109	CLA	CHC-C1C	2.50	1.41	1.35
21	1	1122	CLA	C1C-NC	-2.50	1.34	1.37
21	J	1303	CLA	MG-NC	2.50	2.12	2.06
21	a	1111	CLA	C1C-NC	-2.50	1.34	1.37
21	B	1203	CLA	C1C-C2C	2.50	1.49	1.44
21	B	1219	CLA	C1C-NC	-2.50	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1240	CLA	MG-NC	2.50	2.12	2.06
21	1	1133	CLA	CHC-C1C	2.50	1.41	1.35
21	1	1117	CLA	CHC-C1C	2.50	1.41	1.35
21	b	1212	CLA	C1C-NC	-2.50	1.34	1.37
21	1	1110	CLA	CHC-C1C	2.50	1.41	1.35
21	A	1129	CLA	MG-NC	2.50	2.12	2.06
21	A	1122	CLA	CHC-C1C	2.50	1.41	1.35
21	k	1401	CLA	MG-NC	2.50	2.12	2.06
21	1	1139	CLA	CHC-C1C	2.50	1.41	1.35
21	1	1130	CLA	CHC-C1C	2.50	1.41	1.35
21	B	1220	CLA	C1C-NC	-2.50	1.34	1.37
21	a	1115	CLA	CHC-C1C	2.50	1.41	1.35
21	2	1231	CLA	CHC-C1C	2.50	1.41	1.35
21	a	1106	CLA	CHC-C1C	2.50	1.41	1.35
21	1	1108	CLA	CHC-C1C	2.50	1.41	1.35
21	k	1402	CLA	C3B-C2B	-2.49	1.36	1.40
21	a	1139	CLA	C3B-C2B	-2.49	1.36	1.40
21	A	1112	CLA	MG-NC	2.49	2.12	2.06
21	B	1217	CLA	CHC-C1C	2.49	1.41	1.35
21	A	1107	CLA	CHC-C1C	2.49	1.41	1.35
21	2	1226	CLA	C1C-C2C	2.49	1.49	1.44
21	B	1239	CLA	CHC-C1C	2.49	1.41	1.35
21	1	1118	CLA	C1C-NC	-2.49	1.34	1.37
21	A	1105	CLA	CHC-C1C	2.49	1.41	1.35
21	f	1301	CLA	MG-NC	2.49	2.12	2.06
21	1	1121	CLA	MG-NC	2.49	2.12	2.06
21	2	1239	CLA	C1C-C2C	2.49	1.49	1.44
21	2	1220	CLA	MG-NC	2.49	2.12	2.06
21	A	1122	CLA	C1C-NC	-2.49	1.34	1.37
21	a	1102	CLA	CHC-C1C	2.49	1.41	1.35
21	b	1217	CLA	MG-NC	2.49	2.12	2.06
21	L	1503	CLA	CHC-C1C	2.49	1.41	1.35
21	b	1238	CLA	MG-NC	2.49	2.12	2.06
21	2	1228	CLA	CHC-C1C	2.49	1.41	1.35
21	B	1227	CLA	C1C-NC	-2.49	1.34	1.37
21	1	1113	CLA	MG-NC	2.49	2.12	2.06
21	1	1102	CLA	C1C-C2C	2.49	1.49	1.44
21	a	1109	CLA	CHC-C1C	2.49	1.41	1.35
21	A	1121	CLA	C1C-C2C	2.49	1.49	1.44
21	F	1302	CLA	MG-NC	2.48	2.12	2.06
22	B	2002	PQN	C9-C10	-2.48	1.35	1.39
30	i	4020	ECH	C1-C6	-2.48	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1107	CLA	CHC-C1C	2.48	1.41	1.35
21	B	1232	CLA	C1C-NC	-2.48	1.34	1.37
21	a	1104	CLA	CHC-C1C	2.48	1.41	1.35
21	b	1224	CLA	MG-NC	2.48	2.12	2.06
21	b	1238	CLA	C1C-C2C	2.48	1.49	1.44
21	A	1134	CLA	CHC-C1C	2.48	1.41	1.35
21	B	1221	CLA	CHC-C1C	2.48	1.41	1.35
21	b	1237	CLA	C1C-C2C	2.48	1.49	1.44
21	2	1220	CLA	CHC-C1C	2.48	1.41	1.35
21	a	1111	CLA	CHC-C1C	2.48	1.41	1.35
21	0	1503	CLA	CHC-C1C	2.48	1.41	1.35
21	b	1217	CLA	CHC-C1C	2.48	1.41	1.35
21	A	1116	CLA	C1C-NC	-2.48	1.34	1.37
21	2	1228	CLA	C1C-NC	-2.48	1.34	1.37
21	B	1208	CLA	CHC-C1C	2.48	1.41	1.35
21	b	1209	CLA	CHC-C1C	2.48	1.41	1.35
21	b	1227	CLA	CHC-C1C	2.48	1.41	1.35
21	A	1111	CLA	C1C-NC	-2.48	1.34	1.37
21	1	1112	CLA	MG-NC	2.48	2.12	2.06
21	1	1137	CLA	C3B-C2B	-2.48	1.36	1.40
21	j	1302	CLA	CHC-C1C	2.48	1.41	1.35
21	2	1021	CLA	CHC-C1C	2.48	1.41	1.35
21	0	1502	CLA	C1C-NC	-2.48	1.34	1.37
21	a	1112	CLA	CHC-C1C	2.47	1.41	1.35
21	2	1209	CLA	MG-NC	2.47	2.12	2.06
21	2	1226	CLA	CHC-C1C	2.47	1.41	1.35
21	1	1119	CLA	C1C-NC	-2.47	1.34	1.37
21	B	1222	CLA	C1C-NC	-2.47	1.34	1.37
21	b	1221	CLA	MG-NC	2.47	2.12	2.06
21	a	1135	CLA	CHC-C1C	2.47	1.41	1.35
21	A	1106	CLA	CHC-C1C	2.47	1.41	1.35
21	A	1113	CLA	MG-NC	2.47	2.12	2.06
21	1	1136	CLA	MG-NC	2.47	2.12	2.06
21	6	1301	CLA	CHC-C1C	2.47	1.41	1.35
21	B	1230	CLA	C1C-NC	-2.47	1.34	1.37
21	A	1135	CLA	C1C-C2C	2.47	1.49	1.44
21	1	1120	CLA	MG-NC	2.47	2.12	2.06
21	b	1223	CLA	CHC-C1C	2.47	1.41	1.35
21	B	1236	CLA	C1C-NC	-2.47	1.34	1.37
21	1	1105	CLA	MG-NC	2.47	2.12	2.06
21	b	1232	CLA	MG-NC	2.47	2.12	2.06
21	l	1501	CLA	MG-NC	2.47	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1205	CLA	C3B-C2B	-2.47	1.36	1.40
21	1	1133	CLA	C1C-NC	-2.47	1.34	1.37
21	b	1240	CLA	CHC-C1C	2.47	1.41	1.35
21	1	1104	CLA	CHC-C1C	2.46	1.41	1.35
21	A	1140	CLA	C3B-C2B	-2.46	1.36	1.40
21	b	1236	CLA	C1C-NC	-2.46	1.34	1.37
21	a	1120	CLA	MG-NC	2.46	2.12	2.06
21	L	1501	CLA	CHC-C1C	2.46	1.41	1.35
21	a	1102	CLA	MG-NC	2.46	2.12	2.06
21	B	1219	CLA	CHC-C1C	2.46	1.41	1.35
21	1	1140	CLA	MG-NC	2.46	2.12	2.06
21	2	1223	CLA	CHC-C1C	2.46	1.41	1.35
21	2	1209	CLA	CHC-C1C	2.46	1.41	1.35
21	a	1801	CLA	CHC-C1C	2.46	1.41	1.35
21	a	1012	CLA	CHC-C1C	2.46	1.41	1.35
21	2	1224	CLA	CHC-C1C	2.46	1.41	1.35
21	1	1112	CLA	C3B-C2B	-2.46	1.37	1.40
21	A	1125	CLA	CHC-C1C	2.46	1.41	1.35
21	B	1223	CLA	C1C-NC	-2.46	1.34	1.37
21	B	1205	CLA	MG-NC	2.46	2.12	2.06
21	B	1234	CLA	MG-NC	2.46	2.12	2.06
21	A	1132	CLA	MG-NC	2.46	2.12	2.06
21	K	1401	CLA	CHC-C1C	2.46	1.41	1.35
21	A	1138	CLA	C1C-NC	-2.46	1.34	1.37
21	0	1503	CLA	C1C-NC	-2.46	1.34	1.37
21	1	1109	CLA	MG-NC	2.46	2.12	2.06
21	L	1502	CLA	CHC-C1C	2.46	1.41	1.35
21	B	1218	CLA	C1C-NC	-2.46	1.34	1.37
21	b	1238	CLA	C1C-NC	-2.46	1.34	1.37
21	B	1215	CLA	CHC-C1C	2.46	1.41	1.35
21	2	1210	CLA	MG-NC	2.46	2.12	2.06
21	a	1109	CLA	C1C-C2C	2.46	1.49	1.44
21	A	1112	CLA	CHC-C1C	2.46	1.41	1.35
21	1	1118	CLA	CHC-C1C	2.45	1.41	1.35
21	F	1301	CLA	CHC-C1C	2.45	1.41	1.35
21	a	1135	CLA	MG-NC	2.45	2.12	2.06
21	a	1130	CLA	C1C-NC	-2.45	1.34	1.37
21	b	1023	CLA	C1C-NC	-2.45	1.34	1.37
21	A	1123	CLA	MG-NC	2.45	2.12	2.06
21	a	1134	CLA	C3B-C2B	-2.45	1.37	1.40
21	B	1217	CLA	MG-NC	2.45	2.12	2.06
21	1	1101	CLA	C1C-NC	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1230	CLA	MG-NC	2.45	2.12	2.06
21	a	1105	CLA	MG-NC	2.45	2.12	2.06
36	I	4020	EQ3	C21-C22	-2.45	1.32	1.35
21	b	1228	CLA	CHC-C1C	2.45	1.41	1.35
21	f	1302	CLA	CHC-C1C	2.45	1.41	1.35
21	a	1132	CLA	MG-NC	2.45	2.12	2.06
21	2	1221	CLA	CHC-C1C	2.45	1.41	1.35
21	2	1219	CLA	MG-NC	2.45	2.12	2.06
21	a	1124	CLA	CHC-C1C	2.45	1.41	1.35
21	a	1111	CLA	MG-NC	2.45	2.12	2.06
21	b	1225	CLA	CHC-C1C	2.45	1.41	1.35
21	b	1216	CLA	C1C-NC	-2.45	1.34	1.37
21	2	1217	CLA	CHC-C1C	2.45	1.41	1.35
21	2	1207	CLA	C1C-NC	-2.45	1.34	1.37
21	a	1140	CLA	C1C-NC	-2.45	1.34	1.37
21	2	1219	CLA	CHC-C1C	2.45	1.41	1.35
21	b	1206	CLA	C1C-C2C	2.44	1.49	1.44
21	L	1501	CLA	C1C-NC	-2.44	1.34	1.37
21	1	1124	CLA	CHC-C1C	2.44	1.41	1.35
21	b	1237	CLA	C1C-NC	-2.44	1.34	1.37
21	a	1138	CLA	MG-NC	2.44	2.12	2.06
21	1	1116	CLA	MG-NC	2.44	2.12	2.06
21	a	1139	CLA	MG-NC	2.44	2.12	2.06
21	a	1115	CLA	C1C-NC	-2.44	1.34	1.37
21	A	1106	CLA	C1C-NC	-2.44	1.34	1.37
21	A	1108	CLA	C1C-NC	-2.44	1.34	1.37
21	6	1301	CLA	MG-NC	2.44	2.12	2.06
21	2	1230	CLA	CHC-C1C	2.44	1.41	1.35
21	A	1124	CLA	MG-NC	2.44	2.12	2.06
21	L	1503	CLA	MG-NC	2.44	2.12	2.06
21	a	1113	CLA	MG-NC	2.44	2.12	2.06
21	B	1209	CLA	MG-NC	2.44	2.12	2.06
21	b	1207	CLA	C1C-NC	-2.44	1.34	1.37
21	a	1112	CLA	C1C-NC	-2.44	1.34	1.37
21	a	1137	CLA	C1C-NC	-2.44	1.34	1.37
21	a	1121	CLA	MG-NC	2.44	2.12	2.06
21	1	1101	CLA	CHC-C1C	2.44	1.41	1.35
21	1	1124	CLA	MG-NC	2.44	2.12	2.06
21	A	1103	CLA	CHC-C1C	2.44	1.41	1.35
21	2	1220	CLA	C1C-NC	-2.43	1.34	1.37
21	2	1230	CLA	C1C-NC	-2.43	1.34	1.37
21	L	1501	CLA	MG-NC	2.43	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1238	CLA	C3B-C2B	-2.43	1.37	1.40
21	2	1223	CLA	C1C-NC	-2.43	1.34	1.37
21	a	1122	CLA	CHC-C1C	2.43	1.41	1.35
21	B	1224	CLA	CHC-C1C	2.43	1.41	1.35
21	B	1213	CLA	MG-NC	2.43	2.12	2.06
21	2	1211	CLA	MG-NC	2.43	2.12	2.06
21	1	1125	CLA	MG-NC	2.43	2.12	2.06
21	1	1127	CLA	C1C-NC	-2.43	1.34	1.37
21	A	1128	CLA	C1C-C2C	2.43	1.49	1.44
21	1	1112	CLA	CHC-C1C	2.43	1.41	1.35
21	a	1112	CLA	MG-NC	2.43	2.12	2.06
21	A	1123	CLA	C1C-C2C	2.43	1.49	1.44
21	f	1302	CLA	MG-NC	2.43	2.12	2.06
21	a	1120	CLA	C1C-NC	-2.43	1.34	1.37
21	2	1208	CLA	C1C-NC	-2.43	1.34	1.37
21	2	1227	CLA	C1C-NC	-2.43	1.34	1.37
21	b	1205	CLA	MG-NC	2.43	2.12	2.06
21	A	1127	CLA	MG-NC	2.43	2.12	2.06
21	A	1121	CLA	C1C-NC	-2.43	1.34	1.37
21	2	1206	CLA	CHC-C1C	2.43	1.41	1.35
21	F	1302	CLA	CHC-C1C	2.43	1.41	1.35
21	b	1204	CLA	CHC-C1C	2.43	1.41	1.35
21	1	1135	CLA	CHC-C1C	2.42	1.41	1.35
21	B	1204	CLA	C1C-NC	-2.42	1.34	1.37
21	1	1115	CLA	C3B-C2B	-2.42	1.37	1.40
21	a	1126	CLA	C1C-NC	-2.42	1.34	1.37
21	b	1218	CLA	MG-NC	2.42	2.12	2.06
28	B	4011	45D	C17-C15	2.42	1.52	1.47
21	B	1221	CLA	MG-NC	2.42	2.12	2.06
21	b	1202	CLA	C1C-NC	-2.42	1.34	1.37
21	a	1115	CLA	C3B-C2B	-2.42	1.37	1.40
21	B	1230	CLA	C3B-C2B	-2.42	1.37	1.40
21	B	1209	CLA	C1C-NC	-2.42	1.34	1.37
21	b	1214	CLA	MG-NC	2.42	2.12	2.06
21	K	1401	CLA	C1C-NC	-2.42	1.34	1.37
21	a	1101	CLA	C3B-C2B	-2.42	1.37	1.40
21	B	1022	CLA	MG-NC	2.42	2.12	2.06
21	a	1123	CLA	CHC-C1C	2.42	1.41	1.35
21	B	1229	CLA	C1C-NC	-2.42	1.34	1.37
21	B	1218	CLA	CHC-C1C	2.42	1.41	1.35
21	b	1219	CLA	MG-NC	2.42	2.12	2.06
21	2	1236	CLA	C1C-NC	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1103	CLA	C1C-NC	-2.42	1.34	1.37
21	A	1131	CLA	C1C-NC	-2.42	1.34	1.37
21	A	1116	CLA	C3B-C2B	-2.42	1.37	1.40
21	2	1240	CLA	C3B-C2B	-2.42	1.37	1.40
21	1	1111	CLA	MG-NC	2.42	2.12	2.06
22	B	2002	PQN	C10-C5	-2.42	1.36	1.40
28	h	4020	45D	C18-C16	2.42	1.52	1.47
21	1	1102	CLA	CHC-C1C	2.42	1.41	1.35
21	A	1107	CLA	MG-NC	2.42	2.12	2.06
21	B	1240	CLA	C3B-C2B	-2.41	1.37	1.40
21	a	1127	CLA	C1C-NC	-2.41	1.34	1.37
21	7	1303	CLA	C1C-NC	-2.41	1.34	1.37
21	A	1139	CLA	C1C-NC	-2.41	1.34	1.37
21	1	1138	CLA	MG-NC	2.41	2.12	2.06
21	B	1203	CLA	CHC-C1C	2.41	1.41	1.35
21	8	1402	CLA	MG-NC	2.41	2.12	2.06
21	J	1302	CLA	MG-NC	2.41	2.12	2.06
21	a	1108	CLA	MG-NC	2.41	2.12	2.06
21	1	1122	CLA	CHC-C1C	2.41	1.41	1.35
21	B	1214	CLA	MG-NC	2.41	2.12	2.06
21	1	1117	CLA	C1C-NC	-2.41	1.34	1.37
21	b	1237	CLA	MG-NC	2.41	2.12	2.06
21	b	1203	CLA	CHC-C1C	2.41	1.41	1.35
21	f	1302	CLA	C1C-NC	-2.41	1.34	1.37
21	B	1210	CLA	CHC-C1C	2.41	1.41	1.35
21	2	1207	CLA	CHC-C1C	2.41	1.41	1.35
21	A	1011	CLA	C1C-NC	-2.41	1.34	1.37
21	a	1130	CLA	MG-NC	2.41	2.12	2.06
21	1	1114	CLA	MG-NC	2.41	2.12	2.06
21	B	1216	CLA	MG-NC	2.41	2.12	2.06
21	b	1203	CLA	MG-NC	2.41	2.12	2.06
21	b	1223	CLA	C1C-NC	-2.41	1.34	1.37
21	2	1206	CLA	MG-NC	2.41	2.12	2.06
21	b	1223	CLA	MG-NC	2.41	2.12	2.06
21	b	1236	CLA	CHC-C1C	2.41	1.41	1.35
21	1	1134	CLA	C1C-NC	-2.41	1.34	1.37
21	B	1237	CLA	C1C-C2C	2.41	1.49	1.44
21	b	1239	CLA	CHC-C1C	2.41	1.41	1.35
21	2	1234	CLA	MG-NC	2.41	2.12	2.06
21	a	1103	CLA	C1C-C2C	2.41	1.49	1.44
21	0	1501	CLA	MG-NC	2.40	2.12	2.06
21	2	1236	CLA	MG-NC	2.40	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	1302	CLA	MG-NC	2.40	2.12	2.06
21	j	1302	CLA	C1C-NC	-2.40	1.34	1.37
21	1	1139	CLA	MG-NC	2.40	2.12	2.06
21	b	1225	CLA	MG-NC	2.40	2.12	2.06
21	b	1224	CLA	C1C-NC	-2.40	1.34	1.37
21	A	1115	CLA	C1C-NC	-2.40	1.34	1.37
21	2	1216	CLA	MG-NC	2.40	2.12	2.06
21	B	1232	CLA	CHC-C1C	2.40	1.41	1.35
21	a	1137	CLA	MG-NC	2.40	2.12	2.06
21	A	1107	CLA	C1C-NC	-2.40	1.34	1.37
21	a	1129	CLA	C3B-C2B	-2.40	1.37	1.40
21	1	1115	CLA	C1C-NC	-2.40	1.34	1.37
21	1	1011	CLA	MG-NC	2.40	2.12	2.06
21	1	1128	CLA	MG-NC	2.40	2.12	2.06
21	B	1212	CLA	C1C-NC	-2.39	1.34	1.37
21	A	1124	CLA	C1C-NC	-2.39	1.34	1.37
21	A	1109	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1236	CLA	C3B-C2B	-2.39	1.37	1.40
21	b	1214	CLA	C3B-C2B	-2.39	1.37	1.40
21	b	1206	CLA	CHC-C1C	2.39	1.41	1.35
21	A	1135	CLA	MG-NC	2.39	2.12	2.06
21	2	1222	CLA	MG-NC	2.39	2.12	2.06
21	2	1206	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1205	CLA	C1C-C2C	2.39	1.49	1.44
21	1	1111	CLA	CHC-C1C	2.39	1.41	1.35
21	b	1206	CLA	MG-NC	2.39	2.11	2.06
21	B	1023	CLA	C1C-NC	-2.39	1.34	1.37
21	A	1105	CLA	C1C-NC	-2.39	1.34	1.37
21	a	1122	CLA	MG-NC	2.39	2.11	2.06
21	1	1108	CLA	C1C-NC	-2.39	1.34	1.37
21	B	1201	CLA	C1C-C2C	2.39	1.49	1.44
21	b	1237	CLA	CHC-C1C	2.39	1.41	1.35
21	B	1222	CLA	CHC-C1C	2.39	1.41	1.35
21	a	1102	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1219	CLA	C1C-NC	-2.39	1.34	1.37
21	b	1205	CLA	CHC-C1C	2.39	1.41	1.35
21	2	1223	CLA	MG-NC	2.39	2.11	2.06
21	K	1402	CLA	MG-NC	2.39	2.11	2.06
21	B	1226	CLA	C1C-NC	-2.39	1.34	1.37
21	2	1022	CLA	MG-NC	2.39	2.11	2.06
21	B	1215	CLA	MG-NC	2.39	2.11	2.06
21	b	1209	CLA	C1C-NC	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1138	CLA	C1C-NC	-2.38	1.34	1.37
21	B	1209	CLA	CHC-C1C	2.38	1.41	1.35
21	l	1501	CLA	CHC-C1C	2.38	1.41	1.35
21	2	1224	CLA	MG-NC	2.38	2.11	2.06
21	2	1231	CLA	C1C-NC	-2.38	1.34	1.37
21	1	1012	CLA	MG-NC	2.38	2.11	2.06
21	a	1122	CLA	C1C-NC	-2.38	1.34	1.37
21	K	1401	CLA	MG-NC	2.38	2.11	2.06
21	1	1139	CLA	C3B-C2B	-2.38	1.37	1.40
21	A	1114	CLA	MG-NC	2.38	2.11	2.06
21	2	1218	CLA	MG-NC	2.38	2.11	2.06
21	B	1214	CLA	CHC-C1C	2.38	1.41	1.35
21	2	1022	CLA	C1C-NC	-2.38	1.34	1.37
21	1	1108	CLA	MG-NC	2.38	2.11	2.06
21	b	1228	CLA	MG-NC	2.38	2.11	2.06
21	1	1107	CLA	MG-NC	2.38	2.11	2.06
21	L	1502	CLA	MG-NC	2.38	2.11	2.06
21	j	1302	CLA	MG-NC	2.38	2.11	2.06
21	a	1136	CLA	C1C-NC	-2.38	1.34	1.37
21	f	1302	CLA	C3B-C2B	-2.38	1.37	1.40
21	2	1202	CLA	C1C-NC	-2.38	1.34	1.37
21	b	1221	CLA	CHC-C1C	2.38	1.41	1.35
21	a	1801	CLA	C1C-NC	-2.38	1.34	1.37
21	a	1117	CLA	C1C-NC	-2.38	1.34	1.37
21	2	1209	CLA	C1C-NC	-2.38	1.34	1.37
21	a	1105	CLA	CHC-C1C	2.38	1.41	1.35
21	1	1123	CLA	CHC-C1C	2.38	1.41	1.35
21	A	1128	CLA	MG-NC	2.38	2.11	2.06
21	1	1103	CLA	CHC-C1C	2.38	1.41	1.35
21	a	1128	CLA	C1C-NC	-2.38	1.34	1.37
21	A	1105	CLA	MG-NC	2.38	2.11	2.06
21	b	1224	CLA	CHC-C1C	2.38	1.41	1.35
21	B	1214	CLA	C1C-NC	-2.38	1.34	1.37
21	b	1229	CLA	C1C-NC	-2.38	1.34	1.37
21	1	1120	CLA	C1C-NC	-2.38	1.34	1.37
21	2	1023	CLA	C1C-NC	-2.37	1.34	1.37
21	1	1801	CLA	MG-NC	2.37	2.11	2.06
21	B	1225	CLA	MG-NC	2.37	2.11	2.06
21	a	1136	CLA	MG-NC	2.37	2.11	2.06
21	B	1204	CLA	MG-NC	2.37	2.11	2.06
21	B	1237	CLA	CHC-C1C	2.37	1.41	1.35
21	1	1103	CLA	C1C-C2C	2.37	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1140	CLA	C1C-NC	-2.37	1.34	1.37
21	b	1225	CLA	C1C-NC	-2.37	1.34	1.37
21	b	1022	CLA	C1C-NC	-2.37	1.34	1.37
21	a	1128	CLA	MG-NC	2.37	2.11	2.06
21	2	1205	CLA	CHC-C1C	2.37	1.41	1.35
21	1	1106	CLA	MG-NC	2.37	2.11	2.06
21	a	1108	CLA	C3B-C2B	-2.37	1.37	1.40
21	2	1232	CLA	MG-NC	2.37	2.11	2.06
21	a	1118	CLA	MG-NC	2.37	2.11	2.06
21	6	1302	CLA	MG-NC	2.37	2.11	2.06
21	1	1128	CLA	C1C-C2C	2.37	1.49	1.44
21	A	1104	CLA	MG-NC	2.37	2.11	2.06
21	1	1102	CLA	MG-NC	2.37	2.11	2.06
21	l	1503	CLA	C1C-NC	-2.37	1.34	1.37
21	a	1120	CLA	CHC-C1C	2.37	1.41	1.35
21	A	1116	CLA	MG-NC	2.37	2.11	2.06
21	b	1209	CLA	MG-NC	2.37	2.11	2.06
21	a	1107	CLA	MG-NC	2.37	2.11	2.06
21	2	1021	CLA	C1C-NC	-2.37	1.34	1.37
21	B	1205	CLA	CHC-C1C	2.37	1.41	1.35
21	a	1129	CLA	C1C-NC	-2.37	1.34	1.37
21	7	1303	CLA	CHC-C1C	2.37	1.41	1.35
21	B	1223	CLA	MG-NC	2.37	2.11	2.06
21	a	1101	CLA	MG-NC	2.36	2.11	2.06
21	B	1205	CLA	C1C-NC	-2.36	1.34	1.37
21	B	1226	CLA	CHC-C1C	2.36	1.41	1.35
21	1	1111	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1225	CLA	C1C-NC	-2.36	1.34	1.37
21	8	1401	CLA	C1C-NC	-2.36	1.34	1.37
21	1	1117	CLA	MG-NC	2.36	2.11	2.06
21	a	1012	CLA	MG-NC	2.36	2.11	2.06
21	2	1213	CLA	C1C-NC	-2.36	1.34	1.37
21	b	1204	CLA	C1C-NC	-2.36	1.34	1.37
21	L	1503	CLA	C1C-NC	-2.36	1.34	1.37
21	2	1226	CLA	MG-NC	2.36	2.11	2.06
35	0	6001	LMT	O2B-C2B	-2.36	1.37	1.43
21	B	1235	CLA	C1C-NC	-2.36	1.34	1.37
21	J	1302	CLA	C3B-C2B	-2.36	1.37	1.40
21	b	1239	CLA	C1C-NC	-2.36	1.34	1.37
21	a	1103	CLA	CHC-C1C	2.36	1.41	1.35
21	2	1235	CLA	C1C-NC	-2.36	1.34	1.37
21	a	1105	CLA	C1C-NC	-2.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1225	CLA	MG-NC	2.36	2.11	2.06
21	b	1231	CLA	C1C-NC	-2.36	1.34	1.37
21	1	1128	CLA	CHC-C1C	2.36	1.41	1.35
21	2	1203	CLA	MG-NC	2.36	2.11	2.06
28	h	4020	45D	O02-C18	-2.36	1.18	1.23
21	a	1124	CLA	MG-NC	2.36	2.11	2.06
21	A	1110	CLA	C1C-NC	-2.35	1.34	1.37
21	b	1236	CLA	MG-NC	2.35	2.11	2.06
21	A	1111	CLA	C3B-C2B	-2.35	1.37	1.40
21	2	1221	CLA	C3B-C2B	-2.35	1.37	1.40
21	1	1121	CLA	CHC-C1C	2.35	1.41	1.35
21	B	1216	CLA	C1C-NC	-2.35	1.34	1.37
21	a	1110	CLA	C1C-NC	-2.35	1.34	1.37
21	7	1302	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1205	CLA	C1C-NC	-2.35	1.34	1.37
21	0	1503	CLA	MG-NC	2.35	2.11	2.06
21	1	1110	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1212	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1237	CLA	MG-NC	2.35	2.11	2.06
21	B	1227	CLA	MG-NC	2.35	2.11	2.06
21	a	1110	CLA	MG-NC	2.35	2.11	2.06
21	B	1206	CLA	C1C-NC	-2.35	1.34	1.37
21	1	1101	CLA	MG-NC	2.35	2.11	2.06
21	A	1118	CLA	MG-NC	2.35	2.11	2.06
21	b	1228	CLA	C1C-NC	-2.35	1.34	1.37
21	a	1113	CLA	C1C-NC	-2.35	1.34	1.37
21	B	1208	CLA	MG-NC	2.35	2.11	2.06
21	b	1201	CLA	MG-NC	2.35	2.11	2.06
21	B	1217	CLA	C1C-NC	-2.35	1.34	1.37
21	K	1402	CLA	C1C-NC	-2.35	1.34	1.37
21	B	1213	CLA	C1C-NC	-2.35	1.34	1.37
21	2	1235	CLA	MG-NC	2.35	2.11	2.06
21	B	1238	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1116	CLA	MG-NC	2.34	2.11	2.06
21	B	1215	CLA	C1C-NC	-2.34	1.34	1.37
21	B	1234	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1109	CLA	MG-NC	2.34	2.11	2.06
21	b	1206	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1109	CLA	C1C-NC	-2.34	1.34	1.37
21	b	1201	CLA	C1C-NC	-2.34	1.34	1.37
21	B	1201	CLA	C1C-NC	-2.34	1.34	1.37
21	A	1123	CLA	CHC-C1C	2.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1211	CLA	C1C-NC	-2.34	1.34	1.37
21	1	1118	CLA	MG-NC	2.34	2.11	2.06
21	B	1237	CLA	MG-NC	2.34	2.11	2.06
21	b	1238	CLA	CHC-C1C	2.34	1.41	1.35
22	b	2002	PQN	C10-C5	-2.34	1.36	1.40
21	a	1116	CLA	C1C-NC	-2.34	1.34	1.37
21	a	1111	CLA	C3B-C2B	-2.34	1.37	1.40
21	1	1126	CLA	MG-NC	2.34	2.11	2.06
21	a	1133	CLA	MG-NC	2.34	2.11	2.06
21	B	1203	CLA	C3B-C2B	-2.34	1.37	1.40
21	1	1115	CLA	MG-NC	2.34	2.11	2.06
21	b	1213	CLA	C1C-NC	-2.34	1.34	1.37
36	I	4020	EQ3	C17-C18	2.34	1.38	1.35
21	B	1228	CLA	MG-NC	2.33	2.11	2.06
21	B	1239	CLA	MG-NC	2.33	2.11	2.06
21	B	1239	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1231	CLA	MG-NC	2.33	2.11	2.06
21	2	1234	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1224	CLA	C1C-NC	-2.33	1.34	1.37
21	B	1208	CLA	C1C-NC	-2.33	1.34	1.37
21	A	1139	CLA	C3B-C2B	-2.33	1.37	1.40
21	B	1225	CLA	C1C-NC	-2.33	1.34	1.37
21	1	1133	CLA	MG-NC	2.33	2.11	2.06
21	A	1135	CLA	CHC-C1C	2.33	1.40	1.35
21	b	1204	CLA	MG-NC	2.33	2.11	2.06
21	B	1237	CLA	C1C-NC	-2.33	1.34	1.37
21	1	1130	CLA	C1C-NC	-2.33	1.34	1.37
21	a	1115	CLA	MG-NC	2.33	2.11	2.06
21	B	1206	CLA	MG-NC	2.33	2.11	2.06
21	a	1011	CLA	MG-NC	2.33	2.11	2.06
21	2	1230	CLA	C3B-C2B	-2.33	1.37	1.40
21	B	1220	CLA	MG-NC	2.33	2.11	2.06
21	a	1106	CLA	MG-NC	2.33	2.11	2.06
21	2	1231	CLA	MG-NC	2.33	2.11	2.06
21	1	1122	CLA	MG-NC	2.33	2.11	2.06
21	B	1226	CLA	MG-NC	2.33	2.11	2.06
21	a	1134	CLA	C1C-NC	-2.33	1.34	1.37
21	k	1402	CLA	MG-NC	2.33	2.11	2.06
36	I	4020	EQ3	C27-C26	2.33	1.52	1.47
21	b	1221	CLA	C1C-C2C	2.32	1.49	1.44
21	j	1302	CLA	C3B-C2B	-2.32	1.37	1.40
21	F	1301	CLA	C1C-NC	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1103	CLA	C1C-C2C	2.32	1.49	1.44
21	A	1117	CLA	MG-NC	2.32	2.11	2.06
21	2	1203	CLA	C1C-NC	-2.32	1.34	1.37
21	8	1402	CLA	C1C-NC	-2.32	1.34	1.37
21	b	1227	CLA	MG-NC	2.32	2.11	2.06
21	1	1132	CLA	MG-NC	2.32	2.11	2.06
21	2	1224	CLA	C1C-NC	-2.32	1.34	1.37
21	F	1302	CLA	C1C-NC	-2.32	1.34	1.37
21	a	1117	CLA	MG-NC	2.32	2.11	2.06
21	1	1104	CLA	C1C-NC	-2.32	1.34	1.37
21	A	1121	CLA	CHC-C1C	2.32	1.40	1.35
21	2	1239	CLA	CHC-C1C	2.32	1.40	1.35
21	B	1221	CLA	C3B-C2B	-2.32	1.37	1.40
21	a	1127	CLA	MG-NC	2.32	2.11	2.06
21	b	1207	CLA	MG-NC	2.32	2.11	2.06
21	A	1118	CLA	C1C-NC	-2.32	1.34	1.37
21	2	1239	CLA	MG-NC	2.32	2.11	2.06
21	b	1215	CLA	C1C-NC	-2.32	1.34	1.37
21	b	1221	CLA	C1C-NC	-2.32	1.34	1.37
21	a	1123	CLA	C3B-C2B	-2.32	1.37	1.40
21	A	1115	CLA	MG-NC	2.32	2.11	2.06
35	F	6001	LMT	O3B-C3B	-2.32	1.37	1.43
35	0	6001	LMT	O2'-C2'	-2.32	1.37	1.43
21	l	1501	CLA	C1C-NC	-2.32	1.34	1.37
21	b	1219	CLA	C1C-NC	-2.32	1.34	1.37
21	b	1022	CLA	MG-NC	2.32	2.11	2.06
21	b	1211	CLA	MG-NC	2.32	2.11	2.06
21	b	1239	CLA	MG-NC	2.32	2.11	2.06
21	2	1201	CLA	MG-NC	2.32	2.11	2.06
21	b	1208	CLA	C1C-NC	-2.32	1.34	1.37
21	1	1012	CLA	C1C-NC	-2.32	1.34	1.37
21	2	1202	CLA	MG-NC	2.32	2.11	2.06
21	b	1231	CLA	MG-NC	2.31	2.11	2.06
21	B	1210	CLA	C1C-NC	-2.31	1.34	1.37
21	a	1131	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1140	CLA	C1C-NC	-2.31	1.34	1.37
21	b	1205	CLA	C3B-C2B	-2.31	1.37	1.40
21	A	1108	CLA	MG-NC	2.31	2.11	2.06
21	a	1138	CLA	C1C-NC	-2.31	1.34	1.37
21	b	1240	CLA	C1C-NC	-2.31	1.34	1.37
21	B	1218	CLA	MG-NC	2.31	2.11	2.06
21	2	1212	CLA	MG-NC	2.31	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1112	CLA	C1C-NC	-2.31	1.34	1.37
21	B	1228	CLA	C1C-NC	-2.31	1.34	1.37
21	B	1238	CLA	MG-NC	2.31	2.11	2.06
21	2	1215	CLA	MG-NC	2.31	2.11	2.06
21	a	1125	CLA	MG-NC	2.31	2.11	2.06
21	A	1801	CLA	MG-NC	2.31	2.11	2.06
21	1	1110	CLA	MG-NC	2.31	2.11	2.06
35	F	6001	LMT	O2B-C2B	-2.31	1.37	1.43
21	B	1207	CLA	MG-NC	2.31	2.11	2.06
21	B	1235	CLA	MG-NC	2.31	2.11	2.06
21	1	1013	CLA	C1C-NC	-2.31	1.34	1.37
21	a	1121	CLA	C1C-NC	-2.31	1.34	1.37
21	1	1126	CLA	C1C-NC	-2.31	1.34	1.37
21	2	1237	CLA	C1C-NC	-2.31	1.34	1.37
21	1	1105	CLA	C1C-NC	-2.31	1.34	1.37
21	A	1128	CLA	CHC-C1C	2.31	1.40	1.35
21	2	1232	CLA	C3B-C2B	-2.31	1.37	1.40
21	A	1101	CLA	MG-NC	2.31	2.11	2.06
21	b	1234	CLA	MG-NC	2.30	2.11	2.06
21	a	1126	CLA	MG-NC	2.30	2.11	2.06
21	A	1102	CLA	MG-NC	2.30	2.11	2.06
21	A	1126	CLA	C1C-NC	-2.30	1.34	1.37
21	a	1119	CLA	C1C-NC	-2.30	1.34	1.37
21	B	1201	CLA	MG-NC	2.30	2.11	2.06
21	A	1132	CLA	C3B-C2B	-2.30	1.37	1.40
21	B	1240	CLA	C1C-NC	-2.30	1.34	1.37
21	B	1236	CLA	MG-NC	2.30	2.11	2.06
21	1	1129	CLA	C1C-NC	-2.30	1.34	1.37
21	B	1207	CLA	C1A-CHA	2.30	1.52	1.43
21	1	1013	CLA	C1A-CHA	2.30	1.52	1.43
21	A	1114	CLA	C1C-NC	-2.30	1.34	1.37
21	B	1211	CLA	C1C-NC	-2.30	1.34	1.37
21	1	1108	CLA	C3B-C2B	-2.30	1.37	1.40
21	a	1134	CLA	MG-NC	2.30	2.11	2.06
35	F	6001	LMT	O2'-C2'	-2.30	1.37	1.43
21	a	1011	CLA	C1C-NC	-2.30	1.34	1.37
21	a	1133	CLA	C1C-NC	-2.30	1.34	1.37
21	6	1302	CLA	C1A-CHA	2.30	1.52	1.43
21	a	1131	CLA	MG-NC	2.30	2.11	2.06
21	j	1303	CLA	C3B-C2B	-2.30	1.37	1.40
21	6	1301	CLA	C1C-NC	-2.30	1.34	1.37
21	A	1119	CLA	C1C-NC	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1205	CLA	C1C-C2C	2.29	1.49	1.44
21	2	1238	CLA	MG-NC	2.29	2.11	2.06
21	B	1202	CLA	C1C-NC	-2.29	1.34	1.37
21	B	1224	CLA	MG-NC	2.29	2.11	2.06
21	A	1122	CLA	MG-NC	2.29	2.11	2.06
21	A	1112	CLA	C1C-NC	-2.29	1.34	1.37
21	1	1125	CLA	C1C-NC	-2.29	1.34	1.37
21	1	1102	CLA	C1C-NC	-2.29	1.34	1.37
21	b	1230	CLA	C1C-NC	-2.29	1.34	1.37
21	A	1121	CLA	MG-NC	2.29	2.11	2.06
21	2	1227	CLA	MG-NC	2.29	2.11	2.06
21	a	1114	CLA	C3B-C2B	-2.29	1.37	1.40
21	b	1213	CLA	MG-NC	2.29	2.11	2.06
21	K	1402	CLA	CHC-C1C	2.29	1.40	1.35
21	1	1104	CLA	MG-NC	2.29	2.11	2.06
21	1	1137	CLA	MG-NC	2.29	2.11	2.06
21	B	1231	CLA	C1C-NC	-2.29	1.34	1.37
21	b	1235	CLA	MG-NC	2.29	2.11	2.06
21	B	1219	CLA	MG-NC	2.29	2.11	2.06
21	2	1208	CLA	MG-NC	2.29	2.11	2.06
21	k	1401	CLA	C1C-NC	-2.29	1.34	1.37
21	1	1129	CLA	MG-NC	2.29	2.11	2.06
21	A	1111	CLA	MG-NC	2.29	2.11	2.06
21	a	1140	CLA	MG-NC	2.28	2.11	2.06
21	A	1117	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1130	CLA	C1C-NC	-2.28	1.34	1.37
21	f	1301	CLA	C1C-NC	-2.28	1.34	1.37
21	2	1238	CLA	C1C-NC	-2.28	1.34	1.37
21	1	1107	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1139	CLA	MG-NC	2.28	2.11	2.06
21	1	1134	CLA	MG-NC	2.28	2.11	2.06
21	B	1230	CLA	MG-NC	2.28	2.11	2.06
21	A	1121	CLA	C3B-C2B	-2.28	1.37	1.40
21	1	1130	CLA	MG-NC	2.28	2.11	2.06
21	A	1109	CLA	MG-NC	2.28	2.11	2.06
21	1	1113	CLA	C1C-NC	-2.28	1.34	1.37
21	1	1011	CLA	C1C-NC	-2.28	1.34	1.37
21	1	1131	CLA	MG-NC	2.28	2.11	2.06
21	1	1140	CLA	C3B-C2B	-2.28	1.37	1.40
21	a	1135	CLA	C1C-NC	-2.28	1.34	1.37
21	A	1127	CLA	C1C-NC	-2.28	1.34	1.37
21	L	1502	CLA	C1C-NC	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1104	CLA	MG-NC	2.28	2.11	2.06
21	0	1501	CLA	C1C-NC	-2.28	1.34	1.37
21	B	1021	CLA	C1C-NC	-2.27	1.34	1.37
21	b	1021	CLA	MG-NC	2.27	2.11	2.06
21	k	1402	CLA	C1C-NC	-2.27	1.34	1.37
21	a	1132	CLA	C3B-C2B	-2.27	1.37	1.40
21	b	1205	CLA	C1C-NC	-2.27	1.34	1.37
21	A	1103	CLA	C1D-C2D	2.27	1.47	1.42
21	2	1214	CLA	C1C-NC	-2.27	1.34	1.37
21	1	1116	CLA	C1C-NC	-2.27	1.34	1.37
21	A	1102	CLA	C1C-NC	-2.27	1.34	1.37
21	b	1216	CLA	MG-NC	2.27	2.11	2.06
21	j	1303	CLA	C1C-NC	-2.27	1.34	1.37
21	A	1121	CLA	C1D-C2D	2.27	1.47	1.42
21	B	1212	CLA	MG-NC	2.27	2.11	2.06
21	A	1134	CLA	MG-NC	2.27	2.11	2.06
21	A	1013	CLA	C1C-NC	-2.27	1.34	1.37
21	2	1210	CLA	C3B-C2B	-2.27	1.37	1.40
21	A	1112	CLA	C3B-C2B	-2.27	1.37	1.40
21	A	1123	CLA	C1C-NC	-2.26	1.34	1.37
21	A	1801	CLA	C1C-NC	-2.26	1.34	1.37
21	2	1232	CLA	C1C-NC	-2.26	1.34	1.37
21	2	1201	CLA	C1C-NC	-2.26	1.34	1.37
21	a	1124	CLA	C1C-NC	-2.26	1.34	1.37
21	2	1240	CLA	C1C-NC	-2.26	1.34	1.37
21	a	1104	CLA	C1C-NC	-2.26	1.34	1.37
21	1	1135	CLA	C1D-C2D	2.26	1.47	1.42
21	A	1125	CLA	MG-NC	2.26	2.11	2.06
21	A	1124	CLA	C1D-C2D	2.26	1.47	1.42
21	a	1114	CLA	C1C-NC	-2.26	1.34	1.37
21	l	1503	CLA	MG-NC	2.26	2.11	2.06
21	a	1138	CLA	C3B-C2B	-2.26	1.37	1.40
21	A	1123	CLA	C1A-CHA	2.26	1.52	1.43
21	2	1215	CLA	C1C-NC	-2.26	1.34	1.37
21	a	1139	CLA	C1C-NC	-2.25	1.34	1.37
21	A	1138	CLA	C3B-C2B	-2.25	1.37	1.40
21	B	1023	CLA	MG-NC	2.25	2.11	2.06
21	a	1013	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1114	CLA	C1C-NC	-2.25	1.34	1.37
21	A	1135	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1801	CLA	C1C-NC	-2.25	1.34	1.37
21	b	1208	CLA	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1204	CLA	MG-NC	2.25	2.11	2.06
21	J	1303	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1109	CLA	C3B-C2B	-2.25	1.37	1.40
21	B	1021	CLA	MG-NC	2.25	2.11	2.06
21	a	1119	CLA	MG-NC	2.25	2.11	2.06
21	a	1123	CLA	C1C-NC	-2.25	1.34	1.37
21	b	1232	CLA	C1C-NC	-2.25	1.34	1.37
21	A	1011	CLA	MG-NC	2.25	2.11	2.06
21	B	1232	CLA	MG-NC	2.25	2.11	2.06
21	a	1129	CLA	MG-NC	2.25	2.11	2.06
21	a	1108	CLA	C1C-NC	-2.25	1.34	1.37
21	1	1106	CLA	C1C-NC	-2.24	1.34	1.37
21	A	1128	CLA	C1C-NC	-2.24	1.34	1.37
34	7	4015	ZEX	C1-C6	-2.24	1.50	1.53
21	b	1235	CLA	C1C-NC	-2.24	1.34	1.37
21	1	1131	CLA	C1C-NC	-2.24	1.34	1.37
21	2	1226	CLA	C1C-NC	-2.24	1.34	1.37
21	B	1229	CLA	MG-NC	2.24	2.11	2.06
21	2	1220	CLA	C3B-C2B	-2.24	1.37	1.40
21	0	1503	CLA	C3B-C2B	-2.24	1.37	1.40
21	a	1136	CLA	C1A-CHA	2.24	1.52	1.43
21	b	1203	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1216	CLA	C1D-C2D	2.24	1.47	1.42
21	1	1121	CLA	C1C-NC	-2.24	1.34	1.37
21	2	1021	CLA	MG-NC	2.24	2.11	2.06
21	A	1113	CLA	C1C-NC	-2.24	1.34	1.37
21	A	1104	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1217	CLA	C1C-NC	-2.24	1.34	1.37
21	b	1235	CLA	C1D-C2D	2.24	1.47	1.42
21	a	1106	CLA	C3B-C2B	-2.24	1.37	1.40
21	1	1013	CLA	MG-NC	2.24	2.11	2.06
21	2	1218	CLA	C1C-NC	-2.24	1.34	1.37
21	l	1502	CLA	MG-NC	2.24	2.11	2.06
21	a	1132	CLA	C1C-NC	-2.23	1.34	1.37
21	2	1203	CLA	C3B-C2B	-2.23	1.37	1.40
21	b	1227	CLA	C1C-NC	-2.23	1.34	1.37
21	b	1226	CLA	C1C-NC	-2.23	1.34	1.37
21	A	1120	CLA	MG-NC	2.23	2.11	2.06
21	B	1022	CLA	C1C-NC	-2.23	1.34	1.37
21	b	1214	CLA	C1C-NC	-2.23	1.34	1.37
21	6	1302	CLA	C1C-NC	-2.23	1.34	1.37
21	l	1502	CLA	C1C-NC	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1213	CLA	MG-NC	2.23	2.11	2.06
21	a	1106	CLA	C1C-NC	-2.23	1.34	1.37
21	2	1205	CLA	MG-NC	2.23	2.11	2.06
21	B	1222	CLA	C1C-C2C	2.23	1.48	1.44
21	a	1125	CLA	C3B-C2B	-2.23	1.37	1.40
21	b	1220	CLA	MG-NC	2.23	2.11	2.06
21	a	1107	CLA	C1D-C2D	2.23	1.47	1.42
21	b	1215	CLA	MG-NC	2.23	2.11	2.06
21	A	1138	CLA	MG-NC	2.22	2.11	2.06
21	b	1210	CLA	C1C-NC	-2.22	1.34	1.37
21	2	1204	CLA	C3B-C2B	-2.22	1.37	1.40
21	B	1221	CLA	C1C-NC	-2.22	1.34	1.37
21	b	1222	CLA	C1D-C2D	2.22	1.47	1.42
21	1	1136	CLA	C1D-C2D	2.22	1.47	1.42
21	2	1207	CLA	MG-NC	2.22	2.11	2.06
21	B	1231	CLA	C3B-C2B	-2.22	1.37	1.40
21	2	1217	CLA	C1C-NC	-2.22	1.34	1.37
21	b	1231	CLA	C1D-C2D	2.22	1.47	1.42
21	1	1119	CLA	MG-NC	2.22	2.11	2.06
26	A	5002	LMG	O1-C1	2.22	1.44	1.40
21	A	1101	CLA	C1C-NC	-2.22	1.34	1.37
21	b	1021	CLA	C1C-NC	-2.22	1.34	1.37
21	B	1226	CLA	C1C-C2C	2.22	1.48	1.44
21	b	1204	CLA	C1D-C2D	2.22	1.47	1.42
21	b	1230	CLA	MG-NC	2.22	2.11	2.06
21	1	1123	CLA	C1C-NC	-2.22	1.34	1.37
21	2	1023	CLA	C1A-CHA	2.22	1.52	1.43
21	b	1206	CLA	C3B-C2B	-2.22	1.37	1.40
21	B	1222	CLA	MG-NC	2.22	2.11	2.06
21	A	1110	CLA	C1D-C2D	2.22	1.47	1.42
21	2	1237	CLA	C3B-C2B	-2.22	1.37	1.40
21	B	1210	CLA	C3B-C2B	-2.21	1.37	1.40
21	a	1103	CLA	MG-NC	2.21	2.11	2.06
21	1	1119	CLA	C1D-C2D	2.21	1.47	1.42
35	L	6001	LMT	O2'-C2'	-2.21	1.37	1.43
35	1	6001	LMT	O2'-C2'	-2.21	1.37	1.43
21	b	1229	CLA	MG-NC	2.21	2.11	2.06
21	1	1103	CLA	MG-NC	2.21	2.11	2.06
21	A	1130	CLA	MG-NC	2.21	2.11	2.06
35	1	6001	LMT	O2B-C2B	-2.21	1.37	1.43
21	2	1229	CLA	MG-NC	2.21	2.11	2.06
21	B	1202	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1135	CLA	C1C-NC	-2.21	1.34	1.37
21	a	1118	CLA	C1C-NC	-2.21	1.34	1.37
21	a	1103	CLA	C1D-C2D	2.21	1.47	1.42
21	A	1112	CLA	C1A-CHA	2.20	1.52	1.43
21	A	1138	CLA	C1D-C2D	2.20	1.47	1.42
35	1	6001	LMT	O3B-C3B	-2.20	1.37	1.43
21	a	1120	CLA	C3B-C2B	-2.20	1.37	1.40
21	a	1134	CLA	C1D-C2D	2.20	1.47	1.42
21	A	1113	CLA	C1D-C2D	2.20	1.47	1.42
21	A	1120	CLA	C1D-C2D	2.20	1.47	1.42
21	J	1302	CLA	C1A-CHA	2.20	1.52	1.43
21	1	1114	CLA	C3B-C2B	-2.20	1.37	1.40
21	b	1023	CLA	C1A-CHA	2.20	1.52	1.43
21	b	1235	CLA	C3B-C2B	-2.20	1.37	1.40
21	1	1011	CLA	C1A-CHA	2.20	1.52	1.43
21	2	1232	CLA	C1A-CHA	2.20	1.52	1.43
21	1	1129	CLA	C3B-C2B	-2.20	1.37	1.40
21	a	1123	CLA	C1A-CHA	2.20	1.52	1.43
21	b	1211	CLA	C1C-NC	-2.20	1.34	1.37
21	a	1135	CLA	C1D-C2D	2.20	1.47	1.42
21	a	1101	CLA	C1C-NC	-2.20	1.34	1.37
21	b	1203	CLA	C3B-C2B	-2.19	1.37	1.40
35	0	6001	LMT	O3B-C3B	-2.19	1.37	1.43
21	1	1139	CLA	C1C-NC	-2.19	1.34	1.37
21	b	1236	CLA	C1D-C2D	2.19	1.47	1.42
21	b	1220	CLA	C1A-CHA	2.19	1.52	1.43
21	1	1123	CLA	C3B-C2B	-2.19	1.37	1.40
21	A	1132	CLA	C1C-NC	-2.19	1.34	1.37
21	b	1208	CLA	C3B-C2B	-2.19	1.37	1.40
21	b	1212	CLA	MG-NC	2.19	2.11	2.06
21	A	1134	CLA	C1C-NC	-2.19	1.34	1.37
21	1	1120	CLA	C1A-CHA	2.19	1.52	1.43
21	J	1303	CLA	C3B-C2B	-2.19	1.37	1.40
21	a	1138	CLA	C1A-CHA	2.19	1.52	1.43
21	1	1128	CLA	C1C-NC	-2.18	1.34	1.37
35	1	6001	LMT	O2B-C2B	-2.18	1.37	1.43
21	b	1201	CLA	C1D-C2D	2.18	1.47	1.42
21	B	1206	CLA	C3B-C2B	-2.18	1.37	1.40
21	A	1120	CLA	C1C-NC	-2.18	1.34	1.37
21	a	1011	CLA	C1A-CHA	2.18	1.52	1.43
21	B	1213	CLA	C1A-CHA	2.18	1.52	1.43
21	B	1217	CLA	C1A-CHA	2.18	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1209	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1012	CLA	C1C-NC	-2.18	1.34	1.37
21	A	1119	CLA	MG-NC	2.18	2.11	2.06
21	1	1117	CLA	C1D-C2D	2.18	1.47	1.42
21	B	1204	CLA	C1D-C2D	2.18	1.47	1.42
21	1	1502	CLA	C3B-C2B	-2.17	1.37	1.40
21	2	1205	CLA	C1D-C2D	2.17	1.47	1.42
21	2	1201	CLA	C1A-CHA	2.17	1.52	1.43
21	A	1110	CLA	MG-NC	2.17	2.11	2.06
21	1	1112	CLA	C1A-CHA	2.17	1.52	1.43
28	B	4011	45D	O01-C17	-2.17	1.18	1.23
21	b	1213	CLA	C1D-C2D	2.17	1.47	1.42
21	k	1401	CLA	C1A-CHA	2.17	1.52	1.43
21	A	1129	CLA	C1C-NC	-2.17	1.34	1.37
35	L	6001	LMT	O2B-C2B	-2.17	1.37	1.43
21	1	1102	CLA	C1A-CHA	2.17	1.52	1.43
21	2	1206	CLA	C1A-CHA	2.17	1.52	1.43
21	2	1214	CLA	C3B-C2B	-2.16	1.37	1.40
21	1	1012	CLA	C1A-CHA	2.16	1.52	1.43
21	1	1132	CLA	C1C-NC	-2.16	1.34	1.37
35	1	6001	LMT	O2'-C2'	-2.16	1.37	1.43
21	2	1207	CLA	C1A-CHA	2.16	1.52	1.43
21	7	1303	CLA	C1A-CHA	2.16	1.52	1.43
21	b	1202	CLA	C1D-C2D	2.16	1.47	1.42
21	B	1238	CLA	C1D-C2D	2.16	1.47	1.42
21	a	1801	CLA	C3B-C2B	-2.16	1.37	1.40
21	B	1239	CLA	C1A-CHA	2.16	1.52	1.43
21	A	1131	CLA	MG-NC	2.16	2.11	2.06
21	L	1501	CLA	C1A-CHA	2.16	1.52	1.43
21	b	1240	CLA	C1A-CHA	2.16	1.52	1.43
21	a	1112	CLA	C1A-CHA	2.16	1.52	1.43
21	a	1130	CLA	C3B-C2B	-2.16	1.37	1.40
21	A	1140	CLA	MG-NC	2.16	2.11	2.06
21	A	1012	CLA	C1A-CHA	2.16	1.52	1.43
21	1	1122	CLA	C1D-C2D	2.16	1.47	1.42
21	2	1235	CLA	C3B-C2B	-2.16	1.37	1.40
21	b	1226	CLA	MG-NC	2.16	2.11	2.06
21	2	1215	CLA	C3B-C2B	-2.16	1.37	1.40
21	b	1222	CLA	C1C-NC	-2.16	1.34	1.37
21	A	1122	CLA	C1D-C2D	2.16	1.47	1.42
21	2	1212	CLA	C1A-CHA	2.16	1.52	1.43
21	2	1201	CLA	C1D-C2D	2.16	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1136	CLA	C1C-NC	-2.15	1.34	1.37
21	6	1301	CLA	C1D-C2D	2.15	1.47	1.42
21	b	1201	CLA	C3B-C2B	-2.15	1.37	1.40
21	1	1132	CLA	C3B-C2B	-2.15	1.37	1.40
26	a	5004	LMG	O1-C1	2.15	1.43	1.40
21	j	1302	CLA	C1A-CHA	2.15	1.52	1.43
21	b	1202	CLA	MG-NC	2.15	2.11	2.06
21	2	1221	CLA	C1C-NC	-2.15	1.34	1.37
21	a	1102	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1206	CLA	C1A-CHA	2.15	1.52	1.43
21	a	1122	CLA	C3B-C2B	-2.15	1.37	1.40
21	b	1232	CLA	C3B-C2B	-2.15	1.37	1.40
21	A	1117	CLA	C1D-C2D	2.15	1.47	1.42
21	A	1106	CLA	MG-NC	2.15	2.11	2.06
21	7	1302	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1203	CLA	C1C-NC	-2.14	1.34	1.37
21	1	1111	CLA	C1A-CHA	2.14	1.52	1.43
21	1	1140	CLA	C1D-C2D	2.14	1.47	1.42
30	B	4006	ECH	C25-C26	-2.14	1.32	1.35
21	7	1303	CLA	C1D-C2D	2.14	1.47	1.42
21	b	1218	CLA	C1C-NC	-2.14	1.34	1.37
21	a	1109	CLA	C1A-CHA	2.14	1.52	1.43
21	a	1108	CLA	C1A-CHA	2.14	1.52	1.43
21	1	1110	CLA	C1A-CHA	2.14	1.52	1.43
21	2	1228	CLA	C1A-CHA	2.14	1.52	1.43
21	2	1204	CLA	C1D-C2D	2.14	1.47	1.42
21	1	1121	CLA	C1D-C2D	2.14	1.47	1.42
21	b	1220	CLA	C3B-C2B	-2.14	1.37	1.40
21	a	1103	CLA	C3B-C2B	-2.14	1.37	1.40
21	A	1108	CLA	C3B-C2B	-2.14	1.37	1.40
21	a	1801	CLA	C1A-CHA	2.14	1.52	1.43
21	a	1012	CLA	C1A-CHA	2.14	1.52	1.43
21	b	1218	CLA	C1A-CHA	2.14	1.52	1.43
21	1	1138	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1211	CLA	C1A-CHA	2.14	1.52	1.43
21	2	1206	CLA	C1D-C2D	2.14	1.47	1.42
21	2	1203	CLA	C1D-C2D	2.14	1.47	1.42
21	1	1113	CLA	C1A-CHA	2.13	1.52	1.43
21	a	1122	CLA	C1A-CHA	2.13	1.52	1.43
21	a	1134	CLA	C1A-CHA	2.13	1.52	1.43
21	b	1226	CLA	C1D-C2D	2.13	1.47	1.42
21	B	1210	CLA	C1A-CHA	2.13	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1217	CLA	C1A-CHA	2.13	1.52	1.43
21	1	1137	CLA	C1D-C2D	2.13	1.47	1.42
21	a	1125	CLA	C1A-CHA	2.13	1.51	1.43
21	1	1136	CLA	C1C-NC	-2.13	1.34	1.37
21	2	1239	CLA	C1A-CHA	2.13	1.51	1.43
35	1	6001	LMT	O3B-C3B	-2.13	1.38	1.43
21	2	1228	CLA	MG-NC	2.13	2.11	2.06
21	2	1216	CLA	C1C-NC	-2.13	1.34	1.37
21	1	1113	CLA	C1D-C2D	2.13	1.47	1.42
21	b	1206	CLA	C1A-CHA	2.13	1.51	1.43
21	A	1115	CLA	C3B-C2B	-2.13	1.37	1.40
21	B	1209	CLA	C1A-CHA	2.13	1.51	1.43
21	f	1301	CLA	C1D-C2D	2.13	1.47	1.42
21	2	1227	CLA	C1A-CHA	2.13	1.51	1.43
21	A	1140	CLA	C1D-C2D	2.13	1.47	1.42
21	1	1109	CLA	C1C-NC	-2.13	1.34	1.37
21	2	1220	CLA	C1A-CHA	2.13	1.51	1.43
21	1	1124	CLA	C1C-NC	-2.12	1.34	1.37
21	A	1011	CLA	C1D-C2D	2.12	1.47	1.42
21	b	1023	CLA	C1D-C2D	2.12	1.47	1.42
22	b	2002	PQN	C9-C10	-2.12	1.36	1.39
21	B	1214	CLA	C1D-C2D	2.12	1.47	1.42
21	a	1112	CLA	C3B-C2B	-2.12	1.37	1.40
21	B	1214	CLA	C1A-CHA	2.12	1.51	1.43
21	b	1228	CLA	C1A-CHA	2.12	1.51	1.43
21	b	1222	CLA	MG-NC	2.12	2.11	2.06
21	1	1801	CLA	C3B-C2B	-2.12	1.37	1.40
21	a	1116	CLA	C1A-CHA	2.12	1.51	1.43
21	a	1124	CLA	C1A-CHA	2.12	1.51	1.43
21	a	1124	CLA	C3B-C2B	-2.12	1.37	1.40
21	B	1216	CLA	C1A-CHA	2.12	1.51	1.43
21	1	1122	CLA	C1A-CHA	2.12	1.51	1.43
21	2	1202	CLA	C1A-CHA	2.12	1.51	1.43
21	B	1204	CLA	C3B-C2B	-2.12	1.37	1.40
21	b	1207	CLA	C1A-CHA	2.12	1.51	1.43
21	A	1138	CLA	C1A-CHA	2.12	1.51	1.43
21	a	1133	CLA	C1D-C2D	2.12	1.47	1.42
21	A	1134	CLA	C1D-C2D	2.12	1.47	1.42
21	b	1217	CLA	C1D-C2D	2.12	1.47	1.42
21	2	1222	CLA	C1C-NC	-2.11	1.34	1.37
21	1	1134	CLA	C1D-C2D	2.11	1.47	1.42
21	a	1121	CLA	C1A-CHA	2.11	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1211	CLA	C1D-C2D	2.11	1.47	1.42
21	1	1125	CLA	C1A-CHA	2.11	1.51	1.43
21	a	1120	CLA	C1A-CHA	2.11	1.51	1.43
21	J	1303	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1108	CLA	C1D-C2D	2.11	1.47	1.42
21	7	1302	CLA	C1D-C2D	2.11	1.47	1.42
21	b	1213	CLA	C3B-C2B	-2.11	1.37	1.40
21	1	1123	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1121	CLA	C1A-CHA	2.11	1.51	1.43
21	1	1120	CLA	C3B-C2B	-2.11	1.37	1.40
35	L	6001	LMT	O4'-C4B	-2.11	1.38	1.43
21	b	1022	CLA	C1D-C2D	2.11	1.47	1.42
21	B	1221	CLA	C1D-C2D	2.11	1.47	1.42
21	k	1402	CLA	C1A-CHA	2.11	1.51	1.43
21	B	1231	CLA	C1D-C2D	2.11	1.47	1.42
21	1	1105	CLA	C1D-C2D	2.11	1.47	1.42
21	a	1110	CLA	C1A-CHA	2.11	1.51	1.43
21	B	1023	CLA	C1A-CHA	2.11	1.51	1.43
21	0	1501	CLA	C3B-C2B	-2.11	1.37	1.40
21	1	1109	CLA	C1A-CHA	2.10	1.51	1.43
21	b	1230	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1023	CLA	MG-NC	2.10	2.11	2.06
21	b	1228	CLA	C1D-C2D	2.10	1.47	1.42
21	0	1503	CLA	C1D-C2D	2.10	1.47	1.42
21	B	1220	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1213	CLA	C1A-CHA	2.10	1.51	1.43
21	a	1139	CLA	C1D-C2D	2.10	1.47	1.42
21	a	1013	CLA	MG-NC	2.10	2.11	2.06
21	2	1217	CLA	C1A-CHA	2.10	1.51	1.43
21	a	1111	CLA	C1A-CHA	2.10	1.51	1.43
21	B	1208	CLA	C1D-C2D	2.10	1.47	1.42
21	a	1122	CLA	C1D-C2D	2.10	1.47	1.42
21	b	1210	CLA	C1A-CHA	2.10	1.51	1.43
21	B	1022	CLA	C3B-C2B	-2.10	1.37	1.40
21	1	1112	CLA	C1D-C2D	2.10	1.47	1.42
21	B	1023	CLA	C3B-C2B	-2.10	1.37	1.40
21	B	1217	CLA	C1D-C2D	2.10	1.47	1.42
21	A	1135	CLA	C1D-C2D	2.10	1.47	1.42
21	2	1223	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1227	CLA	C1D-C2D	2.10	1.47	1.42
21	2	1239	CLA	C1D-C2D	2.10	1.47	1.42
21	2	1221	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1215	CLA	C1A-CHA	2.10	1.51	1.43
21	2	1216	CLA	C3B-C2B	-2.10	1.37	1.40
21	A	1123	CLA	C3B-C2B	-2.10	1.37	1.40
21	A	1137	CLA	C1A-CHA	2.10	1.51	1.43
21	l	1501	CLA	C1D-C2D	2.10	1.47	1.42
21	1	1139	CLA	C1A-CHA	2.09	1.51	1.43
21	1	1109	CLA	C1D-C2D	2.09	1.47	1.42
21	L	1503	CLA	C3B-C2B	-2.09	1.37	1.40
21	1	1127	CLA	C1A-CHA	2.09	1.51	1.43
21	A	1134	CLA	C1A-CHA	2.09	1.51	1.43
21	b	1239	CLA	C1D-C2D	2.09	1.47	1.42
21	A	1013	CLA	C1D-C2D	2.09	1.47	1.42
21	A	1108	CLA	C1D-C2D	2.09	1.47	1.42
21	A	1133	CLA	C1C-NC	-2.09	1.34	1.37
21	A	1114	CLA	C1D-C2D	2.09	1.47	1.42
21	A	1117	CLA	C3B-C2B	-2.09	1.37	1.40
21	1	1103	CLA	C1D-C2D	2.09	1.47	1.42
21	6	1302	CLA	C1D-C2D	2.09	1.47	1.42
21	B	1232	CLA	C1A-CHA	2.09	1.51	1.43
30	2	4006	ECH	C1-C6	-2.09	1.50	1.53
21	B	1201	CLA	C3B-C2B	-2.09	1.37	1.40
21	A	1133	CLA	MG-NC	2.09	2.11	2.06
21	1	1101	CLA	C1A-CHA	2.09	1.51	1.43
21	a	1130	CLA	C1A-CHA	2.09	1.51	1.43
21	a	1101	CLA	C1A-CHA	2.09	1.51	1.43
21	B	1215	CLA	C1A-CHA	2.09	1.51	1.43
21	B	1218	CLA	C1D-C2D	2.09	1.47	1.42
21	A	1116	CLA	C1D-C2D	2.08	1.47	1.42
21	1	1110	CLA	C1D-C2D	2.08	1.47	1.42
21	2	1240	CLA	C1D-C2D	2.08	1.47	1.42
21	A	1102	CLA	C1D-C2D	2.08	1.47	1.42
21	2	1231	CLA	C1A-CHA	2.08	1.51	1.43
21	K	1402	CLA	C1D-C2D	2.08	1.47	1.42
21	2	1229	CLA	C1D-C2D	2.08	1.47	1.42
21	1	1115	CLA	C1D-C2D	2.08	1.47	1.42
21	a	1121	CLA	C1D-C2D	2.08	1.47	1.42
21	k	1402	CLA	C1D-C2D	2.08	1.47	1.42
21	2	1232	CLA	C1D-C2D	2.08	1.47	1.42
21	2	1225	CLA	C1D-C2D	2.08	1.47	1.42
21	1	1133	CLA	C1A-CHA	2.08	1.51	1.43
21	b	1232	CLA	C1D-C2D	2.08	1.47	1.42
21	k	1401	CLA	C3B-C2B	-2.08	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1021	CLA	C3B-C2B	-2.08	1.37	1.40
21	l	1501	CLA	C1A-CHA	2.08	1.51	1.43
21	B	1021	CLA	C1A-CHA	2.08	1.51	1.43
21	B	1223	CLA	C1A-CHA	2.08	1.51	1.43
21	b	1213	CLA	C1A-CHA	2.08	1.51	1.43
21	0	1501	CLA	C1D-C2D	2.08	1.47	1.42
21	b	1221	CLA	C1D-C2D	2.08	1.47	1.42
21	1	1118	CLA	C1A-CHA	2.08	1.51	1.43
21	a	1139	CLA	C1A-CHA	2.08	1.51	1.43
21	B	1203	CLA	C1A-CHA	2.08	1.51	1.43
21	8	1402	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1131	CLA	C1D-C2D	2.08	1.47	1.42
21	F	1302	CLA	C1A-CHA	2.08	1.51	1.43
21	F	1301	CLA	C1A-CHA	2.08	1.51	1.43
21	1	1801	CLA	C1A-CHA	2.08	1.51	1.43
21	2	1224	CLA	C1D-C2D	2.08	1.47	1.42
21	1	1111	CLA	C1D-C2D	2.07	1.47	1.42
21	b	1210	CLA	C1D-C2D	2.07	1.47	1.42
21	b	1224	CLA	C1A-CHA	2.07	1.51	1.43
21	J	1303	CLA	C1D-C2D	2.07	1.47	1.42
28	h	4020	45D	O01-C17	-2.07	1.18	1.23
30	b	4011	ECH	C1-C6	-2.07	1.50	1.53
21	B	1218	CLA	C1A-CHA	2.07	1.51	1.43
21	a	1801	CLA	C1D-C2D	2.07	1.47	1.42
21	a	1104	CLA	C1A-CHA	2.07	1.51	1.43
21	A	1102	CLA	C1A-CHA	2.07	1.51	1.43
21	A	1013	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1201	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1227	CLA	C3B-C2B	-2.07	1.37	1.40
21	1	1104	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1212	CLA	C1D-C2D	2.07	1.47	1.42
21	b	1227	CLA	C1D-C2D	2.07	1.47	1.42
21	a	1137	CLA	C1A-CHA	2.07	1.51	1.43
21	a	1117	CLA	C1A-CHA	2.07	1.51	1.43
21	2	1222	CLA	C1D-C2D	2.07	1.47	1.42
21	2	1235	CLA	C1A-CHA	2.07	1.51	1.43
21	2	1230	CLA	C1A-CHA	2.07	1.51	1.43
21	2	1203	CLA	C1A-CHA	2.07	1.51	1.43
21	1	1104	CLA	C3B-C2B	-2.07	1.37	1.40
21	A	1122	CLA	C1A-CHA	2.07	1.51	1.43
21	2	1234	CLA	C1A-CHA	2.07	1.51	1.43
21	B	1228	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1224	CLA	C1D-C2D	2.07	1.47	1.42
21	B	1240	CLA	C1A-CHA	2.06	1.51	1.43
21	1	1114	CLA	C1D-C2D	2.06	1.47	1.42
35	L	6001	LMT	O3B-C3B	-2.06	1.38	1.43
21	2	1208	CLA	C1D-C2D	2.06	1.47	1.42
21	6	1301	CLA	C3B-C2B	-2.06	1.37	1.40
21	2	1220	CLA	C1D-C2D	2.06	1.47	1.42
21	b	1222	CLA	C3B-C2B	-2.06	1.37	1.40
21	b	1212	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1139	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1114	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1129	CLA	C1D-C2D	2.06	1.47	1.42
21	A	1111	CLA	C1A-CHA	2.06	1.51	1.43
21	2	1021	CLA	C1A-CHA	2.06	1.51	1.43
21	1	1130	CLA	C1A-CHA	2.06	1.51	1.43
21	b	1221	CLA	C1A-CHA	2.06	1.51	1.43
21	B	1201	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1114	CLA	C1D-C2D	2.06	1.47	1.42
21	1	1126	CLA	C1A-CHA	2.06	1.51	1.43
21	b	1210	CLA	C3B-C2B	-2.06	1.37	1.40
21	b	1231	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1108	CLA	C1A-CHA	2.06	1.51	1.43
21	B	1213	CLA	C1D-C2D	2.06	1.47	1.42
21	b	1224	CLA	C1D-C2D	2.06	1.47	1.42
21	B	1202	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1119	CLA	C1D-C2D	2.06	1.47	1.42
21	A	1136	CLA	C1A-CHA	2.06	1.51	1.43
21	A	1801	CLA	C1A-CHA	2.06	1.51	1.43
21	B	1222	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1127	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1106	CLA	C1A-CHA	2.06	1.51	1.43
21	2	1213	CLA	C1D-C2D	2.06	1.47	1.42
21	1	1106	CLA	C1D-C2D	2.06	1.47	1.42
21	1	1123	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1117	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1126	CLA	C1A-CHA	2.06	1.51	1.43
21	8	1401	CLA	C1A-CHA	2.06	1.51	1.43
21	a	1101	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1105	CLA	C1D-C2D	2.06	1.47	1.42
21	8	1401	CLA	C1D-C2D	2.06	1.47	1.42
21	B	1021	CLA	C3B-C2B	-2.06	1.37	1.40
21	A	1104	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1209	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1137	CLA	C1D-C2D	2.06	1.47	1.42
21	a	1118	CLA	C3B-C2B	-2.06	1.37	1.40
21	2	1237	CLA	C1D-C2D	2.06	1.47	1.42
21	A	1128	CLA	C1D-C2D	2.06	1.47	1.42
21	f	1302	CLA	C1A-CHA	2.05	1.51	1.43
21	a	1111	CLA	C1D-C2D	2.05	1.47	1.42
21	b	1238	CLA	C1D-C2D	2.05	1.47	1.42
21	b	1216	CLA	C1A-CHA	2.05	1.51	1.43
21	a	1106	CLA	C1D-C2D	2.05	1.47	1.42
21	2	1212	CLA	C1D-C2D	2.05	1.47	1.42
21	a	1131	CLA	C1D-C2D	2.05	1.47	1.42
21	B	1224	CLA	C3B-C2B	-2.05	1.37	1.40
21	B	1212	CLA	C1A-CHA	2.05	1.51	1.43
21	b	1232	CLA	C1A-CHA	2.05	1.51	1.43
21	1	1116	CLA	C1D-C2D	2.05	1.47	1.42
21	1	1124	CLA	C1D-C2D	2.05	1.47	1.42
21	a	1120	CLA	C1D-C2D	2.05	1.47	1.42
21	2	1221	CLA	C1D-C2D	2.05	1.47	1.42
21	2	1211	CLA	C1A-CHA	2.05	1.51	1.43
26	K	5009	LMG	O1-C1	2.05	1.43	1.40
21	1	1801	CLA	C1D-C2D	2.05	1.47	1.42
21	B	1232	CLA	C1D-C2D	2.05	1.47	1.42
21	K	1402	CLA	C1A-CHA	2.05	1.51	1.43
21	2	1235	CLA	C1D-C2D	2.05	1.47	1.42
21	a	1129	CLA	C1D-C2D	2.05	1.47	1.42
35	F	6001	LMT	O4'-C4B	-2.05	1.38	1.43
21	1	1134	CLA	C1A-CHA	2.05	1.51	1.43
21	j	1303	CLA	C1A-CHA	2.05	1.51	1.43
21	A	1127	CLA	C1A-CHA	2.05	1.51	1.43
21	2	1228	CLA	C1D-C2D	2.05	1.47	1.42
21	A	1130	CLA	C1A-CHA	2.05	1.51	1.43
21	1	1131	CLA	C1D-C2D	2.05	1.47	1.42
21	a	1113	CLA	C1A-CHA	2.05	1.51	1.43
21	1	1132	CLA	C1D-C2D	2.04	1.47	1.42
21	A	1107	CLA	C3B-C2B	-2.04	1.37	1.40
21	B	1218	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	1118	CLA	C3B-C2B	-2.04	1.37	1.40
21	2	1240	CLA	C1A-CHA	2.04	1.51	1.43
21	1	1124	CLA	C1A-CHA	2.04	1.51	1.43
21	B	1213	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	1135	CLA	C3B-C2B	-2.04	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1226	CLA	C1D-C2D	2.04	1.47	1.42
21	B	1230	CLA	C1D-C2D	2.04	1.47	1.42
21	l	1503	CLA	C1D-C2D	2.04	1.47	1.42
21	1	1104	CLA	C1D-C2D	2.04	1.47	1.42
21	B	1231	CLA	C1A-CHA	2.04	1.51	1.43
21	A	1101	CLA	C1D-C2D	2.04	1.47	1.42
21	A	1105	CLA	C1D-C2D	2.04	1.47	1.42
21	1	1103	CLA	C1A-CHA	2.04	1.51	1.43
21	a	1131	CLA	C1A-CHA	2.04	1.51	1.43
21	1	1130	CLA	C1D-C2D	2.04	1.47	1.42
21	a	1136	CLA	C1D-C2D	2.04	1.47	1.42
21	a	1013	CLA	C1A-CHA	2.04	1.51	1.43
21	2	1218	CLA	C1A-CHA	2.04	1.51	1.43
21	1	1114	CLA	C1A-CHA	2.04	1.51	1.43
21	b	1223	CLA	C1A-CHA	2.04	1.51	1.43
21	2	1210	CLA	C1D-C2D	2.04	1.47	1.42
21	2	1209	CLA	C1D-C2D	2.04	1.47	1.42
21	A	1118	CLA	C1A-CHA	2.04	1.51	1.43
21	a	1121	CLA	C3B-C2B	-2.04	1.37	1.40
21	1	1138	CLA	C1D-C2D	2.04	1.47	1.42
21	1	1105	CLA	C1A-CHA	2.04	1.51	1.43
21	B	1221	CLA	C1A-CHA	2.04	1.51	1.43
21	a	1013	CLA	C3B-C2B	-2.04	1.37	1.40
21	b	1211	CLA	C3B-C2B	-2.03	1.37	1.40
21	1	1124	CLA	C3B-C2B	-2.03	1.37	1.40
21	a	1127	CLA	C1D-C2D	2.03	1.47	1.42
21	B	1216	CLA	C1D-C2D	2.03	1.47	1.42
21	a	1110	CLA	C1D-C2D	2.03	1.47	1.42
21	b	1219	CLA	C1D-C2D	2.03	1.47	1.42
21	1	1101	CLA	C1D-C2D	2.03	1.47	1.42
21	0	1502	CLA	C3B-C2B	-2.03	1.37	1.40
21	2	1210	CLA	C1A-CHA	2.03	1.51	1.43
21	a	1119	CLA	C3B-C2B	-2.03	1.37	1.40
21	1	1139	CLA	C1D-C2D	2.03	1.47	1.42
21	a	1140	CLA	C1D-C2D	2.03	1.47	1.42
21	2	1218	CLA	C1D-C2D	2.03	1.47	1.42
21	b	1225	CLA	C1D-C2D	2.03	1.47	1.42
21	2	1022	CLA	C1D-C2D	2.03	1.47	1.42
21	2	1226	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1103	CLA	MG-NC	2.03	2.11	2.06
21	2	1214	CLA	C1A-CHA	2.03	1.51	1.43
21	a	1113	CLA	C3B-C2B	-2.03	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	1303	CLA	C1D-C2D	2.03	1.47	1.42
21	b	1203	CLA	C1A-CHA	2.03	1.51	1.43
21	A	1140	CLA	C1A-CHA	2.03	1.51	1.43
21	B	1215	CLA	C1D-C2D	2.03	1.47	1.42
21	1	1107	CLA	C3B-C2B	-2.03	1.37	1.40
21	2	1211	CLA	C3B-C2B	-2.03	1.37	1.40
21	A	1011	CLA	C3B-C2B	-2.03	1.37	1.40
21	B	1240	CLA	C1D-C2D	2.03	1.47	1.42
21	2	1211	CLA	C1D-C2D	2.03	1.47	1.42
21	b	1231	CLA	C3B-C2B	-2.03	1.37	1.40
21	2	1231	CLA	C1D-C2D	2.02	1.47	1.42
21	2	1234	CLA	C1D-C2D	2.02	1.47	1.42
21	b	1215	CLA	C1D-C2D	2.02	1.47	1.42
21	A	1130	CLA	C1D-C2D	2.02	1.47	1.42
21	A	1133	CLA	C1D-C2D	2.02	1.47	1.42
21	b	1021	CLA	C1A-CHA	2.02	1.51	1.43
21	B	1235	CLA	C1A-CHA	2.02	1.51	1.43
21	1	1103	CLA	C3B-C2B	-2.02	1.37	1.40
21	1	1116	CLA	C1A-CHA	2.02	1.51	1.43
21	a	1113	CLA	C1D-C2D	2.02	1.47	1.42
21	B	1229	CLA	C1A-CHA	2.02	1.51	1.43
21	A	1103	CLA	C3B-C2B	-2.02	1.37	1.40
21	f	1302	CLA	C1D-C2D	2.02	1.47	1.42
21	1	1125	CLA	C3B-C2B	-2.02	1.37	1.40
21	2	1224	CLA	C1A-CHA	2.02	1.51	1.43
21	1	1108	CLA	C1A-CHA	2.02	1.51	1.43
21	A	1129	CLA	C1A-CHA	2.02	1.51	1.43
21	a	1140	CLA	C3B-C2B	-2.02	1.37	1.40
21	1	1102	CLA	C1D-C2D	2.02	1.47	1.42
21	a	1108	CLA	C1D-C2D	2.02	1.47	1.42
21	b	1209	CLA	C3B-C2B	-2.02	1.37	1.40
21	A	1137	CLA	MG-NC	2.02	2.11	2.06
21	a	1107	CLA	C1A-CHA	2.02	1.51	1.43
21	L	1503	CLA	C1D-C2D	2.02	1.47	1.42
21	b	1224	CLA	C3B-C2B	-2.02	1.37	1.40
21	A	1101	CLA	C1A-CHA	2.02	1.51	1.43
21	a	1102	CLA	C1D-C2D	2.02	1.47	1.42
21	A	1013	CLA	MG-NC	2.02	2.11	2.06
21	a	1128	CLA	C1A-CHA	2.02	1.51	1.43
21	2	1205	CLA	C1A-CHA	2.02	1.51	1.43
21	B	1237	CLA	C1D-C2D	2.02	1.47	1.42
21	B	1202	CLA	C1A-CHA	2.02	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	1133	CLA	C1A-CHA	2.02	1.51	1.43
21	0	1501	CLA	C1A-CHA	2.02	1.51	1.43
21	A	1116	CLA	C1A-CHA	2.01	1.51	1.43
21	B	1234	CLA	C1A-CHA	2.01	1.51	1.43
21	1	1135	CLA	C3B-C2B	-2.01	1.37	1.40
21	A	1013	CLA	C3B-C2B	-2.01	1.37	1.40
21	a	1123	CLA	C1D-C2D	2.01	1.47	1.42
21	A	1137	CLA	C1D-C2D	2.01	1.47	1.42
21	6	1301	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1240	CLA	C3B-C2B	-2.01	1.37	1.40
28	h	4020	45D	C23-C19	2.01	1.39	1.33
21	2	1214	CLA	C1D-C2D	2.01	1.47	1.42
21	b	1229	CLA	C1D-C2D	2.01	1.47	1.42
21	2	1219	CLA	C1A-CHA	2.01	1.51	1.43
21	B	1225	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1214	CLA	C1D-C2D	2.01	1.47	1.42
21	A	1109	CLA	C1A-CHA	2.01	1.51	1.43
21	a	1112	CLA	C1D-C2D	2.01	1.47	1.42
21	A	1135	CLA	C1A-CHA	2.01	1.51	1.43
21	a	1118	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1239	CLA	C1A-CHA	2.01	1.51	1.43
21	1	1137	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1211	CLA	C1A-CHA	2.01	1.51	1.43
21	1	1128	CLA	C1D-C2D	2.01	1.47	1.42
21	2	1023	CLA	C1D-C2D	2.00	1.47	1.42
21	1	1122	CLA	C3B-C2B	-2.00	1.37	1.40
21	B	1236	CLA	C1A-CHA	2.00	1.51	1.43
21	b	1023	CLA	MG-NC	2.00	2.11	2.06
21	2	1236	CLA	C1A-CHA	2.00	1.51	1.43
21	a	1130	CLA	C1D-C2D	2.00	1.47	1.42
21	2	1216	CLA	C1A-CHA	2.00	1.51	1.43
21	b	1215	CLA	C1A-CHA	2.00	1.51	1.43
21	L	1503	CLA	C1A-CHA	2.00	1.51	1.43
21	A	1113	CLA	C1A-CHA	2.00	1.51	1.43
21	1	1121	CLA	C3B-C2B	-2.00	1.37	1.40
21	1	1128	CLA	C1A-CHA	2.00	1.51	1.43
21	F	1301	CLA	C1D-C2D	2.00	1.47	1.42
21	A	1139	CLA	C1D-C2D	2.00	1.47	1.42
26	1	5002	LMG	C22-C21	-2.00	1.33	1.49
21	2	1215	CLA	C1D-C2D	2.00	1.47	1.42
21	B	1230	CLA	C1A-CHA	2.00	1.51	1.43
21	B	1227	CLA	C1A-CHA	2.00	1.51	1.43

All (3060) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	4016	ZEX	C38-C24-C25	-50.09	31.10	110.87
34	J	4015	ZEX	C38-C24-C25	-49.79	31.58	110.87
34	j	4015	ZEX	C38-C24-C25	-49.78	31.59	110.87
34	7	4015	ZEX	C38-C24-C25	-49.71	31.71	110.87
24	a	4019	BCR	C16-C15-C14	16.68	157.64	123.47
24	b	4018	BCR	C16-C15-C14	16.24	156.75	123.47
24	a	4002	BCR	C16-C15-C14	15.53	155.29	123.47
24	1	4019	BCR	C16-C15-C14	15.42	155.06	123.47
24	i	4018	BCR	C16-C15-C14	14.93	154.06	123.47
24	a	4001	BCR	C16-C15-C14	14.82	153.83	123.47
24	A	4019	BCR	C16-C15-C14	14.62	153.42	123.47
24	h	4018	BCR	C16-C15-C14	14.37	152.91	123.47
24	2	4005	BCR	C16-C15-C14	14.28	152.73	123.47
24	9	4021	BCR	C16-C15-C14	14.23	152.63	123.47
24	2	4018	BCR	C11-C10-C9	14.19	147.57	127.31
24	1	4007	BCR	C16-C15-C14	14.10	152.36	123.47
24	B	4018	BCR	C16-C15-C14	14.08	152.32	123.47
24	2	4010	BCR	C16-C15-C14	14.08	152.32	123.47
24	a	4008	BCR	C16-C15-C14	14.06	152.28	123.47
24	A	4019	BCR	C11-C10-C9	14.06	147.38	127.31
24	1	4001	BCR	C16-C15-C14	13.84	151.83	123.47
24	B	4005	BCR	C16-C15-C14	13.74	151.62	123.47
24	8	4001	BCR	C16-C15-C14	13.71	151.55	123.47
24	1	4002	BCR	C16-C15-C14	13.62	151.38	123.47
24	a	4003	BCR	C16-C15-C14	13.62	151.38	123.47
24	1	4012	BCR	C16-C15-C14	13.49	151.11	123.47
24	1	4008	BCR	C16-C15-C14	13.39	150.90	123.47
24	b	4010	BCR	C21-C20-C19	13.37	164.93	123.22
24	b	4017	BCR	C16-C15-C14	13.36	150.83	123.47
24	2	4010	BCR	C21-C20-C19	13.26	164.61	123.22
24	2	4014	BCR	C21-C20-C19	13.22	164.48	123.22
24	2	4010	BCR	C11-C10-C9	13.20	146.15	127.31
24	1	4002	BCR	C21-C20-C19	13.19	164.37	123.22
24	1	4003	BCR	C16-C15-C14	13.14	150.40	123.47
24	B	4017	BCR	C11-C10-C9	13.08	145.98	127.31
24	k	4001	BCR	C16-C15-C14	13.05	150.21	123.47
24	B	4004	BCR	C16-C15-C14	13.05	150.20	123.47
24	0	4022	BCR	C21-C20-C19	13.03	163.88	123.22
24	1	4003	BCR	C21-C20-C19	13.02	163.86	123.22
24	B	4017	BCR	C16-C15-C14	12.99	150.07	123.47
24	2	4014	BCR	C11-C10-C9	12.96	145.81	127.31
24	6	4016	BCR	C11-C10-C9	12.96	145.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	4022	BCR	C11-C10-C9	12.96	145.81	127.31
24	2	4017	BCR	C11-C10-C9	12.95	145.79	127.31
24	B	4018	BCR	C21-C20-C19	12.92	163.53	123.22
24	2	4004	BCR	C16-C15-C14	12.92	149.93	123.47
24	j	4013	BCR	C21-C20-C19	12.84	163.28	123.22
24	b	4014	BCR	C21-C20-C19	12.80	163.16	123.22
24	K	4001	BCR	C16-C15-C14	12.79	149.68	123.47
24	A	4003	BCR	C21-C20-C19	12.76	163.04	123.22
24	b	4017	BCR	C11-C10-C9	12.74	145.50	127.31
24	2	4004	BCR	C21-C20-C19	12.72	162.92	123.22
24	8	4001	BCR	C21-C20-C19	12.72	162.90	123.22
24	a	4012	BCR	C16-C15-C14	12.70	149.49	123.47
24	b	4004	BCR	C11-C10-C9	12.65	145.36	127.31
24	l	4022	BCR	C21-C20-C19	12.58	162.49	123.22
24	6	4016	BCR	C16-C15-C14	12.57	149.22	123.47
24	A	4012	BCR	C21-C20-C19	12.53	162.33	123.22
24	7	4013	BCR	C21-C20-C19	12.50	162.22	123.22
24	A	4001	BCR	C21-C20-C19	12.49	162.20	123.22
24	B	4014	BCR	C21-C20-C19	12.48	162.17	123.22
24	l	4022	BCR	C11-C10-C9	12.44	145.06	127.31
24	J	4013	BCR	C16-C15-C14	12.43	148.94	123.47
24	6	4016	BCR	C21-C20-C19	12.40	161.91	123.22
24	a	4019	BCR	C11-C10-C9	12.39	145.00	127.31
24	a	4002	BCR	C11-C10-C9	12.37	144.96	127.31
24	B	4010	BCR	C21-C20-C19	12.33	161.68	123.22
24	B	4004	BCR	C21-C20-C19	12.32	161.66	123.22
24	f	4016	BCR	C21-C20-C19	12.31	161.62	123.22
24	0	4019	BCR	C16-C15-C14	12.26	148.60	123.47
24	7	4013	BCR	C16-C15-C14	12.24	148.56	123.47
24	1	4019	BCR	C21-C20-C19	12.22	161.36	123.22
24	a	4007	BCR	C21-C20-C19	12.19	161.27	123.22
24	9	4021	BCR	C11-C10-C9	12.14	144.64	127.31
24	2	4017	BCR	C16-C15-C14	12.13	148.32	123.47
24	b	4005	BCR	C16-C15-C14	12.11	148.28	123.47
24	1	4012	BCR	C21-C20-C19	12.06	160.85	123.22
24	J	4013	BCR	C11-C10-C9	12.05	144.50	127.31
24	b	4010	BCR	C16-C15-C14	12.04	148.14	123.47
24	b	4004	BCR	C21-C20-C19	12.03	160.77	123.22
24	a	4001	BCR	C21-C20-C19	12.02	160.72	123.22
24	i	4018	BCR	C11-C10-C9	12.02	144.46	127.31
24	1	4001	BCR	C11-C10-C9	12.02	144.46	127.31
24	b	4014	BCR	C11-C10-C9	12.00	144.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	4005	BCR	C11-C10-C9	11.93	144.33	127.31
24	1	4008	BCR	C21-C20-C19	11.91	160.39	123.22
24	B	4010	BCR	C16-C15-C14	11.91	147.86	123.47
24	f	4016	BCR	C11-C10-C9	11.89	144.28	127.31
24	7	4013	BCR	C11-C10-C9	11.89	144.28	127.31
21	b	1023	CLA	C4A-NA-C1A	11.84	112.03	106.71
24	2	4018	BCR	C16-C15-C14	11.82	147.68	123.47
24	B	4014	BCR	C11-C10-C9	11.81	144.17	127.31
24	A	4001	BCR	C16-C15-C14	11.76	147.56	123.47
24	A	4019	BCR	C21-C20-C19	11.75	159.90	123.22
24	b	4004	BCR	C16-C15-C14	11.74	147.53	123.47
24	I	4018	BCR	C16-C15-C14	11.74	147.53	123.47
24	b	4005	BCR	C11-C10-C9	11.74	144.06	127.31
24	a	4003	BCR	C21-C20-C19	11.73	159.81	123.22
24	B	4010	BCR	C11-C10-C9	11.63	143.91	127.31
24	k	4001	BCR	C21-C20-C19	11.62	159.47	123.22
24	a	4008	BCR	C11-C10-C9	11.56	143.81	127.31
24	a	4001	BCR	C11-C10-C9	11.56	143.80	127.31
24	B	4018	BCR	C11-C10-C9	11.55	143.80	127.31
21	A	1011	CLA	C4A-NA-C1A	11.55	111.90	106.71
24	h	4018	BCR	C11-C10-C9	11.54	143.78	127.31
21	a	1011	CLA	C4A-NA-C1A	11.54	111.89	106.71
21	2	1023	CLA	C4A-NA-C1A	11.54	111.89	106.71
24	j	4013	BCR	C11-C10-C9	11.53	143.76	127.31
24	a	4002	BCR	C21-C20-C19	11.52	159.17	123.22
24	l	4022	BCR	C16-C15-C14	11.50	147.04	123.47
24	A	4002	BCR	C16-C15-C14	11.48	147.00	123.47
24	a	4007	BCR	C16-C15-C14	11.48	147.00	123.47
24	A	4008	BCR	C21-C20-C19	11.48	159.04	123.22
24	j	4013	BCR	C16-C15-C14	11.47	146.98	123.47
24	L	4022	BCR	C16-C15-C14	11.47	146.97	123.47
24	a	4003	BCR	C11-C10-C9	11.46	143.67	127.31
24	A	4003	BCR	C16-C15-C14	11.42	146.86	123.47
24	2	4004	BCR	C11-C10-C9	11.40	143.58	127.31
24	1	4007	BCR	C21-C20-C19	11.39	158.76	123.22
24	J	4013	BCR	C21-C20-C19	11.37	158.71	123.22
24	A	4012	BCR	C16-C15-C14	11.34	146.71	123.47
21	6	1302	CLA	C4A-NA-C1A	11.33	111.80	106.71
24	f	4016	BCR	C16-C15-C14	11.33	146.68	123.47
24	2	4014	BCR	C16-C15-C14	11.33	146.67	123.47
24	1	4001	BCR	C21-C20-C19	11.31	158.52	123.22
21	a	1109	CLA	C4A-NA-C1A	11.29	111.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4002	BCR	C21-C20-C19	11.29	158.45	123.22
24	L	4022	BCR	C21-C20-C19	11.29	158.44	123.22
24	l	4019	BCR	C21-C20-C19	11.28	158.41	123.22
21	a	1126	CLA	C4A-NA-C1A	11.27	111.77	106.71
24	2	4005	BCR	C21-C20-C19	11.25	158.31	123.22
21	2	1201	CLA	C4A-NA-C1A	11.24	111.76	106.71
24	L	4022	BCR	C11-C10-C9	11.23	143.34	127.31
24	I	4018	BCR	C11-C10-C9	11.21	143.31	127.31
21	1	1012	CLA	C4A-NA-C1A	11.19	111.74	106.71
21	1	1013	CLA	C4A-NA-C1A	11.19	111.74	106.71
24	b	4014	BCR	C16-C15-C14	11.17	146.35	123.47
21	J	1302	CLA	C4A-NA-C1A	11.13	111.71	106.71
24	K	4001	BCR	C21-C20-C19	11.09	157.84	123.22
21	B	1235	CLA	C4A-NA-C1A	11.09	111.69	106.71
21	B	1021	CLA	C4A-NA-C1A	11.08	111.69	106.71
21	1	1011	CLA	C4A-NA-C1A	11.07	111.68	106.71
24	A	4003	BCR	C11-C10-C9	11.04	143.06	127.31
24	a	4012	BCR	C21-C20-C19	11.02	157.62	123.22
24	b	4018	BCR	C21-C20-C19	11.01	157.56	123.22
24	2	4011	BCR	C21-C20-C19	10.97	157.46	123.22
21	b	1202	CLA	C4A-NA-C1A	10.96	111.63	106.71
24	0	4019	BCR	C21-C20-C19	10.95	157.40	123.22
24	1	4003	BCR	C11-C10-C9	10.93	142.91	127.31
21	b	1230	CLA	C4A-NA-C1A	10.93	111.62	106.71
24	h	4018	BCR	C20-C19-C18	10.89	157.01	126.42
21	a	1102	CLA	C4A-NA-C1A	10.86	111.59	106.71
21	A	1112	CLA	C4A-NA-C1A	10.86	111.59	106.71
21	B	1023	CLA	C4A-NA-C1A	10.85	111.59	106.71
24	k	4001	BCR	C11-C10-C9	10.84	142.79	127.31
24	I	4018	BCR	C20-C19-C18	10.84	156.86	126.42
24	A	4007	BCR	C16-C15-C14	10.83	145.67	123.47
21	1	1103	CLA	C4A-NA-C1A	10.81	111.57	106.71
21	a	1013	CLA	C4A-NA-C1A	10.79	111.56	106.71
24	1	4007	BCR	C11-C10-C9	10.79	142.70	127.31
21	1	1112	CLA	C4A-NA-C1A	10.79	111.56	106.71
21	b	1221	CLA	C4A-NA-C1A	10.77	111.55	106.71
24	1	4012	BCR	C11-C10-C9	10.76	142.66	127.31
21	2	1213	CLA	C4A-NA-C1A	10.73	111.53	106.71
21	B	1217	CLA	C4A-NA-C1A	10.73	111.53	106.71
21	a	1112	CLA	C4A-NA-C1A	10.73	111.53	106.71
24	B	4005	BCR	C21-C20-C19	10.72	156.68	123.22
21	B	1207	CLA	C4A-NA-C1A	10.72	111.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	j	1302	CLA	C4A-NA-C1A	10.71	111.52	106.71
21	b	1231	CLA	C4A-NA-C1A	10.69	111.51	106.71
24	l	4019	BCR	C16-C15-C14	10.69	145.38	123.47
24	L	4019	BCR	C21-C20-C19	10.69	156.58	123.22
24	A	4008	BCR	C16-C15-C14	10.69	145.37	123.47
21	2	1216	CLA	C4A-NA-C1A	10.68	111.51	106.71
21	1	1119	CLA	C4A-NA-C1A	10.66	111.50	106.71
21	2	1232	CLA	C4A-NA-C1A	10.66	111.50	106.71
24	A	4007	BCR	C21-C20-C19	10.66	156.49	123.22
21	A	1123	CLA	C4A-NA-C1A	10.65	111.49	106.71
21	a	1106	CLA	C4A-NA-C1A	10.64	111.49	106.71
21	B	1203	CLA	C4A-NA-C1A	10.63	111.49	106.71
21	1	1126	CLA	C4A-NA-C1A	10.63	111.49	106.71
24	A	4002	BCR	C11-C10-C9	10.63	142.48	127.31
21	a	1122	CLA	C4A-NA-C1A	10.61	111.48	106.71
21	2	1021	CLA	C4A-NA-C1A	10.61	111.48	106.71
21	A	1139	CLA	C4A-NA-C1A	10.60	111.47	106.71
21	2	1212	CLA	C4A-NA-C1A	10.58	111.46	106.71
21	A	1108	CLA	C4A-NA-C1A	10.58	111.46	106.71
21	2	1206	CLA	C4A-NA-C1A	10.57	111.46	106.71
21	2	1205	CLA	C4A-NA-C1A	10.57	111.46	106.71
21	b	1207	CLA	C4A-NA-C1A	10.57	111.46	106.71
24	B	4004	BCR	C11-C10-C9	10.55	142.37	127.31
21	J	1303	CLA	C4A-NA-C1A	10.55	111.45	106.71
21	k	1402	CLA	C4A-NA-C1A	10.55	111.45	106.71
24	l	4019	BCR	C11-C10-C9	10.55	142.36	127.31
24	a	4008	BCR	C21-C20-C19	10.55	156.13	123.22
24	K	4001	BCR	C11-C10-C9	10.54	142.36	127.31
21	B	1211	CLA	C4A-NA-C1A	10.53	111.44	106.71
21	a	1801	CLA	C4A-NA-C1A	10.52	111.43	106.71
21	B	1229	CLA	C4A-NA-C1A	10.51	111.43	106.71
24	i	4018	BCR	C20-C19-C18	10.51	155.95	126.42
21	1	1139	CLA	C4A-NA-C1A	10.51	111.43	106.71
24	A	4012	BCR	C11-C10-C9	10.50	142.30	127.31
21	a	1138	CLA	C4A-NA-C1A	10.50	111.43	106.71
24	B	4005	BCR	C11-C10-C9	10.50	142.29	127.31
21	b	1211	CLA	C4A-NA-C1A	10.49	111.42	106.71
21	7	1302	CLA	C4A-NA-C1A	10.49	111.42	106.71
21	A	1126	CLA	C4A-NA-C1A	10.47	111.42	106.71
21	1	1133	CLA	C4A-NA-C1A	10.47	111.41	106.71
21	2	1223	CLA	C4A-NA-C1A	10.43	111.39	106.71
21	2	1022	CLA	C4A-NA-C1A	10.41	111.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1224	CLA	C4A-NA-C1A	10.41	111.39	106.71
21	b	1240	CLA	C4A-NA-C1A	10.39	111.38	106.71
24	1	4008	BCR	C11-C10-C9	10.39	142.13	127.31
21	a	1108	CLA	C4A-NA-C1A	10.37	111.37	106.71
21	A	1111	CLA	C4A-NA-C1A	10.37	111.37	106.71
21	2	1228	CLA	C4A-NA-C1A	10.36	111.36	106.71
24	0	4019	BCR	C11-C10-C9	10.36	142.09	127.31
21	b	1021	CLA	C4A-NA-C1A	10.35	111.36	106.71
21	B	1206	CLA	C4A-NA-C1A	10.35	111.36	106.71
21	B	1215	CLA	C4A-NA-C1A	10.34	111.35	106.71
21	1	1125	CLA	C4A-NA-C1A	10.34	111.35	106.71
21	k	1401	CLA	C4A-NA-C1A	10.33	111.35	106.71
21	a	1103	CLA	C4A-NA-C1A	10.33	111.35	106.71
21	b	1206	CLA	C4A-NA-C1A	10.33	111.35	106.71
21	1	1102	CLA	C4A-NA-C1A	10.32	111.35	106.71
21	b	1220	CLA	C4A-NA-C1A	10.31	111.34	106.71
21	1	1109	CLA	C4A-NA-C1A	10.31	111.34	106.71
24	b	4005	BCR	C21-C20-C19	10.31	155.38	123.22
21	1	1501	CLA	C4A-NA-C1A	10.30	111.34	106.71
21	A	1103	CLA	C4A-NA-C1A	10.29	111.33	106.71
21	A	1102	CLA	C4A-NA-C1A	10.28	111.33	106.71
24	0	4022	BCR	C16-C15-C14	10.28	144.52	123.47
21	A	1012	CLA	C4A-NA-C1A	10.27	111.33	106.71
24	2	4011	BCR	C16-C15-C14	10.27	144.51	123.47
21	1	1118	CLA	C4A-NA-C1A	10.26	111.32	106.71
21	2	1235	CLA	C4A-NA-C1A	10.26	111.32	106.71
21	7	1303	CLA	C4A-NA-C1A	10.25	111.32	106.71
28	h	4020	45D	C42-C38-C36	-10.25	112.69	127.31
21	A	1107	CLA	C4A-NA-C1A	10.24	111.31	106.71
21	A	1138	CLA	C4A-NA-C1A	10.23	111.31	106.71
21	2	1224	CLA	C4A-NA-C1A	10.23	111.31	106.71
24	a	4007	BCR	C11-C10-C9	10.23	141.91	127.31
21	1	1110	CLA	C4A-NA-C1A	10.23	111.30	106.71
21	B	1232	CLA	C4A-NA-C1A	10.22	111.30	106.71
21	B	1205	CLA	C4A-NA-C1A	10.21	111.30	106.71
21	a	1134	CLA	C4A-NA-C1A	10.20	111.29	106.71
21	b	1201	CLA	C4A-NA-C1A	10.20	111.29	106.71
21	2	1209	CLA	C4A-NA-C1A	10.20	111.29	106.71
21	B	1202	CLA	C4A-NA-C1A	10.19	111.29	106.71
21	2	1202	CLA	C4A-NA-C1A	10.19	111.28	106.71
21	B	1222	CLA	C4A-NA-C1A	10.18	111.28	106.71
21	1	1134	CLA	C4A-NA-C1A	10.17	111.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	1501	CLA	C4A-NA-C1A	10.16	111.27	106.71
21	1	1104	CLA	C4A-NA-C1A	10.15	111.27	106.71
21	a	1115	CLA	C4A-NA-C1A	10.14	111.27	106.71
21	a	1124	CLA	C4A-NA-C1A	10.14	111.26	106.71
21	b	1228	CLA	C4A-NA-C1A	10.13	111.26	106.71
21	B	1230	CLA	C4A-NA-C1A	10.12	111.26	106.71
21	2	1240	CLA	C4A-NA-C1A	10.12	111.25	106.71
21	a	1136	CLA	C4A-NA-C1A	10.12	111.25	106.71
21	B	1224	CLA	C4A-NA-C1A	10.11	111.25	106.71
24	a	4019	BCR	C21-C20-C19	10.11	154.78	123.22
21	A	1121	CLA	C4A-NA-C1A	10.11	111.25	106.71
21	2	1222	CLA	C4A-NA-C1A	10.11	111.25	106.71
21	b	1213	CLA	C4A-NA-C1A	10.10	111.25	106.71
24	2	4011	BCR	C11-C10-C9	10.09	141.71	127.31
21	2	1230	CLA	C4A-NA-C1A	10.09	111.24	106.71
21	B	1209	CLA	C4A-NA-C1A	10.08	111.24	106.71
21	B	1221	CLA	C4A-NA-C1A	10.08	111.24	106.71
21	1	1113	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	2	1207	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	a	1139	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	a	1125	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	a	1012	CLA	C4A-NA-C1A	10.07	111.23	106.71
21	B	1231	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	1	1116	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	2	1239	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	2	1234	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	A	1134	CLA	C4A-NA-C1A	10.05	111.22	106.71
21	B	1218	CLA	C4A-NA-C1A	10.05	111.22	106.71
21	B	1220	CLA	C4A-NA-C1A	10.04	111.22	106.71
21	8	1402	CLA	C4A-NA-C1A	10.04	111.22	106.71
21	2	1221	CLA	C4A-NA-C1A	10.02	111.21	106.71
21	b	1216	CLA	C4A-NA-C1A	10.00	111.20	106.71
21	A	1115	CLA	C4A-NA-C1A	10.00	111.20	106.71
21	2	1217	CLA	C4A-NA-C1A	10.00	111.20	106.71
21	A	1013	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	b	1232	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	a	1128	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	2	1231	CLA	C4A-NA-C1A	9.99	111.20	106.71
21	2	1211	CLA	C4A-NA-C1A	9.99	111.20	106.71
24	B	4014	BCR	C16-C15-C14	9.99	143.93	123.47
21	a	1104	CLA	C4A-NA-C1A	9.98	111.19	106.71
21	1	1108	CLA	C4A-NA-C1A	9.98	111.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1239	CLA	C4A-NA-C1A	9.98	111.19	106.71
21	1	1122	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	a	1111	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	1	1106	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	2	1226	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	1	1120	CLA	C4A-NA-C1A	9.96	111.19	106.71
24	8	4001	BCR	C11-C10-C9	9.95	141.52	127.31
21	A	1104	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	a	1120	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	b	1236	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	1	1121	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	b	1218	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	a	1110	CLA	C4A-NA-C1A	9.95	111.18	106.71
21	b	1209	CLA	C4A-NA-C1A	9.94	111.18	106.71
21	8	1401	CLA	C4A-NA-C1A	9.94	111.18	106.71
21	A	1109	CLA	C4A-NA-C1A	9.94	111.18	106.71
21	a	1130	CLA	C4A-NA-C1A	9.94	111.17	106.71
21	B	1239	CLA	C4A-NA-C1A	9.94	111.17	106.71
21	F	1302	CLA	C4A-NA-C1A	9.93	111.17	106.71
21	2	1210	CLA	C4A-NA-C1A	9.93	111.17	106.71
21	2	1220	CLA	C4A-NA-C1A	9.92	111.17	106.71
30	2	4006	ECH	C16-C17-C18	-9.92	113.15	127.31
21	F	1301	CLA	C4A-NA-C1A	9.91	111.16	106.71
21	A	1140	CLA	C4A-NA-C1A	9.91	111.16	106.71
21	a	1101	CLA	C4A-NA-C1A	9.90	111.16	106.71
21	A	1801	CLA	C4A-NA-C1A	9.90	111.16	106.71
21	b	1022	CLA	C4A-NA-C1A	9.90	111.16	106.71
21	a	1113	CLA	C4A-NA-C1A	9.89	111.15	106.71
21	1	1131	CLA	C4A-NA-C1A	9.89	111.15	106.71
21	b	1227	CLA	C4A-NA-C1A	9.89	111.15	106.71
21	2	1204	CLA	C4A-NA-C1A	9.89	111.15	106.71
21	b	1203	CLA	C4A-NA-C1A	9.87	111.14	106.71
21	L	1502	CLA	C4A-NA-C1A	9.87	111.14	106.71
21	a	1131	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	0	1502	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	B	1216	CLA	C4A-NA-C1A	9.85	111.14	106.71
30	i	4020	ECH	C15-C14-C13	-9.84	113.26	127.31
21	B	1223	CLA	C4A-NA-C1A	9.84	111.13	106.71
21	b	1222	CLA	C4A-NA-C1A	9.84	111.13	106.71
21	a	1116	CLA	C4A-NA-C1A	9.83	111.13	106.71
21	b	1208	CLA	C4A-NA-C1A	9.83	111.12	106.71
21	2	1227	CLA	C4A-NA-C1A	9.82	111.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1137	CLA	C4A-NA-C1A	9.82	111.12	106.71
21	a	1123	CLA	C4A-NA-C1A	9.81	111.12	106.71
21	B	1022	CLA	C4A-NA-C1A	9.81	111.12	106.71
21	a	1114	CLA	C4A-NA-C1A	9.80	111.11	106.71
21	1	1101	CLA	C4A-NA-C1A	9.79	111.11	106.71
21	2	1229	CLA	C4A-NA-C1A	9.79	111.11	106.71
21	b	1210	CLA	C4A-NA-C1A	9.78	111.11	106.71
21	B	1201	CLA	C4A-NA-C1A	9.78	111.10	106.71
21	1	1801	CLA	C4A-NA-C1A	9.78	111.10	106.71
28	h	4020	45D	C24-C26-C30	-9.77	103.94	118.94
21	B	1228	CLA	C4A-NA-C1A	9.77	111.10	106.71
21	1	1132	CLA	C4A-NA-C1A	9.77	111.10	106.71
21	2	1219	CLA	C4A-NA-C1A	9.77	111.10	106.71
21	a	1107	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	2	1215	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	a	1117	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	1	1111	CLA	C4A-NA-C1A	9.75	111.09	106.71
21	a	1121	CLA	C4A-NA-C1A	9.74	111.09	106.71
21	a	1140	CLA	C4A-NA-C1A	9.74	111.09	106.71
21	A	1125	CLA	C4A-NA-C1A	9.74	111.09	106.71
24	b	4017	BCR	C21-C20-C19	9.73	153.57	123.22
21	b	1223	CLA	C4A-NA-C1A	9.72	111.08	106.71
21	b	1235	CLA	C4A-NA-C1A	9.72	111.08	106.71
21	A	1116	CLA	C4A-NA-C1A	9.72	111.07	106.71
21	B	1225	CLA	C4A-NA-C1A	9.72	111.07	106.71
21	1	1117	CLA	C4A-NA-C1A	9.71	111.07	106.71
21	L	1503	CLA	C4A-NA-C1A	9.70	111.07	106.71
21	f	1302	CLA	C4A-NA-C1A	9.70	111.07	106.71
21	B	1213	CLA	C4A-NA-C1A	9.70	111.07	106.71
21	A	1110	CLA	C4A-NA-C1A	9.70	111.07	106.71
21	A	1137	CLA	C4A-NA-C1A	9.70	111.07	106.71
21	1	1115	CLA	C4A-NA-C1A	9.69	111.06	106.71
21	B	1234	CLA	C4A-NA-C1A	9.68	111.06	106.71
21	B	1210	CLA	C4A-NA-C1A	9.67	111.05	106.71
21	B	1227	CLA	C4A-NA-C1A	9.67	111.05	106.71
21	B	1237	CLA	C4A-NA-C1A	9.67	111.05	106.71
21	2	1203	CLA	C4A-NA-C1A	9.66	111.05	106.71
21	a	1132	CLA	C4A-NA-C1A	9.65	111.05	106.71
21	1	1136	CLA	C4A-NA-C1A	9.64	111.04	106.71
21	a	1137	CLA	C4A-NA-C1A	9.64	111.04	106.71
21	A	1130	CLA	C4A-NA-C1A	9.61	111.03	106.71
21	1	1107	CLA	C4A-NA-C1A	9.61	111.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1106	CLA	C4A-NA-C1A	9.60	111.02	106.71
24	2	4017	BCR	C21-C20-C19	9.60	153.17	123.22
21	1	1138	CLA	C4A-NA-C1A	9.60	111.02	106.71
21	B	1240	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	a	1105	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	0	1501	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	2	1218	CLA	C4A-NA-C1A	9.59	111.02	106.71
21	1	1105	CLA	C4A-NA-C1A	9.58	111.02	106.71
21	B	1226	CLA	C4A-NA-C1A	9.58	111.01	106.71
21	1	1130	CLA	C4A-NA-C1A	9.58	111.01	106.71
21	2	1208	CLA	C4A-NA-C1A	9.57	111.01	106.71
24	1	4002	BCR	C11-C10-C9	9.57	140.96	127.31
21	1	1127	CLA	C4A-NA-C1A	9.55	111.00	106.71
21	b	1219	CLA	C4A-NA-C1A	9.54	111.00	106.71
21	1	1123	CLA	C4A-NA-C1A	9.53	110.99	106.71
21	a	1127	CLA	C4A-NA-C1A	9.53	110.99	106.71
24	B	4017	BCR	C21-C20-C19	9.52	152.91	123.22
21	a	1119	CLA	C4A-NA-C1A	9.51	110.98	106.71
21	2	1236	CLA	C4A-NA-C1A	9.50	110.98	106.71
21	l	1502	CLA	C4A-NA-C1A	9.49	110.97	106.71
21	K	1402	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	b	1217	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	1	1140	CLA	C4A-NA-C1A	9.47	110.97	106.71
21	A	1131	CLA	C4A-NA-C1A	9.45	110.95	106.71
24	b	4010	BCR	C11-C10-C9	9.45	140.79	127.31
21	a	1118	CLA	C4A-NA-C1A	9.44	110.95	106.71
21	B	1208	CLA	C4A-NA-C1A	9.44	110.95	106.71
21	A	1136	CLA	C4A-NA-C1A	9.44	110.95	106.71
21	b	1229	CLA	C4A-NA-C1A	9.43	110.94	106.71
21	B	1236	CLA	C4A-NA-C1A	9.43	110.94	106.71
21	0	1503	CLA	C4A-NA-C1A	9.43	110.94	106.71
21	B	1212	CLA	C4A-NA-C1A	9.42	110.94	106.71
21	1	1128	CLA	C4A-NA-C1A	9.42	110.94	106.71
21	A	1122	CLA	C4A-NA-C1A	9.42	110.94	106.71
21	b	1237	CLA	C4A-NA-C1A	9.42	110.94	106.71
21	j	1303	CLA	C4A-NA-C1A	9.42	110.94	106.71
21	B	1214	CLA	C4A-NA-C1A	9.41	110.94	106.71
21	A	1118	CLA	C4A-NA-C1A	9.41	110.94	106.71
21	1	1114	CLA	C4A-NA-C1A	9.41	110.94	106.71
21	b	1234	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	b	1215	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	b	1238	CLA	C4A-NA-C1A	9.39	110.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4001	BCR	C11-C10-C9	9.39	140.71	127.31
21	A	1124	CLA	C4A-NA-C1A	9.38	110.92	106.71
21	A	1128	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	K	1401	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	2	1237	CLA	C4A-NA-C1A	9.36	110.92	106.71
21	2	1225	CLA	C4A-NA-C1A	9.35	110.91	106.71
21	A	1114	CLA	C4A-NA-C1A	9.34	110.91	106.71
24	a	4012	BCR	C11-C10-C9	9.34	140.64	127.31
24	b	4018	BCR	C11-C10-C9	9.33	140.63	127.31
21	A	1129	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	A	1127	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	b	1214	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	b	1205	CLA	C4A-NA-C1A	9.32	110.90	106.71
21	A	1117	CLA	C4A-NA-C1A	9.32	110.89	106.71
24	2	4010	BCR	C20-C19-C18	9.32	152.59	126.42
21	b	1225	CLA	C4A-NA-C1A	9.30	110.89	106.71
21	B	1219	CLA	C4A-NA-C1A	9.30	110.89	106.71
24	i	4018	BCR	C21-C20-C19	9.30	152.22	123.22
21	A	1113	CLA	C4A-NA-C1A	9.29	110.88	106.71
24	2	4017	BCR	C20-C19-C18	9.29	152.50	126.42
21	a	1129	CLA	C4A-NA-C1A	9.28	110.88	106.71
21	b	1204	CLA	C4A-NA-C1A	9.26	110.87	106.71
21	f	1301	CLA	C4A-NA-C1A	9.24	110.86	106.71
21	A	1101	CLA	C4A-NA-C1A	9.23	110.86	106.71
21	6	1301	CLA	C4A-NA-C1A	9.23	110.86	106.71
21	A	1132	CLA	C4A-NA-C1A	9.22	110.85	106.71
21	A	1119	CLA	C4A-NA-C1A	9.21	110.84	106.71
24	2	4018	BCR	C21-C20-C19	9.20	151.93	123.22
30	B	4006	ECH	C16-C17-C18	-9.19	114.20	127.31
21	1	1135	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	a	1133	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	l	1503	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	2	1238	CLA	C4A-NA-C1A	9.16	110.83	106.71
24	h	4018	BCR	C21-C20-C19	9.16	151.80	123.22
24	b	4018	BCR	C20-C19-C18	9.14	152.09	126.42
21	1	1129	CLA	C4A-NA-C1A	9.11	110.80	106.71
24	L	4019	BCR	C11-C10-C9	9.11	140.31	127.31
21	A	1120	CLA	C4A-NA-C1A	9.11	110.80	106.71
24	9	4021	BCR	C21-C20-C19	9.06	151.50	123.22
21	1	1124	CLA	C4A-NA-C1A	9.04	110.77	106.71
21	A	1135	CLA	C4A-NA-C1A	9.00	110.75	106.71
24	b	4017	BCR	C20-C19-C18	8.94	151.54	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	4008	BCR	C20-C19-C18	8.92	151.49	126.42
21	A	1105	CLA	C4A-NA-C1A	8.89	110.70	106.71
24	L	4019	BCR	C16-C15-C14	8.88	141.66	123.47
24	2	4011	BCR	C20-C19-C18	8.88	151.35	126.42
24	B	4018	BCR	C20-C19-C18	8.87	151.33	126.42
24	1	4007	BCR	C20-C19-C18	8.86	151.31	126.42
24	A	4007	BCR	C11-C10-C9	8.84	139.92	127.31
24	a	4012	BCR	C20-C19-C18	8.82	151.19	126.42
24	B	4005	BCR	C20-C19-C18	8.81	151.17	126.42
30	b	4011	ECH	C15-C14-C13	-8.81	114.74	127.31
21	a	1135	CLA	C4A-NA-C1A	8.79	110.66	106.71
24	A	4008	BCR	C11-C10-C9	8.77	139.83	127.31
24	a	4002	BCR	C20-C19-C18	8.71	150.88	126.42
21	B	1204	CLA	C4A-NA-C1A	8.70	110.62	106.71
21	b	1212	CLA	C4A-NA-C1A	8.70	110.62	106.71
21	A	1133	CLA	C4A-NA-C1A	8.68	110.61	106.71
30	b	4006	ECH	C20-C21-C22	-8.67	114.94	127.31
24	A	4007	BCR	C20-C19-C18	8.65	150.71	126.42
24	0	4019	BCR	C20-C19-C18	8.64	150.68	126.42
24	B	4017	BCR	C20-C19-C18	8.61	150.60	126.42
21	2	1214	CLA	C4A-NA-C1A	8.61	110.58	106.71
21	B	1238	CLA	C4A-NA-C1A	8.59	110.57	106.71
24	1	4019	BCR	C11-C10-C9	8.49	139.43	127.31
24	2	4005	BCR	C20-C19-C18	8.46	150.19	126.42
24	A	4019	BCR	C20-C19-C18	8.44	150.13	126.42
24	b	4005	BCR	C20-C19-C18	8.43	150.10	126.42
21	b	1226	CLA	C4A-NA-C1A	8.43	110.50	106.71
24	a	4001	BCR	C20-C19-C18	8.32	149.78	126.42
28	h	4020	45D	C32-C34-C36	-8.28	103.16	126.42
24	L	4019	BCR	C20-C19-C18	8.22	149.50	126.42
24	l	4019	BCR	C20-C19-C18	8.07	149.09	126.42
24	1	4019	BCR	C20-C19-C18	8.03	148.99	126.42
34	F	4016	ZEX	C27-C26-C25	-8.03	109.86	122.84
24	K	4001	BCR	C20-C19-C18	8.01	148.91	126.42
24	a	4003	BCR	C20-C19-C18	7.99	148.87	126.42
24	1	4012	BCR	C20-C19-C18	7.99	148.87	126.42
24	J	4013	BCR	C20-C19-C18	7.96	148.79	126.42
24	k	4001	BCR	C20-C19-C18	7.91	148.65	126.42
24	I	4018	BCR	C21-C20-C19	7.89	147.84	123.22
24	6	4016	BCR	C20-C19-C18	7.85	148.47	126.42
24	A	4008	BCR	C20-C19-C18	7.81	148.37	126.42
24	A	4002	BCR	C20-C19-C18	7.79	148.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	4022	BCR	C20-C19-C18	7.73	148.14	126.42
24	1	4008	BCR	C20-C19-C18	7.64	147.87	126.42
24	A	4001	BCR	C20-C19-C18	7.62	147.82	126.42
24	B	4010	BCR	C20-C19-C18	7.58	147.70	126.42
24	f	4016	BCR	C20-C19-C18	7.58	147.70	126.42
24	a	4007	BCR	C20-C19-C18	7.49	147.45	126.42
34	j	4015	ZEX	C27-C26-C25	-7.49	110.73	122.84
24	1	4001	BCR	C20-C19-C18	7.45	147.33	126.42
30	2	4006	ECH	C24-C23-C22	-7.43	115.01	126.23
28	h	4020	45D	C32-C30-C26	7.39	137.86	127.31
24	8	4001	BCR	C20-C19-C18	7.34	147.02	126.42
24	b	4004	BCR	C20-C19-C18	7.19	146.62	126.42
24	2	4004	BCR	C20-C19-C18	7.17	146.57	126.42
24	A	4012	BCR	C20-C19-C18	7.15	146.50	126.42
24	B	4014	BCR	C20-C19-C18	7.09	146.33	126.42
24	l	4022	BCR	C20-C19-C18	7.03	146.17	126.42
21	b	1215	CLA	O2A-C1-C2	7.03	127.10	108.64
24	1	4003	BCR	C20-C19-C18	7.02	146.14	126.42
24	b	4014	BCR	C20-C19-C18	6.89	145.78	126.42
24	B	4004	BCR	C20-C19-C18	6.84	145.64	126.42
24	b	4010	BCR	C20-C19-C18	6.80	145.53	126.42
24	j	4013	BCR	C20-C19-C18	6.80	145.52	126.42
24	7	4013	BCR	C20-C19-C18	6.78	145.47	126.42
24	1	4002	BCR	C20-C19-C18	6.77	145.44	126.42
21	A	1128	CLA	O2A-C1-C2	6.77	126.42	108.64
34	7	4015	ZEX	C27-C26-C25	-6.70	112.01	122.84
24	2	4014	BCR	C20-C19-C18	6.69	145.21	126.42
24	A	4003	BCR	C20-C19-C18	6.64	145.07	126.42
21	B	1239	CLA	O2A-C1-C2	6.63	126.05	108.64
30	B	4006	ECH	C24-C23-C22	-6.60	116.26	126.23
28	h	4020	45D	C24-C20-C08	-6.48	109.00	127.20
34	J	4015	ZEX	C27-C26-C25	-6.40	112.50	122.84
24	a	4019	BCR	C20-C19-C18	6.36	144.29	126.42
21	A	1138	CLA	O2A-C1-C2	6.31	125.23	108.64
21	b	1239	CLA	O2A-C1-C2	6.31	125.21	108.64
21	1	1128	CLA	O2A-C1-C2	6.29	125.17	108.64
21	A	1135	CLA	O2A-C1-C2	6.27	125.11	108.64
28	B	4011	45D	C20-C24-C26	-6.25	116.79	126.23
21	2	1215	CLA	O2A-C1-C2	6.23	125.01	108.64
21	a	1125	CLA	O2A-C1-C2	6.20	124.94	108.64
21	2	1239	CLA	O2A-C1-C2	6.19	124.91	108.64
21	A	1130	CLA	O2A-C1-C2	6.18	124.88	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1011	CLA	C3D-CAD-CBD	-6.18	99.47	107.61
21	B	1206	CLA	O2A-C1-C2	6.14	124.78	108.64
30	i	4020	ECH	C7-C8-C9	-6.11	117.01	126.23
21	1	1012	CLA	O2A-C1-C2	6.10	124.66	108.64
30	b	4011	ECH	C20-C21-C22	-6.03	118.70	127.31
21	A	1107	CLA	O2A-C1-C2	6.01	124.43	108.64
34	F	4016	ZEX	C28-C27-C26	-5.99	116.86	127.09
21	1	1132	CLA	O2A-C1-C2	5.99	124.36	108.64
24	9	4021	BCR	C20-C19-C18	5.98	143.22	126.42
24	0	4022	BCR	C20-C19-C18	5.97	143.19	126.42
21	k	1402	CLA	O2A-C1-C2	5.97	122.93	108.97
21	A	1125	CLA	O2A-C1-C2	5.96	124.29	108.64
28	h	4020	45D	C28-C26-C24	5.91	127.38	118.08
28	B	4011	45D	C41-C37-C35	-5.87	118.94	127.31
21	B	1234	CLA	O2A-C1-C2	5.79	123.85	108.64
21	b	1231	CLA	O2A-C1-C2	5.79	123.84	108.64
21	1	1125	CLA	O2A-C1-C2	5.76	123.77	108.64
21	A	1111	CLA	O2A-C1-C2	5.70	123.62	108.64
21	B	1235	CLA	O2A-C1-C2	5.69	123.58	108.64
21	L	1503	CLA	O2A-C1-C2	5.67	123.55	108.64
21	b	1209	CLA	O2A-C1-C2	5.66	123.50	108.64
30	B	4006	ECH	C16-C15-C14	-5.65	111.89	123.47
21	A	1011	CLA	O2D-CGD-CBD	5.65	121.31	111.27
24	2	4018	BCR	C20-C19-C18	5.65	142.28	126.42
21	A	1120	CLA	O2A-C1-C2	5.65	123.47	108.64
21	a	1138	CLA	O2A-C1-C2	5.62	123.41	108.64
21	l	1503	CLA	O2A-C1-C2	5.61	123.38	108.64
21	B	1213	CLA	O2A-C1-C2	5.59	123.34	108.64
21	B	1231	CLA	O2A-C1-C2	5.59	123.32	108.64
21	a	1140	CLA	O2A-C1-C2	5.59	123.31	108.64
21	B	1216	CLA	O2A-C1-C2	5.58	123.29	108.64
28	h	4020	45D	C20-C24-C26	5.57	134.65	126.23
21	b	1225	CLA	O2A-C1-C2	5.56	123.24	108.64
21	1	1013	CLA	O2A-C1-C2	5.54	123.20	108.64
25	M	5001	LHG	O7-C7-C8	5.53	123.43	111.50
21	0	1503	CLA	O2A-C1-C2	5.53	123.17	108.64
21	a	1127	CLA	O2A-C1-C2	5.52	123.13	108.64
21	1	1112	CLA	O2A-C1-C2	5.51	123.13	108.64
21	2	1225	CLA	O2A-C1-C2	5.51	123.11	108.64
21	b	1220	CLA	O2A-C1-C2	5.51	123.11	108.64
21	1	1135	CLA	O2A-C1-C2	5.50	123.10	108.64
21	1	1138	CLA	O2A-C1-C2	5.49	123.05	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	I	4020	EQ3	C11-C10-C9	-5.48	119.48	127.31
30	B	4006	ECH	C11-C10-C9	-5.47	119.50	127.31
21	B	1023	CLA	O2A-C1-C2	5.47	123.02	108.64
21	A	1109	CLA	O2A-C1-C2	5.47	123.00	108.64
21	a	1101	CLA	O2A-C1-C2	5.46	122.98	108.64
21	b	1219	CLA	O2A-C1-C2	5.45	122.96	108.64
21	b	1234	CLA	O2A-C1-C2	5.45	122.95	108.64
28	B	4011	45D	C31-C29-C25	-5.44	119.54	127.31
21	a	1129	CLA	O2A-C1-C2	5.44	122.94	108.64
21	a	1107	CLA	O2A-C1-C2	5.44	122.94	108.64
21	a	1122	CLA	O2A-C1-C2	5.44	122.94	108.64
21	A	1012	CLA	O2A-C1-C2	5.44	122.93	108.64
21	2	1234	CLA	O2A-C1-C2	5.43	122.91	108.64
21	a	1114	CLA	O2A-C1-C2	5.42	122.88	108.64
21	K	1401	CLA	O2A-C1-C2	5.42	122.87	108.64
21	a	1135	CLA	O2A-C1-C2	5.41	122.85	108.64
21	1	1115	CLA	O2A-C1-C2	5.40	122.84	108.64
21	A	1106	CLA	O2A-C1-C2	5.40	122.82	108.64
21	a	1115	CLA	O2A-C1-C2	5.39	122.79	108.64
21	2	1235	CLA	O2A-C1-C2	5.38	122.78	108.64
21	a	1110	CLA	O2A-C1-C2	5.38	122.78	108.64
21	k	1401	CLA	O2A-C1-C2	5.38	122.77	108.64
21	b	1216	CLA	O2A-C1-C2	5.37	122.76	108.64
21	a	1126	CLA	O2A-C1-C2	5.37	122.76	108.64
21	1	1140	CLA	O2A-C1-C2	5.37	122.75	108.64
21	b	1235	CLA	O2A-C1-C2	5.37	122.75	108.64
21	A	1132	CLA	O2A-C1-C2	5.36	122.71	108.64
21	B	1225	CLA	O2A-C1-C2	5.36	122.71	108.64
21	A	1101	CLA	O2A-C1-C2	5.35	122.70	108.64
21	a	1134	CLA	O2A-C1-C2	5.33	121.44	108.97
21	B	1232	CLA	O2A-C1-C2	5.33	122.64	108.64
21	B	1209	CLA	O2A-C1-C2	5.32	122.62	108.64
21	a	1105	CLA	O2A-C1-C2	5.32	122.61	108.64
21	a	1120	CLA	O2A-C1-C2	5.32	122.61	108.64
21	2	1022	CLA	O2A-C1-C2	5.32	122.61	108.64
21	a	1106	CLA	O2A-C1-C2	5.32	122.61	108.64
21	f	1302	CLA	O2A-C1-C2	5.31	122.59	108.64
21	2	1218	CLA	O2A-C1-C2	5.30	122.57	108.64
21	1	1116	CLA	O2A-C1-C2	5.29	122.55	108.64
21	J	1302	CLA	O2A-C1-C2	5.28	122.50	108.64
36	I	4020	EQ3	C33-C5-C6	-5.28	118.60	124.53
21	1	1801	CLA	O2A-C1-C2	5.27	122.49	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1122	CLA	O2A-C1-C2	5.26	122.45	108.64
21	1	1111	CLA	O2A-C1-C2	5.25	122.44	108.64
21	a	1128	CLA	O2A-C1-C2	5.25	122.44	108.64
21	A	1112	CLA	O2A-C1-C2	5.25	122.42	108.64
21	b	1206	CLA	O2A-C1-C2	5.24	122.42	108.64
21	A	1104	CLA	O2A-C1-C2	5.24	122.41	108.64
21	A	1128	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
21	B	1236	CLA	O2A-C1-C2	5.23	122.38	108.64
21	1	1102	CLA	O2A-C1-C2	5.23	122.38	108.64
34	j	4015	ZEX	C7-C8-C9	-5.22	118.34	126.23
21	0	1502	CLA	O2A-C1-C2	5.22	122.36	108.64
21	a	1012	CLA	O2A-C1-C2	5.22	122.35	108.64
21	A	1115	CLA	O2A-C1-C2	5.21	122.34	108.64
21	a	1136	CLA	O2D-CGD-CBD	5.21	120.53	111.27
21	j	1303	CLA	O2A-C1-C2	5.21	122.32	108.64
21	l	1502	CLA	O2A-C1-C2	5.20	122.31	108.64
21	a	1112	CLA	O2A-C1-C2	5.20	122.30	108.64
21	A	1013	CLA	O2A-C1-C2	5.20	122.30	108.64
21	2	1206	CLA	O2A-C1-C2	5.20	122.29	108.64
21	A	1126	CLA	O2A-C1-C2	5.19	122.28	108.64
21	2	1213	CLA	O2A-C1-C2	5.18	122.24	108.64
21	1	1129	CLA	O2A-C1-C2	5.17	122.23	108.64
21	B	1219	CLA	O2A-C1-C2	5.17	122.21	108.64
21	2	1222	CLA	O2A-C1-C2	5.16	122.21	108.64
21	b	1213	CLA	O2A-C1-C2	5.16	122.20	108.64
21	1	1120	CLA	O2A-C1-C2	5.16	122.19	108.64
21	B	1240	CLA	O2A-C1-C2	5.15	122.17	108.64
21	b	1203	CLA	O2A-C1-C2	5.15	122.17	108.64
21	F	1302	CLA	O2A-C1-C2	5.15	122.16	108.64
21	2	1205	CLA	O2A-C1-C2	5.15	122.16	108.64
21	b	1236	CLA	O2A-C1-C2	5.14	122.14	108.64
21	2	1214	CLA	O2A-C1-C2	5.14	122.14	108.64
21	a	1137	CLA	O2A-C1-C2	5.13	122.13	108.64
21	a	1113	CLA	O2A-C1-C2	5.13	122.13	108.64
21	A	1134	CLA	O2A-C1-C2	5.13	122.12	108.64
25	A	5007	LHG	O7-C7-C8	5.13	122.56	111.50
21	1	1107	CLA	O2A-C1-C2	5.13	122.11	108.64
21	b	1240	CLA	O2A-C1-C2	5.13	122.11	108.64
21	1	1105	CLA	O2A-C1-C2	5.12	122.10	108.64
21	2	1023	CLA	O2A-C1-C2	5.12	122.10	108.64
21	1	1119	CLA	O2A-C1-C2	5.12	122.09	108.64
21	b	1023	CLA	O2A-C1-C2	5.12	122.08	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1139	CLA	O2A-C1-C2	5.11	122.08	108.64
21	1	1101	CLA	O2A-C1-C2	5.11	122.06	108.64
21	a	1133	CLA	O2A-C1-C2	5.10	122.04	108.64
21	0	1501	CLA	O2A-C1-C2	5.10	122.04	108.64
21	f	1301	CLA	O2A-C1-C2	5.10	122.04	108.64
21	2	1237	CLA	O2A-C1-C2	5.09	122.02	108.64
21	1	1133	CLA	O2A-C1-C2	5.09	122.02	108.64
21	B	1209	CLA	O2D-CGD-CBD	5.06	120.27	111.27
21	A	1129	CLA	O2A-C1-C2	5.06	121.94	108.64
21	L	1501	CLA	O2A-C1-C2	5.05	121.92	108.64
21	A	1119	CLA	O2A-C1-C2	5.05	121.90	108.64
21	A	1131	CLA	O2A-C1-C2	5.05	121.90	108.64
21	b	1237	CLA	O2A-C1-C2	5.04	121.88	108.64
21	b	1205	CLA	O2A-C1-C2	5.03	121.86	108.64
21	2	1221	CLA	O2A-C1-C2	5.03	121.86	108.64
21	A	1011	CLA	C4D-C3D-CAD	-5.03	105.67	108.47
21	2	1202	CLA	O2A-C1-C2	5.02	121.84	108.64
21	A	1118	CLA	O2A-C1-C2	5.02	121.84	108.64
21	A	1114	CLA	O2A-C1-C2	5.02	121.83	108.64
21	B	1223	CLA	O2A-C1-C2	5.02	121.82	108.64
21	b	1218	CLA	O2A-C1-C2	5.01	121.81	108.64
21	L	1502	CLA	O2A-C1-C2	5.01	121.80	108.64
21	b	1232	CLA	O2A-C1-C2	5.01	121.80	108.64
21	B	1208	CLA	O2A-C1-C2	5.00	121.79	108.64
21	F	1301	CLA	O2A-C1-C2	5.00	121.79	108.64
21	B	1212	CLA	O2A-C1-C2	5.00	121.78	108.64
21	2	1217	CLA	O2A-C1-C2	5.00	121.77	108.64
21	A	1121	CLA	O2A-C1-C2	4.99	121.75	108.64
21	1	1137	CLA	O2A-C1-C2	4.99	121.74	108.64
21	A	1140	CLA	O2A-C1-C2	4.98	121.74	108.64
21	a	1102	CLA	O2A-C1-C2	4.98	121.73	108.64
21	A	1801	CLA	O2A-C1-C2	4.98	121.73	108.64
21	a	1116	CLA	O2A-C1-C2	4.98	121.72	108.64
26	a	5004	LMG	O7-C10-C11	4.98	122.23	111.50
21	B	1218	CLA	O2A-C1-C2	4.98	121.72	108.64
21	A	1123	CLA	O2A-C1-C2	4.98	121.71	108.64
21	2	1226	CLA	O2A-C1-C2	4.97	121.69	108.64
21	b	1228	CLA	O2A-C1-C2	4.96	121.68	108.64
21	a	1124	CLA	O2A-C1-C2	4.96	121.68	108.64
21	a	1132	CLA	O2A-C1-C2	4.96	121.67	108.64
21	1	1126	CLA	O2A-C1-C2	4.96	121.66	108.64
21	J	1303	CLA	O2A-C1-C2	4.95	121.65	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	1121	CLA	O2A-C1-C2	4.95	121.64	108.64
21	a	1108	CLA	O2A-C1-C2	4.94	121.62	108.64
21	2	1203	CLA	O2A-C1-C2	4.93	121.58	108.64
21	1	1117	CLA	O2A-C1-C2	4.92	121.57	108.64
21	2	1236	CLA	O2A-C1-C2	4.92	121.57	108.64
21	2	1223	CLA	O2A-C1-C2	4.92	121.56	108.64
21	1	1130	CLA	O2A-C1-C2	4.91	121.53	108.64
21	1	1127	CLA	O2A-C1-C2	4.91	121.53	108.64
21	1	1134	CLA	O2A-C1-C2	4.90	121.53	108.64
21	1	1109	CLA	O2A-C1-C2	4.90	121.53	108.64
21	B	1220	CLA	O2A-C1-C2	4.90	121.52	108.64
30	2	4006	ECH	C16-C15-C14	-4.90	113.44	123.47
21	1	1011	CLA	O2A-C1-C2	4.90	121.51	108.64
25	a	5005	LHG	O7-C7-C8	4.90	122.05	111.50
21	B	1224	CLA	O2A-C1-C2	4.89	121.48	108.64
21	1	1110	CLA	O2A-C1-C2	4.88	121.47	108.64
21	1	1121	CLA	O2A-C1-C2	4.88	121.45	108.64
21	a	1139	CLA	O2A-C1-C2	4.87	121.43	108.64
21	B	1022	CLA	O2A-C1-C2	4.86	121.42	108.64
21	2	1224	CLA	O2A-C1-C2	4.85	121.38	108.64
21	2	1228	CLA	O2D-CGD-CBD	4.84	119.88	111.27
21	a	1130	CLA	O2A-C1-C2	4.83	121.34	108.64
21	b	1222	CLA	O2A-C1-C2	4.82	121.29	108.64
26	K	5009	LMG	O7-C10-C11	4.81	121.88	111.50
21	A	1108	CLA	O2A-C1-C2	4.81	121.28	108.64
21	2	1210	CLA	O2A-C1-C2	4.81	121.28	108.64
21	6	1302	CLA	O2D-CGD-CBD	4.79	119.78	111.27
21	1	1136	CLA	O2A-C1-C2	4.79	121.22	108.64
21	B	1205	CLA	O2A-C1-C2	4.78	121.20	108.64
21	B	1217	CLA	O2A-C1-C2	4.78	121.19	108.64
21	b	1223	CLA	O2A-C1-C2	4.78	121.19	108.64
34	7	4015	ZEX	C7-C8-C9	-4.78	119.02	126.23
21	B	1226	CLA	O2A-C1-C2	4.77	121.18	108.64
21	a	1104	CLA	O2A-C1-C2	4.77	121.17	108.64
21	A	1113	CLA	O2A-C1-C2	4.77	121.17	108.64
34	7	4015	ZEX	C38-C24-C23	4.76	119.57	112.20
21	a	1111	CLA	O2A-C1-C2	4.75	121.11	108.64
21	B	1222	CLA	O2A-C1-C2	4.75	121.11	108.64
21	1	1103	CLA	O2A-C1-C2	4.74	121.10	108.64
21	A	1103	CLA	O2A-C1-C2	4.74	121.09	108.64
30	b	4011	ECH	C7-C8-C9	-4.74	119.08	126.23
21	a	1131	CLA	O2A-C1-C2	4.73	121.06	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	4006	ECH	C33-C5-C6	-4.72	119.22	124.53
21	2	1221	CLA	O2D-CGD-CBD	4.72	119.66	111.27
21	1	1104	CLA	O2A-C1-C2	4.71	121.02	108.64
21	a	1128	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
21	a	1136	CLA	O2A-C1-C2	4.71	121.01	108.64
21	1	1123	CLA	O2A-C1-C2	4.71	121.01	108.64
21	2	1211	CLA	O2A-C1-C2	4.70	120.98	108.64
21	B	1201	CLA	O2A-C1-C2	4.69	120.97	108.64
21	A	1133	CLA	O2A-C1-C2	4.69	120.97	108.64
21	A	1102	CLA	O2A-C1-C2	4.69	120.97	108.64
30	b	4006	ECH	C7-C8-C9	-4.69	119.15	126.23
21	1	1501	CLA	O2A-C1-C2	4.69	120.95	108.64
21	2	1208	CLA	O2A-C1-C2	4.67	120.92	108.64
21	a	1119	CLA	O2A-C1-C2	4.67	120.90	108.64
21	B	1204	CLA	O2A-C1-C2	4.66	120.88	108.64
21	2	1219	CLA	O2A-C1-C2	4.66	120.87	108.64
21	B	1221	CLA	O2A-C1-C2	4.65	120.87	108.64
21	A	1105	CLA	O2A-C1-C2	4.65	120.86	108.64
30	B	4006	ECH	C33-C5-C6	-4.64	119.31	124.53
22	B	2002	PQN	C11-C12-C13	-4.64	119.06	126.79
21	b	1221	CLA	O2A-C1-C2	4.64	120.82	108.64
21	2	1229	CLA	O2A-C1-C2	4.63	120.81	108.64
30	b	4006	ECH	C24-C23-C22	-4.63	119.23	126.23
21	b	1214	CLA	O2A-C1-C2	4.63	120.79	108.64
21	2	1238	CLA	O2A-C1-C2	4.62	120.78	108.64
21	A	1137	CLA	O2A-C1-C2	4.62	120.78	108.64
21	a	1117	CLA	O2A-C1-C2	4.62	120.78	108.64
21	1	1118	CLA	O2A-C1-C2	4.62	120.78	108.64
21	B	1229	CLA	O2A-C1-C2	4.61	120.75	108.64
21	a	1103	CLA	O2A-C1-C2	4.61	120.74	108.64
21	b	1221	CLA	O2D-CGD-CBD	4.60	119.45	111.27
21	A	1127	CLA	O2A-C1-C2	4.60	120.72	108.64
21	b	1212	CLA	O2A-C1-C2	4.60	120.72	108.64
34	J	4015	ZEX	C7-C8-C9	-4.59	119.31	126.23
21	1	1106	CLA	O2A-C1-C2	4.57	120.66	108.64
21	A	1122	CLA	O2A-C1-C2	4.56	120.63	108.64
21	B	1211	CLA	O2A-C1-C2	4.56	120.62	108.64
24	6	4016	BCR	C35-C13-C14	-4.56	116.54	122.92
21	b	1229	CLA	O2A-C1-C2	4.55	120.58	108.64
21	2	1201	CLA	O2A-C1-C2	4.54	120.57	108.64
21	b	1202	CLA	O2A-C1-C2	4.53	120.55	108.64
21	B	1227	CLA	O2A-C1-C2	4.52	120.53	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1124	CLA	O2A-C1-C2	4.52	120.51	108.64
21	B	1210	CLA	O2A-C1-C2	4.51	120.50	108.64
30	i	4020	ECH	C15-C16-C17	-4.50	114.25	123.47
21	B	1021	CLA	O2A-C1-C2	4.50	120.47	108.64
21	a	1109	CLA	O2A-C1-C2	4.50	120.47	108.64
21	a	1801	CLA	O2A-C1-C2	4.50	120.46	108.64
21	A	1110	CLA	O2A-C1-C2	4.49	120.44	108.64
21	2	1207	CLA	O2A-C1-C2	4.48	120.42	108.64
21	A	1139	CLA	O2A-C1-C2	4.48	120.42	108.64
21	B	1226	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
21	a	1011	CLA	O2A-C1-C2	4.48	120.40	108.64
21	b	1210	CLA	O2A-C1-C2	4.47	120.39	108.64
36	I	4020	EQ3	C16-C17-C18	-4.47	120.93	127.31
21	A	1136	CLA	O2A-C1-C2	4.45	120.33	108.64
21	B	1240	CLA	O2D-CGD-CBD	4.45	119.17	111.27
21	A	1117	CLA	O2A-C1-C2	4.43	120.29	108.64
30	B	4006	ECH	C20-C21-C22	-4.42	121.00	127.31
21	K	1401	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
21	B	1228	CLA	O2A-C1-C2	4.42	120.24	108.64
30	b	4011	ECH	C12-C13-C14	4.41	125.71	118.94
21	2	1216	CLA	O2A-C1-C2	4.41	120.23	108.64
26	b	5005	LMG	O7-C10-C11	4.40	120.99	111.50
21	a	1013	CLA	O2A-C1-C2	4.39	120.18	108.64
30	2	4006	ECH	C33-C5-C6	-4.39	119.60	124.53
21	2	1021	CLA	O2A-C1-C2	4.39	120.16	108.64
21	b	1227	CLA	O2A-C1-C2	4.39	120.16	108.64
21	B	1214	CLA	O2A-C1-C2	4.38	120.15	108.64
25	A	5006	LHG	O7-C7-C8	4.38	120.94	111.50
21	a	1123	CLA	O2A-C1-C2	4.38	120.15	108.64
21	b	1230	CLA	O2A-C1-C2	4.38	120.14	108.64
21	b	1238	CLA	O2A-C1-C2	4.37	120.12	108.64
30	2	4006	ECH	C7-C8-C9	-4.37	119.63	126.23
21	B	1203	CLA	O2A-C1-C2	4.37	120.12	108.64
21	j	1302	CLA	O2A-C1-C2	4.37	120.11	108.64
21	B	1221	CLA	O2D-CGD-CBD	4.35	119.00	111.27
25	1	5007	LHG	O7-C7-C8	4.35	120.88	111.50
25	1	5005	LHG	O7-C7-C8	4.35	120.87	111.50
21	b	1022	CLA	O2A-C1-C2	4.34	120.05	108.64
30	b	4006	ECH	C15-C14-C13	-4.33	121.14	127.31
25	a	5001	LHG	O7-C7-C8	4.32	120.80	111.50
21	B	1237	CLA	O2A-C1-C2	4.31	119.96	108.64
30	m	4021	ECH	C20-C21-C22	-4.31	121.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	4020	45D	C41-C37-C35	-4.30	121.18	127.31
25	B	5004	LHG	O7-C7-C8	4.29	120.75	111.50
26	A	5002	LMG	O7-C10-C11	4.29	120.75	111.50
25	l	5001	LHG	O7-C7-C8	4.28	120.73	111.50
21	b	1224	CLA	O2A-C1-C2	4.28	119.88	108.64
21	1	1129	CLA	O2D-CGD-CBD	4.28	118.87	111.27
37	L	5004	DGD	O2G-C1B-C2B	4.28	120.72	111.50
25	A	5005	LHG	O7-C7-C8	4.28	120.72	111.50
21	2	1205	CLA	O2D-CGD-CBD	4.27	118.86	111.27
21	2	1213	CLA	O2D-CGD-CBD	4.27	118.86	111.27
21	B	1205	CLA	O2D-CGD-CBD	4.27	118.86	111.27
21	2	1204	CLA	O2A-C1-C2	4.26	119.84	108.64
21	B	1207	CLA	O2A-C1-C2	4.26	119.82	108.64
26	A	5008	LMG	O7-C10-C11	4.25	120.66	111.50
24	f	4016	BCR	C35-C13-C14	-4.25	116.97	122.92
34	j	4015	ZEX	C28-C27-C26	-4.25	119.83	127.09
21	1	1129	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
26	b	5002	LMG	O7-C10-C11	4.21	120.58	111.50
21	2	1202	CLA	O2D-CGD-CBD	4.21	118.75	111.27
25	1	5003	LHG	O7-C7-C8	4.21	120.58	111.50
24	B	4014	BCR	C15-C14-C13	4.19	133.29	127.31
25	2	5004	LHG	O7-C7-C8	4.18	120.52	111.50
21	B	1202	CLA	O2A-C1-C2	4.16	119.58	108.64
21	b	1230	CLA	O2D-CGD-CBD	4.16	118.67	111.27
21	b	1217	CLA	O2A-C1-C2	4.16	119.57	108.64
21	K	1402	CLA	O2D-CGD-CBD	4.16	118.65	111.27
21	a	1102	CLA	O2D-CGD-CBD	4.15	118.64	111.27
25	l	5004	LHG	O7-C7-C8	4.14	120.43	111.50
21	a	1128	CLA	O2D-CGD-CBD	4.14	118.62	111.27
25	1	5001	LHG	O7-C7-C8	4.13	120.40	111.50
21	A	1135	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
25	B	5006	LHG	O7-C7-C8	4.13	120.39	111.50
21	2	1022	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
21	b	1021	CLA	O2A-C1-C2	4.12	119.45	108.64
21	2	1211	CLA	O2D-CGD-CBD	4.11	118.57	111.27
28	h	4020	45D	C28-C26-C30	4.10	128.67	122.92
21	1	1131	CLA	O2A-C1-C2	4.10	119.42	108.64
30	b	4011	ECH	C24-C23-C22	-4.10	120.05	126.23
21	1	1128	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
21	b	1211	CLA	O2A-C1-C2	4.09	119.38	108.64
21	K	1402	CLA	O2A-C1-C2	4.08	119.36	108.64
21	1	1123	CLA	O2D-CGD-CBD	4.08	118.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	l	5002	LHG	O7-C7-C8	4.07	120.27	111.50
22	2	2002	PQN	C11-C12-C13	-4.06	120.03	126.79
21	6	1302	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
21	b	1234	CLA	O2D-CGD-CBD	4.06	118.48	111.27
21	b	1212	CLA	O2D-CGD-CBD	4.06	118.48	111.27
21	B	1213	CLA	O2D-CGD-CBD	4.06	118.48	111.27
21	2	1206	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
25	0	5004	LHG	O7-C7-C8	4.06	120.24	111.50
25	b	5004	LHG	O7-C7-C8	4.05	120.23	111.50
26	B	5005	LMG	O7-C10-C11	4.05	120.23	111.50
21	a	1106	CLA	O2D-CGD-CBD	4.05	118.46	111.27
30	m	4021	ECH	C7-C8-C9	-4.05	120.12	126.23
26	1	5002	LMG	O7-C10-C11	4.04	120.22	111.50
21	B	1202	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
21	2	1230	CLA	O2D-CGD-CBD	4.04	118.44	111.27
21	b	1205	CLA	O2D-CGD-CBD	4.03	118.43	111.27
25	a	5003	LHG	O7-C7-C8	4.03	120.18	111.50
26	a	5002	LMG	O7-C10-C11	4.02	120.16	111.50
21	1	1133	CLA	O2D-CGD-CBD	3.99	118.36	111.27
34	j	4015	ZEX	C31-C32-C33	-3.99	115.21	126.42
21	1	1128	CLA	O2D-CGD-CBD	3.99	118.35	111.27
21	2	1222	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
21	F	1302	CLA	O2D-CGD-CBD	3.98	118.34	111.27
21	A	1012	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
21	A	1801	CLA	O2D-CGD-CBD	3.98	118.34	111.27
21	1	1132	CLA	O2D-CGD-CBD	3.97	118.33	111.27
21	j	1302	CLA	O2D-CGD-CBD	3.97	118.33	111.27
21	A	1116	CLA	O2A-C1-C2	3.97	119.07	108.64
30	b	4011	ECH	C28-C27-C26	-3.97	114.99	118.65
21	B	1215	CLA	O2A-C1-C2	3.97	119.06	108.64
30	M	4021	ECH	C33-C5-C6	-3.96	120.09	124.53
30	M	4021	ECH	C24-C23-C22	-3.95	120.26	126.23
21	B	1230	CLA	O2D-CGD-CBD	3.95	118.28	111.27
21	A	1102	CLA	O2D-CGD-CBD	3.95	118.28	111.27
21	a	1132	CLA	O2D-CGD-CBD	3.95	118.28	111.27
26	1	5004	LMG	O7-C10-C11	3.94	120.00	111.50
35	l	6001	LMT	O5B-C5B-C4B	3.94	116.85	109.69
28	B	4011	45D	C42-C38-C36	-3.94	121.69	127.31
21	a	1013	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	J	1303	CLA	O2D-CGD-CBD	3.93	118.26	111.27
30	M	4021	ECH	C7-C8-C9	-3.92	120.31	126.23
21	K	1401	CLA	O2D-CGD-CBD	3.92	118.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1124	CLA	O2D-CGD-CBD	3.92	118.23	111.27
21	b	1227	CLA	O2D-CGD-CBD	3.92	118.23	111.27
30	i	4020	ECH	C10-C11-C12	-3.91	111.01	123.22
25	A	5003	LHG	O7-C7-C8	3.91	119.93	111.50
21	b	1226	CLA	O2D-CGD-CBD	3.91	118.22	111.27
21	1	1102	CLA	O2D-CGD-CBD	3.91	118.21	111.27
25	a	5007	LHG	O7-C7-C8	3.91	119.92	111.50
26	b	5007	LMG	O7-C10-C11	3.90	119.91	111.50
21	a	1118	CLA	O2A-C1-C2	3.90	118.89	108.64
21	2	1237	CLA	O2D-CGD-CBD	3.90	118.19	111.27
21	1	1113	CLA	O2D-CGD-CBD	3.89	118.19	111.27
26	0	5001	LMG	O7-C10-C11	3.89	119.89	111.50
21	A	1113	CLA	O2D-CGD-CBD	3.89	118.19	111.27
31	F	5001	SQD	O7-S-C6	-3.89	102.31	106.94
21	A	1011	CLA	O2A-C1-C2	3.89	118.86	108.64
34	j	4015	ZEX	C31-C30-C29	-3.89	121.76	127.31
21	2	1210	CLA	O2D-CGD-CBD	3.89	118.18	111.27
30	M	4021	ECH	C20-C21-C22	-3.89	121.76	127.31
21	A	1123	CLA	O2D-CGD-CBD	3.88	118.17	111.27
21	A	1106	CLA	O2D-CGD-CBD	3.88	118.16	111.27
21	A	1128	CLA	O2D-CGD-CBD	3.88	118.16	111.27
25	A	5001	LHG	O7-C7-C8	3.87	119.85	111.50
24	6	4016	BCR	C40-C30-C25	-3.87	104.03	110.30
24	0	4022	BCR	C19-C18-C17	3.87	124.88	118.94
21	A	1124	CLA	O2A-C1-C2	3.86	118.79	108.64
21	A	1125	CLA	O2D-CGD-CBD	3.86	118.13	111.27
21	b	1204	CLA	O2A-C1-C2	3.86	118.78	108.64
21	A	1129	CLA	O2D-CGD-CBD	3.86	118.12	111.27
21	b	1201	CLA	O2A-C1-C2	3.85	118.75	108.64
21	B	1230	CLA	O2A-C1-C2	3.84	118.73	108.64
21	B	1239	CLA	O2D-CGD-CBD	3.84	118.09	111.27
21	a	1137	CLA	O2D-CGD-CBD	3.84	118.08	111.27
21	L	1503	CLA	O2D-CGD-CBD	3.84	118.08	111.27
26	2	5005	LMG	O7-C10-C11	3.83	119.76	111.50
21	1	1106	CLA	O2D-CGD-CBD	3.82	118.05	111.27
21	B	1226	CLA	O2D-CGD-CBD	3.82	118.05	111.27
21	j	1303	CLA	O2D-CGD-CBD	3.81	118.05	111.27
21	1	1105	CLA	O2D-CGD-CBD	3.81	118.04	111.27
21	1	1134	CLA	O2D-CGD-CBD	3.81	118.04	111.27
25	l	5003	LHG	O7-C7-C8	3.80	119.70	111.50
26	A	5004	LMG	O7-C10-C11	3.80	119.70	111.50
30	m	4021	ECH	C33-C5-C6	-3.80	120.26	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1228	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
21	a	1121	CLA	O2D-CGD-CBD	3.79	118.01	111.27
21	1	1135	CLA	O2D-CGD-CBD	3.79	118.01	111.27
25	0	5002	LHG	O7-C7-C8	3.79	119.67	111.50
21	2	1238	CLA	O2D-CGD-CBD	3.79	118.00	111.27
21	a	1129	CLA	O2D-CGD-CBD	3.79	118.00	111.27
21	l	1502	CLA	O2D-CGD-CBD	3.79	118.00	111.27
21	a	1105	CLA	O2D-CGD-CBD	3.78	117.99	111.27
21	a	1120	CLA	O2D-CGD-CBD	3.78	117.99	111.27
21	A	1110	CLA	O2D-CGD-CBD	3.78	117.98	111.27
21	a	1123	CLA	O2D-CGD-CBD	3.77	117.97	111.27
24	9	4021	BCR	C30-C25-C26	-3.77	117.31	122.61
30	2	4006	ECH	C19-C18-C17	3.77	124.72	118.94
24	a	4003	BCR	C30-C25-C26	-3.76	117.31	122.61
21	1	1130	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	A	1116	CLA	O2D-CGD-CBD	3.76	117.95	111.27
21	2	1021	CLA	O2D-CGD-CBD	3.76	117.94	111.27
21	b	1238	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
24	A	4008	BCR	C39-C30-C25	-3.75	104.22	110.30
21	1	1110	CLA	O2D-CGD-CBD	3.75	117.93	111.27
21	l	1501	CLA	O2D-CGD-CBD	3.75	117.93	111.27
21	a	1012	CLA	O2D-CGD-CBD	3.74	117.92	111.27
28	h	4020	45D	C30-C32-C34	3.74	134.90	123.22
21	a	1110	CLA	O2D-CGD-CBD	3.74	117.92	111.27
36	I	4020	EQ3	C15-C14-C13	-3.74	121.98	127.31
21	1	1119	CLA	O2D-CGD-CBD	3.73	117.90	111.27
30	b	4011	ECH	C33-C5-C6	-3.73	120.34	124.53
21	1	1106	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	m	4021	ECH	C15-C14-C13	-3.73	121.99	127.31
21	2	1204	CLA	O2D-CGD-CBD	3.73	117.89	111.27
21	A	1111	CLA	O2D-CGD-CBD	3.73	117.89	111.27
26	B	5002	LMG	O7-C10-C11	3.72	119.52	111.50
21	B	1208	CLA	O2D-CGD-CBD	3.72	117.88	111.27
21	b	1226	CLA	O2A-C1-C2	3.72	118.41	108.64
24	b	4004	BCR	C39-C30-C25	-3.72	104.27	110.30
21	1	1012	CLA	O2D-CGD-CBD	3.71	117.86	111.27
21	6	1301	CLA	O2D-CGD-CBD	3.71	117.86	111.27
21	B	1222	CLA	O2D-CGD-CBD	3.70	117.85	111.27
21	b	1229	CLA	O2D-CGD-CBD	3.70	117.85	111.27
21	B	1228	CLA	O2D-CGD-CBD	3.70	117.84	111.27
28	B	4011	45D	C21-C15-C17	3.70	120.98	115.48
21	B	1227	CLA	O2D-CGD-CBD	3.70	117.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	1101	CLA	O2D-CGD-CBD	3.70	117.83	111.27
34	j	4015	ZEX	C38-C24-C23	3.70	117.92	112.20
21	b	1211	CLA	O2D-CGD-CBD	3.69	117.83	111.27
36	I	4020	EQ3	C7-C8-C9	-3.69	120.65	126.23
25	F	5002	LHG	O7-C7-C8	3.69	119.46	111.50
21	B	1224	CLA	O2D-CGD-CBD	3.69	117.83	111.27
28	h	4020	45D	C40-C36-C38	-3.69	117.75	122.92
21	A	1140	CLA	O2D-CGD-CBD	3.69	117.83	111.27
21	1	1120	CLA	O2D-CGD-CBD	3.69	117.82	111.27
24	0	4022	BCR	C36-C18-C19	-3.69	112.27	118.08
21	2	1208	CLA	O2D-CGD-CBD	3.68	117.82	111.27
24	7	4013	BCR	C38-C26-C25	-3.68	120.39	124.53
21	A	1133	CLA	O2D-CGD-CBD	3.68	117.80	111.27
21	l	1503	CLA	O2D-CGD-CBD	3.67	117.79	111.27
28	h	4020	45D	C23-C19-C07	-3.67	116.90	127.20
30	i	4020	ECH	C12-C13-C14	3.67	124.57	118.94
21	b	1206	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
21	1	1103	CLA	O2D-CGD-CBD	3.67	117.78	111.27
21	a	1138	CLA	O2D-CGD-CBD	3.66	117.78	111.27
21	8	1401	CLA	O2D-CGD-CBD	3.66	117.76	111.27
21	a	1140	CLA	O2D-CGD-CBD	3.65	117.76	111.27
21	1	1107	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
21	J	1302	CLA	O2D-CGD-CBD	3.65	117.75	111.27
21	2	1212	CLA	O2D-CGD-CBD	3.65	117.75	111.27
26	2	5002	LMG	O7-C10-C11	3.65	119.36	111.50
21	6	1301	CLA	O2A-C1-C2	3.64	121.81	108.42
36	I	4020	EQ3	C23-C24-C25	-3.64	116.97	127.20
21	b	1237	CLA	O2D-CGD-CBD	3.64	117.74	111.27
21	A	1120	CLA	O2D-CGD-CBD	3.64	117.74	111.27
21	0	1502	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
21	b	1202	CLA	O2D-CGD-CBD	3.64	117.73	111.27
21	1	1101	CLA	O2D-CGD-CBD	3.64	117.73	111.27
21	A	1105	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	a	1119	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	B	1204	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	B	1234	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	B	1021	CLA	O2D-CGD-CBD	3.63	117.71	111.27
31	b	5006	SQD	O7-S-C6	-3.63	102.63	106.94
21	A	1109	CLA	O2D-CGD-CBD	3.63	117.71	111.27
21	B	1206	CLA	O2D-CGD-CBD	3.62	117.70	111.27
21	2	1216	CLA	O2D-CGD-CBD	3.62	117.70	111.27
21	A	1101	CLA	O2D-CGD-CBD	3.62	117.69	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1239	CLA	O2D-CGD-CBD	3.61	117.69	111.27
21	A	1126	CLA	O2D-CGD-CBD	3.61	117.68	111.27
21	a	1108	CLA	O2D-CGD-CBD	3.61	117.68	111.27
21	A	1132	CLA	O2D-CGD-CBD	3.61	117.68	111.27
31	L	5001	SQD	O7-S-C6	-3.61	102.65	106.94
21	a	1116	CLA	O2D-CGD-CBD	3.60	117.67	111.27
21	A	1801	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
21	b	1226	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
21	b	1219	CLA	O2D-CGD-CBD	3.60	117.67	111.27
21	A	1101	CLA	CAA-C2A-C3A	-3.60	102.93	112.78
30	B	4006	ECH	C20-C19-C18	-3.60	116.32	126.42
21	a	1114	CLA	O2D-CGD-CBD	3.59	117.66	111.27
36	I	4020	EQ3	C8-C7-C6	-3.59	117.11	127.20
21	a	1126	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
24	2	4018	BCR	C38-C26-C25	-3.59	120.50	124.53
34	F	4016	ZEX	C38-C24-C23	3.58	117.75	112.20
21	1	1139	CLA	O2D-CGD-CBD	3.58	117.63	111.27
21	1	1140	CLA	O2D-CGD-CBD	3.58	117.63	111.27
24	B	4005	BCR	C38-C26-C25	-3.58	120.51	124.53
21	b	1209	CLA	O2D-CGD-CBD	3.57	117.61	111.27
21	B	1238	CLA	O2A-C1-C2	3.57	118.01	108.64
30	i	4020	ECH	C33-C5-C6	-3.56	120.53	124.53
21	A	1012	CLA	O2D-CGD-CBD	3.56	117.60	111.27
21	a	1131	CLA	O2D-CGD-CBD	3.56	117.59	111.27
21	b	1231	CLA	O2D-CGD-CBD	3.56	117.59	111.27
24	a	4019	BCR	C15-C14-C13	-3.56	122.23	127.31
24	j	4013	BCR	C38-C26-C25	-3.56	120.53	124.53
21	B	1219	CLA	O2D-CGD-CBD	3.56	117.59	111.27
21	a	1113	CLA	O2D-CGD-CBD	3.56	117.59	111.27
21	1	1113	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
21	1	1116	CLA	O2D-CGD-CBD	3.54	117.56	111.27
21	B	1211	CLA	O2D-CGD-CBD	3.54	117.56	111.27
35	0	6001	LMT	C3'-C4'-C5'	-3.54	102.80	110.93
21	a	1133	CLA	O2D-CGD-CBD	3.54	117.56	111.27
21	B	1217	CLA	O2D-CGD-CBD	3.54	117.56	111.27
30	b	4011	ECH	C10-C11-C12	-3.54	112.17	123.22
21	1	1112	CLA	O2D-CGD-CBD	3.54	117.56	111.27
21	b	1214	CLA	O2D-CGD-CBD	3.54	117.56	111.27
24	A	4002	BCR	C15-C14-C13	3.54	132.36	127.31
31	f	5001	SQD	O7-S-C6	-3.53	102.74	106.94
21	a	1127	CLA	O2D-CGD-CBD	3.53	117.55	111.27
21	b	1217	CLA	O2D-CGD-CBD	3.53	117.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1130	CLA	O2D-CGD-CBD	3.53	117.54	111.27
21	B	1229	CLA	O2D-CGD-CBD	3.53	117.54	111.27
21	j	1302	CLA	CMA-C3A-C4A	3.53	121.26	111.77
21	a	1101	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
21	a	1134	CLA	O2D-CGD-CBD	3.52	117.53	111.27
21	b	1222	CLA	O2D-CGD-CBD	3.52	117.53	111.27
21	2	1214	CLA	O2D-CGD-CBD	3.52	117.52	111.27
21	1	1801	CLA	O2D-CGD-CBD	3.52	117.52	111.27
24	A	4008	BCR	C15-C14-C13	3.52	132.33	127.31
21	A	1013	CLA	O2D-CGD-CBD	3.52	117.52	111.27
21	a	1117	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
21	L	1502	CLA	O2D-CGD-CBD	3.51	117.51	111.27
24	2	4014	BCR	C15-C14-C13	3.51	132.32	127.31
24	J	4013	BCR	C38-C26-C25	-3.51	120.58	124.53
21	0	1501	CLA	O2D-CGD-CBD	3.51	117.51	111.27
21	B	1212	CLA	O2D-CGD-CBD	3.51	117.50	111.27
21	b	1208	CLA	O2D-CGD-CBD	3.51	117.50	111.27
25	L	5005	LHG	O7-C7-C8	3.51	119.06	111.50
21	b	1204	CLA	O2D-CGD-CBD	3.50	117.50	111.27
21	2	1230	CLA	O2A-C1-C2	3.50	121.30	108.42
21	1	1126	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
21	1	1108	CLA	O2D-CGD-CBD	3.50	117.49	111.27
21	B	1231	CLA	O2D-CGD-CBD	3.50	117.48	111.27
21	2	1219	CLA	O2D-CGD-CBD	3.50	117.48	111.27
21	A	1117	CLA	O2D-CGD-CBD	3.50	117.48	111.27
30	b	4011	ECH	C15-C16-C17	-3.50	116.31	123.47
21	A	1119	CLA	O2D-CGD-CBD	3.50	117.48	111.27
21	2	1215	CLA	O2D-CGD-CBD	3.49	117.47	111.27
21	A	1113	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
34	F	4016	ZEX	C7-C8-C9	-3.49	120.96	126.23
21	b	1240	CLA	O2D-CGD-CBD	3.49	117.47	111.27
21	0	1502	CLA	O2D-CGD-CBD	3.49	117.47	111.27
21	a	1135	CLA	O2D-CGD-CBD	3.49	117.46	111.27
21	1	1138	CLA	O2D-CGD-CBD	3.48	117.46	111.27
24	2	4011	BCR	C15-C14-C13	3.48	132.28	127.31
21	2	1226	CLA	O2D-CGD-CBD	3.48	117.46	111.27
21	2	1201	CLA	O2D-CGD-CBD	3.48	117.45	111.27
21	1	1107	CLA	O2D-CGD-CBD	3.48	117.45	111.27
30	B	4006	ECH	C28-C27-C26	-3.47	115.45	118.65
21	2	1203	CLA	O2D-CGD-CBD	3.47	117.44	111.27
21	a	1104	CLA	O2D-CGD-CBD	3.47	117.44	111.27
21	a	1125	CLA	O2D-CGD-CBD	3.47	117.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	5009	LMG	C1-C2-C3	3.47	117.22	110.00
21	a	1111	CLA	O2D-CGD-CBD	3.47	117.43	111.27
28	h	4020	45D	C34-C36-C38	3.47	124.26	118.94
21	B	1206	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
21	a	1118	CLA	O2D-CGD-CBD	3.46	117.41	111.27
21	A	1122	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
21	a	1109	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
21	f	1301	CLA	O2D-CGD-CBD	3.45	117.40	111.27
21	7	1302	CLA	O2D-CGD-CBD	3.45	117.40	111.27
21	2	1217	CLA	O2D-CGD-CBD	3.45	117.40	111.27
24	9	4021	BCR	C35-C13-C14	-3.45	118.09	122.92
21	A	1107	CLA	O2D-CGD-CBD	3.45	117.40	111.27
30	b	4011	ECH	C35-C13-C12	-3.45	112.64	118.08
21	1	1124	CLA	O2D-CGD-CBD	3.44	117.39	111.27
21	b	1210	CLA	O2D-CGD-CBD	3.44	117.39	111.27
21	b	1213	CLA	O2D-CGD-CBD	3.44	117.38	111.27
26	a	5004	LMG	O1-C1-C2	3.44	113.67	108.30
34	j	4015	ZEX	C39-C29-C30	-3.44	118.11	122.92
24	A	4003	BCR	C1-C6-C5	-3.44	117.77	122.61
21	2	1022	CLA	O2D-CGD-CBD	3.44	117.38	111.27
24	2	4005	BCR	C40-C30-C25	-3.44	104.72	110.30
21	a	1115	CLA	O2D-CGD-CBD	3.44	117.37	111.27
21	A	1137	CLA	O2D-CGD-CBD	3.44	117.37	111.27
28	B	4011	45D	C23-C19-C07	-3.43	117.56	127.20
28	B	4011	45D	C05-C03-C07	3.43	115.77	110.48
24	8	4001	BCR	C40-C30-C25	-3.43	104.73	110.30
21	0	1503	CLA	O2D-CGD-CBD	3.43	117.37	111.27
22	b	2002	PQN	C14-C13-C15	3.43	121.04	115.27
21	1	1126	CLA	O2D-CGD-CBD	3.43	117.36	111.27
21	2	1220	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
21	B	1202	CLA	O2D-CGD-CBD	3.43	117.36	111.27
21	b	1203	CLA	O2D-CGD-CBD	3.43	117.36	111.27
21	a	1103	CLA	O2D-CGD-CBD	3.42	117.35	111.27
21	B	1235	CLA	O2D-CGD-CBD	3.42	117.35	111.27
21	A	1131	CLA	O2D-CGD-CBD	3.42	117.35	111.27
30	2	4006	ECH	C28-C27-C26	-3.42	115.50	118.65
21	A	1115	CLA	O2D-CGD-CBD	3.42	117.34	111.27
21	1	1119	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
21	2	1218	CLA	O2D-CGD-CBD	3.41	117.33	111.27
21	b	1223	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	B	1216	CLA	O2D-CGD-CBD	3.41	117.33	111.27
21	a	1126	CLA	O2D-CGD-CBD	3.40	117.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2001	PQN	C14-C13-C15	3.40	120.99	115.27
21	1	1013	CLA	O2D-CGD-CBD	3.40	117.31	111.27
21	a	1112	CLA	O2D-CGD-CBD	3.40	117.30	111.27
21	f	1302	CLA	O2D-CGD-CBD	3.40	117.30	111.27
21	2	1231	CLA	O2D-CGD-CBD	3.39	117.30	111.27
21	1	1101	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
24	L	4019	BCR	C15-C14-C13	3.39	132.14	127.31
21	F	1301	CLA	O2D-CGD-CBD	3.39	117.28	111.27
21	B	1218	CLA	O2D-CGD-CBD	3.39	117.28	111.27
21	2	1240	CLA	O2D-CGD-CBD	3.39	117.28	111.27
21	A	1106	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
21	A	1103	CLA	O2D-CGD-CBD	3.38	117.28	111.27
21	1	1125	CLA	O2D-CGD-CBD	3.38	117.27	111.27
21	2	1229	CLA	O2D-CGD-CBD	3.38	117.27	111.27
24	L	4019	BCR	C40-C30-C25	-3.38	104.82	110.30
21	7	1303	CLA	O2D-CGD-CBD	3.37	117.26	111.27
21	b	1232	CLA	O2D-CGD-CBD	3.37	117.26	111.27
30	i	4020	ECH	C20-C21-C22	-3.37	122.50	127.31
21	2	1209	CLA	O2D-CGD-CBD	3.37	117.25	111.27
21	A	1117	CLA	CMA-C3A-C4A	3.37	120.82	111.77
21	1	1136	CLA	O2D-CGD-CBD	3.36	117.25	111.27
21	1	1104	CLA	O2D-CGD-CBD	3.36	117.23	111.27
30	M	4021	ECH	C16-C17-C18	-3.35	122.52	127.31
30	B	4006	ECH	C11-C12-C13	-3.35	117.00	126.42
24	a	4019	BCR	C40-C30-C25	-3.35	104.86	110.30
24	2	4004	BCR	C40-C30-C25	-3.35	104.87	110.30
34	J	4015	ZEX	C38-C24-C23	3.35	117.38	112.20
21	1	1131	CLA	O2D-CGD-CBD	3.35	117.21	111.27
21	B	1223	CLA	O2D-CGD-CBD	3.35	117.21	111.27
21	B	1215	CLA	O2D-CGD-CBD	3.34	117.21	111.27
21	B	1203	CLA	O2D-CGD-CBD	3.34	117.21	111.27
24	a	4002	BCR	C40-C30-C25	-3.34	104.88	110.30
21	1	1115	CLA	O2D-CGD-CBD	3.34	117.20	111.27
21	B	1210	CLA	O2D-CGD-CBD	3.34	117.20	111.27
30	M	4021	ECH	C15-C14-C13	-3.34	122.55	127.31
24	a	4007	BCR	C40-C30-C25	-3.34	104.89	110.30
21	a	1109	CLA	O2D-CGD-CBD	3.34	117.20	111.27
22	A	2001	PQN	C11-C12-C13	-3.34	121.24	126.79
21	b	1215	CLA	O2D-CGD-CBD	3.33	117.19	111.27
21	A	1139	CLA	O2D-CGD-CBD	3.33	117.18	111.27
21	2	1227	CLA	O2D-CGD-CBD	3.33	117.18	111.27
31	0	5005	SQD	O7-S-C6	-3.33	102.98	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	f	4016	BCR	C12-C13-C14	3.33	124.04	118.94
21	2	1220	CLA	O2D-CGD-CBD	3.32	117.17	111.27
21	B	1225	CLA	O2D-CGD-CBD	3.32	117.17	111.27
24	b	4004	BCR	C30-C25-C24	3.32	125.17	115.78
30	B	4006	ECH	C7-C8-C9	-3.32	121.22	126.23
21	1	1114	CLA	O2D-CGD-CBD	3.32	117.16	111.27
30	b	4011	ECH	C20-C19-C18	-3.32	117.10	126.42
21	2	1239	CLA	O2D-CGD-CBD	3.31	117.15	111.27
21	1	1118	CLA	O2D-CGD-CBD	3.31	117.14	111.27
21	1	1127	CLA	O2D-CGD-CBD	3.31	117.14	111.27
21	b	1022	CLA	O2D-CGD-CBD	3.31	117.14	111.27
21	a	1801	CLA	O2D-CGD-CBD	3.30	117.14	111.27
21	A	1112	CLA	O2D-CGD-CBD	3.30	117.14	111.27
21	8	1402	CLA	O2D-CGD-CBD	3.30	117.14	111.27
22	1	2001	PQN	C14-C13-C15	3.29	120.81	115.27
21	b	1208	CLA	O2A-C1-C2	3.29	117.29	108.64
21	B	1232	CLA	O2D-CGD-CBD	3.29	117.12	111.27
21	L	1501	CLA	O2D-CGD-CBD	3.29	117.12	111.27
21	A	1134	CLA	O2D-CGD-CBD	3.29	117.11	111.27
21	1	1121	CLA	O2D-CGD-CBD	3.29	117.11	111.27
21	a	1124	CLA	O2D-CGD-CBD	3.28	117.10	111.27
21	b	1235	CLA	O2D-CGD-CBD	3.28	117.10	111.27
21	b	1215	CLA	C1-O2A-CGA	3.28	125.05	116.44
21	2	1225	CLA	O2D-CGD-CBD	3.28	117.09	111.27
24	b	4017	BCR	C39-C30-C25	-3.27	104.99	110.30
21	2	1023	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
21	1	1137	CLA	O2D-CGD-CBD	3.27	117.08	111.27
21	a	1123	CLA	CMA-C3A-C4A	3.27	120.56	111.77
24	b	4005	BCR	C40-C30-C25	-3.27	105.00	110.30
31	L	5002	SQD	O7-S-C6	-3.26	103.06	106.94
21	a	1139	CLA	O2D-CGD-CBD	3.26	117.07	111.27
24	1	4002	BCR	C38-C26-C25	-3.26	120.86	124.53
21	a	1130	CLA	O2D-CGD-CBD	3.26	117.06	111.27
21	1	1109	CLA	CMA-C3A-C4A	3.26	120.54	111.77
21	A	1104	CLA	O2D-CGD-CBD	3.26	117.06	111.27
24	a	4012	BCR	C39-C30-C25	-3.26	105.01	110.30
21	1	1117	CLA	CMA-C3A-C4A	3.26	120.52	111.77
21	a	1120	CLA	CMA-C3A-C4A	3.25	120.51	111.77
21	A	1114	CLA	O2D-CGD-CBD	3.25	117.04	111.27
21	a	1107	CLA	O2D-CGD-CBD	3.25	117.04	111.27
21	0	1502	CLA	CMA-C3A-C4A	3.25	120.50	111.77
21	2	1223	CLA	O2D-CGD-CBD	3.25	117.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	f	4016	BCR	C40-C30-C25	-3.25	105.03	110.30
26	0	5001	LMG	O6-C5-C4	3.25	115.59	109.69
21	B	1236	CLA	O2D-CGD-CBD	3.24	117.03	111.27
21	B	1220	CLA	O2D-CGD-CBD	3.24	117.02	111.27
24	h	4018	BCR	C40-C30-C25	-3.23	105.05	110.30
30	b	4006	ECH	C19-C18-C17	-3.23	113.98	118.94
21	a	1109	CLA	CMA-C3A-C4A	3.23	120.45	111.77
21	B	1208	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
21	2	1222	CLA	O2D-CGD-CBD	3.23	117.00	111.27
21	2	1240	CLA	CMA-C3A-C4A	3.23	120.44	111.77
21	a	1117	CLA	O2D-CGD-CBD	3.23	117.00	111.27
24	A	4002	BCR	C40-C30-C25	-3.22	105.07	110.30
21	b	1206	CLA	O2D-CGD-CBD	3.22	116.99	111.27
21	a	1136	CLA	CMA-C3A-C4A	3.22	120.42	111.77
21	a	1108	CLA	CMA-C3A-C4A	3.22	120.42	111.77
21	b	1236	CLA	O2D-CGD-CBD	3.22	116.98	111.27
21	2	1215	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
21	b	1021	CLA	O2D-CGD-CBD	3.22	116.98	111.27
24	a	4001	BCR	C30-C25-C26	-3.21	118.09	122.61
21	A	1011	CLA	CHA-C1A-NA	-3.21	119.04	126.40
24	l	4019	BCR	C34-C9-C10	-3.21	118.42	122.92
25	l	5002	LHG	C5-O7-C7	-3.21	109.89	117.79
24	B	4005	BCR	C40-C30-C25	-3.21	105.10	110.30
30	2	4006	ECH	C21-C20-C19	-3.21	113.21	123.22
21	1	1109	CLA	O2D-CGD-CBD	3.21	116.97	111.27
31	B	5008	SQD	O7-S-C6	-3.20	103.13	106.94
21	A	1130	CLA	O2A-CGA-CBA	3.20	121.95	111.91
21	a	1117	CLA	CMA-C3A-C4A	3.20	120.38	111.77
34	7	4015	ZEX	C31-C32-C33	-3.19	117.44	126.42
30	m	4021	ECH	C16-C17-C18	-3.19	122.75	127.31
26	b	5007	LMG	O1-C1-C2	3.19	113.29	108.30
21	2	1234	CLA	CMA-C3A-C4A	3.19	120.35	111.77
30	i	4020	ECH	C23-C24-C25	-3.19	118.24	127.20
21	k	1402	CLA	O2D-CGD-CBD	3.19	116.94	111.27
21	A	1139	CLA	CMA-C3A-C4A	3.19	120.35	111.77
30	m	4021	ECH	C24-C23-C22	-3.19	121.42	126.23
21	B	1237	CLA	O2D-CGD-CBD	3.18	116.92	111.27
34	J	4015	ZEX	C31-C32-C33	-3.18	117.50	126.42
21	B	1215	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
24	b	4005	BCR	C38-C26-C25	-3.17	120.97	124.53
21	2	1224	CLA	O2D-CGD-CBD	3.17	116.90	111.27
34	J	4015	ZEX	C39-C29-C30	-3.17	118.48	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1108	CLA	CMA-C3A-C4A	3.17	120.28	111.77
21	A	1129	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
21	b	1215	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
21	B	1234	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
24	1	4002	BCR	C40-C30-C25	-3.16	105.17	110.30
21	1	1139	CLA	CMA-C3A-C4A	3.16	120.25	111.77
21	2	1211	CLA	CMA-C3A-C4A	3.15	120.25	111.77
21	1	1122	CLA	O2D-CGD-CBD	3.15	116.86	111.27
21	8	1401	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	a	1135	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	B	1240	CLA	CMA-C3A-C4A	3.14	120.22	111.77
21	7	1303	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
21	2	1212	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
21	2	1207	CLA	O2D-CGD-CBD	3.14	116.85	111.27
24	f	4016	BCR	C15-C14-C13	3.14	131.79	127.31
25	A	5001	LHG	O8-C23-C24	3.14	121.75	111.91
21	A	1117	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
21	2	1236	CLA	CMA-C3A-C4A	3.13	120.19	111.77
21	A	1102	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
35	l	6001	LMT	C3'-C4'-C5'	-3.13	103.75	110.93
24	h	4018	BCR	C39-C30-C25	-3.13	105.23	110.30
21	b	1209	CLA	CMA-C3A-C4A	3.13	120.18	111.77
21	b	1224	CLA	O2D-CGD-CBD	3.13	116.82	111.27
21	B	1231	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
21	2	1220	CLA	CMA-C3A-C4A	3.12	120.17	111.77
21	2	1218	CLA	CMA-C3A-C4A	3.12	120.16	111.77
26	0	5001	LMG	C1-O6-C5	3.12	119.81	113.69
21	a	1011	CLA	C3D-CAD-CBD	-3.12	103.50	107.61
21	B	1210	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
24	2	4011	BCR	C39-C30-C25	-3.11	105.25	110.30
21	A	1109	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
21	B	1220	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
21	b	1223	CLA	O2D-CGD-CBD	3.11	116.79	111.27
21	1	1126	CLA	CMA-C3A-C4A	3.11	120.12	111.77
21	b	1219	CLA	CMA-C3A-C4A	3.10	120.11	111.77
21	6	1302	CLA	CMA-C3A-C4A	3.10	120.10	111.77
21	A	1121	CLA	O2D-CGD-CBD	3.10	116.77	111.27
21	A	1127	CLA	O2D-CGD-CBD	3.09	116.77	111.27
28	h	4020	45D	C31-C29-C25	-3.09	122.90	127.31
24	0	4022	BCR	C40-C30-C25	-3.09	105.29	110.30
21	1	1801	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
21	2	1232	CLA	O2D-CGD-CBD	3.09	116.75	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1209	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	7	1303	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	J	1302	CLA	CMA-C3A-C4A	3.08	120.05	111.77
21	B	1022	CLA	O2D-CGD-CBD	3.08	116.74	111.27
21	B	1237	CLA	O2A-CGA-CBA	3.08	121.57	111.91
21	A	1119	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
21	B	1220	CLA	CMA-C3A-C4A	3.07	120.03	111.77
21	j	1303	CLA	CMA-C3A-C4A	3.07	120.02	111.77
24	A	4001	BCR	C34-C9-C10	-3.07	118.62	122.92
21	B	1214	CLA	O2D-CGD-CBD	3.07	116.72	111.27
21	a	1126	CLA	CMA-C3A-C4A	3.07	120.02	111.77
21	1	1113	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	2	1223	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	2	1208	CLA	CMA-C3A-C4A	3.06	120.01	111.77
21	B	1207	CLA	O2A-CGA-CBA	3.06	121.52	111.91
21	1	1136	CLA	CMA-C3A-C4A	3.06	120.01	111.77
24	1	4008	BCR	C40-C30-C25	-3.06	105.33	110.30
30	b	4006	ECH	C21-C20-C19	3.06	132.78	123.22
21	A	1011	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
21	b	1207	CLA	C1-O2A-CGA	3.06	124.47	116.44
21	1	1120	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	2	1217	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	1	1122	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	2	1235	CLA	O2D-CGD-CBD	3.06	116.70	111.27
22	B	2002	PQN	C14-C13-C15	3.05	120.41	115.27
21	1	1120	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
21	a	1122	CLA	O2D-CGD-CBD	3.05	116.69	111.27
30	b	4006	ECH	C28-C27-C26	-3.05	115.84	118.65
21	b	1209	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
36	I	4020	EQ3	C24-C23-C22	-3.04	121.64	126.23
21	b	1238	CLA	O2D-CGD-CBD	3.04	116.67	111.27
26	b	5002	LMG	O8-C28-C29	3.04	121.45	111.91
21	1	1110	CLA	CMA-C3A-C4A	3.04	119.94	111.77
24	A	4003	BCR	C40-C30-C25	-3.04	105.37	110.30
35	L	6001	LMT	C1B-C2B-C3B	3.04	116.32	110.00
36	I	4020	EQ3	C16-C15-C14	-3.03	117.26	123.47
21	A	1108	CLA	O2D-CGD-CBD	3.03	116.66	111.27
21	b	1216	CLA	O2D-CGD-CBD	3.03	116.65	111.27
21	1	1114	CLA	CMA-C3A-C4A	3.03	119.92	111.77
21	B	1207	CLA	CAC-C3C-C2C	3.03	132.70	127.53
21	1	1105	CLA	CMA-C3A-C4A	3.03	119.90	111.77
21	a	1121	CLA	CMA-C3A-C4A	3.02	119.90	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1225	CLA	O2D-CGD-CBD	3.02	116.64	111.27
24	7	4013	BCR	C34-C9-C10	-3.02	118.70	122.92
21	B	1207	CLA	CMA-C3A-C4A	3.02	119.88	111.77
21	A	1122	CLA	CMA-C3A-C4A	3.02	119.88	111.77
22	b	2002	PQN	C17-C16-C15	-3.01	105.17	113.36
21	a	1139	CLA	CMA-C3A-C4A	3.01	119.87	111.77
25	A	5001	LHG	C5-O7-C7	-3.01	110.37	117.79
34	J	4015	ZEX	C37-C21-C26	-3.01	105.42	110.30
21	A	1114	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	J	1303	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	B	1232	CLA	CMA-C3A-C4A	3.01	119.86	111.77
24	f	4016	BCR	C2-C1-C6	3.01	115.11	110.48
21	B	1225	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	a	1138	CLA	CMA-C3A-C4A	3.01	119.85	111.77
24	A	4019	BCR	C8-C9-C10	3.00	123.55	118.94
34	j	4015	ZEX	C28-C29-C30	3.00	123.55	118.94
21	1	1112	CLA	CMA-C3A-C4A	3.00	119.84	111.77
21	2	1219	CLA	CMA-C3A-C4A	3.00	119.83	111.77
21	1	1140	CLA	CMA-C3A-C4A	3.00	119.83	111.77
24	L	4019	BCR	C39-C30-C25	-3.00	105.44	110.30
21	b	1232	CLA	CMA-C3A-C4A	3.00	119.82	111.77
21	A	1011	CLA	C2A-C1A-CHA	2.99	129.09	123.86
30	2	4006	ECH	C23-C22-C21	-2.99	114.35	118.94
21	a	1127	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	1	1101	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	b	1210	CLA	CMA-C3A-C4A	2.99	119.80	111.77
21	A	1013	CLA	CMB-C2B-C3B	2.99	130.26	124.68
21	A	1136	CLA	O2D-CGD-CBD	2.98	116.57	111.27
21	B	1224	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	2	1204	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	F	1302	CLA	CMA-C3A-C4A	2.98	119.79	111.77
36	I	4020	EQ3	C21-C20-C19	-2.98	113.91	123.22
21	2	1225	CLA	CMA-C3A-C4A	2.98	119.79	111.77
22	2	2002	PQN	C14-C13-C15	2.98	120.28	115.27
21	a	1801	CLA	CMA-C3A-C4A	2.98	119.78	111.77
21	1	1011	CLA	O2D-CGD-CBD	2.98	116.56	111.27
24	2	4018	BCR	C19-C18-C17	2.98	123.51	118.94
21	a	1112	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
21	a	1122	CLA	CMA-C3A-C4A	2.98	119.77	111.77
28	h	4020	45D	C21-C15-C17	2.97	119.90	115.48
21	A	1102	CLA	O2A-CGA-CBA	2.97	121.23	111.91
21	k	1401	CLA	O2D-CGD-CBD	2.97	116.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	k	1401	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	l	1125	CLA	CMA-C3A-C4A	2.97	119.75	111.77
21	b	1234	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
35	L	6001	LMT	O5B-C1B-C2B	2.97	116.63	110.35
24	B	4004	BCR	C38-C26-C25	-2.97	121.20	124.53
21	2	1206	CLA	O2D-CGD-CBD	2.96	116.52	111.27
21	b	1220	CLA	O2D-CGD-CBD	2.96	116.52	111.27
21	A	1124	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
21	2	1238	CLA	CMA-C3A-C4A	2.95	119.71	111.77
21	b	1217	CLA	CMA-C3A-C4A	2.95	119.70	111.77
21	b	1022	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
24	j	4013	BCR	C34-C9-C10	-2.95	118.80	122.92
21	a	1114	CLA	CMA-C3A-C4A	2.95	119.69	111.77
26	0	5001	LMG	C3-C4-C5	2.95	115.50	110.24
26	A	5002	LMG	O8-C28-C29	2.95	121.15	111.91
21	b	1237	CLA	O2A-CGA-CBA	2.95	121.15	111.91
21	1	1123	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
21	2	1231	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
24	9	4021	BCR	C40-C30-C25	-2.94	105.53	110.30
24	9	4021	BCR	C12-C13-C14	2.94	123.45	118.94
24	a	4008	BCR	C38-C26-C25	-2.94	121.23	124.53
34	7	4015	ZEX	C17-C1-C6	-2.94	105.53	110.30
21	b	1207	CLA	CMA-C3A-C4A	2.94	119.67	111.77
21	1	1123	CLA	CMA-C3A-C4A	2.94	119.67	111.77
24	l	4022	BCR	C40-C30-C25	-2.94	105.54	110.30
21	b	1021	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
25	1	5003	LHG	C5-O7-C7	-2.93	110.57	117.79
21	a	1113	CLA	CMA-C3A-C4A	2.93	119.66	111.77
21	1	1124	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	B	1214	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	b	1202	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
21	A	1108	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	b	1238	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	1	1117	CLA	O2D-CGD-CBD	2.93	116.47	111.27
26	a	5004	LMG	O8-C28-C29	2.93	121.09	111.91
21	B	1223	CLA	CMA-C3A-C4A	2.92	119.63	111.77
30	b	4011	ECH	C23-C24-C25	-2.92	119.00	127.20
22	2	2002	PQN	C2M-C2-C3	-2.92	119.64	124.40
21	a	1124	CLA	CMA-C3A-C4A	2.92	119.61	111.77
24	I	4018	BCR	C35-C13-C12	2.92	122.67	118.08
21	a	1116	CLA	CMA-C3A-C4A	2.92	119.61	111.77
21	2	1021	CLA	CMB-C2B-C1B	-2.91	123.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1223	CLA	CMA-C3A-C4A	2.91	119.60	111.77
21	a	1011	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
21	b	1214	CLA	CMA-C3A-C4A	2.91	119.59	111.77
21	2	1212	CLA	CMA-C3A-C4A	2.91	119.58	111.77
21	A	1119	CLA	CMB-C2B-C3B	2.90	130.11	124.68
21	1	1102	CLA	O2A-CGA-CBA	2.90	121.02	111.91
21	2	1023	CLA	O2D-CGD-CBD	2.90	116.43	111.27
24	K	4001	BCR	C40-C30-C25	-2.90	105.59	110.30
21	a	1136	CLA	O2A-CGA-CBA	2.90	121.02	111.91
24	2	4010	BCR	C15-C14-C13	2.90	131.45	127.31
28	h	4020	45D	C19-C23-C25	-2.90	121.85	126.23
21	B	1219	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	A	1105	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	a	1125	CLA	OBD-CAD-C3D	-2.90	123.17	127.98
21	B	1211	CLA	CMA-C3A-C4A	2.90	119.56	111.77
24	I	4018	BCR	C15-C14-C13	2.90	131.44	127.31
28	B	4011	45D	O02-C18-C16	-2.89	118.40	120.96
36	I	4020	EQ3	C20-C21-C22	-2.89	123.18	127.31
25	B	5006	LHG	O8-C23-C24	2.89	120.99	111.91
21	a	1125	CLA	CMA-C3A-C4A	2.89	119.55	111.77
24	A	4003	BCR	C19-C18-C17	2.89	123.38	118.94
21	a	1107	CLA	CMA-C3A-C4A	2.89	119.54	111.77
28	B	4011	45D	C31-C33-C35	-2.89	118.30	126.42
24	B	4014	BCR	C39-C30-C25	-2.89	105.61	110.30
21	2	1207	CLA	O2A-CGA-CBA	2.89	120.97	111.91
21	A	1118	CLA	O2D-CGD-CBD	2.89	116.40	111.27
24	7	4013	BCR	C40-C30-C25	-2.89	105.62	110.30
25	a	5003	LHG	O8-C23-C24	2.89	120.97	111.91
21	b	1221	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
21	B	1202	CLA	O2A-CGA-CBA	2.89	120.96	111.91
35	F	6001	LMT	C3'-C4'-C5'	-2.88	104.31	110.93
24	B	4014	BCR	C19-C18-C17	2.88	123.36	118.94
21	7	1302	CLA	CMA-C3A-C4A	2.88	119.52	111.77
21	2	1203	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
21	A	1123	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	a	1012	CLA	CMB-C2B-C3B	2.88	130.06	124.68
24	0	4019	BCR	C40-C30-C25	-2.87	105.64	110.30
21	1	1138	CLA	CMA-C3A-C4A	2.87	119.50	111.77
21	B	1212	CLA	CMA-C3A-C4A	2.87	119.50	111.77
24	1	4003	BCR	C1-C6-C5	-2.87	118.57	122.61
21	B	1201	CLA	O2D-CGD-CBD	2.87	116.37	111.27
21	2	1229	CLA	CMA-C3A-C4A	2.87	119.49	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	I	4020	EQ3	C35-C13-C12	2.87	122.60	118.08
21	1	1127	CLA	CMA-C3A-C4A	2.87	119.49	111.77
24	B	4018	BCR	C15-C14-C13	-2.87	123.22	127.31
25	1	5003	LHG	O8-C23-C24	2.86	120.88	111.91
21	1	1117	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
21	8	1401	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
21	2	1239	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	1	1115	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	1	1121	CLA	CMA-C3A-C4A	2.85	119.44	111.77
24	A	4012	BCR	C38-C26-C25	-2.85	121.33	124.53
24	0	4019	BCR	C34-C9-C10	-2.85	118.93	122.92
24	I	4018	BCR	C40-C30-C25	-2.85	105.68	110.30
24	b	4014	BCR	C19-C18-C17	2.85	123.31	118.94
24	b	4014	BCR	C39-C30-C25	-2.85	105.68	110.30
21	A	1140	CLA	CMA-C3A-C4A	2.85	119.42	111.77
26	B	5002	LMG	O8-C28-C29	2.85	120.84	111.91
24	j	4013	BCR	C39-C30-C25	-2.84	105.69	110.30
24	j	4013	BCR	C8-C9-C10	2.84	123.30	118.94
21	B	1209	CLA	CMA-C3A-C4A	2.84	119.41	111.77
21	a	1011	CLA	CHA-C1A-NA	-2.84	119.89	126.40
24	9	4021	BCR	C30-C25-C24	2.84	123.81	115.78
21	B	1021	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
21	b	1231	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
21	b	1209	CLA	C1-O2A-CGA	2.84	123.89	116.44
21	A	1109	CLA	O2A-CGA-CBA	2.84	120.81	111.91
21	A	1113	CLA	CMA-C3A-C4A	2.84	119.39	111.77
21	2	1215	CLA	C1-O2A-CGA	2.83	123.88	116.44
21	b	1220	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
24	a	4003	BCR	C27-C26-C25	-2.83	118.62	122.73
21	A	1130	CLA	C1-O2A-CGA	2.83	123.88	116.44
21	2	1215	CLA	CMA-C3A-C4A	2.83	119.38	111.77
24	i	4018	BCR	C40-C30-C25	-2.83	105.71	110.30
21	1	1137	CLA	O2A-CGA-CBA	2.83	120.78	111.91
21	1	1137	CLA	CMA-C3A-C4A	2.83	119.37	111.77
21	b	1224	CLA	O2A-CGA-CBA	2.82	120.77	111.91
24	0	4019	BCR	C38-C26-C25	-2.82	121.36	124.53
24	a	4002	BCR	C34-C9-C10	-2.82	118.97	122.92
21	A	1136	CLA	CMA-C3A-C4A	2.82	119.36	111.77
30	2	4006	ECH	C37-C22-C21	2.82	126.87	122.92
21	a	1125	CLA	C1-O2A-CGA	2.82	123.84	116.44
21	b	1240	CLA	CMA-C3A-C4A	2.82	119.34	111.77
25	a	5001	LHG	C5-O7-C7	-2.81	110.86	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1205	CLA	CMA-C3A-C4A	2.81	119.33	111.77
21	1	1107	CLA	CMA-C3A-C4A	2.81	119.32	111.77
24	2	4010	BCR	C34-C9-C10	-2.81	118.99	122.92
21	B	1215	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	2	1204	CLA	C1-O2A-CGA	2.81	123.81	116.44
22	a	2001	PQN	C14-C13-C15	2.81	119.99	115.27
25	0	5002	LHG	O8-C23-C24	2.81	120.72	111.91
21	a	1105	CLA	CMA-C3A-C4A	2.81	119.31	111.77
36	I	4020	EQ3	C10-C11-C12	-2.81	114.46	123.22
26	b	5002	LMG	C7-O1-C1	-2.81	108.26	113.74
21	1	1128	CLA	CMA-C3A-C4A	2.80	119.31	111.77
34	7	4015	ZEX	C39-C29-C30	-2.80	119.00	122.92
21	B	1213	CLA	CMA-C3A-C4A	2.80	119.30	111.77
21	b	1205	CLA	O2A-CGA-CBA	2.80	120.69	111.91
21	B	1212	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
21	1	1135	CLA	CMA-C3A-C4A	2.80	119.29	111.77
21	f	1301	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
21	a	1140	CLA	CMA-C3A-C4A	2.80	119.29	111.77
21	B	1210	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	1	1111	CLA	O2D-CGD-CBD	2.79	116.23	111.27
21	b	1221	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	1	1124	CLA	O2A-CGA-CBA	2.79	120.67	111.91
21	a	1110	CLA	CMA-C3A-C4A	2.79	119.28	111.77
35	1	6001	LMT	C1'-O5'-C5'	-2.79	108.21	113.69
21	B	1208	CLA	CMA-C3A-C4A	2.79	119.27	111.77
24	2	4018	BCR	C36-C18-C19	-2.79	113.68	118.08
21	2	1237	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	a	1101	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	B	1238	CLA	CMA-C3A-C4A	2.79	119.26	111.77
24	A	4002	BCR	C34-C9-C10	-2.78	119.02	122.92
28	h	4020	45D	C31-C33-C35	-2.78	118.60	126.42
21	A	1110	CLA	CMA-C3A-C4A	2.78	119.24	111.77
24	J	4013	BCR	C39-C30-C25	-2.78	105.79	110.30
21	b	1228	CLA	O2D-CGD-CBD	2.78	116.21	111.27
21	f	1302	CLA	CMA-C3A-C4A	2.78	119.24	111.77
26	0	5001	LMG	O8-C28-C29	2.78	120.62	111.91
21	b	1234	CLA	CMA-C3A-C4A	2.78	119.23	111.77
21	A	1125	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
21	A	1112	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
21	b	1207	CLA	O2A-C1-C2	2.77	115.92	108.64
25	A	5006	LHG	O8-C23-C24	2.77	120.60	111.91
21	K	1402	CLA	CMA-C3A-C4A	2.77	119.22	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	1402	CLA	O2A-CGA-CBA	2.77	120.60	111.91
21	2	1239	CLA	O2A-CGA-CBA	2.77	120.59	111.91
21	b	1207	CLA	O2D-CGD-CBD	2.77	116.19	111.27
21	A	1118	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
21	a	1140	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
21	A	1106	CLA	O2A-CGA-CBA	2.77	120.59	111.91
21	A	1122	CLA	O2D-CGD-CBD	2.77	116.18	111.27
21	a	1114	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
21	b	1202	CLA	O2A-CGA-CBA	2.76	120.58	111.91
21	A	1121	CLA	CMA-C3A-C4A	2.76	119.20	111.77
34	7	4015	ZEX	C37-C21-C26	-2.76	105.82	110.30
24	B	4004	BCR	C40-C30-C25	-2.76	105.82	110.30
35	L	6001	LMT	C3B-C4B-C5B	-2.76	105.31	110.24
21	A	1011	CLA	CED-O2D-CGD	-2.76	109.69	115.94
24	1	4007	BCR	C40-C30-C25	-2.76	105.83	110.30
21	B	1234	CLA	CMA-C3A-C4A	2.76	119.18	111.77
24	2	4005	BCR	C38-C26-C25	-2.75	121.44	124.53
21	1	1134	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	2	1226	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	1	1011	CLA	CHA-C1A-NA	-2.75	120.09	126.40
26	K	5009	LMG	O8-C28-C29	2.75	120.55	111.91
22	a	2001	PQN	C12-C11-C3	-2.75	104.63	112.05
21	1	1102	CLA	CMB-C2B-C3B	2.75	129.83	124.68
24	1	4002	BCR	C34-C9-C10	-2.75	119.07	122.92
21	A	1124	CLA	CMB-C2B-C3B	2.75	129.82	124.68
28	B	4011	45D	C28-C26-C30	-2.75	119.07	122.92
24	A	4019	BCR	C8-C7-C6	2.75	134.92	127.20
24	b	4005	BCR	C37-C22-C23	2.75	122.41	118.08
21	A	1120	CLA	CMA-C3A-C4A	2.74	119.15	111.77
24	6	4016	BCR	C12-C13-C14	2.74	123.15	118.94
21	1	1137	CLA	CAA-CBA-CGA	-2.74	105.24	113.25
21	2	1232	CLA	CMA-C3A-C4A	2.74	119.14	111.77
34	F	4016	ZEX	C1-C6-C5	-2.74	118.75	122.61
21	b	1201	CLA	O2D-CGD-CBD	2.74	116.14	111.27
24	I	4018	BCR	C39-C30-C25	-2.74	105.86	110.30
24	a	4008	BCR	C39-C30-C25	-2.74	105.86	110.30
21	A	1120	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
21	A	1112	CLA	O2A-CGA-CBA	2.74	120.49	111.91
21	2	1205	CLA	O2A-CGA-CBA	2.74	120.49	111.91
21	1	1140	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
24	A	4012	BCR	C39-C30-C25	-2.73	105.86	110.30
25	a	5007	LHG	O8-C23-C24	2.73	120.49	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1101	CLA	CHA-C1A-NA	-2.73	120.14	126.40
21	A	1129	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
21	b	1218	CLA	CMB-C2B-C3B	2.73	129.79	124.68
21	1	1118	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
21	b	1218	CLA	CMA-C3A-C4A	2.73	119.11	111.77
24	2	4018	BCR	C29-C28-C27	2.73	117.48	111.38
24	a	4012	BCR	C8-C9-C10	2.73	123.13	118.94
21	2	1219	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	B	4018	BCR	C38-C26-C25	-2.73	121.46	124.53
21	B	1240	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
24	2	4014	BCR	C40-C30-C25	-2.73	105.88	110.30
24	A	4003	BCR	C36-C18-C19	-2.72	113.78	118.08
25	b	5004	LHG	O8-C23-C24	2.72	120.46	111.91
21	A	1107	CLA	CMA-C3A-C4A	2.72	119.09	111.77
21	a	1011	CLA	C2A-C1A-CHA	2.72	128.62	123.86
21	B	1216	CLA	CMA-C3A-C4A	2.72	119.09	111.77
21	B	1238	CLA	O2D-CGD-CBD	2.72	116.10	111.27
21	l	1502	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	1	1116	CLA	CMA-C3A-C4A	2.72	119.08	111.77
26	b	5005	LMG	O8-C28-C29	2.72	120.43	111.91
21	b	1230	CLA	CMA-C3A-C4A	2.71	119.07	111.77
26	A	5008	LMG	O8-C28-C29	2.71	120.42	111.91
24	B	4014	BCR	C36-C18-C19	-2.71	113.81	118.08
26	b	5007	LMG	O8-C28-C29	2.71	120.40	111.91
24	1	4007	BCR	C38-C26-C25	-2.70	121.49	124.53
21	b	1218	CLA	O2D-CGD-CBD	2.70	116.07	111.27
21	2	1234	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
25	a	5001	LHG	O8-C23-C24	2.70	120.39	111.91
21	a	1114	CLA	O2A-CGA-CBA	2.70	120.38	111.91
21	1	1116	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
21	2	1202	CLA	CMA-C3A-C4A	2.70	119.03	111.77
30	m	4021	ECH	C37-C22-C23	-2.70	113.83	118.08
25	A	5005	LHG	C5-O7-C7	-2.70	111.15	117.79
21	2	1201	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
21	B	1022	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
24	f	4016	BCR	C32-C1-C6	-2.70	105.93	110.30
24	B	4017	BCR	C19-C18-C17	2.69	123.08	118.94
24	b	4004	BCR	C38-C26-C25	-2.69	121.50	124.53
24	b	4005	BCR	C39-C30-C25	-2.69	105.93	110.30
21	2	1206	CLA	CMA-C3A-C4A	2.69	119.01	111.77
21	B	1217	CLA	CMA-C3A-C4A	2.69	119.01	111.77
21	a	1115	CLA	CMA-C3A-C4A	2.69	119.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	4001	BCR	C34-C9-C10	-2.69	119.15	122.92
24	a	4007	BCR	C38-C26-C25	-2.69	121.51	124.53
21	a	1119	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
21	L	1501	CLA	CMA-C3A-C4A	2.69	119.00	111.77
24	A	4019	BCR	C34-C9-C10	-2.69	119.16	122.92
21	1	1801	CLA	O2A-CGA-CBA	2.69	120.34	111.91
21	A	1011	CLA	OBD-CAD-CBD	2.69	129.74	125.89
36	I	4020	EQ3	C15-C16-C17	-2.69	117.97	123.47
24	K	4001	BCR	C23-C24-C25	-2.69	119.66	127.20
26	A	5004	LMG	O1-C1-C2	2.69	112.50	108.30
21	a	1119	CLA	CMA-C3A-C4A	2.68	118.99	111.77
21	a	1101	CLA	CHA-C1A-NA	-2.68	120.25	126.40
21	a	1134	CLA	CMA-C3A-C4A	2.68	118.98	111.77
21	2	1211	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
28	B	4011	45D	C19-C23-C25	-2.68	122.18	126.23
21	2	1210	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
24	l	4019	BCR	C40-C30-C25	-2.68	105.95	110.30
21	b	1202	CLA	C1-O2A-CGA	2.68	123.47	116.44
24	b	4017	BCR	C38-C26-C25	-2.68	121.52	124.53
21	K	1401	CLA	CMA-C3A-C4A	2.68	118.97	111.77
24	I	4018	BCR	C12-C13-C14	-2.68	114.83	118.94
24	I	4018	BCR	C2-C1-C6	2.68	114.60	110.48
24	b	4014	BCR	C36-C18-C19	-2.68	113.86	118.08
21	2	1213	CLA	CMA-C3A-C4A	2.68	118.96	111.77
21	2	1220	CLA	CAA-CBA-CGA	-2.67	107.84	113.59
26	2	5005	LMG	O8-C28-C29	2.67	120.30	111.91
24	b	4018	BCR	C38-C26-C25	-2.67	121.53	124.53
21	B	1231	CLA	C1-O2A-CGA	2.67	123.45	116.44
21	1	1106	CLA	CMA-C3A-C4A	2.67	118.95	111.77
21	A	1135	CLA	CMA-C3A-C4A	2.67	118.94	111.77
21	A	1124	CLA	CMA-C3A-C4A	2.67	118.94	111.77
21	B	1230	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
21	8	1402	CLA	CMA-C3A-C4A	2.66	118.93	111.77
21	A	1128	CLA	O2A-CGA-CBA	2.66	120.26	111.91
21	a	1124	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	b	4017	BCR	C34-C9-C10	-2.66	119.19	122.92
34	J	4015	ZEX	C31-C30-C29	-2.66	123.51	127.31
21	1	1130	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	B	1235	CLA	CMA-C3A-C4A	2.66	118.92	111.77
26	1	5004	LMG	O8-C28-C29	2.66	120.25	111.91
21	a	1112	CLA	CMA-C3A-C4A	2.66	118.92	111.77
21	B	1239	CLA	O2A-CGA-CBA	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	i	4018	BCR	C39-C30-C25	-2.66	105.99	110.30
21	0	1501	CLA	CMA-C3A-C4A	2.66	118.91	111.77
24	1	4012	BCR	C39-C30-C25	-2.66	105.99	110.30
25	F	5002	LHG	O8-C23-C24	2.65	120.24	111.91
24	b	4014	BCR	C15-C14-C13	2.65	131.10	127.31
21	A	1130	CLA	CMB-C2B-C3B	2.65	129.64	124.68
21	2	1234	CLA	O2D-CGD-CBD	2.65	115.98	111.27
24	A	4007	BCR	C40-C30-C25	-2.65	106.00	110.30
24	B	4018	BCR	C39-C30-C25	-2.65	106.00	110.30
30	b	4006	ECH	C36-C18-C19	2.65	122.25	118.08
26	A	5004	LMG	O8-C28-C29	2.65	120.22	111.91
24	k	4001	BCR	C40-C30-C25	-2.65	106.01	110.30
21	a	1130	CLA	CMA-C3A-C4A	2.65	118.89	111.77
21	F	1301	CLA	CMB-C2B-C1B	-2.65	124.40	128.46
21	2	1201	CLA	CMA-C3A-C4A	2.65	118.88	111.77
21	B	1218	CLA	CMA-C3A-C4A	2.65	118.88	111.77
24	1	4003	BCR	C39-C30-C25	-2.64	106.01	110.30
24	2	4018	BCR	C34-C9-C10	-2.64	119.22	122.92
24	A	4019	BCR	C35-C13-C14	-2.64	119.22	122.92
24	A	4001	BCR	C35-C13-C12	2.64	122.24	118.08
28	B	4011	45D	C09-C05-C03	2.64	117.42	113.18
21	b	1239	CLA	O2A-CGA-CBA	2.64	120.19	111.91
21	B	1201	CLA	O2A-CGA-CBA	2.64	120.19	111.91
24	b	4010	BCR	C40-C30-C25	-2.64	106.02	110.30
21	b	1204	CLA	C1-O2A-CGA	2.64	123.37	116.44
21	b	1220	CLA	O2A-CGA-CBA	2.64	120.19	111.91
24	2	4014	BCR	C39-C30-C25	-2.64	106.02	110.30
24	L	4019	BCR	C37-C22-C23	2.64	122.23	118.08
26	B	5005	LMG	O8-C28-C29	2.64	120.18	111.91
25	0	5004	LHG	O8-C23-C24	2.64	120.18	111.91
24	A	4002	BCR	C8-C9-C10	2.64	122.98	118.94
24	0	4022	BCR	C34-C9-C10	-2.63	119.24	122.92
25	1	5001	LHG	O8-C23-C24	2.63	120.17	111.91
24	B	4017	BCR	C38-C26-C25	-2.63	121.57	124.53
21	a	1129	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
21	a	1128	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	b	1231	CLA	C1-O2A-CGA	2.63	123.34	116.44
25	1	5001	LHG	C5-O7-C7	-2.63	111.32	117.79
21	J	1302	CLA	C1-O2A-CGA	2.63	123.34	116.44
21	2	1201	CLA	O2A-CGA-CBA	2.63	120.15	111.91
21	B	1023	CLA	CMA-C3A-C4A	2.63	118.83	111.77
25	a	5005	LHG	O8-C23-C24	2.63	120.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	5005	LMG	O1-C7-C8	-2.62	104.57	110.90
24	i	4018	BCR	C38-C26-C25	-2.62	121.58	124.53
21	1	1011	CLA	C2A-C1A-CHA	2.62	128.44	123.86
21	2	1235	CLA	CMA-C3A-C4A	2.62	118.82	111.77
21	1	1801	CLA	CMA-C3A-C4A	2.62	118.81	111.77
24	9	4021	BCR	C34-C9-C10	-2.62	119.26	122.92
30	B	4006	ECH	C8-C7-C6	-2.62	119.86	127.20
21	1	1101	CLA	CHA-C1A-NA	-2.62	120.41	126.40
24	0	4022	BCR	C29-C28-C27	2.62	117.22	111.38
21	k	1402	CLA	O2A-CGA-CBA	2.61	120.11	111.91
24	7	4013	BCR	C8-C9-C10	2.61	122.95	118.94
21	1	1107	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
24	A	4001	BCR	C40-C30-C25	-2.61	106.06	110.30
21	A	1127	CLA	CMB-C2B-C3B	2.61	129.56	124.68
21	k	1402	CLA	CMA-C3A-C4A	2.61	118.79	111.77
21	A	1013	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
21	2	1022	CLA	CMA-C3A-C4A	2.61	118.78	111.77
22	b	2002	PQN	C2M-C2-C3	-2.61	120.15	124.40
21	B	1204	CLA	O2A-CGA-CBA	2.61	120.08	111.91
25	l	5001	LHG	O8-C23-C24	2.61	120.08	111.91
21	B	1023	CLA	O2D-CGD-CBD	2.60	115.90	111.27
21	a	1102	CLA	CMA-C3A-C4A	2.60	118.77	111.77
21	b	1237	CLA	C1-O2A-CGA	2.60	123.28	116.44
21	A	1801	CLA	O2A-CGA-CBA	2.60	120.08	111.91
21	B	1217	CLA	C1-O2A-CGA	2.60	123.28	116.44
21	b	1023	CLA	O2D-CGD-CBD	2.60	115.89	111.27
21	b	1219	CLA	O2A-CGA-CBA	2.60	120.07	111.91
21	A	1138	CLA	CMA-C3A-C4A	2.60	118.77	111.77
21	1	1102	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
21	2	1219	CLA	CHA-C1A-NA	-2.60	120.44	126.40
24	J	4013	BCR	C40-C30-C25	-2.60	106.09	110.30
24	b	4004	BCR	C30-C25-C26	-2.60	118.96	122.61
21	a	1118	CLA	CMA-C3A-C4A	2.60	118.75	111.77
21	2	1224	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	a	4008	BCR	C40-C30-C25	-2.60	106.09	110.30
21	B	1202	CLA	C1-O2A-CGA	2.60	123.25	116.44
21	a	1114	CLA	C1-O2A-CGA	2.59	123.25	116.44
30	b	4006	ECH	C20-C19-C18	2.59	133.71	126.42
21	A	1125	CLA	OBD-CAD-C3D	-2.59	123.67	127.98
24	B	4017	BCR	C36-C18-C19	-2.59	113.99	118.08
21	B	1206	CLA	C1-O2A-CGA	2.59	123.25	116.44
21	a	1122	CLA	CMB-C2B-C1B	-2.59	124.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1125	CLA	C1-O2A-CGA	2.59	123.25	116.44
24	2	4010	BCR	C8-C9-C10	2.59	122.91	118.94
21	b	1229	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	L	1502	CLA	CMA-C3A-C4A	2.59	118.73	111.77
25	l	5004	LHG	O8-C23-C24	2.59	120.03	111.91
21	B	1227	CLA	CMA-C3A-C4A	2.59	118.73	111.77
24	2	4018	BCR	C23-C24-C25	2.59	134.47	127.20
21	2	1230	CLA	CMA-C3A-C4A	2.59	118.72	111.77
24	a	4002	BCR	C8-C9-C10	2.59	122.91	118.94
21	1	1129	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
21	B	1204	CLA	C1-O2A-CGA	2.59	123.23	116.44
24	1	4007	BCR	C39-C30-C25	-2.59	106.11	110.30
21	2	1222	CLA	CMA-C3A-C4A	2.58	118.72	111.77
30	m	4021	ECH	C28-C27-C26	-2.58	116.27	118.65
21	A	1115	CLA	CMA-C3A-C4A	2.58	118.72	111.77
21	b	1203	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
21	f	1301	CLA	CMA-C3A-C4A	2.58	118.71	111.77
21	0	1501	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
25	L	5005	LHG	O8-C23-C24	2.58	120.00	111.91
24	b	4004	BCR	C34-C9-C10	-2.58	119.31	122.92
21	2	1223	CLA	O2A-CGA-CBA	2.58	120.00	111.91
34	7	4015	ZEX	C31-C30-C29	-2.58	123.63	127.31
21	2	1202	CLA	O2A-CGA-CBA	2.58	120.00	111.91
24	A	4007	BCR	C34-C9-C10	-2.58	119.31	122.92
24	1	4019	BCR	C40-C30-C25	-2.58	106.12	110.30
24	A	4002	BCR	C35-C13-C12	2.58	122.14	118.08
36	I	4020	EQ3	C38-C26-C27	2.58	119.31	115.48
36	I	4020	EQ3	C29-C30-C25	2.57	114.44	110.48
21	l	1503	CLA	CMB-C2B-C3B	2.57	129.49	124.68
21	a	1112	CLA	O2A-CGA-CBA	2.57	119.98	111.91
25	l	5003	LHG	O8-C23-C24	2.57	119.98	111.91
21	A	1012	CLA	CHA-C1A-NA	-2.57	120.51	126.40
21	6	1301	CLA	CMA-C3A-C4A	2.57	118.69	111.77
21	1	1011	CLA	O2A-CGA-CBA	2.57	119.98	111.91
21	B	1213	CLA	CMB-C2B-C3B	2.57	129.49	124.68
24	A	4019	BCR	C15-C14-C13	-2.57	123.65	127.31
21	K	1401	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
21	2	1230	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
21	B	1221	CLA	CMA-C3A-C4A	2.56	118.67	111.77
21	b	1236	CLA	O2A-CGA-CBA	2.56	119.94	111.91
21	B	1214	CLA	O2A-CGA-CBA	2.56	119.94	111.91
24	a	4012	BCR	C34-C9-C10	-2.56	119.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	J	4015	ZEX	C40-C33-C34	-2.56	119.34	122.92
21	b	1225	CLA	CMA-C3A-C4A	2.56	118.65	111.77
25	A	5007	LHG	O7-C7-O9	-2.56	117.53	123.70
24	B	4017	BCR	C40-C30-C25	-2.56	106.15	110.30
24	a	4003	BCR	C39-C30-C25	-2.55	106.16	110.30
21	B	1201	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
24	6	4016	BCR	C30-C25-C26	-2.55	119.02	122.61
25	1	5005	LHG	O8-C23-C24	2.55	119.92	111.91
30	i	4020	ECH	C28-C27-C26	-2.55	116.30	118.65
21	b	1226	CLA	CMA-C3A-C4A	2.55	118.63	111.77
21	2	1222	CLA	O2A-CGA-CBA	2.55	119.91	111.91
21	B	1238	CLA	C1-O2A-CGA	2.55	123.13	116.44
21	B	1210	CLA	CAC-C3C-C4C	2.55	128.12	124.81
21	2	1221	CLA	CMB-C2B-C1B	-2.55	124.55	128.46
30	2	4006	ECH	C8-C7-C6	-2.55	120.05	127.20
21	1	1101	CLA	O2A-CGA-CBA	2.55	119.90	111.91
24	9	4021	BCR	C8-C9-C10	2.55	122.85	118.94
21	a	1137	CLA	O2A-CGA-CBA	2.54	119.89	111.91
21	2	1214	CLA	CMA-C3A-C4A	2.54	118.61	111.77
21	A	1134	CLA	CMA-C3A-C4A	2.54	118.60	111.77
21	B	1239	CLA	CMA-C3A-C4A	2.54	118.60	111.77
24	2	4018	BCR	C30-C25-C24	2.54	122.96	115.78
25	A	5007	LHG	O8-C23-C24	2.54	119.88	111.91
24	L	4022	BCR	C39-C30-C25	-2.54	106.18	110.30
21	b	1236	CLA	CMA-C3A-C4A	2.54	118.59	111.77
25	l	5002	LHG	O8-C23-C24	2.54	119.87	111.91
24	A	4019	BCR	C30-C25-C26	-2.53	119.04	122.61
21	1	1128	CLA	O2A-CGA-CBA	2.53	119.86	111.91
24	1	4012	BCR	C40-C30-C25	-2.53	106.19	110.30
21	2	1207	CLA	CMA-C3A-C4A	2.53	118.58	111.77
21	A	1138	CLA	C1-O2A-CGA	2.53	123.09	116.44
24	1	4001	BCR	C40-C30-C25	-2.53	106.19	110.30
24	A	4003	BCR	C39-C30-C25	-2.53	106.19	110.30
21	6	1302	CLA	CHA-C1A-NA	-2.53	120.60	126.40
21	b	1238	CLA	C1-O2A-CGA	2.53	123.08	116.44
21	1	1128	CLA	C1-O2A-CGA	2.53	123.08	116.44
21	a	1105	CLA	O2A-CGA-CBA	2.53	119.85	111.91
36	I	4020	EQ3	C7-C6-C5	-2.53	115.33	121.46
21	b	1214	CLA	O2A-CGA-CBA	2.53	119.84	111.91
24	B	4014	BCR	C40-C30-C25	-2.53	106.20	110.30
24	b	4014	BCR	C40-C30-C25	-2.53	106.20	110.30
21	a	1136	CLA	C1-O2A-CGA	2.53	123.07	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1127	CLA	CMA-C3A-C4A	2.52	118.56	111.77
30	2	4006	ECH	C11-C10-C9	-2.52	123.71	127.31
21	A	1138	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
24	2	4010	BCR	C39-C30-C25	-2.52	106.21	110.30
21	b	1206	CLA	C1-O2A-CGA	2.52	123.06	116.44
21	1	1111	CLA	CMA-C3A-C4A	2.52	118.55	111.77
21	a	1104	CLA	CMA-C3A-C4A	2.52	118.55	111.77
30	i	4020	ECH	C28-C29-C30	-2.52	109.14	113.18
30	i	4020	ECH	C29-C30-C25	-2.52	106.60	110.48
21	A	1112	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	l	1503	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	B	1211	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
21	a	1116	CLA	O2A-CGA-CBA	2.52	119.81	111.91
24	a	4001	BCR	C40-C30-C25	-2.52	106.22	110.30
37	L	5004	DGD	O1G-C1A-C2A	2.52	119.80	111.91
21	a	1129	CLA	C1-O2A-CGA	2.52	123.04	116.44
21	2	1236	CLA	O2D-CGD-CBD	2.51	115.74	111.27
21	A	1134	CLA	O2A-CGA-CBA	2.51	119.79	111.91
21	2	1210	CLA	CMA-C3A-C4A	2.51	118.53	111.77
25	A	5003	LHG	C5-O7-C7	-2.51	111.61	117.79
21	A	1120	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	A	4002	BCR	C38-C26-C25	-2.51	121.71	124.53
21	6	1302	CLA	C2A-C1A-CHA	2.51	128.25	123.86
21	A	1116	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	a	4008	BCR	C40-C30-C29	2.51	118.94	108.91
21	a	1139	CLA	C1-O2A-CGA	2.51	123.02	116.44
21	A	1013	CLA	C1-O2A-CGA	2.51	123.02	116.44
21	b	1218	CLA	O2A-CGA-CBA	2.51	119.77	111.91
24	B	4010	BCR	C39-C30-C25	-2.51	106.23	110.30
21	B	1225	CLA	O2A-CGA-CBA	2.50	119.76	111.91
21	a	1118	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
21	1	1104	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
21	b	1206	CLA	CMA-C3A-C4A	2.50	118.49	111.77
24	A	4001	BCR	C8-C9-C10	2.50	122.77	118.94
28	B	4011	45D	C30-C32-C34	-2.50	115.42	123.22
24	1	4012	BCR	C40-C30-C29	2.50	118.89	108.91
30	i	4020	ECH	C24-C23-C22	-2.50	122.46	126.23
21	B	1223	CLA	O2A-CGA-CBA	2.50	119.74	111.91
21	b	1225	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
21	2	1227	CLA	CMA-C3A-C4A	2.49	118.48	111.77
21	l	1501	CLA	CMA-C3A-C4A	2.49	118.48	111.77
21	b	1207	CLA	O2A-CGA-CBA	2.49	119.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	M	5001	LHG	O8-C23-C24	2.49	119.73	111.91
24	2	4010	BCR	C38-C26-C25	-2.49	121.73	124.53
21	A	1128	CLA	C1-O2A-CGA	2.49	122.98	116.44
21	1	1111	CLA	CAC-C3C-C4C	2.49	128.04	124.81
21	B	1237	CLA	CMA-C3A-C4A	2.49	118.46	111.77
25	A	5005	LHG	O8-C23-C24	2.49	119.72	111.91
25	M	5001	LHG	O7-C7-O9	-2.49	117.69	123.70
21	2	1214	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
21	a	1134	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
28	h	4020	45D	C21-C15-C07	-2.49	120.11	124.11
21	1	1012	CLA	CHA-C1A-NA	-2.49	120.70	126.40
21	a	1106	CLA	CMA-C3A-C4A	2.49	118.46	111.77
25	B	5004	LHG	C5-O7-C7	-2.49	111.67	117.79
21	b	1208	CLA	C1-O2A-CGA	2.49	122.97	116.44
21	A	1101	CLA	O2A-CGA-CBA	2.48	119.71	111.91
21	1	1126	CLA	O2A-CGA-CBA	2.48	119.71	111.91
21	F	1301	CLA	CMA-C3A-C4A	2.48	118.45	111.77
24	A	4012	BCR	C40-C30-C29	2.48	118.84	108.91
21	2	1213	CLA	O2A-CGA-CBA	2.48	119.70	111.91
21	B	1204	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	L	1503	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	A	1127	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
24	h	4018	BCR	C40-C30-C29	2.48	118.82	108.91
25	a	5003	LHG	C5-O7-C7	-2.48	111.69	117.79
34	j	4015	ZEX	C19-C9-C10	-2.48	119.45	122.92
21	A	1011	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
24	0	4022	BCR	C38-C26-C25	-2.48	121.75	124.53
21	a	1133	CLA	CMA-C3A-C4A	2.48	118.43	111.77
24	b	4018	BCR	C40-C30-C29	2.47	118.80	108.91
24	a	4002	BCR	C38-C26-C25	-2.47	121.75	124.53
24	L	4019	BCR	C34-C9-C10	-2.47	119.46	122.92
26	a	5002	LMG	O8-C28-C29	2.47	119.66	111.91
24	i	4018	BCR	C37-C22-C23	2.47	121.97	118.08
21	2	1237	CLA	O2A-CGA-CBA	2.47	119.65	111.91
21	b	1240	CLA	O2A-CGA-CBA	2.47	119.65	111.91
26	2	5002	LMG	O8-C28-C29	2.47	119.65	111.91
21	0	1503	CLA	O2A-CGA-CBA	2.47	119.65	111.91
24	a	4001	BCR	C40-C30-C29	2.47	118.78	108.91
21	b	1208	CLA	CMA-C3A-C4A	2.47	118.41	111.77
21	a	1012	CLA	CMA-C3A-C4A	2.47	118.41	111.77
24	1	4007	BCR	C40-C30-C29	2.47	118.77	108.91
21	1	1127	CLA	O2A-CGA-CBA	2.47	119.65	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	4013	BCR	C40-C30-C29	2.46	118.76	108.91
21	A	1101	CLA	C1-O2A-CGA	2.46	122.91	116.44
24	L	4022	BCR	C35-C13-C12	2.46	121.96	118.08
24	A	4003	BCR	C40-C30-C29	2.46	118.75	108.91
24	i	4018	BCR	C40-C30-C29	2.46	118.75	108.91
21	b	1212	CLA	CHA-C1A-NA	-2.46	120.76	126.40
24	b	4004	BCR	C40-C30-C29	2.46	118.75	108.91
24	I	4018	BCR	C40-C30-C29	2.46	118.75	108.91
24	2	4014	BCR	C40-C30-C29	2.46	118.75	108.91
24	2	4017	BCR	C40-C30-C29	2.46	118.75	108.91
24	B	4014	BCR	C34-C9-C10	-2.46	119.48	122.92
24	a	4019	BCR	C40-C30-C29	2.46	118.74	108.91
24	2	4005	BCR	C40-C30-C29	2.46	118.74	108.91
24	9	4021	BCR	C40-C30-C29	2.46	118.73	108.91
24	b	4014	BCR	C40-C30-C29	2.46	118.73	108.91
24	b	4017	BCR	C40-C30-C29	2.46	118.73	108.91
25	A	5003	LHG	O8-C23-C24	2.46	119.61	111.91
34	F	4016	ZEX	C11-C12-C13	-2.46	119.52	126.42
24	a	4002	BCR	C40-C30-C29	2.46	118.73	108.91
24	B	4005	BCR	C40-C30-C29	2.45	118.72	108.91
24	6	4016	BCR	C40-C30-C29	2.45	118.72	108.91
24	J	4013	BCR	C40-C30-C29	2.45	118.72	108.91
21	2	1210	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	l	4019	BCR	C40-C30-C29	2.45	118.72	108.91
24	A	4001	BCR	C40-C30-C29	2.45	118.72	108.91
21	b	1022	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	0	4022	BCR	C40-C30-C29	2.45	118.71	108.91
21	1	1118	CLA	CMA-C3A-C4A	2.45	118.36	111.77
24	A	4007	BCR	C40-C30-C29	2.45	118.71	108.91
21	j	1303	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
24	b	4005	BCR	C40-C30-C29	2.45	118.71	108.91
24	a	4007	BCR	C40-C30-C29	2.45	118.70	108.91
24	1	4003	BCR	C40-C30-C29	2.45	118.70	108.91
21	a	1138	CLA	O2A-CGA-CBA	2.45	119.59	111.91
21	a	1133	CLA	O2A-CGA-CBA	2.45	119.59	111.91
21	1	1011	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
21	b	1220	CLA	CMA-C3A-C4A	2.45	118.35	111.77
21	1	1013	CLA	CMB-C2B-C3B	2.45	129.26	124.68
24	L	4022	BCR	C40-C30-C29	2.45	118.69	108.91
24	8	4001	BCR	C40-C30-C29	2.45	118.69	108.91
21	a	1012	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
24	2	4018	BCR	C40-C30-C29	2.45	118.69	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	4017	BCR	C40-C30-C29	2.45	118.69	108.91
24	B	4018	BCR	C40-C30-C29	2.45	118.69	108.91
24	1	4003	BCR	C40-C30-C25	-2.45	106.33	110.30
24	K	4001	BCR	C40-C30-C29	2.45	118.69	108.91
24	a	4003	BCR	C40-C30-C29	2.45	118.69	108.91
24	A	4002	BCR	C40-C30-C29	2.44	118.68	108.91
24	B	4004	BCR	C40-C30-C29	2.44	118.68	108.91
21	2	1236	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	8	4001	BCR	C29-C28-C27	2.44	116.84	111.38
24	2	4011	BCR	C40-C30-C29	2.44	118.68	108.91
21	b	1228	CLA	CMA-C3A-C4A	2.44	118.34	111.77
24	7	4013	BCR	C40-C30-C29	2.44	118.68	108.91
24	f	4016	BCR	C40-C30-C29	2.44	118.67	108.91
24	2	4010	BCR	C40-C30-C29	2.44	118.67	108.91
24	k	4001	BCR	C38-C26-C25	-2.44	121.79	124.53
24	l	4019	BCR	C38-C26-C25	-2.44	121.79	124.53
24	1	4002	BCR	C40-C30-C29	2.44	118.67	108.91
21	B	1222	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
24	l	4022	BCR	C40-C30-C29	2.44	118.66	108.91
36	I	4020	EQ3	C38-C26-C25	-2.44	120.19	124.11
30	i	4020	ECH	C8-C9-C10	-2.44	115.20	118.94
21	B	1232	CLA	O2A-CGA-CBA	2.44	119.56	111.91
21	A	1138	CLA	O2D-CGD-CBD	2.44	115.60	111.27
24	1	4019	BCR	C40-C30-C29	2.44	118.65	108.91
21	b	1235	CLA	CMA-C3A-C4A	2.44	118.32	111.77
21	2	1204	CLA	CMA-C3A-C4A	2.44	118.32	111.77
30	2	4006	ECH	C36-C18-C19	-2.44	114.24	118.08
24	1	4008	BCR	C37-C22-C23	2.44	121.91	118.08
24	1	4008	BCR	C40-C30-C29	2.43	118.64	108.91
21	K	1401	CLA	CAA-C2A-C1A	-2.43	104.00	111.97
21	1	1112	CLA	O2A-CGA-CBA	2.43	119.54	111.91
21	1	1119	CLA	CMA-C3A-C4A	2.43	118.31	111.77
21	1	1115	CLA	C1-O2A-CGA	2.43	122.82	116.44
21	1	1132	CLA	CMB-C2B-C3B	2.43	129.22	124.68
24	L	4019	BCR	C40-C30-C29	2.43	118.62	108.91
24	0	4019	BCR	C40-C30-C29	2.43	118.62	108.91
21	A	1105	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	1	5007	LHG	O8-C23-C24	2.43	119.53	111.91
24	2	4004	BCR	C38-C26-C25	-2.43	121.80	124.53
24	2	4014	BCR	C19-C18-C17	2.43	122.67	118.94
24	J	4013	BCR	C34-C9-C10	-2.43	119.52	122.92
24	L	4022	BCR	C15-C14-C13	2.43	130.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	4001	BCR	C30-C25-C26	-2.43	119.19	122.61
21	A	1104	CLA	CMB-C2B-C3B	2.43	129.22	124.68
24	A	4019	BCR	C40-C30-C29	2.43	118.61	108.91
24	A	4002	BCR	C37-C22-C23	2.43	121.90	118.08
21	a	1118	CLA	O2A-CGA-CBA	2.43	119.52	111.91
24	1	4001	BCR	C40-C30-C29	2.43	118.61	108.91
21	b	1232	CLA	O2A-CGA-CBA	2.43	119.52	111.91
24	a	4012	BCR	C40-C30-C29	2.43	118.61	108.91
24	a	4019	BCR	C35-C13-C14	-2.42	119.53	122.92
21	a	1103	CLA	CMA-C3A-C4A	2.42	118.28	111.77
21	2	1218	CLA	O2A-CGA-CBA	2.42	119.51	111.91
21	A	1117	CLA	O2A-CGA-CBA	2.42	119.50	111.91
24	B	4010	BCR	C40-C30-C29	2.42	118.58	108.91
25	a	5007	LHG	C5-O7-C7	-2.42	111.84	117.79
24	b	4010	BCR	C40-C30-C29	2.42	118.58	108.91
24	B	4014	BCR	C40-C30-C29	2.42	118.58	108.91
30	B	4006	ECH	C12-C13-C14	2.42	122.65	118.94
24	1	4008	BCR	C38-C26-C25	-2.42	121.81	124.53
30	i	4020	ECH	C7-C6-C5	-2.42	115.61	121.46
24	B	4010	BCR	C34-C9-C10	-2.42	119.54	122.92
24	a	4003	BCR	C40-C30-C25	-2.42	106.38	110.30
28	h	4020	45D	C10-C18-C16	2.42	120.88	118.65
24	2	4010	BCR	C19-C18-C17	2.42	122.65	118.94
24	2	4004	BCR	C40-C30-C29	2.41	118.56	108.91
21	1	1136	CLA	O2A-CGA-CBA	2.41	119.48	111.91
21	a	1136	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
21	2	1209	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
21	b	1217	CLA	O2A-CGA-CBA	2.41	119.47	111.91
30	M	4021	ECH	C23-C24-C25	-2.41	120.44	127.20
21	1	1135	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
25	B	5006	LHG	C5-O7-C7	-2.41	111.87	117.79
21	A	1103	CLA	CMB-C2B-C3B	2.41	129.18	124.68
21	b	1230	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
21	B	1239	CLA	C1-O2A-CGA	2.40	122.75	116.44
25	B	5004	LHG	O8-C23-C24	2.40	119.45	111.91
21	1	1503	CLA	O2A-CGA-CBA	2.40	119.45	111.91
21	2	1206	CLA	O2A-CGA-CBA	2.40	119.45	111.91
21	A	1127	CLA	O2A-CGA-CBA	2.40	119.45	111.91
21	a	1113	CLA	CMB-C2B-C3B	2.40	129.17	124.68
21	b	1201	CLA	CMA-C3A-C4A	2.40	118.23	111.77
21	J	1303	CLA	O2A-CGA-CBA	2.40	119.44	111.91
21	B	1206	CLA	CMA-C3A-C4A	2.40	118.22	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	4017	BCR	C40-C30-C25	-2.40	106.41	110.30
28	B	4011	45D	C24-C26-C30	2.40	122.62	118.94
21	1	1116	CLA	O2A-CGA-CBA	2.40	119.43	111.91
21	B	1023	CLA	O2A-CGA-CBA	2.39	119.42	111.91
21	a	1012	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	A	4008	BCR	C40-C30-C29	2.39	118.48	108.91
24	a	4019	BCR	C30-C25-C26	-2.39	119.24	122.61
24	7	4013	BCR	C29-C28-C27	2.39	116.73	111.38
21	b	1227	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	f	1302	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	b	1212	CLA	C1-O2A-CGA	2.39	122.72	116.44
24	k	4001	BCR	C40-C30-C29	2.39	118.47	108.91
21	b	1213	CLA	C1-O2A-CGA	2.39	122.72	116.44
31	f	5001	SQD	O3-C3-C2	-2.39	104.82	110.35
21	1	1801	CLA	C1-O2A-CGA	2.39	122.72	116.44
24	a	4012	BCR	C30-C25-C26	-2.39	119.25	122.61
21	1	1102	CLA	C1-O2A-CGA	2.39	122.71	116.44
26	b	5005	LMG	O6-C1-O1	-2.39	104.32	109.97
28	B	4011	45D	C21-C15-C07	-2.39	120.27	124.11
24	a	4007	BCR	C34-C9-C10	-2.38	119.58	122.92
21	b	1210	CLA	O2A-CGA-CBA	2.38	119.39	111.91
21	2	1216	CLA	CHA-C1A-NA	-2.38	120.94	126.40
21	b	1225	CLA	CMB-C2B-C3B	2.38	129.13	124.68
21	a	1128	CLA	O2A-CGA-CBA	2.38	119.38	111.91
21	a	1121	CLA	CMB-C2B-C3B	2.38	129.13	124.68
21	A	1129	CLA	CMB-C2B-C3B	2.38	129.13	124.68
21	l	1503	CLA	C1-O2A-CGA	2.38	122.69	116.44
21	b	1227	CLA	CMA-C3A-C4A	2.38	118.17	111.77
21	2	1239	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
21	a	1115	CLA	OBD-CAD-C3D	-2.38	124.03	127.98
25	b	5004	LHG	C5-O7-C7	-2.38	111.94	117.79
21	B	1205	CLA	O2A-CGA-CBA	2.38	119.36	111.91
21	B	1209	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
21	2	1023	CLA	O2A-CGA-CBA	2.37	119.36	111.91
21	B	1206	CLA	O2A-CGA-CBA	2.37	119.36	111.91
24	A	4003	BCR	C1-C6-C7	2.37	122.50	115.78
21	L	1501	CLA	CMB-C2B-C3B	2.37	129.12	124.68
36	I	4020	EQ3	C37-C22-C23	2.37	121.82	118.08
24	b	4018	BCR	C29-C28-C27	2.37	116.68	111.38
21	A	1012	CLA	C2A-C1A-CHA	2.37	128.01	123.86
21	1	1013	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
21	b	1219	CLA	C1-O2A-CGA	2.37	122.66	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	1102	CLA	O2A-CGA-CBA	2.37	119.35	111.91
21	1	1121	CLA	CHA-C1A-NA	-2.37	120.97	126.40
21	A	1113	CLA	O2A-CGA-CBA	2.37	119.34	111.91
24	B	4014	BCR	C8-C9-C10	2.37	122.58	118.94
25	2	5004	LHG	C5-O7-C7	-2.37	111.96	117.79
34	7	4015	ZEX	C40-C33-C34	-2.37	119.61	122.92
21	A	1012	CLA	O2A-CGA-CBA	2.37	119.34	111.91
21	a	1106	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
36	I	4020	EQ3	C12-C13-C14	-2.37	115.31	118.94
24	A	4012	BCR	C34-C9-C10	-2.37	119.61	122.92
24	a	4001	BCR	C27-C26-C25	-2.36	119.30	122.73
21	2	1203	CLA	CMA-C3A-C4A	2.36	118.13	111.77
22	B	2002	PQN	O4-C4-C5	-2.36	117.73	121.56
24	1	4008	BCR	C29-C28-C27	2.36	116.66	111.38
25	2	5004	LHG	O8-C23-C24	2.36	119.33	111.91
21	b	1216	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	B	1220	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	b	1223	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	2	1219	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
21	A	1129	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	1	1139	CLA	C1-O2A-CGA	2.36	122.64	116.44
21	A	1120	CLA	C1-O2A-CGA	2.36	122.64	116.44
24	0	4022	BCR	C8-C9-C10	2.36	122.56	118.94
28	h	4020	45D	C03-C07-C19	2.36	122.45	115.78
21	a	1111	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	2	1214	CLA	CHA-C1A-NA	-2.36	121.00	126.40
21	B	1210	CLA	CHA-C1A-NA	-2.36	121.00	126.40
21	A	1134	CLA	CHA-C1A-NA	-2.36	121.00	126.40
22	b	2002	PQN	O1-C1-C10	-2.36	117.74	121.56
21	1	1111	CLA	CHA-C1A-NA	-2.36	121.00	126.40
24	I	4018	BCR	C32-C1-C6	-2.36	106.47	110.30
21	k	1402	CLA	C1-O2A-CGA	2.36	122.63	116.44
21	A	1125	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	b	1209	CLA	O2A-CGA-CBA	2.36	119.31	111.91
21	B	1205	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	b	1022	CLA	CMA-C3A-C4A	2.36	118.11	111.77
24	B	4005	BCR	C34-C9-C10	-2.36	119.62	122.92
24	a	4002	BCR	C29-C28-C27	2.36	116.64	111.38
24	0	4019	BCR	C32-C1-C6	-2.36	106.48	110.30
24	2	4014	BCR	C36-C18-C19	-2.36	114.36	118.08
21	a	1103	CLA	CMB-C2B-C3B	2.36	129.09	124.68
21	B	1213	CLA	CHA-C1A-NA	-2.35	121.01	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	1121	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
21	b	1225	CLA	O2A-CGA-CBA	2.35	119.29	111.91
21	2	1212	CLA	CAA-C2A-C3A	-2.35	110.61	116.10
21	b	1239	CLA	CMA-C3A-C4A	2.35	118.09	111.77
24	b	4017	BCR	C40-C30-C25	-2.35	106.48	110.30
30	M	4021	ECH	C28-C27-C26	-2.35	116.48	118.65
21	2	1218	CLA	CMB-C2B-C3B	2.35	129.08	124.68
24	2	4018	BCR	C40-C30-C25	-2.35	106.49	110.30
21	0	1503	CLA	CMA-C3A-C4A	2.35	118.09	111.77
21	a	1011	CLA	O2A-CGA-CBA	2.35	119.28	111.91
21	b	1212	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
21	1	1130	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	2	1234	CLA	O2A-CGA-CBA	2.35	119.28	111.91
24	2	4018	BCR	C8-C9-C10	2.35	122.54	118.94
21	B	1210	CLA	O2A-CGA-CBA	2.35	119.28	111.91
21	L	1503	CLA	O2A-CGA-CBA	2.35	119.27	111.91
22	A	2001	PQN	C2M-C2-C3	-2.35	120.57	124.40
21	b	1204	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	B	1229	CLA	O2A-CGA-CBA	2.35	119.27	111.91
21	1	1133	CLA	CMA-C3A-C4A	2.34	118.07	111.77
21	1	1130	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
21	1	1111	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
24	a	4008	BCR	C32-C1-C6	-2.34	106.50	110.30
21	A	1135	CLA	O2D-CGD-CBD	2.34	115.43	111.27
21	1	1124	CLA	C1-O2A-CGA	2.34	122.58	116.44
21	b	1022	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	A	1011	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
21	2	1226	CLA	O2A-CGA-CBA	2.34	119.24	111.91
21	1	1105	CLA	O2A-CGA-CBA	2.34	119.24	111.91
21	B	1208	CLA	O2A-CGA-CBA	2.34	119.24	111.91
30	M	4021	ECH	C8-C7-C6	-2.34	120.64	127.20
21	A	1109	CLA	CMA-C3A-C4A	2.34	118.05	111.77
21	B	1207	CLA	C1-O2A-CGA	2.34	122.57	116.44
24	A	4008	BCR	C32-C1-C6	-2.33	106.51	110.30
30	m	4021	ECH	C23-C24-C25	-2.33	120.65	127.20
21	1	1013	CLA	CMA-C3A-C4A	2.33	118.04	111.77
31	B	5008	SQD	O3-C3-C2	-2.33	104.96	110.35
30	b	4006	ECH	C15-C16-C17	-2.33	118.70	123.47
21	A	1106	CLA	CMA-C3A-C4A	2.33	118.04	111.77
24	a	4007	BCR	C35-C13-C12	2.33	121.75	118.08
24	2	4010	BCR	C36-C18-C19	-2.33	114.40	118.08
21	b	1218	CLA	CMB-C2B-C1B	-2.33	124.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1104	CLA	CMA-C3A-C4A	2.33	118.04	111.77
30	i	4020	ECH	C35-C13-C12	-2.33	114.41	118.08
24	K	4001	BCR	C34-C9-C10	-2.33	119.66	122.92
24	B	4005	BCR	C39-C30-C25	-2.33	106.52	110.30
21	2	1216	CLA	CMA-C3A-C4A	2.33	118.03	111.77
21	2	1236	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
21	2	1224	CLA	CMA-C3A-C4A	2.33	118.03	111.77
24	b	4004	BCR	C24-C25-C26	-2.33	115.83	121.46
21	a	1113	CLA	O2A-CGA-CBA	2.33	119.21	111.91
24	B	4018	BCR	C34-C9-C10	-2.33	119.66	122.92
21	a	1012	CLA	CHA-C1A-NA	-2.33	121.07	126.40
24	2	4014	BCR	C8-C9-C10	2.33	122.51	118.94
24	a	4001	BCR	C39-C30-C25	-2.33	106.53	110.30
21	a	1121	CLA	CHA-C1A-NA	-2.32	121.07	126.40
21	l	1501	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
21	1	1102	CLA	CAA-CBA-CGA	-2.32	106.46	113.25
21	b	1215	CLA	O2A-CGA-CBA	2.32	119.19	111.91
21	1	1107	CLA	O2A-CGA-CBA	2.32	119.19	111.91
21	1	1133	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	2	4018	BCR	C37-C22-C23	2.32	121.73	118.08
21	b	1221	CLA	C6-C7-C8	-2.32	108.42	115.92
21	l	1501	CLA	O2A-CGA-CBA	2.32	119.19	111.91
34	j	4015	ZEX	C11-C12-C13	-2.32	119.90	126.42
26	1	5002	LMG	O8-C28-C29	2.32	119.18	111.91
21	a	1122	CLA	C1-O2A-CGA	2.32	122.53	116.44
25	a	5005	LHG	O7-C7-O9	-2.32	118.10	123.70
21	b	1021	CLA	O2A-CGA-CBA	2.32	119.18	111.91
21	b	1201	CLA	O2A-CGA-CBA	2.32	119.18	111.91
21	2	1221	CLA	CMA-C3A-C4A	2.32	118.00	111.77
21	b	1234	CLA	CMB-C2B-C3B	2.32	129.01	124.68
21	A	1111	CLA	CMA-C3A-C4A	2.32	118.00	111.77
25	0	5004	LHG	C5-O7-C7	-2.31	112.09	117.79
24	b	4004	BCR	C19-C18-C17	2.31	122.49	118.94
21	A	1104	CLA	CHA-C1A-NA	-2.31	121.10	126.40
21	A	1137	CLA	O2A-CGA-CBA	2.31	119.17	111.91
21	a	1125	CLA	O2A-CGA-CBA	2.31	119.17	111.91
24	L	4022	BCR	C12-C13-C14	-2.31	115.39	118.94
24	2	4017	BCR	C39-C30-C25	-2.31	106.55	110.30
24	a	4019	BCR	C34-C9-C10	-2.31	119.68	122.92
26	B	5002	LMG	C7-O1-C1	-2.31	109.22	113.74
21	1	1111	CLA	C1-O2A-CGA	2.31	122.51	116.44
24	1	4012	BCR	C37-C22-C23	2.31	121.72	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1023	CLA	CMB-C2B-C3B	2.31	129.00	124.68
21	a	1119	CLA	CMB-C2B-C3B	2.31	129.00	124.68
21	2	1021	CLA	O2A-CGA-CBA	2.31	119.16	111.91
21	B	1222	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
21	B	1219	CLA	O2A-CGA-CBA	2.31	119.15	111.91
21	2	1224	CLA	CHA-C1A-NA	-2.31	121.11	126.40
21	B	1228	CLA	CMA-C3A-C4A	2.31	117.97	111.77
21	a	1107	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
21	2	1022	CLA	OBD-CAD-C3D	-2.31	124.15	127.98
21	A	1125	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
24	6	4016	BCR	C37-C22-C23	2.30	121.71	118.08
30	m	4021	ECH	C8-C7-C6	-2.30	120.73	127.20
35	L	6001	LMT	C3'-C4'-C5'	-2.30	105.65	110.93
24	B	4017	BCR	C34-C9-C10	-2.30	119.70	122.92
24	B	4017	BCR	C39-C30-C25	-2.30	106.57	110.30
24	j	4013	BCR	C37-C22-C23	2.30	121.70	118.08
21	1	1121	CLA	CMB-C2B-C3B	2.30	128.98	124.68
21	b	1237	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
24	B	4004	BCR	C19-C18-C17	2.30	122.47	118.94
24	A	4019	BCR	C40-C30-C25	-2.30	106.57	110.30
21	1	1134	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	a	1134	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	2	1207	CLA	CHA-C1A-NA	-2.30	121.13	126.40
21	7	1302	CLA	CAA-C2A-C3A	-2.30	110.74	116.10
21	B	1228	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	K	1401	CLA	C1-O2A-CGA	2.30	122.47	116.44
21	b	1213	CLA	CBA-CAA-C2A	2.30	120.64	113.86
21	A	1107	CLA	O2A-CGA-CBA	2.30	119.11	111.91
21	b	1023	CLA	O2A-CGA-CBA	2.29	119.11	111.91
21	b	1021	CLA	CHA-C1A-NA	-2.29	121.14	126.40
36	I	4020	EQ3	C3-C4-C5	2.29	116.42	111.85
21	1	1012	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	a	4008	BCR	C35-C13-C12	2.29	121.69	118.08
21	k	1401	CLA	O2A-CGA-CBA	2.29	119.10	111.91
21	2	1023	CLA	CHA-C1A-NA	-2.29	121.15	126.40
34	F	4016	ZEX	C40-C33-C34	-2.29	119.72	122.92
25	l	5004	LHG	C5-O7-C7	-2.29	112.15	117.79
24	9	4021	BCR	C27-C26-C25	-2.29	119.41	122.73
21	1	1135	CLA	CMB-C2B-C3B	2.29	128.96	124.68
21	a	1124	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
21	1	1111	CLA	CMB-C2B-C3B	2.29	128.96	124.68
21	b	1214	CLA	CMB-C2B-C1B	-2.29	124.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1123	CLA	CHA-C1A-NA	-2.29	121.16	126.40
26	b	5002	LMG	O7-C10-O9	-2.29	118.17	123.70
21	B	1222	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
24	f	4016	BCR	C29-C28-C27	2.29	116.48	111.38
21	B	1207	CLA	O2D-CGD-CBD	2.28	115.33	111.27
28	h	4020	45D	C27-C25-C23	2.28	121.68	118.08
21	k	1401	CLA	CHA-C1A-NA	-2.28	121.17	126.40
22	1	2001	PQN	C2M-C2-C3	-2.28	120.67	124.40
21	a	1131	CLA	CMA-C3A-C4A	2.28	117.91	111.77
21	b	1023	CLA	CHA-C1A-NA	-2.28	121.17	126.40
21	2	1023	CLA	C2A-C1A-CHA	2.28	127.85	123.86
24	a	4012	BCR	C27-C26-C25	-2.28	119.42	122.73
21	A	1136	CLA	OBD-CAD-C3D	-2.28	124.20	127.98
21	a	1115	CLA	C1-O2A-CGA	2.28	122.42	116.44
24	J	4013	BCR	C37-C22-C23	2.28	121.67	118.08
24	A	4007	BCR	C37-C22-C23	2.28	121.67	118.08
24	l	4019	BCR	C39-C30-C25	-2.28	106.61	110.30
21	b	1229	CLA	C1-O2A-CGA	2.28	122.42	116.44
21	B	1213	CLA	CBA-CAA-C2A	2.28	120.58	113.86
24	2	4005	BCR	C39-C30-C25	-2.28	106.61	110.30
24	2	4014	BCR	C34-C9-C10	-2.28	119.73	122.92
21	a	1012	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
21	B	1219	CLA	CHA-C1A-NA	-2.27	121.19	126.40
21	A	1118	CLA	O2A-CGA-CBA	2.27	119.04	111.91
21	1	1129	CLA	CHA-C1A-NA	-2.27	121.20	126.40
21	1	1012	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
21	B	1236	CLA	O2A-CGA-CBA	2.27	119.03	111.91
21	A	1128	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
21	2	1238	CLA	CHA-C1A-NA	-2.27	121.20	126.40
21	a	1107	CLA	C1-O2A-CGA	2.27	122.40	116.44
24	K	4001	BCR	C37-C22-C23	2.27	121.65	118.08
21	2	1230	CLA	O2A-CGA-CBA	2.27	119.03	111.91
21	a	1108	CLA	CHA-C1A-NA	-2.27	121.20	126.40
31	0	5005	SQD	O3-C3-C2	-2.27	105.11	110.35
21	A	1124	CLA	C1-O2A-CGA	2.27	122.39	116.44
24	K	4001	BCR	C38-C26-C27	2.27	117.97	113.62
21	a	1103	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
21	A	1121	CLA	O2A-CGA-CBA	2.26	119.01	111.91
21	a	1132	CLA	OBD-CAD-C3D	-2.26	124.22	127.98
24	a	4012	BCR	C40-C30-C25	-2.26	106.63	110.30
21	1	1119	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	B	4004	BCR	C29-C28-C27	2.26	116.43	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1104	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
21	1	1129	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	1	1102	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	a	1101	CLA	C1-O2A-CGA	2.26	122.38	116.44
21	a	1140	CLA	C1-O2A-CGA	2.26	122.38	116.44
21	B	1240	CLA	O2A-CGA-CBA	2.26	119.00	111.91
21	2	1226	CLA	CHA-C1A-NA	-2.26	121.23	126.40
24	b	4018	BCR	C37-C22-C23	2.26	121.64	118.08
21	a	1120	CLA	CHA-C1A-NA	-2.26	121.23	126.40
21	L	1502	CLA	O2A-CGA-CBA	2.26	118.99	111.91
21	2	1237	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
21	1	1012	CLA	C2A-C1A-CHA	2.26	127.80	123.86
21	a	1114	CLA	CHA-C1A-NA	-2.25	121.23	126.40
21	a	1104	CLA	O2A-CGA-CBA	2.25	118.98	111.91
21	a	1118	CLA	CHA-C1A-NA	-2.25	121.23	126.40
21	A	1122	CLA	CMB-C2B-C3B	2.25	128.89	124.68
30	B	4006	ECH	C23-C24-C25	-2.25	120.88	127.20
24	B	4004	BCR	C34-C9-C10	-2.25	119.77	122.92
21	B	1237	CLA	C1-O2A-CGA	2.25	122.35	116.44
21	1	1013	CLA	CHA-C1A-NA	-2.25	121.24	126.40
21	a	1101	CLA	O2A-CGA-CBA	2.25	118.97	111.91
21	A	1109	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
21	A	1120	CLA	OBD-CAD-C3D	-2.25	124.25	127.98
21	J	1302	CLA	O2A-CGA-CBA	2.25	118.97	111.91
21	a	1101	CLA	CBA-CAA-C2A	2.25	120.50	113.86
24	1	4002	BCR	C31-C1-C6	-2.25	106.65	110.30
21	k	1401	CLA	C1-O2A-CGA	2.25	122.34	116.44
21	b	1226	CLA	C1-O2A-CGA	2.25	122.34	116.44
21	a	1011	CLA	O2D-CGD-CBD	2.25	115.26	111.27
21	B	1217	CLA	C1-C2-C3	2.25	129.93	126.04
24	A	4012	BCR	C37-C22-C23	2.25	121.62	118.08
30	b	4006	ECH	C37-C22-C23	-2.25	114.54	118.08
21	2	1227	CLA	CHA-C1A-NA	-2.24	121.26	126.40
21	b	1229	CLA	C6-C7-C8	-2.24	108.66	115.92
21	a	1121	CLA	O2A-CGA-CBA	2.24	118.95	111.91
21	2	1022	CLA	CHA-C1A-NA	-2.24	121.26	126.40
21	b	1237	CLA	CMA-C3A-C4A	2.24	117.80	111.77
24	b	4014	BCR	C34-C9-C10	-2.24	119.78	122.92
21	B	1207	CLA	CHA-C1A-NA	-2.24	121.26	126.40
24	a	4001	BCR	C37-C22-C23	2.24	121.61	118.08
21	a	1119	CLA	O2A-CGA-CBA	2.24	118.94	111.91
24	2	4018	BCR	C35-C13-C12	2.24	121.61	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1115	CLA	C1-O2A-CGA	2.24	122.33	116.44
28	B	4011	45D	C06-C04-C08	2.24	113.93	110.48
21	B	1229	CLA	CMA-C3A-C4A	2.24	117.80	111.77
30	2	4006	ECH	C12-C13-C14	-2.24	115.50	118.94
24	A	4012	BCR	C40-C30-C25	-2.24	106.67	110.30
24	k	4001	BCR	C37-C22-C23	2.24	121.61	118.08
21	b	1235	CLA	O2A-CGA-CBA	2.24	118.94	111.91
21	2	1210	CLA	CHA-C1A-NA	-2.24	121.27	126.40
21	A	1112	CLA	CHA-C1A-NA	-2.24	121.27	126.40
30	b	4006	ECH	C23-C24-C25	-2.24	120.92	127.20
24	A	4003	BCR	C34-C9-C10	-2.24	119.79	122.92
24	a	4003	BCR	C35-C13-C14	-2.24	119.79	122.92
24	1	4007	BCR	C37-C22-C23	2.24	121.60	118.08
24	1	4001	BCR	C15-C14-C13	-2.24	124.12	127.31
21	2	1214	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
21	B	1222	CLA	CMA-C3A-C4A	2.24	117.78	111.77
24	B	4018	BCR	C12-C13-C14	2.24	122.37	118.94
21	A	1102	CLA	CMB-C2B-C3B	2.24	128.86	124.68
24	B	4017	BCR	C32-C1-C6	-2.23	106.67	110.30
24	B	4010	BCR	C37-C22-C23	2.23	121.60	118.08
21	B	1235	CLA	O2A-CGA-CBA	2.23	118.92	111.91
21	1	1129	CLA	O2A-CGA-CBA	2.23	118.92	111.91
21	a	1104	CLA	CMB-C2B-C3B	2.23	128.85	124.68
24	0	4019	BCR	C39-C30-C25	-2.23	106.68	110.30
21	B	1214	CLA	CHA-C1A-NA	-2.23	121.29	126.40
24	A	4002	BCR	C12-C13-C14	-2.23	115.52	118.94
21	A	1130	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
24	l	4022	BCR	C19-C18-C17	2.23	122.36	118.94
21	a	1013	CLA	O2A-CGA-CBA	2.23	118.90	111.91
21	B	1022	CLA	O2A-CGA-CBA	2.23	118.90	111.91
21	A	1104	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
24	b	4017	BCR	C15-C14-C13	2.23	130.49	127.31
21	1	1112	CLA	CHA-C1A-NA	-2.23	121.30	126.40
21	b	1205	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
21	b	1213	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
26	K	5009	LMG	O7-C10-O9	-2.23	118.32	123.70
21	b	1234	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
21	2	1236	CLA	CHA-C1A-NA	-2.22	121.30	126.40
21	b	1203	CLA	CMA-C3A-C4A	2.22	117.75	111.77
21	b	1221	CLA	O2A-CGA-CBA	2.22	118.89	111.91
26	K	5009	LMG	O6-C1-C2	2.22	115.06	110.35
21	2	1209	CLA	CHA-C1A-NA	-2.22	121.31	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	5002	LMG	O1-C1-C2	2.22	111.77	108.30
21	A	1104	CLA	O2A-CGA-CBA	2.22	118.88	111.91
21	A	1103	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
28	h	4020	45D	C42-C41-C37	-2.22	118.92	123.47
24	a	4008	BCR	C37-C22-C23	2.22	121.58	118.08
21	l	1503	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
21	2	1240	CLA	CHA-C1A-NA	-2.22	121.31	126.40
21	A	1126	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	a	1139	CLA	CHA-C1A-NA	-2.22	121.31	126.40
21	1	1114	CLA	CHA-C1A-NA	-2.22	121.31	126.40
24	b	4005	BCR	C35-C13-C12	2.22	121.57	118.08
21	f	1302	CLA	O2A-CGA-CBA	2.22	118.87	111.91
21	1	1120	CLA	CHA-C1A-NA	-2.22	121.32	126.40
21	2	1228	CLA	CHA-C1A-NA	-2.22	121.32	126.40
21	2	1219	CLA	CBA-CAA-C2A	2.22	120.41	113.86
24	1	4001	BCR	C30-C25-C26	-2.22	119.49	122.61
21	2	1234	CLA	CMB-C2B-C3B	2.22	128.82	124.68
24	a	4008	BCR	C34-C9-C10	-2.22	119.82	122.92
21	B	1207	CLA	CAC-C3C-C4C	-2.22	121.94	124.81
21	l	1501	CLA	CMB-C2B-C3B	2.22	128.82	124.68
21	B	1023	CLA	CHA-C1A-NA	-2.21	121.33	126.40
21	b	1226	CLA	CHA-C1A-NA	-2.21	121.33	126.40
21	B	1226	CLA	O2A-CGA-CBA	2.21	118.86	111.91
24	B	4004	BCR	C36-C18-C19	-2.21	114.59	118.08
21	1	1118	CLA	O2A-CGA-CBA	2.21	118.85	111.91
30	b	4006	ECH	C8-C7-C6	-2.21	120.99	127.20
21	1	1118	CLA	CMB-C2B-C3B	2.21	128.82	124.68
28	B	4011	45D	C10-C18-C16	2.21	120.70	118.65
21	A	1107	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
24	a	4019	BCR	C37-C22-C23	2.21	121.56	118.08
24	7	4013	BCR	C19-C18-C17	2.21	122.34	118.94
21	a	1126	CLA	O2A-CGA-CBA	2.21	118.85	111.91
21	2	1220	CLA	CHA-C1A-NA	-2.21	121.33	126.40
24	a	4001	BCR	C2-C1-C6	2.21	113.88	110.48
21	a	1013	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	B	4010	BCR	C35-C13-C12	2.21	121.56	118.08
21	1	1135	CLA	O2A-CGA-CBA	2.21	118.84	111.91
21	1	1138	CLA	O2A-CGA-CBA	2.21	118.84	111.91
21	1	1012	CLA	CMA-C3A-C4A	2.21	117.71	111.77
21	8	1401	CLA	CAA-CBA-CGA	-2.21	108.84	113.59
21	2	1211	CLA	O2A-CGA-CBA	2.21	118.84	111.91
34	7	4015	ZEX	C11-C12-C13	-2.21	120.21	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1208	CLA	O2A-CGA-CBA	2.21	118.84	111.91
31	F	5001	SQD	O3-C3-C2	-2.21	105.25	110.35
21	1	1112	CLA	C1-O2A-CGA	2.21	122.23	116.44
24	2	4017	BCR	C30-C25-C26	-2.21	119.50	122.61
21	B	1221	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
21	b	1231	CLA	O2A-CGA-CBA	2.21	118.83	111.91
21	B	1237	CLA	CMB-C2B-C3B	2.21	128.80	124.68
21	A	1114	CLA	CHA-C1A-NA	-2.21	121.35	126.40
24	b	4010	BCR	C39-C30-C25	-2.20	106.72	110.30
21	2	1021	CLA	CHA-C1A-NA	-2.20	121.35	126.40
21	b	1213	CLA	CMA-C3A-C4A	2.20	117.70	111.77
31	L	5001	SQD	O3-C3-C2	-2.20	105.25	110.35
21	8	1402	CLA	CHA-C1A-NA	-2.20	121.35	126.40
21	a	1801	CLA	CHA-C1A-NA	-2.20	121.35	126.40
24	2	4018	BCR	C15-C14-C13	2.20	130.46	127.31
21	1	1104	CLA	O2A-CGA-CBA	2.20	118.82	111.91
21	a	1132	CLA	CMA-C3A-C4A	2.20	117.69	111.77
24	9	4021	BCR	C38-C26-C27	2.20	117.84	113.62
21	8	1401	CLA	CHA-C1A-NA	-2.20	121.36	126.40
24	1	4012	BCR	C8-C9-C10	2.20	122.32	118.94
24	2	4010	BCR	C40-C30-C25	-2.20	106.73	110.30
21	L	1503	CLA	C6-C7-C8	-2.20	108.81	115.92
24	1	4002	BCR	C29-C28-C27	2.20	116.29	111.38
21	B	1218	CLA	CHA-C1A-NA	-2.20	121.36	126.40
21	A	1116	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	i	4018	BCR	C2-C1-C6	2.20	113.87	110.48
28	B	4011	45D	C41-C42-C38	-2.20	118.97	123.47
24	6	4016	BCR	C15-C14-C13	2.20	130.45	127.31
21	a	1104	CLA	CHA-C1A-NA	-2.20	121.37	126.40
21	B	1021	CLA	CHA-C1A-NA	-2.20	121.37	126.40
21	a	1133	CLA	CHA-C1A-NA	-2.20	121.37	126.40
21	a	1111	CLA	CAC-C3C-C4C	2.20	127.66	124.81
21	J	1303	CLA	CHA-C1A-NA	-2.19	121.37	126.40
21	a	1134	CLA	CHA-C1A-NA	-2.19	121.37	126.40
21	f	1301	CLA	CHA-C1A-NA	-2.19	121.37	126.40
21	b	1222	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
25	l	5003	LHG	C5-O7-C7	-2.19	112.39	117.79
24	1	4001	BCR	C29-C28-C27	2.19	116.28	111.38
21	a	1137	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	A	1134	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
21	F	1302	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	A	1135	CLA	CHA-C1A-NA	-2.19	121.38	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	1102	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	1	1132	CLA	O2A-CGA-CBA	2.19	118.78	111.91
21	B	1216	CLA	O2A-CGA-CBA	2.19	118.78	111.91
21	1	1118	CLA	CHA-C1A-NA	-2.19	121.38	126.40
24	2	4018	BCR	C10-C11-C12	-2.19	116.39	123.22
21	B	1023	CLA	CAC-C3C-C4C	2.19	127.65	124.81
21	1	1128	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	a	4002	BCR	C31-C1-C6	-2.19	106.75	110.30
21	1	1131	CLA	O2A-CGA-CBA	2.19	118.77	111.91
21	1	1140	CLA	CHA-C1A-NA	-2.19	121.39	126.40
21	A	1118	CLA	CHA-C1A-NA	-2.19	121.39	126.40
21	A	1130	CLA	CMA-C3A-C4A	2.19	117.65	111.77
21	B	1213	CLA	C1-O2A-CGA	2.19	122.18	116.44
21	2	1224	CLA	CMB-C2B-C3B	2.18	128.77	124.68
24	A	4002	BCR	C38-C26-C27	2.18	117.81	113.62
24	b	4014	BCR	C8-C9-C10	2.18	122.29	118.94
24	B	4018	BCR	C40-C30-C25	-2.18	106.76	110.30
21	J	1302	CLA	CHA-C1A-NA	-2.18	121.40	126.40
21	2	1238	CLA	C1-O2A-CGA	2.18	122.17	116.44
24	1	4002	BCR	C37-C22-C23	2.18	121.52	118.08
21	A	1011	CLA	C2A-C3A-C4A	2.18	105.39	101.87
21	a	1120	CLA	C1-O2A-CGA	2.18	122.17	116.44
21	b	1237	CLA	CAC-C3C-C4C	2.18	127.64	124.81
21	k	1402	CLA	CHA-C1A-NA	-2.18	121.40	126.40
24	B	4010	BCR	C40-C30-C25	-2.18	106.76	110.30
21	L	1501	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
21	a	1129	CLA	CHA-C1A-NA	-2.18	121.40	126.40
24	A	4001	BCR	C29-C28-C27	2.18	116.25	111.38
21	A	1113	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
21	A	1130	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
21	a	1123	CLA	O2A-CGA-CBA	2.18	118.75	111.91
21	B	1240	CLA	CHA-C1A-NA	-2.18	121.41	126.40
21	A	1122	CLA	CHA-C1A-NA	-2.18	121.41	126.40
21	B	1218	CLA	O2A-CGA-CBA	2.18	118.74	111.91
21	B	1231	CLA	CMA-C3A-C4A	2.18	117.63	111.77
21	A	1133	CLA	C1-C2-C3	-2.18	122.28	126.04
24	a	4001	BCR	C23-C24-C25	2.18	133.32	127.20
21	B	1021	CLA	O2A-CGA-CBA	2.18	118.74	111.91
24	i	4018	BCR	C34-C9-C10	-2.18	119.87	122.92
21	a	1125	CLA	CHA-C1A-NA	-2.18	121.41	126.40
21	b	1215	CLA	CMA-C3A-C4A	2.18	117.62	111.77
21	a	1108	CLA	C1-O2A-CGA	2.18	122.15	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1223	CLA	CHA-C1A-NA	-2.17	121.42	126.40
21	l	1502	CLA	O2A-CGA-CBA	2.17	118.73	111.91
21	b	1238	CLA	CHA-C1A-NA	-2.17	121.42	126.40
21	B	1226	CLA	CAC-C3C-C4C	2.17	127.63	124.81
21	a	1137	CLA	CMA-C3A-C4A	2.17	117.61	111.77
21	b	1228	CLA	O2A-CGA-CBA	2.17	118.72	111.91
21	A	1125	CLA	C1-O2A-CGA	2.17	122.14	116.44
21	2	1217	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	1	2001	PQN	C12-C11-C3	-2.17	106.19	112.05
25	1	5001	LHG	C6-C5-C4	-2.17	106.65	111.79
21	b	1229	CLA	O2A-CGA-CBA	2.17	118.72	111.91
21	J	1303	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
24	A	4019	BCR	C37-C22-C23	2.17	121.50	118.08
30	b	4011	ECH	C7-C6-C5	-2.17	116.21	121.46
21	A	1111	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
21	2	1214	CLA	O2A-CGA-CBA	2.17	118.71	111.91
21	6	1301	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	2	1223	CLA	CHA-C1A-NA	-2.17	121.44	126.40
21	2	1202	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
21	a	1112	CLA	CHA-C1A-NA	-2.17	121.44	126.40
24	a	4012	BCR	C37-C22-C23	2.17	121.49	118.08
21	A	1136	CLA	O2A-CGA-CBA	2.17	118.70	111.91
21	2	1231	CLA	CHA-C1A-NA	-2.17	121.44	126.40
21	2	1201	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	b	1022	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	A	1132	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	1	1102	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	B	1206	CLA	CHA-C1A-NA	-2.16	121.44	126.40
24	h	4018	BCR	C30-C25-C26	-2.16	119.57	122.61
21	2	1206	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	a	1128	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
21	b	1209	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	a	1013	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
21	b	1023	CLA	CMA-C3A-C4A	2.16	117.59	111.77
21	A	1113	CLA	CHA-C1A-NA	-2.16	121.45	126.40
21	a	1132	CLA	CHA-C1A-NA	-2.16	121.45	126.40
21	j	1303	CLA	CHA-C1A-NA	-2.16	121.45	126.40
21	b	1232	CLA	CMB-C2B-C3B	2.16	128.72	124.68
24	h	4018	BCR	C32-C1-C6	-2.16	106.80	110.30
21	A	1105	CLA	CHA-C1A-NA	-2.16	121.45	126.40
24	A	4007	BCR	C35-C13-C12	2.16	121.48	118.08
24	l	4022	BCR	C34-C9-C10	-2.16	119.90	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1124	CLA	CHA-C1A-NA	-2.16	121.46	126.40
21	2	1229	CLA	C1-O2A-CGA	2.16	122.11	116.44
24	7	4013	BCR	C30-C25-C24	2.16	121.88	115.78
34	F	4016	ZEX	C31-C32-C33	-2.16	120.36	126.42
21	2	1217	CLA	O2A-CGA-CBA	2.16	118.68	111.91
25	1	5005	LHG	O7-C7-O9	-2.16	118.49	123.70
21	a	1111	CLA	CHA-C1A-NA	-2.16	121.46	126.40
30	B	4006	ECH	C19-C18-C17	2.16	122.25	118.94
21	2	1225	CLA	O2A-CGA-CBA	2.16	118.67	111.91
24	j	4013	BCR	C24-C25-C26	-2.16	116.24	121.46
21	a	1113	CLA	CHA-C1A-NA	-2.16	121.46	126.40
24	8	4001	BCR	C38-C26-C25	-2.16	122.11	124.53
24	A	4007	BCR	C15-C14-C13	2.15	130.38	127.31
24	K	4001	BCR	C39-C30-C25	-2.15	106.81	110.30
24	l	4019	BCR	C35-C13-C12	2.15	121.47	118.08
21	1	1138	CLA	CHA-C1A-NA	-2.15	121.47	126.40
21	B	1224	CLA	CMA-C3A-C4A	2.15	117.56	111.77
21	b	1226	CLA	O2A-CGA-CBA	2.15	118.67	111.91
24	b	4005	BCR	C24-C25-C26	-2.15	116.25	121.46
21	K	1401	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	2	4014	BCR	C37-C22-C23	2.15	121.47	118.08
21	A	1130	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
21	a	1135	CLA	O2A-CGA-CBA	2.15	118.66	111.91
24	k	4001	BCR	C34-C9-C10	-2.15	119.91	122.92
21	2	1202	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
31	b	5006	SQD	O3-C3-C2	-2.15	105.38	110.35
21	A	1013	CLA	CHA-C1A-NA	-2.15	121.47	126.40
21	b	1223	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	1	4008	BCR	C39-C30-C25	-2.15	106.81	110.30
24	2	4017	BCR	C35-C13-C12	2.15	121.47	118.08
21	A	1011	CLA	O2A-CGA-CBA	2.15	118.66	111.91
21	B	1212	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	2	1221	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	2	1217	CLA	CAC-C3C-C4C	2.15	127.60	124.81
21	b	1218	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	A	2001	PQN	C17-C16-C15	-2.15	107.53	113.36
21	F	1301	CLA	O2A-CGA-CBA	2.15	118.64	111.91
24	i	4018	BCR	C15-C14-C13	2.15	130.37	127.31
21	2	1218	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	2	1215	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	6	1301	CLA	O2A-CGA-CBA	2.14	118.64	111.91
21	1	1109	CLA	CHA-C1A-NA	-2.14	121.49	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	2002	PQN	C11-C12-C13	-2.14	123.22	126.79
21	a	1116	CLA	OBD-CAD-C3D	-2.14	124.42	127.98
21	a	1107	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
21	a	1102	CLA	CMB-C2B-C3B	2.14	128.69	124.68
24	a	4003	BCR	C34-C9-C10	-2.14	119.92	122.92
21	b	1228	CLA	CHA-C1A-NA	-2.14	121.49	126.40
24	K	4001	BCR	C10-C11-C12	-2.14	116.53	123.22
21	2	1232	CLA	CHA-C1A-NA	-2.14	121.50	126.40
24	L	4019	BCR	C38-C26-C25	-2.14	122.12	124.53
24	b	4004	BCR	C36-C18-C19	-2.14	114.70	118.08
24	2	4004	BCR	C39-C30-C25	-2.14	106.83	110.30
21	b	1222	CLA	CMA-C3A-C4A	2.14	117.53	111.77
24	L	4019	BCR	C32-C1-C6	-2.14	106.83	110.30
21	B	1215	CLA	O2A-CGA-CBA	2.14	118.62	111.91
24	A	4003	BCR	C35-C13-C12	2.14	121.45	118.08
21	A	1115	CLA	O2A-CGA-CBA	2.14	118.62	111.91
34	F	4016	ZEX	C27-C28-C29	2.14	129.47	126.23
21	1	1012	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
21	2	1221	CLA	O2A-CGA-CBA	2.14	118.62	111.91
21	a	1131	CLA	O2A-CGA-CBA	2.14	118.61	111.91
21	b	1230	CLA	O2A-CGA-CBA	2.14	118.61	111.91
21	0	1502	CLA	O2A-CGA-CBA	2.14	118.61	111.91
21	A	1137	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
21	b	1203	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
21	a	1135	CLA	CHA-C1A-NA	-2.14	121.51	126.40
21	b	1205	CLA	OBD-CAD-C3D	-2.14	124.44	127.98
24	A	4002	BCR	C39-C30-C25	-2.14	106.84	110.30
21	a	1105	CLA	CHA-C1A-NA	-2.13	121.51	126.40
21	b	1206	CLA	CHA-C1A-NA	-2.13	121.51	126.40
21	b	1237	CLA	CHA-C1A-NA	-2.13	121.51	126.40
34	F	4016	ZEX	C39-C29-C28	2.13	121.44	118.08
24	b	4005	BCR	C30-C25-C24	2.13	121.81	115.78
36	I	4020	EQ3	C36-C18-C19	2.13	121.44	118.08
30	b	4006	ECH	C11-C10-C9	-2.13	124.27	127.31
24	1	4003	BCR	C34-C9-C10	-2.13	119.94	122.92
21	1	1121	CLA	O2A-CGA-CBA	2.13	118.59	111.91
21	A	1013	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
21	7	1302	CLA	CHA-C1A-NA	-2.13	121.52	126.40
21	B	1218	CLA	CMB-C2B-C3B	2.13	128.66	124.68
26	a	5004	LMG	O7-C10-O9	-2.13	118.56	123.70
21	2	1208	CLA	CHA-C1A-NA	-2.13	121.52	126.40
21	a	1132	CLA	CMB-C2B-C1B	-2.13	125.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	4022	BCR	C37-C22-C23	2.13	121.43	118.08
35	0	6001	LMT	O1B-C4'-C3'	2.13	112.94	107.28
21	B	1234	CLA	CHA-C1A-NA	-2.13	121.52	126.40
24	a	4001	BCR	C32-C1-C6	-2.13	106.85	110.30
21	A	1114	CLA	O2A-CGA-CBA	2.13	118.58	111.91
21	2	1218	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
24	L	4019	BCR	C23-C24-C25	2.13	133.18	127.20
21	l	1501	CLA	CAC-C3C-C4C	2.13	127.57	124.81
24	6	4016	BCR	C27-C26-C25	-2.13	119.64	122.73
24	a	4007	BCR	C30-C25-C26	-2.13	119.62	122.61
21	1	1127	CLA	CHA-C1A-NA	-2.13	121.53	126.40
21	a	1140	CLA	CHA-C1A-NA	-2.13	121.53	126.40
21	a	1105	CLA	CAC-C3C-C4C	2.13	127.57	124.81
21	1	1135	CLA	CHA-C1A-NA	-2.13	121.53	126.40
24	1	4019	BCR	C39-C30-C25	-2.13	106.85	110.30
30	b	4011	ECH	C19-C18-C17	2.12	122.20	118.94
21	A	1106	CLA	CAA-C2A-C1A	-2.12	105.01	111.97
21	b	1023	CLA	C2A-C1A-CHA	2.12	127.57	123.86
21	b	1234	CLA	O2A-CGA-CBA	2.12	118.57	111.91
21	1	1104	CLA	CHA-C1A-NA	-2.12	121.53	126.40
21	a	1136	CLA	CHA-C1A-NA	-2.12	121.53	126.40
21	b	1222	CLA	O2A-CGA-CBA	2.12	118.57	111.91
21	1	1013	CLA	O2A-CGA-CBA	2.12	118.57	111.91
21	1	1140	CLA	C1-O2A-CGA	2.12	122.01	116.44
21	B	1220	CLA	CHA-C1A-NA	-2.12	121.54	126.40
24	a	4012	BCR	C38-C26-C27	2.12	117.69	113.62
21	B	1239	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
24	a	4007	BCR	C38-C26-C27	2.12	117.69	113.62
21	A	1126	CLA	O2A-CGA-CBA	2.12	118.56	111.91
21	A	1124	CLA	O2A-CGA-CBA	2.12	118.56	111.91
21	F	1301	CLA	CHA-C1A-NA	-2.12	121.54	126.40
21	a	1119	CLA	CHA-C1A-NA	-2.12	121.55	126.40
21	1	1125	CLA	CMB-C2B-C3B	2.12	128.64	124.68
21	B	1218	CLA	C1-O2A-CGA	2.12	122.00	116.44
24	l	4019	BCR	C32-C1-C6	-2.12	106.86	110.30
21	b	1240	CLA	CHA-C1A-NA	-2.12	121.55	126.40
21	a	1127	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	j	4013	BCR	C19-C18-C17	2.12	122.19	118.94
21	b	1237	CLA	CMB-C2B-C3B	2.12	128.64	124.68
21	B	1231	CLA	O2A-CGA-CBA	2.12	118.55	111.91
21	A	1131	CLA	O2A-CGA-CBA	2.12	118.55	111.91
21	2	1237	CLA	CHA-C1A-NA	-2.12	121.55	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	4020	ECH	C34-C9-C10	2.12	125.89	122.92
24	a	4002	BCR	C37-C22-C23	2.11	121.41	118.08
21	2	1212	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	7	4013	BCR	C37-C22-C23	2.11	121.41	118.08
21	A	1135	CLA	O2A-CGA-CBA	2.11	118.54	111.91
21	A	1120	CLA	O2A-CGA-CBA	2.11	118.54	111.91
21	A	1136	CLA	C1-O2A-CGA	2.11	121.99	116.44
21	B	1238	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	2	1222	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	B	4018	BCR	C11-C12-C13	-2.11	120.48	126.42
21	6	1301	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	B	1217	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	A	1102	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
21	A	1121	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	b	1216	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	I	4018	BCR	C38-C26-C25	-2.11	122.16	124.53
30	2	4006	ECH	C15-C16-C17	2.11	127.80	123.47
21	A	1128	CLA	OBD-CAD-CBD	-2.11	122.88	125.89
35	0	6001	LMT	C1'-C2'-C3'	2.11	114.39	110.00
21	B	1022	CLA	CMA-C3A-C4A	2.11	117.44	111.77
21	8	1401	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
24	8	4001	BCR	C37-C22-C23	2.10	121.39	118.08
21	A	1111	CLA	C1-O2A-CGA	2.10	121.97	116.44
24	A	4007	BCR	C38-C26-C25	-2.10	122.17	124.53
21	b	1219	CLA	CHA-C1A-NA	-2.10	121.58	126.40
24	A	4001	BCR	C37-C22-C23	2.10	121.39	118.08
24	l	4019	BCR	C37-C22-C23	2.10	121.39	118.08
21	2	1235	CLA	O2A-CGA-CBA	2.10	118.51	111.91
21	a	1128	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	2	1239	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
24	l	4022	BCR	C37-C22-C23	2.10	121.39	118.08
21	1	1123	CLA	O2A-CGA-CBA	2.10	118.51	111.91
24	l	4022	BCR	C35-C13-C12	2.10	121.39	118.08
21	2	1214	CLA	CMB-C2B-C3B	2.10	128.61	124.68
21	1	1139	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	b	1215	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	A	1125	CLA	CHA-C1A-NA	-2.10	121.59	126.40
21	a	1122	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	L	4019	BCR	C35-C13-C12	2.10	121.39	118.08
30	2	4006	ECH	C29-C30-C25	-2.10	107.25	110.48
24	l	4022	BCR	C32-C1-C6	-2.10	106.89	110.30
21	1	1801	CLA	CHA-C1A-NA	-2.10	121.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	5005	LMG	O7-C10-O9	-2.10	118.63	123.70
21	a	1012	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	b	1207	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	1	4003	BCR	C37-C22-C23	2.10	121.38	118.08
21	1	1013	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	B	1217	CLA	CAC-C3C-C4C	2.10	127.53	124.81
21	1	1132	CLA	CMA-C3A-C4A	2.10	117.41	111.77
21	B	1211	CLA	CHA-C1A-NA	-2.10	121.60	126.40
30	B	4006	ECH	C37-C22-C21	2.10	125.86	122.92
21	B	1227	CLA	O2A-CGA-CBA	2.09	118.48	111.91
24	K	4001	BCR	C12-C13-C14	-2.09	115.73	118.94
21	b	1224	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
21	b	1222	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
21	2	1228	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
26	A	5002	LMG	O7-C10-O9	-2.09	118.64	123.70
21	f	1301	CLA	O2A-CGA-CBA	2.09	118.47	111.91
24	9	4021	BCR	C8-C7-C6	2.09	133.08	127.20
24	0	4022	BCR	C15-C14-C13	2.09	130.29	127.31
21	A	1120	CLA	CHA-C1A-NA	-2.09	121.61	126.40
31	L	5002	SQD	O3-C3-C2	-2.09	105.52	110.35
21	2	1215	CLA	O2A-CGA-CBA	2.09	118.47	111.91
21	A	1129	CLA	CMA-C3A-C4A	2.09	117.39	111.77
21	6	1302	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
21	a	1123	CLA	CHA-C1A-NA	-2.09	121.61	126.40
21	8	1402	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
21	a	1103	CLA	O2A-CGA-CBA	2.09	118.47	111.91
21	j	1303	CLA	O2A-CGA-CBA	2.09	118.47	111.91
21	a	1107	CLA	CHA-C1A-NA	-2.09	121.61	126.40
26	b	5002	LMG	C30-C29-C28	-2.09	106.03	113.62
34	J	4015	ZEX	C23-C24-C25	-2.09	106.36	109.33
21	b	1222	CLA	CMB-C2B-C3B	2.09	128.59	124.68
21	a	1109	CLA	CHA-C1A-NA	-2.09	121.62	126.40
24	k	4001	BCR	C29-C28-C27	2.09	116.04	111.38
21	a	1130	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
21	2	1240	CLA	CAA-C2A-C3A	-2.09	111.23	116.10
24	A	4002	BCR	C31-C1-C6	-2.09	106.91	110.30
21	b	1217	CLA	CHA-C1A-NA	-2.09	121.62	126.40
21	a	1127	CLA	C1-O2A-CGA	2.09	121.92	116.44
21	1	1109	CLA	CAC-C3C-C4C	2.09	127.52	124.81
21	A	1137	CLA	CMA-C3A-C4A	2.09	117.38	111.77
21	A	1107	CLA	C1-O2A-CGA	2.09	121.92	116.44
21	K	1401	CLA	O2A-CGA-CBA	2.09	118.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	5005	LHG	O7-C7-O9	-2.09	118.66	123.70
21	a	1113	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
21	A	1140	CLA	C1-O2A-CGA	2.09	121.92	116.44
21	j	1302	CLA	CHA-C1A-NA	-2.08	121.62	126.40
26	B	5002	LMG	C30-C29-C28	-2.08	106.04	113.62
31	L	5001	SQD	O8-S-C6	-2.08	102.42	105.74
24	B	4018	BCR	C35-C13-C14	-2.08	120.00	122.92
21	B	1023	CLA	CMB-C2B-C3B	2.08	128.58	124.68
21	b	1222	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
24	A	4007	BCR	C39-C30-C25	-2.08	106.92	110.30
21	2	1230	CLA	CHA-C1A-NA	-2.08	121.63	126.40
21	a	1110	CLA	CHA-C1A-NA	-2.08	121.63	126.40
24	7	4013	BCR	C36-C18-C19	-2.08	114.80	118.08
21	B	1222	CLA	O2A-CGA-CBA	2.08	118.44	111.91
21	1	1113	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	l	4022	BCR	C36-C18-C19	-2.08	114.80	118.08
21	2	1238	CLA	O2A-CGA-CBA	2.08	118.43	111.91
21	a	1124	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	b	1213	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	b	1202	CLA	CMA-C3A-C4A	2.08	117.36	111.77
21	a	1107	CLA	O2A-CGA-CBA	2.08	118.43	111.91
21	7	1303	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	7	1303	CLA	CAA-C2A-C3A	-2.08	111.25	116.10
21	2	1226	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
21	b	1227	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	1	1125	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	6	1301	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
21	1	1122	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	b	1224	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	6	4016	BCR	C38-C26-C27	2.08	117.60	113.62
21	B	1228	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	B	1022	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	B	4010	BCR	C38-C26-C25	-2.07	122.20	124.53
21	b	1206	CLA	CAC-C3C-C4C	2.07	127.50	124.81
21	2	1234	CLA	CHA-C1A-NA	-2.07	121.65	126.40
21	l	1502	CLA	CHA-C1A-NA	-2.07	121.65	126.40
26	B	5002	LMG	O7-C10-O9	-2.07	118.69	123.70
34	j	4015	ZEX	C40-C33-C34	-2.07	120.02	122.92
24	2	4005	BCR	C37-C22-C23	2.07	121.34	118.08
24	0	4019	BCR	C8-C9-C10	2.07	122.12	118.94
21	B	1218	CLA	OBD-CAD-C3D	-2.07	124.54	127.98
24	b	4004	BCR	C35-C13-C12	2.07	121.34	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1215	CLA	CAC-C3C-C4C	2.07	127.50	124.81
21	2	1211	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	A	1127	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	1	1137	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	b	1220	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	A	1138	CLA	CHA-C1A-NA	-2.07	121.67	126.40
24	1	4019	BCR	C37-C22-C23	2.07	121.33	118.08
21	2	1205	CLA	CBC-CAC-C3C	-2.07	106.74	112.43
31	0	5005	SQD	O8-S-C6	-2.07	102.45	105.74
24	2	4011	BCR	C37-C22-C23	2.06	121.33	118.08
21	A	1012	CLA	CMA-C3A-C4A	2.06	117.32	111.77
34	F	4016	ZEX	C20-C13-C14	-2.06	120.03	122.92
21	A	1111	CLA	CAC-C3C-C4C	2.06	127.49	124.81
21	1	1107	CLA	CHA-C1A-NA	-2.06	121.67	126.40
21	B	1236	CLA	CHA-C1A-NA	-2.06	121.67	126.40
21	A	1140	CLA	O2A-CGA-CBA	2.06	118.38	111.91
30	b	4011	ECH	O27-C27-C26	2.06	122.79	120.96
21	B	1236	CLA	CMA-C3A-C4A	2.06	117.31	111.77
21	2	1218	CLA	C1-O2A-CGA	2.06	121.85	116.44
21	1	1130	CLA	CHA-C1A-NA	-2.06	121.68	126.40
21	K	1402	CLA	CHA-C1A-NA	-2.06	121.68	126.40
21	B	1203	CLA	CMA-C3A-C4A	2.06	117.31	111.77
24	j	4013	BCR	C40-C30-C25	-2.06	106.96	110.30
21	2	1207	CLA	CMA-C3A-C2A	2.06	122.14	113.83
21	B	1202	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
21	b	1240	CLA	CMB-C2B-C3B	2.06	128.53	124.68
21	1	1136	CLA	CHA-C1A-NA	-2.06	121.68	126.40
21	b	1204	CLA	O2A-CGA-CBA	2.06	118.37	111.91
35	l	6001	LMT	C1B-O5B-C5B	2.06	117.73	113.69
30	M	4021	ECH	C11-C10-C9	-2.06	124.37	127.31
21	A	1123	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
21	B	1221	CLA	O2A-CGA-CBA	2.06	118.36	111.91
21	b	1221	CLA	CHA-C1A-NA	-2.06	121.69	126.40
21	2	1219	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
21	a	1110	CLA	O2A-CGA-CBA	2.06	118.36	111.91
35	1	6001	LMT	O5B-C5B-C6B	2.06	111.55	106.44
21	L	1503	CLA	CHA-C1A-NA	-2.06	121.69	126.40
21	B	1215	CLA	CHA-C1A-NA	-2.06	121.69	126.40
21	A	1128	CLA	CMA-C3A-C4A	2.06	117.30	111.77
25	A	5003	LHG	O8-C23-O10	-2.06	118.40	123.59
24	h	4018	BCR	C38-C26-C25	-2.06	122.22	124.53
21	B	1216	CLA	CHA-C1A-NA	-2.06	121.69	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1111	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	9	4021	BCR	C39-C30-C25	-2.05	106.97	110.30
21	2	1221	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
21	A	1101	CLA	C2A-C1A-CHA	2.05	127.45	123.86
25	A	5006	LHG	O7-C7-O9	-2.05	118.74	123.70
24	2	4004	BCR	C37-C22-C23	2.05	121.31	118.08
21	b	1239	CLA	CHA-C1A-NA	-2.05	121.70	126.40
21	l	1501	CLA	CHA-C1A-NA	-2.05	121.70	126.40
21	B	1205	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
21	b	1223	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
24	K	4001	BCR	C35-C13-C12	2.05	121.31	118.08
21	A	1124	CLA	CHA-C1A-NA	-2.05	121.70	126.40
21	b	1227	CLA	O2A-CGA-CBA	2.05	118.34	111.91
21	L	1502	CLA	CHA-C1A-NA	-2.05	121.70	126.40
21	a	1116	CLA	CHA-C1A-NA	-2.05	121.70	126.40
21	b	1217	CLA	C1-O2A-CGA	2.05	121.82	116.44
21	B	1203	CLA	O2A-CGA-CBA	2.05	118.34	111.91
31	L	5001	SQD	O5-C1-O6	-2.05	105.12	109.97
21	1	1011	CLA	C3D-CAD-CBD	-2.05	104.91	107.61
21	b	1210	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
21	B	1211	CLA	O2A-CGA-CBA	2.05	118.34	111.91
21	2	1202	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	A	1101	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
34	j	4015	ZEX	C17-C1-C6	-2.05	106.98	110.30
21	a	1106	CLA	O2A-CGA-CBA	2.05	118.33	111.91
21	1	1108	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	L	5002	SQD	O8-S-C6	-2.05	102.48	105.74
24	A	4007	BCR	C2-C1-C6	2.05	113.63	110.48
21	L	1502	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	A	1131	CLA	CHA-C1A-NA	-2.05	121.71	126.40
24	2	4017	BCR	C34-C9-C10	-2.05	120.06	122.92
21	A	1122	CLA	C1-O2A-CGA	2.05	121.81	116.44
21	b	1204	CLA	CAC-C3C-C4C	2.04	127.46	124.81
21	B	1226	CLA	CMA-C3A-C4A	2.04	117.27	111.77
21	B	1208	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	b	1210	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	2	1226	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
21	B	1201	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
21	A	1125	CLA	O2A-CGA-CBA	2.04	118.32	111.91
24	B	4004	BCR	C37-C22-C23	2.04	121.30	118.08
21	B	1217	CLA	O2A-CGA-CBA	2.04	118.32	111.91
21	b	1235	CLA	CMB-C2B-C3B	2.04	128.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1132	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
30	i	4020	ECH	C16-C15-C14	2.04	127.66	123.47
21	2	1232	CLA	CAA-CBA-CGA	-2.04	109.20	113.59
21	2	1231	CLA	CMA-C3A-C4A	2.04	117.26	111.77
24	2	4005	BCR	C34-C9-C10	-2.04	120.06	122.92
21	a	1132	CLA	O2A-CGA-CBA	2.04	118.31	111.91
21	1	1132	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	2	1222	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
21	b	1206	CLA	O2A-CGA-CBA	2.04	118.31	111.91
21	A	1801	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	2	4018	BCR	C30-C25-C26	-2.04	119.74	122.61
21	1	1131	CLA	CMA-C3A-C4A	2.04	117.25	111.77
24	B	4018	BCR	C37-C22-C23	2.04	121.29	118.08
24	a	4012	BCR	C32-C1-C6	-2.04	107.00	110.30
21	2	1207	CLA	C1-O2A-CGA	2.04	121.79	116.44
21	F	1302	CLA	O2A-CGA-CBA	2.04	118.30	111.91
35	1	6001	LMT	C3'-C4'-C5'	-2.04	106.26	110.93
24	9	4021	BCR	C23-C24-C25	2.04	132.92	127.20
21	A	1116	CLA	CHA-C1A-NA	-2.04	121.73	126.40
30	M	4021	ECH	C7-C6-C5	-2.04	116.53	121.46
21	2	1022	CLA	C1-O2A-CGA	2.03	121.78	116.44
21	1	1115	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
24	K	4001	BCR	C27-C26-C25	-2.03	119.78	122.73
21	A	1013	CLA	O2A-CGA-CBA	2.03	118.29	111.91
24	2	4010	BCR	C1-C6-C5	-2.03	119.75	122.61
21	B	1213	CLA	C2A-C1A-CHA	2.03	127.42	123.86
21	a	1136	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
24	1	4003	BCR	C1-C6-C7	2.03	121.53	115.78
21	A	1104	CLA	CMA-C3A-C4A	2.03	117.23	111.77
24	K	4001	BCR	C38-C26-C25	-2.03	122.25	124.53
21	1	1133	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	A	4002	BCR	C30-C25-C26	-2.03	119.75	122.61
24	7	4013	BCR	C39-C30-C25	-2.03	107.00	110.30
21	f	1302	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	b	1232	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	a	1108	CLA	O2A-CGA-CBA	2.03	118.28	111.91
21	1	1116	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	B	1221	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	1	4001	BCR	C37-C22-C23	2.03	121.28	118.08
21	a	1136	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
21	1	1117	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	2	1203	CLA	O2A-CGA-CBA	2.03	118.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1119	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	0	1501	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
21	1	1126	CLA	CHA-C1A-NA	-2.03	121.75	126.40
34	7	4015	ZEX	C23-C24-C25	-2.03	106.44	109.33
21	a	1129	CLA	CMA-C3A-C4A	2.03	117.22	111.77
34	F	4016	ZEX	C31-C30-C29	2.03	130.20	127.31
21	B	1209	CLA	O2A-CGA-CBA	2.03	118.27	111.91
21	2	1239	CLA	C1-O2A-CGA	2.03	121.76	116.44
24	A	4008	BCR	C37-C22-C23	2.03	121.27	118.08
24	a	4007	BCR	C37-C22-C23	2.03	121.27	118.08
21	1	1109	CLA	CMD-C2D-C3D	-2.03	120.89	124.68
21	L	1503	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
21	b	1236	CLA	CHA-C1A-NA	-2.02	121.76	126.40
21	B	1234	CLA	O2A-CGA-CBA	2.02	118.26	111.91
21	a	1128	CLA	OBD-CAD-CBD	-2.02	123.00	125.89
21	1	1105	CLA	CHA-C1A-NA	-2.02	121.76	126.40
21	B	1240	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
31	b	5006	SQD	O8-S-C6	-2.02	102.52	105.74
21	A	1801	CLA	C1-O2A-CGA	2.02	121.75	116.44
21	a	1125	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
21	a	1124	CLA	CMB-C2B-C3B	2.02	128.46	124.68
21	1	1110	CLA	CHA-C1A-NA	-2.02	121.77	126.40
21	A	1123	CLA	C1-O2A-CGA	2.02	121.75	116.44
21	1	1134	CLA	CHA-C1A-NA	-2.02	121.77	126.40
21	A	1102	CLA	CMA-C3A-C4A	2.02	117.20	111.77
24	A	4019	BCR	C1-C6-C5	-2.02	119.77	122.61
24	a	4019	BCR	C19-C18-C17	2.02	122.04	118.94
21	B	1209	CLA	C1-O2A-CGA	2.02	121.74	116.44
21	A	1107	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
21	a	1129	CLA	O2A-CGA-CBA	2.02	118.24	111.91
24	1	4007	BCR	C31-C1-C6	-2.02	107.03	110.30
21	B	1231	CLA	CHA-C1A-NA	-2.02	121.78	126.40
21	A	1132	CLA	O2A-CGA-CBA	2.02	118.24	111.91
21	B	1237	CLA	CHA-C1A-NA	-2.02	121.78	126.40
21	B	1226	CLA	CHA-C1A-NA	-2.02	121.78	126.40
24	J	4013	BCR	C8-C9-C10	2.02	122.03	118.94
24	J	4013	BCR	C35-C13-C14	-2.02	120.10	122.92
21	b	1201	CLA	CHA-C1A-NA	-2.02	121.78	126.40
21	B	1224	CLA	CHA-C1A-NA	-2.02	121.78	126.40
21	A	1119	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	A	1132	CLA	CMA-C3A-C4A	2.01	117.18	111.77
21	2	1225	CLA	CHA-C1A-NA	-2.01	121.79	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	4018	BCR	C10-C11-C12	-2.01	116.94	123.22
21	l	1501	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
21	2	1203	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	L	1503	CLA	C1-O2A-CGA	2.01	121.72	116.44
31	B	5008	SQD	O8-S-C6	-2.01	102.54	105.74
21	B	1201	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	1	1114	CLA	CMB-C2B-C3B	2.01	128.44	124.68
21	b	1224	CLA	CMA-C3A-C4A	2.01	117.17	111.77
24	B	4005	BCR	C37-C22-C23	2.01	121.24	118.08
21	L	1502	CLA	C11-C12-C13	-2.01	109.43	115.92
21	b	1234	CLA	CHA-C1A-NA	-2.01	121.80	126.40
21	a	1109	CLA	O2A-CGA-CBA	2.01	118.21	111.91
21	A	1115	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	2	4011	BCR	C38-C26-C25	-2.01	122.27	124.53
24	2	4017	BCR	C8-C9-C10	2.01	122.02	118.94
21	B	1226	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
21	1	1136	CLA	C1-O2A-CGA	2.01	121.71	116.44
21	A	1123	CLA	CMA-C3A-C2A	2.01	121.92	113.83
21	A	1140	CLA	CHA-C1A-NA	-2.01	121.80	126.40
21	2	1228	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
24	2	4017	BCR	C38-C26-C25	-2.01	122.28	124.53
21	a	1120	CLA	CAC-C3C-C4C	2.01	127.41	124.81
24	a	4001	BCR	C34-C9-C10	-2.01	120.11	122.92
21	A	1108	CLA	O2A-CGA-CBA	2.00	118.20	111.91
21	2	1229	CLA	O2A-CGA-CBA	2.00	118.20	111.91
21	A	1129	CLA	CHA-C1A-NA	-2.00	121.81	126.40
21	B	1232	CLA	CHA-C1A-NA	-2.00	121.81	126.40
21	2	1239	CLA	CHA-C1A-NA	-2.00	121.81	126.40
26	b	5002	LMG	O1-C1-C2	2.00	111.43	108.30
24	0	4022	BCR	C1-C6-C5	-2.00	119.79	122.61
28	h	4020	45D	C23-C25-C29	-2.00	115.87	118.94
21	a	1011	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
21	b	1230	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
26	0	5001	LMG	O6-C5-C6	2.00	111.41	106.44
21	b	1214	CLA	CHA-C1A-NA	-2.00	121.82	126.40
21	b	1209	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (799) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1012	CLA	NA
21	A	1012	CLA	ND

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Mol	Chain	Res	Type	Atom
21	2	1220	CLA	NC
21	2	1220	CLA	ND
21	2	1220	CLA	NA
21	B	1214	CLA	NC
21	B	1214	CLA	ND
21	B	1214	CLA	NA
21	1	1112	CLA	NC
21	1	1112	CLA	ND
21	1	1112	CLA	NA
21	1	1139	CLA	NC
21	1	1139	CLA	ND
21	1	1139	CLA	NA
21	b	1235	CLA	NC
21	b	1235	CLA	ND
21	b	1235	CLA	NA
21	1	1011	CLA	NC
21	1	1011	CLA	ND
21	1	1011	CLA	NA
21	2	1231	CLA	NC
21	2	1231	CLA	ND
21	2	1231	CLA	NA
21	b	1220	CLA	NC
21	b	1220	CLA	ND
21	b	1220	CLA	NA
21	2	1213	CLA	NC
21	2	1213	CLA	ND
21	2	1213	CLA	NA
21	B	1204	CLA	ND
21	B	1204	CLA	NA
21	2	1229	CLA	NC
21	2	1229	CLA	ND
21	2	1229	CLA	NA
21	2	1214	CLA	NC
21	2	1214	CLA	ND
21	2	1214	CLA	NA
21	a	1102	CLA	NC
21	a	1102	CLA	ND
21	a	1102	CLA	NA
21	B	1220	CLA	NC
21	B	1220	CLA	ND
21	B	1220	CLA	NA
21	1	1131	CLA	NC

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Mol	Chain	Res	Type	Atom
21	1	1131	CLA	ND
21	1	1131	CLA	NA
21	A	1801	CLA	NC
21	A	1801	CLA	ND
21	A	1801	CLA	NA
21	j	1302	CLA	NC
21	j	1302	CLA	ND
21	j	1302	CLA	NA
21	b	1225	CLA	NC
21	b	1225	CLA	ND
21	b	1225	CLA	NA
21	b	1202	CLA	ND
21	b	1202	CLA	NA
21	A	1114	CLA	NC
21	A	1114	CLA	ND
21	A	1114	CLA	NA
21	a	1116	CLA	ND
21	a	1116	CLA	NA
21	b	1216	CLA	NC
21	b	1216	CLA	ND
21	b	1216	CLA	NA
21	b	1211	CLA	NC
21	b	1211	CLA	ND
21	b	1211	CLA	NA
21	A	1101	CLA	NA
21	B	1213	CLA	NC
21	B	1213	CLA	ND
21	B	1213	CLA	NA
21	2	1236	CLA	NC
21	2	1236	CLA	ND
21	2	1236	CLA	NA
21	B	1216	CLA	NC
21	B	1216	CLA	ND
21	B	1216	CLA	NA
21	B	1237	CLA	NC
21	B	1237	CLA	ND
21	B	1237	CLA	NA
21	1	1013	CLA	NC
21	1	1013	CLA	ND
21	1	1013	CLA	NA
21	2	1206	CLA	NC
21	2	1206	CLA	ND

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Mol	Chain	Res	Type	Atom
21	2	1206	CLA	NA
21	2	1022	CLA	NC
21	2	1022	CLA	ND
21	2	1022	CLA	NA
21	a	1101	CLA	NC
21	a	1101	CLA	NA
21	a	1121	CLA	NC
21	a	1121	CLA	ND
21	a	1121	CLA	NA
21	B	1219	CLA	NC
21	B	1219	CLA	NA
21	A	1126	CLA	NC
21	A	1126	CLA	ND
21	A	1126	CLA	NA
21	B	1240	CLA	NC
21	B	1240	CLA	ND
21	B	1240	CLA	NA
21	b	1214	CLA	NC
21	b	1214	CLA	ND
21	b	1214	CLA	NA
21	1	1122	CLA	NC
21	1	1122	CLA	ND
21	1	1122	CLA	NA
21	2	1230	CLA	NC
21	2	1230	CLA	ND
21	2	1230	CLA	NA
21	B	1217	CLA	NC
21	B	1217	CLA	ND
21	B	1217	CLA	NA
21	A	1116	CLA	NC
21	A	1116	CLA	ND
21	A	1116	CLA	NA
21	f	1301	CLA	NC
21	f	1301	CLA	ND
21	f	1301	CLA	NA
21	a	1115	CLA	NC
21	a	1115	CLA	NA
21	b	1227	CLA	NC
21	b	1227	CLA	ND
21	b	1227	CLA	NA
21	2	1234	CLA	NC
21	2	1234	CLA	ND

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Mol	Chain	Res	Type	Atom
21	2	1234	CLA	NA
21	b	1208	CLA	NC
21	b	1208	CLA	ND
21	b	1208	CLA	NA
21	1	1127	CLA	NC
21	1	1127	CLA	ND
21	1	1127	CLA	NA
21	b	1203	CLA	NC
21	b	1203	CLA	ND
21	b	1203	CLA	NA
21	B	1207	CLA	NC
21	B	1207	CLA	NA
21	a	1011	CLA	NC
21	a	1011	CLA	ND
21	a	1011	CLA	NA
21	2	1237	CLA	NC
21	2	1237	CLA	ND
21	2	1237	CLA	NA
21	2	1210	CLA	NC
21	2	1210	CLA	NA
21	k	1401	CLA	NC
21	k	1401	CLA	ND
21	k	1401	CLA	NA
21	1	1104	CLA	NC
21	1	1104	CLA	ND
21	1	1104	CLA	NA
21	1	1134	CLA	NC
21	1	1134	CLA	ND
21	1	1134	CLA	NA
21	A	1110	CLA	NC
21	A	1110	CLA	ND
21	A	1110	CLA	NA
21	1	1124	CLA	NC
21	1	1124	CLA	ND
21	1	1124	CLA	NA
21	2	1201	CLA	NC
21	2	1201	CLA	ND
21	2	1201	CLA	NA
21	2	1216	CLA	NC
21	2	1216	CLA	NA
21	2	1216	CLA	ND
21	A	1113	CLA	NC

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Mol	Chain	Res	Type	Atom
21	A	1113	CLA	ND
21	A	1113	CLA	NA
21	B	1231	CLA	NA
21	b	1240	CLA	NC
21	b	1240	CLA	ND
21	b	1240	CLA	NA
21	b	1222	CLA	NC
21	b	1222	CLA	ND
21	b	1222	CLA	NA
21	a	1133	CLA	NC
21	a	1133	CLA	NA
21	b	1229	CLA	NC
21	b	1229	CLA	ND
21	b	1229	CLA	NA
21	2	1235	CLA	NC
21	2	1235	CLA	ND
21	2	1235	CLA	NA
21	1	1115	CLA	NC
21	1	1115	CLA	ND
21	1	1115	CLA	NA
21	1	1106	CLA	NC
21	1	1106	CLA	ND
21	1	1106	CLA	NA
21	2	1211	CLA	NC
21	2	1211	CLA	ND
21	2	1211	CLA	NA
21	1	1113	CLA	NC
21	1	1113	CLA	ND
21	1	1113	CLA	NA
21	A	1123	CLA	ND
21	A	1123	CLA	NA
21	a	1013	CLA	NC
21	a	1013	CLA	ND
21	a	1013	CLA	NA
21	2	1226	CLA	NC
21	2	1226	CLA	ND
21	2	1226	CLA	NA
21	B	1023	CLA	NC
21	B	1023	CLA	ND
21	B	1023	CLA	NA
21	b	1224	CLA	NC
21	b	1224	CLA	ND

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Mol	Chain	Res	Type	Atom
21	b	1224	CLA	NA
21	1	1111	CLA	NC
21	1	1111	CLA	ND
21	1	1111	CLA	NA
21	2	1225	CLA	NC
21	2	1225	CLA	ND
21	2	1225	CLA	NA
21	b	1022	CLA	ND
21	b	1022	CLA	NA
21	1	1116	CLA	NC
21	1	1116	CLA	ND
21	1	1116	CLA	NA
21	a	1131	CLA	NC
21	a	1131	CLA	ND
21	a	1131	CLA	NA
21	1	1119	CLA	NC
21	1	1119	CLA	ND
21	1	1119	CLA	NA
21	F	1302	CLA	NC
21	F	1302	CLA	ND
21	F	1302	CLA	NA
21	2	1223	CLA	NC
21	2	1223	CLA	NA
21	a	1123	CLA	ND
21	a	1123	CLA	NA
21	A	1112	CLA	NC
21	A	1112	CLA	ND
21	A	1112	CLA	NA
21	A	1103	CLA	NC
21	A	1103	CLA	ND
21	A	1103	CLA	NA
21	a	1107	CLA	NC
21	a	1107	CLA	ND
21	a	1107	CLA	NA
21	a	1122	CLA	NC
21	a	1122	CLA	ND
21	a	1122	CLA	NA
21	B	1211	CLA	NC
21	B	1211	CLA	ND
21	B	1211	CLA	NA
21	B	1239	CLA	NC
21	B	1239	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	1239	CLA	NA
21	B	1236	CLA	NC
21	B	1236	CLA	ND
21	B	1236	CLA	NA
21	8	1402	CLA	NC
21	8	1402	CLA	ND
21	8	1402	CLA	NA
21	7	1302	CLA	ND
21	7	1302	CLA	NA
21	L	1503	CLA	NC
21	L	1503	CLA	NA
21	B	1224	CLA	NC
21	B	1224	CLA	ND
21	B	1224	CLA	NA
21	a	1127	CLA	NC
21	a	1127	CLA	ND
21	a	1127	CLA	NA
21	A	1011	CLA	NC
21	A	1011	CLA	ND
21	A	1011	CLA	NA
21	a	1105	CLA	NC
21	a	1105	CLA	ND
21	a	1105	CLA	NA
21	a	1132	CLA	NC
21	a	1132	CLA	ND
21	a	1132	CLA	NA
21	K	1401	CLA	NC
21	K	1401	CLA	ND
21	K	1401	CLA	NA
21	1	1137	CLA	NC
21	1	1137	CLA	ND
21	1	1137	CLA	NA
21	2	1238	CLA	NC
21	2	1238	CLA	ND
21	2	1238	CLA	NA
21	a	1128	CLA	NC
21	a	1128	CLA	ND
21	a	1128	CLA	NA
21	B	1208	CLA	NC
21	B	1208	CLA	ND
21	B	1208	CLA	NA
21	1	1107	CLA	NC

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Mol	Chain	Res	Type	Atom
21	1	1107	CLA	ND
21	1	1107	CLA	NA
21	a	1106	CLA	NC
21	a	1106	CLA	ND
21	a	1106	CLA	NA
21	b	1212	CLA	NC
21	b	1212	CLA	NA
21	1	1101	CLA	NA
21	a	1103	CLA	ND
21	a	1103	CLA	NA
21	1	1132	CLA	NC
21	1	1132	CLA	ND
21	1	1132	CLA	NA
21	B	1226	CLA	NC
21	B	1226	CLA	ND
21	B	1226	CLA	NA
21	A	1105	CLA	NC
21	A	1105	CLA	ND
21	A	1105	CLA	NA
21	b	1228	CLA	NC
21	b	1228	CLA	ND
21	b	1228	CLA	NA
21	b	1206	CLA	NC
21	b	1206	CLA	ND
21	b	1206	CLA	NA
21	B	1215	CLA	NC
21	B	1215	CLA	ND
21	B	1215	CLA	NA
21	1	1118	CLA	NC
21	1	1118	CLA	ND
21	1	1118	CLA	NA
21	1	1503	CLA	NC
21	1	1503	CLA	ND
21	1	1503	CLA	NA
21	1	1103	CLA	ND
21	1	1103	CLA	NA
21	k	1402	CLA	NC
21	k	1402	CLA	ND
21	k	1402	CLA	NA
21	0	1502	CLA	NC
21	0	1502	CLA	ND
21	0	1502	CLA	NA

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Mol	Chain	Res	Type	Atom
21	B	1202	CLA	ND
21	B	1202	CLA	NA
21	L	1502	CLA	NC
21	L	1502	CLA	ND
21	L	1502	CLA	NA
21	B	1222	CLA	NC
21	B	1222	CLA	ND
21	B	1222	CLA	NA
21	B	1230	CLA	NC
21	B	1230	CLA	ND
21	B	1230	CLA	NA
21	b	1234	CLA	NC
21	b	1234	CLA	ND
21	b	1234	CLA	NA
21	1	1129	CLA	NC
21	1	1129	CLA	ND
21	1	1129	CLA	NA
21	B	1212	CLA	NC
21	B	1212	CLA	ND
21	B	1212	CLA	NA
21	A	1122	CLA	NC
21	A	1122	CLA	ND
21	A	1122	CLA	NA
21	B	1238	CLA	NC
21	B	1238	CLA	ND
21	B	1238	CLA	NA
21	A	1121	CLA	NC
21	A	1121	CLA	ND
21	A	1121	CLA	NA
21	B	1209	CLA	NC
21	B	1209	CLA	NA
21	a	1111	CLA	NC
21	a	1111	CLA	ND
21	a	1111	CLA	NA
21	1	1130	CLA	NC
21	1	1130	CLA	ND
21	1	1130	CLA	NA
21	l	1501	CLA	NC
21	l	1501	CLA	ND
21	l	1501	CLA	NA
21	a	1113	CLA	NC
21	a	1113	CLA	ND

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Mol	Chain	Res	Type	Atom
21	a	1113	CLA	NA
21	F	1301	CLA	NC
21	F	1301	CLA	ND
21	F	1301	CLA	NA
21	B	1228	CLA	NC
21	B	1228	CLA	ND
21	B	1228	CLA	NA
21	A	1106	CLA	NC
21	A	1106	CLA	ND
21	A	1106	CLA	NA
21	A	1138	CLA	NC
21	A	1138	CLA	ND
21	A	1138	CLA	NA
21	b	1239	CLA	NC
21	b	1239	CLA	ND
21	b	1239	CLA	NA
21	a	1129	CLA	NC
21	a	1129	CLA	ND
21	a	1129	CLA	NA
21	A	1136	CLA	NC
21	A	1136	CLA	ND
21	A	1136	CLA	NA
21	b	1021	CLA	NC
21	b	1021	CLA	ND
21	b	1021	CLA	NA
21	1	1105	CLA	NC
21	1	1105	CLA	ND
21	1	1105	CLA	NA
21	B	1210	CLA	NC
21	B	1210	CLA	NA
21	2	1207	CLA	NC
21	2	1207	CLA	NA
21	b	1226	CLA	NC
21	b	1226	CLA	ND
21	b	1226	CLA	NA
21	b	1205	CLA	NC
21	b	1205	CLA	NA
21	b	1205	CLA	ND
21	B	1234	CLA	NA
21	2	1208	CLA	NC
21	2	1208	CLA	ND
21	2	1208	CLA	NA

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Mol	Chain	Res	Type	Atom
21	1	1123	CLA	NA
21	a	1130	CLA	NC
21	a	1130	CLA	ND
21	a	1130	CLA	NA
21	B	1223	CLA	NC
21	B	1223	CLA	ND
21	B	1223	CLA	NA
21	a	1140	CLA	NC
21	a	1140	CLA	ND
21	a	1140	CLA	NA
21	2	1021	CLA	NC
21	2	1021	CLA	ND
21	2	1021	CLA	NA
21	1	1135	CLA	NA
21	b	1201	CLA	NC
21	b	1201	CLA	ND
21	b	1201	CLA	NA
21	a	1109	CLA	NC
21	a	1109	CLA	ND
21	a	1109	CLA	NA
21	2	1204	CLA	NC
21	2	1204	CLA	ND
21	2	1204	CLA	NA
21	A	1135	CLA	NA
21	A	1104	CLA	ND
21	A	1104	CLA	NA
21	2	1227	CLA	NC
21	2	1227	CLA	ND
21	2	1227	CLA	NA
21	b	1217	CLA	NC
21	b	1217	CLA	ND
21	b	1217	CLA	NA
21	a	1112	CLA	NC
21	a	1112	CLA	ND
21	a	1112	CLA	NA
21	J	1303	CLA	NC
21	J	1303	CLA	ND
21	J	1303	CLA	NA
21	b	1236	CLA	NC
21	b	1236	CLA	ND
21	b	1236	CLA	NA
21	1	1133	CLA	NC

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Mol	Chain	Res	Type	Atom
21	1	1133	CLA	ND
21	1	1133	CLA	NA
21	2	1205	CLA	NC
21	2	1205	CLA	ND
21	2	1205	CLA	NA
21	a	1801	CLA	NC
21	a	1801	CLA	ND
21	a	1801	CLA	NA
21	0	1501	CLA	NC
21	0	1501	CLA	ND
21	0	1501	CLA	NA
21	1	1801	CLA	NC
21	1	1801	CLA	ND
21	1	1801	CLA	NA
21	2	1219	CLA	NC
21	2	1219	CLA	NA
21	a	1012	CLA	NC
21	a	1012	CLA	ND
21	a	1012	CLA	NA
21	2	1217	CLA	NC
21	2	1217	CLA	ND
21	2	1217	CLA	NA
34	F	4016	ZEX	C24
21	1	1121	CLA	NC
21	1	1121	CLA	ND
21	1	1121	CLA	NA
21	A	1137	CLA	NC
21	A	1137	CLA	ND
21	A	1137	CLA	NA
21	B	1201	CLA	NC
21	B	1201	CLA	ND
21	B	1201	CLA	NA
21	A	1132	CLA	NC
21	A	1132	CLA	ND
21	A	1132	CLA	NA
21	B	1229	CLA	NC
21	B	1229	CLA	ND
21	B	1229	CLA	NA
21	b	1218	CLA	NC
21	b	1218	CLA	ND
21	b	1218	CLA	NA
21	a	1104	CLA	NC

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Mol	Chain	Res	Type	Atom
21	a	1104	CLA	ND
21	a	1104	CLA	NA
21	1	1125	CLA	NC
21	1	1125	CLA	ND
21	1	1125	CLA	NA
21	b	1231	CLA	NC
21	b	1231	CLA	ND
21	b	1231	CLA	NA
21	A	1129	CLA	NC
21	A	1129	CLA	NA
21	A	1111	CLA	NC
21	A	1111	CLA	ND
21	A	1111	CLA	NA
21	b	1215	CLA	NC
21	b	1215	CLA	ND
21	b	1215	CLA	NA
21	L	1501	CLA	NC
21	L	1501	CLA	ND
21	L	1501	CLA	NA
21	A	1134	CLA	NC
21	A	1134	CLA	ND
21	A	1134	CLA	NA
21	1	1110	CLA	NC
21	1	1110	CLA	ND
21	1	1110	CLA	NA
21	0	1503	CLA	NC
21	0	1503	CLA	ND
21	0	1503	CLA	NA
21	f	1302	CLA	NC
21	f	1302	CLA	ND
21	f	1302	CLA	NA
21	2	1202	CLA	ND
21	2	1202	CLA	NA
21	b	1204	CLA	NC
21	b	1204	CLA	ND
21	b	1204	CLA	NA
21	A	1130	CLA	NC
21	A	1130	CLA	ND
21	A	1130	CLA	NA
21	6	1302	CLA	NC
21	6	1302	CLA	ND
21	6	1302	CLA	NA

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Mol	Chain	Res	Type	Atom
21	A	1107	CLA	NC
21	A	1107	CLA	ND
21	A	1107	CLA	NA
21	b	1237	CLA	NC
21	b	1237	CLA	ND
21	b	1237	CLA	NA
21	2	1215	CLA	NC
21	2	1215	CLA	ND
21	2	1215	CLA	NA
21	B	1235	CLA	NC
21	B	1235	CLA	ND
21	B	1235	CLA	NA
21	A	1133	CLA	NC
21	A	1133	CLA	ND
21	A	1133	CLA	NA
21	2	1232	CLA	ND
21	2	1232	CLA	NA
21	a	1139	CLA	NC
21	a	1139	CLA	ND
21	a	1139	CLA	NA
21	B	1221	CLA	NC
21	B	1221	CLA	ND
21	B	1221	CLA	NA
21	1	1126	CLA	NC
21	1	1126	CLA	ND
21	1	1126	CLA	NA
21	a	1124	CLA	NC
21	a	1124	CLA	ND
21	a	1124	CLA	NA
21	2	1023	CLA	NC
21	2	1023	CLA	ND
21	2	1023	CLA	NA
21	A	1115	CLA	NC
21	A	1115	CLA	ND
21	A	1115	CLA	NA
21	2	1222	CLA	NC
21	2	1222	CLA	ND
21	2	1222	CLA	NA
21	B	1218	CLA	NC
21	B	1218	CLA	ND
21	B	1218	CLA	NA
21	a	1117	CLA	NC

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Mol	Chain	Res	Type	Atom
21	a	1117	CLA	ND
21	a	1117	CLA	NA
21	7	1303	CLA	NC
21	7	1303	CLA	ND
21	7	1303	CLA	NA
21	b	1207	CLA	NC
21	b	1207	CLA	NA
21	1	1109	CLA	NC
21	1	1109	CLA	ND
21	1	1109	CLA	NA
21	2	1212	CLA	NC
21	2	1212	CLA	ND
21	2	1212	CLA	NA
21	2	1218	CLA	NC
21	2	1218	CLA	ND
21	2	1218	CLA	NA
21	B	1021	CLA	NC
21	B	1021	CLA	ND
21	B	1021	CLA	NA
21	B	1227	CLA	NC
21	B	1227	CLA	NA
21	A	1131	CLA	NC
21	A	1131	CLA	ND
21	A	1131	CLA	NA
21	j	1303	CLA	NC
21	j	1303	CLA	ND
21	j	1303	CLA	NA
21	A	1117	CLA	NC
21	A	1117	CLA	ND
21	A	1117	CLA	NA
21	A	1128	CLA	NC
21	A	1128	CLA	ND
21	A	1128	CLA	NA
21	b	1238	CLA	NC
21	b	1238	CLA	ND
21	b	1238	CLA	NA
21	l	1502	CLA	NC
21	l	1502	CLA	ND
21	l	1502	CLA	NA
21	B	1022	CLA	NC
21	B	1022	CLA	ND
21	B	1022	CLA	NA

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Mol	Chain	Res	Type	Atom
21	2	1240	CLA	NC
21	2	1240	CLA	NA
21	K	1402	CLA	NA
21	a	1110	CLA	NC
21	a	1110	CLA	ND
21	a	1110	CLA	NA
21	b	1221	CLA	NC
21	b	1221	CLA	ND
21	b	1221	CLA	NA
21	b	1210	CLA	NC
21	b	1210	CLA	NA
21	B	1203	CLA	ND
21	B	1203	CLA	NA
21	A	1119	CLA	NC
21	A	1119	CLA	ND
21	A	1119	CLA	NA
21	1	1140	CLA	NC
21	1	1140	CLA	ND
21	1	1140	CLA	NA
21	1	1114	CLA	NC
21	1	1114	CLA	ND
21	1	1114	CLA	NA
21	b	1209	CLA	NC
21	b	1209	CLA	NA
21	A	1139	CLA	NC
21	A	1139	CLA	ND
21	A	1139	CLA	NA
21	a	1118	CLA	NC
21	a	1118	CLA	ND
21	a	1118	CLA	NA
21	1	1102	CLA	NC
21	1	1102	CLA	ND
21	1	1102	CLA	NA
21	A	1125	CLA	NC
21	A	1125	CLA	NA
21	6	1301	CLA	NC
21	6	1301	CLA	ND
21	6	1301	CLA	NA
21	B	1232	CLA	NC
21	B	1232	CLA	ND
21	B	1232	CLA	NA
21	2	1228	CLA	NC

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Mol	Chain	Res	Type	Atom
21	2	1228	CLA	ND
21	2	1228	CLA	NA
21	a	1136	CLA	NC
21	a	1136	CLA	ND
21	a	1136	CLA	NA
21	A	1140	CLA	NC
21	A	1140	CLA	ND
21	A	1140	CLA	NA
21	1	1136	CLA	NC
21	1	1136	CLA	ND
21	1	1136	CLA	NA
21	2	1209	CLA	NA
21	2	1203	CLA	NC
21	2	1203	CLA	ND
21	2	1203	CLA	NA
21	8	1401	CLA	NC
21	8	1401	CLA	ND
21	8	1401	CLA	NA
21	A	1108	CLA	NC
21	A	1108	CLA	ND
21	A	1108	CLA	NA
21	2	1239	CLA	NC
21	2	1239	CLA	ND
21	2	1239	CLA	NA
21	1	1108	CLA	NC
21	1	1108	CLA	ND
21	1	1108	CLA	NA
21	A	1013	CLA	NC
21	A	1013	CLA	ND
21	A	1013	CLA	NA
21	1	1138	CLA	NC
21	1	1138	CLA	ND
21	1	1138	CLA	NA
21	b	1223	CLA	ND
21	b	1223	CLA	NA
21	2	1221	CLA	NC
21	2	1221	CLA	ND
21	2	1221	CLA	NA
21	A	1120	CLA	NC
21	A	1120	CLA	ND
21	A	1120	CLA	NA
21	B	1205	CLA	NC

Continued on next page...

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Mol	Chain	Res	Type	Atom
21	B	1205	CLA	NA
21	B	1205	CLA	ND
21	1	1012	CLA	NA
21	1	1012	CLA	ND
21	b	1023	CLA	NC
21	b	1023	CLA	ND
21	b	1023	CLA	NA
21	B	1225	CLA	NC
21	B	1225	CLA	ND
21	B	1225	CLA	NA
21	b	1230	CLA	NC
21	b	1230	CLA	ND
21	b	1230	CLA	NA
21	a	1137	CLA	NC
21	a	1137	CLA	ND
21	a	1137	CLA	NA
21	A	1102	CLA	NC
21	A	1102	CLA	ND
21	A	1102	CLA	NA
21	b	1219	CLA	NC
21	b	1219	CLA	ND
21	b	1219	CLA	NA
21	a	1134	CLA	NC
21	a	1134	CLA	ND
21	a	1134	CLA	NA
21	1	1120	CLA	NC
21	1	1120	CLA	ND
21	1	1120	CLA	NA
21	b	1232	CLA	NC
21	b	1232	CLA	ND
21	b	1232	CLA	NA
21	A	1124	CLA	NC
21	A	1124	CLA	ND
21	A	1124	CLA	NA
21	2	1224	CLA	NC
21	2	1224	CLA	ND
21	2	1224	CLA	NA
21	A	1109	CLA	NC
21	A	1109	CLA	ND
21	A	1109	CLA	NA
21	J	1302	CLA	NC
21	J	1302	CLA	ND

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Mol	Chain	Res	Type	Atom
21	J	1302	CLA	NA
21	a	1135	CLA	ND
21	a	1135	CLA	NA
21	a	1138	CLA	NC
21	a	1138	CLA	ND
21	a	1138	CLA	NA
21	b	1213	CLA	NC
21	b	1213	CLA	ND
21	b	1213	CLA	NA
21	1	1117	CLA	NC
21	1	1117	CLA	ND
21	1	1117	CLA	NA
21	a	1114	CLA	NC
21	a	1114	CLA	ND
21	a	1114	CLA	NA
21	B	1206	CLA	NC
21	B	1206	CLA	ND
21	B	1206	CLA	NA
21	A	1127	CLA	NC
21	A	1127	CLA	ND
21	A	1127	CLA	NA
21	1	1128	CLA	NC
21	1	1128	CLA	ND
21	1	1128	CLA	NA
21	a	1126	CLA	NC
21	a	1126	CLA	NA
21	a	1126	CLA	ND
21	A	1118	CLA	NC
21	A	1118	CLA	ND
21	A	1118	CLA	NA
21	a	1108	CLA	NC
21	a	1108	CLA	ND
21	a	1108	CLA	NA
21	a	1125	CLA	NC
21	a	1125	CLA	ND
21	a	1125	CLA	NA
21	a	1120	CLA	NC
21	a	1120	CLA	NA
21	a	1119	CLA	NC
21	a	1119	CLA	ND
21	a	1119	CLA	NA

All (6201) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	1012	CLA	CHA-CBD-CGD-O1D
21	A	1012	CLA	CHA-CBD-CGD-O2D
21	A	1012	CLA	CAD-CBD-CGD-O1D
21	A	1012	CLA	CAD-CBD-CGD-O2D
21	A	1012	CLA	C2-C3-C5-C6
21	A	1012	CLA	C4-C3-C5-C6
26	0	5001	LMG	C2-C1-O1-C7
26	0	5001	LMG	O6-C1-O1-C7
21	B	1214	CLA	C6-C7-C8-C9
21	1	1112	CLA	C1A-C2A-CAA-CBA
21	1	1112	CLA	C3A-C2A-CAA-CBA
21	1	1112	CLA	C2-C1-O2A-CGA
21	1	1112	CLA	CBD-CGD-O2D-CED
21	1	1139	CLA	CHA-CBD-CGD-O1D
21	1	1139	CLA	CHA-CBD-CGD-O2D
21	1	1139	CLA	CBD-CGD-O2D-CED
21	1	1011	CLA	C1A-C2A-CAA-CBA
24	a	4001	BCR	C11-C10-C9-C8
24	a	4001	BCR	C11-C10-C9-C34
24	a	4001	BCR	C10-C11-C12-C13
24	a	4001	BCR	C11-C12-C13-C14
24	a	4001	BCR	C11-C12-C13-C35
24	a	4001	BCR	C17-C18-C19-C20
24	a	4001	BCR	C36-C18-C19-C20
37	L	5004	DGD	C2B-C1B-O2G-C2G
37	L	5004	DGD	C2D-C1D-O3G-C3G
37	L	5004	DGD	O6D-C1D-O3G-C3G
37	L	5004	DGD	C4D-C5D-C6D-O5D
37	L	5004	DGD	O6E-C1E-O5D-C6D
21	2	1231	CLA	CBD-CGD-O2D-CED
21	b	1220	CLA	CBD-CGD-O2D-CED
21	2	1213	CLA	CHA-CBD-CGD-O1D
21	2	1213	CLA	CHA-CBD-CGD-O2D
21	B	1204	CLA	CHA-CBD-CGD-O1D
21	2	1229	CLA	C1A-C2A-CAA-CBA
21	2	1229	CLA	C3A-C2A-CAA-CBA
21	2	1229	CLA	CBD-CGD-O2D-CED
21	2	1229	CLA	C11-C12-C13-C15
21	B	1220	CLA	C6-C7-C8-C9
35	F	6001	LMT	C2-C1-O1'-C1'
21	A	1801	CLA	CHA-CBD-CGD-O1D
21	A	1801	CLA	CHA-CBD-CGD-O2D
21	A	1801	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	j	1302	CLA	C2-C1-O2A-CGA
25	l	5002	LHG	C1-C2-C3-O3
25	l	5002	LHG	C4-O6-P-O4
25	l	5002	LHG	C4-O6-P-O5
25	l	5002	LHG	O6-C4-C5-O7
24	1	4001	BCR	C11-C10-C9-C8
24	1	4001	BCR	C11-C10-C9-C34
24	1	4001	BCR	C10-C11-C12-C13
24	6	4016	BCR	C10-C11-C12-C13
24	6	4016	BCR	C11-C12-C13-C14
24	6	4016	BCR	C11-C12-C13-C35
24	6	4016	BCR	C36-C18-C19-C20
24	6	4016	BCR	C21-C22-C23-C24
24	6	4016	BCR	C37-C22-C23-C24
21	b	1225	CLA	C1A-C2A-CAA-CBA
21	b	1225	CLA	C3A-C2A-CAA-CBA
25	M	5001	LHG	C4-O6-P-O3
25	M	5001	LHG	C4-O6-P-O4
25	M	5001	LHG	C4-O6-P-O5
25	M	5001	LHG	O9-C7-O7-C5
25	M	5001	LHG	C8-C7-O7-C5
25	2	5004	LHG	C4-O6-P-O3
21	b	1202	CLA	C3A-C2A-CAA-CBA
21	A	1114	CLA	CBD-CGD-O2D-CED
24	B	4010	BCR	C11-C10-C9-C8
24	B	4010	BCR	C11-C10-C9-C34
24	B	4010	BCR	C10-C11-C12-C13
24	B	4010	BCR	C17-C18-C19-C20
24	B	4010	BCR	C36-C18-C19-C20
21	a	1116	CLA	C3A-C2A-CAA-CBA
21	a	1116	CLA	CBD-CGD-O2D-CED
21	a	1116	CLA	C2-C3-C5-C6
21	a	1116	CLA	C4-C3-C5-C6
34	7	4015	ZEX	C21-C26-C27-C28
34	7	4015	ZEX	C7-C8-C9-C19
34	7	4015	ZEX	C7-C8-C9-C10
34	j	4015	ZEX	C25-C26-C27-C28
34	j	4015	ZEX	C31-C32-C33-C34
34	j	4015	ZEX	C31-C32-C33-C40
21	b	1216	CLA	C1A-C2A-CAA-CBA
21	b	1216	CLA	C3A-C2A-CAA-CBA
21	b	1216	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	b	1216	CLA	C4-C3-C5-C6
28	B	4011	45D	C19-C23-C25-C27
28	B	4011	45D	C19-C23-C25-C29
28	B	4011	45D	C31-C33-C35-C37
28	B	4011	45D	C31-C33-C35-C39
21	B	1213	CLA	C1A-C2A-CAA-CBA
21	2	1236	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	C1A-C2A-CAA-CBA
21	B	1216	CLA	C3A-C2A-CAA-CBA
21	B	1237	CLA	CBA-CGA-O2A-C1
21	B	1237	CLA	O1A-CGA-O2A-C1
21	B	1237	CLA	C2-C3-C5-C6
21	B	1237	CLA	C4-C3-C5-C6
25	B	5004	LHG	C3-O3-P-O6
25	B	5004	LHG	C4-O6-P-O3
25	B	5004	LHG	C4-O6-P-O4
25	B	5004	LHG	C4-O6-P-O5
21	2	1206	CLA	C2-C1-O2A-CGA
21	2	1206	CLA	C14-C13-C15-C16
24	1	4007	BCR	C11-C10-C9-C8
24	1	4007	BCR	C11-C10-C9-C34
24	1	4007	BCR	C21-C22-C23-C24
24	1	4007	BCR	C37-C22-C23-C24
24	1	4007	BCR	C23-C24-C25-C30
24	A	4008	BCR	C23-C24-C25-C26
21	a	1121	CLA	C1A-C2A-CAA-CBA
21	a	1121	CLA	C2-C3-C5-C6
21	a	1121	CLA	C4-C3-C5-C6
21	B	1219	CLA	C1A-C2A-CAA-CBA
21	B	1219	CLA	CBA-CGA-O2A-C1
21	B	1219	CLA	O1A-CGA-O2A-C1
21	A	1126	CLA	C2-C1-O2A-CGA
21	A	1126	CLA	CBD-CGD-O2D-CED
21	B	1240	CLA	C1A-C2A-CAA-CBA
21	B	1240	CLA	C3A-C2A-CAA-CBA
21	b	1214	CLA	C6-C7-C8-C9
21	1	1122	CLA	CHA-CBD-CGD-O1D
21	1	1122	CLA	CHA-CBD-CGD-O2D
21	2	1230	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	C1A-C2A-CAA-CBA
21	B	1217	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	1116	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	C2-C3-C5-C6
21	A	1116	CLA	C4-C3-C5-C6
21	f	1301	CLA	CBD-CGD-O2D-CED
21	2	1234	CLA	C1A-C2A-CAA-CBA
21	2	1234	CLA	C3A-C2A-CAA-CBA
21	2	1234	CLA	CHA-CBD-CGD-O1D
21	2	1234	CLA	CHA-CBD-CGD-O2D
21	b	1208	CLA	C1A-C2A-CAA-CBA
21	b	1208	CLA	C3A-C2A-CAA-CBA
21	b	1208	CLA	C2-C3-C5-C6
21	b	1208	CLA	C4-C3-C5-C6
24	A	4012	BCR	C5-C6-C7-C8
24	A	4012	BCR	C11-C10-C9-C8
24	A	4012	BCR	C11-C10-C9-C34
24	A	4012	BCR	C11-C12-C13-C14
24	A	4012	BCR	C11-C12-C13-C35
24	1	4003	BCR	C1-C6-C7-C8
24	1	4003	BCR	C11-C10-C9-C8
24	1	4003	BCR	C11-C10-C9-C34
21	1	1127	CLA	C2-C3-C5-C6
21	1	1127	CLA	C4-C3-C5-C6
21	B	1207	CLA	C11-C12-C13-C14
24	f	4016	BCR	C10-C11-C12-C13
24	f	4016	BCR	C11-C12-C13-C14
24	f	4016	BCR	C11-C12-C13-C35
24	f	4016	BCR	C21-C22-C23-C24
24	f	4016	BCR	C37-C22-C23-C24
21	2	1210	CLA	C1A-C2A-CAA-CBA
21	2	1210	CLA	C3A-C2A-CAA-CBA
21	k	1401	CLA	CHA-CBD-CGD-O1D
21	k	1401	CLA	CHA-CBD-CGD-O2D
21	1	1104	CLA	CBD-CGD-O2D-CED
24	l	4022	BCR	C7-C8-C9-C10
24	l	4022	BCR	C7-C8-C9-C34
24	l	4022	BCR	C10-C11-C12-C13
24	l	4022	BCR	C11-C12-C13-C14
24	l	4022	BCR	C11-C12-C13-C35
24	l	4022	BCR	C21-C22-C23-C24
24	l	4022	BCR	C37-C22-C23-C24
21	1	1134	CLA	C2-C1-O2A-CGA
21	1	1134	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	1134	CLA	C4-C3-C5-C6
24	k	4001	BCR	C11-C10-C9-C8
24	k	4001	BCR	C11-C10-C9-C34
24	k	4001	BCR	C10-C11-C12-C13
24	k	4001	BCR	C17-C18-C19-C20
24	k	4001	BCR	C36-C18-C19-C20
24	2	4018	BCR	C1-C6-C7-C8
24	2	4018	BCR	C11-C10-C9-C8
24	2	4018	BCR	C17-C18-C19-C20
24	2	4018	BCR	C36-C18-C19-C20
24	2	4018	BCR	C23-C24-C25-C26
24	2	4018	BCR	C23-C24-C25-C30
21	A	1110	CLA	C1A-C2A-CAA-CBA
21	A	1110	CLA	C3A-C2A-CAA-CBA
21	1	1124	CLA	C6-C7-C8-C9
36	I	4020	EQ3	C21-C22-C23-C24
36	I	4020	EQ3	C37-C22-C23-C24
21	A	1113	CLA	CHA-CBD-CGD-O1D
21	A	1113	CLA	C2-C3-C5-C6
21	A	1113	CLA	C4-C3-C5-C6
21	B	1231	CLA	C2-C1-O2A-CGA
25	1	5001	LHG	O1-C1-C2-C3
25	1	5001	LHG	C1-C2-C3-O3
25	1	5001	LHG	O7-C5-C6-O8
21	b	1240	CLA	C3A-C2A-CAA-CBA
21	b	1240	CLA	CAD-CBD-CGD-O1D
21	b	1240	CLA	CAD-CBD-CGD-O2D
24	0	4022	BCR	C11-C10-C9-C8
24	0	4022	BCR	C11-C10-C9-C34
24	0	4022	BCR	C10-C11-C12-C13
21	b	1222	CLA	C2-C3-C5-C6
21	b	1222	CLA	C4-C3-C5-C6
21	a	1133	CLA	C2-C1-O2A-CGA
21	a	1133	CLA	C4-C3-C5-C6
21	b	1229	CLA	C1A-C2A-CAA-CBA
21	b	1229	CLA	C3A-C2A-CAA-CBA
21	b	1229	CLA	CBD-CGD-O2D-CED
21	2	1235	CLA	CHA-CBD-CGD-O1D
21	2	1235	CLA	CHA-CBD-CGD-O2D
21	1	1106	CLA	C1A-C2A-CAA-CBA
21	1	1106	CLA	C3A-C2A-CAA-CBA
21	1	1106	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	1	1106	CLA	CHA-CBD-CGD-O2D
21	1	1106	CLA	C14-C13-C15-C16
21	2	1211	CLA	C1A-C2A-CAA-CBA
21	2	1211	CLA	C3A-C2A-CAA-CBA
21	2	1211	CLA	CHA-CBD-CGD-O1D
21	2	1211	CLA	CHA-CBD-CGD-O2D
21	1	1113	CLA	C2A-CAA-CBA-CGA
21	a	1013	CLA	C2-C1-O2A-CGA
21	a	1013	CLA	CHA-CBD-CGD-O1D
21	a	1013	CLA	CHA-CBD-CGD-O2D
24	B	4014	BCR	C11-C10-C9-C8
24	B	4014	BCR	C11-C10-C9-C34
24	B	4014	BCR	C21-C22-C23-C24
24	B	4014	BCR	C37-C22-C23-C24
21	2	1226	CLA	CHA-CBD-CGD-O1D
21	2	1226	CLA	CHA-CBD-CGD-O2D
21	2	1226	CLA	CAD-CBD-CGD-O1D
21	b	1224	CLA	C3A-C2A-CAA-CBA
21	b	1224	CLA	CBD-CGD-O2D-CED
24	h	4018	BCR	C1-C6-C7-C8
24	h	4018	BCR	C11-C10-C9-C8
24	h	4018	BCR	C11-C10-C9-C34
24	h	4018	BCR	C10-C11-C12-C13
24	h	4018	BCR	C11-C12-C13-C14
24	h	4018	BCR	C11-C12-C13-C35
24	h	4018	BCR	C17-C18-C19-C20
24	h	4018	BCR	C36-C18-C19-C20
21	1	1111	CLA	C3A-C2A-CAA-CBA
21	1	1111	CLA	CHA-CBD-CGD-O1D
21	1	1111	CLA	CHA-CBD-CGD-O2D
25	F	5002	LHG	O1-C1-C2-C3
25	F	5002	LHG	O2-C2-C3-O3
25	F	5002	LHG	C4-O6-P-O3
25	F	5002	LHG	C4-O6-P-O4
25	F	5002	LHG	C4-O6-P-O5
21	2	1225	CLA	C1A-C2A-CAA-CBA
21	2	1225	CLA	C3A-C2A-CAA-CBA
21	1	1116	CLA	C1A-C2A-CAA-CBA
21	1	1116	CLA	C3A-C2A-CAA-CBA
21	1	1116	CLA	CBD-CGD-O2D-CED
21	1	1116	CLA	C6-C7-C8-C9
31	F	5001	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
21	F	1302	CLA	C1A-C2A-CAA-CBA
21	F	1302	CLA	C3A-C2A-CAA-CBA
21	F	1302	CLA	CHA-CBD-CGD-O1D
21	F	1302	CLA	CHA-CBD-CGD-O2D
21	2	1223	CLA	CHA-CBD-CGD-O1D
21	2	1223	CLA	CHA-CBD-CGD-O2D
21	a	1123	CLA	C2-C1-O2A-CGA
24	J	4013	BCR	C1-C6-C7-C8
24	J	4013	BCR	C7-C8-C9-C34
24	J	4013	BCR	C11-C10-C9-C8
24	J	4013	BCR	C11-C10-C9-C34
24	J	4013	BCR	C10-C11-C12-C13
24	J	4013	BCR	C15-C16-C17-C18
24	J	4013	BCR	C17-C18-C19-C20
24	J	4013	BCR	C36-C18-C19-C20
21	A	1112	CLA	C1A-C2A-CAA-CBA
21	A	1112	CLA	C3A-C2A-CAA-CBA
21	A	1103	CLA	C1A-C2A-CAA-CBA
21	A	1103	CLA	C3A-C2A-CAA-CBA
21	A	1103	CLA	CHA-CBD-CGD-O1D
21	A	1103	CLA	CHA-CBD-CGD-O2D
21	A	1103	CLA	CAD-CBD-CGD-O1D
21	a	1107	CLA	CBD-CGD-O2D-CED
21	a	1122	CLA	C1A-C2A-CAA-CBA
21	a	1122	CLA	CHA-CBD-CGD-O1D
21	a	1122	CLA	CHA-CBD-CGD-O2D
21	B	1239	CLA	C1A-C2A-CAA-CBA
21	B	1239	CLA	C3A-C2A-CAA-CBA
21	B	1239	CLA	C2-C1-O2A-CGA
21	B	1236	CLA	C2-C1-O2A-CGA
24	A	4001	BCR	C11-C10-C9-C8
24	A	4001	BCR	C11-C10-C9-C34
24	A	4001	BCR	C11-C12-C13-C14
24	A	4001	BCR	C11-C12-C13-C35
21	8	1402	CLA	CBA-CGA-O2A-C1
21	7	1302	CLA	CBD-CGD-O2D-CED
21	L	1503	CLA	C1A-C2A-CAA-CBA
21	L	1503	CLA	C2-C3-C5-C6
21	L	1503	CLA	C4-C3-C5-C6
24	1	4002	BCR	C11-C10-C9-C8
24	1	4002	BCR	C11-C10-C9-C34
24	1	4002	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	1	4002	BCR	C17-C18-C19-C20
24	1	4002	BCR	C36-C18-C19-C20
24	1	4002	BCR	C21-C22-C23-C24
24	1	4002	BCR	C37-C22-C23-C24
21	B	1224	CLA	C1A-C2A-CAA-CBA
21	B	1224	CLA	C3A-C2A-CAA-CBA
21	B	1224	CLA	CBD-CGD-O2D-CED
21	a	1132	CLA	CHA-CBD-CGD-O1D
21	a	1132	CLA	CHA-CBD-CGD-O2D
25	A	5007	LHG	O1-C1-C2-C3
25	A	5007	LHG	O2-C2-C3-O3
25	A	5007	LHG	C3-O3-P-O5
25	A	5007	LHG	O9-C7-O7-C5
25	A	5007	LHG	C8-C7-O7-C5
21	1	1137	CLA	CHA-CBD-CGD-O1D
24	b	4010	BCR	C17-C18-C19-C20
24	b	4010	BCR	C36-C18-C19-C20
24	b	4017	BCR	C11-C10-C9-C8
24	b	4017	BCR	C11-C10-C9-C34
24	b	4017	BCR	C11-C12-C13-C14
24	b	4017	BCR	C17-C18-C19-C20
24	b	4017	BCR	C36-C18-C19-C20
24	2	4011	BCR	C7-C8-C9-C10
24	2	4011	BCR	C7-C8-C9-C34
24	2	4011	BCR	C17-C18-C19-C20
24	2	4011	BCR	C36-C18-C19-C20
24	2	4011	BCR	C21-C22-C23-C24
24	2	4011	BCR	C37-C22-C23-C24
21	a	1128	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	CBD-CGD-O2D-CED
21	1	1107	CLA	C1A-C2A-CAA-CBA
21	a	1106	CLA	C3A-C2A-CAA-CBA
21	a	1106	CLA	CHA-CBD-CGD-O1D
21	a	1106	CLA	CHA-CBD-CGD-O2D
34	J	4015	ZEX	C21-C26-C27-C28
25	1	5001	LHG	O1-C1-C2-C3
25	1	5001	LHG	O2-C2-C3-O3
25	1	5001	LHG	C4-O6-P-O3
25	1	5001	LHG	C4-O6-P-O4
25	1	5001	LHG	C4-O6-P-O5
21	a	1103	CLA	C1A-C2A-CAA-CBA
21	a	1103	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	a	1103	CLA	CHA-CBD-CGD-O1D
21	a	1103	CLA	CAD-CBD-CGD-O1D
21	a	1103	CLA	CAD-CBD-CGD-O2D
21	a	1103	CLA	C2-C3-C5-C6
21	a	1103	CLA	C4-C3-C5-C6
26	b	5005	LMG	O6-C1-O1-C7
26	b	5005	LMG	C11-C10-O7-C8
21	1	1132	CLA	CHA-CBD-CGD-O1D
21	1	1132	CLA	CHA-CBD-CGD-O2D
21	B	1226	CLA	C4-C3-C5-C6
21	B	1226	CLA	C14-C13-C15-C16
21	b	1228	CLA	C1A-C2A-CAA-CBA
21	b	1206	CLA	C2-C1-O2A-CGA
21	B	1215	CLA	C1A-C2A-CAA-CBA
21	B	1215	CLA	C3A-C2A-CAA-CBA
21	B	1215	CLA	CBD-CGD-O2D-CED
21	B	1215	CLA	C2-C3-C5-C6
21	B	1215	CLA	C4-C3-C5-C6
25	A	5001	LHG	O1-C1-C2-C3
25	A	5001	LHG	C3-O3-P-O5
25	A	5001	LHG	C4-O6-P-O4
21	l	1503	CLA	CBD-CGD-O2D-CED
21	1	1103	CLA	C1A-C2A-CAA-CBA
21	1	1103	CLA	C3A-C2A-CAA-CBA
21	1	1103	CLA	CHA-CBD-CGD-O1D
24	I	4018	BCR	C11-C10-C9-C34
24	I	4018	BCR	C19-C20-C21-C22
21	k	1402	CLA	C2-C1-O2A-CGA
21	k	1402	CLA	CHA-CBD-CGD-O1D
21	k	1402	CLA	CHA-CBD-CGD-O2D
21	B	1202	CLA	C3A-C2A-CAA-CBA
21	B	1202	CLA	CHA-CBD-CGD-O1D
21	B	1202	CLA	CHA-CBD-CGD-O2D
21	B	1202	CLA	CAD-CBD-CGD-O1D
21	L	1502	CLA	C1A-C2A-CAA-CBA
21	L	1502	CLA	C3A-C2A-CAA-CBA
26	1	5002	LMG	C2-C1-O1-C7
26	1	5002	LMG	O6-C1-O1-C7
26	1	5002	LMG	C11-C10-O7-C8
24	B	4005	BCR	C11-C10-C9-C8
24	B	4005	BCR	C11-C10-C9-C34
24	B	4005	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	4005	BCR	C17-C18-C19-C20
24	B	4005	BCR	C36-C18-C19-C20
24	B	4005	BCR	C37-C22-C23-C24
21	B	1230	CLA	C1A-C2A-CAA-CBA
21	B	1230	CLA	C3A-C2A-CAA-CBA
21	1	1129	CLA	C1A-C2A-CAA-CBA
21	1	1129	CLA	C3A-C2A-CAA-CBA
24	2	4005	BCR	C11-C10-C9-C8
24	2	4005	BCR	C11-C10-C9-C34
24	2	4005	BCR	C10-C11-C12-C13
24	2	4005	BCR	C17-C18-C19-C20
24	2	4005	BCR	C36-C18-C19-C20
24	2	4005	BCR	C21-C22-C23-C24
24	2	4005	BCR	C37-C22-C23-C24
24	0	4019	BCR	C11-C10-C9-C8
24	0	4019	BCR	C11-C10-C9-C34
24	0	4019	BCR	C23-C24-C25-C26
26	2	5005	LMG	C2-C1-O1-C7
26	2	5005	LMG	O6-C1-O1-C7
21	B	1212	CLA	CHA-CBD-CGD-O1D
21	B	1212	CLA	CBD-CGD-O2D-CED
21	A	1122	CLA	C1A-C2A-CAA-CBA
21	A	1122	CLA	C2A-CAA-CBA-CGA
21	A	1122	CLA	CHA-CBD-CGD-O1D
21	A	1122	CLA	CHA-CBD-CGD-O2D
25	a	5005	LHG	C1-C2-C3-O3
25	a	5005	LHG	C2-C3-O3-P
25	a	5005	LHG	C4-O6-P-O3
25	a	5005	LHG	C4-O6-P-O5
25	a	5005	LHG	O9-C7-O7-C5
25	a	5005	LHG	C8-C7-O7-C5
24	a	4008	BCR	C11-C10-C9-C8
24	a	4008	BCR	C11-C10-C9-C34
24	a	4008	BCR	C13-C14-C15-C16
24	a	4008	BCR	C17-C18-C19-C20
24	a	4008	BCR	C36-C18-C19-C20
24	a	4008	BCR	C23-C24-C25-C30
21	A	1121	CLA	C1A-C2A-CAA-CBA
21	A	1121	CLA	C6-C7-C8-C9
21	B	1209	CLA	C1A-C2A-CAA-CBA
21	B	1209	CLA	C3A-C2A-CAA-CBA
21	B	1209	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	1209	CLA	C11-C10-C8-C9
21	a	1111	CLA	C3A-C2A-CAA-CBA
21	a	1111	CLA	CHA-CBD-CGD-O1D
21	a	1111	CLA	CHA-CBD-CGD-O2D
21	a	1111	CLA	C2-C3-C5-C6
21	a	1111	CLA	C4-C3-C5-C6
21	1	1130	CLA	C2-C3-C5-C6
21	1	1130	CLA	C4-C3-C5-C6
21	l	1501	CLA	C3A-C2A-CAA-CBA
21	l	1501	CLA	C2-C1-O2A-CGA
21	a	1113	CLA	CHA-CBD-CGD-O1D
21	a	1113	CLA	CHA-CBD-CGD-O2D
21	F	1301	CLA	C11-C10-C8-C7
21	A	1106	CLA	C1A-C2A-CAA-CBA
21	A	1106	CLA	CHA-CBD-CGD-O2D
24	9	4021	BCR	C1-C6-C7-C8
24	9	4021	BCR	C5-C6-C7-C8
24	9	4021	BCR	C11-C10-C9-C8
24	9	4021	BCR	C11-C10-C9-C34
24	9	4021	BCR	C10-C11-C12-C13
24	9	4021	BCR	C11-C12-C13-C14
24	9	4021	BCR	C11-C12-C13-C35
24	9	4021	BCR	C21-C22-C23-C24
21	A	1138	CLA	CHA-CBD-CGD-O1D
21	A	1138	CLA	CHA-CBD-CGD-O2D
21	b	1239	CLA	C1A-C2A-CAA-CBA
21	b	1239	CLA	C3A-C2A-CAA-CBA
21	b	1239	CLA	C2-C1-O2A-CGA
21	a	1129	CLA	C3A-C2A-CAA-CBA
21	b	1021	CLA	C4-C3-C5-C6
24	K	4001	BCR	C1-C6-C7-C8
24	K	4001	BCR	C11-C10-C9-C8
24	K	4001	BCR	C11-C10-C9-C34
24	K	4001	BCR	C15-C16-C17-C18
24	K	4001	BCR	C17-C18-C19-C20
24	K	4001	BCR	C36-C18-C19-C20
30	M	4021	ECH	C21-C22-C23-C24
30	M	4021	ECH	C37-C22-C23-C24
30	M	4021	ECH	C23-C24-C25-C26
21	B	1210	CLA	C1A-C2A-CAA-CBA
24	a	4002	BCR	C11-C10-C9-C8
24	a	4002	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	a	4002	BCR	C11-C12-C13-C14
24	a	4002	BCR	C11-C12-C13-C35
24	a	4002	BCR	C21-C22-C23-C24
24	a	4002	BCR	C37-C22-C23-C24
21	2	1207	CLA	CBD-CGD-O2D-CED
30	b	4011	ECH	C21-C22-C23-C24
30	b	4011	ECH	C23-C24-C25-C30
21	b	1205	CLA	CHA-CBD-CGD-O1D
21	b	1205	CLA	CHA-CBD-CGD-O2D
21	B	1234	CLA	C1A-C2A-CAA-CBA
21	2	1208	CLA	CBD-CGD-O2D-CED
21	1	1123	CLA	C2-C1-O2A-CGA
26	K	5009	LMG	O6-C1-O1-C7
26	K	5009	LMG	O9-C10-O7-C8
26	K	5009	LMG	C11-C10-O7-C8
21	a	1130	CLA	C4-C3-C5-C6
21	a	1140	CLA	CBD-CGD-O2D-CED
24	b	4014	BCR	C11-C10-C9-C8
24	b	4014	BCR	C11-C10-C9-C34
24	b	4014	BCR	C21-C22-C23-C24
24	b	4014	BCR	C37-C22-C23-C24
21	2	1021	CLA	CHA-CBD-CGD-O1D
21	2	1021	CLA	CHA-CBD-CGD-O2D
21	1	1135	CLA	C4-C3-C5-C6
21	1	1135	CLA	C3-C5-C6-C7
21	a	1109	CLA	C1A-C2A-CAA-CBA
21	a	1109	CLA	C3A-C2A-CAA-CBA
21	a	1109	CLA	CHA-CBD-CGD-O1D
21	a	1109	CLA	CHA-CBD-CGD-O2D
21	a	1109	CLA	CBD-CGD-O2D-CED
21	2	1204	CLA	CHA-CBD-CGD-O1D
21	2	1204	CLA	CHA-CBD-CGD-O2D
21	A	1135	CLA	CBD-CGD-O2D-CED
35	L	6001	LMT	C2'-C1'-O1'-C1
35	L	6001	LMT	O5'-C1'-O1'-C1
24	A	4002	BCR	C1-C6-C7-C8
24	A	4002	BCR	C11-C10-C9-C8
24	A	4002	BCR	C11-C10-C9-C34
24	A	4002	BCR	C11-C12-C13-C14
24	A	4002	BCR	C11-C12-C13-C35
24	A	4003	BCR	C1-C6-C7-C8
24	A	4003	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	A	4003	BCR	C11-C10-C9-C34
24	A	4003	BCR	C13-C14-C15-C16
24	A	4003	BCR	C36-C18-C19-C20
24	A	4003	BCR	C21-C22-C23-C24
24	A	4003	BCR	C37-C22-C23-C24
21	2	1227	CLA	CHA-CBD-CGD-O1D
21	2	1227	CLA	CHA-CBD-CGD-O2D
21	b	1217	CLA	C3A-C2A-CAA-CBA
21	b	1217	CLA	C2-C3-C5-C6
21	b	1217	CLA	C4-C3-C5-C6
21	a	1112	CLA	C1A-C2A-CAA-CBA
21	a	1112	CLA	C3A-C2A-CAA-CBA
21	a	1112	CLA	C2-C1-O2A-CGA
21	a	1112	CLA	CBD-CGD-O2D-CED
21	J	1303	CLA	C2A-CAA-CBA-CGA
21	J	1303	CLA	CHA-CBD-CGD-O1D
21	J	1303	CLA	CHA-CBD-CGD-O2D
21	J	1303	CLA	C12-C13-C15-C16
21	1	1133	CLA	C2-C1-O2A-CGA
26	A	5008	LMG	C2-C1-O1-C7
26	A	5008	LMG	O6-C1-O1-C7
26	A	5008	LMG	O9-C10-O7-C8
26	A	5008	LMG	C11-C10-O7-C8
21	a	1801	CLA	C1A-C2A-CAA-CBA
21	a	1801	CLA	C3A-C2A-CAA-CBA
21	a	1801	CLA	CBD-CGD-O2D-CED
21	0	1501	CLA	C1A-C2A-CAA-CBA
21	0	1501	CLA	C3A-C2A-CAA-CBA
21	1	1801	CLA	CBA-CGA-O2A-C1
21	1	1801	CLA	O1A-CGA-O2A-C1
21	1	1801	CLA	CAD-CBD-CGD-O1D
21	1	1801	CLA	CAD-CBD-CGD-O2D
21	2	1219	CLA	C1A-C2A-CAA-CBA
21	2	1219	CLA	C2-C1-O2A-CGA
21	a	1012	CLA	CAD-CBD-CGD-O1D
21	a	1012	CLA	CAD-CBD-CGD-O2D
21	a	1012	CLA	C2-C3-C5-C6
21	a	1012	CLA	C4-C3-C5-C6
24	2	4010	BCR	C11-C10-C9-C8
24	2	4010	BCR	C11-C10-C9-C34
24	2	4010	BCR	C11-C12-C13-C14
24	2	4010	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
24	2	4010	BCR	C17-C18-C19-C20
24	2	4010	BCR	C36-C18-C19-C20
24	2	4010	BCR	C18-C19-C20-C21
31	B	5008	SQD	C2-C1-O6-C44
31	B	5008	SQD	O5-C1-O6-C44
21	2	1217	CLA	C1A-C2A-CAA-CBA
21	2	1217	CLA	C3A-C2A-CAA-CBA
21	2	1217	CLA	CBD-CGD-O2D-CED
34	F	4016	ZEX	C1-C6-C7-C8
34	F	4016	ZEX	C5-C6-C7-C8
34	F	4016	ZEX	C25-C26-C27-C28
34	F	4016	ZEX	C7-C8-C9-C19
34	F	4016	ZEX	C7-C8-C9-C10
21	1	1121	CLA	C1A-C2A-CAA-CBA
21	1	1121	CLA	C3A-C2A-CAA-CBA
21	1	1121	CLA	CBD-CGD-O2D-CED
25	1	5003	LHG	O1-C1-C2-C3
25	1	5003	LHG	C1-C2-C3-O3
25	1	5003	LHG	C4-O6-P-O4
25	1	5003	LHG	C4-O6-P-O5
24	8	4001	BCR	C11-C10-C9-C8
24	8	4001	BCR	C11-C10-C9-C34
24	8	4001	BCR	C11-C12-C13-C14
24	8	4001	BCR	C11-C12-C13-C35
24	8	4001	BCR	C21-C22-C23-C24
24	8	4001	BCR	C37-C22-C23-C24
21	A	1137	CLA	CHA-CBD-CGD-O1D
21	A	1137	CLA	CHA-CBD-CGD-O2D
21	B	1201	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	CHA-CBD-CGD-O1D
21	A	1132	CLA	CHA-CBD-CGD-O2D
21	B	1229	CLA	C1A-C2A-CAA-CBA
21	B	1229	CLA	C3A-C2A-CAA-CBA
21	1	1125	CLA	C1A-C2A-CAA-CBA
21	1	1125	CLA	C3A-C2A-CAA-CBA
21	b	1231	CLA	C2-C1-O2A-CGA
21	b	1231	CLA	CBD-CGD-O2D-CED
21	A	1129	CLA	C6-C7-C8-C9
24	j	4013	BCR	C11-C10-C9-C8
24	j	4013	BCR	C11-C10-C9-C34
24	j	4013	BCR	C23-C24-C25-C26
24	j	4013	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	a	5003	LHG	O1-C1-C2-C3
25	a	5003	LHG	C4-O6-P-O3
25	a	5003	LHG	C4-O6-P-O4
25	a	5003	LHG	C4-O6-P-O5
25	a	5003	LHG	O7-C5-C6-O8
21	A	1111	CLA	C3A-C2A-CAA-CBA
21	b	1215	CLA	C1A-C2A-CAA-CBA
21	b	1215	CLA	C3A-C2A-CAA-CBA
21	b	1215	CLA	C2-C1-O2A-CGA
21	L	1501	CLA	C1A-C2A-CAA-CBA
21	L	1501	CLA	C3A-C2A-CAA-CBA
21	A	1134	CLA	C1A-C2A-CAA-CBA
21	A	1134	CLA	CHA-CBD-CGD-O1D
21	A	1134	CLA	CHA-CBD-CGD-O2D
21	1	1110	CLA	C1A-C2A-CAA-CBA
21	1	1110	CLA	C3A-C2A-CAA-CBA
24	B	4017	BCR	C11-C10-C9-C8
24	B	4017	BCR	C11-C10-C9-C34
24	B	4017	BCR	C10-C11-C12-C13
24	B	4017	BCR	C11-C12-C13-C14
24	B	4017	BCR	C11-C12-C13-C35
24	B	4017	BCR	C17-C18-C19-C20
24	B	4017	BCR	C36-C18-C19-C20
21	f	1302	CLA	CHA-CBD-CGD-O1D
21	f	1302	CLA	CHA-CBD-CGD-O2D
21	f	1302	CLA	CAD-CBD-CGD-O1D
21	f	1302	CLA	CAD-CBD-CGD-O2D
21	f	1302	CLA	C6-C7-C8-C9
21	2	1202	CLA	C3A-C2A-CAA-CBA
31	b	5006	SQD	C8-C7-O47-C45
31	b	5006	SQD	O5-C5-C6-S
21	A	1107	CLA	C1A-C2A-CAA-CBA
21	A	1107	CLA	C2-C1-O2A-CGA
21	A	1107	CLA	CBD-CGD-O2D-CED
21	b	1237	CLA	CBA-CGA-O2A-C1
21	b	1237	CLA	O1A-CGA-O2A-C1
21	b	1237	CLA	CBD-CGD-O2D-CED
21	2	1215	CLA	C1A-C2A-CAA-CBA
21	2	1215	CLA	C3A-C2A-CAA-CBA
21	2	1215	CLA	C2-C1-O2A-CGA
21	2	1232	CLA	CBD-CGD-O2D-CED
21	B	1221	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	1	1126	CLA	C1A-C2A-CAA-CBA
21	1	1126	CLA	C3A-C2A-CAA-CBA
21	1	1126	CLA	CBD-CGD-O2D-CED
21	1	1126	CLA	C2-C3-C5-C6
21	1	1126	CLA	C4-C3-C5-C6
24	b	4005	BCR	C1-C6-C7-C8
24	b	4005	BCR	C11-C10-C9-C8
24	b	4005	BCR	C11-C10-C9-C34
24	b	4005	BCR	C10-C11-C12-C13
24	b	4005	BCR	C36-C18-C19-C20
21	2	1023	CLA	CHA-CBD-CGD-O1D
21	2	1023	CLA	CBD-CGD-O2D-CED
21	2	1222	CLA	C3A-C2A-CAA-CBA
21	B	1218	CLA	C1A-C2A-CAA-CBA
24	a	4003	BCR	C11-C10-C9-C8
24	a	4003	BCR	C11-C10-C9-C34
21	a	1117	CLA	C1A-C2A-CAA-CBA
21	a	1117	CLA	C3A-C2A-CAA-CBA
21	a	1117	CLA	CHA-CBD-CGD-O1D
21	a	1117	CLA	CHA-CBD-CGD-O2D
21	7	1303	CLA	CBD-CGD-O2D-CED
26	b	5007	LMG	O6-C1-O1-C7
26	b	5007	LMG	C11-C10-O7-C8
25	A	5003	LHG	C4-O6-P-O4
25	a	5007	LHG	O1-C1-C2-C3
25	a	5007	LHG	C4-O6-P-O3
25	a	5007	LHG	C4-O6-P-O4
25	a	5007	LHG	C4-O6-P-O5
21	1	1109	CLA	CBD-CGD-O2D-CED
21	1	1109	CLA	C4-C3-C5-C6
21	2	1212	CLA	CBD-CGD-O2D-CED
21	2	1218	CLA	C3A-C2A-CAA-CBA
21	2	1218	CLA	CBA-CGA-O2A-C1
21	2	1218	CLA	O1A-CGA-O2A-C1
21	2	1218	CLA	CBD-CGD-O2D-CED
21	2	1218	CLA	C14-C13-C15-C16
21	B	1021	CLA	CBD-CGD-O2D-CED
21	B	1021	CLA	C2-C3-C5-C6
21	B	1021	CLA	C4-C3-C5-C6
21	B	1227	CLA	C1A-C2A-CAA-CBA
21	B	1227	CLA	C3A-C2A-CAA-CBA
21	B	1227	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	A	1131	CLA	C6-C7-C8-C9
24	a	4019	BCR	C11-C10-C9-C8
24	a	4019	BCR	C11-C10-C9-C34
24	a	4019	BCR	C10-C11-C12-C13
24	a	4019	BCR	C17-C18-C19-C20
24	a	4019	BCR	C36-C18-C19-C20
24	a	4019	BCR	C21-C22-C23-C24
24	a	4019	BCR	C37-C22-C23-C24
21	j	1303	CLA	C2-C1-O2A-CGA
21	A	1117	CLA	CHA-CBD-CGD-O1D
21	A	1117	CLA	CHA-CBD-CGD-O2D
24	B	4018	BCR	C17-C18-C19-C20
24	B	4018	BCR	C36-C18-C19-C20
24	B	4018	BCR	C18-C19-C20-C21
21	A	1128	CLA	C2-C1-O2A-CGA
21	A	1128	CLA	CHA-CBD-CGD-O1D
21	A	1128	CLA	CHA-CBD-CGD-O2D
21	A	1128	CLA	C2-C3-C5-C6
21	A	1128	CLA	C4-C3-C5-C6
25	1	5007	LHG	C3-O3-P-O4
25	1	5007	LHG	C3-O3-P-O5
25	1	5007	LHG	C3-O3-P-O6
25	1	5007	LHG	C4-O6-P-O3
25	1	5007	LHG	C8-C7-O7-C5
24	l	4019	BCR	C7-C8-C9-C10
24	l	4019	BCR	C7-C8-C9-C34
24	l	4019	BCR	C23-C24-C25-C26
21	l	1502	CLA	CHA-CBD-CGD-O1D
21	l	1502	CLA	CHA-CBD-CGD-O2D
24	2	4017	BCR	C11-C10-C9-C8
24	2	4017	BCR	C11-C10-C9-C34
24	2	4017	BCR	C17-C18-C19-C20
24	2	4017	BCR	C36-C18-C19-C20
21	a	1110	CLA	C1A-C2A-CAA-CBA
21	a	1110	CLA	C3A-C2A-CAA-CBA
28	h	4020	45D	C19-C23-C25-C27
28	h	4020	45D	C19-C23-C25-C29
28	h	4020	45D	C31-C33-C35-C37
28	h	4020	45D	C31-C33-C35-C39
28	h	4020	45D	C35-C37-C41-C42
24	2	4014	BCR	C11-C10-C9-C8
24	2	4014	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	2	4014	BCR	C21-C22-C23-C24
24	2	4014	BCR	C37-C22-C23-C24
24	1	4012	BCR	C11-C10-C9-C8
24	1	4012	BCR	C11-C10-C9-C34
24	1	4012	BCR	C11-C12-C13-C14
24	1	4012	BCR	C11-C12-C13-C35
24	1	4012	BCR	C21-C22-C23-C24
31	L	5002	SQD	O5-C5-C6-S
21	b	1210	CLA	C1A-C2A-CAA-CBA
26	a	5002	LMG	C2-C1-O1-C7
26	a	5002	LMG	O6-C1-O1-C7
26	a	5002	LMG	O9-C10-O7-C8
26	a	5002	LMG	C11-C10-O7-C8
24	L	4019	BCR	C7-C8-C9-C34
21	B	1203	CLA	CBD-CGD-O2D-CED
30	2	4006	ECH	C23-C24-C25-C26
21	A	1119	CLA	C1A-C2A-CAA-CBA
21	A	1119	CLA	C3A-C2A-CAA-CBA
21	A	1119	CLA	C11-C10-C8-C9
21	1	1140	CLA	C2-C1-O2A-CGA
21	1	1140	CLA	CBD-CGD-O2D-CED
25	B	5006	LHG	O1-C1-C2-C3
25	B	5006	LHG	C3-O3-P-O4
25	B	5006	LHG	C3-O3-P-O5
25	B	5006	LHG	O9-C7-O7-C5
21	b	1209	CLA	C1A-C2A-CAA-CBA
21	b	1209	CLA	C3A-C2A-CAA-CBA
21	b	1209	CLA	C4-C3-C5-C6
21	b	1209	CLA	C6-C7-C8-C9
21	A	1139	CLA	CBD-CGD-O2D-CED
24	a	4007	BCR	C11-C10-C9-C8
24	a	4007	BCR	C11-C10-C9-C34
24	a	4007	BCR	C17-C18-C19-C20
24	a	4007	BCR	C36-C18-C19-C20
24	b	4004	BCR	C1-C6-C7-C8
24	b	4004	BCR	C5-C6-C7-C8
24	b	4004	BCR	C11-C10-C9-C8
24	b	4004	BCR	C11-C10-C9-C34
24	b	4004	BCR	C10-C11-C12-C13
24	b	4004	BCR	C23-C24-C25-C26
24	b	4004	BCR	C23-C24-C25-C30
21	a	1118	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	1102	CLA	C3A-C2A-CAA-CBA
21	1	1102	CLA	CBA-CGA-O2A-C1
21	1	1102	CLA	O1A-CGA-O2A-C1
21	1	1102	CLA	CHA-CBD-CGD-O1D
21	1	1102	CLA	CHA-CBD-CGD-O2D
21	1	1102	CLA	CAD-CBD-CGD-O1D
24	7	4013	BCR	C11-C10-C9-C8
24	7	4013	BCR	C11-C10-C9-C34
24	7	4013	BCR	C11-C12-C13-C35
24	7	4013	BCR	C23-C24-C25-C26
24	7	4013	BCR	C23-C24-C25-C30
24	A	4019	BCR	C7-C8-C9-C10
24	A	4019	BCR	C7-C8-C9-C34
21	2	1228	CLA	C1A-C2A-CAA-CBA
21	2	1228	CLA	C3A-C2A-CAA-CBA
21	2	1228	CLA	CHA-CBD-CGD-O1D
21	2	1228	CLA	CHA-CBD-CGD-O2D
25	A	5006	LHG	O1-C1-C2-C3
25	A	5006	LHG	C3-O3-P-O5
25	A	5006	LHG	C3-O3-P-O6
25	A	5006	LHG	O9-C7-O7-C5
25	A	5006	LHG	C8-C7-O7-C5
21	A	1140	CLA	C2-C1-O2A-CGA
21	A	1140	CLA	C11-C12-C13-C14
26	a	5004	LMG	C2-C1-O1-C7
26	a	5004	LMG	O6-C1-O1-C7
26	a	5004	LMG	C11-C10-O7-C8
21	1	1136	CLA	CHA-CBD-CGD-O1D
21	1	1136	CLA	CHA-CBD-CGD-O2D
21	2	1209	CLA	C1A-C2A-CAA-CBA
21	2	1209	CLA	C3A-C2A-CAA-CBA
21	2	1203	CLA	C2-C3-C5-C6
21	2	1203	CLA	C4-C3-C5-C6
21	8	1401	CLA	C1A-C2A-CAA-CBA
21	8	1401	CLA	C3A-C2A-CAA-CBA
21	A	1108	CLA	C1A-C2A-CAA-CBA
21	2	1239	CLA	C1A-C2A-CAA-CBA
21	2	1239	CLA	C3A-C2A-CAA-CBA
21	2	1239	CLA	C2-C1-O2A-CGA
21	2	1239	CLA	CHA-CBD-CGD-O1D
21	1	1108	CLA	C1A-C2A-CAA-CBA
21	1	1108	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	1	1108	CLA	CHA-CBD-CGD-O2D
21	1	1108	CLA	CBD-CGD-O2D-CED
21	1	1138	CLA	C2-C1-O2A-CGA
21	1	1138	CLA	CBD-CGD-O2D-CED
21	b	1223	CLA	CHA-CBD-CGD-O1D
21	b	1223	CLA	CHA-CBD-CGD-O2D
30	m	4021	ECH	C21-C22-C23-C24
30	m	4021	ECH	C37-C22-C23-C24
30	m	4021	ECH	C23-C24-C25-C26
25	0	5002	LHG	O1-C1-C2-C3
24	b	4018	BCR	C23-C24-C25-C26
24	b	4018	BCR	C23-C24-C25-C30
21	2	1221	CLA	CHA-CBD-CGD-O2D
24	L	4022	BCR	C1-C6-C7-C8
24	L	4022	BCR	C11-C10-C9-C8
24	L	4022	BCR	C11-C10-C9-C34
24	L	4022	BCR	C10-C11-C12-C13
24	L	4022	BCR	C17-C18-C19-C20
24	L	4022	BCR	C36-C18-C19-C20
21	1	1012	CLA	CHA-CBD-CGD-O1D
21	1	1012	CLA	CHA-CBD-CGD-O2D
21	1	1012	CLA	CAD-CBD-CGD-O1D
21	1	1012	CLA	CAD-CBD-CGD-O2D
21	1	1012	CLA	C4-C3-C5-C6
21	B	1225	CLA	C1A-C2A-CAA-CBA
21	B	1225	CLA	C3A-C2A-CAA-CBA
25	A	5005	LHG	C1-C2-C3-O3
25	A	5005	LHG	C4-O6-P-O3
25	A	5005	LHG	C4-O6-P-O4
25	A	5005	LHG	C4-O6-P-O5
25	A	5005	LHG	O9-C7-O7-C5
25	A	5005	LHG	C8-C7-O7-C5
21	b	1230	CLA	C3A-C2A-CAA-CBA
21	b	1230	CLA	C2-C1-O2A-CGA
21	b	1230	CLA	C2-C3-C5-C6
21	b	1230	CLA	C4-C3-C5-C6
26	A	5002	LMG	O6-C1-O1-C7
26	A	5002	LMG	O1-C7-C8-O7
26	A	5002	LMG	O9-C10-O7-C8
26	A	5002	LMG	C11-C10-O7-C8
21	A	1102	CLA	C11-C10-C8-C9
25	l	5004	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	i	4020	ECH	C1-C6-C7-C8
30	i	4020	ECH	C5-C6-C7-C8
30	i	4020	ECH	C7-C8-C9-C10
30	i	4020	ECH	C37-C22-C23-C24
25	1	5005	LHG	O1-C1-C2-C3
25	1	5005	LHG	C3-O3-P-O6
25	1	5005	LHG	O9-C7-O7-C5
25	1	5005	LHG	C8-C7-O7-C5
21	b	1219	CLA	C3A-C2A-CAA-CBA
21	b	1219	CLA	C2-C3-C5-C6
21	b	1219	CLA	C4-C3-C5-C6
24	A	4007	BCR	C11-C12-C13-C14
24	A	4007	BCR	C11-C12-C13-C35
21	a	1134	CLA	C1A-C2A-CAA-CBA
21	a	1134	CLA	CHA-CBD-CGD-O1D
21	a	1134	CLA	CHA-CBD-CGD-O2D
25	1	5003	LHG	O1-C1-C2-C3
25	1	5003	LHG	C3-O3-P-O5
25	1	5003	LHG	C4-O6-P-O4
21	b	1232	CLA	C1A-C2A-CAA-CBA
21	b	1232	CLA	C3A-C2A-CAA-CBA
25	a	5001	LHG	O1-C1-C2-C3
25	a	5001	LHG	C1-C2-C3-O3
25	a	5001	LHG	C4-O6-P-O3
21	A	1124	CLA	C11-C12-C13-C14
21	2	1224	CLA	C1A-C2A-CAA-CBA
21	2	1224	CLA	C3A-C2A-CAA-CBA
35	0	6001	LMT	C2-C1-O1'-C1'
21	a	1135	CLA	CHA-CBD-CGD-O1D
21	a	1135	CLA	CHA-CBD-CGD-O2D
21	a	1138	CLA	C2-C1-O2A-CGA
21	b	1213	CLA	C1A-C2A-CAA-CBA
21	b	1213	CLA	CBD-CGD-O2D-CED
24	1	4019	BCR	C7-C8-C9-C10
24	1	4019	BCR	C7-C8-C9-C34
24	1	4019	BCR	C10-C11-C12-C13
24	1	4019	BCR	C17-C18-C19-C20
24	1	4019	BCR	C36-C18-C19-C20
21	1	1117	CLA	C1A-C2A-CAA-CBA
21	1	1117	CLA	C3A-C2A-CAA-CBA
21	1	1117	CLA	CHA-CBD-CGD-O1D
21	1	1117	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	a	4012	BCR	C1-C6-C7-C8
24	a	4012	BCR	C11-C10-C9-C8
24	a	4012	BCR	C11-C10-C9-C34
21	a	1114	CLA	C1A-C2A-CAA-CBA
21	a	1114	CLA	CBA-CGA-O2A-C1
21	a	1114	CLA	O1A-CGA-O2A-C1
21	a	1114	CLA	C3-C5-C6-C7
21	B	1206	CLA	C2-C1-O2A-CGA
31	L	5001	SQD	C2-C1-O6-C44
31	L	5001	SQD	O5-C1-O6-C44
31	L	5001	SQD	O5-C5-C6-S
31	L	5001	SQD	C5-C6-S-O7
31	L	5001	SQD	C5-C6-S-O8
31	L	5001	SQD	C5-C6-S-O9
21	A	1127	CLA	C2A-CAA-CBA-CGA
24	i	4018	BCR	C11-C10-C9-C8
24	i	4018	BCR	C11-C10-C9-C34
24	i	4018	BCR	C10-C11-C12-C13
24	i	4018	BCR	C11-C12-C13-C35
24	i	4018	BCR	C17-C18-C19-C20
24	i	4018	BCR	C36-C18-C19-C20
21	1	1128	CLA	C2-C1-O2A-CGA
21	1	1128	CLA	CHA-CBD-CGD-O1D
21	1	1128	CLA	CHA-CBD-CGD-O2D
21	a	1126	CLA	CBD-CGD-O2D-CED
31	0	5005	SQD	O5-C5-C6-S
24	B	4004	BCR	C1-C6-C7-C8
24	B	4004	BCR	C5-C6-C7-C8
24	B	4004	BCR	C7-C8-C9-C34
24	B	4004	BCR	C11-C10-C9-C8
24	B	4004	BCR	C11-C10-C9-C34
24	B	4004	BCR	C11-C12-C13-C14
24	B	4004	BCR	C11-C12-C13-C35
24	B	4004	BCR	C21-C22-C23-C24
24	B	4004	BCR	C37-C22-C23-C24
24	B	4004	BCR	C23-C24-C25-C26
24	B	4004	BCR	C23-C24-C25-C30
21	A	1118	CLA	CBD-CGD-O2D-CED
21	a	1108	CLA	C1A-C2A-CAA-CBA
21	a	1108	CLA	CHA-CBD-CGD-O1D
21	a	1108	CLA	CHA-CBD-CGD-O2D
21	a	1125	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	a	1120	CLA	C1A-C2A-CAA-CBA
24	2	4004	BCR	C1-C6-C7-C8
24	2	4004	BCR	C5-C6-C7-C8
24	2	4004	BCR	C7-C8-C9-C10
24	2	4004	BCR	C7-C8-C9-C34
24	2	4004	BCR	C11-C10-C9-C8
24	2	4004	BCR	C11-C10-C9-C34
24	2	4004	BCR	C11-C12-C13-C14
24	2	4004	BCR	C11-C12-C13-C35
24	2	4004	BCR	C17-C18-C19-C20
24	2	4004	BCR	C36-C18-C19-C20
21	a	1119	CLA	CBD-CGD-O2D-CED
21	B	1227	CLA	O1D-CGD-O2D-CED
21	a	1138	CLA	O1D-CGD-O2D-CED
21	K	1402	CLA	C15-C16-C17-C18
21	2	1220	CLA	O1D-CGD-O2D-CED
21	B	1220	CLA	O1D-CGD-O2D-CED
21	8	1402	CLA	O1D-CGD-O2D-CED
21	2	1021	CLA	O1D-CGD-O2D-CED
21	A	1104	CLA	O1D-CGD-O2D-CED
21	b	1218	CLA	O1D-CGD-O2D-CED
21	a	1104	CLA	O1D-CGD-O2D-CED
21	1	1138	CLA	O1D-CGD-O2D-CED
21	2	1220	CLA	CBD-CGD-O2D-CED
21	B	1214	CLA	CBD-CGD-O2D-CED
21	b	1235	CLA	CBD-CGD-O2D-CED
21	1	1011	CLA	CBD-CGD-O2D-CED
21	2	1213	CLA	CBD-CGD-O2D-CED
21	B	1204	CLA	CBD-CGD-O2D-CED
21	2	1214	CLA	CBD-CGD-O2D-CED
21	B	1220	CLA	CBD-CGD-O2D-CED
21	1	1131	CLA	CBD-CGD-O2D-CED
21	j	1302	CLA	CBD-CGD-O2D-CED
21	a	1121	CLA	CBD-CGD-O2D-CED
21	B	1219	CLA	CBD-CGD-O2D-CED
21	B	1240	CLA	CBD-CGD-O2D-CED
21	B	1217	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	CBD-CGD-O2D-CED
21	b	1227	CLA	CBD-CGD-O2D-CED
21	b	1203	CLA	CBD-CGD-O2D-CED
21	2	1210	CLA	CBD-CGD-O2D-CED
21	2	1201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1231	CLA	CBD-CGD-O2D-CED
21	a	1133	CLA	CBD-CGD-O2D-CED
21	1	1106	CLA	CBD-CGD-O2D-CED
21	2	1211	CLA	CBD-CGD-O2D-CED
21	1	1113	CLA	CBD-CGD-O2D-CED
21	b	1022	CLA	CBD-CGD-O2D-CED
21	F	1302	CLA	CBD-CGD-O2D-CED
21	a	1122	CLA	CBD-CGD-O2D-CED
21	8	1402	CLA	CBD-CGD-O2D-CED
21	L	1503	CLA	CBD-CGD-O2D-CED
21	a	1132	CLA	CBD-CGD-O2D-CED
21	1	1137	CLA	CBD-CGD-O2D-CED
21	1	1107	CLA	CBD-CGD-O2D-CED
21	a	1106	CLA	CBD-CGD-O2D-CED
21	a	1103	CLA	CBD-CGD-O2D-CED
21	A	1105	CLA	CBD-CGD-O2D-CED
21	b	1206	CLA	CBD-CGD-O2D-CED
21	1	1118	CLA	CBD-CGD-O2D-CED
21	1	1103	CLA	CBD-CGD-O2D-CED
21	B	1238	CLA	CBD-CGD-O2D-CED
21	A	1121	CLA	CBD-CGD-O2D-CED
21	1	1130	CLA	CBD-CGD-O2D-CED
21	l	1501	CLA	CBD-CGD-O2D-CED
21	a	1113	CLA	CBD-CGD-O2D-CED
21	F	1301	CLA	CBD-CGD-O2D-CED
21	A	1138	CLA	CBD-CGD-O2D-CED
21	b	1239	CLA	CBD-CGD-O2D-CED
21	2	1021	CLA	CBD-CGD-O2D-CED
21	b	1201	CLA	CBD-CGD-O2D-CED
21	A	1104	CLA	CBD-CGD-O2D-CED
21	b	1217	CLA	CBD-CGD-O2D-CED
21	2	1219	CLA	CBD-CGD-O2D-CED
21	B	1229	CLA	CBD-CGD-O2D-CED
21	b	1218	CLA	CBD-CGD-O2D-CED
21	a	1104	CLA	CBD-CGD-O2D-CED
21	1	1125	CLA	CBD-CGD-O2D-CED
21	b	1215	CLA	CBD-CGD-O2D-CED
21	1	1110	CLA	CBD-CGD-O2D-CED
21	f	1302	CLA	CBD-CGD-O2D-CED
21	2	1215	CLA	CBD-CGD-O2D-CED
21	B	1235	CLA	CBD-CGD-O2D-CED
21	a	1139	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1115	CLA	CBD-CGD-O2D-CED
21	B	1218	CLA	CBD-CGD-O2D-CED
21	a	1117	CLA	CBD-CGD-O2D-CED
21	B	1227	CLA	CBD-CGD-O2D-CED
21	j	1303	CLA	CBD-CGD-O2D-CED
21	B	1022	CLA	CBD-CGD-O2D-CED
21	2	1240	CLA	CBD-CGD-O2D-CED
21	A	1119	CLA	CBD-CGD-O2D-CED
21	1	1114	CLA	CBD-CGD-O2D-CED
21	6	1301	CLA	CBD-CGD-O2D-CED
21	B	1232	CLA	CBD-CGD-O2D-CED
21	2	1228	CLA	CBD-CGD-O2D-CED
21	a	1136	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	CBD-CGD-O2D-CED
21	2	1203	CLA	CBD-CGD-O2D-CED
21	8	1401	CLA	CBD-CGD-O2D-CED
21	2	1239	CLA	CBD-CGD-O2D-CED
21	b	1223	CLA	CBD-CGD-O2D-CED
21	A	1120	CLA	CBD-CGD-O2D-CED
21	b	1230	CLA	CBD-CGD-O2D-CED
21	a	1137	CLA	CBD-CGD-O2D-CED
21	b	1219	CLA	CBD-CGD-O2D-CED
21	b	1232	CLA	CBD-CGD-O2D-CED
21	2	1224	CLA	CBD-CGD-O2D-CED
21	A	1109	CLA	CBD-CGD-O2D-CED
21	J	1302	CLA	CBD-CGD-O2D-CED
21	a	1138	CLA	CBD-CGD-O2D-CED
21	a	1114	CLA	CBD-CGD-O2D-CED
21	B	1206	CLA	CBD-CGD-O2D-CED
21	a	1120	CLA	CBD-CGD-O2D-CED
21	A	1801	CLA	O1A-CGA-O2A-C1
21	A	1114	CLA	O1A-CGA-O2A-C1
26	2	5005	LMG	O10-C28-O8-C9
21	2	1204	CLA	O1A-CGA-O2A-C1
21	2	1219	CLA	O1A-CGA-O2A-C1
21	1	1109	CLA	O1A-CGA-O2A-C1
31	f	5001	SQD	O10-C23-O48-C46
21	a	1110	CLA	O1A-CGA-O2A-C1
26	a	5002	LMG	O10-C28-O8-C9
26	A	5002	LMG	O10-C28-O8-C9
26	B	5005	LMG	O10-C28-O8-C9
25	1	5005	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
21	b	1219	CLA	O1A-CGA-O2A-C1
21	8	1402	CLA	O1A-CGA-O2A-C1
21	B	1207	CLA	C4C-C3C-CAC-CBC
21	2	1231	CLA	O1D-CGD-O2D-CED
21	2	1214	CLA	O1D-CGD-O2D-CED
21	B	1219	CLA	O1D-CGD-O2D-CED
21	F	1301	CLA	O1D-CGD-O2D-CED
21	2	1219	CLA	O1D-CGD-O2D-CED
21	f	1302	CLA	O1D-CGD-O2D-CED
21	a	1139	CLA	O1D-CGD-O2D-CED
21	B	1218	CLA	O1D-CGD-O2D-CED
21	B	1203	CLA	O1D-CGD-O2D-CED
21	1	1114	CLA	O1D-CGD-O2D-CED
21	b	1219	CLA	O1D-CGD-O2D-CED
21	2	1231	CLA	CBA-CGA-O2A-C1
21	1	1139	CLA	O1D-CGD-O2D-CED
21	b	1220	CLA	O1D-CGD-O2D-CED
21	A	1114	CLA	O1D-CGD-O2D-CED
21	f	1301	CLA	O1D-CGD-O2D-CED
21	b	1229	CLA	O1D-CGD-O2D-CED
21	a	1107	CLA	O1D-CGD-O2D-CED
21	7	1302	CLA	O1D-CGD-O2D-CED
21	B	1212	CLA	O1D-CGD-O2D-CED
21	2	1207	CLA	O1D-CGD-O2D-CED
21	2	1208	CLA	O1D-CGD-O2D-CED
21	a	1801	CLA	O1D-CGD-O2D-CED
21	2	1217	CLA	O1D-CGD-O2D-CED
21	B	1201	CLA	O1D-CGD-O2D-CED
21	b	1231	CLA	O1D-CGD-O2D-CED
21	A	1107	CLA	O1D-CGD-O2D-CED
21	1	1126	CLA	O1D-CGD-O2D-CED
21	7	1303	CLA	O1D-CGD-O2D-CED
21	1	1109	CLA	O1D-CGD-O2D-CED
21	2	1212	CLA	O1D-CGD-O2D-CED
21	2	1218	CLA	O1D-CGD-O2D-CED
21	B	1021	CLA	O1D-CGD-O2D-CED
21	2	1240	CLA	O1D-CGD-O2D-CED
21	A	1139	CLA	O1D-CGD-O2D-CED
21	a	1118	CLA	O1D-CGD-O2D-CED
21	B	1232	CLA	O1D-CGD-O2D-CED
21	1	1108	CLA	O1D-CGD-O2D-CED
21	2	1224	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1118	CLA	O1D-CGD-O2D-CED
21	A	1801	CLA	CBA-CGA-O2A-C1
26	2	5005	LMG	C29-C28-O8-C9
21	2	1219	CLA	CBA-CGA-O2A-C1
21	1	1109	CLA	CBA-CGA-O2A-C1
31	f	5001	SQD	C24-C23-O48-C46
21	a	1110	CLA	CBA-CGA-O2A-C1
26	a	5002	LMG	C29-C28-O8-C9
26	A	5002	LMG	C29-C28-O8-C9
26	B	5005	LMG	C29-C28-O8-C9
25	1	5005	LHG	C24-C23-O8-C6
21	b	1219	CLA	CBA-CGA-O2A-C1
21	A	1012	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	CBD-CGD-O2D-CED
21	2	1022	CLA	CBD-CGD-O2D-CED
21	b	1214	CLA	CBD-CGD-O2D-CED
21	2	1230	CLA	CBD-CGD-O2D-CED
21	a	1115	CLA	CBD-CGD-O2D-CED
21	b	1208	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	CBD-CGD-O2D-CED
21	b	1240	CLA	CBD-CGD-O2D-CED
21	2	1235	CLA	CBD-CGD-O2D-CED
21	a	1013	CLA	CBD-CGD-O2D-CED
21	1	1119	CLA	CBD-CGD-O2D-CED
21	A	1112	CLA	CBD-CGD-O2D-CED
21	A	1103	CLA	CBD-CGD-O2D-CED
21	a	1127	CLA	CBD-CGD-O2D-CED
21	a	1105	CLA	CBD-CGD-O2D-CED
21	a	1128	CLA	CBD-CGD-O2D-CED
21	1	1132	CLA	CBD-CGD-O2D-CED
21	b	1228	CLA	CBD-CGD-O2D-CED
21	B	1210	CLA	CBD-CGD-O2D-CED
21	b	1226	CLA	CBD-CGD-O2D-CED
21	B	1234	CLA	CBD-CGD-O2D-CED
21	1	1123	CLA	CBD-CGD-O2D-CED
21	1	1135	CLA	CBD-CGD-O2D-CED
21	2	1204	CLA	CBD-CGD-O2D-CED
21	J	1303	CLA	CBD-CGD-O2D-CED
21	2	1205	CLA	CBD-CGD-O2D-CED
21	1	1801	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	CBD-CGD-O2D-CED
21	0	1503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	b	1204	CLA	CBD-CGD-O2D-CED
21	a	1124	CLA	CBD-CGD-O2D-CED
21	2	1222	CLA	CBD-CGD-O2D-CED
21	K	1402	CLA	CBD-CGD-O2D-CED
21	a	1110	CLA	CBD-CGD-O2D-CED
21	1	1102	CLA	CBD-CGD-O2D-CED
21	1	1012	CLA	CBD-CGD-O2D-CED
21	A	1102	CLA	CBD-CGD-O2D-CED
21	1	1120	CLA	CBD-CGD-O2D-CED
21	a	1135	CLA	CBD-CGD-O2D-CED
21	1	1128	CLA	CBD-CGD-O2D-CED
21	B	1207	CLA	C2C-C3C-CAC-CBC
35	0	6001	LMT	C3'-C4'-O1B-C1B
21	b	1235	CLA	O1A-CGA-O2A-C1
21	B	1204	CLA	O1A-CGA-O2A-C1
26	A	5004	LMG	O10-C28-O8-C9
21	1	1013	CLA	O1A-CGA-O2A-C1
21	b	1214	CLA	O1A-CGA-O2A-C1
21	b	1227	CLA	O1A-CGA-O2A-C1
21	2	1237	CLA	O1A-CGA-O2A-C1
21	1	1104	CLA	O1A-CGA-O2A-C1
21	A	1110	CLA	O1A-CGA-O2A-C1
21	2	1235	CLA	O1A-CGA-O2A-C1
26	1	5004	LMG	O10-C28-O8-C9
21	k	1402	CLA	O1A-CGA-O2A-C1
26	1	5002	LMG	O10-C28-O8-C9
21	l	1501	CLA	O1A-CGA-O2A-C1
21	b	1218	CLA	O1A-CGA-O2A-C1
21	a	1104	CLA	O1A-CGA-O2A-C1
21	A	1129	CLA	O1A-CGA-O2A-C1
21	1	1110	CLA	O1A-CGA-O2A-C1
21	f	1302	CLA	O1A-CGA-O2A-C1
21	A	1130	CLA	O1A-CGA-O2A-C1
21	B	1235	CLA	O1A-CGA-O2A-C1
21	B	1227	CLA	O1A-CGA-O2A-C1
21	a	1136	CLA	O1A-CGA-O2A-C1
21	2	1221	CLA	O1A-CGA-O2A-C1
21	A	1109	CLA	O1A-CGA-O2A-C1
21	B	1206	CLA	O1A-CGA-O2A-C1
31	0	5005	SQD	O10-C23-O48-C46
21	2	1229	CLA	O1D-CGD-O2D-CED
21	2	1236	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	1104	CLA	O1D-CGD-O2D-CED
21	b	1224	CLA	O1D-CGD-O2D-CED
21	1	1116	CLA	O1D-CGD-O2D-CED
21	l	1503	CLA	O1D-CGD-O2D-CED
21	A	1135	CLA	O1D-CGD-O2D-CED
21	a	1112	CLA	O1D-CGD-O2D-CED
21	1	1121	CLA	O1D-CGD-O2D-CED
21	b	1237	CLA	O1D-CGD-O2D-CED
21	1	1140	CLA	O1D-CGD-O2D-CED
21	a	1126	CLA	O1D-CGD-O2D-CED
26	0	5001	LMG	O6-C5-C6-O5
21	1	1112	CLA	O1D-CGD-O2D-CED
21	a	1116	CLA	O1D-CGD-O2D-CED
21	1	1134	CLA	O1D-CGD-O2D-CED
21	B	1208	CLA	O1D-CGD-O2D-CED
21	B	1215	CLA	O1D-CGD-O2D-CED
21	a	1140	CLA	O1D-CGD-O2D-CED
21	a	1109	CLA	O1D-CGD-O2D-CED
21	2	1232	CLA	O1D-CGD-O2D-CED
21	2	1023	CLA	O1D-CGD-O2D-CED
21	b	1213	CLA	O1D-CGD-O2D-CED
21	B	1206	CLA	O1D-CGD-O2D-CED
21	a	1119	CLA	O1D-CGD-O2D-CED
21	a	1101	CLA	CBD-CGD-O2D-CED
21	2	1216	CLA	CBD-CGD-O2D-CED
21	B	1239	CLA	CBD-CGD-O2D-CED
21	1	1101	CLA	CBD-CGD-O2D-CED
21	B	1226	CLA	CBD-CGD-O2D-CED
21	1	1105	CLA	CBD-CGD-O2D-CED
21	A	1131	CLA	CBD-CGD-O2D-CED
21	A	1126	CLA	O1D-CGD-O2D-CED
21	B	1224	CLA	O1D-CGD-O2D-CED
21	1	1107	CLA	O1D-CGD-O2D-CED
21	a	1103	CLA	O1D-CGD-O2D-CED
21	A	1138	CLA	O1D-CGD-O2D-CED
21	b	1201	CLA	O1D-CGD-O2D-CED
21	b	1215	CLA	O1D-CGD-O2D-CED
21	8	1401	CLA	O1D-CGD-O2D-CED
21	b	1223	CLA	O1D-CGD-O2D-CED
21	A	1120	CLA	O1D-CGD-O2D-CED
21	J	1302	CLA	O1D-CGD-O2D-CED
26	1	5002	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	b	5006	SQD	O49-C7-O47-C45
25	1	5007	LHG	O9-C7-O7-C5
26	a	5004	LMG	O9-C10-O7-C8
21	B	1212	CLA	O1A-CGA-O2A-C1
21	L	1501	CLA	O1A-CGA-O2A-C1
21	b	1203	CLA	O1D-CGD-O2D-CED
21	A	1114	CLA	C3-C5-C6-C7
21	2	1206	CLA	C3-C5-C6-C7
21	1	1122	CLA	C3-C5-C6-C7
21	A	1116	CLA	C3-C5-C6-C7
21	a	1115	CLA	C3-C5-C6-C7
21	a	1011	CLA	C3-C5-C6-C7
21	2	1237	CLA	C3-C5-C6-C7
21	1	1104	CLA	C3-C5-C6-C7
21	1	1124	CLA	C3-C5-C6-C7
21	b	1240	CLA	C3-C5-C6-C7
21	b	1224	CLA	C3-C5-C6-C7
21	1	1111	CLA	C3-C5-C6-C7
21	1	1116	CLA	C3-C5-C6-C7
21	a	1127	CLA	C3-C5-C6-C7
21	2	1238	CLA	C3-C5-C6-C7
21	b	1206	CLA	C3-C5-C6-C7
21	l	1503	CLA	C3-C5-C6-C7
21	1	1103	CLA	C3-C5-C6-C7
21	B	1209	CLA	C3-C5-C6-C7
21	B	1228	CLA	C3-C5-C6-C7
21	2	1021	CLA	C3-C5-C6-C7
21	1	1133	CLA	C3-C5-C6-C7
21	2	1205	CLA	C3-C5-C6-C7
21	a	1801	CLA	C3-C5-C6-C7
21	A	1137	CLA	C3-C5-C6-C7
21	b	1231	CLA	C3-C5-C6-C7
21	a	1124	CLA	C3-C5-C6-C7
21	A	1115	CLA	C3-C5-C6-C7
21	B	1218	CLA	C3-C5-C6-C7
21	b	1207	CLA	C3-C5-C6-C7
21	2	1218	CLA	C3-C5-C6-C7
21	b	1221	CLA	C3-C5-C6-C7
21	2	1203	CLA	C3-C5-C6-C7
21	A	1108	CLA	C3-C5-C6-C7
21	A	1120	CLA	C3-C5-C6-C7
21	1	1120	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	1109	CLA	C3-C5-C6-C7
21	a	1108	CLA	C3-C5-C6-C7
21	a	1120	CLA	C3-C5-C6-C7
21	b	1235	CLA	CBA-CGA-O2A-C1
26	A	5004	LMG	C29-C28-O8-C9
21	A	1114	CLA	CBA-CGA-O2A-C1
21	b	1214	CLA	CBA-CGA-O2A-C1
21	2	1237	CLA	CBA-CGA-O2A-C1
21	1	1134	CLA	CBA-CGA-O2A-C1
21	A	1110	CLA	CBA-CGA-O2A-C1
21	2	1235	CLA	CBA-CGA-O2A-C1
26	1	5004	LMG	C29-C28-O8-C9
26	1	5002	LMG	C29-C28-O8-C9
21	B	1230	CLA	CBA-CGA-O2A-C1
21	1	1130	CLA	CBA-CGA-O2A-C1
21	l	1501	CLA	CBA-CGA-O2A-C1
21	B	1228	CLA	CBA-CGA-O2A-C1
21	2	1207	CLA	CBA-CGA-O2A-C1
21	2	1204	CLA	CBA-CGA-O2A-C1
21	J	1303	CLA	CBA-CGA-O2A-C1
21	0	1501	CLA	CBA-CGA-O2A-C1
21	A	1129	CLA	CBA-CGA-O2A-C1
21	1	1110	CLA	CBA-CGA-O2A-C1
21	f	1302	CLA	CBA-CGA-O2A-C1
21	A	1130	CLA	CBA-CGA-O2A-C1
21	1	1126	CLA	CBA-CGA-O2A-C1
21	a	1124	CLA	CBA-CGA-O2A-C1
21	B	1227	CLA	CBA-CGA-O2A-C1
21	2	1221	CLA	CBA-CGA-O2A-C1
21	A	1109	CLA	CBA-CGA-O2A-C1
21	6	1301	CLA	C2-C1-O2A-CGA
35	l	6001	LMT	O5B-C5B-C6B-O6B
25	B	5006	LHG	C8-C7-O7-C5
21	1	1011	CLA	O1D-CGD-O2D-CED
21	b	1239	CLA	O1D-CGD-O2D-CED
21	A	1140	CLA	O1D-CGD-O2D-CED
21	B	1211	CLA	CBD-CGD-O2D-CED
21	B	1209	CLA	CBD-CGD-O2D-CED
21	b	1207	CLA	CBD-CGD-O2D-CED
21	A	1128	CLA	CBD-CGD-O2D-CED
21	A	1124	CLA	CBD-CGD-O2D-CED
21	A	1127	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	1230	CLA	C2-C1-O2A-CGA
21	b	1202	CLA	O1A-CGA-O2A-C1
21	j	1303	CLA	O1A-CGA-O2A-C1
21	2	1231	CLA	O1A-CGA-O2A-C1
21	1	1108	CLA	CBA-CGA-O2A-C1
21	a	1129	CLA	C3-C5-C6-C7
21	2	1217	CLA	C3-C5-C6-C7
21	b	1235	CLA	C4-C3-C5-C6
21	2	1226	CLA	C4-C3-C5-C6
21	a	1127	CLA	C4-C3-C5-C6
21	a	1128	CLA	C4-C3-C5-C6
21	a	1104	CLA	C4-C3-C5-C6
21	B	1235	CLA	C4-C3-C5-C6
21	B	1225	CLA	C4-C3-C5-C6
21	b	1216	CLA	C2-C3-C5-C6
21	1	1134	CLA	C2-C3-C5-C6
21	a	1133	CLA	C2-C3-C5-C6
21	a	1128	CLA	C2-C3-C5-C6
21	B	1226	CLA	C2-C3-C5-C6
21	b	1021	CLA	C2-C3-C5-C6
21	a	1130	CLA	C2-C3-C5-C6
21	1	1135	CLA	C2-C3-C5-C6
21	a	1104	CLA	C2-C3-C5-C6
21	1	1012	CLA	C2-C3-C5-C6
21	2	1206	CLA	CBD-CGD-O2D-CED
21	1	1122	CLA	CBD-CGD-O2D-CED
21	a	1011	CLA	CBD-CGD-O2D-CED
21	1	1115	CLA	CBD-CGD-O2D-CED
21	k	1402	CLA	CBD-CGD-O2D-CED
21	a	1129	CLA	CBD-CGD-O2D-CED
21	a	1012	CLA	CBD-CGD-O2D-CED
21	1	1136	CLA	CBD-CGD-O2D-CED
21	2	1214	CLA	C2A-CAA-CBA-CGA
21	A	1801	CLA	C2A-CAA-CBA-CGA
21	b	1216	CLA	C2A-CAA-CBA-CGA
21	B	1240	CLA	C2A-CAA-CBA-CGA
21	b	1214	CLA	C2A-CAA-CBA-CGA
21	2	1237	CLA	C2A-CAA-CBA-CGA
21	A	1113	CLA	C2A-CAA-CBA-CGA
21	F	1302	CLA	C2A-CAA-CBA-CGA
21	8	1402	CLA	C2A-CAA-CBA-CGA
21	2	1238	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	k	1402	CLA	C2A-CAA-CBA-CGA
21	B	1238	CLA	C2A-CAA-CBA-CGA
21	1	1135	CLA	C2A-CAA-CBA-CGA
21	a	1109	CLA	C2A-CAA-CBA-CGA
21	A	1135	CLA	C2A-CAA-CBA-CGA
21	0	1503	CLA	C2A-CAA-CBA-CGA
21	b	1238	CLA	C2A-CAA-CBA-CGA
21	B	1225	CLA	C2A-CAA-CBA-CGA
21	a	1114	CLA	C2A-CAA-CBA-CGA
21	2	1215	CLA	O1D-CGD-O2D-CED
21	j	1303	CLA	O1D-CGD-O2D-CED
26	0	5001	LMG	C20-C21-C22-C23
26	0	5001	LMG	C23-C24-C25-C26
26	0	5001	LMG	C38-C39-C40-C41
37	L	5004	DGD	C8A-C9A-CAA-CBA
37	L	5004	DGD	CEA-CFA-CGA-CHA
37	L	5004	DGD	CEB-CFB-CGB-CHB
26	A	5004	LMG	C17-C18-C19-C20
26	A	5004	LMG	C23-C24-C25-C26
26	1	5004	LMG	C23-C24-C25-C26
26	1	5004	LMG	C35-C36-C37-C38
26	b	5005	LMG	C38-C39-C40-C41
26	b	5005	LMG	C41-C42-C43-C44
26	B	5002	LMG	C20-C21-C22-C23
26	B	5002	LMG	C23-C24-C25-C26
26	B	5002	LMG	C35-C36-C37-C38
26	1	5002	LMG	C17-C18-C19-C20
26	1	5002	LMG	C38-C39-C40-C41
26	1	5002	LMG	C41-C42-C43-C44
26	2	5005	LMG	C38-C39-C40-C41
26	2	5005	LMG	C41-C42-C43-C44
26	b	5002	LMG	C20-C21-C22-C23
26	b	5002	LMG	C23-C24-C25-C26
26	b	5002	LMG	C35-C36-C37-C38
26	A	5008	LMG	C20-C21-C22-C23
26	A	5008	LMG	C35-C36-C37-C38
26	b	5007	LMG	C20-C21-C22-C23
26	b	5007	LMG	C23-C24-C25-C26
26	b	5007	LMG	C35-C36-C37-C38
26	b	5007	LMG	C41-C42-C43-C44
26	a	5002	LMG	C17-C18-C19-C20
26	a	5002	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
26	a	5002	LMG	C41-C42-C43-C44
26	a	5004	LMG	C17-C18-C19-C20
26	a	5004	LMG	C20-C21-C22-C23
26	A	5002	LMG	C17-C18-C19-C20
26	A	5002	LMG	C38-C39-C40-C41
26	A	5002	LMG	C41-C42-C43-C44
26	B	5005	LMG	C38-C39-C40-C41
26	B	5005	LMG	C41-C42-C43-C44
26	2	5002	LMG	C20-C21-C22-C23
26	2	5002	LMG	C23-C24-C25-C26
26	2	5002	LMG	C35-C36-C37-C38
21	1	1139	CLA	C3-C5-C6-C7
21	A	1113	CLA	C3-C5-C6-C7
21	L	1503	CLA	C3-C5-C6-C7
21	a	1128	CLA	C3-C5-C6-C7
21	2	1207	CLA	C3-C5-C6-C7
21	1	1125	CLA	C3-C5-C6-C7
21	f	1302	CLA	C3-C5-C6-C7
21	b	1237	CLA	C3-C5-C6-C7
21	2	1215	CLA	C3-C5-C6-C7
21	j	1303	CLA	C3-C5-C6-C7
21	A	1128	CLA	C3-C5-C6-C7
21	b	1232	CLA	C3-C5-C6-C7
21	a	1126	CLA	C3-C5-C6-C7
21	B	1204	CLA	CBA-CGA-O2A-C1
21	1	1013	CLA	CBA-CGA-O2A-C1
21	b	1227	CLA	CBA-CGA-O2A-C1
21	1	1104	CLA	CBA-CGA-O2A-C1
21	1	1124	CLA	CBA-CGA-O2A-C1
21	a	1013	CLA	CBA-CGA-O2A-C1
21	k	1402	CLA	CBA-CGA-O2A-C1
21	B	1202	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	CBA-CGA-O2A-C1
21	A	1104	CLA	CBA-CGA-O2A-C1
21	1	1121	CLA	CBA-CGA-O2A-C1
21	b	1218	CLA	CBA-CGA-O2A-C1
21	a	1104	CLA	CBA-CGA-O2A-C1
21	L	1501	CLA	CBA-CGA-O2A-C1
31	b	5006	SQD	C24-C23-O48-C46
21	B	1235	CLA	CBA-CGA-O2A-C1
21	B	1218	CLA	CBA-CGA-O2A-C1
25	a	5007	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
21	a	1136	CLA	CBA-CGA-O2A-C1
21	B	1206	CLA	CBA-CGA-O2A-C1
31	0	5005	SQD	C24-C23-O48-C46
25	l	5001	LHG	C31-C32-C33-C34
21	B	1204	CLA	O1D-CGD-O2D-CED
21	B	1240	CLA	O1D-CGD-O2D-CED
21	A	1116	CLA	O1D-CGD-O2D-CED
21	2	1210	CLA	O1D-CGD-O2D-CED
21	1	1113	CLA	O1D-CGD-O2D-CED
21	1	1137	CLA	O1D-CGD-O2D-CED
21	b	1217	CLA	O1D-CGD-O2D-CED
21	B	1022	CLA	O1D-CGD-O2D-CED
21	a	1136	CLA	O1D-CGD-O2D-CED
21	a	1137	CLA	O1D-CGD-O2D-CED
21	b	1232	CLA	O1D-CGD-O2D-CED
21	a	1114	CLA	O1D-CGD-O2D-CED
21	2	1237	CLA	CBD-CGD-O2D-CED
21	B	1202	CLA	CBD-CGD-O2D-CED
21	2	1202	CLA	CBD-CGD-O2D-CED
21	a	1125	CLA	CBD-CGD-O2D-CED
21	B	1217	CLA	O1D-CGD-O2D-CED
21	2	1201	CLA	O1D-CGD-O2D-CED
21	a	1122	CLA	O1D-CGD-O2D-CED
21	A	1121	CLA	O1D-CGD-O2D-CED
21	l	1501	CLA	O1D-CGD-O2D-CED
21	a	1113	CLA	O1D-CGD-O2D-CED
21	a	1117	CLA	O1D-CGD-O2D-CED
21	A	1119	CLA	O1D-CGD-O2D-CED
21	2	1203	CLA	O1D-CGD-O2D-CED
37	L	5004	DGD	O1B-C1B-O2G-C2G
26	b	5005	LMG	O9-C10-O7-C8
26	b	5007	LMG	O9-C10-O7-C8
21	B	1214	CLA	O1A-CGA-O2A-C1
21	a	1121	CLA	O1A-CGA-O2A-C1
21	a	1013	CLA	O1A-CGA-O2A-C1
21	B	1202	CLA	O1A-CGA-O2A-C1
21	B	1209	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	O1A-CGA-O2A-C1
21	2	1207	CLA	O1A-CGA-O2A-C1
21	J	1303	CLA	O1A-CGA-O2A-C1
21	1	1121	CLA	O1A-CGA-O2A-C1
21	1	1126	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	1218	CLA	O1A-CGA-O2A-C1
21	1	1138	CLA	O1A-CGA-O2A-C1
25	0	5002	LHG	O10-C23-O8-C6
21	A	1102	CLA	O1A-CGA-O2A-C1
21	1	1108	CLA	O1A-CGA-O2A-C1
21	j	1302	CLA	O1D-CGD-O2D-CED
21	A	1105	CLA	O1D-CGD-O2D-CED
21	1	1118	CLA	O1D-CGD-O2D-CED
21	1	1130	CLA	O1D-CGD-O2D-CED
21	1	1125	CLA	O1D-CGD-O2D-CED
24	h	4018	BCR	C13-C14-C15-C16
24	b	4017	BCR	C13-C14-C15-C16
24	I	4018	BCR	C13-C14-C15-C16
24	0	4019	BCR	C13-C14-C15-C16
24	A	4002	BCR	C13-C14-C15-C16
24	B	4017	BCR	C13-C14-C15-C16
24	B	4018	BCR	C19-C20-C21-C22
24	2	4017	BCR	C13-C14-C15-C16
28	h	4020	45D	C26-C30-C32-C34
24	b	4018	BCR	C13-C14-C15-C16
24	i	4018	BCR	C13-C14-C15-C16
24	i	4018	BCR	C15-C16-C17-C18
21	B	1237	CLA	CBD-CGD-O2D-CED
21	B	1207	CLA	CBD-CGD-O2D-CED
21	A	1110	CLA	CBD-CGD-O2D-CED
21	2	1238	CLA	CBD-CGD-O2D-CED
21	b	1212	CLA	CBD-CGD-O2D-CED
21	B	1230	CLA	CBD-CGD-O2D-CED
21	b	1234	CLA	CBD-CGD-O2D-CED
21	1	1129	CLA	CBD-CGD-O2D-CED
21	A	1136	CLA	CBD-CGD-O2D-CED
21	a	1130	CLA	CBD-CGD-O2D-CED
21	A	1111	CLA	CBD-CGD-O2D-CED
21	L	1501	CLA	CBD-CGD-O2D-CED
21	6	1302	CLA	CBD-CGD-O2D-CED
21	A	1133	CLA	CBD-CGD-O2D-CED
21	A	1117	CLA	CBD-CGD-O2D-CED
21	1	1502	CLA	CBD-CGD-O2D-CED
21	b	1209	CLA	CBD-CGD-O2D-CED
21	2	1209	CLA	CBD-CGD-O2D-CED
21	1	1131	CLA	O1D-CGD-O2D-CED
21	B	1229	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	5001	LHG	O2-C2-C3-O3
25	6	5001	LHG	O2-C2-C3-O3
25	L	5005	LHG	O2-C2-C3-O3
25	A	5006	LHG	O2-C2-C3-O3
25	A	5005	LHG	O2-C2-C3-O3
25	l	5004	LHG	O2-C2-C3-O3
25	1	5005	LHG	O2-C2-C3-O3
25	0	5004	LHG	O2-C2-C3-O3
21	b	1227	CLA	C3-C5-C6-C7
21	2	1226	CLA	C3-C5-C6-C7
21	a	1105	CLA	C3-C5-C6-C7
21	K	1401	CLA	C3-C5-C6-C7
21	F	1301	CLA	C3-C5-C6-C7
21	b	1205	CLA	C3-C5-C6-C7
21	b	1236	CLA	C3-C5-C6-C7
21	b	1218	CLA	C3-C5-C6-C7
21	A	1111	CLA	C3-C5-C6-C7
21	0	1503	CLA	C3-C5-C6-C7
21	2	1221	CLA	C3-C5-C6-C7
21	B	1205	CLA	C3-C5-C6-C7
21	a	1121	CLA	CBA-CGA-O2A-C1
21	B	1207	CLA	CBA-CGA-O2A-C1
21	L	1503	CLA	CBA-CGA-O2A-C1
21	1	1135	CLA	CBA-CGA-O2A-C1
21	a	1117	CLA	CBA-CGA-O2A-C1
21	j	1303	CLA	CBA-CGA-O2A-C1
21	A	1102	CLA	CBA-CGA-O2A-C1
21	a	1134	CLA	CBA-CGA-O2A-C1
21	a	1138	CLA	CBA-CGA-O2A-C1
21	1	1117	CLA	CBA-CGA-O2A-C1
21	B	1207	CLA	O1A-CGA-O2A-C1
21	1	1134	CLA	O1A-CGA-O2A-C1
21	1	1124	CLA	O1A-CGA-O2A-C1
21	B	1230	CLA	O1A-CGA-O2A-C1
21	1	1130	CLA	O1A-CGA-O2A-C1
21	A	1104	CLA	O1A-CGA-O2A-C1
21	0	1501	CLA	O1A-CGA-O2A-C1
31	b	5006	SQD	O10-C23-O48-C46
21	a	1124	CLA	O1A-CGA-O2A-C1
35	0	6001	LMT	O5B-C5B-C6B-O6B
26	0	5001	LMG	C4-C5-C6-O5
21	b	1235	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	1213	CLA	O1D-CGD-O2D-CED
21	b	1227	CLA	O1D-CGD-O2D-CED
21	B	1231	CLA	O1D-CGD-O2D-CED
21	a	1133	CLA	O1D-CGD-O2D-CED
21	1	1106	CLA	O1D-CGD-O2D-CED
21	b	1022	CLA	O1D-CGD-O2D-CED
21	F	1302	CLA	O1D-CGD-O2D-CED
21	b	1206	CLA	O1D-CGD-O2D-CED
21	6	1301	CLA	O1D-CGD-O2D-CED
21	a	1102	CLA	CBD-CGD-O2D-CED
21	b	1236	CLA	CBD-CGD-O2D-CED
21	A	1129	CLA	CBD-CGD-O2D-CED
21	b	1210	CLA	CBD-CGD-O2D-CED
21	1	1117	CLA	CBD-CGD-O2D-CED
21	a	1108	CLA	CBD-CGD-O2D-CED
25	a	5007	LHG	C30-C31-C32-C33
21	B	1214	CLA	O1D-CGD-O2D-CED
21	a	1138	CLA	O1A-CGA-O2A-C1
25	b	5004	LHG	C13-C14-C15-C16
26	2	5005	LMG	C32-C33-C34-C35
25	a	5007	LHG	C13-C14-C15-C16
26	a	5004	LMG	C36-C37-C38-C39
25	1	5004	LHG	C28-C29-C30-C31
21	a	1106	CLA	O1D-CGD-O2D-CED
21	B	1238	CLA	O1D-CGD-O2D-CED
21	1	1110	CLA	O1D-CGD-O2D-CED
21	2	1228	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	O1D-CGD-O2D-CED
21	a	1120	CLA	O1D-CGD-O2D-CED
25	2	5004	LHG	C7-C8-C9-C10
25	1	5003	LHG	C33-C34-C35-C36
21	1	1127	CLA	CBD-CGD-O2D-CED
21	b	1021	CLA	CBD-CGD-O2D-CED
21	B	1205	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	C3-C5-C6-C7
21	F	1302	CLA	C3-C5-C6-C7
21	B	1215	CLA	C3-C5-C6-C7
21	B	1203	CLA	C3-C5-C6-C7
21	A	1140	CLA	C3-C5-C6-C7
21	1	1012	CLA	C3-C5-C6-C7
21	b	1230	CLA	C3-C5-C6-C7
21	B	1214	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	b	1202	CLA	CBA-CGA-O2A-C1
21	A	1126	CLA	CBA-CGA-O2A-C1
21	B	1209	CLA	CBA-CGA-O2A-C1
21	1	1138	CLA	CBA-CGA-O2A-C1
25	0	5002	LHG	C24-C23-O8-C6
21	a	1126	CLA	CBA-CGA-O2A-C1
21	a	1121	CLA	O1D-CGD-O2D-CED
21	B	1235	CLA	O1D-CGD-O2D-CED
35	1	6001	LMT	O5B-C5B-C6B-O6B
35	l	6001	LMT	C4B-C5B-C6B-O6B
25	l	5004	LHG	C2-C3-O3-P
21	L	1503	CLA	O1A-CGA-O2A-C1
25	a	5007	LHG	O10-C23-O8-C6
21	a	1134	CLA	O1A-CGA-O2A-C1
21	a	1106	CLA	C5-C6-C7-C8
21	b	1225	CLA	C4-C3-C5-C6
21	A	1126	CLA	C4-C3-C5-C6
21	2	1237	CLA	C4-C3-C5-C6
21	1	1116	CLA	C4-C3-C5-C6
21	a	1122	CLA	C4-C3-C5-C6
21	B	1212	CLA	C4-C3-C5-C6
21	A	1121	CLA	C4-C3-C5-C6
21	a	1140	CLA	C4-C3-C5-C6
21	2	1217	CLA	C4-C3-C5-C6
21	1	1121	CLA	C4-C3-C5-C6
21	b	1215	CLA	C4-C3-C5-C6
21	A	1134	CLA	C4-C3-C5-C6
21	0	1503	CLA	C4-C3-C5-C6
21	A	1107	CLA	C4-C3-C5-C6
21	b	1237	CLA	C4-C3-C5-C6
21	A	1133	CLA	C4-C3-C5-C6
21	2	1218	CLA	C4-C3-C5-C6
21	B	1203	CLA	C4-C3-C5-C6
21	1	1140	CLA	C4-C3-C5-C6
21	a	1135	CLA	C4-C3-C5-C6
21	b	1225	CLA	C2-C3-C5-C6
21	A	1126	CLA	C2-C3-C5-C6
21	2	1237	CLA	C2-C3-C5-C6
21	1	1116	CLA	C2-C3-C5-C6
21	a	1122	CLA	C2-C3-C5-C6
21	A	1121	CLA	C2-C3-C5-C6
21	a	1140	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	1217	CLA	C2-C3-C5-C6
21	1	1121	CLA	C2-C3-C5-C6
21	b	1215	CLA	C2-C3-C5-C6
21	A	1134	CLA	C2-C3-C5-C6
21	0	1503	CLA	C2-C3-C5-C6
21	A	1107	CLA	C2-C3-C5-C6
21	b	1237	CLA	C2-C3-C5-C6
21	B	1235	CLA	C2-C3-C5-C6
21	A	1133	CLA	C2-C3-C5-C6
21	1	1109	CLA	C2-C3-C5-C6
21	2	1218	CLA	C2-C3-C5-C6
21	B	1203	CLA	C2-C3-C5-C6
21	1	1140	CLA	C2-C3-C5-C6
21	b	1209	CLA	C2-C3-C5-C6
21	a	1135	CLA	C2-C3-C5-C6
21	B	1214	CLA	C2A-CAA-CBA-CGA
21	2	1213	CLA	C2A-CAA-CBA-CGA
21	B	1216	CLA	C2A-CAA-CBA-CGA
21	1	1106	CLA	C2A-CAA-CBA-CGA
21	2	1225	CLA	C2A-CAA-CBA-CGA
21	B	1239	CLA	C2A-CAA-CBA-CGA
21	b	1237	CLA	C2A-CAA-CBA-CGA
21	B	1218	CLA	C2A-CAA-CBA-CGA
21	A	1108	CLA	C2A-CAA-CBA-CGA
21	2	1211	CLA	O1D-CGD-O2D-CED
21	L	1503	CLA	O1D-CGD-O2D-CED
21	a	1132	CLA	O1D-CGD-O2D-CED
21	A	1115	CLA	O1D-CGD-O2D-CED
21	2	1239	CLA	O1D-CGD-O2D-CED
21	b	1230	CLA	O1D-CGD-O2D-CED
21	A	1126	CLA	O1A-CGA-O2A-C1
21	b	1206	CLA	O1A-CGA-O2A-C1
21	a	1126	CLA	O1A-CGA-O2A-C1
31	b	5006	SQD	O5-C1-O6-C44
21	a	1103	CLA	C3-C5-C6-C7
21	2	1206	CLA	CBA-CGA-O2A-C1
37	L	5004	DGD	O6D-C5D-C6D-O5D
21	a	1013	CLA	O1D-CGD-O2D-CED
21	a	1105	CLA	O1D-CGD-O2D-CED
21	1	1103	CLA	O1D-CGD-O2D-CED
21	J	1303	CLA	O1D-CGD-O2D-CED
21	a	1124	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1102	CLA	O1D-CGD-O2D-CED
21	1	1120	CLA	O1D-CGD-O2D-CED
21	1	1128	CLA	O1D-CGD-O2D-CED
21	1	1135	CLA	O1A-CGA-O2A-C1
21	a	1117	CLA	O1A-CGA-O2A-C1
21	1	1117	CLA	O1A-CGA-O2A-C1
25	A	5001	LHG	C11-C12-C13-C14
21	A	1012	CLA	O1D-CGD-O2D-CED
21	b	1214	CLA	O1D-CGD-O2D-CED
21	2	1230	CLA	O1D-CGD-O2D-CED
21	b	1240	CLA	O1D-CGD-O2D-CED
21	2	1235	CLA	O1D-CGD-O2D-CED
21	1	1123	CLA	O1D-CGD-O2D-CED
21	1	1135	CLA	O1D-CGD-O2D-CED
21	0	1503	CLA	O1D-CGD-O2D-CED
21	b	1204	CLA	O1D-CGD-O2D-CED
21	B	1222	CLA	CBD-CGD-O2D-CED
25	2	5004	LHG	C1-C2-C3-O3
25	B	5004	LHG	C1-C2-C3-O3
25	F	5002	LHG	C1-C2-C3-O3
25	a	5003	LHG	C1-C2-C3-O3
25	a	5007	LHG	C1-C2-C3-O3
25	1	5007	LHG	C1-C2-C3-O3
25	A	5006	LHG	C1-C2-C3-O3
25	1	5005	LHG	C1-C2-C3-O3
25	l	5003	LHG	C1-C2-C3-O3
21	2	1210	CLA	O1A-CGA-O2A-C1
21	b	1239	CLA	O1A-CGA-O2A-C1
21	A	1801	CLA	C3-C5-C6-C7
21	b	1208	CLA	C3-C5-C6-C7
21	B	1231	CLA	C3-C5-C6-C7
21	B	1226	CLA	C3-C5-C6-C7
21	b	1238	CLA	C3-C5-C6-C7
21	b	1208	CLA	O1D-CGD-O2D-CED
21	a	1127	CLA	O1D-CGD-O2D-CED
21	b	1228	CLA	O1D-CGD-O2D-CED
21	K	1402	CLA	O1D-CGD-O2D-CED
21	1	1102	CLA	O1D-CGD-O2D-CED
21	1	1012	CLA	O1D-CGD-O2D-CED
26	0	5001	LMG	C29-C28-O8-C9
21	b	1216	CLA	CBA-CGA-O2A-C1
21	2	1236	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	2	1210	CLA	CBA-CGA-O2A-C1
21	2	1201	CLA	CBA-CGA-O2A-C1
21	b	1240	CLA	CBA-CGA-O2A-C1
21	a	1123	CLA	CBA-CGA-O2A-C1
21	B	1239	CLA	CBA-CGA-O2A-C1
21	a	1128	CLA	CBA-CGA-O2A-C1
21	B	1208	CLA	CBA-CGA-O2A-C1
21	b	1212	CLA	CBA-CGA-O2A-C1
21	b	1206	CLA	CBA-CGA-O2A-C1
21	l	1503	CLA	CBA-CGA-O2A-C1
21	A	1121	CLA	CBA-CGA-O2A-C1
21	b	1239	CLA	CBA-CGA-O2A-C1
21	1	1123	CLA	CBA-CGA-O2A-C1
26	K	5009	LMG	C29-C28-O8-C9
21	a	1130	CLA	CBA-CGA-O2A-C1
21	A	1135	CLA	CBA-CGA-O2A-C1
21	a	1112	CLA	CBA-CGA-O2A-C1
21	2	1202	CLA	CBA-CGA-O2A-C1
21	2	1023	CLA	CBA-CGA-O2A-C1
21	l	1502	CLA	CBA-CGA-O2A-C1
21	b	1221	CLA	CBA-CGA-O2A-C1
21	2	1239	CLA	CBA-CGA-O2A-C1
21	b	1023	CLA	CBA-CGA-O2A-C1
21	a	1137	CLA	CBA-CGA-O2A-C1
21	1	1128	CLA	CBA-CGA-O2A-C1
21	a	1133	CLA	C8-C10-C11-C12
21	K	1401	CLA	CBD-CGD-O2D-CED
21	A	1013	CLA	CBD-CGD-O2D-CED
24	h	4018	BCR	C15-C16-C17-C18
25	b	5004	LHG	C23-C24-C25-C26
21	b	1214	CLA	C13-C15-C16-C17
21	F	1302	CLA	C8-C10-C11-C12
21	K	1401	CLA	C13-C15-C16-C17
21	1	1118	CLA	C15-C16-C17-C18
21	A	1136	CLA	C15-C16-C17-C18
21	B	1223	CLA	C8-C10-C11-C12
21	b	1237	CLA	C5-C6-C7-C8
21	A	1133	CLA	C15-C16-C17-C18
21	B	1203	CLA	C13-C15-C16-C17
21	a	1136	CLA	C13-C15-C16-C17
21	b	1213	CLA	C5-C6-C7-C8
21	1	1123	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	0	6001	LMT	C4B-C5B-C6B-O6B
21	b	1225	CLA	C5-C6-C7-C8
21	B	1213	CLA	C15-C16-C17-C18
21	B	1240	CLA	C15-C16-C17-C18
21	2	1210	CLA	C13-C15-C16-C17
21	1	1134	CLA	C8-C10-C11-C12
21	F	1302	CLA	C15-C16-C17-C18
21	B	1208	CLA	C5-C6-C7-C8
21	a	1111	CLA	C10-C11-C12-C13
21	b	1021	CLA	C5-C6-C7-C8
21	J	1303	CLA	C8-C10-C11-C12
21	1	1801	CLA	C5-C6-C7-C8
21	A	1132	CLA	C13-C15-C16-C17
21	1	1125	CLA	C10-C11-C12-C13
21	b	1231	CLA	C5-C6-C7-C8
21	0	1503	CLA	C10-C11-C12-C13
21	A	1133	CLA	C8-C10-C11-C12
21	1	1126	CLA	C13-C15-C16-C17
21	b	1207	CLA	C10-C11-C12-C13
21	B	1205	CLA	C8-C10-C11-C12
21	b	1232	CLA	C15-C16-C17-C18
21	a	1135	CLA	C13-C15-C16-C17
21	b	1213	CLA	C15-C16-C17-C18
25	2	5004	LHG	O2-C2-C3-O3
25	B	5004	LHG	O2-C2-C3-O3
25	a	5005	LHG	O2-C2-C3-O3
25	a	5003	LHG	O2-C2-C3-O3
25	1	5007	LHG	O2-C2-C3-O3
25	l	5003	LHG	O2-C2-C3-O3
25	a	5001	LHG	O2-C2-C3-O3
25	a	5007	LHG	C7-C8-C9-C10
26	b	5005	LMG	C2-C1-O1-C7
26	b	5007	LMG	C2-C1-O1-C7
26	A	5002	LMG	C2-C1-O1-C7
21	b	1216	CLA	O1A-CGA-O2A-C1
21	2	1236	CLA	O1A-CGA-O2A-C1
21	b	1240	CLA	O1A-CGA-O2A-C1
21	a	1123	CLA	O1A-CGA-O2A-C1
21	b	1221	CLA	O1A-CGA-O2A-C1
21	b	1023	CLA	O1A-CGA-O2A-C1
21	f	1302	CLA	C4-C3-C5-C6
21	b	1235	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	1226	CLA	C2-C3-C5-C6
21	a	1127	CLA	C2-C3-C5-C6
21	A	1012	CLA	C11-C10-C8-C9
21	A	1012	CLA	C11-C12-C13-C14
21	b	1202	CLA	C14-C13-C15-C16
21	b	1211	CLA	C11-C12-C13-C14
21	2	1022	CLA	C11-C12-C13-C14
21	A	1126	CLA	C14-C13-C15-C16
21	1	1122	CLA	C6-C7-C8-C9
21	A	1116	CLA	C6-C7-C8-C9
21	A	1116	CLA	C11-C10-C8-C9
21	a	1115	CLA	C11-C12-C13-C14
21	b	1208	CLA	C6-C7-C8-C9
21	2	1210	CLA	C6-C7-C8-C9
21	A	1110	CLA	C6-C7-C8-C9
21	b	1222	CLA	C11-C12-C13-C14
21	1	1115	CLA	C6-C7-C8-C9
21	a	1013	CLA	C14-C13-C15-C16
21	B	1023	CLA	C11-C12-C13-C14
21	a	1131	CLA	C6-C7-C8-C9
21	F	1302	CLA	C11-C12-C13-C14
21	a	1123	CLA	C6-C7-C8-C9
21	a	1122	CLA	C14-C13-C15-C16
21	a	1128	CLA	C11-C12-C13-C14
21	a	1106	CLA	C14-C13-C15-C16
21	b	1206	CLA	C14-C13-C15-C16
21	B	1215	CLA	C6-C7-C8-C9
21	l	1503	CLA	C14-C13-C15-C16
21	0	1502	CLA	C6-C7-C8-C9
21	L	1502	CLA	C6-C7-C8-C9
21	a	1111	CLA	C11-C12-C13-C14
21	F	1301	CLA	C14-C13-C15-C16
21	B	1228	CLA	C6-C7-C8-C9
21	A	1106	CLA	C14-C13-C15-C16
21	a	1130	CLA	C6-C7-C8-C9
21	a	1130	CLA	C11-C12-C13-C14
21	a	1140	CLA	C11-C12-C13-C14
21	1	1133	CLA	C11-C10-C8-C9
21	1	1133	CLA	C14-C13-C15-C16
21	a	1012	CLA	C11-C10-C8-C9
21	a	1012	CLA	C11-C12-C13-C14
21	A	1137	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	1201	CLA	C11-C10-C8-C9
21	b	1231	CLA	C14-C13-C15-C16
21	A	1129	CLA	C11-C10-C8-C9
21	A	1134	CLA	C14-C13-C15-C16
21	A	1107	CLA	C6-C7-C8-C9
21	A	1107	CLA	C14-C13-C15-C16
21	B	1221	CLA	C11-C12-C13-C14
21	1	1126	CLA	C6-C7-C8-C9
21	a	1117	CLA	C14-C13-C15-C16
21	A	1131	CLA	C11-C10-C8-C9
21	a	1110	CLA	C6-C7-C8-C9
21	a	1118	CLA	C11-C12-C13-C14
21	A	1125	CLA	C14-C13-C15-C16
21	b	1219	CLA	C11-C10-C8-C9
21	1	1120	CLA	C11-C12-C13-C14
21	b	1232	CLA	C6-C7-C8-C9
21	B	1206	CLA	C14-C13-C15-C16
21	1	1128	CLA	C11-C10-C8-C9
21	a	1126	CLA	C11-C12-C13-C14
21	a	1126	CLA	C14-C13-C15-C16
21	A	1118	CLA	C11-C10-C8-C9
22	b	2002	PQN	C21-C22-C23-C24
21	a	1119	CLA	C11-C10-C8-C9
21	2	1022	CLA	O1D-CGD-O2D-CED
21	a	1115	CLA	O1D-CGD-O2D-CED
21	2	1204	CLA	O1D-CGD-O2D-CED
21	A	1132	CLA	O1D-CGD-O2D-CED
21	a	1110	CLA	O1D-CGD-O2D-CED
21	A	1106	CLA	CBD-CGD-O2D-CED
21	L	1503	CLA	C8-C10-C11-C12
21	a	1106	CLA	C10-C11-C12-C13
21	1	1101	CLA	C10-C11-C12-C13
21	A	1131	CLA	C5-C6-C7-C8
21	B	1203	CLA	C10-C11-C12-C13
21	1	1128	CLA	C8-C10-C11-C12
21	b	1225	CLA	C2A-CAA-CBA-CGA
21	l	1501	CLA	C2A-CAA-CBA-CGA
24	a	4001	BCR	C37-C22-C23-C24
24	1	4001	BCR	C11-C12-C13-C35
24	1	4007	BCR	C7-C8-C9-C34
24	1	4003	BCR	C11-C12-C13-C35
24	1	4003	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
36	I	4020	EQ3	C7-C8-C9-C34
24	0	4022	BCR	C37-C22-C23-C24
24	B	4014	BCR	C7-C8-C9-C34
24	B	4014	BCR	C11-C12-C13-C35
24	J	4013	BCR	C11-C12-C13-C35
24	b	4010	BCR	C37-C22-C23-C24
24	b	4017	BCR	C11-C12-C13-C35
24	I	4018	BCR	C36-C18-C19-C20
24	0	4019	BCR	C11-C12-C13-C35
24	0	4019	BCR	C37-C22-C23-C24
24	a	4008	BCR	C37-C22-C23-C24
24	9	4021	BCR	C37-C22-C23-C24
30	b	4011	ECH	C7-C8-C9-C34
30	b	4011	ECH	C37-C22-C23-C24
24	b	4014	BCR	C11-C12-C13-C35
24	A	4003	BCR	C7-C8-C9-C34
24	1	4008	BCR	C36-C18-C19-C20
24	j	4013	BCR	C11-C12-C13-C35
30	b	4006	ECH	C37-C22-C23-C24
24	2	4017	BCR	C11-C12-C13-C35
24	2	4014	BCR	C11-C12-C13-C35
24	1	4012	BCR	C37-C22-C23-C24
30	2	4006	ECH	C7-C8-C9-C34
30	2	4006	ECH	C36-C18-C19-C20
30	2	4006	ECH	C37-C22-C23-C24
24	b	4004	BCR	C11-C12-C13-C35
24	b	4004	BCR	C37-C22-C23-C24
24	7	4013	BCR	C37-C22-C23-C24
24	b	4018	BCR	C37-C22-C23-C24
30	i	4020	ECH	C11-C12-C13-C35
24	A	4007	BCR	C37-C22-C23-C24
24	B	4004	BCR	C36-C18-C19-C20
24	2	4004	BCR	C37-C22-C23-C24
24	1	4001	BCR	C11-C12-C13-C14
24	B	4014	BCR	C11-C12-C13-C14
24	J	4013	BCR	C11-C12-C13-C14
24	b	4010	BCR	C21-C22-C23-C24
24	I	4018	BCR	C17-C18-C19-C20
24	B	4005	BCR	C21-C22-C23-C24
24	0	4019	BCR	C11-C12-C13-C14
24	0	4019	BCR	C21-C22-C23-C24
30	b	4011	ECH	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	b	4014	BCR	C11-C12-C13-C14
24	j	4013	BCR	C11-C12-C13-C14
24	2	4017	BCR	C11-C12-C13-C14
24	2	4014	BCR	C11-C12-C13-C14
30	2	4006	ECH	C17-C18-C19-C20
30	2	4006	ECH	C21-C22-C23-C24
24	b	4004	BCR	C11-C12-C13-C14
24	b	4004	BCR	C21-C22-C23-C24
24	7	4013	BCR	C11-C12-C13-C14
24	7	4013	BCR	C21-C22-C23-C24
24	b	4018	BCR	C21-C22-C23-C24
30	i	4020	ECH	C11-C12-C13-C14
24	i	4018	BCR	C11-C12-C13-C14
25	F	5002	LHG	C8-C7-O7-C5
25	l	5001	LHG	C23-C24-C25-C26
25	a	5003	LHG	C23-C24-C25-C26
25	1	5007	LHG	C7-C8-C9-C10
21	2	1201	CLA	O1A-CGA-O2A-C1
21	b	1212	CLA	O1A-CGA-O2A-C1
21	l	1503	CLA	O1A-CGA-O2A-C1
21	A	1121	CLA	O1A-CGA-O2A-C1
21	a	1130	CLA	O1A-CGA-O2A-C1
21	a	1112	CLA	O1A-CGA-O2A-C1
21	2	1023	CLA	O1A-CGA-O2A-C1
21	1	1128	CLA	O1A-CGA-O2A-C1
21	B	1240	CLA	C13-C15-C16-C17
21	A	1116	CLA	C5-C6-C7-C8
21	l	1503	CLA	C10-C11-C12-C13
21	B	1209	CLA	C15-C16-C17-C18
21	b	1239	CLA	C8-C10-C11-C12
21	A	1111	CLA	C15-C16-C17-C18
21	L	1501	CLA	C13-C15-C16-C17
21	A	1130	CLA	C5-C6-C7-C8
22	2	2002	PQN	C23-C25-C26-C27
21	B	1218	CLA	C5-C6-C7-C8
21	B	1218	CLA	C10-C11-C12-C13
21	a	1118	CLA	C5-C6-C7-C8
21	1	1012	CLA	C5-C6-C7-C8
21	B	1225	CLA	C5-C6-C7-C8
21	B	1225	CLA	C13-C15-C16-C17
21	B	1213	CLA	O1D-CGD-O2D-CED
21	2	1205	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	b	1203	CLA	C3-C5-C6-C7
21	L	1502	CLA	C3-C5-C6-C7
21	B	1210	CLA	C3-C5-C6-C7
21	b	1215	CLA	C3-C5-C6-C7
21	b	1210	CLA	C3-C5-C6-C7
21	b	1232	CLA	CBA-CGA-O2A-C1
21	A	1012	CLA	C5-C6-C7-C8
21	B	1214	CLA	C13-C15-C16-C17
21	B	1214	CLA	C15-C16-C17-C18
21	j	1302	CLA	C5-C6-C7-C8
21	A	1101	CLA	C10-C11-C12-C13
21	b	1214	CLA	C8-C10-C11-C12
21	B	1217	CLA	C10-C11-C12-C13
21	B	1207	CLA	C13-C15-C16-C17
21	2	1210	CLA	C8-C10-C11-C12
21	1	1134	CLA	C5-C6-C7-C8
21	A	1110	CLA	C8-C10-C11-C12
21	A	1110	CLA	C10-C11-C12-C13
21	A	1113	CLA	C13-C15-C16-C17
21	a	1013	CLA	C10-C11-C12-C13
21	a	1013	CLA	C13-C15-C16-C17
21	2	1225	CLA	C5-C6-C7-C8
21	a	1131	CLA	C10-C11-C12-C13
21	A	1103	CLA	C13-C15-C16-C17
21	a	1127	CLA	C15-C16-C17-C18
21	b	1228	CLA	C5-C6-C7-C8
21	b	1228	CLA	C13-C15-C16-C17
21	B	1215	CLA	C13-C15-C16-C17
21	1	1118	CLA	C10-C11-C12-C13
21	1	1103	CLA	C5-C6-C7-C8
21	B	1228	CLA	C15-C16-C17-C18
21	A	1106	CLA	C8-C10-C11-C12
21	A	1106	CLA	C15-C16-C17-C18
21	a	1130	CLA	C15-C16-C17-C18
21	A	1104	CLA	C15-C16-C17-C18
21	2	1205	CLA	C8-C10-C11-C12
21	A	1137	CLA	C8-C10-C11-C12
21	2	1202	CLA	C13-C15-C16-C17
21	2	1215	CLA	C8-C10-C11-C12
21	a	1117	CLA	C13-C15-C16-C17
21	1	1109	CLA	C10-C11-C12-C13
21	A	1125	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	A	1140	CLA	C8-C10-C11-C12
21	1	1136	CLA	C8-C10-C11-C12
21	b	1223	CLA	C15-C16-C17-C18
21	A	1102	CLA	C10-C11-C12-C13
21	a	1135	CLA	C10-C11-C12-C13
21	B	1206	CLA	C10-C11-C12-C13
21	a	1125	CLA	C13-C15-C16-C17
25	1	5003	LHG	C9-C10-C11-C12
31	L	5002	SQD	C7-C8-C9-C10
25	A	5006	LHG	C7-C8-C9-C10
25	1	5005	LHG	C7-C8-C9-C10
21	A	1103	CLA	O1D-CGD-O2D-CED
21	2	1222	CLA	O1D-CGD-O2D-CED
21	B	1228	CLA	CBD-CGD-O2D-CED
21	1	1133	CLA	CBD-CGD-O2D-CED
21	b	1220	CLA	C15-C16-C17-C18
21	1	1131	CLA	C5-C6-C7-C8
21	b	1216	CLA	C5-C6-C7-C8
21	B	1216	CLA	C15-C16-C17-C18
21	a	1121	CLA	C10-C11-C12-C13
21	1	1122	CLA	C10-C11-C12-C13
21	b	1208	CLA	C8-C10-C11-C12
21	A	1110	CLA	C5-C6-C7-C8
21	A	1110	CLA	C13-C15-C16-C17
21	b	1240	CLA	C8-C10-C11-C12
21	b	1222	CLA	C10-C11-C12-C13
21	a	1133	CLA	C15-C16-C17-C18
21	1	1106	CLA	C13-C15-C16-C17
21	a	1123	CLA	C15-C16-C17-C18
21	A	1103	CLA	C15-C16-C17-C18
21	a	1122	CLA	C13-C15-C16-C17
21	B	1211	CLA	C8-C10-C11-C12
21	L	1503	CLA	C15-C16-C17-C18
21	K	1401	CLA	C5-C6-C7-C8
21	B	1208	CLA	C15-C16-C17-C18
21	A	1105	CLA	C15-C16-C17-C18
21	B	1215	CLA	C5-C6-C7-C8
21	B	1215	CLA	C10-C11-C12-C13
21	a	1111	CLA	C5-C6-C7-C8
21	A	1106	CLA	C13-C15-C16-C17
21	B	1234	CLA	C10-C11-C12-C13
21	2	1208	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	a	1112	CLA	C5-C6-C7-C8
21	B	1201	CLA	C10-C11-C12-C13
21	B	1229	CLA	C8-C10-C11-C12
21	b	1218	CLA	C10-C11-C12-C13
21	b	1218	CLA	C13-C15-C16-C17
21	b	1231	CLA	C15-C16-C17-C18
21	b	1215	CLA	C5-C6-C7-C8
21	A	1134	CLA	C5-C6-C7-C8
21	A	1134	CLA	C8-C10-C11-C12
21	A	1134	CLA	C15-C16-C17-C18
21	A	1107	CLA	C5-C6-C7-C8
21	a	1139	CLA	C13-C15-C16-C17
21	B	1221	CLA	C15-C16-C17-C18
21	1	1126	CLA	C10-C11-C12-C13
21	a	1124	CLA	C5-C6-C7-C8
21	B	1218	CLA	C13-C15-C16-C17
21	j	1303	CLA	C5-C6-C7-C8
21	K	1402	CLA	C13-C15-C16-C17
21	b	1209	CLA	C15-C16-C17-C18
21	A	1013	CLA	C10-C11-C12-C13
21	A	1120	CLA	C13-C15-C16-C17
21	J	1302	CLA	C8-C10-C11-C12
21	1	1117	CLA	C15-C16-C17-C18
21	A	1118	CLA	C5-C6-C7-C8
21	a	1135	CLA	O1D-CGD-O2D-CED
25	0	5002	LHG	O1-C1-C2-O2
21	A	1135	CLA	O1A-CGA-O2A-C1
21	2	1239	CLA	O1A-CGA-O2A-C1
25	F	5002	LHG	C23-C24-C25-C26
25	A	5007	LHG	C23-C24-C25-C26
25	l	5001	LHG	C7-C8-C9-C10
25	A	5001	LHG	C23-C24-C25-C26
26	1	5002	LMG	C28-C29-C30-C31
25	a	5005	LHG	C7-C8-C9-C10
26	b	5007	LMG	C28-C29-C30-C31
25	1	5007	LHG	C23-C24-C25-C26
25	1	5005	LHG	C23-C24-C25-C26
25	l	5003	LHG	C23-C24-C25-C26
25	a	5001	LHG	C7-C8-C9-C10
25	0	5004	LHG	C23-C24-C25-C26
21	b	1202	CLA	CBD-CGD-O2D-CED
21	1	1132	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	1131	CLA	C13-C15-C16-C17
21	j	1302	CLA	C10-C11-C12-C13
21	A	1114	CLA	C10-C11-C12-C13
21	B	1216	CLA	C8-C10-C11-C12
21	B	1023	CLA	C8-C10-C11-C12
21	b	1224	CLA	C5-C6-C7-C8
21	K	1401	CLA	C15-C16-C17-C18
21	1	1101	CLA	C15-C16-C17-C18
21	B	1238	CLA	C5-C6-C7-C8
21	A	1136	CLA	C5-C6-C7-C8
21	B	1234	CLA	C5-C6-C7-C8
21	B	1223	CLA	C5-C6-C7-C8
21	b	1201	CLA	C13-C15-C16-C17
22	1	2001	PQN	C18-C20-C21-C22
21	1	1133	CLA	C15-C16-C17-C18
21	B	1229	CLA	C5-C6-C7-C8
21	b	1218	CLA	C5-C6-C7-C8
21	1	1125	CLA	C15-C16-C17-C18
21	b	1219	CLA	C8-C10-C11-C12
21	1	1128	CLA	C10-C11-C12-C13
21	A	1130	CLA	C3-C5-C6-C7
21	j	1302	CLA	CBA-CGA-O2A-C1
21	2	1234	CLA	CBA-CGA-O2A-C1
21	A	1113	CLA	CBA-CGA-O2A-C1
25	F	5002	LHG	C24-C23-O8-C6
25	a	5005	LHG	C24-C23-O8-C6
21	a	1113	CLA	CBA-CGA-O2A-C1
21	b	1201	CLA	CBA-CGA-O2A-C1
21	b	1217	CLA	CBA-CGA-O2A-C1
21	A	1134	CLA	CBA-CGA-O2A-C1
21	b	1209	CLA	CBA-CGA-O2A-C1
21	A	1139	CLA	CBA-CGA-O2A-C1
21	1	1801	CLA	O1D-CGD-O2D-CED
21	1	1139	CLA	C2-C1-O2A-CGA
21	2	1229	CLA	C2-C1-O2A-CGA
21	2	1214	CLA	C2-C1-O2A-CGA
21	A	1101	CLA	C2-C1-O2A-CGA
21	1	1013	CLA	C2-C1-O2A-CGA
21	2	1022	CLA	C2-C1-O2A-CGA
21	1	1122	CLA	C2-C1-O2A-CGA
21	f	1301	CLA	C2-C1-O2A-CGA
21	b	1227	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	1	1104	CLA	C2-C1-O2A-CGA
21	b	1229	CLA	C2-C1-O2A-CGA
21	A	1123	CLA	C2-C1-O2A-CGA
21	1	1111	CLA	C2-C1-O2A-CGA
21	A	1112	CLA	C2-C1-O2A-CGA
21	a	1107	CLA	C2-C1-O2A-CGA
21	1	1137	CLA	C2-C1-O2A-CGA
21	1	1101	CLA	C2-C1-O2A-CGA
21	1	1118	CLA	C2-C1-O2A-CGA
21	a	1111	CLA	C2-C1-O2A-CGA
21	B	1228	CLA	C2-C1-O2A-CGA
21	A	1138	CLA	C2-C1-O2A-CGA
21	a	1129	CLA	C2-C1-O2A-CGA
21	a	1140	CLA	C2-C1-O2A-CGA
21	A	1104	CLA	C2-C1-O2A-CGA
21	2	1217	CLA	C2-C1-O2A-CGA
21	A	1137	CLA	C2-C1-O2A-CGA
21	B	1229	CLA	C2-C1-O2A-CGA
21	a	1104	CLA	C2-C1-O2A-CGA
21	1	1125	CLA	C2-C1-O2A-CGA
21	A	1111	CLA	C2-C1-O2A-CGA
21	a	1139	CLA	C2-C1-O2A-CGA
21	1	1126	CLA	C2-C1-O2A-CGA
21	2	1023	CLA	C2-C1-O2A-CGA
21	B	1203	CLA	C2-C1-O2A-CGA
21	A	1119	CLA	C2-C1-O2A-CGA
21	b	1209	CLA	C2-C1-O2A-CGA
21	A	1139	CLA	C2-C1-O2A-CGA
21	a	1118	CLA	C2-C1-O2A-CGA
21	2	1203	CLA	C2-C1-O2A-CGA
21	A	1108	CLA	C2-C1-O2A-CGA
21	b	1023	CLA	C2-C1-O2A-CGA
21	J	1302	CLA	C2-C1-O2A-CGA
21	a	1126	CLA	C2-C1-O2A-CGA
21	a	1108	CLA	C2-C1-O2A-CGA
21	a	1119	CLA	C2-C1-O2A-CGA
35	F	6001	LMT	O1'-C1-C2-C3
21	B	1214	CLA	C8-C10-C11-C12
21	a	1102	CLA	C5-C6-C7-C8
21	B	1213	CLA	C13-C15-C16-C17
21	a	1121	CLA	C8-C10-C11-C12
21	2	1210	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	b	1206	CLA	C15-C16-C17-C18
21	1	1103	CLA	C15-C16-C17-C18
21	B	1202	CLA	C15-C16-C17-C18
21	b	1201	CLA	C8-C10-C11-C12
21	b	1236	CLA	C13-C15-C16-C17
21	b	1231	CLA	C13-C15-C16-C17
21	l	1502	CLA	C5-C6-C7-C8
21	l	1502	CLA	C10-C11-C12-C13
21	B	1205	CLA	C5-C6-C7-C8
21	A	1112	CLA	O1D-CGD-O2D-CED
25	A	5003	LHG	C7-C8-C9-C10
25	A	5003	LHG	C23-C24-C25-C26
25	a	5007	LHG	C23-C24-C25-C26
25	B	5006	LHG	C7-C8-C9-C10
25	l	5004	LHG	C23-C24-C25-C26
31	0	5005	SQD	C23-C24-C25-C26
21	2	1234	CLA	CBD-CGD-O2D-CED
21	2	1223	CLA	CBD-CGD-O2D-CED
21	A	1108	CLA	CBD-CGD-O2D-CED
35	L	6001	LMT	C5'-C4'-O1B-C1B
21	2	1201	CLA	C13-C15-C16-C17
21	a	1106	CLA	C13-C15-C16-C17
21	A	1138	CLA	C8-C10-C11-C12
21	B	1234	CLA	C8-C10-C11-C12
21	2	1205	CLA	C13-C15-C16-C17
21	A	1137	CLA	C13-C15-C16-C17
21	B	1229	CLA	C10-C11-C12-C13
21	A	1131	CLA	C13-C15-C16-C17
21	A	1140	CLA	C10-C11-C12-C13
21	b	1214	CLA	C4-C3-C5-C6
21	2	1216	CLA	O1D-CGD-O2D-CED
21	A	1113	CLA	O1D-CGD-O2D-CED
21	1	1101	CLA	O1D-CGD-O2D-CED
21	A	1012	CLA	C6-C7-C8-C10
21	1	1131	CLA	C6-C7-C8-C10
21	b	1211	CLA	C11-C10-C8-C7
21	B	1216	CLA	C11-C12-C13-C15
21	a	1121	CLA	C11-C12-C13-C15
21	b	1208	CLA	C11-C10-C8-C7
21	2	1210	CLA	C11-C12-C13-C15
21	1	1104	CLA	C11-C12-C13-C15
21	A	1110	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	A	1113	CLA	C6-C7-C8-C10
21	B	1211	CLA	C11-C10-C8-C7
21	B	1224	CLA	C6-C7-C8-C10
21	1	1101	CLA	C11-C12-C13-C15
21	l	1503	CLA	C11-C12-C13-C15
21	l	1501	CLA	C11-C12-C13-C15
21	A	1136	CLA	C12-C13-C15-C16
21	b	1021	CLA	C11-C12-C13-C15
21	1	1133	CLA	C6-C7-C8-C10
21	a	1104	CLA	C6-C7-C8-C10
21	a	1117	CLA	C11-C10-C8-C7
21	A	1117	CLA	C11-C10-C8-C7
21	b	1210	CLA	C11-C10-C8-C7
21	A	1125	CLA	C6-C7-C8-C10
21	a	1136	CLA	C11-C10-C8-C7
21	A	1120	CLA	C6-C7-C8-C10
21	1	1120	CLA	C11-C12-C13-C15
21	a	1125	CLA	C11-C12-C13-C15
21	B	1204	CLA	C3-C5-C6-C7
21	B	1237	CLA	C3-C5-C6-C7
21	a	1122	CLA	C3-C5-C6-C7
21	2	1204	CLA	C3-C5-C6-C7
21	B	1227	CLA	C3-C5-C6-C7
21	2	1206	CLA	O1A-CGA-O2A-C1
21	a	1137	CLA	O1A-CGA-O2A-C1
24	1	4007	BCR	C13-C14-C15-C16
24	A	4001	BCR	C19-C20-C21-C22
24	2	4011	BCR	C19-C20-C21-C22
24	I	4018	BCR	C15-C16-C17-C18
24	2	4010	BCR	C19-C20-C21-C22
24	1	4008	BCR	C13-C14-C15-C16
24	a	4003	BCR	C13-C14-C15-C16
24	B	4018	BCR	C13-C14-C15-C16
24	1	4019	BCR	C9-C10-C11-C12
21	1	1013	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	CBA-CGA-O2A-C1
21	A	1012	CLA	C2A-CAA-CBA-CGA
21	B	1204	CLA	C2A-CAA-CBA-CGA
21	1	1127	CLA	C2A-CAA-CBA-CGA
21	b	1240	CLA	C2A-CAA-CBA-CGA
21	2	1211	CLA	C2A-CAA-CBA-CGA
21	B	1229	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	a	1101	CLA	O1D-CGD-O2D-CED
21	1	1119	CLA	O1D-CGD-O2D-CED
21	B	1239	CLA	O1D-CGD-O2D-CED
21	a	1128	CLA	O1D-CGD-O2D-CED
21	B	1226	CLA	O1D-CGD-O2D-CED
21	B	1210	CLA	O1D-CGD-O2D-CED
21	b	1226	CLA	O1D-CGD-O2D-CED
21	B	1234	CLA	O1D-CGD-O2D-CED
21	A	1131	CLA	O1D-CGD-O2D-CED
21	B	1214	CLA	C5-C6-C7-C8
21	b	1225	CLA	C13-C15-C16-C17
21	A	1126	CLA	C10-C11-C12-C13
21	b	1214	CLA	C5-C6-C7-C8
21	1	1127	CLA	C15-C16-C17-C18
21	B	1231	CLA	C5-C6-C7-C8
21	1	1106	CLA	C15-C16-C17-C18
21	a	1131	CLA	C8-C10-C11-C12
21	B	1224	CLA	C10-C11-C12-C13
21	a	1103	CLA	C13-C15-C16-C17
21	b	1228	CLA	C10-C11-C12-C13
21	F	1301	CLA	C15-C16-C17-C18
21	b	1205	CLA	C10-C11-C12-C13
21	a	1130	CLA	C13-C15-C16-C17
21	0	1501	CLA	C13-C15-C16-C17
22	a	2001	PQN	C18-C20-C21-C22
21	f	1302	CLA	C5-C6-C7-C8
21	b	1207	CLA	C8-C10-C11-C12
21	a	1138	CLA	C15-C16-C17-C18
21	a	1120	CLA	C5-C6-C7-C8
25	1	5003	LHG	C17-C18-C19-C20
21	B	1208	CLA	O1A-CGA-O2A-C1
26	K	5009	LMG	O10-C28-O8-C9
21	b	1216	CLA	CBD-CGD-O2D-CED
21	F	1301	CLA	C13-C15-C16-C17
21	b	1021	CLA	C13-C15-C16-C17
21	b	1201	CLA	C10-C11-C12-C13
21	A	1139	CLA	C8-C10-C11-C12
21	B	1211	CLA	O1D-CGD-O2D-CED
21	b	1207	CLA	O1D-CGD-O2D-CED
25	B	5004	LHG	C23-C24-C25-C26
26	A	5008	LMG	C28-C29-C30-C31
24	1	4003	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	1	4002	BCR	C10-C11-C12-C13
24	b	4017	BCR	C10-C11-C12-C13
24	B	4005	BCR	C10-C11-C12-C13
24	0	4019	BCR	C10-C11-C12-C13
24	K	4001	BCR	C10-C11-C12-C13
24	A	4003	BCR	C10-C11-C12-C13
24	2	4010	BCR	C10-C11-C12-C13
24	1	4008	BCR	C10-C11-C12-C13
24	a	4003	BCR	C10-C11-C12-C13
24	B	4018	BCR	C10-C11-C12-C13
24	2	4017	BCR	C10-C11-C12-C13
24	7	4013	BCR	C10-C11-C12-C13
24	b	4018	BCR	C10-C11-C12-C13
35	L	6001	LMT	O5B-C5B-C6B-O6B
25	l	5002	LHG	O2-C2-C3-O3
25	1	5003	LHG	O2-C2-C3-O3
25	A	5003	LHG	O2-C2-C3-O3
25	a	5007	LHG	O2-C2-C3-O3
25	B	5006	LHG	O2-C2-C3-O3
25	F	5002	LHG	O9-C7-O7-C5
21	a	1106	CLA	C3-C5-C6-C7
21	B	1220	CLA	C8-C10-C11-C12
21	6	1302	CLA	C2A-CAA-CBA-CGA
21	b	1220	CLA	C5-C6-C7-C8
21	1	1134	CLA	C15-C16-C17-C18
21	A	1113	CLA	C5-C6-C7-C8
21	a	1133	CLA	C5-C6-C7-C8
21	1	1106	CLA	C10-C11-C12-C13
21	a	1105	CLA	C5-C6-C7-C8
21	1	1118	CLA	C8-C10-C11-C12
21	0	1502	CLA	C13-C15-C16-C17
21	B	1210	CLA	C10-C11-C12-C13
21	1	1125	CLA	C8-C10-C11-C12
21	A	1111	CLA	C10-C11-C12-C13
21	b	1221	CLA	C15-C16-C17-C18
21	1	1136	CLA	C13-C15-C16-C17
21	2	1221	CLA	C13-C15-C16-C17
21	b	1232	CLA	C10-C11-C12-C13
21	a	1108	CLA	C5-C6-C7-C8
21	2	1208	CLA	CBA-CGA-O2A-C1
21	a	1109	CLA	CBA-CGA-O2A-C1
26	A	5002	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
21	A	1125	CLA	CBD-CGD-O2D-CED
26	0	5001	LMG	O10-C28-O8-C9
21	2	1234	CLA	O1A-CGA-O2A-C1
21	B	1239	CLA	O1A-CGA-O2A-C1
21	a	1128	CLA	O1A-CGA-O2A-C1
21	a	1113	CLA	O1A-CGA-O2A-C1
21	2	1202	CLA	O1A-CGA-O2A-C1
21	l	1502	CLA	O1A-CGA-O2A-C1
25	1	5003	LHG	C23-C24-C25-C26
31	f	5001	SQD	C28-C29-C30-C31
21	b	1235	CLA	C15-C16-C17-C18
21	a	1102	CLA	C10-C11-C12-C13
21	B	1216	CLA	C10-C11-C12-C13
21	A	1116	CLA	C8-C10-C11-C12
21	2	1201	CLA	C10-C11-C12-C13
21	1	1106	CLA	C5-C6-C7-C8
21	B	1215	CLA	C8-C10-C11-C12
21	A	1121	CLA	C8-C10-C11-C12
21	A	1121	CLA	C15-C16-C17-C18
21	B	1228	CLA	C5-C6-C7-C8
21	A	1135	CLA	C15-C16-C17-C18
21	b	1236	CLA	C10-C11-C12-C13
21	a	1104	CLA	C5-C6-C7-C8
21	L	1501	CLA	C10-C11-C12-C13
21	0	1503	CLA	C5-C6-C7-C8
21	0	1503	CLA	C13-C15-C16-C17
21	f	1302	CLA	C15-C16-C17-C18
21	2	1202	CLA	C10-C11-C12-C13
21	b	1204	CLA	C13-C15-C16-C17
21	a	1117	CLA	C5-C6-C7-C8
21	A	1125	CLA	C15-C16-C17-C18
21	2	1203	CLA	C13-C15-C16-C17
21	A	1013	CLA	C13-C15-C16-C17
21	1	1120	CLA	C5-C6-C7-C8
21	b	1213	CLA	C13-C15-C16-C17
21	B	1206	CLA	C15-C16-C17-C18
21	a	1126	CLA	C8-C10-C11-C12
25	2	5004	LHG	C34-C35-C36-C37
21	1	1122	CLA	O1D-CGD-O2D-CED
21	a	1011	CLA	O1D-CGD-O2D-CED
21	B	1209	CLA	O1D-CGD-O2D-CED
21	1	1105	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	a	1012	CLA	O1D-CGD-O2D-CED
21	A	1127	CLA	O1D-CGD-O2D-CED
21	1	1124	CLA	CBD-CGD-O2D-CED
21	b	1217	CLA	O1A-CGA-O2A-C1
21	A	1139	CLA	O1A-CGA-O2A-C1
26	2	5005	LMG	C11-C10-O7-C8
25	0	5002	LHG	C5-C6-O8-C23
21	1	1139	CLA	C13-C15-C16-C17
21	2	1229	CLA	C15-C16-C17-C18
21	A	1101	CLA	C8-C10-C11-C12
21	2	1206	CLA	C13-C15-C16-C17
21	B	1219	CLA	C13-C15-C16-C17
21	1	1122	CLA	C5-C6-C7-C8
21	b	1203	CLA	C13-C15-C16-C17
21	A	1110	CLA	C15-C16-C17-C18
21	b	1240	CLA	C10-C11-C12-C13
21	F	1302	CLA	C10-C11-C12-C13
21	A	1122	CLA	C10-C11-C12-C13
21	a	1111	CLA	C13-C15-C16-C17
21	2	1208	CLA	C10-C11-C12-C13
21	J	1303	CLA	C13-C15-C16-C17
21	0	1501	CLA	C15-C16-C17-C18
21	2	1215	CLA	C10-C11-C12-C13
22	A	2001	PQN	C18-C20-C21-C22
21	a	1110	CLA	C5-C6-C7-C8
21	A	1119	CLA	C5-C6-C7-C8
21	2	1221	CLA	C10-C11-C12-C13
21	B	1205	CLA	C10-C11-C12-C13
21	b	1230	CLA	C8-C10-C11-C12
21	A	1124	CLA	C8-C10-C11-C12
21	A	1109	CLA	C13-C15-C16-C17
21	a	1138	CLA	C13-C15-C16-C17
22	b	2002	PQN	C18-C20-C21-C22
25	l	5002	LHG	C3-O3-P-O6
25	l	5002	LHG	C4-O6-P-O3
25	2	5004	LHG	C3-O3-P-O6
25	F	5002	LHG	C3-O3-P-O6
25	A	5007	LHG	C3-O3-P-O6
25	A	5007	LHG	C4-O6-P-O3
25	l	5001	LHG	C3-O3-P-O6
25	A	5001	LHG	C4-O6-P-O3
25	a	5005	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	1	5003	LHG	C3-O3-P-O6
25	1	5003	LHG	C4-O6-P-O3
25	a	5003	LHG	C3-O3-P-O6
25	A	5003	LHG	C3-O3-P-O6
25	L	5005	LHG	C3-O3-P-O6
25	B	5006	LHG	C3-O3-P-O6
25	B	5006	LHG	C4-O6-P-O3
25	0	5002	LHG	C3-O3-P-O6
25	l	5003	LHG	C3-O3-P-O6
25	l	5003	LHG	C4-O6-P-O3
25	0	5004	LHG	C3-O3-P-O6
25	l	5003	LHG	C7-C8-C9-C10
21	1	1127	CLA	C3-C5-C6-C7
21	b	1209	CLA	C3-C5-C6-C7
21	2	1216	CLA	CBA-CGA-O2A-C1
21	A	1123	CLA	CBA-CGA-O2A-C1
21	B	1210	CLA	CBA-CGA-O2A-C1
21	b	1226	CLA	CBA-CGA-O2A-C1
21	1	1133	CLA	CBA-CGA-O2A-C1
21	B	1201	CLA	CBA-CGA-O2A-C1
21	2	1222	CLA	CBA-CGA-O2A-C1
21	a	1118	CLA	CBA-CGA-O2A-C1
21	1	1136	CLA	CBA-CGA-O2A-C1
21	a	1135	CLA	CBA-CGA-O2A-C1
21	k	1402	CLA	O1D-CGD-O2D-CED
21	A	1124	CLA	O1D-CGD-O2D-CED
21	b	1211	CLA	C5-C6-C7-C8
21	1	1104	CLA	C10-C11-C12-C13
21	2	1202	CLA	C15-C16-C17-C18
21	b	1210	CLA	C8-C10-C11-C12
21	A	1120	CLA	C15-C16-C17-C18
21	1	1115	CLA	O1D-CGD-O2D-CED
21	A	1128	CLA	O1D-CGD-O2D-CED
34	7	4015	ZEX	C25-C26-C27-C28
34	J	4015	ZEX	C25-C26-C27-C28
25	A	5007	LHG	C1-C2-C3-O3
25	l	5001	LHG	C1-C2-C3-O3
26	K	5009	LMG	O6-C5-C6-O5
25	A	5003	LHG	C1-C2-C3-O3
25	L	5005	LHG	C1-C2-C3-O3
25	B	5006	LHG	C1-C2-C3-O3
26	a	5004	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
26	2	5005	LMG	O9-C10-O7-C8
21	1	1139	CLA	C4-C3-C5-C6
21	B	1216	CLA	C4-C3-C5-C6
21	a	1101	CLA	C4-C3-C5-C6
21	l	1503	CLA	C4-C3-C5-C6
21	2	1208	CLA	C4-C3-C5-C6
21	b	1211	CLA	C15-C16-C17-C18
21	1	1124	CLA	C5-C6-C7-C8
21	A	1109	CLA	C15-C16-C17-C18
21	J	1302	CLA	C5-C6-C7-C8
21	a	1129	CLA	O1D-CGD-O2D-CED
21	1	1136	CLA	O1D-CGD-O2D-CED
21	b	1235	CLA	C2A-CAA-CBA-CGA
21	B	1237	CLA	C2A-CAA-CBA-CGA
21	1	1013	CLA	C2A-CAA-CBA-CGA
21	a	1127	CLA	C2A-CAA-CBA-CGA
21	1	1136	CLA	C2A-CAA-CBA-CGA
21	1	1138	CLA	C2A-CAA-CBA-CGA
21	2	1224	CLA	C2A-CAA-CBA-CGA
21	a	1135	CLA	C2A-CAA-CBA-CGA
21	a	1138	CLA	C2A-CAA-CBA-CGA
21	a	1108	CLA	C2A-CAA-CBA-CGA
21	A	1801	CLA	C16-C17-C18-C19
21	A	1107	CLA	C16-C17-C18-C19
21	A	1117	CLA	C16-C17-C18-C20
21	A	1125	CLA	C16-C17-C18-C20
21	2	1224	CLA	C6-C7-C8-C9
21	a	1102	CLA	CBA-CGA-O2A-C1
21	A	1136	CLA	CBA-CGA-O2A-C1
21	A	1137	CLA	CBA-CGA-O2A-C1
21	b	1231	CLA	CBA-CGA-O2A-C1
21	B	1221	CLA	CBA-CGA-O2A-C1
21	B	1232	CLA	CBA-CGA-O2A-C1
21	1	1120	CLA	CBA-CGA-O2A-C1
21	B	1238	CLA	C8-C10-C11-C12
21	b	1232	CLA	O1A-CGA-O2A-C1
21	b	1222	CLA	C8-C10-C11-C12
21	L	1502	CLA	C13-C15-C16-C17
25	a	5003	LHG	C29-C30-C31-C32
24	2	4010	BCR	C13-C14-C15-C16
24	8	4001	BCR	C19-C20-C21-C22
24	a	4019	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	M	5001	LHG	C23-C24-C25-C26
25	1	5001	LHG	C7-C8-C9-C10
31	F	5001	SQD	C12-C13-C14-C15
31	B	5008	SQD	C13-C14-C15-C16
25	B	5006	LHG	C26-C27-C28-C29
25	1	5003	LHG	C32-C33-C34-C35
25	0	5004	LHG	C24-C25-C26-C27
31	0	5005	SQD	C31-C32-C33-C34
21	2	1226	CLA	CBD-CGD-O2D-CED
25	1	5001	LHG	C8-C7-O7-C5
31	f	5001	SQD	C8-C7-O47-C45
21	A	1114	CLA	C5-C6-C7-C8
24	6	4016	BCR	C11-C10-C9-C34
24	f	4016	BCR	C11-C10-C9-C34
24	2	4018	BCR	C11-C10-C9-C34
24	b	4010	BCR	C11-C10-C9-C34
24	2	4011	BCR	C11-C10-C9-C34
26	A	5008	LMG	O6-C5-C6-O5
24	A	4019	BCR	C11-C10-C9-C34
24	A	4007	BCR	C11-C10-C9-C34
24	1	4019	BCR	C11-C10-C9-C34
21	A	1012	CLA	C3-C5-C6-C7
21	1	1121	CLA	C3-C5-C6-C7
21	B	1229	CLA	C3-C5-C6-C7
26	0	5001	LMG	C39-C40-C41-C42
25	B	5004	LHG	C11-C12-C13-C14
25	F	5002	LHG	C17-C18-C19-C20
25	F	5002	LHG	C29-C30-C31-C32
26	B	5002	LMG	C22-C23-C24-C25
26	A	5008	LMG	C21-C22-C23-C24
26	A	5008	LMG	C36-C37-C38-C39
21	a	1110	CLA	C10-C11-C12-C13
25	A	5006	LHG	C13-C14-C15-C16
25	A	5006	LHG	C25-C26-C27-C28
25	A	5006	LHG	C28-C29-C30-C31
25	1	5004	LHG	C25-C26-C27-C28
25	1	5003	LHG	C29-C30-C31-C32
25	a	5001	LHG	C11-C12-C13-C14
21	A	1113	CLA	O1A-CGA-O2A-C1
25	a	5005	LHG	O10-C23-O8-C6
21	b	1201	CLA	O1A-CGA-O2A-C1
21	b	1209	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	2	1206	CLA	O1D-CGD-O2D-CED
21	b	1216	CLA	C16-C17-C18-C20
21	1	1013	CLA	C16-C17-C18-C20
21	1	1122	CLA	C11-C12-C13-C14
21	A	1116	CLA	C16-C17-C18-C19
21	1	1127	CLA	C16-C17-C18-C20
21	A	1110	CLA	C16-C17-C18-C20
21	2	1226	CLA	C6-C7-C8-C10
21	2	1223	CLA	C6-C7-C8-C10
21	B	1228	CLA	C16-C17-C18-C20
21	A	1135	CLA	C16-C17-C18-C20
21	J	1303	CLA	C16-C17-C18-C19
21	1	1133	CLA	C16-C17-C18-C19
21	a	1801	CLA	C6-C7-C8-C10
21	a	1012	CLA	C16-C17-C18-C20
21	b	1218	CLA	C16-C17-C18-C20
21	b	1231	CLA	C16-C17-C18-C20
21	B	1203	CLA	C16-C17-C18-C20
21	1	1140	CLA	C16-C17-C18-C19
21	A	1139	CLA	C16-C17-C18-C19
21	A	1140	CLA	C16-C17-C18-C20
21	2	1203	CLA	C16-C17-C18-C20
21	A	1102	CLA	C16-C17-C18-C19
21	J	1302	CLA	C16-C17-C18-C19
21	1	1112	CLA	CBA-CGA-O2A-C1
21	1	1137	CLA	CBA-CGA-O2A-C1
25	1	5002	LHG	C13-C14-C15-C16
25	2	5004	LHG	C13-C14-C15-C16
25	F	5002	LHG	C31-C32-C33-C34
25	a	5005	LHG	C11-C10-C9-C8
35	L	6001	LMT	C3'-C4'-O1B-C1B
31	B	5008	SQD	C31-C32-C33-C34
25	1	5003	LHG	C9-C10-C11-C12
25	1	5003	LHG	C13-C14-C15-C16
25	a	5007	LHG	C31-C32-C33-C34
31	f	5001	SQD	C24-C25-C26-C27
25	A	5006	LHG	C11-C10-C9-C8
25	1	5005	LHG	C28-C29-C30-C31
21	B	1237	CLA	O1D-CGD-O2D-CED
21	B	1202	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	O1D-CGD-O2D-CED
21	2	1209	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	5001	LHG	O9-C7-O7-C5
31	f	5001	SQD	O49-C7-O47-C45
21	A	1112	CLA	C15-C16-C17-C18
21	b	1212	CLA	C8-C10-C11-C12
21	1	1109	CLA	C5-C6-C7-C8
31	b	5006	SQD	C7-C8-C9-C10
31	F	5001	SQD	C11-C12-C13-C14
25	A	5007	LHG	C13-C14-C15-C16
25	a	5005	LHG	C17-C18-C19-C20
25	a	5005	LHG	C24-C25-C26-C27
25	B	5006	LHG	C11-C12-C13-C14
25	B	5006	LHG	C31-C32-C33-C34
26	A	5002	LMG	C15-C16-C17-C18
26	B	5005	LMG	C21-C22-C23-C24
25	1	5004	LHG	C11-C12-C13-C14
21	2	1237	CLA	O1D-CGD-O2D-CED
21	a	1125	CLA	O1D-CGD-O2D-CED
25	B	5004	LHG	C34-C35-C36-C37
25	1	5001	LHG	C28-C29-C30-C31
25	A	5007	LHG	C30-C31-C32-C33
25	1	5001	LHG	C13-C14-C15-C16
26	1	5004	LMG	C29-C30-C31-C32
25	L	5005	LHG	C11-C12-C13-C14
25	L	5005	LHG	C13-C14-C15-C16
25	L	5005	LHG	C32-C33-C34-C35
21	2	1238	CLA	O1D-CGD-O2D-CED
25	1	5002	LHG	C11-C12-C13-C14
25	M	5001	LHG	C24-C25-C26-C27
25	A	5007	LHG	C12-C13-C14-C15
25	a	5007	LHG	C25-C26-C27-C28
21	1	1115	CLA	C3-C5-C6-C7
21	B	1201	CLA	C3-C5-C6-C7
25	2	5004	LHG	C23-C24-C25-C26
25	0	5002	LHG	C23-C24-C25-C26
21	2	1202	CLA	O1D-CGD-O2D-CED
21	6	1302	CLA	O1D-CGD-O2D-CED
21	A	1117	CLA	O1D-CGD-O2D-CED
24	6	4016	BCR	C11-C10-C9-C8
24	f	4016	BCR	C11-C10-C9-C8
24	b	4010	BCR	C11-C10-C9-C8
24	2	4011	BCR	C11-C10-C9-C8
24	I	4018	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	A	4019	BCR	C11-C10-C9-C8
26	B	5005	LMG	C2-C1-O1-C7
24	A	4007	BCR	C11-C10-C9-C8
24	1	4019	BCR	C11-C10-C9-C8
21	A	1120	CLA	CBA-CGA-O2A-C1
37	L	5004	DGD	C3A-C4A-C5A-C6A
37	L	5004	DGD	C6A-C7A-C8A-C9A
25	F	5002	LHG	C34-C35-C36-C37
25	A	5007	LHG	C34-C35-C36-C37
26	1	5002	LMG	C14-C15-C16-C17
26	A	5008	LMG	C14-C15-C16-C17
25	1	5003	LHG	C30-C31-C32-C33
25	a	5003	LHG	C17-C18-C19-C20
26	b	5007	LMG	C22-C23-C24-C25
25	A	5005	LHG	C16-C17-C18-C19
26	A	5002	LMG	C30-C31-C32-C33
25	1	5005	LHG	C13-C14-C15-C16
21	b	1235	CLA	C13-C15-C16-C17
21	a	1132	CLA	C5-C6-C7-C8
21	B	1202	CLA	C13-C15-C16-C17
21	j	1302	CLA	O1A-CGA-O2A-C1
25	F	5002	LHG	O10-C23-O8-C6
21	A	1134	CLA	O1A-CGA-O2A-C1
21	B	1232	CLA	O1A-CGA-O2A-C1
21	A	1114	CLA	C16-C17-C18-C20
21	b	1211	CLA	C16-C17-C18-C20
21	B	1208	CLA	C16-C17-C18-C19
21	b	1212	CLA	C16-C17-C18-C19
21	B	1215	CLA	C16-C17-C18-C19
21	A	1139	CLA	C16-C17-C18-C20
21	A	1127	CLA	C16-C17-C18-C19
21	L	1501	CLA	O1D-CGD-O2D-CED
21	B	1229	CLA	C4-C3-C5-C6
26	0	5001	LMG	C29-C30-C31-C32
25	a	5005	LHG	C11-C12-C13-C14
25	a	5005	LHG	C13-C14-C15-C16
35	1	6001	LMT	C4-C5-C6-C7
25	1	5003	LHG	C27-C28-C29-C30
31	b	5006	SQD	C28-C29-C30-C31
25	1	5007	LHG	C32-C33-C34-C35
31	L	5002	SQD	C10-C11-C12-C13
25	a	5001	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	L	5001	SQD	C16-C17-C18-C19
21	B	1225	CLA	C2-C3-C5-C6
21	j	1302	CLA	C11-C10-C8-C9
21	A	1126	CLA	C6-C7-C8-C9
21	1	1134	CLA	C14-C13-C15-C16
21	A	1110	CLA	C14-C13-C15-C16
21	L	1503	CLA	C11-C10-C8-C9
21	b	1212	CLA	C14-C13-C15-C16
21	1	1118	CLA	C11-C10-C8-C9
21	B	1230	CLA	C11-C10-C8-C9
21	a	1012	CLA	C6-C7-C8-C9
21	b	1218	CLA	C11-C10-C8-C9
21	b	1215	CLA	C11-C10-C8-C9
22	2	2002	PQN	C21-C22-C23-C24
21	K	1402	CLA	C11-C10-C8-C9
21	A	1125	CLA	C6-C7-C8-C9
21	2	1203	CLA	C6-C7-C8-C9
21	1	1012	CLA	C6-C7-C8-C9
22	b	2002	PQN	C19-C18-C20-C21
21	a	1125	CLA	C11-C12-C13-C14
21	a	1130	CLA	O1D-CGD-O2D-CED
21	l	1502	CLA	O1D-CGD-O2D-CED
25	l	5002	LHG	C23-C24-C25-C26
25	a	5001	LHG	C23-C24-C25-C26
31	F	5001	SQD	C10-C11-C12-C13
25	l	5001	LHG	C26-C27-C28-C29
25	b	5004	LHG	C29-C30-C31-C32
26	2	5005	LMG	C31-C32-C33-C34
26	b	5002	LMG	C21-C22-C23-C24
25	A	5003	LHG	C11-C12-C13-C14
25	a	5007	LHG	C10-C11-C12-C13
25	1	5005	LHG	C11-C12-C13-C14
25	0	5004	LHG	C25-C26-C27-C28
21	B	1204	CLA	C5-C6-C7-C8
21	b	1211	CLA	C8-C10-C11-C12
21	b	1206	CLA	C10-C11-C12-C13
21	a	1801	CLA	C5-C6-C7-C8
21	a	1104	CLA	C15-C16-C17-C18
21	b	1215	CLA	C8-C10-C11-C12
21	2	1236	CLA	C2A-CAA-CBA-CGA
21	L	1503	CLA	C2A-CAA-CBA-CGA
21	a	1128	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	a	1106	CLA	C2A-CAA-CBA-CGA
21	b	1239	CLA	C2A-CAA-CBA-CGA
21	A	1119	CLA	C2A-CAA-CBA-CGA
21	A	1125	CLA	C2A-CAA-CBA-CGA
21	a	1136	CLA	C2A-CAA-CBA-CGA
21	B	1216	CLA	O1A-CGA-O2A-C1
21	A	1136	CLA	O1A-CGA-O2A-C1
21	2	1208	CLA	O1A-CGA-O2A-C1
21	a	1109	CLA	O1A-CGA-O2A-C1
21	B	1201	CLA	O1A-CGA-O2A-C1
21	b	1231	CLA	O1A-CGA-O2A-C1
21	2	1222	CLA	O1A-CGA-O2A-C1
21	1	1136	CLA	O1A-CGA-O2A-C1
21	1	1120	CLA	O1A-CGA-O2A-C1
24	B	4010	BCR	C37-C22-C23-C24
24	1	4007	BCR	C36-C18-C19-C20
24	A	4008	BCR	C37-C22-C23-C24
24	A	4012	BCR	C37-C22-C23-C24
24	0	4022	BCR	C11-C12-C13-C35
24	K	4001	BCR	C11-C12-C13-C35
24	a	4002	BCR	C36-C18-C19-C20
30	b	4011	ECH	C11-C12-C13-C35
24	A	4003	BCR	C11-C12-C13-C35
24	j	4013	BCR	C37-C22-C23-C24
24	b	4005	BCR	C37-C22-C23-C24
24	a	4003	BCR	C11-C12-C13-C35
24	a	4003	BCR	C37-C22-C23-C24
24	l	4019	BCR	C37-C22-C23-C24
24	L	4019	BCR	C37-C22-C23-C24
24	A	4019	BCR	C36-C18-C19-C20
30	i	4020	ECH	C7-C8-C9-C34
24	1	4019	BCR	C37-C22-C23-C24
24	a	4012	BCR	C11-C12-C13-C35
25	l	5001	LHG	C34-C35-C36-C37
25	A	5001	LHG	C26-C27-C28-C29
26	A	5008	LMG	C13-C14-C15-C16
25	1	5003	LHG	C16-C17-C18-C19
26	a	5004	LMG	C21-C22-C23-C24
26	B	5005	LMG	C15-C16-C17-C18
25	l	5003	LHG	C13-C14-C15-C16
25	a	5001	LHG	C12-C13-C14-C15
25	M	5001	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	2	5004	LHG	O1-C1-C2-C3
25	B	5004	LHG	O1-C1-C2-C3
25	b	5004	LHG	O1-C1-C2-C3
25	A	5005	LHG	O1-C1-C2-C3
25	l	5004	LHG	O1-C1-C2-C3
25	0	5004	LHG	O1-C1-C2-C3
24	a	4001	BCR	C21-C22-C23-C24
24	B	4010	BCR	C21-C22-C23-C24
24	A	4008	BCR	C21-C22-C23-C24
24	1	4003	BCR	C11-C12-C13-C14
24	1	4003	BCR	C21-C22-C23-C24
24	0	4022	BCR	C11-C12-C13-C14
24	0	4022	BCR	C21-C22-C23-C24
24	J	4013	BCR	C7-C8-C9-C10
24	K	4001	BCR	C11-C12-C13-C14
30	b	4011	ECH	C11-C12-C13-C14
24	A	4003	BCR	C11-C12-C13-C14
24	j	4013	BCR	C21-C22-C23-C24
24	b	4005	BCR	C21-C22-C23-C24
24	a	4003	BCR	C11-C12-C13-C14
24	a	4003	BCR	C21-C22-C23-C24
30	b	4006	ECH	C21-C22-C23-C24
24	l	4019	BCR	C21-C22-C23-C24
24	L	4019	BCR	C21-C22-C23-C24
24	A	4019	BCR	C17-C18-C19-C20
30	i	4020	ECH	C21-C22-C23-C24
24	1	4019	BCR	C21-C22-C23-C24
24	a	4012	BCR	C11-C12-C13-C14
24	2	4004	BCR	C21-C22-C23-C24
21	2	1229	CLA	C3-C5-C6-C7
21	A	1133	CLA	C3-C5-C6-C7
21	A	1114	CLA	C15-C16-C17-C18
21	B	1217	CLA	C5-C6-C7-C8
21	1	1115	CLA	C8-C10-C11-C12
21	2	1205	CLA	C10-C11-C12-C13
21	1	1140	CLA	C13-C15-C16-C17
35	F	6001	LMT	C2-C3-C4-C5
26	2	5005	LMG	C13-C14-C15-C16
25	a	5003	LHG	C13-C14-C15-C16
25	l	5004	LHG	C13-C14-C15-C16
25	0	5004	LHG	C11-C12-C13-C14
26	K	5009	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	1	5003	LHG	C7-C8-C9-C10
25	A	5006	LHG	C23-C24-C25-C26
21	B	1230	CLA	O1D-CGD-O2D-CED
21	b	1209	CLA	O1D-CGD-O2D-CED
25	l	5001	LHG	C11-C12-C13-C14
25	a	5005	LHG	C18-C19-C20-C21
25	A	5003	LHG	C13-C14-C15-C16
25	L	5005	LHG	C34-C35-C36-C37
31	L	5002	SQD	C34-C35-C36-C37
25	0	5002	LHG	C13-C14-C15-C16
25	0	5002	LHG	C28-C29-C30-C31
25	a	5001	LHG	C28-C29-C30-C31
25	0	5004	LHG	C26-C27-C28-C29
21	A	1123	CLA	O1A-CGA-O2A-C1
21	1	1011	CLA	C16-C17-C18-C19
21	1	1011	CLA	C16-C17-C18-C20
21	1	1122	CLA	C11-C12-C13-C15
21	2	1237	CLA	C16-C17-C18-C20
21	1	1134	CLA	C16-C17-C18-C20
21	A	1110	CLA	C16-C17-C18-C19
21	2	1223	CLA	C6-C7-C8-C9
21	b	1212	CLA	C16-C17-C18-C20
21	B	1209	CLA	C16-C17-C18-C19
21	a	1140	CLA	C16-C17-C18-C19
21	a	1140	CLA	C16-C17-C18-C20
21	2	1021	CLA	C16-C17-C18-C19
21	a	1012	CLA	C16-C17-C18-C19
21	1	1121	CLA	C6-C7-C8-C10
21	2	1202	CLA	C16-C17-C18-C19
21	a	1117	CLA	C16-C17-C18-C19
21	a	1117	CLA	C16-C17-C18-C20
21	B	1203	CLA	C16-C17-C18-C19
21	A	1125	CLA	C16-C17-C18-C19
21	A	1120	CLA	C16-C17-C18-C19
31	0	5005	SQD	O5-C1-O6-C44
21	2	1214	CLA	C5-C6-C7-C8
21	B	1217	CLA	C8-C10-C11-C12
21	b	1224	CLA	C10-C11-C12-C13
21	a	1106	CLA	C8-C10-C11-C12
21	0	1503	CLA	C8-C10-C11-C12
21	B	1207	CLA	O1D-CGD-O2D-CED
25	M	5001	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	M	5001	LHG	C31-C32-C33-C34
31	F	5001	SQD	C14-C15-C16-C17
25	l	5001	LHG	C11-C10-C9-C8
25	b	5004	LHG	C30-C31-C32-C33
35	L	6001	LMT	C6-C7-C8-C9
26	B	5005	LMG	C39-C40-C41-C42
35	L	6001	LMT	C1-C2-C3-C4
35	F	6001	LMT	O5'-C5'-C6'-O6'
21	b	1212	CLA	O1D-CGD-O2D-CED
21	A	1133	CLA	O1D-CGD-O2D-CED
25	F	5002	LHG	C11-C12-C13-C14
25	A	5003	LHG	C9-C10-C11-C12
26	A	5002	LMG	C37-C38-C39-C40
25	l	5003	LHG	C11-C12-C13-C14
25	0	5004	LHG	C11-C10-C9-C8
25	0	5004	LHG	C7-C8-C9-C10
21	2	1237	CLA	C13-C15-C16-C17
21	1	1116	CLA	C13-C15-C16-C17
21	1	1012	CLA	C8-C10-C11-C12
21	B	1210	CLA	O1A-CGA-O2A-C1
25	1	5001	LHG	C11-C12-C13-C14
25	F	5002	LHG	C13-C14-C15-C16
25	l	5001	LHG	C30-C31-C32-C33
25	A	5001	LHG	C13-C14-C15-C16
31	b	5006	SQD	C26-C27-C28-C29
25	L	5005	LHG	C27-C28-C29-C30
25	0	5002	LHG	C34-C35-C36-C37
31	L	5001	SQD	C13-C14-C15-C16
21	b	1228	CLA	C3-C5-C6-C7
21	A	1122	CLA	C3-C5-C6-C7
21	b	1210	CLA	CBA-CGA-O2A-C1
25	A	5003	LHG	C34-C35-C36-C37
25	A	5006	LHG	C16-C17-C18-C19
21	A	1111	CLA	O1D-CGD-O2D-CED
21	b	1210	CLA	O1D-CGD-O2D-CED
21	1	1011	CLA	C3A-C2A-CAA-CBA
21	B	1213	CLA	C3A-C2A-CAA-CBA
21	a	1121	CLA	C3A-C2A-CAA-CBA
21	1	1104	CLA	C3A-C2A-CAA-CBA
21	b	1022	CLA	C3A-C2A-CAA-CBA
21	a	1107	CLA	C3A-C2A-CAA-CBA
21	a	1122	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	L	1503	CLA	C3A-C2A-CAA-CBA
21	1	1107	CLA	C3A-C2A-CAA-CBA
21	b	1228	CLA	C3A-C2A-CAA-CBA
21	b	1234	CLA	C3A-C2A-CAA-CBA
21	A	1121	CLA	C3A-C2A-CAA-CBA
21	a	1113	CLA	C3A-C2A-CAA-CBA
21	B	1210	CLA	C3A-C2A-CAA-CBA
21	B	1234	CLA	C3A-C2A-CAA-CBA
21	1	1135	CLA	C3A-C2A-CAA-CBA
21	A	1135	CLA	C3A-C2A-CAA-CBA
21	A	1104	CLA	C3A-C2A-CAA-CBA
21	2	1219	CLA	C3A-C2A-CAA-CBA
21	a	1104	CLA	C3A-C2A-CAA-CBA
21	A	1134	CLA	C3A-C2A-CAA-CBA
21	A	1107	CLA	C3A-C2A-CAA-CBA
21	b	1210	CLA	C3A-C2A-CAA-CBA
21	A	1125	CLA	C3A-C2A-CAA-CBA
21	1	1108	CLA	C3A-C2A-CAA-CBA
21	a	1134	CLA	C3A-C2A-CAA-CBA
21	a	1135	CLA	C3A-C2A-CAA-CBA
21	b	1213	CLA	C3A-C2A-CAA-CBA
21	a	1108	CLA	C3A-C2A-CAA-CBA
21	b	1222	CLA	C13-C15-C16-C17
21	B	1021	CLA	C5-C6-C7-C8
21	a	1136	CLA	C5-C6-C7-C8
21	1	1120	CLA	C15-C16-C17-C18
21	B	1206	CLA	C13-C15-C16-C17
24	1	4001	BCR	C13-C14-C15-C16
24	1	4003	BCR	C13-C14-C15-C16
24	a	4002	BCR	C13-C14-C15-C16
35	L	6001	LMT	C2-C1-O1'-C1'
26	0	5001	LMG	C21-C22-C23-C24
25	M	5001	LHG	C30-C31-C32-C33
25	1	5003	LHG	C10-C11-C12-C13
25	a	5007	LHG	C11-C12-C13-C14
25	A	5005	LHG	C31-C32-C33-C34
25	l	5003	LHG	C28-C29-C30-C31
21	b	1234	CLA	O1D-CGD-O2D-CED
21	b	1226	CLA	O1A-CGA-O2A-C1
21	1	1133	CLA	O1A-CGA-O2A-C1
21	B	1221	CLA	O1A-CGA-O2A-C1
21	A	1114	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	b	1216	CLA	C16-C17-C18-C19
21	1	1013	CLA	C16-C17-C18-C19
21	A	1116	CLA	C16-C17-C18-C20
21	1	1127	CLA	C16-C17-C18-C19
21	2	1226	CLA	C6-C7-C8-C9
21	A	1103	CLA	C16-C17-C18-C19
21	a	1132	CLA	C16-C17-C18-C19
21	a	1132	CLA	C16-C17-C18-C20
21	B	1209	CLA	C16-C17-C18-C20
21	B	1228	CLA	C16-C17-C18-C19
21	A	1135	CLA	C16-C17-C18-C19
21	J	1303	CLA	C16-C17-C18-C20
21	a	1801	CLA	C6-C7-C8-C9
21	b	1218	CLA	C16-C17-C18-C19
21	A	1107	CLA	C16-C17-C18-C20
21	1	1140	CLA	C16-C17-C18-C20
21	A	1140	CLA	C16-C17-C18-C19
21	A	1102	CLA	C16-C17-C18-C20
25	1	5002	LHG	C26-C27-C28-C29
25	A	5003	LHG	C28-C29-C30-C31
25	L	5005	LHG	C33-C34-C35-C36
31	L	5002	SQD	C30-C31-C32-C33
25	0	5004	LHG	C29-C30-C31-C32
21	A	1110	CLA	O1D-CGD-O2D-CED
21	1	1129	CLA	O1D-CGD-O2D-CED
21	a	1108	CLA	O1D-CGD-O2D-CED
26	0	5001	LMG	C22-C23-C24-C25
25	A	5003	LHG	C33-C34-C35-C36
25	A	5006	LHG	C9-C10-C11-C12
25	1	5005	LHG	C12-C13-C14-C15
21	1	1117	CLA	O1D-CGD-O2D-CED
21	a	1101	CLA	C3-C5-C6-C7
21	a	1013	CLA	C3-C5-C6-C7
21	1	1501	CLA	C3-C5-C6-C7
21	b	1204	CLA	C3-C5-C6-C7
21	a	1135	CLA	C3-C5-C6-C7
25	A	5001	LHG	C28-C29-C30-C31
25	1	5007	LHG	C16-C17-C18-C19
21	a	1118	CLA	O1A-CGA-O2A-C1
21	a	1135	CLA	O1A-CGA-O2A-C1
21	b	1236	CLA	C5-C6-C7-C8
21	B	1240	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	a	1132	CLA	C4-C3-C5-C6
21	1	1123	CLA	C4-C3-C5-C6
21	A	1117	CLA	C4-C3-C5-C6
21	1	1122	CLA	CBA-CGA-O2A-C1
21	2	1230	CLA	CBA-CGA-O2A-C1
21	1	1119	CLA	CBA-CGA-O2A-C1
21	B	1240	CLA	C2-C3-C5-C6
21	a	1132	CLA	C2-C3-C5-C6
21	B	1212	CLA	C2-C3-C5-C6
21	1	1123	CLA	C2-C3-C5-C6
21	A	1117	CLA	C2-C3-C5-C6
21	l	1502	CLA	C2-C3-C5-C6
26	1	5004	LMG	C11-C10-O7-C8
25	A	5001	LHG	C8-C7-O7-C5
31	0	5005	SQD	C8-C7-O47-C45
26	1	5004	LMG	C21-C22-C23-C24
25	M	5001	LHG	O1-C1-C2-O2
25	2	5004	LHG	O1-C1-C2-O2
25	B	5004	LHG	O1-C1-C2-O2
25	1	5001	LHG	O1-C1-C2-O2
25	F	5002	LHG	O1-C1-C2-O2
25	A	5007	LHG	O1-C1-C2-O2
25	b	5004	LHG	O1-C1-C2-O2
25	1	5003	LHG	O1-C1-C2-O2
25	A	5006	LHG	O1-C1-C2-O2
25	A	5005	LHG	O1-C1-C2-O2
25	1	5005	LHG	O1-C1-C2-O2
25	l	5003	LHG	O1-C1-C2-O2
25	a	5001	LHG	O1-C1-C2-O2
25	0	5004	LHG	O1-C1-C2-O2
25	l	5002	LHG	C25-C26-C27-C28
25	M	5001	LHG	C11-C10-C9-C8
25	M	5001	LHG	C25-C26-C27-C28
25	a	5003	LHG	C11-C12-C13-C14
26	a	5002	LMG	C39-C40-C41-C42
25	0	5002	LHG	C11-C12-C13-C14
25	l	5003	LHG	C11-C10-C9-C8
21	a	1102	CLA	O1A-CGA-O2A-C1
21	2	1237	CLA	C16-C17-C18-C19
21	A	1127	CLA	C16-C17-C18-C20
31	b	5006	SQD	C12-C13-C14-C15
31	L	5001	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	M	5001	LHG	O2-C2-C3-O3
21	a	1122	CLA	C5-C6-C7-C8
25	M	5001	LHG	C11-C12-C13-C14
25	b	5004	LHG	C11-C12-C13-C14
25	a	5003	LHG	C10-C11-C12-C13
37	L	5004	DGD	CCA-CDA-CEA-CFA
21	1	1112	CLA	O1A-CGA-O2A-C1
21	2	1216	CLA	O1A-CGA-O2A-C1
21	1	1137	CLA	O1A-CGA-O2A-C1
21	A	1137	CLA	O1A-CGA-O2A-C1
21	A	1120	CLA	O1A-CGA-O2A-C1
21	B	1237	CLA	C5-C6-C7-C8
21	a	1103	CLA	C10-C11-C12-C13
25	M	5001	LHG	C1-C2-C3-O3
25	M	5001	LHG	C13-C14-C15-C16
25	A	5007	LHG	C11-C12-C13-C14
26	1	5002	LMG	C36-C37-C38-C39
25	b	5004	LHG	C10-C11-C12-C13
26	K	5009	LMG	C40-C41-C42-C43
25	a	5003	LHG	C34-C35-C36-C37
31	b	5006	SQD	C16-C17-C18-C19
26	B	5005	LMG	C11-C12-C13-C14
26	1	5004	LMG	O9-C10-O7-C8
31	0	5005	SQD	O49-C7-O47-C45
21	b	1235	CLA	C2-C1-O2A-CGA
21	B	1220	CLA	C2-C1-O2A-CGA
21	2	1236	CLA	C2-C1-O2A-CGA
21	B	1216	CLA	C2-C1-O2A-CGA
21	a	1101	CLA	C2-C1-O2A-CGA
21	k	1401	CLA	C2-C1-O2A-CGA
21	B	1023	CLA	C2-C1-O2A-CGA
21	a	1122	CLA	C2-C1-O2A-CGA
21	a	1127	CLA	C2-C1-O2A-CGA
21	1	1107	CLA	C2-C1-O2A-CGA
21	B	1230	CLA	C2-C1-O2A-CGA
21	1	1105	CLA	C2-C1-O2A-CGA
21	a	1109	CLA	C2-C1-O2A-CGA
21	b	1236	CLA	C2-C1-O2A-CGA
21	0	1503	CLA	C2-C1-O2A-CGA
21	B	1218	CLA	C2-C1-O2A-CGA
21	A	1125	CLA	C2-C1-O2A-CGA
21	A	1013	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	a	1137	CLA	C2-C1-O2A-CGA
21	A	1118	CLA	C2-C1-O2A-CGA
25	A	5001	LHG	C24-C25-C26-C27
25	a	5007	LHG	C28-C29-C30-C31
25	l	5003	LHG	C10-C11-C12-C13
25	a	5001	LHG	C9-C10-C11-C12
26	A	5004	LMG	O6-C5-C6-O5
21	1	1134	CLA	C10-C11-C12-C13
21	B	1231	CLA	C10-C11-C12-C13
21	a	1103	CLA	C15-C16-C17-C18
21	A	1122	CLA	C8-C10-C11-C12
21	A	1136	CLA	C8-C10-C11-C12
21	2	1204	CLA	C5-C6-C7-C8
21	A	1119	CLA	C13-C15-C16-C17
21	b	1209	CLA	C13-C15-C16-C17
21	a	1118	CLA	C8-C10-C11-C12
21	a	1135	CLA	C5-C6-C7-C8
34	j	4015	ZEX	C21-C26-C27-C28
21	b	1210	CLA	O1A-CGA-O2A-C1
25	2	5004	LHG	C11-C10-C9-C8
26	B	5002	LMG	C32-C33-C34-C35
31	B	5008	SQD	C30-C31-C32-C33
25	1	5003	LHG	C11-C12-C13-C14
31	L	5002	SQD	C11-C12-C13-C14
25	A	5005	LHG	C11-C12-C13-C14
25	l	5003	LHG	C34-C35-C36-C37
21	B	1204	CLA	C16-C17-C18-C20
21	1	1121	CLA	C6-C7-C8-C9
21	J	1302	CLA	C16-C17-C18-C20
25	1	5001	LHG	C23-C24-C25-C26
24	a	4001	BCR	C23-C24-C25-C26
24	B	4010	BCR	C23-C24-C25-C26
24	B	4010	BCR	C23-C24-C25-C30
28	B	4011	45D	C03-C07-C19-C23
28	B	4011	45D	C15-C07-C19-C23
24	1	4007	BCR	C23-C24-C25-C26
24	A	4008	BCR	C23-C24-C25-C30
24	A	4012	BCR	C1-C6-C7-C8
24	A	4012	BCR	C23-C24-C25-C26
24	A	4012	BCR	C23-C24-C25-C30
24	1	4003	BCR	C5-C6-C7-C8
24	l	4022	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	k	4001	BCR	C23-C24-C25-C26
24	k	4001	BCR	C23-C24-C25-C30
24	2	4018	BCR	C5-C6-C7-C8
36	I	4020	EQ3	C1-C6-C7-C8
24	0	4022	BCR	C1-C6-C7-C8
24	0	4022	BCR	C5-C6-C7-C8
24	J	4013	BCR	C5-C6-C7-C8
24	1	4002	BCR	C1-C6-C7-C8
24	1	4002	BCR	C5-C6-C7-C8
24	1	4002	BCR	C23-C24-C25-C26
24	1	4002	BCR	C23-C24-C25-C30
24	2	4011	BCR	C23-C24-C25-C26
24	2	4011	BCR	C23-C24-C25-C30
24	B	4005	BCR	C1-C6-C7-C8
24	B	4005	BCR	C5-C6-C7-C8
24	2	4005	BCR	C1-C6-C7-C8
24	2	4005	BCR	C5-C6-C7-C8
24	0	4019	BCR	C23-C24-C25-C30
24	K	4001	BCR	C5-C6-C7-C8
30	M	4021	ECH	C5-C6-C7-C8
30	b	4011	ECH	C5-C6-C7-C8
30	b	4011	ECH	C23-C24-C25-C26
21	A	1135	CLA	C3-C5-C6-C7
24	A	4002	BCR	C5-C6-C7-C8
24	A	4003	BCR	C5-C6-C7-C8
30	B	4006	ECH	C23-C24-C25-C26
24	b	4005	BCR	C5-C6-C7-C8
30	b	4006	ECH	C5-C6-C7-C8
24	l	4019	BCR	C23-C24-C25-C30
24	1	4012	BCR	C1-C6-C7-C8
24	1	4012	BCR	C5-C6-C7-C8
24	L	4019	BCR	C23-C24-C25-C26
24	L	4019	BCR	C23-C24-C25-C30
24	a	4007	BCR	C23-C24-C25-C26
24	a	4007	BCR	C23-C24-C25-C30
30	m	4021	ECH	C5-C6-C7-C8
30	m	4021	ECH	C23-C24-C25-C30
24	L	4022	BCR	C5-C6-C7-C8
24	1	4019	BCR	C1-C6-C7-C8
24	a	4012	BCR	C5-C6-C7-C8
25	1	5003	LHG	C25-C26-C27-C28
25	A	5005	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	0	5004	LHG	C33-C34-C35-C36
21	b	1222	CLA	CBA-CGA-O2A-C1
21	K	1401	CLA	CBA-CGA-O2A-C1
21	K	1402	CLA	CBA-CGA-O2A-C1
21	2	1201	CLA	C8-C10-C11-C12
21	2	1225	CLA	C15-C16-C17-C18
21	2	1238	CLA	C13-C15-C16-C17
21	a	1106	CLA	C15-C16-C17-C18
21	b	1212	CLA	C15-C16-C17-C18
21	B	1209	CLA	C5-C6-C7-C8
21	b	1236	CLA	C15-C16-C17-C18
21	2	1205	CLA	C5-C6-C7-C8
21	0	1501	CLA	C10-C11-C12-C13
21	a	1104	CLA	C8-C10-C11-C12
21	B	1205	CLA	C13-C15-C16-C17
21	A	1127	CLA	C15-C16-C17-C18
21	1	1128	CLA	C5-C6-C7-C8
25	0	5002	LHG	C8-C7-O7-C5
25	a	5001	LHG	C8-C7-O7-C5
26	K	5009	LMG	C33-C34-C35-C36
25	B	5004	LHG	C28-C29-C30-C31
21	a	1110	CLA	C11-C12-C13-C14
21	2	1228	CLA	C2A-CAA-CBA-CGA
25	A	5006	LHG	C35-C36-C37-C38
21	1	1119	CLA	C10-C11-C12-C13
21	B	1239	CLA	C8-C10-C11-C12
21	a	1109	CLA	C15-C16-C17-C18
21	a	1118	CLA	C10-C11-C12-C13
21	b	1021	CLA	O1D-CGD-O2D-CED
31	B	5008	SQD	C12-C13-C14-C15
21	l	1502	CLA	C4-C3-C5-C6
21	A	1139	CLA	C4-C3-C5-C6
21	1	1127	CLA	O1D-CGD-O2D-CED
21	2	1206	CLA	C11-C10-C8-C7
21	1	1122	CLA	C6-C7-C8-C10
21	A	1110	CLA	C12-C13-C15-C16
21	1	1124	CLA	C6-C7-C8-C10
21	b	1222	CLA	C11-C12-C13-C15
21	a	1133	CLA	C11-C12-C13-C15
21	a	1131	CLA	C6-C7-C8-C10
21	a	1123	CLA	C6-C7-C8-C10
21	a	1123	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	A	1112	CLA	C6-C7-C8-C10
21	B	1211	CLA	C6-C7-C8-C10
21	B	1211	CLA	C12-C13-C15-C16
21	a	1132	CLA	C12-C13-C15-C16
21	b	1212	CLA	C12-C13-C15-C16
21	A	1121	CLA	C12-C13-C15-C16
21	F	1301	CLA	C11-C12-C13-C15
21	B	1210	CLA	C2-C3-C5-C6
21	B	1210	CLA	C12-C13-C15-C16
21	2	1205	CLA	C6-C7-C8-C10
21	A	1137	CLA	C11-C12-C13-C15
21	B	1201	CLA	C6-C7-C8-C10
21	B	1229	CLA	C2-C3-C5-C6
21	b	1218	CLA	C11-C10-C8-C7
21	b	1231	CLA	C2-C3-C5-C6
21	b	1231	CLA	C11-C10-C8-C7
21	b	1231	CLA	C11-C12-C13-C15
21	A	1134	CLA	C11-C10-C8-C7
21	b	1204	CLA	C11-C10-C8-C7
22	2	2002	PQN	C21-C22-C23-C25
21	B	1218	CLA	C6-C7-C8-C10
22	A	2001	PQN	C17-C18-C20-C21
21	B	1227	CLA	C2-C3-C5-C6
21	A	1119	CLA	C12-C13-C15-C16
21	b	1209	CLA	C11-C12-C13-C15
21	a	1118	CLA	C12-C13-C15-C16
21	1	1136	CLA	C2-C3-C5-C6
21	2	1203	CLA	C6-C7-C8-C10
21	2	1203	CLA	C11-C10-C8-C7
21	A	1120	CLA	C12-C13-C15-C16
21	b	1023	CLA	C11-C10-C8-C7
21	A	1102	CLA	C6-C7-C8-C10
21	b	1219	CLA	C11-C10-C8-C7
21	b	1232	CLA	C6-C7-C8-C10
21	B	1206	CLA	C6-C7-C8-C10
21	B	1206	CLA	C12-C13-C15-C16
21	A	1127	CLA	C11-C12-C13-C15
22	b	2002	PQN	C17-C18-C20-C21
22	b	2002	PQN	C21-C22-C23-C25
21	1	1122	CLA	O1A-CGA-O2A-C1
21	2	1230	CLA	O1A-CGA-O2A-C1
21	B	1231	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	1	1119	CLA	O1A-CGA-O2A-C1
21	B	1213	CLA	C5-C6-C7-C8
21	1	1104	CLA	C5-C6-C7-C8
21	1	1119	CLA	C13-C15-C16-C17
21	1	1103	CLA	C8-C10-C11-C12
21	a	1012	CLA	C5-C6-C7-C8
21	B	1203	CLA	C5-C6-C7-C8
24	1	4002	BCR	C19-C20-C21-C22
24	B	4017	BCR	C15-C16-C17-C18
28	h	4020	45D	C25-C29-C31-C33
24	1	4019	BCR	C13-C14-C15-C16
24	a	4012	BCR	C19-C20-C21-C22
21	B	1215	CLA	C16-C17-C18-C20
21	2	1202	CLA	C16-C17-C18-C20
21	a	1102	CLA	O1D-CGD-O2D-CED
21	A	1129	CLA	O1D-CGD-O2D-CED
25	0	5004	LHG	O9-C7-O7-C5
26	b	5005	LMG	C28-C29-C30-C31
25	L	5005	LHG	C7-C8-C9-C10
21	A	1116	CLA	CBA-CGA-O2A-C1
21	B	1231	CLA	CBA-CGA-O2A-C1
21	a	1133	CLA	CBA-CGA-O2A-C1
21	2	1226	CLA	CBA-CGA-O2A-C1
21	F	1302	CLA	CBA-CGA-O2A-C1
21	B	1236	CLA	CBA-CGA-O2A-C1
21	A	1011	CLA	CBA-CGA-O2A-C1
21	b	1228	CLA	CBA-CGA-O2A-C1
21	F	1301	CLA	CBA-CGA-O2A-C1
21	A	1106	CLA	CBA-CGA-O2A-C1
21	2	1021	CLA	CBA-CGA-O2A-C1
21	b	1236	CLA	CBA-CGA-O2A-C1
21	b	1230	CLA	CBA-CGA-O2A-C1
21	a	1119	CLA	CBA-CGA-O2A-C1
26	a	5002	LMG	C11-C12-C13-C14
25	B	5006	LHG	C35-C36-C37-C38
21	A	1106	CLA	C2A-CAA-CBA-CGA
21	2	1204	CLA	C2A-CAA-CBA-CGA
21	b	1217	CLA	C2A-CAA-CBA-CGA
21	1	1110	CLA	C2A-CAA-CBA-CGA
21	1	1012	CLA	C2A-CAA-CBA-CGA
21	a	1101	CLA	C15-C16-C17-C18
21	a	1103	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	1137	CLA	C10-C11-C12-C13
35	F	6001	LMT	C6-C7-C8-C9
31	F	5001	SQD	C29-C30-C31-C32
25	A	5001	LHG	C25-C26-C27-C28
25	A	5003	LHG	C10-C11-C12-C13
25	0	5002	LHG	C26-C27-C28-C29
25	1	5005	LHG	C35-C36-C37-C38
21	B	1231	CLA	C13-C15-C16-C17
21	b	1224	CLA	C13-C15-C16-C17
21	2	1225	CLA	C8-C10-C11-C12
21	1	1119	CLA	C15-C16-C17-C18
21	A	1105	CLA	C13-C15-C16-C17
21	J	1303	CLA	C10-C11-C12-C13
21	l	1502	CLA	C13-C15-C16-C17
21	a	1126	CLA	C5-C6-C7-C8
25	2	5004	LHG	C11-C12-C13-C14
25	l	5003	LHG	C26-C27-C28-C29
25	0	5004	LHG	C13-C14-C15-C16
25	0	5004	LHG	C28-C29-C30-C31
35	0	6001	LMT	C4-C5-C6-C7
21	A	1011	CLA	C3-C5-C6-C7
21	A	1102	CLA	C3-C5-C6-C7
25	b	5004	LHG	C9-C10-C11-C12
26	b	5007	LMG	C40-C41-C42-C43
31	L	5001	SQD	C14-C15-C16-C17
21	b	1221	CLA	CBD-CGD-O2D-CED
21	B	1203	CLA	CBA-CGA-O2A-C1
21	1	1132	CLA	C16-C17-C18-C20
21	0	1502	CLA	C16-C17-C18-C19
21	B	1221	CLA	C16-C17-C18-C19
21	B	1239	CLA	C10-C11-C12-C13
21	1	1133	CLA	C13-C15-C16-C17
21	A	1139	CLA	C13-C15-C16-C17
25	F	5002	LHG	C26-C27-C28-C29
25	l	5003	LHG	C30-C31-C32-C33
26	b	5002	LMG	C10-C11-C12-C13
25	A	5005	LHG	C23-C24-C25-C26
26	A	5004	LMG	C11-C10-O7-C8
31	F	5001	SQD	C8-C7-O47-C45
31	B	5008	SQD	C8-C7-O47-C45
25	a	5003	LHG	C8-C7-O7-C5
25	L	5005	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	0	5004	LHG	C8-C7-O7-C5
25	F	5002	LHG	O6-C4-C5-O7
25	1	5005	LHG	O6-C4-C5-O7
24	a	4007	BCR	C10-C11-C12-C13
21	b	1236	CLA	O1D-CGD-O2D-CED
25	B	5004	LHG	C29-C30-C31-C32
25	1	5007	LHG	C12-C13-C14-C15
35	l	6001	LMT	O1'-C1-C2-C3
25	A	5006	LHG	C29-C30-C31-C32
26	2	5002	LMG	C13-C14-C15-C16
21	b	1211	CLA	C13-C15-C16-C17
21	b	1214	CLA	C15-C16-C17-C18
21	B	1225	CLA	C15-C16-C17-C18
21	a	1123	CLA	CBD-CGD-O2D-CED
25	F	5002	LHG	C30-C31-C32-C33
25	1	5007	LHG	C34-C35-C36-C37
31	L	5001	SQD	C15-C16-C17-C18
26	A	5004	LMG	O9-C10-O7-C8
31	F	5001	SQD	O49-C7-O47-C45
25	A	5001	LHG	O9-C7-O7-C5
25	L	5005	LHG	O9-C7-O7-C5
25	0	5002	LHG	O9-C7-O7-C5
21	b	1216	CLA	C3-C5-C6-C7
21	a	1139	CLA	C3-C5-C6-C7
25	A	5001	LHG	C35-C36-C37-C38
26	2	5002	LMG	C36-C37-C38-C39
31	L	5001	SQD	C29-C30-C31-C32
21	a	1135	CLA	C15-C16-C17-C18
25	l	5001	LHG	O7-C5-C6-O8
31	L	5001	SQD	O6-C44-C45-O47
21	B	1214	CLA	C16-C17-C18-C20
21	B	1229	CLA	C16-C17-C18-C19
21	2	1224	CLA	C6-C7-C8-C10
25	l	5002	LHG	C34-C35-C36-C37
25	b	5004	LHG	C28-C29-C30-C31
26	b	5002	LMG	C32-C33-C34-C35
25	A	5003	LHG	C25-C26-C27-C28
25	L	5005	LHG	C28-C29-C30-C31
31	0	5005	SQD	C24-C25-C26-C27
21	B	1201	CLA	C15-C16-C17-C18
21	b	1204	CLA	C5-C6-C7-C8
21	a	1110	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	1140	CLA	C13-C15-C16-C17
21	B	1210	CLA	C4-C3-C5-C6
21	1	1139	CLA	C2-C3-C5-C6
21	a	1101	CLA	C2-C3-C5-C6
21	l	1503	CLA	C2-C3-C5-C6
21	2	1208	CLA	C2-C3-C5-C6
21	f	1302	CLA	C2-C3-C5-C6
21	A	1139	CLA	C2-C3-C5-C6
25	1	5005	LHG	C31-C32-C33-C34
21	A	1012	CLA	C6-C7-C8-C9
21	2	1229	CLA	C14-C13-C15-C16
21	j	1302	CLA	C6-C7-C8-C9
21	b	1211	CLA	C11-C10-C8-C9
21	B	1216	CLA	C11-C12-C13-C14
21	2	1206	CLA	C11-C10-C8-C9
21	a	1121	CLA	C14-C13-C15-C16
21	1	1104	CLA	C11-C12-C13-C14
21	A	1113	CLA	C6-C7-C8-C9
21	a	1133	CLA	C11-C12-C13-C14
21	b	1224	CLA	C11-C12-C13-C14
21	1	1111	CLA	C6-C7-C8-C9
22	B	2002	PQN	C21-C22-C23-C24
21	a	1131	CLA	C11-C12-C13-C14
21	a	1123	CLA	C11-C10-C8-C9
21	A	1112	CLA	C6-C7-C8-C9
21	B	1211	CLA	C6-C7-C8-C9
21	B	1211	CLA	C11-C10-C8-C9
21	B	1211	CLA	C14-C13-C15-C16
21	B	1224	CLA	C6-C7-C8-C9
21	a	1127	CLA	C14-C13-C15-C16
21	a	1132	CLA	C14-C13-C15-C16
21	0	1502	CLA	C14-C13-C15-C16
21	A	1122	CLA	C6-C7-C8-C9
21	l	1501	CLA	C11-C12-C13-C14
21	A	1136	CLA	C14-C13-C15-C16
21	B	1210	CLA	C14-C13-C15-C16
21	b	1226	CLA	C11-C10-C8-C9
21	B	1234	CLA	C11-C12-C13-C14
21	2	1204	CLA	C6-C7-C8-C9
21	A	1104	CLA	C11-C12-C13-C14
21	1	1133	CLA	C6-C7-C8-C9
21	B	1201	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	a	1104	CLA	C6-C7-C8-C9
21	b	1231	CLA	C11-C10-C8-C9
21	b	1231	CLA	C11-C12-C13-C14
21	A	1134	CLA	C11-C10-C8-C9
21	b	1204	CLA	C11-C10-C8-C9
21	b	1237	CLA	C6-C7-C8-C9
21	a	1117	CLA	C11-C10-C8-C9
22	A	2001	PQN	C19-C18-C20-C21
21	2	1218	CLA	C11-C12-C13-C14
21	A	1131	CLA	C14-C13-C15-C16
21	A	1128	CLA	C6-C7-C8-C9
21	A	1119	CLA	C11-C12-C13-C14
21	A	1119	CLA	C14-C13-C15-C16
21	b	1209	CLA	C11-C12-C13-C14
21	A	1139	CLA	C6-C7-C8-C9
21	1	1136	CLA	C11-C12-C13-C14
21	A	1120	CLA	C6-C7-C8-C9
21	1	1012	CLA	C11-C10-C8-C9
21	b	1023	CLA	C11-C10-C8-C9
21	A	1124	CLA	C14-C13-C15-C16
21	B	1206	CLA	C6-C7-C8-C9
21	A	1127	CLA	C11-C12-C13-C14
21	a	1119	CLA	C14-C13-C15-C16
21	A	1013	CLA	O1D-CGD-O2D-CED
31	B	5008	SQD	C14-C15-C16-C17
21	A	1108	CLA	O1D-CGD-O2D-CED
21	A	1116	CLA	C2A-CAA-CBA-CGA
21	A	1110	CLA	C2A-CAA-CBA-CGA
21	B	1236	CLA	C2A-CAA-CBA-CGA
21	A	1138	CLA	C2A-CAA-CBA-CGA
21	B	1022	CLA	C2A-CAA-CBA-CGA
25	L	5005	LHG	C17-C18-C19-C20
31	L	5002	SQD	C29-C30-C31-C32
26	b	5007	LMG	O6-C5-C6-O5
34	j	4015	ZEX	C27-C28-C29-C39
21	B	1211	CLA	C15-C16-C17-C18
21	l	1501	CLA	C13-C15-C16-C17
25	a	5003	LHG	C31-C32-C33-C34
31	f	5001	SQD	C32-C33-C34-C35
25	0	5002	LHG	C33-C34-C35-C36
34	j	4015	ZEX	C27-C28-C29-C30
24	A	4012	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	A	4003	BCR	C17-C18-C19-C20
24	b	4005	BCR	C17-C18-C19-C20
35	F	6001	LMT	C1-C2-C3-C4
21	b	1222	CLA	O1A-CGA-O2A-C1
21	2	1226	CLA	O1A-CGA-O2A-C1
21	B	1236	CLA	O1A-CGA-O2A-C1
21	K	1401	CLA	O1A-CGA-O2A-C1
21	F	1301	CLA	O1A-CGA-O2A-C1
21	K	1402	CLA	O1A-CGA-O2A-C1
21	b	1220	CLA	C1A-C2A-CAA-CBA
21	B	1220	CLA	C1A-C2A-CAA-CBA
21	A	1801	CLA	C1A-C2A-CAA-CBA
21	b	1202	CLA	C1A-C2A-CAA-CBA
21	a	1116	CLA	C1A-C2A-CAA-CBA
21	2	1236	CLA	C1A-C2A-CAA-CBA
21	2	1230	CLA	C1A-C2A-CAA-CBA
21	A	1116	CLA	C1A-C2A-CAA-CBA
21	1	1127	CLA	C1A-C2A-CAA-CBA
21	k	1401	CLA	C1A-C2A-CAA-CBA
21	1	1104	CLA	C1A-C2A-CAA-CBA
21	1	1134	CLA	C1A-C2A-CAA-CBA
21	2	1216	CLA	C1A-C2A-CAA-CBA
21	b	1240	CLA	C1A-C2A-CAA-CBA
21	1	1113	CLA	C1A-C2A-CAA-CBA
21	b	1224	CLA	C1A-C2A-CAA-CBA
21	1	1111	CLA	C1A-C2A-CAA-CBA
21	a	1107	CLA	C1A-C2A-CAA-CBA
21	B	1236	CLA	C1A-C2A-CAA-CBA
21	a	1106	CLA	C1A-C2A-CAA-CBA
21	b	1212	CLA	C1A-C2A-CAA-CBA
21	A	1105	CLA	C1A-C2A-CAA-CBA
21	B	1202	CLA	C1A-C2A-CAA-CBA
21	b	1234	CLA	C1A-C2A-CAA-CBA
21	a	1111	CLA	C1A-C2A-CAA-CBA
21	1	1130	CLA	C1A-C2A-CAA-CBA
21	l	1501	CLA	C1A-C2A-CAA-CBA
21	a	1113	CLA	C1A-C2A-CAA-CBA
21	a	1129	CLA	C1A-C2A-CAA-CBA
21	2	1208	CLA	C1A-C2A-CAA-CBA
21	a	1130	CLA	C1A-C2A-CAA-CBA
21	1	1135	CLA	C1A-C2A-CAA-CBA
21	A	1135	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	1104	CLA	C1A-C2A-CAA-CBA
21	b	1217	CLA	C1A-C2A-CAA-CBA
21	b	1236	CLA	C1A-C2A-CAA-CBA
21	A	1137	CLA	C1A-C2A-CAA-CBA
21	a	1104	CLA	C1A-C2A-CAA-CBA
21	A	1111	CLA	C1A-C2A-CAA-CBA
21	2	1202	CLA	C1A-C2A-CAA-CBA
21	6	1302	CLA	C1A-C2A-CAA-CBA
21	2	1222	CLA	C1A-C2A-CAA-CBA
21	1	1109	CLA	C1A-C2A-CAA-CBA
21	2	1218	CLA	C1A-C2A-CAA-CBA
21	1	1114	CLA	C1A-C2A-CAA-CBA
21	1	1102	CLA	C1A-C2A-CAA-CBA
21	A	1125	CLA	C1A-C2A-CAA-CBA
21	A	1120	CLA	C1A-C2A-CAA-CBA
21	b	1230	CLA	C1A-C2A-CAA-CBA
21	b	1219	CLA	C1A-C2A-CAA-CBA
21	1	1120	CLA	C1A-C2A-CAA-CBA
21	a	1135	CLA	C1A-C2A-CAA-CBA
21	B	1204	CLA	C16-C17-C18-C19
21	b	1211	CLA	C16-C17-C18-C19
21	B	1208	CLA	C16-C17-C18-C20
21	1	1132	CLA	C16-C17-C18-C19
21	b	1021	CLA	C16-C17-C18-C19
21	1	1133	CLA	C16-C17-C18-C20
21	b	1231	CLA	C16-C17-C18-C19
31	B	5008	SQD	O49-C7-O47-C45
25	a	5001	LHG	O9-C7-O7-C5
25	l	5002	LHG	C28-C29-C30-C31
25	M	5001	LHG	C27-C28-C29-C30
25	1	5003	LHG	C24-C25-C26-C27
25	1	5003	LHG	C28-C29-C30-C31
25	B	5006	LHG	C13-C14-C15-C16
25	B	5006	LHG	C17-C18-C19-C20
26	a	5004	LMG	C15-C16-C17-C18
25	A	5005	LHG	C28-C29-C30-C31
24	b	4017	BCR	C15-C16-C17-C18
24	B	4005	BCR	C15-C16-C17-C18
24	K	4001	BCR	C13-C14-C15-C16
24	7	4013	BCR	C19-C20-C21-C22
24	b	4018	BCR	C19-C20-C21-C22
21	j	1302	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	1	1134	CLA	C13-C15-C16-C17
21	a	1104	CLA	C13-C15-C16-C17
21	2	1239	CLA	C10-C11-C12-C13
21	1	1117	CLA	C5-C6-C7-C8
21	a	1126	CLA	C10-C11-C12-C13
25	2	5004	LHG	C30-C31-C32-C33
25	a	5003	LHG	C33-C34-C35-C36
26	B	5002	LMG	O6-C5-C6-O5
26	b	5002	LMG	O6-C5-C6-O5
21	a	1140	CLA	C3-C5-C6-C7
21	K	1401	CLA	O1D-CGD-O2D-CED
21	B	1205	CLA	O1D-CGD-O2D-CED
25	M	5001	LHG	C34-C35-C36-C37
21	a	1133	CLA	O1A-CGA-O2A-C1
21	A	1011	CLA	O1A-CGA-O2A-C1
21	2	1206	CLA	C10-C11-C12-C13
21	1	1101	CLA	C8-C10-C11-C12
21	A	1135	CLA	C13-C15-C16-C17
21	1	1126	CLA	C15-C16-C17-C18
21	a	1125	CLA	C15-C16-C17-C18
21	a	1111	CLA	CBA-CGA-O2A-C1
25	l	5002	LHG	O6-C4-C5-C6
25	1	5001	LHG	O6-C4-C5-C6
25	F	5002	LHG	O6-C4-C5-C6
25	A	5007	LHG	O6-C4-C5-C6
25	b	5004	LHG	O6-C4-C5-C6
25	0	5002	LHG	C31-C32-C33-C34
25	a	5001	LHG	C25-C26-C27-C28
26	K	5009	LMG	C10-C11-C12-C13
21	B	1222	CLA	O1D-CGD-O2D-CED
31	f	5001	SQD	C10-C11-C12-C13
25	A	5005	LHG	C17-C18-C19-C20
26	B	5005	LMG	C14-C15-C16-C17
21	a	1128	CLA	C15-C16-C17-C18
21	b	1210	CLA	C15-C16-C17-C18
21	1	1134	CLA	C16-C17-C18-C19
21	A	1132	CLA	C16-C17-C18-C20
21	A	1013	CLA	C16-C17-C18-C20
25	l	5001	LHG	C28-C29-C30-C31
31	b	5006	SQD	C13-C14-C15-C16
21	b	1216	CLA	O1D-CGD-O2D-CED
21	2	1224	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	1128	CLA	CBA-CGA-O2A-C1
21	b	1231	CLA	C4-C3-C5-C6
21	B	1227	CLA	C4-C3-C5-C6
21	1	1136	CLA	C4-C3-C5-C6
25	M	5001	LHG	C12-C13-C14-C15
31	L	5002	SQD	C31-C32-C33-C34
25	B	5006	LHG	C9-C10-C11-C12
21	a	1115	CLA	C15-C16-C17-C18
21	B	1208	CLA	C8-C10-C11-C12
21	b	1232	CLA	C13-C15-C16-C17
37	L	5004	DGD	C7B-C8B-C9B-CAB
25	b	5004	LHG	C25-C26-C27-C28
31	B	5008	SQD	C33-C34-C35-C36
25	a	5003	LHG	C26-C27-C28-C29
25	L	5005	LHG	C12-C13-C14-C15
25	B	5006	LHG	C27-C28-C29-C30
35	0	6001	LMT	C7-C8-C9-C10
21	b	1228	CLA	O1A-CGA-O2A-C1
21	b	1230	CLA	O1A-CGA-O2A-C1
25	a	5003	LHG	C11-C10-C9-C8
21	A	1117	CLA	C16-C17-C18-C19
21	2	1203	CLA	C16-C17-C18-C19
25	1	5001	LHG	C4-C5-C6-O8
25	A	5007	LHG	C4-C5-C6-O8
26	1	5002	LMG	C7-C8-C9-O8
25	b	5004	LHG	C4-C5-C6-O8
31	b	5006	SQD	O6-C44-C45-C46
25	1	5007	LHG	C33-C34-C35-C36
25	L	5005	LHG	C4-C5-C6-O8
25	1	5005	LHG	C4-C5-C6-O8
31	L	5001	SQD	C44-C45-C46-O48
31	0	5005	SQD	O6-C44-C45-C46
21	b	1216	CLA	C8-C10-C11-C12
21	a	1109	CLA	C8-C10-C11-C12
21	2	1214	CLA	C11-C12-C13-C14
21	A	1116	CLA	O1A-CGA-O2A-C1
21	2	1021	CLA	O1A-CGA-O2A-C1
26	A	5008	LMG	C8-C7-O1-C1
26	b	5007	LMG	C8-C7-O1-C1
31	0	5005	SQD	C45-C44-O6-C1
25	2	5004	LHG	C26-C27-C28-C29
35	1	6001	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	a	5007	LHG	C29-C30-C31-C32
21	j	1302	CLA	C15-C16-C17-C18
21	A	1118	CLA	C13-C15-C16-C17
26	A	5004	LMG	C16-C17-C18-C19
25	A	5001	LHG	C33-C34-C35-C36
31	L	5002	SQD	C25-C26-C27-C28
26	a	5002	LMG	C10-C11-C12-C13
21	F	1302	CLA	O1A-CGA-O2A-C1
21	A	1128	CLA	O1A-CGA-O2A-C1
21	B	1203	CLA	O1A-CGA-O2A-C1
25	1	5005	LHG	C32-C33-C34-C35
35	1	6001	LMT	C4B-C5B-C6B-O6B
25	a	5003	LHG	O1-C1-C2-O2
25	a	5007	LHG	O1-C1-C2-O2
25	B	5006	LHG	O1-C1-C2-O2
25	l	5004	LHG	O1-C1-C2-O2
31	0	5005	SQD	C32-C33-C34-C35
21	a	1133	CLA	C10-C11-C12-C13
21	a	1111	CLA	O1A-CGA-O2A-C1
21	b	1236	CLA	O1A-CGA-O2A-C1
21	a	1119	CLA	O1A-CGA-O2A-C1
26	1	5002	LMG	C10-C11-C12-C13
25	a	5003	LHG	C9-C10-C11-C12
25	l	5004	LHG	C8-C7-O7-C5
25	a	5003	LHG	C19-C20-C21-C22
21	2	1223	CLA	O1D-CGD-O2D-CED
21	A	1106	CLA	O1D-CGD-O2D-CED
21	1	1133	CLA	O1D-CGD-O2D-CED
21	a	1121	CLA	C13-C15-C16-C17
21	a	1121	CLA	C15-C16-C17-C18
21	1	1103	CLA	C10-C11-C12-C13
21	a	1012	CLA	C13-C15-C16-C17
22	b	2002	PQN	C20-C21-C22-C23
26	a	5002	LMG	O6-C5-C6-O5
21	1	1131	CLA	C4-C3-C5-C6
21	b	1202	CLA	C4-C3-C5-C6
21	1	1119	CLA	C4-C3-C5-C6
21	B	1202	CLA	C4-C3-C5-C6
25	2	5004	LHG	C28-C29-C30-C31
25	F	5002	LHG	C19-C20-C21-C22
25	l	5001	LHG	C9-C10-C11-C12
21	B	1224	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	A	1120	CLA	C16-C17-C18-C20
21	B	1211	CLA	CBA-CGA-O2A-C1
21	0	1503	CLA	CBA-CGA-O2A-C1
21	a	1125	CLA	CBA-CGA-O2A-C1
21	a	1131	CLA	CBD-CGD-O2D-CED
21	1	1116	CLA	C5-C6-C7-C8
21	a	1111	CLA	C8-C10-C11-C12
21	a	1130	CLA	C8-C10-C11-C12
21	2	1203	CLA	C15-C16-C17-C18
21	2	1221	CLA	C5-C6-C7-C8
21	A	1127	CLA	C5-C6-C7-C8
25	A	5007	LHG	C28-C29-C30-C31
26	A	5008	LMG	C12-C13-C14-C15
31	L	5002	SQD	C16-C17-C18-C19
25	F	5002	LHG	C6-C5-O7-C7
26	a	5004	LMG	C7-C8-O7-C10
21	B	1228	CLA	O1D-CGD-O2D-CED
21	2	1023	CLA	C2A-CAA-CBA-CGA
21	B	1215	CLA	C15-C16-C17-C18
21	2	1203	CLA	C8-C10-C11-C12
21	a	1102	CLA	C2-C1-O2A-CGA
21	b	1225	CLA	C2-C1-O2A-CGA
21	a	1121	CLA	C2-C1-O2A-CGA
21	b	1203	CLA	C2-C1-O2A-CGA
21	B	1207	CLA	C2-C1-O2A-CGA
21	2	1225	CLA	C2-C1-O2A-CGA
21	b	1022	CLA	C2-C1-O2A-CGA
21	1	1119	CLA	C2-C1-O2A-CGA
21	A	1129	CLA	C2-C1-O2A-CGA
21	1	1110	CLA	C2-C1-O2A-CGA
31	L	5002	SQD	C32-C33-C34-C35
25	1	5005	LHG	C33-C34-C35-C36
21	1	1013	CLA	O1D-CGD-O2D-CED
25	1	5007	LHG	C11-C12-C13-C14
21	a	1121	CLA	C5-C6-C7-C8
21	A	1113	CLA	C10-C11-C12-C13
21	B	1230	CLA	C8-C10-C11-C12
21	A	1125	CLA	C10-C11-C12-C13
25	1	5001	LHG	C35-C36-C37-C38
31	b	5006	SQD	C31-C32-C33-C34
31	L	5002	SQD	C24-C25-C26-C27
25	1	5004	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
21	1	1116	CLA	CBA-CGA-O2A-C1
21	0	1502	CLA	CBA-CGA-O2A-C1
21	B	1222	CLA	CBA-CGA-O2A-C1
21	1	1129	CLA	CBA-CGA-O2A-C1
21	2	1203	CLA	CBA-CGA-O2A-C1
25	a	5001	LHG	O6-C4-C5-O7
21	A	1011	CLA	CAA-CBA-CGA-O2A
25	a	5003	LHG	O8-C23-C24-C25
21	B	1221	CLA	C16-C17-C18-C20
21	b	1221	CLA	C16-C17-C18-C19
25	2	5004	LHG	C29-C30-C31-C32
25	A	5001	LHG	C34-C35-C36-C37
25	a	5007	LHG	C19-C20-C21-C22
21	l	1501	CLA	C10-C11-C12-C13
21	A	1109	CLA	C8-C10-C11-C12
25	A	5003	LHG	C19-C20-C21-C22
25	A	5005	LHG	C35-C36-C37-C38
25	0	5004	LHG	C30-C31-C32-C33
25	1	5003	LHG	C29-C30-C31-C32
26	A	5002	LMG	C28-C29-C30-C31
21	1	1101	CLA	C13-C15-C16-C17
21	B	1201	CLA	C13-C15-C16-C17
21	A	1129	CLA	C5-C6-C7-C8
21	b	1209	CLA	C8-C10-C11-C12
21	b	1023	CLA	C10-C11-C12-C13
37	L	5004	DGD	C2E-C1E-O5D-C6D
26	K	5009	LMG	C2-C1-O1-C7
31	f	5001	SQD	C2-C1-O6-C44
31	0	5005	SQD	C2-C1-O6-C44
25	a	5001	LHG	O7-C5-C6-O8
25	A	5001	LHG	C19-C20-C21-C22
31	b	5006	SQD	C10-C11-C12-C13
25	0	5004	LHG	C9-C10-C11-C12
25	a	5003	LHG	O9-C7-O7-C5
21	B	1226	CLA	C5-C6-C7-C8
21	B	1209	CLA	C10-C11-C12-C13
21	b	1218	CLA	C8-C10-C11-C12
21	2	1239	CLA	C13-C15-C16-C17
21	a	1125	CLA	O1A-CGA-O2A-C1
21	B	1214	CLA	C16-C17-C18-C19
21	b	1203	CLA	C16-C17-C18-C20
26	A	5008	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	a	5003	LHG	C28-C29-C30-C31
25	l	5003	LHG	C35-C36-C37-C38
21	b	1204	CLA	C4-C3-C5-C6
21	K	1402	CLA	C4-C3-C5-C6
21	A	1108	CLA	C4-C3-C5-C6
21	A	1012	CLA	C11-C10-C8-C7
21	A	1012	CLA	C11-C12-C13-C15
21	b	1235	CLA	C6-C7-C8-C10
21	2	1229	CLA	C12-C13-C15-C16
21	1	1131	CLA	C2-C3-C5-C6
21	j	1302	CLA	C6-C7-C8-C10
21	j	1302	CLA	C11-C10-C8-C7
21	b	1202	CLA	C2-C3-C5-C6
21	b	1211	CLA	C6-C7-C8-C10
21	b	1211	CLA	C11-C12-C13-C15
21	B	1213	CLA	C11-C12-C13-C15
21	B	1216	CLA	C2-C3-C5-C6
21	1	1013	CLA	C6-C7-C8-C10
21	a	1121	CLA	C12-C13-C15-C16
21	A	1126	CLA	C12-C13-C15-C16
21	B	1217	CLA	C12-C13-C15-C16
21	1	1127	CLA	C12-C13-C15-C16
21	a	1011	CLA	C12-C13-C15-C16
21	2	1210	CLA	C6-C7-C8-C10
21	1	1104	CLA	C12-C13-C15-C16
21	b	1240	CLA	C12-C13-C15-C16
21	B	1023	CLA	C11-C12-C13-C15
21	b	1224	CLA	C11-C12-C13-C15
21	1	1111	CLA	C6-C7-C8-C10
21	1	1111	CLA	C11-C10-C8-C7
22	B	2002	PQN	C21-C22-C23-C25
21	a	1131	CLA	C11-C12-C13-C15
21	F	1302	CLA	C11-C12-C13-C15
21	A	1112	CLA	C11-C10-C8-C7
21	a	1122	CLA	C12-C13-C15-C16
21	B	1239	CLA	C11-C12-C13-C15
21	a	1127	CLA	C6-C7-C8-C10
21	a	1127	CLA	C12-C13-C15-C16
21	b	1212	CLA	C11-C10-C8-C7
21	a	1103	CLA	C6-C7-C8-C10
21	a	1103	CLA	C11-C10-C8-C7
21	B	1226	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	b	1206	CLA	C12-C13-C15-C16
21	B	1215	CLA	C6-C7-C8-C10
21	1	1118	CLA	C11-C12-C13-C15
21	l	1503	CLA	C6-C7-C8-C10
21	1	1103	CLA	C12-C13-C15-C16
21	0	1502	CLA	C12-C13-C15-C16
21	B	1202	CLA	C2-C3-C5-C6
21	A	1122	CLA	C6-C7-C8-C10
21	A	1121	CLA	C6-C7-C8-C10
21	l	1501	CLA	C12-C13-C15-C16
21	b	1021	CLA	C11-C10-C8-C7
21	b	1226	CLA	C11-C10-C8-C7
21	1	1123	CLA	C11-C10-C8-C7
21	a	1130	CLA	C11-C12-C13-C15
21	b	1201	CLA	C11-C10-C8-C7
21	A	1135	CLA	C11-C10-C8-C7
21	A	1104	CLA	C11-C12-C13-C15
21	a	1112	CLA	C11-C10-C8-C7
21	a	1112	CLA	C12-C13-C15-C16
21	J	1303	CLA	C6-C7-C8-C10
21	J	1303	CLA	C11-C12-C13-C15
21	1	1133	CLA	C11-C12-C13-C15
21	2	1205	CLA	C11-C10-C8-C7
21	0	1501	CLA	C12-C13-C15-C16
21	a	1012	CLA	C6-C7-C8-C10
21	a	1012	CLA	C11-C10-C8-C7
21	b	1218	CLA	C12-C13-C15-C16
21	a	1104	CLA	C11-C12-C13-C15
21	A	1129	CLA	C11-C10-C8-C7
22	a	2001	PQN	C21-C22-C23-C25
21	b	1215	CLA	C11-C10-C8-C7
21	L	1501	CLA	C11-C12-C13-C15
21	0	1503	CLA	C11-C12-C13-C15
21	f	1302	CLA	C6-C7-C8-C10
21	A	1107	CLA	C11-C12-C13-C15
21	b	1237	CLA	C6-C7-C8-C10
21	B	1235	CLA	C12-C13-C15-C16
22	2	2002	PQN	C17-C18-C20-C21
21	1	1126	CLA	C6-C7-C8-C10
21	2	1023	CLA	C11-C10-C8-C7
21	a	1117	CLA	C12-C13-C15-C16
22	A	2001	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
21	b	1207	CLA	C6-C7-C8-C10
21	1	1109	CLA	C11-C10-C8-C7
21	1	1109	CLA	C11-C12-C13-C15
21	2	1218	CLA	C11-C10-C8-C7
21	2	1218	CLA	C11-C12-C13-C15
21	A	1131	CLA	C6-C7-C8-C10
21	A	1131	CLA	C11-C10-C8-C7
21	A	1131	CLA	C12-C13-C15-C16
21	A	1128	CLA	C6-C7-C8-C10
21	l	1502	CLA	C12-C13-C15-C16
21	K	1402	CLA	C2-C3-C5-C6
21	a	1110	CLA	C6-C7-C8-C10
21	B	1203	CLA	C11-C10-C8-C7
21	A	1119	CLA	C11-C12-C13-C15
21	A	1139	CLA	C6-C7-C8-C10
21	A	1139	CLA	C12-C13-C15-C16
21	1	1136	CLA	C11-C12-C13-C15
21	2	1239	CLA	C6-C7-C8-C10
21	b	1023	CLA	C6-C7-C8-C10
21	b	1219	CLA	C6-C7-C8-C10
21	1	1120	CLA	C12-C13-C15-C16
21	A	1124	CLA	C11-C10-C8-C7
21	1	1117	CLA	C12-C13-C15-C16
21	a	1119	CLA	C12-C13-C15-C16
21	b	1220	CLA	C3-C5-C6-C7
25	1	5007	LHG	C29-C30-C31-C32
21	b	1235	CLA	C6-C7-C8-C9
21	B	1204	CLA	C11-C10-C8-C9
21	1	1131	CLA	C6-C7-C8-C9
21	1	1131	CLA	C14-C13-C15-C16
21	b	1202	CLA	C11-C12-C13-C14
21	b	1211	CLA	C6-C7-C8-C9
21	B	1216	CLA	C14-C13-C15-C16
21	1	1013	CLA	C6-C7-C8-C9
21	a	1121	CLA	C11-C12-C13-C14
21	B	1240	CLA	C11-C10-C8-C9
21	b	1227	CLA	C11-C12-C13-C14
21	1	1127	CLA	C14-C13-C15-C16
21	a	1011	CLA	C11-C10-C8-C9
21	1	1104	CLA	C14-C13-C15-C16
21	B	1231	CLA	C6-C7-C8-C9
21	b	1240	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	1123	CLA	C11-C10-C8-C9
21	1	1111	CLA	C11-C10-C8-C9
21	2	1225	CLA	C6-C7-C8-C9
21	2	1225	CLA	C14-C13-C15-C16
21	B	1239	CLA	C11-C10-C8-C9
21	B	1239	CLA	C11-C12-C13-C14
21	K	1401	CLA	C6-C7-C8-C9
21	a	1128	CLA	C6-C7-C8-C9
21	a	1103	CLA	C6-C7-C8-C9
21	a	1103	CLA	C11-C10-C8-C9
21	a	1103	CLA	C11-C12-C13-C14
21	1	1118	CLA	C11-C12-C13-C14
21	l	1503	CLA	C6-C7-C8-C9
21	L	1502	CLA	C14-C13-C15-C16
21	B	1238	CLA	C11-C10-C8-C9
21	A	1121	CLA	C14-C13-C15-C16
21	B	1209	CLA	C11-C12-C13-C14
21	A	1138	CLA	C11-C10-C8-C9
21	b	1021	CLA	C11-C10-C8-C9
21	b	1021	CLA	C11-C12-C13-C14
21	1	1123	CLA	C11-C10-C8-C9
21	b	1201	CLA	C11-C10-C8-C9
21	A	1135	CLA	C11-C10-C8-C9
22	1	2001	PQN	C21-C22-C23-C24
21	a	1112	CLA	C14-C13-C15-C16
21	J	1303	CLA	C11-C12-C13-C14
21	2	1205	CLA	C11-C10-C8-C9
21	0	1501	CLA	C14-C13-C15-C16
21	A	1132	CLA	C14-C13-C15-C16
21	B	1229	CLA	C6-C7-C8-C9
21	b	1218	CLA	C14-C13-C15-C16
22	a	2001	PQN	C21-C22-C23-C24
21	L	1501	CLA	C11-C12-C13-C14
21	0	1503	CLA	C14-C13-C15-C16
21	f	1302	CLA	C11-C10-C8-C9
21	B	1235	CLA	C14-C13-C15-C16
21	1	1126	CLA	C14-C13-C15-C16
21	2	1023	CLA	C11-C10-C8-C9
21	B	1218	CLA	C11-C10-C8-C9
22	A	2001	PQN	C21-C22-C23-C24
21	b	1207	CLA	C11-C12-C13-C14
21	2	1218	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	1128	CLA	C11-C12-C13-C14
21	l	1502	CLA	C14-C13-C15-C16
21	b	1221	CLA	C6-C7-C8-C9
21	b	1210	CLA	C11-C10-C8-C9
21	A	1139	CLA	C14-C13-C15-C16
21	2	1203	CLA	C14-C13-C15-C16
21	A	1013	CLA	C14-C13-C15-C16
21	b	1223	CLA	C14-C13-C15-C16
21	b	1230	CLA	C11-C10-C8-C9
21	a	1135	CLA	C11-C10-C8-C9
21	l	1117	CLA	C14-C13-C15-C16
21	A	1127	CLA	C14-C13-C15-C16
21	a	1108	CLA	C6-C7-C8-C9
24	a	4001	BCR	C13-C14-C15-C16
25	M	5001	LHG	C14-C15-C16-C17
31	L	5002	SQD	C15-C16-C17-C18
25	B	5006	LHG	C29-C30-C31-C32
21	B	1240	CLA	CBA-CGA-O2A-C1
21	l	1118	CLA	CBA-CGA-O2A-C1
21	B	1214	CLA	C10-C11-C12-C13
21	B	1219	CLA	C10-C11-C12-C13
21	a	1122	CLA	C8-C10-C11-C12
21	2	1238	CLA	C8-C10-C11-C12
25	a	5007	LHG	C26-C27-C28-C29
31	f	5001	SQD	C34-C35-C36-C37
26	a	5002	LMG	C37-C38-C39-C40
25	a	5001	LHG	C35-C36-C37-C38
21	l	1131	CLA	C8-C10-C11-C12
21	a	1115	CLA	C16-C17-C18-C19
21	l	1111	CLA	C16-C17-C18-C20
21	a	1127	CLA	C16-C17-C18-C20
21	A	1013	CLA	C16-C17-C18-C19
31	F	5001	SQD	C35-C36-C37-C38
21	l	1124	CLA	O1D-CGD-O2D-CED
30	B	4006	ECH	C21-C22-C23-C24
24	B	4018	BCR	C21-C22-C23-C24
24	L	4019	BCR	C7-C8-C9-C10
24	B	4004	BCR	C7-C8-C9-C10
25	B	5004	LHG	C9-C10-C11-C12
31	b	5006	SQD	C14-C15-C16-C17
25	B	5006	LHG	C14-C15-C16-C17
21	a	1111	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	2	1208	CLA	C3-C5-C6-C7
21	2	1234	CLA	O1D-CGD-O2D-CED
21	2	1226	CLA	O1D-CGD-O2D-CED
21	2	1237	CLA	C5-C6-C7-C8
21	1	1130	CLA	C5-C6-C7-C8
21	A	1013	CLA	C8-C10-C11-C12
31	f	5001	SQD	C26-C27-C28-C29
25	1	5007	LHG	C25-C26-C27-C28
25	0	5004	LHG	C35-C36-C37-C38
21	a	1127	CLA	CBA-CGA-O2A-C1
25	1	5003	LHG	C35-C36-C37-C38
21	B	1231	CLA	C15-C16-C17-C18
21	B	1230	CLA	C5-C6-C7-C8
21	F	1301	CLA	C10-C11-C12-C13
26	2	5005	LMG	C42-C43-C44-C45
31	b	5006	SQD	C9-C10-C11-C12
31	F	5001	SQD	C17-C18-C19-C20
21	B	1224	CLA	C16-C17-C18-C19
21	B	1216	CLA	C13-C15-C16-C17
21	A	1140	CLA	C15-C16-C17-C18
25	2	5004	LHG	O6-C4-C5-C6
25	1	5005	LHG	O6-C4-C5-C6
25	a	5001	LHG	O6-C4-C5-C6
25	0	5004	LHG	O6-C4-C5-C6
21	1	1140	CLA	C3-C5-C6-C7
25	F	5002	LHG	C25-C26-C27-C28
25	1	5001	LHG	C33-C34-C35-C36
26	K	5009	LMG	C32-C33-C34-C35
21	1	1140	CLA	CBA-CGA-O2A-C1
21	A	1013	CLA	CBA-CGA-O2A-C1
24	2	4018	BCR	C10-C11-C12-C13
21	B	1230	CLA	C13-C15-C16-C17
21	F	1301	CLA	C8-C10-C11-C12
21	b	1202	CLA	O1D-CGD-O2D-CED
21	A	1125	CLA	O1D-CGD-O2D-CED
25	F	5002	LHG	C35-C36-C37-C38
26	1	5002	LMG	C15-C16-C17-C18
21	B	1231	CLA	C4-C3-C5-C6
21	b	1223	CLA	C4-C3-C5-C6
21	b	1214	CLA	C2-C3-C5-C6
21	1	1119	CLA	C2-C3-C5-C6
21	b	1204	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	1108	CLA	C2-C3-C5-C6
26	0	5001	LMG	C28-C29-C30-C31
25	B	5006	LHG	C23-C24-C25-C26
21	1	1111	CLA	C10-C11-C12-C13
21	A	1106	CLA	O1A-CGA-O2A-C1
21	0	1503	CLA	O1A-CGA-O2A-C1
26	b	5007	LMG	C21-C22-C23-C24
21	A	1112	CLA	C16-C17-C18-C20
21	1	1103	CLA	C16-C17-C18-C19
21	0	1503	CLA	C16-C17-C18-C20
21	j	1303	CLA	C6-C7-C8-C10
25	B	5004	LHG	C30-C31-C32-C33
21	2	1229	CLA	C8-C10-C11-C12
21	2	1225	CLA	C13-C15-C16-C17
21	2	1204	CLA	C15-C16-C17-C18
21	b	1237	CLA	C13-C15-C16-C17
21	B	1226	CLA	CBA-CGA-O2A-C1
21	2	1217	CLA	CBA-CGA-O2A-C1
21	A	1117	CLA	CBA-CGA-O2A-C1
25	1	5007	LHG	C24-C23-O8-C6
26	0	5001	LMG	C18-C19-C20-C21
21	2	1210	CLA	C2C-C3C-CAC-CBC
26	1	5004	LMG	C16-C17-C18-C19
26	a	5002	LMG	C34-C35-C36-C37
21	A	1801	CLA	C3A-C2A-CAA-CBA
21	1	1127	CLA	C3A-C2A-CAA-CBA
21	1	1119	CLA	C3A-C2A-CAA-CBA
21	A	1105	CLA	C3A-C2A-CAA-CBA
21	A	1106	CLA	C3A-C2A-CAA-CBA
21	B	1218	CLA	C3A-C2A-CAA-CBA
21	A	1140	CLA	C3A-C2A-CAA-CBA
21	1	1128	CLA	C3A-C2A-CAA-CBA
26	0	5001	LMG	C24-C25-C26-C27
26	b	5002	LMG	C11-C12-C13-C14
25	1	5003	LHG	C33-C34-C35-C36
25	a	5003	LHG	C30-C31-C32-C33
31	L	5002	SQD	C35-C36-C37-C38
31	0	5005	SQD	C29-C30-C31-C32
34	j	4015	ZEX	C29-C30-C31-C32
28	B	4011	45D	C25-C29-C31-C33
24	h	4018	BCR	C19-C20-C21-C22
24	1	4002	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	A	4003	BCR	C15-C16-C17-C18
24	j	4013	BCR	C19-C20-C21-C22
24	b	4005	BCR	C13-C14-C15-C16
24	1	4012	BCR	C13-C14-C15-C16
25	2	5004	LHG	C35-C36-C37-C38
31	F	5001	SQD	C13-C14-C15-C16
26	1	5002	LMG	C30-C31-C32-C33
21	B	1222	CLA	O1A-CGA-O2A-C1
26	A	5004	LMG	C14-C15-C16-C17
31	F	5001	SQD	C9-C10-C11-C12
26	B	5002	LMG	C15-C16-C17-C18
25	1	5007	LHG	C13-C14-C15-C16
21	b	1240	CLA	C16-C17-C18-C19
21	B	1229	CLA	C16-C17-C18-C20
21	1	1011	CLA	CBA-CGA-O2A-C1
21	a	1801	CLA	CBA-CGA-O2A-C1
21	A	1140	CLA	CBA-CGA-O2A-C1
25	1	5001	LHG	C25-C26-C27-C28
21	B	1220	CLA	C5-C6-C7-C8
21	a	1116	CLA	C5-C6-C7-C8
21	B	1223	CLA	C13-C15-C16-C17
26	0	5001	LMG	C7-C8-C9-O8
25	l	5001	LHG	C4-C5-C6-O8
31	b	5006	SQD	C44-C45-C46-O48
25	a	5007	LHG	C4-C5-C6-O8
25	A	5006	LHG	C4-C5-C6-O8
25	A	5005	LHG	C4-C5-C6-O8
25	a	5001	LHG	C4-C5-C6-O8
25	l	5002	LHG	C31-C32-C33-C34
25	l	5003	LHG	C27-C28-C29-C30
25	b	5004	LHG	C7-C8-C9-C10
35	1	6001	LMT	C2-C3-C4-C5
31	L	5002	SQD	C11-C10-C9-C8
25	A	5005	LHG	C33-C34-C35-C36
21	1	1127	CLA	C13-C15-C16-C17
22	a	2001	PQN	C25-C26-C27-C28
31	f	5001	SQD	C25-C26-C27-C28
21	j	1302	CLA	C3-C5-C6-C7
21	0	1502	CLA	C3-C5-C6-C7
25	F	5002	LHG	C10-C11-C12-C13
25	a	5005	LHG	C35-C36-C37-C38
35	0	6001	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	0	1502	CLA	O1A-CGA-O2A-C1
21	B	1214	CLA	C4-C3-C5-C6
21	1	1132	CLA	C4-C3-C5-C6
21	A	1122	CLA	C4-C3-C5-C6
21	J	1303	CLA	C4-C3-C5-C6
21	2	1023	CLA	C4-C3-C5-C6
21	b	1210	CLA	C4-C3-C5-C6
21	A	1118	CLA	CBA-CGA-O2A-C1
21	A	1801	CLA	C16-C17-C18-C20
21	A	1112	CLA	C16-C17-C18-C19
21	b	1228	CLA	C16-C17-C18-C19
21	j	1303	CLA	C6-C7-C8-C9
26	a	5002	LMG	C42-C43-C44-C45
26	2	5002	LMG	C32-C33-C34-C35
25	a	5007	LHG	C11-C10-C9-C8
21	B	1227	CLA	C5-C6-C7-C8
25	A	5003	LHG	C4-O6-P-O3
25	1	5007	LHG	C10-C11-C12-C13
21	b	1221	CLA	O1D-CGD-O2D-CED
21	b	1211	CLA	C3-C5-C6-C7
21	A	1104	CLA	C3-C5-C6-C7
21	1	1119	CLA	C2A-CAA-CBA-CGA
21	a	1113	CLA	C2A-CAA-CBA-CGA
21	B	1228	CLA	C2A-CAA-CBA-CGA
25	l	5002	LHG	O1-C1-C2-O2
25	l	5001	LHG	O1-C1-C2-O2
21	A	1103	CLA	C10-C11-C12-C13
37	L	5004	DGD	CFB-CGB-CHB-CIB
31	L	5002	SQD	C27-C28-C29-C30
25	B	5004	LHG	O6-C4-C5-O7
25	A	5007	LHG	O6-C4-C5-O7
25	l	5001	LHG	O6-C4-C5-O7
25	b	5004	LHG	O6-C4-C5-O7
21	B	1240	CLA	O1A-CGA-O2A-C1
21	1	1116	CLA	O1A-CGA-O2A-C1
21	B	1211	CLA	O1A-CGA-O2A-C1
21	1	1129	CLA	O1A-CGA-O2A-C1
21	2	1203	CLA	O1A-CGA-O2A-C1
21	a	1115	CLA	C16-C17-C18-C20
21	b	1203	CLA	C16-C17-C18-C19
21	A	1104	CLA	C16-C17-C18-C19
21	A	1135	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	1221	CLA	C8-C10-C11-C12
21	a	1126	CLA	C15-C16-C17-C18
31	F	5001	SQD	C11-C10-C9-C8
31	B	5008	SQD	O47-C7-C8-C9
25	0	5004	LHG	O8-C23-C24-C25
31	F	5001	SQD	C16-C17-C18-C19
21	a	1123	CLA	O1D-CGD-O2D-CED
21	B	1239	CLA	C15-C16-C17-C18
21	A	1137	CLA	C15-C16-C17-C18
21	1	1118	CLA	O1A-CGA-O2A-C1
25	1	5001	LHG	C26-C27-C28-C29
26	b	5007	LMG	C24-C25-C26-C27
26	0	5001	LMG	O7-C8-C9-O8
25	A	5007	LHG	O7-C5-C6-O8
26	b	5005	LMG	O7-C8-C9-O8
25	A	5001	LHG	O7-C5-C6-O8
31	b	5006	SQD	O6-C44-C45-O47
25	A	5005	LHG	O7-C5-C6-O8
25	1	5003	LHG	O7-C5-C6-O8
21	1	1127	CLA	CBA-CGA-O2A-C1
21	A	1131	CLA	CBA-CGA-O2A-C1
21	6	1301	CLA	CBA-CGA-O2A-C1
21	b	1229	CLA	C5-C6-C7-C8
21	B	1218	CLA	C15-C16-C17-C18
21	b	1210	CLA	C13-C15-C16-C17
21	a	1119	CLA	C5-C6-C7-C8
25	2	5004	LHG	C15-C16-C17-C18
25	A	5006	LHG	C32-C33-C34-C35
21	A	1103	CLA	C16-C17-C18-C20
21	b	1021	CLA	C16-C17-C18-C20
35	0	6001	LMT	C3-C4-C5-C6
31	0	5005	SQD	C30-C31-C32-C33
31	F	5001	SQD	O5-C1-O6-C44
21	A	1107	CLA	C8-C10-C11-C12
25	6	5001	LHG	C1-C2-C3-O3
25	1	5004	LHG	C1-C2-C3-O3
25	0	5004	LHG	C1-C2-C3-O3
25	a	5005	LHG	C19-C20-C21-C22
21	2	1214	CLA	C4-C3-C5-C6
21	L	1501	CLA	C4-C3-C5-C6
21	a	1126	CLA	C4-C3-C5-C6
21	2	1210	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	L	1502	CLA	C2-C1-O2A-CGA
21	2	1207	CLA	C2-C1-O2A-CGA
21	2	1208	CLA	C2-C1-O2A-CGA
21	a	1801	CLA	C2-C1-O2A-CGA
21	A	1131	CLA	C2-C1-O2A-CGA
21	b	1235	CLA	C11-C10-C8-C9
21	b	1235	CLA	C11-C12-C13-C14
21	2	1229	CLA	C6-C7-C8-C9
21	A	1801	CLA	C6-C7-C8-C9
21	B	1219	CLA	C11-C12-C13-C14
21	b	1203	CLA	C6-C7-C8-C9
21	2	1201	CLA	C14-C13-C15-C16
21	B	1231	CLA	C11-C10-C8-C9
21	b	1222	CLA	C6-C7-C8-C9
21	A	1123	CLA	C11-C12-C13-C14
21	2	1225	CLA	C11-C12-C13-C14
21	F	1302	CLA	C14-C13-C15-C16
21	B	1224	CLA	C11-C12-C13-C14
21	B	1208	CLA	C11-C10-C8-C9
21	B	1226	CLA	C11-C10-C8-C9
21	0	1502	CLA	C11-C10-C8-C9
21	B	1230	CLA	C11-C12-C13-C14
21	B	1228	CLA	C11-C10-C8-C9
21	b	1021	CLA	C14-C13-C15-C16
21	b	1226	CLA	C11-C12-C13-C14
21	J	1303	CLA	C6-C7-C8-C9
21	1	1133	CLA	C11-C12-C13-C14
21	b	1218	CLA	C6-C7-C8-C9
21	a	1104	CLA	C11-C12-C13-C14
21	f	1302	CLA	C11-C12-C13-C14
21	B	1235	CLA	C11-C10-C8-C9
21	A	1115	CLA	C11-C12-C13-C14
21	1	1109	CLA	C11-C12-C13-C14
21	A	1117	CLA	C11-C10-C8-C9
21	B	1205	CLA	C11-C12-C13-C14
21	b	1219	CLA	C6-C7-C8-C9
21	A	1124	CLA	C11-C10-C8-C9
21	A	1109	CLA	C11-C12-C13-C14
21	J	1302	CLA	C11-C12-C13-C14
21	a	1138	CLA	C14-C13-C15-C16
21	1	1128	CLA	C11-C12-C13-C14
21	a	1126	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	5004	LHG	C11-C10-C9-C8
21	b	1022	CLA	C15-C16-C17-C18
21	a	1132	CLA	C13-C15-C16-C17
21	a	1140	CLA	C5-C6-C7-C8
25	F	5002	LHG	C2-C3-O3-P
25	1	5005	LHG	C2-C3-O3-P
25	0	5004	LHG	C2-C3-O3-P
21	A	1013	CLA	O1A-CGA-O2A-C1
25	b	5004	LHG	C31-C32-C33-C34
31	b	5006	SQD	C25-C26-C27-C28
21	A	1131	CLA	C2A-CAA-CBA-CGA
21	a	1110	CLA	C2A-CAA-CBA-CGA
21	a	1121	CLA	C16-C17-C18-C20
21	1	1111	CLA	C16-C17-C18-C19
21	a	1128	CLA	C16-C17-C18-C20
21	0	1502	CLA	C16-C17-C18-C20
21	2	1021	CLA	C16-C17-C18-C20
21	A	1132	CLA	C16-C17-C18-C19
21	K	1402	CLA	C16-C17-C18-C19
21	1	1011	CLA	C3-C5-C6-C7
24	a	4001	BCR	C23-C24-C25-C30
24	6	4016	BCR	C1-C6-C7-C8
24	6	4016	BCR	C5-C6-C7-C8
24	1	4003	BCR	C23-C24-C25-C30
24	f	4016	BCR	C1-C6-C7-C8
24	f	4016	BCR	C5-C6-C7-C8
24	l	4022	BCR	C5-C6-C7-C8
24	k	4001	BCR	C1-C6-C7-C8
24	k	4001	BCR	C5-C6-C7-C8
24	h	4018	BCR	C5-C6-C7-C8
24	b	4010	BCR	C23-C24-C25-C26
24	b	4010	BCR	C23-C24-C25-C30
24	2	4011	BCR	C1-C6-C7-C8
24	2	4011	BCR	C5-C6-C7-C8
24	B	4005	BCR	C23-C24-C25-C26
24	B	4005	BCR	C23-C24-C25-C30
24	a	4008	BCR	C1-C6-C7-C8
24	a	4008	BCR	C5-C6-C7-C8
21	1	1130	CLA	C3-C5-C6-C7
30	M	4021	ECH	C23-C24-C25-C30
24	b	4014	BCR	C23-C24-C25-C30
21	a	1012	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	2	4010	BCR	C23-C24-C25-C26
24	2	4010	BCR	C23-C24-C25-C30
24	a	4003	BCR	C23-C24-C25-C26
30	b	4006	ECH	C23-C24-C25-C26
24	2	4017	BCR	C5-C6-C7-C8
28	h	4020	45D	C03-C07-C19-C23
28	h	4020	45D	C15-C07-C19-C23
28	h	4020	45D	C04-C08-C20-C24
24	1	4012	BCR	C23-C24-C25-C26
24	1	4012	BCR	C23-C24-C25-C30
30	2	4006	ECH	C5-C6-C7-C8
30	2	4006	ECH	C23-C24-C25-C30
21	B	1216	CLA	C5-C6-C7-C8
21	2	1201	CLA	C15-C16-C17-C18
21	B	1226	CLA	C15-C16-C17-C18
21	A	1105	CLA	C5-C6-C7-C8
21	1	1103	CLA	C13-C15-C16-C17
21	b	1210	CLA	C5-C6-C7-C8
25	a	5005	LHG	C16-C17-C18-C19
25	a	5001	LHG	O8-C23-C24-C25
28	h	4020	45D	C20-C24-C26-C28
21	A	1107	CLA	CBA-CGA-O2A-C1
21	2	1224	CLA	CBA-CGA-O2A-C1
24	6	4016	BCR	C17-C18-C19-C20
24	B	4014	BCR	C7-C8-C9-C10
24	A	4003	BCR	C7-C8-C9-C10
24	1	4008	BCR	C17-C18-C19-C20
28	h	4020	45D	C32-C34-C36-C38
30	2	4006	ECH	C7-C8-C9-C10
24	B	4004	BCR	C17-C18-C19-C20
21	A	1012	CLA	C10-C11-C12-C13
21	1	1115	CLA	C15-C16-C17-C18
21	1	1121	CLA	C5-C6-C7-C8
21	2	1023	CLA	C10-C11-C12-C13
21	1	1109	CLA	C15-C16-C17-C18
21	b	1230	CLA	C10-C11-C12-C13
21	1	1120	CLA	C13-C15-C16-C17
22	b	2002	PQN	C23-C25-C26-C27
25	M	5001	LHG	C19-C20-C21-C22
31	0	5005	SQD	C27-C28-C29-C30
26	0	5001	LMG	O9-C10-O7-C8
21	A	1129	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	1	1011	CLA	O1A-CGA-O2A-C1
21	b	1229	CLA	C2C-C3C-CAC-CBC
21	a	1121	CLA	C16-C17-C18-C19
21	b	1221	CLA	C16-C17-C18-C20
21	2	1221	CLA	C16-C17-C18-C20
21	b	1212	CLA	C3-C5-C6-C7
25	A	5005	LHG	C10-C11-C12-C13
21	1	1013	CLA	C5-C6-C7-C8
21	l	1501	CLA	C8-C10-C11-C12
21	A	1111	CLA	C13-C15-C16-C17
25	A	5007	LHG	C9-C10-C11-C12
25	a	5005	LHG	C26-C27-C28-C29
21	B	1224	CLA	C15-C16-C17-C18
21	B	1230	CLA	C10-C11-C12-C13
25	A	5001	LHG	O6-C4-C5-C6
25	B	5006	LHG	O6-C4-C5-C6
25	l	5003	LHG	O6-C4-C5-C6
25	a	5005	LHG	C10-C11-C12-C13
21	B	1214	CLA	C6-C7-C8-C10
21	b	1235	CLA	C11-C10-C8-C7
21	b	1235	CLA	C11-C12-C13-C15
21	2	1229	CLA	C6-C7-C8-C10
21	1	1131	CLA	C12-C13-C15-C16
21	b	1202	CLA	C11-C12-C13-C15
21	A	1114	CLA	C12-C13-C15-C16
21	A	1101	CLA	C11-C12-C13-C15
21	B	1216	CLA	C6-C7-C8-C10
21	B	1216	CLA	C12-C13-C15-C16
21	2	1206	CLA	C12-C13-C15-C16
21	A	1126	CLA	C11-C12-C13-C15
21	B	1240	CLA	C11-C10-C8-C7
21	b	1214	CLA	C6-C7-C8-C10
21	B	1207	CLA	C11-C12-C13-C15
21	a	1011	CLA	C11-C10-C8-C7
21	A	1113	CLA	C12-C13-C15-C16
21	B	1231	CLA	C2-C3-C5-C6
21	B	1231	CLA	C6-C7-C8-C10
21	B	1231	CLA	C11-C10-C8-C7
21	A	1123	CLA	C11-C10-C8-C7
21	2	1225	CLA	C6-C7-C8-C10
21	2	1225	CLA	C12-C13-C15-C16
21	1	1116	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	F	1302	CLA	C12-C13-C15-C16
21	A	1103	CLA	C11-C12-C13-C15
21	A	1103	CLA	C12-C13-C15-C16
21	a	1122	CLA	C11-C10-C8-C7
21	B	1239	CLA	C6-C7-C8-C10
21	B	1224	CLA	C11-C12-C13-C15
21	K	1401	CLA	C6-C7-C8-C10
21	a	1128	CLA	C6-C7-C8-C10
21	a	1128	CLA	C11-C12-C13-C15
21	B	1208	CLA	C11-C10-C8-C7
21	a	1103	CLA	C11-C12-C13-C15
21	1	1132	CLA	C2-C3-C5-C6
21	B	1226	CLA	C11-C10-C8-C7
21	B	1226	CLA	C12-C13-C15-C16
21	b	1206	CLA	C6-C7-C8-C10
21	b	1206	CLA	C11-C10-C8-C7
21	l	1503	CLA	C12-C13-C15-C16
21	0	1502	CLA	C11-C10-C8-C7
21	L	1502	CLA	C12-C13-C15-C16
21	B	1230	CLA	C6-C7-C8-C10
21	B	1238	CLA	C11-C10-C8-C7
21	B	1209	CLA	C11-C10-C8-C7
21	B	1209	CLA	C11-C12-C13-C15
21	a	1111	CLA	C11-C12-C13-C15
21	A	1106	CLA	C12-C13-C15-C16
21	A	1138	CLA	C11-C10-C8-C7
21	A	1138	CLA	C11-C12-C13-C15
21	A	1136	CLA	C11-C12-C13-C15
21	b	1021	CLA	C12-C13-C15-C16
21	2	1021	CLA	C6-C7-C8-C10
21	a	1109	CLA	C12-C13-C15-C16
22	1	2001	PQN	C21-C22-C23-C25
21	1	1133	CLA	C11-C10-C8-C7
21	A	1132	CLA	C12-C13-C15-C16
21	B	1229	CLA	C6-C7-C8-C10
21	a	1104	CLA	C11-C10-C8-C7
21	L	1501	CLA	C2-C3-C5-C6
21	L	1501	CLA	C12-C13-C15-C16
21	f	1302	CLA	C11-C10-C8-C7
21	A	1107	CLA	C12-C13-C15-C16
21	B	1235	CLA	C11-C10-C8-C7
21	1	1126	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	1218	CLA	C11-C10-C8-C7
21	b	1207	CLA	C11-C12-C13-C15
21	a	1110	CLA	C11-C10-C8-C7
21	b	1221	CLA	C6-C7-C8-C10
21	b	1210	CLA	C2-C3-C5-C6
21	b	1209	CLA	C6-C7-C8-C10
21	a	1118	CLA	C11-C10-C8-C7
21	A	1140	CLA	C11-C12-C13-C15
21	1	1012	CLA	C11-C12-C13-C15
21	b	1230	CLA	C11-C10-C8-C7
21	A	1102	CLA	C11-C10-C8-C7
21	A	1124	CLA	C11-C12-C13-C15
21	A	1109	CLA	C11-C12-C13-C15
21	J	1302	CLA	C11-C12-C13-C15
21	a	1135	CLA	C11-C10-C8-C7
21	A	1127	CLA	C12-C13-C15-C16
21	a	1126	CLA	C11-C10-C8-C7
21	a	1119	CLA	C11-C10-C8-C7
26	2	5002	LMG	C24-C25-C26-C27
21	A	1123	CLA	C13-C15-C16-C17
21	A	1125	CLA	C13-C15-C16-C17
21	A	1102	CLA	C5-C6-C7-C8
24	B	4010	BCR	C19-C20-C21-C22
24	h	4018	BCR	C9-C10-C11-C12
24	2	4005	BCR	C13-C14-C15-C16
24	2	4017	BCR	C19-C20-C21-C22
21	a	1127	CLA	C16-C17-C18-C19
21	1	1103	CLA	C16-C17-C18-C20
21	A	1133	CLA	C16-C17-C18-C19
21	b	1232	CLA	C16-C17-C18-C20
26	B	5002	LMG	C16-C17-C18-C19
25	l	5004	LHG	O9-C7-O7-C5
25	A	5005	LHG	C24-C23-O8-C6
25	A	5003	LHG	C35-C36-C37-C38
21	L	1503	CLA	C13-C15-C16-C17
21	a	1127	CLA	O1A-CGA-O2A-C1
21	a	1129	CLA	C2A-CAA-CBA-CGA
21	b	1201	CLA	C2A-CAA-CBA-CGA
21	1	1801	CLA	C2A-CAA-CBA-CGA
26	0	5001	LMG	C11-C10-O7-C8
21	b	1240	CLA	C5-C6-C7-C8
21	A	1128	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	1	1140	CLA	C15-C16-C17-C18
25	A	5006	LHG	C11-C12-C13-C14
21	B	1231	CLA	C16-C17-C18-C19
21	b	1207	CLA	CBA-CGA-O2A-C1
21	A	1116	CLA	CAA-CBA-CGA-O2A
26	a	5004	LMG	O7-C10-C11-C12
21	2	1224	CLA	CAA-CBA-CGA-O2A
25	1	5001	LHG	C17-C18-C19-C20
25	A	5003	LHG	C31-C32-C33-C34
25	a	5007	LHG	C24-C25-C26-C27
25	l	5004	LHG	C35-C36-C37-C38
25	A	5006	LHG	C24-C25-C26-C27
25	0	5004	LHG	C16-C17-C18-C19
21	A	1113	CLA	C8-C10-C11-C12
21	A	1115	CLA	C10-C11-C12-C13
21	a	1136	CLA	C8-C10-C11-C12
21	A	1801	CLA	CAD-CBD-CGD-O2D
21	1	1124	CLA	CAD-CBD-CGD-O2D
21	2	1216	CLA	CAD-CBD-CGD-O2D
21	2	1226	CLA	CAD-CBD-CGD-O2D
21	A	1103	CLA	CAD-CBD-CGD-O2D
21	B	1202	CLA	CAD-CBD-CGD-O2D
21	2	1217	CLA	CAD-CBD-CGD-O2D
21	a	1124	CLA	CAD-CBD-CGD-O2D
21	K	1402	CLA	CAD-CBD-CGD-O2D
21	a	1137	CLA	CAD-CBD-CGD-O2D
21	A	1102	CLA	CAD-CBD-CGD-O2D
31	b	5006	SQD	C27-C28-C29-C30
21	A	1116	CLA	C13-C15-C16-C17
21	B	1208	CLA	C10-C11-C12-C13
21	1	1109	CLA	C8-C10-C11-C12
35	L	6001	LMT	C4B-C5B-C6B-O6B
26	K	5009	LMG	C30-C31-C32-C33
21	2	1205	CLA	C4-C3-C5-C6
21	A	1012	CLA	C16-C17-C18-C20
37	L	5004	DGD	C2A-C3A-C4A-C5A
25	A	5001	LHG	C17-C18-C19-C20
21	b	1203	CLA	C15-C16-C17-C18
21	b	1219	CLA	C5-C6-C7-C8
21	A	1136	CLA	C2-C3-C5-C6
21	2	1205	CLA	C2-C3-C5-C6
31	b	5006	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	l	5002	LHG	C4-C5-C6-O8
26	A	5008	LMG	C7-C8-C9-O8
31	B	5008	SQD	O6-C44-C45-C46
26	A	5002	LMG	O1-C7-C8-C9
21	1	1127	CLA	O1A-CGA-O2A-C1
21	A	1107	CLA	O1A-CGA-O2A-C1
25	1	5007	LHG	O10-C23-O8-C6
31	b	5006	SQD	C18-C19-C20-C21
31	0	5005	SQD	C12-C13-C14-C15
25	1	5001	LHG	O6-C4-C5-O7
25	a	5003	LHG	O6-C4-C5-O7
25	A	5006	LHG	O6-C4-C5-O7
21	b	1225	CLA	C15-C16-C17-C18
22	B	2002	PQN	C15-C16-C17-C18
21	a	1101	CLA	CAA-CBA-CGA-O2A
21	b	1215	CLA	CAA-CBA-CGA-O2A
21	b	1225	CLA	O1D-CGD-O2D-CED
21	a	1131	CLA	O1D-CGD-O2D-CED
31	0	5005	SQD	C18-C19-C20-C21
21	b	1229	CLA	C2A-CAA-CBA-CGA
21	1	1116	CLA	C2A-CAA-CBA-CGA
21	1	1125	CLA	C2A-CAA-CBA-CGA
25	B	5006	LHG	C28-C29-C30-C31
21	a	1011	CLA	C16-C17-C18-C19
21	1	1125	CLA	C16-C17-C18-C19
21	0	1503	CLA	C16-C17-C18-C19
21	B	1021	CLA	C16-C17-C18-C20
21	b	1232	CLA	C16-C17-C18-C19
21	a	1135	CLA	C16-C17-C18-C19
21	a	1135	CLA	C16-C17-C18-C20
21	2	1220	CLA	CHA-CBD-CGD-O1D
21	2	1220	CLA	CHA-CBD-CGD-O2D
21	b	1220	CLA	CHA-CBD-CGD-O1D
21	b	1220	CLA	CHA-CBD-CGD-O2D
21	B	1204	CLA	CHA-CBD-CGD-O2D
21	a	1102	CLA	CHA-CBD-CGD-O1D
21	a	1102	CLA	CHA-CBD-CGD-O2D
21	B	1220	CLA	CHA-CBD-CGD-O1D
21	B	1220	CLA	CHA-CBD-CGD-O2D
21	b	1202	CLA	CHA-CBD-CGD-O1D
21	b	1202	CLA	CHA-CBD-CGD-O2D
21	B	1213	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	B	1213	CLA	CHA-CBD-CGD-O2D
21	B	1240	CLA	CHA-CBD-CGD-O1D
21	B	1240	CLA	CHA-CBD-CGD-O2D
21	2	1230	CLA	CHA-CBD-CGD-O1D
21	2	1230	CLA	CHA-CBD-CGD-O2D
21	1	1127	CLA	CHA-CBD-CGD-O1D
21	1	1127	CLA	CHA-CBD-CGD-O2D
21	2	1210	CLA	CHA-CBD-CGD-O1D
21	1	1134	CLA	CHA-CBD-CGD-O1D
21	1	1134	CLA	CHA-CBD-CGD-O2D
21	A	1113	CLA	CHA-CBD-CGD-O2D
21	1	1113	CLA	CHA-CBD-CGD-O1D
21	1	1113	CLA	CHA-CBD-CGD-O2D
21	A	1123	CLA	CHA-CBD-CGD-O1D
21	A	1123	CLA	CHA-CBD-CGD-O2D
21	B	1211	CLA	CHA-CBD-CGD-O1D
21	8	1402	CLA	CHA-CBD-CGD-O1D
21	1	1137	CLA	CHA-CBD-CGD-O2D
21	a	1128	CLA	CHA-CBD-CGD-O1D
21	a	1128	CLA	CHA-CBD-CGD-O2D
21	a	1103	CLA	CHA-CBD-CGD-O2D
21	B	1226	CLA	CHA-CBD-CGD-O1D
21	B	1226	CLA	CHA-CBD-CGD-O2D
21	1	1103	CLA	CHA-CBD-CGD-O2D
21	B	1212	CLA	CHA-CBD-CGD-O2D
21	B	1209	CLA	CHA-CBD-CGD-O1D
21	1	1501	CLA	CHA-CBD-CGD-O1D
21	1	1501	CLA	CHA-CBD-CGD-O2D
21	A	1106	CLA	CHA-CBD-CGD-O1D
21	b	1226	CLA	CHA-CBD-CGD-O1D
21	b	1226	CLA	CHA-CBD-CGD-O2D
21	2	1205	CLA	CHA-CBD-CGD-O1D
21	2	1205	CLA	CHA-CBD-CGD-O2D
21	A	1111	CLA	CHA-CBD-CGD-O1D
21	A	1111	CLA	CHA-CBD-CGD-O2D
21	2	1202	CLA	CHA-CBD-CGD-O1D
21	2	1202	CLA	CHA-CBD-CGD-O2D
21	b	1237	CLA	CHA-CBD-CGD-O2D
21	B	1221	CLA	CHA-CBD-CGD-O1D
21	2	1023	CLA	CHA-CBD-CGD-O2D
21	B	1218	CLA	CHA-CBD-CGD-O1D
21	B	1218	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	2	1212	CLA	CHA-CBD-CGD-O1D
21	2	1212	CLA	CHA-CBD-CGD-O2D
21	B	1021	CLA	CHA-CBD-CGD-O1D
21	B	1227	CLA	CHA-CBD-CGD-O1D
21	B	1227	CLA	CHA-CBD-CGD-O2D
21	b	1221	CLA	CHA-CBD-CGD-O1D
21	b	1221	CLA	CHA-CBD-CGD-O2D
21	2	1239	CLA	CHA-CBD-CGD-O2D
21	1	1138	CLA	CHA-CBD-CGD-O1D
21	1	1138	CLA	CHA-CBD-CGD-O2D
21	2	1221	CLA	CHA-CBD-CGD-O1D
21	B	1205	CLA	CHA-CBD-CGD-O1D
21	B	1205	CLA	CHA-CBD-CGD-O2D
21	b	1230	CLA	CHA-CBD-CGD-O1D
21	b	1230	CLA	CHA-CBD-CGD-O2D
21	a	1138	CLA	CHA-CBD-CGD-O1D
21	a	1138	CLA	CHA-CBD-CGD-O2D
21	b	1213	CLA	CHA-CBD-CGD-O1D
21	a	1126	CLA	CHA-CBD-CGD-O1D
25	1	5007	LHG	C35-C36-C37-C38
25	A	5006	LHG	C17-C18-C19-C20
21	a	1130	CLA	C3-C5-C6-C7
21	2	1217	CLA	O1A-CGA-O2A-C1
21	1	1140	CLA	O1A-CGA-O2A-C1
21	A	1140	CLA	O1A-CGA-O2A-C1
21	A	1118	CLA	O1A-CGA-O2A-C1
25	L	5005	LHG	C35-C36-C37-C38
21	1	1123	CLA	C13-C15-C16-C17
35	F	6001	LMT	C11-C10-C9-C8
26	A	5008	LMG	O7-C8-C9-O8
31	B	5008	SQD	O6-C44-C45-O47
31	b	5006	SQD	O47-C45-C46-O48
31	f	5001	SQD	O47-C45-C46-O48
25	L	5005	LHG	O7-C5-C6-O8
25	1	5005	LHG	O7-C5-C6-O8
21	F	1302	CLA	C13-C15-C16-C17
21	a	1801	CLA	O1A-CGA-O2A-C1
21	A	1131	CLA	O1A-CGA-O2A-C1
21	A	1117	CLA	O1A-CGA-O2A-C1
21	6	1301	CLA	O1A-CGA-O2A-C1
21	2	1224	CLA	O1A-CGA-O2A-C1
25	B	5006	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
21	b	1227	CLA	C16-C17-C18-C20
21	B	1230	CLA	C16-C17-C18-C19
25	A	5001	LHG	O1-C1-C2-O2
25	L	5005	LHG	O1-C1-C2-O2
21	A	1132	CLA	C3-C5-C6-C7
21	l	1127	CLA	C5-C6-C7-C8
21	a	1140	CLA	C10-C11-C12-C13
21	A	1123	CLA	C4-C3-C5-C6
21	a	1123	CLA	C4-C3-C5-C6
21	A	1136	CLA	C4-C3-C5-C6
37	L	5004	DGD	C6B-C7B-C8B-C9B
21	B	1226	CLA	O1A-CGA-O2A-C1
25	B	5006	LHG	C19-C20-C21-C22
21	b	1226	CLA	C8-C10-C11-C12
21	B	1202	CLA	CAA-CBA-CGA-O2A
21	2	1229	CLA	C11-C10-C8-C9
21	2	1229	CLA	C11-C12-C13-C14
21	A	1114	CLA	C14-C13-C15-C16
21	B	1216	CLA	C6-C7-C8-C9
21	A	1113	CLA	C14-C13-C15-C16
21	l	1111	CLA	C11-C12-C13-C14
21	a	1127	CLA	C11-C12-C13-C14
21	b	1206	CLA	C6-C7-C8-C9
21	l	1118	CLA	C14-C13-C15-C16
21	l	1503	CLA	C11-C10-C8-C9
21	F	1301	CLA	C11-C10-C8-C9
21	J	1303	CLA	C14-C13-C15-C16
21	b	1236	CLA	C6-C7-C8-C9
22	a	2001	PQN	C19-C18-C20-C21
21	l	1012	CLA	C11-C12-C13-C14
21	B	1206	CLA	C11-C10-C8-C9
31	0	5005	SQD	C13-C14-C15-C16
21	b	1222	CLA	CBD-CGD-O2D-CED
21	B	1023	CLA	C2C-C3C-CAC-CBC
26	a	5004	LMG	C32-C33-C34-C35
31	b	5006	SQD	C4-C5-C6-S
21	b	1240	CLA	C16-C17-C18-C20
31	F	5001	SQD	O47-C7-C8-C9
21	B	1210	CLA	C5-C6-C7-C8
25	l	5007	LHG	C26-C27-C28-C29
24	l	4007	BCR	C11-C12-C13-C35
30	B	4006	ECH	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	B	4018	BCR	C37-C22-C23-C24
24	b	4004	BCR	C7-C8-C9-C34
30	i	4020	ECH	C36-C18-C19-C20
21	B	1224	CLA	C13-C15-C16-C17
21	2	1221	CLA	C15-C16-C17-C18
21	A	1118	CLA	C8-C10-C11-C12
24	1	4007	BCR	C7-C8-C9-C10
24	a	4008	BCR	C21-C22-C23-C24
24	A	4007	BCR	C21-C22-C23-C24
21	a	1104	CLA	C3-C5-C6-C7
31	F	5001	SQD	C33-C34-C35-C36
21	B	1204	CLA	C1A-C2A-CAA-CBA
21	1	1119	CLA	C1A-C2A-CAA-CBA
21	A	1011	CLA	C1A-C2A-CAA-CBA
21	B	1212	CLA	C1A-C2A-CAA-CBA
21	2	1204	CLA	C1A-C2A-CAA-CBA
21	A	1106	CLA	C16-C17-C18-C19
22	2	2002	PQN	C26-C27-C28-C30
21	1	1120	CLA	C16-C17-C18-C20
21	2	1226	CLA	C5-C6-C7-C8
21	B	1219	CLA	C2-C1-O2A-CGA
21	2	1021	CLA	C2-C1-O2A-CGA
21	1	1135	CLA	C2-C1-O2A-CGA
21	B	1225	CLA	C2-C1-O2A-CGA
21	A	1109	CLA	C2-C1-O2A-CGA
35	1	6001	LMT	C3-C4-C5-C6
24	l	4022	BCR	C9-C10-C11-C12
24	b	4010	BCR	C19-C20-C21-C22
21	a	1012	CLA	C10-C11-C12-C13
25	6	5001	LHG	C4-O6-P-O3
25	b	5004	LHG	C4-O6-P-O3
25	A	5005	LHG	C3-O3-P-O6
25	1	5005	LHG	C4-O6-P-O3
25	a	5001	LHG	C3-O3-P-O6
26	K	5009	LMG	C4-C5-C6-O5
31	F	5001	SQD	C26-C27-C28-C29
21	A	1801	CLA	C4-C3-C5-C6
21	b	1203	CLA	C4-C3-C5-C6
21	a	1136	CLA	C4-C3-C5-C6
25	B	5004	LHG	C5-C4-O6-P
25	l	5001	LHG	C5-C4-O6-P
25	1	5007	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
21	b	1223	CLA	C2-C3-C5-C6
35	0	6001	LMT	C5'-C4'-O1B-C1B
31	0	5005	SQD	C19-C20-C21-C22
25	1	5002	LHG	C3-O3-P-O5
25	2	5004	LHG	C3-O3-P-O5
25	2	5004	LHG	C4-O6-P-O4
25	B	5004	LHG	C3-O3-P-O4
25	F	5002	LHG	C3-O3-P-O4
25	A	5007	LHG	C3-O3-P-O4
25	A	5007	LHG	C4-O6-P-O4
25	1	5001	LHG	C3-O3-P-O5
25	A	5001	LHG	C4-O6-P-O5
25	a	5005	LHG	C3-O3-P-O5
25	1	5003	LHG	C3-O3-P-O5
25	a	5003	LHG	C3-O3-P-O5
25	A	5003	LHG	C3-O3-P-O5
25	A	5003	LHG	C4-O6-P-O5
25	1	5007	LHG	C4-O6-P-O4
25	L	5005	LHG	C3-O3-P-O5
25	B	5006	LHG	C4-O6-P-O5
25	0	5002	LHG	C3-O3-P-O4
25	1	5004	LHG	C3-O3-P-O4
25	1	5005	LHG	C3-O3-P-O4
25	1	5003	LHG	C3-O3-P-O4
25	a	5001	LHG	C4-O6-P-O4
25	0	5004	LHG	C3-O3-P-O5
21	b	1214	CLA	C16-C17-C18-C20
21	A	1122	CLA	C11-C12-C13-C14
21	b	1205	CLA	C16-C17-C18-C20
21	A	1104	CLA	C16-C17-C18-C20
21	A	1137	CLA	C16-C17-C18-C19
21	f	1302	CLA	C16-C17-C18-C20
22	A	2001	PQN	C26-C27-C28-C30
21	a	1138	CLA	C16-C17-C18-C19
26	A	5002	LMG	C10-C11-C12-C13
25	1	5005	LHG	C9-C10-C11-C12
21	a	1134	CLA	O2A-C1-C2-C3
21	b	1206	CLA	C13-C15-C16-C17
21	1	1503	CLA	C13-C15-C16-C17
21	2	1213	CLA	CBA-CGA-O2A-C1
25	1	5001	LHG	O6-C4-C5-C6
25	a	5003	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	5006	LHG	O6-C4-C5-C6
26	1	5004	LMG	C22-C23-C24-C25
26	1	5002	LMG	C32-C33-C34-C35
25	A	5005	LHG	C15-C16-C17-C18
25	a	5001	LHG	C31-C32-C33-C34
21	2	1207	CLA	C5-C6-C7-C8
21	2	1235	CLA	C2A-CAA-CBA-CGA
21	A	1134	CLA	C2A-CAA-CBA-CGA
21	A	1120	CLA	C2A-CAA-CBA-CGA
21	1	1134	CLA	C3-C5-C6-C7
31	B	5008	SQD	C18-C19-C20-C21
26	B	5005	LMG	C30-C31-C32-C33
21	2	1210	CLA	C16-C17-C18-C19
21	a	1122	CLA	C16-C17-C18-C20
21	B	1212	CLA	C6-C7-C8-C10
21	2	1205	CLA	C16-C17-C18-C20
21	2	1210	CLA	C4C-C3C-CAC-CBC
21	2	1220	CLA	CAD-CBD-CGD-O1D
21	b	1220	CLA	CAD-CBD-CGD-O1D
21	B	1220	CLA	CAD-CBD-CGD-O1D
21	b	1202	CLA	CAD-CBD-CGD-O1D
21	b	1211	CLA	CAD-CBD-CGD-O1D
21	2	1210	CLA	CAD-CBD-CGD-O1D
21	A	1113	CLA	CAD-CBD-CGD-O1D
21	1	1113	CLA	CAD-CBD-CGD-O1D
21	B	1211	CLA	CAD-CBD-CGD-O1D
21	7	1302	CLA	CAD-CBD-CGD-O1D
21	1	1137	CLA	C2-C3-C5-C6
21	B	1226	CLA	CAD-CBD-CGD-O1D
21	1	1103	CLA	CAD-CBD-CGD-O1D
21	1	1501	CLA	CAD-CBD-CGD-O1D
21	B	1210	CLA	CAD-CBD-CGD-O1D
21	b	1226	CLA	CAD-CBD-CGD-O1D
21	B	1234	CLA	CAD-CBD-CGD-O1D
21	1	1123	CLA	CAD-CBD-CGD-O1D
21	b	1217	CLA	CAD-CBD-CGD-O1D
21	a	1801	CLA	CAD-CBD-CGD-O1D
21	1	1125	CLA	CAD-CBD-CGD-O1D
21	A	1111	CLA	CAD-CBD-CGD-O1D
21	2	1202	CLA	CAD-CBD-CGD-O1D
21	7	1303	CLA	CAD-CBD-CGD-O1D
21	2	1212	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	b	1210	CLA	CAD-CBD-CGD-O1D
21	A	1125	CLA	CAD-CBD-CGD-O1D
21	A	1101	CLA	CAA-CBA-CGA-O2A
21	b	1202	CLA	C8-C10-C11-C12
21	a	1127	CLA	C5-C6-C7-C8
21	B	1238	CLA	C10-C11-C12-C13
21	a	1112	CLA	C15-C16-C17-C18
21	B	1221	CLA	C10-C11-C12-C13
21	A	1140	CLA	C5-C6-C7-C8
26	b	5005	LMG	C14-C15-C16-C17
31	B	5008	SQD	C34-C35-C36-C37
25	A	5005	LHG	C7-C8-C9-C10
26	A	5008	LMG	C33-C34-C35-C36
21	1	1139	CLA	CBA-CGA-O2A-C1
21	A	1112	CLA	CBA-CGA-O2A-C1
21	A	1119	CLA	CBA-CGA-O2A-C1
21	a	1127	CLA	C13-C15-C16-C17
21	a	1140	CLA	C15-C16-C17-C18
25	1	5001	LHG	C9-C10-C11-C12
21	a	1119	CLA	C16-C17-C18-C19
21	1	1139	CLA	C12-C13-C15-C16
21	b	1220	CLA	C11-C12-C13-C15
21	2	1229	CLA	C11-C10-C8-C7
21	2	1214	CLA	C6-C7-C8-C10
25	2	5004	LHG	O6-C4-C5-O7
21	A	1114	CLA	C6-C7-C8-C10
21	b	1216	CLA	C6-C7-C8-C10
21	B	1219	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	C11-C10-C8-C7
21	b	1227	CLA	C11-C12-C13-C15
21	a	1123	CLA	C2-C3-C5-C6
21	A	1112	CLA	C11-C12-C13-C15
21	K	1401	CLA	C12-C13-C15-C16
21	B	1208	CLA	C12-C13-C15-C16
21	a	1106	CLA	C12-C13-C15-C16
21	1	1103	CLA	C6-C7-C8-C10
21	L	1502	CLA	C6-C7-C8-C10
21	B	1230	CLA	C11-C12-C13-C15
21	l	1501	CLA	C11-C10-C8-C7
21	F	1301	CLA	C12-C13-C15-C16
21	A	1106	CLA	C6-C7-C8-C10
21	A	1104	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	a	1112	CLA	C11-C12-C13-C15
21	b	1236	CLA	C6-C7-C8-C10
21	0	1501	CLA	C11-C12-C13-C15
21	a	1012	CLA	C11-C12-C13-C15
21	B	1201	CLA	C11-C10-C8-C7
21	b	1231	CLA	C6-C7-C8-C10
21	A	1129	CLA	C6-C7-C8-C10
21	A	1134	CLA	C12-C13-C15-C16
21	A	1130	CLA	C11-C10-C8-C7
21	A	1107	CLA	C6-C7-C8-C10
21	a	1139	CLA	C12-C13-C15-C16
21	B	1221	CLA	C11-C12-C13-C15
21	2	1023	CLA	C6-C7-C8-C10
21	a	1117	CLA	C6-C7-C8-C10
21	K	1402	CLA	C12-C13-C15-C16
25	B	5006	LHG	O6-C4-C5-O7
21	A	1125	CLA	C12-C13-C15-C16
21	1	1136	CLA	C6-C7-C8-C10
21	1	1138	CLA	C11-C10-C8-C7
21	A	1120	CLA	C11-C10-C8-C7
21	b	1230	CLA	C6-C7-C8-C10
21	1	1120	CLA	C6-C7-C8-C10
21	b	1232	CLA	C11-C12-C13-C15
25	0	5004	LHG	O6-C4-C5-O7
21	a	1135	CLA	C12-C13-C15-C16
21	b	1213	CLA	C11-C12-C13-C15
21	1	1117	CLA	C6-C7-C8-C10
21	B	1206	CLA	C11-C10-C8-C7
21	1	1128	CLA	C11-C10-C8-C7
21	A	1118	CLA	C11-C12-C13-C15
25	F	5002	LHG	C11-C10-C9-C8
26	a	5002	LMG	C33-C34-C35-C36
21	A	1013	CLA	C3-C5-C6-C7
21	b	1219	CLA	C3-C5-C6-C7
21	b	1207	CLA	O1A-CGA-O2A-C1
25	1	5003	LHG	C31-C32-C33-C34
21	b	1202	CLA	CAA-CBA-CGA-O2A
21	a	1011	CLA	CAA-CBA-CGA-O2A
25	B	5006	LHG	O8-C23-C24-C25
25	1	5005	LHG	C27-C28-C29-C30
21	B	1202	CLA	C8-C10-C11-C12
21	a	1139	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	A	1112	CLA	O1A-CGA-O2A-C1
25	A	5005	LHG	O10-C23-O8-C6
21	j	1302	CLA	C8-C10-C11-C12
22	A	2001	PQN	C23-C25-C26-C27
21	2	1239	CLA	C2A-CAA-CBA-CGA
21	b	1023	CLA	C2A-CAA-CBA-CGA
21	a	1126	CLA	C2A-CAA-CBA-CGA
21	a	1119	CLA	C2A-CAA-CBA-CGA
21	0	1501	CLA	C16-C17-C18-C20
25	2	5004	LHG	C25-C26-C27-C28
25	1	5001	LHG	C19-C20-C21-C22
25	b	5004	LHG	C35-C36-C37-C38
26	A	5008	LMG	C15-C16-C17-C18
21	A	1127	CLA	CAA-CBA-CGA-O2A
26	1	5004	LMG	C14-C15-C16-C17
26	1	5002	LMG	C34-C35-C36-C37
25	a	5003	LHG	C4-C5-C6-O8
31	L	5001	SQD	O6-C44-C45-C46
31	L	5001	SQD	O49-C7-O47-C45
25	b	5004	LHG	O7-C5-C6-O8
25	a	5007	LHG	O7-C5-C6-O8
25	1	5007	LHG	O7-C5-C6-O8
25	A	5006	LHG	O7-C5-C6-O8
31	L	5001	SQD	O47-C45-C46-O48
31	0	5005	SQD	O6-C44-C45-O47
26	0	5001	LMG	C34-C35-C36-C37
21	2	1215	CLA	CAA-CBA-CGA-O2A
21	b	1228	CLA	C16-C17-C18-C20
21	1	1126	CLA	C16-C17-C18-C20
21	K	1402	CLA	C16-C17-C18-C20
21	1	1013	CLA	C8-C10-C11-C12
21	b	1208	CLA	C5-C6-C7-C8
25	l	5002	LHG	C24-C25-C26-C27
25	l	5004	LHG	C11-C10-C9-C8
25	M	5001	LHG	C5-C4-O6-P
25	L	5005	LHG	C2-C3-O3-P
25	l	5002	LHG	C35-C36-C37-C38
21	1	1139	CLA	O1A-CGA-O2A-C1
21	A	1138	CLA	O1A-CGA-O2A-C1
21	B	1219	CLA	C4-C3-C5-C6
21	B	1205	CLA	C4-C3-C5-C6
25	A	5001	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
21	b	1222	CLA	C5-C6-C7-C8
21	L	1503	CLA	C5-C6-C7-C8
21	B	1213	CLA	C11-C12-C13-C14
21	a	1101	CLA	C6-C7-C8-C9
21	A	1126	CLA	C11-C12-C13-C14
21	b	1208	CLA	C11-C10-C8-C9
21	A	1123	CLA	C14-C13-C15-C16
21	A	1103	CLA	C11-C12-C13-C14
21	a	1122	CLA	C11-C10-C8-C9
21	B	1239	CLA	C6-C7-C8-C9
21	1	1101	CLA	C11-C12-C13-C14
21	A	1105	CLA	C11-C10-C8-C9
21	b	1206	CLA	C11-C10-C8-C9
21	l	1503	CLA	C11-C12-C13-C14
21	B	1230	CLA	C6-C7-C8-C9
21	A	1138	CLA	C11-C12-C13-C14
21	A	1136	CLA	C11-C12-C13-C14
21	2	1208	CLA	C6-C7-C8-C9
21	1	1123	CLA	C11-C12-C13-C14
21	2	1021	CLA	C6-C7-C8-C9
21	a	1109	CLA	C14-C13-C15-C16
21	a	1104	CLA	C11-C10-C8-C9
21	L	1501	CLA	C14-C13-C15-C16
21	a	1118	CLA	C11-C10-C8-C9
21	2	1239	CLA	C6-C7-C8-C9
21	B	1205	CLA	C14-C13-C15-C16
21	b	1023	CLA	C6-C7-C8-C9
21	1	1120	CLA	C6-C7-C8-C9
21	1	1120	CLA	C14-C13-C15-C16
21	A	1109	CLA	C6-C7-C8-C9
21	a	1126	CLA	C6-C7-C8-C9
25	A	5001	LHG	C12-C13-C14-C15
21	1	1132	CLA	C3-C5-C6-C7
21	1	1127	CLA	CAA-CBA-CGA-O2A
21	A	1112	CLA	C5-C6-C7-C8
25	l	5003	LHG	C24-C25-C26-C27
24	a	4001	BCR	C18-C19-C20-C21
24	1	4001	BCR	C18-C19-C20-C21
24	k	4001	BCR	C18-C19-C20-C21
24	2	4018	BCR	C18-C19-C20-C21
24	9	4021	BCR	C18-C19-C20-C21
24	a	4019	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	b	4006	ECH	C18-C19-C20-C21
24	A	4019	BCR	C18-C19-C20-C21
24	a	4007	BCR	C19-C20-C21-C22
25	l	5004	LHG	C26-C27-C28-C29
21	B	1217	CLA	C3-C5-C6-C7
21	2	1206	CLA	C15-C16-C17-C18
21	f	1302	CLA	C16-C17-C18-C19
25	A	5007	LHG	C33-C34-C35-C36
25	1	5003	LHG	C11-C10-C9-C8
25	a	5007	LHG	C34-C35-C36-C37
36	I	4020	EQ3	C7-C8-C9-C10
24	a	4002	BCR	C17-C18-C19-C20
21	j	1302	CLA	CAA-CBA-CGA-O2A
21	a	1011	CLA	C5-C6-C7-C8
21	b	1230	CLA	C13-C15-C16-C17
35	l	6001	LMT	C2B-C1B-O1B-C4'
25	a	5005	LHG	C25-C26-C27-C28
21	b	1235	CLA	C3-C5-C6-C7
21	B	1207	CLA	C3-C5-C6-C7
21	1	1102	CLA	C3-C5-C6-C7
21	a	1118	CLA	C4-C3-C5-C6
21	2	1213	CLA	O1A-CGA-O2A-C1
21	a	1011	CLA	O1A-CGA-O2A-C1
21	A	1124	CLA	O1A-CGA-O2A-C1
21	1	1123	CLA	C5-C6-C7-C8
21	a	1118	CLA	C16-C17-C18-C19
25	1	5001	LHG	C13-C14-C15-C16
35	1	6001	LMT	C11-C10-C9-C8
25	A	5005	LHG	C26-C27-C28-C29
31	f	5001	SQD	C11-C10-C9-C8
21	k	1402	CLA	C1-C2-C3-C4
21	a	1134	CLA	C1-C2-C3-C4
21	A	1119	CLA	O1A-CGA-O2A-C1
21	B	1206	CLA	C3-C5-C6-C7
25	B	5004	LHG	C26-C27-C28-C29
25	1	5007	LHG	C15-C16-C17-C18
21	B	1217	CLA	C15-C16-C17-C18
21	2	1021	CLA	C13-C15-C16-C17
21	A	1127	CLA	C13-C15-C16-C17
26	1	5002	LMG	C9-C8-O7-C10
25	B	5004	LHG	O6-C4-C5-C6
21	b	1225	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	L	1502	CLA	C2A-CAA-CBA-CGA
21	2	1217	CLA	C2A-CAA-CBA-CGA
21	A	1012	CLA	C2-C1-O2A-CGA
21	1	1131	CLA	C2-C1-O2A-CGA
21	b	1202	CLA	C2-C1-O2A-CGA
21	a	1011	CLA	C2-C1-O2A-CGA
21	K	1401	CLA	C2-C1-O2A-CGA
21	A	1105	CLA	C2-C1-O2A-CGA
21	A	1121	CLA	C2-C1-O2A-CGA
21	F	1301	CLA	C2-C1-O2A-CGA
21	f	1302	CLA	C2-C1-O2A-CGA
21	2	1218	CLA	C2-C1-O2A-CGA
21	b	1232	CLA	C2-C1-O2A-CGA
21	2	1224	CLA	C2-C1-O2A-CGA
21	B	1231	CLA	C16-C17-C18-C20
21	a	1128	CLA	C16-C17-C18-C19
21	A	1137	CLA	C16-C17-C18-C20
31	f	5001	SQD	C7-C8-C9-C10
25	0	5004	LHG	C12-C13-C14-C15
31	L	5001	SQD	C8-C7-O47-C45
25	l	5001	LHG	C35-C36-C37-C38
25	a	5003	LHG	C7-C8-C9-C10
25	6	5001	LHG	C2-C3-O3-P
25	a	5003	LHG	C2-C3-O3-P
25	a	5007	LHG	C5-C4-O6-P
25	l	5003	LHG	C2-C3-O3-P
24	a	4001	BCR	C15-C16-C17-C18
24	b	4005	BCR	C15-C16-C17-C18
25	A	5001	LHG	O6-C4-C5-O7
25	l	5003	LHG	O6-C4-C5-O7
21	2	1021	CLA	C15-C16-C17-C18
21	2	1207	CLA	C4-C3-C5-C6
21	a	1109	CLA	C4-C3-C5-C6
31	L	5001	SQD	C9-C10-C11-C12
24	1	4003	BCR	C23-C24-C25-C26
24	b	4017	BCR	C5-C6-C7-C8
24	a	4008	BCR	C23-C24-C25-C26
24	a	4002	BCR	C1-C6-C7-C8
24	a	4002	BCR	C5-C6-C7-C8
24	a	4002	BCR	C23-C24-C25-C26
24	a	4002	BCR	C23-C24-C25-C30
24	2	4017	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	1	4019	BCR	C5-C6-C7-C8
24	i	4018	BCR	C1-C6-C7-C8
21	1	1011	CLA	C5-C6-C7-C8
31	F	5001	SQD	C7-C8-C9-C10
21	1	1118	CLA	CAA-CBA-CGA-O2A
21	A	1118	CLA	CAA-CBA-CGA-O2A
25	0	5004	LHG	C34-C35-C36-C37
21	A	1012	CLA	C16-C17-C18-C19
21	b	1227	CLA	C16-C17-C18-C19
21	b	1215	CLA	C16-C17-C18-C20
21	1	1117	CLA	C16-C17-C18-C20
21	b	1229	CLA	C3-C5-C6-C7
21	B	1212	CLA	C3-C5-C6-C7
26	1	5004	LMG	O6-C1-O1-C7
21	b	1022	CLA	C2A-CAA-CBA-CGA
21	b	1228	CLA	C2A-CAA-CBA-CGA
25	1	5002	LHG	O7-C5-C6-O8
26	A	5004	LMG	O1-C7-C8-O7
26	1	5002	LMG	O7-C8-C9-O8
21	b	1021	CLA	C15-C16-C17-C18
25	A	5003	LHG	C15-C16-C17-C18
25	M	5001	LHG	C3-O3-P-O6
25	1	5001	LHG	C3-O3-P-O6
25	6	5001	LHG	C3-O3-P-O6
25	A	5001	LHG	C3-O3-P-O6
25	b	5004	LHG	C3-O3-P-O6
25	a	5007	LHG	C3-O3-P-O6
25	A	5006	LHG	C4-O6-P-O3
25	1	5004	LHG	C4-O6-P-O3
25	0	5004	LHG	C4-O6-P-O3
25	B	5004	LHG	C35-C36-C37-C38
25	F	5002	LHG	C28-C29-C30-C31
26	2	5005	LMG	C29-C30-C31-C32
21	1	1102	CLA	C6-C7-C8-C9
31	B	5008	SQD	C11-C10-C9-C8
26	b	5007	LMG	C12-C13-C14-C15
25	B	5006	LHG	C11-C10-C9-C8
25	A	5007	LHG	C16-C17-C18-C19
25	0	5002	LHG	C4-C5-C6-O8
21	1	1123	CLA	C15-C16-C17-C18
21	B	1204	CLA	C11-C10-C8-C7
21	2	1206	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	1	1127	CLA	C6-C7-C8-C10
21	b	1203	CLA	C11-C10-C8-C7
21	1	1106	CLA	C11-C10-C8-C7
21	A	1123	CLA	C2-C3-C5-C6
21	L	1503	CLA	C11-C10-C8-C7
21	1	1118	CLA	C12-C13-C15-C16
21	B	1228	CLA	C11-C10-C8-C7
21	2	1204	CLA	C6-C7-C8-C10
21	a	1112	CLA	C6-C7-C8-C10
21	2	1023	CLA	C2-C3-C5-C6
21	1	1012	CLA	C6-C7-C8-C10
21	1	1012	CLA	C11-C10-C8-C7
21	B	1206	CLA	C11-C12-C13-C15
26	1	5004	LMG	C30-C31-C32-C33
21	a	1127	CLA	CAA-CBA-CGA-O2A
21	B	1230	CLA	C3-C5-C6-C7
21	A	1114	CLA	C6-C7-C8-C9
21	b	1216	CLA	C6-C7-C8-C9
21	2	1210	CLA	C11-C12-C13-C14
21	a	1133	CLA	C11-C10-C8-C9
21	A	1112	CLA	C11-C10-C8-C9
21	B	1226	CLA	C6-C7-C8-C9
21	1	1103	CLA	C6-C7-C8-C9
21	1	1103	CLA	C14-C13-C15-C16
21	l	1501	CLA	C14-C13-C15-C16
21	A	1104	CLA	C14-C13-C15-C16
21	a	1112	CLA	C11-C10-C8-C9
21	2	1215	CLA	C11-C10-C8-C9
21	1	1109	CLA	C11-C10-C8-C9
21	b	1238	CLA	C11-C10-C8-C9
21	K	1402	CLA	C14-C13-C15-C16
21	a	1136	CLA	C11-C10-C8-C9
21	A	1120	CLA	C11-C10-C8-C9
21	b	1232	CLA	C11-C12-C13-C14
21	1	1117	CLA	C6-C7-C8-C9
24	1	4012	BCR	C19-C20-C21-C22
24	i	4018	BCR	C19-C20-C21-C22
21	2	1210	CLA	C16-C17-C18-C20
21	B	1230	CLA	C16-C17-C18-C20
21	B	1212	CLA	C6-C7-C8-C9
21	A	1136	CLA	C16-C17-C18-C19
21	a	1138	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	M	5001	LHG	C33-C34-C35-C36
26	a	5002	LMG	C14-C15-C16-C17
26	b	5005	LMG	C30-C31-C32-C33
21	A	1138	CLA	CBA-CGA-O2A-C1
21	b	1022	CLA	C13-C15-C16-C17
21	a	1119	CLA	C8-C10-C11-C12
21	b	1222	CLA	O1D-CGD-O2D-CED
25	1	5005	LHG	C30-C31-C32-C33
26	A	5008	LMG	C4-C5-C6-O5
21	j	1302	CLA	C2A-CAA-CBA-CGA
21	2	1201	CLA	C2A-CAA-CBA-CGA
21	a	1013	CLA	C2A-CAA-CBA-CGA
25	A	5005	LHG	C9-C10-C11-C12
21	a	1011	CLA	C16-C17-C18-C20
21	2	1238	CLA	C16-C17-C18-C19
21	A	1122	CLA	C11-C12-C13-C15
21	2	1215	CLA	C11-C12-C13-C15
21	a	1120	CLA	C6-C7-C8-C9
25	1	5002	LHG	C15-C16-C17-C18
21	A	1124	CLA	CBA-CGA-O2A-C1
25	a	5005	LHG	O1-C1-C2-C3
21	f	1301	CLA	O1A-CGA-O2A-C1
28	h	4020	45D	C20-C24-C26-C30
21	a	1117	CLA	C10-C11-C12-C13
21	A	1109	CLA	C4-C3-C5-C6
21	a	1122	CLA	O1A-CGA-O2A-C1
21	1	1101	CLA	CAA-CBA-CGA-O2A
21	A	1801	CLA	C2-C3-C5-C6
21	b	1229	CLA	C2-C3-C5-C6
21	b	1214	CLA	C16-C17-C18-C19
21	b	1222	CLA	C16-C17-C18-C19
21	2	1205	CLA	C16-C17-C18-C19
21	1	1138	CLA	C11-C12-C13-C15
21	f	1301	CLA	CBA-CGA-O2A-C1
21	a	1011	CLA	CBA-CGA-O2A-C1
31	F	5001	SQD	C24-C23-O48-C46
21	2	1223	CLA	CBA-CGA-O2A-C1
21	a	1122	CLA	CBA-CGA-O2A-C1
26	b	5005	LMG	C29-C28-O8-C9
21	a	1120	CLA	CBA-CGA-O2A-C1
21	a	1120	CLA	O1A-CGA-O2A-C1
31	f	5001	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	b	5002	LMG	C40-C41-C42-C43
21	1	1132	CLA	C13-C15-C16-C17
21	A	1117	CLA	C15-C16-C17-C18
21	2	1223	CLA	O1A-CGA-O2A-C1
26	b	5005	LMG	O10-C28-O8-C9
26	b	5005	LMG	C39-C40-C41-C42
21	2	1022	CLA	C2A-CAA-CBA-CGA
21	A	1136	CLA	C2A-CAA-CBA-CGA
21	b	1205	CLA	C16-C17-C18-C19
21	A	1011	CLA	CAA-CBA-CGA-O1A
24	A	4008	BCR	C19-C20-C21-C22
24	J	4013	BCR	C13-C14-C15-C16
24	2	4005	BCR	C15-C16-C17-C18
28	h	4020	45D	C36-C38-C42-C41
24	a	4007	BCR	C15-C16-C17-C18
24	A	4007	BCR	C9-C10-C11-C12
24	B	4004	BCR	C19-C20-C21-C22
25	a	5007	LHG	C35-C36-C37-C38
21	2	1225	CLA	C3-C5-C6-C7
26	a	5004	LMG	C33-C34-C35-C36
25	F	5002	LHG	C9-C10-C11-C12
25	0	5002	LHG	O6-C4-C5-O7
25	1	5002	LHG	C14-C15-C16-C17
25	A	5003	LHG	C27-C28-C29-C30
24	I	4018	BCR	C10-C11-C12-C13
24	a	4008	BCR	C10-C11-C12-C13
24	1	4012	BCR	C10-C11-C12-C13
26	2	5005	LMG	C10-C11-C12-C13
21	2	1221	CLA	C16-C17-C18-C19
25	1	5001	LHG	O8-C23-C24-C25
26	1	5004	LMG	C33-C34-C35-C36
21	b	1229	CLA	C4-C3-C5-C6
21	B	1224	CLA	C4-C3-C5-C6
21	a	1105	CLA	C4-C3-C5-C6
21	1	1103	CLA	C4-C3-C5-C6
21	A	1132	CLA	C2-C3-C5-C6
21	a	1126	CLA	C2-C3-C5-C6
31	F	5001	SQD	O10-C23-O48-C46
25	0	5002	LHG	C15-C16-C17-C18
21	a	1011	CLA	C10-C11-C12-C13
21	B	1224	CLA	C5-C6-C7-C8
21	f	1302	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	1218	CLA	C8-C10-C11-C12
25	A	5005	LHG	C19-C20-C21-C22
25	1	5005	LHG	C26-C27-C28-C29
21	A	1011	CLA	C2-C1-O2A-CGA
21	1	1103	CLA	C2-C1-O2A-CGA
26	b	5002	LMG	C22-C23-C24-C25
21	2	1232	CLA	C2A-CAA-CBA-CGA
21	a	1122	CLA	C16-C17-C18-C19
25	A	5006	LHG	C27-C28-C29-C30
26	1	5004	LMG	C2-C1-O1-C7
21	B	1224	CLA	C8-C10-C11-C12
37	L	5004	DGD	O1G-C1G-C2G-O2G
21	l	1503	CLA	C2A-CAA-CBA-CGA
21	a	1111	CLA	C2A-CAA-CBA-CGA
21	L	1501	CLA	C2A-CAA-CBA-CGA
35	l	6001	LMT	C5-C6-C7-C8
25	a	5005	LHG	C31-C32-C33-C34
25	M	5001	LHG	C2-C3-O3-P
25	l	5004	LHG	C5-C4-O6-P
25	0	5002	LHG	C11-C10-C9-C8
21	b	1211	CLA	C3A-C2A-CAA-CBA
21	1	1013	CLA	C3A-C2A-CAA-CBA
21	b	1214	CLA	C3A-C2A-CAA-CBA
21	8	1402	CLA	C3A-C2A-CAA-CBA
21	k	1402	CLA	C3A-C2A-CAA-CBA
21	B	1228	CLA	C3A-C2A-CAA-CBA
21	A	1108	CLA	C3A-C2A-CAA-CBA
21	A	1102	CLA	C3A-C2A-CAA-CBA
21	A	1101	CLA	C16-C17-C18-C20
21	1	1126	CLA	CAA-CBA-CGA-O2A
25	1	5001	LHG	C31-C32-C33-C34
34	7	4015	ZEX	C33-C34-C35-C15
24	1	4007	BCR	C15-C16-C17-C18
24	A	4012	BCR	C19-C20-C21-C22
24	9	4021	BCR	C19-C20-C21-C22
21	B	1223	CLA	O1A-CGA-O2A-C1
37	L	5004	DGD	C5B-C6B-C7B-C8B
35	0	6001	LMT	O1'-C1-C2-C3
21	2	1022	CLA	C4-C3-C5-C6
21	a	1131	CLA	C4-C3-C5-C6
21	B	1211	CLA	C4-C3-C5-C6
21	2	1229	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	F	5002	LHG	C15-C16-C17-C18
21	B	1204	CLA	C6-C7-C8-C9
21	a	1121	CLA	C11-C10-C8-C9
21	B	1219	CLA	C11-C10-C8-C9
21	A	1126	CLA	C11-C10-C8-C9
21	a	1133	CLA	C14-C13-C15-C16
21	b	1229	CLA	C6-C7-C8-C9
21	a	1131	CLA	C11-C10-C8-C9
21	A	1103	CLA	C11-C10-C8-C9
21	1	1132	CLA	C14-C13-C15-C16
21	A	1105	CLA	C14-C13-C15-C16
21	A	1121	CLA	C11-C10-C8-C9
21	B	1234	CLA	C11-C10-C8-C9
21	A	1137	CLA	C14-C13-C15-C16
21	B	1201	CLA	C14-C13-C15-C16
21	A	1111	CLA	C11-C12-C13-C14
21	A	1133	CLA	C6-C7-C8-C9
21	a	1139	CLA	C6-C7-C8-C9
21	B	1218	CLA	C6-C7-C8-C9
21	b	1238	CLA	C14-C13-C15-C16
21	K	1402	CLA	C11-C12-C13-C14
21	1	1140	CLA	C11-C12-C13-C14
21	A	1125	CLA	C11-C12-C13-C14
21	2	1221	CLA	C14-C13-C15-C16
21	a	1135	CLA	C11-C12-C13-C14
22	b	2002	PQN	C24-C23-C25-C26
22	A	2001	PQN	C26-C27-C28-C29
21	B	1225	CLA	C16-C17-C18-C20
25	a	5007	LHG	C14-C15-C16-C17
25	2	5004	LHG	C16-C17-C18-C19
25	A	5007	LHG	C27-C28-C29-C30
25	A	5005	LHG	C30-C31-C32-C33
21	b	1229	CLA	C10-C11-C12-C13
24	6	4016	BCR	C35-C13-C14-C15
28	B	4011	45D	C28-C26-C30-C32
28	B	4011	45D	C39-C35-C37-C41
24	f	4016	BCR	C35-C13-C14-C15
24	1	4022	BCR	C11-C10-C9-C34
24	2	4018	BCR	C20-C21-C22-C37
36	I	4020	EQ3	C11-C10-C9-C34
24	2	4011	BCR	C16-C17-C18-C36
26	b	5005	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
25	A	5001	LHG	C4-C5-C6-O8
24	9	4021	BCR	C35-C13-C14-C15
30	M	4021	ECH	C11-C10-C9-C34
30	b	4011	ECH	C16-C17-C18-C36
34	F	4016	ZEX	C20-C13-C14-C15
30	B	4006	ECH	C11-C10-C9-C34
30	B	4006	ECH	C35-C13-C14-C15
30	b	4006	ECH	C11-C10-C9-C34
30	2	4006	ECH	C11-C10-C9-C34
30	m	4021	ECH	C11-C10-C9-C34
26	2	5005	LMG	C40-C41-C42-C43
25	L	5005	LHG	C16-C17-C18-C19
25	0	5004	LHG	C10-C11-C12-C13
21	A	1132	CLA	C5-C6-C7-C8
21	2	1239	CLA	C15-C16-C17-C18
26	2	5005	LMG	C30-C31-C32-C33
25	a	5003	LHG	O10-C23-C24-C25
22	B	2002	PQN	C26-C27-C28-C30
21	A	1012	CLA	O2A-C1-C2-C3
21	1	1012	CLA	O2A-C1-C2-C3
21	B	1223	CLA	CBA-CGA-O2A-C1
25	A	5005	LHG	C13-C14-C15-C16
24	2	4018	BCR	C37-C22-C23-C24
24	b	4014	BCR	C7-C8-C9-C34
24	1	4008	BCR	C37-C22-C23-C24
28	h	4020	45D	C32-C34-C36-C40
25	2	5004	LHG	C33-C34-C35-C36
21	A	1104	CLA	C10-C11-C12-C13
21	b	1205	CLA	CBD-CGD-O2D-CED
31	f	5001	SQD	C15-C16-C17-C18
21	B	1220	CLA	C4-C3-C5-C6
21	A	1132	CLA	C4-C3-C5-C6
21	B	1237	CLA	C1A-C2A-CAA-CBA
21	1	1013	CLA	C1A-C2A-CAA-CBA
21	a	1011	CLA	C1A-C2A-CAA-CBA
21	b	1022	CLA	C1A-C2A-CAA-CBA
21	8	1402	CLA	C1A-C2A-CAA-CBA
21	k	1402	CLA	C1A-C2A-CAA-CBA
21	B	1222	CLA	C1A-C2A-CAA-CBA
21	b	1021	CLA	C1A-C2A-CAA-CBA
21	B	1223	CLA	C1A-C2A-CAA-CBA
21	B	1021	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	1140	CLA	C1A-C2A-CAA-CBA
21	b	1215	CLA	C16-C17-C18-C19
21	2	1215	CLA	C11-C12-C13-C14
21	a	1124	CLA	C6-C7-C8-C9
21	b	1216	CLA	C12-C13-C15-C16
21	B	1240	CLA	C6-C7-C8-C10
21	B	1217	CLA	C11-C10-C8-C7
21	A	1116	CLA	C6-C7-C8-C10
21	b	1208	CLA	C6-C7-C8-C10
21	b	1203	CLA	C6-C7-C8-C10
22	B	2002	PQN	C17-C18-C20-C21
21	1	1116	CLA	C11-C12-C13-C15
21	A	1103	CLA	C11-C10-C8-C7
21	a	1127	CLA	C11-C12-C13-C15
21	a	1106	CLA	C6-C7-C8-C10
21	1	1103	CLA	C11-C12-C13-C15
21	a	1111	CLA	C12-C13-C15-C16
21	A	1106	CLA	C11-C10-C8-C7
21	a	1109	CLA	C11-C10-C8-C7
21	1	1133	CLA	C12-C13-C15-C16
21	a	1104	CLA	C12-C13-C15-C16
22	a	2001	PQN	C17-C18-C20-C21
22	2	2002	PQN	C16-C17-C18-C20
22	A	2001	PQN	C22-C23-C25-C26
21	2	1203	CLA	C12-C13-C15-C16
21	2	1221	CLA	C6-C7-C8-C10
21	B	1205	CLA	C6-C7-C8-C10
21	a	1119	CLA	C6-C7-C8-C10
21	1	1106	CLA	C8-C10-C11-C12
21	a	1136	CLA	C10-C11-C12-C13
24	7	4013	BCR	C15-C16-C17-C18
25	a	5005	LHG	C12-C13-C14-C15
25	l	5004	LHG	C9-C10-C11-C12
21	2	1238	CLA	O1A-CGA-O2A-C1
21	b	1223	CLA	O1A-CGA-O2A-C1
22	B	2002	PQN	C26-C27-C28-C29
21	a	1105	CLA	C10-C11-C12-C13
21	b	1224	CLA	C2A-CAA-CBA-CGA
21	0	1501	CLA	C2A-CAA-CBA-CGA
21	a	1012	CLA	C2A-CAA-CBA-CGA
21	b	1204	CLA	C2A-CAA-CBA-CGA
21	2	1215	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	2	1218	CLA	C2A-CAA-CBA-CGA
21	1	1128	CLA	C2A-CAA-CBA-CGA
21	A	1801	CLA	C5-C6-C7-C8
21	2	1237	CLA	C8-C10-C11-C12
21	a	1123	CLA	C10-C11-C12-C13
22	a	2001	PQN	C23-C25-C26-C27
21	1	1128	CLA	C13-C15-C16-C17
21	a	1116	CLA	CAA-CBA-CGA-O2A
26	A	5002	LMG	C13-C14-C15-C16
21	a	1131	CLA	C15-C16-C17-C18
21	b	1205	CLA	C5-C6-C7-C8
21	b	1223	CLA	CBA-CGA-O2A-C1
25	A	5005	LHG	C14-C15-C16-C17
21	b	1022	CLA	C16-C17-C18-C20
21	l	1503	CLA	C16-C17-C18-C20
21	1	1116	CLA	C15-C16-C17-C18
21	a	1127	CLA	C10-C11-C12-C13
21	b	1231	CLA	C10-C11-C12-C13
21	2	1235	CLA	C5-C6-C7-C8
21	1	1013	CLA	C4-C3-C5-C6
21	b	1205	CLA	C4-C3-C5-C6
21	B	1219	CLA	C5-C6-C7-C8
21	b	1227	CLA	C10-C11-C12-C13
21	b	1240	CLA	C13-C15-C16-C17
21	2	1202	CLA	C2-C3-C5-C6
25	a	5001	LHG	C15-C16-C17-C18
25	A	5007	LHG	C31-C32-C33-C34
21	b	1202	CLA	C15-C16-C17-C18
21	a	1118	CLA	C15-C16-C17-C18
21	a	1133	CLA	C3-C5-C6-C7
21	A	1105	CLA	C3-C5-C6-C7
21	b	1021	CLA	C3-C5-C6-C7
25	l	5003	LHG	O9-C7-O7-C5
21	A	1011	CLA	C16-C17-C18-C19
24	6	4016	BCR	C12-C13-C14-C15
28	B	4011	45D	C24-C26-C30-C32
28	B	4011	45D	C33-C35-C37-C41
24	f	4016	BCR	C12-C13-C14-C15
24	l	4022	BCR	C11-C10-C9-C8
24	2	4018	BCR	C20-C21-C22-C23
36	I	4020	EQ3	C11-C10-C9-C8
24	2	4011	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	9	4021	BCR	C12-C13-C14-C15
30	M	4021	ECH	C11-C10-C9-C8
30	b	4011	ECH	C16-C17-C18-C19
34	F	4016	ZEX	C12-C13-C14-C15
30	B	4006	ECH	C11-C10-C9-C8
30	B	4006	ECH	C12-C13-C14-C15
30	b	4006	ECH	C11-C10-C9-C8
30	2	4006	ECH	C11-C10-C9-C8
30	m	4021	ECH	C11-C10-C9-C8
26	1	5004	LMG	O7-C8-C9-O8
34	7	4015	ZEX	C29-C30-C31-C32
24	a	4008	BCR	C19-C20-C21-C22
24	1	4008	BCR	C15-C16-C17-C18
24	8	4001	BCR	C15-C16-C17-C18
24	B	4018	BCR	C15-C16-C17-C18
24	2	4017	BCR	C15-C16-C17-C18
25	F	5002	LHG	C16-C17-C18-C19
25	B	5006	LHG	C10-C11-C12-C13
21	b	1023	CLA	C15-C16-C17-C18
31	B	5008	SQD	C17-C18-C19-C20
21	b	1021	CLA	O1A-CGA-O2A-C1
25	b	5004	LHG	C1-C2-C3-O3
25	1	5005	LHG	C19-C20-C21-C22
21	J	1303	CLA	C3-C5-C6-C7
21	2	1229	CLA	C4-C3-C5-C6
21	2	1202	CLA	C4-C3-C5-C6
21	A	1118	CLA	C4-C3-C5-C6
25	B	5006	LHG	C33-C34-C35-C36
35	0	6001	LMT	C1-C2-C3-C4
21	2	1238	CLA	C2-C1-O2A-CGA
21	B	1208	CLA	C2-C1-O2A-CGA
21	B	1226	CLA	C2-C1-O2A-CGA
21	K	1402	CLA	C2-C1-O2A-CGA
21	2	1022	CLA	C2-C3-C5-C6
21	B	1211	CLA	C2-C3-C5-C6
21	B	1224	CLA	C2-C3-C5-C6
21	B	1205	CLA	C2-C3-C5-C6
21	b	1238	CLA	CBD-CGD-O2D-CED
26	A	5008	LMG	C18-C19-C20-C21
21	1	1103	CLA	CAA-CBA-CGA-O2A
21	A	1114	CLA	C11-C10-C8-C9
21	A	1112	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	b	1228	CLA	C11-C12-C13-C14
21	B	1215	CLA	C11-C10-C8-C9
21	K	1402	CLA	C6-C7-C8-C9
21	2	1211	CLA	O1A-CGA-O2A-C1
21	1	1107	CLA	O1A-CGA-O2A-C1
35	F	6001	LMT	O5B-C1B-O1B-C4'
21	1	1137	CLA	C4-C3-C5-C6
31	b	5006	SQD	C15-C16-C17-C18
25	l	5004	LHG	C27-C28-C29-C30
21	b	1210	CLA	C10-C11-C12-C13
21	2	1229	CLA	C2A-CAA-CBA-CGA
21	a	1102	CLA	C2A-CAA-CBA-CGA
21	A	1112	CLA	C2A-CAA-CBA-CGA
21	B	1224	CLA	C2A-CAA-CBA-CGA
21	J	1302	CLA	C2A-CAA-CBA-CGA
24	a	4001	BCR	C1-C6-C7-C8
24	1	4001	BCR	C1-C6-C7-C8
24	1	4007	BCR	C1-C6-C7-C8
36	I	4020	EQ3	C23-C24-C25-C30
24	J	4013	BCR	C23-C24-C25-C30
24	b	4017	BCR	C1-C6-C7-C8
24	I	4018	BCR	C1-C6-C7-C8
24	b	4014	BCR	C23-C24-C25-C26
24	1	4008	BCR	C1-C6-C7-C8
24	8	4001	BCR	C1-C6-C7-C8
24	b	4005	BCR	C23-C24-C25-C30
24	a	4003	BCR	C1-C6-C7-C8
24	a	4003	BCR	C23-C24-C25-C30
24	B	4018	BCR	C23-C24-C25-C30
24	A	4019	BCR	C23-C24-C25-C30
24	L	4022	BCR	C23-C24-C25-C30
24	A	4007	BCR	C23-C24-C25-C30
24	1	4019	BCR	C23-C24-C25-C30
21	B	1219	CLA	C15-C16-C17-C18
21	a	1801	CLA	CAA-CBA-CGA-O2A
21	2	1202	CLA	CAA-CBA-CGA-O2A
25	l	5004	LHG	O8-C23-C24-C25
24	I	4018	BCR	C7-C8-C9-C34
26	A	5004	LMG	O1-C7-C8-C9
26	A	5004	LMG	C11-C12-C13-C14
21	b	1222	CLA	C15-C16-C17-C18
24	1	4001	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	K	4001	BCR	C19-C20-C21-C22
24	a	4002	BCR	C9-C10-C11-C12
24	a	4002	BCR	C19-C20-C21-C22
25	l	5002	LHG	C33-C34-C35-C36
25	1	5001	LHG	C33-C34-C35-C36
21	2	1235	CLA	C4-C3-C5-C6
21	0	1501	CLA	C4-C3-C5-C6
21	a	1110	CLA	C4-C3-C5-C6
21	B	1219	CLA	C2-C3-C5-C6
21	a	1131	CLA	C2-C3-C5-C6
21	a	1105	CLA	C2-C3-C5-C6
21	2	1207	CLA	C2-C3-C5-C6
21	a	1118	CLA	C2-C3-C5-C6
21	1	1011	CLA	CAA-CBA-CGA-O2A
25	a	5005	LHG	O8-C23-C24-C25
25	A	5005	LHG	C32-C33-C34-C35
21	a	1104	CLA	C10-C11-C12-C13
25	A	5001	LHG	C9-C10-C11-C12
25	a	5003	LHG	C25-C26-C27-C28
21	a	1116	CLA	C11-C12-C13-C14
21	B	1213	CLA	C16-C17-C18-C20
21	A	1113	CLA	C16-C17-C18-C19
21	B	1223	CLA	C16-C17-C18-C20
21	2	1204	CLA	C16-C17-C18-C20
21	B	1235	CLA	C16-C17-C18-C20
21	b	1209	CLA	C16-C17-C18-C19
21	1	1136	CLA	C16-C17-C18-C19
21	A	1133	CLA	C10-C11-C12-C13
25	A	5003	LHG	O6-C4-C5-O7
21	B	1201	CLA	C2A-CAA-CBA-CGA
25	1	5003	LHG	C24-C23-O8-C6
25	1	5005	LHG	C34-C35-C36-C37
21	B	1211	CLA	C3-C5-C6-C7
25	B	5004	LHG	C24-C25-C26-C27
26	A	5008	LMG	C19-C20-C21-C22
21	L	1501	CLA	C5-C6-C7-C8
21	B	1203	CLA	C15-C16-C17-C18
22	B	2002	PQN	C14-C13-C15-C16
21	F	1302	CLA	C4-C3-C5-C6
21	b	1206	CLA	C4-C3-C5-C6
21	1	1120	CLA	C4-C3-C5-C6
21	a	1108	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	K	5009	LMG	C24-C25-C26-C27
21	a	1101	CLA	C6-C7-C8-C10
21	a	1121	CLA	C11-C10-C8-C7
21	B	1219	CLA	C11-C12-C13-C15
21	2	1225	CLA	C11-C12-C13-C15
21	1	1132	CLA	C12-C13-C15-C16
21	A	1105	CLA	C11-C12-C13-C15
21	1	1103	CLA	C11-C10-C8-C7
21	A	1122	CLA	C2-C3-C5-C6
21	B	1228	CLA	C6-C7-C8-C10
21	b	1205	CLA	C2-C3-C5-C6
21	J	1303	CLA	C2-C3-C5-C6
21	0	1501	CLA	C2-C3-C5-C6
21	b	1218	CLA	C11-C12-C13-C15
21	f	1302	CLA	C11-C12-C13-C15
21	a	1139	CLA	C6-C7-C8-C10
21	A	1131	CLA	C2-C3-C5-C6
21	b	1238	CLA	C11-C10-C8-C7
21	b	1210	CLA	C11-C12-C13-C15
21	1	1128	CLA	C12-C13-C15-C16
25	B	5004	LHG	C33-C34-C35-C36
24	L	4022	BCR	C13-C14-C15-C16
24	A	4007	BCR	C19-C20-C21-C22
24	2	4004	BCR	C13-C14-C15-C16
26	0	5001	LMG	O7-C10-C11-C12
21	a	1103	CLA	CAA-CBA-CGA-O2A
21	B	1217	CLA	C16-C17-C18-C20
21	a	1109	CLA	C13-C15-C16-C17
25	M	5001	LHG	O7-C5-C6-O8
25	F	5002	LHG	O7-C5-C6-O8
26	A	5008	LMG	O10-C28-O8-C9
21	1	1107	CLA	CBA-CGA-O2A-C1
25	B	5004	LHG	C32-C33-C34-C35
25	F	5002	LHG	O8-C23-C24-C25
21	a	1129	CLA	CAA-CBA-CGA-O2A
25	a	5003	LHG	O7-C7-C8-C9
21	b	1224	CLA	C8-C10-C11-C12
21	K	1401	CLA	C8-C10-C11-C12
25	a	5003	LHG	C14-C15-C16-C17
21	1	1138	CLA	C11-C12-C13-C14
21	1	1117	CLA	C16-C17-C18-C19
21	b	1238	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	L	5002	SQD	C28-C29-C30-C31
25	l	5004	LHG	C19-C20-C21-C22
24	B	4018	BCR	C11-C10-C9-C34
25	B	5006	LHG	C25-C26-C27-C28
24	b	4018	BCR	C11-C10-C9-C34
31	B	5008	SQD	C7-C8-C9-C10
26	B	5002	LMG	O7-C10-C11-C12
21	l	1503	CLA	CAA-CBA-CGA-O2A
21	K	1401	CLA	C4-C3-C5-C6
21	b	1226	CLA	C4-C3-C5-C6
21	b	1207	CLA	C4-C3-C5-C6
21	A	1013	CLA	C4-C3-C5-C6
21	2	1224	CLA	C4-C3-C5-C6
21	1	1013	CLA	C13-C15-C16-C17
21	a	1105	CLA	C8-C10-C11-C12
21	B	1022	CLA	C8-C10-C11-C12
21	b	1213	CLA	O1A-CGA-O2A-C1
21	j	1302	CLA	C2-C3-C5-C6
21	1	1013	CLA	C2-C3-C5-C6
21	a	1109	CLA	C2-C3-C5-C6
21	a	1136	CLA	C2-C3-C5-C6
21	A	1109	CLA	C2-C3-C5-C6
25	1	5001	LHG	C12-C13-C14-C15
21	b	1213	CLA	C10-C11-C12-C13
25	A	5001	LHG	O7-C7-C8-C9
21	1	1125	CLA	CAA-CBA-CGA-O2A
21	b	1219	CLA	CAA-CBA-CGA-O2A
31	B	5008	SQD	C15-C16-C17-C18
21	1	1139	CLA	C14-C13-C15-C16
21	b	1220	CLA	C11-C12-C13-C14
21	2	1214	CLA	C6-C7-C8-C9
21	a	1102	CLA	C11-C12-C13-C14
21	b	1216	CLA	C14-C13-C15-C16
21	B	1237	CLA	C11-C10-C8-C9
21	B	1217	CLA	C11-C10-C8-C9
21	b	1203	CLA	C14-C13-C15-C16
21	a	1011	CLA	C14-C13-C15-C16
21	1	1106	CLA	C11-C10-C8-C9
22	B	2002	PQN	C16-C17-C18-C19
21	A	1103	CLA	C14-C13-C15-C16
21	K	1401	CLA	C14-C13-C15-C16
21	B	1208	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	a	1106	CLA	C6-C7-C8-C9
21	1	1103	CLA	C11-C12-C13-C14
21	l	1501	CLA	C11-C10-C8-C9
21	A	1106	CLA	C11-C10-C8-C9
21	a	1112	CLA	C11-C12-C13-C14
21	2	1205	CLA	C6-C7-C8-C9
21	0	1501	CLA	C11-C12-C13-C14
21	a	1104	CLA	C14-C13-C15-C16
21	b	1231	CLA	C6-C7-C8-C9
21	A	1130	CLA	C11-C10-C8-C9
21	a	1139	CLA	C14-C13-C15-C16
21	2	1023	CLA	C6-C7-C8-C9
21	a	1117	CLA	C6-C7-C8-C9
21	l	1502	CLA	C6-C7-C8-C9
21	a	1118	CLA	C14-C13-C15-C16
21	1	1136	CLA	C6-C7-C8-C9
21	1	1138	CLA	C11-C10-C8-C9
21	b	1230	CLA	C6-C7-C8-C9
21	a	1135	CLA	C14-C13-C15-C16
21	b	1213	CLA	C11-C12-C13-C14
21	A	1118	CLA	C11-C12-C13-C14
26	a	5004	LMG	C29-C30-C31-C32
26	2	5002	LMG	C22-C23-C24-C25
21	A	1126	CLA	C3A-C2A-CAA-CBA
21	a	1011	CLA	C3A-C2A-CAA-CBA
21	A	1011	CLA	C3A-C2A-CAA-CBA
21	a	1128	CLA	C3A-C2A-CAA-CBA
21	A	1138	CLA	C3A-C2A-CAA-CBA
21	b	1021	CLA	C3A-C2A-CAA-CBA
21	B	1223	CLA	C3A-C2A-CAA-CBA
21	2	1232	CLA	C3A-C2A-CAA-CBA
21	B	1022	CLA	C3A-C2A-CAA-CBA
21	a	1120	CLA	C3A-C2A-CAA-CBA
25	a	5003	LHG	C27-C28-C29-C30
25	b	5004	LHG	O2-C2-C3-O3
21	2	1214	CLA	O1A-CGA-O2A-C1
21	2	1230	CLA	CAA-CBA-CGA-O2A
25	l	5001	LHG	O7-C7-C8-C9
21	1	1108	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	C30-C31-C32-C33
21	1	1112	CLA	CAD-CBD-CGD-O2D
21	b	1227	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	8	1402	CLA	CAD-CBD-CGD-O2D
21	A	1011	CLA	CAD-CBD-CGD-O2D
21	B	1222	CLA	CAD-CBD-CGD-O2D
21	L	1501	CLA	CAD-CBD-CGD-O2D
21	6	1302	CLA	CAD-CBD-CGD-O2D
21	B	1218	CLA	CAD-CBD-CGD-O2D
21	6	1301	CLA	CAD-CBD-CGD-O2D
21	2	1209	CLA	CAD-CBD-CGD-O2D
21	1	1138	CLA	CAD-CBD-CGD-O2D
21	1	1120	CLA	CAD-CBD-CGD-O2D
21	a	1125	CLA	CAD-CBD-CGD-O2D
21	B	1225	CLA	C16-C17-C18-C19
31	0	5005	SQD	C14-C15-C16-C17
21	b	1212	CLA	C10-C11-C12-C13
21	a	1132	CLA	C2A-CAA-CBA-CGA
21	b	1215	CLA	C2A-CAA-CBA-CGA
25	A	5005	LHG	C29-C30-C31-C32
21	a	1123	CLA	C13-C15-C16-C17
21	l	1502	CLA	C15-C16-C17-C18
21	B	1204	CLA	C2-C1-O2A-CGA
25	M	5001	LHG	O7-C7-C8-C9
21	b	1216	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	O8-C23-C24-C25
21	k	1402	CLA	CAA-CBA-CGA-O2A
26	2	5002	LMG	O7-C10-C11-C12
21	a	1117	CLA	C15-C16-C17-C18
21	1	1124	CLA	C4-C3-C5-C6
21	B	1220	CLA	C2-C3-C5-C6
21	2	1224	CLA	C2-C3-C5-C6
21	A	1118	CLA	C2-C3-C5-C6
21	2	1214	CLA	CAA-CBA-CGA-O2A
25	l	5002	LHG	O7-C7-C8-C9
21	a	1128	CLA	CAA-CBA-CGA-O2A
26	0	5001	LMG	C19-C20-C21-C22
25	B	5006	LHG	C30-C31-C32-C33
25	l	5004	LHG	C24-C25-C26-C27
31	0	5005	SQD	C28-C29-C30-C31
24	1	4007	BCR	C11-C12-C13-C14
24	1	4007	BCR	C17-C18-C19-C20
24	b	4014	BCR	C7-C8-C9-C10
24	1	4008	BCR	C21-C22-C23-C24
24	b	4004	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	i	4020	ECH	C17-C18-C19-C20
21	1	1801	CLA	C11-C10-C8-C9
37	L	5004	DGD	O1G-C1G-C2G-C3G
26	1	5004	LMG	C7-C8-C9-O8
25	1	5007	LHG	C4-C5-C6-O8
25	1	5003	LHG	O10-C23-O8-C6
21	A	1121	CLA	C3-C5-C6-C7
26	A	5004	LMG	O8-C28-C29-C30
21	1	1136	CLA	CAA-CBA-CGA-O2A
26	A	5002	LMG	O8-C28-C29-C30
21	a	1122	CLA	O2A-C1-C2-C3
37	L	5004	DGD	CAB-CBB-CCB-CDB
25	B	5004	LHG	C10-C11-C12-C13
21	2	1211	CLA	CBA-CGA-O2A-C1
21	2	1238	CLA	CBA-CGA-O2A-C1
21	a	1116	CLA	C2A-CAA-CBA-CGA
21	2	1202	CLA	C2A-CAA-CBA-CGA
21	1	1106	CLA	C3-C5-C6-C7
21	A	1011	CLA	C16-C17-C18-C20
21	b	1201	CLA	C16-C17-C18-C19
21	A	1133	CLA	C16-C17-C18-C20
31	0	5005	SQD	C11-C10-C9-C8
25	B	5004	LHG	C16-C17-C18-C19
21	1	1011	CLA	CHA-CBD-CGD-O2D
21	2	1214	CLA	CHA-CBD-CGD-O1D
21	2	1214	CLA	CHA-CBD-CGD-O2D
21	b	1225	CLA	CHA-CBD-CGD-O1D
21	b	1225	CLA	CHA-CBD-CGD-O2D
21	A	1114	CLA	CHA-CBD-CGD-O2D
21	b	1211	CLA	CHA-CBD-CGD-O1D
21	2	1236	CLA	CHA-CBD-CGD-O1D
21	2	1236	CLA	CHA-CBD-CGD-O2D
21	B	1216	CLA	CHA-CBD-CGD-O1D
21	B	1216	CLA	CHA-CBD-CGD-O2D
21	a	1121	CLA	CHA-CBD-CGD-O1D
21	a	1121	CLA	CHA-CBD-CGD-O2D
21	A	1126	CLA	CHA-CBD-CGD-O1D
21	A	1126	CLA	CHA-CBD-CGD-O2D
21	B	1217	CLA	CHA-CBD-CGD-O2D
21	a	1011	CLA	CHA-CBD-CGD-O1D
21	a	1011	CLA	CHA-CBD-CGD-O2D
21	2	1201	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	a	1133	CLA	CHA-CBD-CGD-O2D
21	1	1119	CLA	CHA-CBD-CGD-O1D
21	1	1119	CLA	CHA-CBD-CGD-O2D
21	a	1123	CLA	CHA-CBD-CGD-O1D
21	a	1123	CLA	CHA-CBD-CGD-O2D
21	B	1211	CLA	CHA-CBD-CGD-O2D
21	8	1402	CLA	CHA-CBD-CGD-O2D
21	B	1224	CLA	CHA-CBD-CGD-O1D
21	B	1224	CLA	CHA-CBD-CGD-O2D
21	a	1127	CLA	CHA-CBD-CGD-O1D
21	a	1127	CLA	CHA-CBD-CGD-O2D
21	b	1212	CLA	CHA-CBD-CGD-O2D
21	b	1206	CLA	CHA-CBD-CGD-O1D
21	b	1206	CLA	CHA-CBD-CGD-O2D
21	1	1118	CLA	CHA-CBD-CGD-O1D
21	1	1118	CLA	CHA-CBD-CGD-O2D
21	B	1230	CLA	CHA-CBD-CGD-O1D
21	a	1129	CLA	CHA-CBD-CGD-O2D
21	A	1136	CLA	CHA-CBD-CGD-O1D
21	A	1136	CLA	CHA-CBD-CGD-O2D
21	2	1207	CLA	CHA-CBD-CGD-O1D
21	2	1207	CLA	CHA-CBD-CGD-O2D
21	1	1123	CLA	CHA-CBD-CGD-O1D
21	B	1223	CLA	CHA-CBD-CGD-O1D
21	B	1223	CLA	CHA-CBD-CGD-O2D
21	0	1501	CLA	CHA-CBD-CGD-O2D
21	1	1801	CLA	CHA-CBD-CGD-O1D
21	1	1801	CLA	CHA-CBD-CGD-O2D
21	B	1201	CLA	CHA-CBD-CGD-O2D
21	a	1104	CLA	CHA-CBD-CGD-O1D
21	a	1104	CLA	CHA-CBD-CGD-O2D
21	1	1125	CLA	CHA-CBD-CGD-O1D
21	b	1204	CLA	CHA-CBD-CGD-O1D
21	b	1204	CLA	CHA-CBD-CGD-O2D
21	b	1237	CLA	CHA-CBD-CGD-O1D
21	2	1215	CLA	CHA-CBD-CGD-O2D
21	B	1235	CLA	CHA-CBD-CGD-O1D
21	B	1235	CLA	CHA-CBD-CGD-O2D
21	a	1139	CLA	CHA-CBD-CGD-O2D
21	1	1126	CLA	CHA-CBD-CGD-O1D
21	1	1126	CLA	CHA-CBD-CGD-O2D
21	b	1207	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	1021	CLA	CHA-CBD-CGD-O2D
21	2	1240	CLA	CHA-CBD-CGD-O1D
21	2	1240	CLA	CHA-CBD-CGD-O2D
21	A	1119	CLA	CHA-CBD-CGD-O2D
21	1	1114	CLA	CHA-CBD-CGD-O1D
21	1	1114	CLA	CHA-CBD-CGD-O2D
21	A	1125	CLA	CHA-CBD-CGD-O1D
24	A	4019	BCR	C19-C20-C21-C22
21	a	1136	CLA	CHA-CBD-CGD-O1D
21	a	1136	CLA	CHA-CBD-CGD-O2D
21	A	1108	CLA	CHA-CBD-CGD-O2D
21	A	1013	CLA	CHA-CBD-CGD-O1D
21	A	1013	CLA	CHA-CBD-CGD-O2D
21	b	1023	CLA	CHA-CBD-CGD-O2D
21	B	1225	CLA	CHA-CBD-CGD-O1D
21	B	1225	CLA	CHA-CBD-CGD-O2D
21	a	1137	CLA	CHA-CBD-CGD-O1D
21	2	1224	CLA	CHA-CBD-CGD-O1D
21	2	1224	CLA	CHA-CBD-CGD-O2D
21	b	1213	CLA	CHA-CBD-CGD-O2D
21	A	1127	CLA	CHA-CBD-CGD-O1D
21	A	1127	CLA	CHA-CBD-CGD-O2D
21	a	1126	CLA	CHA-CBD-CGD-O2D
21	A	1118	CLA	CHA-CBD-CGD-O1D
21	A	1118	CLA	CHA-CBD-CGD-O2D
21	a	1120	CLA	CHA-CBD-CGD-O2D
21	a	1119	CLA	CHA-CBD-CGD-O2D
21	A	1115	CLA	C15-C16-C17-C18
21	a	1112	CLA	C4-C3-C5-C6
26	A	5004	LMG	O7-C10-C11-C12
25	a	5005	LHG	O7-C7-C8-C9
21	2	1219	CLA	CAA-CBA-CGA-O2A
26	A	5008	LMG	C29-C28-O8-C9
21	1	1124	CLA	C2-C3-C5-C6
21	1	1139	CLA	C10-C11-C12-C13
25	0	5002	LHG	O6-C4-C5-C6
24	B	4018	BCR	C11-C10-C9-C8
24	b	4018	BCR	C11-C10-C9-C8
21	B	1237	CLA	C16-C17-C18-C19
25	B	5004	LHG	O8-C23-C24-C25
25	a	5007	LHG	O7-C7-C8-C9
25	l	5004	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	b	5006	SQD	C24-C25-C26-C27
31	B	5008	SQD	O49-C7-C8-C9
35	1	6001	LMT	C9-C10-C11-C12
25	l	5002	LHG	O9-C7-O7-C5
21	b	1239	CLA	C15-C16-C17-C18
31	F	5001	SQD	O48-C23-C24-C25
21	a	1122	CLA	CAA-CBA-CGA-O2A
21	1	1107	CLA	CAA-CBA-CGA-O2A
21	L	1502	CLA	CAA-CBA-CGA-O2A
21	b	1210	CLA	CAA-CBA-CGA-O2A
21	A	1134	CLA	O1D-CGD-O2D-CED
21	B	1226	CLA	C8-C10-C11-C12
25	A	5001	LHG	C24-C23-O8-C6
25	l	5003	LHG	C8-C7-O7-C5
21	A	1801	CLA	CAA-CBA-CGA-O2A
21	B	1210	CLA	CAA-CBA-CGA-O2A
21	B	1222	CLA	C4-C3-C5-C6
21	J	1302	CLA	C4-C3-C5-C6
21	a	1139	CLA	O1A-CGA-O2A-C1
21	b	1227	CLA	C5-C6-C7-C8
21	B	1214	CLA	C2-C3-C5-C6
21	2	1214	CLA	C2-C3-C5-C6
21	A	1801	CLA	C11-C12-C13-C15
21	a	1115	CLA	C11-C12-C13-C15
21	L	1503	CLA	C11-C12-C13-C15
21	l	1503	CLA	C11-C10-C8-C7
21	b	1226	CLA	C2-C3-C5-C6
21	a	1130	CLA	C6-C7-C8-C10
21	2	1205	CLA	C11-C12-C13-C15
21	b	1218	CLA	C6-C7-C8-C10
21	A	1111	CLA	C11-C12-C13-C15
21	2	1202	CLA	C12-C13-C15-C16
21	2	1215	CLA	C11-C10-C8-C7
21	A	1117	CLA	C6-C7-C8-C10
21	A	1117	CLA	C12-C13-C15-C16
21	a	1118	CLA	C11-C12-C13-C15
21	J	1302	CLA	C6-C7-C8-C10
21	a	1126	CLA	C11-C12-C13-C15
21	a	1108	CLA	C2-C3-C5-C6
21	B	1213	CLA	C16-C17-C18-C19
21	2	1238	CLA	C16-C17-C18-C20
21	B	1210	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	a	1128	CLA	C5-C6-C7-C8
21	2	1210	CLA	CAA-CBA-CGA-O2A
21	A	1136	CLA	CAA-CBA-CGA-O2A
26	K	5009	LMG	O7-C10-C11-C12
26	b	5002	LMG	O7-C10-C11-C12
21	b	1230	CLA	CAA-CBA-CGA-O2A
31	L	5001	SQD	O47-C7-C8-C9
21	A	1801	CLA	C11-C12-C13-C14
21	1	1134	CLA	C11-C10-C8-C9
21	b	1240	CLA	C11-C12-C13-C14
21	1	1116	CLA	C11-C12-C13-C14
21	L	1503	CLA	C11-C12-C13-C14
21	b	1212	CLA	C11-C10-C8-C9
21	1	1101	CLA	C11-C10-C8-C9
21	b	1239	CLA	C14-C13-C15-C16
21	A	1111	CLA	C6-C7-C8-C9
21	A	1134	CLA	C11-C12-C13-C14
21	A	1107	CLA	C11-C12-C13-C14
22	2	2002	PQN	C16-C17-C18-C19
22	A	2001	PQN	C24-C23-C25-C26
21	A	1117	CLA	C14-C13-C15-C16
21	a	1110	CLA	C11-C10-C8-C9
21	2	1203	CLA	C11-C10-C8-C9
21	2	1239	CLA	C11-C12-C13-C14
21	b	1223	CLA	C6-C7-C8-C9
21	2	1221	CLA	C6-C7-C8-C9
21	A	1120	CLA	C14-C13-C15-C16
21	A	1102	CLA	C14-C13-C15-C16
21	J	1302	CLA	C6-C7-C8-C9
25	1	5007	LHG	C5-C6-O8-C23
24	l	4022	BCR	C19-C20-C21-C22
24	b	4018	BCR	C15-C16-C17-C18
21	b	1203	CLA	CBA-CGA-O2A-C1
21	b	1021	CLA	CBA-CGA-O2A-C1
21	a	1139	CLA	CBA-CGA-O2A-C1
21	b	1213	CLA	CBA-CGA-O2A-C1
21	a	1128	CLA	C13-C15-C16-C17
21	a	1107	CLA	CAA-CBA-CGA-O2A
26	b	5005	LMG	O8-C28-C29-C30
25	A	5001	LHG	O10-C23-C24-C25
25	0	5004	LHG	O10-C23-C24-C25
31	f	5001	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
31	0	5005	SQD	C4-C5-C6-S
21	L	1503	CLA	C16-C17-C18-C20
21	2	1202	CLA	C3-C5-C6-C7
25	l	5002	LHG	C8-C7-O7-C5
21	b	1220	CLA	C2A-CAA-CBA-CGA
25	a	5003	LHG	O9-C7-C8-C9
21	A	1113	CLA	CAA-CBA-CGA-O2A
25	A	5006	LHG	C15-C16-C17-C18
31	0	5005	SQD	C35-C36-C37-C38
21	b	1022	CLA	C16-C17-C18-C19
25	l	5002	LHG	O1-C1-C2-C3
25	L	5005	LHG	O1-C1-C2-C3
21	B	1021	CLA	O1A-CGA-O2A-C1
26	1	5004	LMG	O7-C10-C11-C12
25	0	5002	LHG	C19-C20-C21-C22
26	0	5001	LMG	O9-C10-C11-C12
21	2	1214	CLA	CAA-CBA-CGA-O1A
25	l	5002	LHG	O9-C7-C8-C9
25	M	5001	LHG	O9-C7-C8-C9
25	F	5002	LHG	O10-C23-C24-C25
25	A	5001	LHG	O9-C7-C8-C9
34	7	4015	ZEX	C31-C32-C33-C34
24	2	4018	BCR	C21-C22-C23-C24
31	B	5008	SQD	C9-C10-C11-C12
25	1	5003	LHG	C19-C20-C21-C22
21	1	1115	CLA	C10-C11-C12-C13
21	A	1131	CLA	C10-C11-C12-C13
25	A	5001	LHG	O10-C23-O8-C6
21	2	1229	CLA	C2C-C3C-CAC-CBC
26	b	5005	LMG	C11-C12-C13-C14
21	A	1114	CLA	C1A-C2A-CAA-CBA
21	A	1101	CLA	C1A-C2A-CAA-CBA
21	b	1214	CLA	C1A-C2A-CAA-CBA
21	1	1101	CLA	C1A-C2A-CAA-CBA
21	l	1503	CLA	C1A-C2A-CAA-CBA
21	B	1228	CLA	C1A-C2A-CAA-CBA
21	1	1105	CLA	C1A-C2A-CAA-CBA
21	0	1503	CLA	C1A-C2A-CAA-CBA
21	2	1232	CLA	C1A-C2A-CAA-CBA
21	a	1124	CLA	C1A-C2A-CAA-CBA
21	B	1022	CLA	C1A-C2A-CAA-CBA
21	2	1203	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	1	1012	CLA	C1A-C2A-CAA-CBA
21	A	1102	CLA	C1A-C2A-CAA-CBA
21	1	1128	CLA	C1A-C2A-CAA-CBA
25	1	5005	LHG	C10-C11-C12-C13
31	0	5005	SQD	C16-C17-C18-C19
21	B	1222	CLA	C6-C7-C8-C9
21	k	1402	CLA	CAA-CBA-CGA-O1A
21	1	1125	CLA	CAA-CBA-CGA-O1A
26	2	5002	LMG	C40-C41-C42-C43
21	b	1203	CLA	O1A-CGA-O2A-C1
21	B	1202	CLA	C2-C1-O2A-CGA
21	B	1235	CLA	C2-C1-O2A-CGA
25	1	5001	LHG	C18-C19-C20-C21
26	1	5004	LMG	C34-C35-C36-C37
21	2	1214	CLA	CBA-CGA-O2A-C1
26	A	5004	LMG	O10-C28-C29-C30
21	l	1503	CLA	CAA-CBA-CGA-O1A
25	a	5005	LHG	O9-C7-C8-C9
21	2	1219	CLA	CAA-CBA-CGA-O1A
21	b	1219	CLA	CAA-CBA-CGA-O1A
31	B	5008	SQD	C28-C29-C30-C31
25	F	5002	LHG	C4-C5-C6-O8
31	L	5002	SQD	O6-C44-C45-C46
21	A	1114	CLA	CAA-CBA-CGA-O2A
21	2	1211	CLA	CAA-CBA-CGA-O2A
25	A	5007	LHG	O7-C7-C8-C9
25	A	5003	LHG	C24-C25-C26-C27
25	l	5004	LHG	C29-C30-C31-C32
21	A	1114	CLA	C13-C15-C16-C17
25	L	5005	LHG	C29-C30-C31-C32
21	a	1129	CLA	CAA-CBA-CGA-O1A
21	1	1136	CLA	CAA-CBA-CGA-O1A
21	A	1112	CLA	C10-C11-C12-C13
25	1	5005	LHG	C5-C6-O8-C23
25	A	5005	LHG	C25-C26-C27-C28
21	1	1129	CLA	CAA-CBA-CGA-O2A
21	1	1132	CLA	C5-C6-C7-C8
25	l	5001	LHG	O9-C7-O7-C5
21	b	1216	CLA	CAA-CBA-CGA-O1A
25	B	5004	LHG	O10-C23-C24-C25
21	2	1230	CLA	CAA-CBA-CGA-O1A
21	A	1113	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	l	5001	LHG	O9-C7-C8-C9
26	B	5002	LMG	O9-C10-C11-C12
26	A	5002	LMG	O10-C28-C29-C30
21	2	1209	CLA	C2A-CAA-CBA-CGA
35	0	6001	LMT	C2'-C1'-O1'-C1
21	1	1101	CLA	C5-C6-C7-C8
25	M	5001	LHG	C3-O3-P-O5
25	6	5001	LHG	C3-O3-P-O5
25	a	5007	LHG	C3-O3-P-O5
25	A	5003	LHG	C14-C15-C16-C17
25	a	5001	LHG	C26-C27-C28-C29
26	A	5004	LMG	O9-C10-C11-C12
21	2	1210	CLA	CAA-CBA-CGA-O1A
21	1	1107	CLA	CAA-CBA-CGA-O1A
26	b	5002	LMG	O9-C10-C11-C12
21	b	1215	CLA	CAA-CBA-CGA-O1A
21	b	1230	CLA	CAA-CBA-CGA-O1A
21	j	1303	CLA	CAA-CBA-CGA-O2A
24	a	4001	BCR	C5-C6-C7-C8
24	1	4001	BCR	C5-C6-C7-C8
24	1	4007	BCR	C5-C6-C7-C8
30	M	4021	ECH	C1-C6-C7-C8
24	1	4008	BCR	C5-C6-C7-C8
24	8	4001	BCR	C5-C6-C7-C8
24	a	4003	BCR	C5-C6-C7-C8
24	B	4018	BCR	C23-C24-C25-C26
24	A	4019	BCR	C23-C24-C25-C26
24	L	4022	BCR	C23-C24-C25-C26
21	A	1127	CLA	C3-C5-C6-C7
24	i	4018	BCR	C5-C6-C7-C8
21	1	1111	CLA	C15-C16-C17-C18
21	L	1502	CLA	CAA-CBA-CGA-O1A
21	1	1108	CLA	CAA-CBA-CGA-O1A
26	2	5002	LMG	O9-C10-C11-C12
26	A	5004	LMG	C13-C14-C15-C16
21	B	1204	CLA	CAA-CBA-CGA-O2A
21	b	1211	CLA	CAA-CBA-CGA-O2A
21	2	1234	CLA	CAA-CBA-CGA-O2A
21	a	1136	CLA	CAA-CBA-CGA-O2A
21	1	1109	CLA	C16-C17-C18-C20
26	b	5007	LMG	C18-C19-C20-C21
24	l	4019	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	1209	CLA	C2A-CAA-CBA-CGA
21	A	1128	CLA	C2A-CAA-CBA-CGA
21	A	1116	CLA	CAA-CBA-CGA-O1A
21	a	1128	CLA	CAA-CBA-CGA-O1A
21	A	1136	CLA	CAA-CBA-CGA-O1A
25	l	5004	LHG	O9-C7-C8-C9
21	b	1221	CLA	C10-C11-C12-C13
21	B	1214	CLA	CAA-CBA-CGA-O2A
21	1	1115	CLA	CAA-CBA-CGA-O2A
21	b	1021	CLA	C8-C10-C11-C12
25	a	5001	LHG	O10-C23-C24-C25
21	j	1302	CLA	C4-C3-C5-C6
21	A	1131	CLA	C4-C3-C5-C6
21	B	1206	CLA	C4-C3-C5-C6
24	A	4019	BCR	C13-C14-C15-C16
25	A	5005	LHG	C24-C25-C26-C27
21	1	1011	CLA	CAD-CBD-CGD-O1D
21	2	1213	CLA	CAD-CBD-CGD-O1D
21	A	1114	CLA	CAD-CBD-CGD-O1D
21	B	1240	CLA	CAD-CBD-CGD-O1D
21	1	1134	CLA	CAD-CBD-CGD-O1D
21	2	1201	CLA	CAD-CBD-CGD-O1D
21	a	1133	CLA	CAD-CBD-CGD-O1D
21	B	1224	CLA	CAD-CBD-CGD-O1D
21	A	1121	CLA	CAD-CBD-CGD-O1D
21	b	1231	CLA	CAD-CBD-CGD-O1D
21	2	1215	CLA	CAD-CBD-CGD-O1D
21	1	1109	CLA	CAD-CBD-CGD-O1D
31	f	5001	SQD	O5-C5-C6-S
21	A	1119	CLA	CAD-CBD-CGD-O1D
21	A	1108	CLA	CAD-CBD-CGD-O1D
21	a	1119	CLA	CAD-CBD-CGD-O1D
25	A	5007	LHG	O9-C7-C8-C9
25	F	5002	LHG	O7-C7-C8-C9
21	A	1106	CLA	CAA-CBA-CGA-O2A
21	b	1021	CLA	CAA-CBA-CGA-O2A
25	1	5005	LHG	O8-C23-C24-C25
21	B	1219	CLA	C8-C10-C11-C12
21	1	1104	CLA	C15-C16-C17-C18
21	a	1131	CLA	C13-C15-C16-C17
21	a	1011	CLA	C11-C12-C13-C14
21	2	1237	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	B	1231	CLA	C11-C12-C13-C14
22	B	2002	PQN	C24-C23-C25-C26
21	A	1105	CLA	C6-C7-C8-C9
21	1	1103	CLA	C11-C10-C8-C9
21	B	1202	CLA	C11-C12-C13-C14
21	b	1201	CLA	C11-C12-C13-C14
21	2	1204	CLA	C11-C12-C13-C14
21	2	1205	CLA	C11-C12-C13-C14
21	A	1134	CLA	C6-C7-C8-C9
21	2	1202	CLA	C14-C13-C15-C16
22	2	2002	PQN	C19-C18-C20-C21
21	b	1207	CLA	C6-C7-C8-C9
21	b	1213	CLA	C6-C7-C8-C9
21	a	1119	CLA	C6-C7-C8-C9
31	F	5001	SQD	O10-C23-C24-C25
21	2	1224	CLA	CAA-CBA-CGA-O1A
25	1	5002	LHG	C29-C30-C31-C32
26	2	5005	LMG	C16-C17-C18-C19
21	B	1213	CLA	C3-C5-C6-C7
21	B	1220	CLA	CAA-CBA-CGA-O2A
21	B	1216	CLA	CAA-CBA-CGA-O2A
21	L	1503	CLA	CAA-CBA-CGA-O2A
25	b	5004	LHG	O8-C23-C24-C25
21	b	1226	CLA	CAA-CBA-CGA-O2A
21	a	1134	CLA	CAA-CBA-CGA-O2A
21	2	1023	CLA	C8-C10-C11-C12
25	1	5005	LHG	O10-C23-C24-C25
37	L	5004	DGD	CDA-CEA-CFA-CGA
25	1	5001	LHG	C24-C25-C26-C27
35	0	6001	LMT	C6-C7-C8-C9
21	B	1217	CLA	CAA-CBA-CGA-O2A
21	8	1402	CLA	CAA-CBA-CGA-O2A
21	B	1226	CLA	CAA-CBA-CGA-O2A
21	A	1135	CLA	CAA-CBA-CGA-O2A
25	1	5003	LHG	O7-C7-C8-C9
21	A	1128	CLA	CAA-CBA-CGA-O2A
25	1	5003	LHG	O8-C23-C24-C25
21	a	1111	CLA	C15-C16-C17-C18
26	K	5009	LMG	O9-C10-C11-C12
31	L	5001	SQD	O49-C7-C8-C9
26	A	5004	LMG	C4-C5-C6-O5
21	B	1221	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	1	1140	CLA	C5-C6-C7-C8
21	B	1220	CLA	C6-C7-C8-C10
21	B	1220	CLA	C11-C10-C8-C7
21	A	1101	CLA	C3A-C2A-CAA-CBA
21	b	1203	CLA	C2-C3-C5-C6
21	b	1203	CLA	C11-C12-C13-C15
21	1	1134	CLA	C11-C10-C8-C7
21	A	1110	CLA	C11-C12-C13-C15
21	B	1231	CLA	C11-C12-C13-C15
21	b	1240	CLA	C11-C12-C13-C15
21	b	1229	CLA	C6-C7-C8-C10
21	1	1115	CLA	C6-C7-C8-C10
21	1	1106	CLA	C12-C13-C15-C16
22	B	2002	PQN	C16-C17-C18-C20
21	a	1131	CLA	C11-C10-C8-C7
21	1	1101	CLA	C3A-C2A-CAA-CBA
21	1	1101	CLA	C11-C10-C8-C7
21	A	1105	CLA	C6-C7-C8-C10
21	b	1228	CLA	C6-C7-C8-C10
21	0	1502	CLA	C6-C7-C8-C10
21	B	1202	CLA	C11-C12-C13-C15
21	L	1502	CLA	C11-C12-C13-C15
21	A	1121	CLA	C11-C10-C8-C7
21	b	1239	CLA	C12-C13-C15-C16
21	2	1207	CLA	C6-C7-C8-C10
21	2	1208	CLA	C6-C7-C8-C10
21	b	1201	CLA	C11-C12-C13-C15
21	A	1111	CLA	C6-C7-C8-C10
21	A	1115	CLA	C12-C13-C15-C16
21	2	1218	CLA	C12-C13-C15-C16
21	a	1110	CLA	C2-C3-C5-C6
21	A	1119	CLA	C11-C10-C8-C7
21	A	1125	CLA	C11-C12-C13-C15
21	a	1136	CLA	C11-C12-C13-C15
21	2	1239	CLA	C11-C12-C13-C15
21	b	1223	CLA	C6-C7-C8-C10
21	2	1221	CLA	C11-C10-C8-C7
21	B	1205	CLA	C12-C13-C15-C16
21	1	1012	CLA	C3A-C2A-CAA-CBA
21	A	1102	CLA	C12-C13-C15-C16
21	b	1213	CLA	C6-C7-C8-C10
21	b	1213	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	a	1114	CLA	C3A-C2A-CAA-CBA
21	A	1127	CLA	C6-C7-C8-C10
21	A	1118	CLA	C11-C10-C8-C7
21	a	1125	CLA	C12-C13-C15-C16
21	A	1801	CLA	CAA-CBA-CGA-O1A
21	a	1101	CLA	CAA-CBA-CGA-O1A
21	a	1122	CLA	CAA-CBA-CGA-O1A
21	b	1226	CLA	CAA-CBA-CGA-O1A
21	0	1503	CLA	CAA-CBA-CGA-O1A
21	b	1210	CLA	CAA-CBA-CGA-O1A
21	a	1134	CLA	CAA-CBA-CGA-O1A
21	2	1229	CLA	CAA-CBA-CGA-O2A
21	b	1208	CLA	CAA-CBA-CGA-O2A
21	B	1208	CLA	CAA-CBA-CGA-O2A
21	2	1207	CLA	CAA-CBA-CGA-O2A
21	1	1135	CLA	CAA-CBA-CGA-O2A
25	A	5003	LHG	O7-C7-C8-C9
25	a	5007	LHG	O8-C23-C24-C25
21	b	1232	CLA	CAA-CBA-CGA-O2A
31	B	5008	SQD	C27-C28-C29-C30
21	A	1109	CLA	C5-C6-C7-C8
24	1	4003	BCR	C17-C18-C19-C20
24	2	4014	BCR	C17-C18-C19-C20
24	1	4012	BCR	C17-C18-C19-C20
24	7	4013	BCR	C17-C18-C19-C20
21	b	1208	CLA	CAA-CBA-CGA-O1A
21	B	1210	CLA	CAA-CBA-CGA-O1A
21	2	1207	CLA	CAA-CBA-CGA-O1A
21	A	1135	CLA	CAA-CBA-CGA-O1A
21	j	1303	CLA	CAA-CBA-CGA-O1A
24	l	4022	BCR	C13-C14-C15-C16
34	J	4015	ZEX	C33-C34-C35-C15
21	l	1503	CLA	C16-C17-C18-C19
35	l	6001	LMT	C2-C1-O1'-C1'
21	J	1303	CLA	CAA-CBA-CGA-O2A
21	0	1503	CLA	CAA-CBA-CGA-O2A
26	A	5002	LMG	C14-C15-C16-C17
35	0	6001	LMT	O5'-C1'-O1'-C1
21	B	1211	CLA	C5-C6-C7-C8
21	2	1218	CLA	C8-C10-C11-C12
21	b	1223	CLA	C10-C11-C12-C13
21	b	1219	CLA	C10-C11-C12-C13

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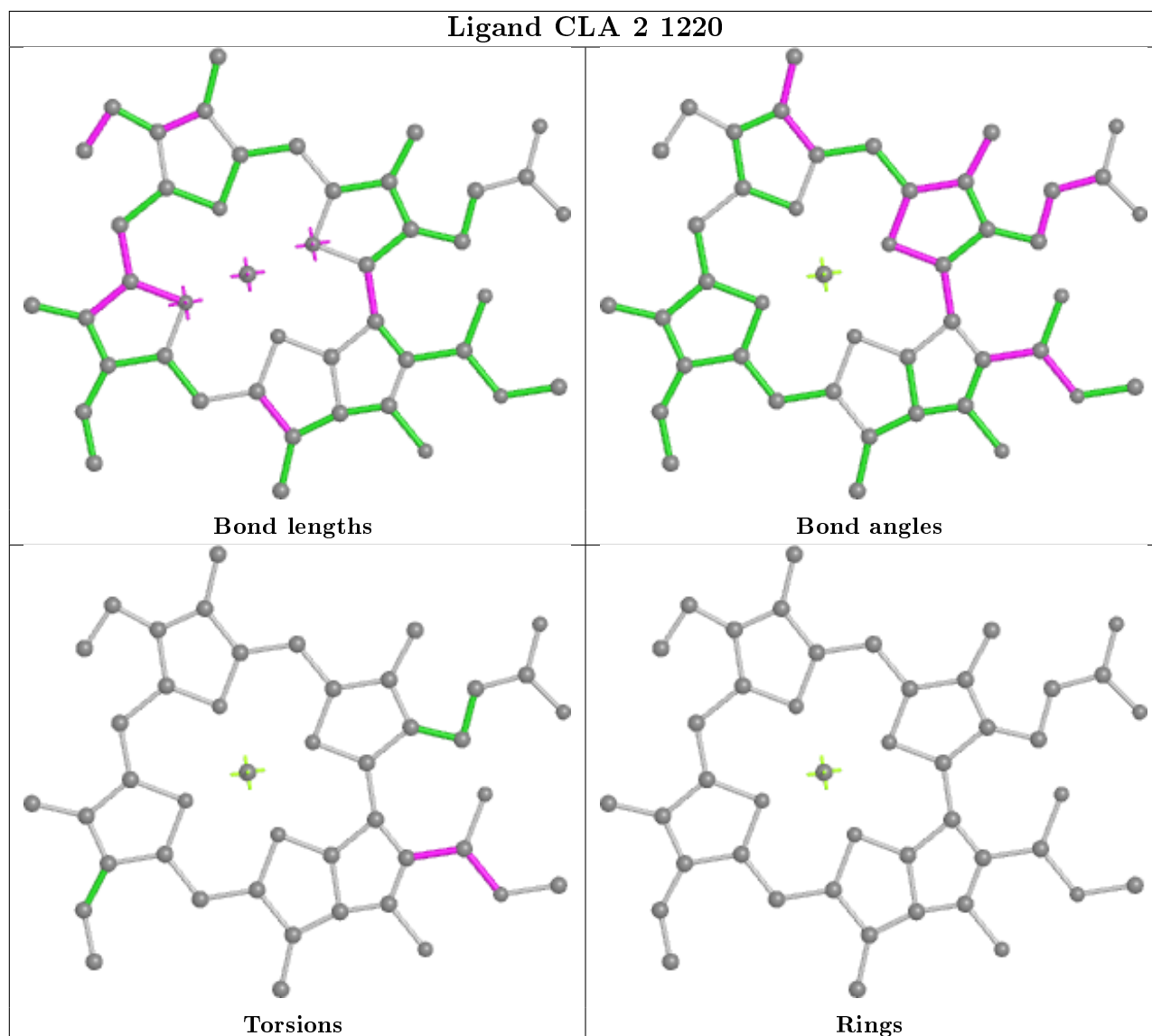
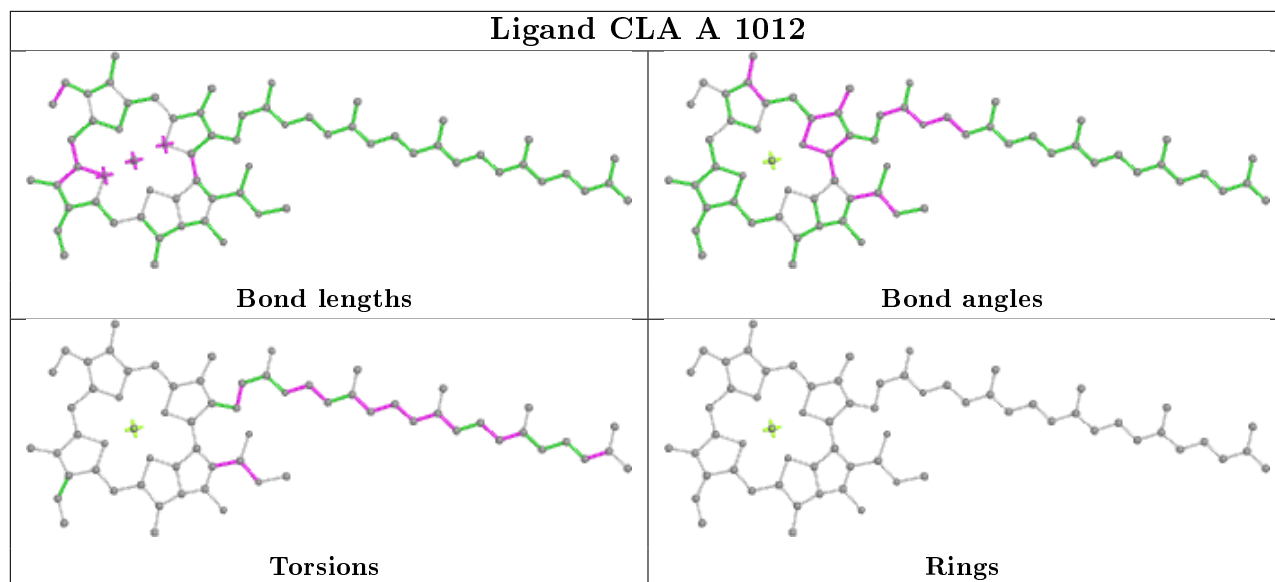
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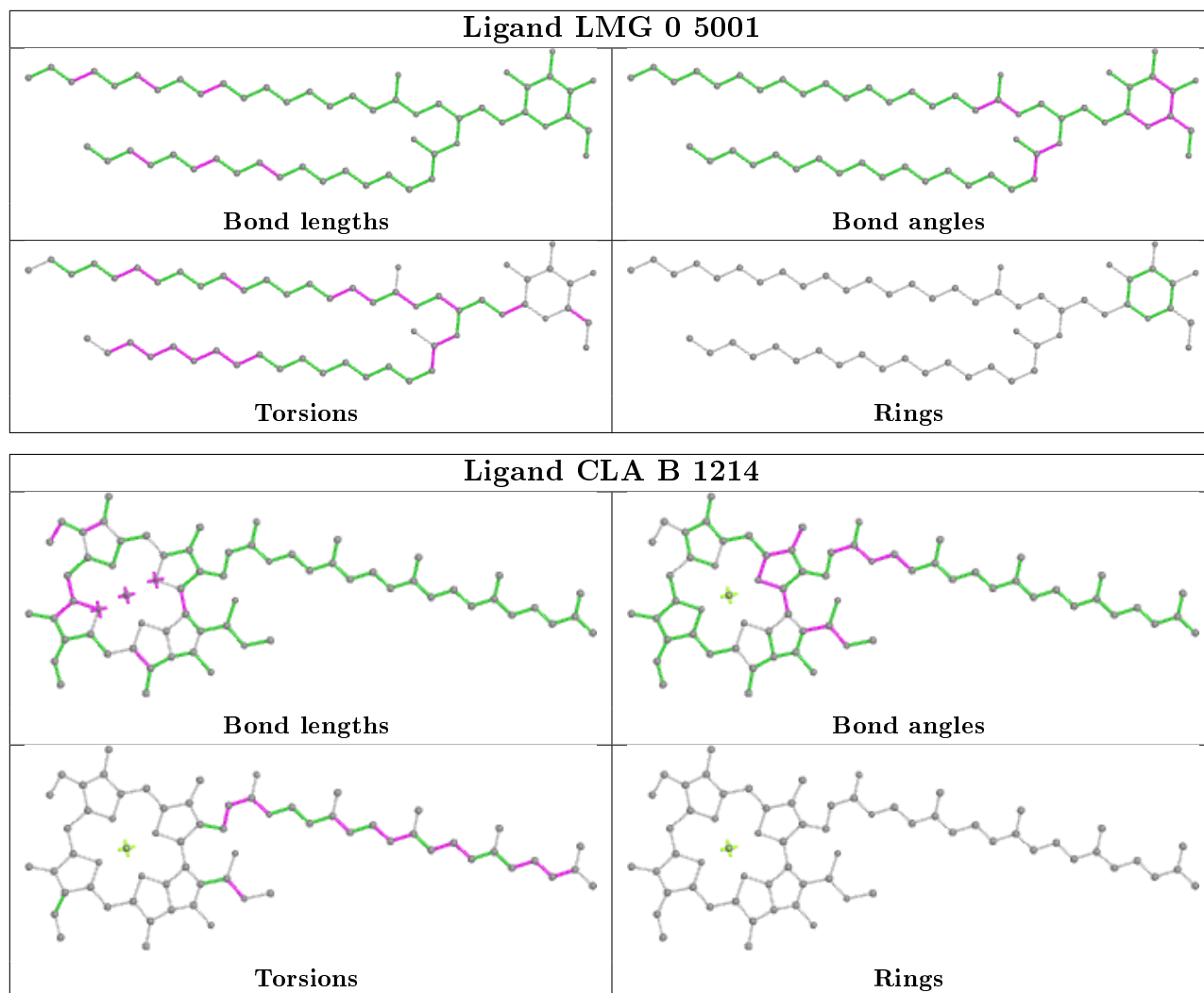
Mol	Chain	Res	Type	Atoms
21	A	1114	CLA	CAA-CBA-CGA-O1A
26	b	5005	LMG	O10-C28-C29-C30
21	B	1226	CLA	CAA-CBA-CGA-O1A
25	1	5003	LHG	O9-C7-C8-C9
25	A	5003	LHG	O9-C7-C8-C9
25	a	5007	LHG	O9-C7-C8-C9
25	l	5002	LHG	C9-C10-C11-C12
21	b	1203	CLA	CAA-CBA-CGA-O2A
21	k	1401	CLA	CAA-CBA-CGA-O2A
21	2	1226	CLA	CAA-CBA-CGA-O2A
21	B	1239	CLA	CAA-CBA-CGA-O2A
21	B	1234	CLA	CAA-CBA-CGA-O2A
21	a	1118	CLA	CAA-CBA-CGA-O2A
21	A	1125	CLA	CAA-CBA-CGA-O2A
25	0	5002	LHG	O7-C7-C8-C9
21	B	1205	CLA	CAA-CBA-CGA-O2A
21	A	1105	CLA	C10-C11-C12-C13
21	1	1120	CLA	C8-C10-C11-C12
21	a	1107	CLA	CAA-CBA-CGA-O1A
21	B	1208	CLA	CAA-CBA-CGA-O1A
26	1	5004	LMG	O9-C10-C11-C12
25	b	5004	LHG	O10-C23-C24-C25
21	A	1102	CLA	C13-C15-C16-C17
26	b	5007	LMG	C30-C31-C32-C33
21	A	1126	CLA	CAA-CBA-CGA-O2A
21	b	1205	CLA	CAA-CBA-CGA-O2A

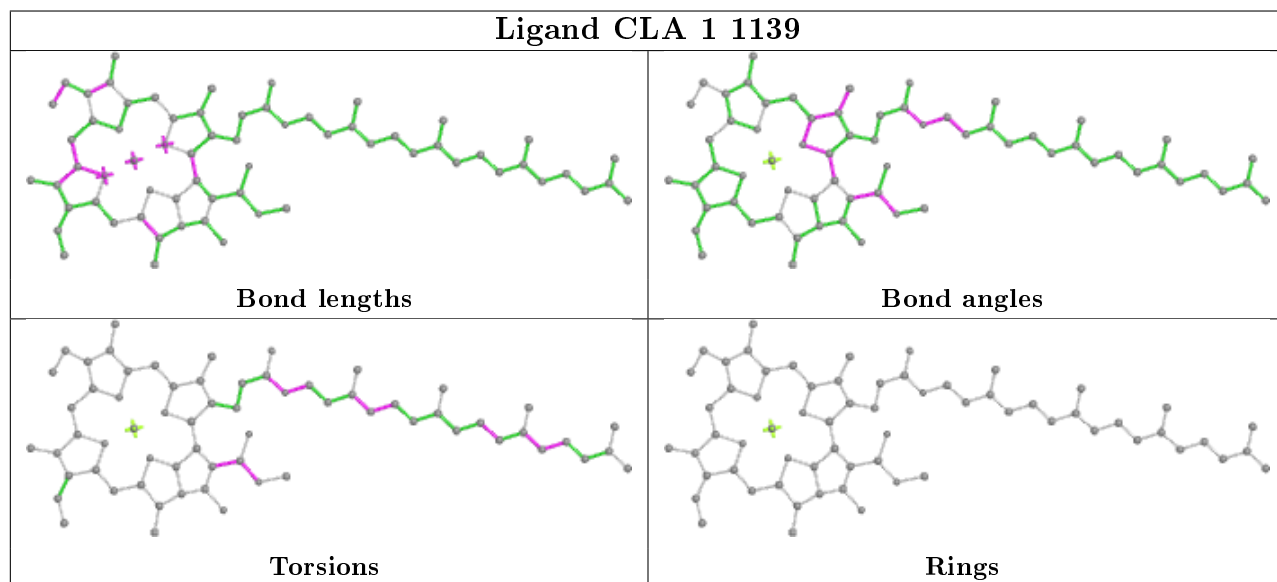
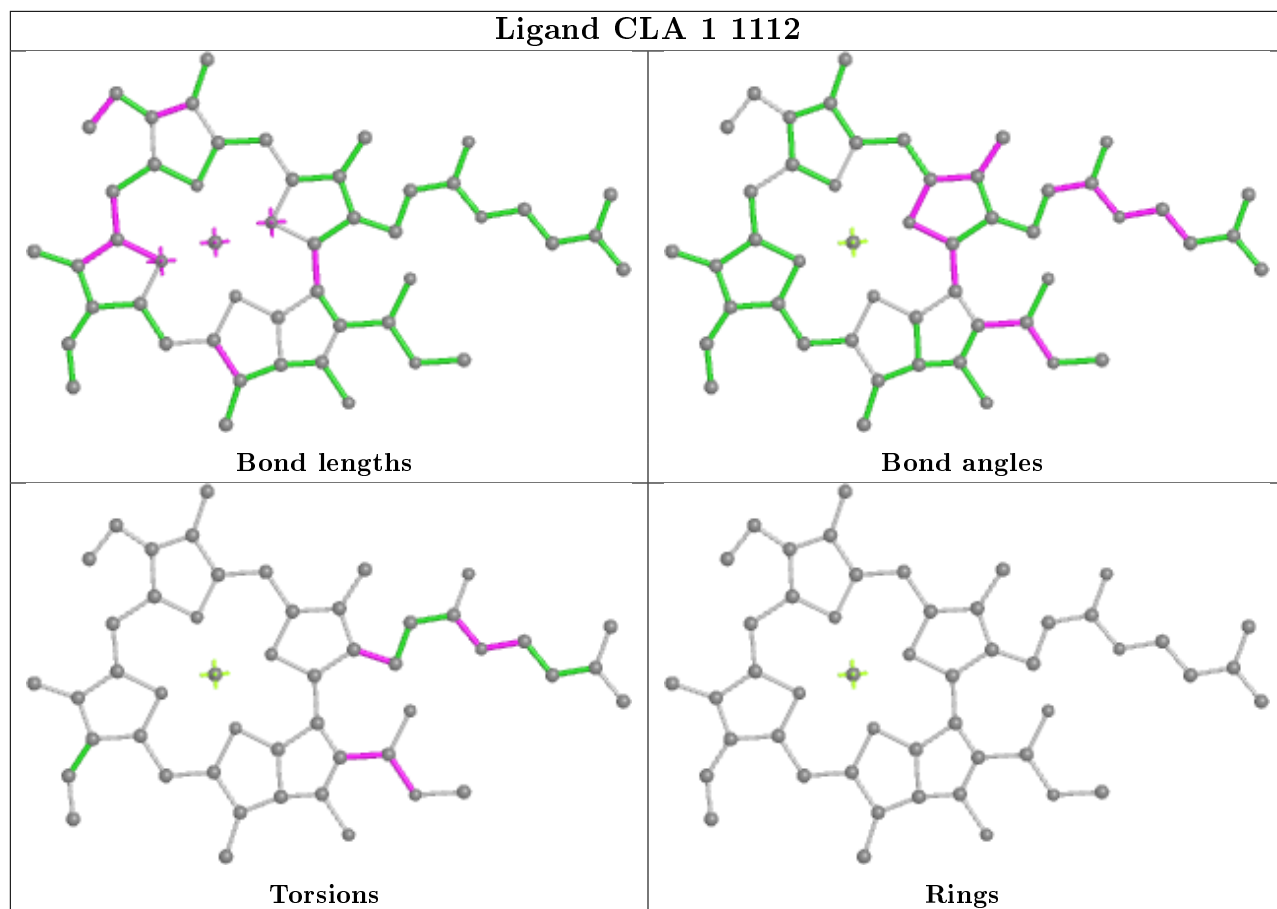
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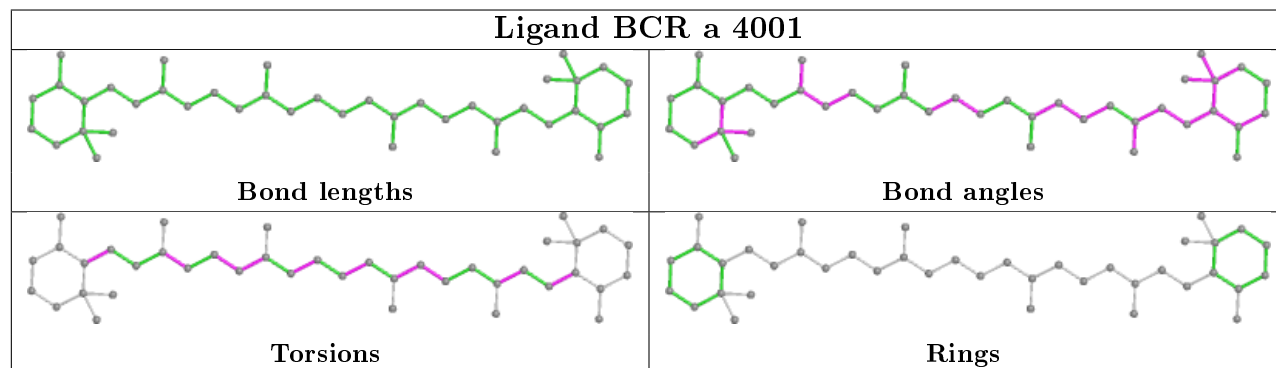
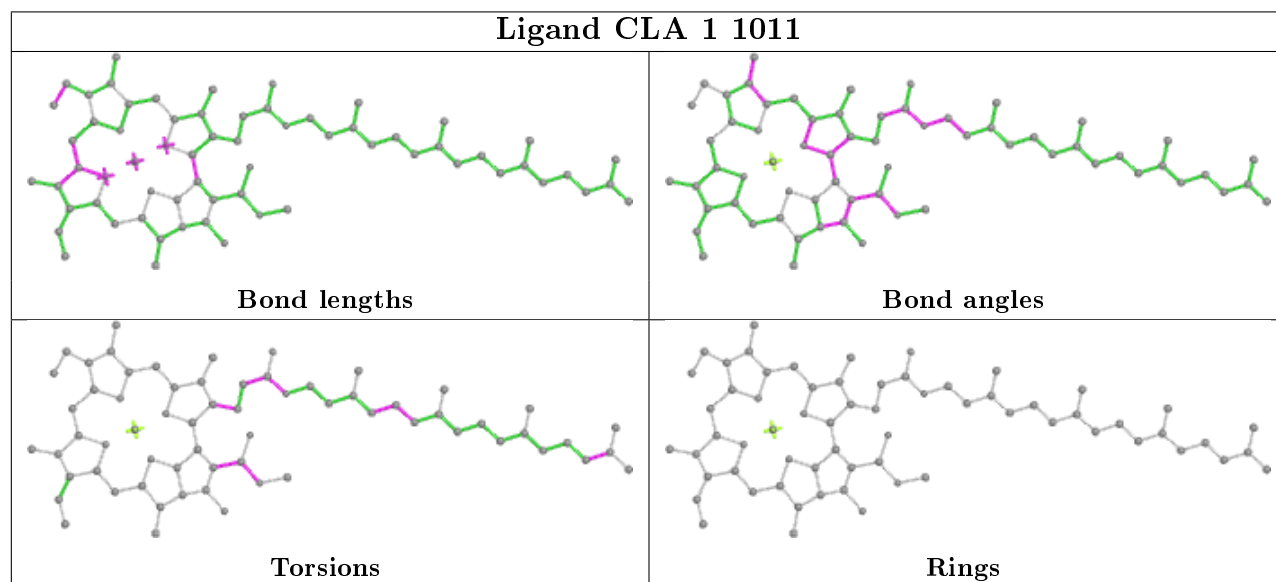
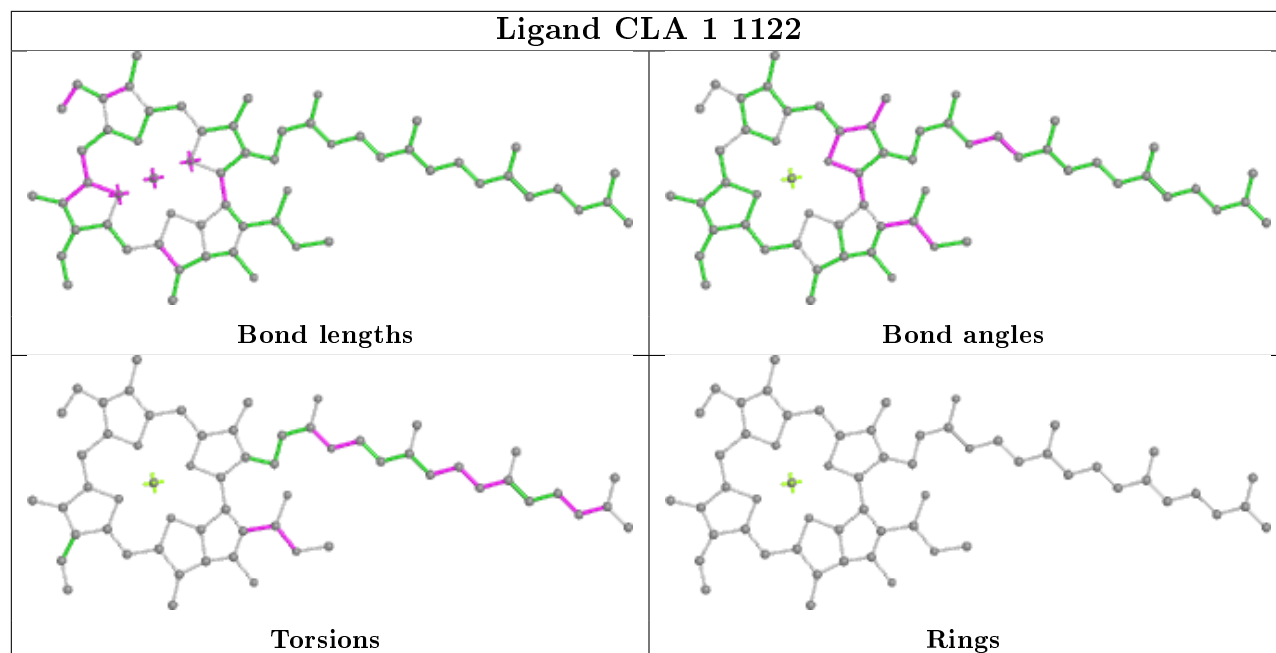
No monomer is involved in short contacts.

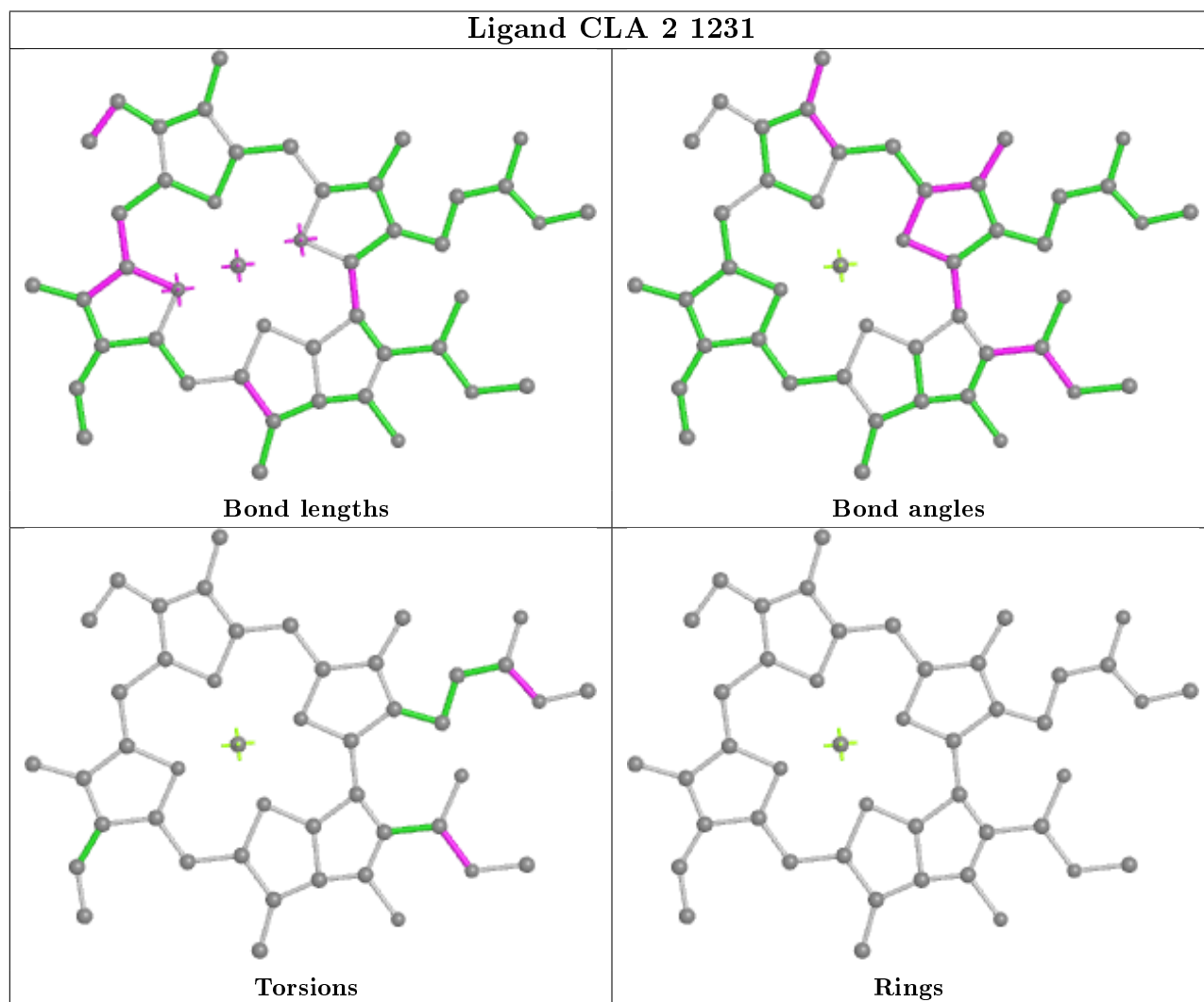
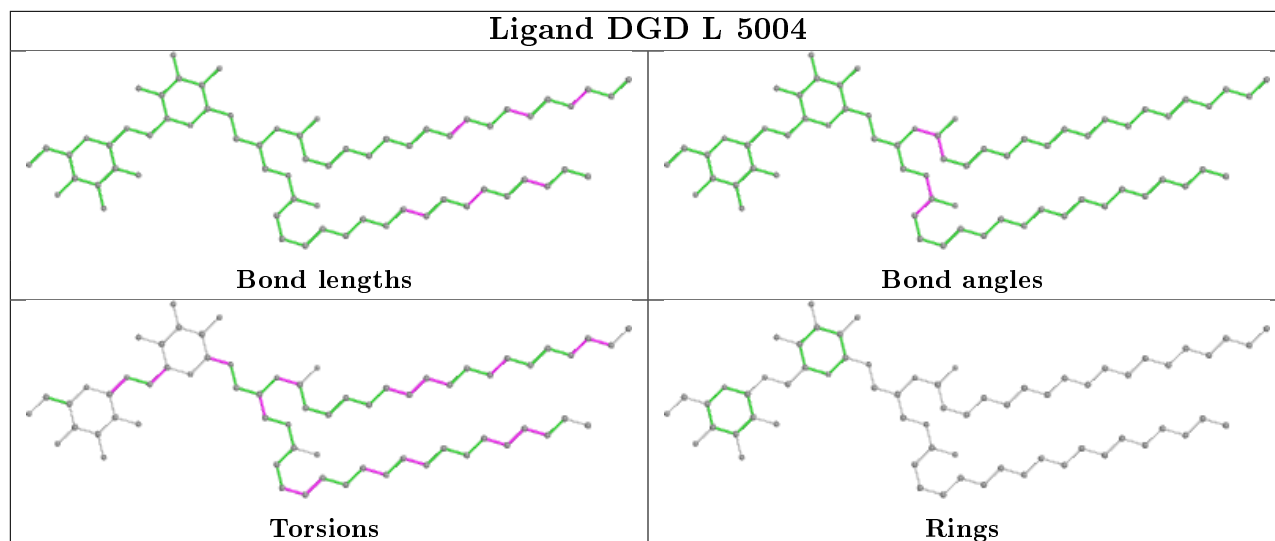
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

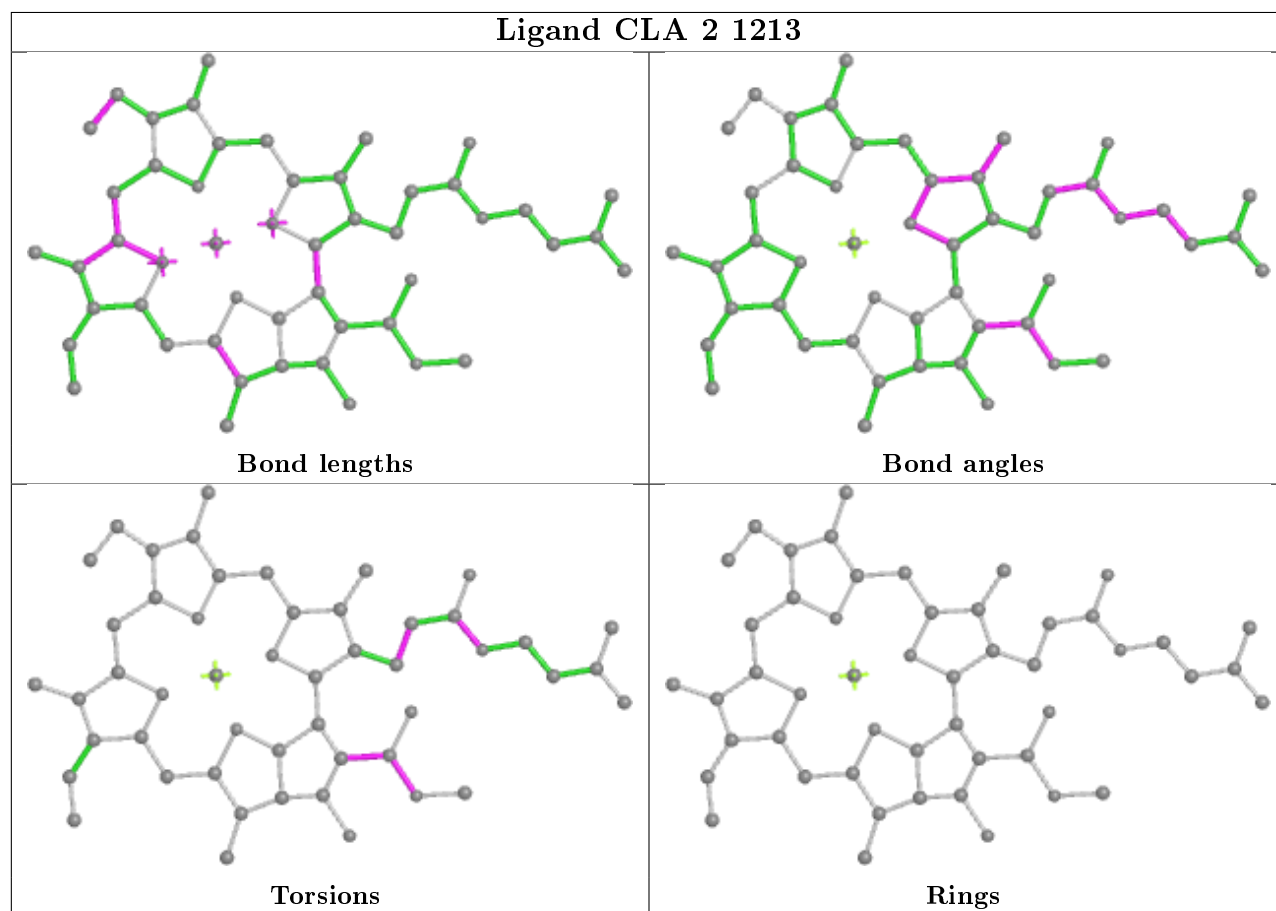
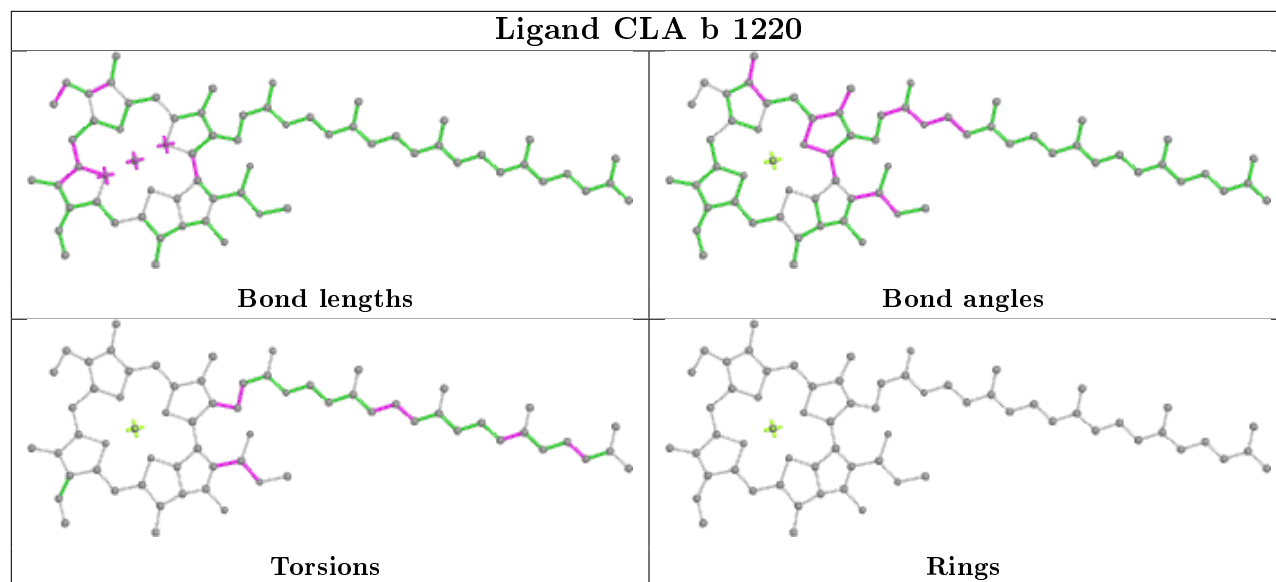


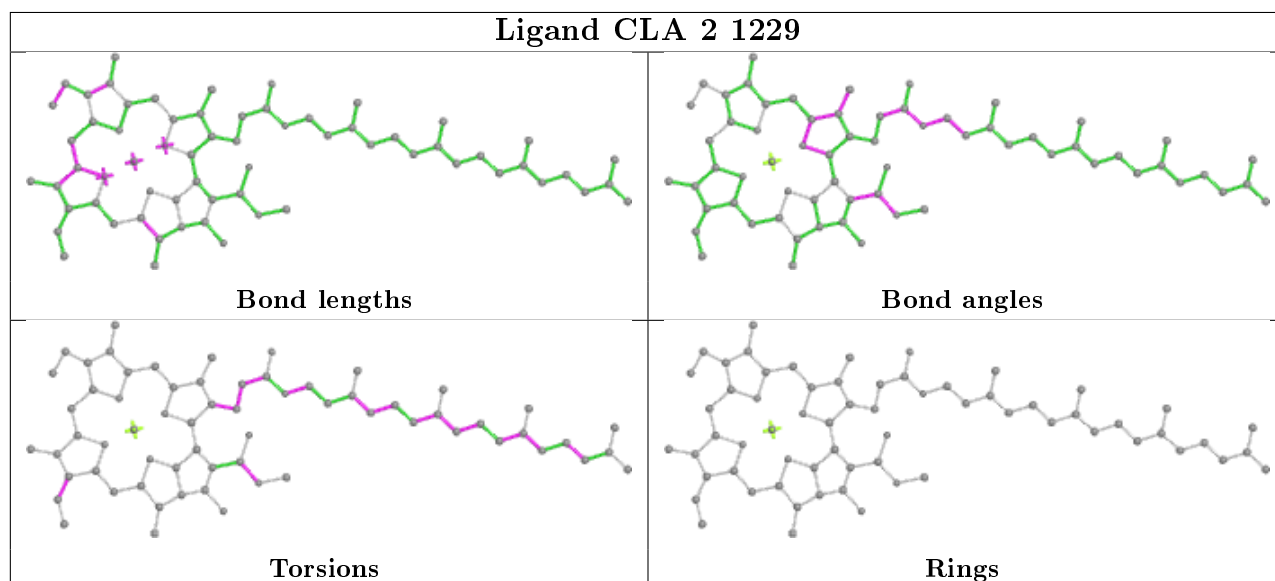
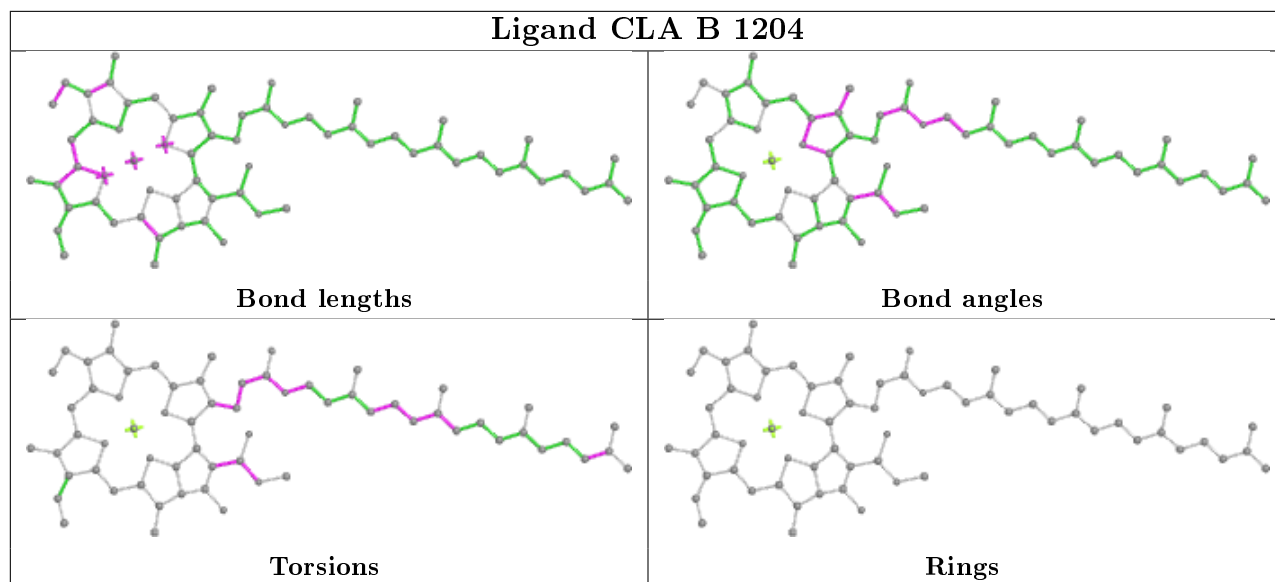


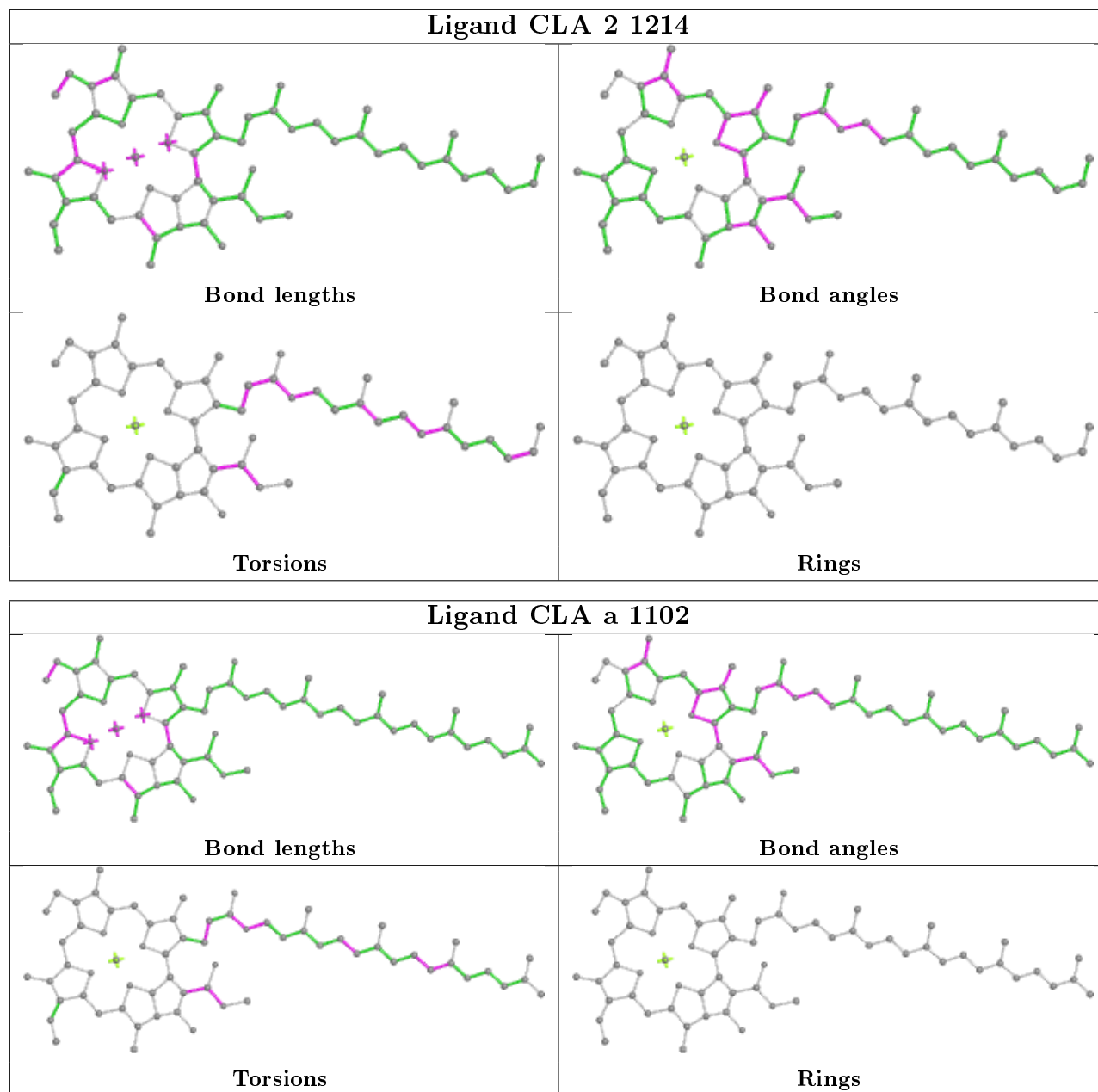


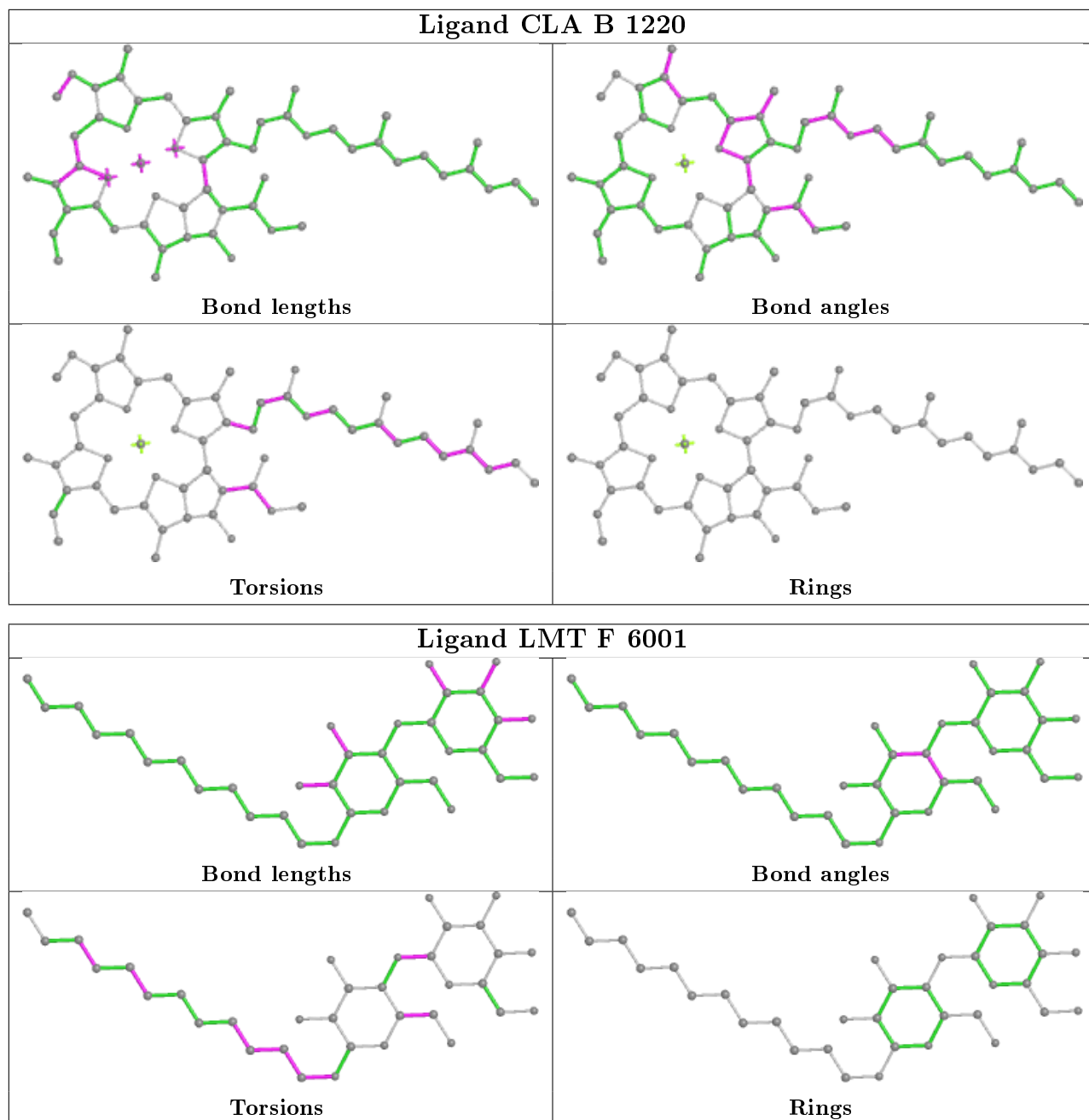


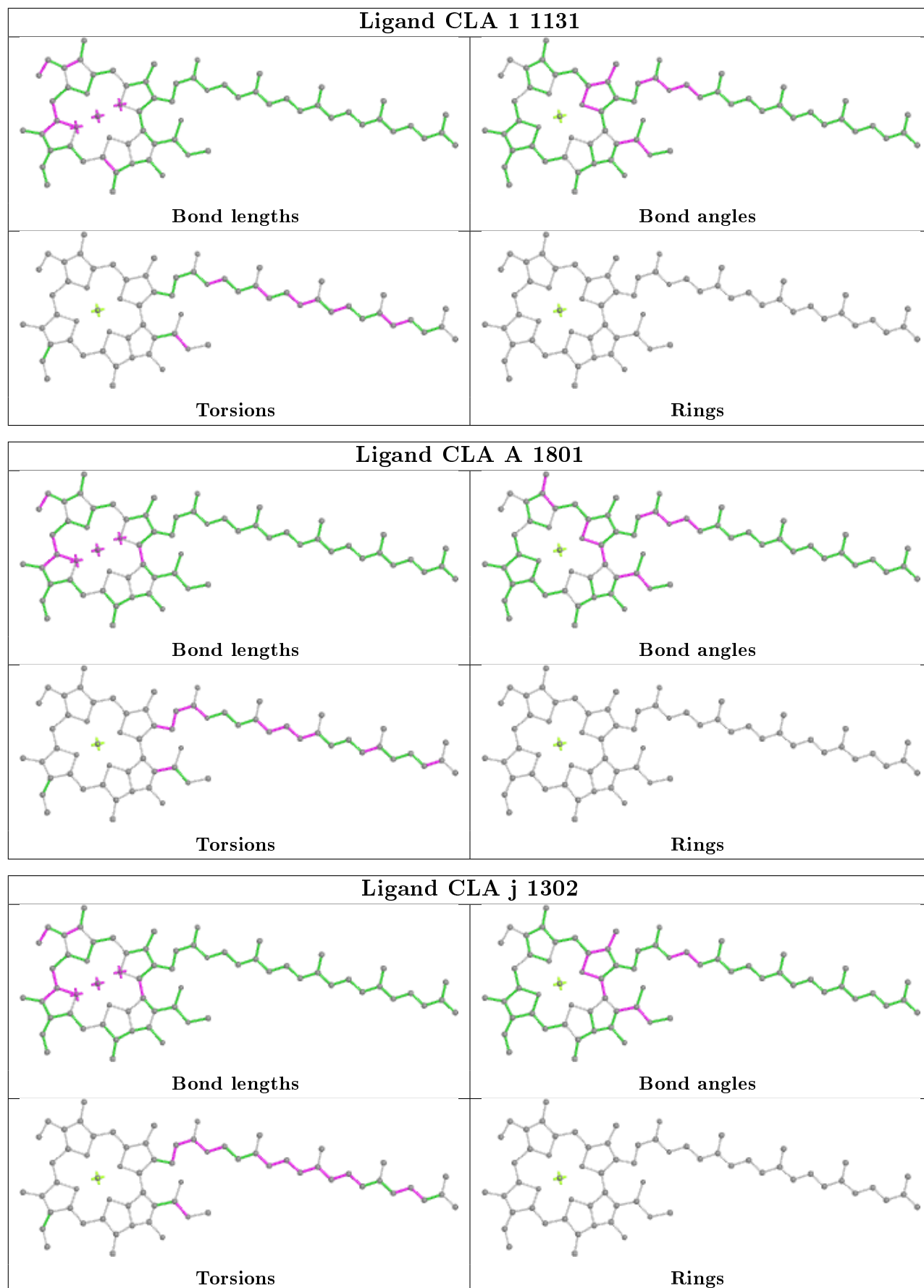


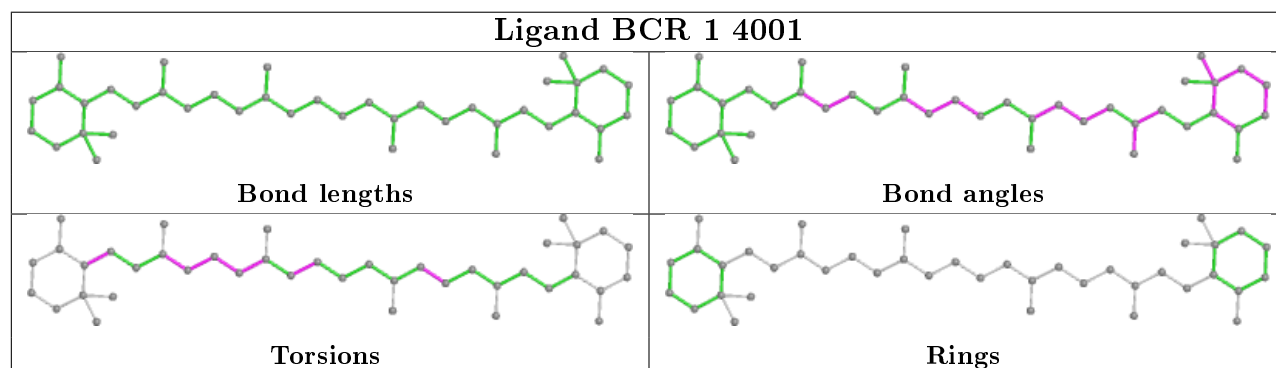
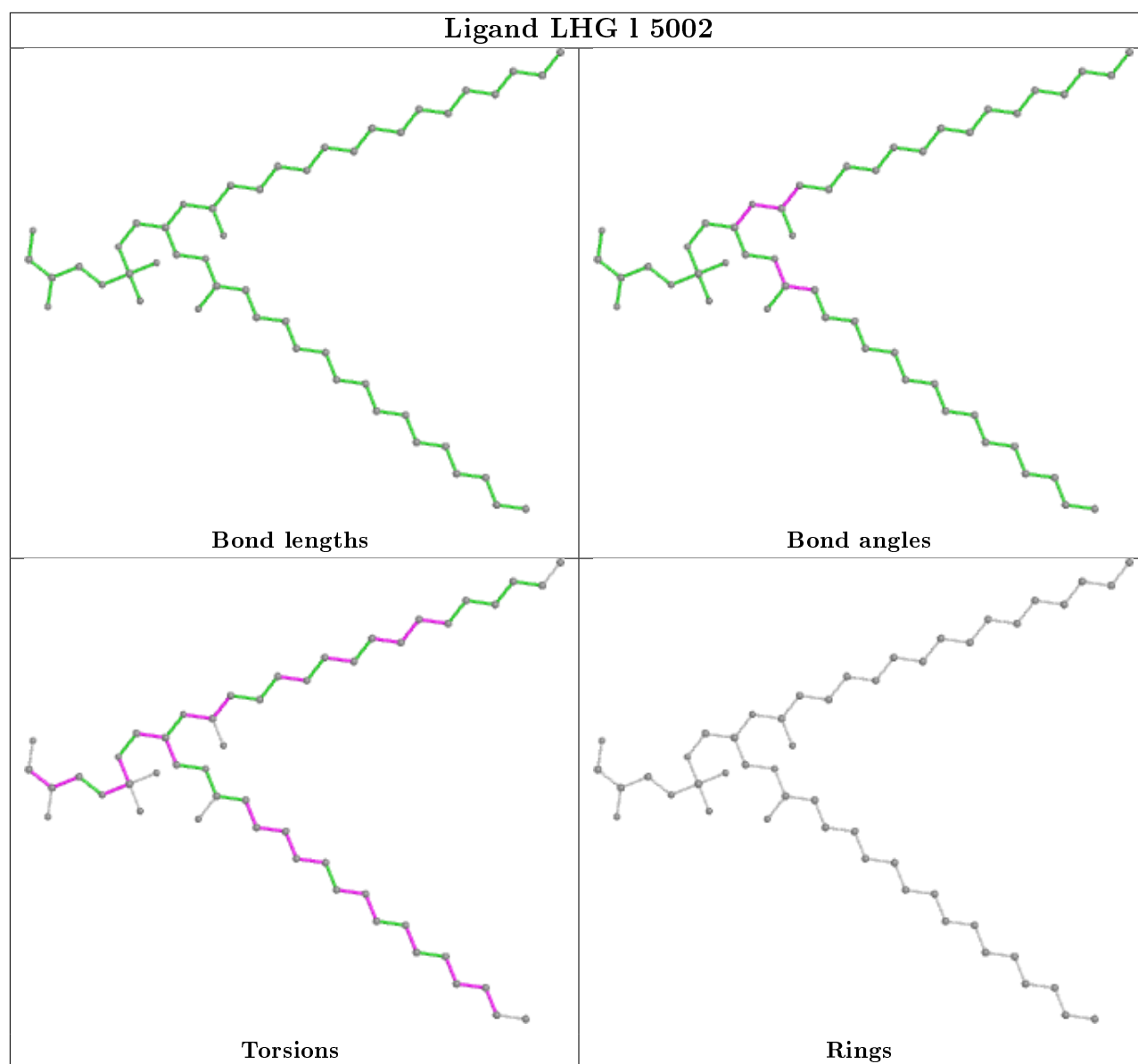


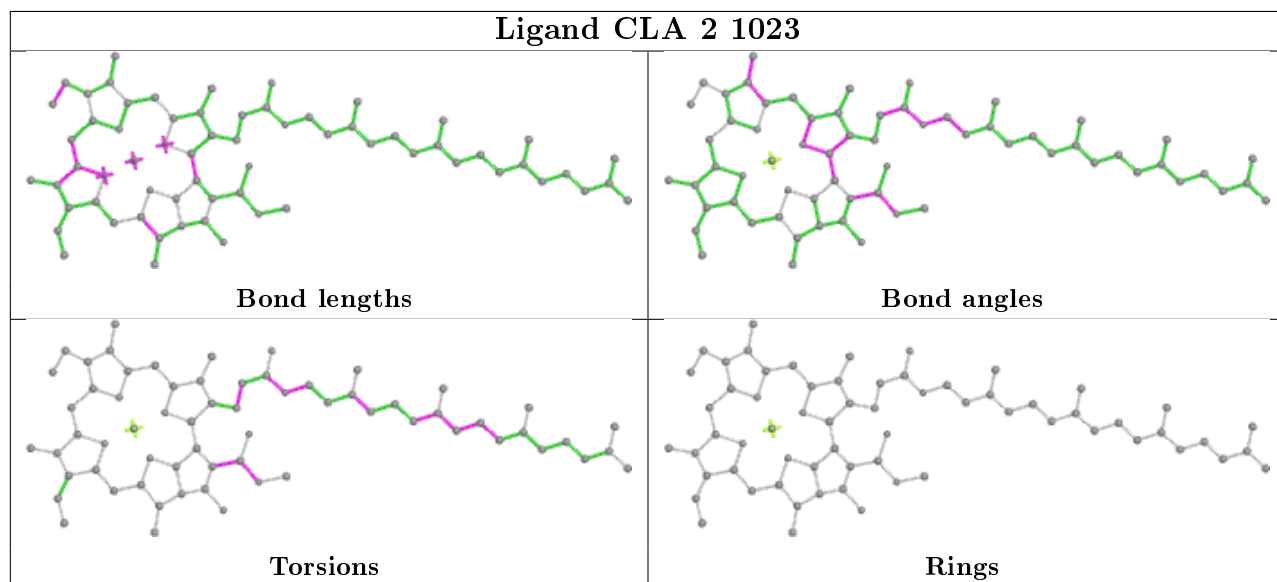
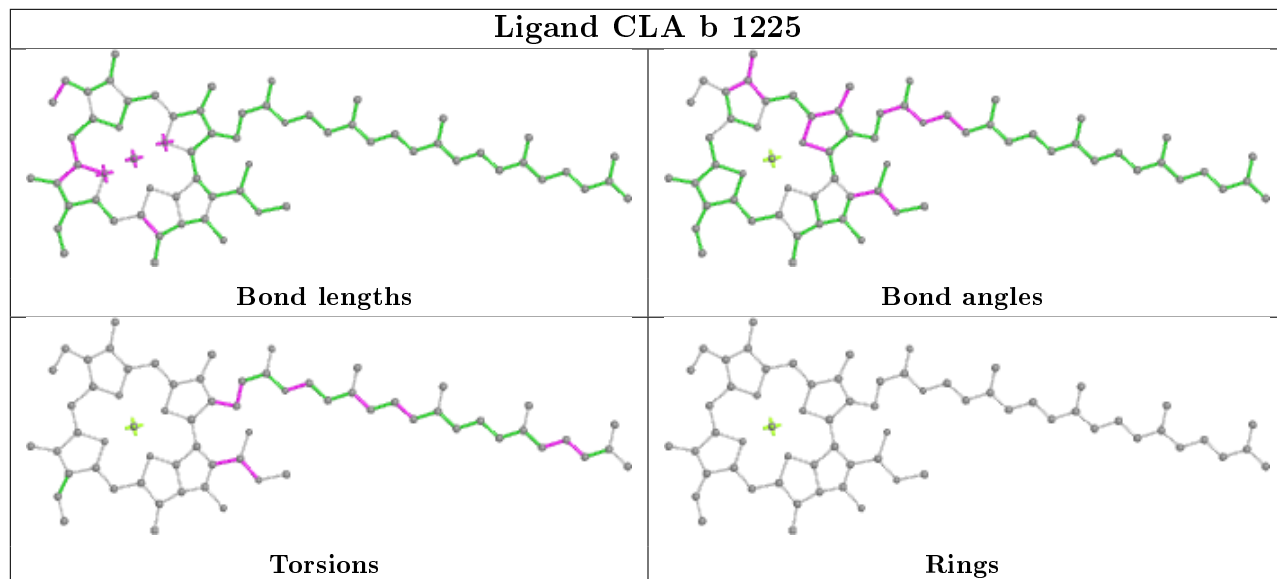
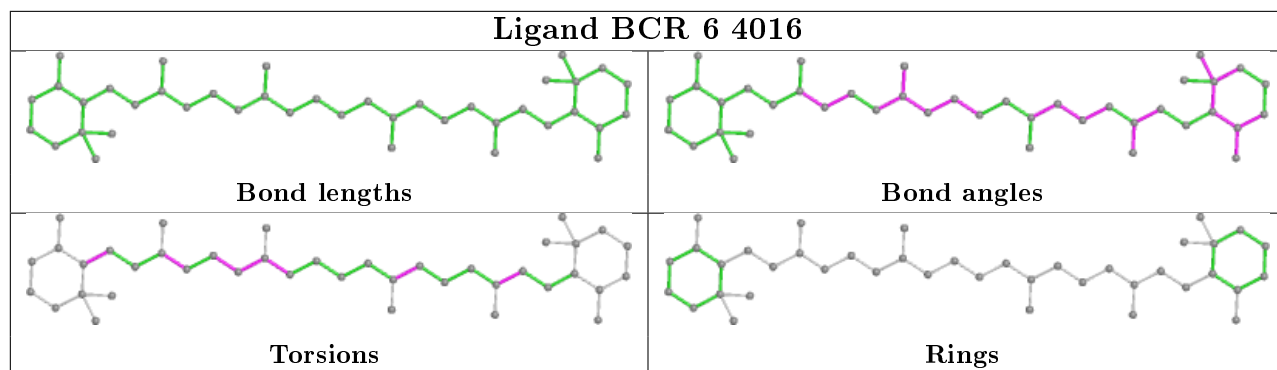


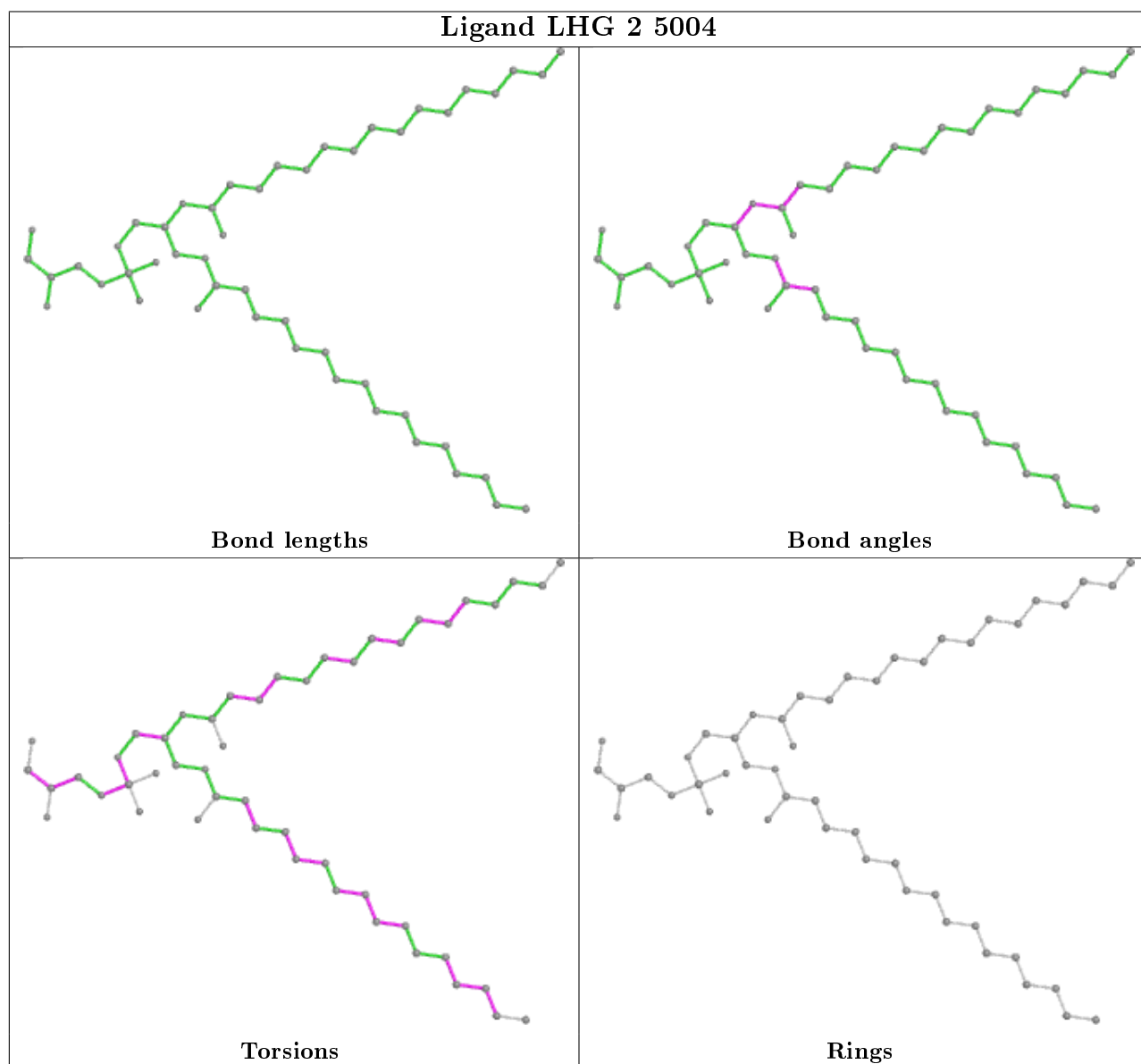
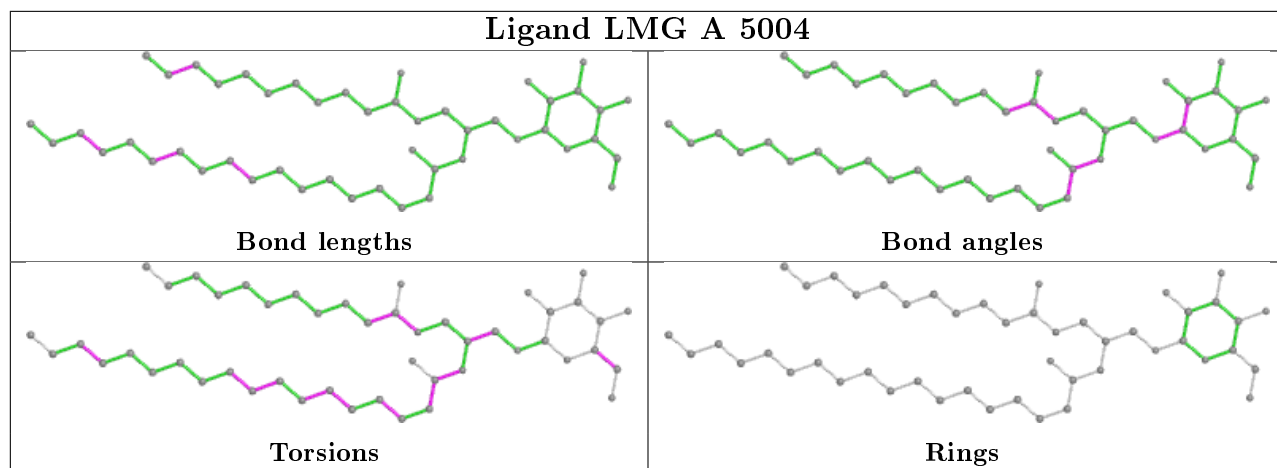


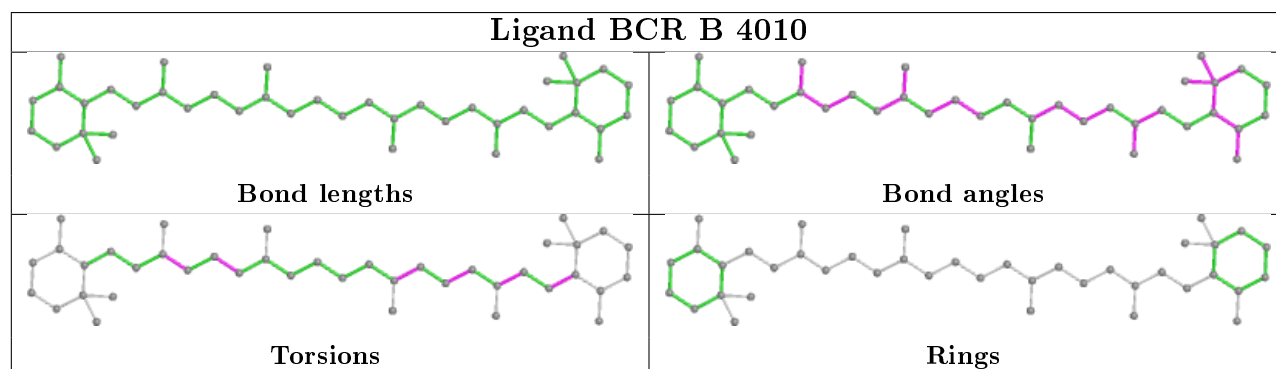
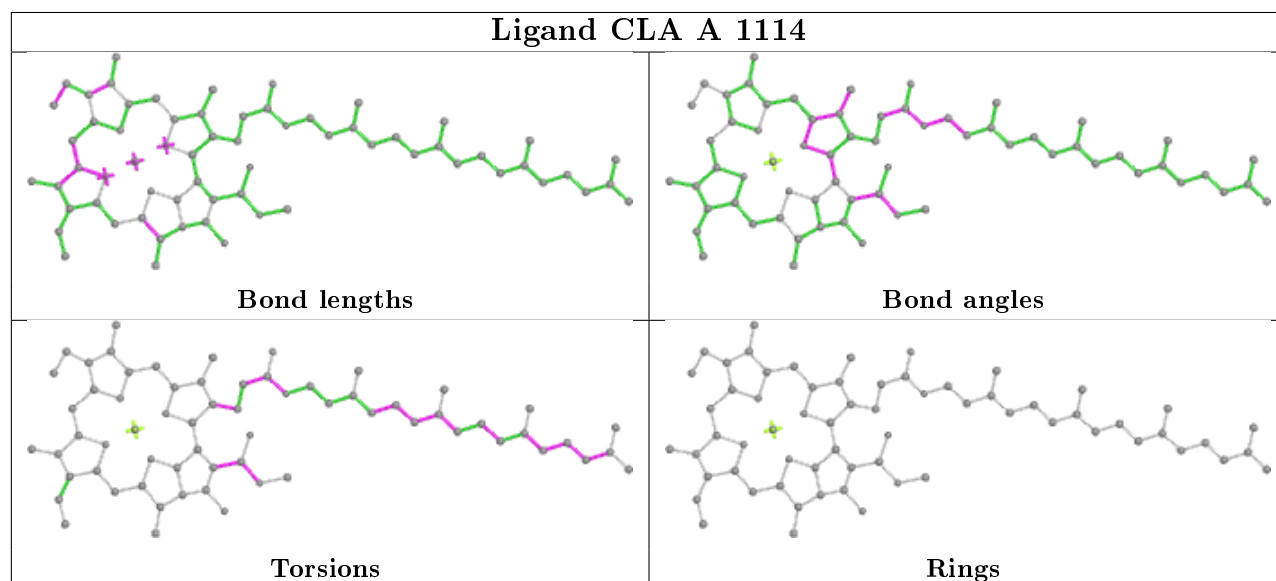
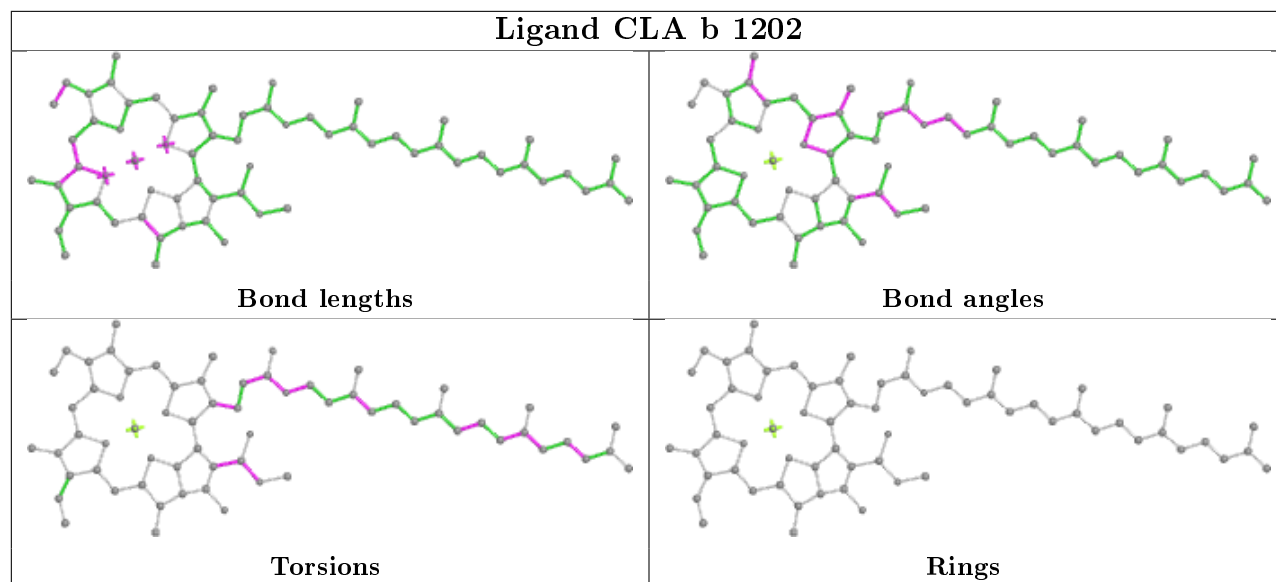


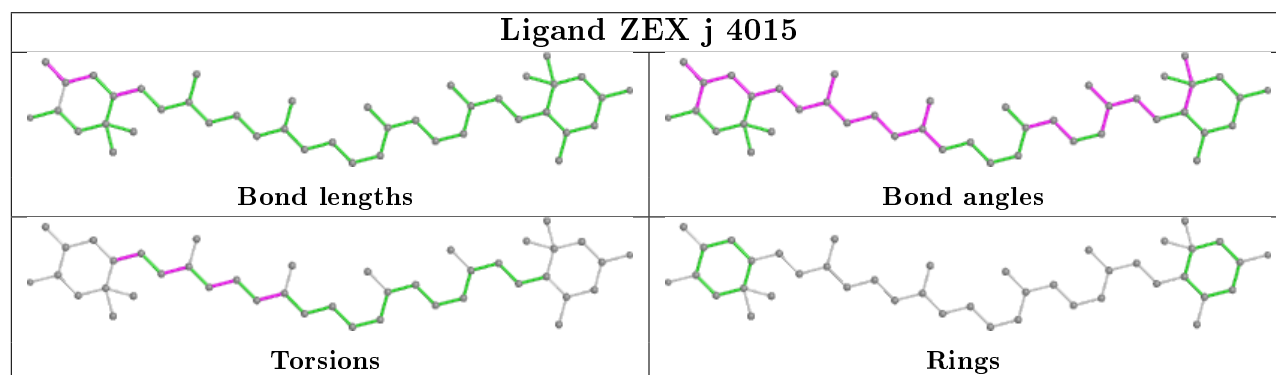
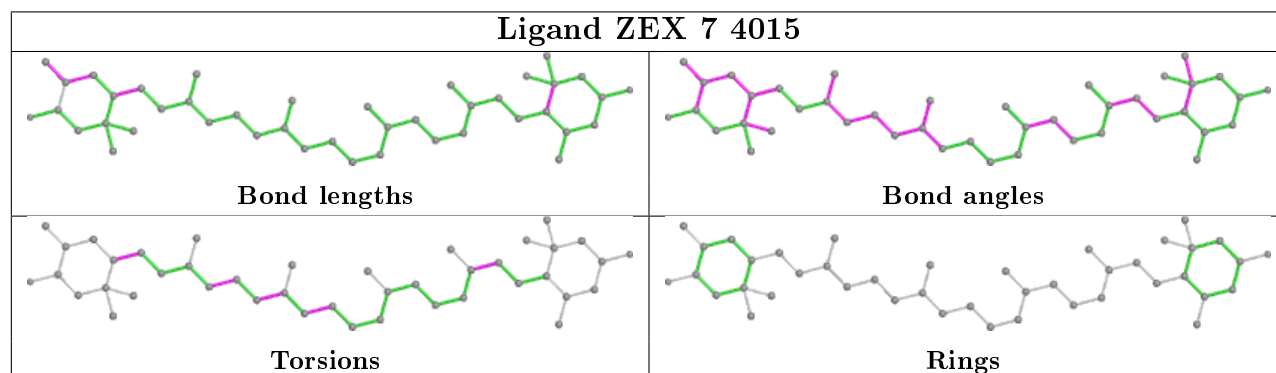
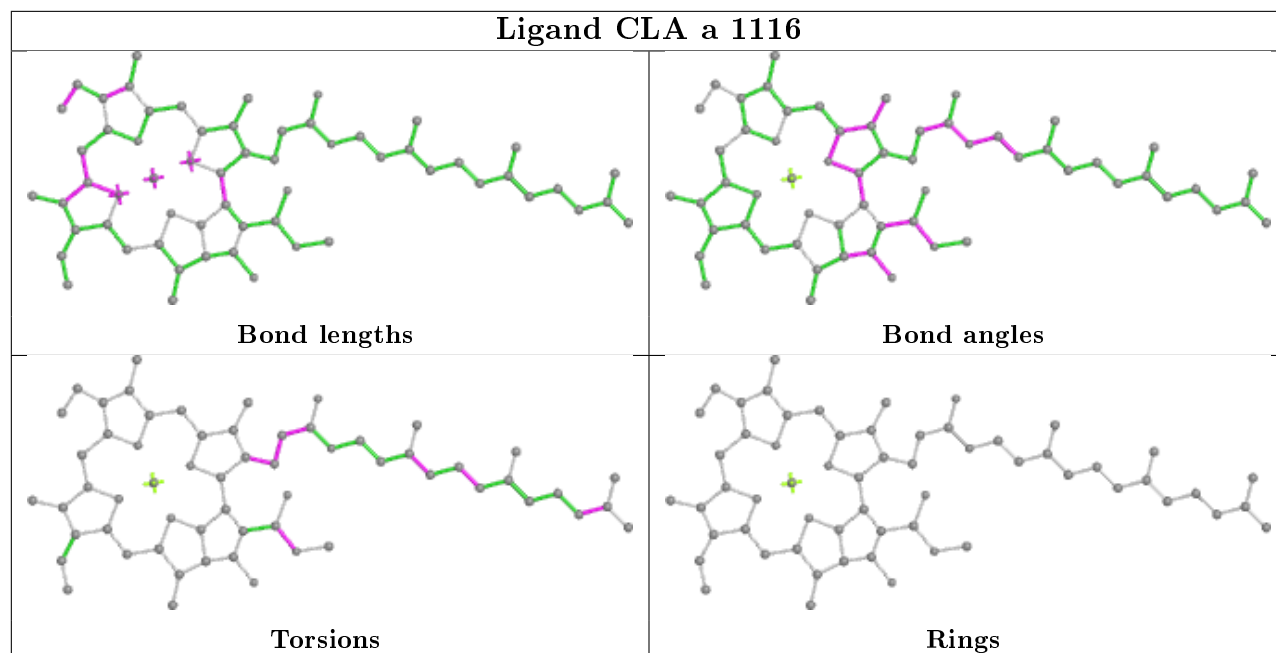


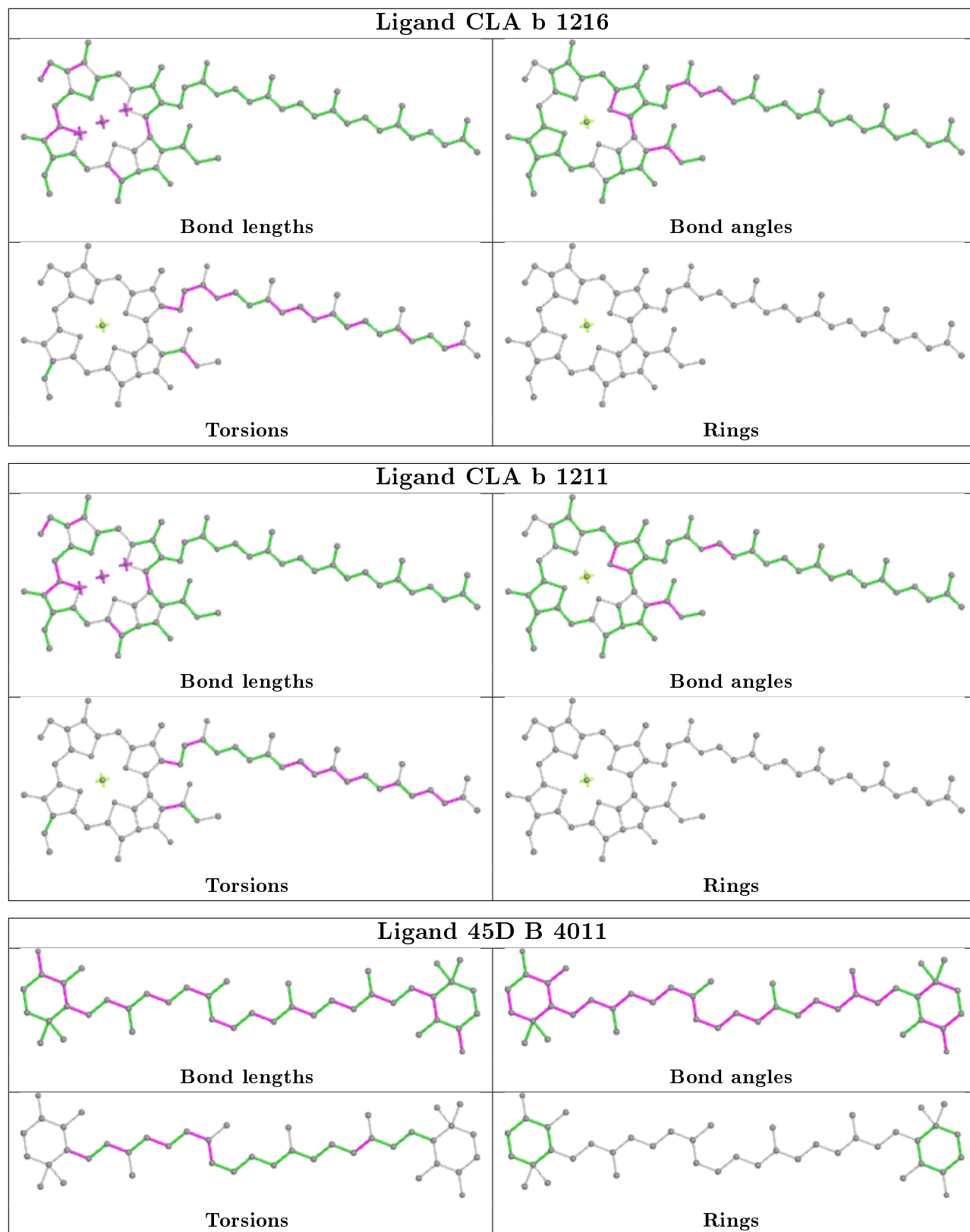


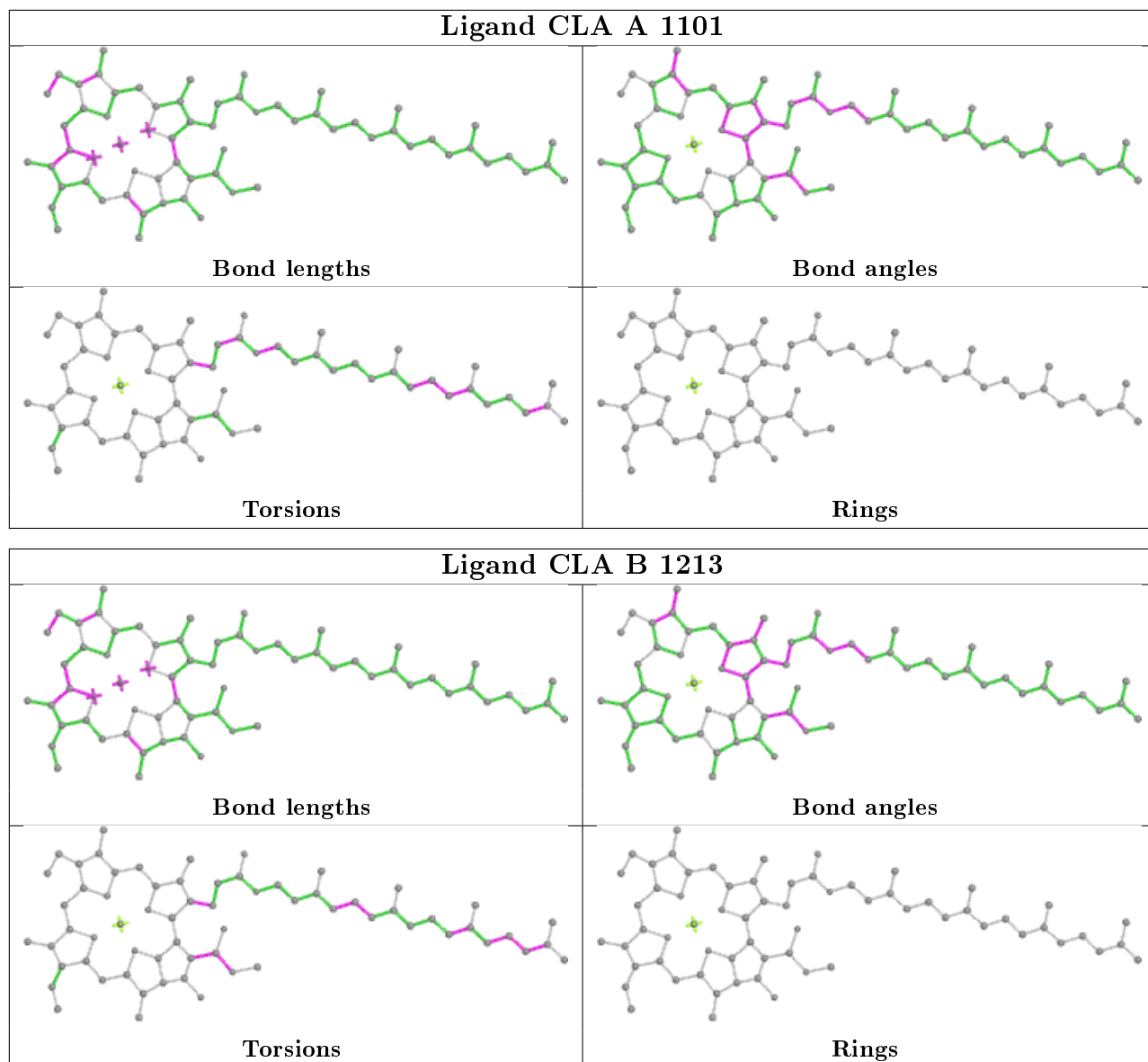


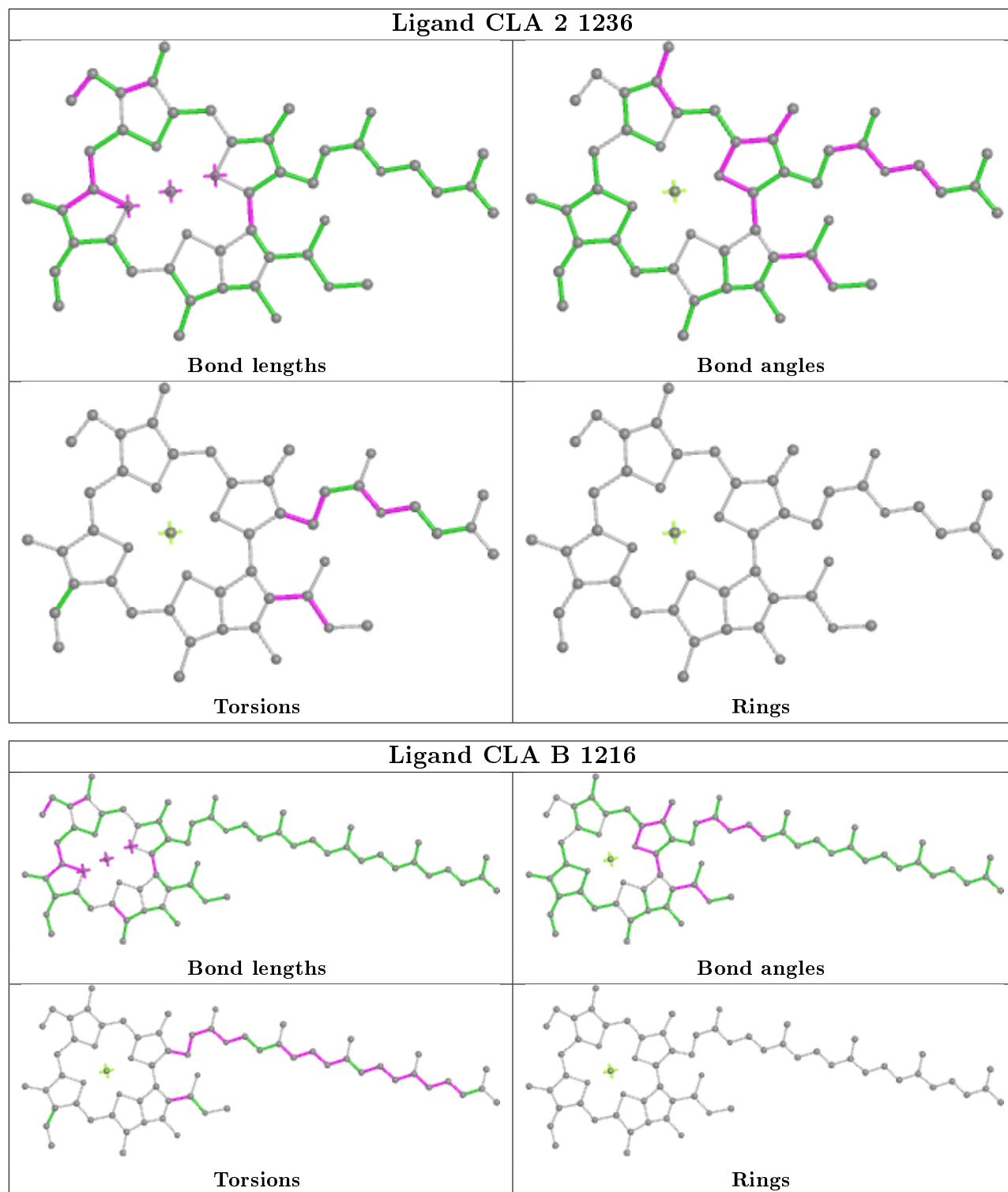


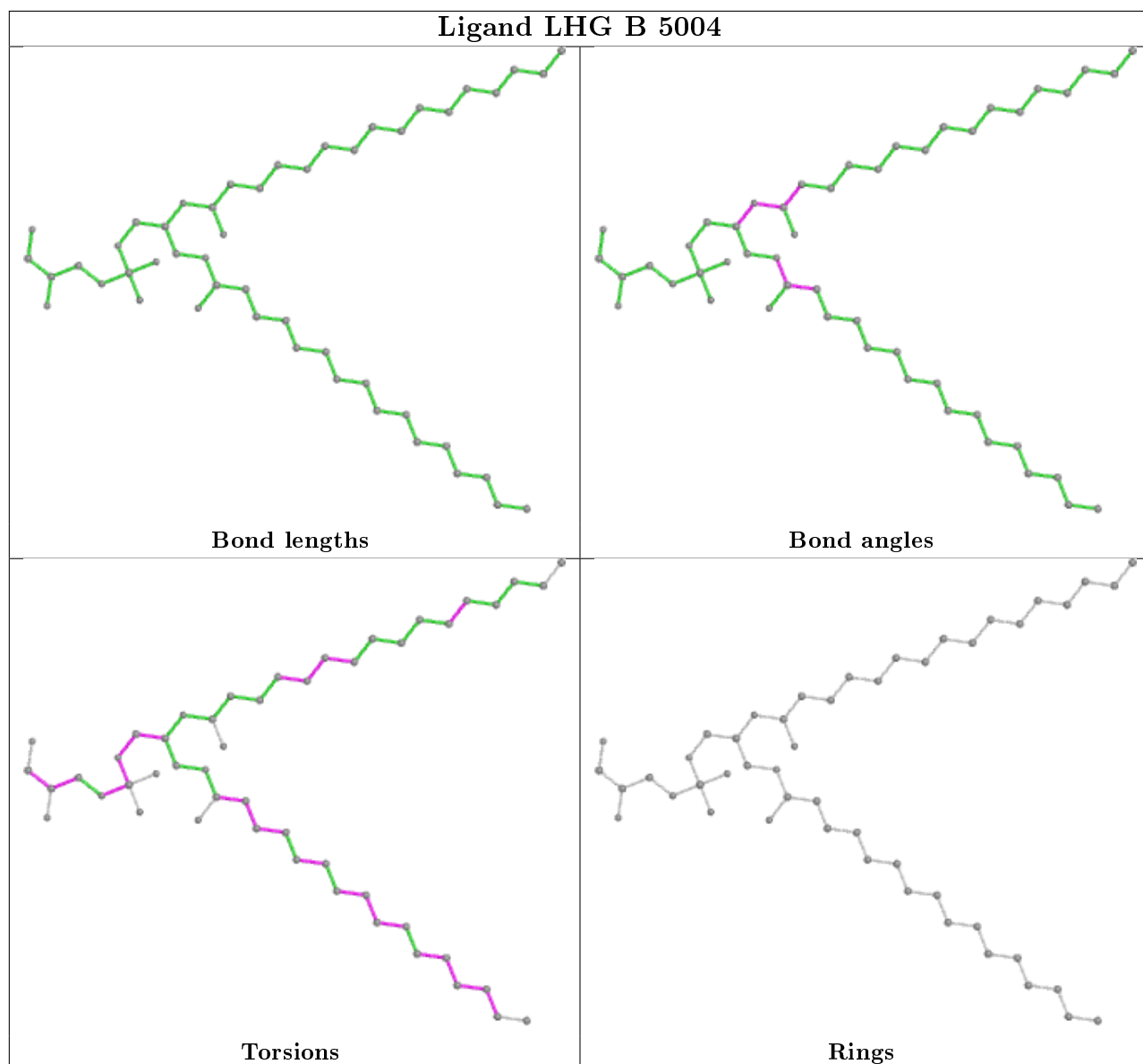
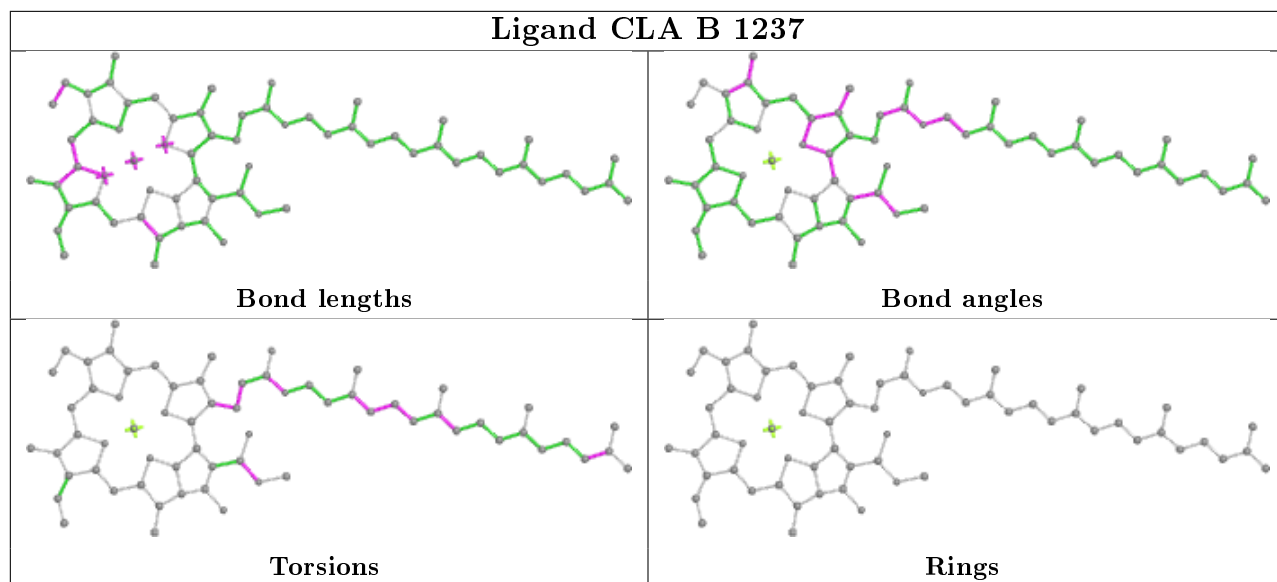


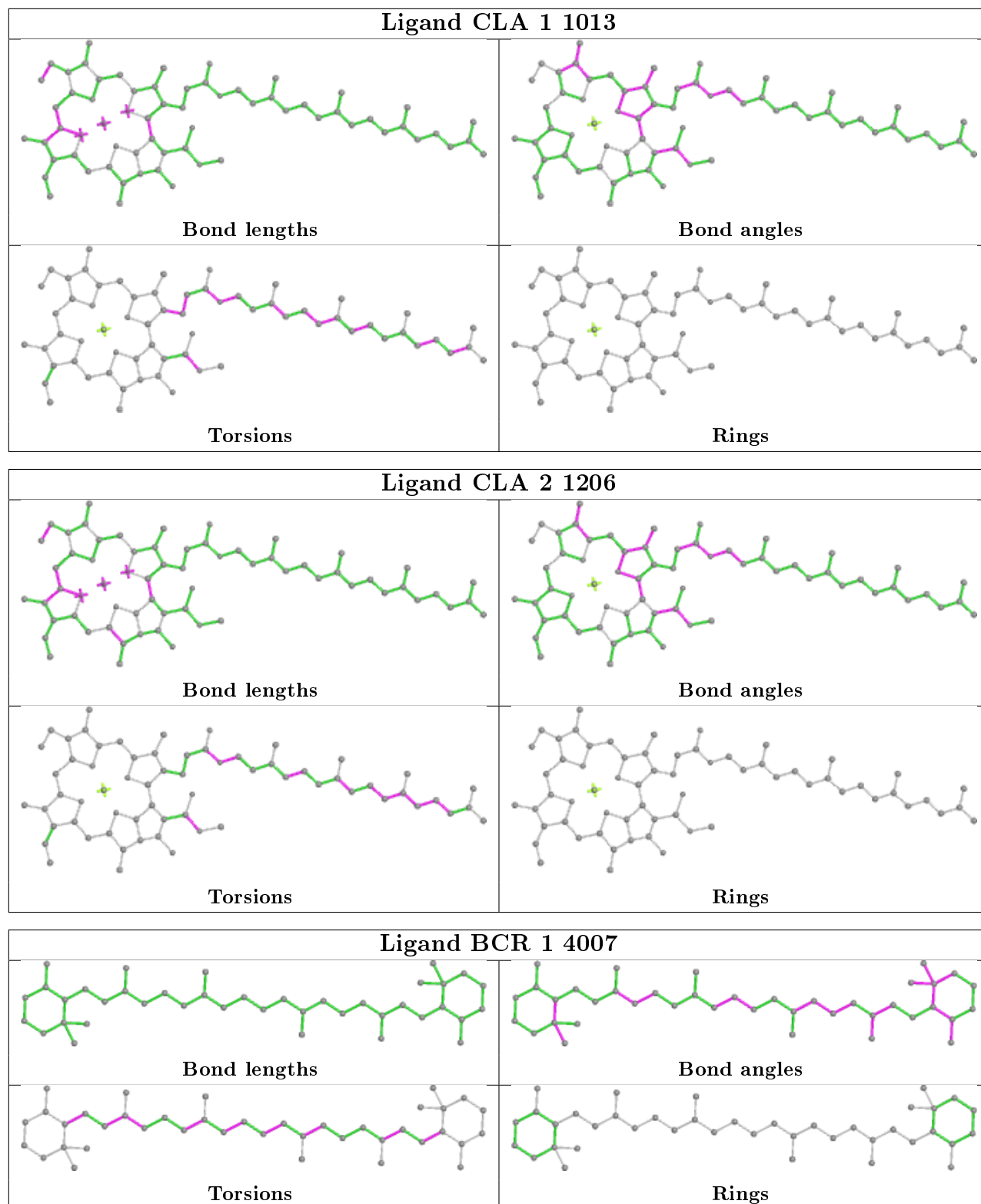


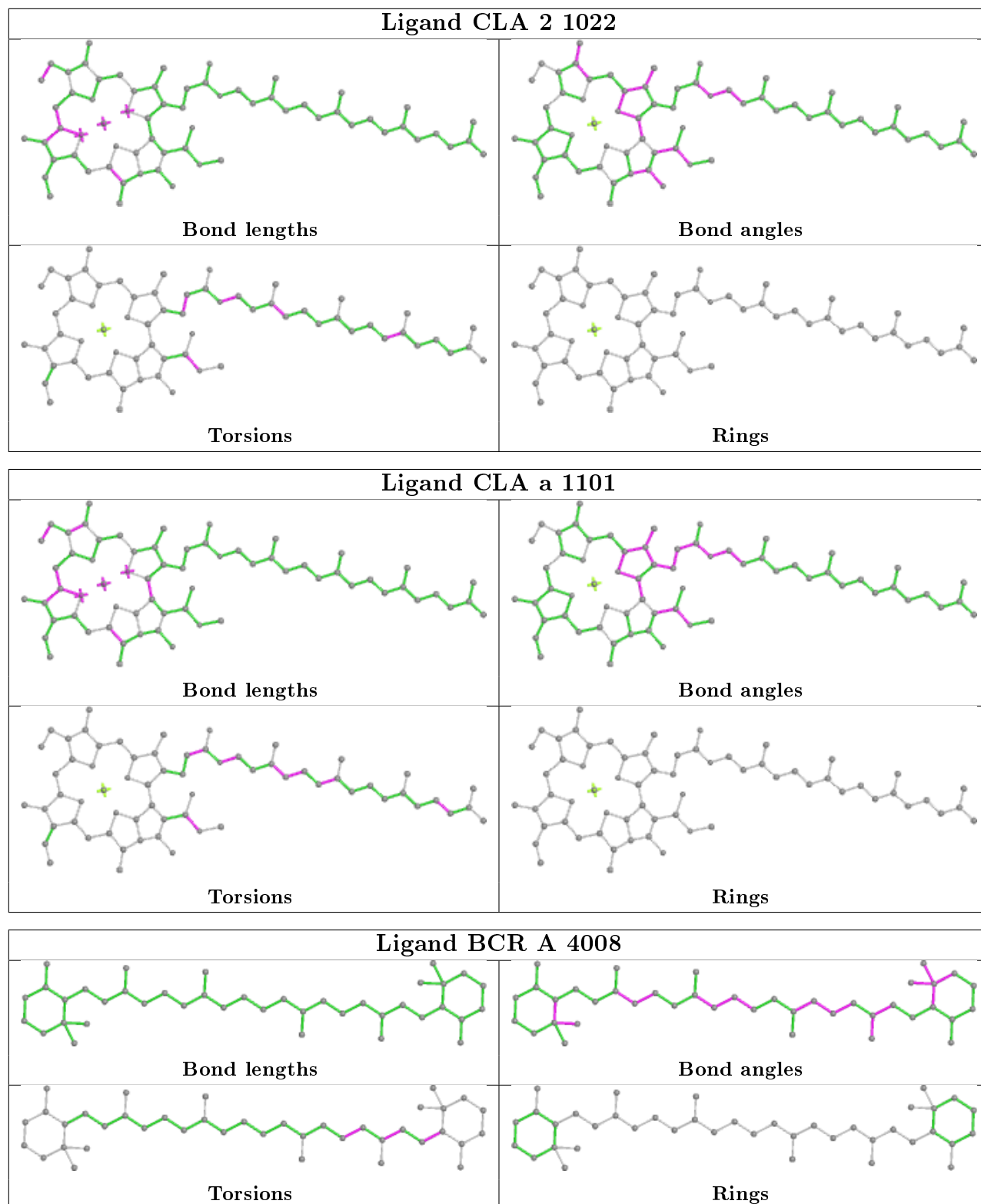


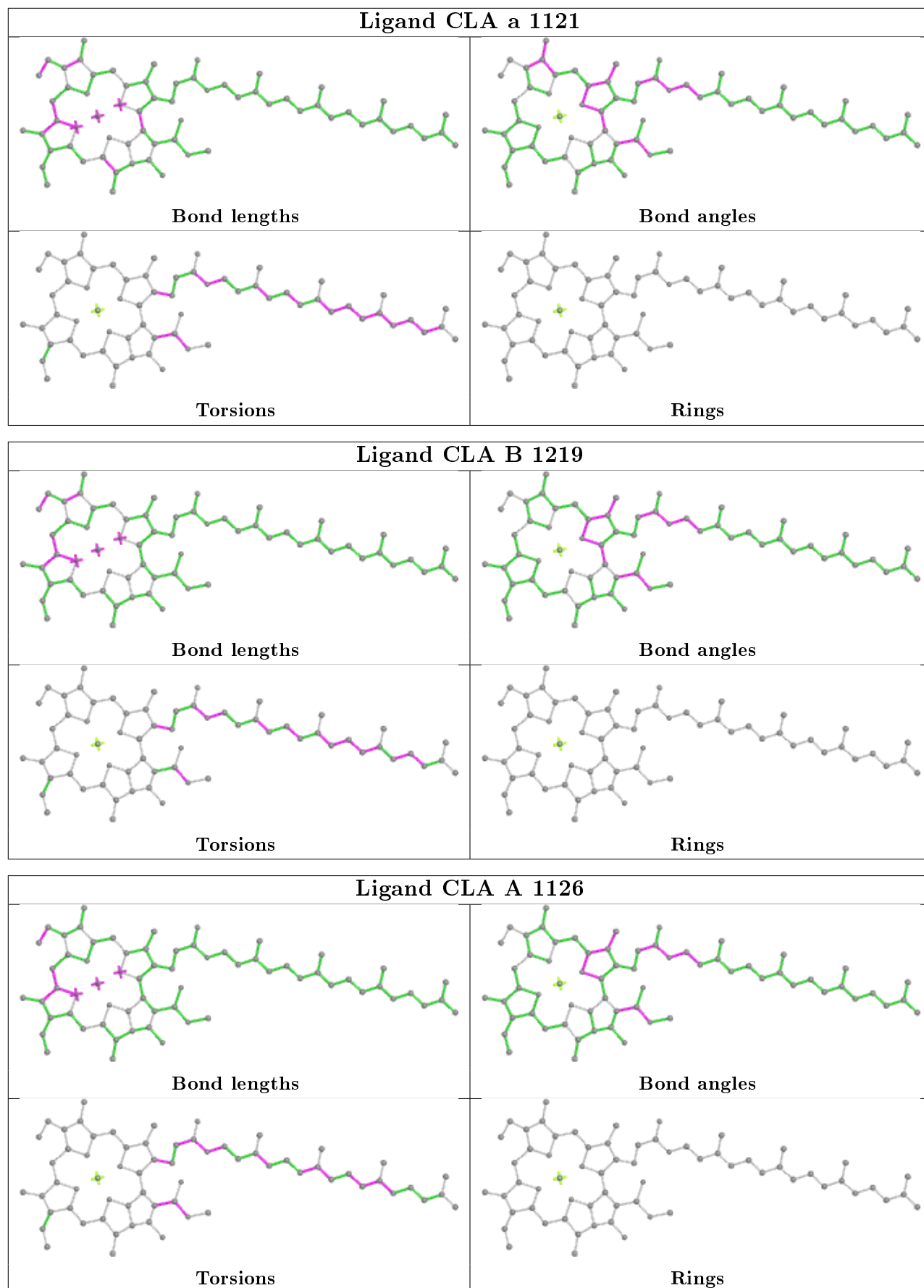


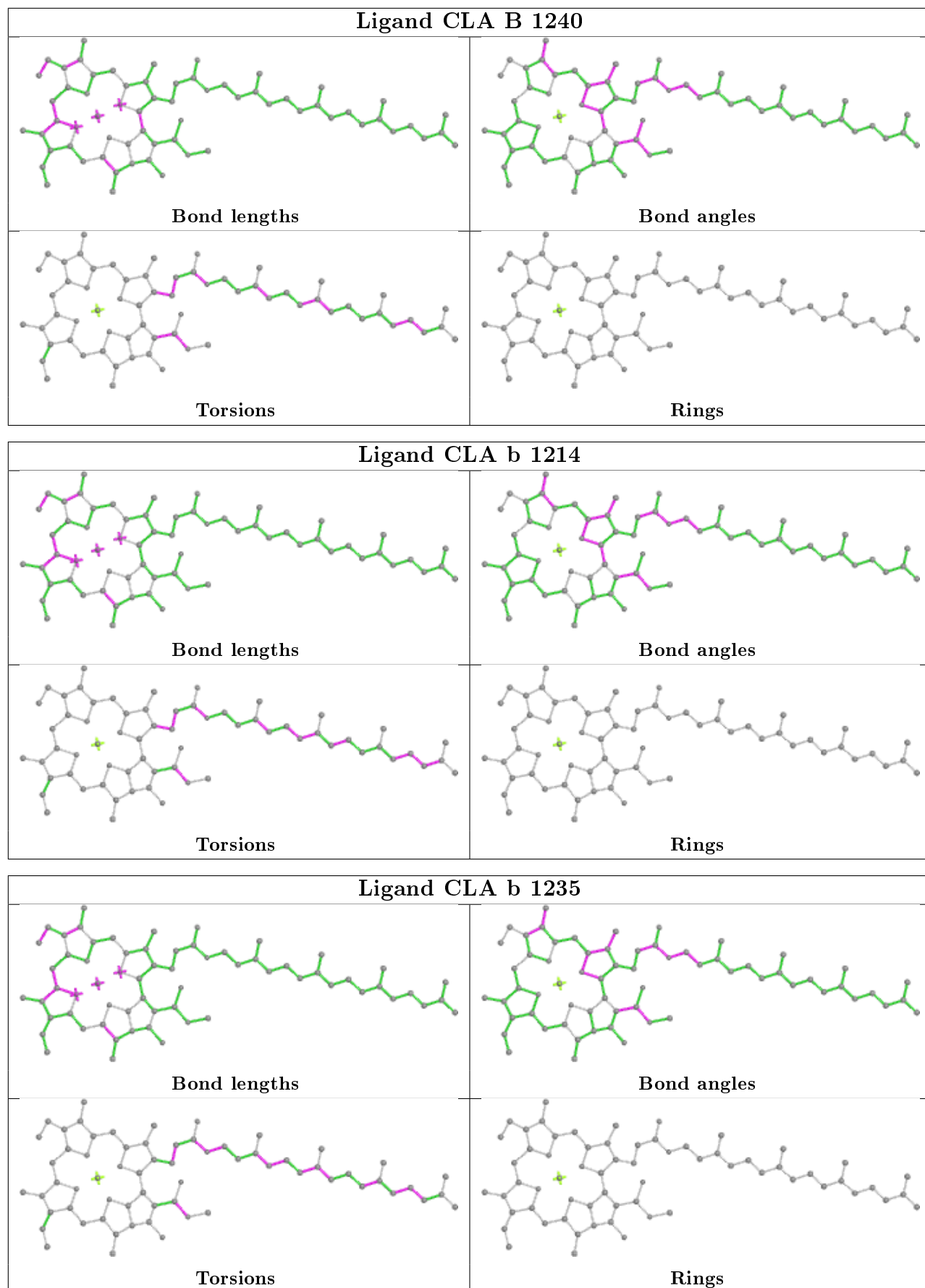


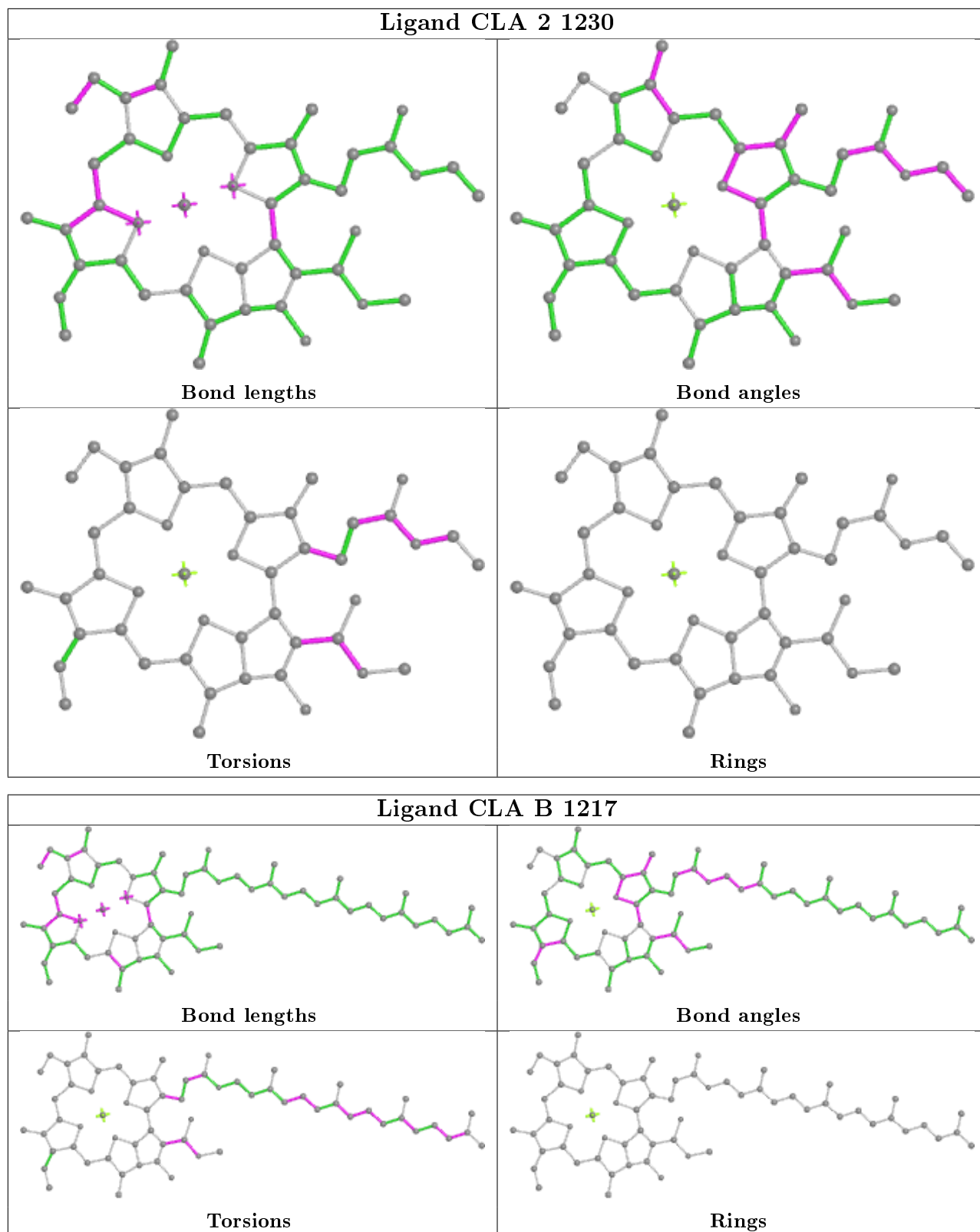


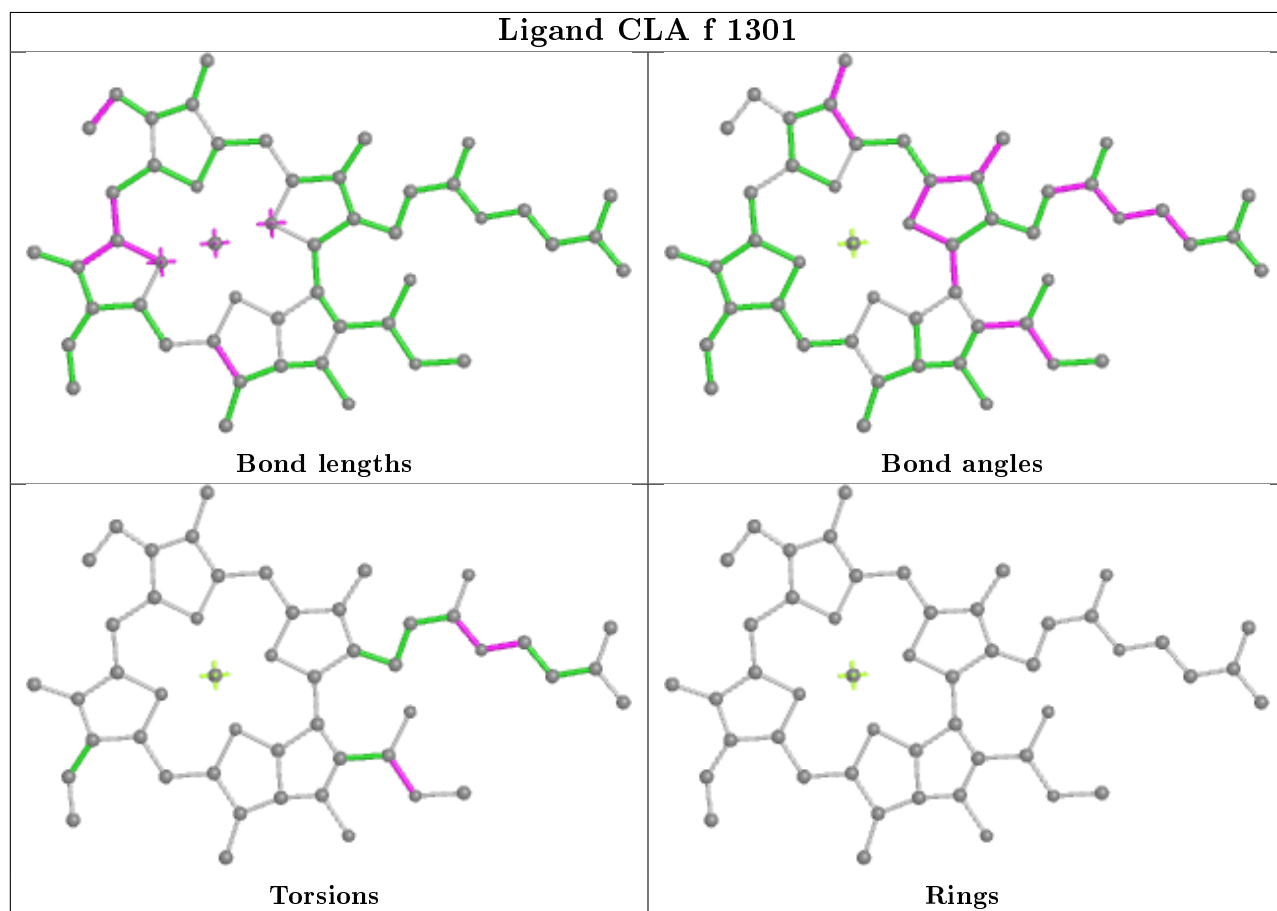
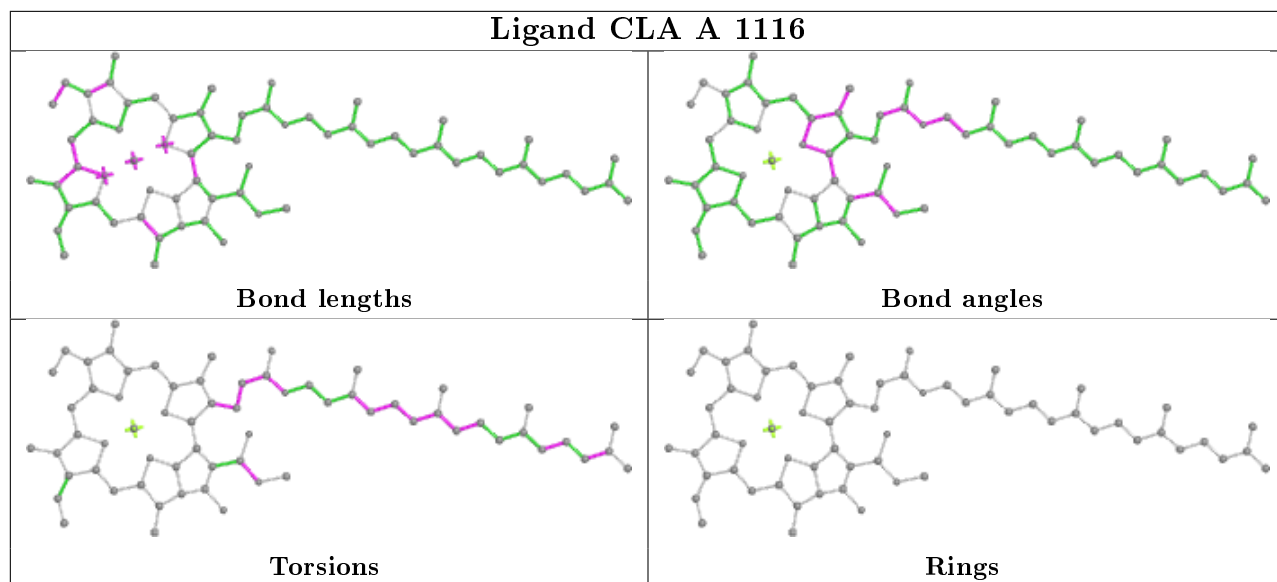


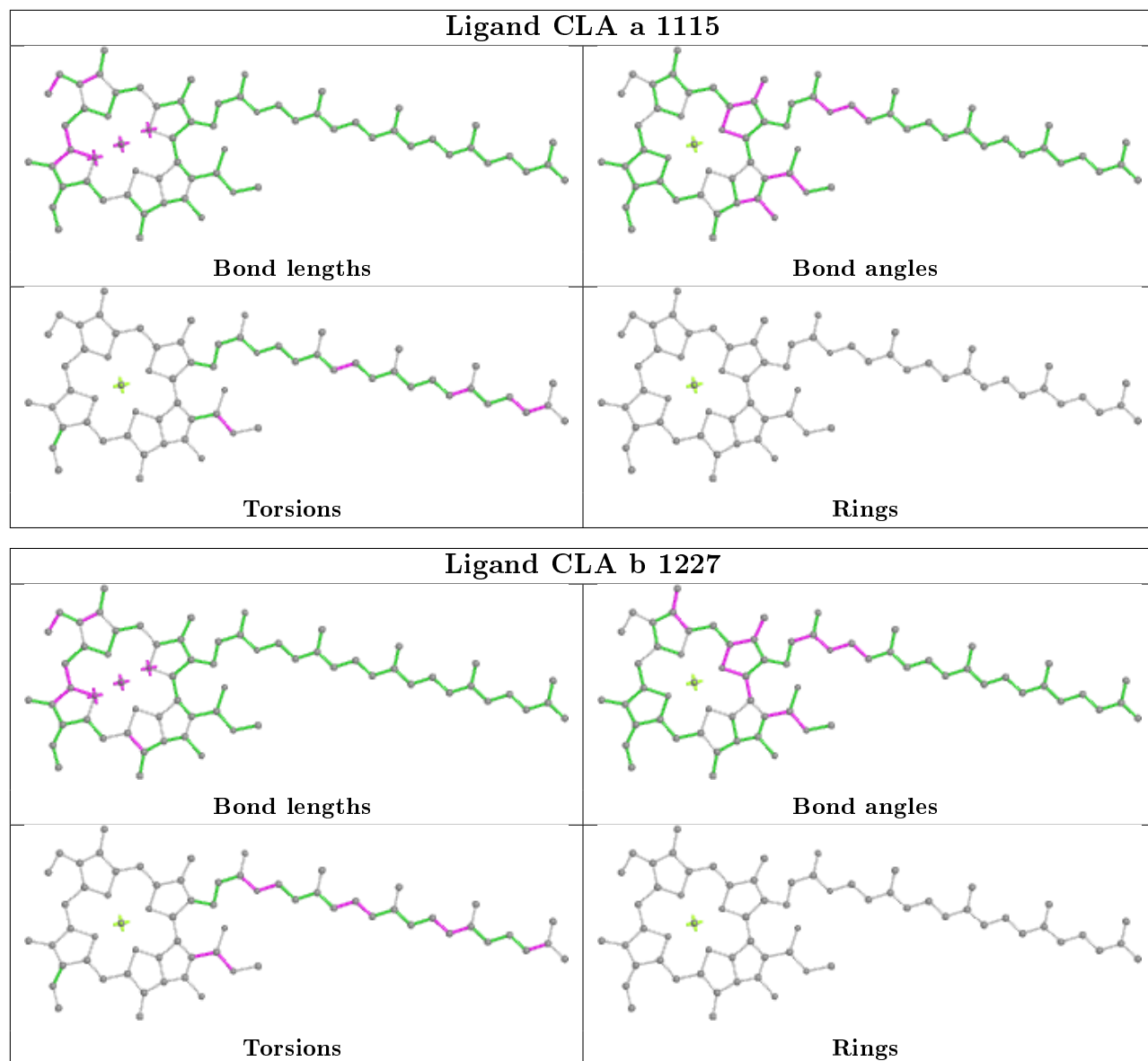


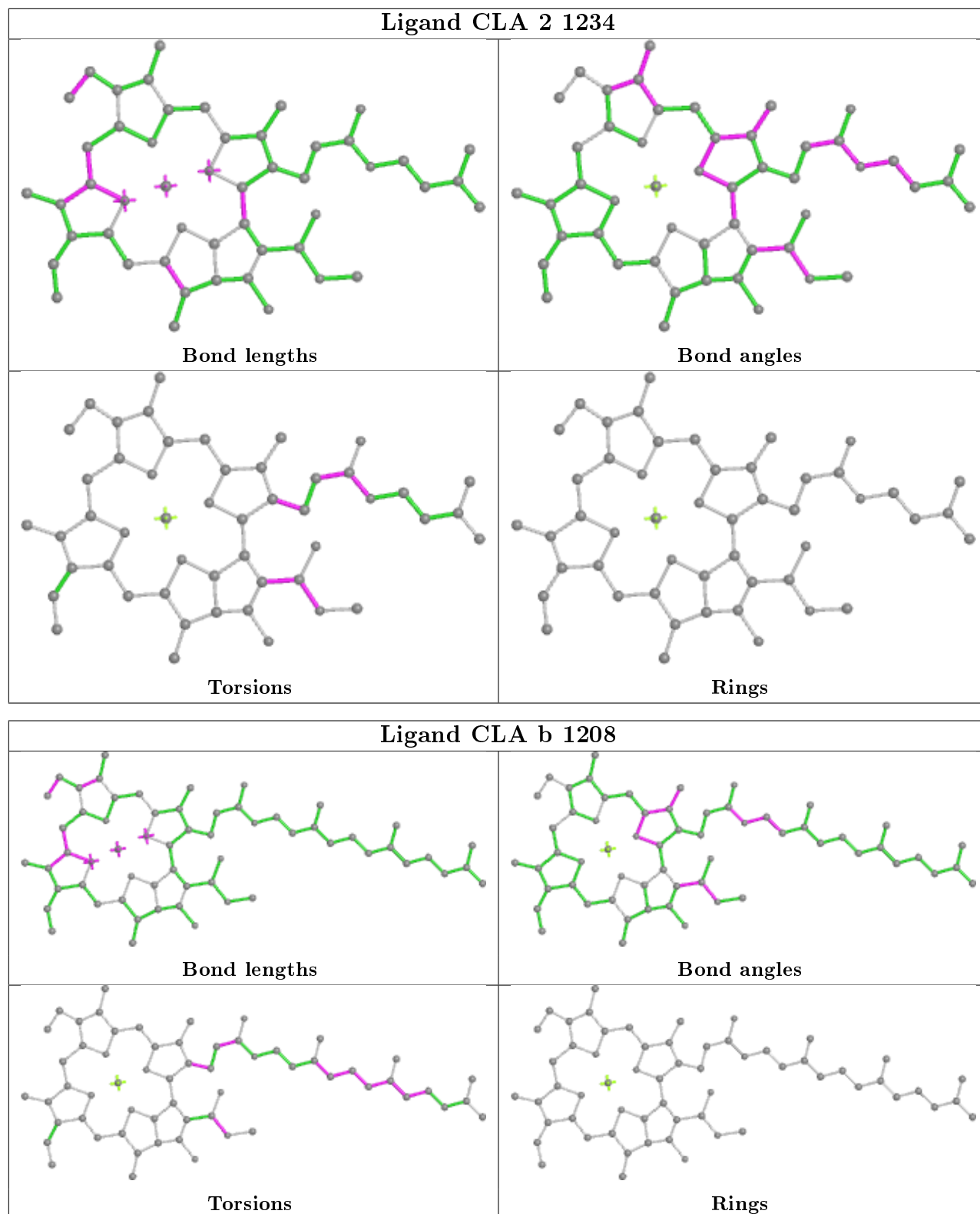


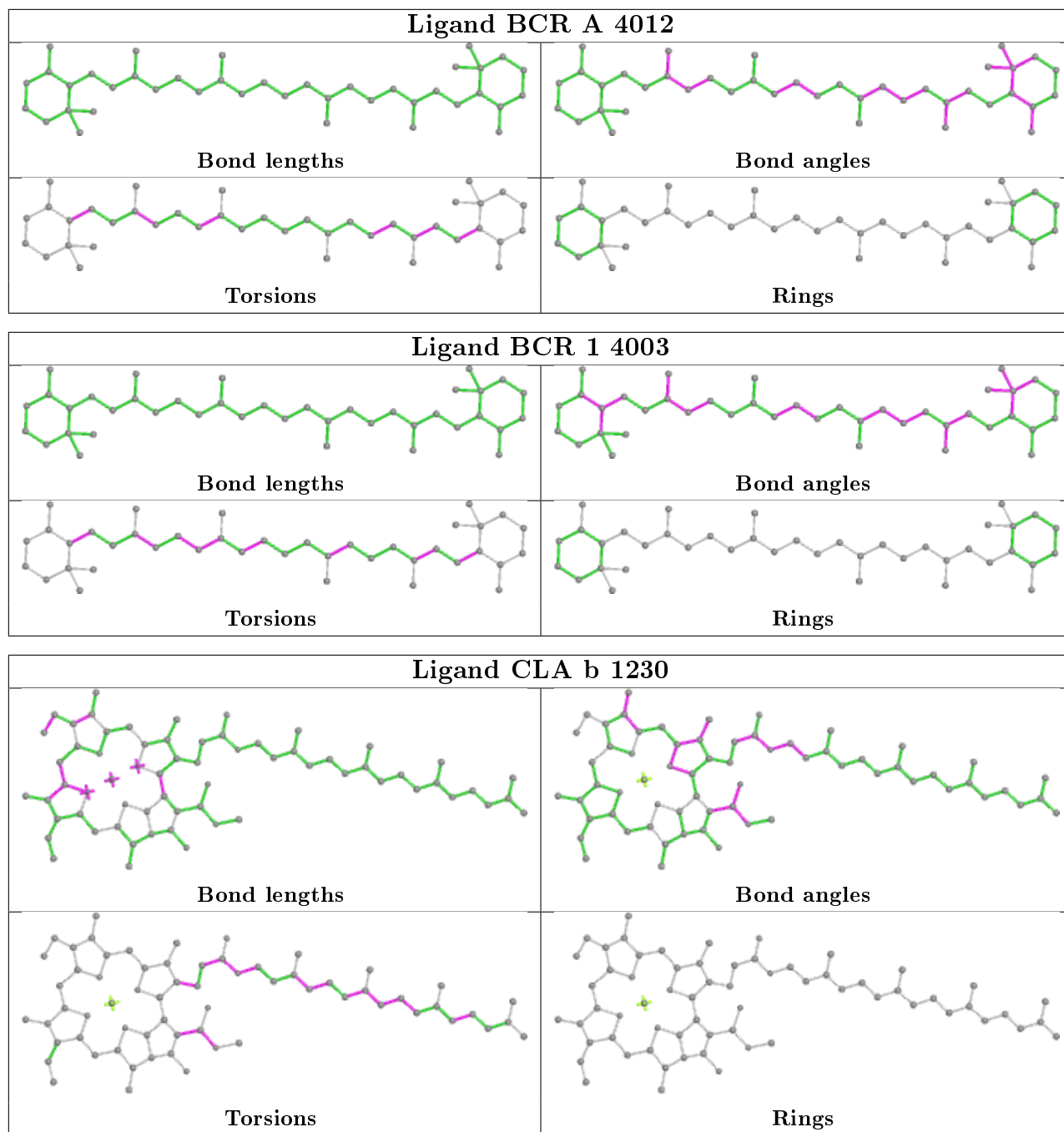


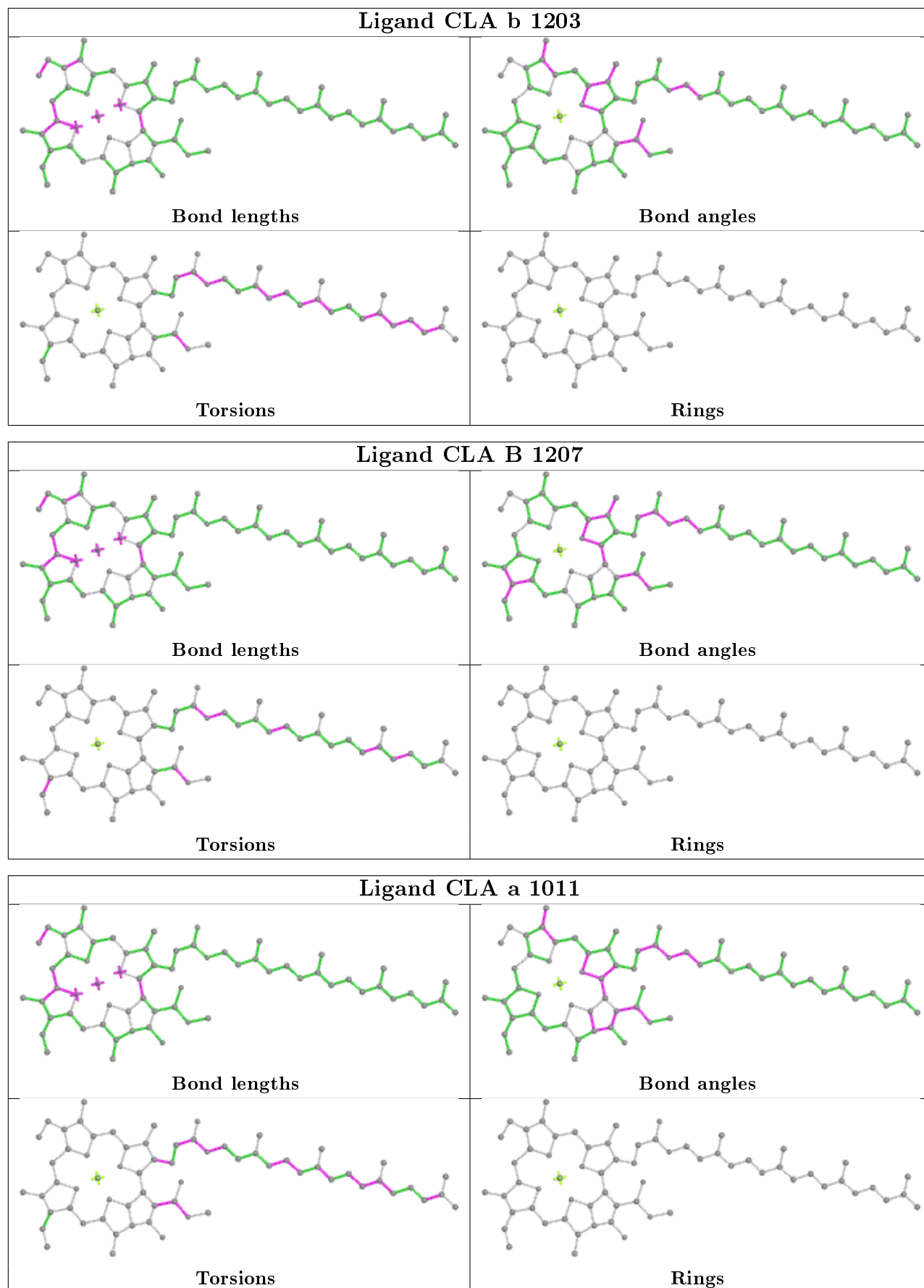


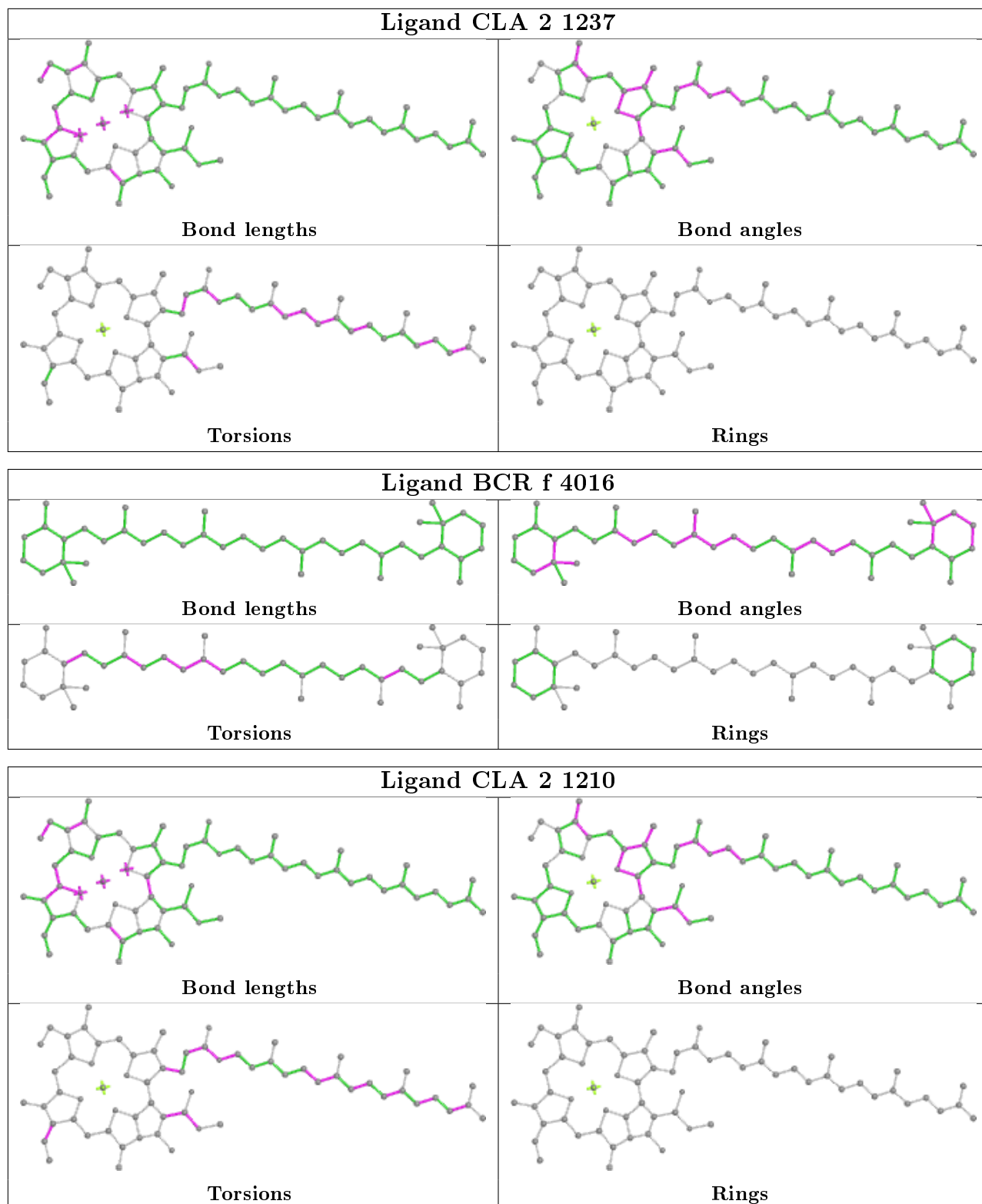


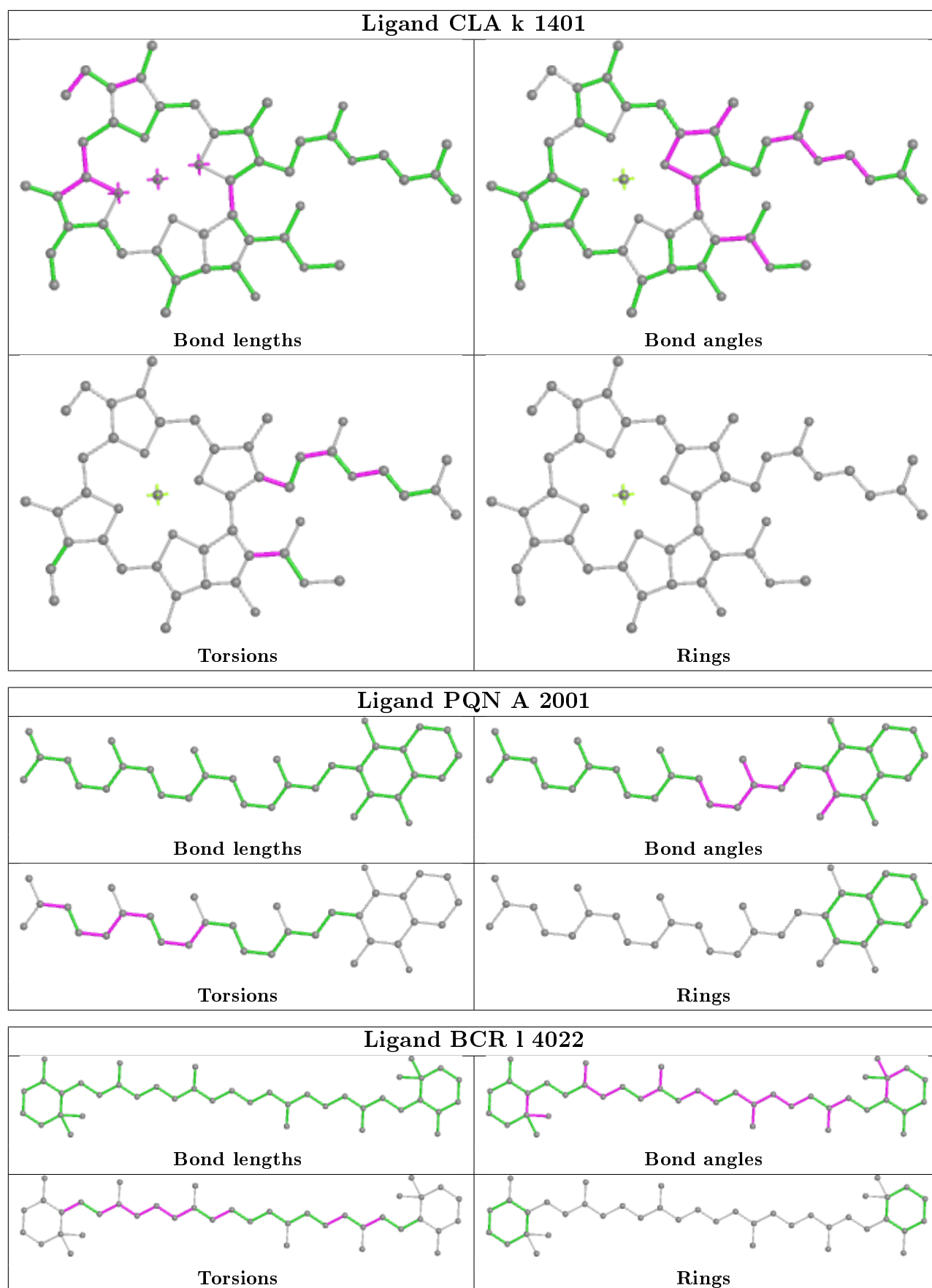


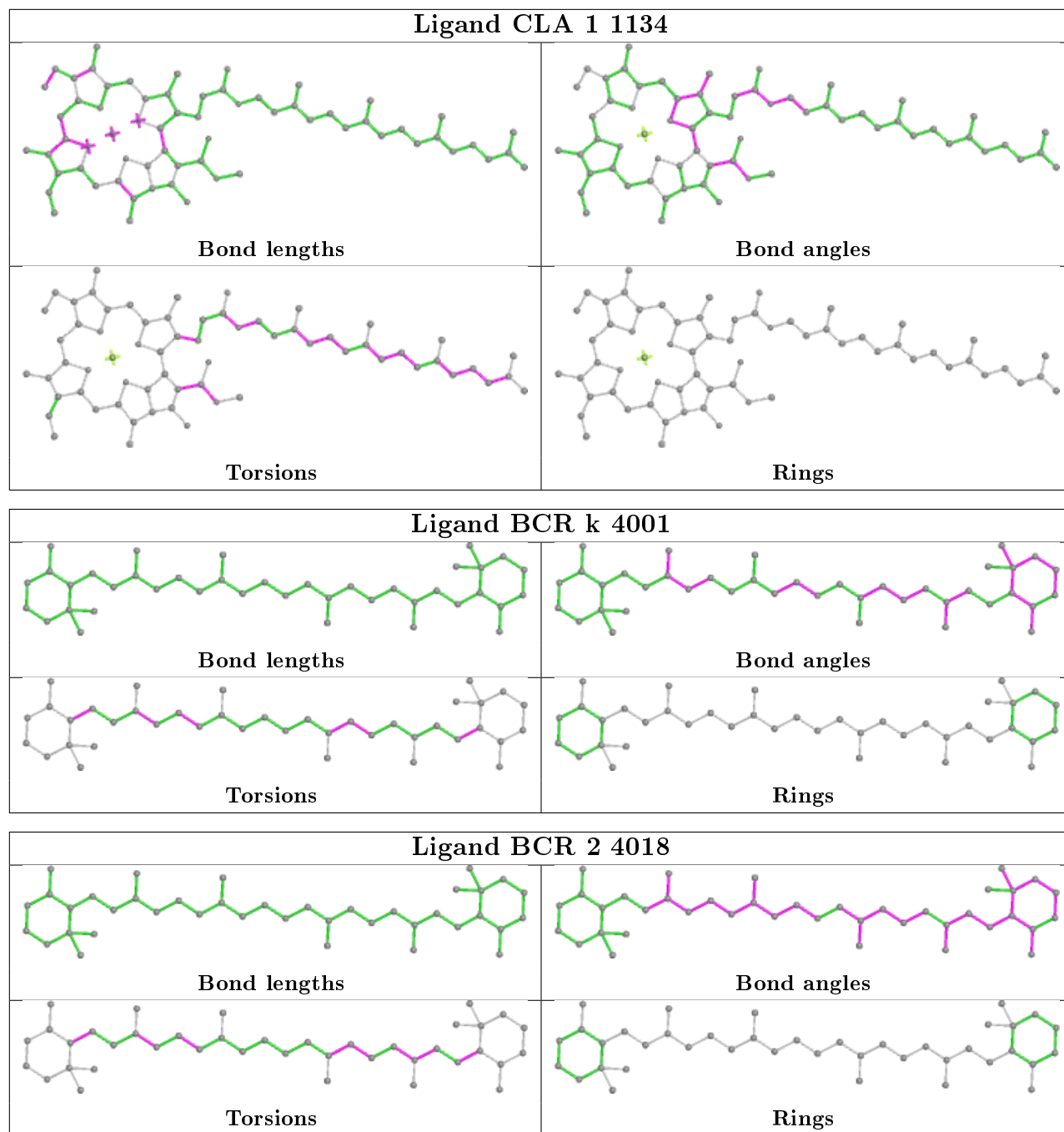


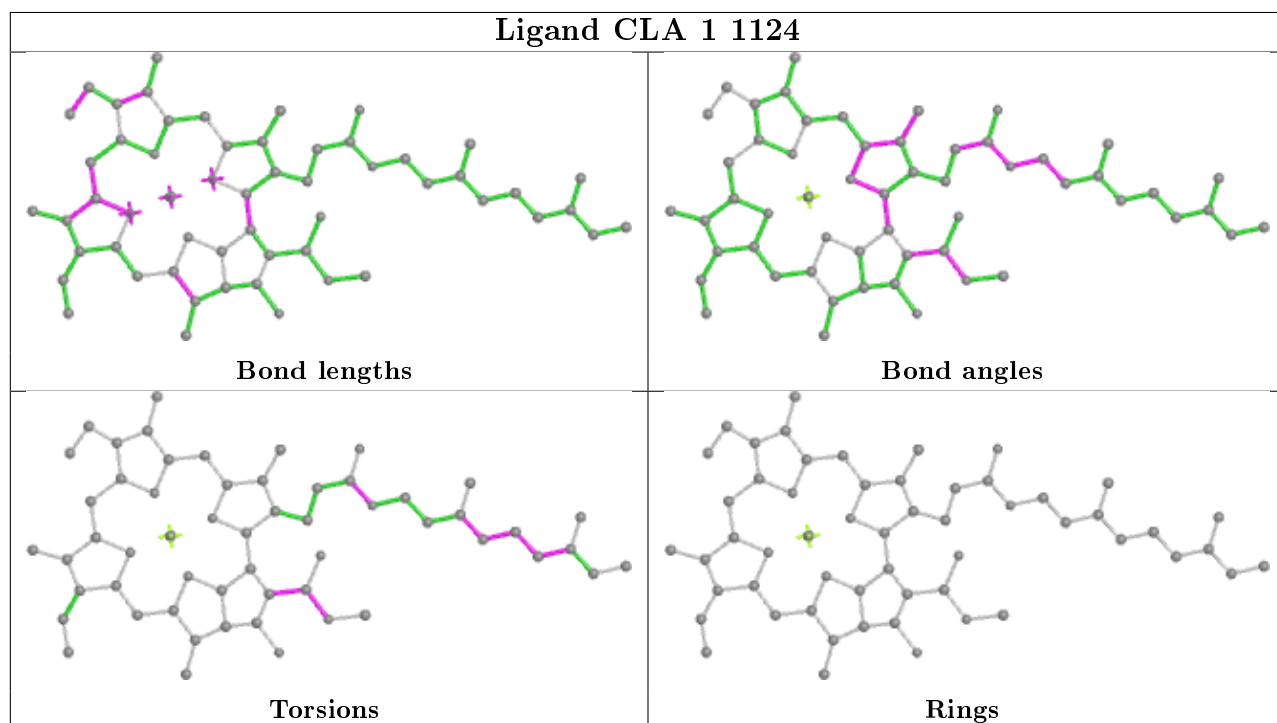
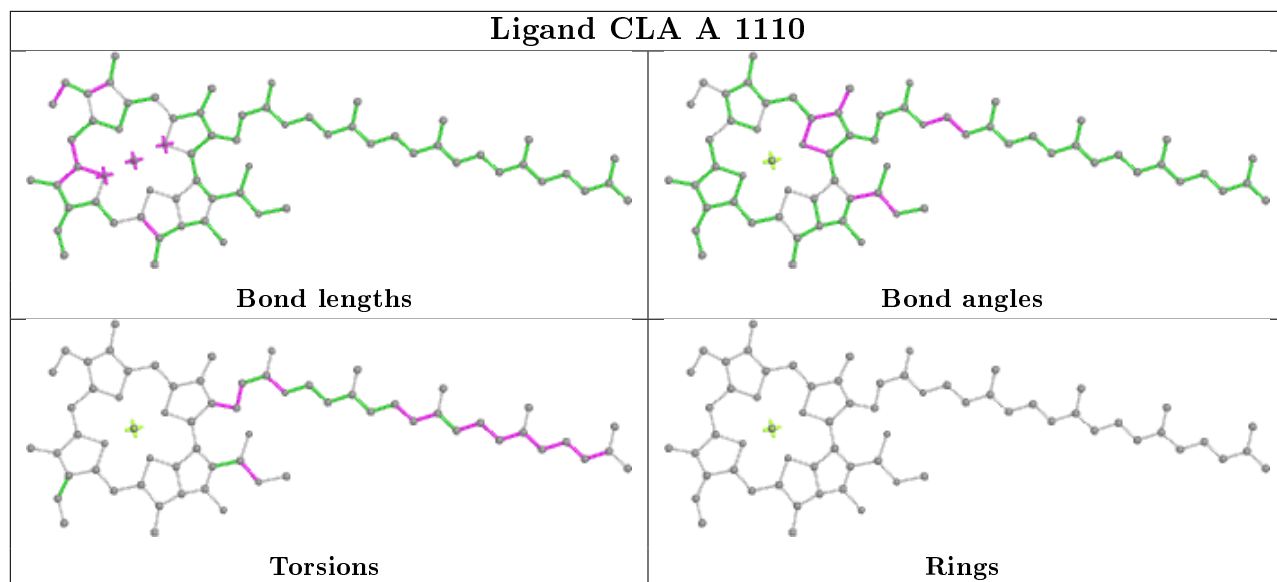


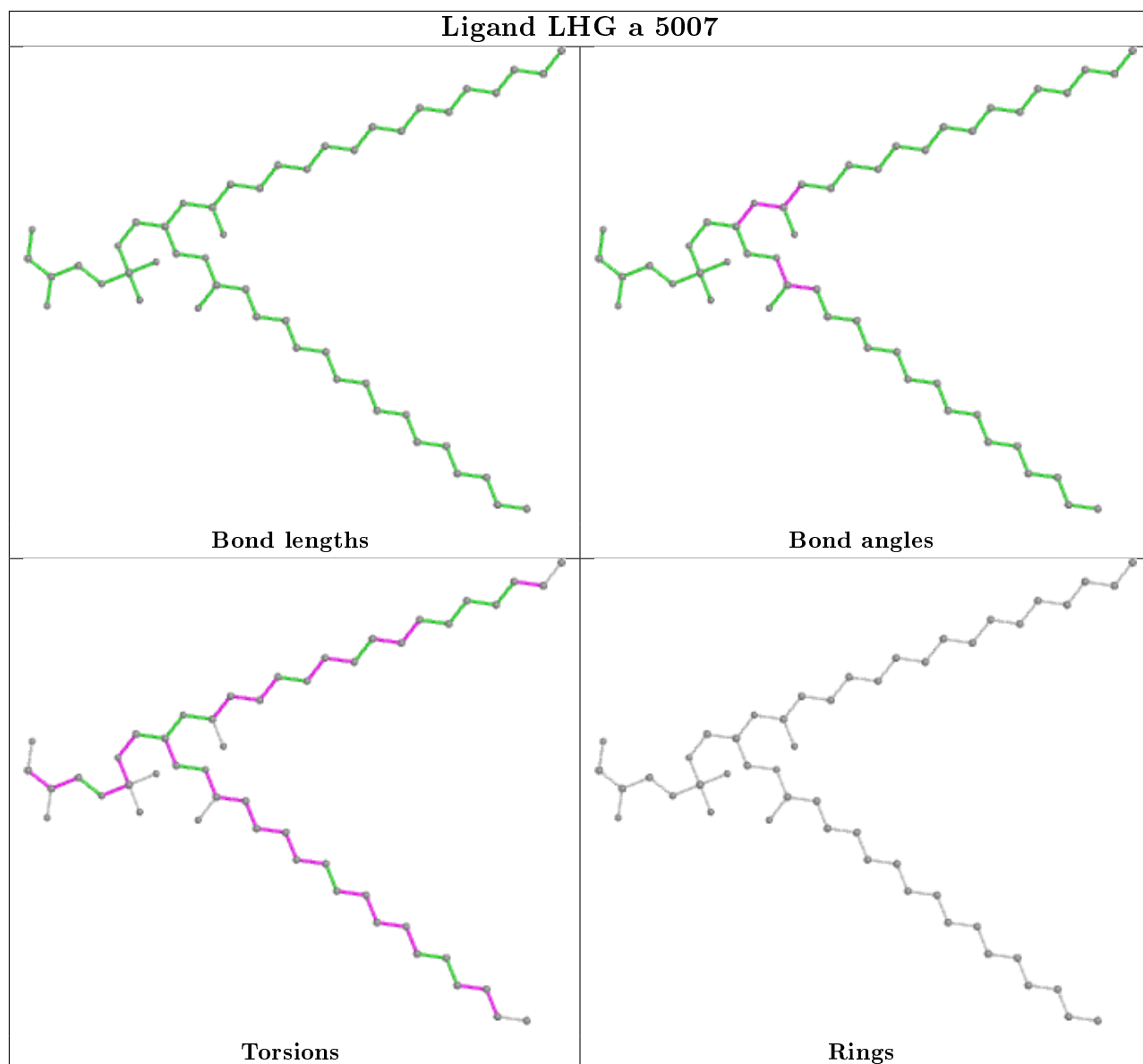
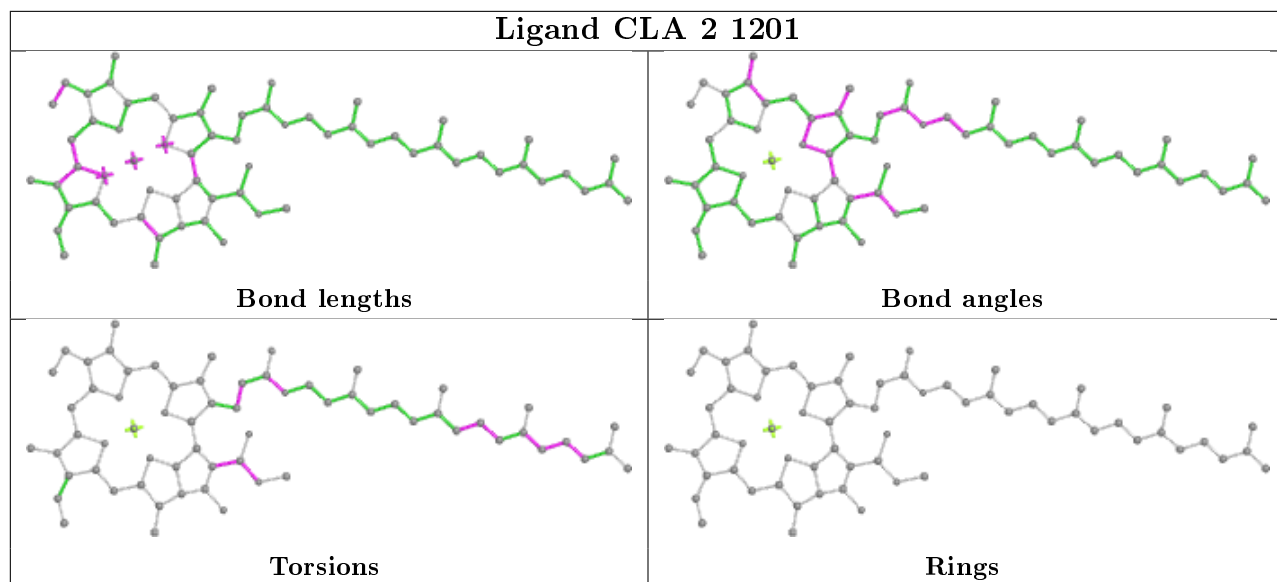


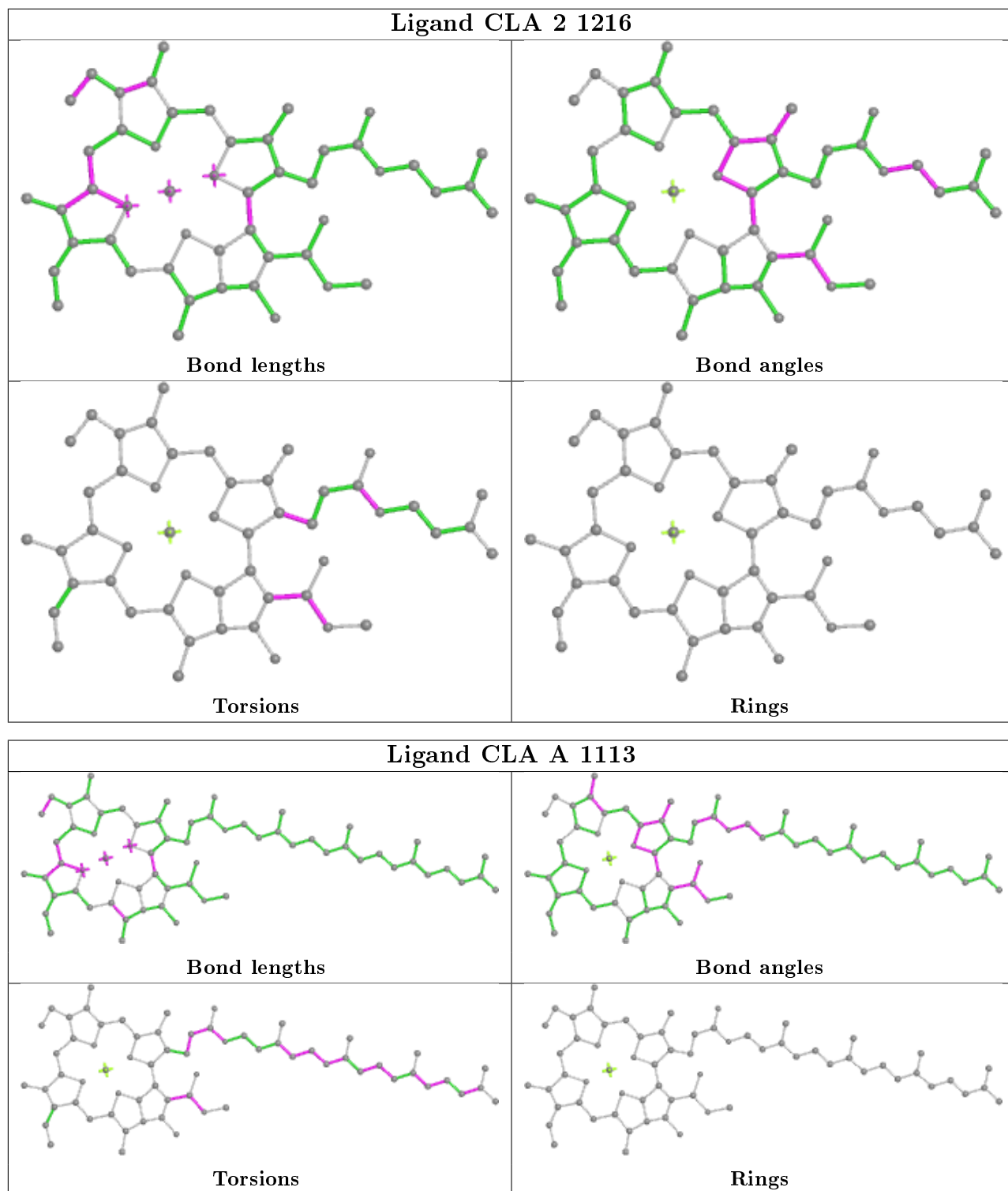


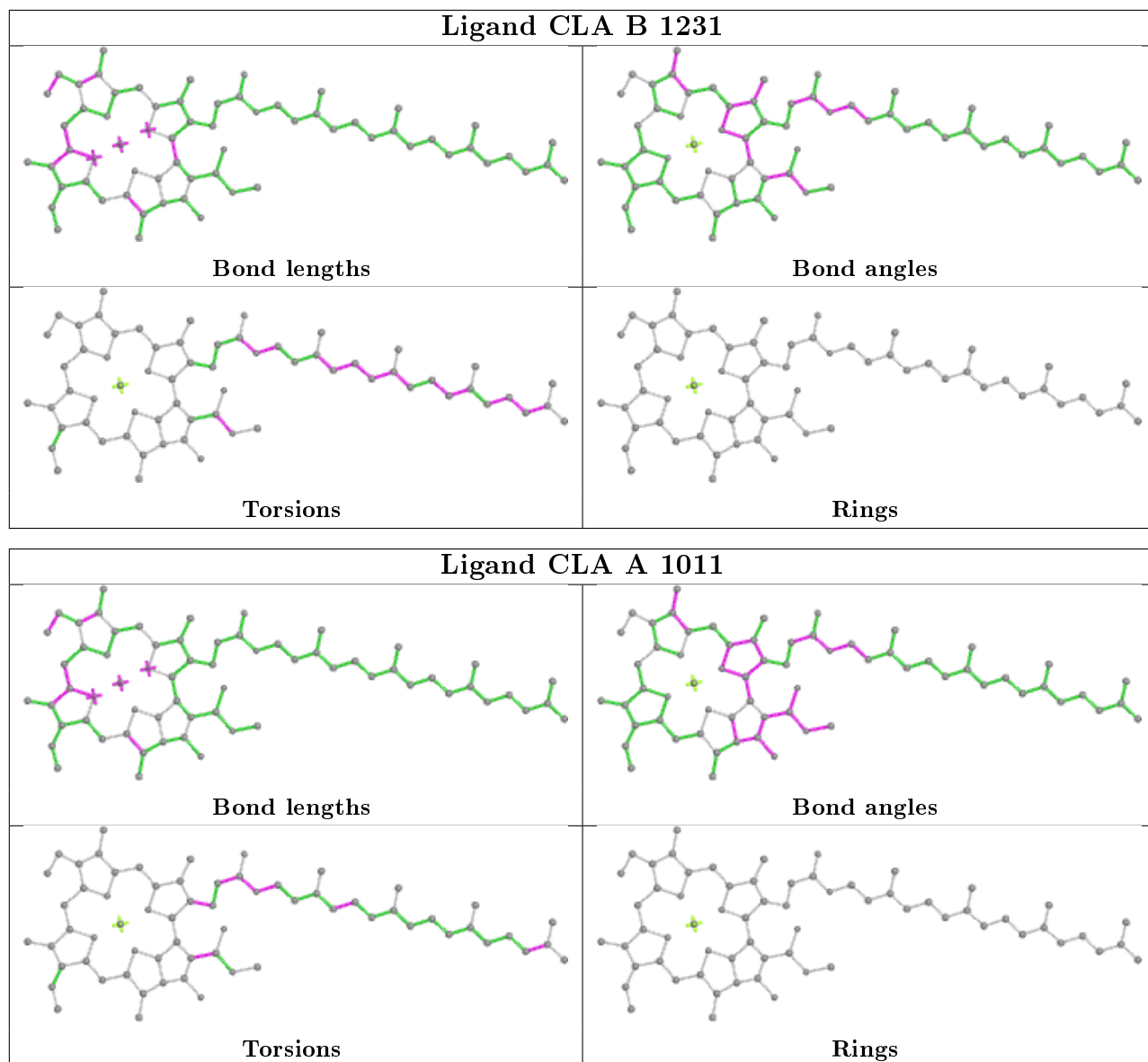


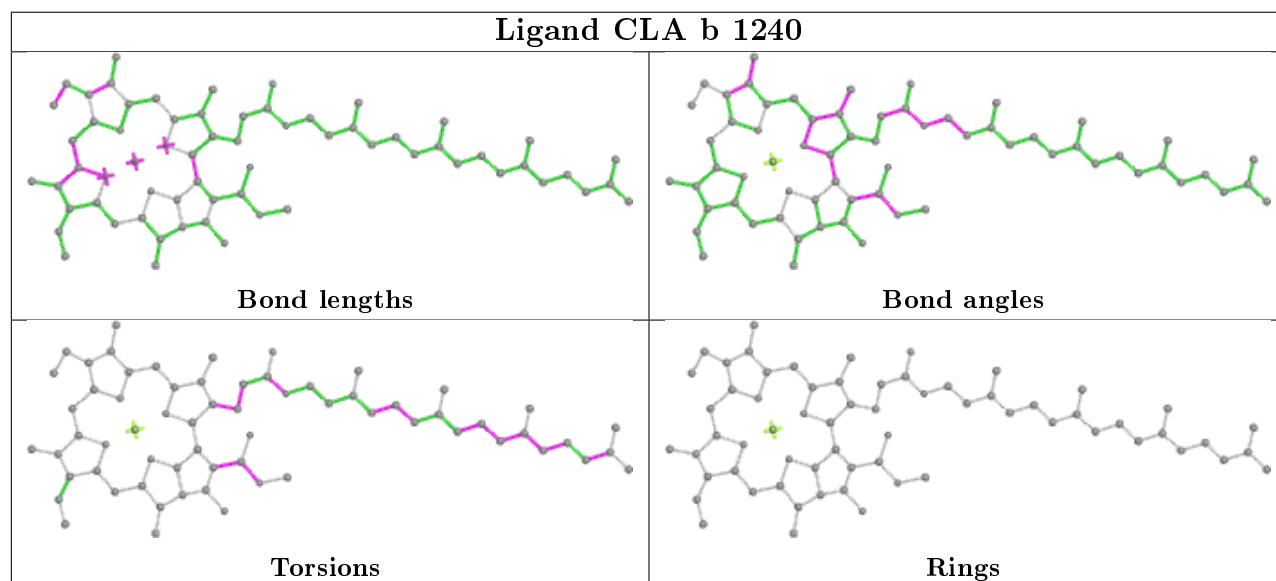
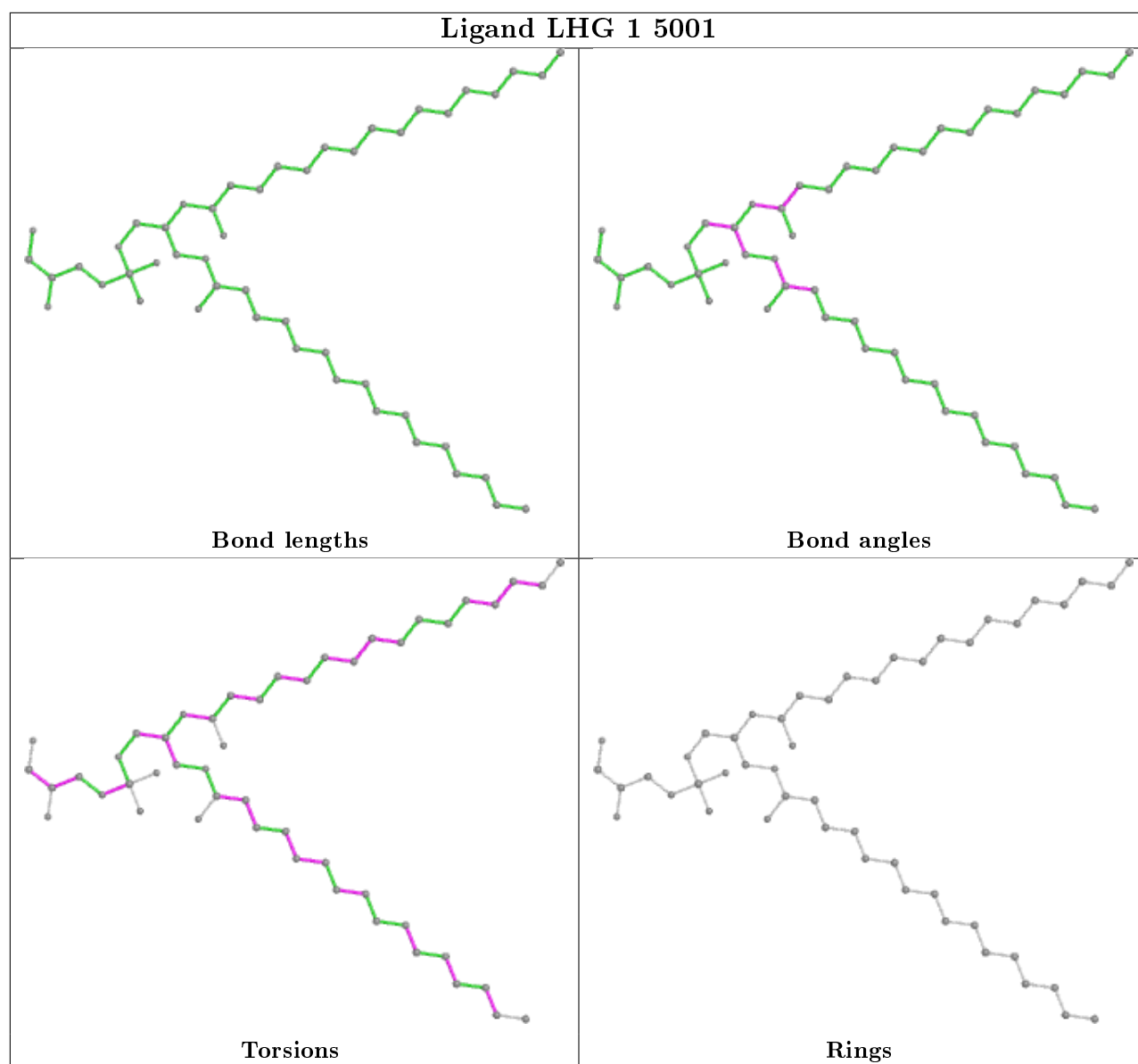


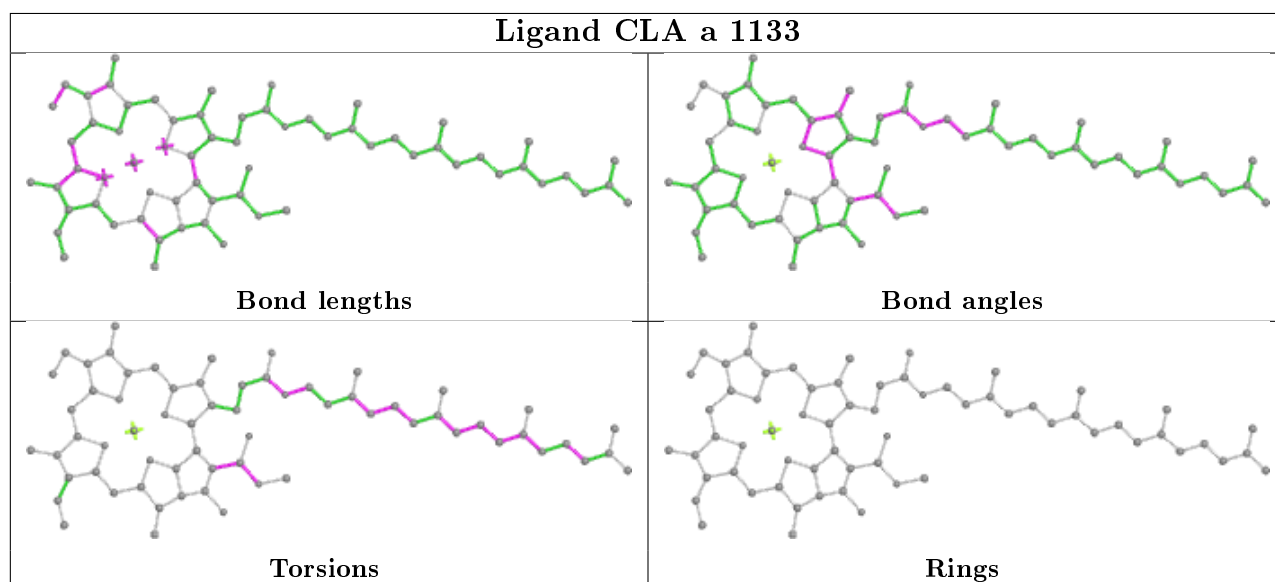
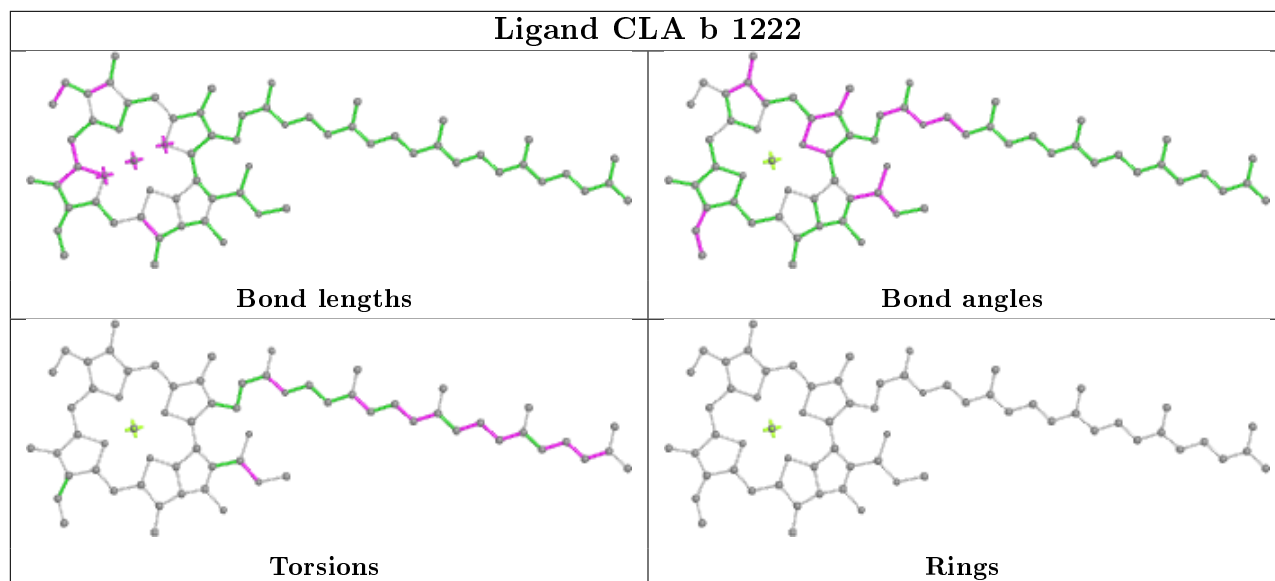
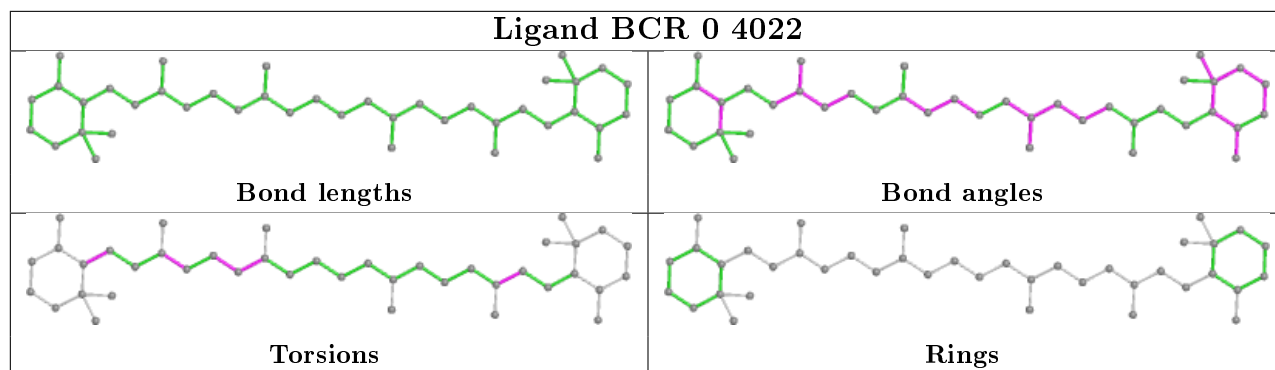


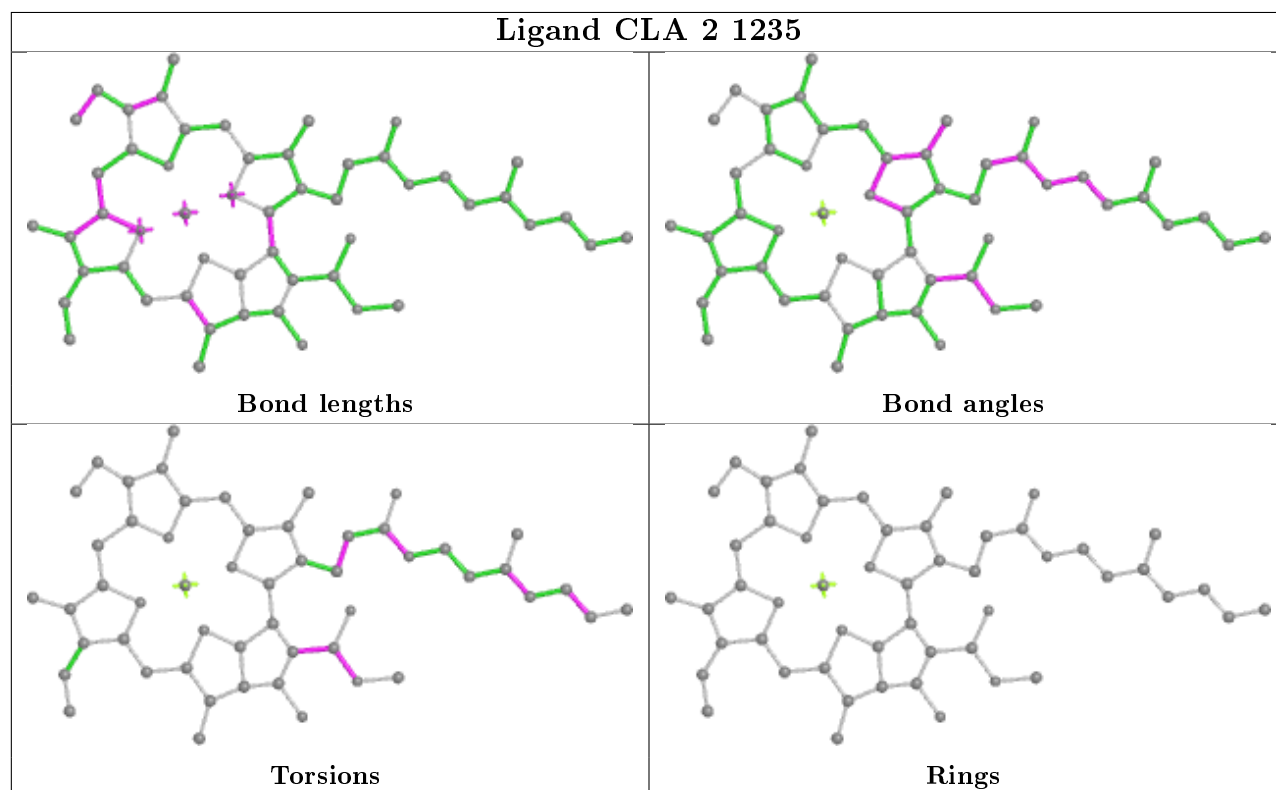
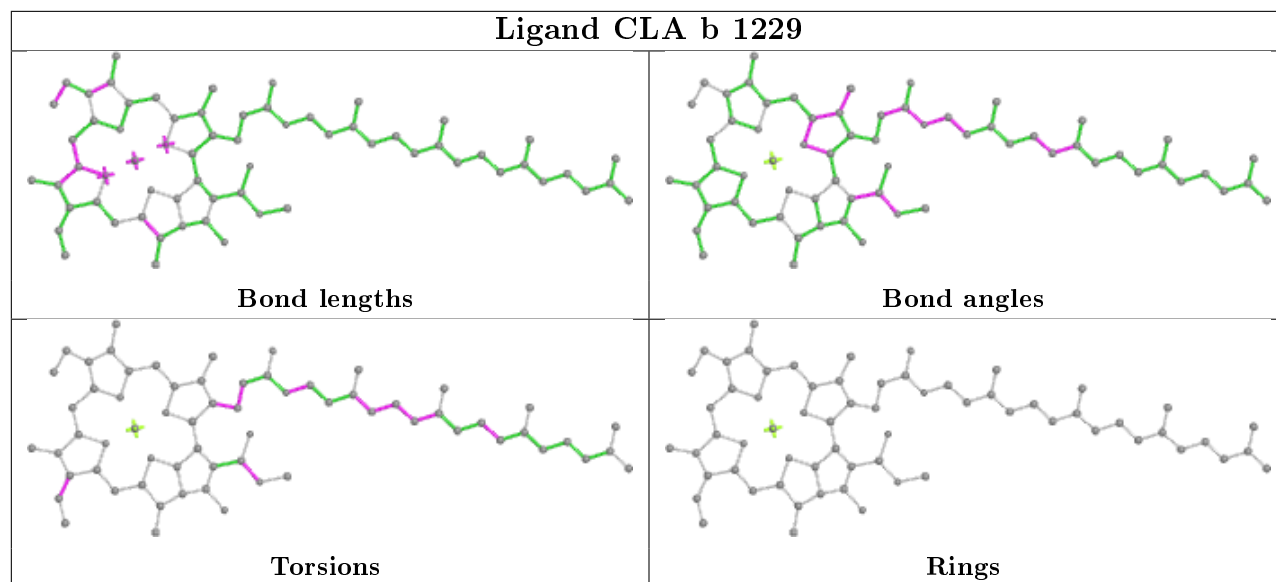


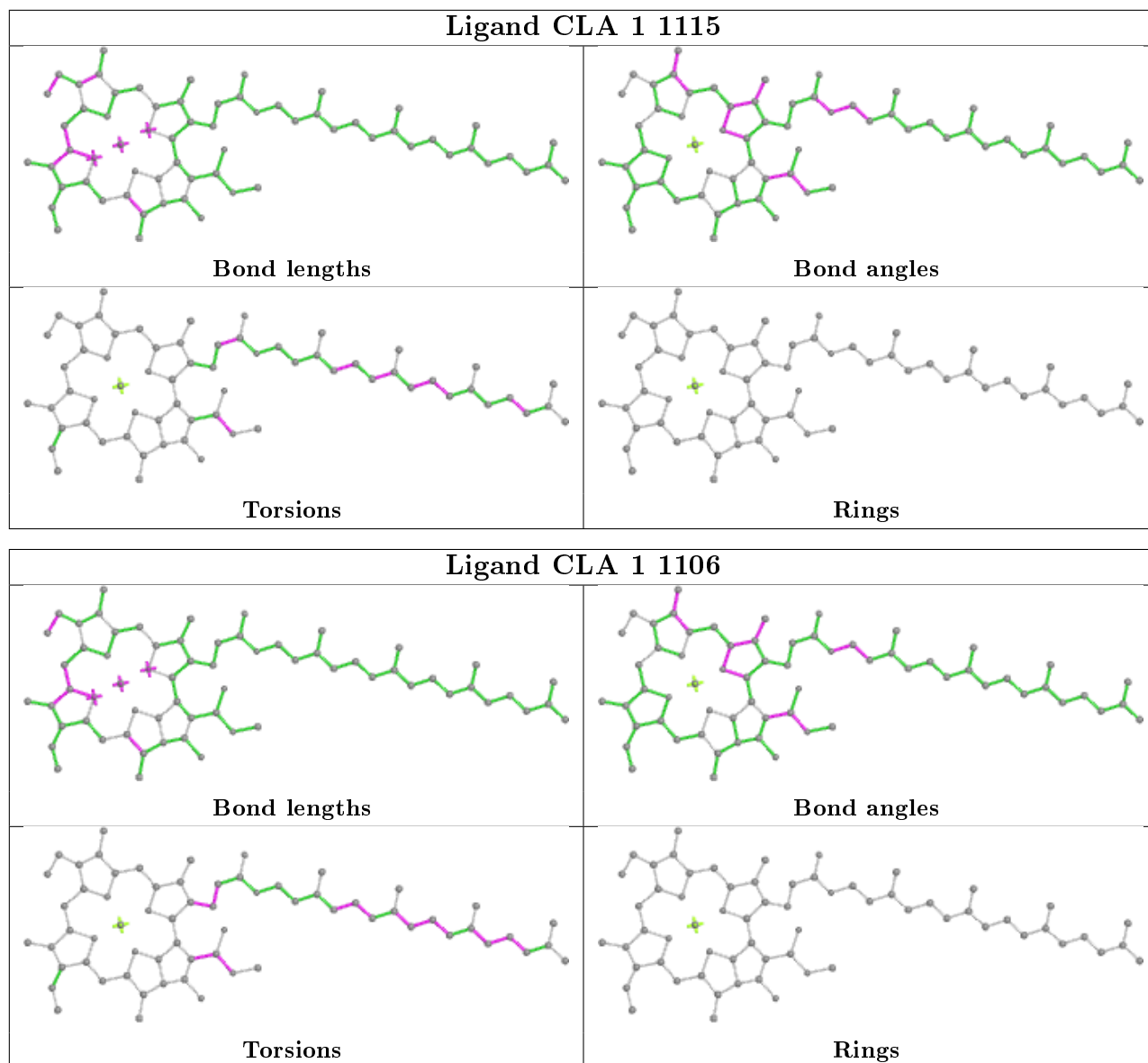


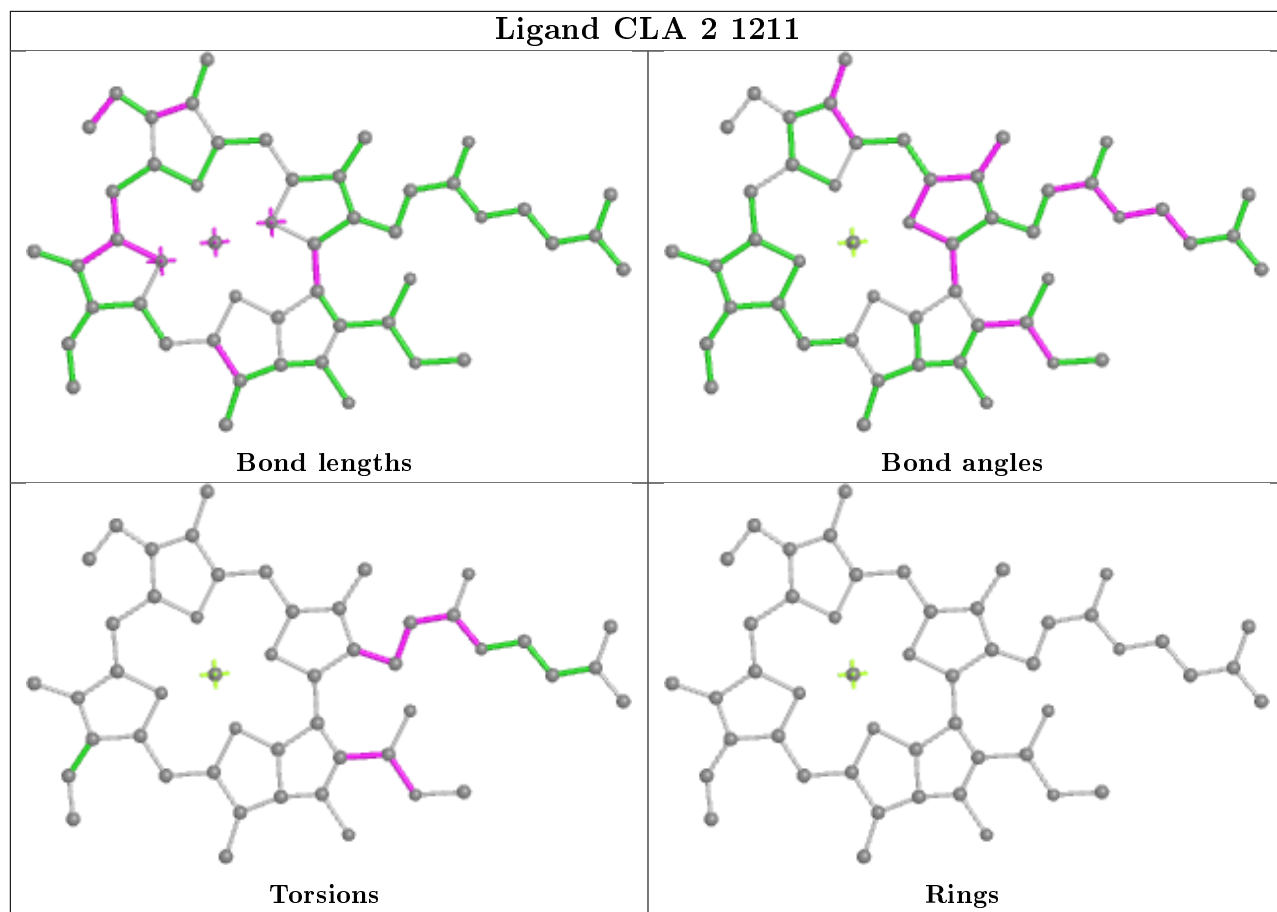


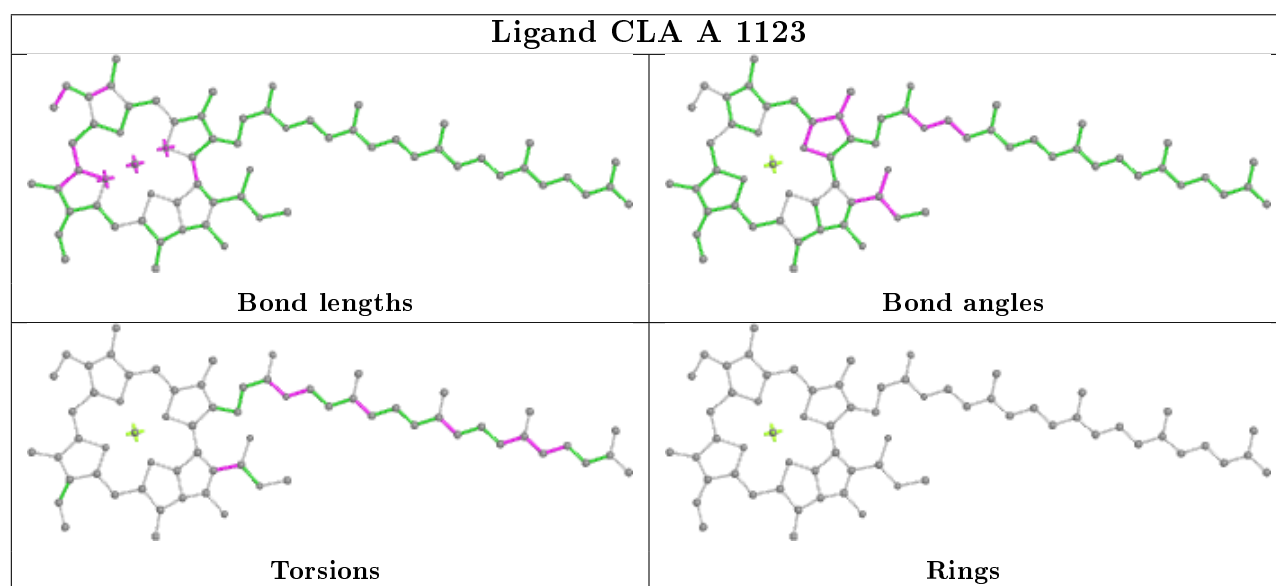
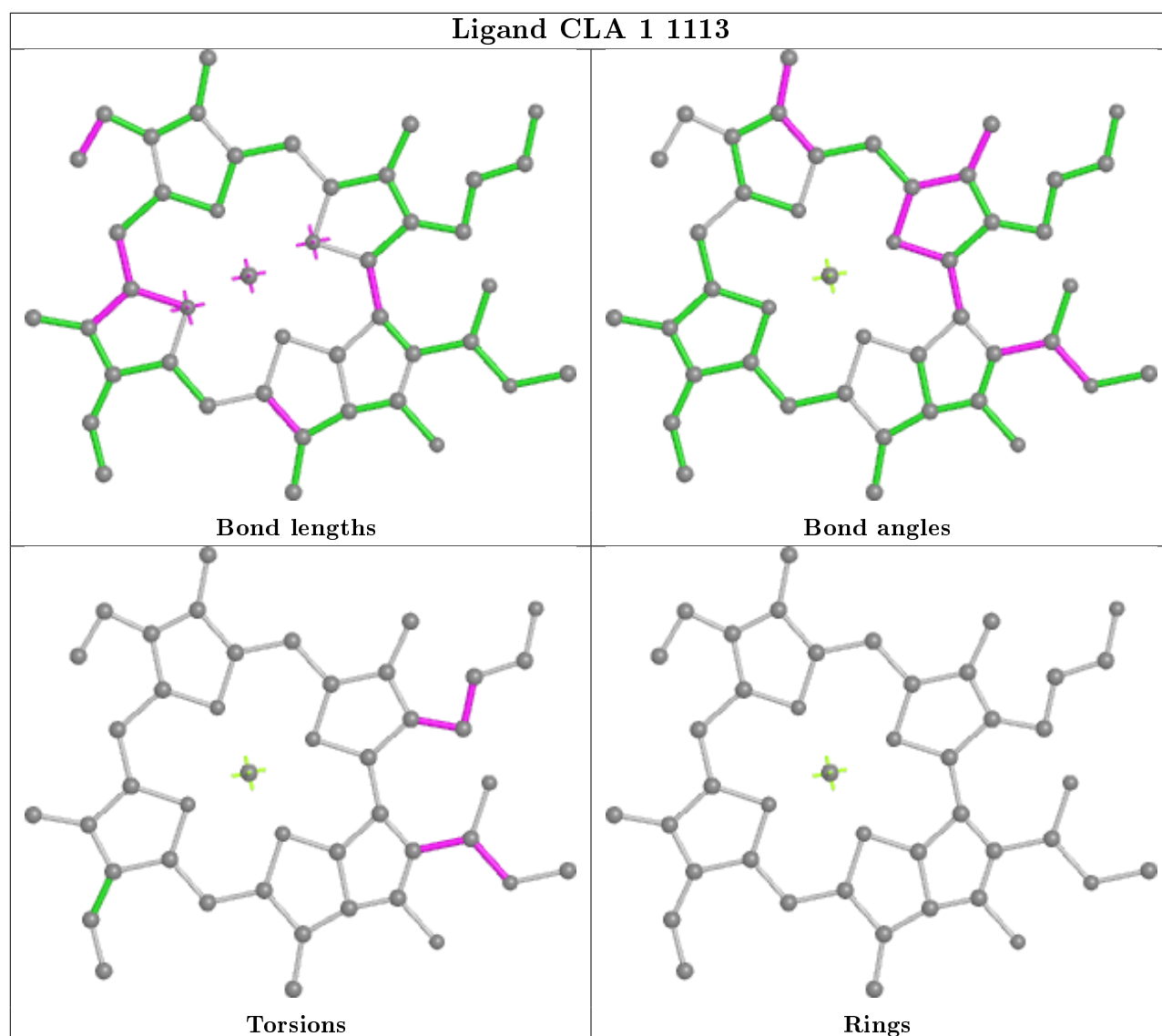


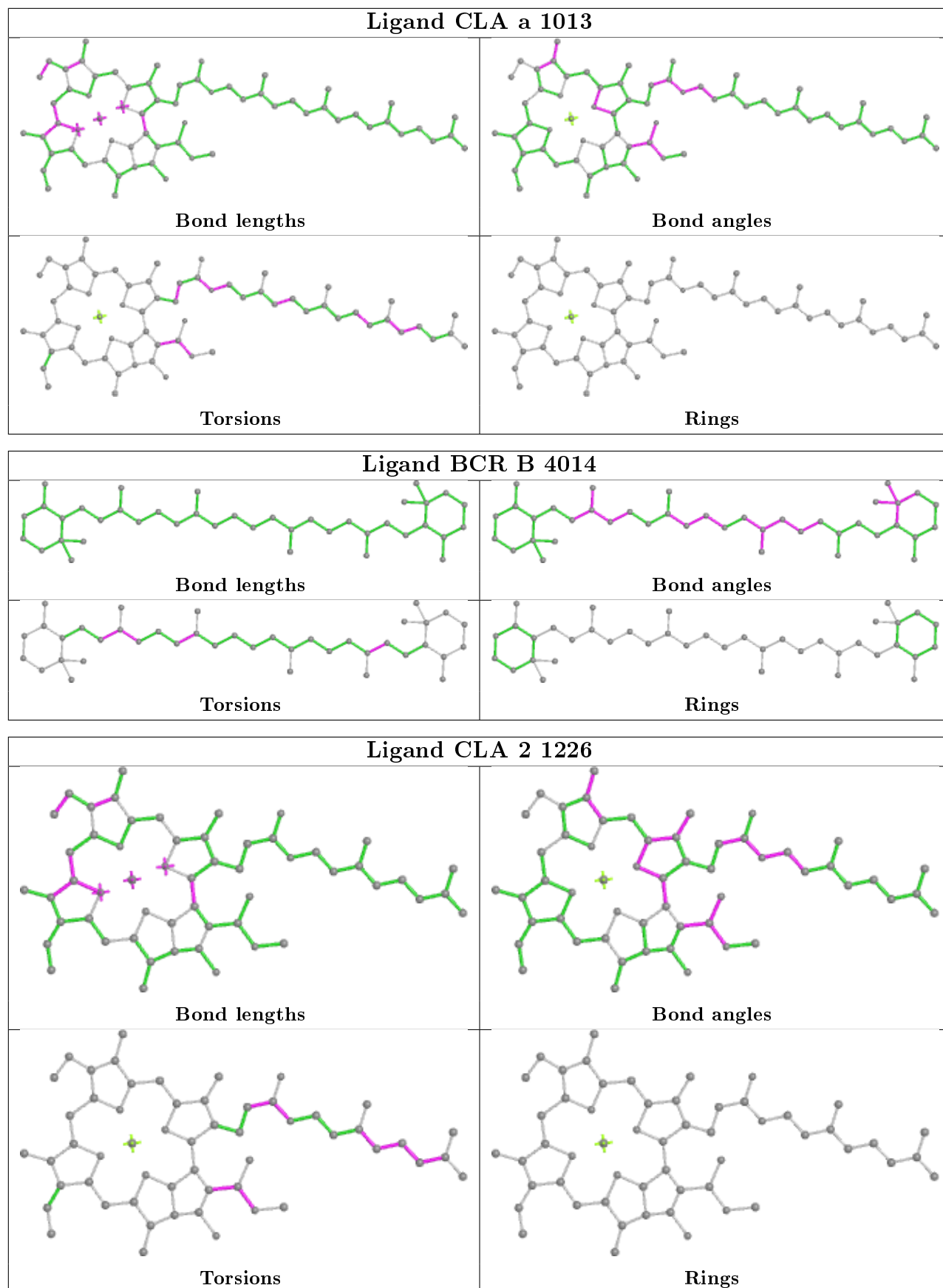


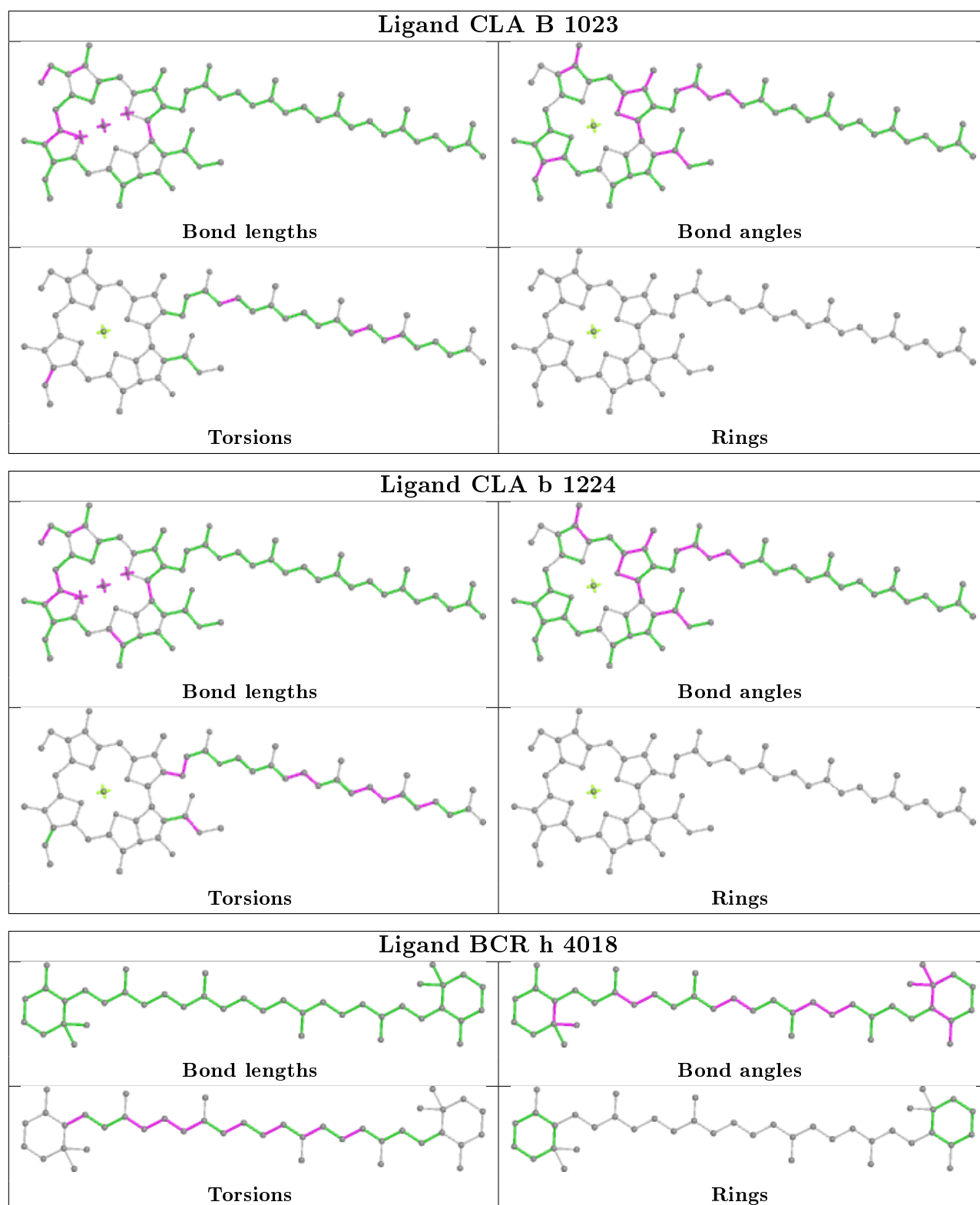


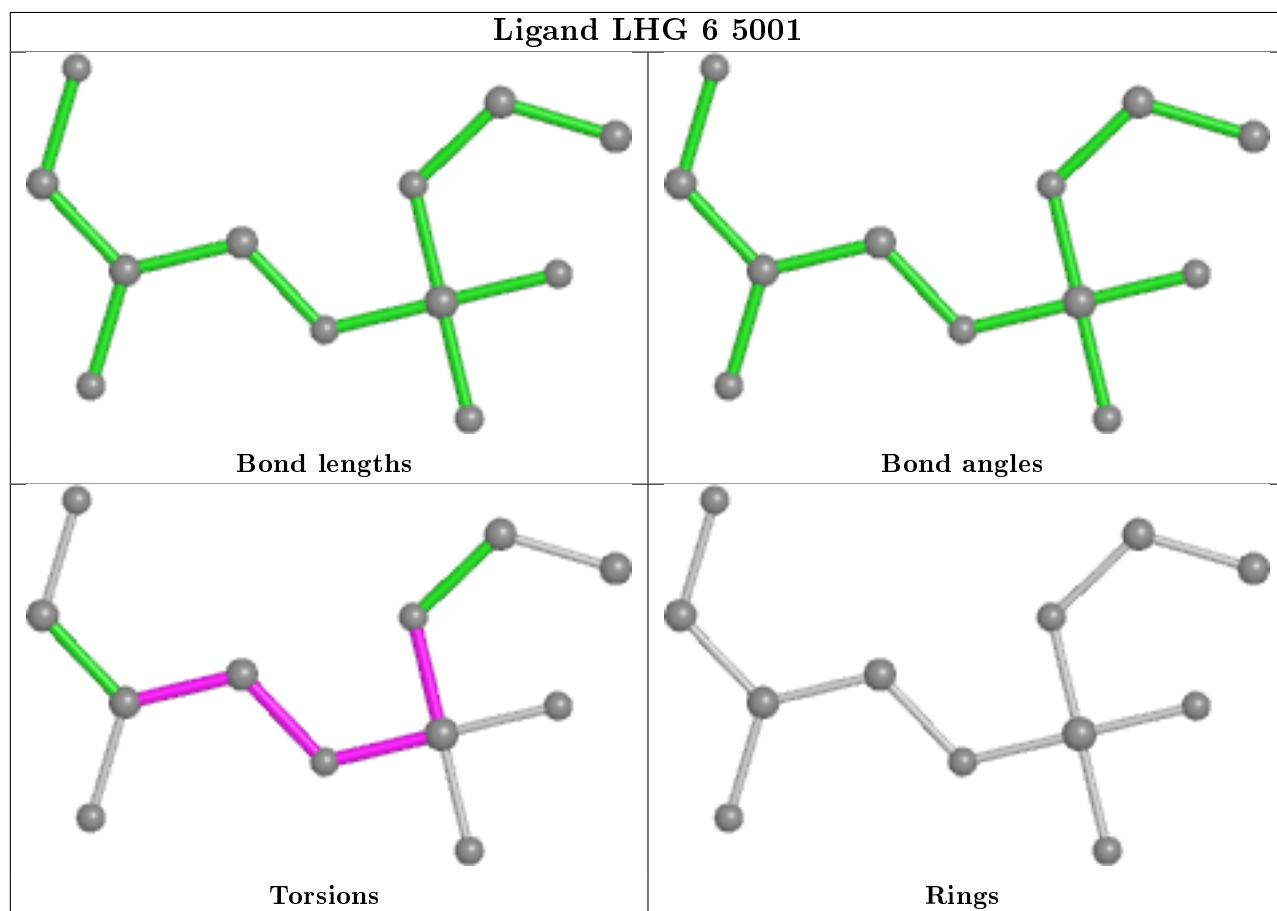
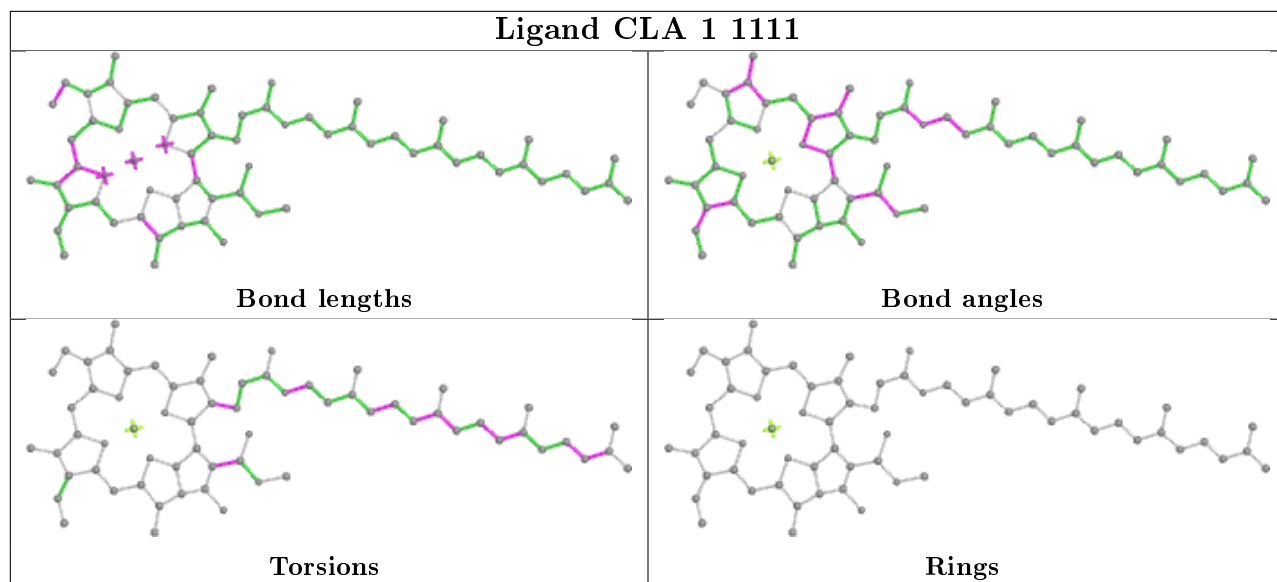


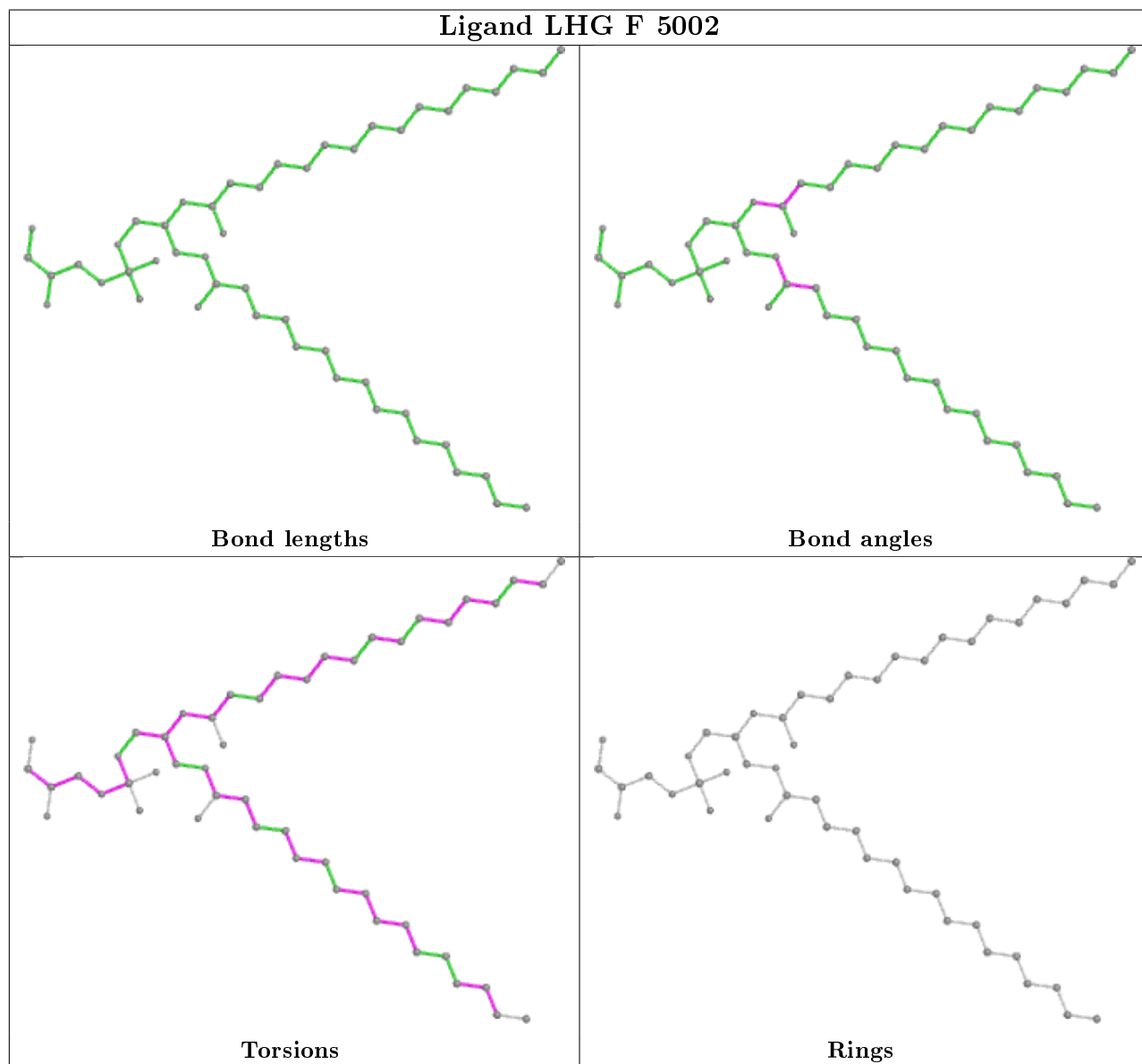
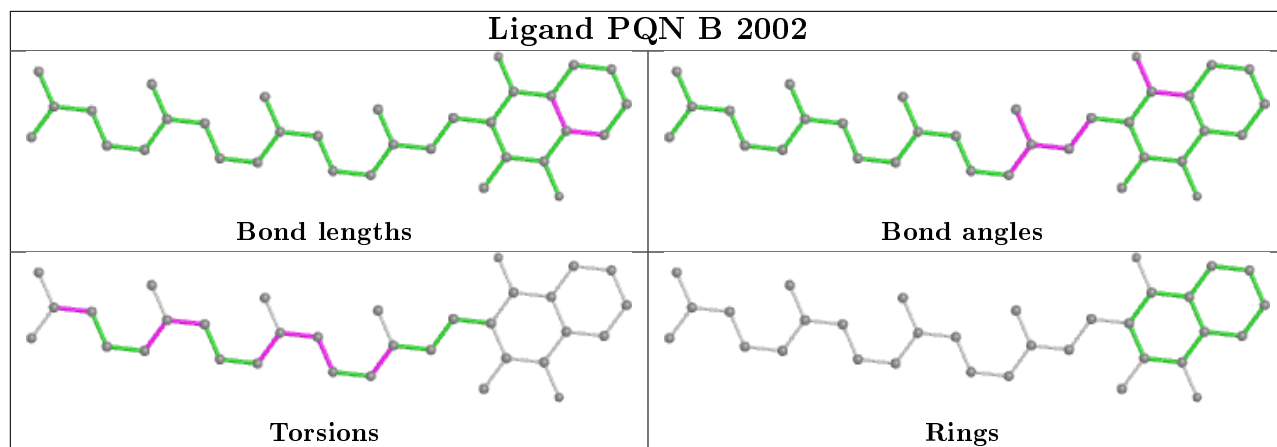


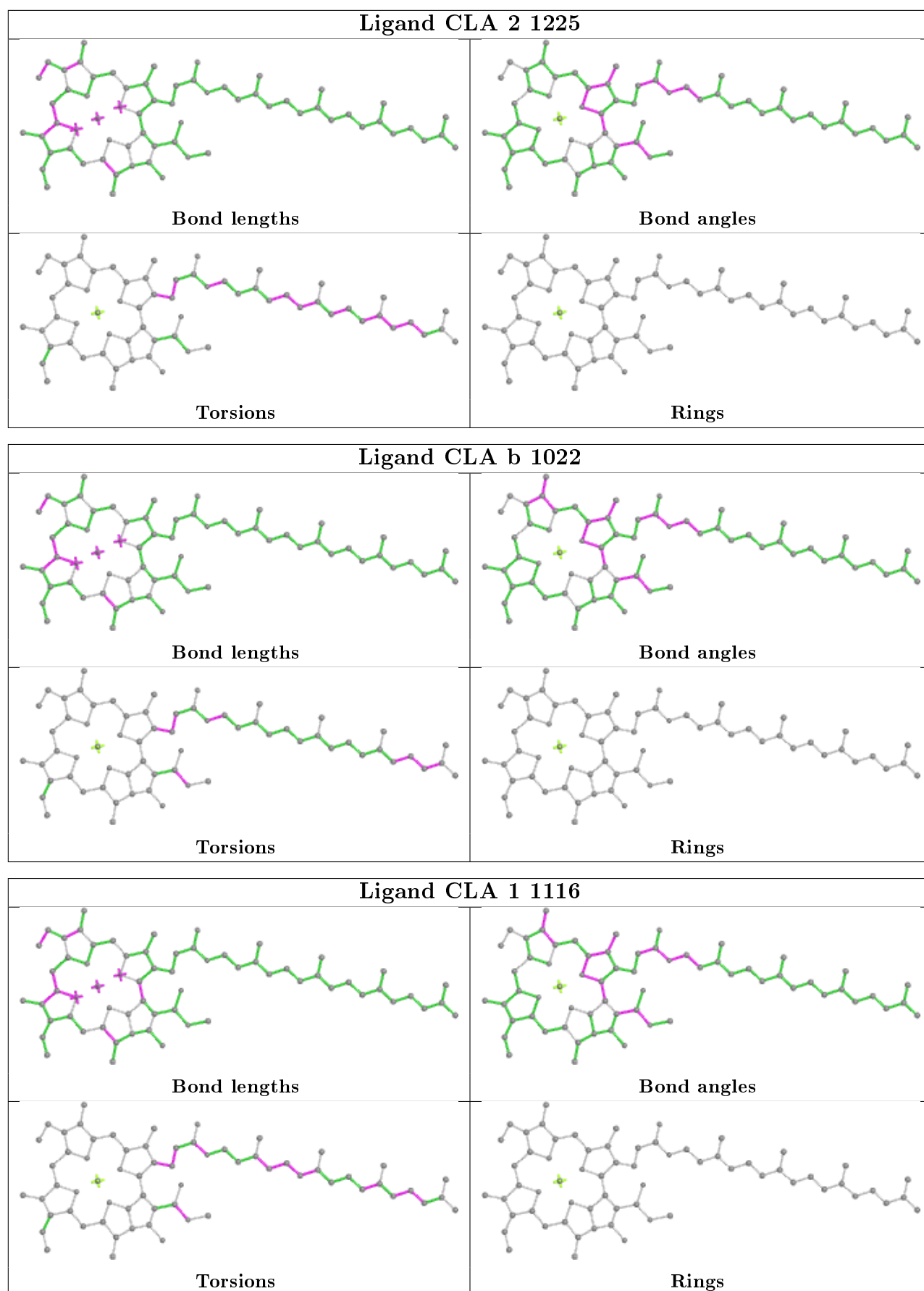


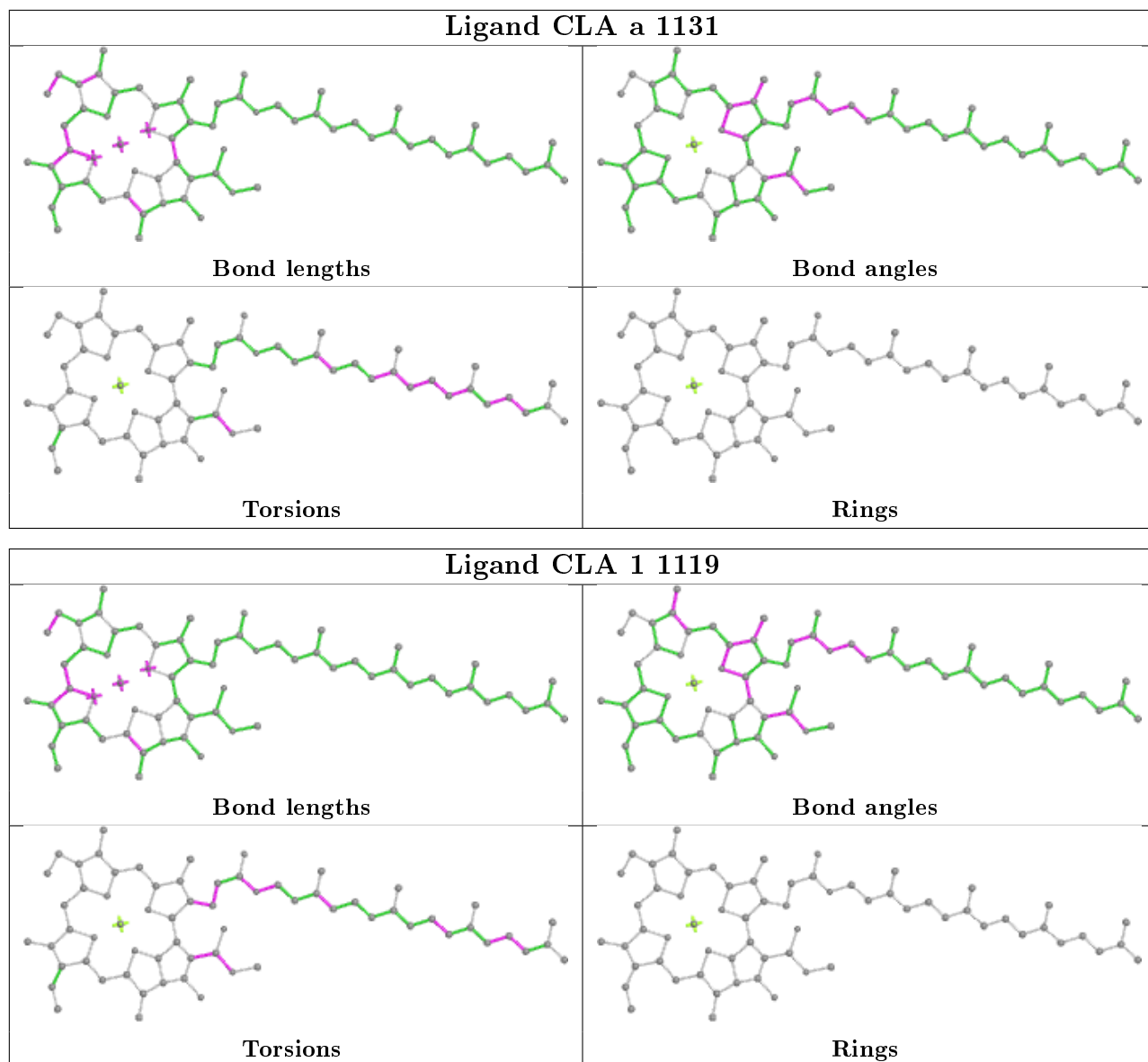


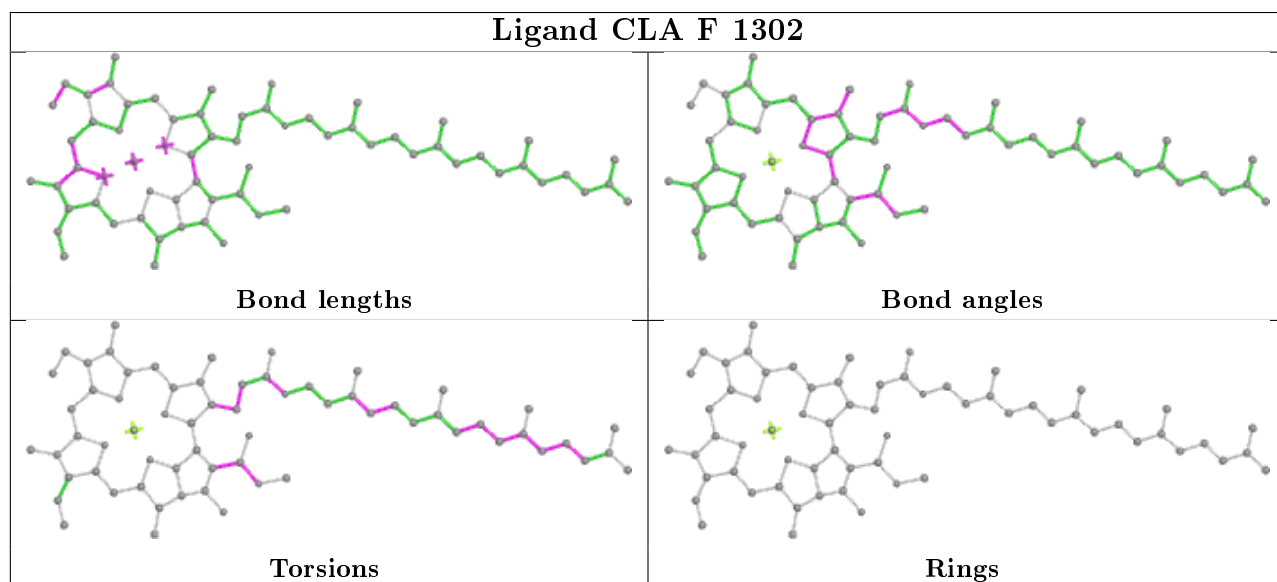
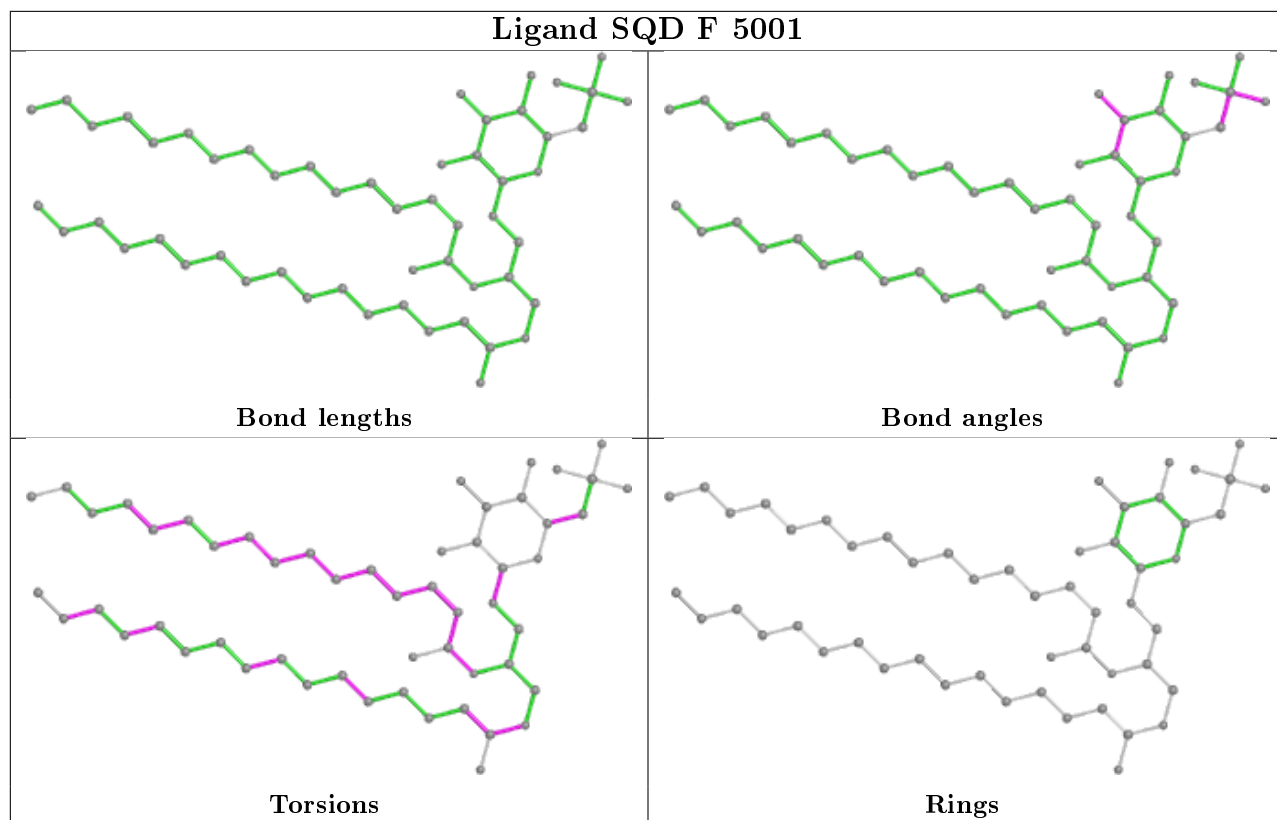


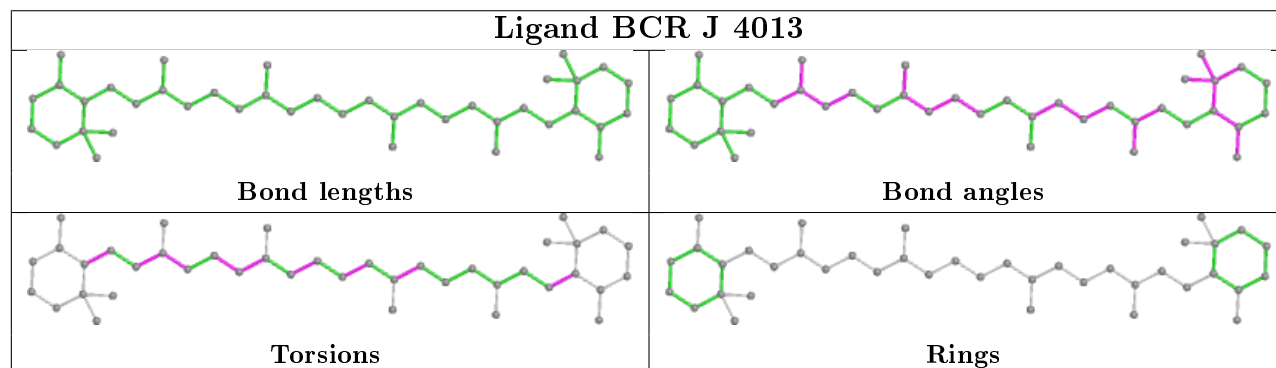
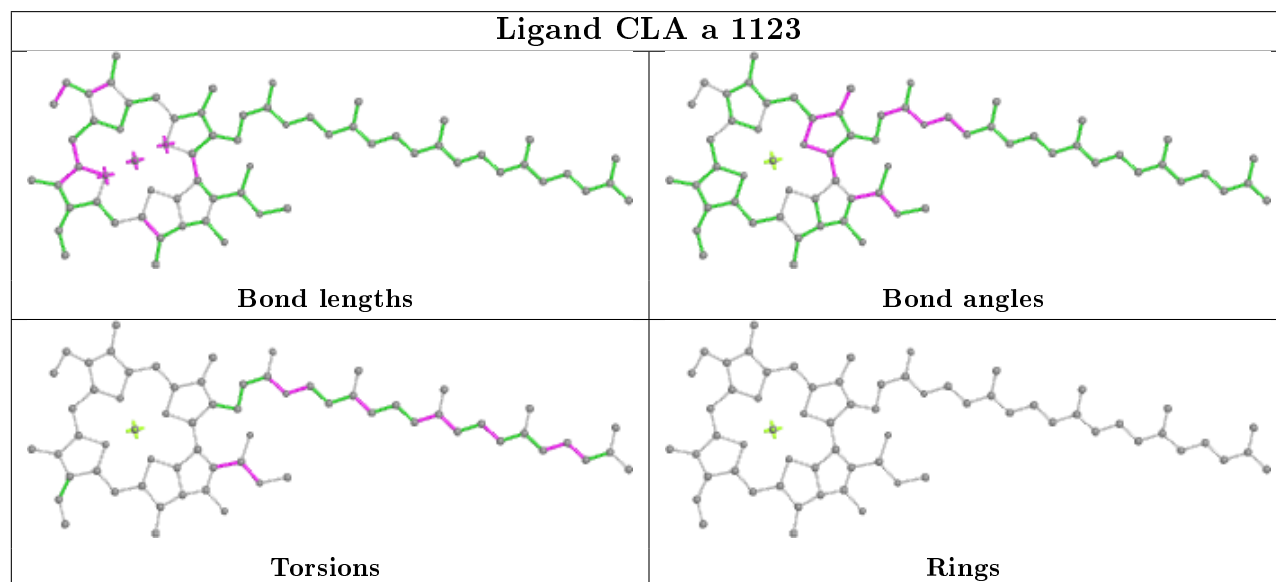
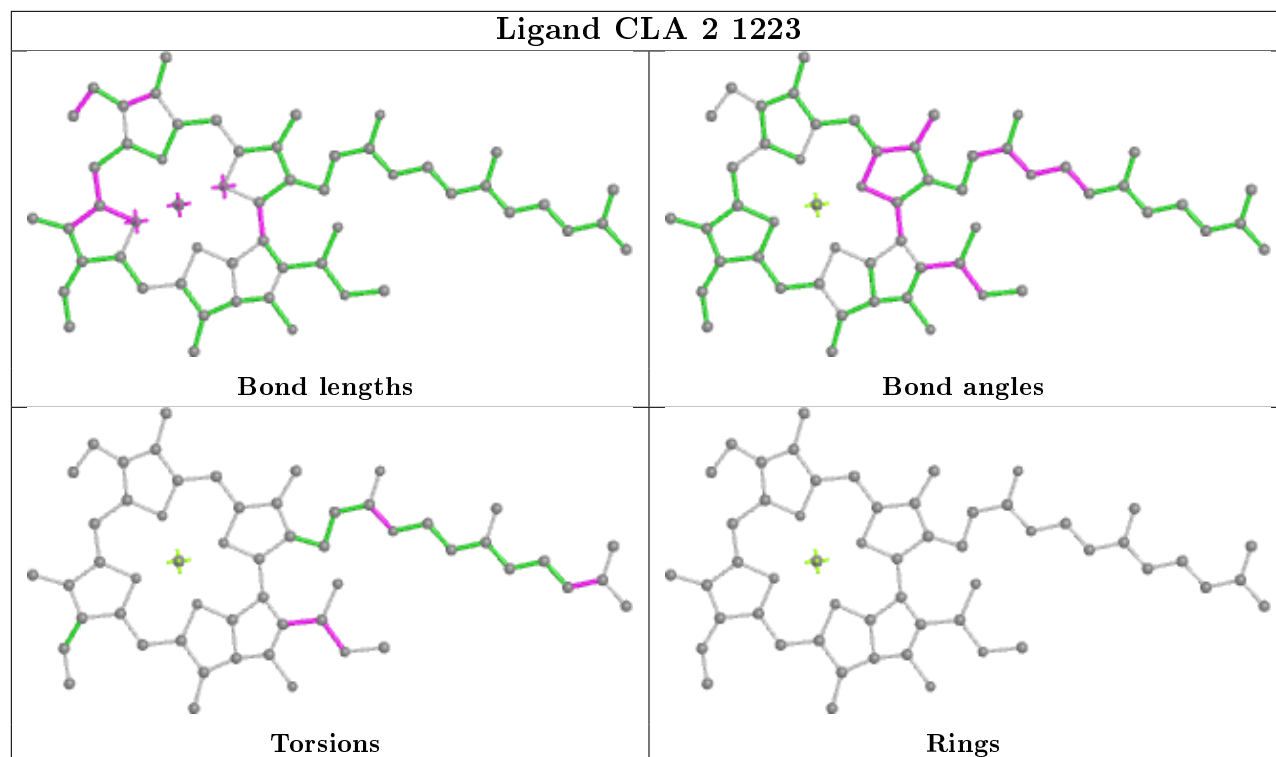


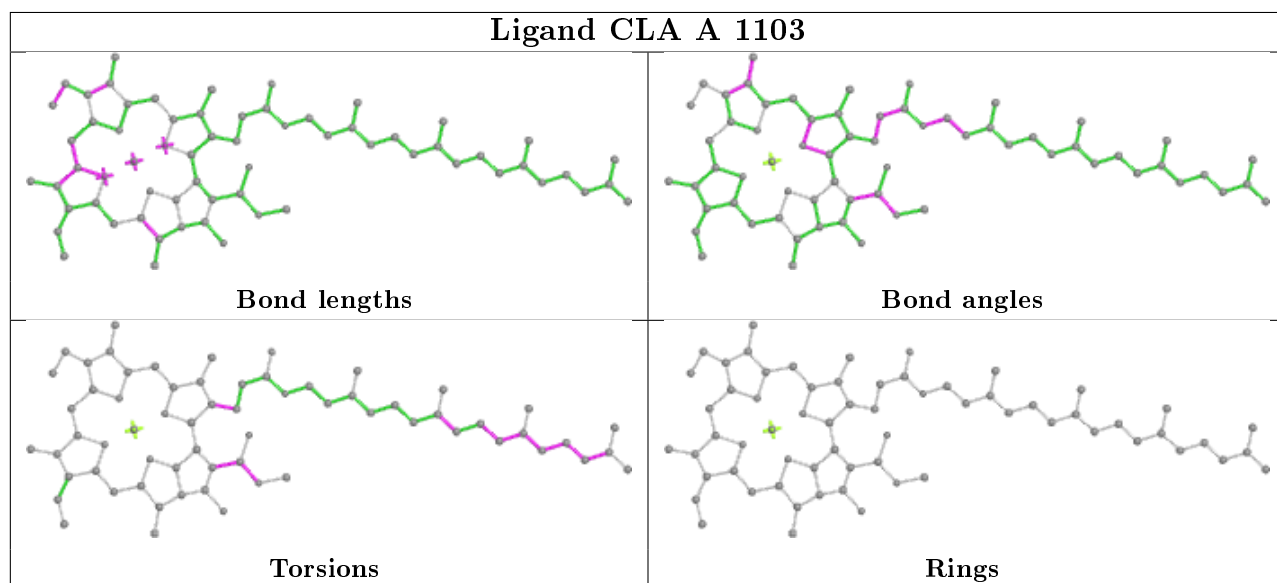
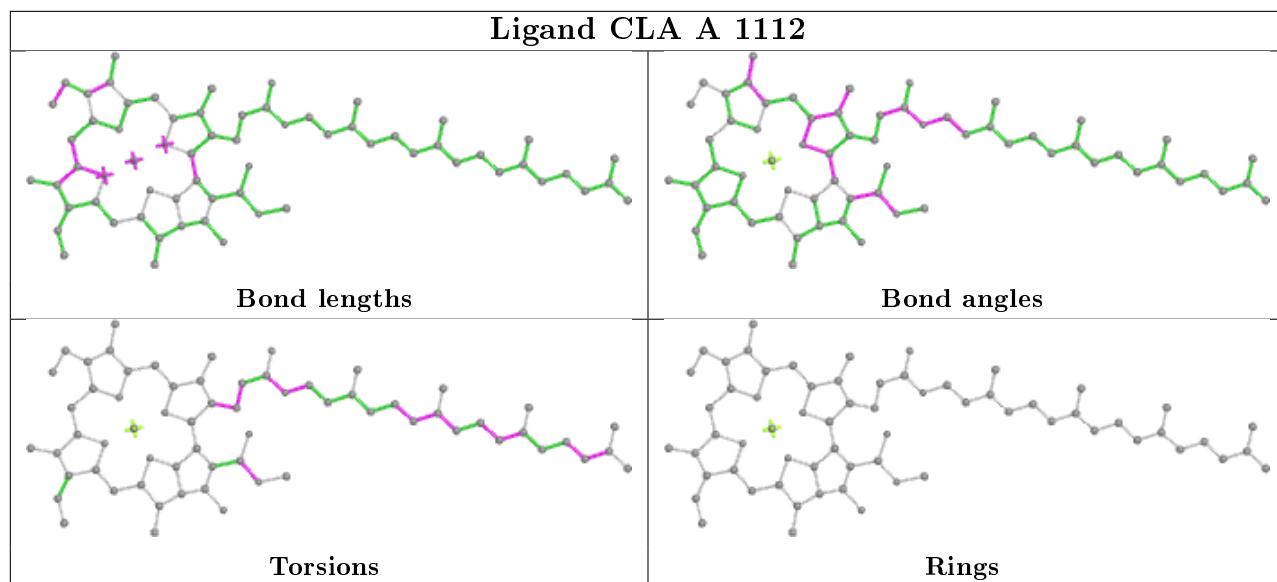


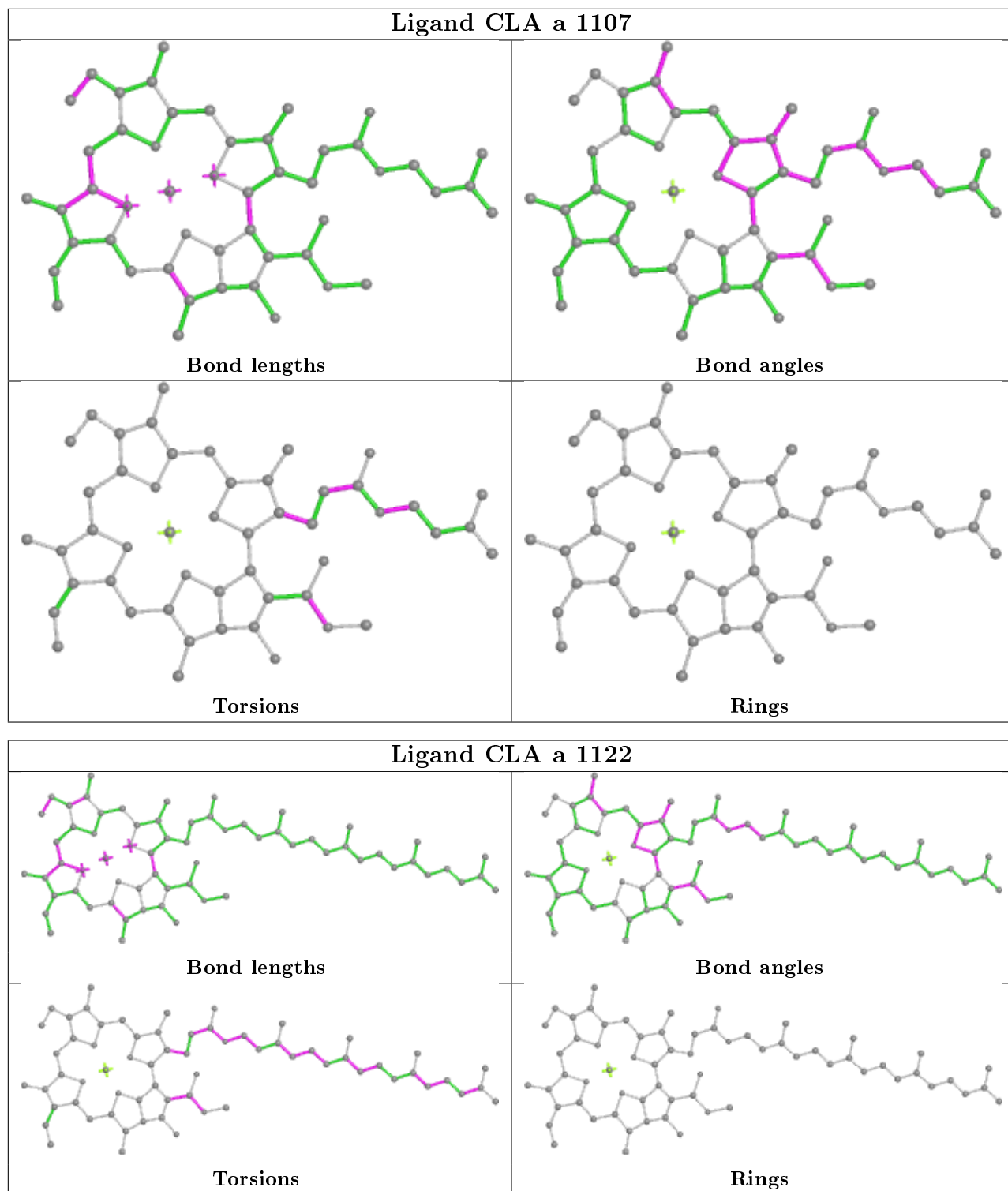


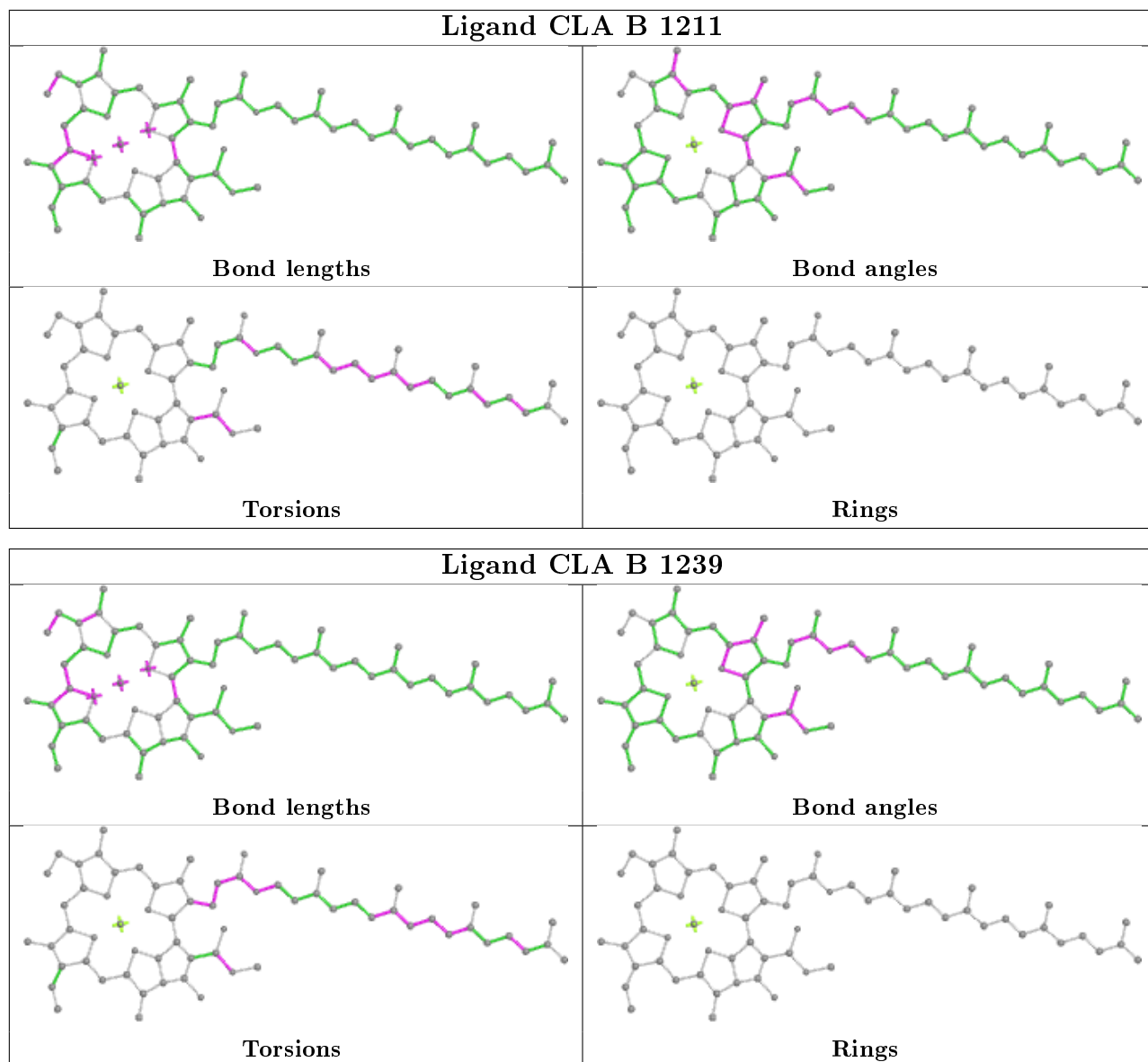


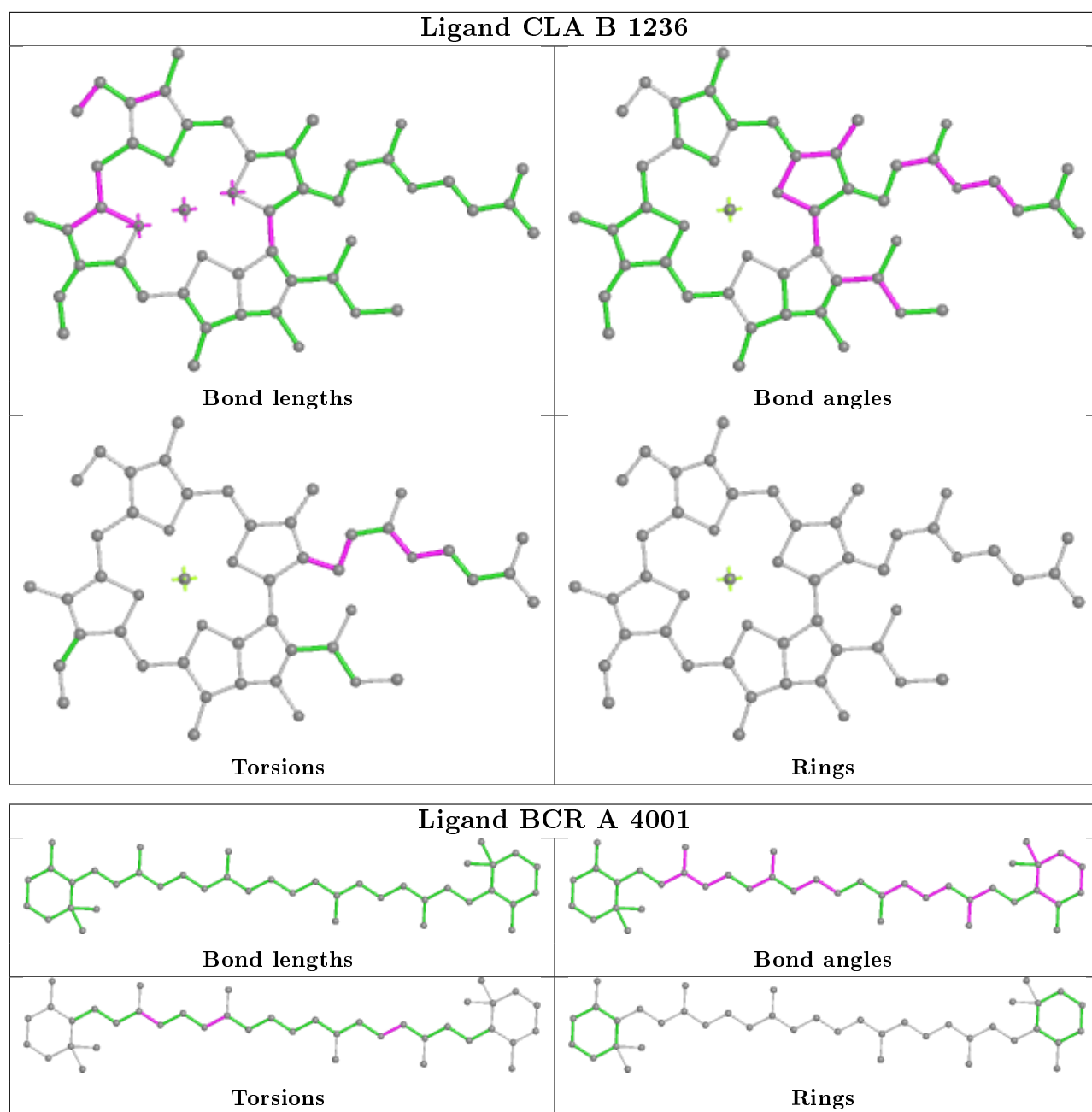


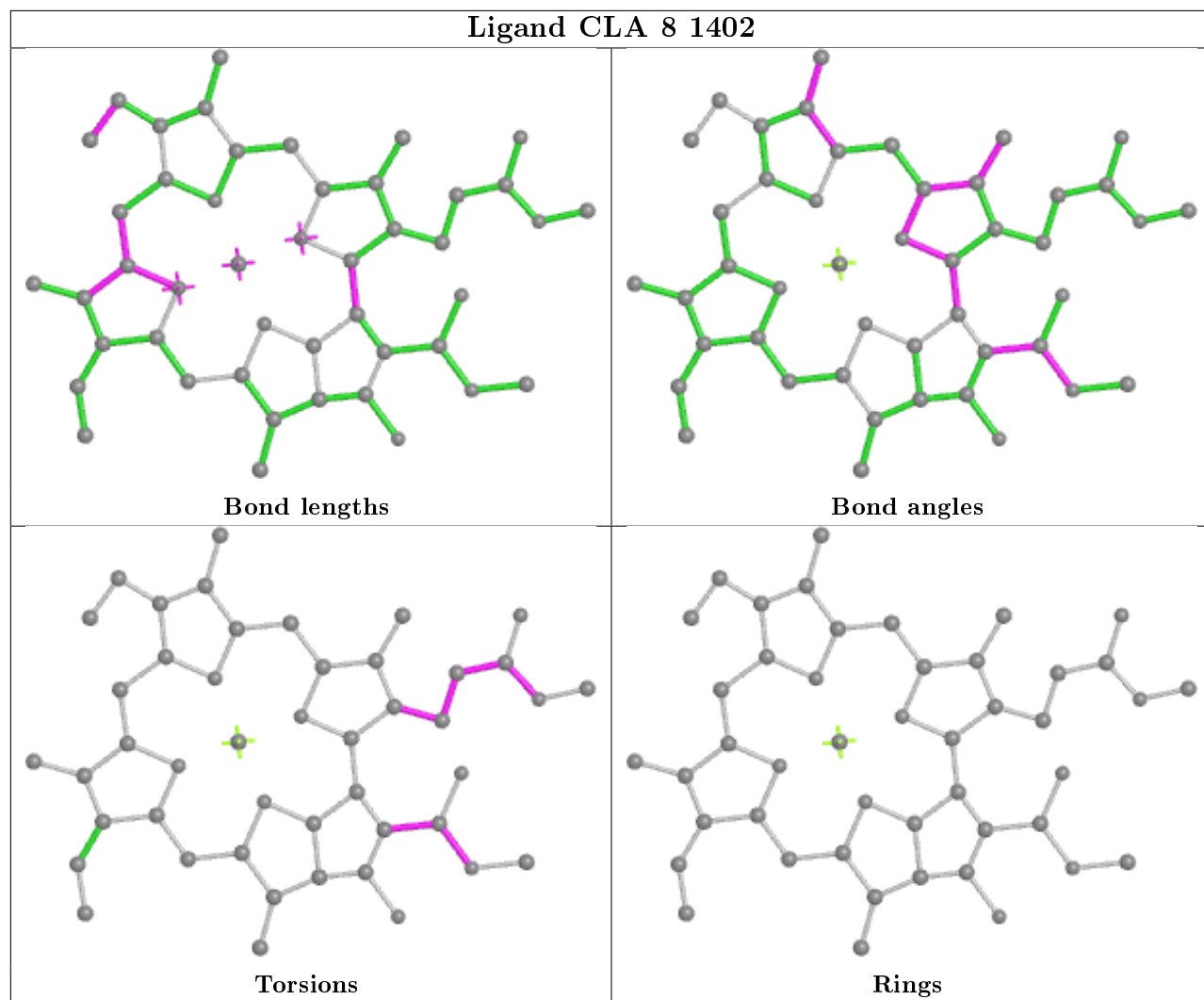


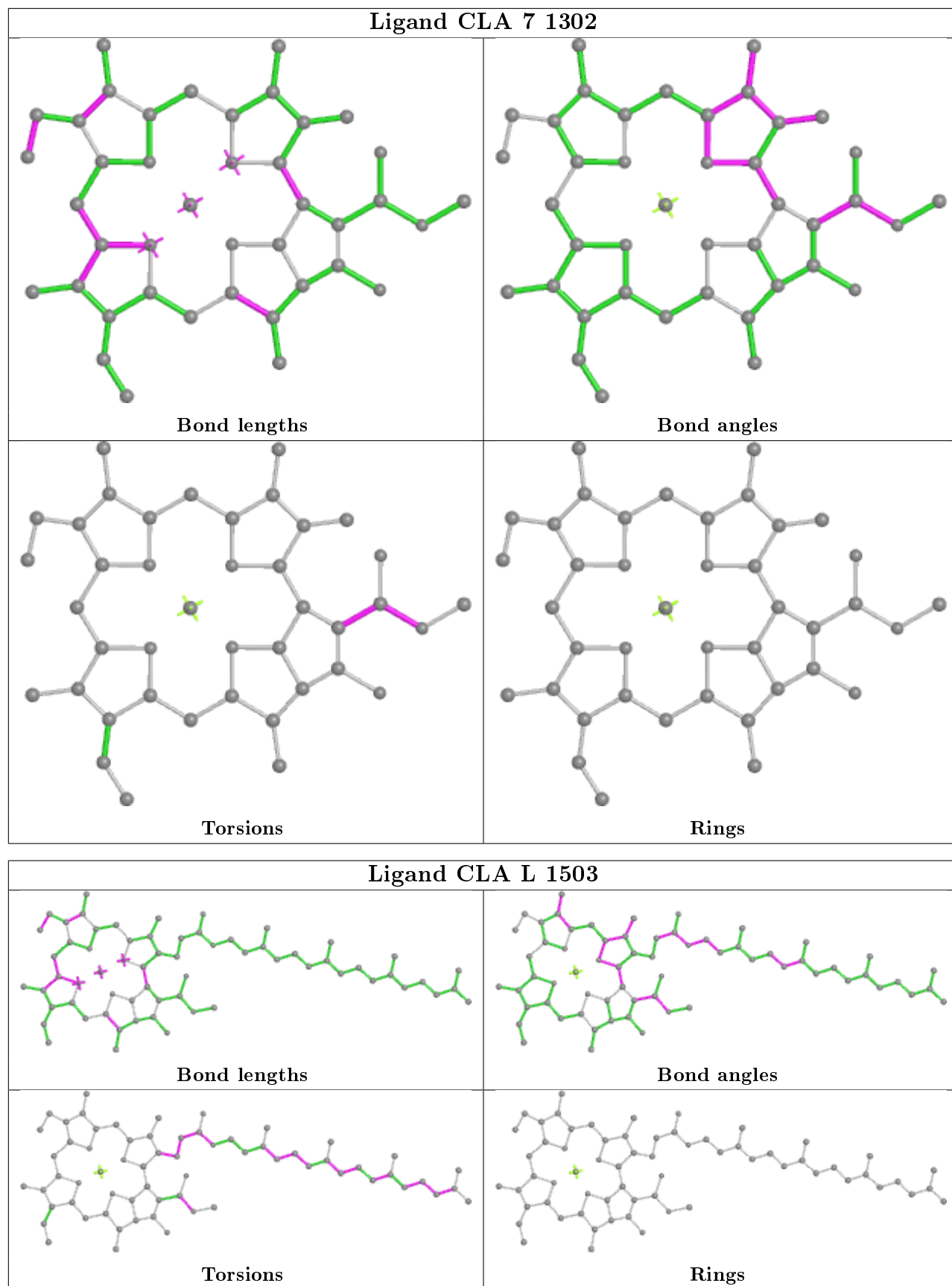


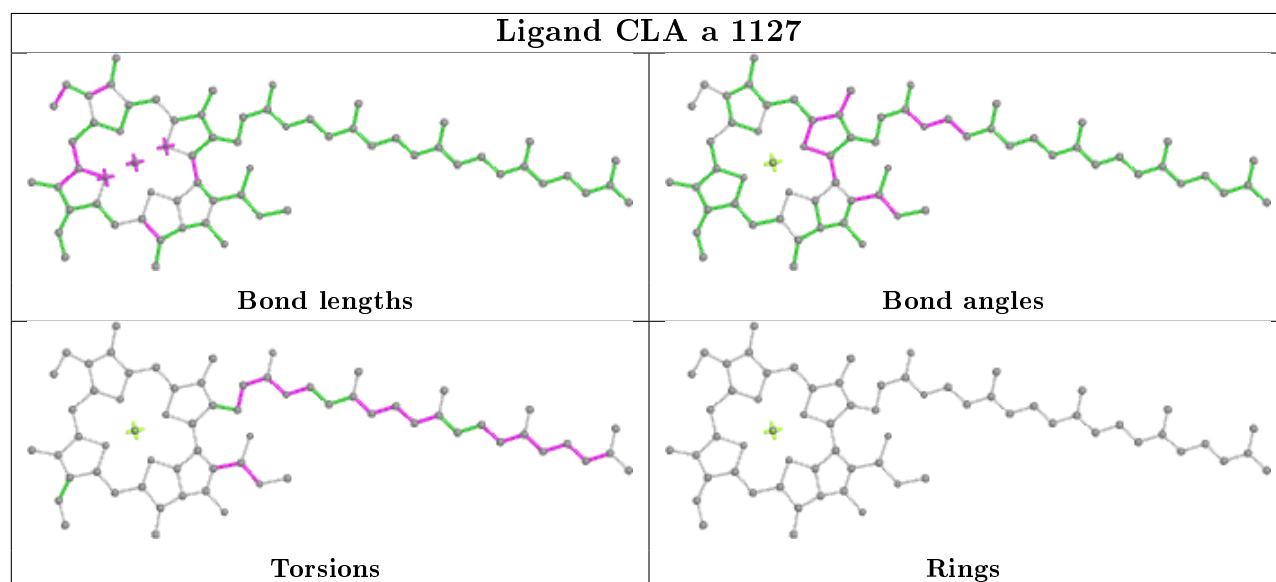
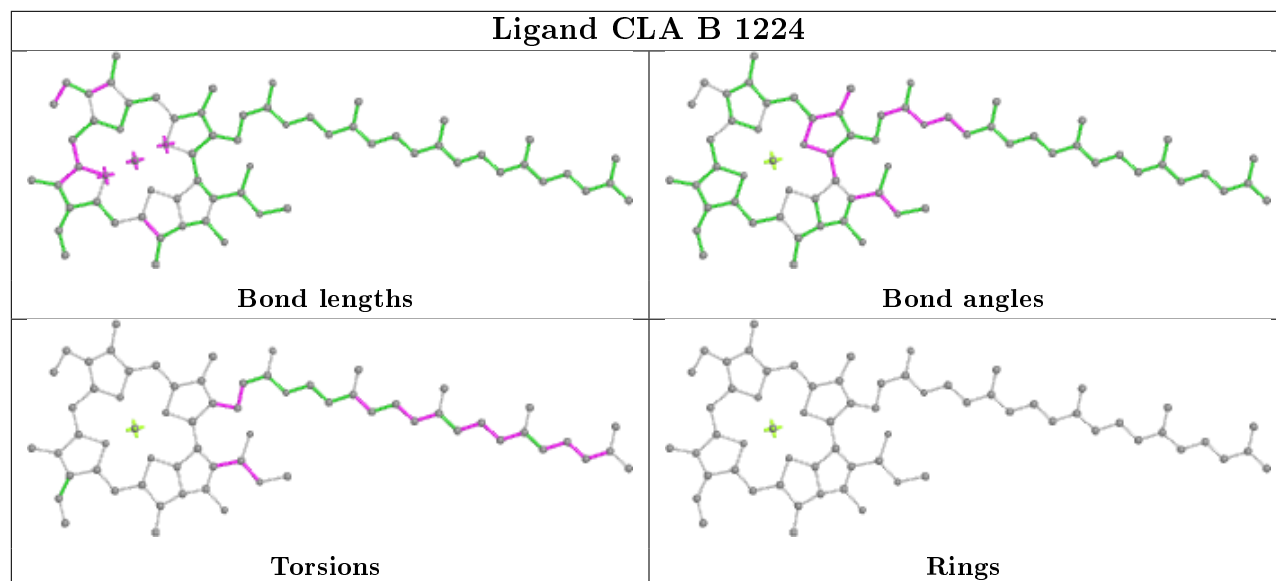
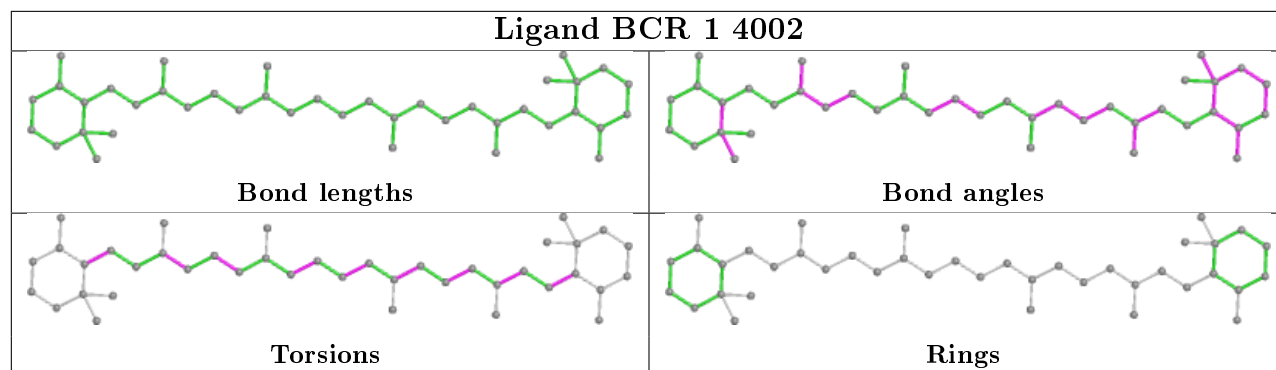


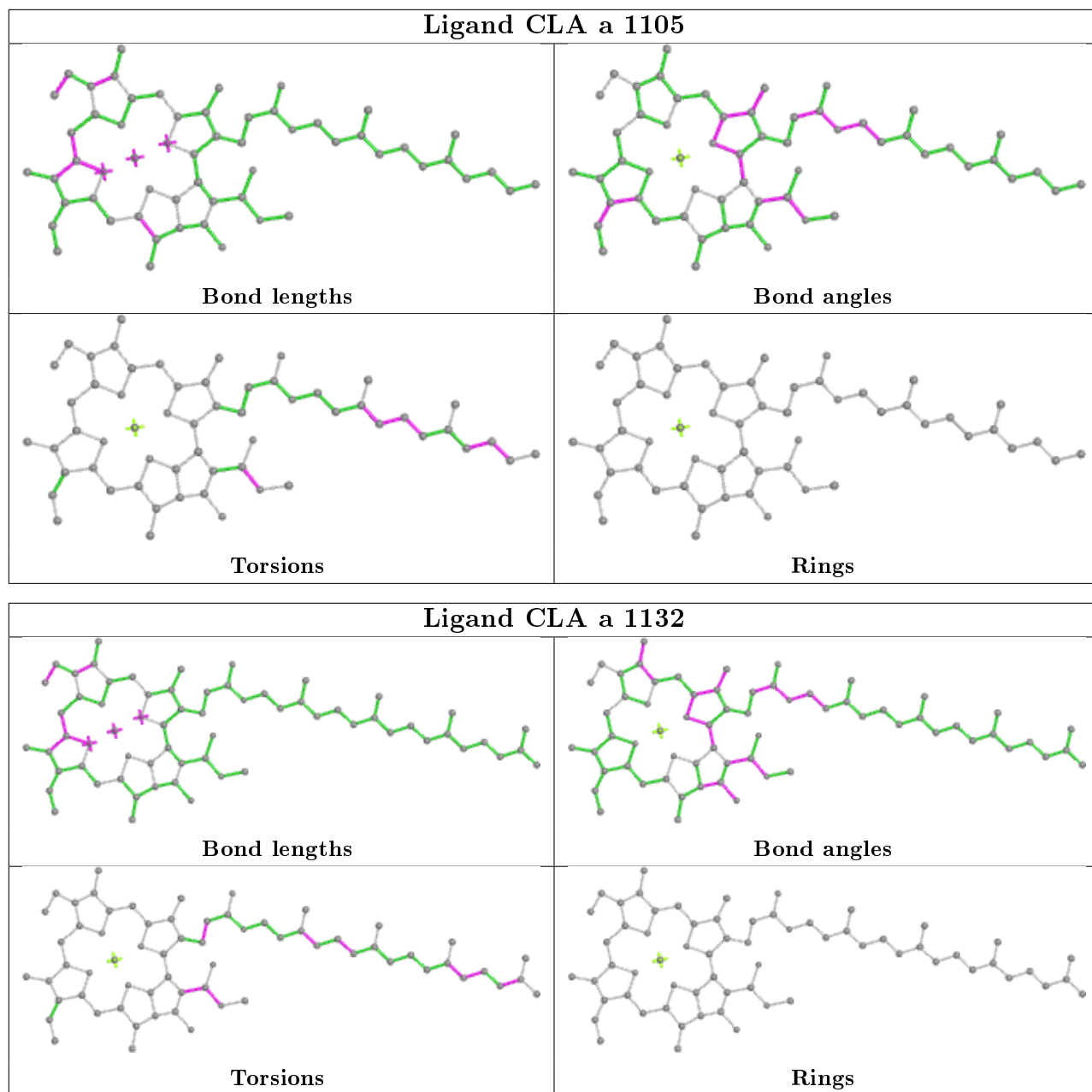


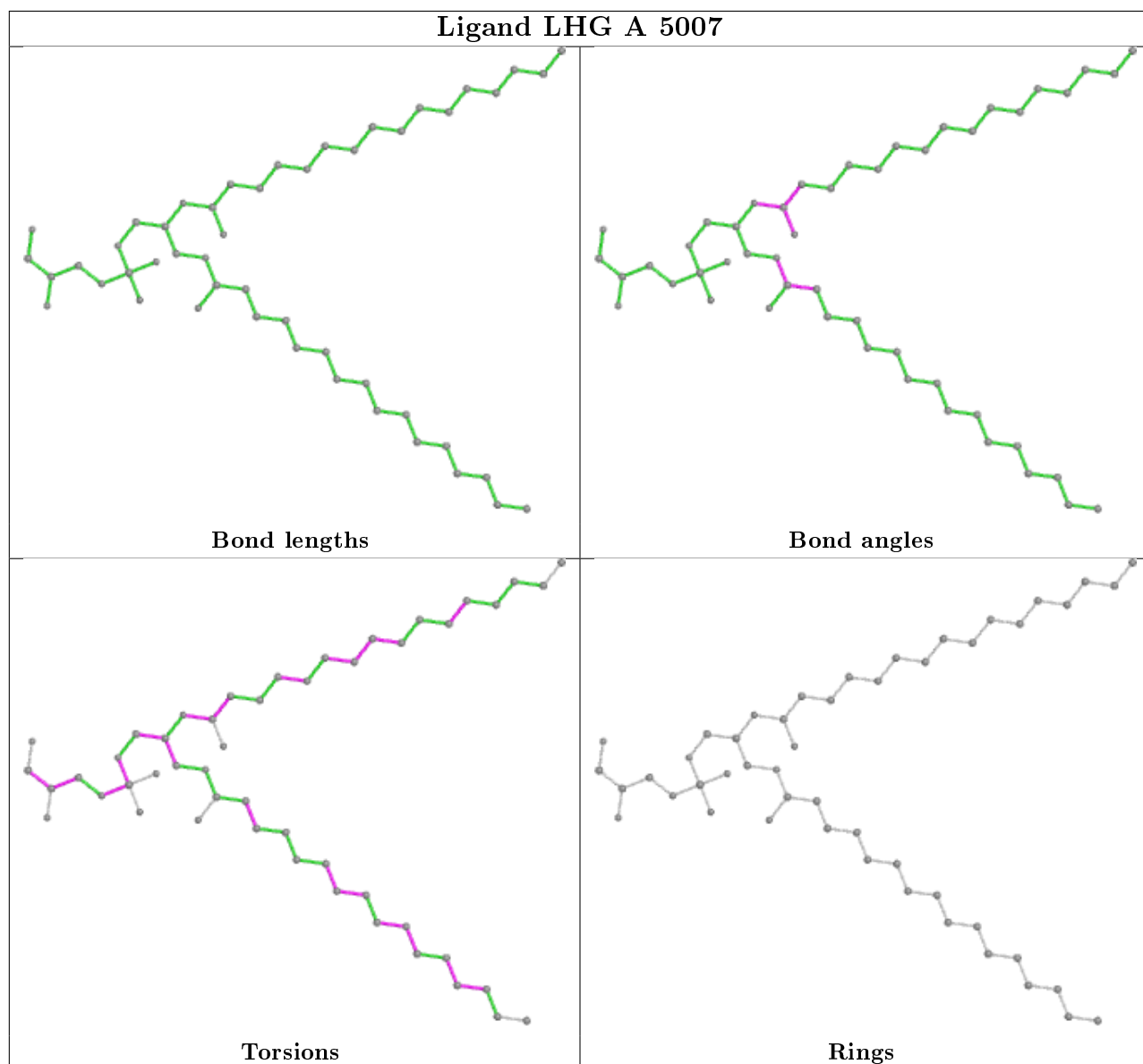
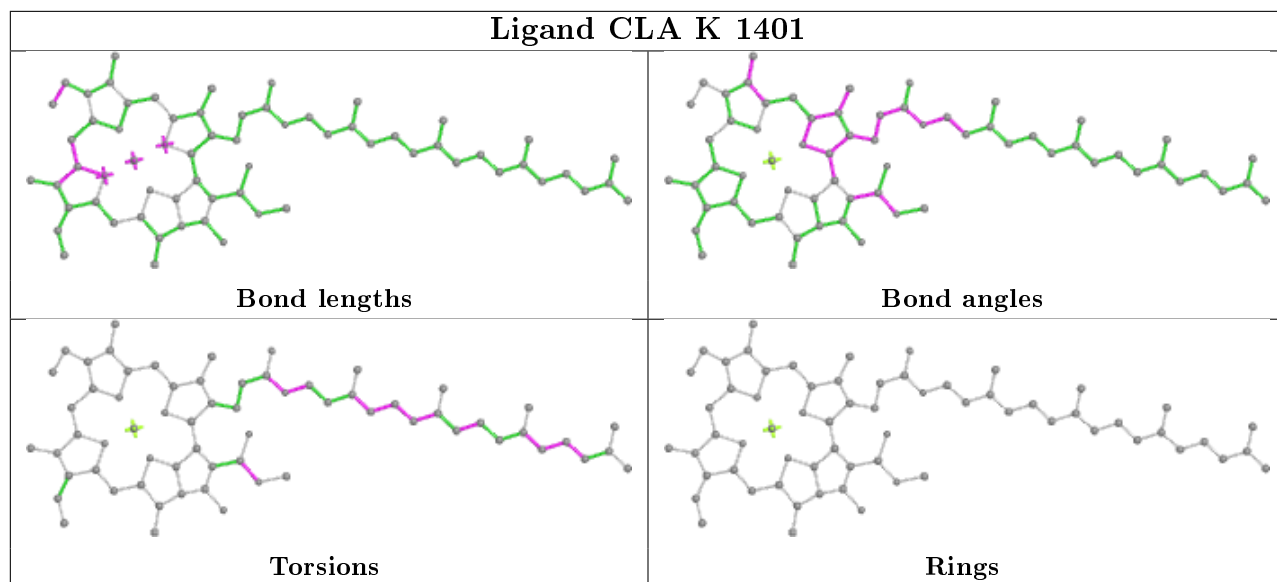


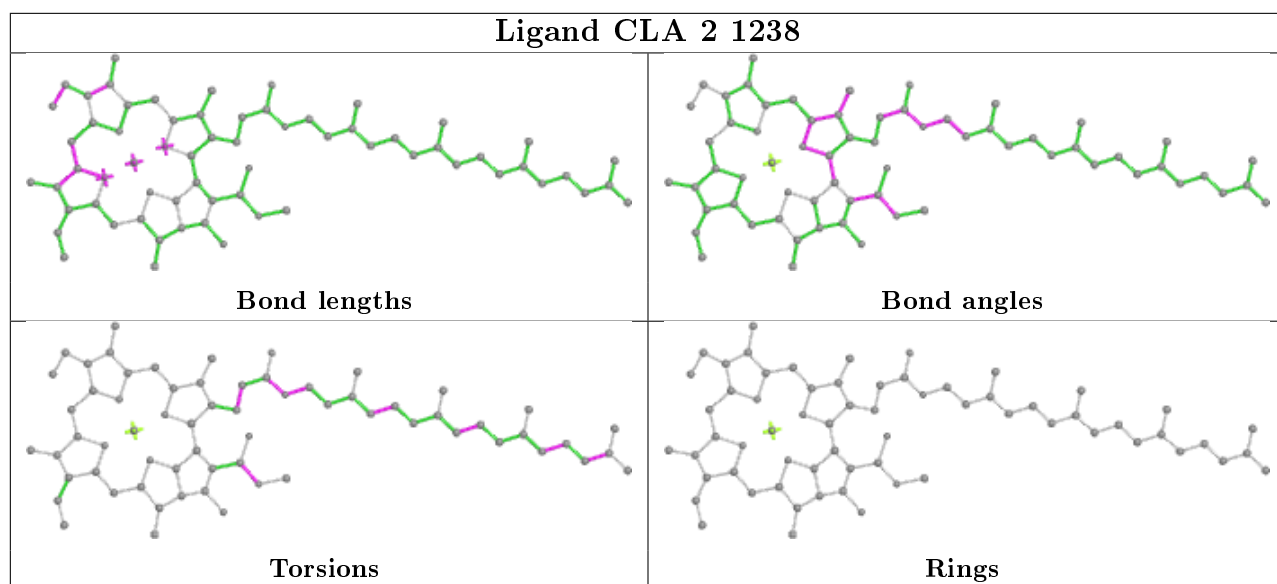
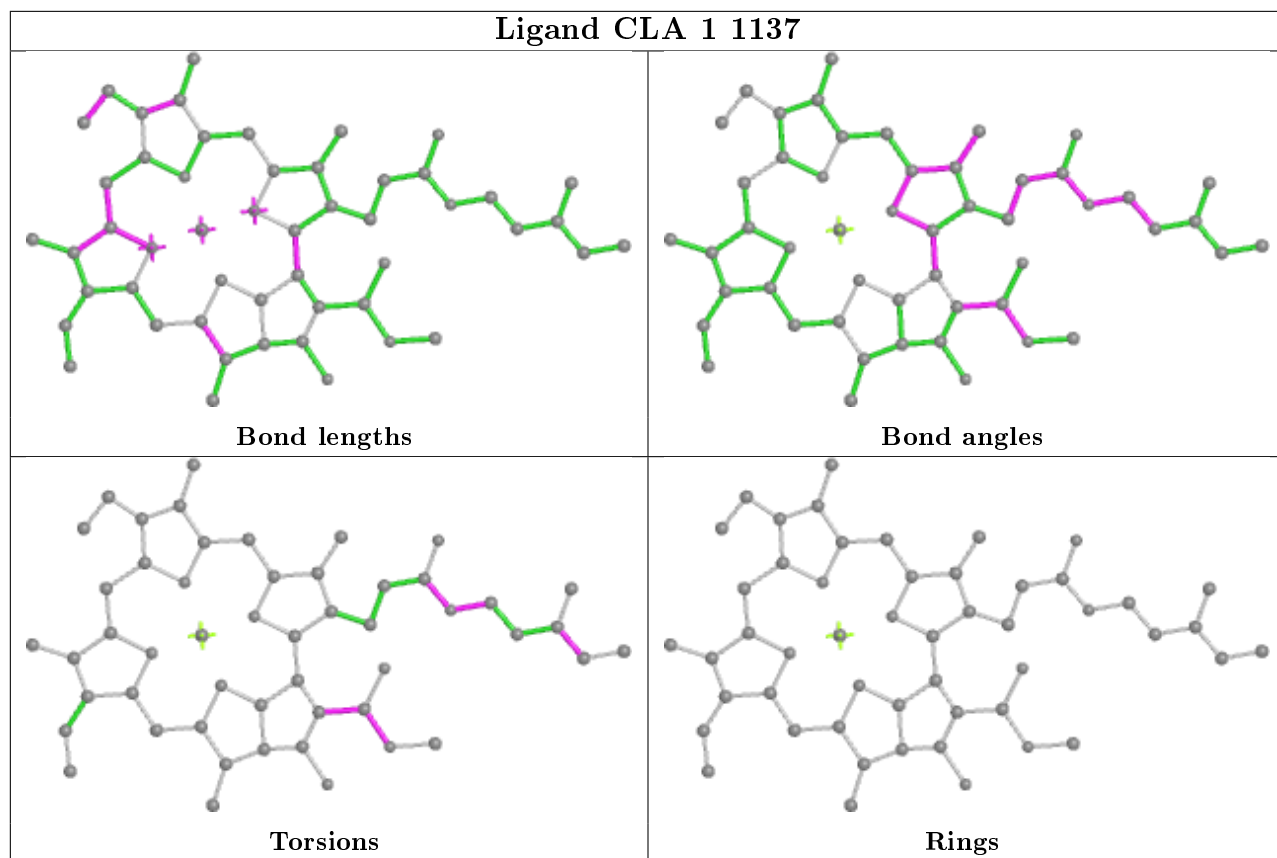


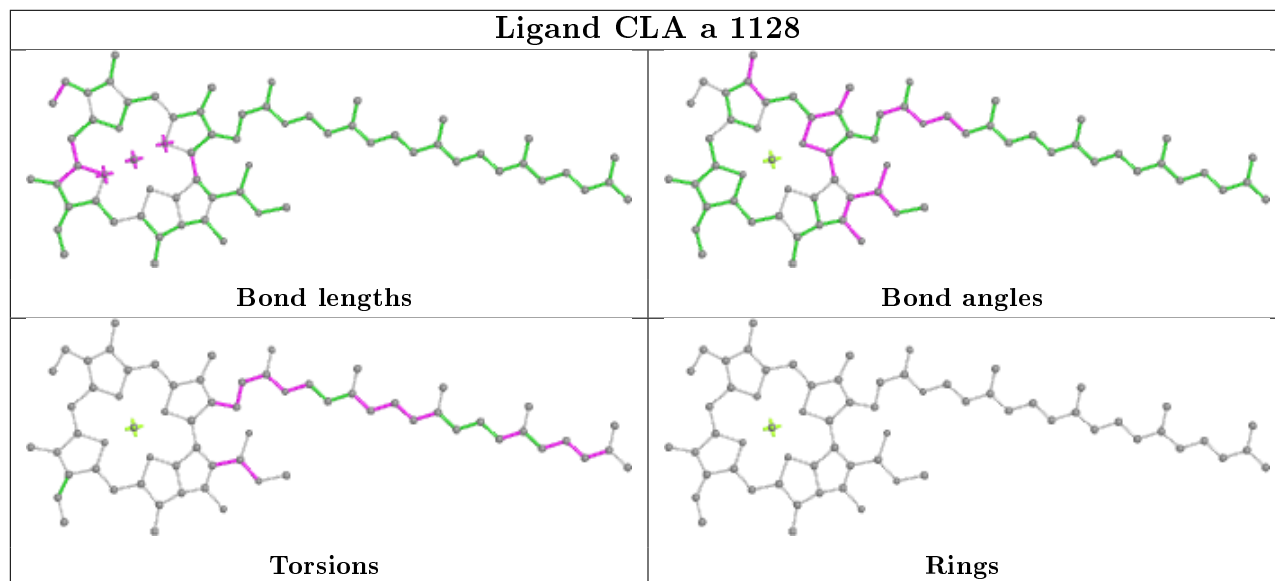
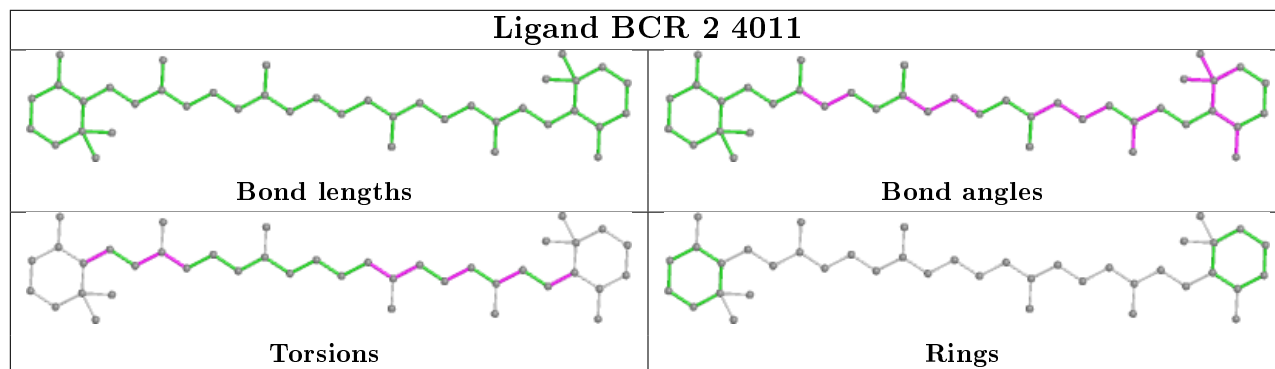
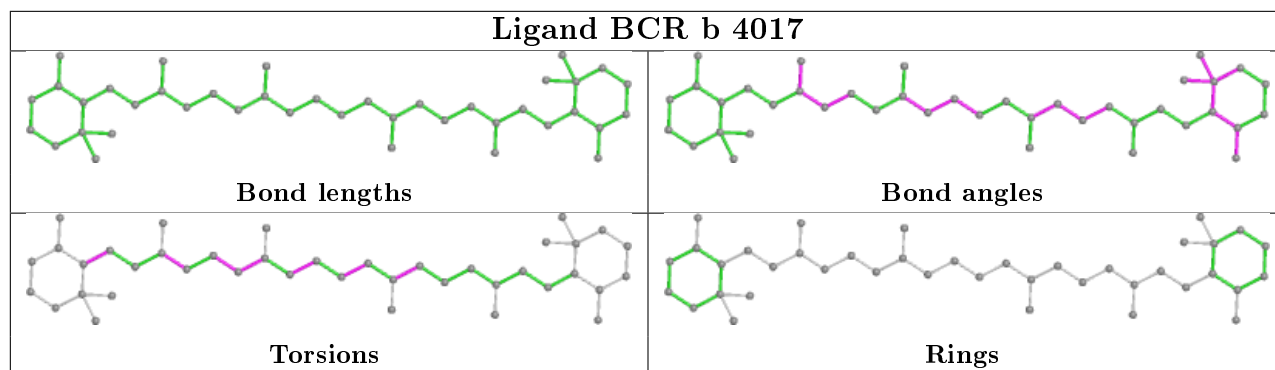
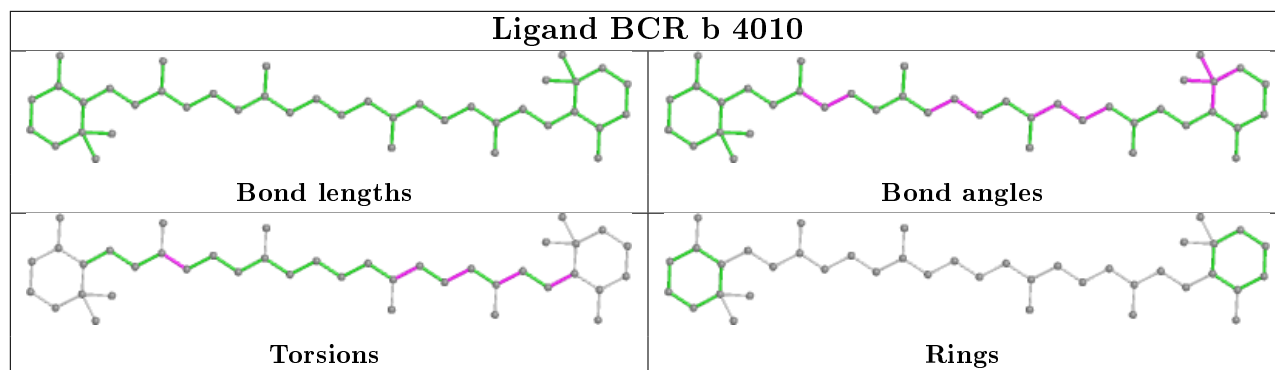


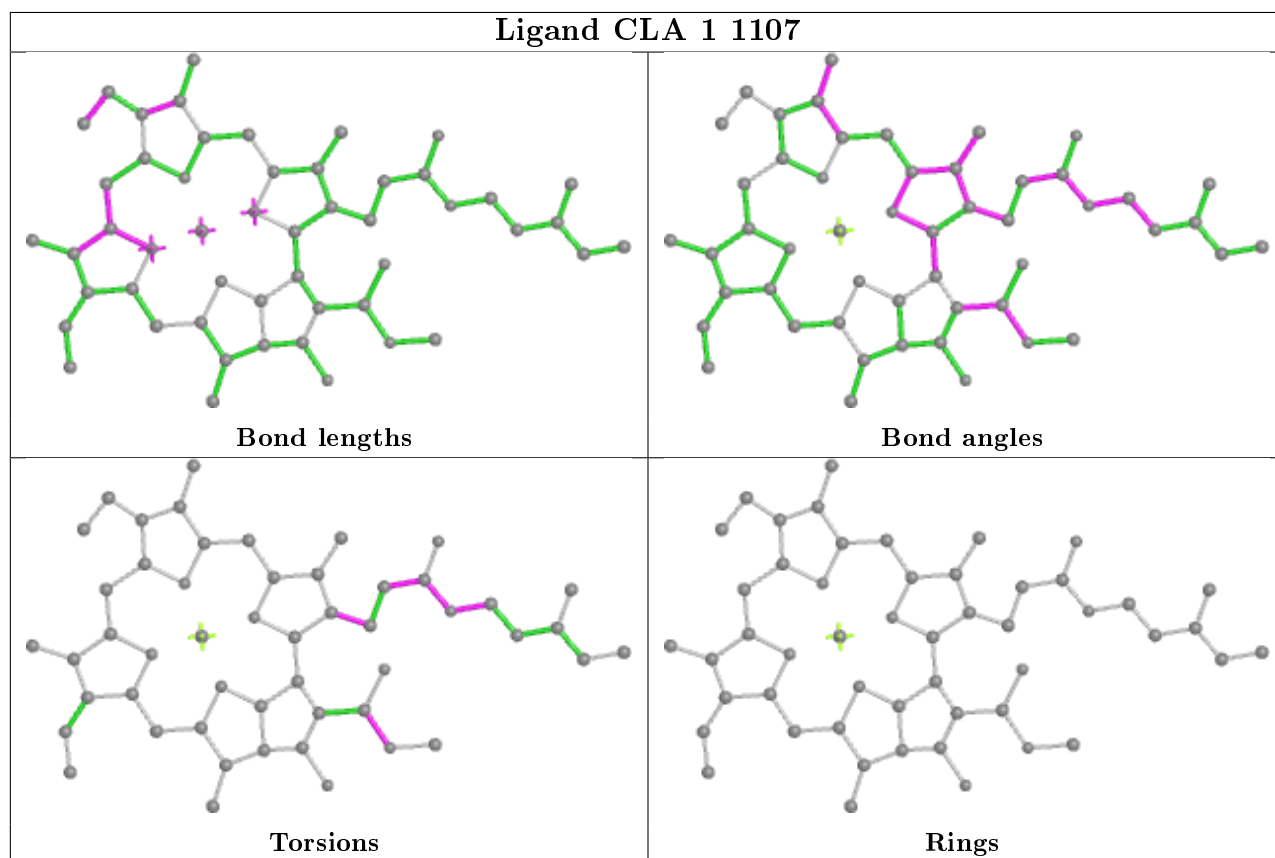
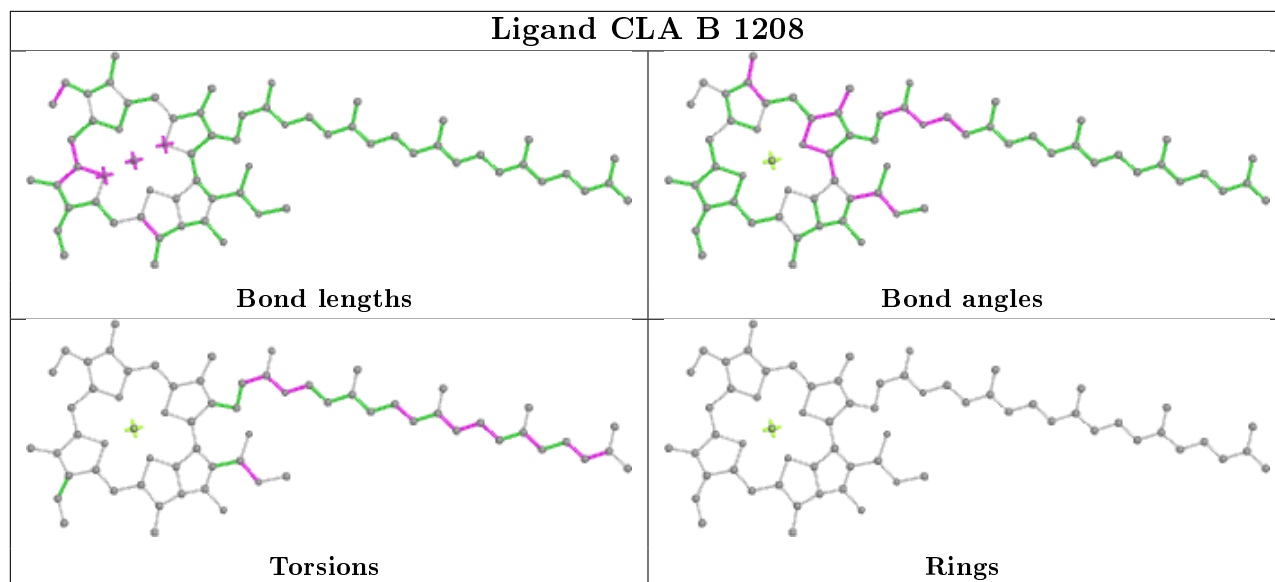


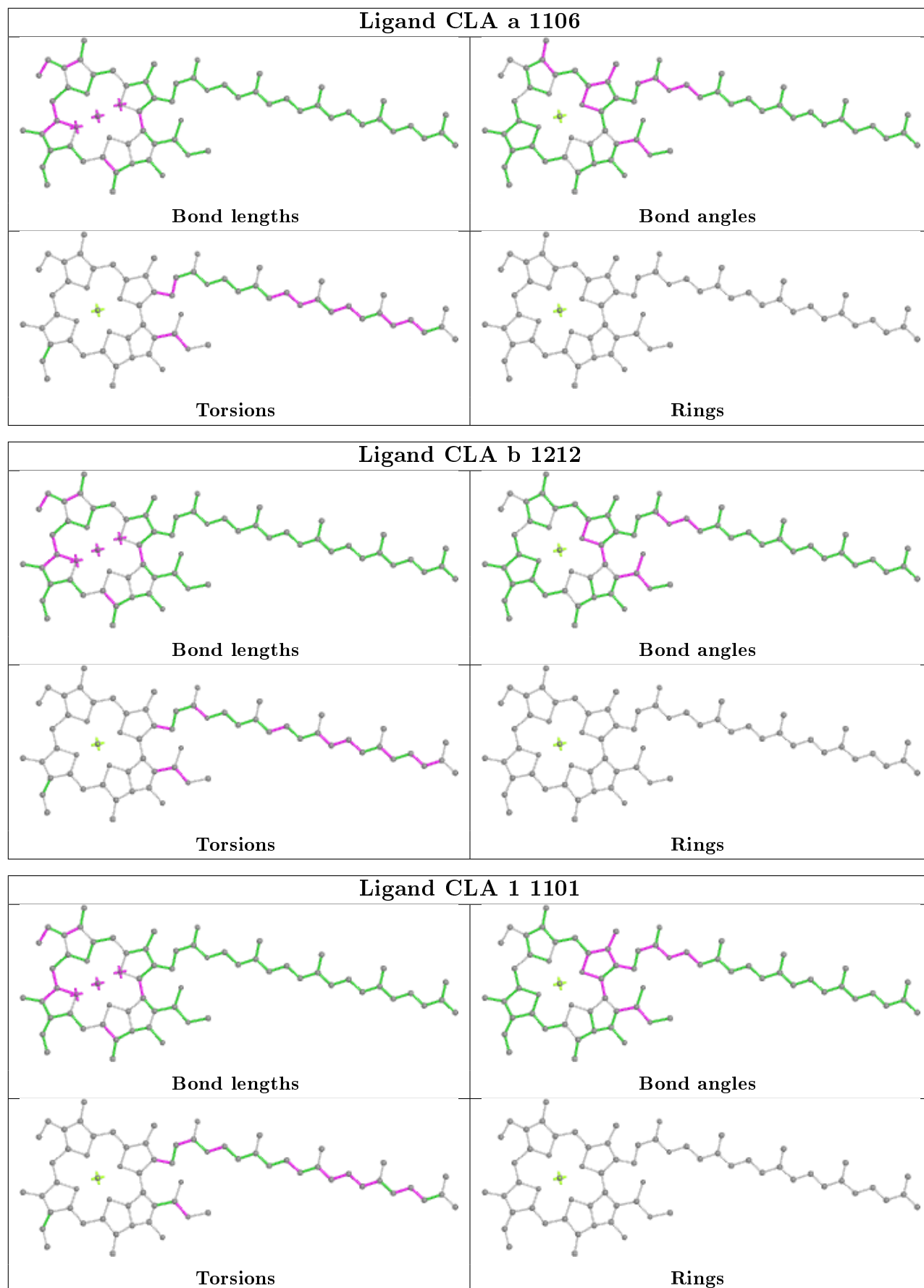


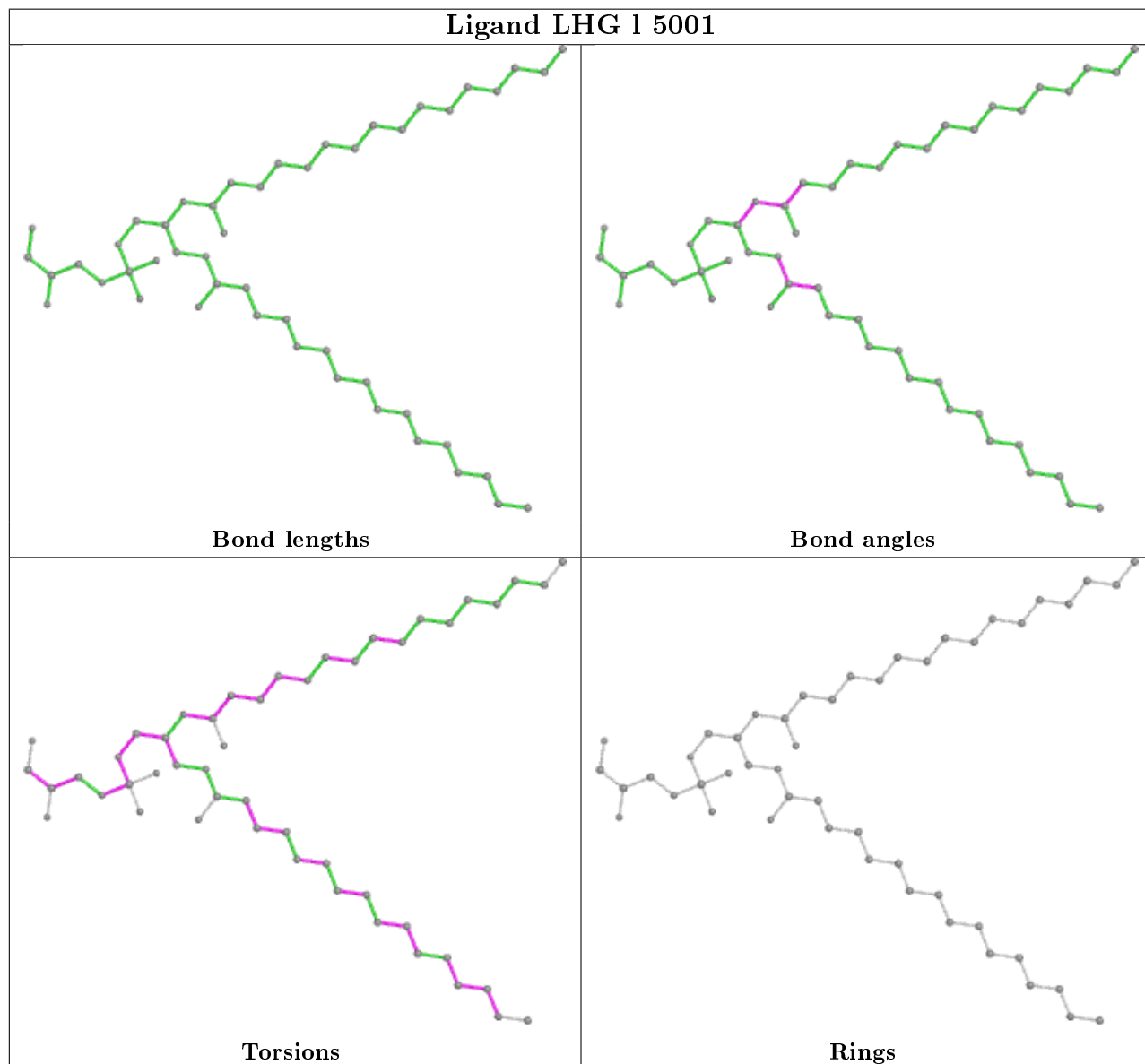
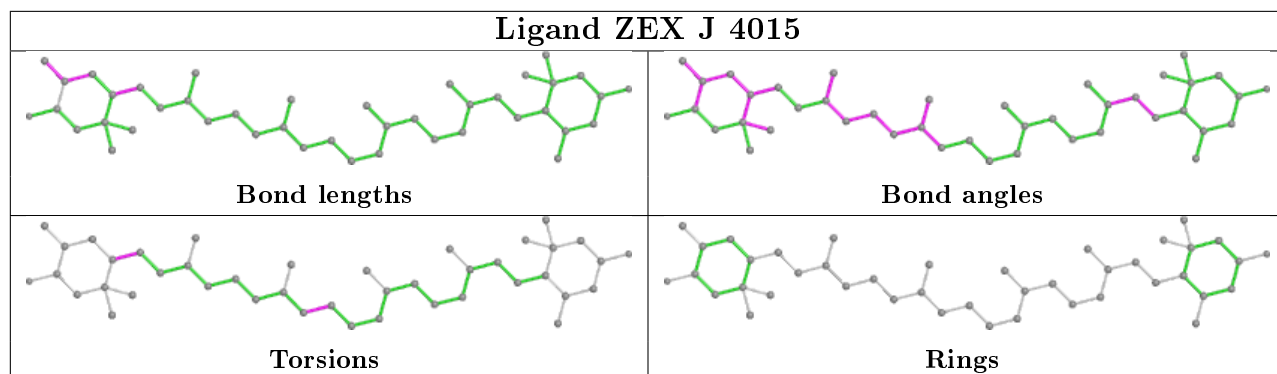


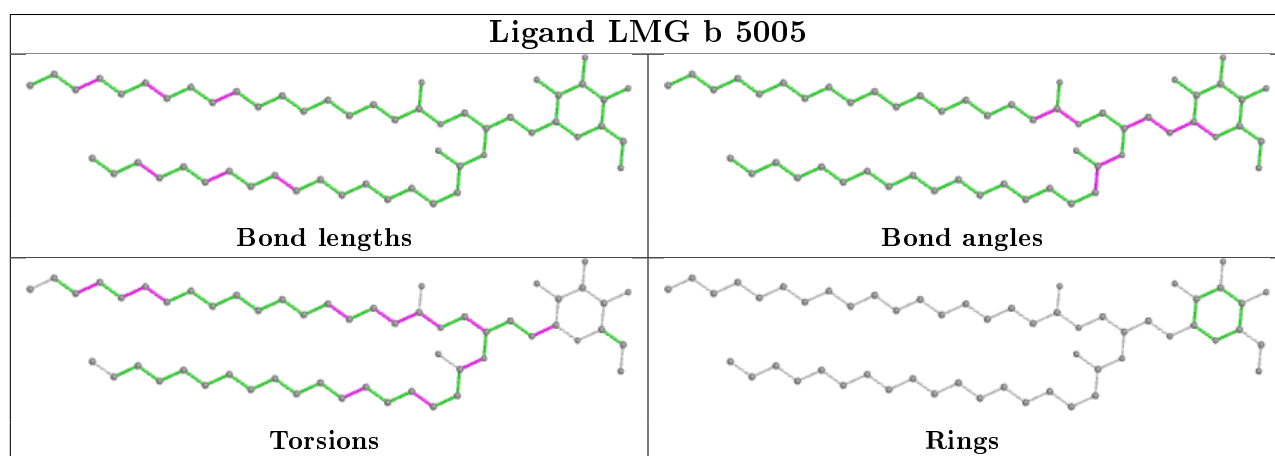
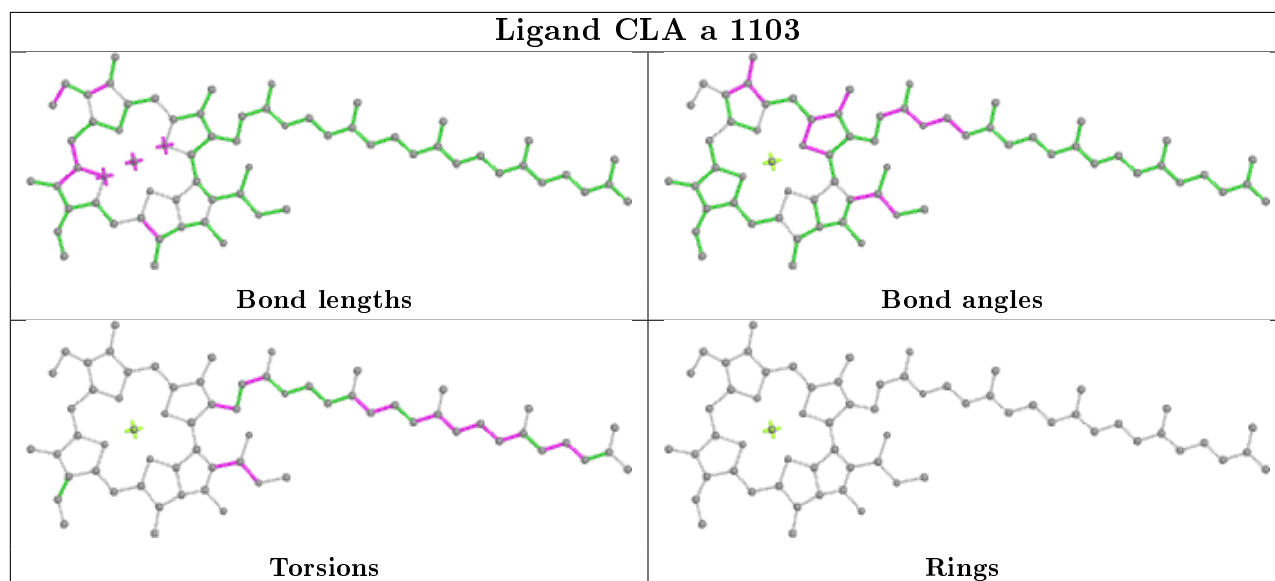
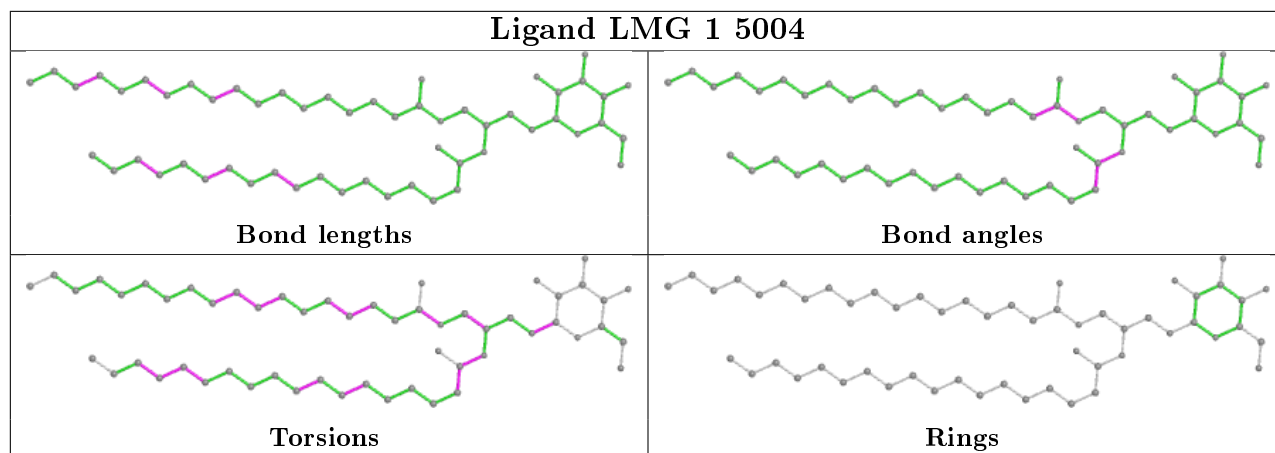


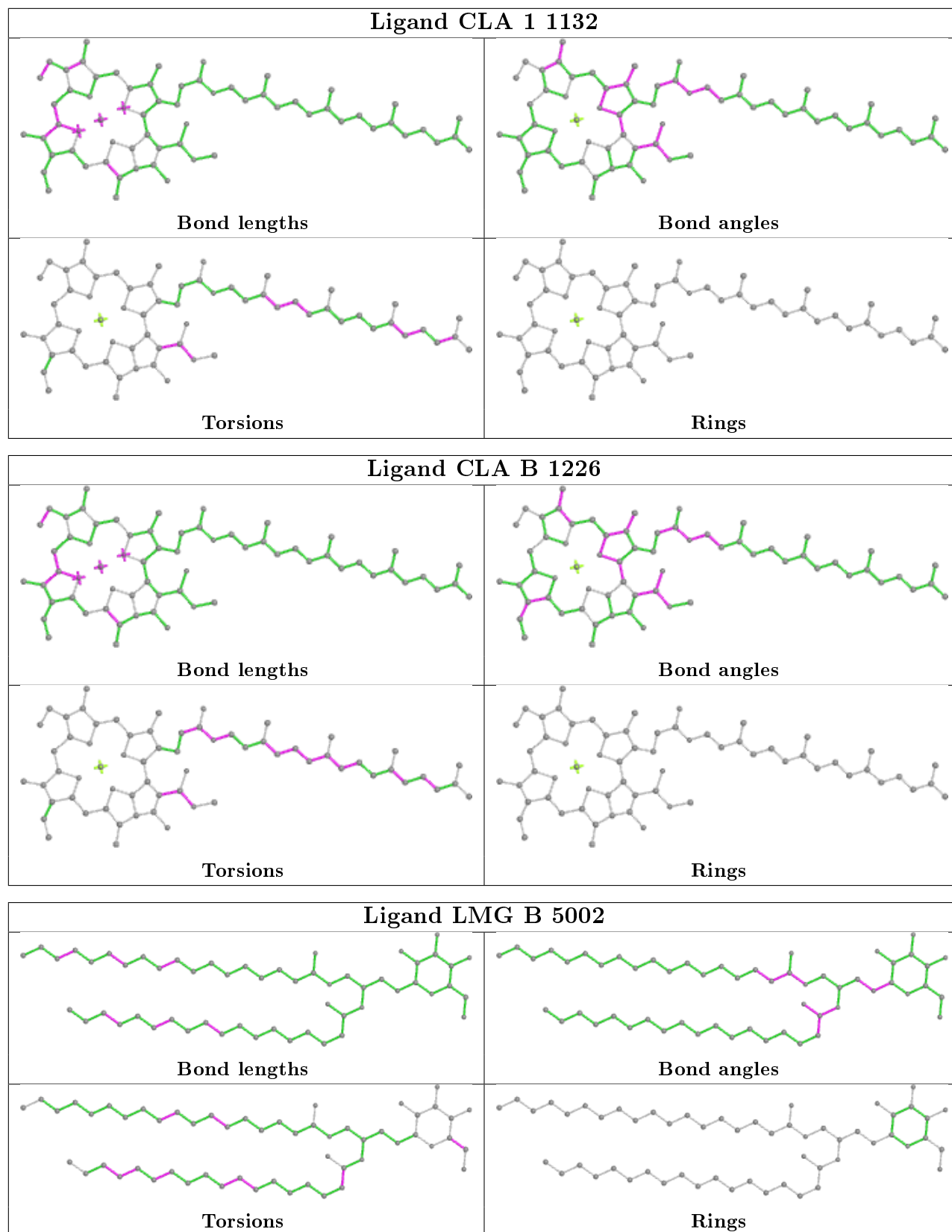


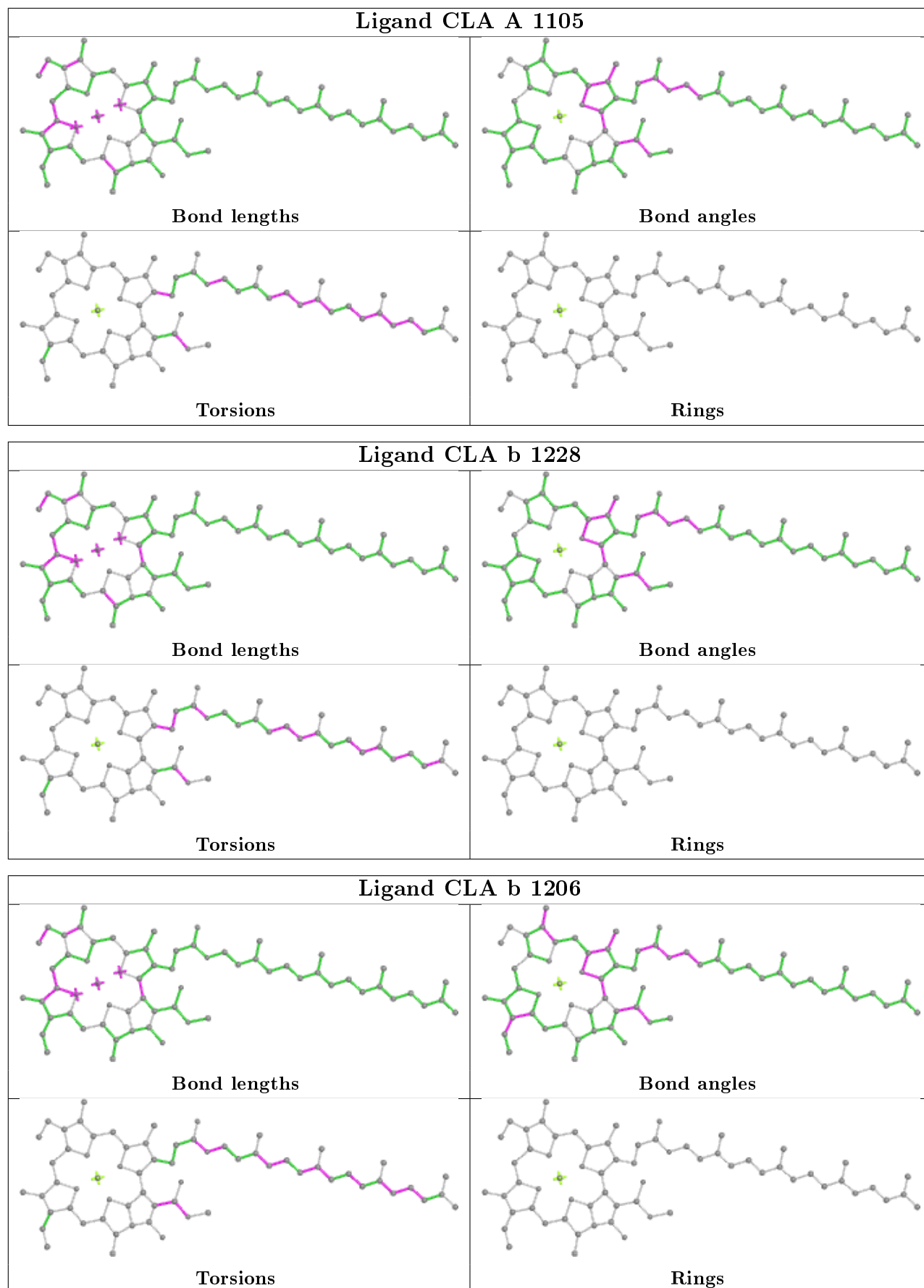


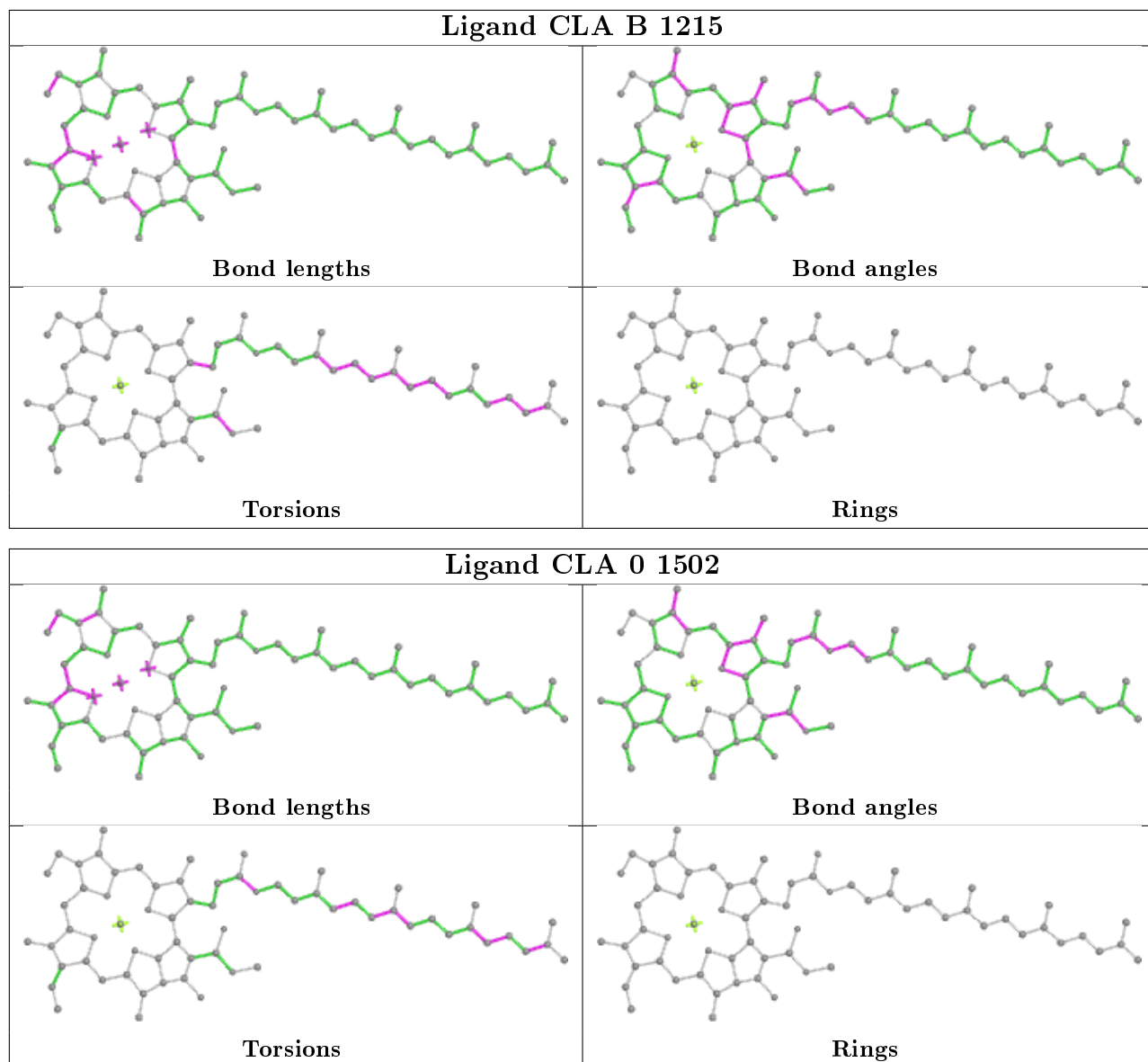


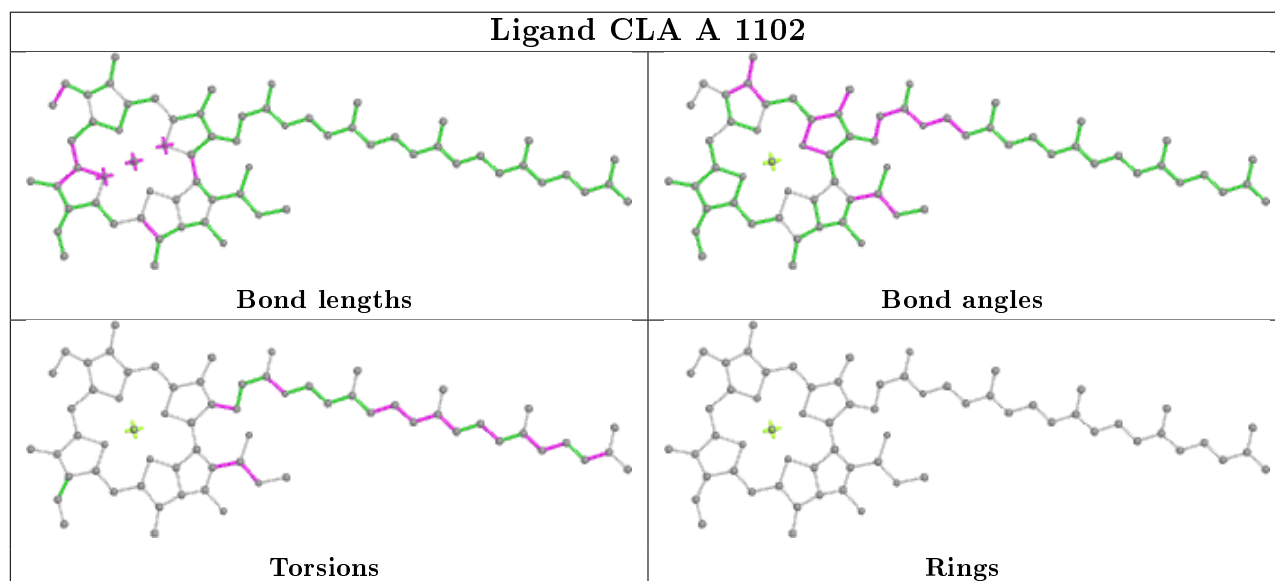
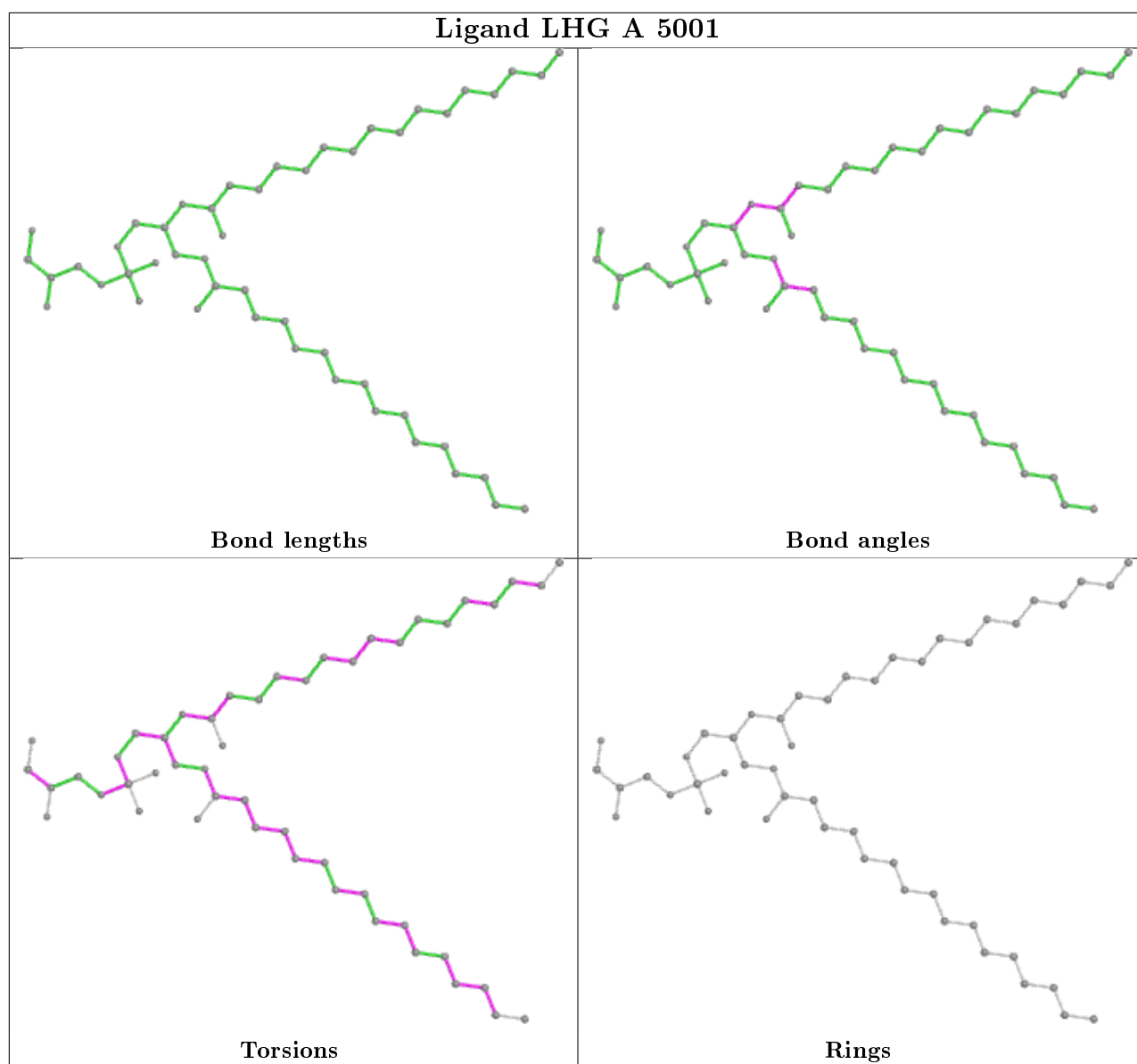


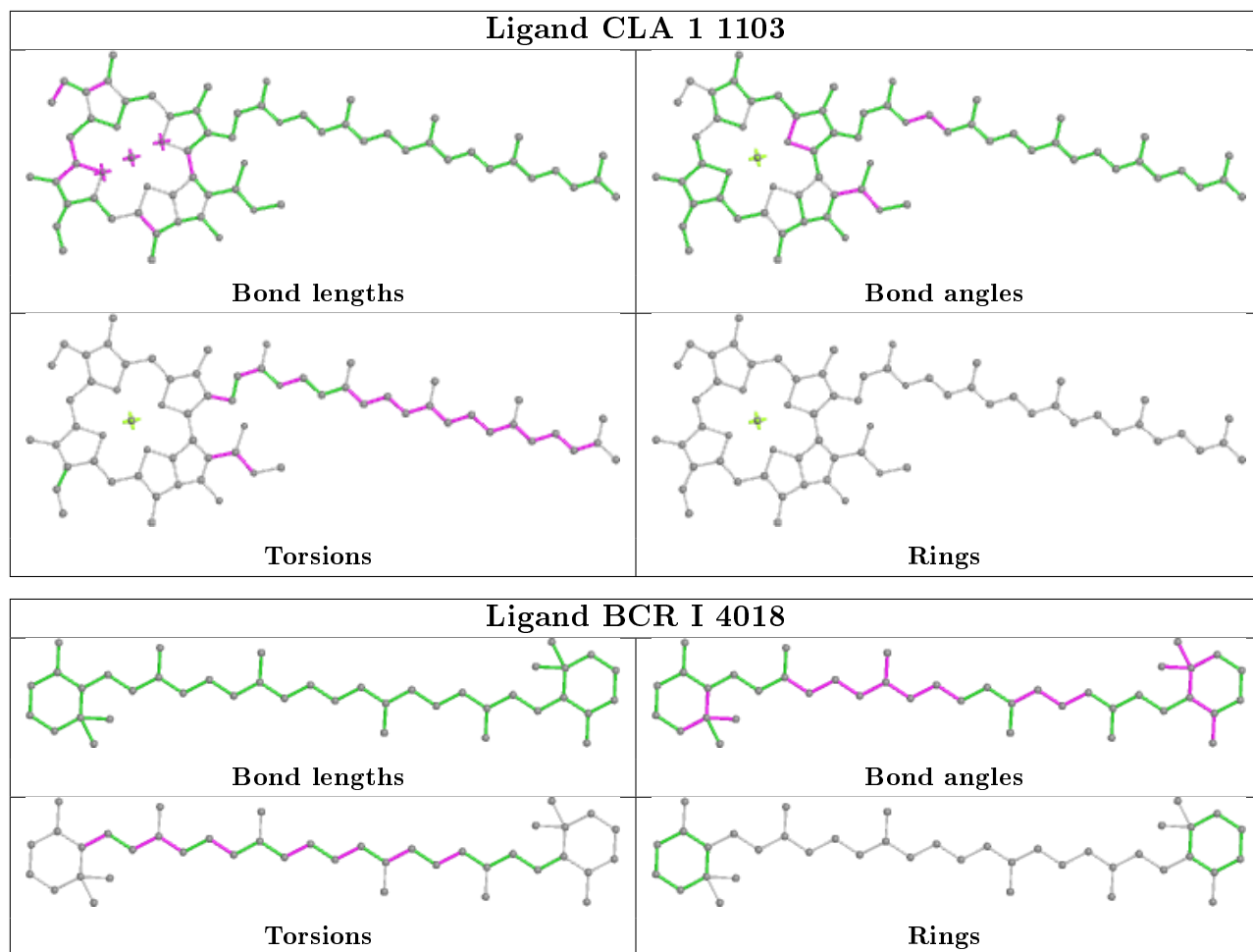


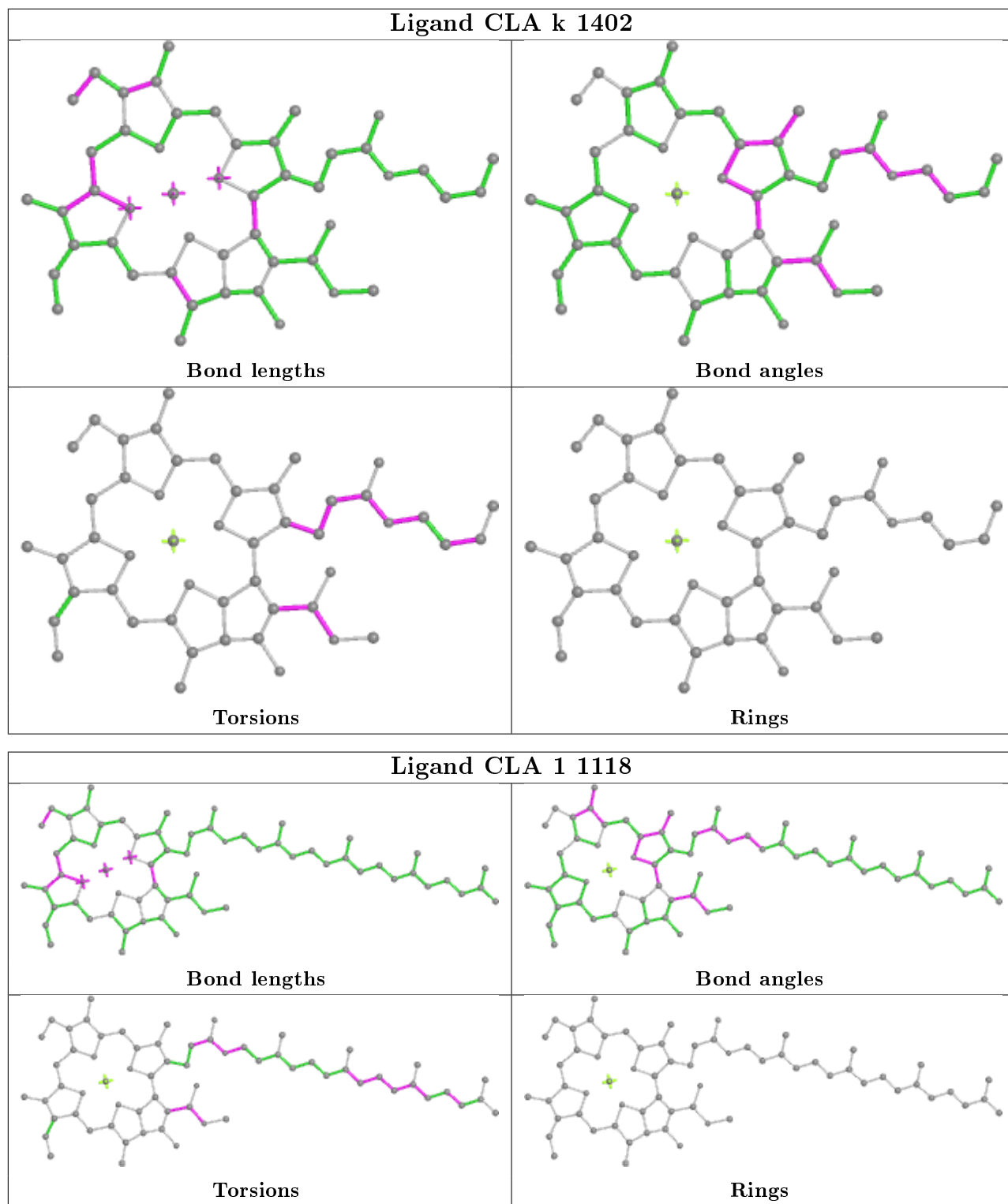


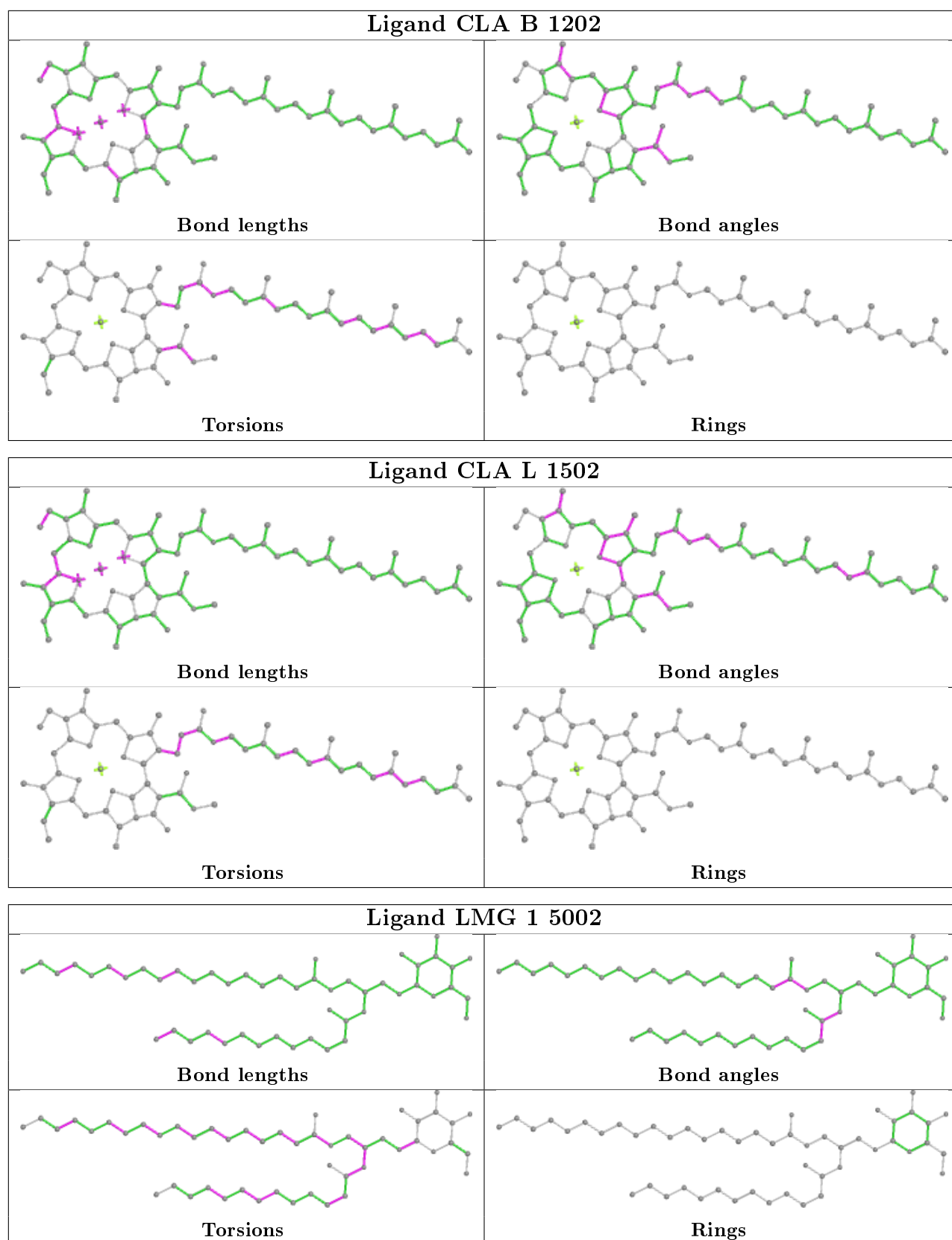


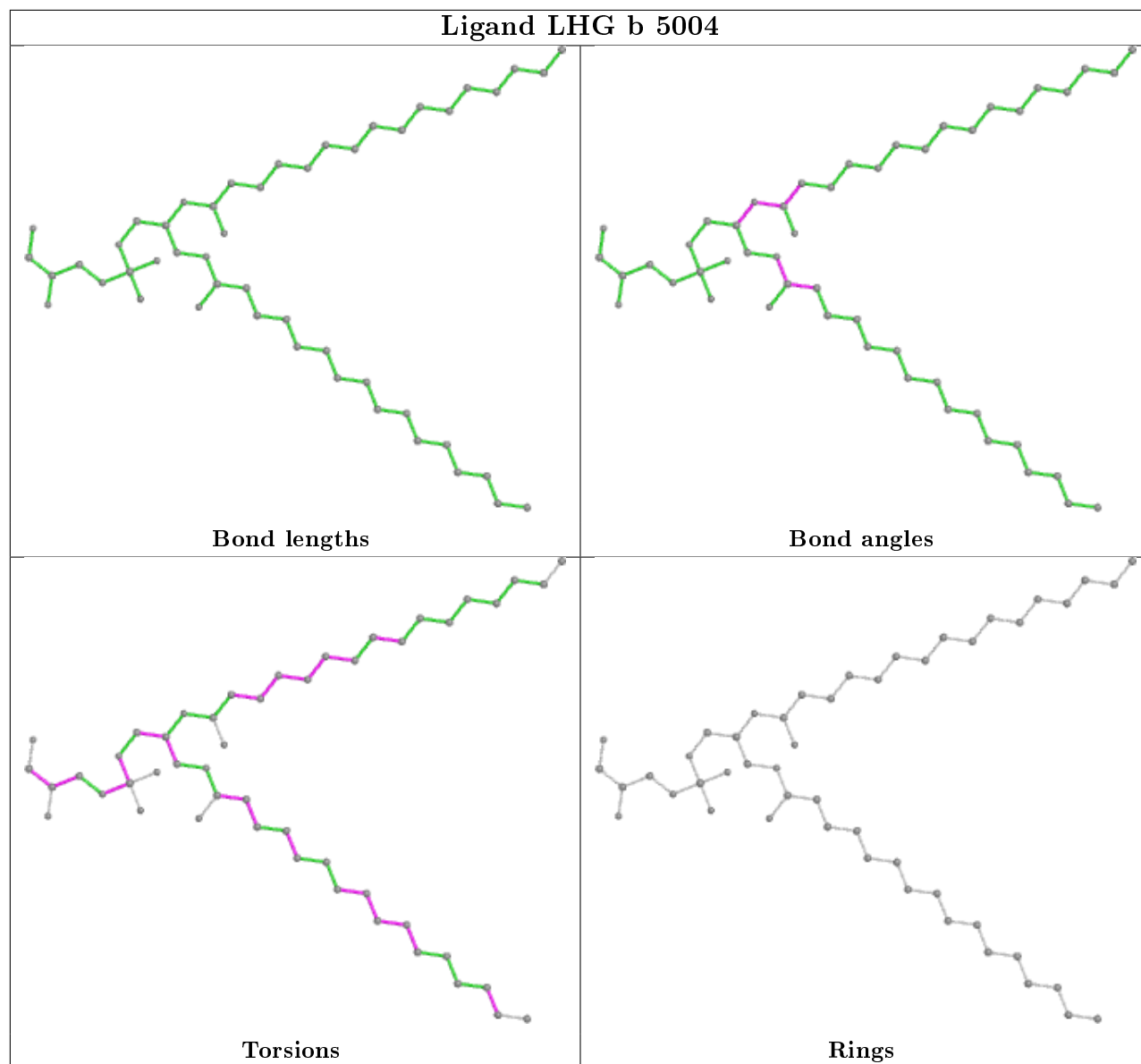


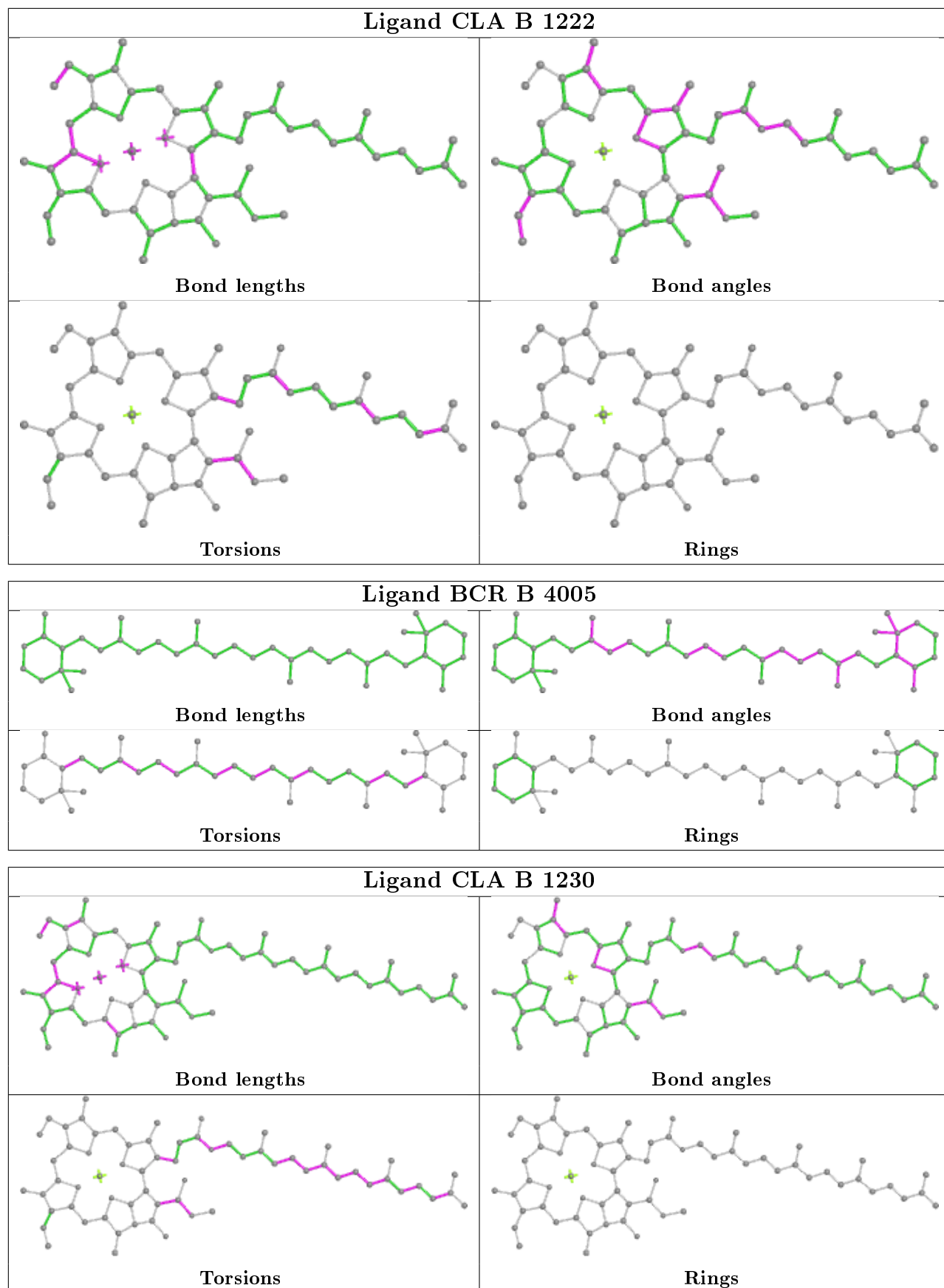


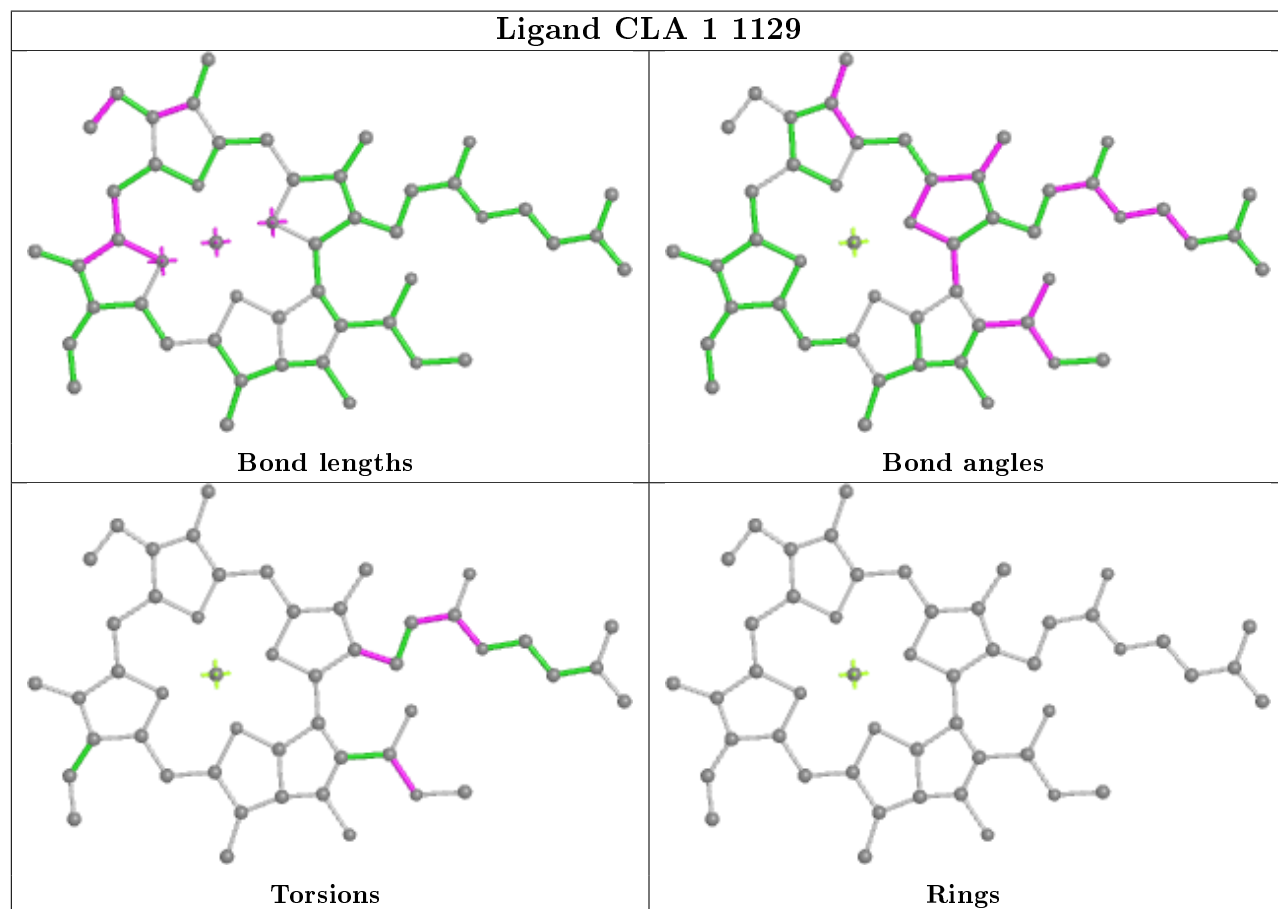
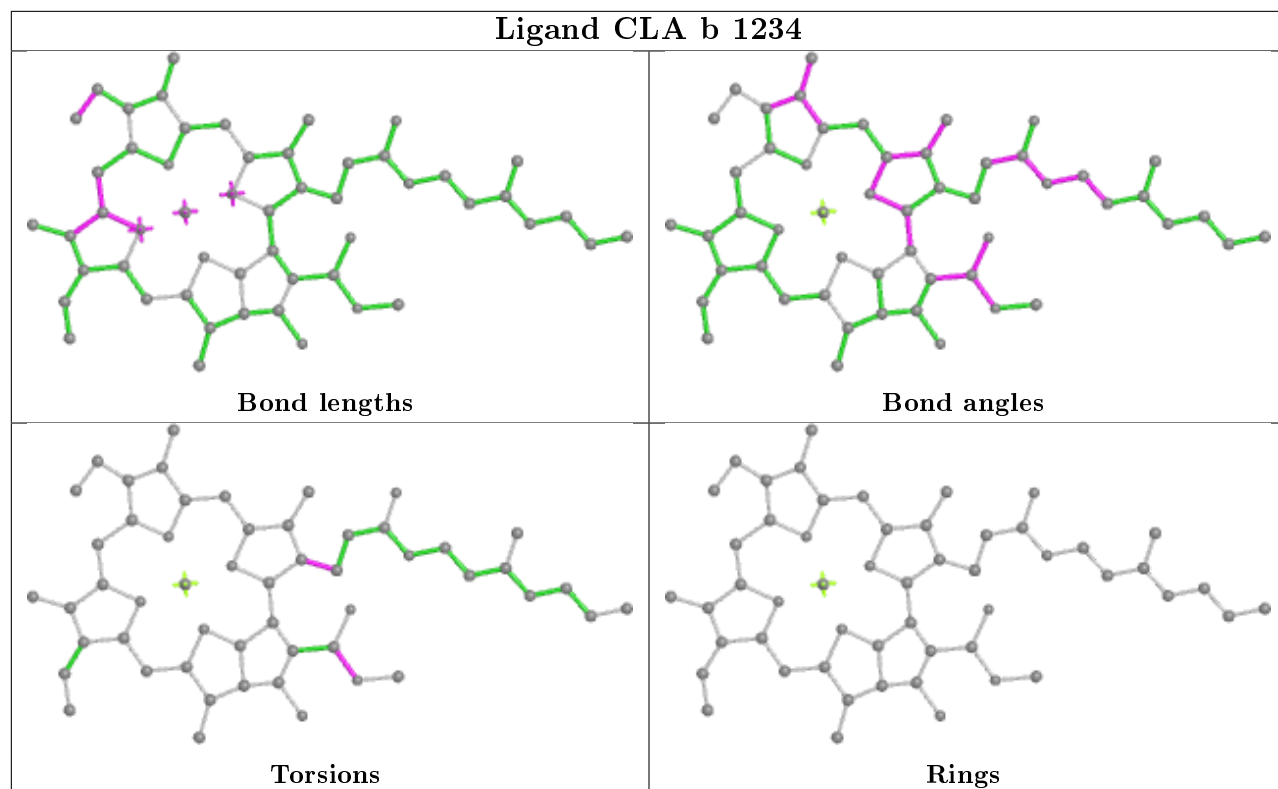


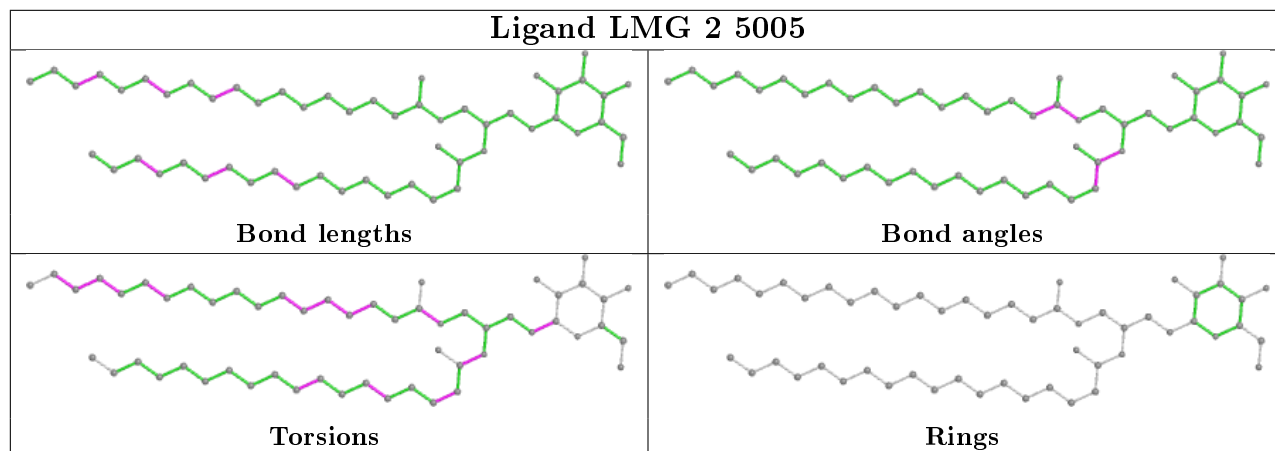
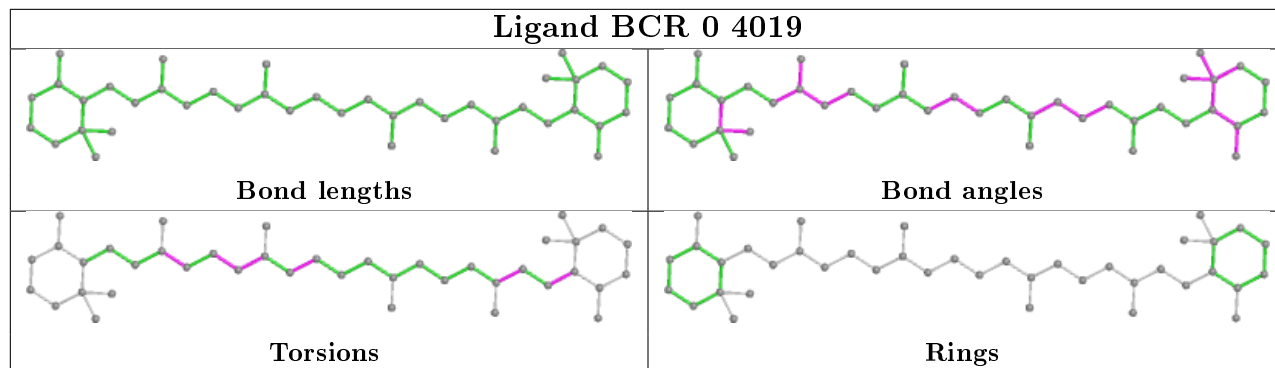
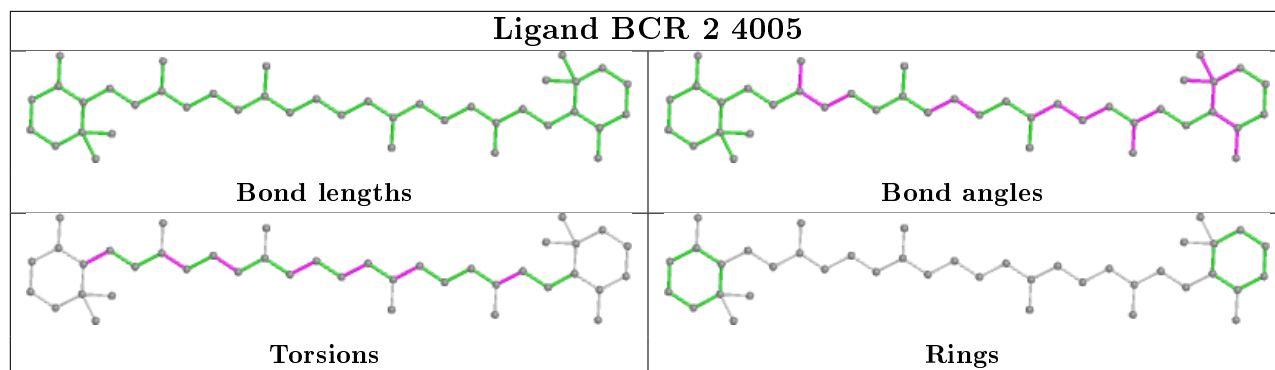


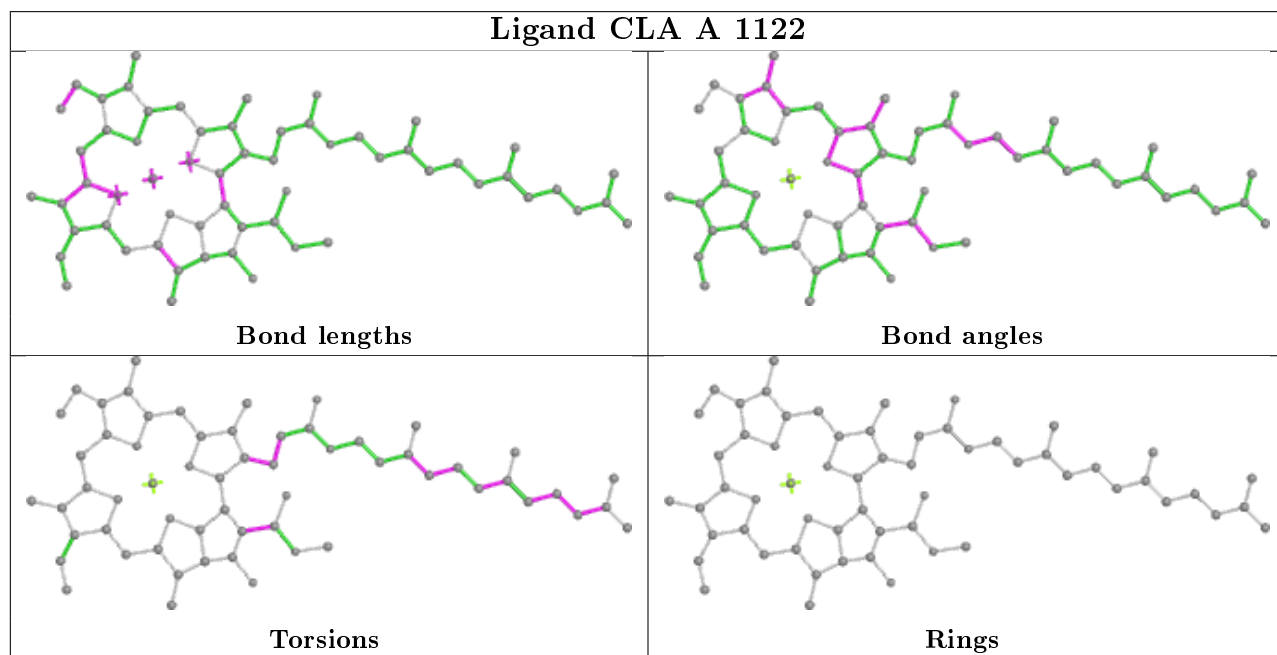
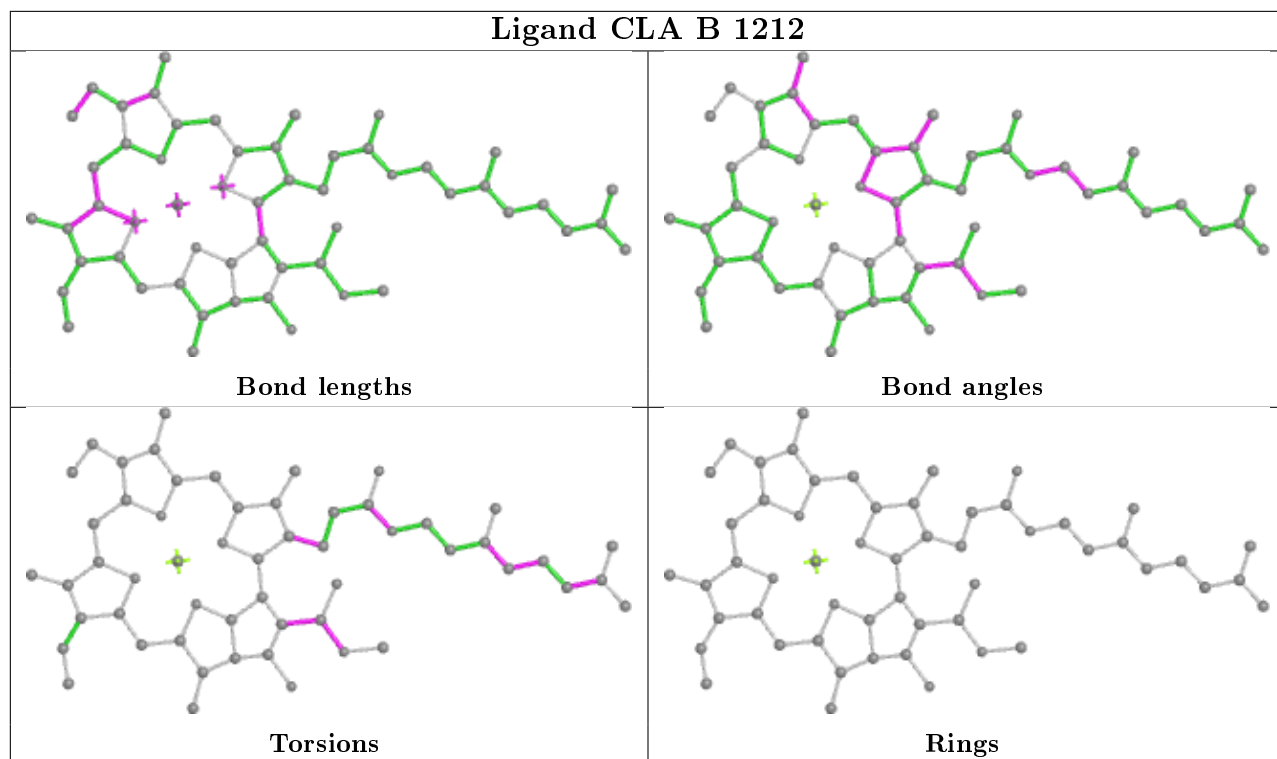


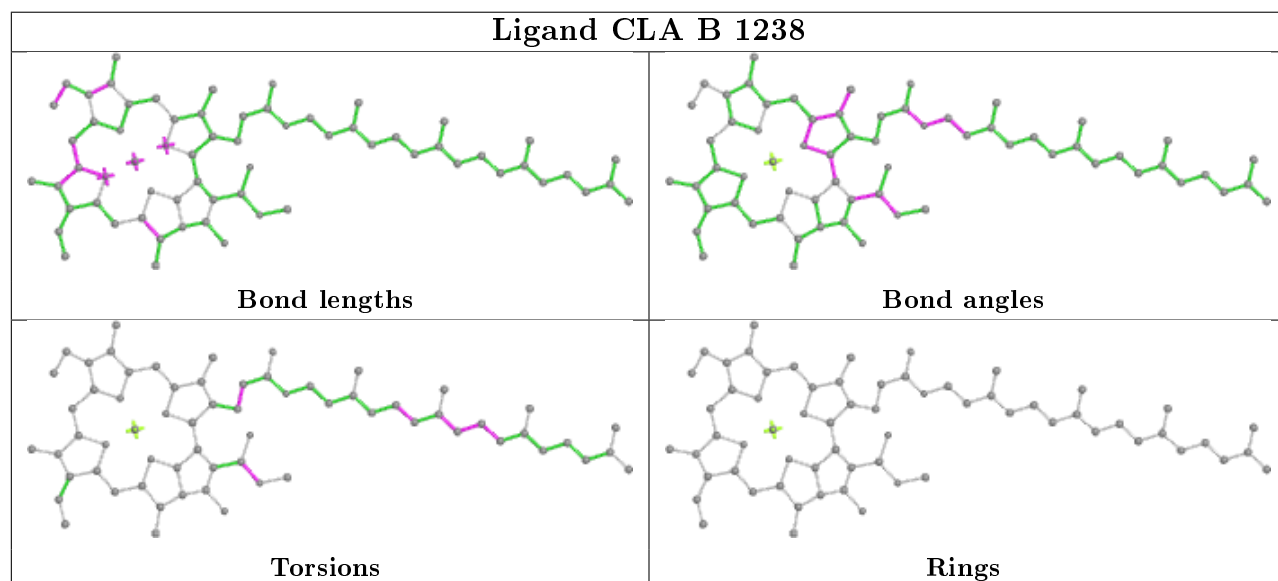
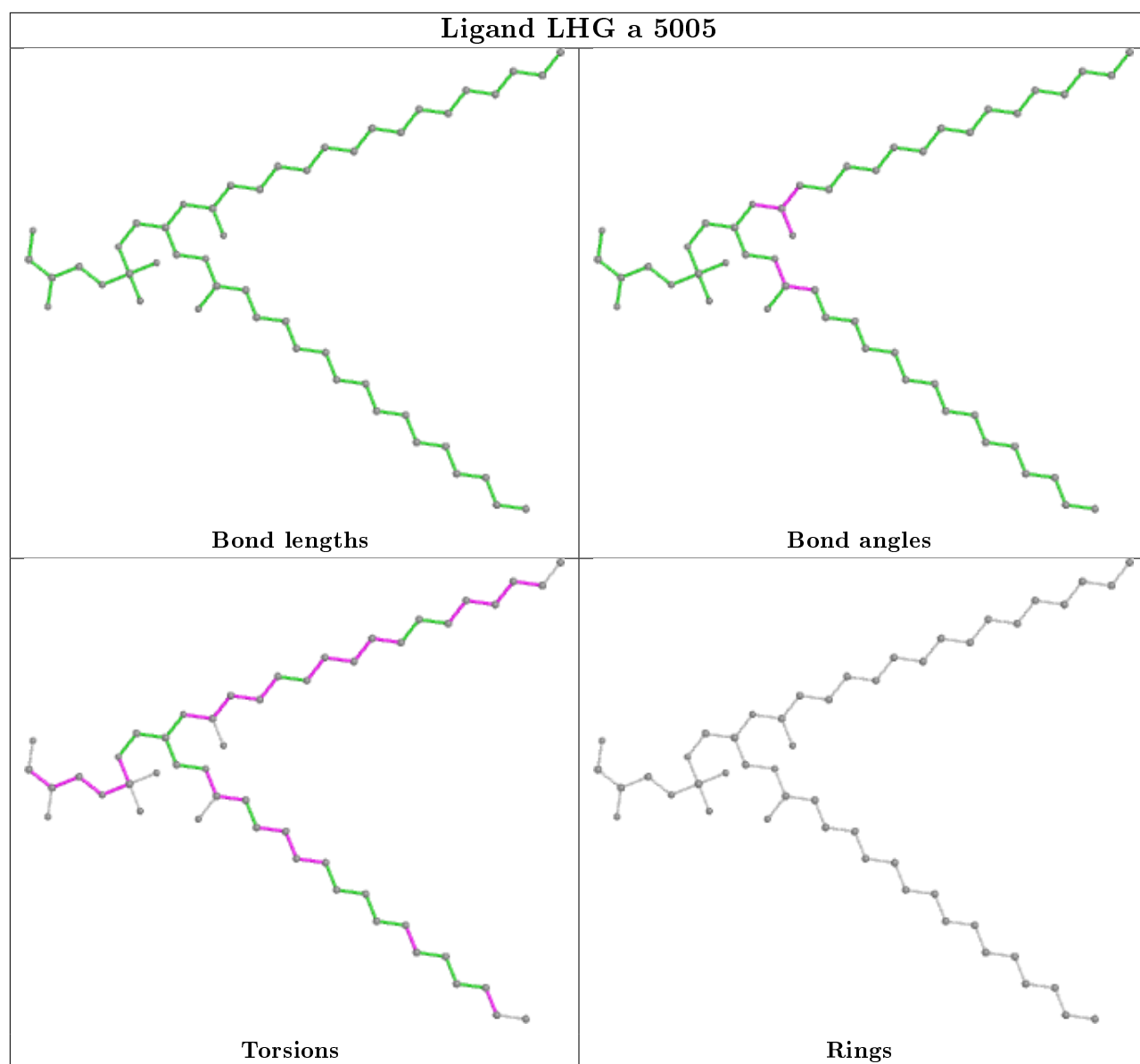


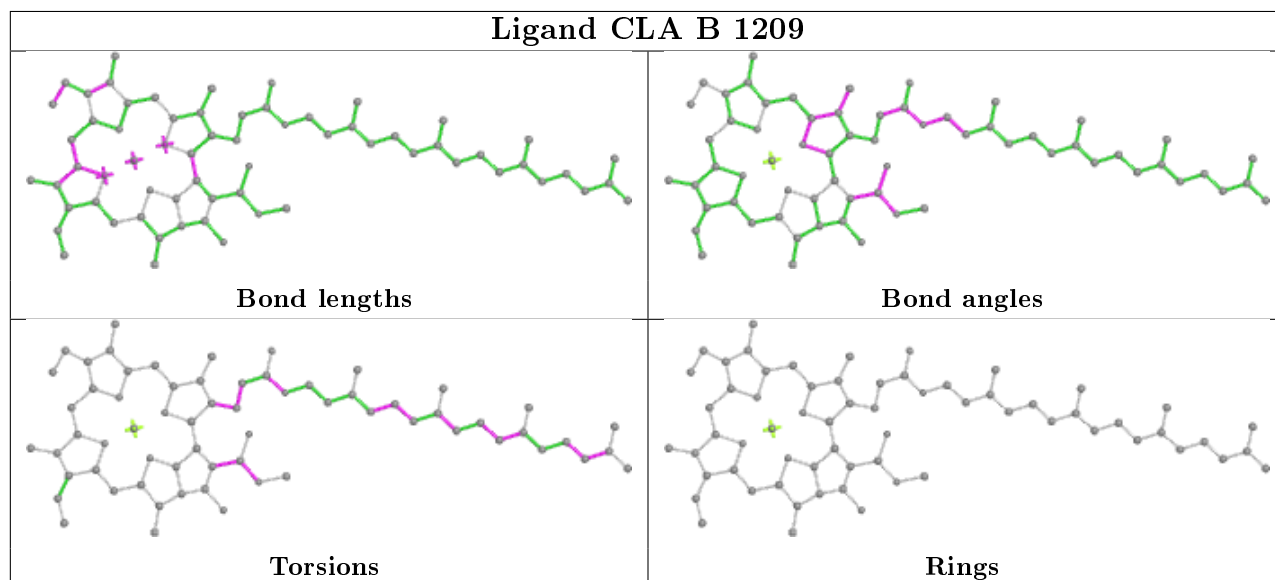
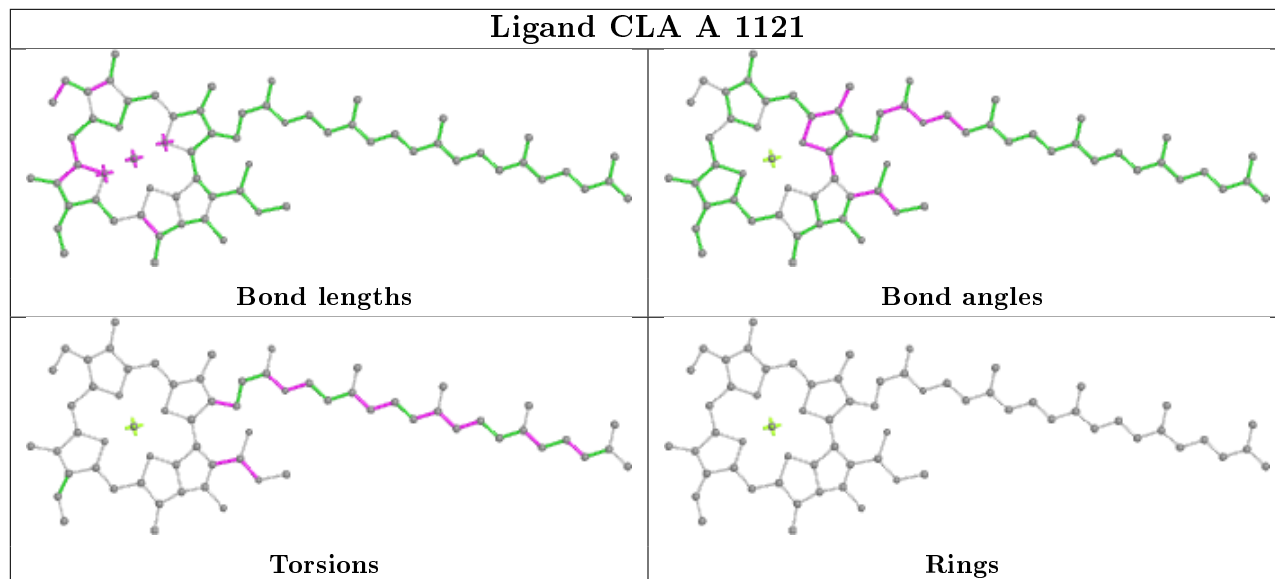
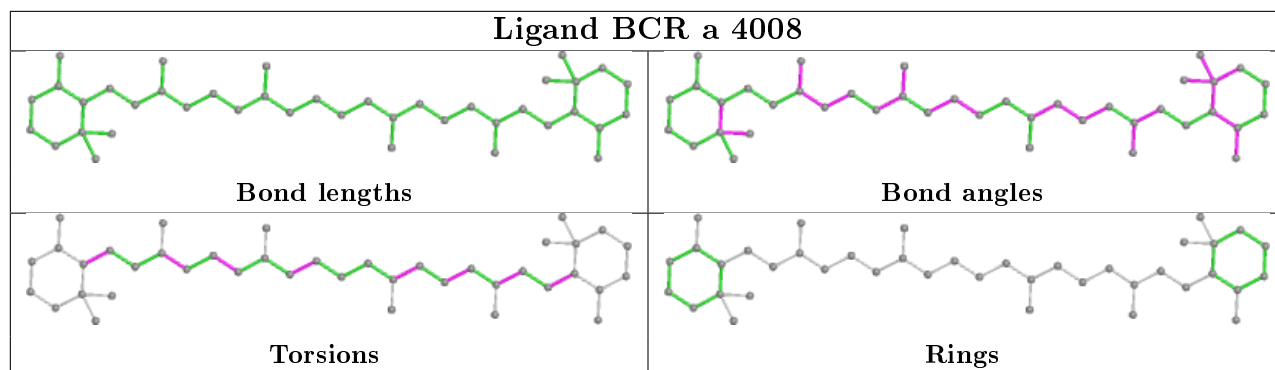


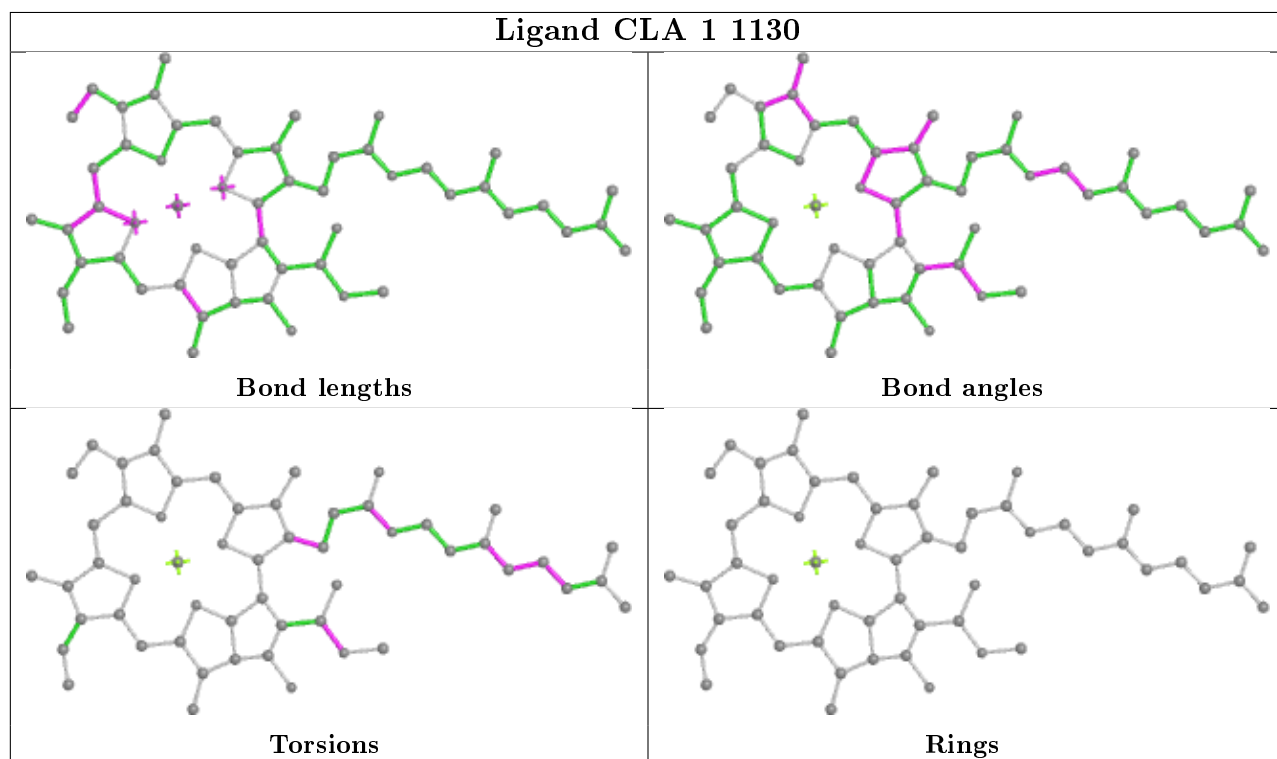
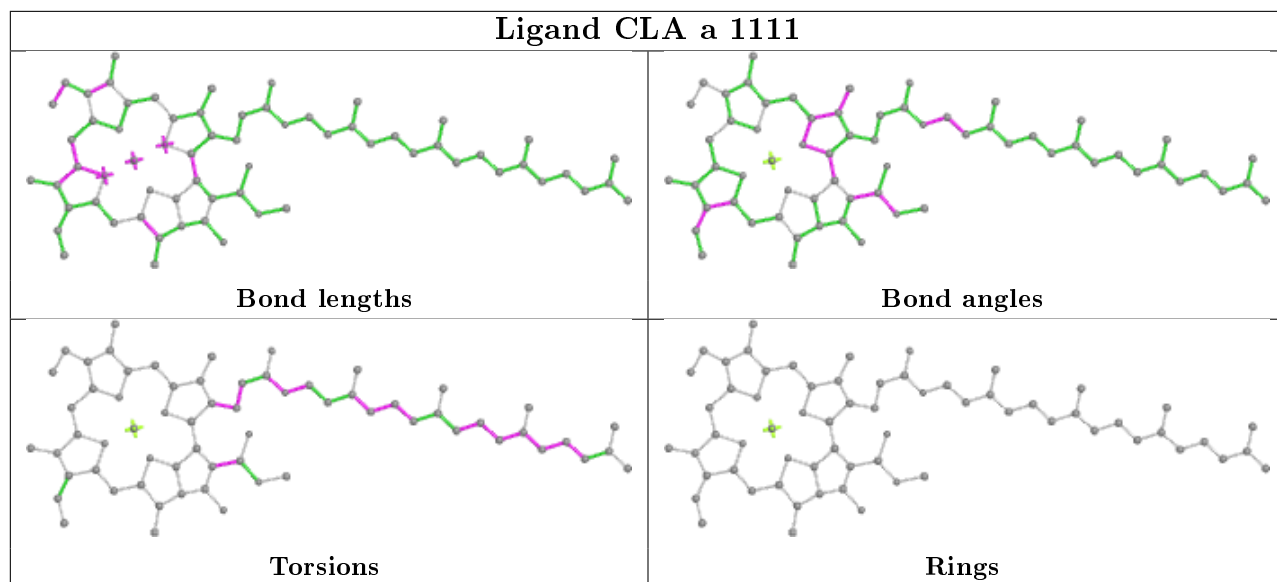


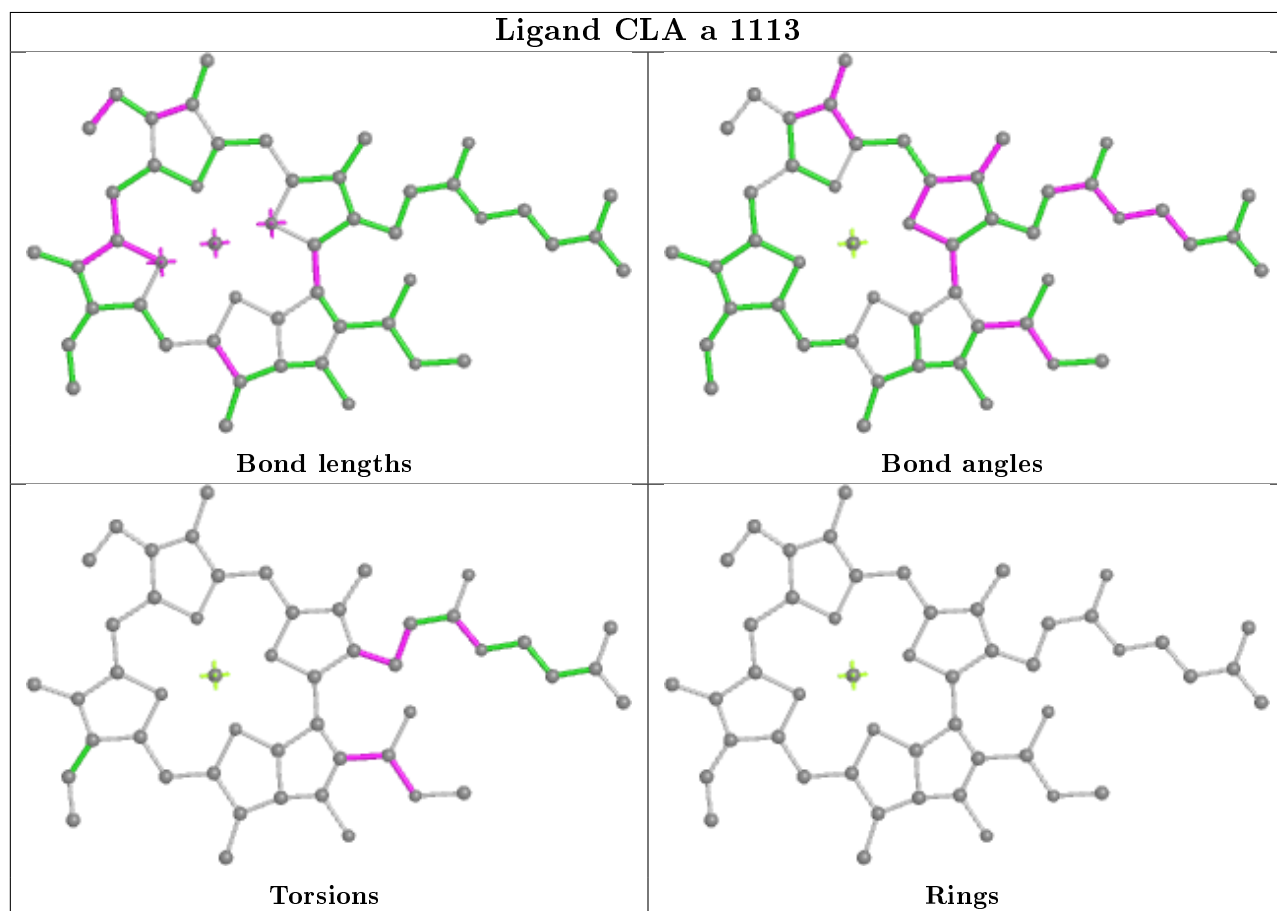
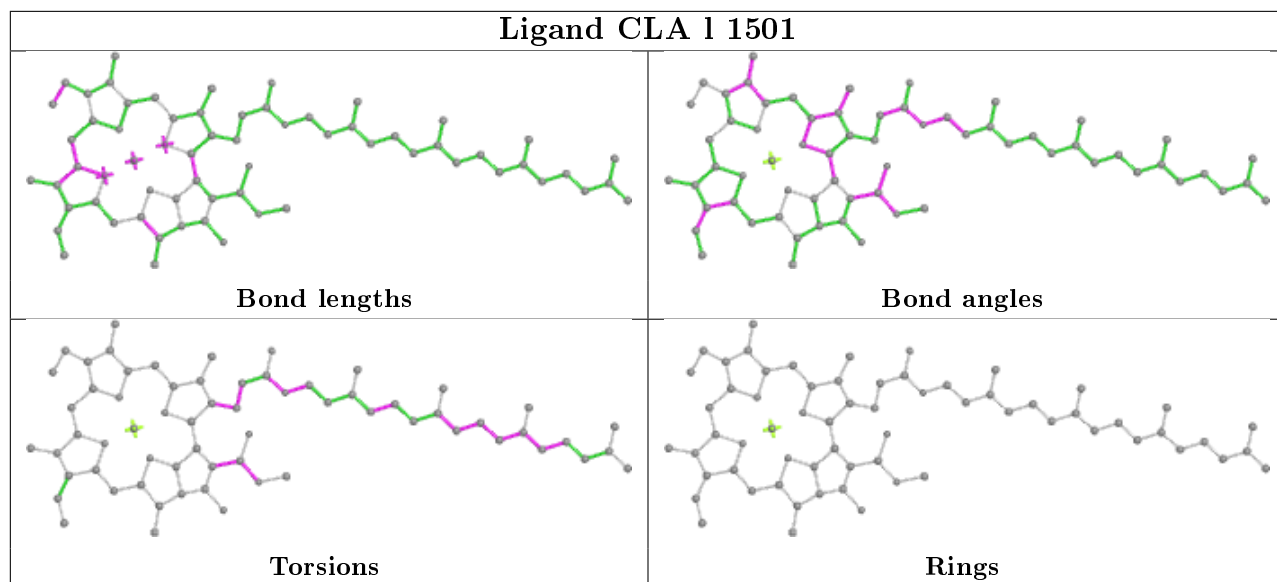


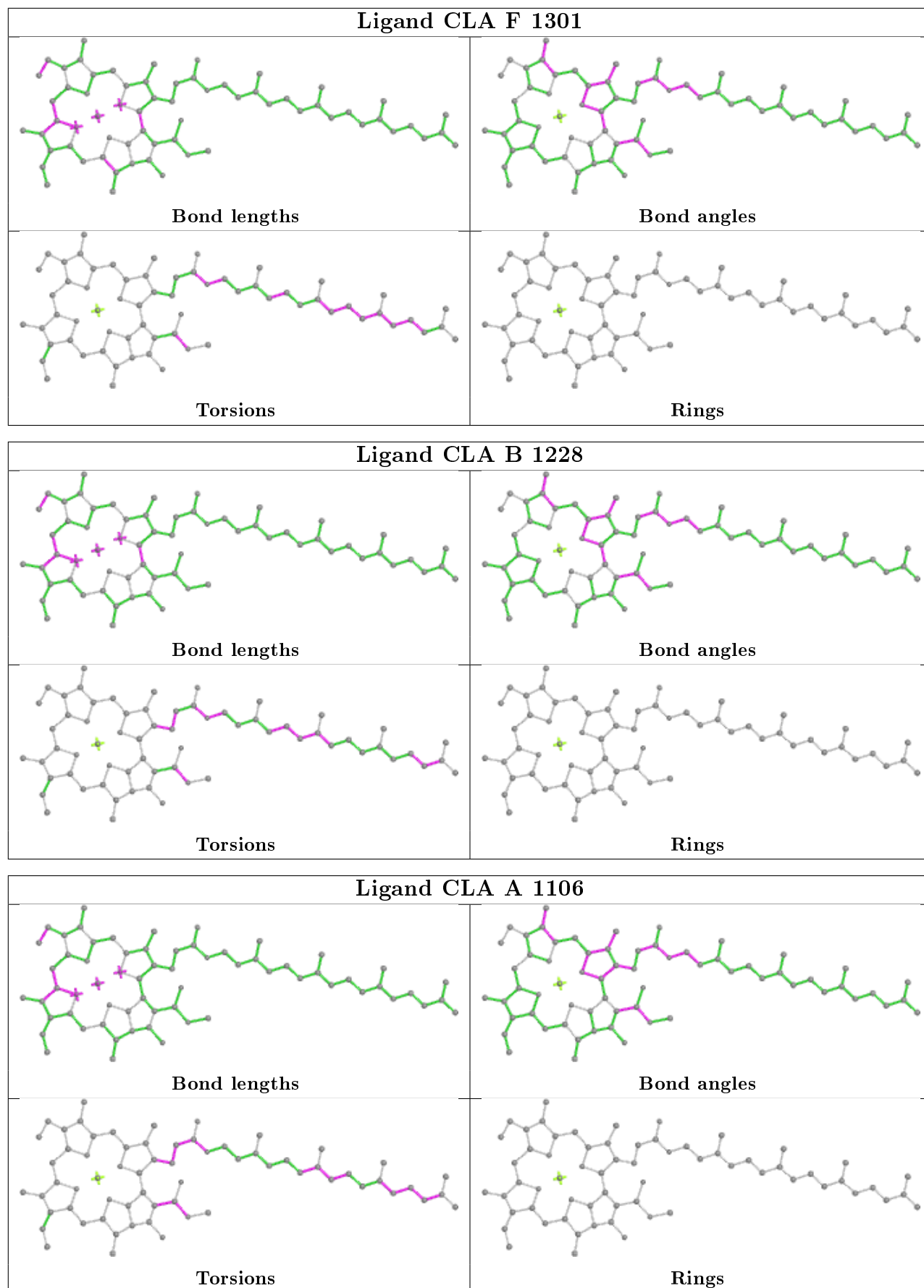


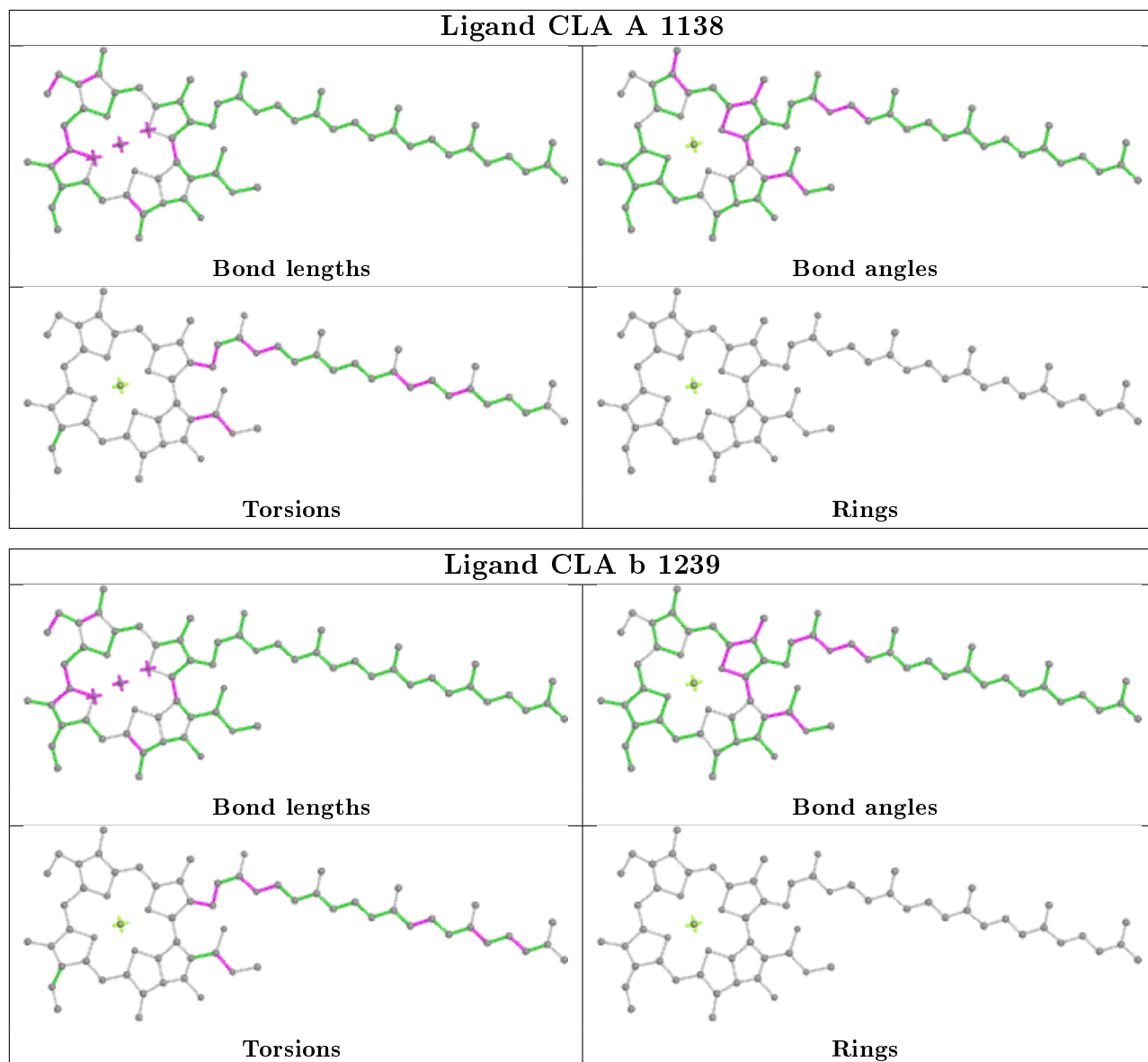


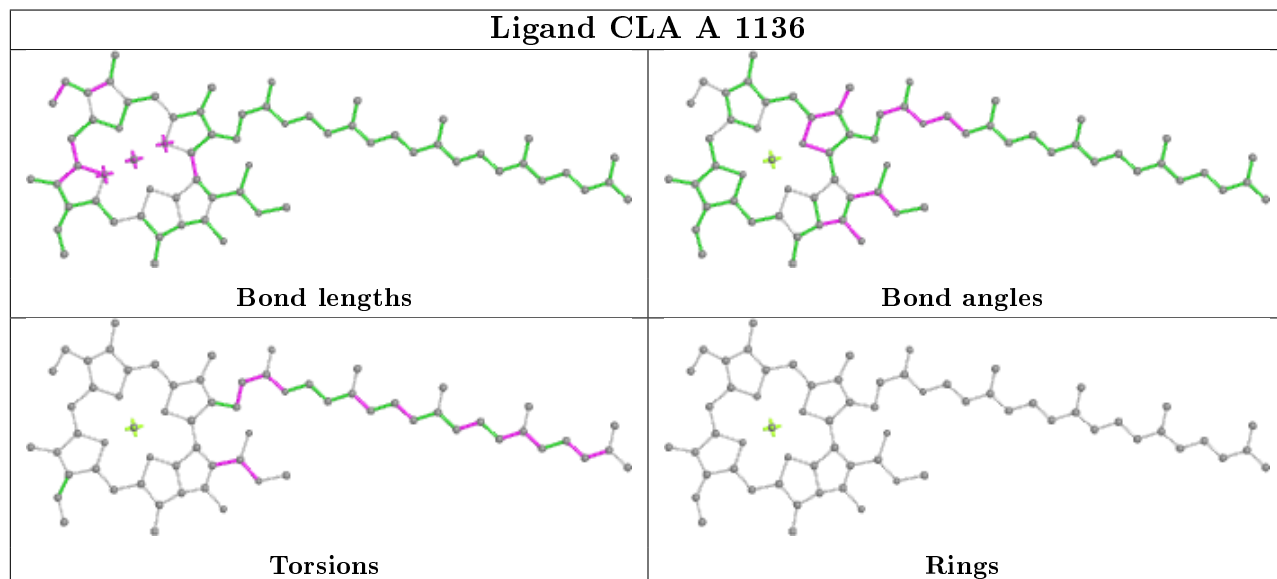
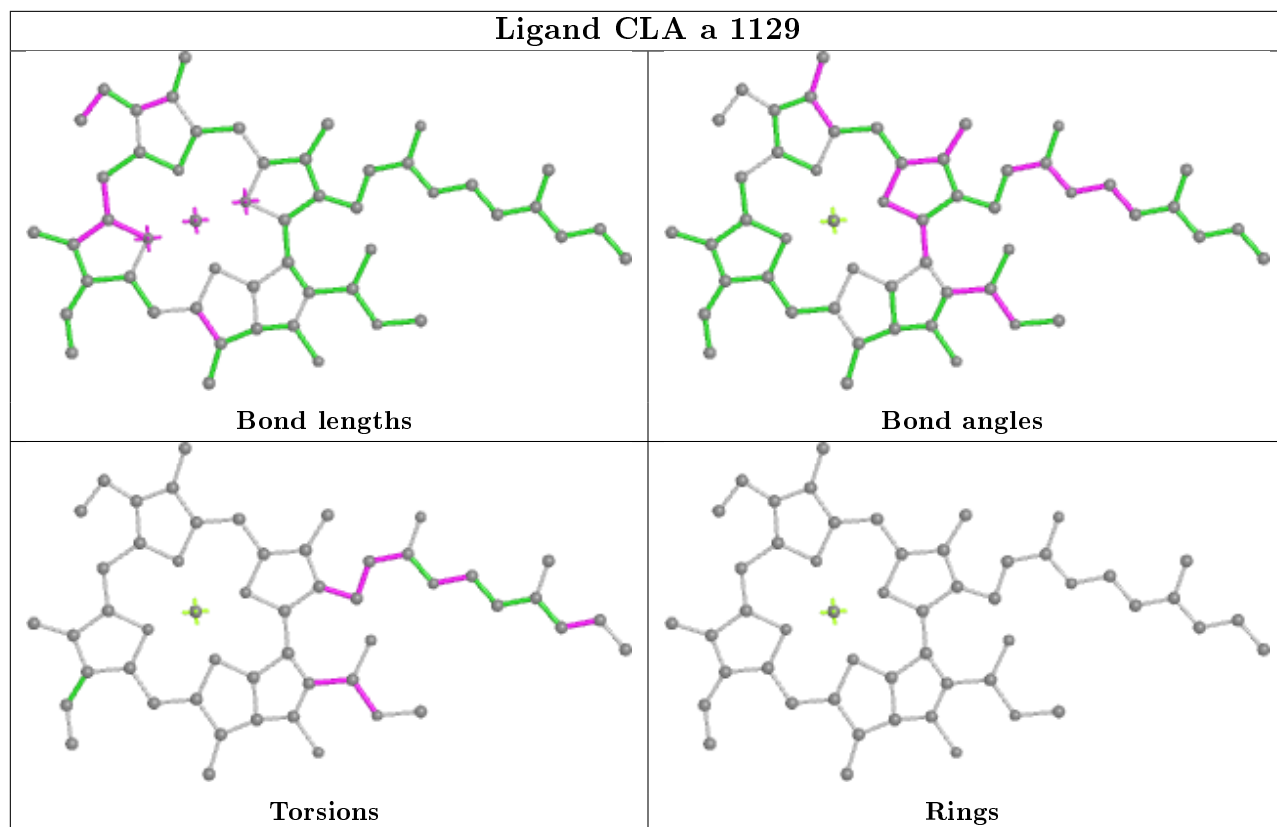


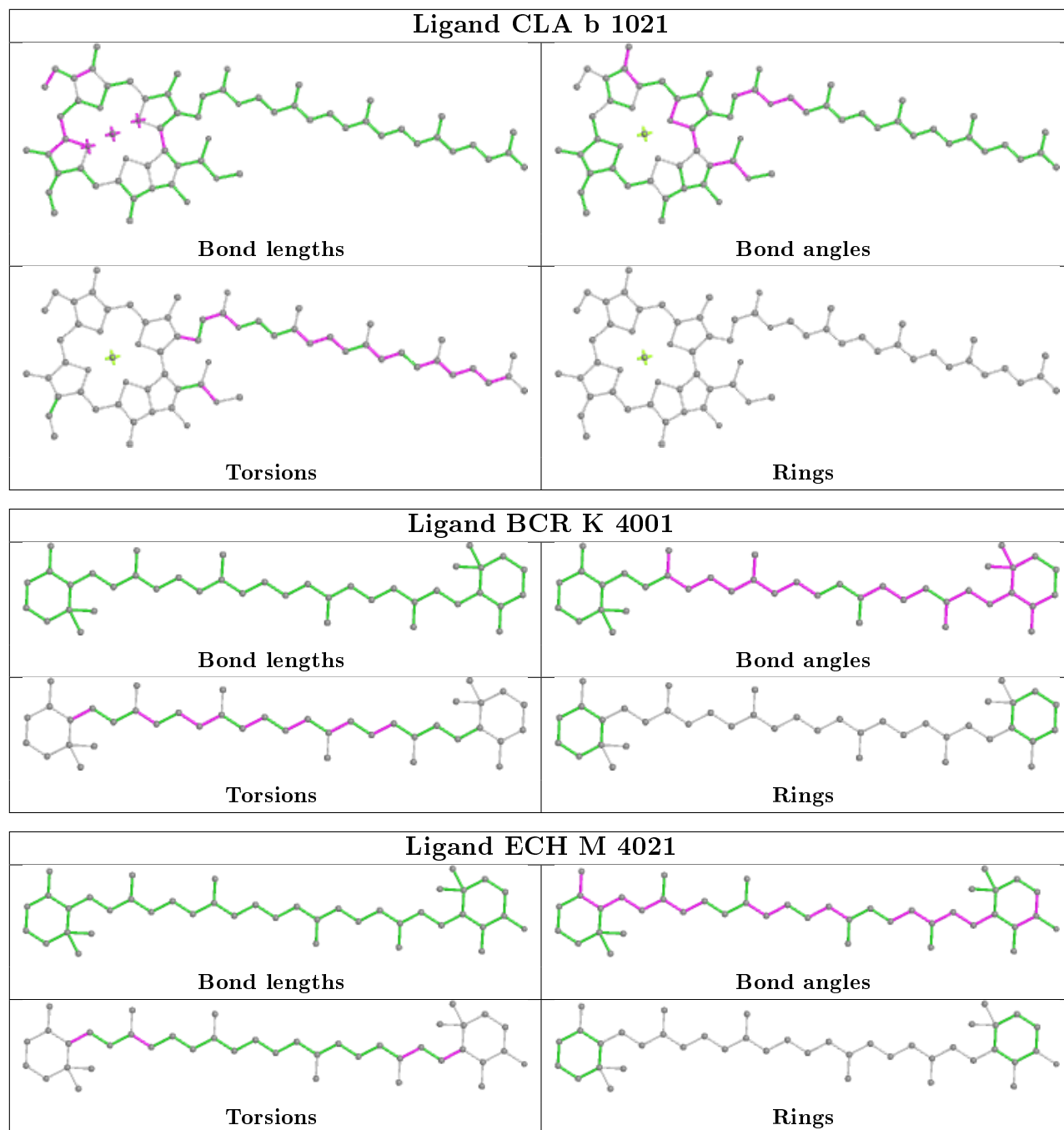


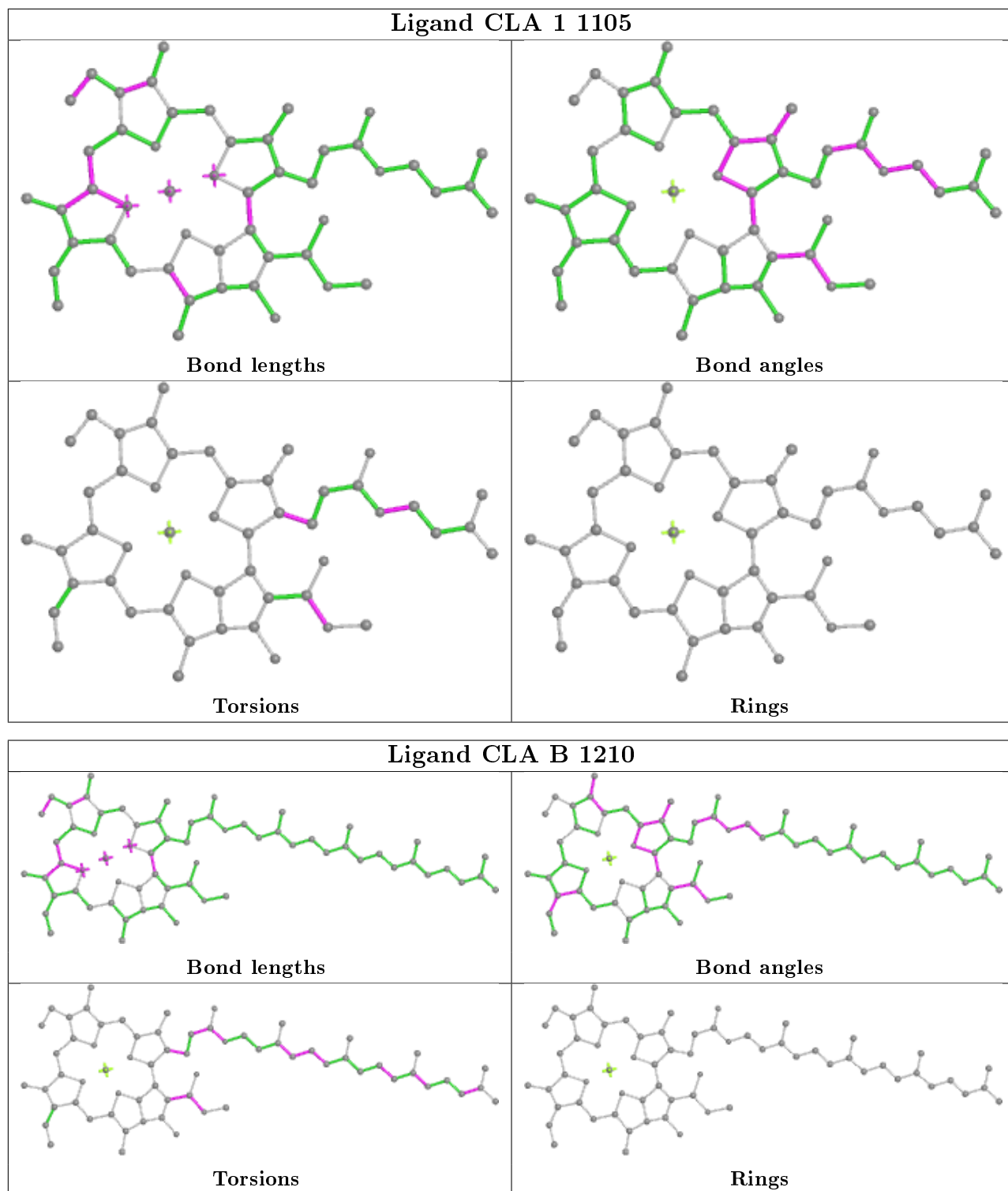


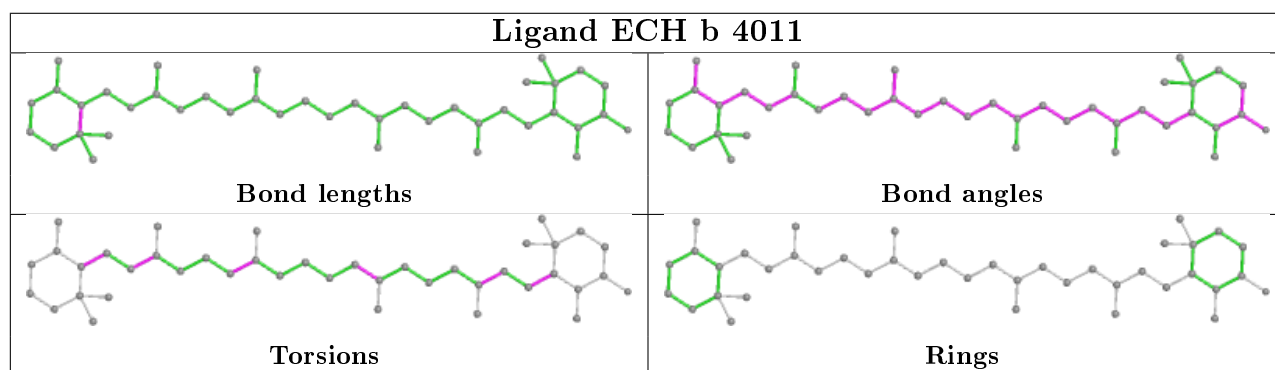
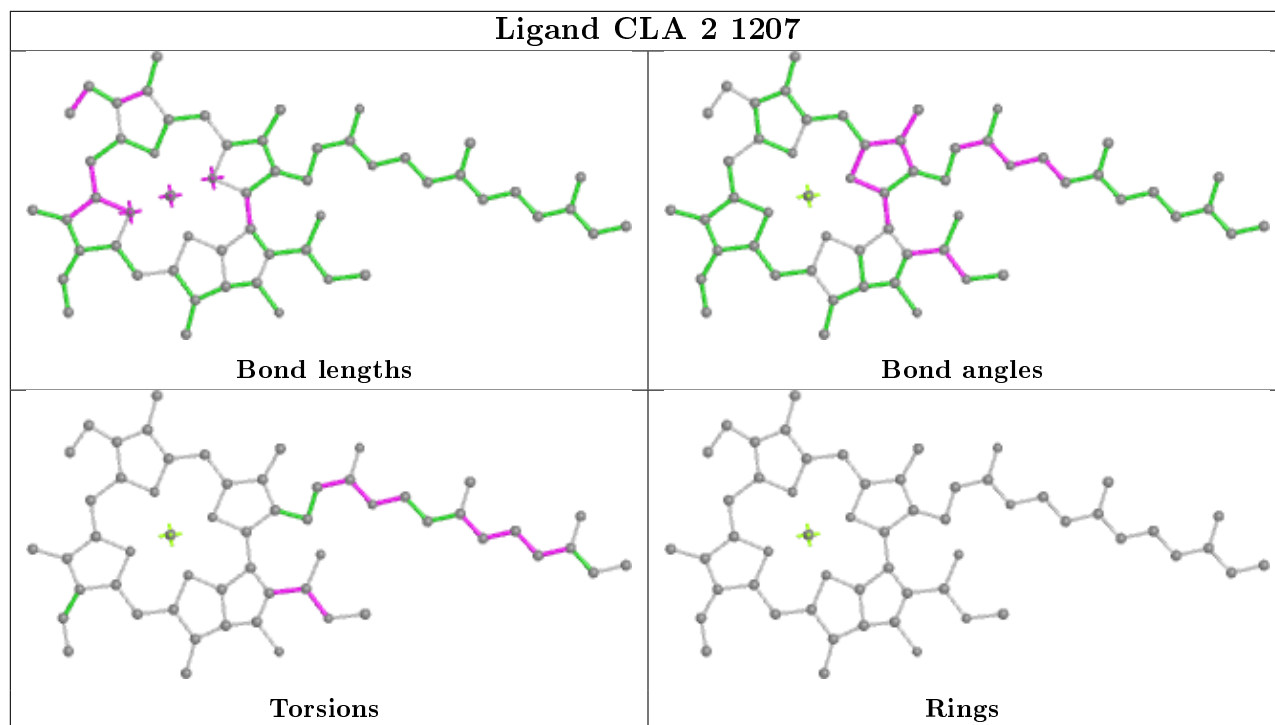
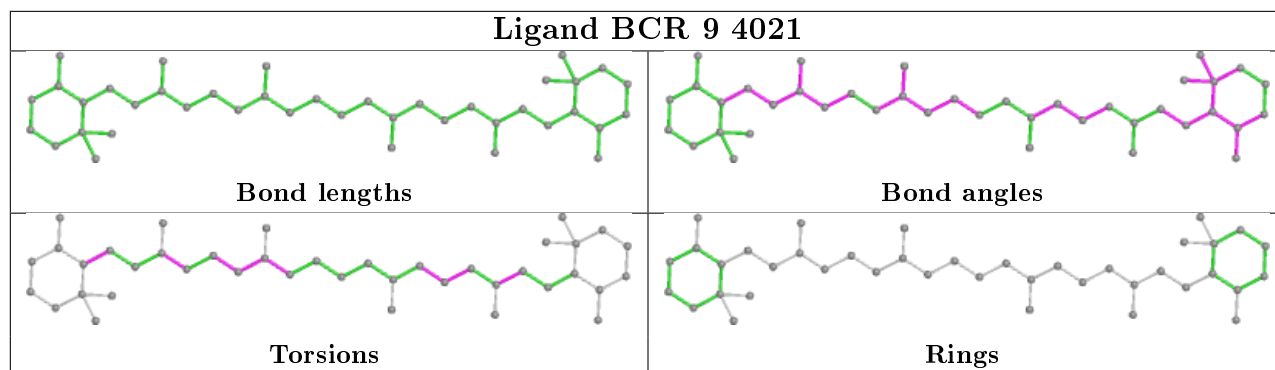


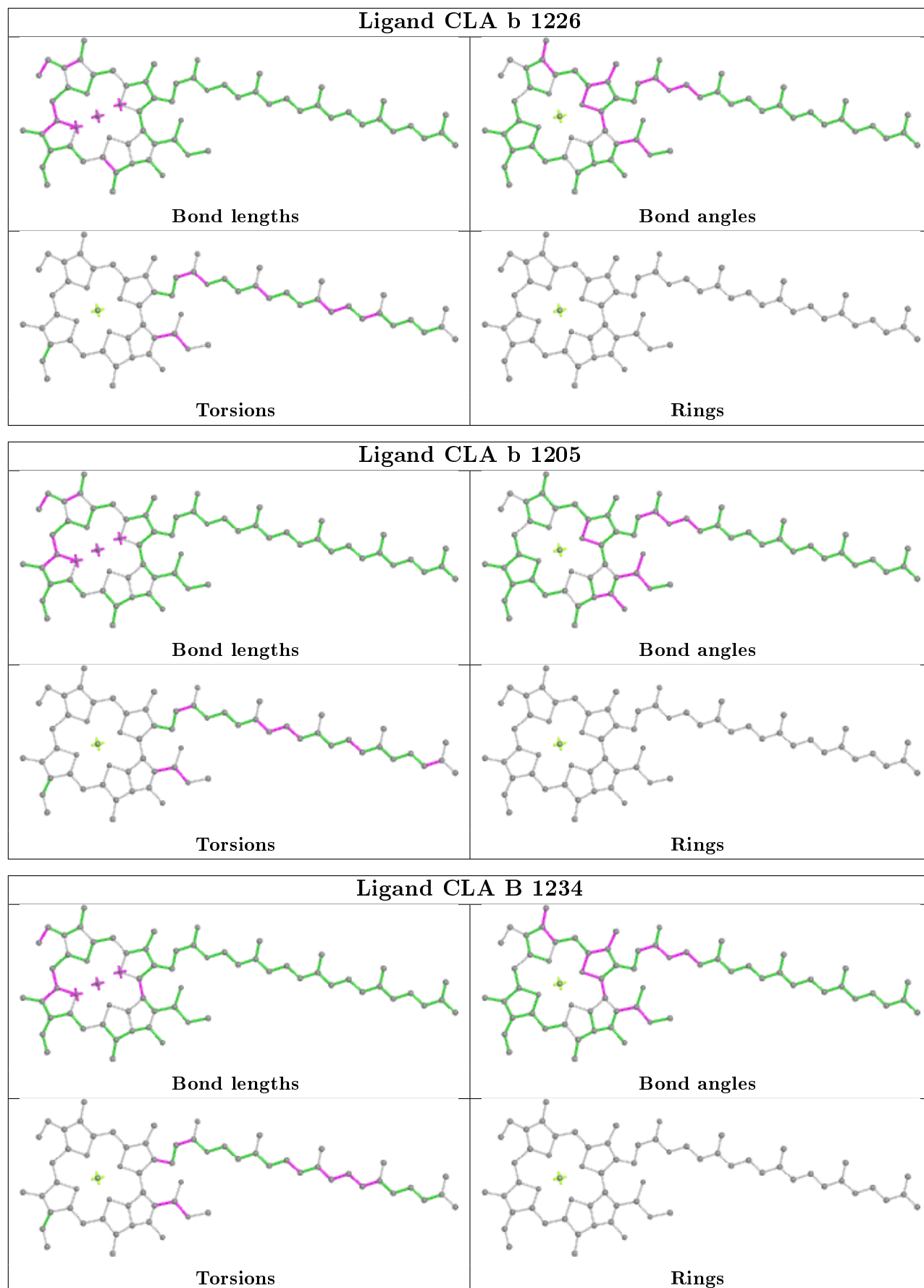


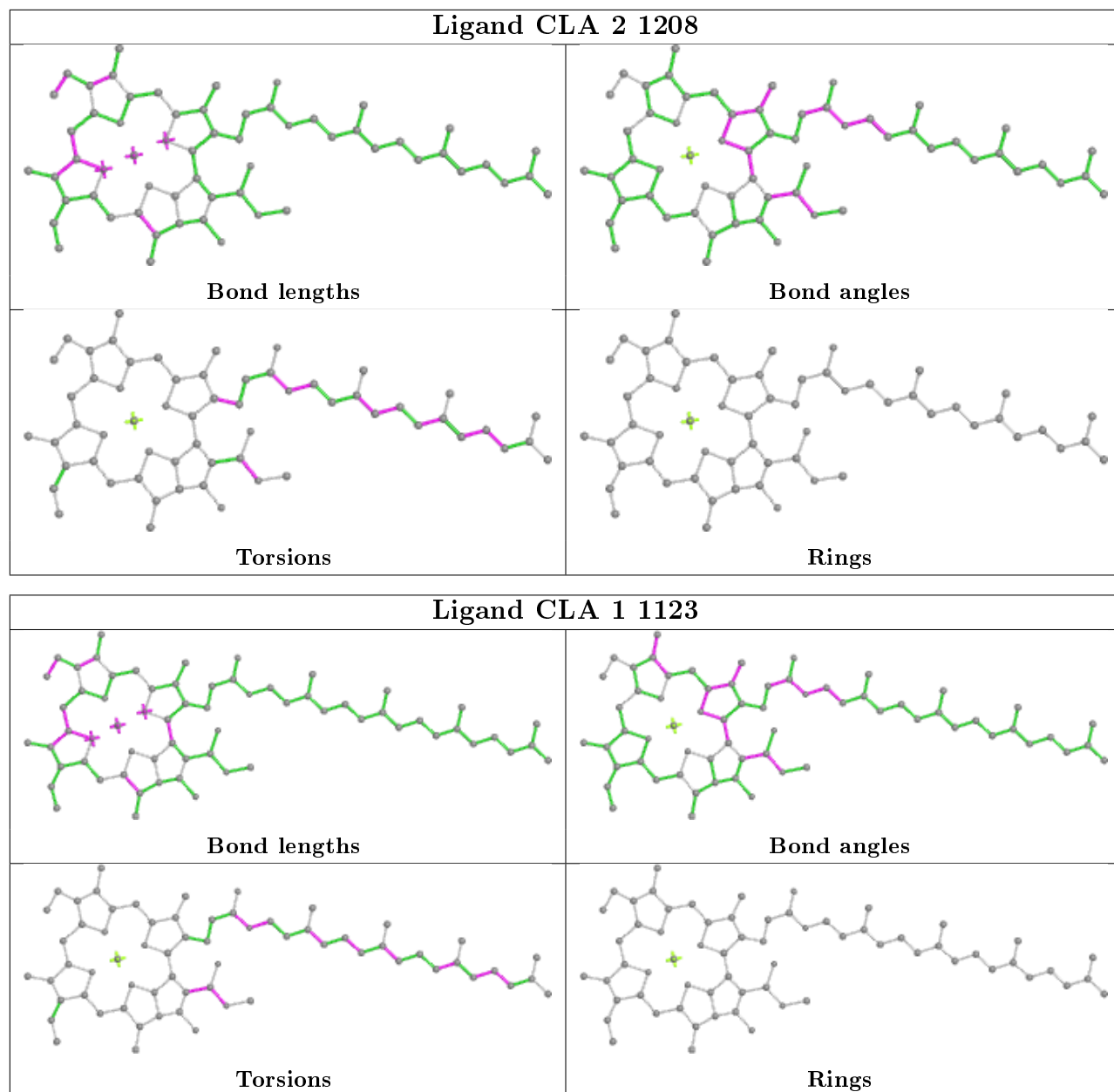


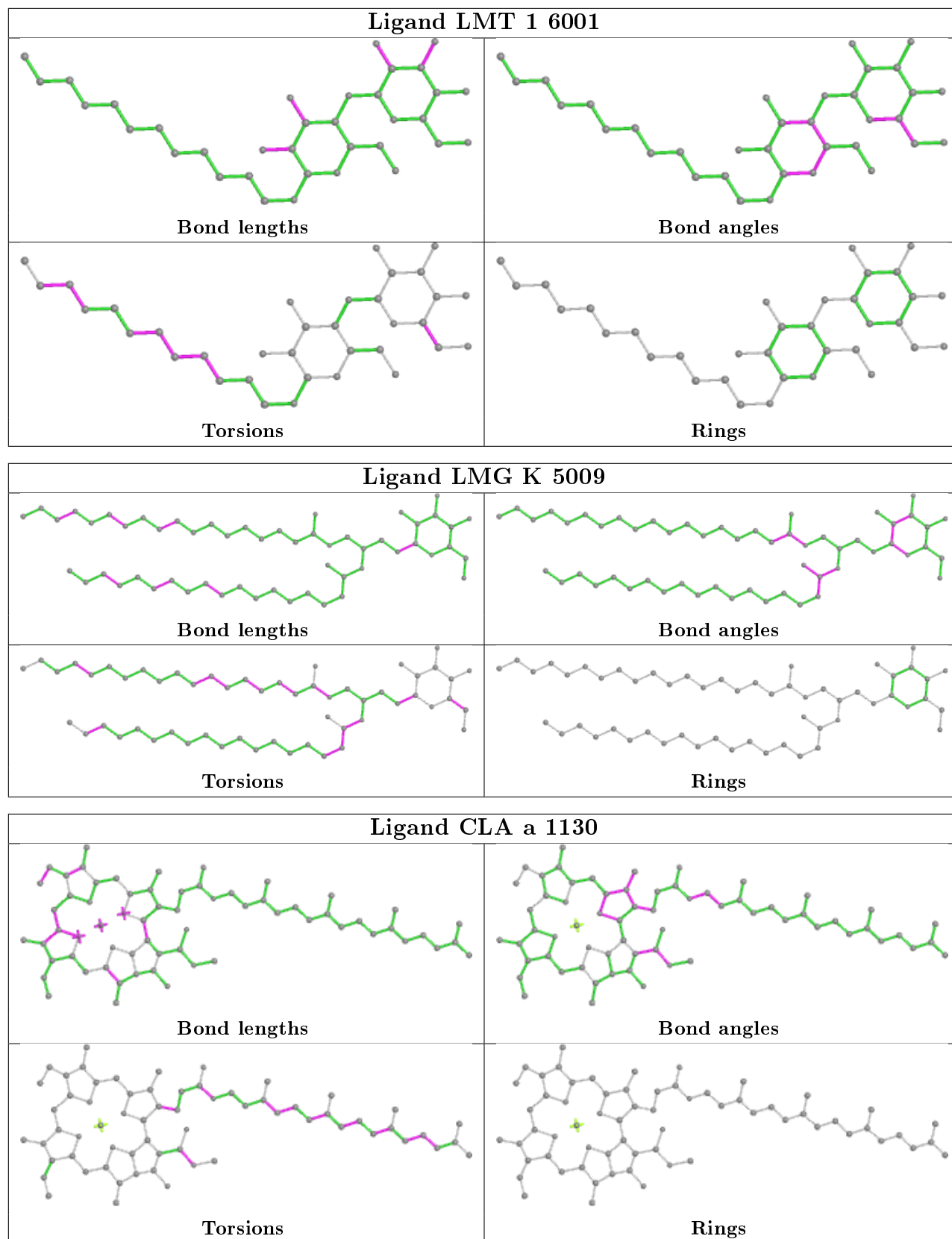


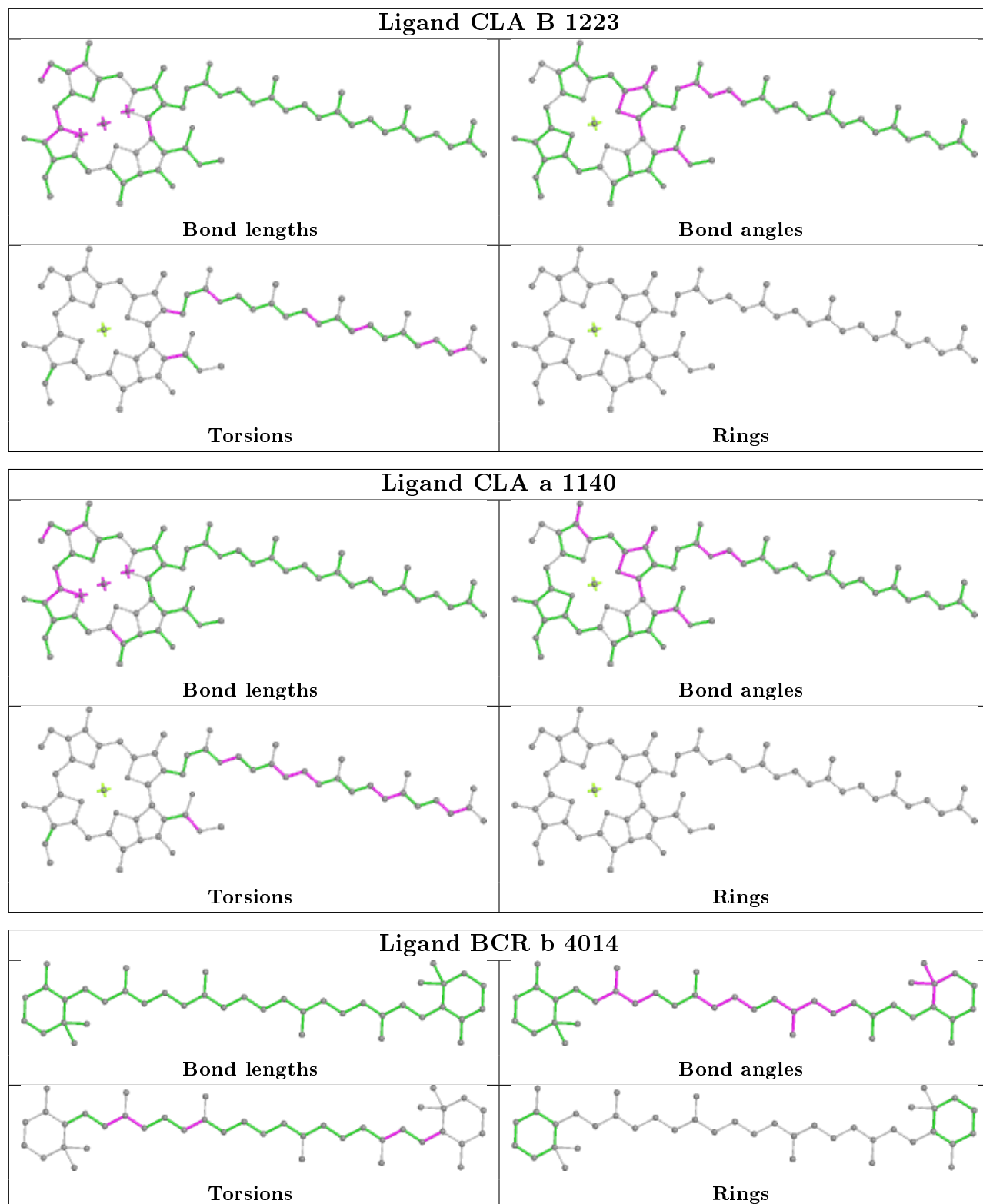


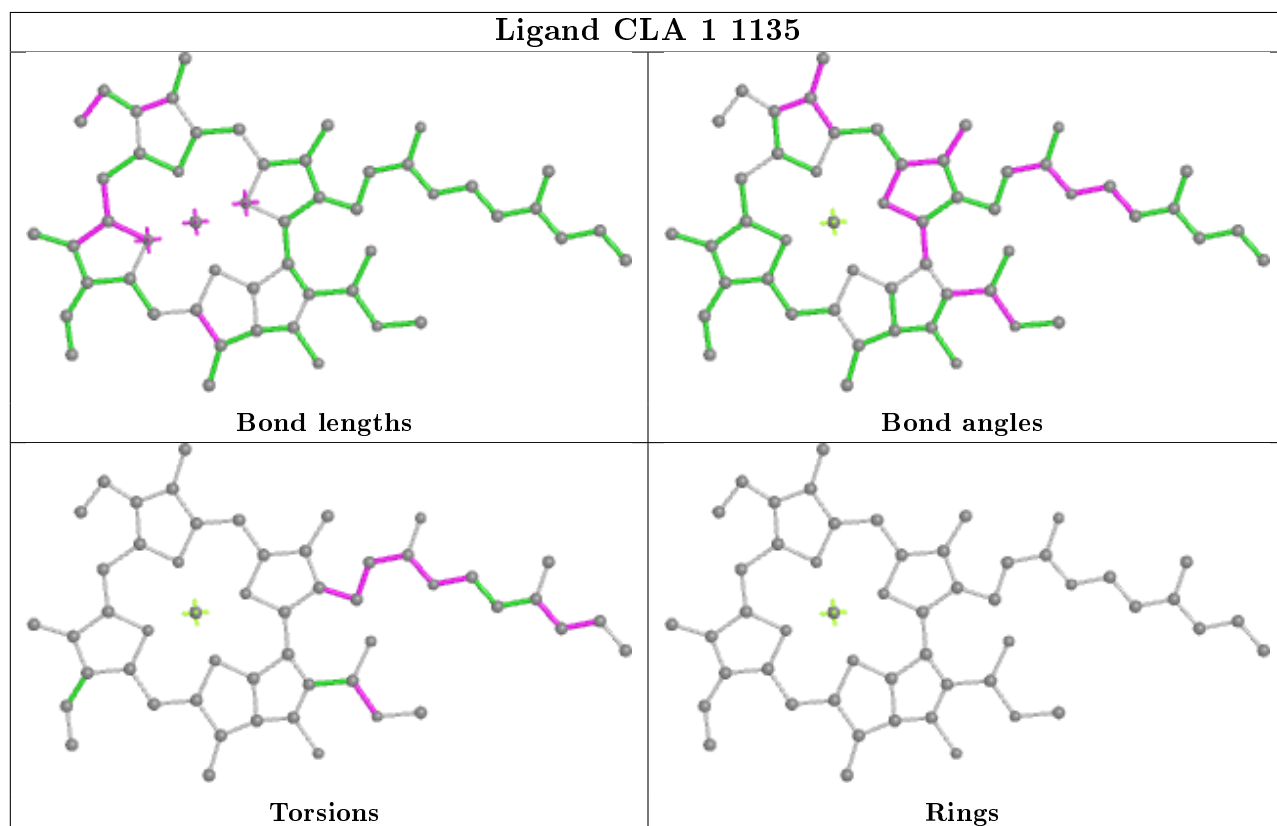
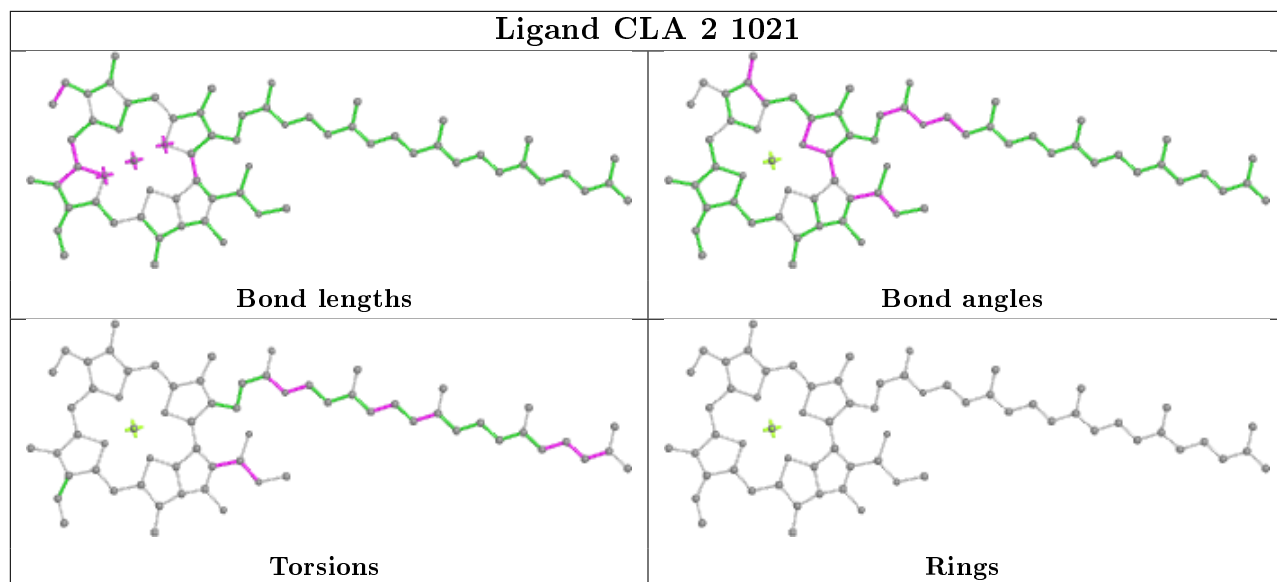


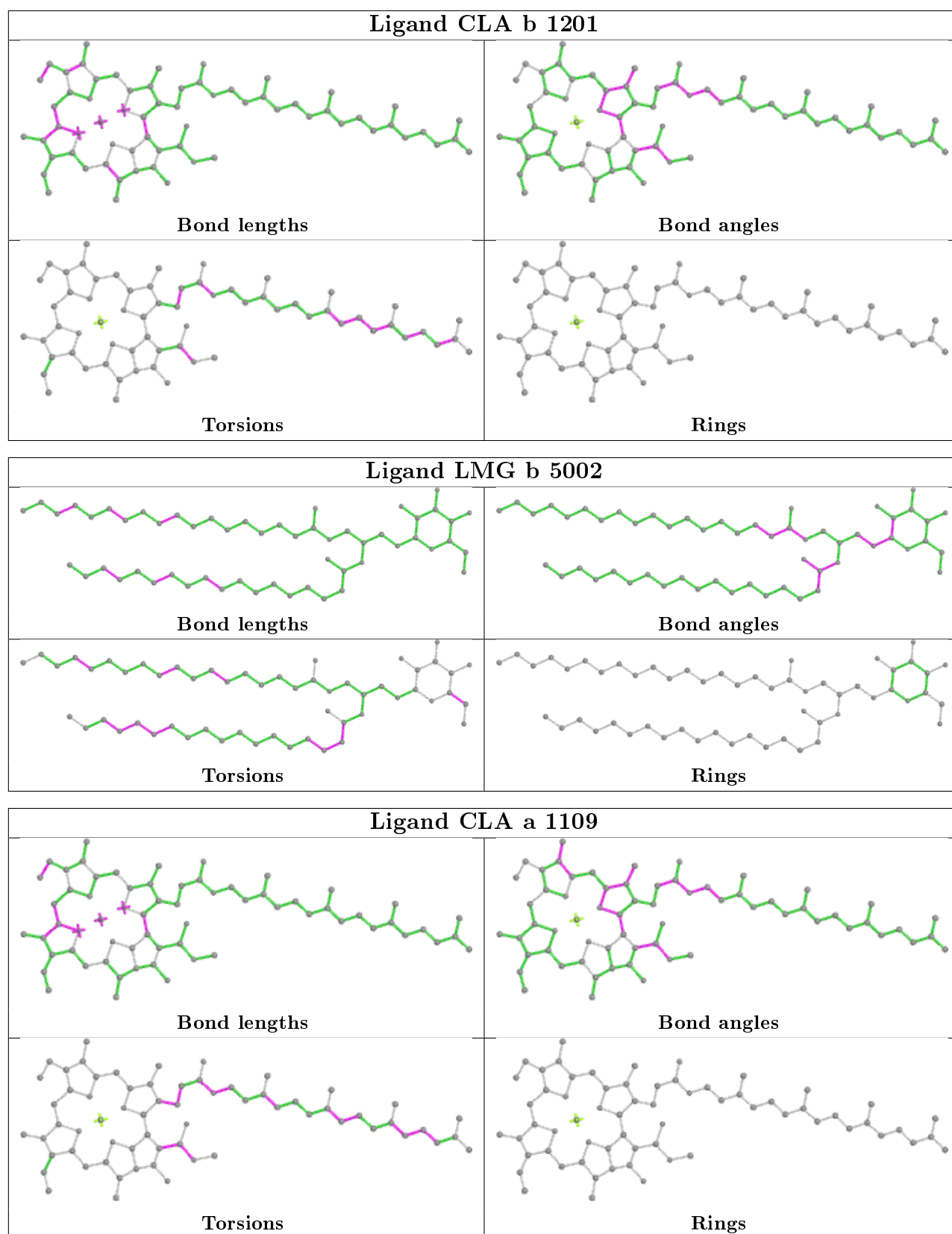


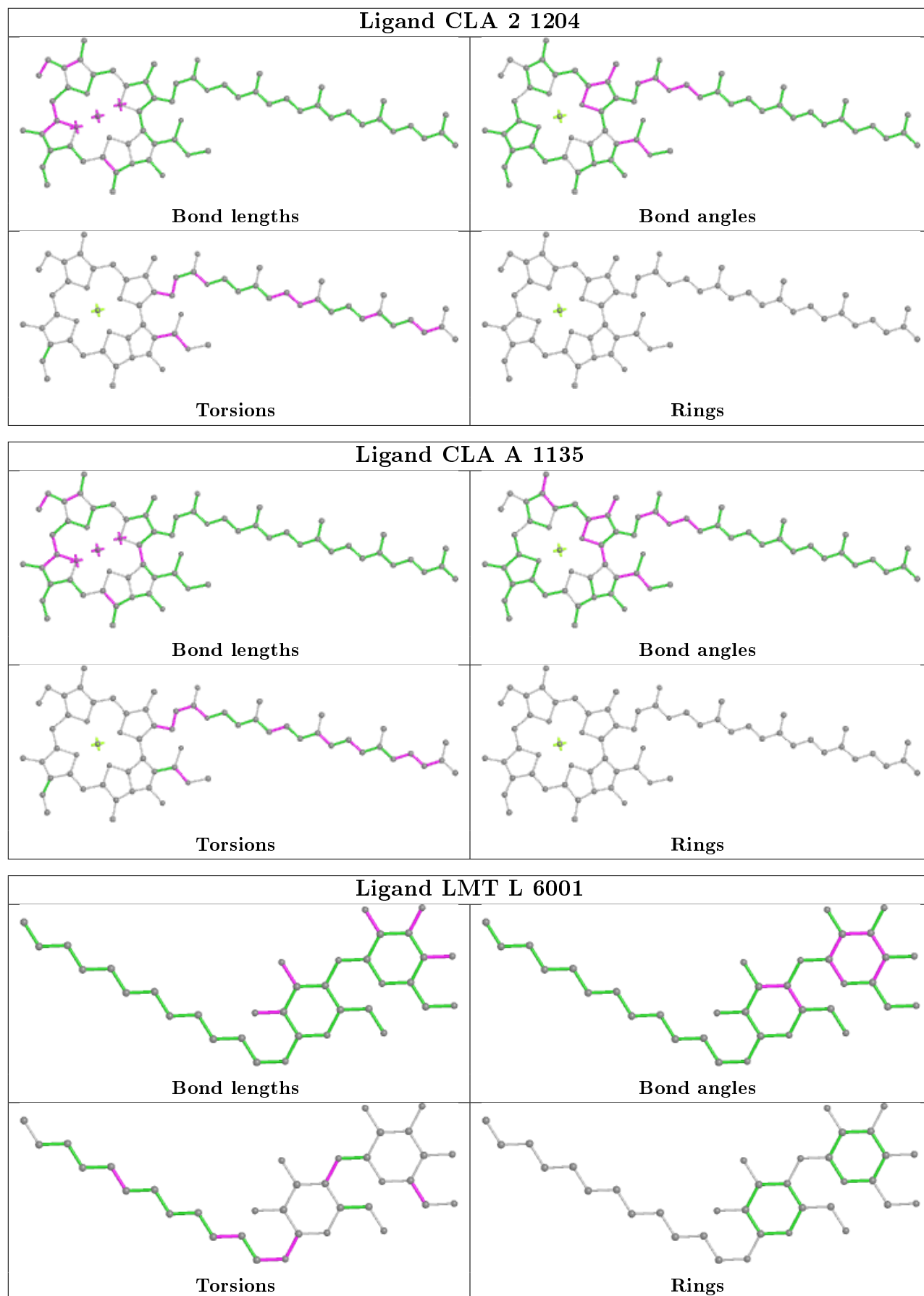


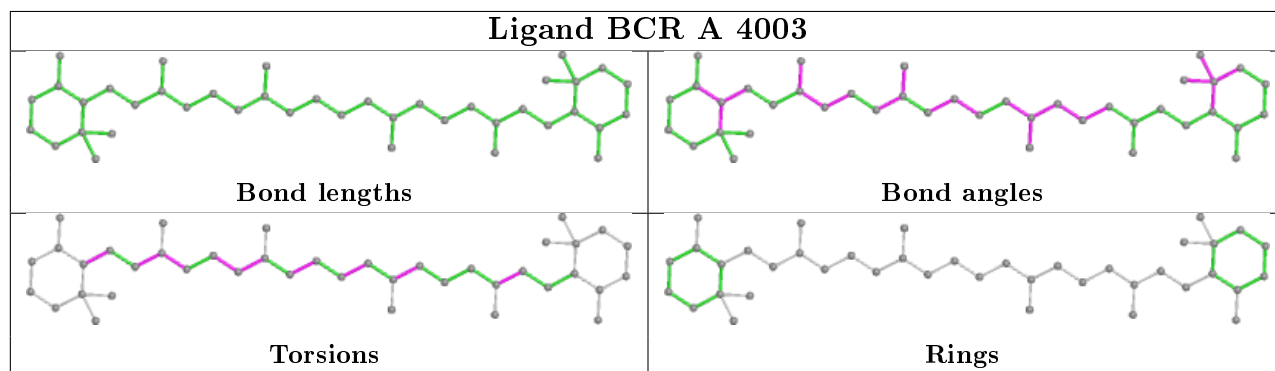
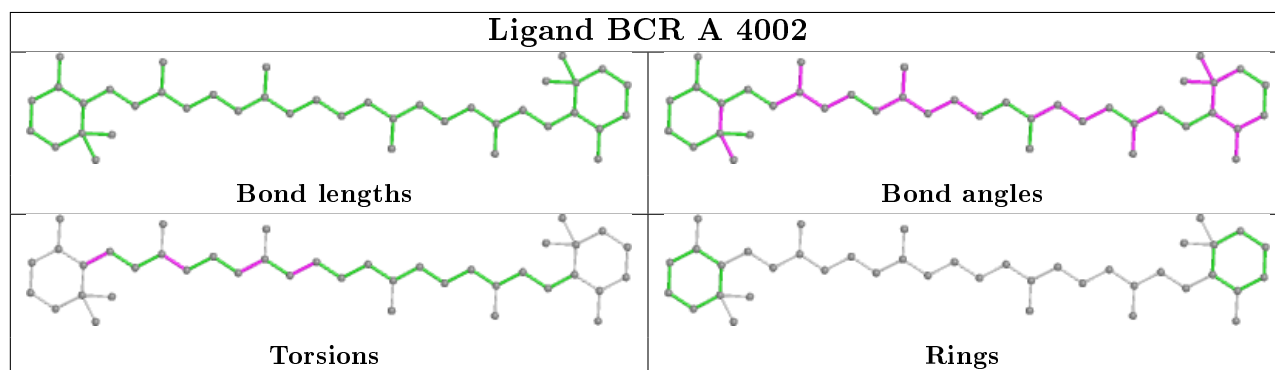
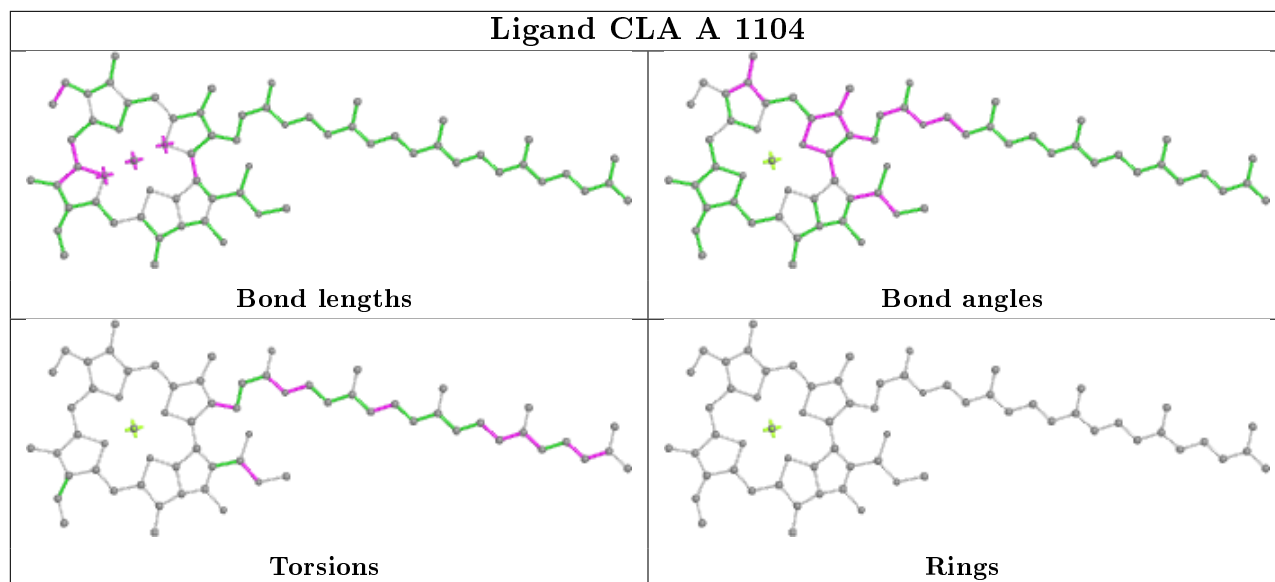


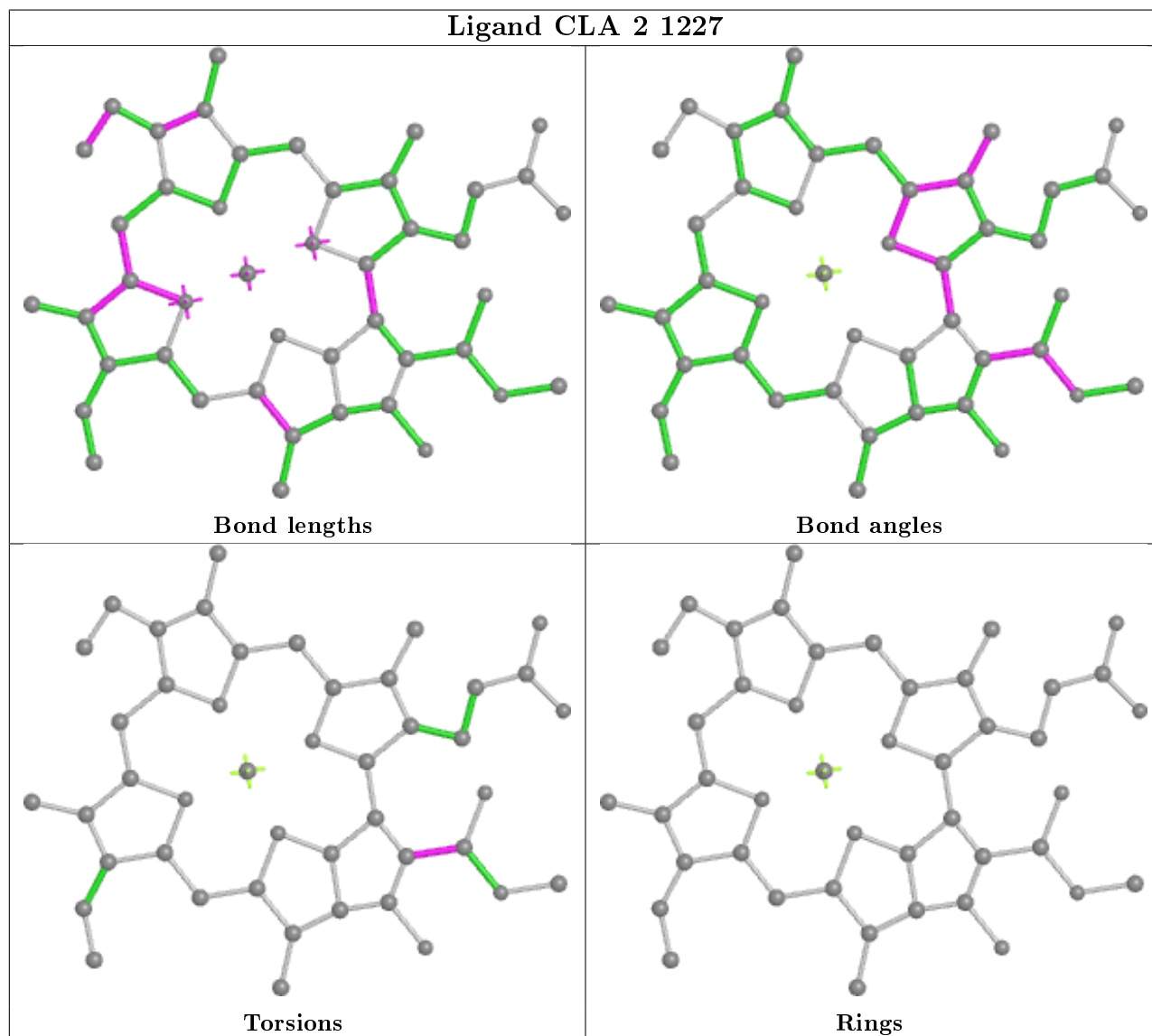
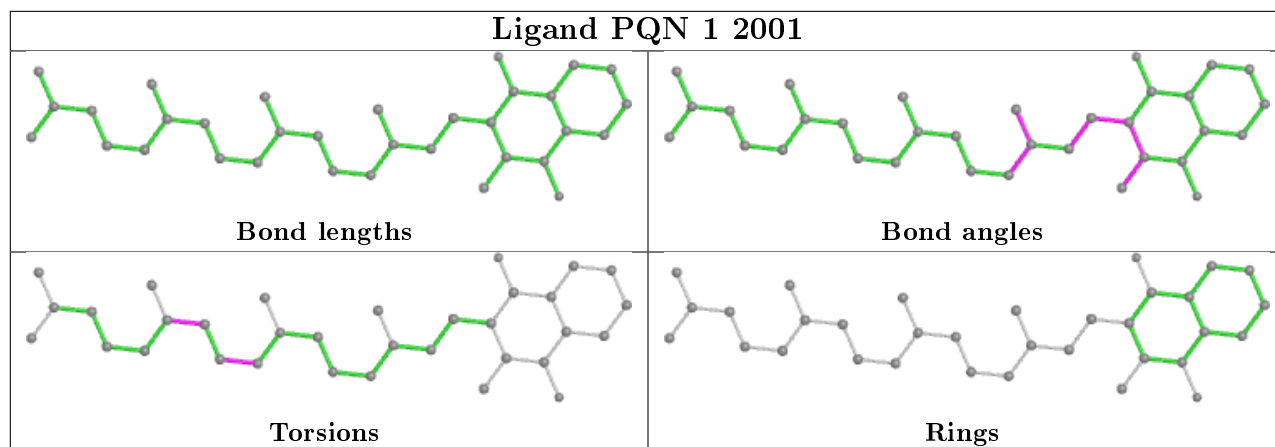


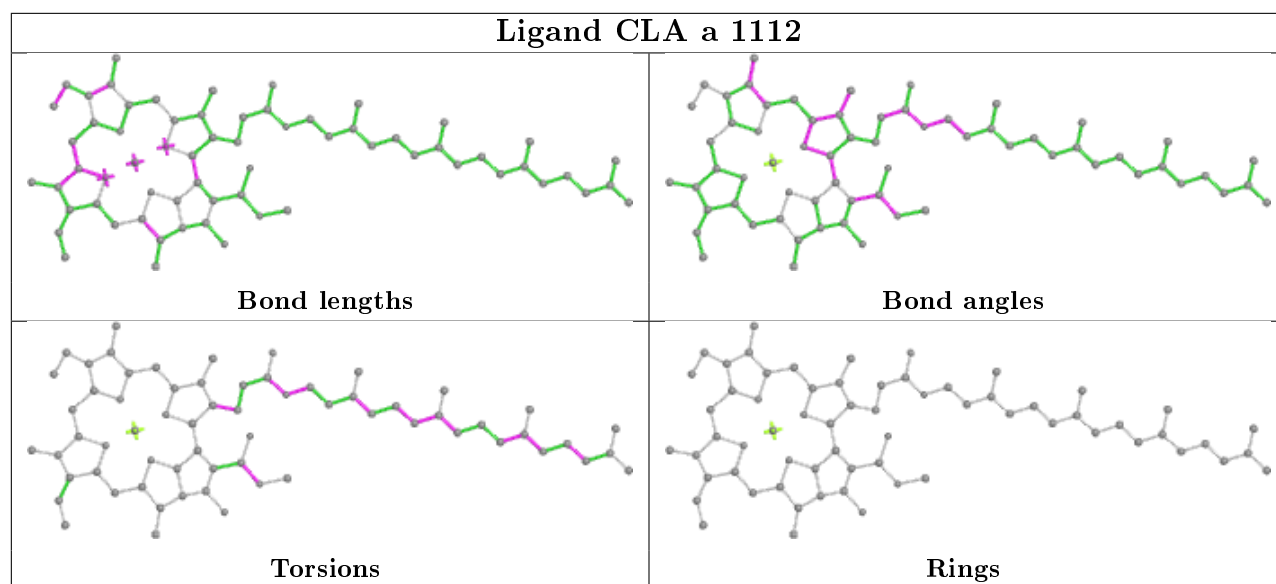
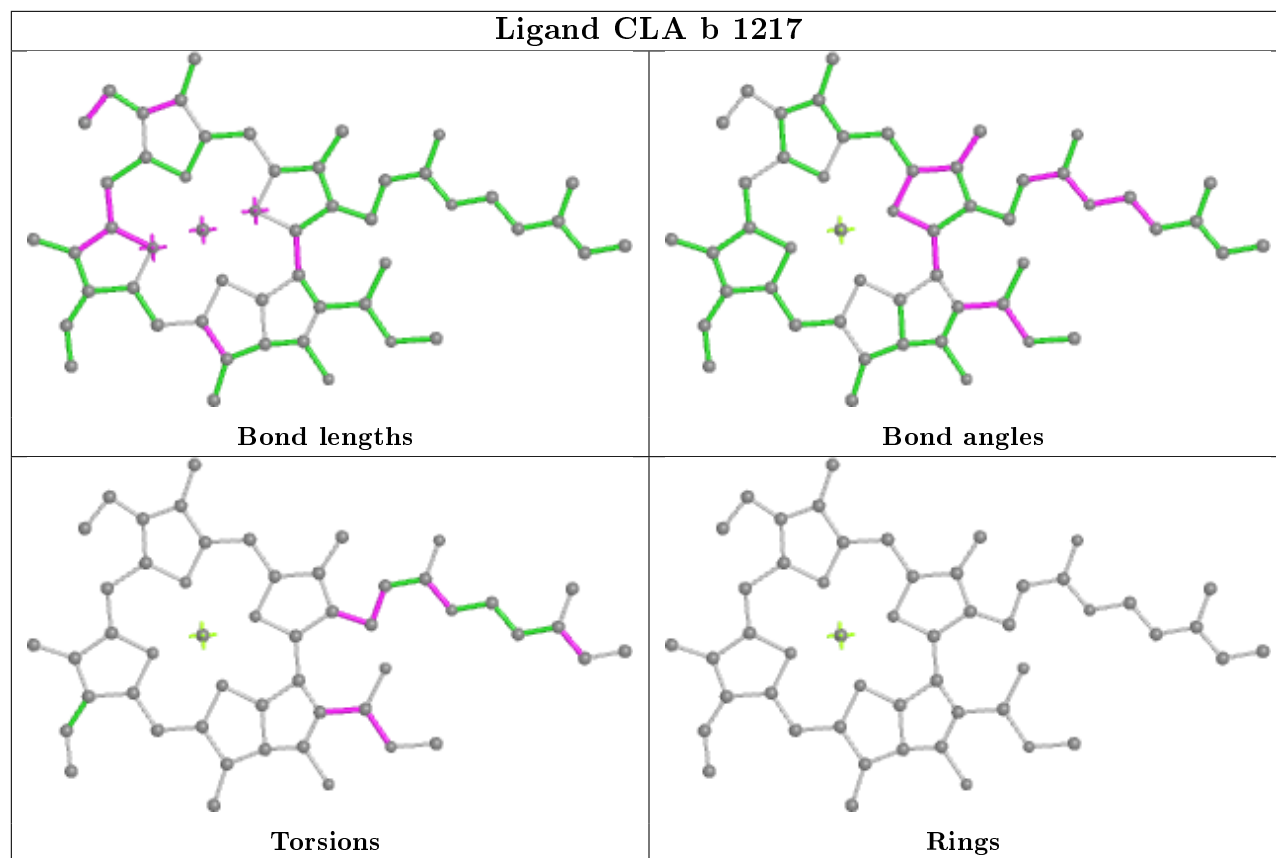


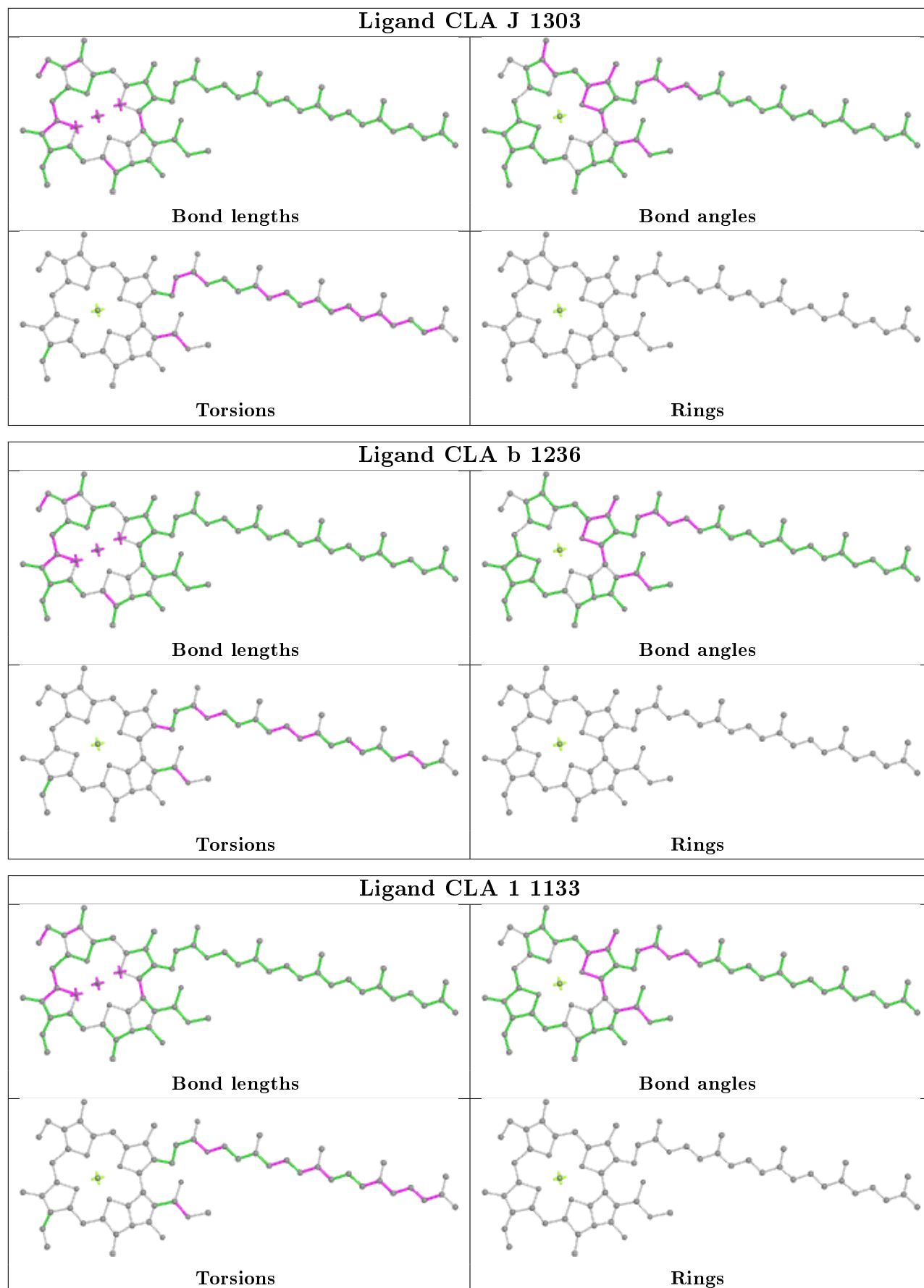


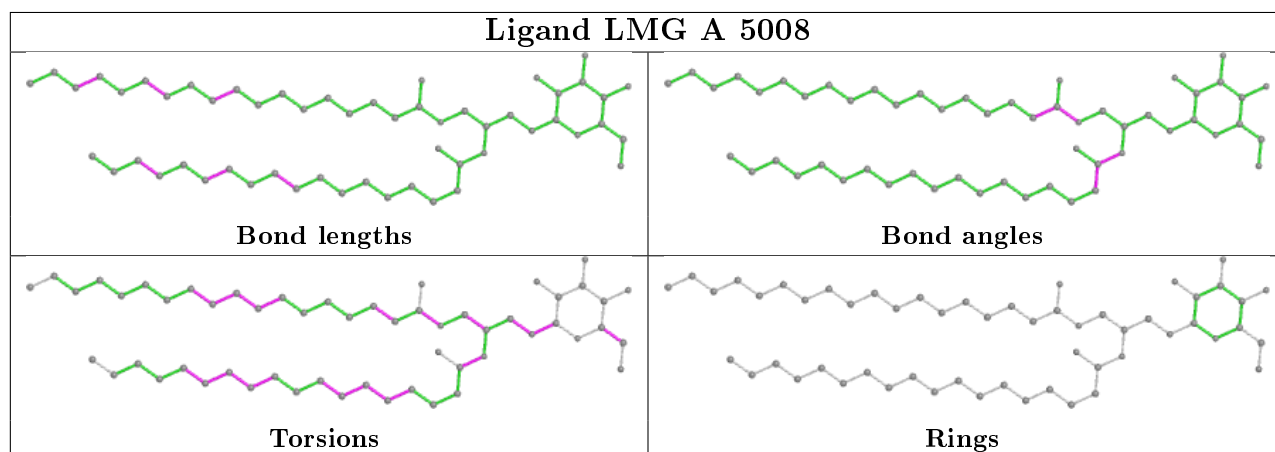
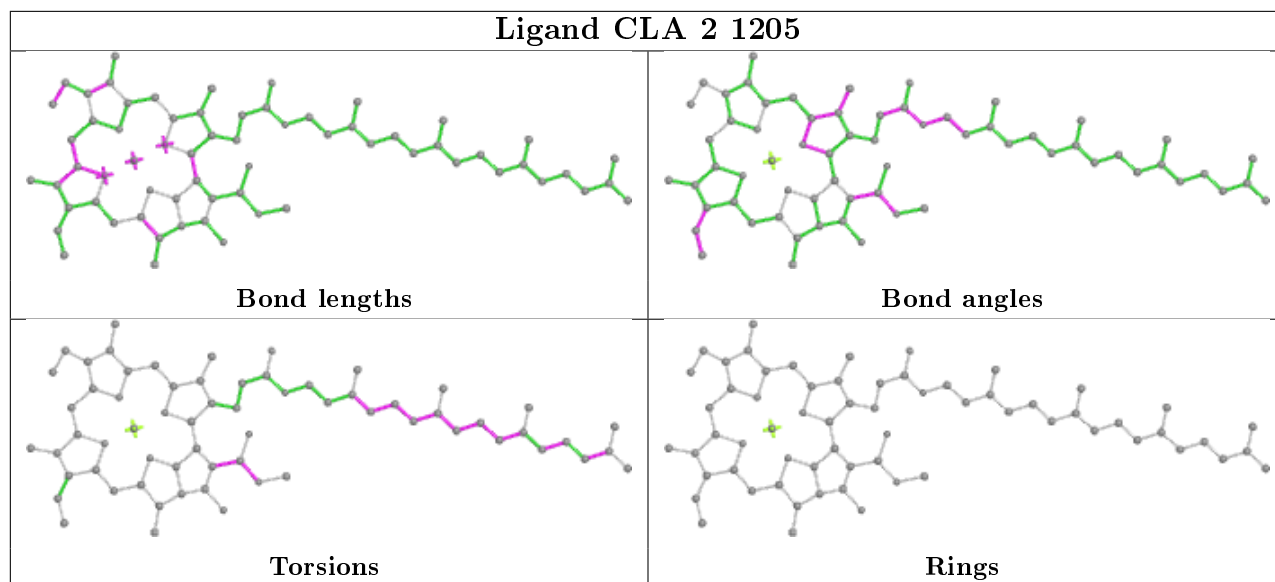


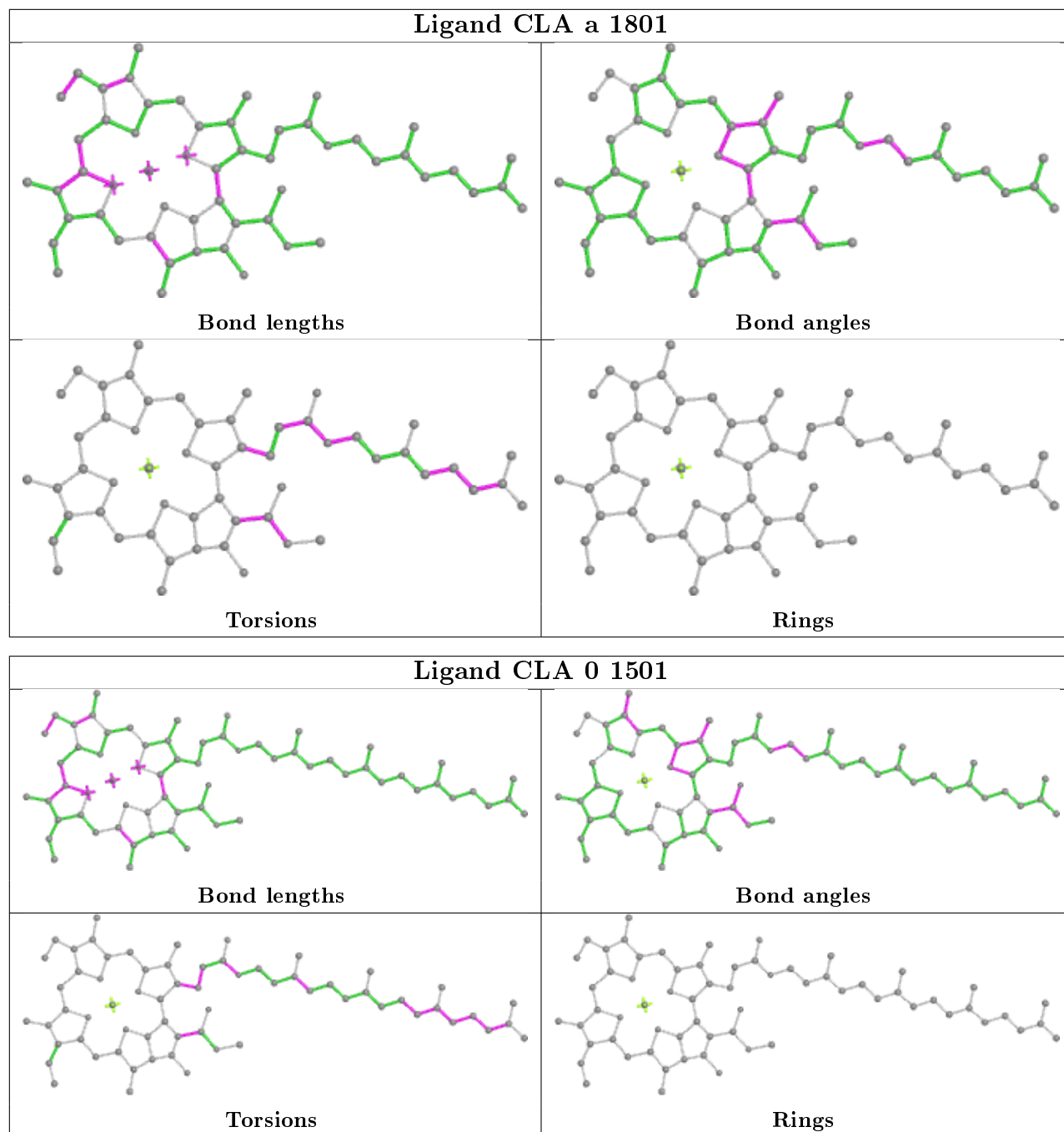


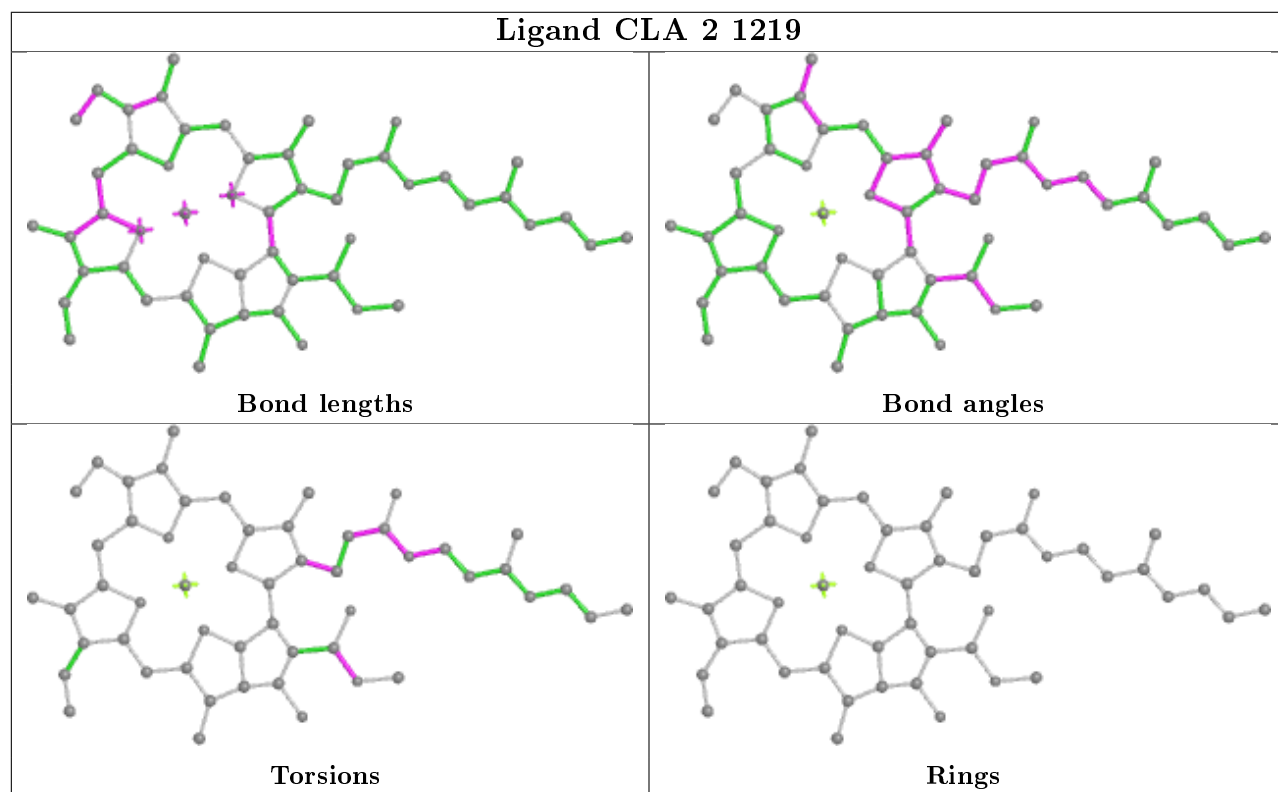
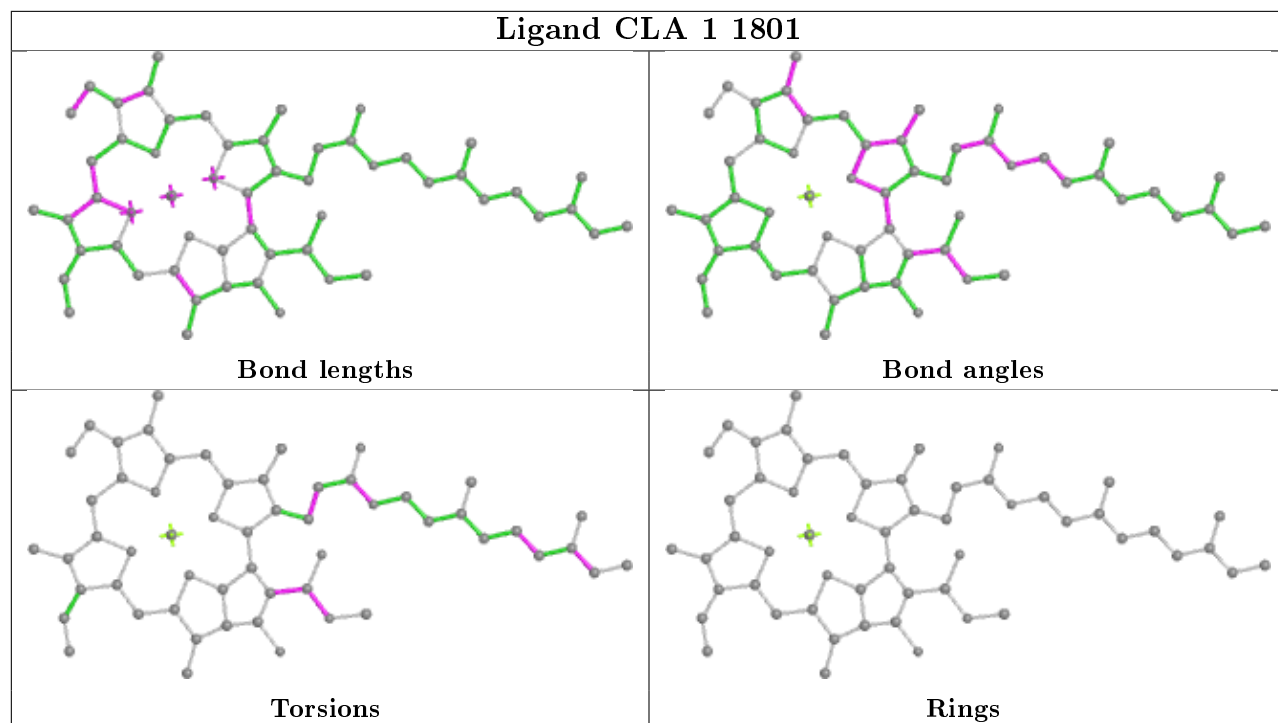


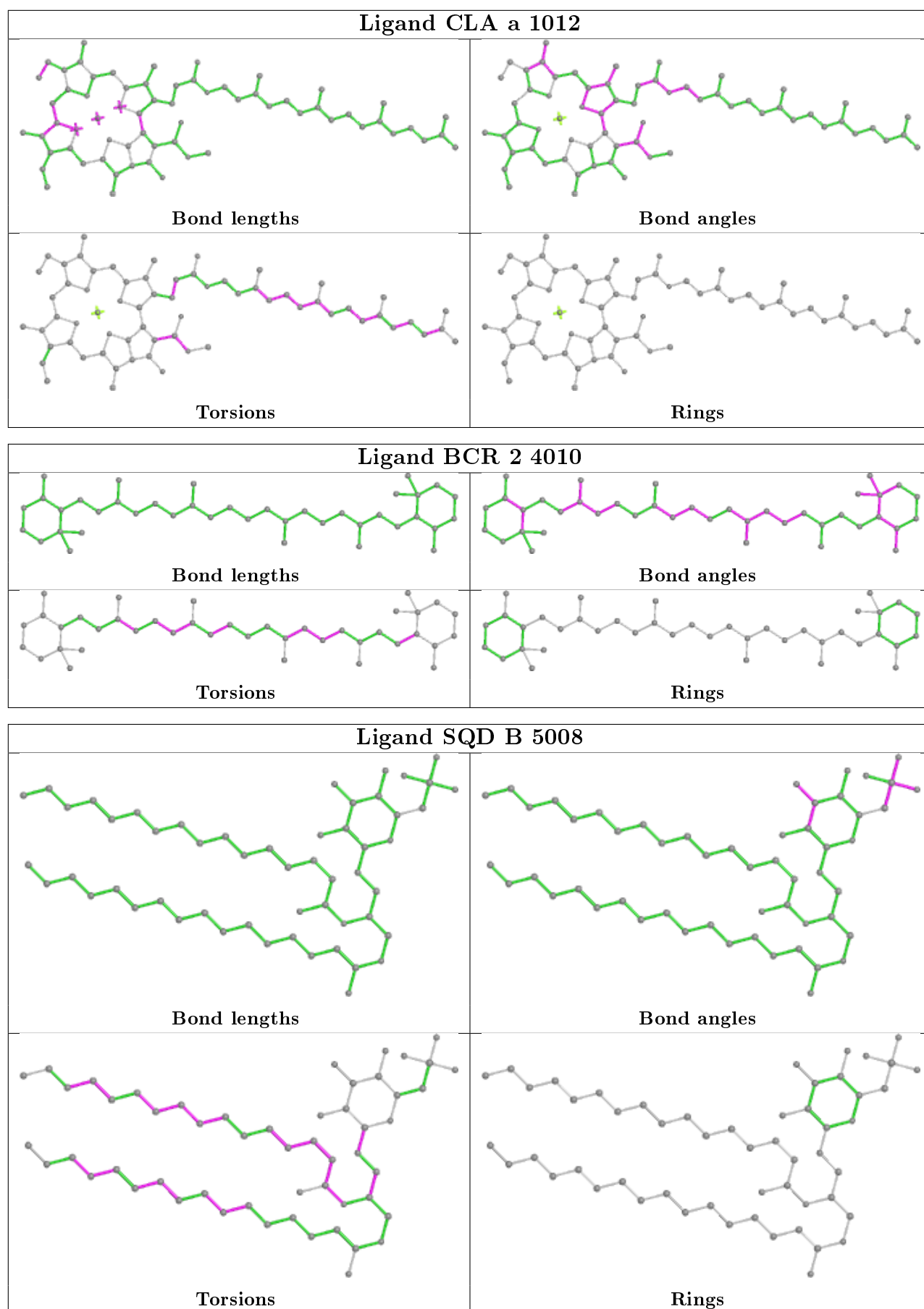


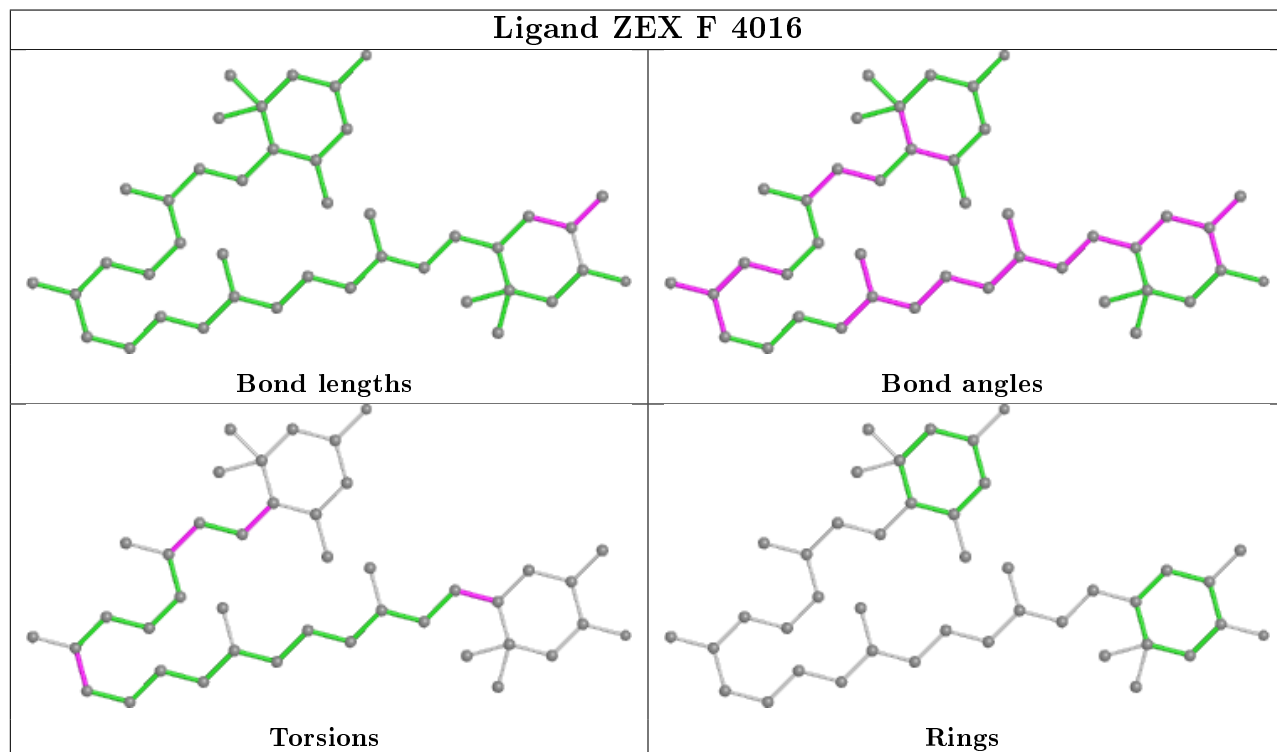
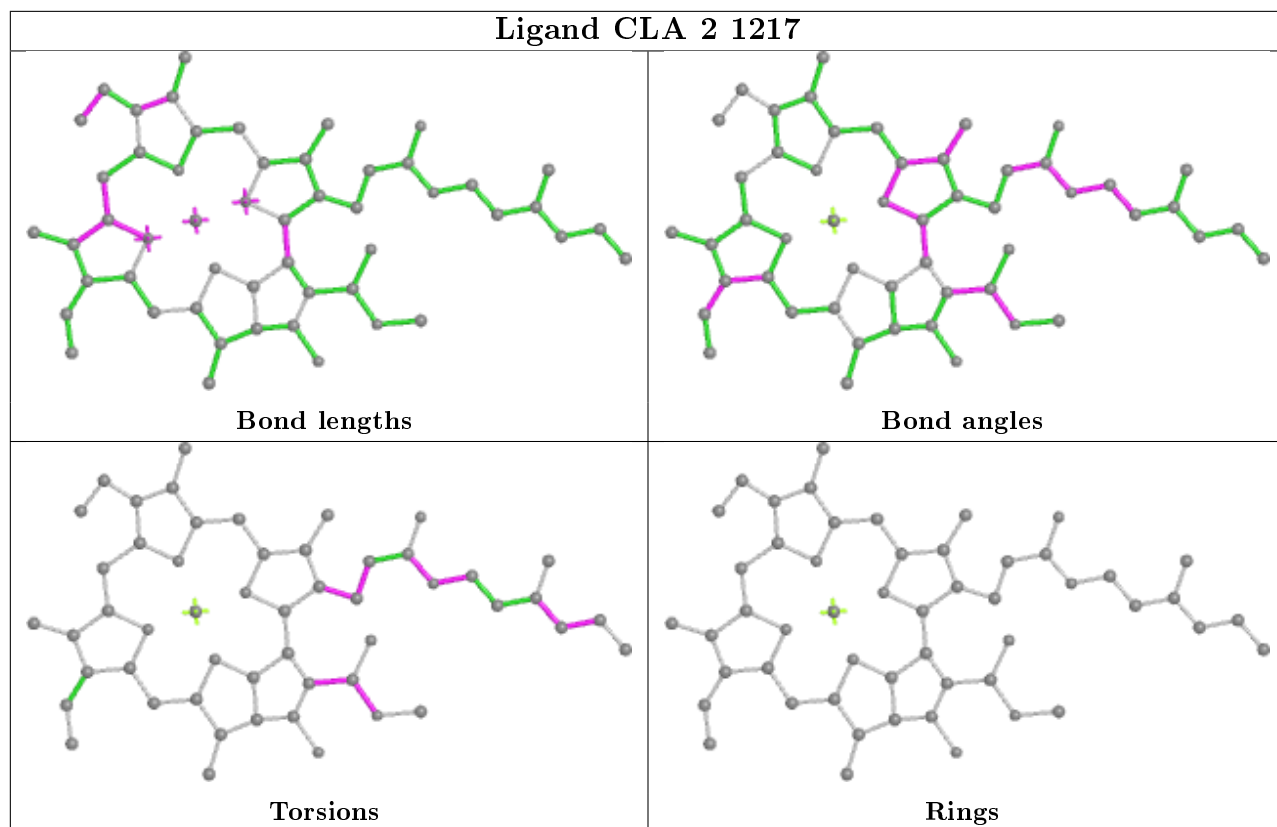


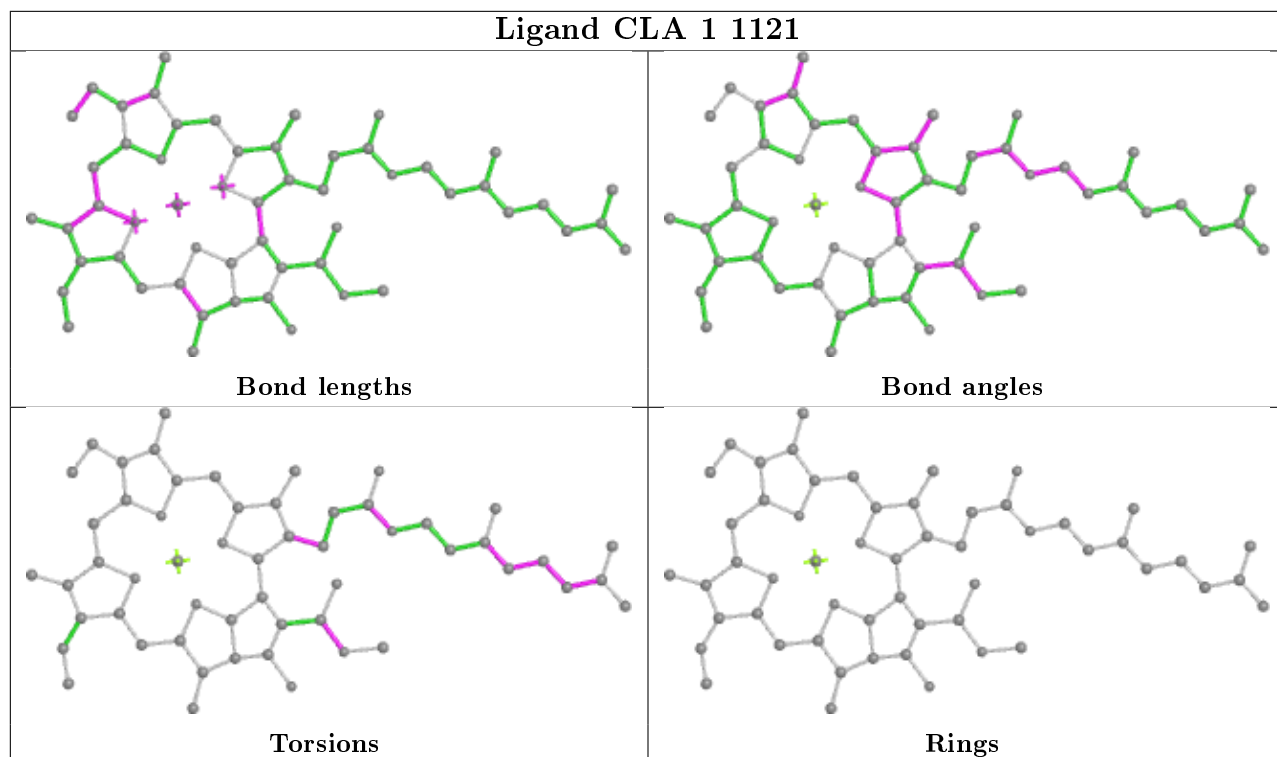
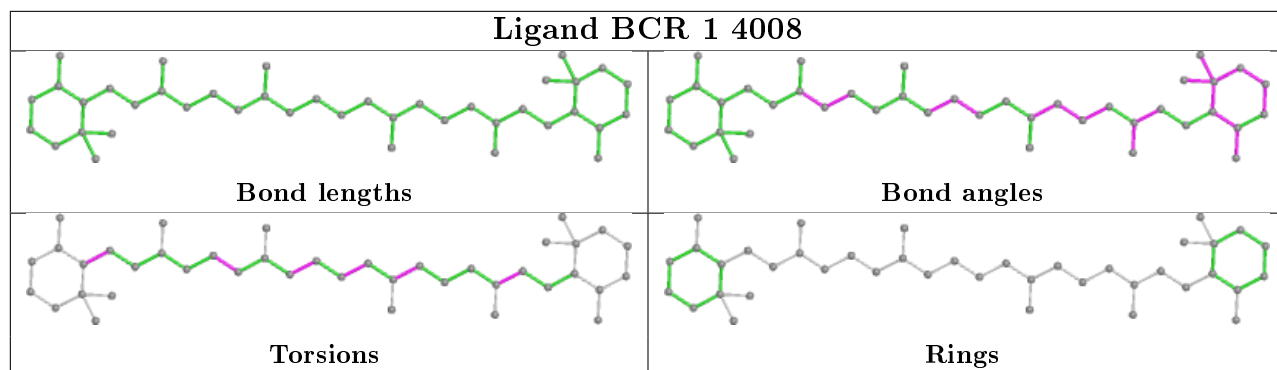


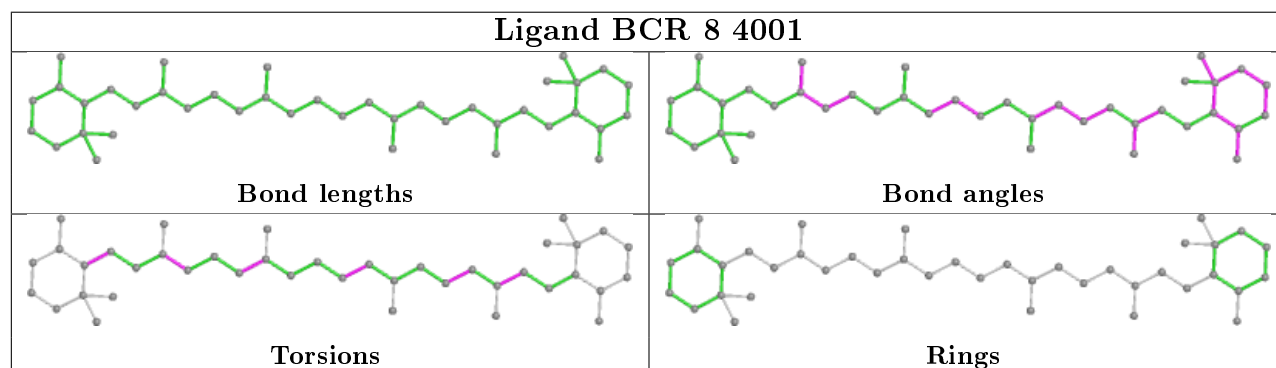
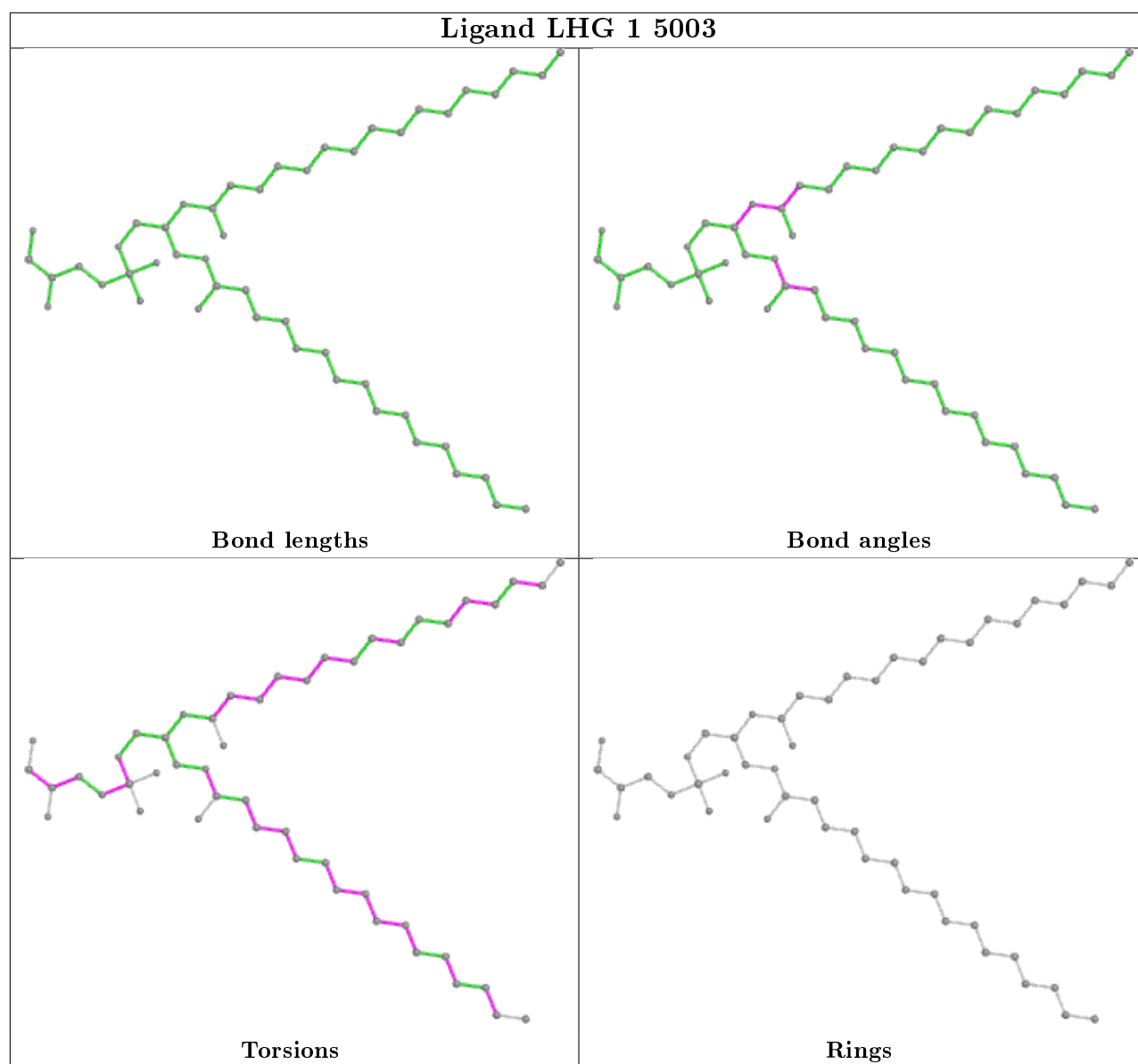


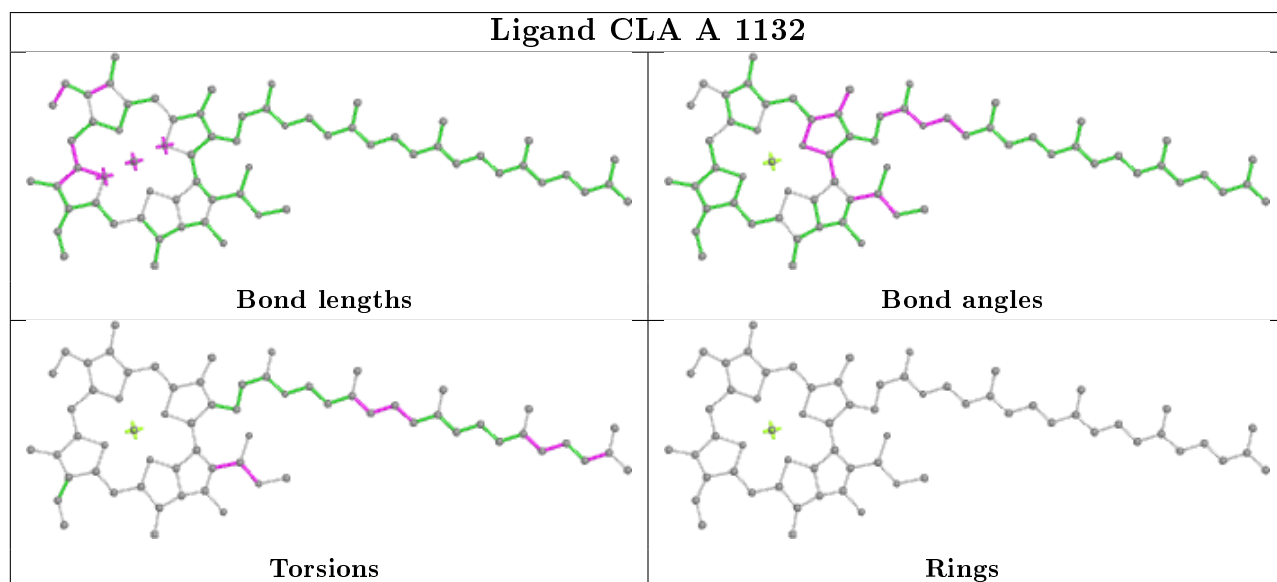
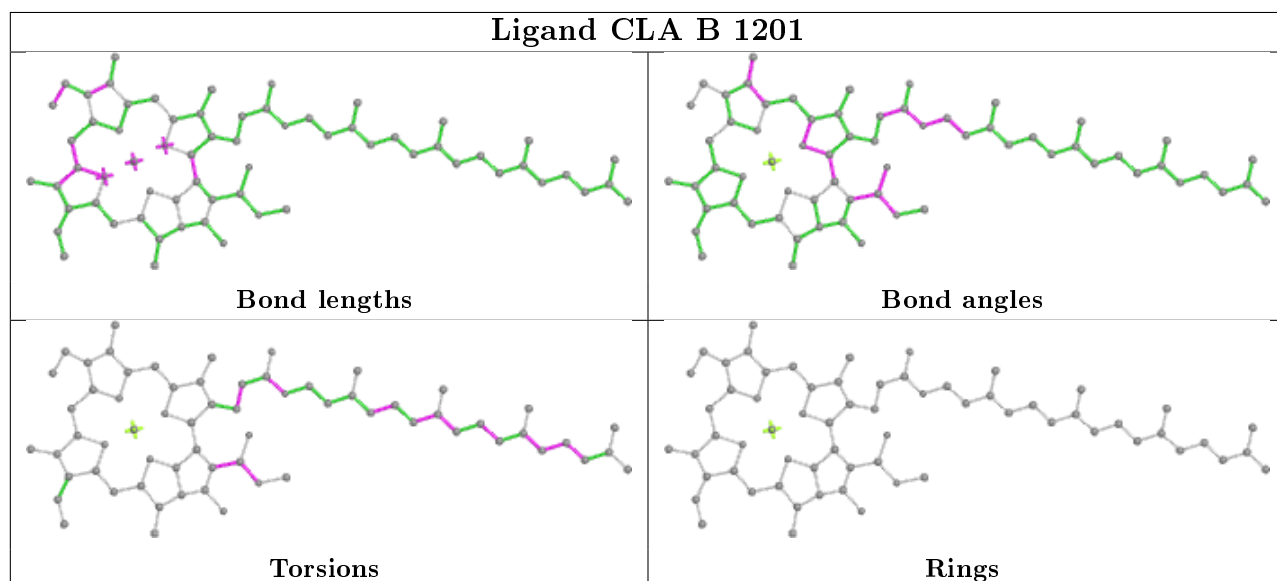
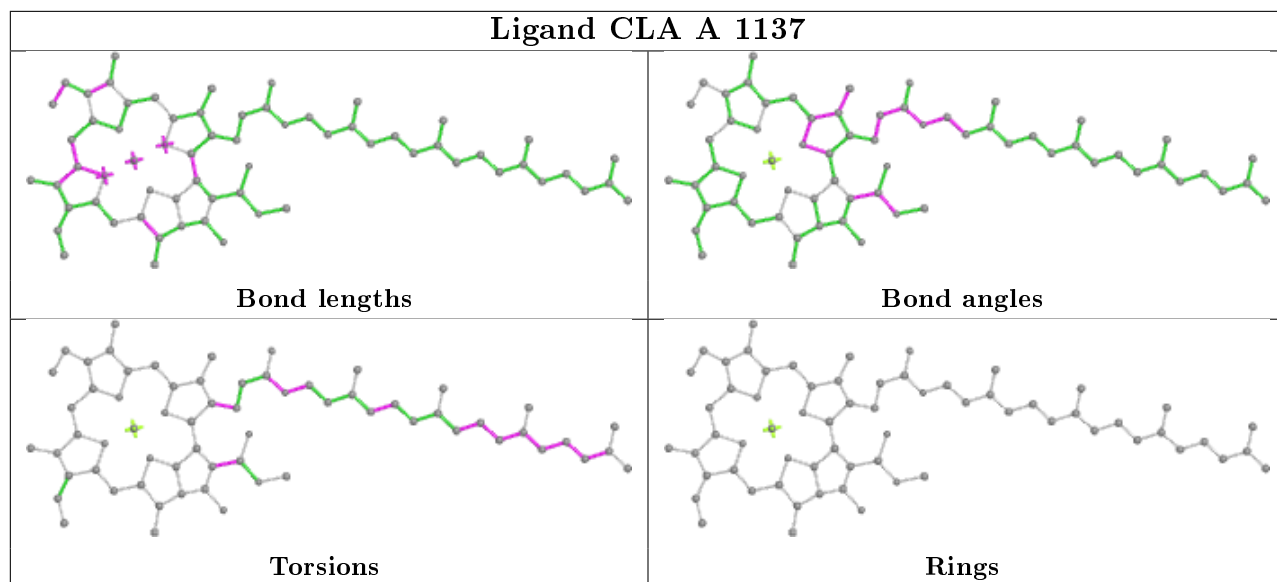


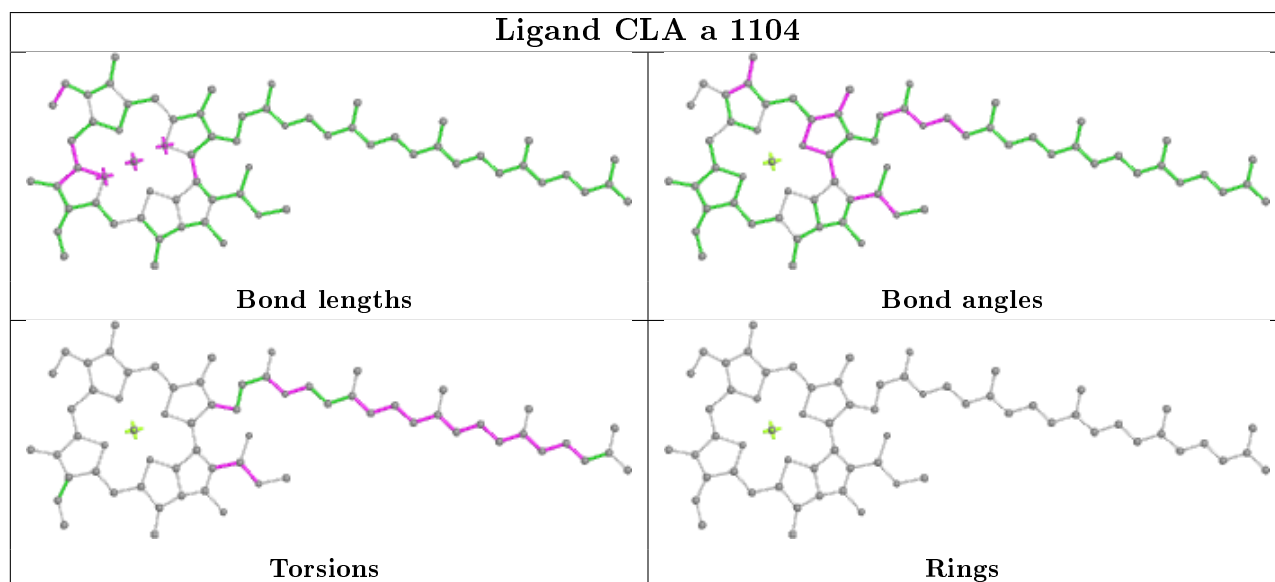
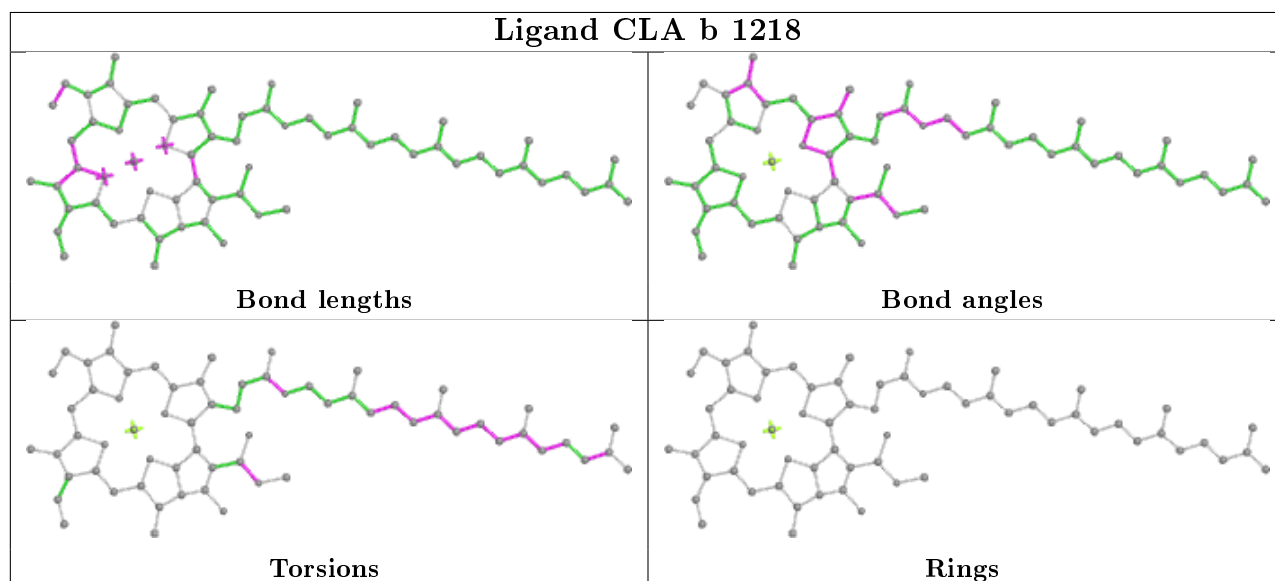
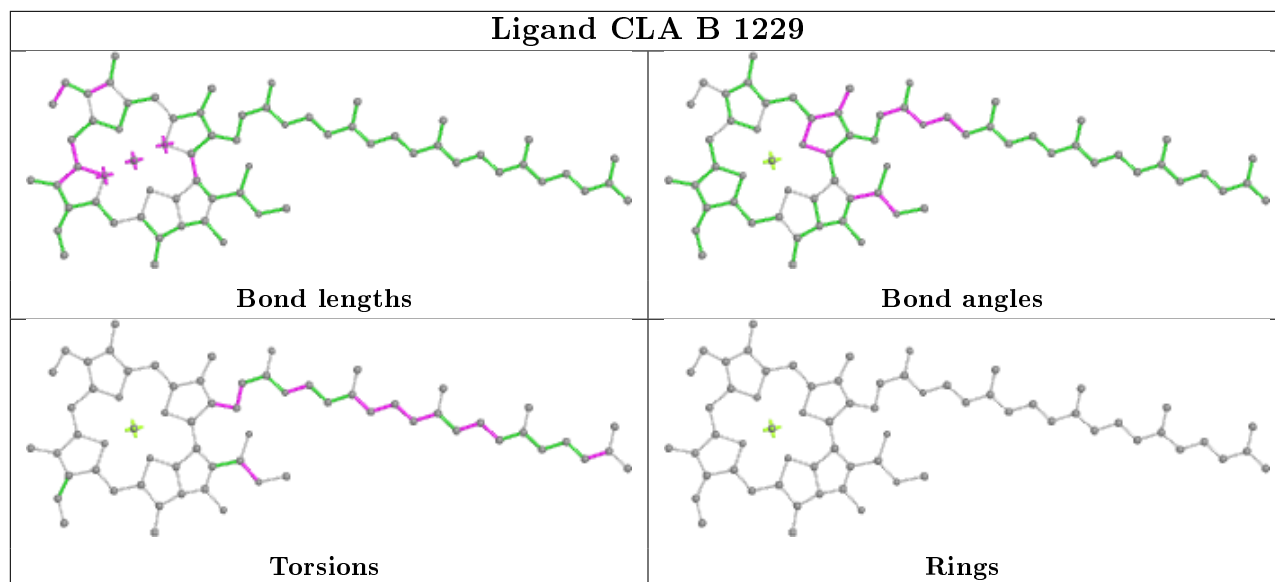


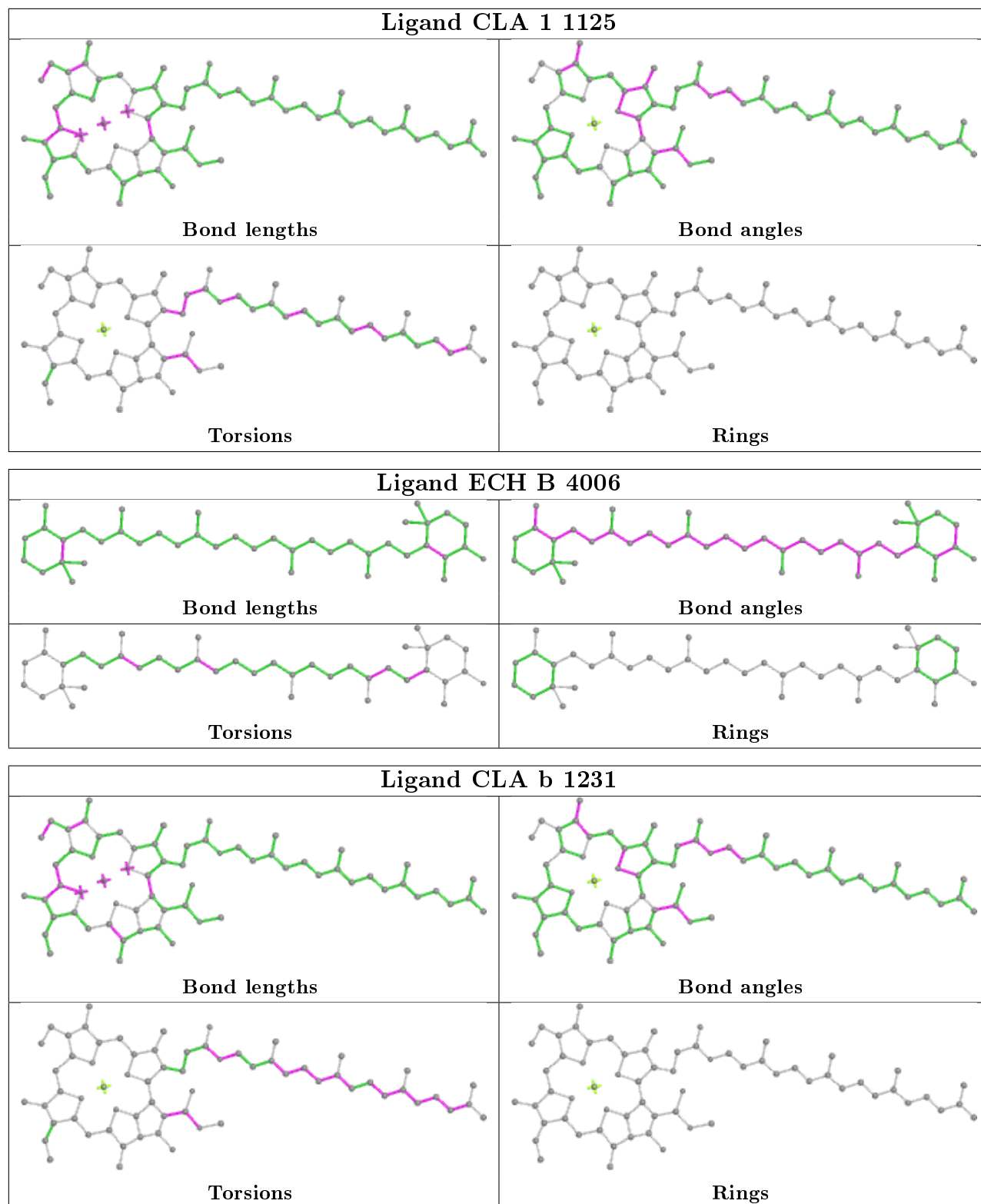


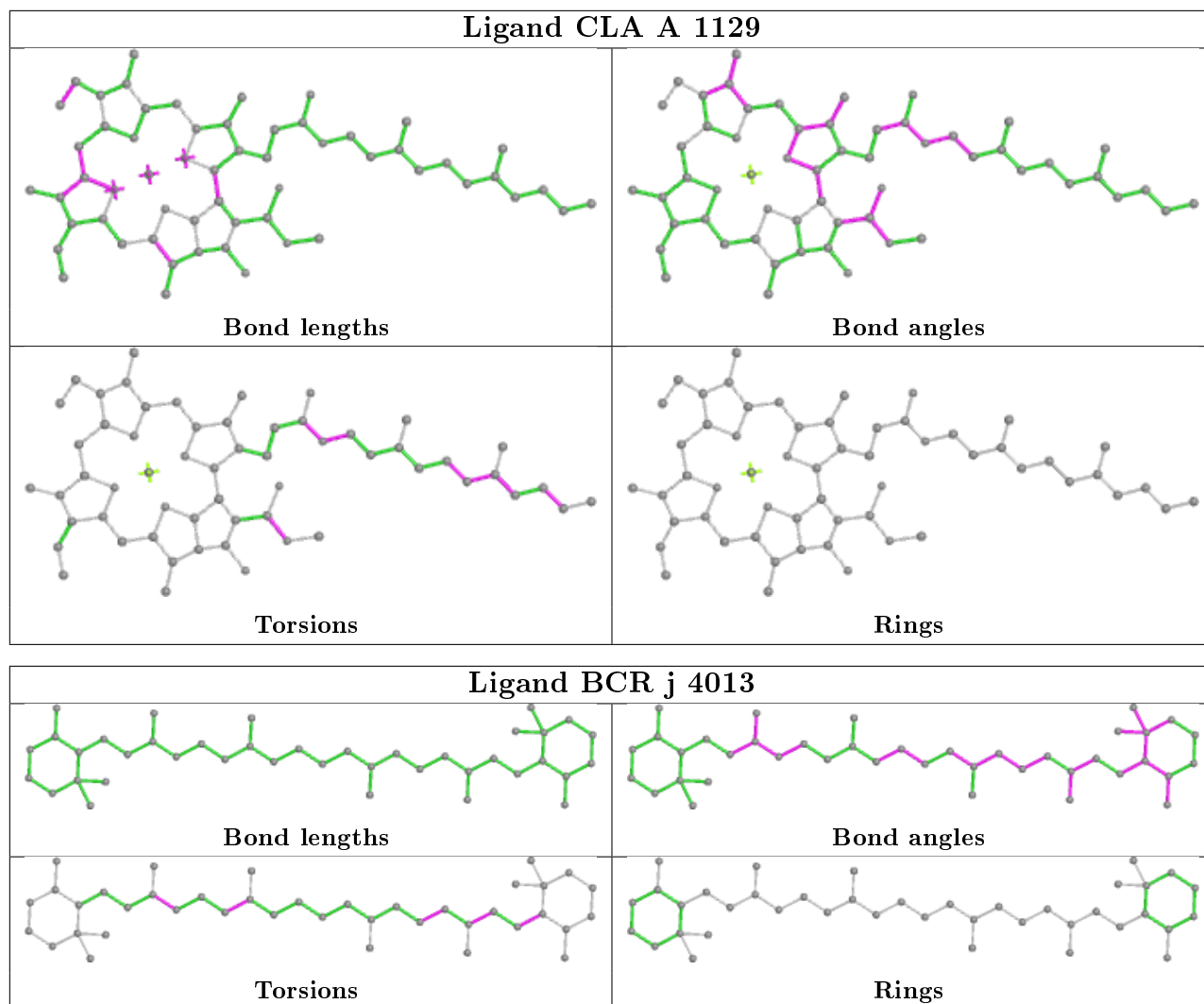


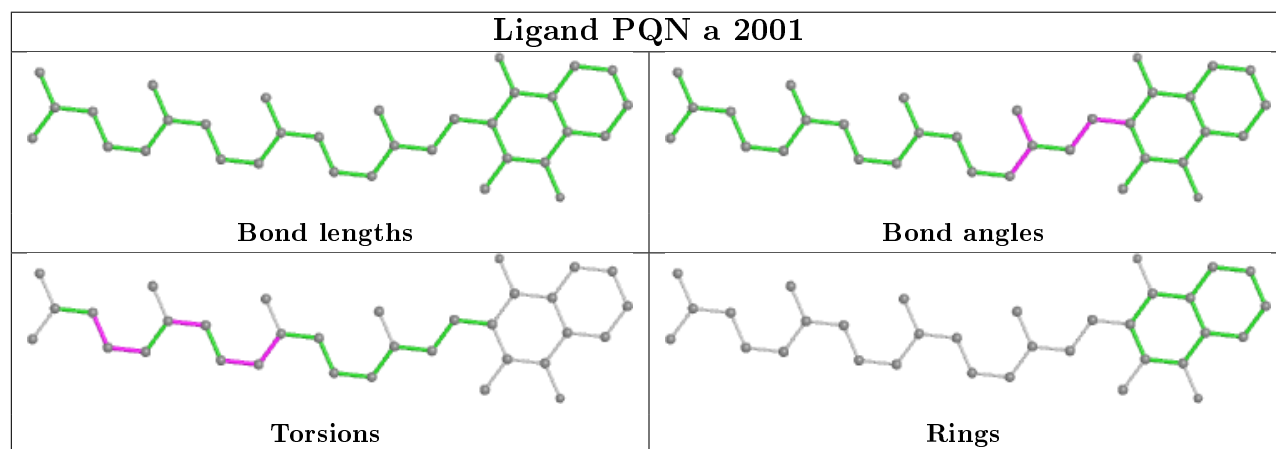
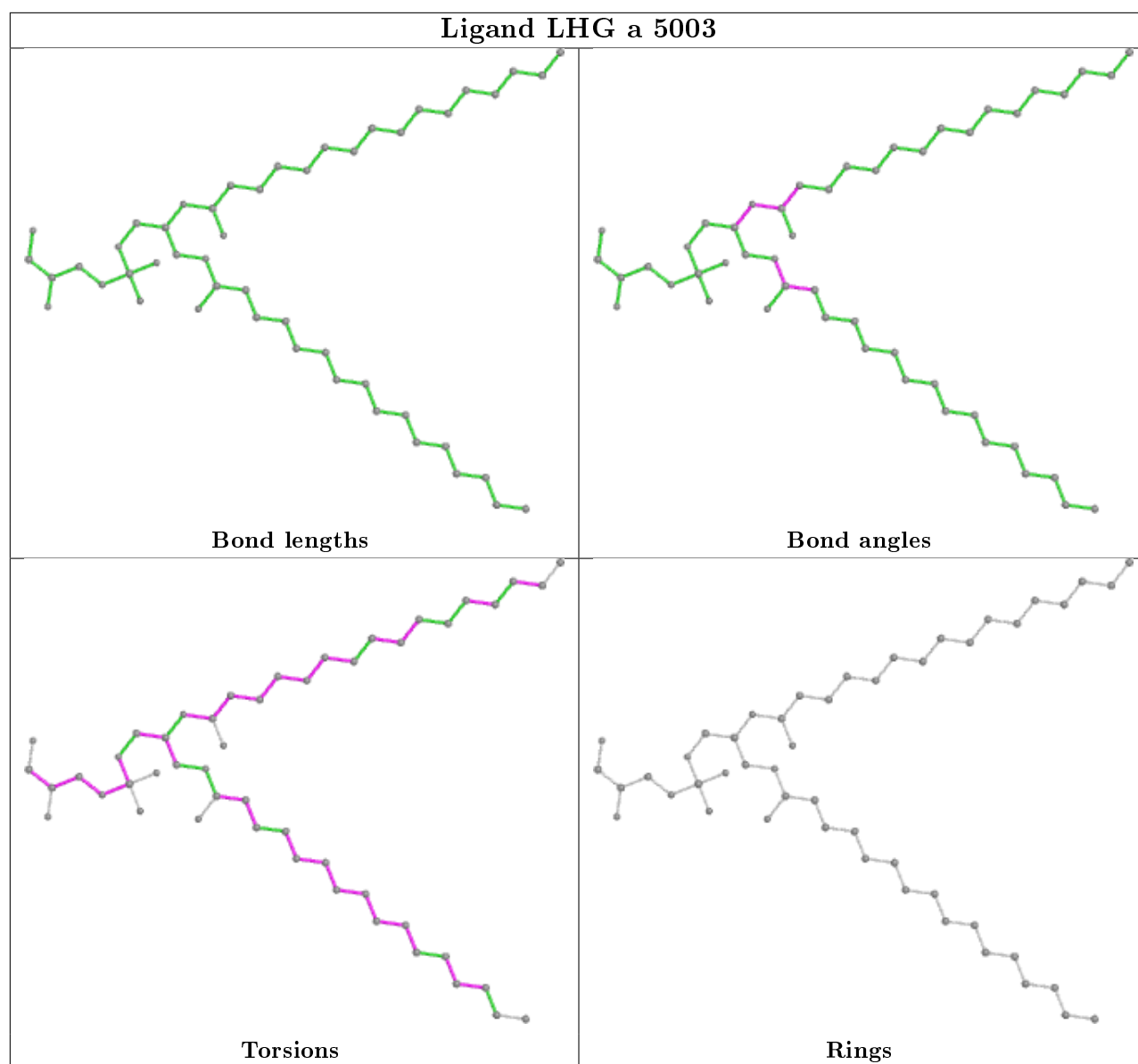


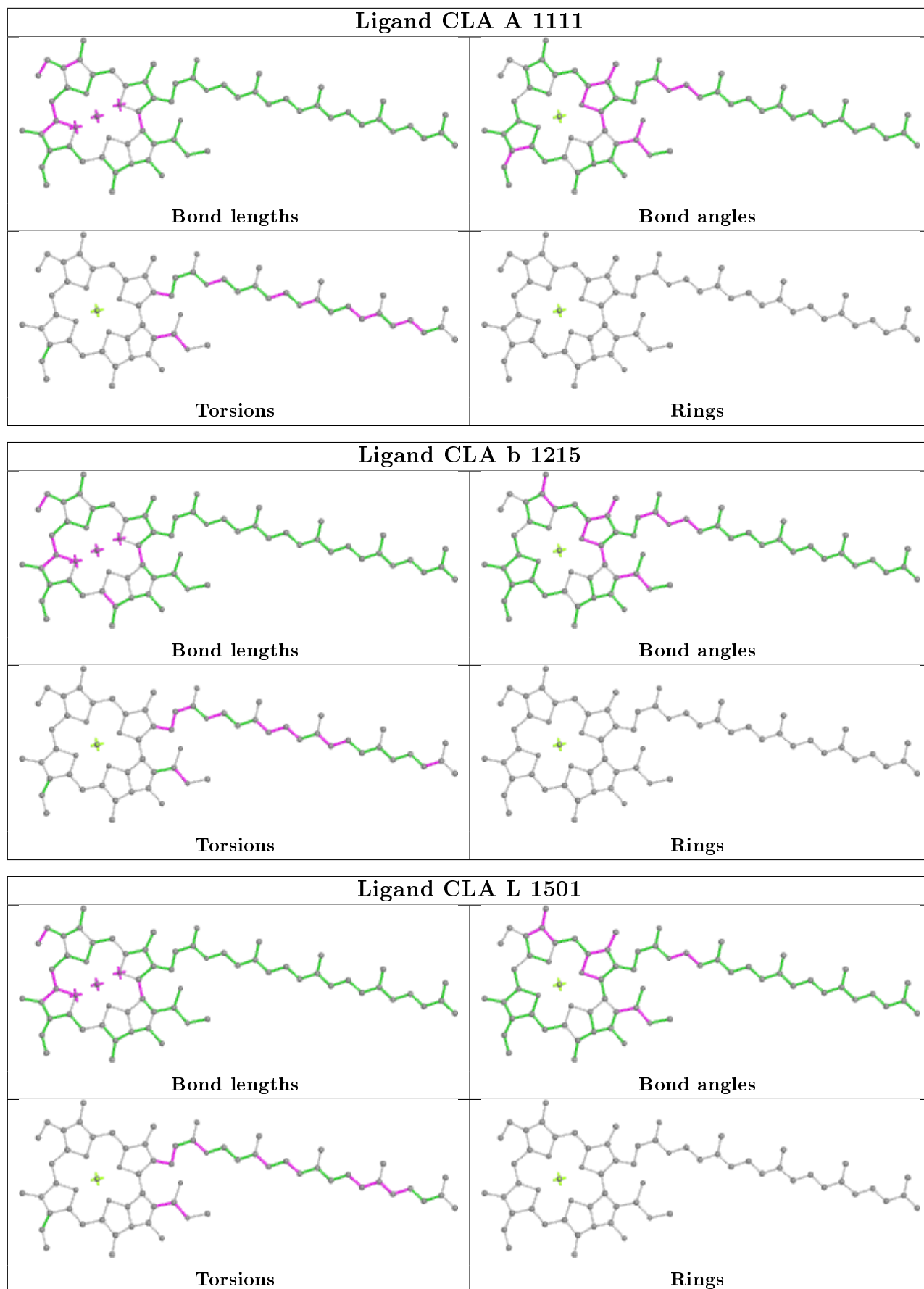


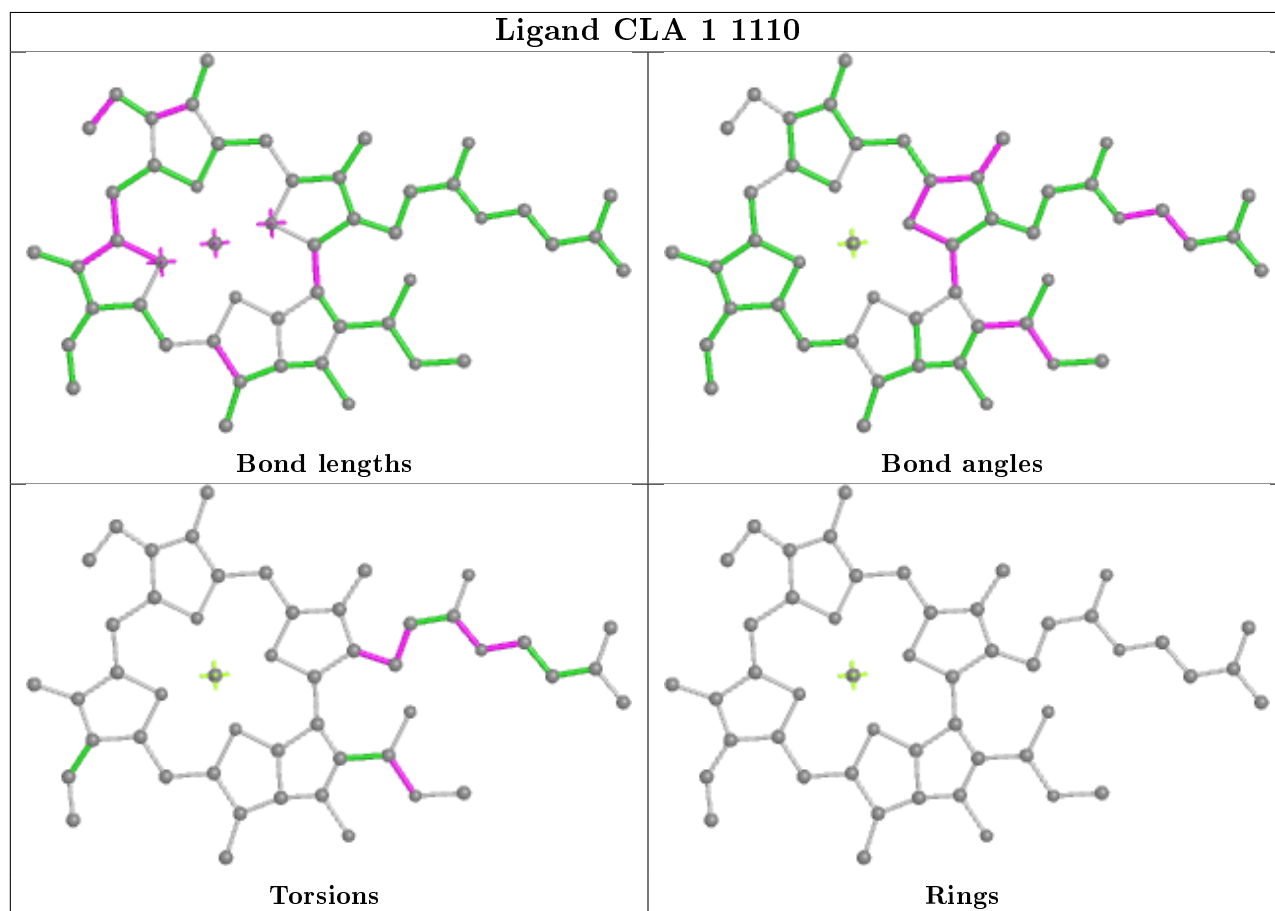
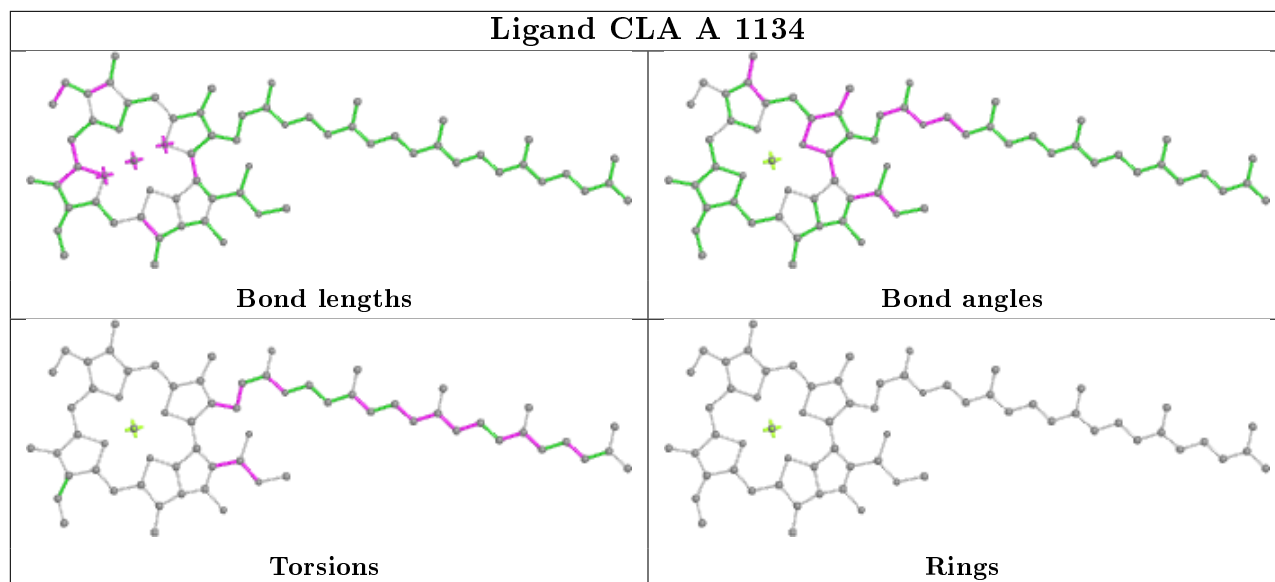


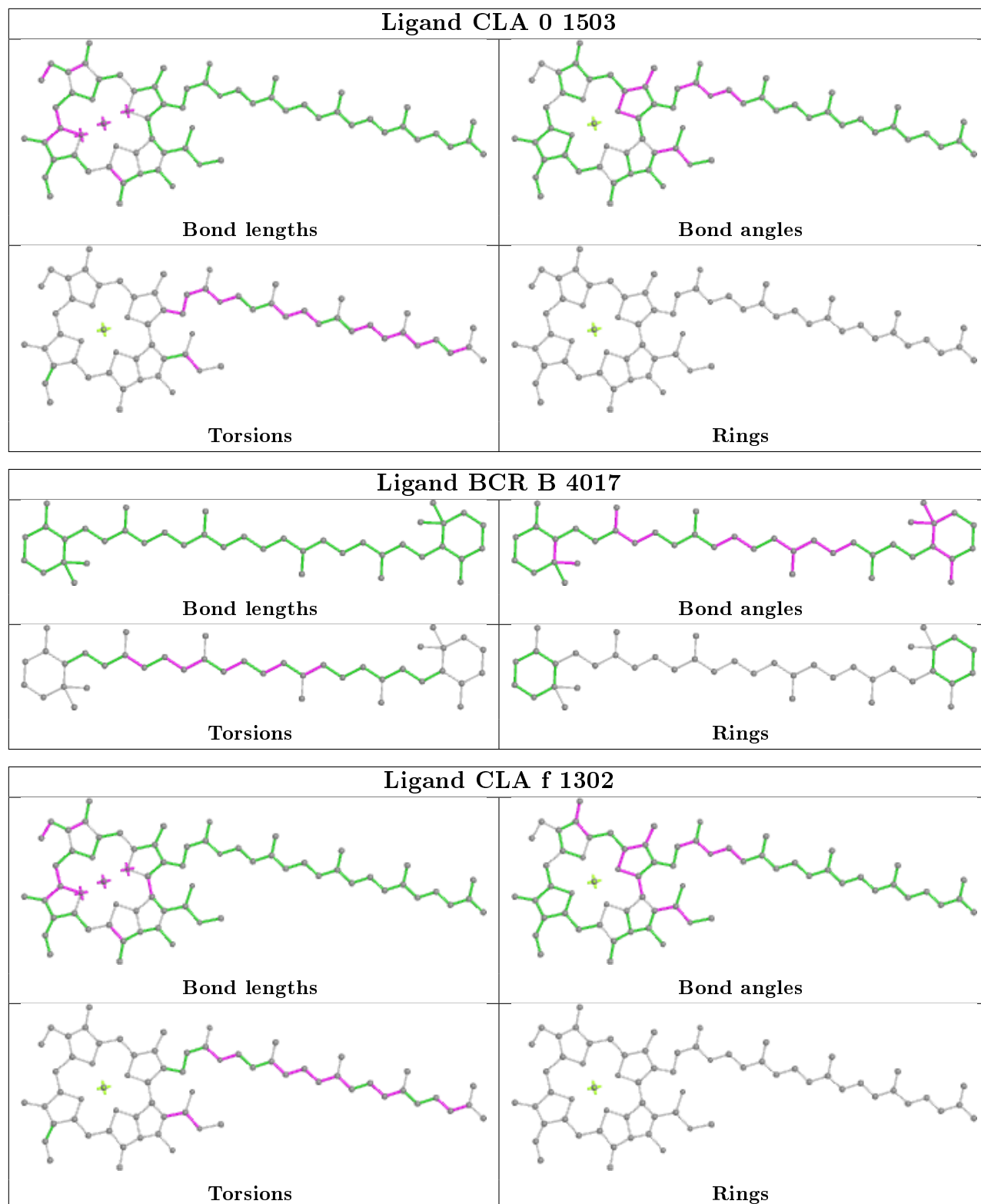


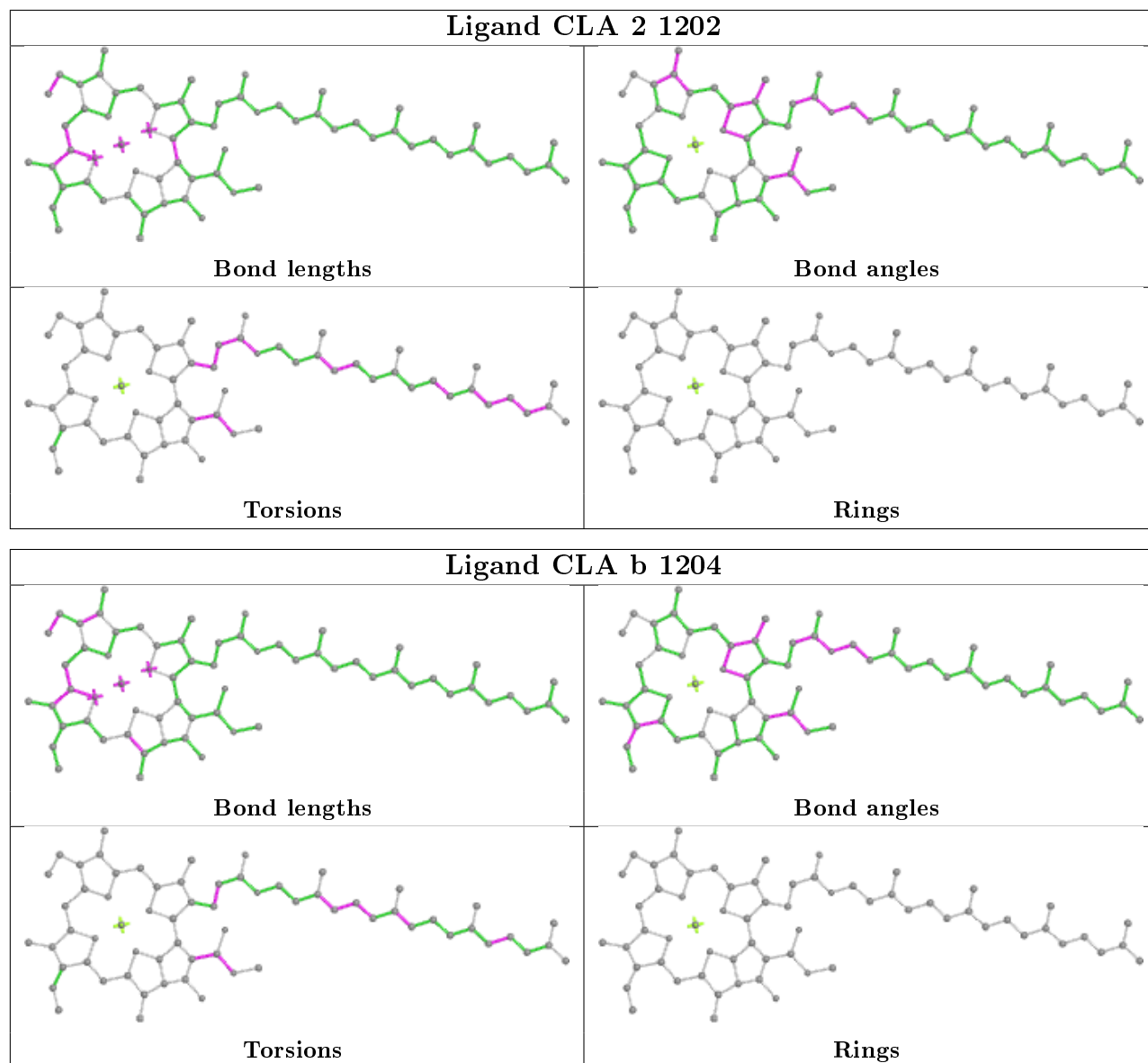


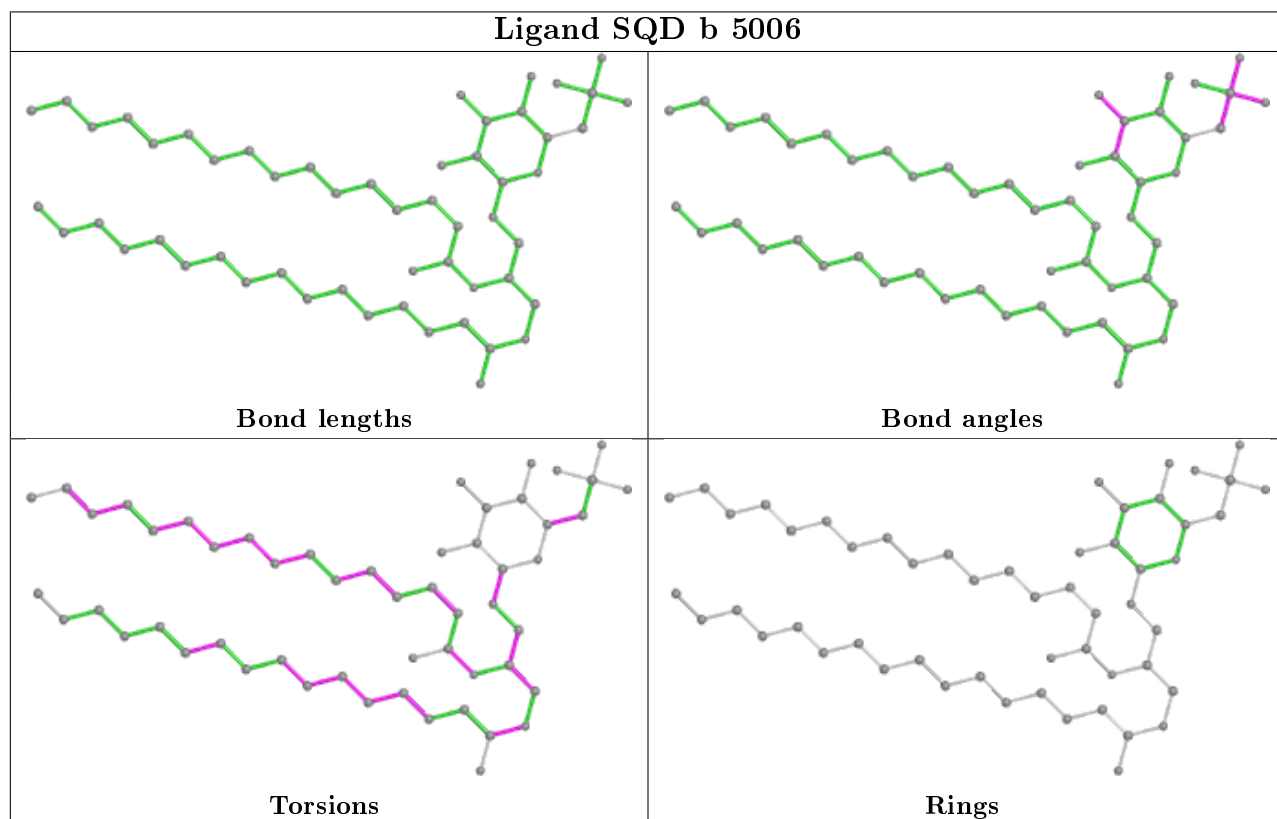
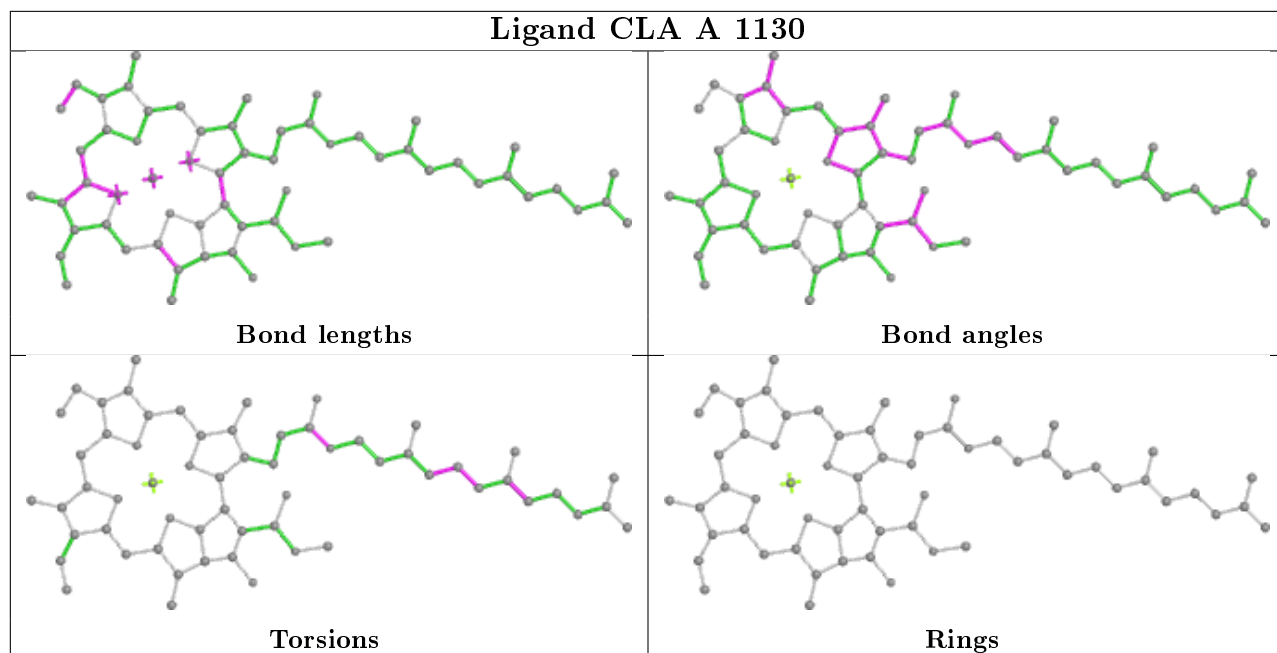


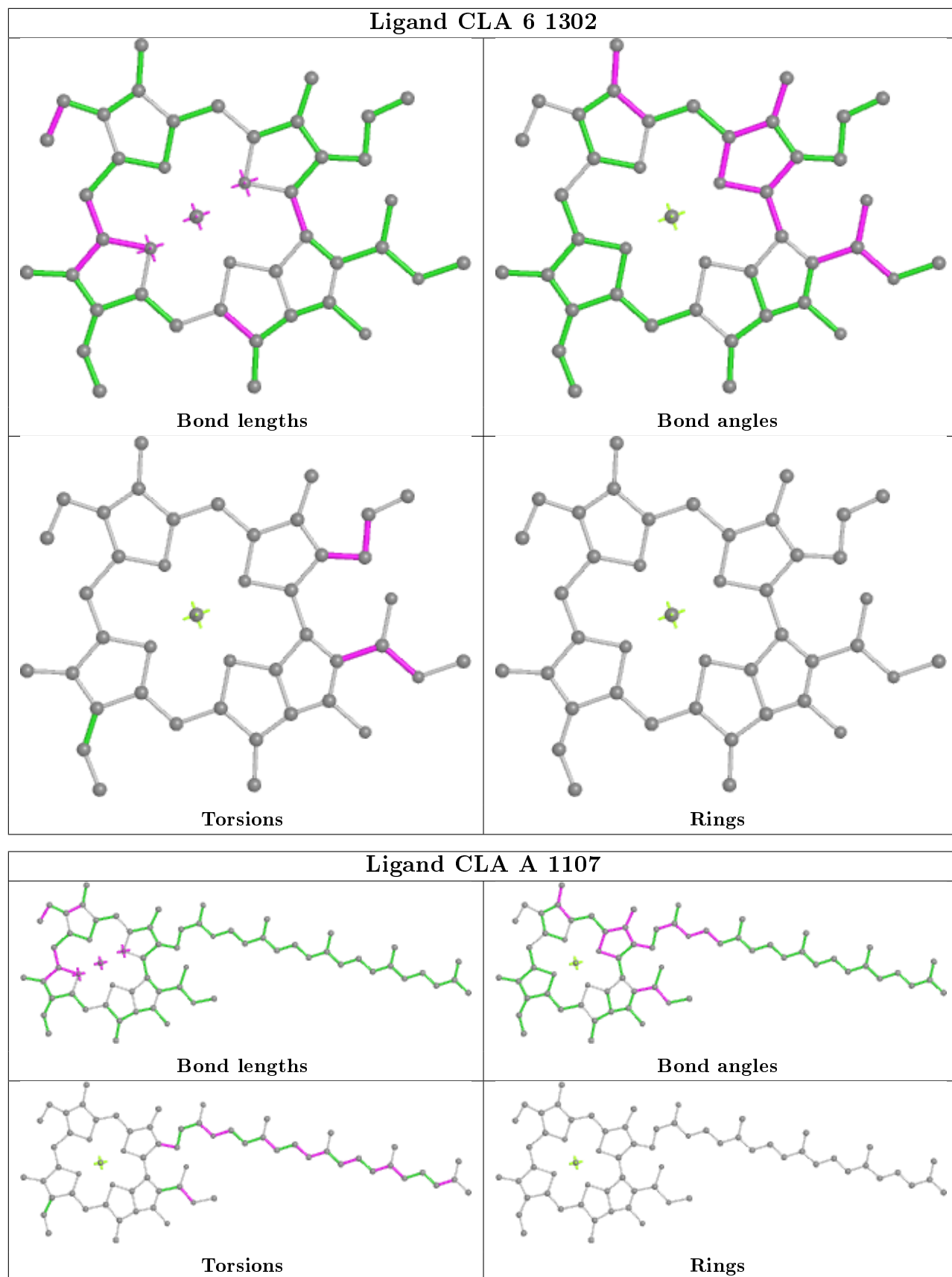


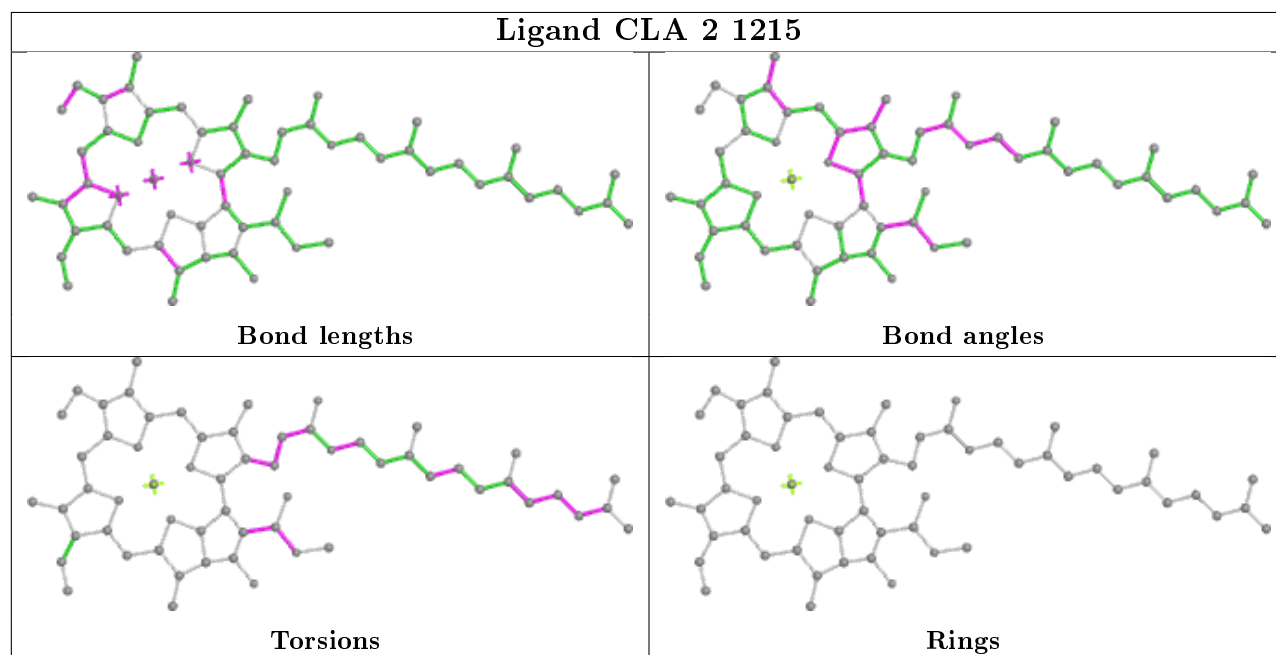
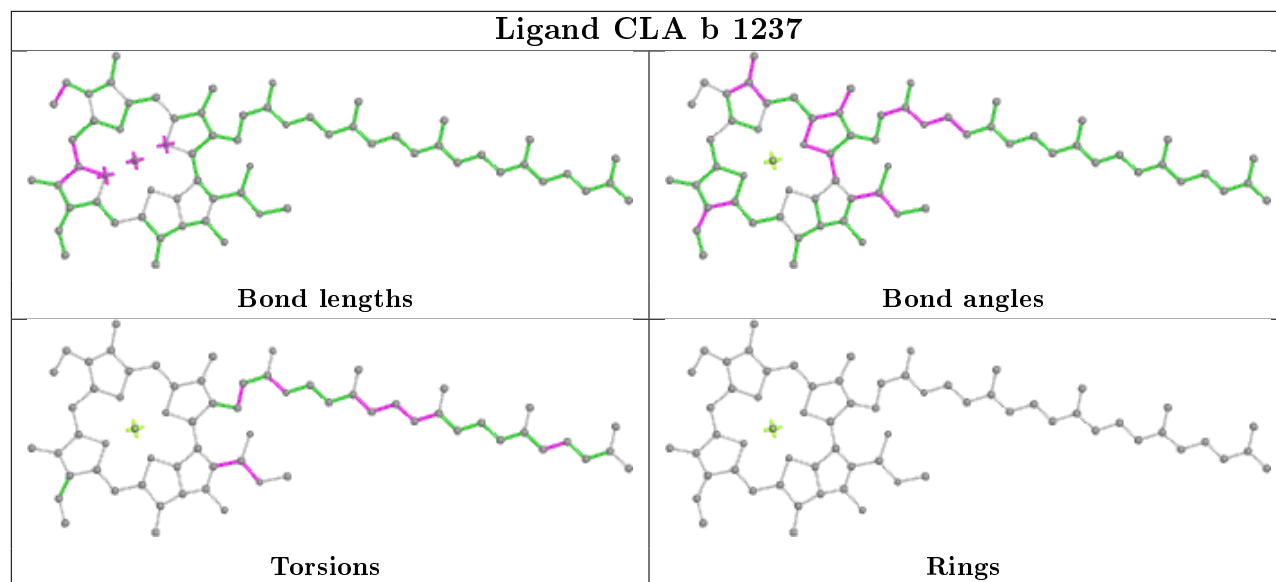


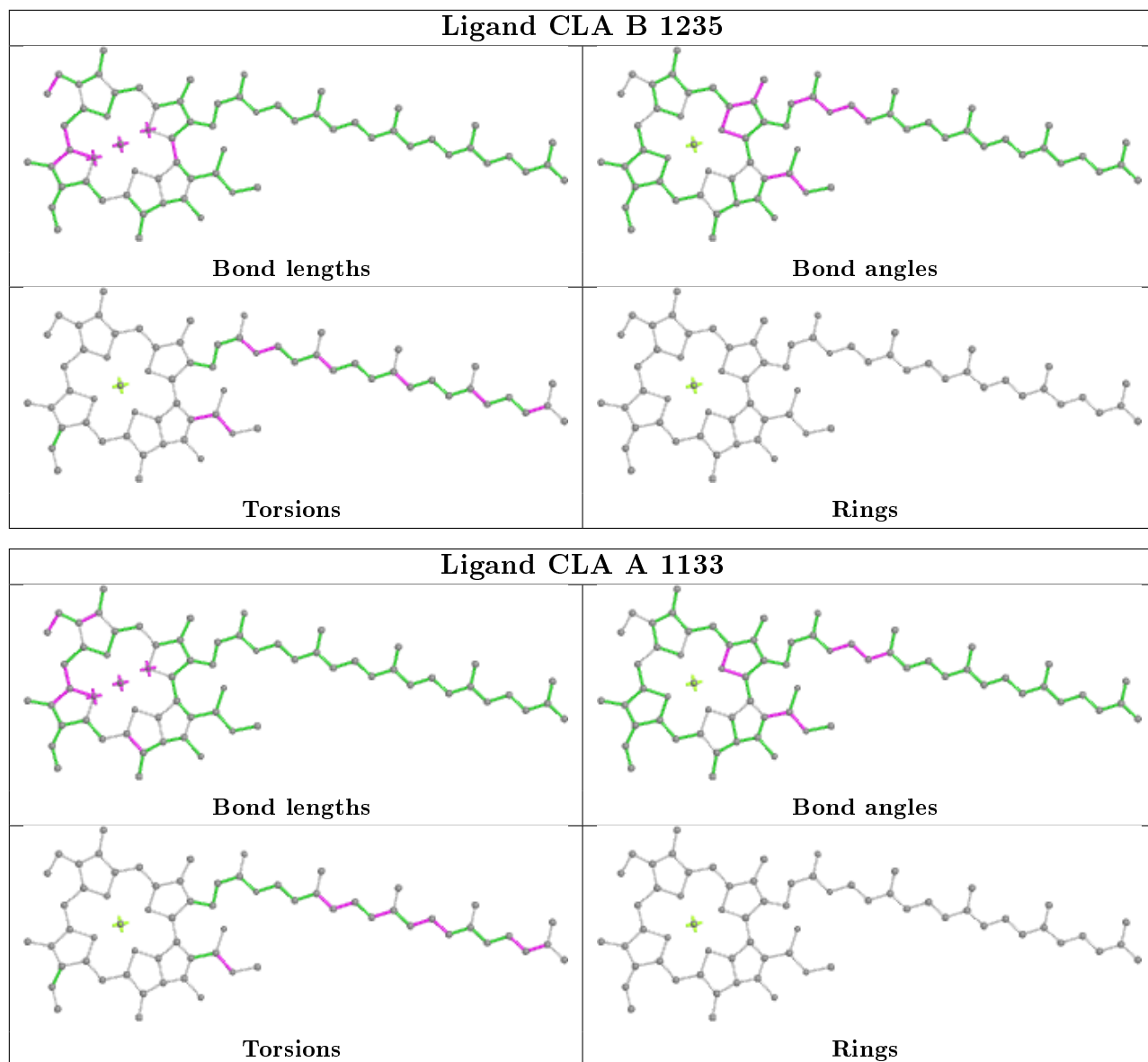


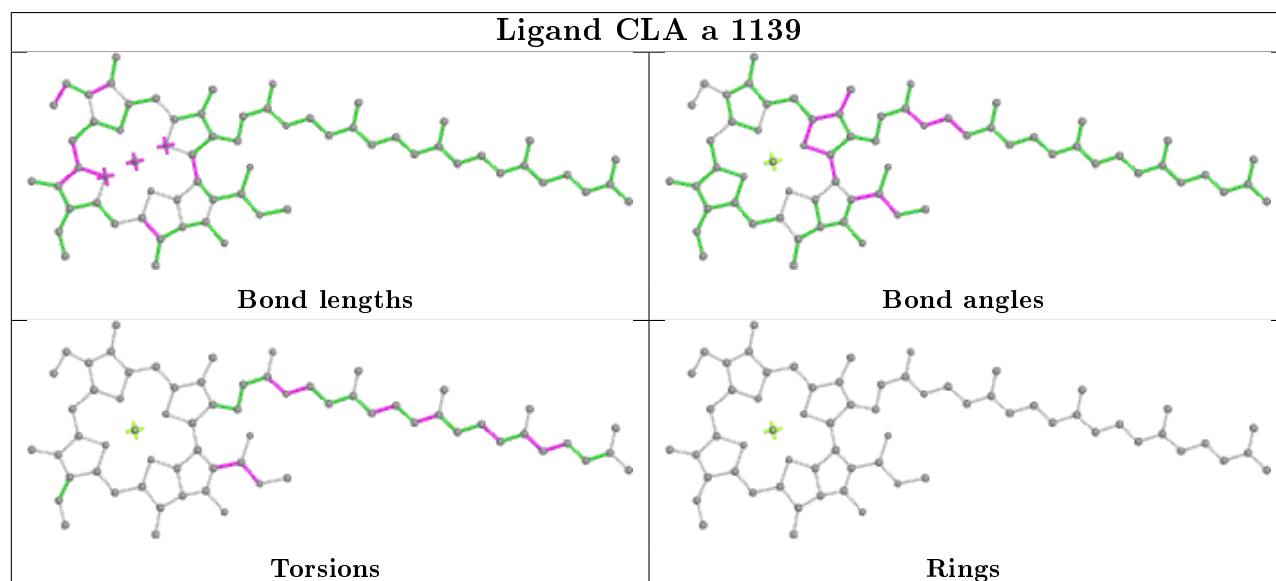
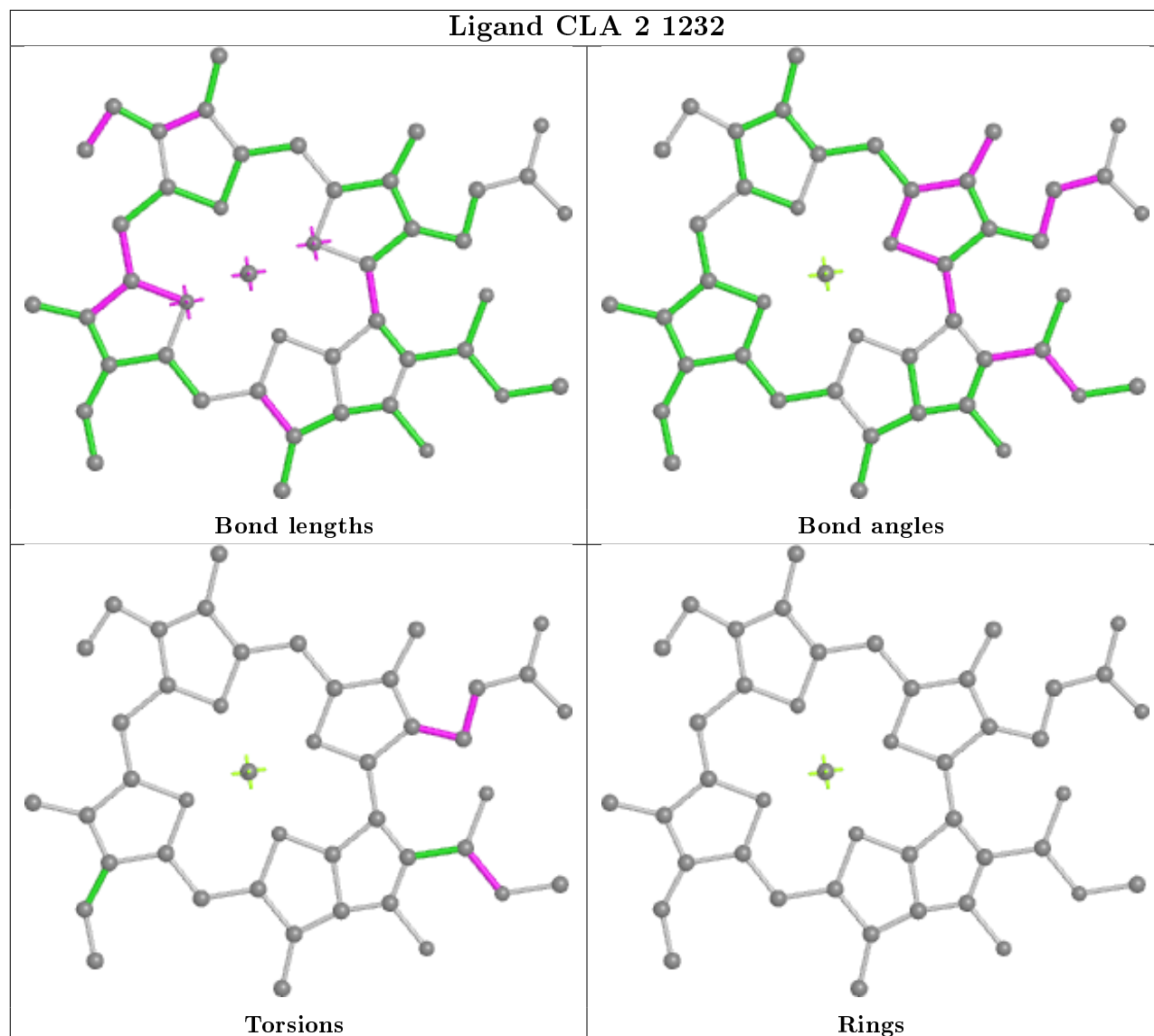


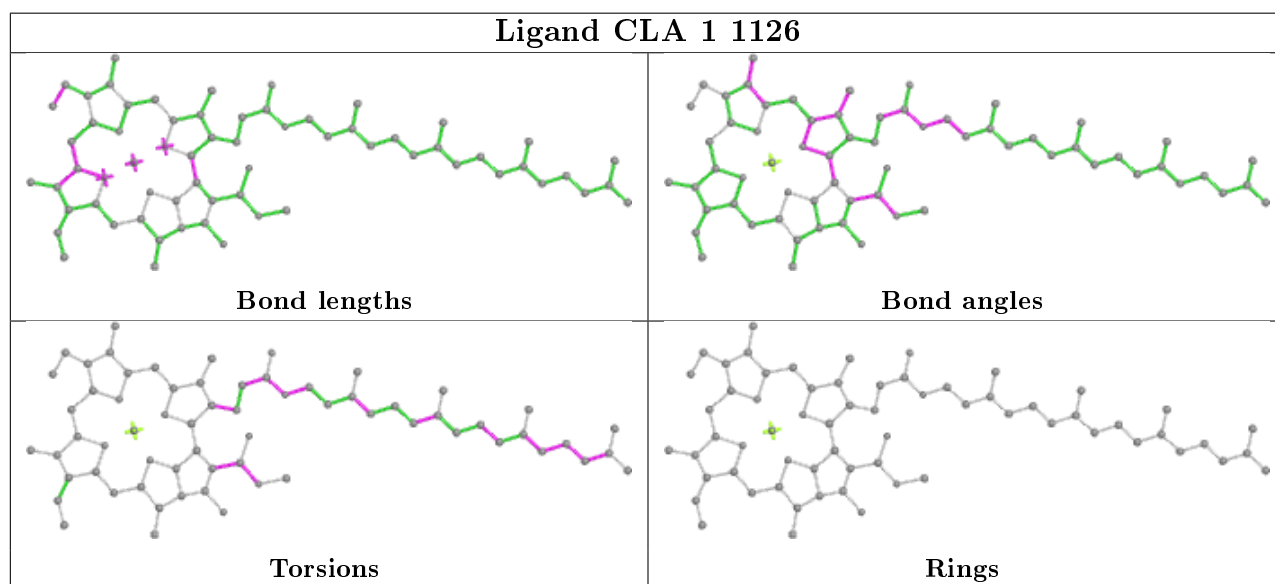
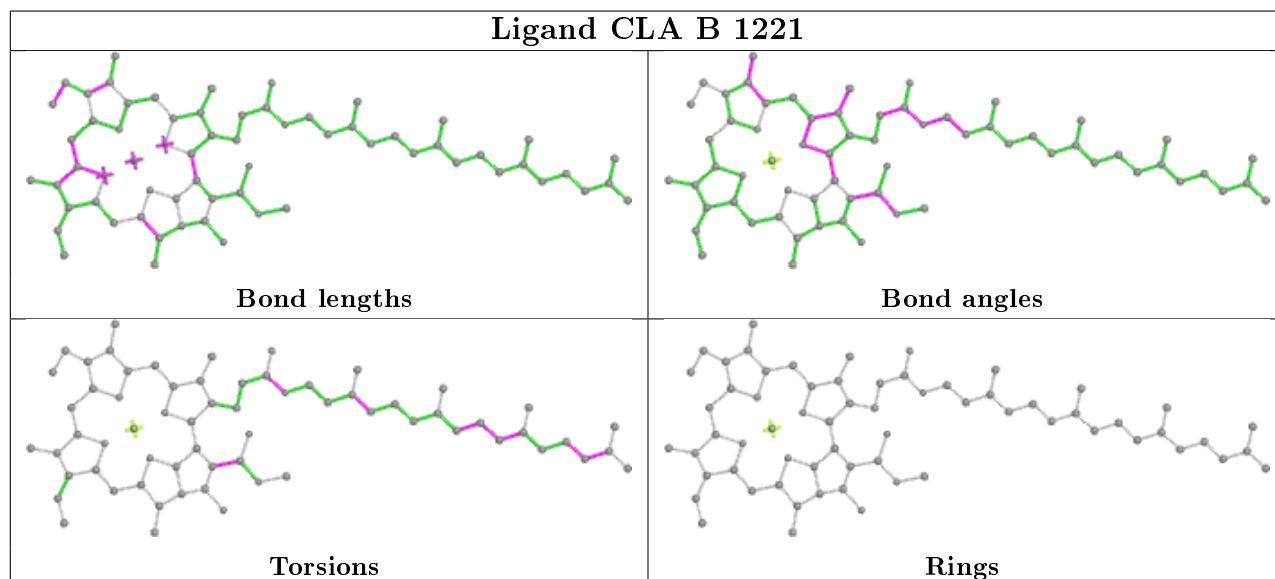
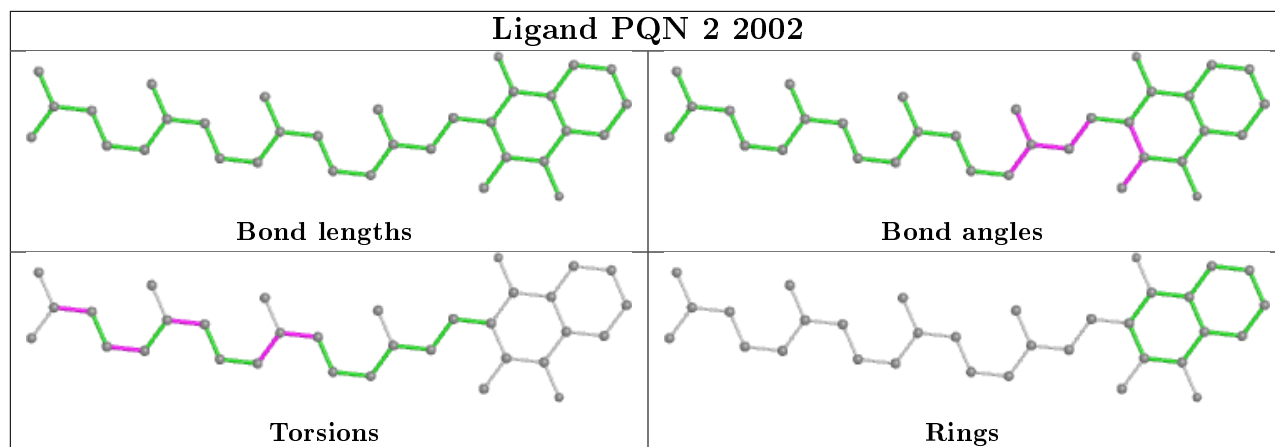


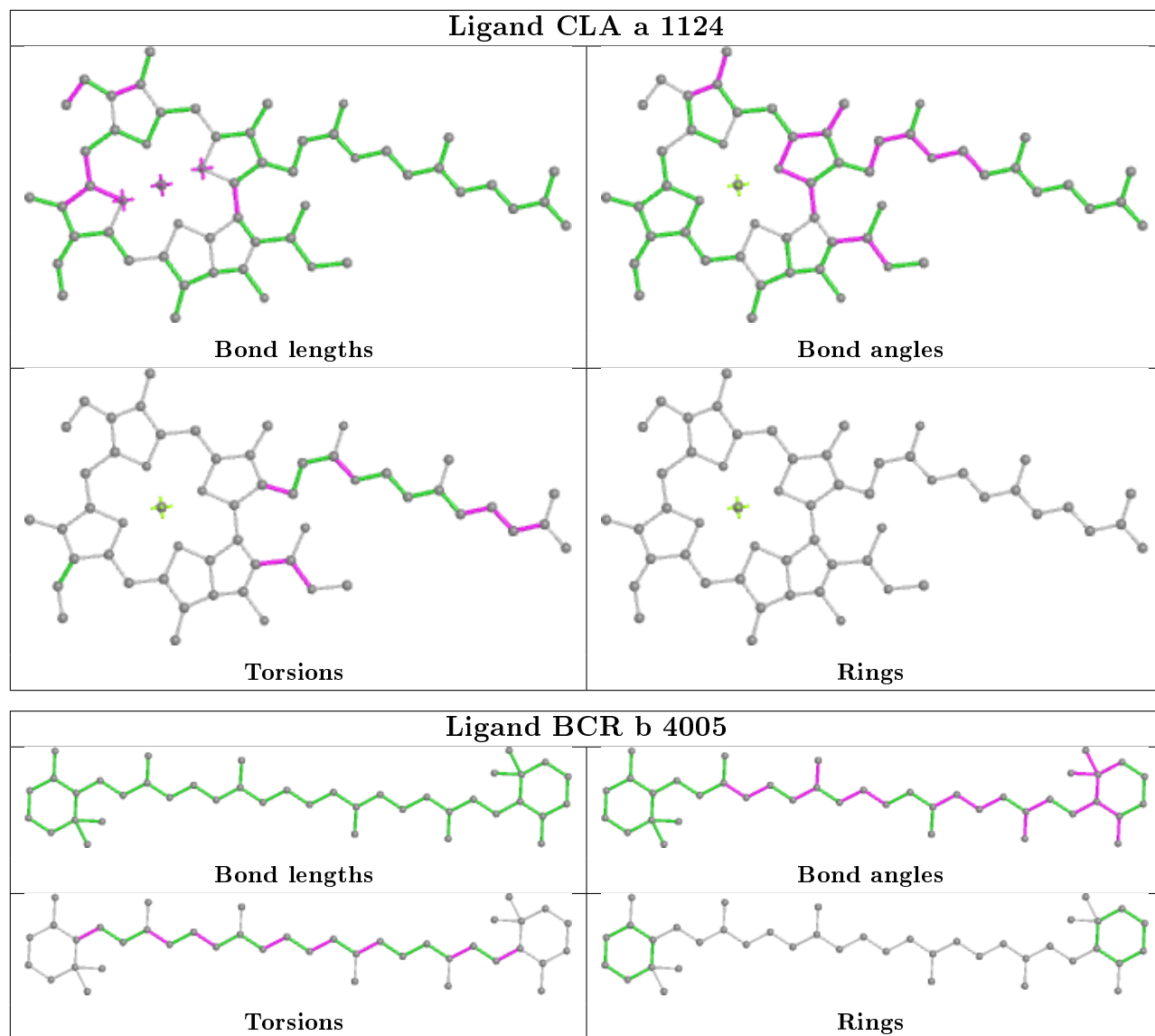


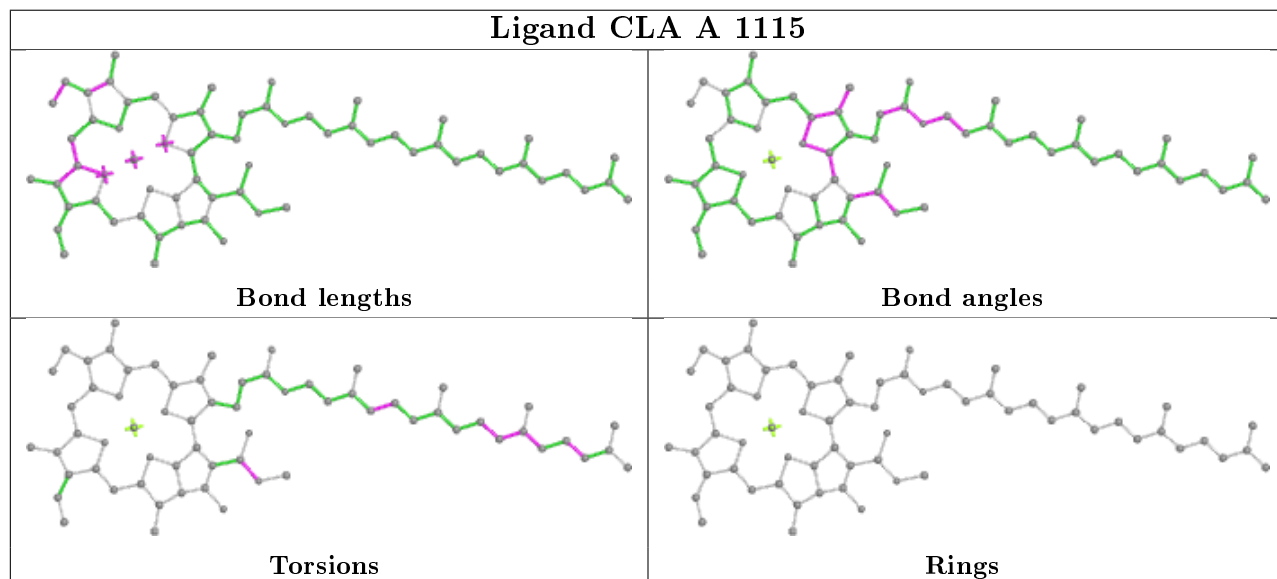
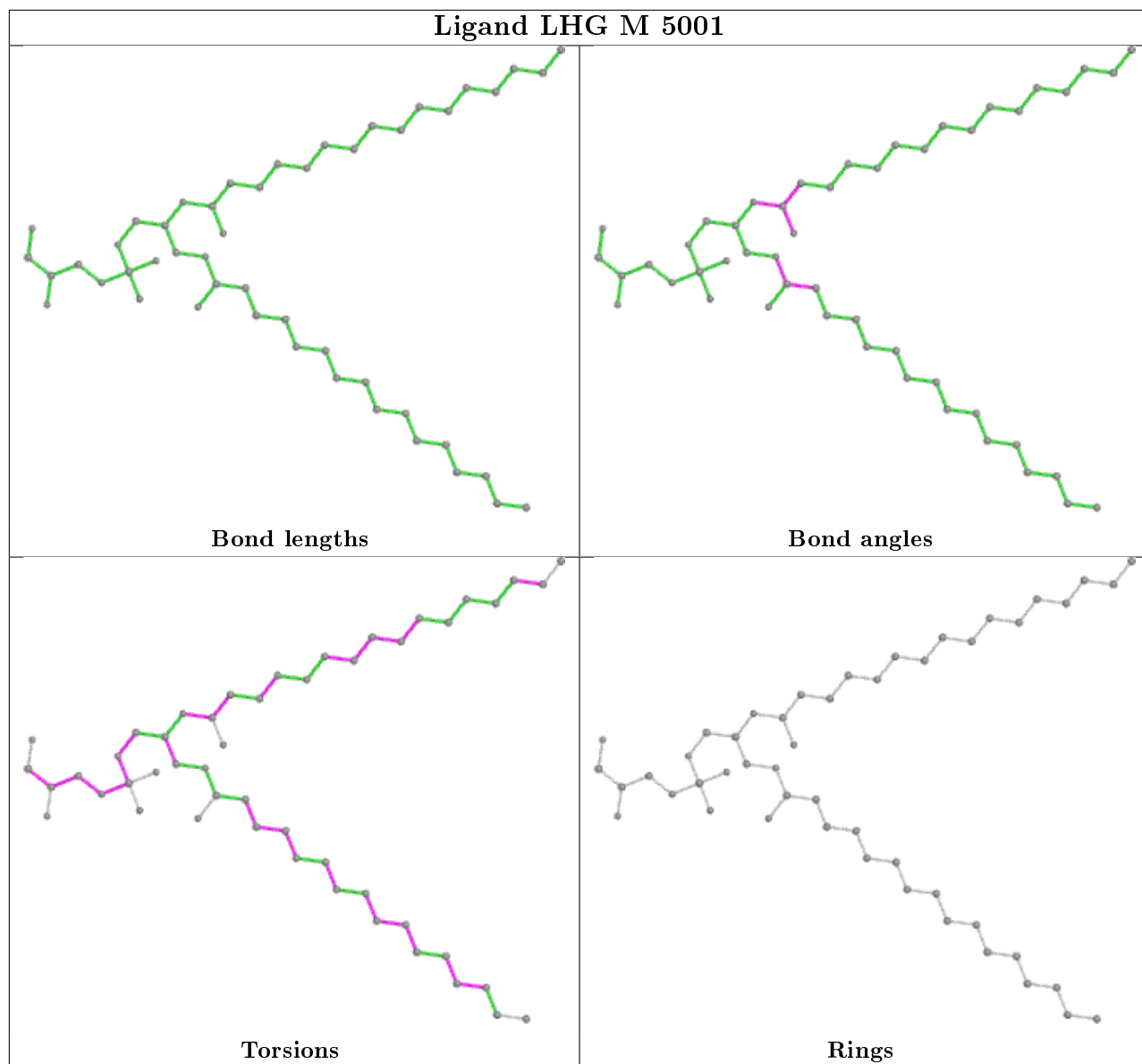


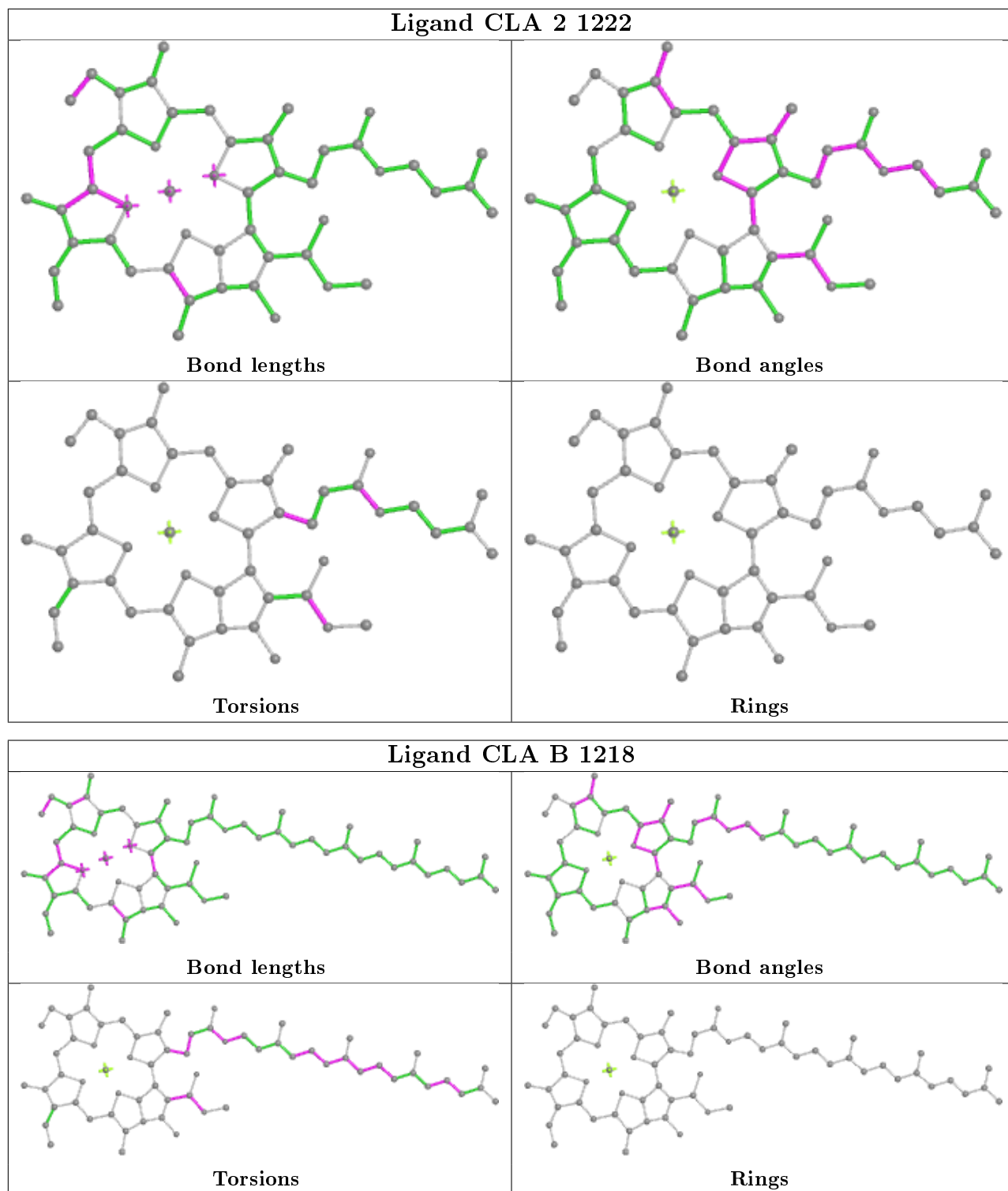


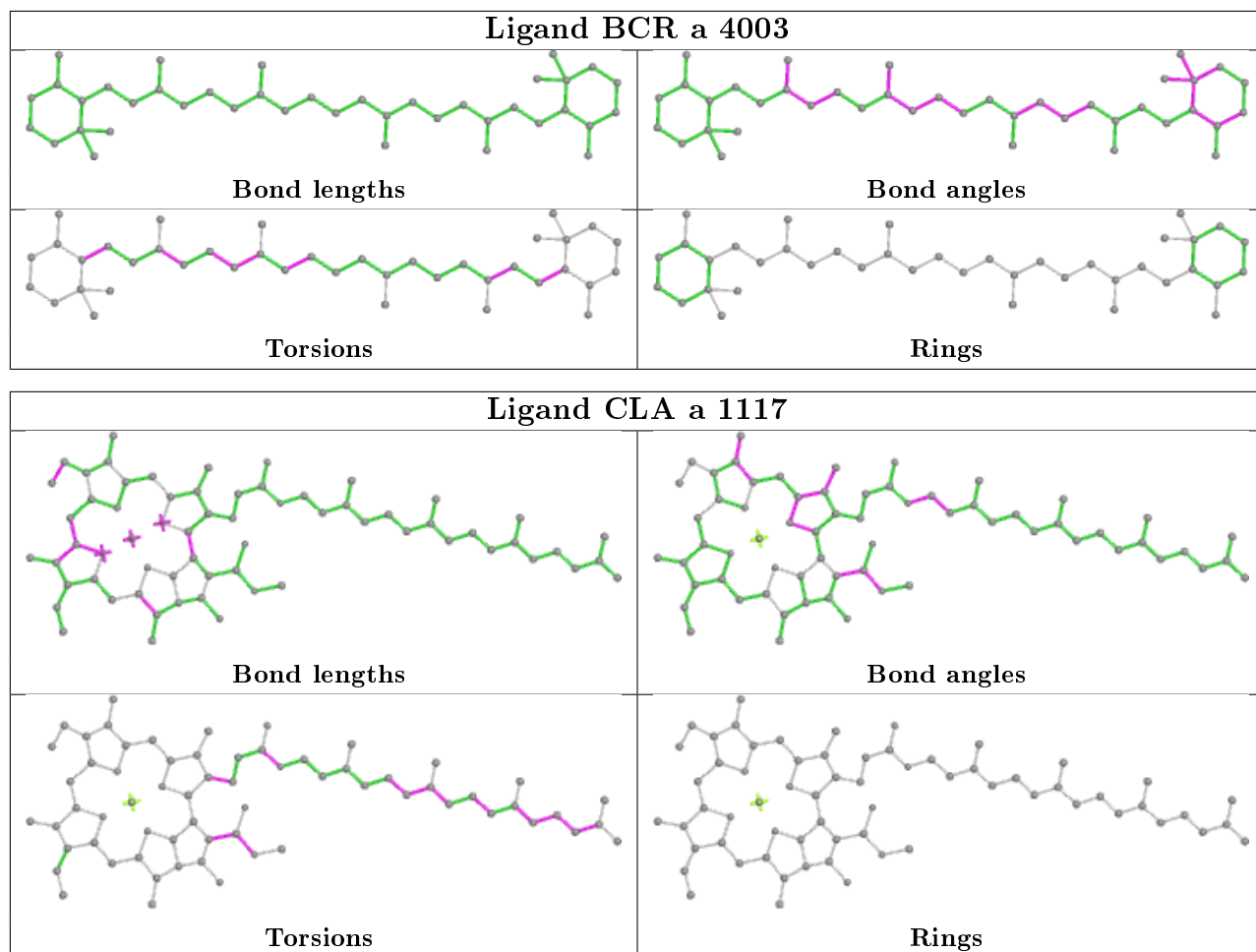


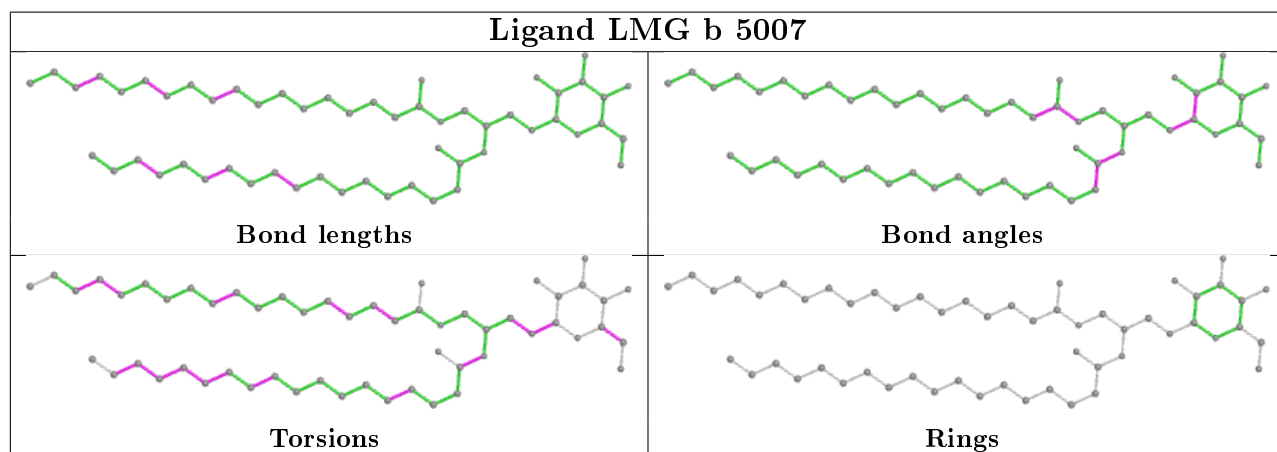
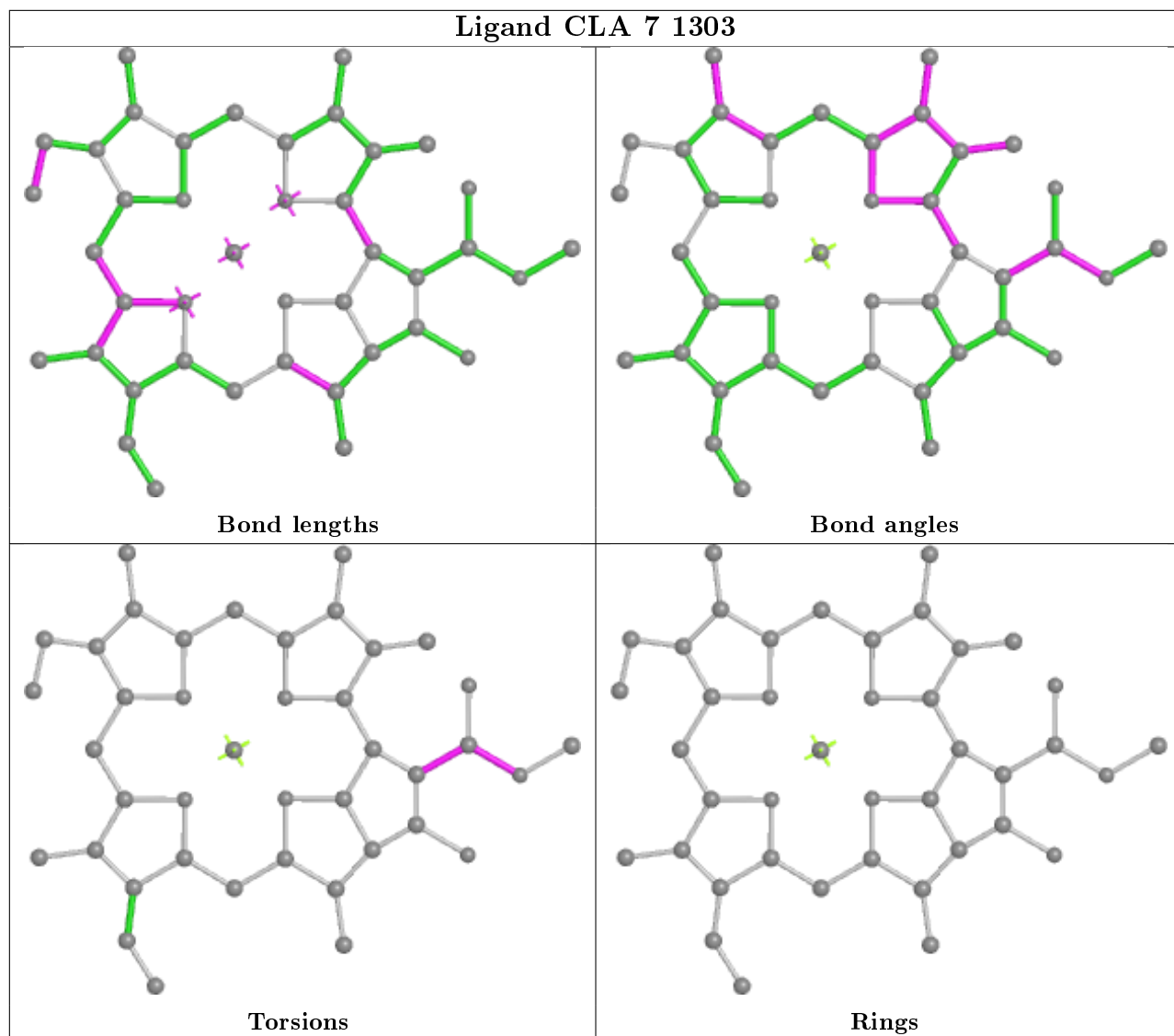


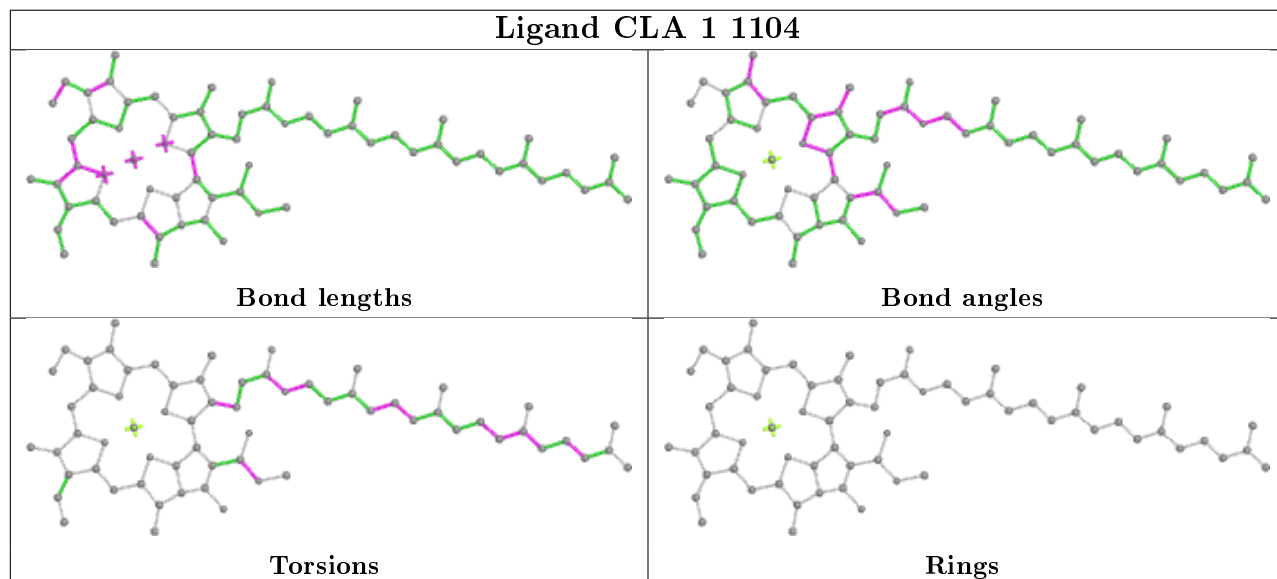
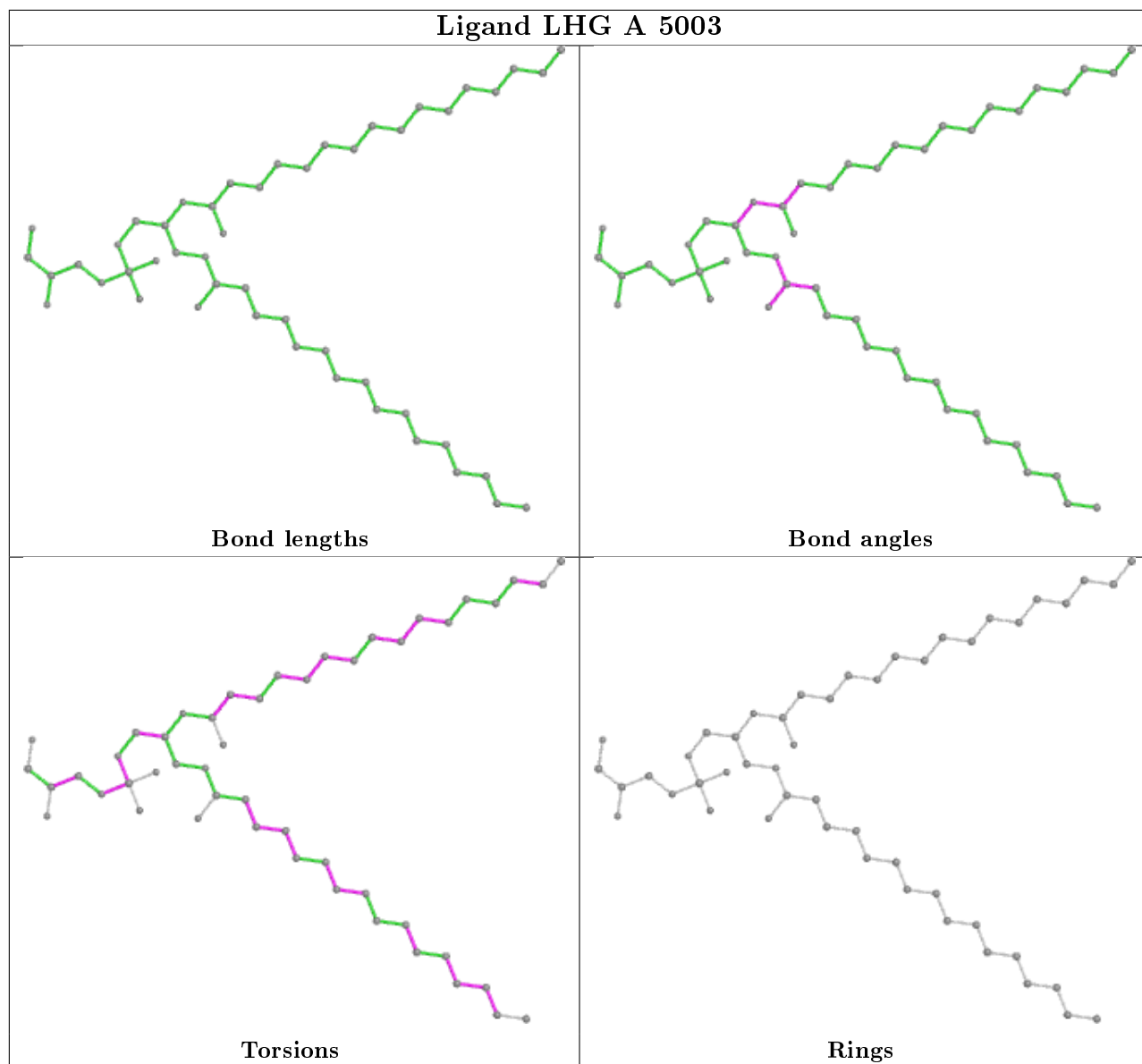


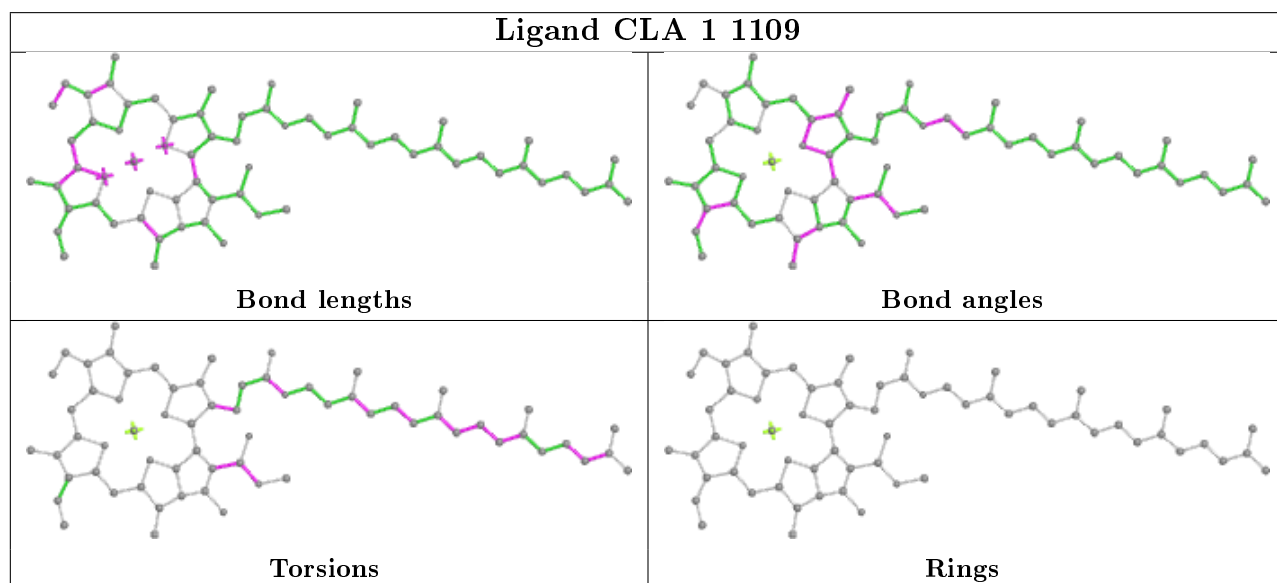
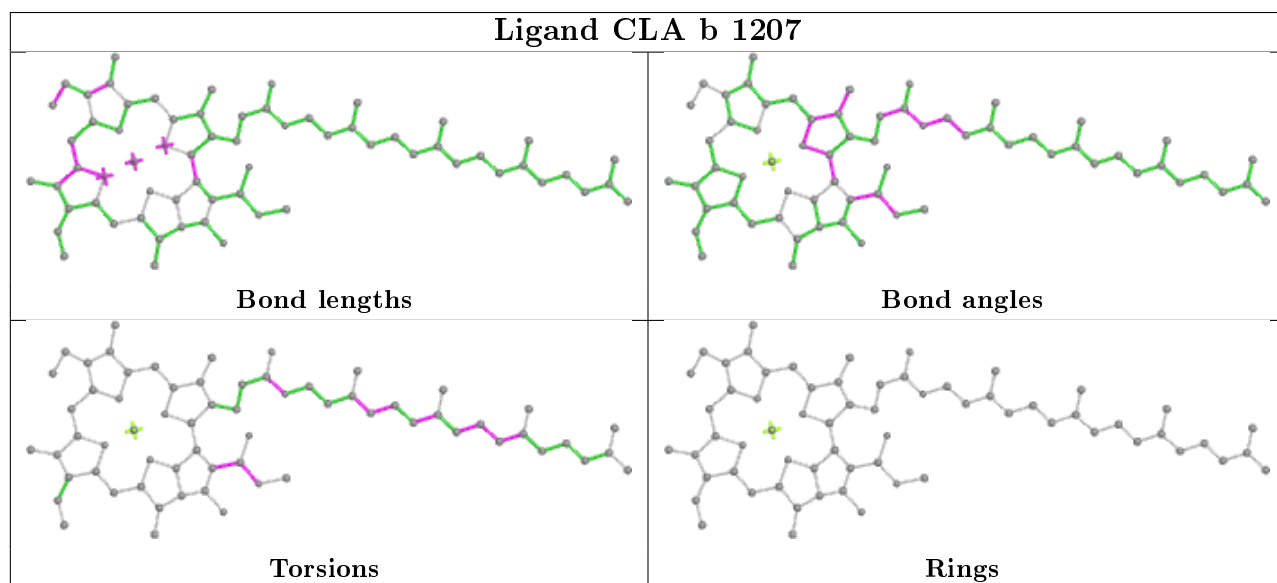
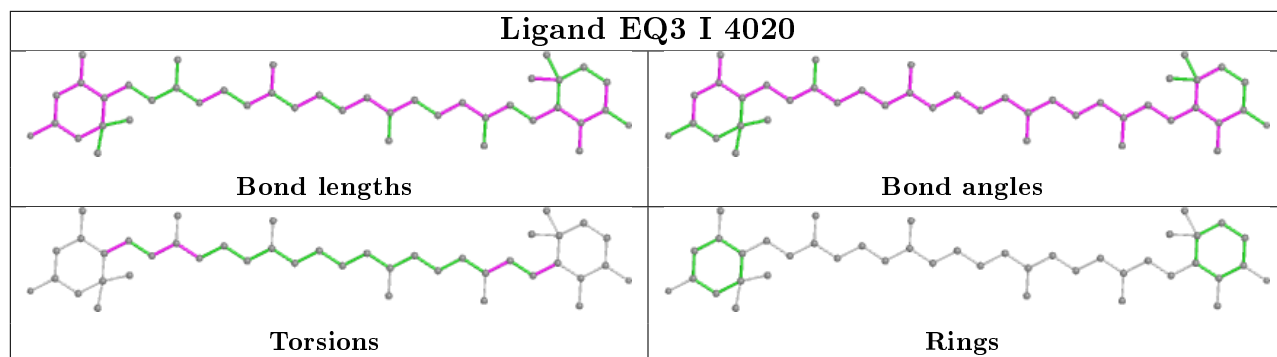


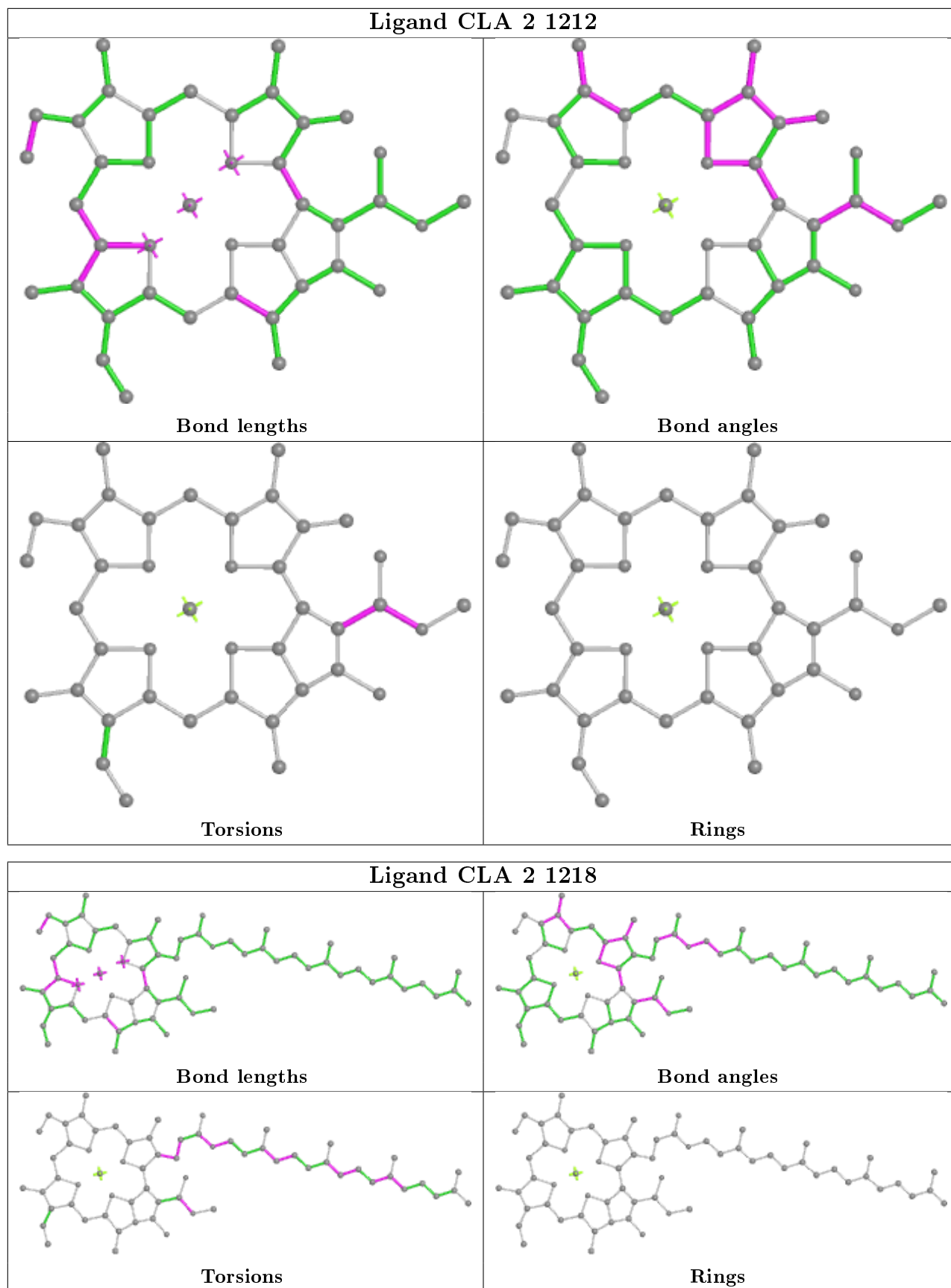


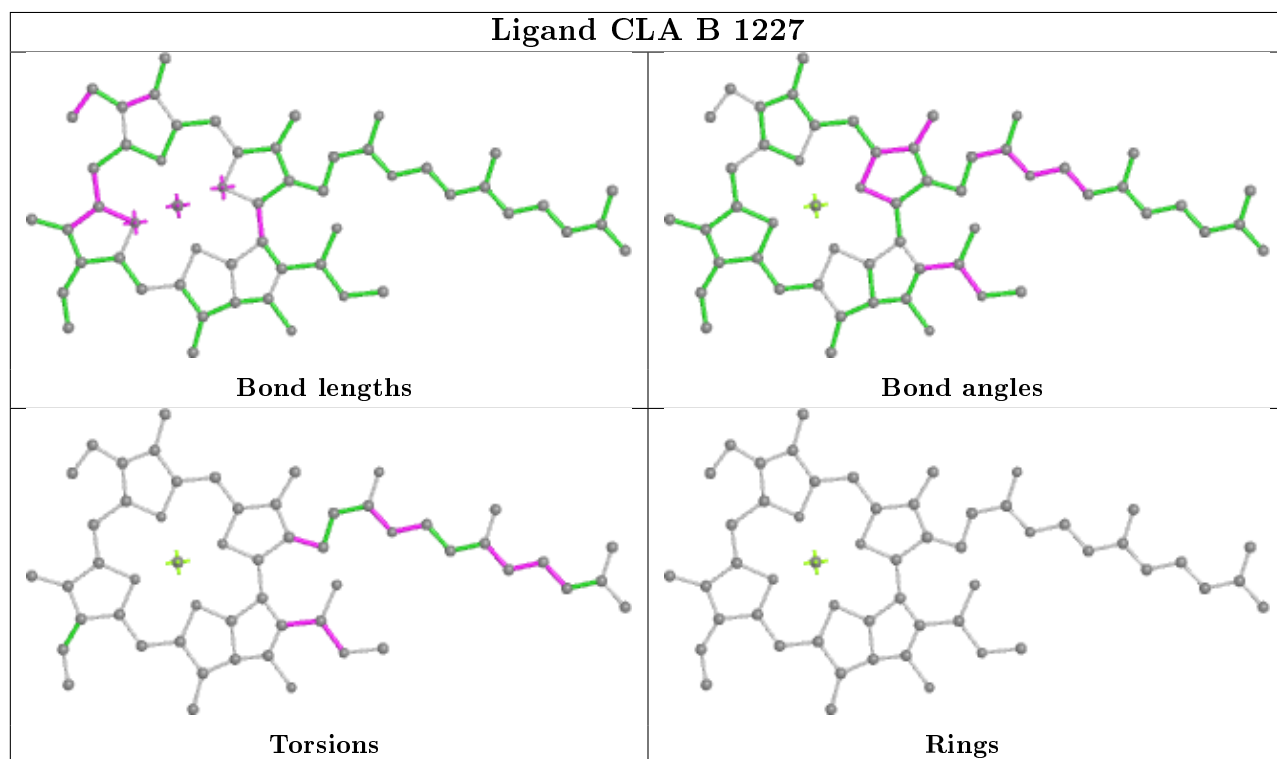
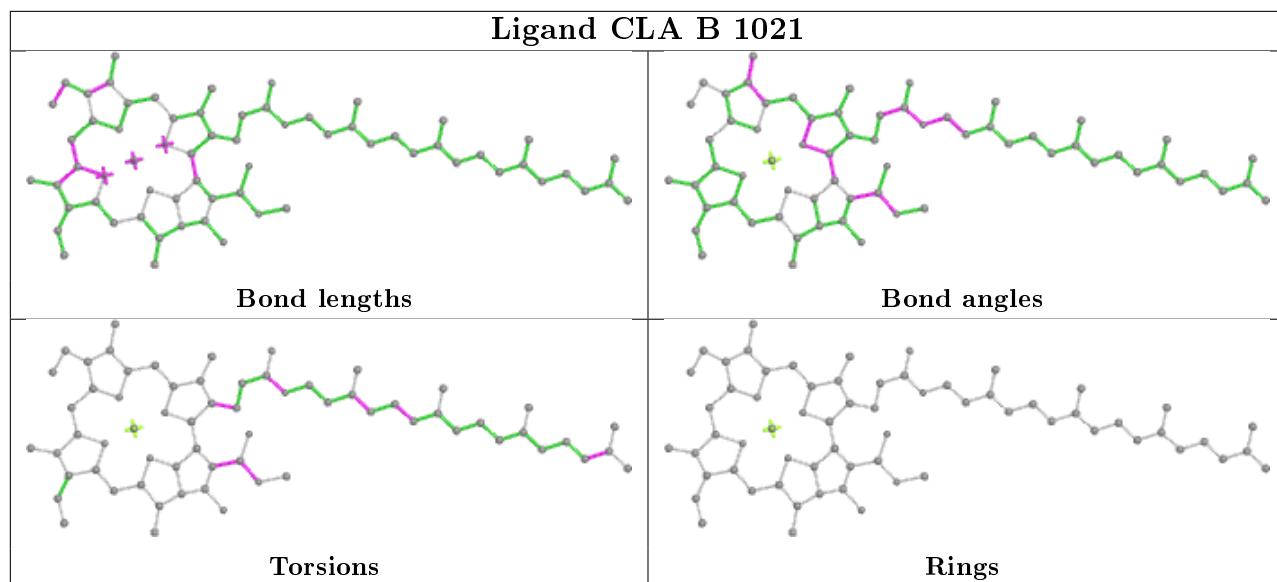


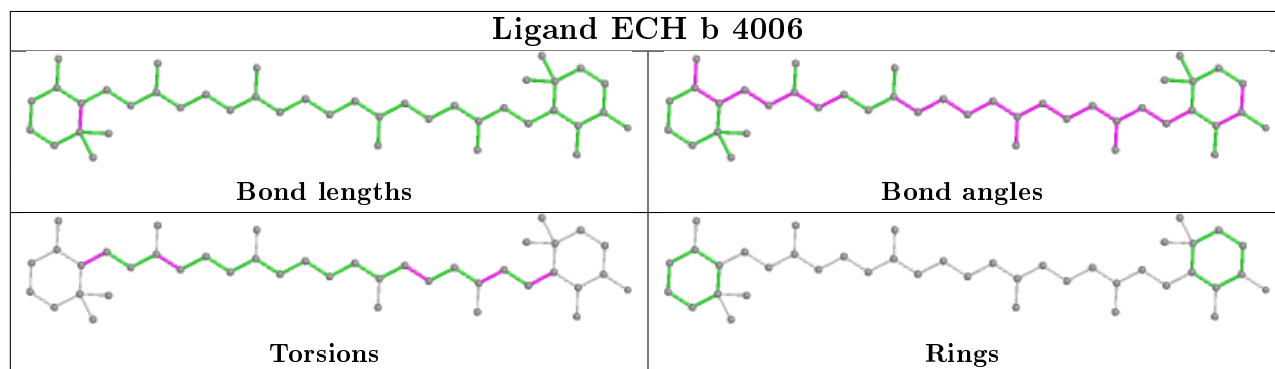
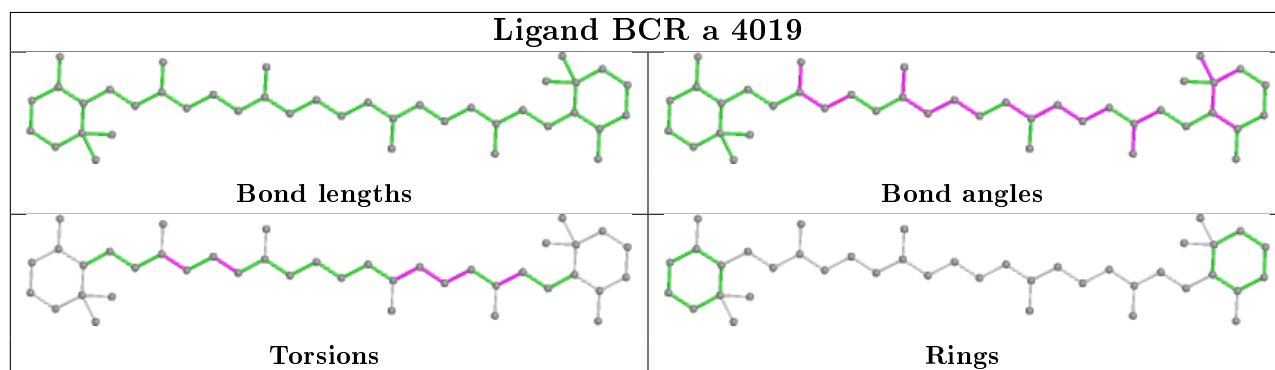
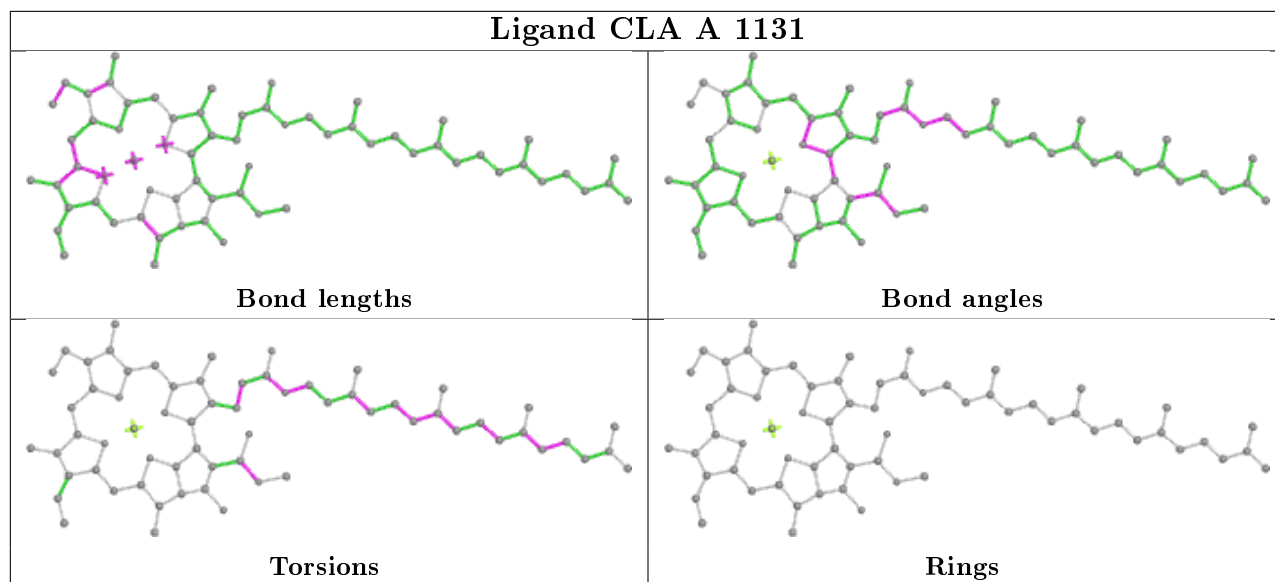


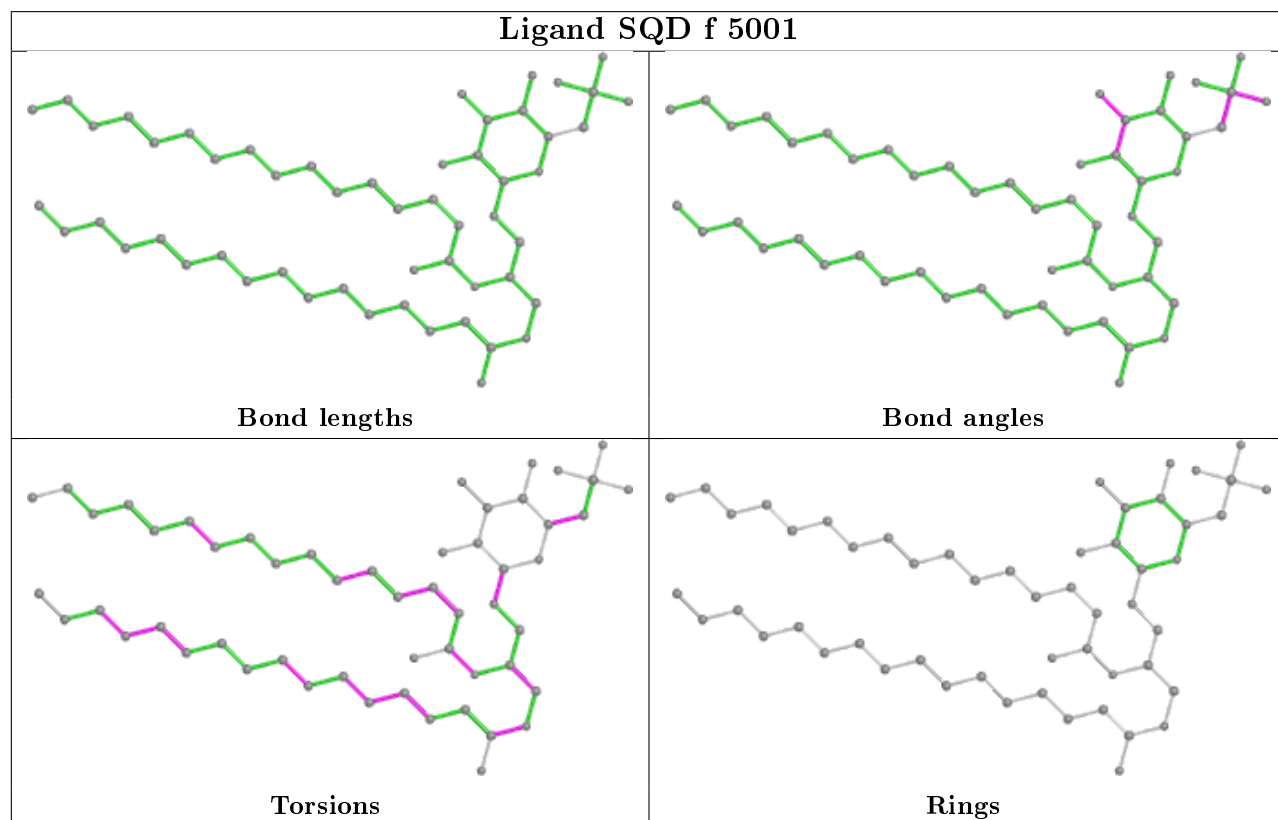
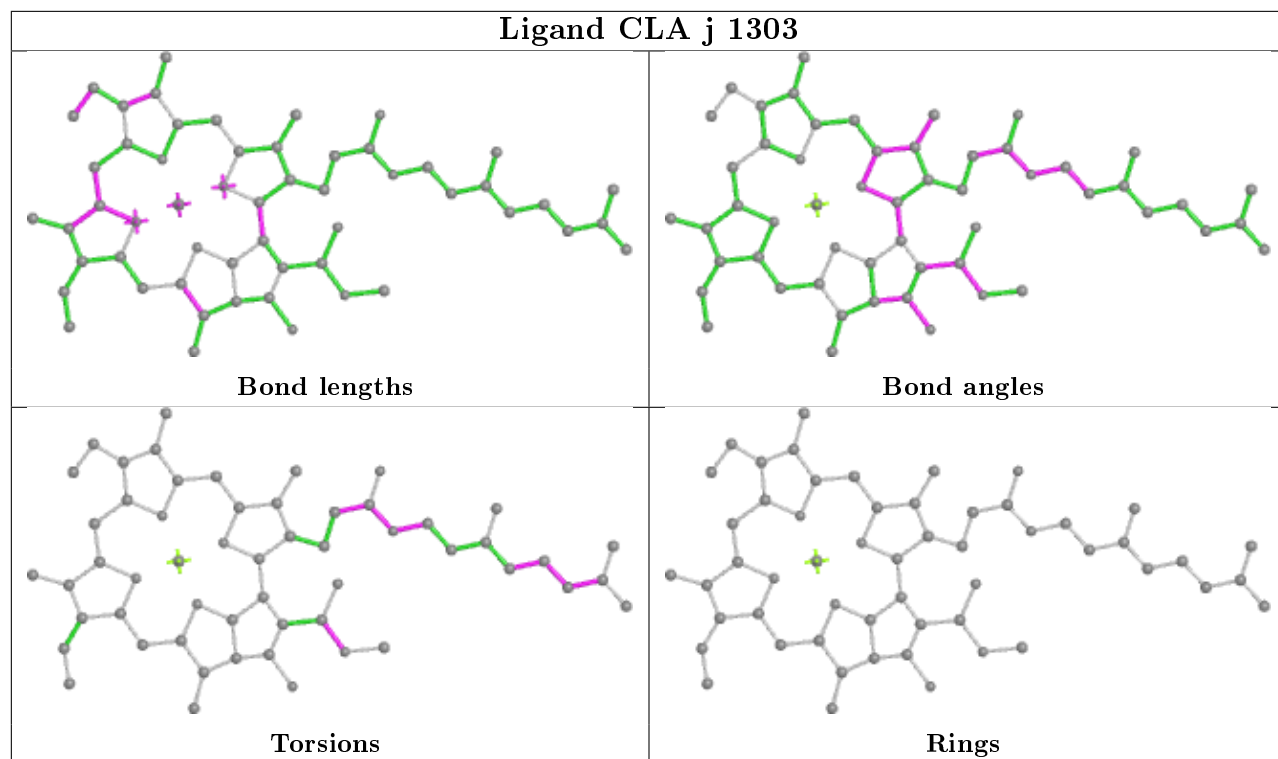


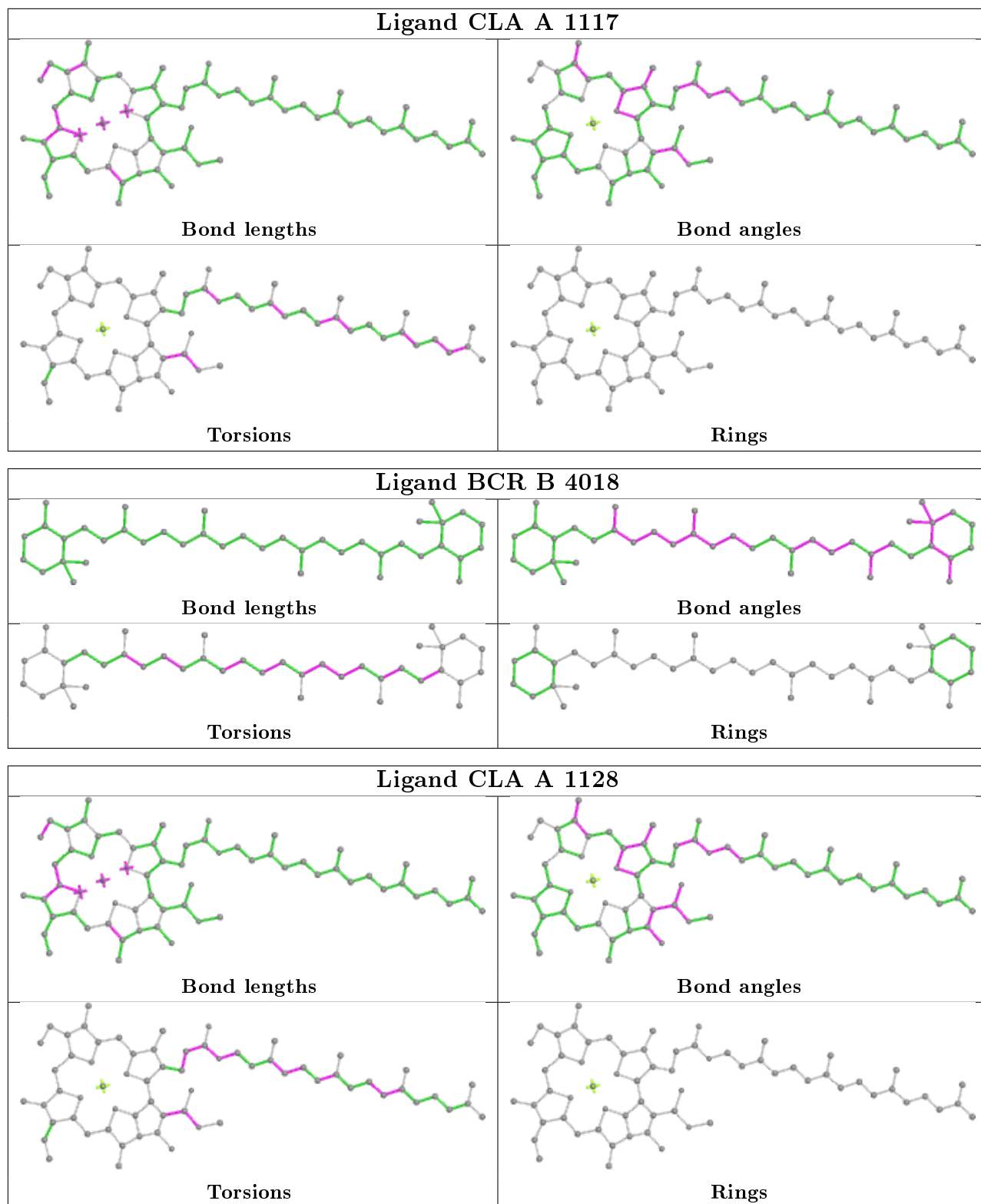


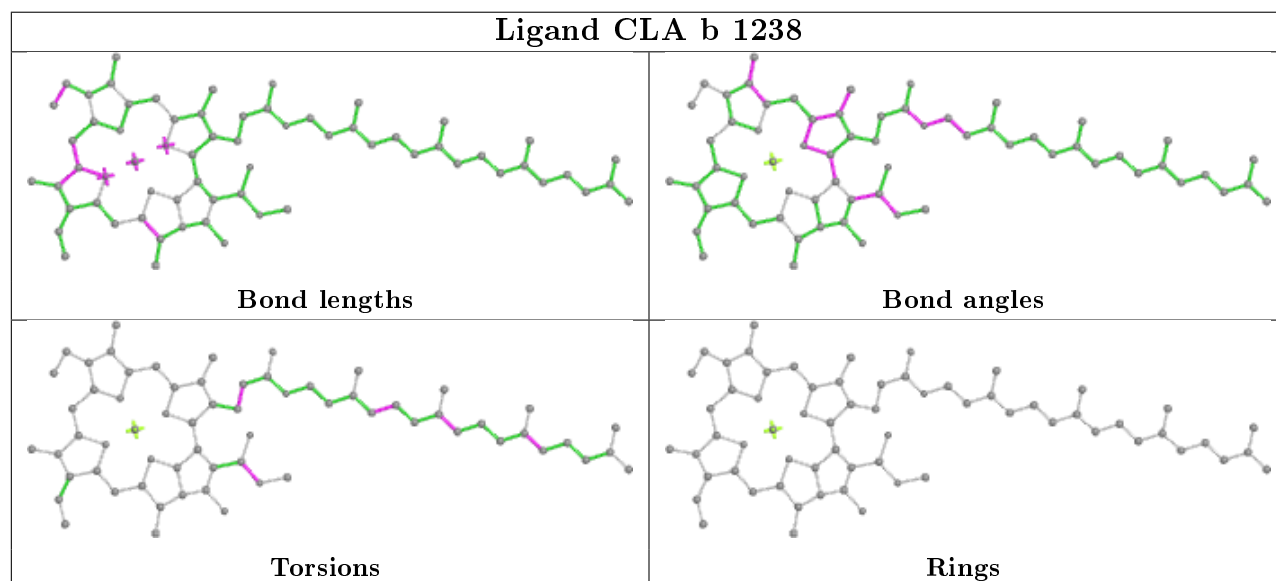
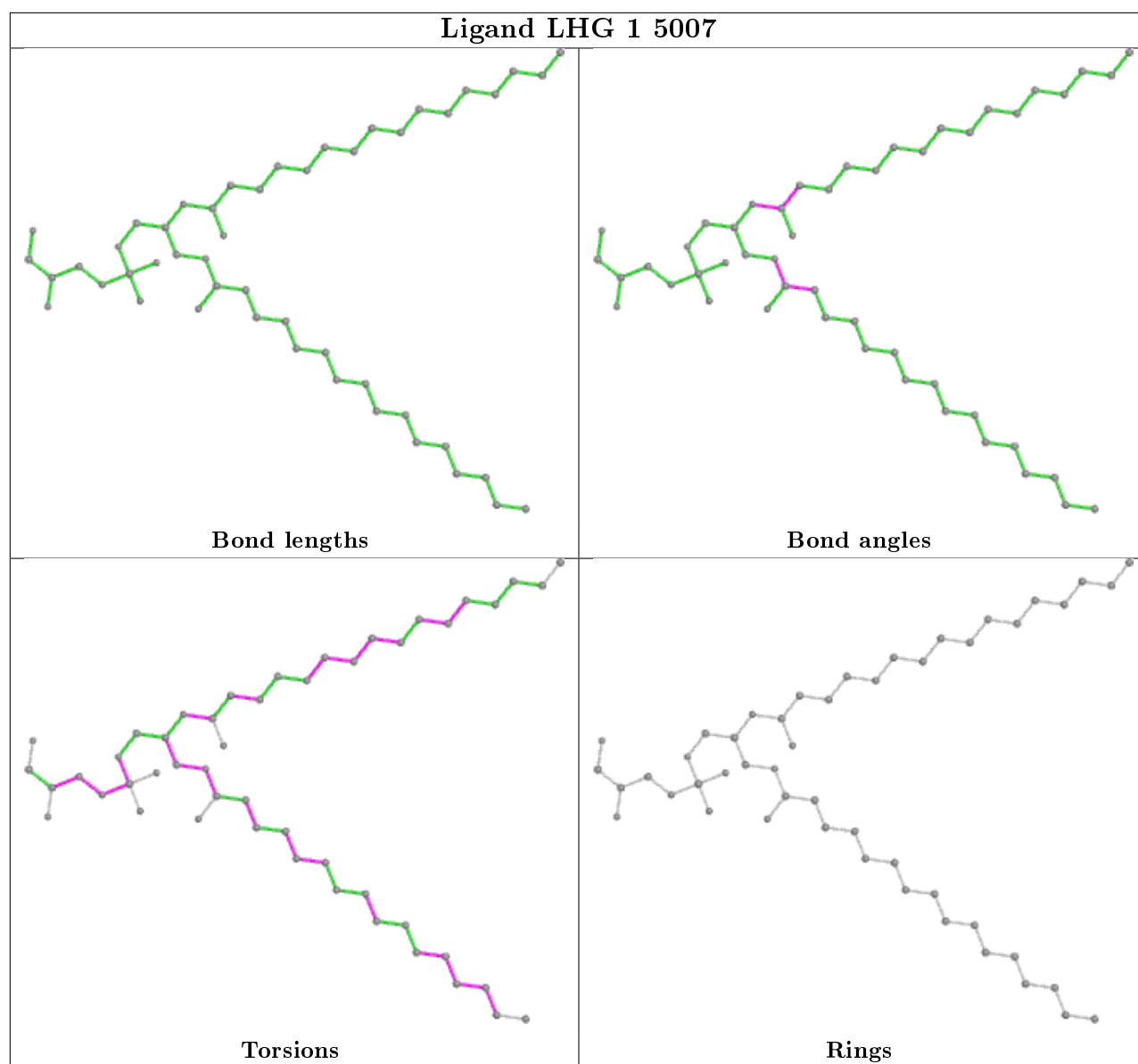


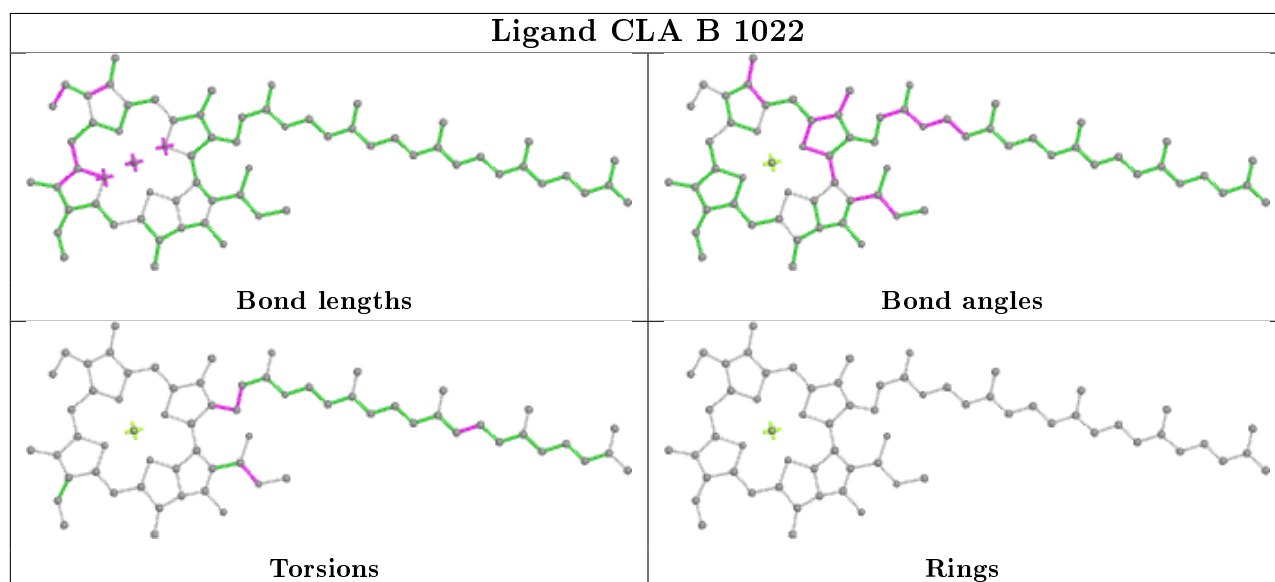
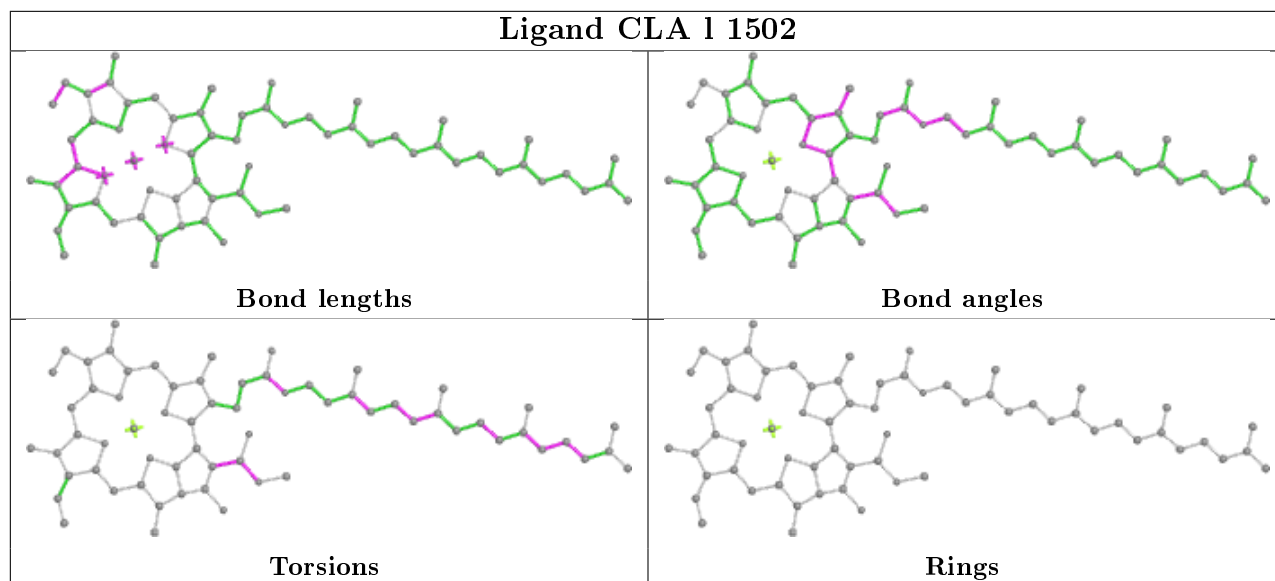
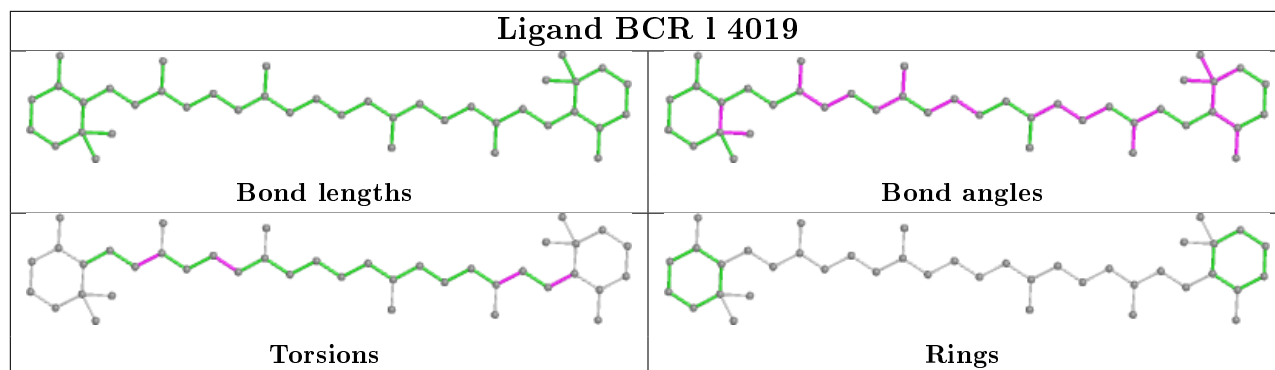


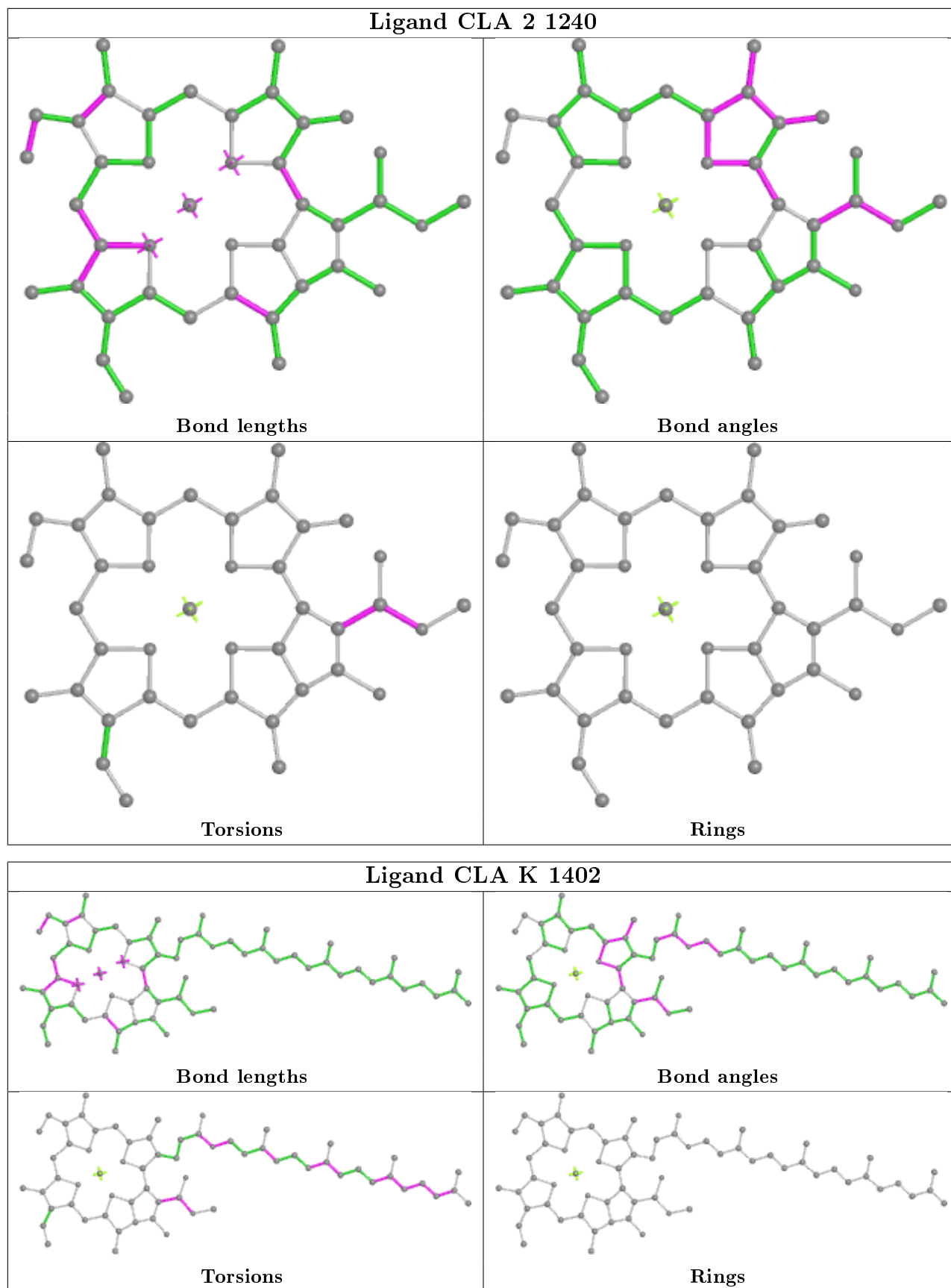


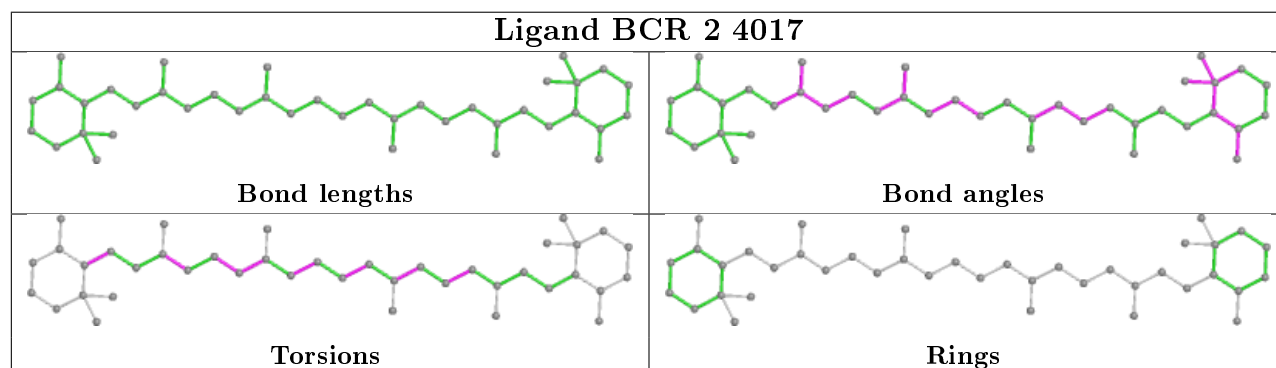
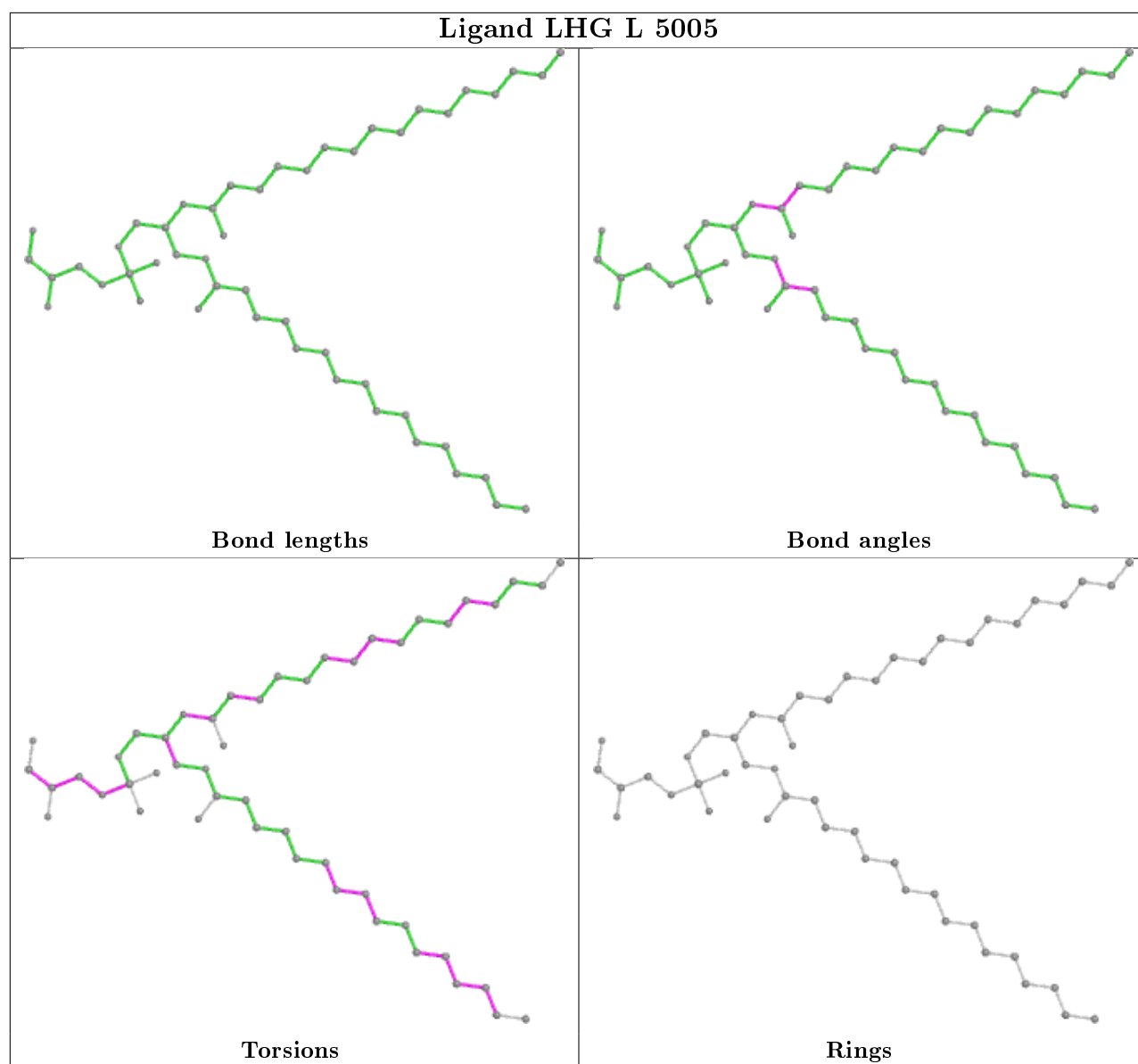


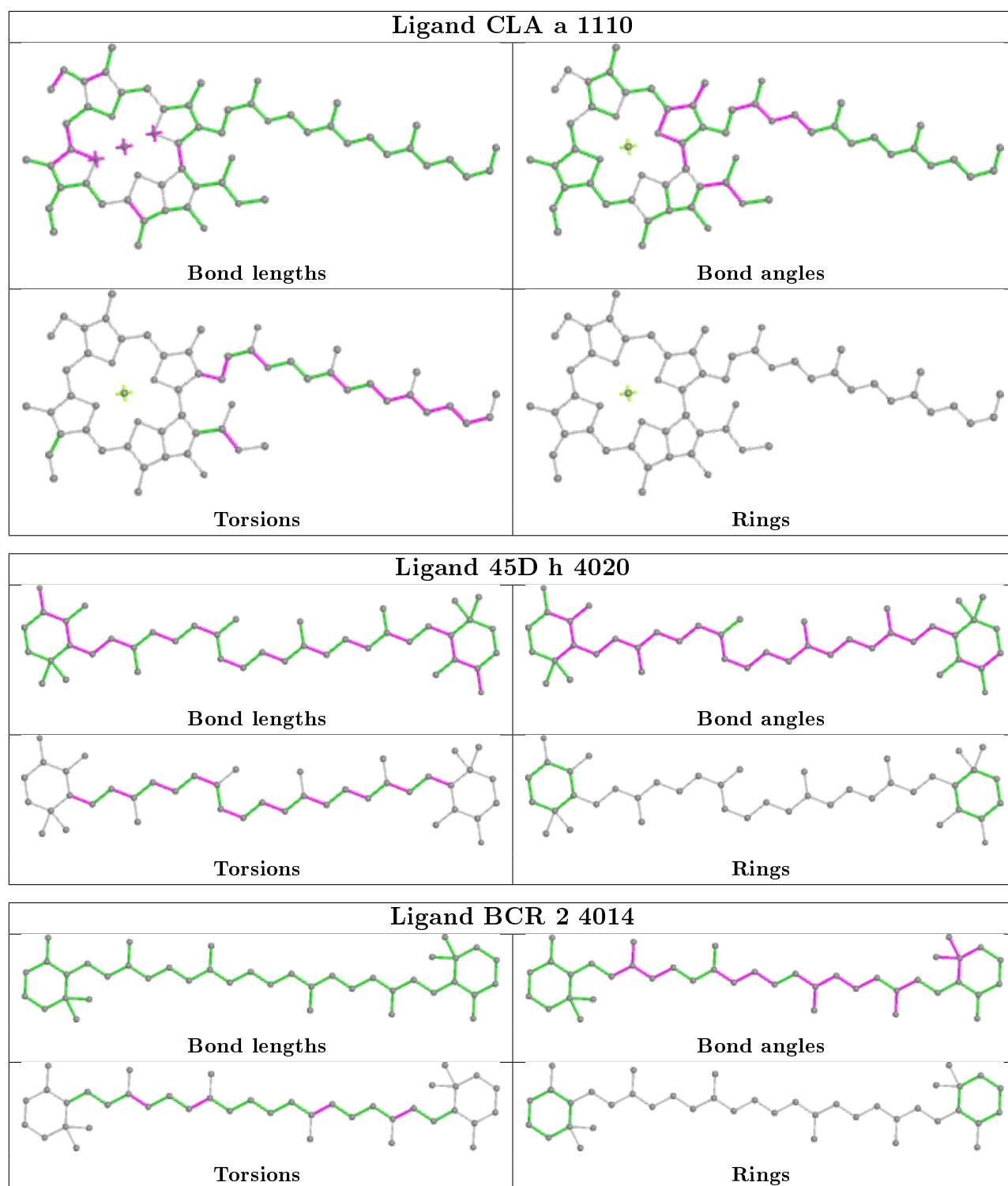


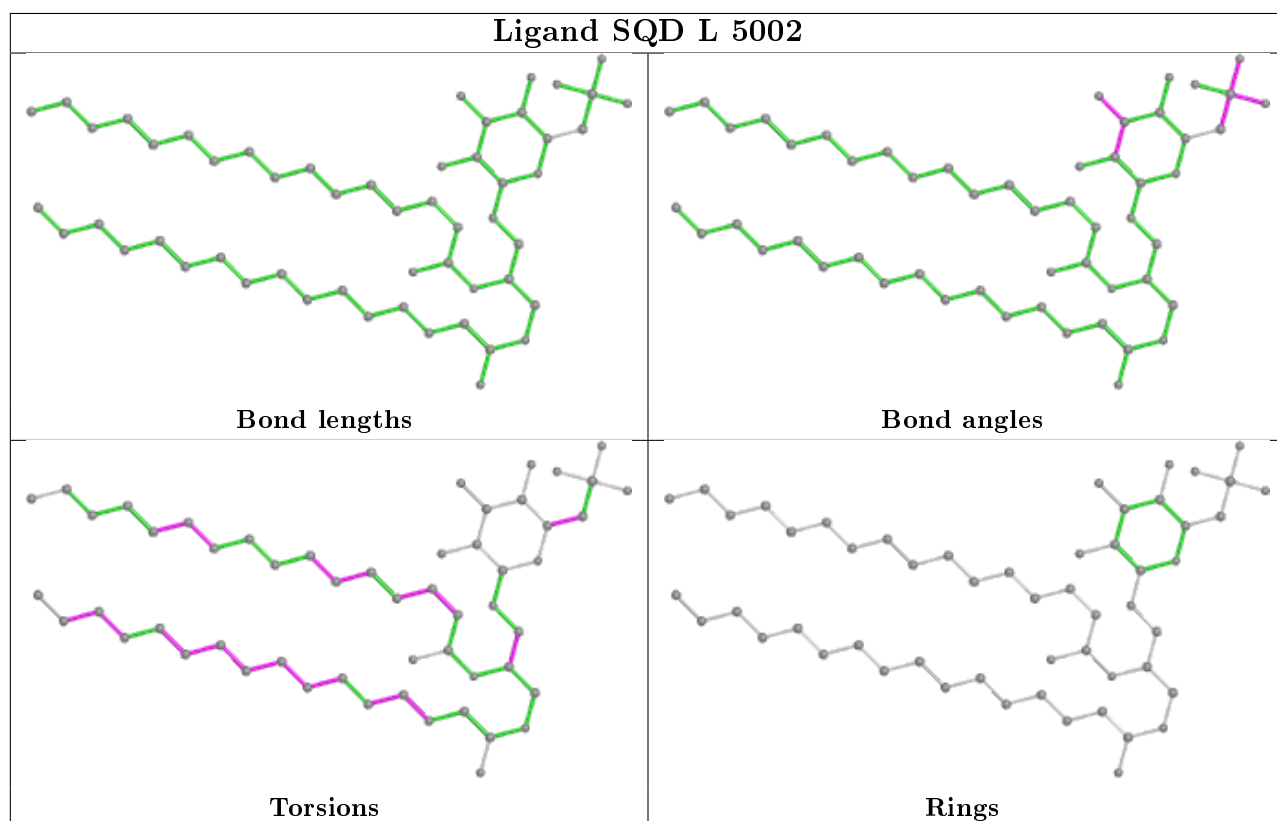
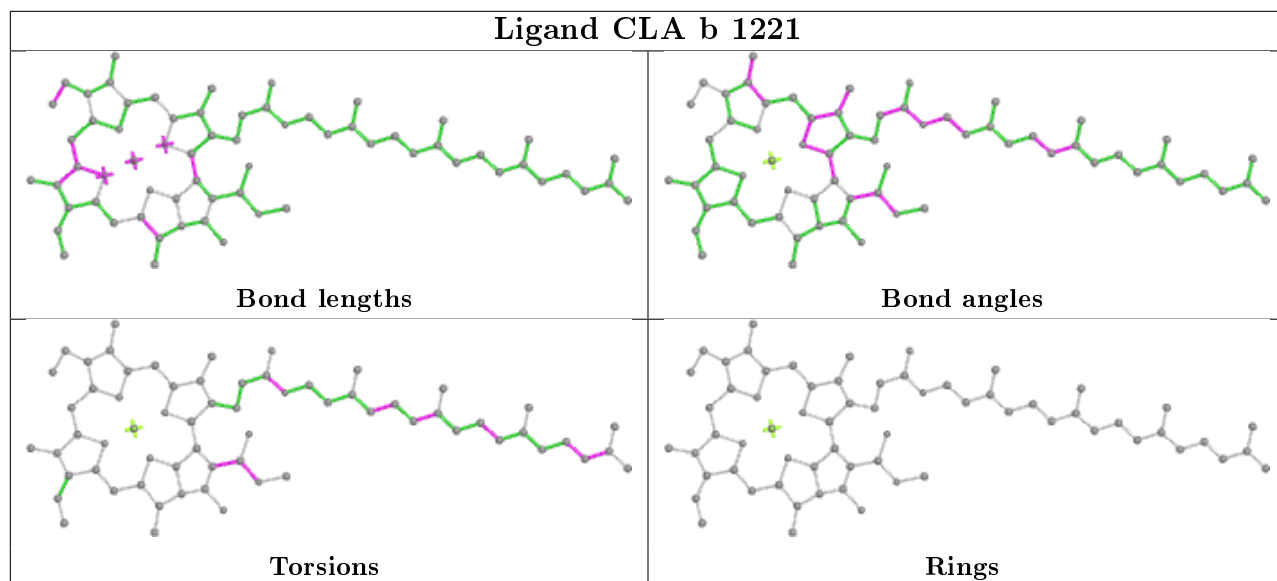
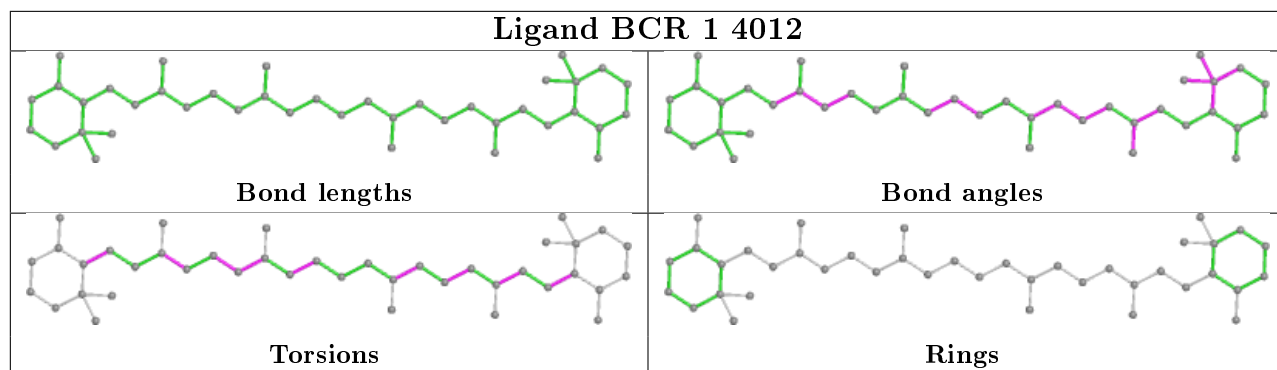


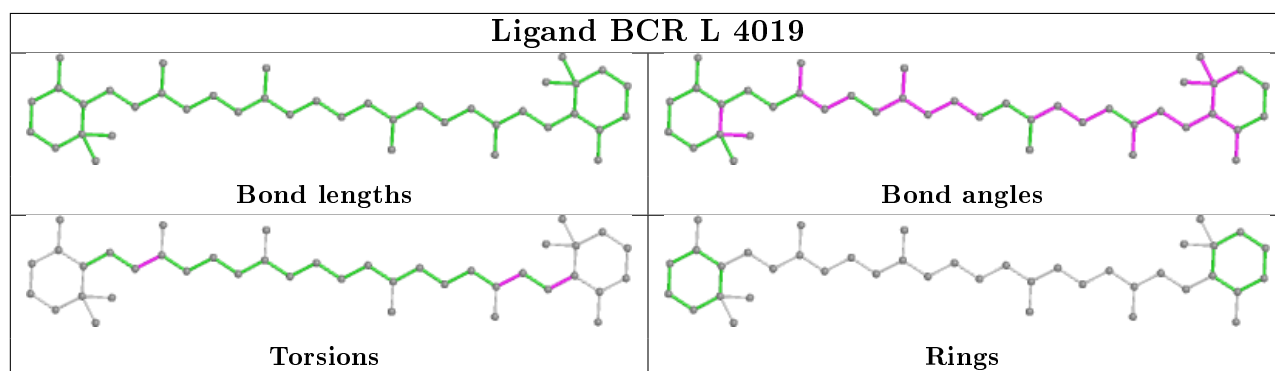
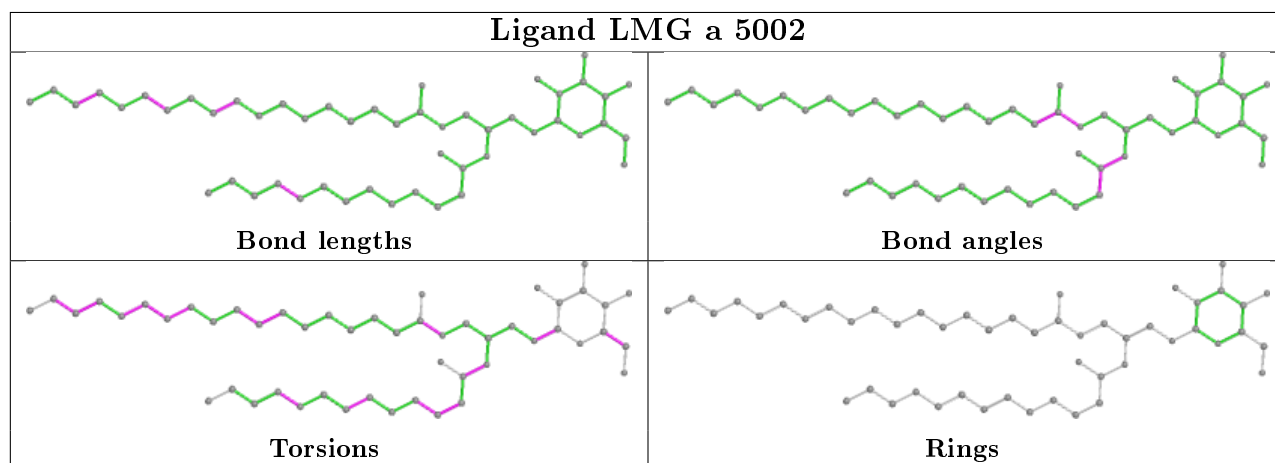
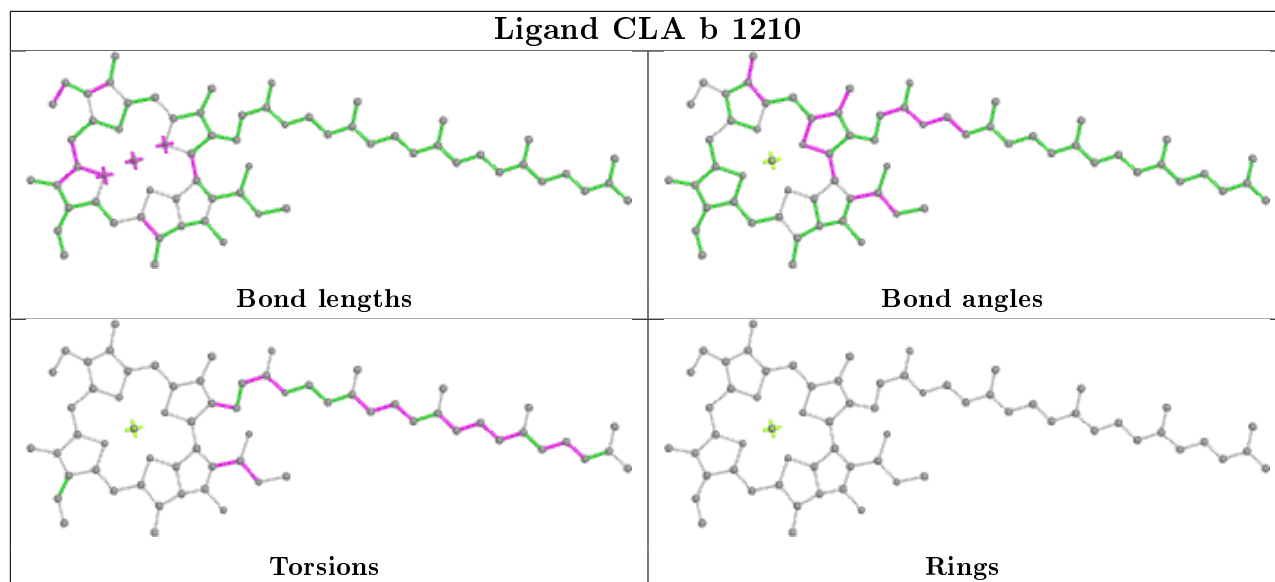


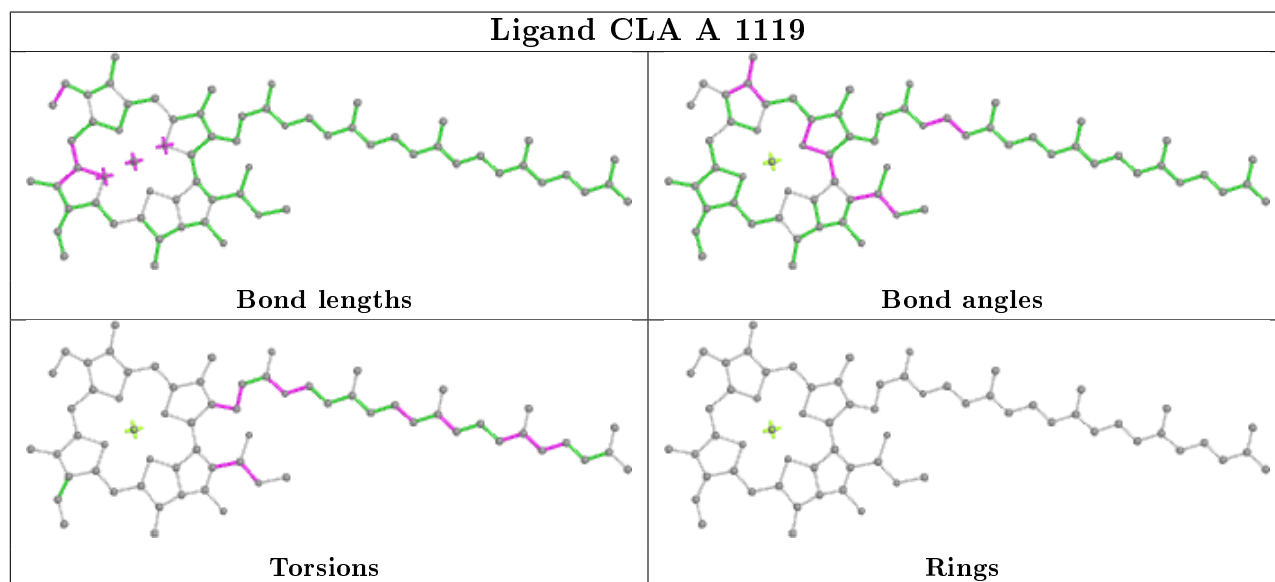
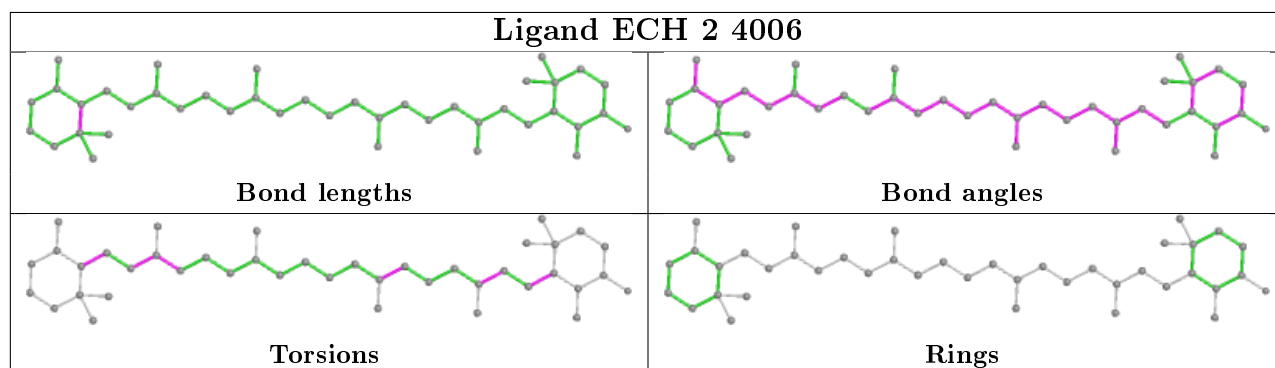
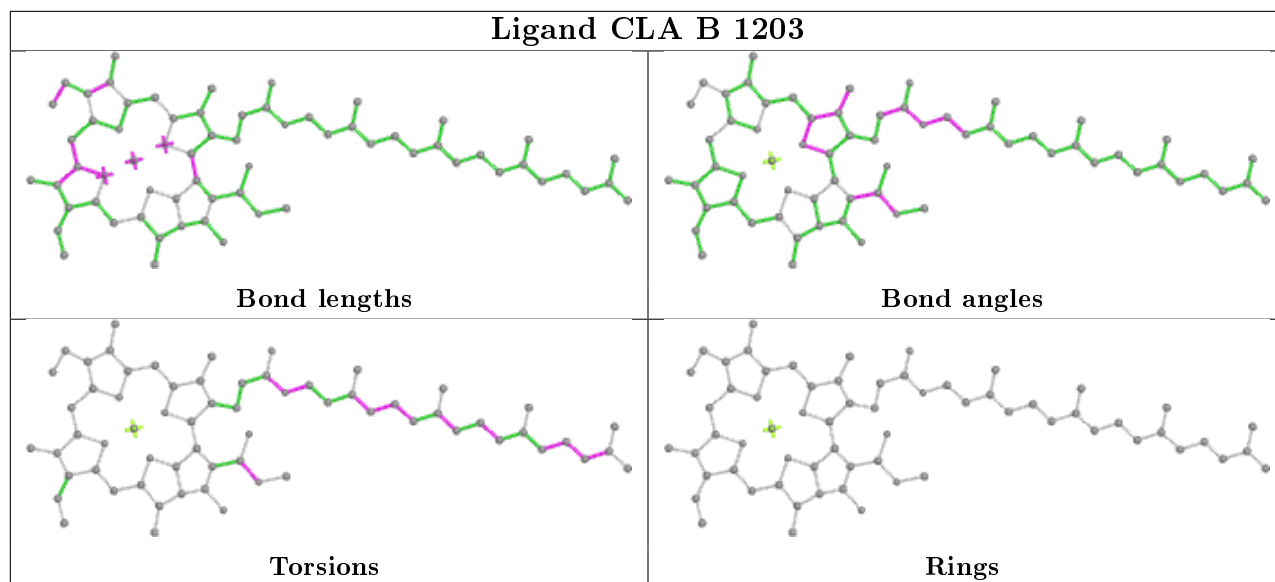


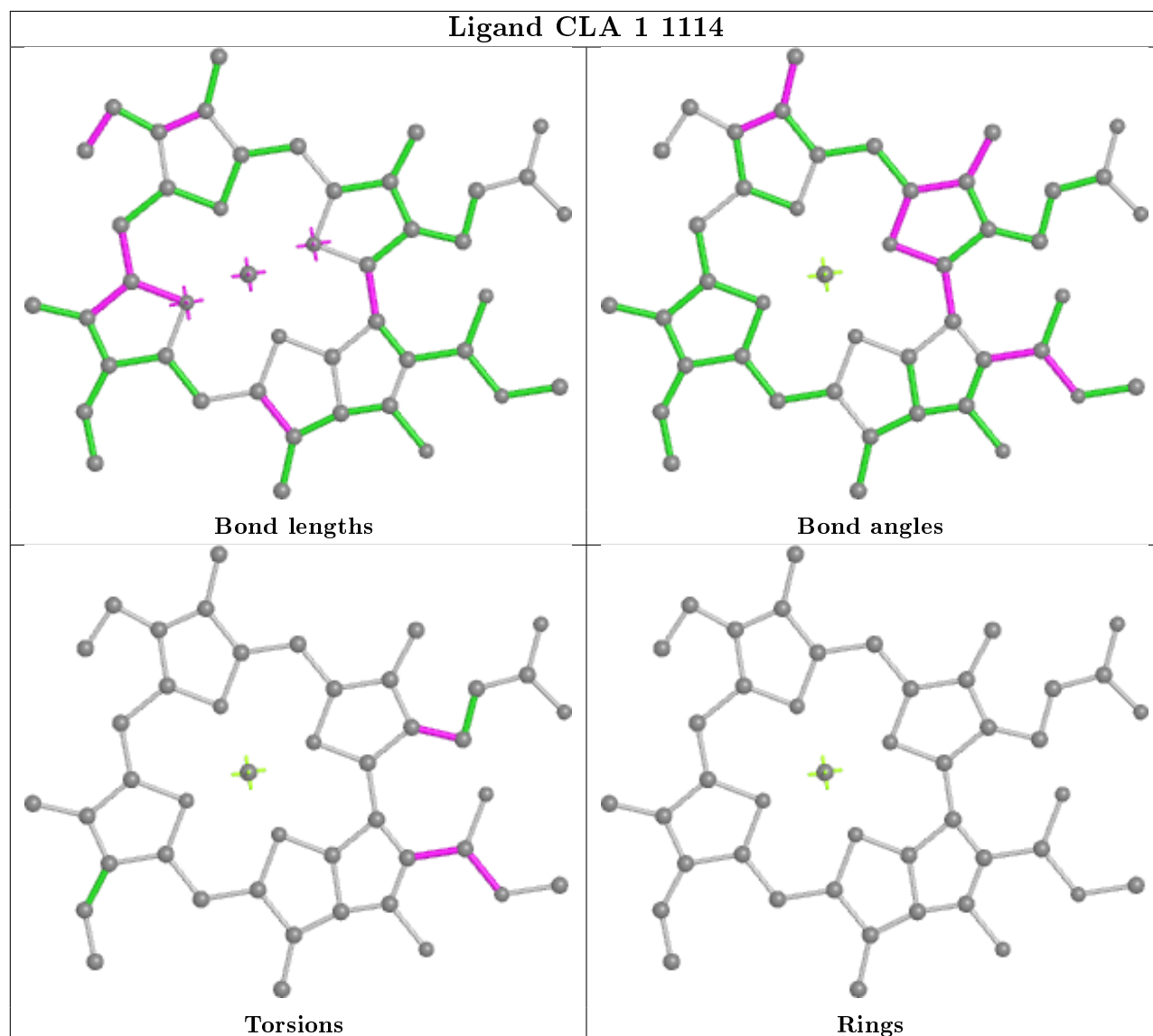
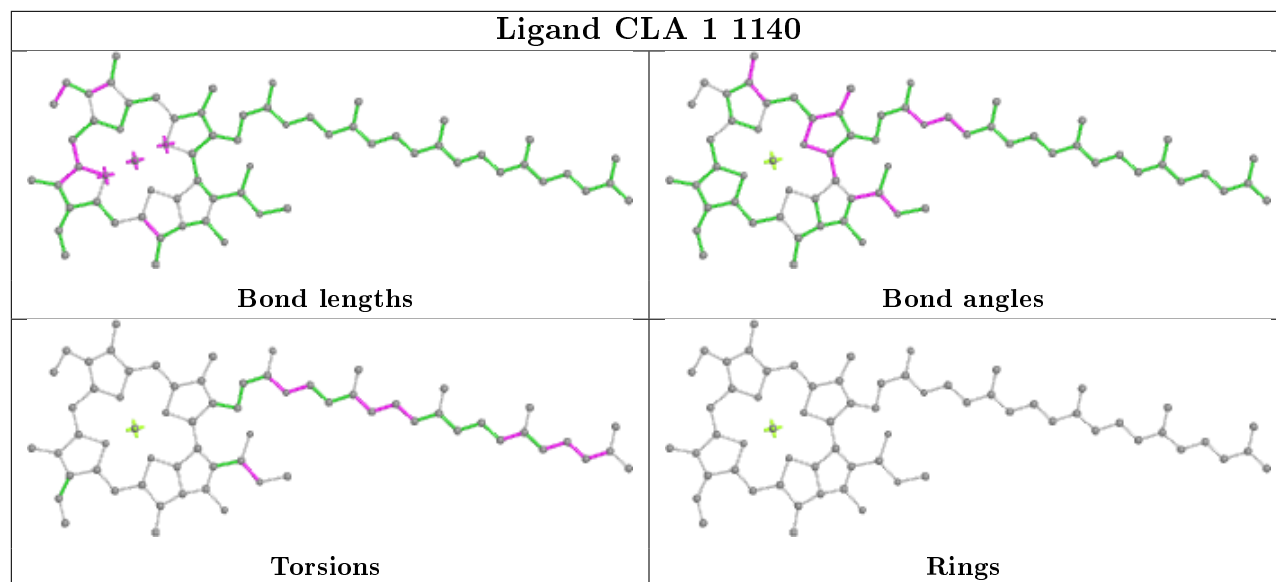


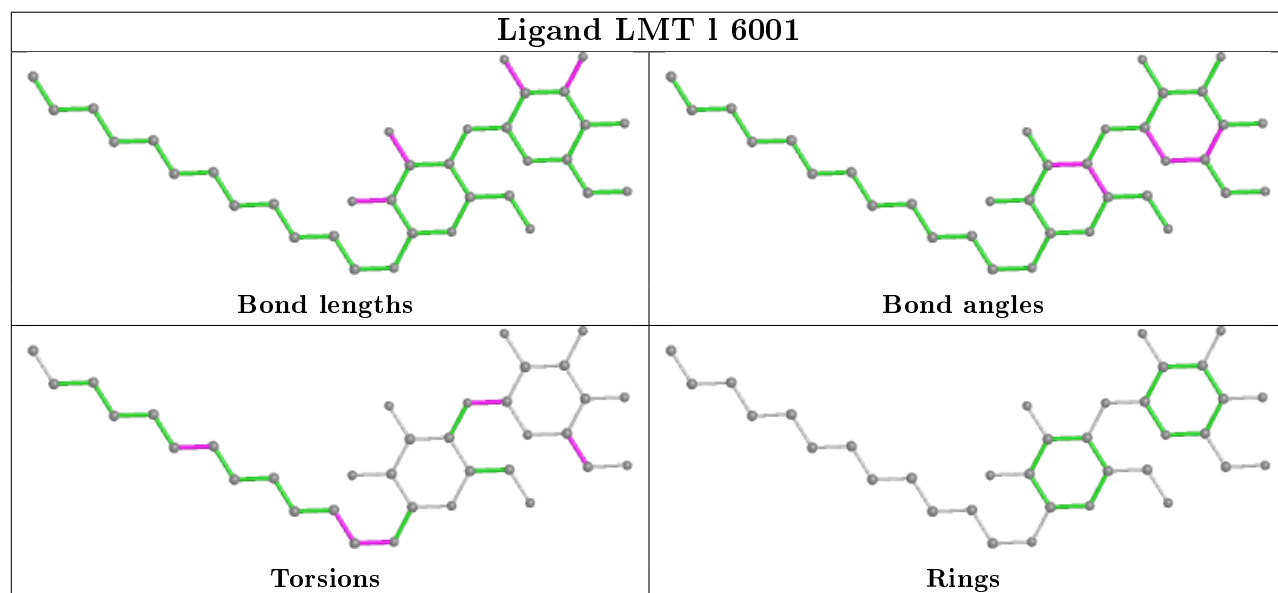
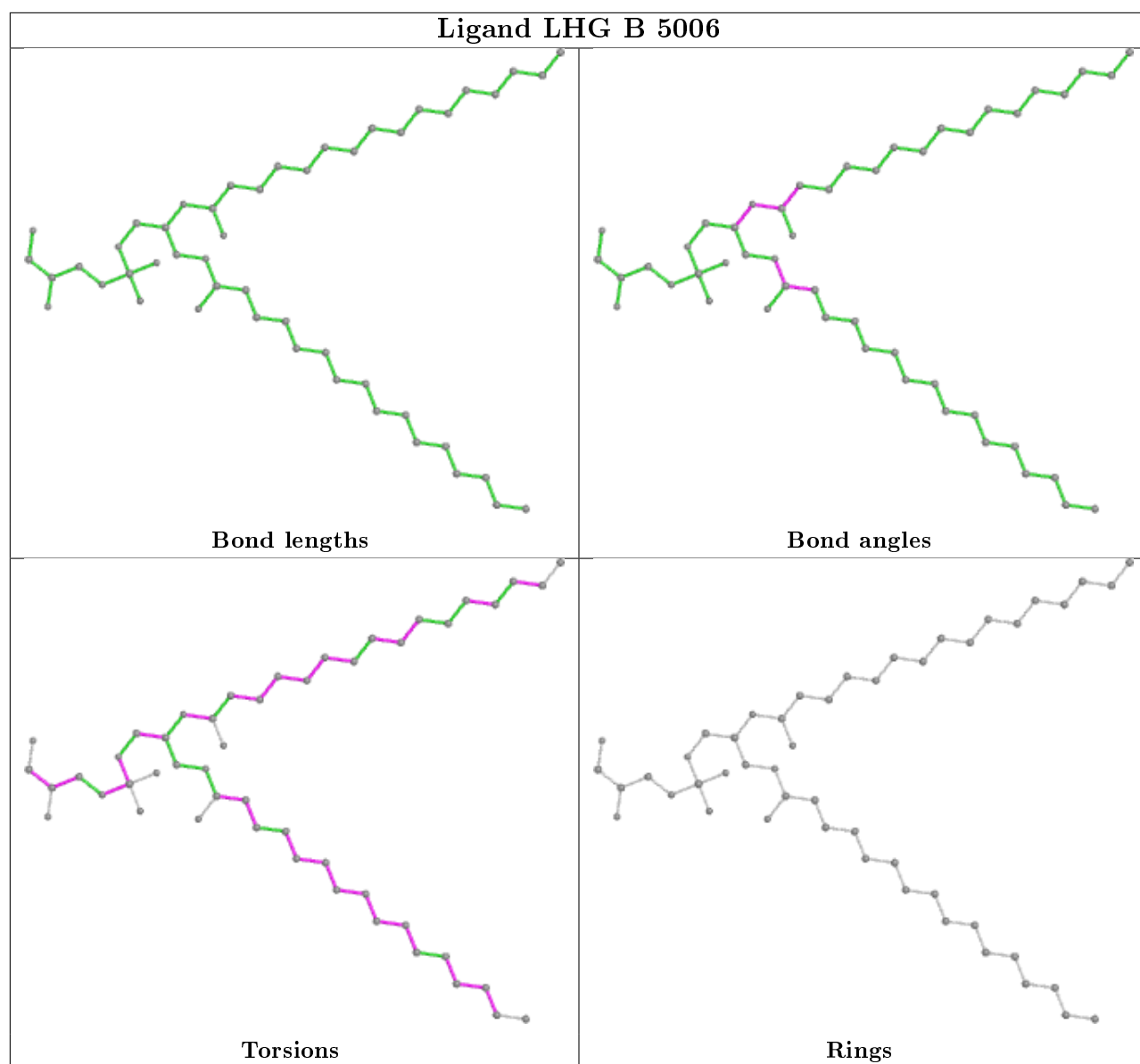


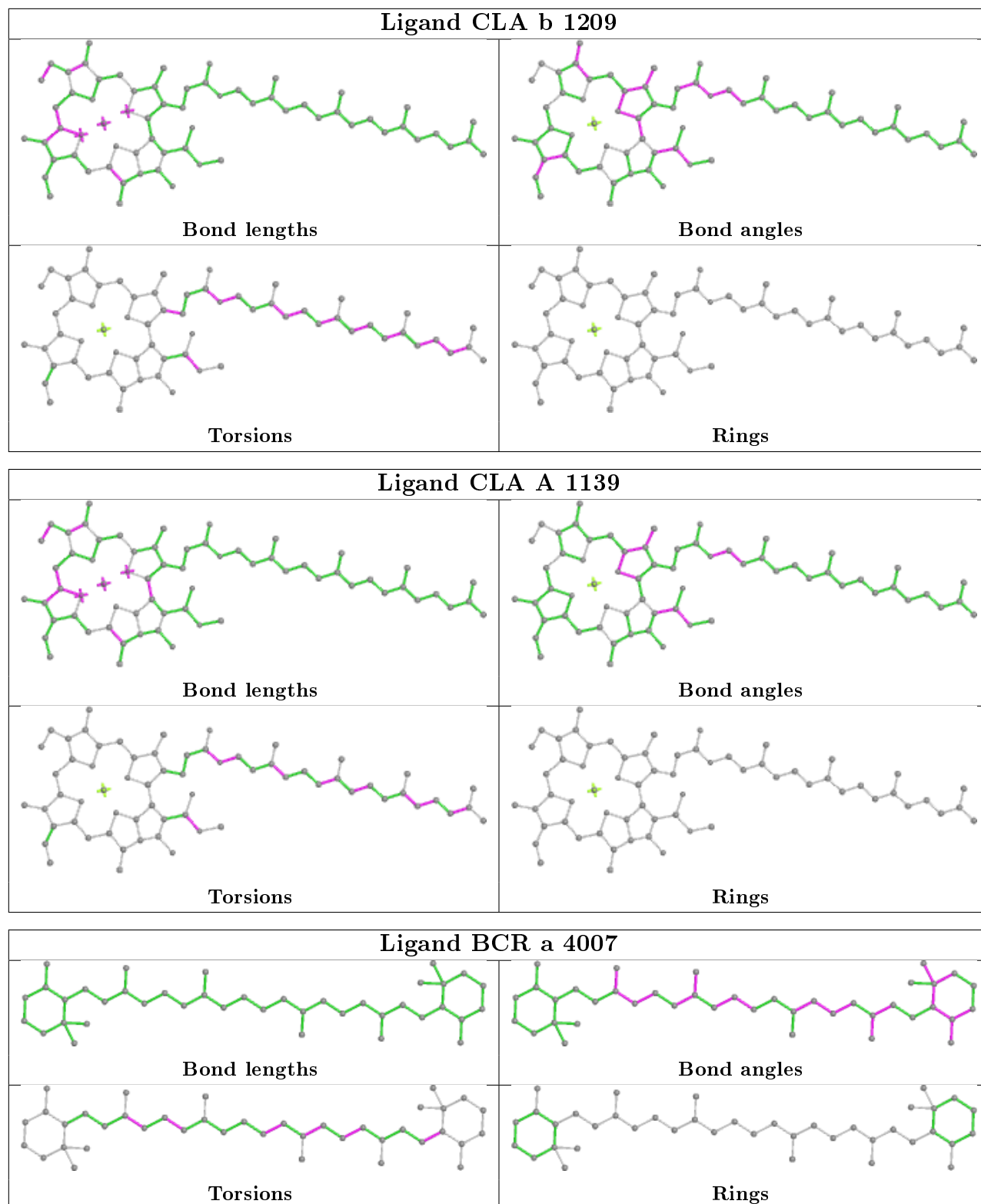


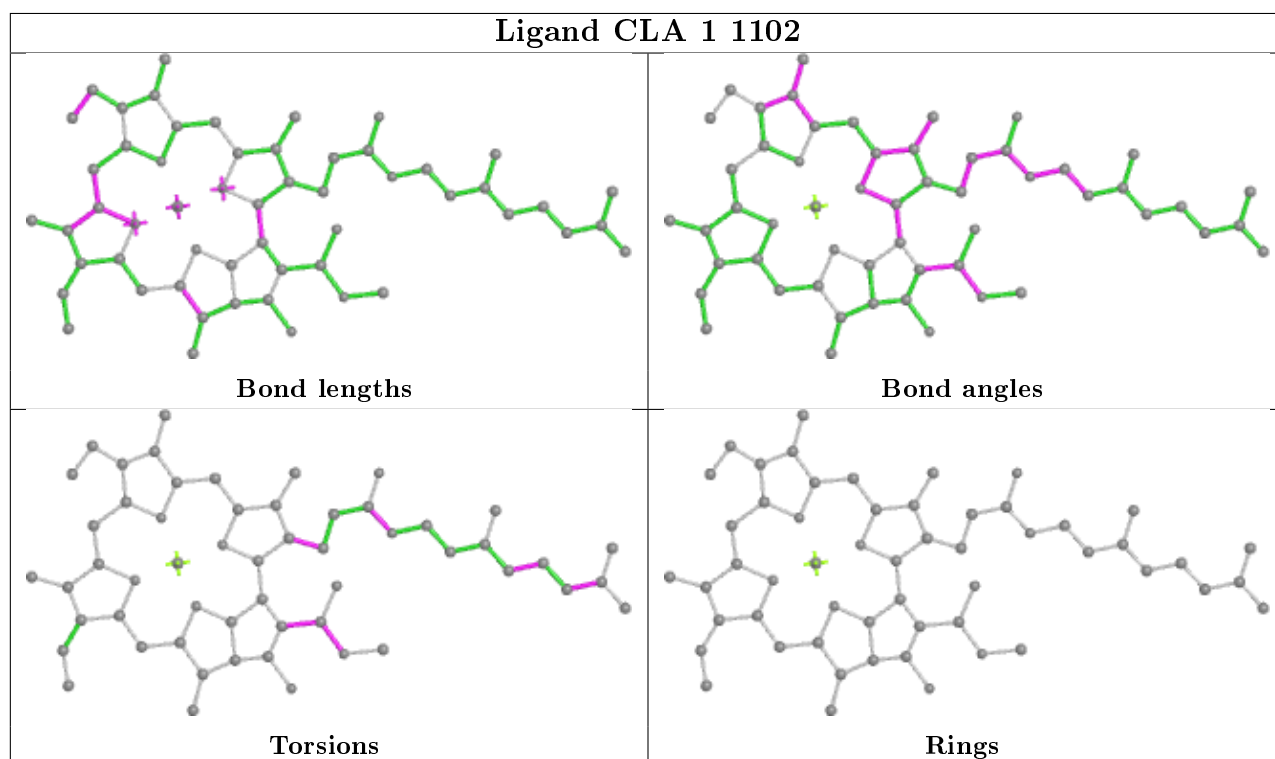
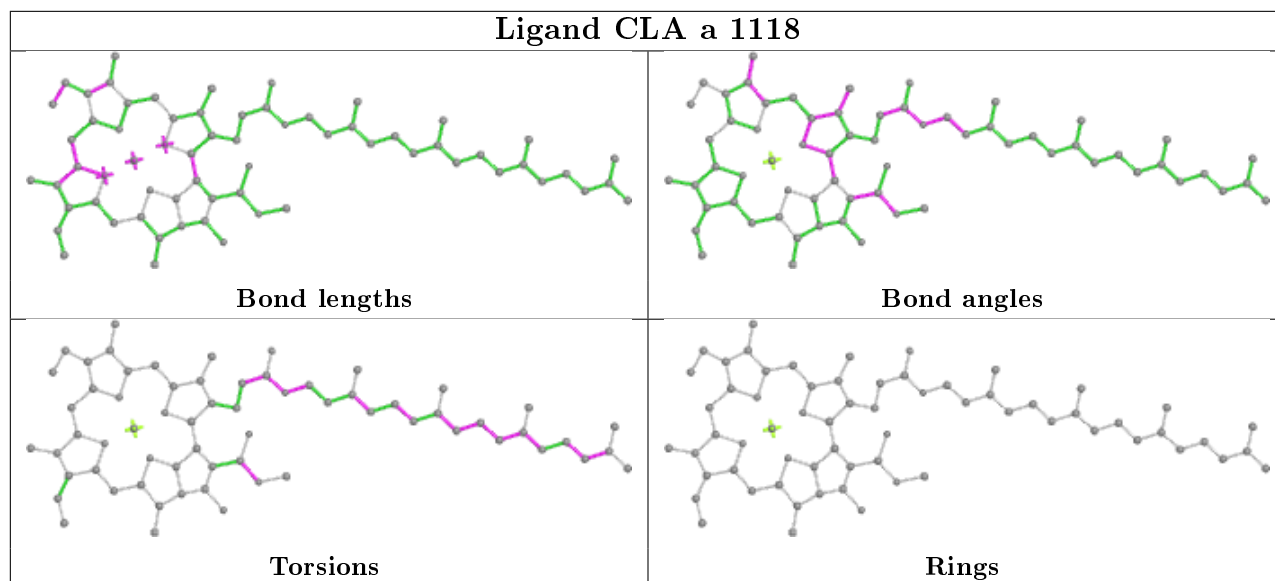
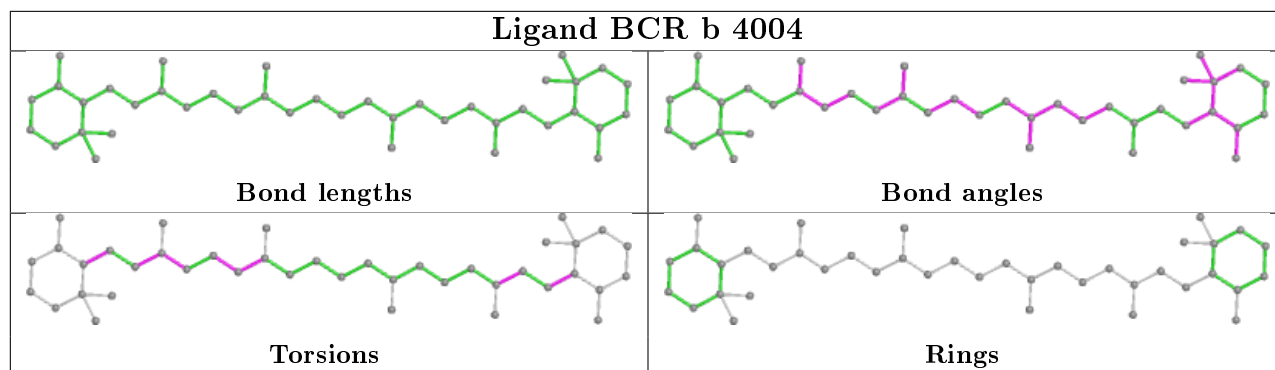


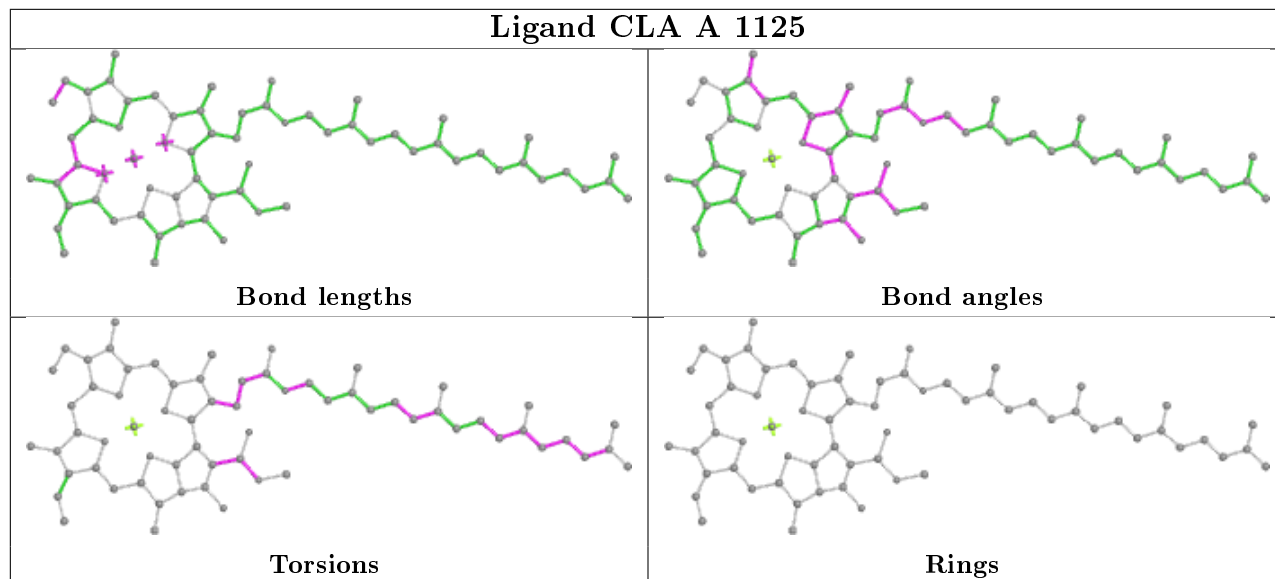
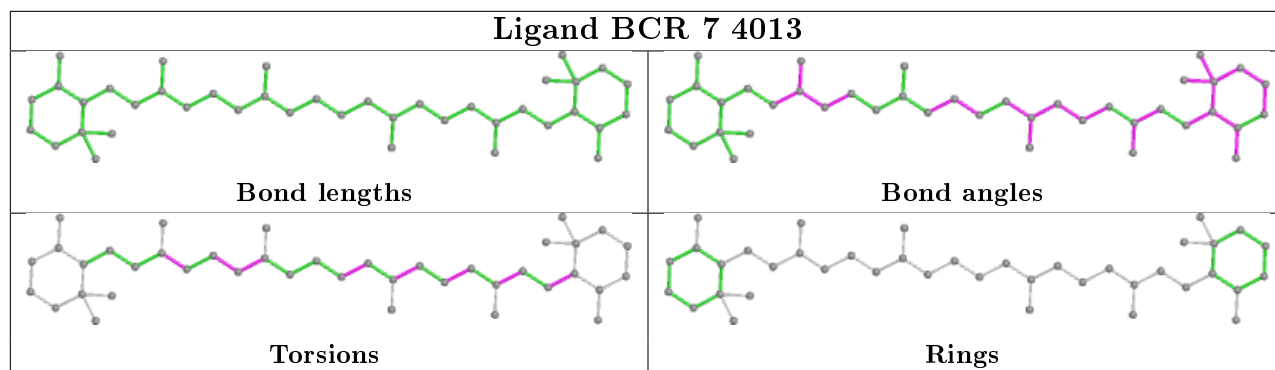


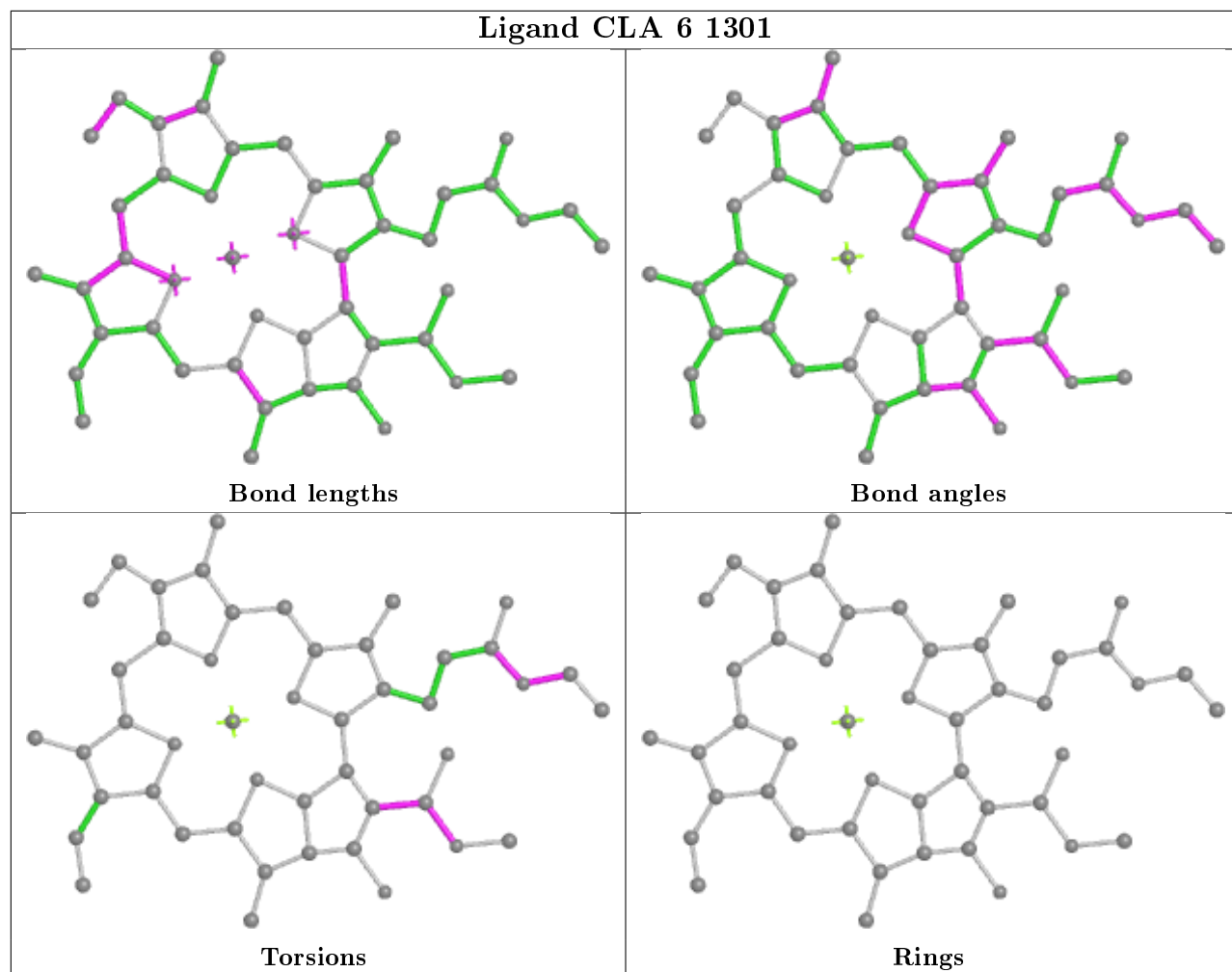


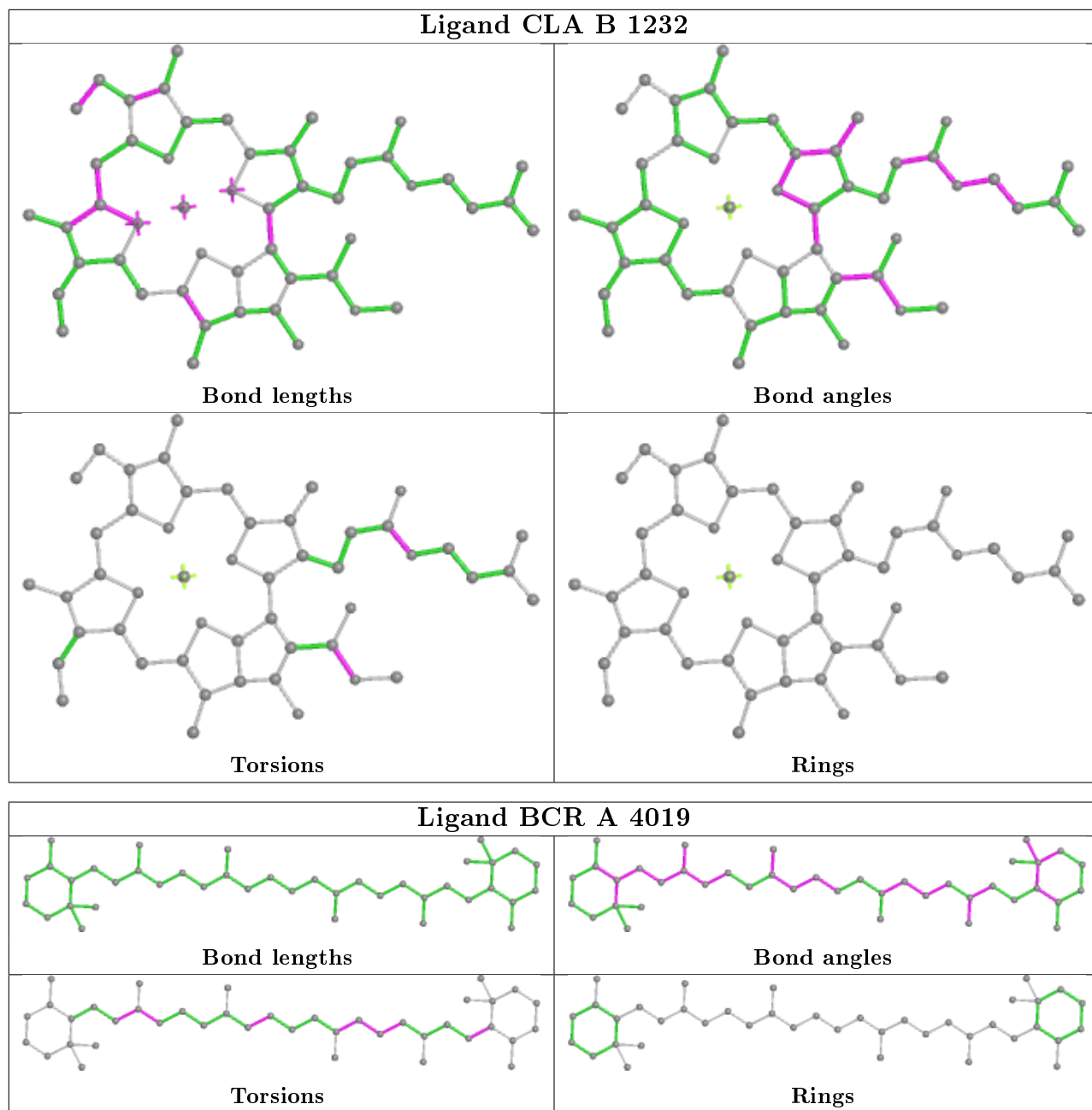


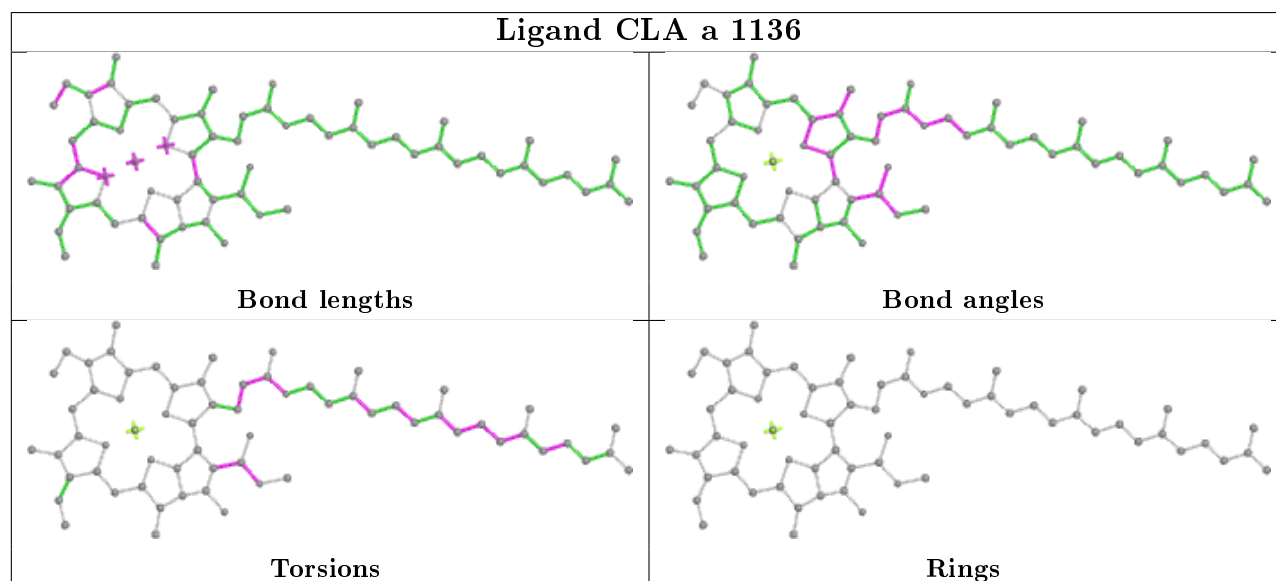
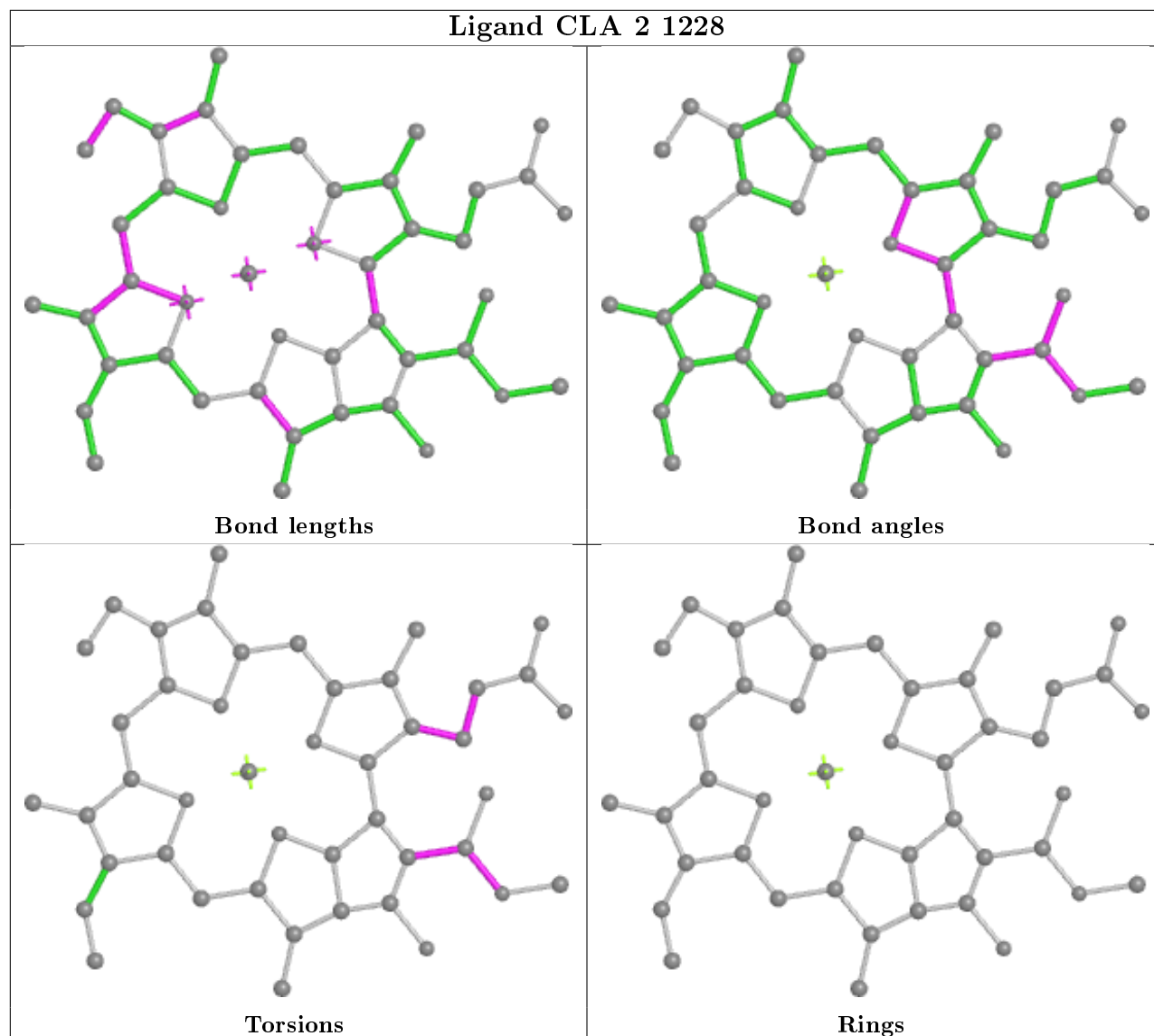


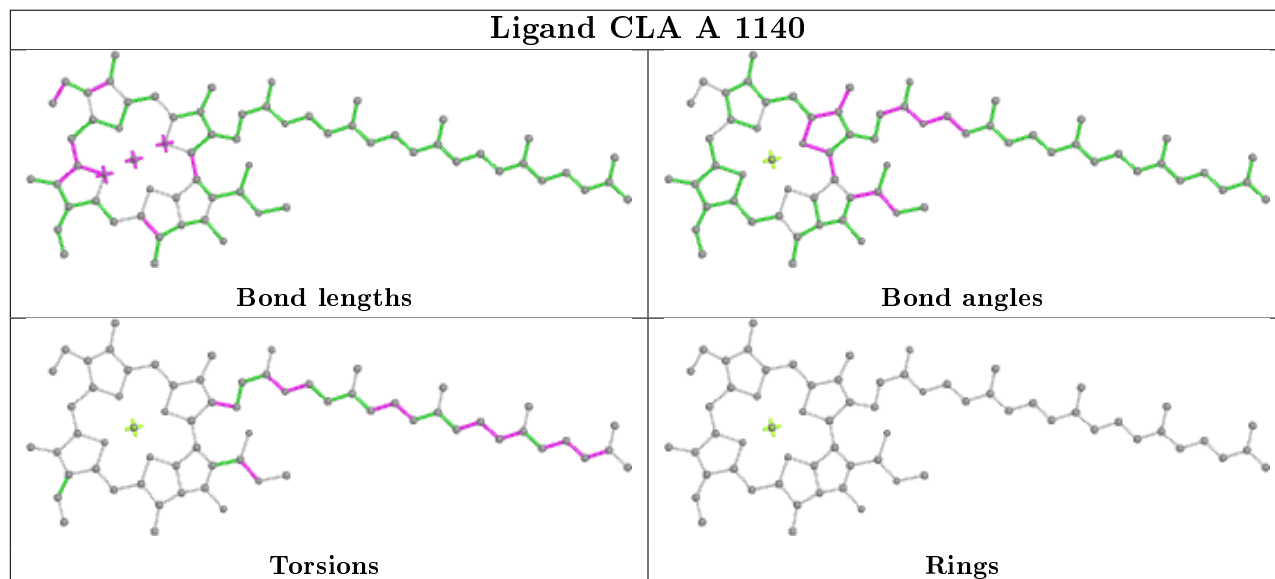
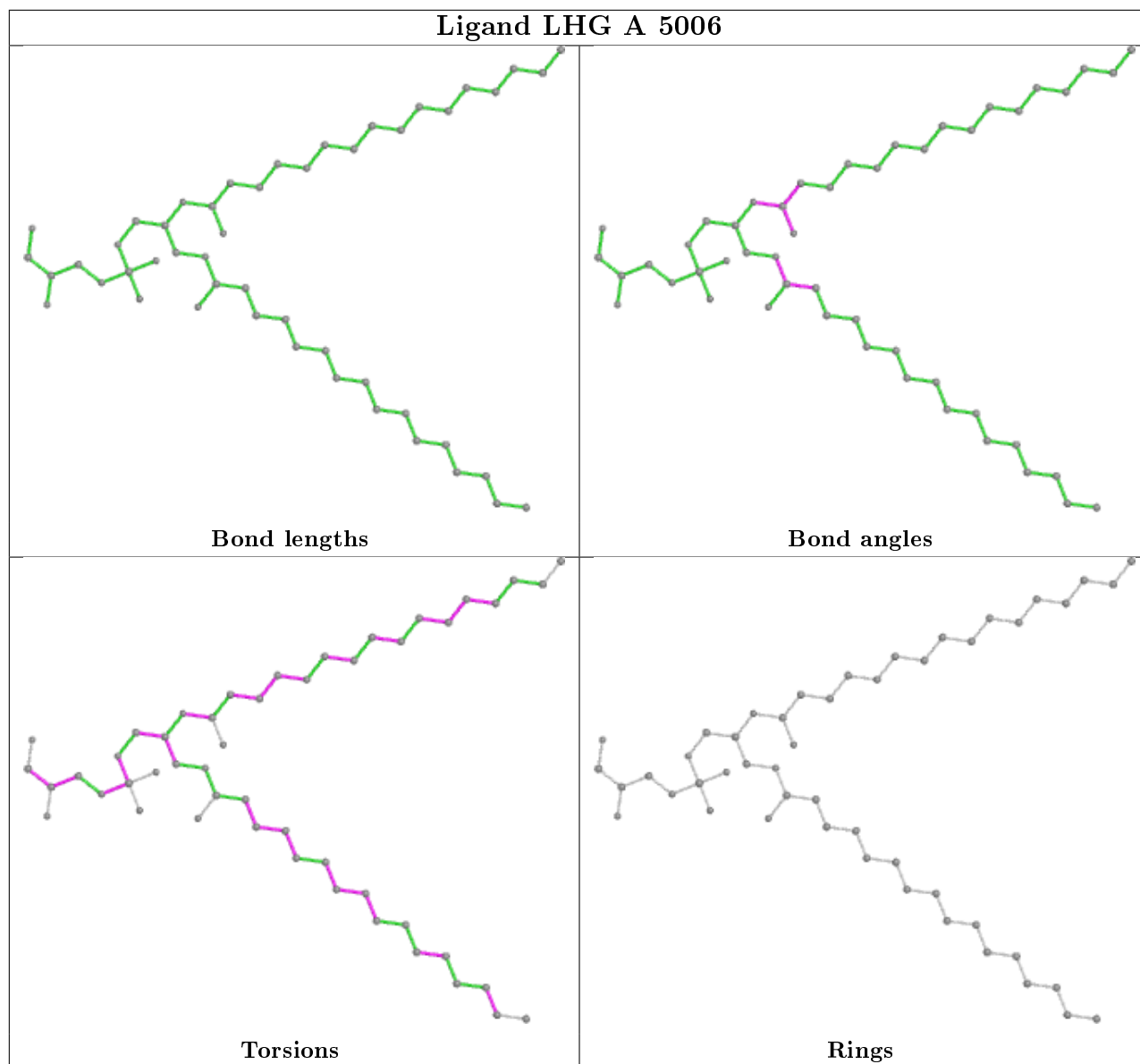


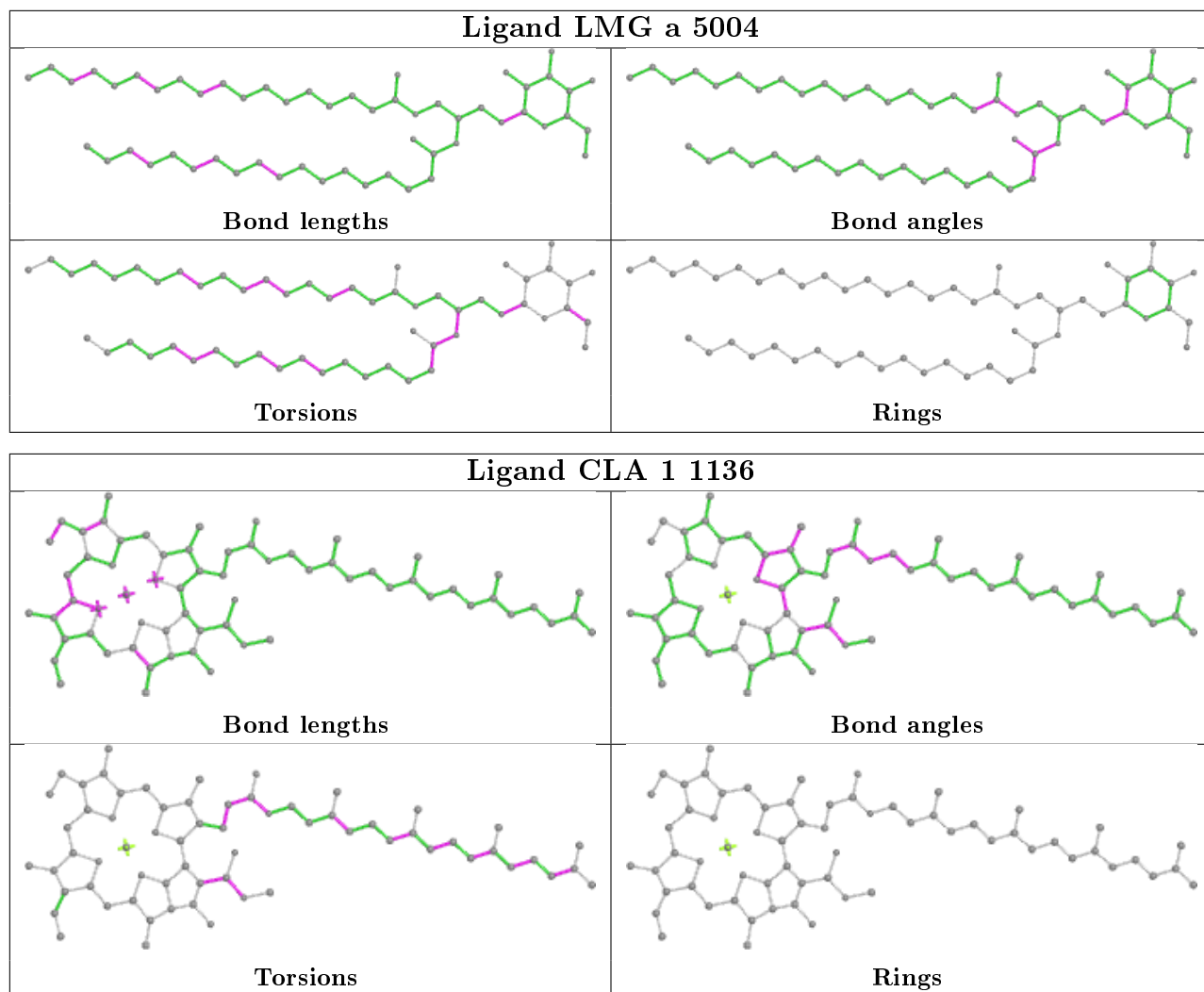


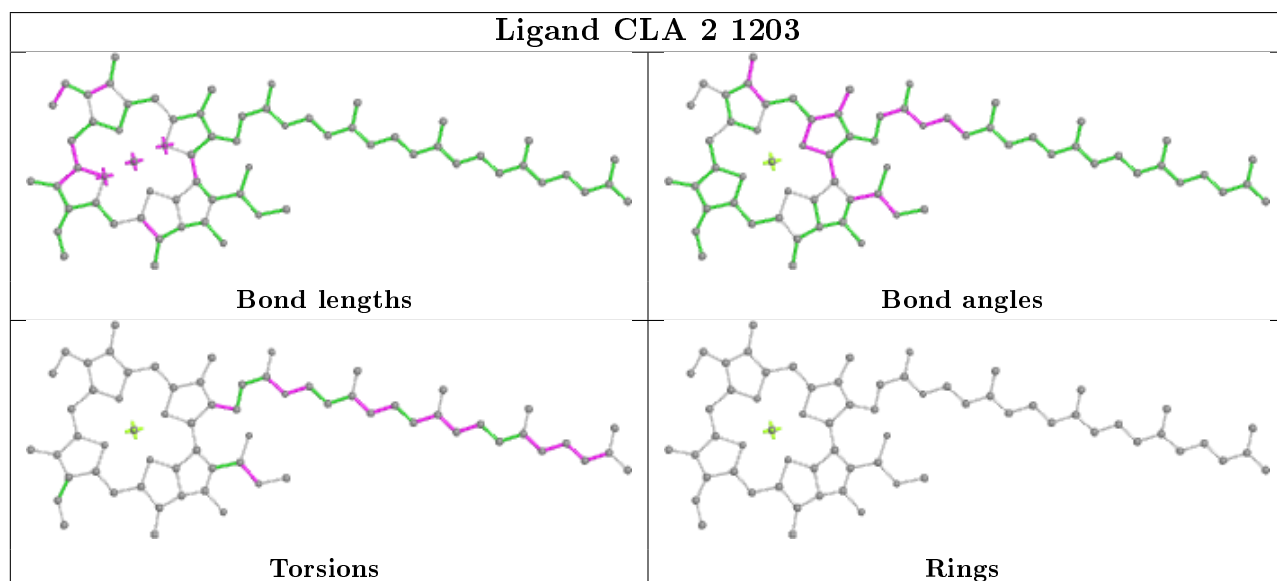
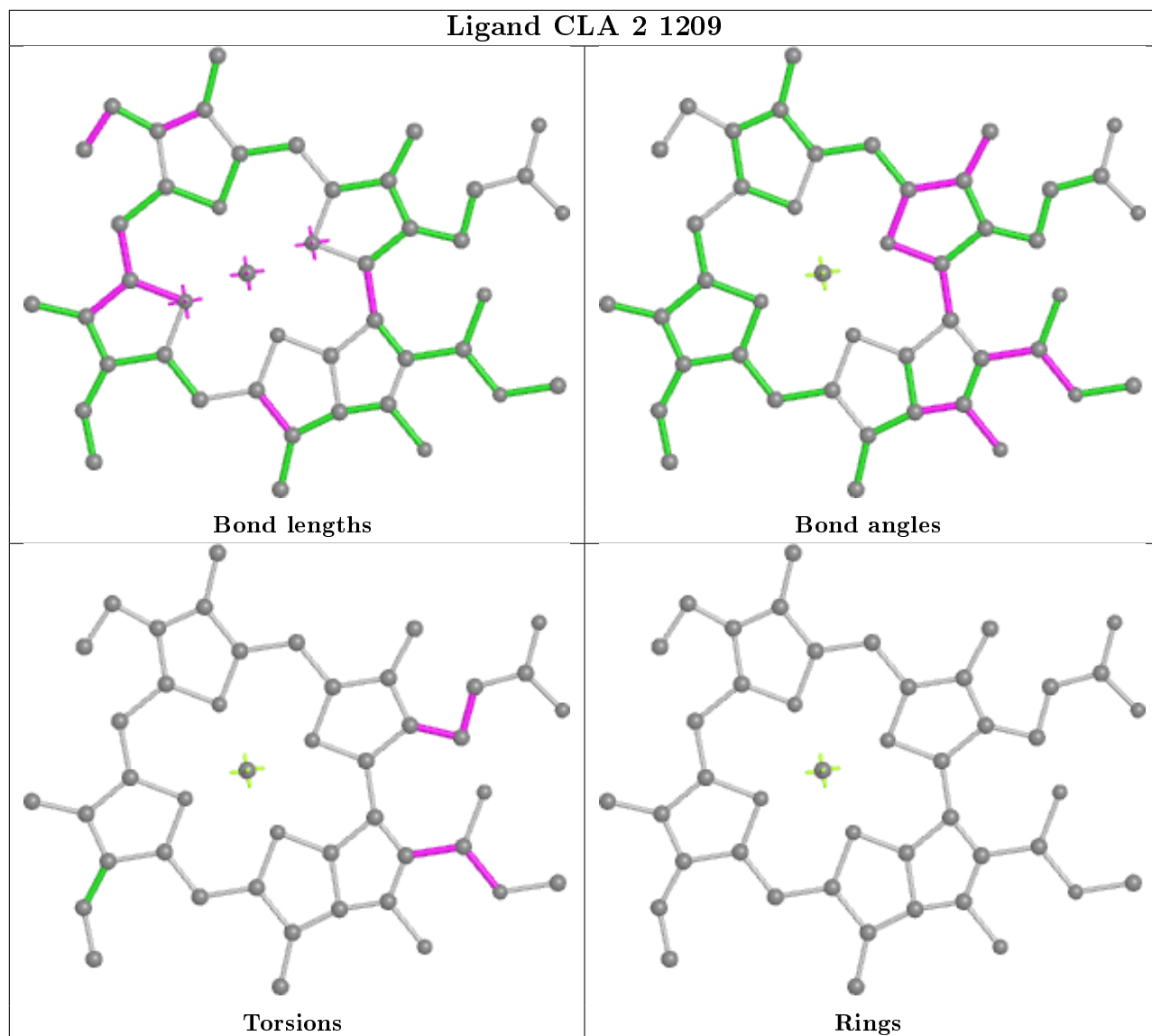


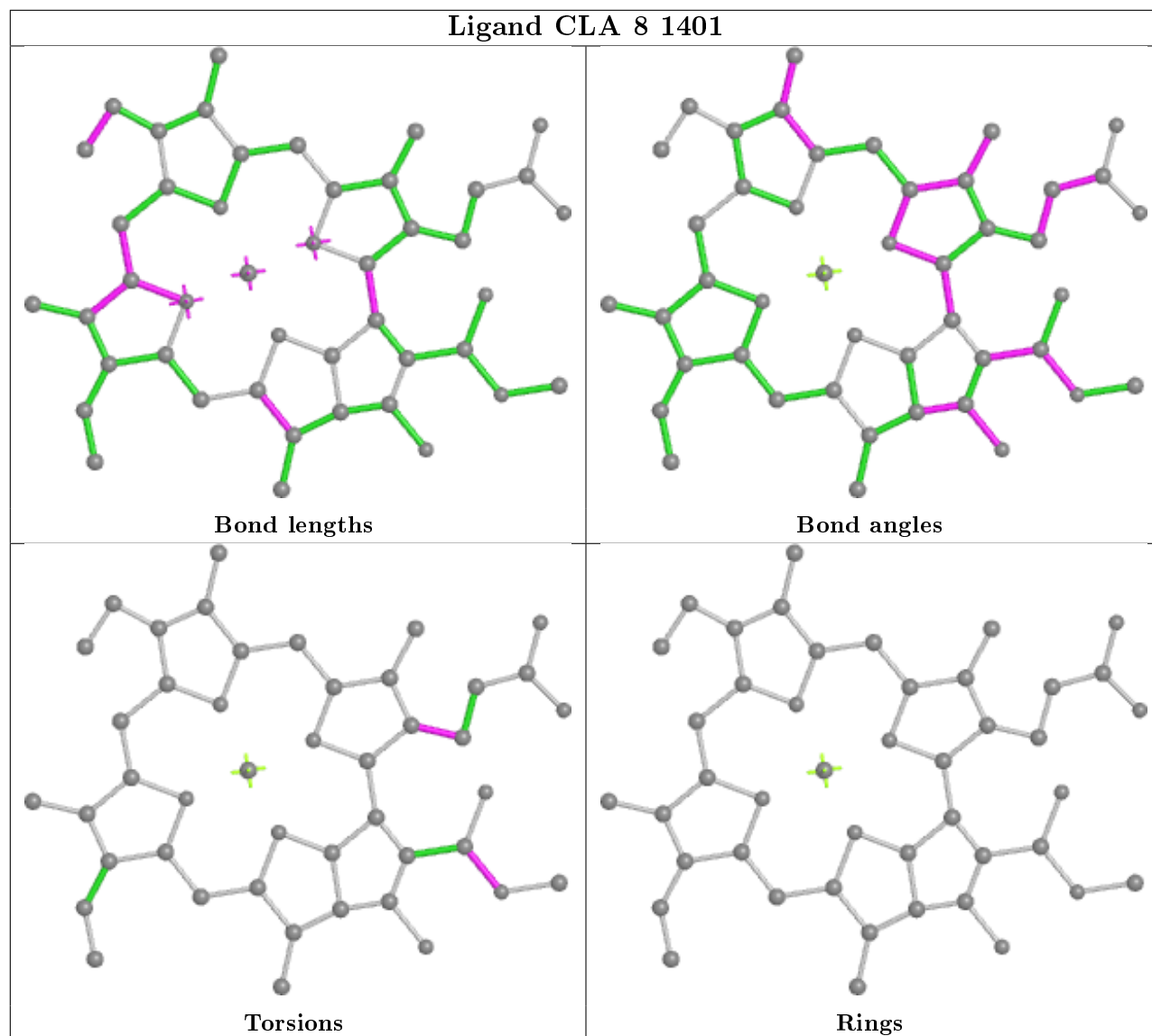


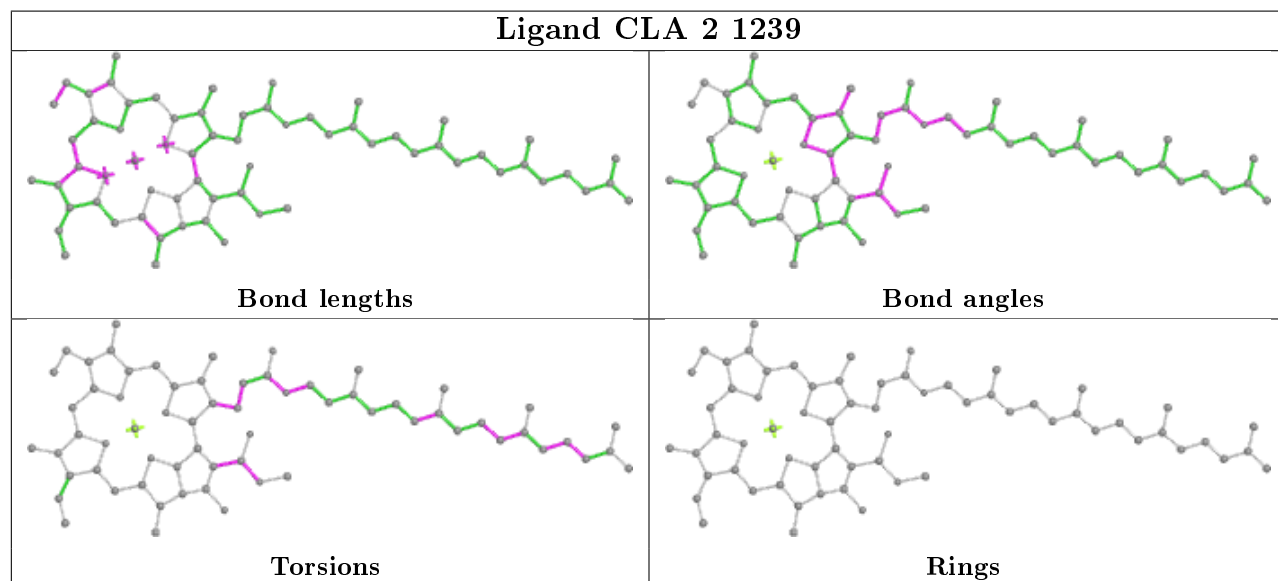
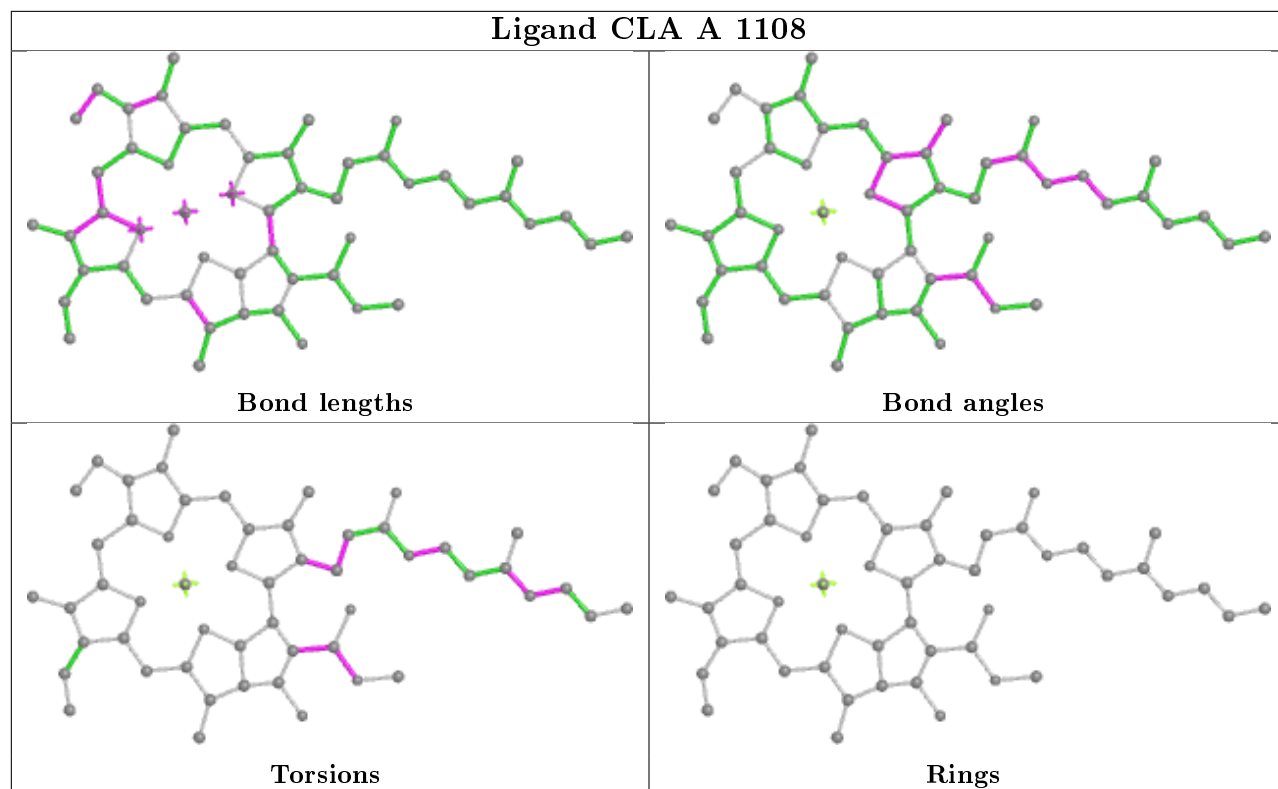


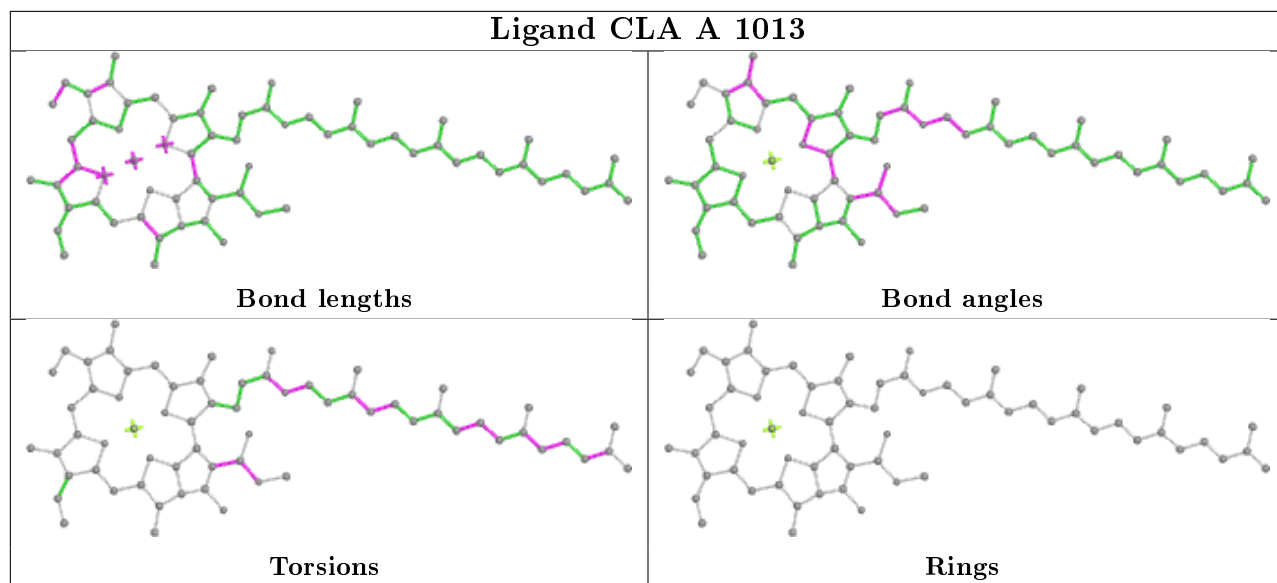
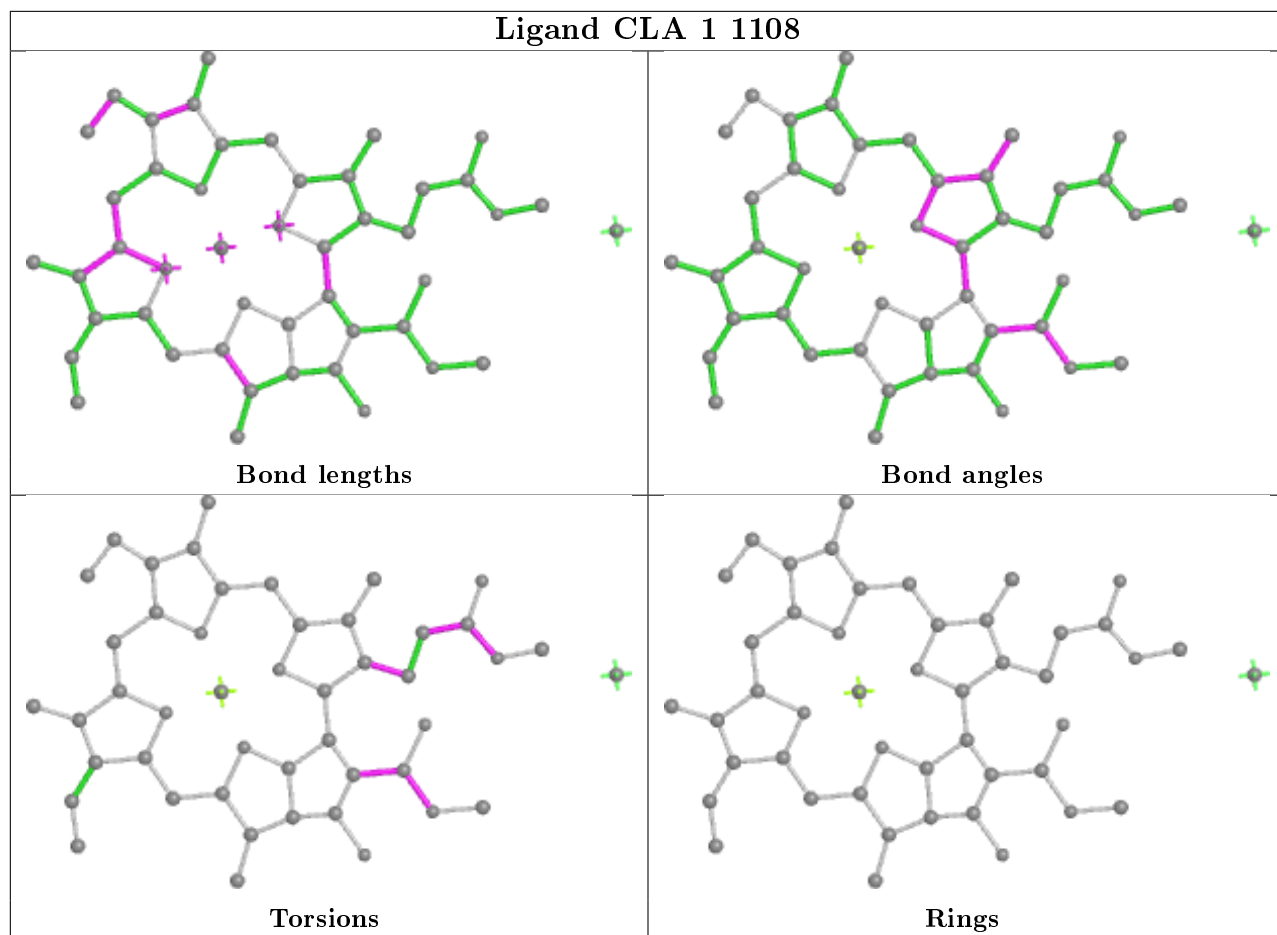


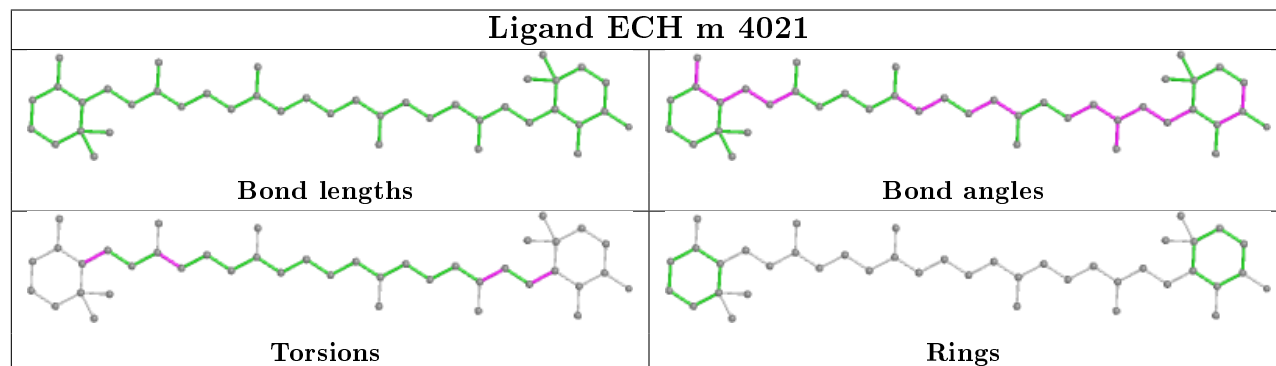
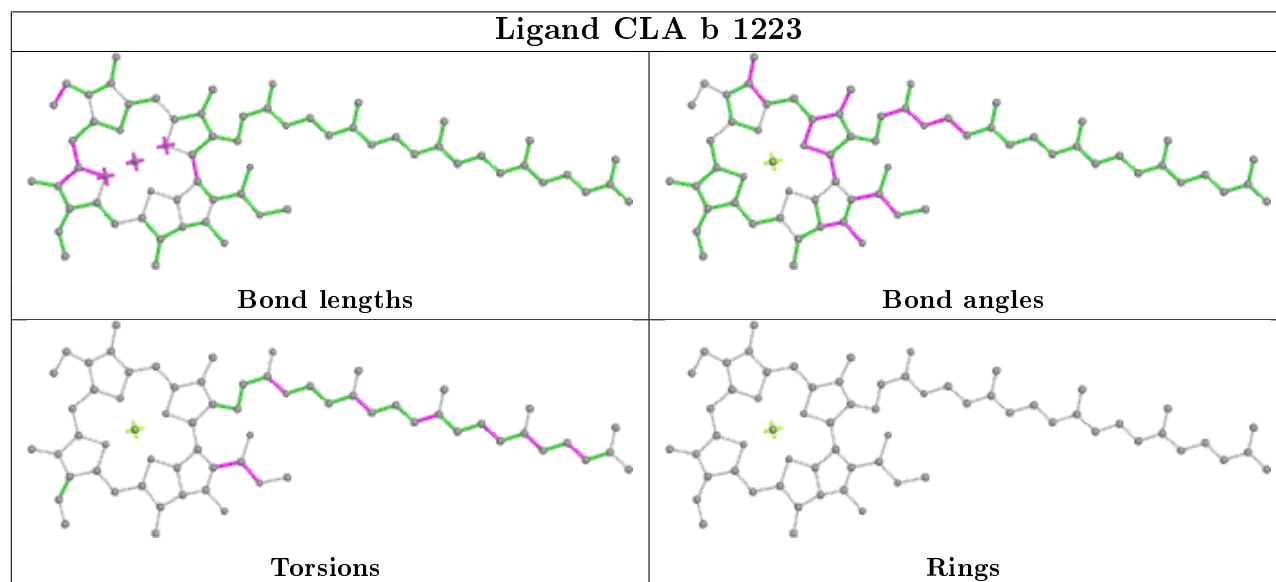
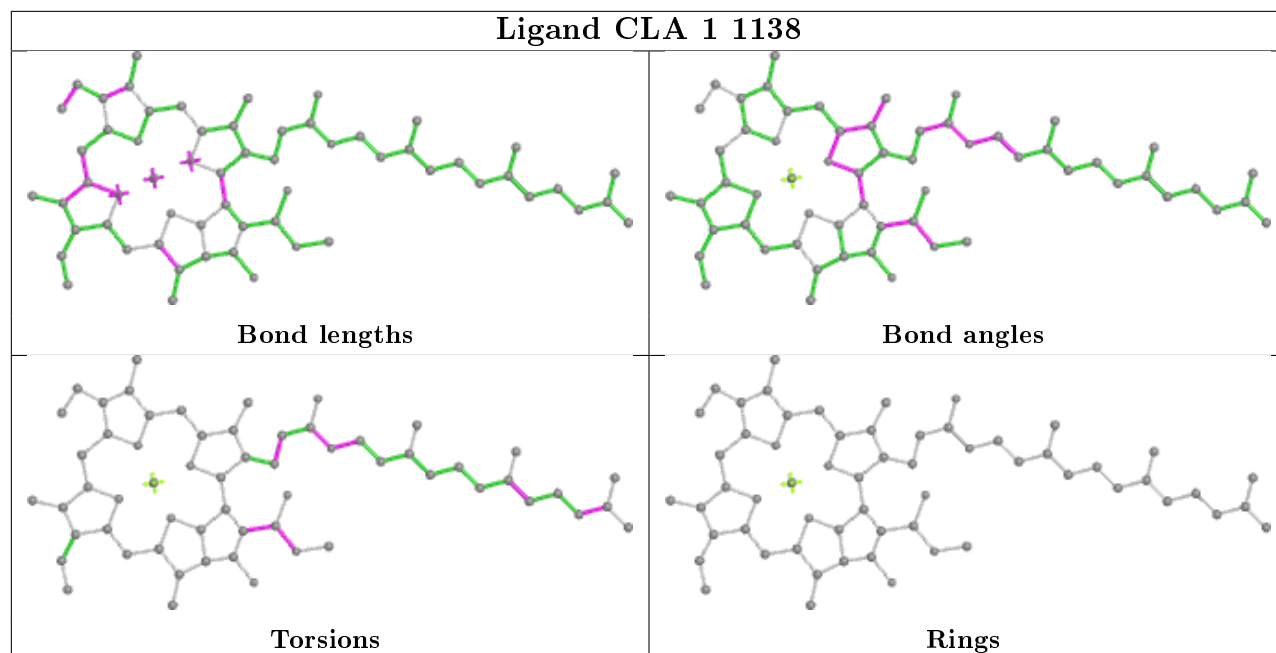


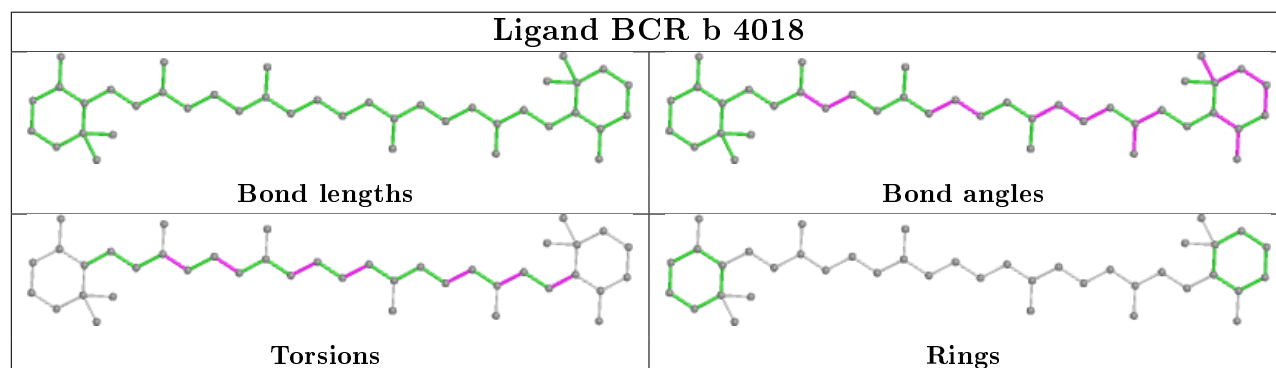
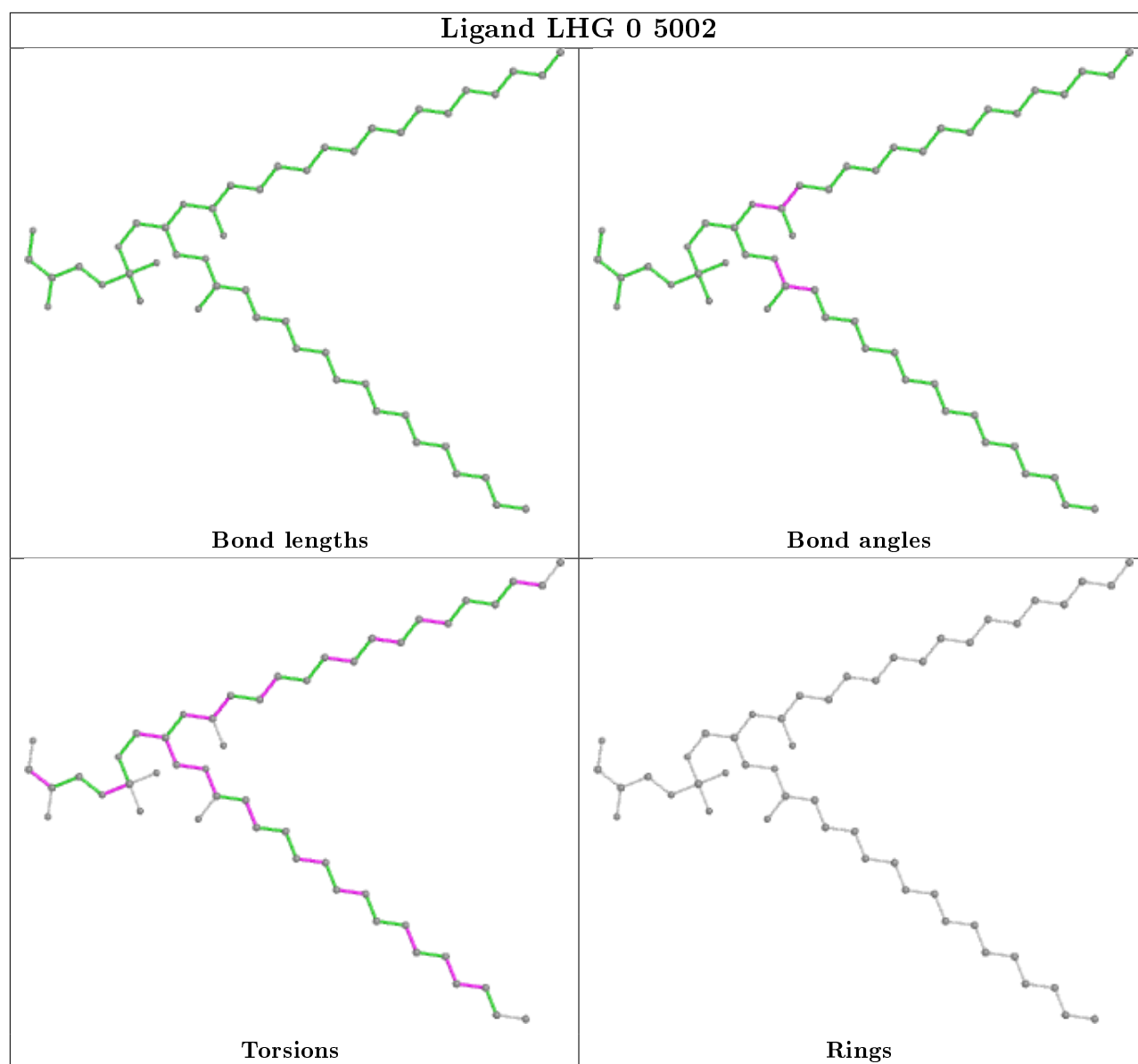


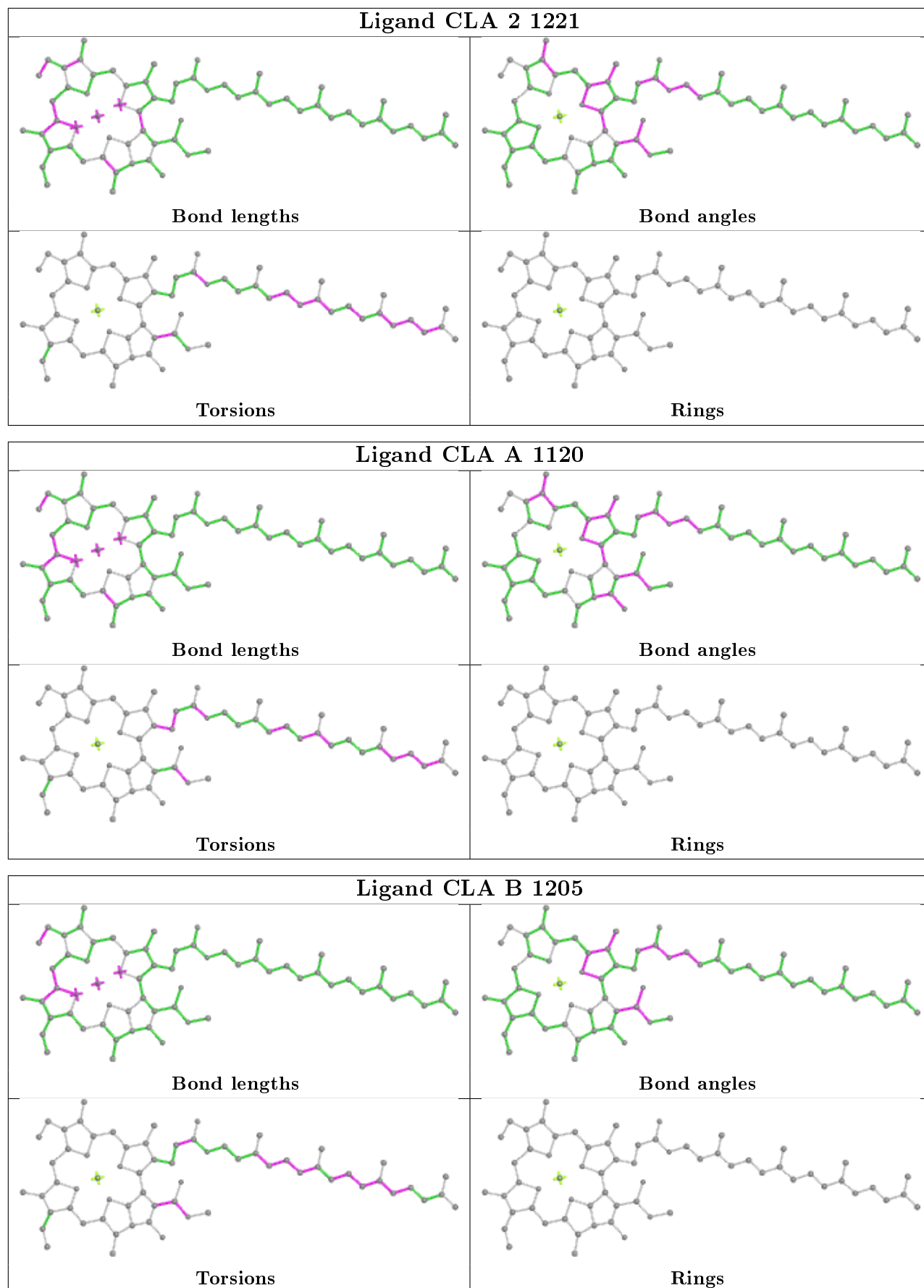


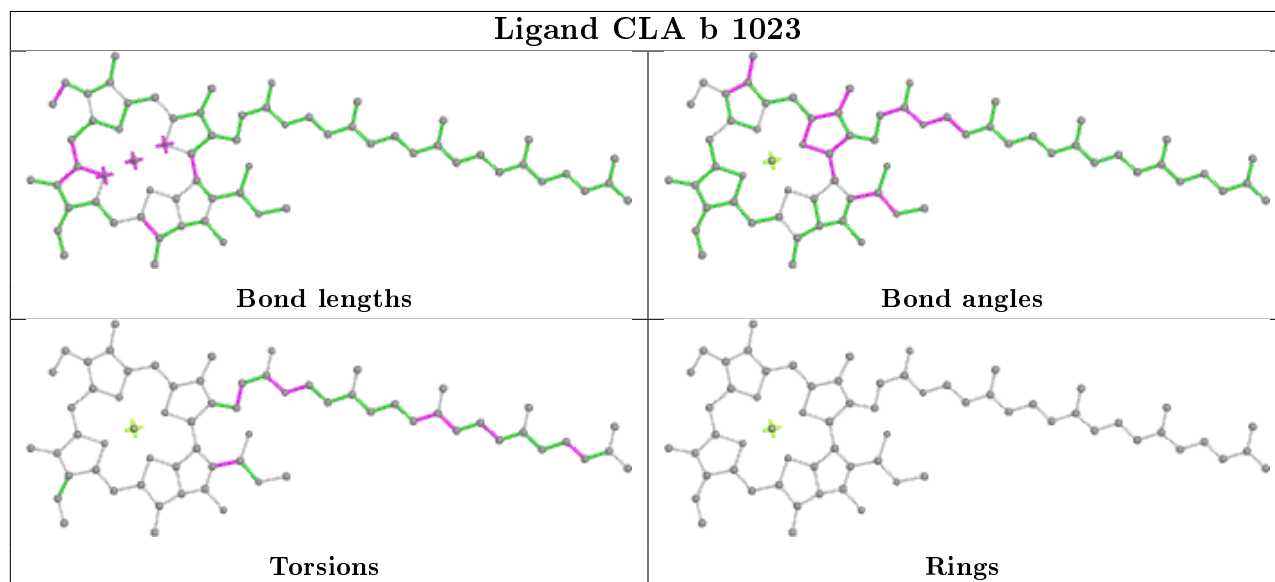
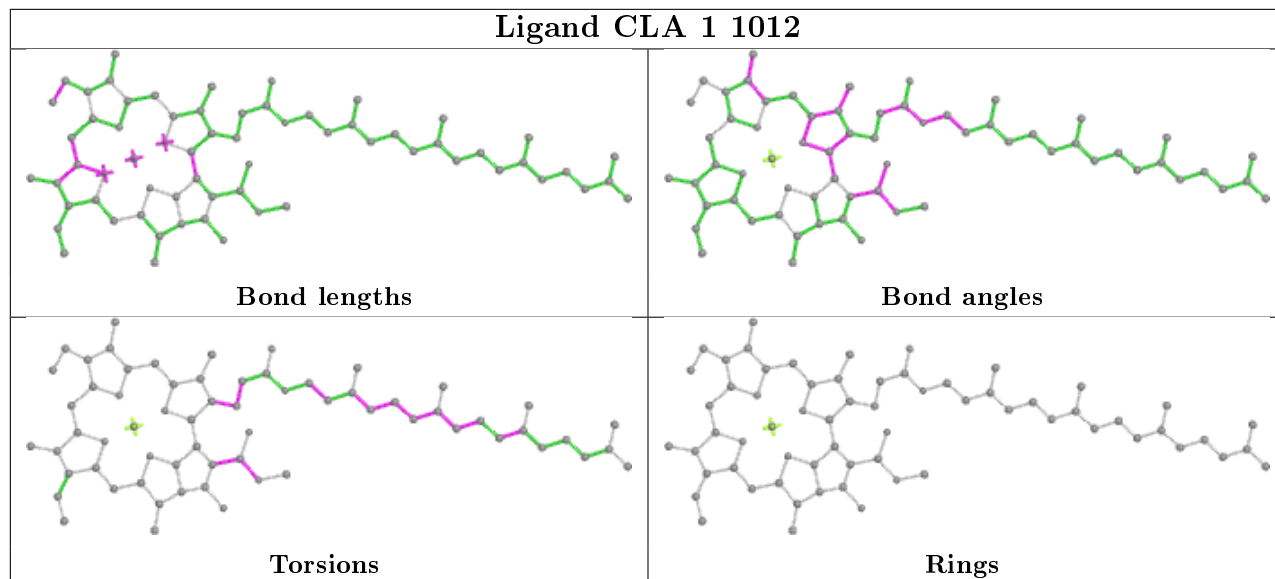
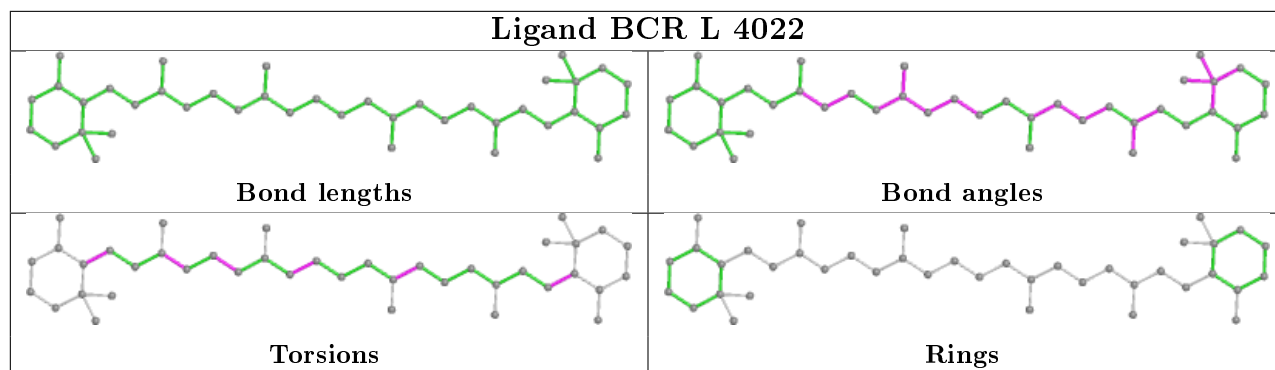


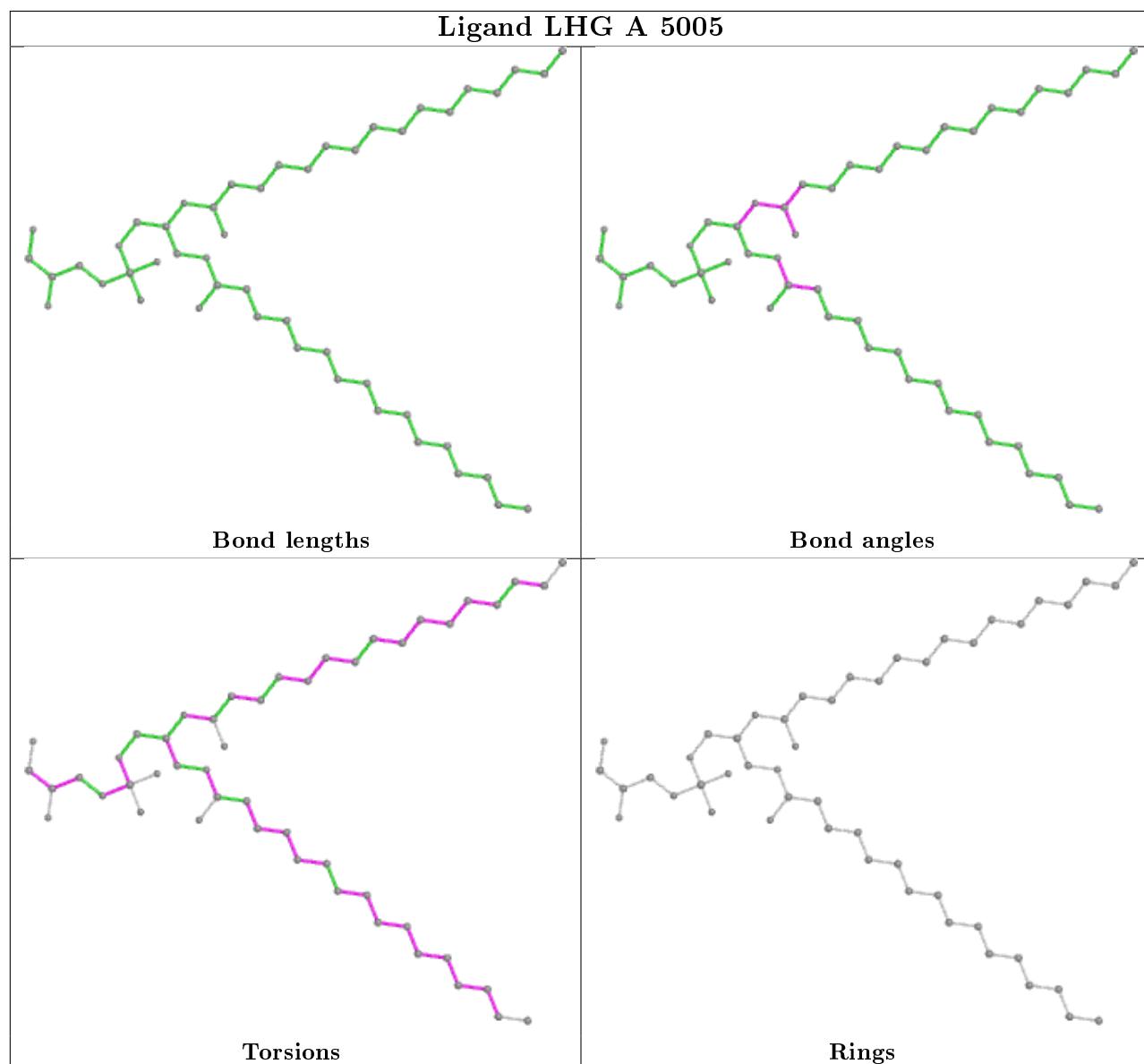
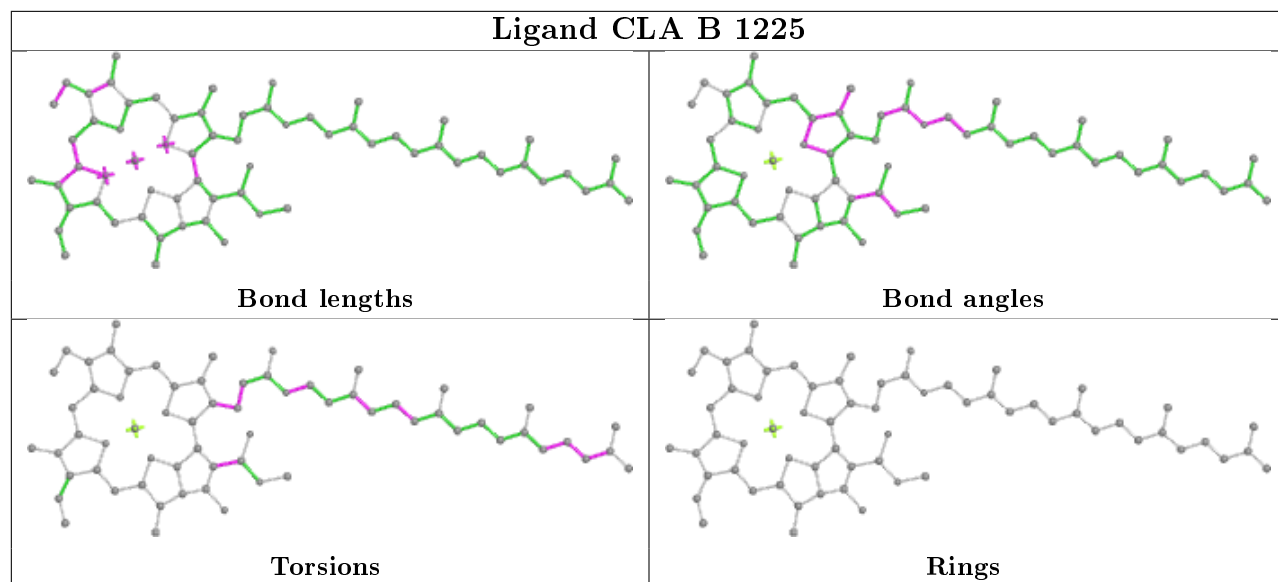


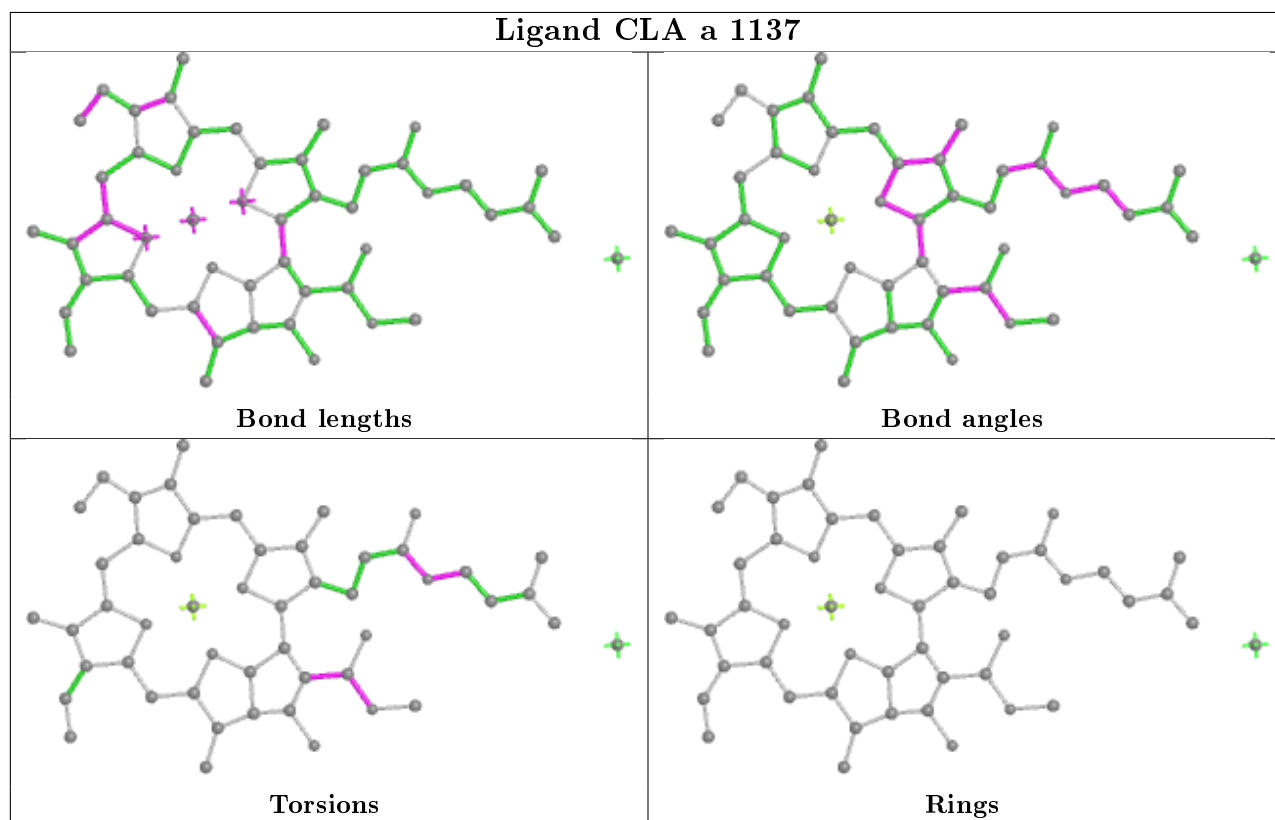
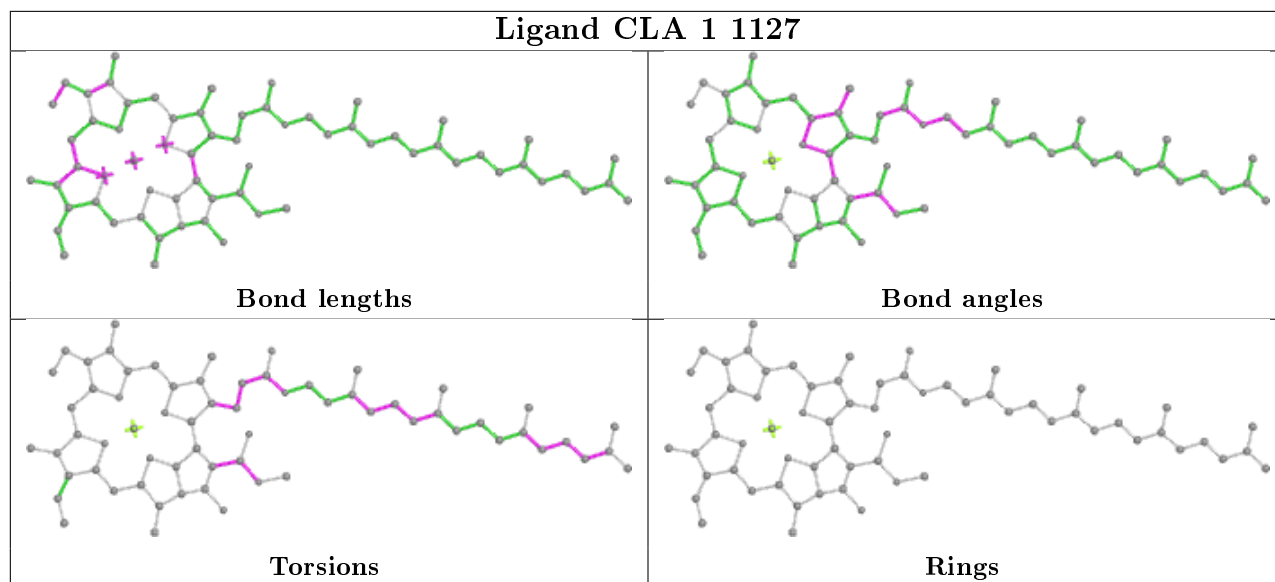


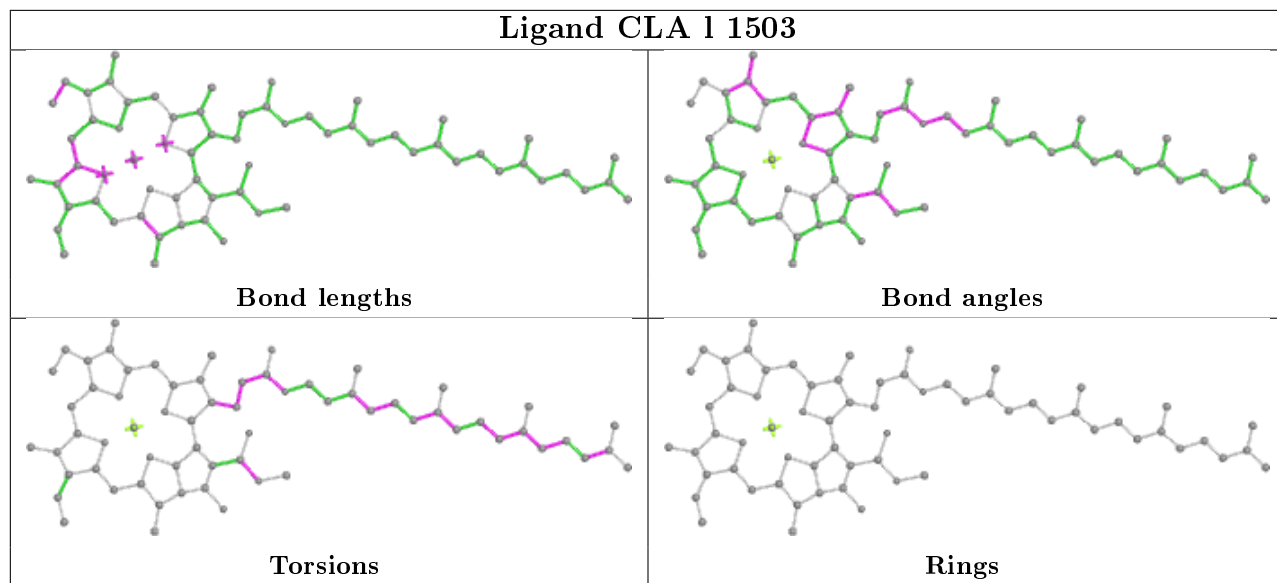
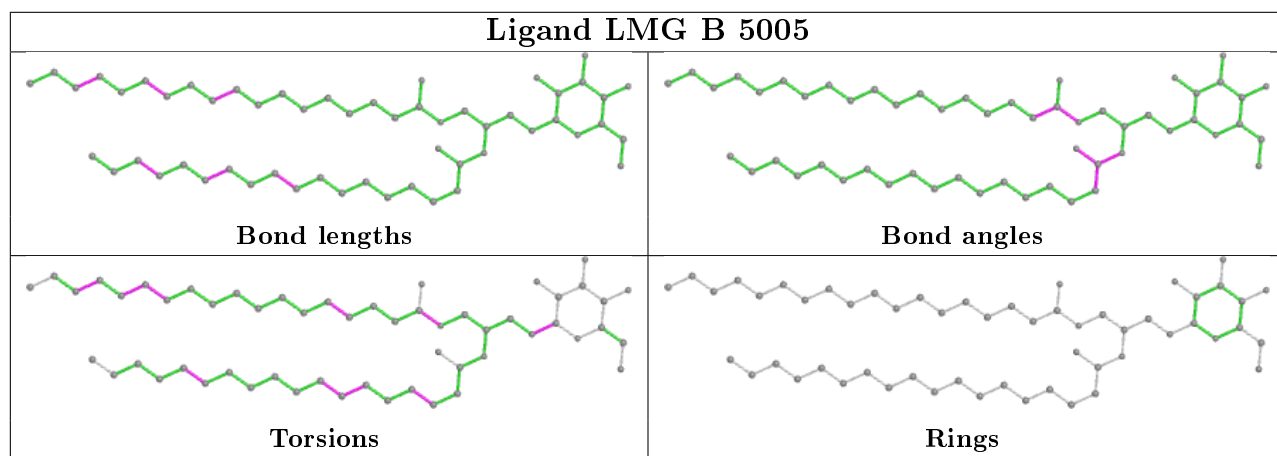
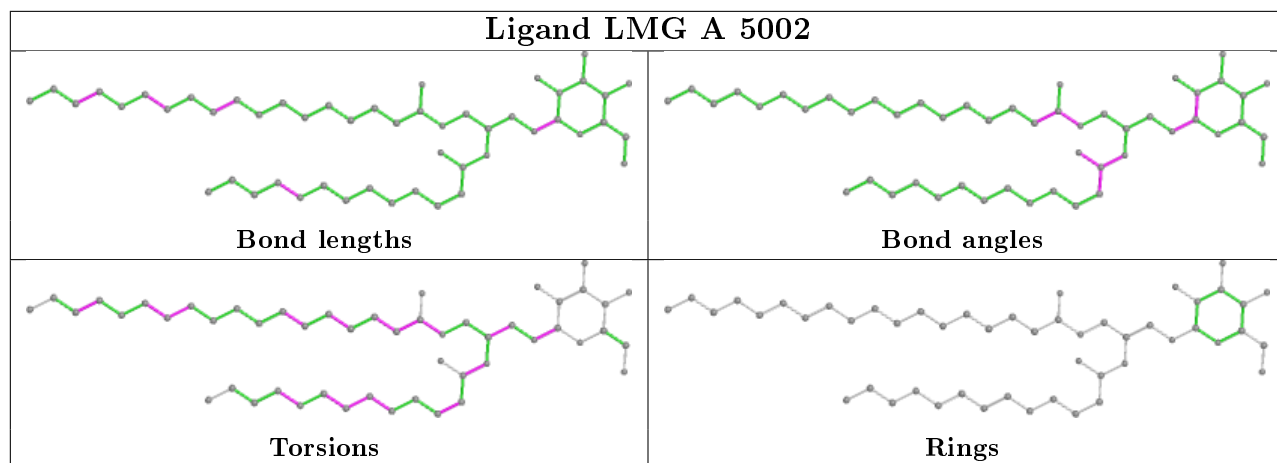


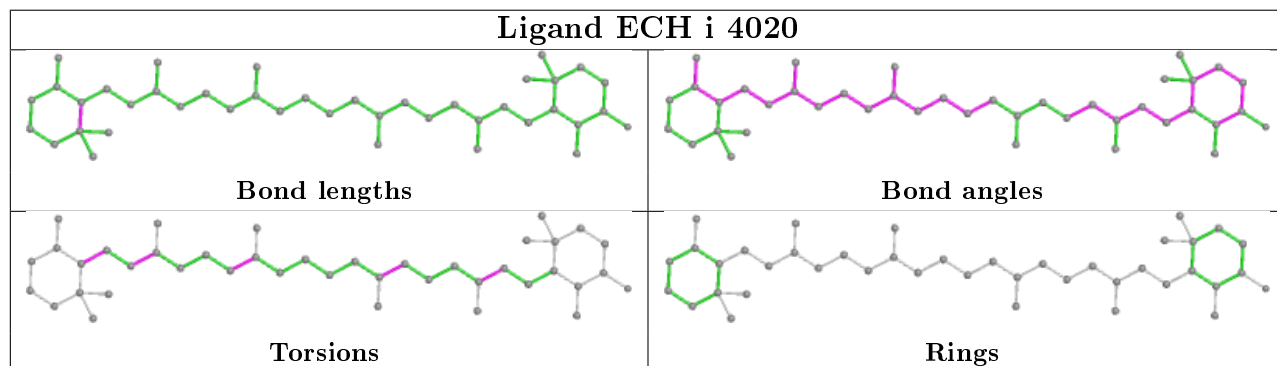
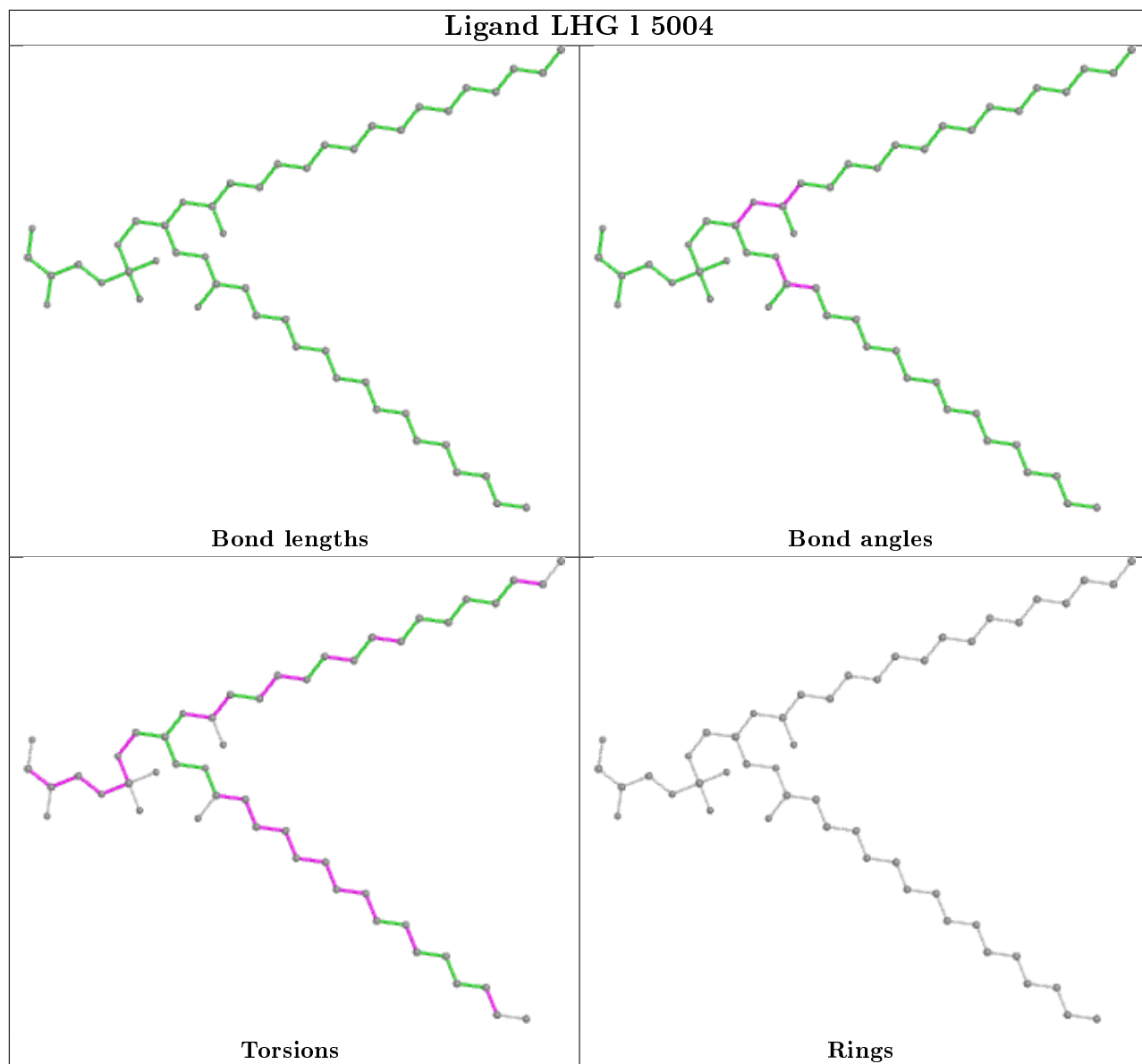


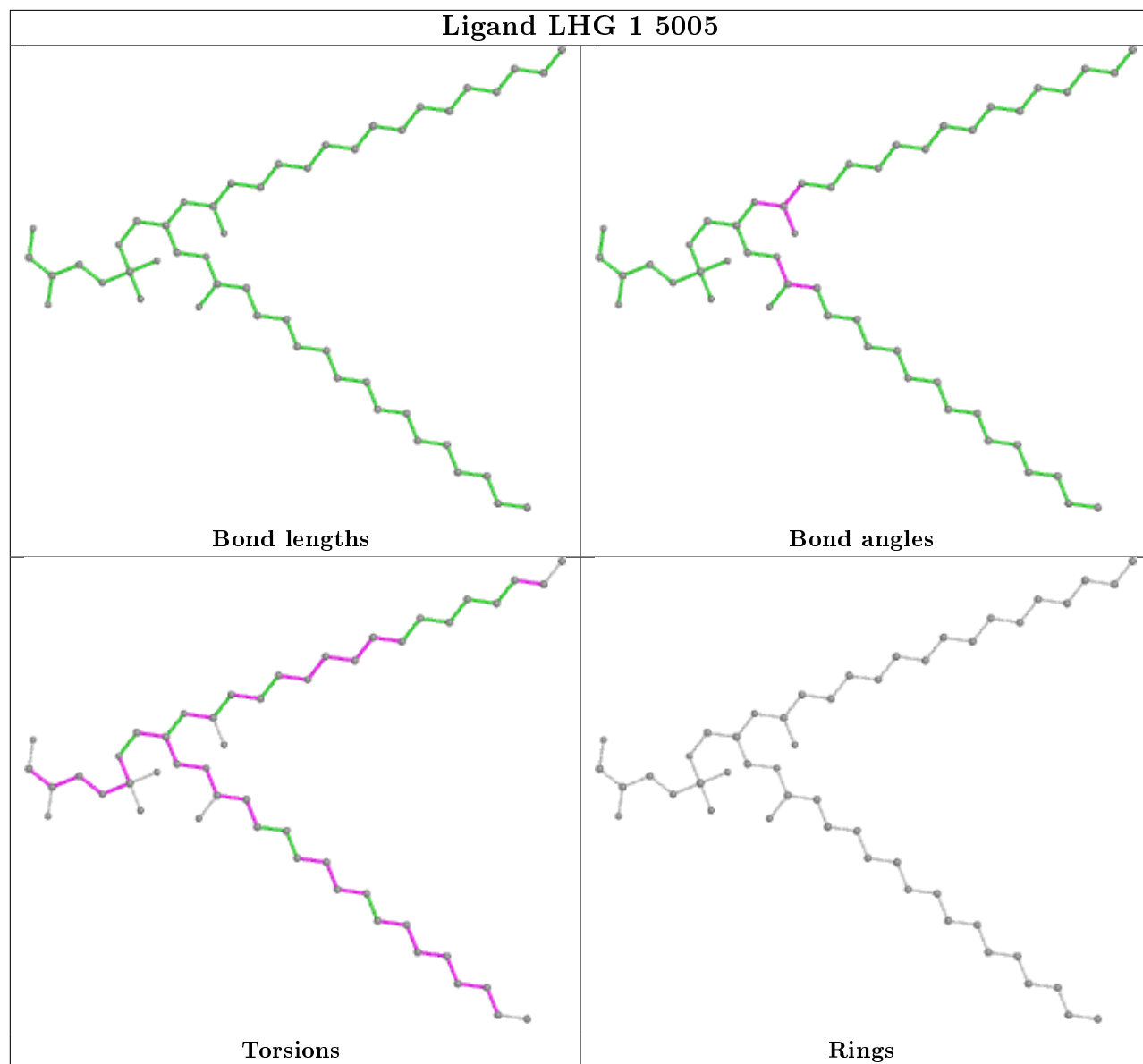


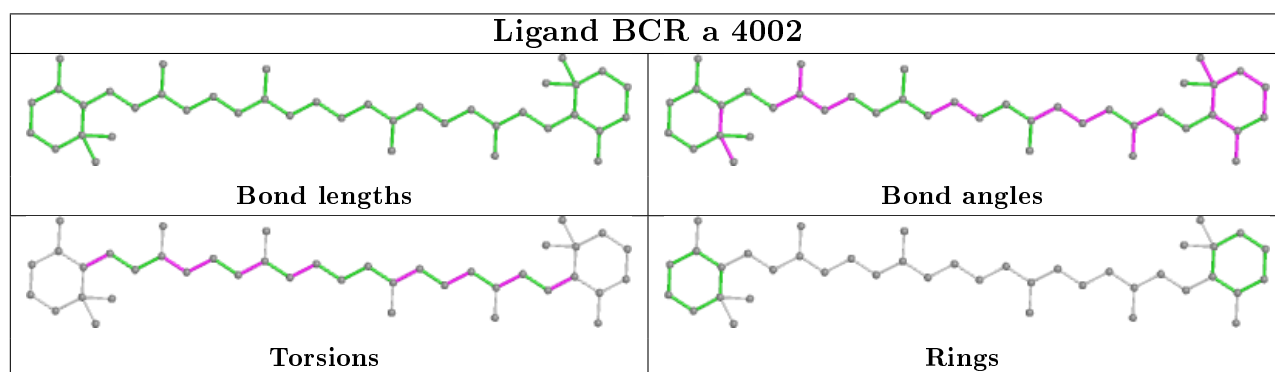
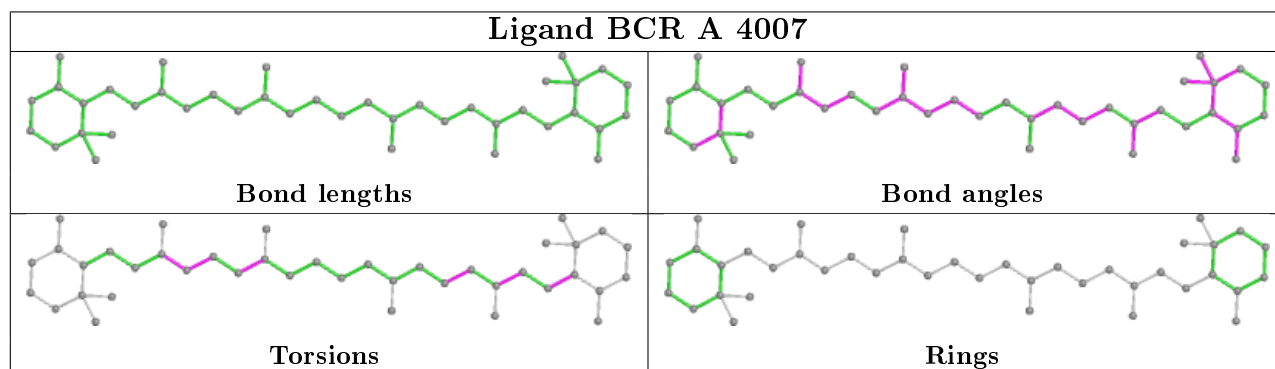
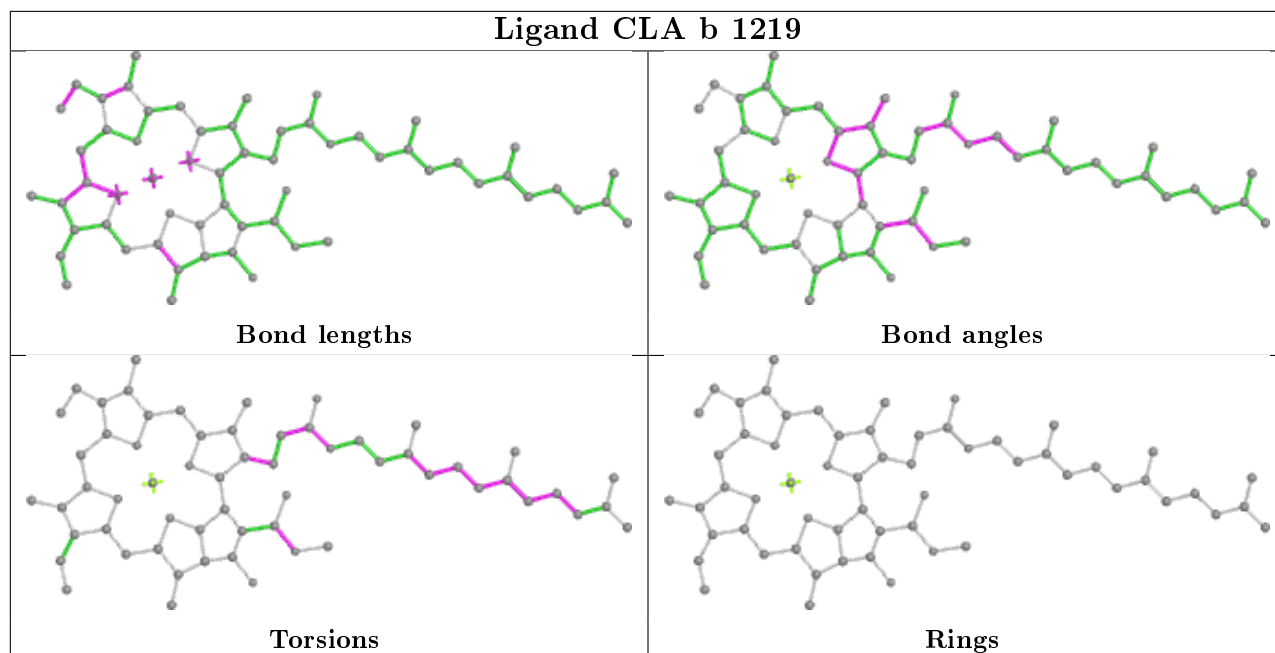


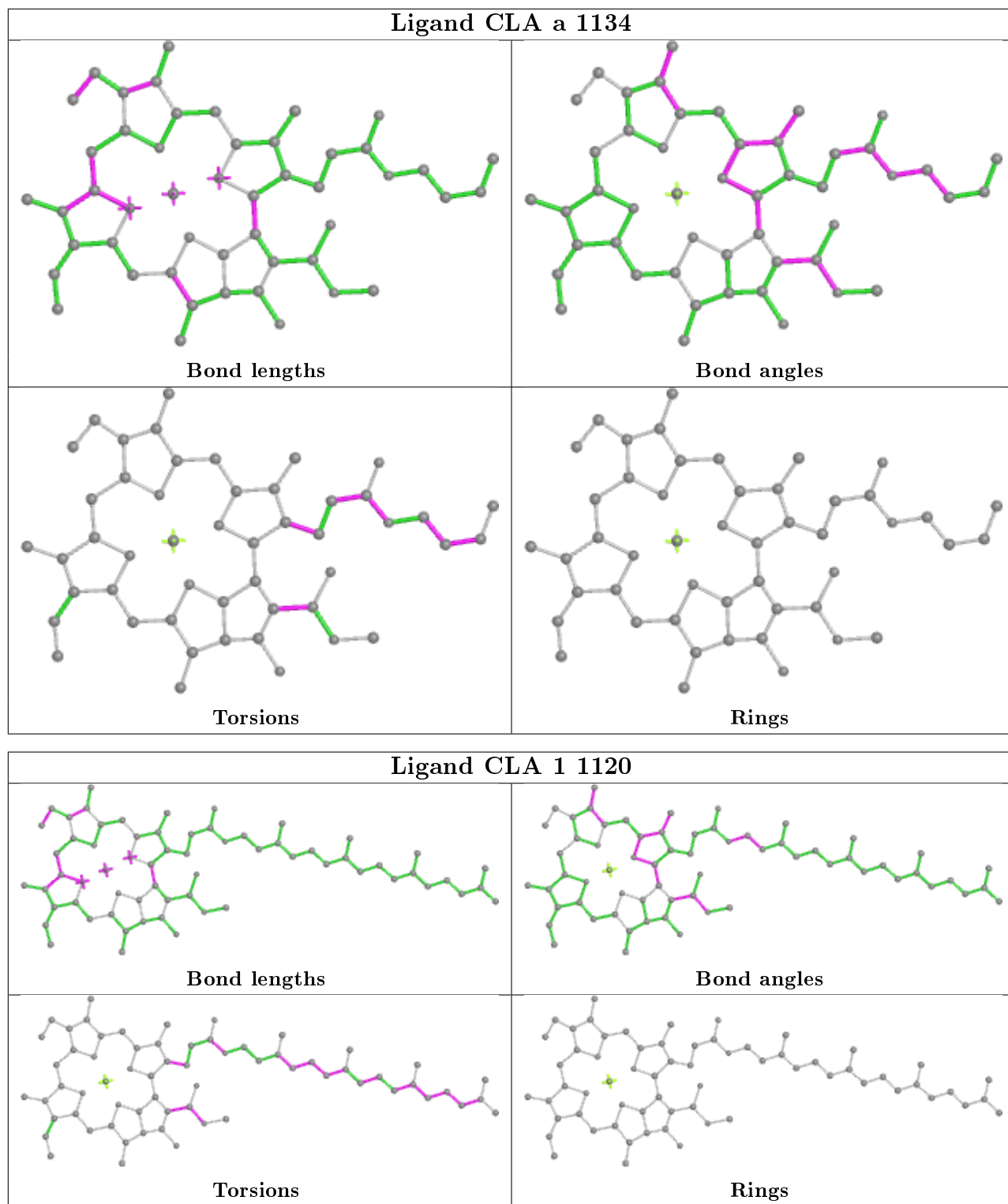


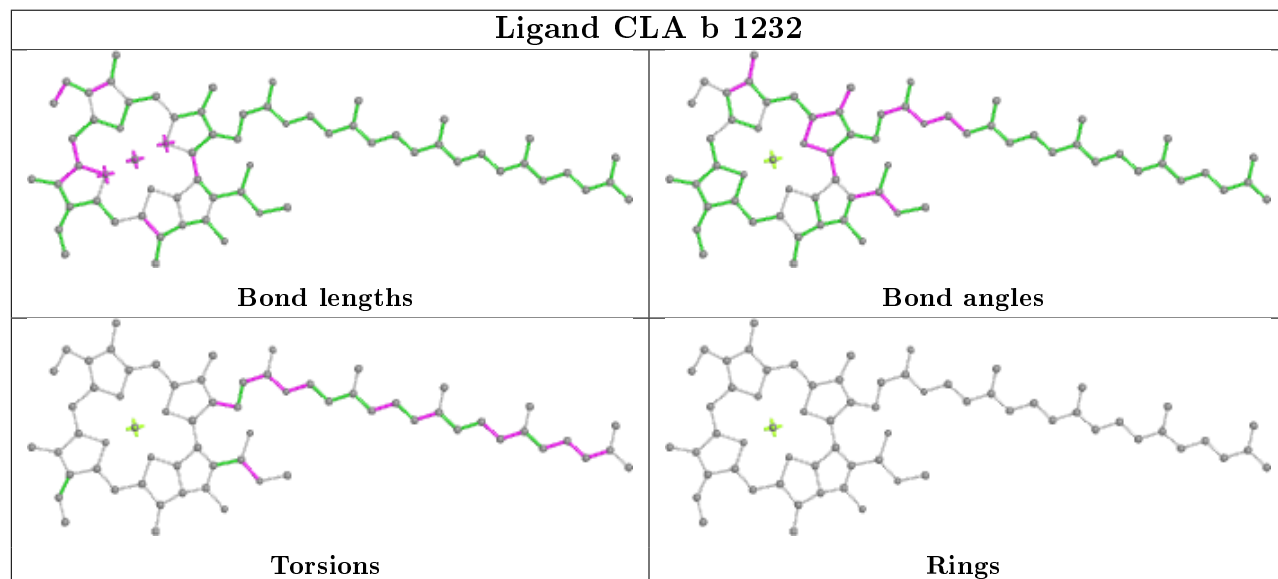
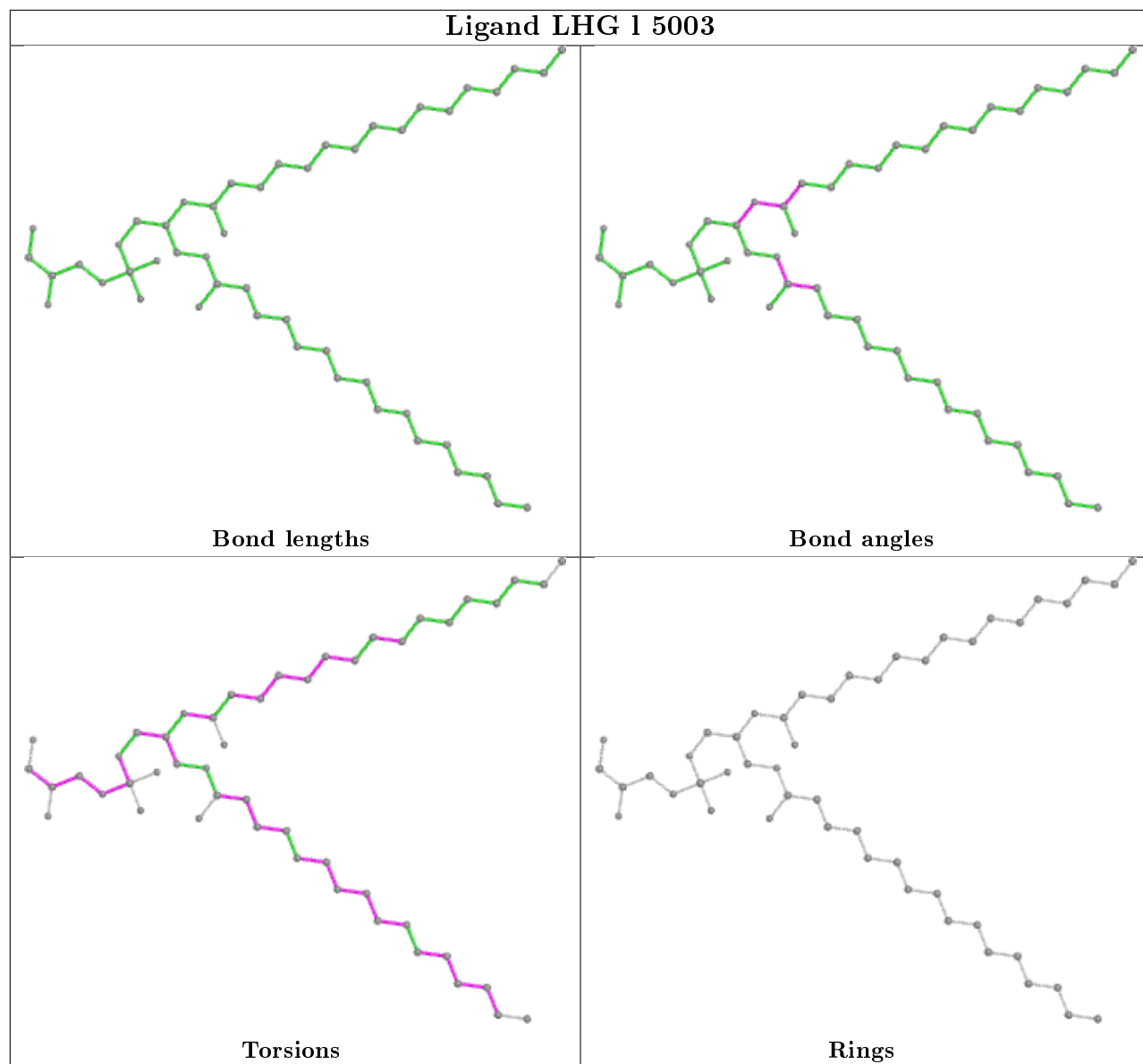


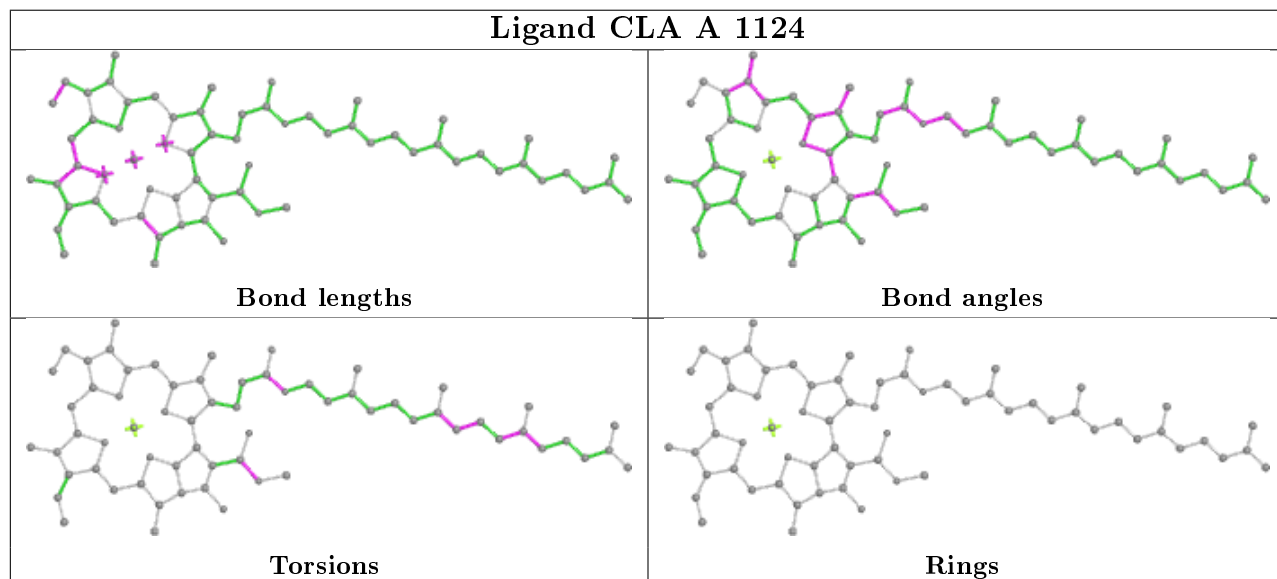
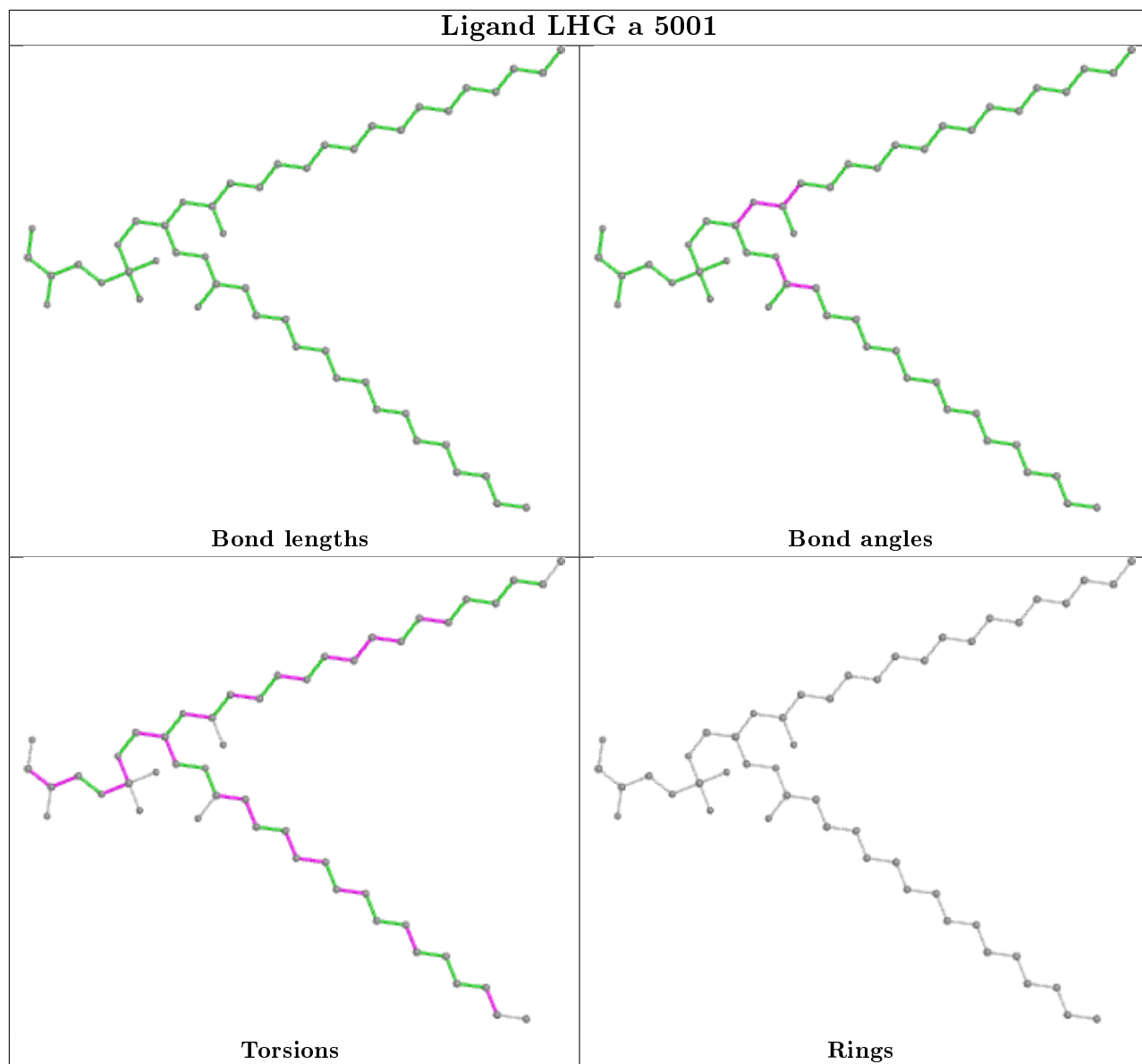


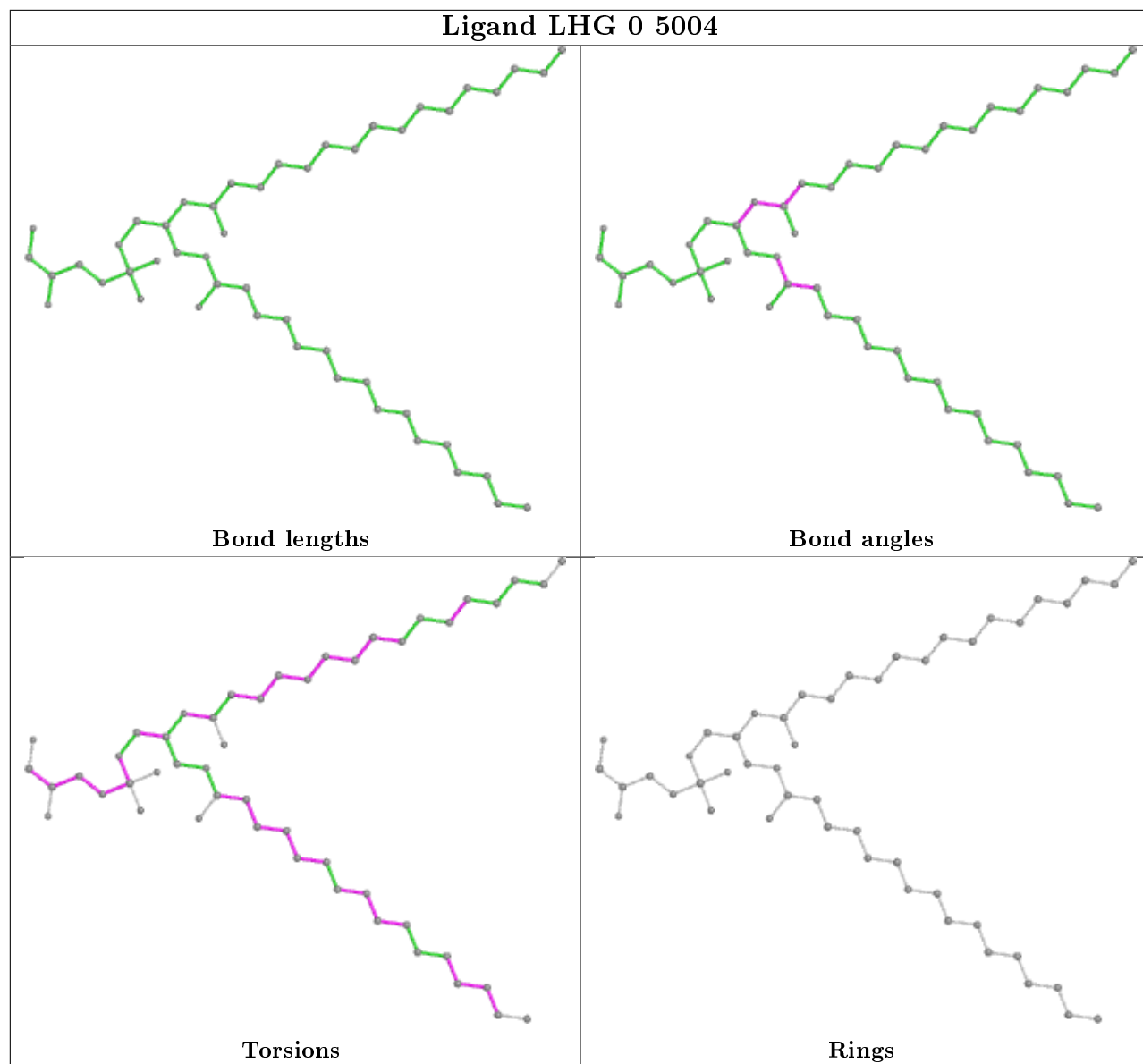


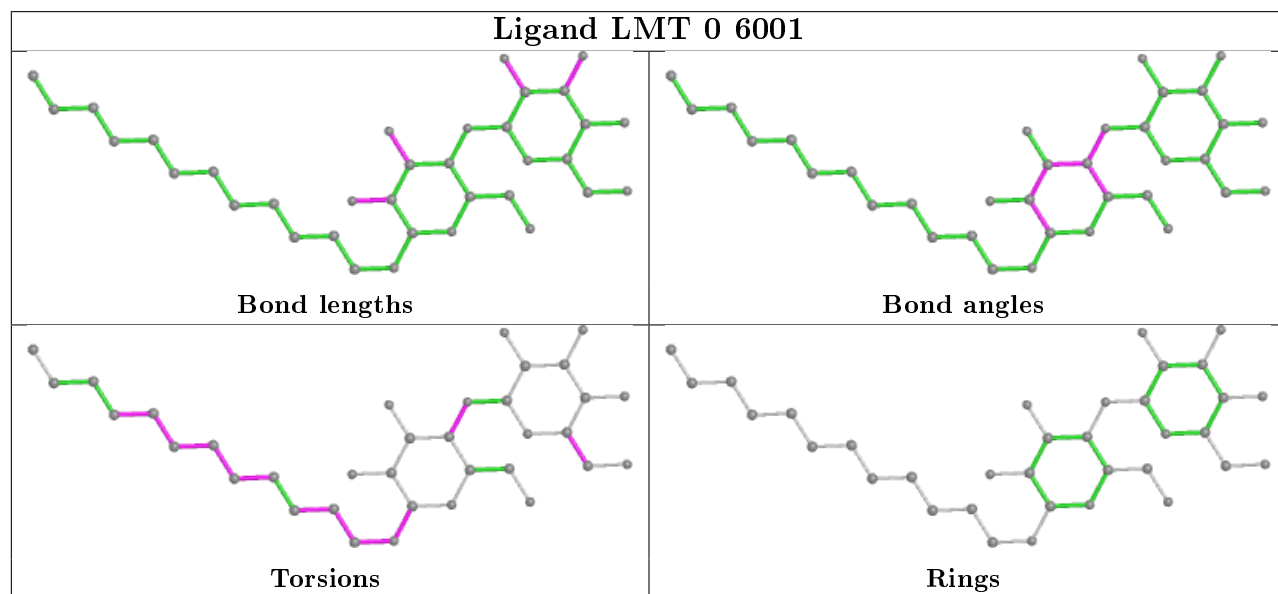
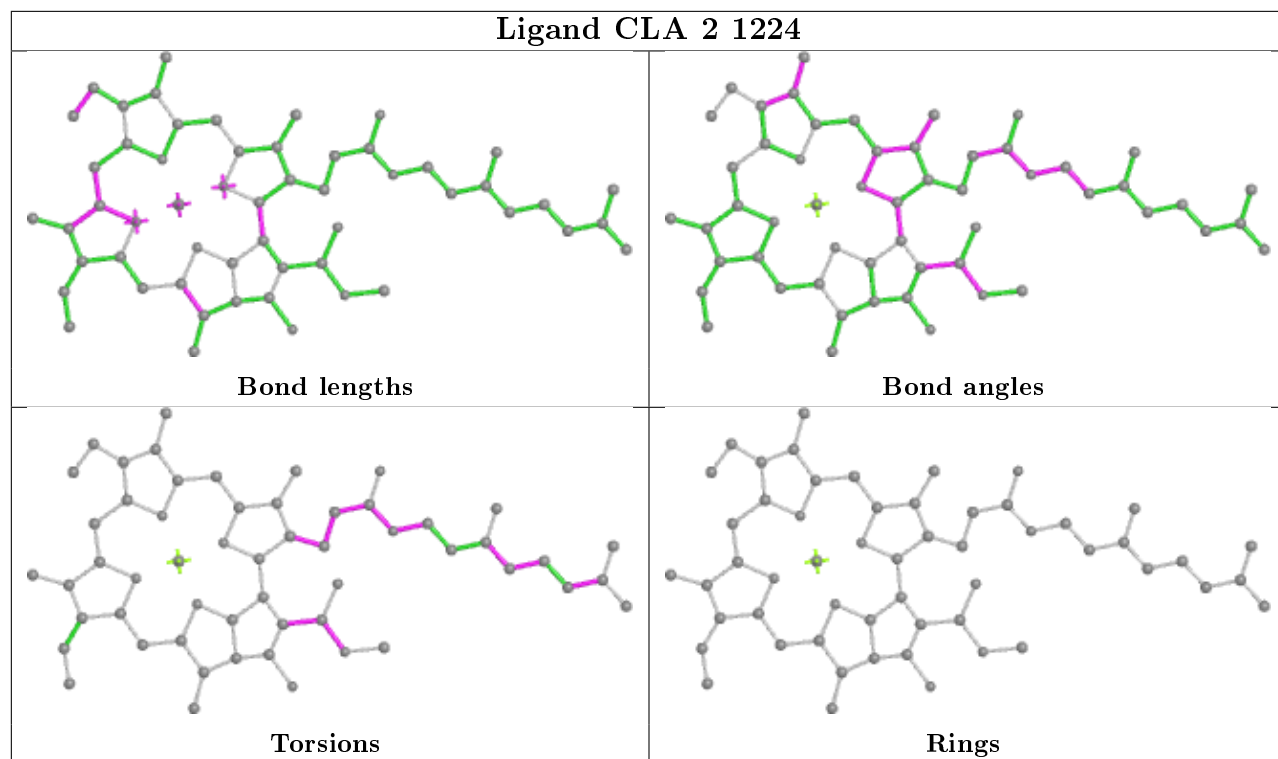


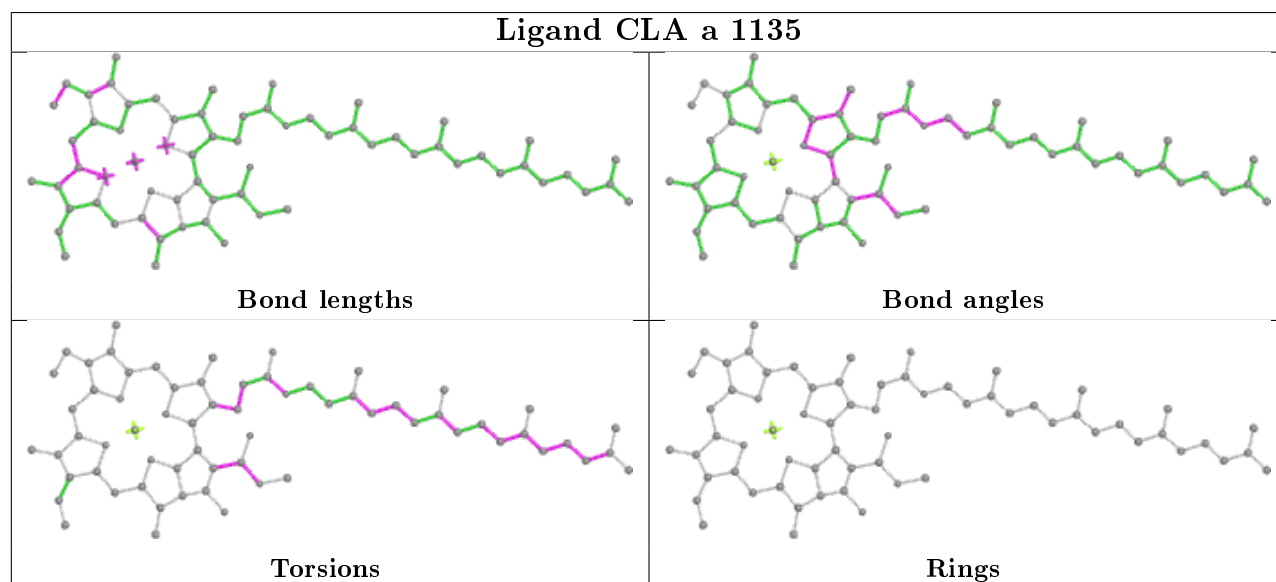
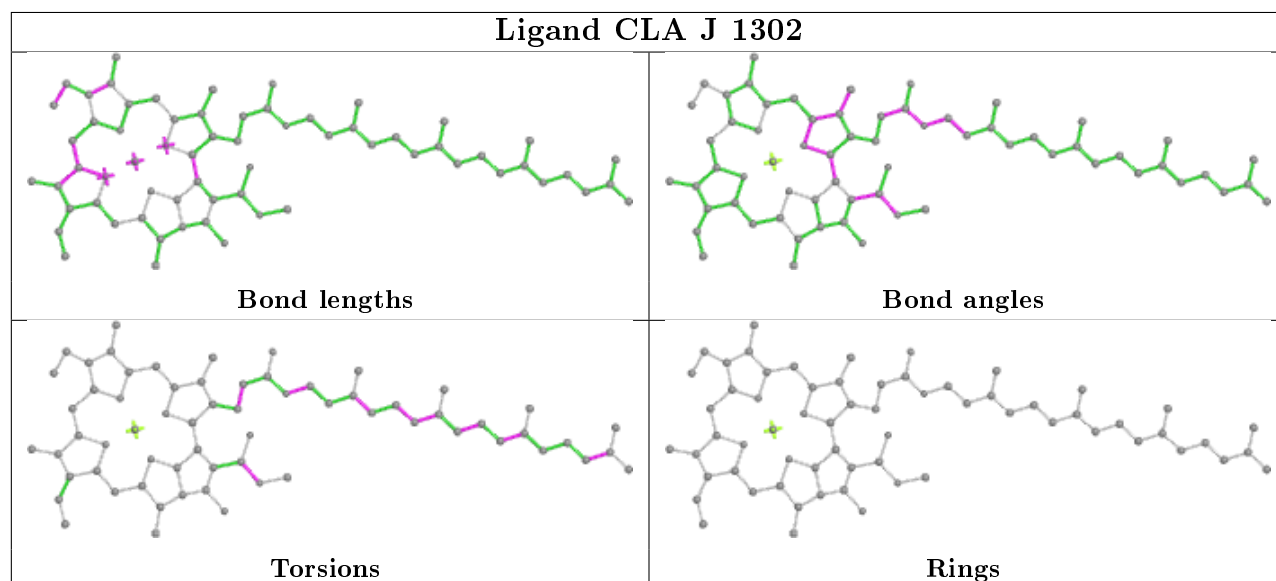
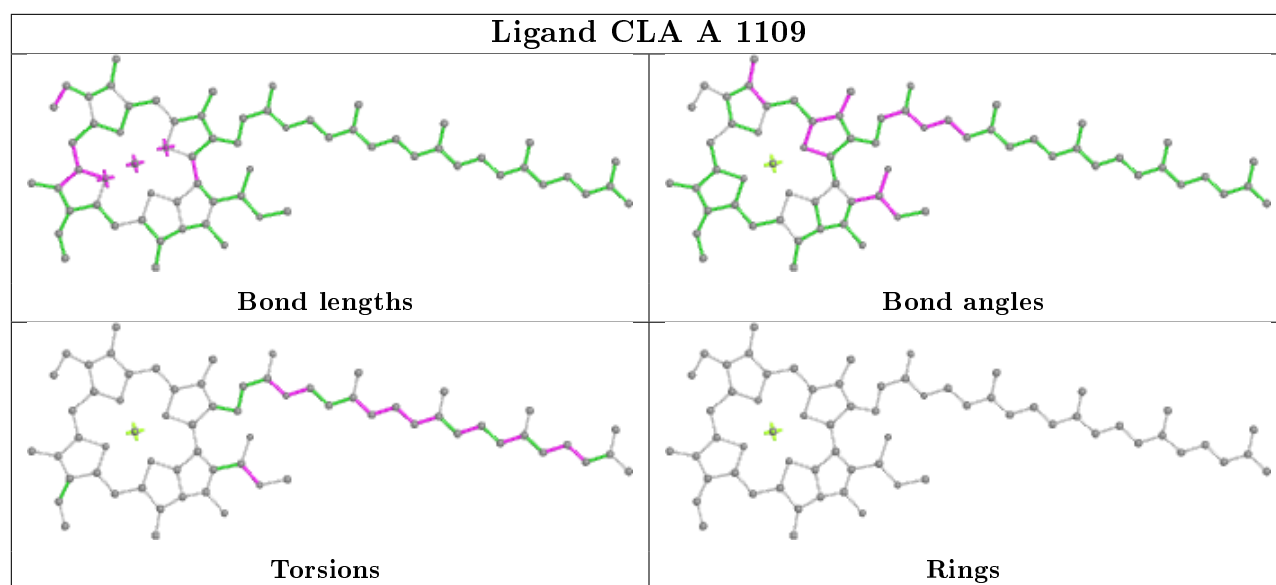


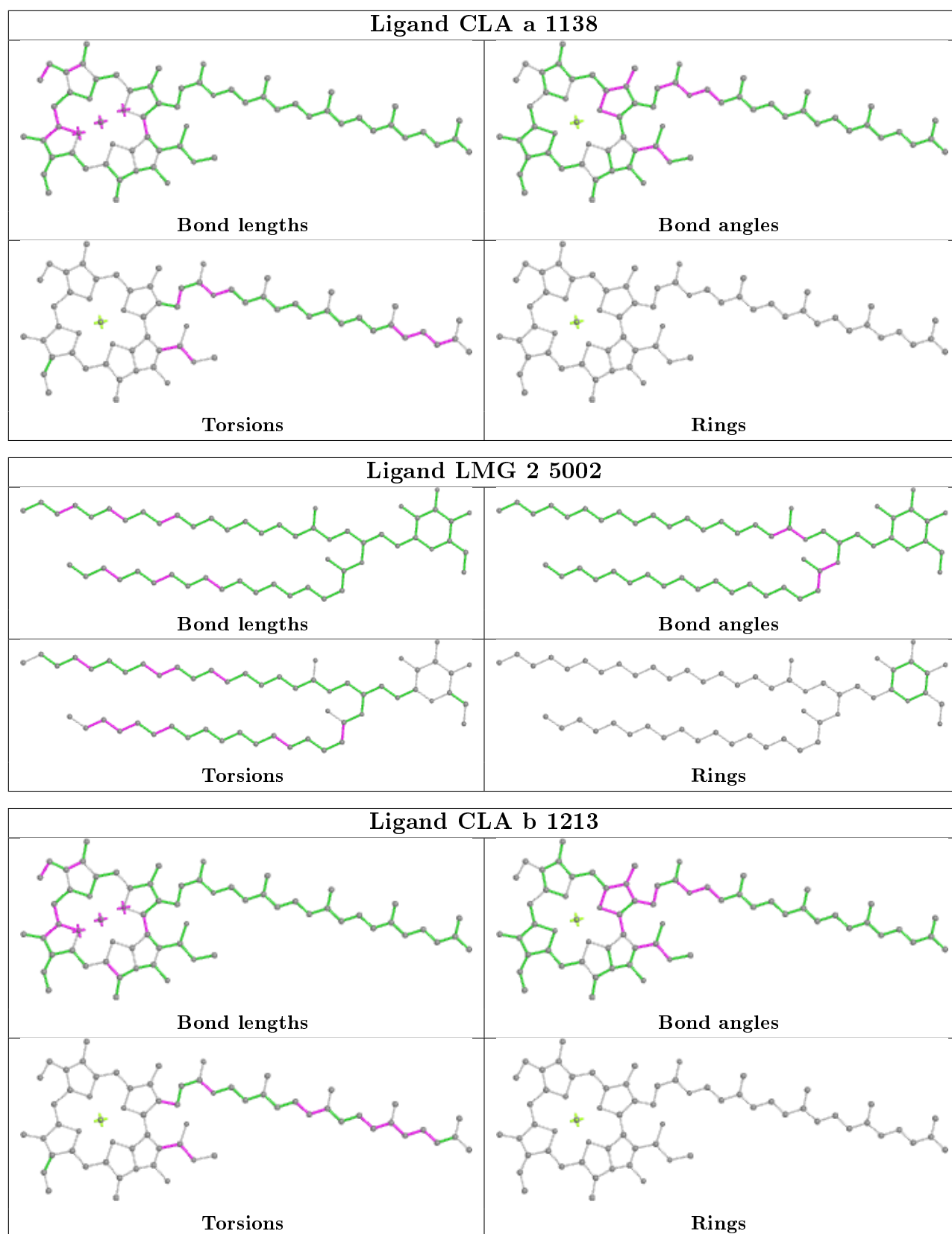


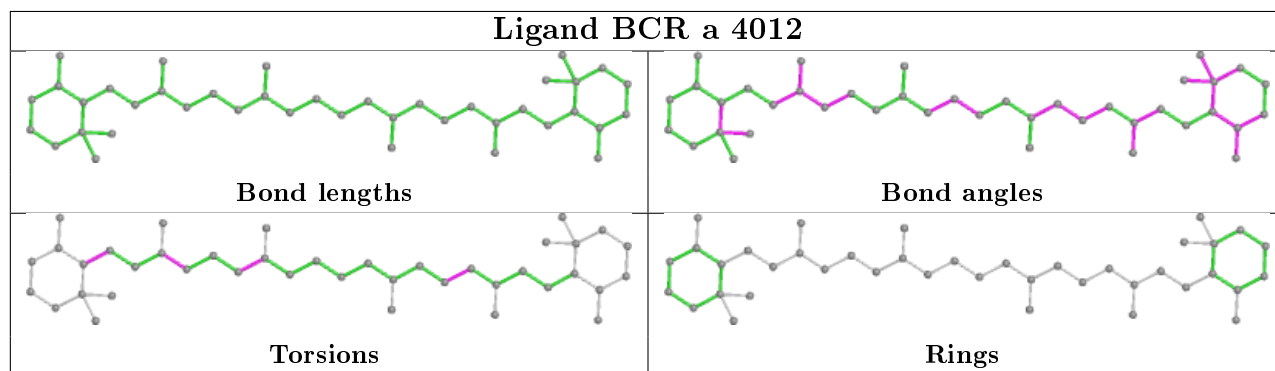
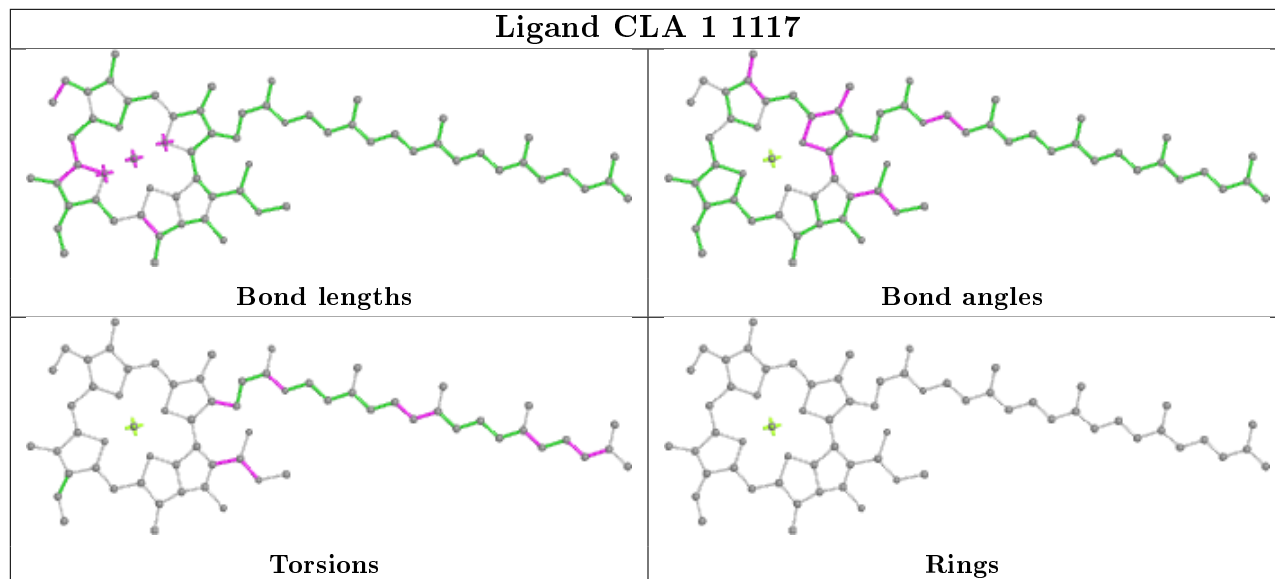
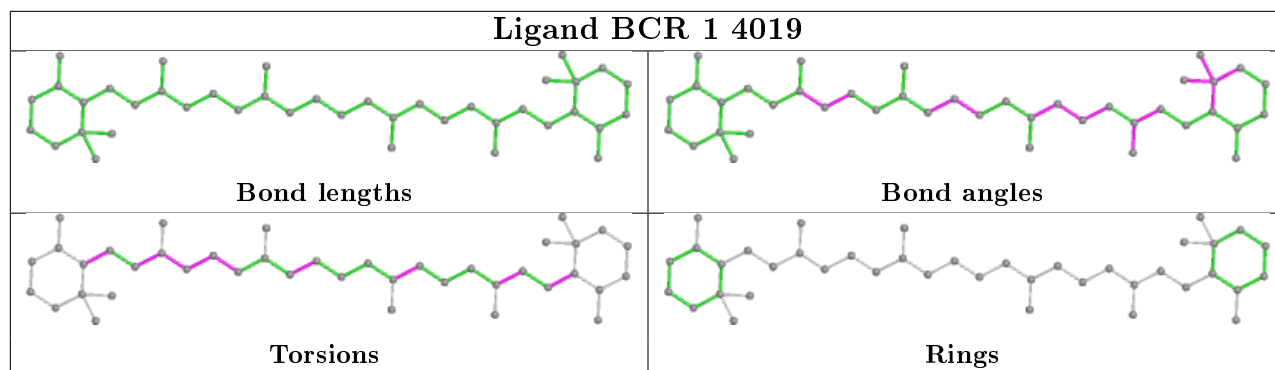


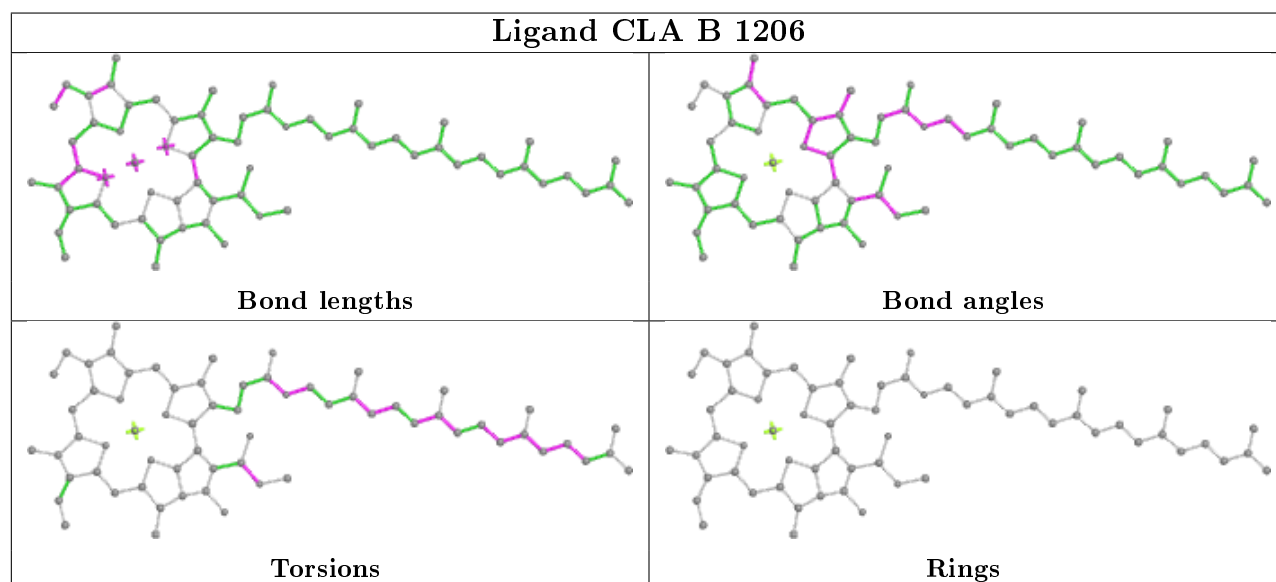
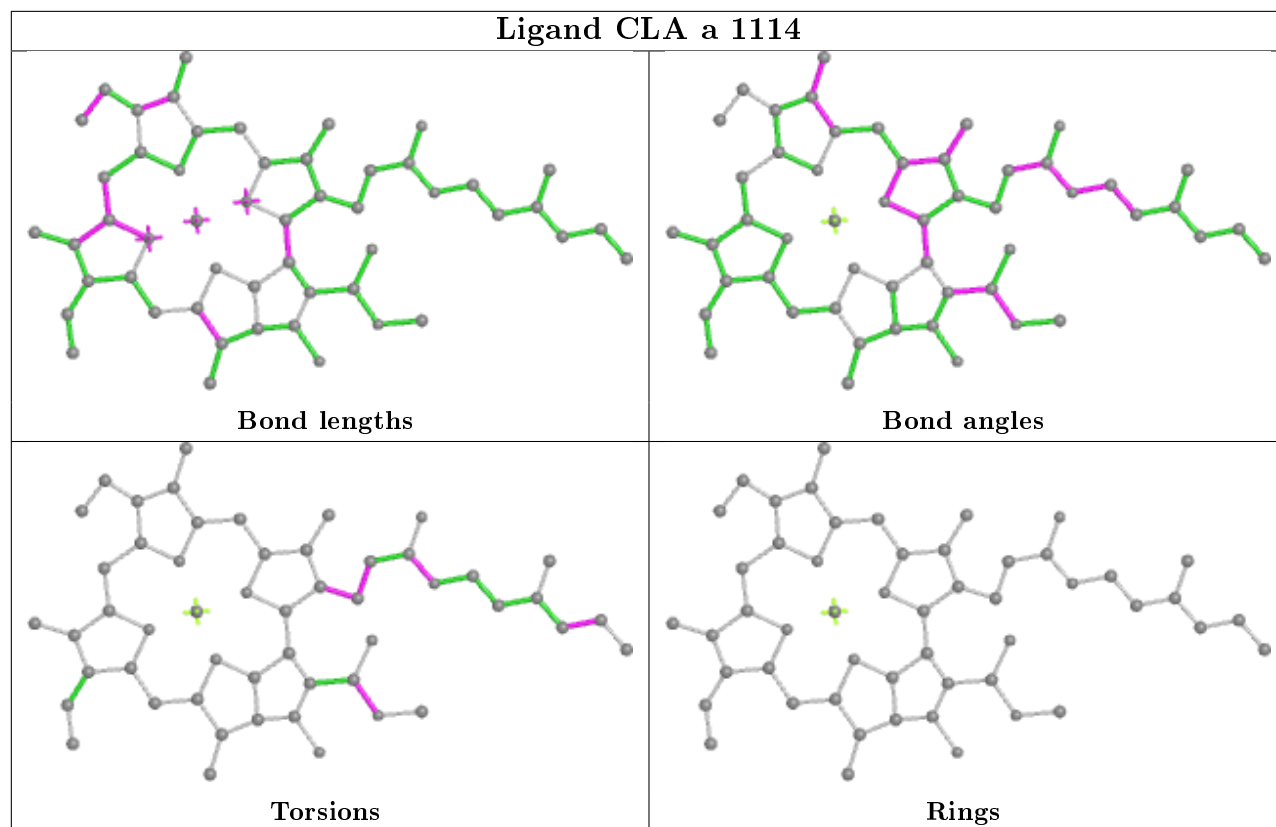


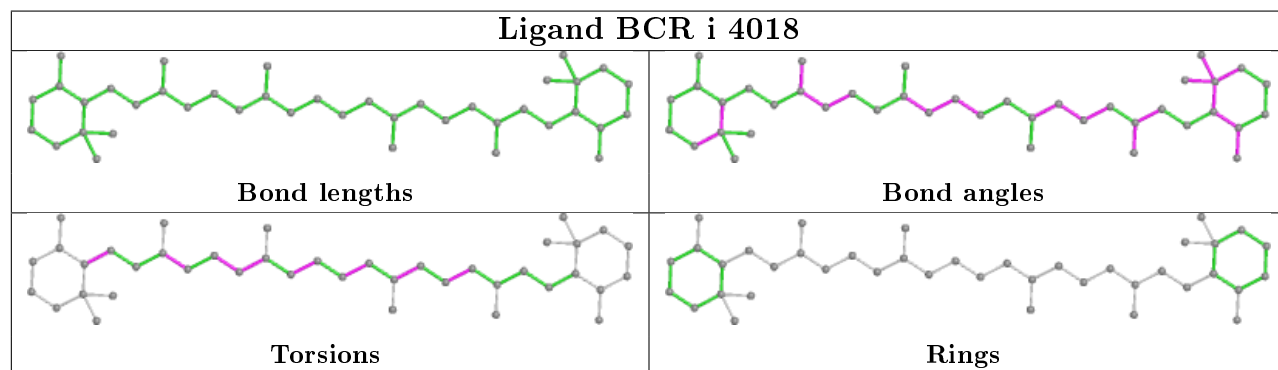
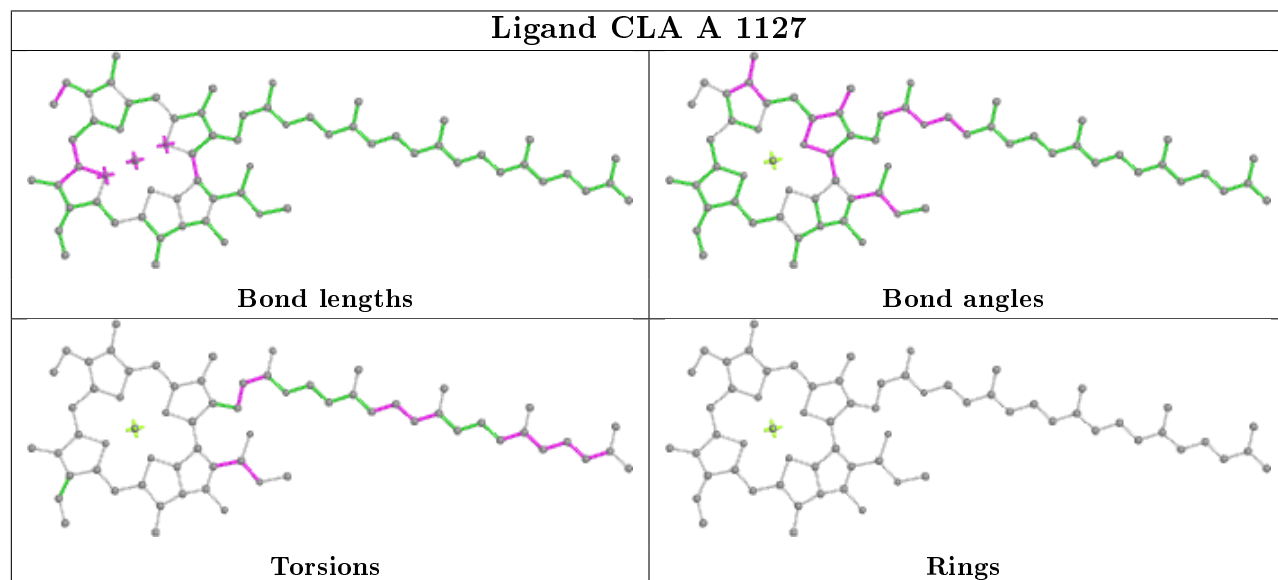
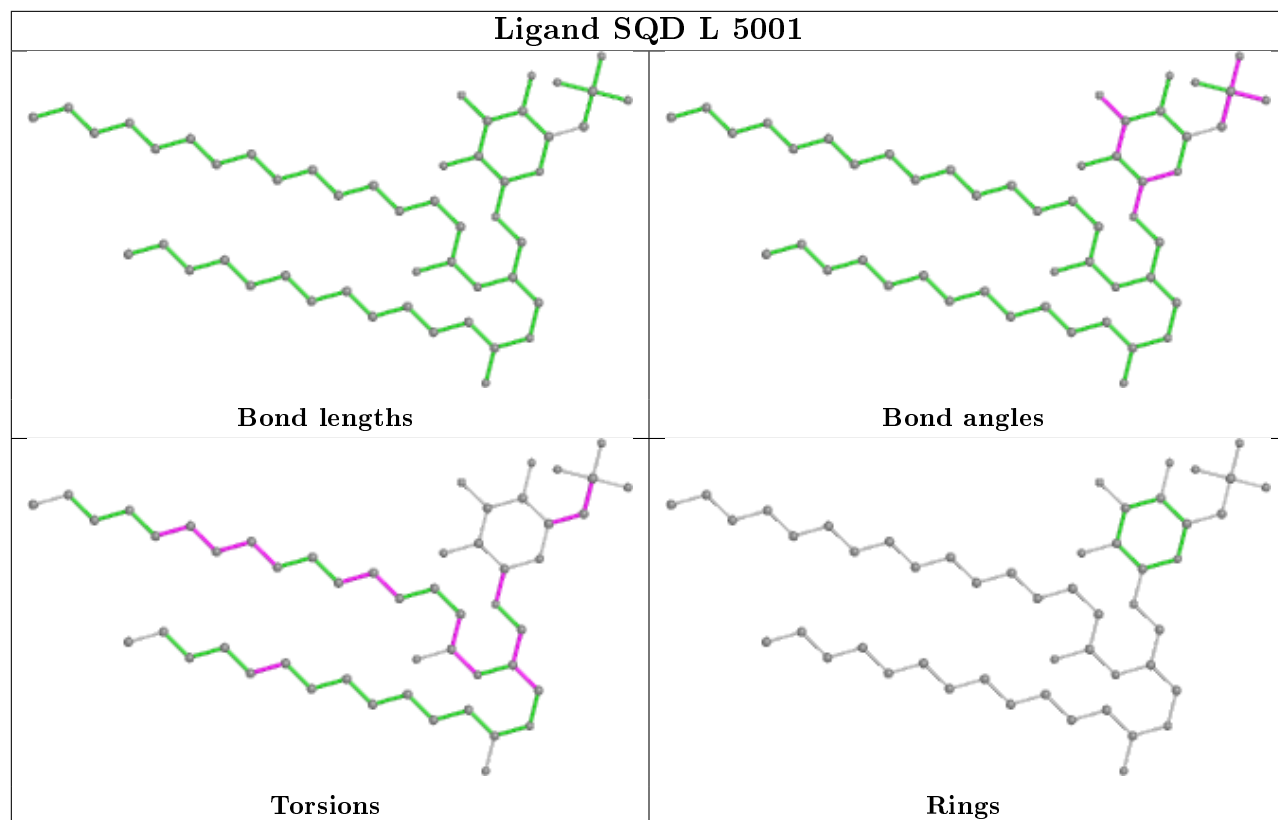


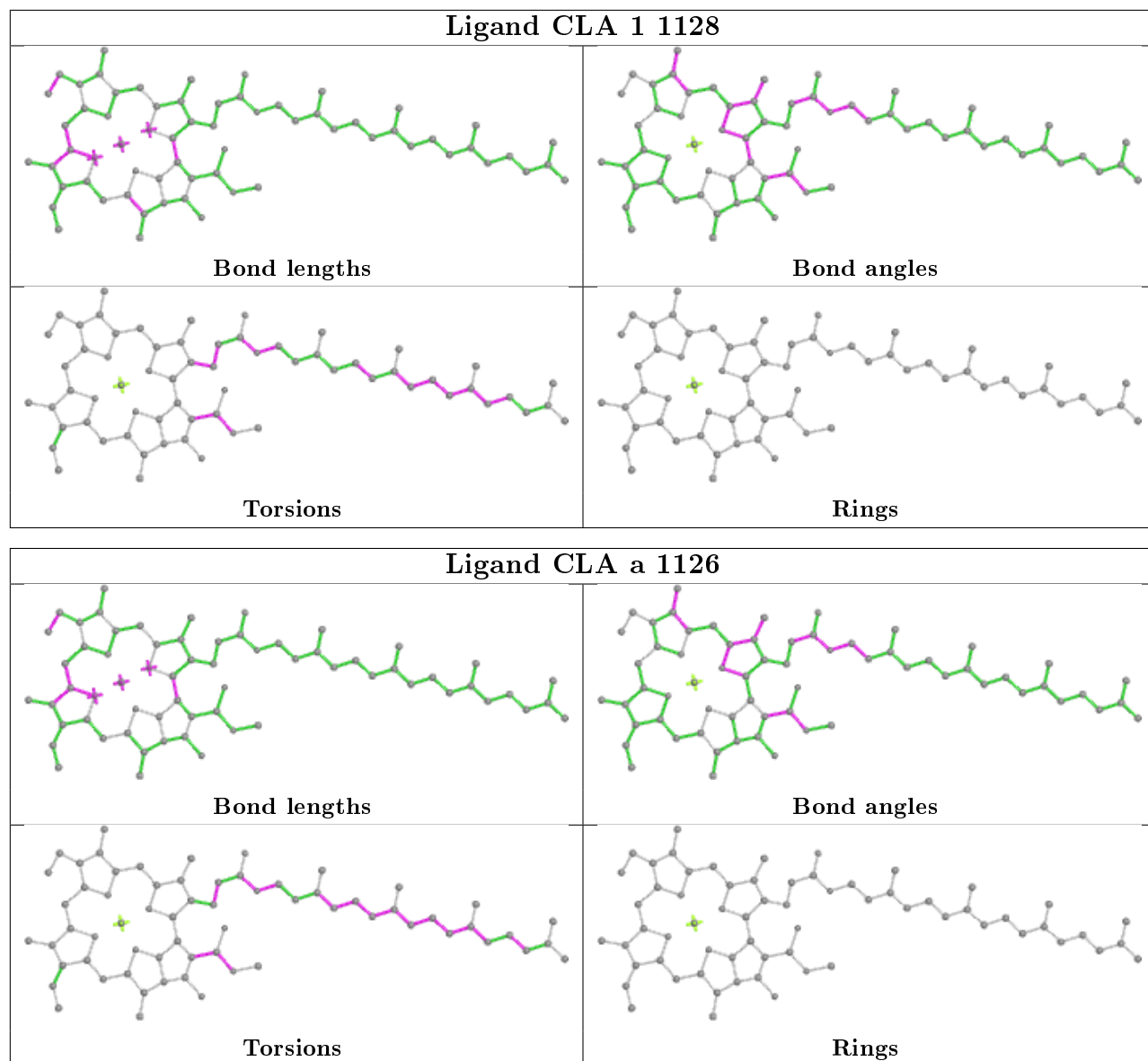


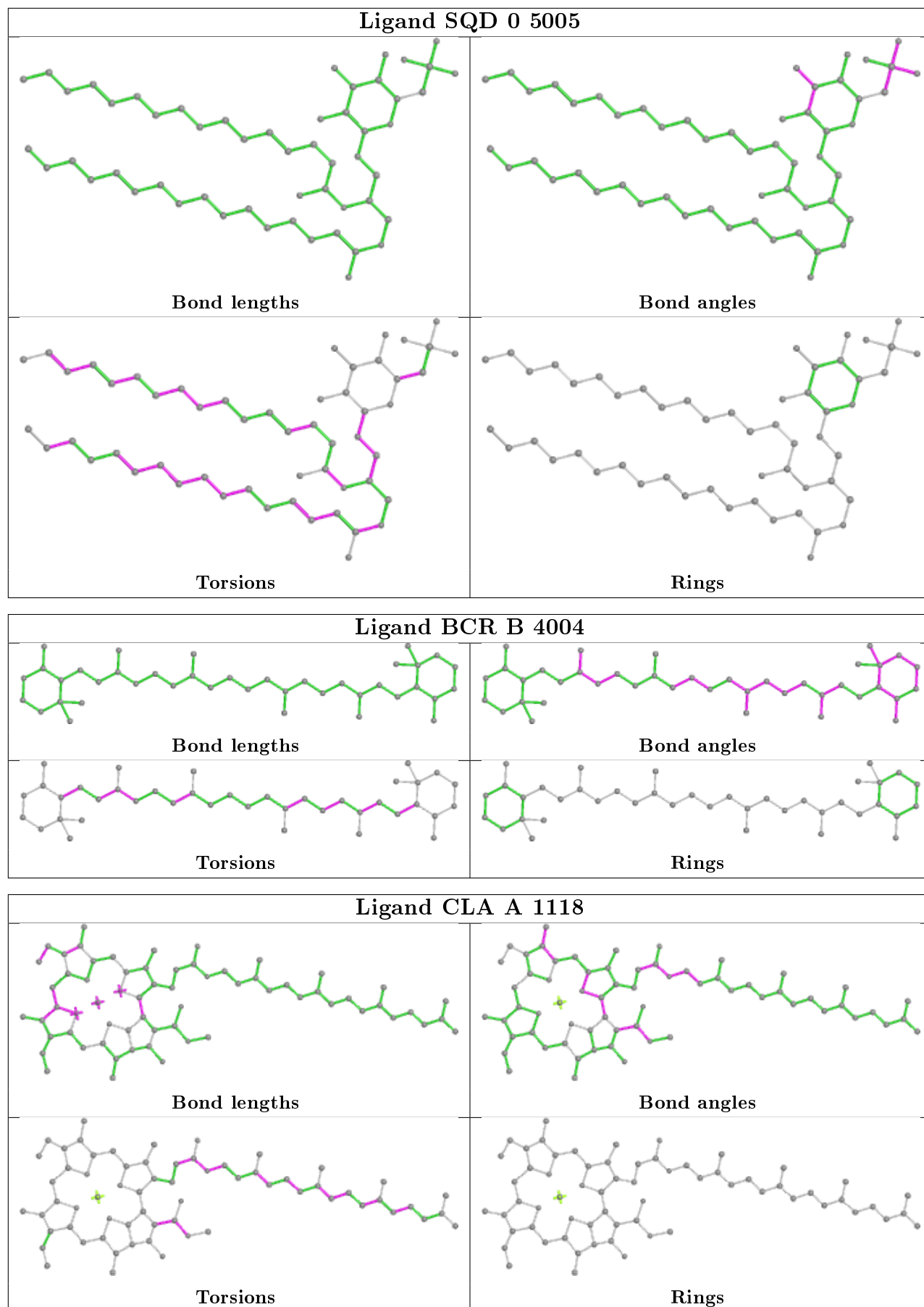


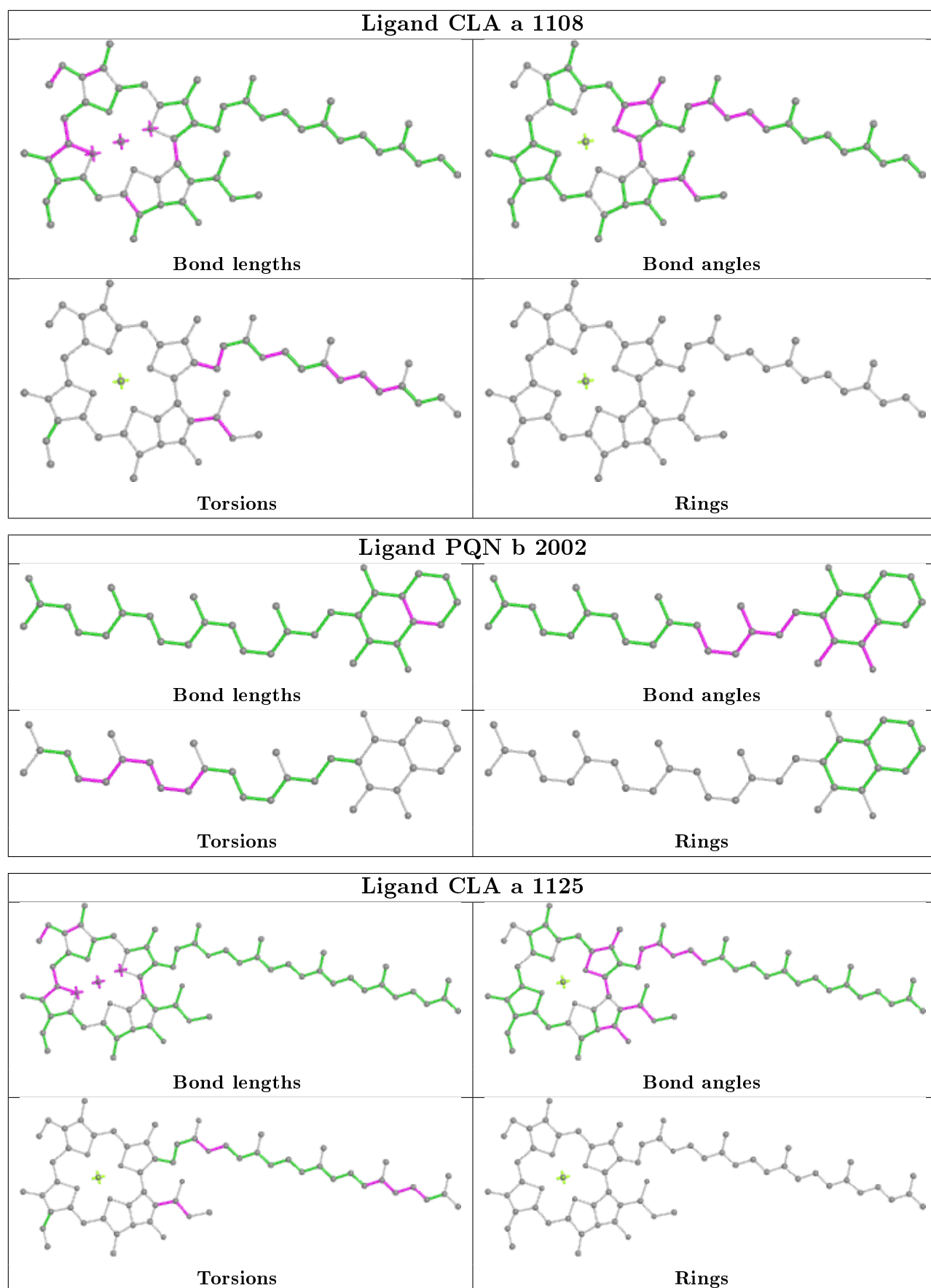


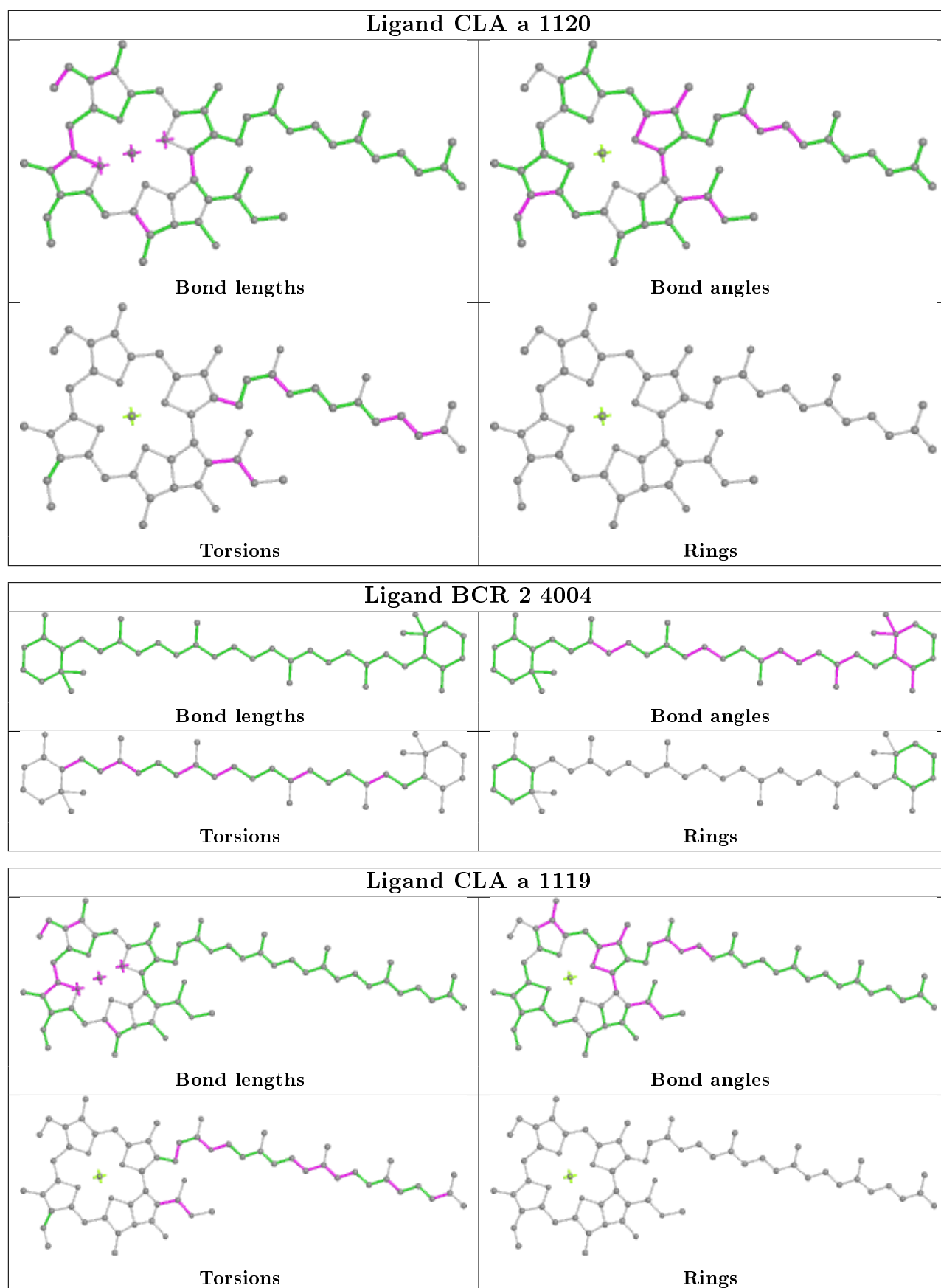












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/751 (100%)	-0.19	20 (2%) 54 58	29, 47, 72, 134	0
1	a	751/751 (100%)	0.97	140 (18%) 1 1	48, 95, 149, 209	0
2	2	731/731 (100%)	0.85	131 (17%) 1 1	43, 101, 146, 169	0
2	B	731/731 (100%)	0.06	42 (5%) 23 25	29, 56, 90, 152	0
3	3	80/80 (100%)	1.51	23 (28%) 0 0	54, 84, 110, 119	0
3	C	80/80 (100%)	-0.47	1 (1%) 77 79	33, 45, 59, 81	0
4	D	141/141 (100%)	-0.24	7 (4%) 28 30	30, 44, 70, 120	0
4	d	141/141 (100%)	0.81	27 (19%) 1 1	56, 82, 106, 136	0
5	5	69/69 (100%)	1.53	16 (23%) 0 0	75, 109, 122, 128	0
5	E	69/69 (100%)	0.59	10 (14%) 2 2	45, 62, 91, 97	0
6	6	143/143 (100%)	2.13	62 (43%) 0 0	114, 141, 158, 189	0
6	F	143/143 (100%)	-0.03	7 (4%) 29 31	56, 78, 94, 130	0
6	f	143/143 (100%)	0.86	27 (18%) 1 1	60, 97, 112, 132	0
7	I	40/40 (100%)	-0.02	0 100 100	36, 49, 87, 107	0
7	i	40/40 (100%)	0.48	3 (7%) 14 14	41, 49, 103, 132	0
8	7	40/40 (100%)	1.29	13 (32%) 0 0	109, 128, 152, 165	0
8	J	40/40 (100%)	-0.13	2 (5%) 28 30	54, 69, 95, 101	0
8	j	40/40 (100%)	0.81	8 (20%) 1 0	87, 98, 117, 132	0
9	K	80/80 (100%)	1.71	27 (33%) 0 0	53, 72, 127, 146	38 (47%)
10	L	157/157 (100%)	-0.03	6 (3%) 40 43	36, 43, 64, 131	0
10	l	157/157 (100%)	0.36	14 (8%) 9 9	45, 60, 107, 184	0
11	9	31/31 (100%)	0.30	3 (9%) 7 7	78, 86, 98, 111	0
11	M	31/31 (100%)	-0.30	1 (3%) 47 51	49, 58, 66, 96	0
11	m	31/31 (100%)	-0.58	0 100 100	38, 43, 55, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	b	729/729 (100%)	-0.11	12 (1%) 72 74	39, 54, 75, 93	0
13	c	81/81 (100%)	0.25	4 (4%) 29 31	54, 69, 83, 96	0
14	e	68/68 (100%)	2.09	33 (48%) 0 0	63, 79, 100, 108	0
15	k	78/78 (100%)	4.54	61 (78%) 0 0	140, 160, 200, 208	38 (48%)
16	1	744/744 (100%)	1.09	150 (20%) 1 0	42, 90, 121, 151	0
17	4	140/140 (100%)	0.68	27 (19%) 1 1	51, 76, 105, 120	0
18	h	38/38 (100%)	0.60	7 (18%) 1 1	54, 68, 95, 96	0
19	8	79/79 (100%)	3.23	43 (54%) 0 0	103, 127, 168, 172	39 (49%)
20	0	154/154 (100%)	-0.26	3 (1%) 66 69	38, 51, 73, 108	0
All	All	6771/6771 (100%)	0.57	930 (13%) 3 2	29, 70, 138, 209	115 (1%)

All (930) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	4	SER	15.3
15	k	81	VAL	14.4
15	k	15	THR	13.7
1	a	6	PRO	12.8
1	a	5	PRO	12.1
9	K	52	LEU	11.8
15	k	14	THR	11.7
16	1	239	PRO	11.5
19	8	55	LEU	11.4
1	a	256	PHE	11.2
15	k	38	TYR	11.2
1	a	3	ILE	11.1
1	a	268	TRP	10.9
2	2	1	MET	10.8
16	1	12	ALA	10.7
19	8	56	ALA	10.6
15	k	50	LEU	10.5
15	k	12	SER	10.5
1	a	271	TYR	10.4
15	k	18	TRP	10.2
15	k	39	PHE	10.1
19	8	58	LYS	10.0
7	i	39	GLU	10.0
19	8	48	LYS	9.7
16	1	243	ILE	9.7

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Mol	Chain	Res	Type	RSRZ
1	a	257	ALA	9.5
15	k	11	ALA	9.4
19	8	39	PHE	9.4
1	a	244	LEU	9.3
19	8	15	THR	9.3
19	8	38	TYR	9.2
6	6	1	ALA	9.2
19	8	57	SER	9.2
2	B	1	MET	8.9
6	6	90	ILE	8.8
1	a	265	THR	8.7
1	a	751	GLY	8.6
19	8	50	LEU	8.5
15	k	56	ALA	8.4
15	k	53	PRO	8.4
15	k	55	LEU	8.2
6	6	92	GLU	8.1
6	6	103	ILE	8.0
2	2	314	GLY	8.0
3	3	65	ILE	8.0
19	8	18	TRP	8.0
2	2	312	LEU	7.9
9	K	56	ALA	7.8
19	8	87	SER	7.8
15	k	13	PRO	7.5
16	1	246	PRO	7.5
15	k	16	ALA	7.5
15	k	19	SER	7.5
4	d	1	MET	7.5
6	6	102	VAL	7.4
1	a	2	THR	7.4
16	1	286	GLY	7.4
4	d	2	THR	7.4
16	1	11	LYS	7.4
6	6	106	PRO	7.2
10	1	2	ALA	7.2
2	2	225	PHE	7.1
5	5	31	SER	7.1
7	i	40	GLY	7.1
5	E	32	GLY	7.0
15	k	36	ILE	6.9
19	8	14	THR	6.9

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Mol	Chain	Res	Type	RSRZ
16	1	244	LEU	6.9
1	a	7	GLU	6.9
6	6	99	GLN	6.9
1	a	243	ILE	6.9
1	a	270	VAL	6.9
15	k	60	THR	6.9
3	3	30	PRO	6.8
6	6	107	LEU	6.8
6	6	89	GLU	6.8
1	a	519	LYS	6.8
16	1	279	GLY	6.8
13	c	1	MET	6.8
16	1	183	LYS	6.7
16	1	30	LYS	6.7
16	1	623	PRO	6.7
15	k	44	THR	6.7
15	k	21	SER	6.7
16	1	249	MET	6.7
6	6	101	VAL	6.6
15	k	46	LYS	6.6
1	a	274	PHE	6.6
2	2	310	GLY	6.6
2	2	311	PRO	6.6
1	a	231	VAL	6.6
16	1	14	VAL	6.6
2	2	2	ALA	6.5
19	8	60	THR	6.5
19	8	59	LYS	6.4
1	a	621	VAL	6.4
6	6	93	SER	6.3
19	8	46	LYS	6.3
15	k	70	MET	6.3
3	3	14	CYS	6.3
9	K	51	ALA	6.3
16	1	10	ALA	6.2
14	e	26	ALA	6.2
19	8	35	VAL	6.1
14	e	38	ILE	6.1
15	k	24	ILE	6.1
6	F	2	ASP	6.1
9	K	53	PRO	6.1
6	6	120	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
16	1	100	TYR	6.1
2	2	226	PHE	6.0
5	5	43	ARG	6.0
14	e	9	VAL	6.0
16	1	15	SER	6.0
12	b	730	PHE	5.9
16	1	18	ASN	5.9
5	5	19	TYR	5.9
2	2	295	TRP	5.9
2	2	731	GLY	5.8
6	6	11	SER	5.8
16	1	21	VAL	5.8
1	a	266	LEU	5.8
16	1	31	PRO	5.8
16	1	16	VAL	5.8
1	a	10	ALA	5.7
1	a	518	GLY	5.7
1	a	1	MET	5.7
19	8	9	ALA	5.7
2	2	215	THR	5.7
14	e	30	LYS	5.7
1	a	12	ALA	5.7
9	K	57	SER	5.7
1	a	205	LEU	5.6
16	1	51	LEU	5.6
2	2	470	TYR	5.6
1	a	255	SER	5.6
16	1	238	LEU	5.6
15	k	51	ALA	5.5
1	a	108	THR	5.5
16	1	92	PHE	5.4
14	e	31	SER	5.4
9	K	59	LYS	5.4
14	e	3	LEU	5.4
16	1	515	ALA	5.4
10	l	7	VAL	5.4
16	1	103	TRP	5.4
15	k	83	GLY	5.4
19	8	19	SER	5.3
6	6	61	HIS	5.3
17	4	2	THR	5.3
19	8	52	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
2	2	504	SER	5.2
14	e	23	GLY	5.2
15	k	79	GLY	5.2
8	7	1	MET	5.2
9	K	50	LEU	5.2
15	k	85	ALA	5.2
16	1	505	ALA	5.2
9	K	45	GLY	5.2
10	L	1	MET	5.2
5	5	22	VAL	5.2
19	8	84	LEU	5.2
16	1	160	CYS	5.1
16	1	256	PHE	5.1
6	6	59	PHE	5.1
16	1	182	VAL	5.1
1	A	2	THR	5.1
8	7	2	ASP	5.0
11	9	2	ALA	5.0
2	2	524	LEU	5.0
6	6	4	PHE	5.0
3	3	26	LEU	5.0
12	b	731	GLY	5.0
9	K	46	LYS	5.0
1	a	272	SER	5.0
15	k	57	SER	5.0
15	k	20	LEU	5.0
10	l	1	MET	5.0
9	K	44	THR	5.0
16	1	184	ALA	5.0
1	a	520	VAL	5.0
15	k	68	ALA	4.9
16	1	29	GLY	4.9
16	1	242	PHE	4.9
9	K	60	THR	4.9
16	1	9	GLU	4.9
16	1	363	THR	4.9
19	8	44	THR	4.9
4	d	68	LEU	4.9
5	E	66	LEU	4.9
6	6	104	ASN	4.9
16	1	22	PRO	4.9
6	F	1	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	2	216	PRO	4.9
14	e	39	VAL	4.9
19	8	34	PHE	4.9
15	k	86	SER	4.9
2	2	205	GLN	4.8
6	f	16	TYR	4.8
8	j	40	PRO	4.8
16	1	34	PHE	4.8
6	6	2	ASP	4.8
5	5	62	ALA	4.8
1	a	40	ARG	4.8
9	K	48	LYS	4.8
2	B	480	ASP	4.8
14	e	29	GLU	4.7
3	3	40	ALA	4.7
6	f	1	ALA	4.7
1	a	378	TYR	4.7
19	8	45	GLY	4.7
6	6	105	VAL	4.7
16	1	248	LYS	4.7
6	6	87	LEU	4.7
1	a	323	GLU	4.7
6	6	63	GLY	4.7
6	6	19	LYS	4.7
1	a	41	GLY	4.7
14	e	37	VAL	4.7
7	i	38	GLY	4.6
16	1	19	ASN	4.6
6	6	98	MET	4.6
19	8	47	GLY	4.6
2	2	520	ILE	4.6
4	D	2	THR	4.6
15	k	43	LYS	4.6
16	1	496	ALA	4.6
1	a	500	ASN	4.6
16	1	8	ARG	4.6
1	a	47	TRP	4.5
10	1	4	SER	4.5
2	2	456	VAL	4.5
2	2	579	TRP	4.5
14	e	60	ASN	4.5
1	a	253	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
17	4	114	ALA	4.5
16	1	231	VAL	4.5
17	4	103	VAL	4.5
16	1	288	LEU	4.5
1	a	383	TYR	4.5
2	2	222	LEU	4.5
15	k	25	ILE	4.5
16	1	709	VAL	4.5
1	a	249	MET	4.5
1	a	267	ASN	4.4
1	a	207	LEU	4.4
19	8	20	LEU	4.4
2	2	263	PRO	4.4
6	f	59	PHE	4.4
19	8	36	ILE	4.4
1	a	748	LEU	4.4
1	a	613	MET	4.4
2	2	166	ALA	4.4
3	3	57	ALA	4.4
15	k	10	GLN	4.4
2	2	286	ILE	4.4
1	a	38	LEU	4.4
8	7	38	PHE	4.4
1	a	269	GLY	4.3
6	6	38	GLU	4.3
1	A	12	ALA	4.3
1	a	8	ARG	4.3
8	7	9	SER	4.3
1	a	247	SER	4.3
15	k	28	LEU	4.3
5	5	32	GLY	4.3
2	2	471	GLY	4.3
16	1	266	LEU	4.3
16	1	180	TYR	4.3
15	k	35	VAL	4.3
15	k	32	PHE	4.3
15	k	72	PHE	4.3
2	B	342	ILE	4.3
14	e	40	ARG	4.3
15	k	29	CYS	4.3
3	3	13	GLY	4.2
10	l	43	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
6	6	134	LYS	4.2
4	d	56	LEU	4.2
19	8	51	ALA	4.2
3	3	12	ILE	4.2
1	A	359	LEU	4.2
2	2	441	VAL	4.2
9	K	55	LEU	4.2
3	3	29	VAL	4.2
10	l	3	GLU	4.2
1	a	273	ASP	4.2
2	2	218	HIS	4.2
2	B	244	PHE	4.2
8	j	32	PHE	4.2
3	3	63	LEU	4.2
2	2	217	PRO	4.2
14	e	33	ILE	4.1
16	1	396	ILE	4.1
5	5	20	GLY	4.1
1	a	9	GLU	4.1
17	4	141	VAL	4.1
1	a	275	LEU	4.1
16	1	270	VAL	4.1
3	3	41	SER	4.1
9	K	42	GLN	4.1
1	a	36	ARG	4.1
16	1	38	LEU	4.1
15	k	40	ALA	4.1
14	e	32	GLY	4.1
8	7	33	TYR	4.0
2	2	527	THR	4.0
5	5	23	GLY	4.0
10	L	2	ALA	4.0
1	a	92	PHE	4.0
6	6	17	LEU	4.0
1	a	156	TYR	4.0
16	1	240	HIS	4.0
16	1	504	THR	4.0
10	l	5	ASN	4.0
4	d	104	PHE	4.0
9	K	8	LEU	4.0
16	1	705	ASN	4.0
19	8	64	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
3	3	62	PHE	4.0
2	B	213	LEU	4.0
2	2	460	TRP	4.0
1	a	206	GLY	4.0
14	e	24	THR	4.0
6	6	131	LEU	3.9
5	5	10	ARG	3.9
6	f	94	LYS	3.9
16	1	156	TYR	3.9
2	2	232	VAL	3.9
19	8	53	PRO	3.9
2	2	427	LEU	3.9
2	B	243	ILE	3.9
2	2	501	GLY	3.9
15	k	45	GLY	3.9
16	1	234	LYS	3.9
4	d	40	PHE	3.9
1	a	254	PRO	3.9
2	2	396	TYR	3.9
9	K	34	PHE	3.9
8	J	32	PHE	3.9
1	a	37	THR	3.9
16	1	680	ALA	3.9
14	e	8	LYS	3.9
11	9	3	LEU	3.9
13	c	62	PHE	3.9
17	4	107	LYS	3.9
1	a	623	PRO	3.8
2	2	398	PRO	3.8
16	1	163	ILE	3.8
15	k	34	PHE	3.8
4	D	1	MET	3.8
15	k	54	GLN	3.8
1	a	624	ASP	3.8
4	d	83	TYR	3.8
1	a	105	ALA	3.8
1	a	107	PRO	3.8
1	a	750	ILE	3.8
6	6	3	ASP	3.8
4	d	86	TYR	3.8
9	K	54	GLN	3.8
2	2	214	SER	3.8

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Mol	Chain	Res	Type	RSRZ
16	1	255	SER	3.8
16	1	257	ALA	3.8
15	k	37	GLY	3.8
6	6	110	LYS	3.8
5	E	3	LEU	3.8
1	A	6	PRO	3.8
8	j	1	MET	3.8
2	2	423	VAL	3.8
2	B	343	THR	3.8
1	a	263	PHE	3.7
9	K	23	GLY	3.7
19	8	49	ASP	3.7
2	2	472	PHE	3.7
16	1	360	GLY	3.7
17	4	110	GLU	3.7
15	k	58	LYS	3.7
2	2	528	ALA	3.7
1	a	204	LEU	3.7
2	2	316	GLY	3.7
6	6	21	LYS	3.7
3	3	39	ILE	3.7
9	K	24	ILE	3.7
3	3	5	VAL	3.7
2	2	424	SER	3.7
2	2	525	HIS	3.7
1	a	208	GLY	3.7
15	k	82	LEU	3.7
17	4	113	GLU	3.7
1	a	34	PHE	3.6
14	e	18	TRP	3.6
14	e	27	SER	3.6
1	a	261	THR	3.6
19	8	24	ILE	3.6
16	1	665	LEU	3.6
1	a	39	ALA	3.6
6	6	62	ALA	3.6
16	1	710	ALA	3.6
1	a	233	PRO	3.6
5	5	7	ASP	3.6
1	a	301	ALA	3.6
16	1	500	ASN	3.6
18	h	38	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	a	617	VAL	3.6
10	L	3	GLU	3.6
16	1	522	MET	3.6
8	7	3	GLY	3.6
16	1	250	ALA	3.6
6	6	113	LEU	3.5
1	a	250	ALA	3.5
1	a	367	ALA	3.5
16	1	516	VAL	3.5
17	4	77	LYS	3.5
6	6	91	ARG	3.5
15	k	78	ALA	3.5
16	1	285	THR	3.5
16	1	378	TYR	3.5
9	K	19	SER	3.5
8	7	32	PHE	3.5
1	a	259	GLY	3.5
1	a	303	LEU	3.5
4	d	77	LYS	3.5
6	6	50	TYR	3.5
1	A	3	ILE	3.5
16	1	514	ILE	3.5
6	6	18	ALA	3.4
2	2	341	VAL	3.4
1	a	264	PHE	3.4
15	k	61	PHE	3.4
16	1	201	LEU	3.4
15	k	27	CYS	3.4
16	1	251	GLU	3.4
2	2	399	VAL	3.4
1	a	258	GLN	3.4
10	l	6	GLN	3.4
16	1	177	TRP	3.4
6	F	113	LEU	3.4
2	B	2	ALA	3.4
6	6	94	LYS	3.4
19	8	54	GLN	3.4
2	2	82	LEU	3.4
19	8	23	GLY	3.4
3	3	8	TYR	3.4
2	2	523	GLY	3.3
2	2	530	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	3	27	GLU	3.3
6	6	51	PRO	3.3
6	6	86	TYR	3.3
15	k	9	ALA	3.3
8	j	2	ASP	3.3
10	l	91	VAL	3.3
19	8	81	VAL	3.3
4	d	92	GLY	3.3
2	2	522	LEU	3.3
9	K	61	PHE	3.3
16	1	204	LEU	3.3
1	a	618	TRP	3.3
6	f	15	ALA	3.3
18	h	2	ASP	3.3
16	1	25	PHE	3.3
16	1	152	PHE	3.3
6	F	94	LYS	3.3
2	2	618	ARG	3.3
10	L	110	SER	3.3
2	2	313	THR	3.3
16	1	161	THR	3.3
19	8	32	PHE	3.3
16	1	96	LYS	3.3
6	6	117	LEU	3.3
6	6	130	LYS	3.3
6	6	43	ALA	3.3
6	6	10	CYS	3.3
14	e	5	ARG	3.3
2	2	422	TRP	3.3
6	6	132	VAL	3.3
2	2	519	ALA	3.2
4	d	30	ILE	3.2
1	a	209	SER	3.2
2	B	295	TRP	3.2
6	f	37	ALA	3.2
16	1	17	ASP	3.2
15	k	80	MET	3.2
6	f	95	ASN	3.2
14	e	59	ASN	3.2
1	a	619	GLY	3.2
8	j	4	LEU	3.2
1	a	202	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	3	7	ILE	3.2
16	1	393	HIS	3.2
16	1	364	ILE	3.2
2	B	312	LEU	3.2
16	1	359	LEU	3.2
17	4	83	TYR	3.1
1	a	203	GLY	3.1
1	a	286	GLY	3.1
4	d	4	LEU	3.1
16	1	281	LEU	3.1
16	1	503	ALA	3.1
17	4	96	TYR	3.1
1	a	242	PHE	3.1
16	1	47	TRP	3.1
2	B	239	THR	3.1
5	5	2	ALA	3.1
2	2	243	ILE	3.1
16	1	289	TRP	3.1
4	d	46	GLY	3.1
6	f	2	ASP	3.1
2	2	227	THR	3.1
2	2	337	ALA	3.1
6	6	22	ASN	3.1
6	6	41	ALA	3.1
16	1	501	ALA	3.1
2	2	297	ILE	3.1
14	e	11	ILE	3.1
16	1	390	PHE	3.1
17	4	85	ILE	3.1
2	2	343	THR	3.1
2	2	526	THR	3.1
6	f	129	GLY	3.1
5	E	70	GLN	3.1
3	3	38	GLN	3.0
16	1	159	TYR	3.0
6	F	134	LYS	3.0
4	d	47	ALA	3.0
3	3	32	ASP	3.0
4	D	136	LYS	3.0
4	d	29	ALA	3.0
15	k	69	THR	3.0
3	3	43	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
17	4	98	HIS	3.0
8	7	6	SER	3.0
5	E	69	VAL	3.0
1	a	304	PHE	3.0
17	4	102	GLY	3.0
16	1	367	ALA	3.0
1	a	31	PRO	3.0
4	d	84	LYS	3.0
1	a	300	ILE	3.0
6	6	16	TYR	3.0
12	b	635	TYR	3.0
16	1	247	SER	3.0
16	1	507	TYR	3.0
2	2	476	LEU	3.0
11	M	1	MET	3.0
2	B	345	LEU	3.0
5	E	68	LEU	3.0
16	1	391	THR	3.0
16	1	655	ALA	3.0
1	a	637	GLN	3.0
2	2	494	TRP	3.0
1	A	300	ILE	2.9
1	a	11	LYS	2.9
15	k	48	LYS	2.9
6	f	41	ALA	2.9
16	1	717	ALA	2.9
17	4	117	THR	2.9
19	8	31	VAL	2.9
16	1	174	PHE	2.9
19	8	61	PHE	2.9
16	1	245	GLU	2.9
2	B	495	LEU	2.9
16	1	712	ALA	2.9
17	4	97	LEU	2.9
1	a	338	LYS	2.9
2	2	230	TRP	2.9
1	a	163	ILE	2.9
2	B	339	LEU	2.9
14	e	34	LEU	2.9
19	8	22	VAL	2.9
1	a	381	ILE	2.9
2	2	573	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
6	f	19	LYS	2.9
2	2	428	GLY	2.9
2	2	582	ASN	2.9
6	f	39	ARG	2.9
6	f	53	LEU	2.9
1	a	145	TYR	2.9
1	a	678	VAL	2.9
2	B	338	SER	2.9
14	e	20	GLY	2.9
6	6	44	LEU	2.9
13	c	36	ALA	2.9
8	7	40	PRO	2.8
17	4	101	ASP	2.8
19	8	12	SER	2.8
2	B	730	PHE	2.8
6	f	30	PRO	2.8
2	2	710	PHE	2.8
4	D	110	GLU	2.8
6	6	111	LYS	2.8
8	J	33	TYR	2.8
1	A	548	ILE	2.8
16	1	743	PHE	2.8
1	a	235	ASP	2.8
6	6	127	THR	2.8
14	e	68	LEU	2.8
16	1	356	LEU	2.8
16	1	397	GLY	2.8
16	1	398	GLY	2.8
2	2	330	PHE	2.8
6	6	49	GLY	2.8
16	1	298	LEU	2.8
16	1	400	LEU	2.8
17	4	108	VAL	2.8
2	2	586	TRP	2.8
2	2	654	TRP	2.8
4	d	95	GLN	2.8
1	a	305	ILE	2.8
6	f	42	SER	2.8
2	2	282	VAL	2.7
4	d	39	VAL	2.7
16	1	94	GLY	2.7
2	B	488	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	2	426	PHE	2.7
1	a	201	LEU	2.7
2	2	361	GLN	2.7
6	f	34	LYS	2.7
16	1	151	GLY	2.7
2	B	377	ALA	2.7
16	1	395	TRP	2.7
1	a	366	VAL	2.7
14	e	22	VAL	2.7
1	a	396	ILE	2.7
2	2	567	ILE	2.7
6	f	60	THR	2.7
2	2	268	LEU	2.7
2	2	505	LEU	2.7
6	f	10	CYS	2.7
17	4	33	THR	2.7
4	D	133	PHE	2.7
14	e	41	PHE	2.7
2	B	204	GLY	2.7
2	B	297	ILE	2.7
3	C	62	PHE	2.7
2	2	420	LEU	2.7
6	6	67	ILE	2.7
8	7	7	PHE	2.7
5	E	12	LYS	2.7
1	a	96	LYS	2.6
2	2	431	THR	2.6
8	7	10	THR	2.6
2	B	380	LEU	2.6
15	k	77	GLY	2.6
2	2	605	GLN	2.6
4	d	70	THR	2.6
1	a	733	LEU	2.6
2	2	320	LEU	2.6
16	1	381	ILE	2.6
17	4	30	ILE	2.6
2	B	215	THR	2.6
5	5	4	ASN	2.6
16	1	517	ALA	2.6
9	K	63	LEU	2.6
16	1	377	PRO	2.6
6	f	40	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	2	247	SER	2.6
16	1	521	ALA	2.6
19	8	16	ALA	2.6
16	1	187	LEU	2.6
16	1	683	LEU	2.6
1	a	283	PRO	2.6
2	B	472	PHE	2.6
2	B	344	SER	2.6
2	2	518	HIS	2.6
2	B	341	VAL	2.6
2	2	307	ALA	2.6
1	a	411	PHE	2.6
13	c	35	LYS	2.6
15	k	42	GLN	2.6
2	2	43	TYR	2.6
1	a	630	VAL	2.6
1	a	26	GLU	2.6
16	1	304	PHE	2.6
1	a	616	ASP	2.6
17	4	116	GLY	2.6
6	f	27	THR	2.5
14	e	2	ALA	2.5
16	1	27	LYS	2.5
5	5	11	ILE	2.5
16	1	61	GLN	2.5
10	L	106	GLY	2.5
16	1	91	TYR	2.5
1	A	327	ALA	2.5
1	A	358	LEU	2.5
2	B	264	GLN	2.5
15	k	64	PRO	2.5
2	2	336	LEU	2.5
2	2	223	MET	2.5
2	2	467	LYS	2.5
16	1	13	LYS	2.5
1	a	229	ALA	2.5
2	B	346	VAL	2.5
16	1	430	LEU	2.5
8	j	3	GLY	2.5
2	B	214	SER	2.5
18	h	1	MET	2.5
6	f	55	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
8	7	4	LEU	2.5
1	A	360	GLY	2.5
6	F	128	SER	2.5
20	0	4	SER	2.5
6	6	39	ARG	2.5
2	2	164	SER	2.5
2	2	344	SER	2.5
10	1	9	GLN	2.5
16	1	110	ILE	2.5
3	3	58	CYS	2.5
2	2	502	THR	2.5
2	2	204	GLY	2.5
3	3	31	TRP	2.5
5	5	68	LEU	2.5
16	1	226	LEU	2.5
6	6	137	GLU	2.5
18	h	4	SER	2.5
17	4	133	PHE	2.5
16	1	64	ASP	2.5
2	B	499	ASN	2.5
2	2	601	GLY	2.5
15	k	84	LEU	2.4
1	a	159	TYR	2.4
2	2	68	VAL	2.4
12	b	662	ILE	2.4
2	2	712	VAL	2.4
1	A	9	GLU	2.4
6	f	98	MET	2.4
15	k	26	MET	2.4
3	3	36	ALA	2.4
14	e	7	ASP	2.4
2	2	92	TRP	2.4
2	B	216	PRO	2.4
2	2	163	PRO	2.4
6	6	9	PRO	2.4
20	0	74	SER	2.4
14	e	28	VAL	2.4
1	a	734	GLY	2.4
16	1	20	PRO	2.4
1	a	200	HIS	2.4
6	6	52	HIS	2.4
6	f	130	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	2	203	ARG	2.4
16	1	713	ILE	2.4
1	a	174	PHE	2.4
1	a	611	TRP	2.4
20	0	113	THR	2.4
2	2	584	LEU	2.4
16	1	502	LEU	2.4
1	a	27	LYS	2.4
2	2	233	TYR	2.4
6	6	58	ARG	2.4
8	j	31	ARG	2.4
2	2	711	THR	2.4
6	F	127	THR	2.4
6	f	38	GLU	2.4
17	4	109	ASN	2.3
4	d	94	VAL	2.3
16	1	115	GLN	2.3
9	K	58	LYS	2.3
2	B	524	LEU	2.3
2	2	419	HIS	2.3
19	8	42	GLN	2.3
4	d	67	ALA	2.3
6	f	18	ALA	2.3
6	6	20	SER	2.3
2	B	259	GLY	2.3
1	a	362	LEU	2.3
2	2	53	HIS	2.3
16	1	58	PHE	2.3
2	B	240	ALA	2.3
2	2	352	SER	2.3
4	d	96	TYR	2.3
2	2	445	GLY	2.3
11	9	5	ASP	2.3
1	a	43	LYS	2.3
1	a	284	VAL	2.3
9	K	18	TRP	2.3
14	e	61	PHE	2.3
2	2	418	SER	2.3
6	6	108	ALA	2.3
16	1	282	ASN	2.3
1	a	276	THR	2.3
2	B	487	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
16	1	271	TYR	2.3
2	B	182	LEU	2.3
2	2	397	ASP	2.3
2	2	531	LEU	2.3
15	k	52	LEU	2.3
16	1	65	LEU	2.3
12	b	341	VAL	2.3
1	a	197	MET	2.3
2	2	577	MET	2.3
1	a	521	ALA	2.3
5	E	2	ALA	2.3
1	a	668	TYR	2.3
1	a	199	HIS	2.3
2	2	491	LEU	2.3
16	1	208	GLY	2.3
2	2	358	PHE	2.3
1	A	502	LEU	2.3
1	a	726	VAL	2.2
2	2	706	GLY	2.2
5	E	67	GLU	2.2
17	4	3	GLU	2.2
1	a	593	LEU	2.2
1	a	723	GLY	2.2
16	1	132	GLY	2.2
6	f	127	THR	2.2
12	b	710	PHE	2.2
16	1	519	LYS	2.2
16	1	687	PHE	2.2
1	a	492	LEU	2.2
2	2	507	LEU	2.2
6	6	13	ASN	2.2
16	1	253	TYR	2.2
2	2	566	ASP	2.2
2	2	594	LYS	2.2
19	8	27	CYS	2.2
2	2	156	HIS	2.2
10	l	16	PHE	2.2
12	b	524	LEU	2.2
6	6	12	GLU	2.2
1	A	208	GLY	2.2
15	k	49	ASP	2.2
2	2	292	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	a	677	PHE	2.2
2	2	462	GLN	2.2
14	e	21	ASP	2.2
9	K	38	TYR	2.2
2	2	242	HIS	2.2
1	a	307	ALA	2.2
4	d	48	ALA	2.2
6	f	21	LYS	2.2
9	K	49	ASP	2.2
16	1	144	PHE	2.2
1	a	222	PRO	2.2
2	B	479	PRO	2.2
2	B	731	GLY	2.2
1	A	297	HIS	2.2
1	a	684	MET	2.2
2	B	473	ASP	2.2
2	2	57	ILE	2.2
12	b	297	ILE	2.2
10	L	107	GLU	2.2
1	a	68	VAL	2.1
4	d	32	TRP	2.1
1	A	751	GLY	2.1
2	B	227	THR	2.1
2	B	252	THR	2.1
2	2	130	THR	2.1
4	D	92	GLY	2.1
1	a	635	PHE	2.1
16	1	748	LEU	2.1
17	4	81	GLN	2.1
2	B	423	VAL	2.1
14	e	25	VAL	2.1
15	k	73	GLY	2.1
16	1	229	ALA	2.1
16	1	241	GLU	2.1
2	2	588	THR	2.1
1	a	25	PHE	2.1
2	2	457	PHE	2.1
2	2	345	LEU	2.1
1	A	355	ASN	2.1
8	7	5	LYS	2.1
16	1	136	GLY	2.1
1	a	729	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	2	576	ALA	2.1
18	h	7	ALA	2.1
16	1	23	THR	2.1
1	a	548	ILE	2.1
4	d	97	LEU	2.1
16	1	361	SER	2.1
17	4	118	LYS	2.1
10	l	92	ALA	2.1
14	e	53	ALA	2.1
16	1	265	THR	2.1
4	d	3	GLU	2.1
5	5	12	LYS	2.1
15	k	74	HIS	2.1
5	5	47	ASN	2.1
1	a	308	GLY	2.1
2	2	315	ALA	2.1
16	1	213	ALA	2.1
18	h	6	ALA	2.1
1	a	363	THR	2.1
2	B	431	THR	2.1
12	b	620	TYR	2.1
16	1	236	ILE	2.1
1	a	369	HIS	2.1
1	a	747	SER	2.1
10	l	20	LEU	2.1
1	A	485	TRP	2.1
16	1	708	ASN	2.1
1	a	675	GLY	2.1
19	8	80	MET	2.1
2	2	219	PRO	2.1
12	b	576	ALA	2.1
17	4	51	ASN	2.1
1	A	10	ALA	2.0
2	2	511	PRO	2.0
16	1	299	ALA	2.0
1	a	622	SER	2.0
4	D	89	TYR	2.0
10	l	89	ILE	2.0
16	1	632	LEU	2.0
16	1	686	LEU	2.0
17	4	115	GLN	2.0
18	h	3	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	ASP	2.0
6	6	64	ASP	2.0
2	2	655	ALA	2.0
2	2	293	THR	2.0
16	1	109	HIS	2.0
16	1	617	VAL	2.0
1	a	24	SER	2.0
8	j	6	SER	2.0
1	A	362	LEU	2.0
2	2	157	LEU	2.0
4	d	122	ILE	2.0
16	1	145	TYR	2.0
12	b	577	MET	2.0
2	2	264	GLN	2.0
2	2	340	GLY	2.0
2	2	568	SER	2.0
9	K	87	SER	2.0
12	b	418	SER	2.0
16	1	366	VAL	2.0
1	a	340	LEU	2.0
2	2	342	ILE	2.0
5	E	34	LEU	2.0
6	6	40	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	k	4001	40/40	0.22	0.61	119,152,167,168	0
24	BCR	8	4001	40/40	0.53	0.54	105,124,139,140	0
34	ZEX	7	4015	42/42	0.54	0.43	100,131,150,152	0
27	ACT	a	7001	4/4	0.55	0.18	128,130,130,131	0
24	BCR	2	4004	40/40	0.56	0.86	105,125,145,147	0
25	LHG	B	5006	49/49	0.60	0.90	84,117,143,146	0
26	LMG	A	5008	55/55	0.60	0.65	72,119,146,146	0
26	LMG	b	5007	55/55	0.62	0.61	76,97,115,116	0
24	BCR	B	4018	40/40	0.62	0.61	64,85,115,121	0
21	CLA	a	1113	50/65	0.62	0.47	116,145,155,159	0
24	BCR	K	4001	40/40	0.62	0.38	40,73,103,106	0
25	LHG	1	5005	49/49	0.63	0.38	90,126,165,169	0
25	LHG	F	5002	49/49	0.64	0.41	73,110,175,181	0
24	BCR	1	4001	40/40	0.65	0.50	90,109,136,137	0
24	BCR	1	4019	40/40	0.66	0.63	106,122,142,143	0
24	BCR	b	4018	40/40	0.67	0.45	53,76,95,100	0
24	BCR	2	4018	40/40	0.67	0.81	83,136,143,144	0
24	BCR	2	4005	40/40	0.68	0.34	81,113,134,136	0
21	CLA	6	1302	43/65	0.68	0.56	116,141,171,178	0
26	LMG	B	5005	55/55	0.68	0.40	71,110,133,137	0
34	ZEX	j	4015	42/42	0.69	0.37	51,97,113,117	0
24	BCR	7	4013	40/40	0.69	0.39	78,113,122,124	0
25	LHG	l	5004	49/49	0.69	0.26	48,75,159,163	0
25	LHG	a	5007	49/49	0.70	0.70	100,139,169,175	0
25	LHG	l	5002	49/49	0.70	0.29	65,87,148,157	0
21	CLA	2	1217	52/65	0.71	0.34	99,130,138,139	0
25	LHG	a	5005	49/49	0.71	0.25	51,107,175,183	0
25	LHG	1	5007	49/49	0.72	0.46	80,102,149,154	0
26	LMG	2	5005	55/55	0.72	0.54	105,127,150,153	0
37	DGD	L	5004	66/66	0.72	0.33	42,87,116,121	0
31	SQD	b	5006	54/54	0.72	0.32	46,81,138,143	0
27	ACT	B	7001	4/4	0.72	0.38	57,71,71,74	0
24	BCR	a	4003	40/40	0.72	0.39	81,121,142,146	0
24	BCR	a	4001	40/40	0.72	0.34	89,142,156,156	0
35	LMT	1	6001	35/35	0.72	0.40	76,127,136,141	0
25	LHG	M	5001	49/49	0.72	0.24	51,97,144,149	0
25	LHG	0	5004	49/49	0.73	0.30	55,96,124,136	0
26	LMG	a	5002	50/55	0.73	0.23	54,78,109,110	0
25	LHG	A	5006	49/49	0.73	0.36	44,81,137,147	0
24	BCR	a	4019	40/40	0.74	0.53	98,114,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	a	4002	40/40	0.74	0.27	108,123,141,142	0
25	LHG	2	5004	49/49	0.74	0.41	92,108,152,153	0
24	BCR	A	4019	40/40	0.74	0.55	72,84,114,114	0
21	CLA	2	1209	45/65	0.75	0.36	104,130,139,142	0
23	SF4	C	3002	8/8	0.75	0.23	43,65,114,208	0
31	SQD	f	5001	54/54	0.75	0.36	42,100,123,132	0
25	LHG	6	5001	12/49	0.75	0.23	80,131,152,159	0
26	LMG	A	5002	50/55	0.76	0.23	40,72,99,106	0
24	BCR	1	4003	40/40	0.76	0.32	71,105,134,138	0
34	ZEX	J	4015	42/42	0.76	0.30	55,68,112,116	0
35	LMT	l	6001	35/35	0.76	0.36	55,95,118,120	0
21	CLA	1	1108	47/65	0.76	0.33	50,112,123,128	0
21	CLA	2	1240	41/65	0.76	0.48	131,137,146,150	0
31	SQD	0	5005	54/54	0.76	0.23	59,91,141,148	0
25	LHG	A	5005	49/49	0.76	0.27	48,72,132,139	0
25	LHG	l	5001	49/49	0.77	0.37	64,92,141,144	0
21	CLA	k	1402	49/65	0.77	0.26	134,158,161,161	8
24	BCR	6	4016	40/40	0.77	0.42	59,91,128,129	0
21	CLA	2	1216	50/65	0.77	0.32	91,127,138,139	0
25	LHG	l	5003	49/49	0.77	0.36	81,111,137,138	0
25	LHG	A	5007	49/49	0.77	0.32	46,85,113,121	0
21	CLA	B	1240	65/65	0.77	0.40	76,105,133,136	0
30	ECH	2	4006	41/41	0.77	0.34	65,122,132,133	0
21	CLA	2	1212	41/65	0.77	0.34	100,132,137,144	0
24	BCR	j	4013	40/40	0.78	0.32	72,90,121,123	0
21	CLA	2	1231	46/65	0.78	0.27	84,122,128,129	0
21	CLA	a	1114	52/65	0.78	0.34	119,138,150,152	0
26	LMG	1	5002	50/55	0.78	0.31	44,94,119,120	0
24	BCR	B	4004	40/40	0.78	0.31	63,93,109,110	0
26	LMG	K	5009	55/55	0.78	0.24	41,80,106,107	0
21	CLA	J	1302	65/65	0.79	0.32	75,95,121,137	0
24	BCR	1	4012	40/40	0.79	0.33	100,112,124,125	0
31	SQD	F	5001	54/54	0.79	0.42	66,93,129,134	0
21	CLA	a	1112	65/65	0.80	0.26	74,129,135,137	0
26	LMG	b	5005	55/55	0.80	0.36	54,79,114,116	0
21	CLA	1	1105	50/65	0.80	0.28	96,116,123,126	0
21	CLA	a	1118	65/65	0.80	0.24	102,119,142,150	0
21	CLA	1	1139	65/65	0.80	0.28	75,115,124,125	0
21	CLA	k	1401	50/65	0.80	0.24	84,137,147,152	5
21	CLA	a	1115	65/65	0.80	0.28	89,133,152,154	0
21	CLA	a	1120	55/65	0.80	0.27	98,124,129,138	0
26	LMG	a	5004	55/55	0.80	0.26	85,112,130,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	2	1234	50/65	0.81	0.25	90,107,111,113	0
21	CLA	2	1213	50/65	0.81	0.35	99,122,130,139	0
21	CLA	J	1303	65/65	0.81	0.34	93,112,125,127	0
21	CLA	2	1232	45/65	0.81	0.25	101,128,147,151	0
26	LMG	1	5004	55/55	0.81	0.36	83,97,112,118	0
21	CLA	2	1219	53/65	0.81	0.24	108,125,148,156	0
21	CLA	1	1138	60/65	0.81	0.28	84,118,134,136	0
24	BCR	2	4010	40/40	0.81	0.32	66,101,136,136	0
21	CLA	a	1102	65/65	0.81	0.33	68,92,118,128	0
21	CLA	a	1108	57/65	0.81	0.22	91,124,129,130	0
21	CLA	2	1218	65/65	0.81	0.31	91,133,158,162	0
21	CLA	1	1134	65/65	0.81	0.24	89,105,120,125	0
21	CLA	j	1302	65/65	0.82	0.35	77,110,125,133	0
24	BCR	B	4005	40/40	0.82	0.27	45,78,102,103	0
21	CLA	7	1303	41/65	0.82	0.39	133,150,155,157	0
21	CLA	1	1113	44/65	0.82	0.31	83,124,133,135	0
27	ACT	A	7001	4/4	0.82	0.33	28,55,63,71	0
21	CLA	1	1109	65/65	0.82	0.45	72,109,120,122	0
24	BCR	b	4014	40/40	0.82	0.29	59,79,88,92	0
31	SQD	L	5002	54/54	0.83	0.23	33,61,95,99	0
21	CLA	2	1202	65/65	0.83	0.26	56,94,106,108	0
21	CLA	2	1235	53/65	0.83	0.24	82,112,122,123	0
23	SF4	A	3001	8/8	0.83	0.27	40,87,137,173	0
26	LMG	0	5001	55/55	0.83	0.28	34,74,99,107	0
21	CLA	a	1123	65/65	0.83	0.30	55,105,117,121	0
21	CLA	1	1120	65/65	0.83	0.20	85,102,126,128	0
24	BCR	2	4014	40/40	0.83	0.35	78,113,132,136	0
21	CLA	j	1303	55/65	0.83	0.42	97,117,130,137	0
21	CLA	2	1214	59/65	0.84	0.25	70,109,135,159	0
21	CLA	1	1123	65/65	0.84	0.28	49,86,107,115	0
21	CLA	6	1301	47/65	0.84	0.22	99,128,135,136	0
31	SQD	B	5008	54/54	0.84	0.32	61,86,107,113	0
21	CLA	1	1103	65/65	0.84	0.25	63,87,101,103	0
21	CLA	1	1114	45/65	0.84	0.36	107,117,125,129	0
26	LMG	A	5004	48/55	0.84	0.31	37,84,102,107	0
21	CLA	a	1801	55/65	0.84	0.24	83,118,128,133	0
24	BCR	a	4007	40/40	0.84	0.37	69,87,144,147	0
24	BCR	A	4003	40/40	0.85	0.26	32,53,89,91	0
24	BCR	1	4002	40/40	0.85	0.24	89,100,119,123	0
24	BCR	1	4007	40/40	0.85	0.32	55,73,127,132	0
21	CLA	1	1013	65/65	0.85	0.28	73,91,97,104	0
24	BCR	a	4008	40/40	0.85	0.28	51,82,109,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	l	4022	40/40	0.85	0.25	57,74,97,100	0
24	BCR	9	4021	40/40	0.85	0.29	58,80,116,118	0
21	CLA	7	1302	41/65	0.85	0.42	120,130,140,143	0
21	CLA	2	1229	65/65	0.86	0.26	83,109,124,136	0
22	PQN	1	2001	33/33	0.86	0.29	67,88,108,108	0
24	BCR	b	4004	40/40	0.86	0.21	36,60,76,87	0
21	CLA	2	1230	47/65	0.86	0.18	89,114,127,129	0
21	CLA	1	1115	65/65	0.86	0.23	78,119,130,131	0
25	LHG	B	5004	49/49	0.86	0.25	73,87,96,101	0
21	CLA	B	1232	50/65	0.86	0.23	81,92,105,108	0
21	CLA	2	1222	50/65	0.86	0.32	69,105,119,122	0
26	LMG	2	5002	55/55	0.86	0.26	55,72,93,107	0
33	MG	B	6002	1/1	0.86	0.23	69,69,69,69	0
21	CLA	1	1117	65/65	0.86	0.31	57,99,112,123	0
21	CLA	a	1116	60/65	0.86	0.27	79,99,109,110	0
31	SQD	L	5001	51/54	0.86	0.21	42,80,104,107	0
21	CLA	2	1220	45/65	0.86	0.27	114,124,128,132	0
21	CLA	a	1011	65/65	0.86	0.20	40,58,71,96	0
21	CLA	1	1116	65/65	0.86	0.22	75,95,118,121	0
25	LHG	0	5002	49/49	0.86	0.17	44,63,131,140	0
21	CLA	a	1111	65/65	0.86	0.28	76,106,131,133	0
21	CLA	b	1231	65/65	0.86	0.20	50,69,93,98	0
21	CLA	2	1215	60/65	0.87	0.23	73,100,112,118	0
21	CLA	F	1302	65/65	0.87	0.22	70,93,105,114	0
21	CLA	a	1139	65/65	0.87	0.20	64,86,103,105	0
25	LHG	L	5005	49/49	0.87	0.22	46,75,102,104	0
21	CLA	B	1231	65/65	0.87	0.22	66,84,101,104	0
35	LMT	L	6001	35/35	0.87	0.27	55,79,90,97	0
21	CLA	1	1104	65/65	0.87	0.27	65,91,99,106	0
21	CLA	a	1101	65/65	0.87	0.21	50,83,91,100	0
21	CLA	1	1118	65/65	0.87	0.22	79,103,130,134	0
21	CLA	2	1236	50/65	0.87	0.27	75,110,117,124	0
25	LHG	a	5003	49/49	0.87	0.36	76,96,106,109	0
21	CLA	2	1221	65/65	0.87	0.25	84,95,132,137	0
21	CLA	f	1302	65/65	0.87	0.35	67,99,109,115	0
21	CLA	b	1236	65/65	0.87	0.25	48,74,118,122	0
21	CLA	B	1209	65/65	0.87	0.23	67,88,123,127	0
21	CLA	A	1113	65/65	0.87	0.31	41,64,105,111	0
21	CLA	2	1225	65/65	0.88	0.22	52,92,111,114	0
21	CLA	2	1227	45/65	0.88	0.18	81,94,127,131	0
21	CLA	a	1105	58/65	0.88	0.25	78,110,122,129	0
30	ECH	b	4011	41/41	0.88	0.28	60,81,90,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	2	1208	60/65	0.88	0.18	63,88,138,142	0
21	CLA	1	1133	65/65	0.88	0.20	73,87,99,107	0
21	CLA	a	1121	65/65	0.88	0.28	94,117,142,146	0
24	BCR	a	4012	40/40	0.88	0.26	66,95,106,110	0
21	CLA	B	1219	65/65	0.88	0.19	73,94,125,126	0
24	BCR	2	4011	40/40	0.88	0.26	60,93,104,109	0
24	BCR	f	4016	40/40	0.88	0.22	66,81,104,107	0
21	CLA	2	1210	65/65	0.88	0.23	75,107,116,119	0
24	BCR	B	4010	40/40	0.88	0.32	51,66,81,84	0
25	LHG	1	5003	49/49	0.88	0.33	62,83,96,99	0
21	CLA	a	1125	65/65	0.88	0.24	64,91,106,111	0
21	CLA	a	1110	59/65	0.88	0.23	77,109,156,159	0
21	CLA	a	1134	49/65	0.88	0.17	73,118,128,132	0
21	CLA	a	1119	65/65	0.88	0.27	54,82,128,133	0
21	CLA	a	1107	50/65	0.89	0.18	68,88,108,112	0
21	CLA	a	1122	65/65	0.89	0.23	61,95,108,113	0
24	BCR	0	4022	40/40	0.89	0.24	41,60,87,92	0
32	CA	2	6001	1/1	0.89	0.06	112,112,112,112	0
21	CLA	B	1216	65/65	0.89	0.24	65,85,101,106	0
21	CLA	a	1109	65/65	0.89	0.20	65,102,118,124	0
21	CLA	F	1301	65/65	0.89	0.22	53,77,121,124	0
21	CLA	a	1117	65/65	0.89	0.38	64,89,103,112	0
24	BCR	1	4008	40/40	0.89	0.24	49,69,93,95	0
24	BCR	A	4002	40/40	0.89	0.24	33,60,75,82	0
21	CLA	1	1112	50/65	0.89	0.23	83,109,122,126	0
24	BCR	L	4022	40/40	0.89	0.21	41,57,81,86	0
30	ECH	B	4006	41/41	0.89	0.19	45,86,105,108	0
21	CLA	1	1127	65/65	0.89	0.28	64,86,112,118	0
21	CLA	b	1227	65/65	0.89	0.25	58,73,120,124	0
24	BCR	b	4010	40/40	0.89	0.21	41,58,68,71	0
21	CLA	b	1240	65/65	0.89	0.23	60,88,134,154	0
21	CLA	1	1107	51/65	0.89	0.17	83,102,117,121	0
21	CLA	2	1211	50/65	0.90	0.16	80,110,117,123	0
25	LHG	1	5001	49/49	0.90	0.24	64,84,101,104	0
21	CLA	a	1128	65/65	0.90	0.20	59,86,97,102	0
21	CLA	1	1102	55/65	0.90	0.21	50,81,117,120	0
21	CLA	1	1121	55/65	0.90	0.20	58,96,124,128	0
21	CLA	1	1126	65/65	0.90	0.23	58,94,108,115	0
21	CLA	b	1232	65/65	0.90	0.22	64,79,121,123	0
24	BCR	l	4019	40/40	0.90	0.23	29,44,54,56	0
24	BCR	b	4005	40/40	0.90	0.19	30,47,90,91	0
21	CLA	b	1222	65/65	0.90	0.25	38,54,114,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	B	1218	65/65	0.90	0.25	62,91,123,125	0
28	45D	h	4020	42/42	0.90	0.19	33,55,68,75	0
21	CLA	2	1203	65/65	0.90	0.26	57,88,101,105	0
21	CLA	a	1106	65/65	0.90	0.24	58,95,106,112	0
25	LHG	b	5004	49/49	0.90	0.23	63,80,101,105	0
21	CLA	a	1133	65/65	0.90	0.19	70,95,114,117	0
21	CLA	1	1128	65/65	0.90	0.21	62,79,99,113	0
21	CLA	2	1205	65/65	0.90	0.20	54,77,89,91	0
21	CLA	a	1129	52/65	0.90	0.17	64,85,95,98	0
21	CLA	B	1217	65/65	0.90	0.23	64,93,113,116	0
21	CLA	1	1012	65/65	0.90	0.26	72,88,98,101	0
21	CLA	b	1021	65/65	0.90	0.18	36,52,66,72	0
21	CLA	b	1230	65/65	0.90	0.22	53,86,120,125	0
35	LMT	F	6001	35/35	0.90	0.28	57,88,112,115	0
21	CLA	1	1101	65/65	0.91	0.22	58,88,120,123	0
21	CLA	B	1234	65/65	0.91	0.22	39,73,95,100	0
21	CLA	B	1214	65/65	0.91	0.22	48,81,89,92	0
21	CLA	B	1213	65/65	0.91	0.18	58,80,112,120	0
21	CLA	b	1208	60/65	0.91	0.15	36,53,91,103	0
21	CLA	b	1220	65/65	0.91	0.20	48,64,100,103	0
21	CLA	l	1501	65/65	0.91	0.21	48,69,110,117	0
30	ECH	i	4020	41/41	0.91	0.22	38,53,83,90	0
26	LMG	b	5002	55/55	0.91	0.20	36,55,84,89	0
26	LMG	B	5002	55/55	0.91	0.19	36,52,81,89	0
21	CLA	b	1228	65/65	0.91	0.18	58,73,117,121	0
29	CL	2	6000	1/1	0.91	0.31	74,74,74,74	0
21	CLA	1	1125	65/65	0.91	0.28	56,78,91,94	0
25	LHG	a	5001	49/49	0.91	0.25	57,72,117,128	0
21	CLA	B	1228	65/65	0.91	0.20	44,66,113,122	0
21	CLA	2	1223	55/65	0.91	0.26	64,99,141,145	0
21	CLA	B	1227	55/65	0.91	0.26	67,76,102,107	0
21	CLA	1	1111	65/65	0.91	0.19	63,85,113,118	0
30	ECH	b	4006	41/41	0.91	0.16	32,47,97,99	0
21	CLA	2	1228	45/65	0.91	0.16	53,67,126,132	0
24	BCR	J	4013	40/40	0.91	0.19	48,69,89,91	0
22	PQN	a	2001	33/33	0.91	0.24	39,65,84,87	0
27	ACT	B	7002	4/4	0.91	0.11	78,82,83,84	0
24	BCR	B	4017	40/40	0.91	0.25	22,44,56,57	0
21	CLA	A	1112	65/65	0.91	0.17	39,62,94,98	0
21	CLA	a	1126	65/65	0.91	0.24	71,91,104,105	0
21	CLA	8	1401	45/65	0.91	0.12	83,101,137,143	3
21	CLA	f	1301	50/65	0.91	0.15	74,93,114,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	2	1206	65/65	0.91	0.17	44,66,80,88	0
30	ECH	m	4021	41/41	0.91	0.19	23,49,80,80	0
21	CLA	K	1402	65/65	0.91	0.20	50,71,111,115	10
21	CLA	B	1210	65/65	0.91	0.16	38,67,90,92	0
21	CLA	B	1211	65/65	0.91	0.17	45,76,102,107	0
21	CLA	B	1212	55/65	0.92	0.17	70,82,128,132	0
21	CLA	2	1023	65/65	0.92	0.20	46,60,68,82	0
21	CLA	A	1122	60/65	0.92	0.16	25,42,70,83	0
34	ZEX	F	4016	42/42	0.92	0.16	46,72,98,103	0
21	CLA	1	1119	65/65	0.92	0.27	53,75,92,112	0
21	CLA	A	1123	65/65	0.92	0.18	25,38,52,60	0
21	CLA	b	1229	65/65	0.92	0.22	54,68,97,108	0
21	CLA	2	1021	65/65	0.92	0.24	45,67,114,117	0
24	BCR	B	4014	40/40	0.92	0.21	35,57,80,84	0
21	CLA	2	1226	55/65	0.92	0.20	55,70,91,97	0
21	CLA	A	1125	65/65	0.92	0.21	22,46,61,65	0
21	CLA	b	1206	65/65	0.92	0.17	28,48,62,80	0
35	LMT	0	6001	35/35	0.92	0.21	51,72,84,90	0
24	BCR	h	4018	40/40	0.92	0.21	36,60,75,79	0
21	CLA	a	1135	65/65	0.92	0.22	42,69,151,157	0
21	CLA	a	1138	65/65	0.92	0.16	50,77,85,90	0
24	BCR	b	4017	40/40	0.92	0.22	35,52,61,64	0
21	CLA	b	1213	65/65	0.92	0.28	39,64,89,93	0
21	CLA	b	1235	65/65	0.92	0.19	45,80,93,97	0
21	CLA	a	1136	65/65	0.92	0.19	44,73,87,100	0
21	CLA	B	1202	65/65	0.92	0.17	32,54,66,69	0
21	CLA	A	1134	65/65	0.92	0.19	25,57,107,111	0
21	CLA	1	1110	50/65	0.92	0.15	70,91,137,157	0
23	SF4	C	3003	8/8	0.92	0.14	53,74,78,84	0
24	BCR	i	4018	40/40	0.92	0.22	29,52,63,69	0
21	CLA	1	1106	65/65	0.92	0.21	49,91,119,122	0
21	CLA	B	1222	55/65	0.92	0.32	50,68,84,89	0
30	ECH	M	4021	41/41	0.92	0.15	45,61,74,81	0
21	CLA	1	1124	56/65	0.92	0.22	44,66,87,93	0
21	CLA	B	1230	65/65	0.92	0.21	29,68,110,114	0
21	CLA	B	1235	65/65	0.92	0.26	45,66,92,94	0
21	CLA	A	1133	65/65	0.92	0.19	28,48,78,81	0
24	BCR	A	4012	40/40	0.92	0.19	43,60,73,73	0
24	BCR	0	4019	40/40	0.92	0.17	35,57,67,69	0
21	CLA	L	1503	65/65	0.92	0.18	35,54,82,87	0
21	CLA	A	1107	65/65	0.93	0.17	42,56,121,124	0
21	CLA	A	1120	65/65	0.93	0.13	30,53,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CLA	b	1237	65/65	0.93	0.16	36,55,71,76	0
24	BCR	2	4017	40/40	0.93	0.19	31,56,72,76	0
21	CLA	B	1225	65/65	0.93	0.25	41,61,70,76	0
21	CLA	8	1402	46/65	0.93	0.18	103,119,135,139	5
21	CLA	b	1234	53/65	0.93	0.19	40,57,75,91	0
21	CLA	b	1212	65/65	0.93	0.17	41,53,87,97	0
21	CLA	B	1220	57/65	0.93	0.17	53,78,101,108	0
21	CLA	b	1226	65/65	0.93	0.17	26,50,71,76	0
21	CLA	B	1221	65/65	0.93	0.18	50,62,95,98	0
21	CLA	2	1201	65/65	0.93	0.16	61,77,86,90	0
21	CLA	b	1219	60/65	0.93	0.22	33,66,132,132	0
21	CLA	A	1119	65/65	0.93	0.18	27,39,52,56	0
21	CLA	1	1140	65/65	0.93	0.20	60,77,119,120	0
21	CLA	a	1124	55/65	0.93	0.20	45,59,117,127	0
21	CLA	b	1214	65/65	0.93	0.20	33,49,89,98	0
21	CLA	b	1224	65/65	0.93	0.19	33,48,83,87	0
21	CLA	b	1209	65/65	0.93	0.14	40,57,100,107	0
21	CLA	2	1224	55/65	0.93	0.21	53,70,95,110	0
21	CLA	A	1139	65/65	0.93	0.17	43,59,83,91	0
21	CLA	A	1109	65/65	0.93	0.17	36,54,65,74	0
21	CLA	A	1115	65/65	0.93	0.21	41,57,69,72	0
21	CLA	B	1224	65/65	0.93	0.20	28,52,78,87	0
21	CLA	B	1226	65/65	0.93	0.18	31,51,70,79	0
21	CLA	A	1121	65/65	0.93	0.17	28,48,130,132	0
21	CLA	1	1122	60/65	0.93	0.18	47,75,101,106	0
21	CLA	1	1135	52/65	0.93	0.17	53,69,89,108	0
21	CLA	b	1218	65/65	0.93	0.19	46,66,101,102	0
25	LHG	A	5003	49/49	0.93	0.21	29,62,101,107	0
21	CLA	A	1105	65/65	0.93	0.16	44,68,92,95	0
21	CLA	b	1216	65/65	0.93	0.16	41,57,91,102	0
21	CLA	2	1204	65/65	0.93	0.17	35,67,89,91	0
21	CLA	A	1127	65/65	0.93	0.24	22,42,59,64	0
21	CLA	K	1401	65/65	0.93	0.22	33,63,97,102	15
21	CLA	A	1104	65/65	0.93	0.21	19,41,62,64	0
21	CLA	1	1011	65/65	0.93	0.18	38,62,88,103	0
21	CLA	1	1137	51/65	0.93	0.18	48,65,76,87	0
21	CLA	A	1114	65/65	0.93	0.18	56,75,111,116	0
21	CLA	A	1108	53/65	0.93	0.20	30,57,91,92	0
21	CLA	A	1126	65/65	0.93	0.15	28,48,62,75	0
21	CLA	2	1237	65/65	0.93	0.18	30,51,61,76	0
21	CLA	B	1236	50/65	0.93	0.27	44,63,96,101	0
21	CLA	B	1208	65/65	0.93	0.16	53,76,108,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	A	4001	40/40	0.93	0.15	35,52,68,68	0
36	EQ3	I	4020	42/42	0.94	0.22	24,37,48,66	0
21	CLA	0	1503	65/65	0.94	0.15	43,56,82,99	0
24	BCR	A	4007	40/40	0.94	0.19	31,46,106,108	0
21	CLA	b	1202	65/65	0.94	0.16	26,43,52,57	0
21	CLA	A	1116	65/65	0.94	0.26	36,53,86,90	0
21	CLA	b	1211	65/65	0.94	0.14	29,46,98,103	0
21	CLA	B	1215	65/65	0.94	0.26	33,57,92,99	0
21	CLA	B	1207	65/65	0.94	0.17	28,39,61,68	0
21	CLA	1	1801	56/65	0.94	0.15	62,76,106,112	0
21	CLA	l	1503	65/65	0.94	0.20	31,54,99,101	0
21	CLA	A	1128	65/65	0.94	0.17	29,43,62,86	0
21	CLA	2	1022	65/65	0.94	0.18	34,62,74,74	0
21	CLA	b	1238	65/65	0.94	0.17	30,52,63,69	0
21	CLA	a	1130	65/65	0.94	0.15	52,68,111,119	0
23	SF4	1	3001	8/8	0.94	0.17	57,66,94,130	0
21	CLA	B	1223	65/65	0.94	0.27	54,67,78,95	0
24	BCR	I	4018	40/40	0.94	0.21	24,45,59,67	0
21	CLA	A	1103	65/65	0.94	0.20	25,41,61,66	0
21	CLA	2	1239	65/65	0.94	0.18	39,57,93,104	0
22	PQN	2	2002	33/33	0.94	0.18	42,57,70,78	0
21	CLA	0	1502	65/65	0.94	0.16	32,49,77,84	0
21	CLA	a	1127	65/65	0.94	0.31	50,80,108,110	0
21	CLA	A	1011	65/65	0.94	0.15	20,37,61,79	0
21	CLA	A	1138	65/65	0.94	0.16	46,61,68,73	0
21	CLA	A	1135	65/65	0.94	0.17	25,42,100,107	0
21	CLA	b	1210	65/65	0.94	0.14	31,43,63,68	0
21	CLA	a	1104	65/65	0.94	0.23	40,68,105,111	0
28	45D	B	4011	42/42	0.94	0.18	31,49,61,69	0
23	SF4	3	3002	8/8	0.94	0.13	65,73,110,240	0
24	BCR	A	4008	40/40	0.94	0.25	17,46,78,82	0
21	CLA	A	1118	65/65	0.94	0.19	38,52,84,89	0
21	CLA	A	1129	58/65	0.94	0.17	20,42,92,96	0
22	PQN	b	2002	33/33	0.94	0.24	36,51,69,69	0
21	CLA	a	1103	65/65	0.94	0.26	49,67,130,133	0
21	CLA	a	1013	65/65	0.94	0.25	34,53,90,92	0
21	CLA	1	1132	65/65	0.94	0.14	23,48,63,71	0
21	CLA	A	1801	65/65	0.94	0.14	22,47,108,110	0
21	CLA	A	1102	65/65	0.95	0.14	32,49,106,120	0
21	CLA	b	1022	65/65	0.95	0.21	37,49,59,65	0
21	CLA	L	1502	65/65	0.95	0.20	21,36,98,103	0
21	CLA	b	1201	65/65	0.95	0.15	30,44,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	MG	b	6002	1/1	0.95	0.12	54,54,54,54	0
21	CLA	A	1117	65/65	0.95	0.29	31,46,56,59	0
25	LHG	A	5001	49/49	0.95	0.18	31,47,61,64	0
21	CLA	0	1501	65/65	0.95	0.18	37,47,74,82	0
21	CLA	A	1106	65/65	0.95	0.14	26,45,71,87	0
21	CLA	B	1204	65/65	0.95	0.16	32,50,67,83	0
21	CLA	B	1238	65/65	0.95	0.19	17,35,46,56	0
21	CLA	A	1124	65/65	0.95	0.19	23,35,118,122	0
21	CLA	l	1502	65/65	0.95	0.19	30,55,103,110	0
21	CLA	A	1111	65/65	0.95	0.17	31,48,81,86	0
21	CLA	b	1215	65/65	0.95	0.17	28,48,68,83	0
21	CLA	A	1140	65/65	0.95	0.18	25,43,66,76	0
21	CLA	L	1501	65/65	0.95	0.18	33,51,91,94	0
21	CLA	l	1136	65/65	0.95	0.13	46,66,77,83	0
21	CLA	b	1239	65/65	0.95	0.23	36,51,62,84	0
21	CLA	l	1131	65/65	0.95	0.17	35,47,69,74	0
21	CLA	B	1237	65/65	0.95	0.21	21,34,54,61	0
21	CLA	b	1225	65/65	0.95	0.21	23,41,59,63	0
21	CLA	A	1012	65/65	0.95	0.17	31,44,63,73	0
21	CLA	b	1217	51/65	0.95	0.11	32,56,86,95	0
21	CLA	A	1013	65/65	0.95	0.21	23,47,57,65	0
21	CLA	b	1221	65/65	0.95	0.15	31,50,85,99	0
21	CLA	b	1204	65/65	0.95	0.15	26,40,78,108	0
22	PQN	A	2001	33/33	0.95	0.18	30,46,57,64	0
21	CLA	A	1130	60/65	0.95	0.17	21,39,93,95	0
24	BCR	L	4019	40/40	0.95	0.17	24,38,45,52	0
21	CLA	B	1203	65/65	0.95	0.21	33,50,69,75	0
21	CLA	B	1205	65/65	0.95	0.15	34,43,69,74	0
21	CLA	b	1207	65/65	0.95	0.16	32,50,71,81	0
21	CLA	a	1140	65/65	0.95	0.21	48,70,93,95	0
21	CLA	b	1023	65/65	0.95	0.23	34,51,66,80	0
21	CLA	l	1130	55/65	0.95	0.14	29,53,83,95	0
21	CLA	B	1201	65/65	0.95	0.14	37,48,80,91	0
21	CLA	B	1021	65/65	0.95	0.14	30,42,53,61	0
21	CLA	a	1137	51/65	0.95	0.17	43,63,109,113	0
21	CLA	B	1229	65/65	0.95	0.19	40,60,80,85	0
21	CLA	A	1131	65/65	0.95	0.21	27,38,59,76	0
21	CLA	A	1101	65/65	0.96	0.15	32,50,68,74	0
21	CLA	2	1207	56/65	0.96	0.14	29,46,78,86	0
21	CLA	a	1012	65/65	0.96	0.22	25,57,101,103	0
21	CLA	B	1206	65/65	0.96	0.15	31,43,60,72	0
21	CLA	B	1023	65/65	0.96	0.22	21,33,45,55	0

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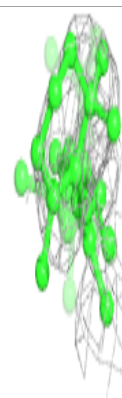
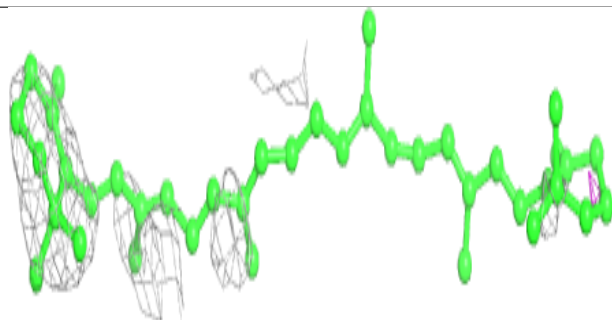
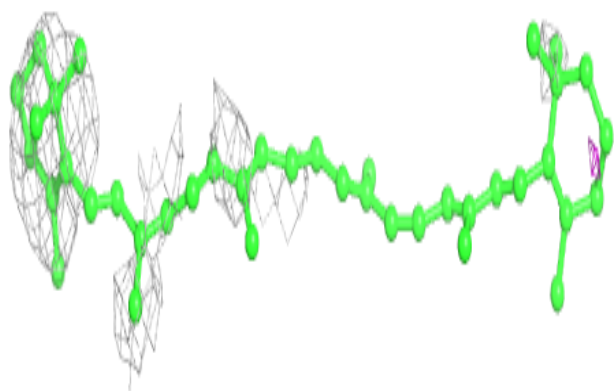
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	B	1022	65/65	0.96	0.19	19,36,44,51	0
21	CLA	a	1131	65/65	0.96	0.17	36,58,68,71	0
21	CLA	b	1205	65/65	0.96	0.13	28,43,59,65	0
21	CLA	2	1238	65/65	0.96	0.15	36,52,61,75	0
32	CA	l	1001	1/1	0.96	0.04	55,55,55,55	0
21	CLA	A	1136	65/65	0.96	0.13	21,42,68,77	0
21	CLA	A	1110	65/65	0.96	0.22	30,47,124,127	0
21	CLA	b	1203	65/65	0.96	0.19	25,45,60,64	0
21	CLA	a	1132	65/65	0.96	0.14	37,57,66,71	0
21	CLA	B	1239	65/65	0.96	0.24	11,39,59,85	0
21	CLA	A	1137	65/65	0.96	0.20	24,38,111,116	0
21	CLA	1	1129	50/65	0.96	0.15	49,63,76,78	0
32	CA	b	6001	1/1	0.96	0.06	61,61,61,61	0
21	CLA	A	1132	65/65	0.96	0.15	21,35,44,51	0
21	CLA	b	1223	65/65	0.96	0.18	33,55,83,86	0
29	CL	b	6000	1/1	0.97	0.11	53,53,53,53	0
22	PQN	B	2002	33/33	0.97	0.17	24,35,39,48	0
23	SF4	c	3003	8/8	0.98	0.09	57,78,82,85	0
32	CA	0	1001	1/1	0.98	0.04	56,56,56,56	0
32	CA	L	1001	1/1	0.98	0.08	44,44,44,44	0
23	SF4	3	3003	8/8	0.98	0.07	75,88,175,321	0
23	SF4	c	3002	8/8	0.98	0.11	53,57,64,76	0
32	CA	B	6001	1/1	0.98	0.10	80,80,80,80	0
23	SF4	a	3001	8/8	0.99	0.16	61,65,75,77	0
29	CL	B	6000	1/1	0.99	0.04	36,36,36,36	0

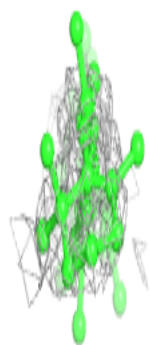
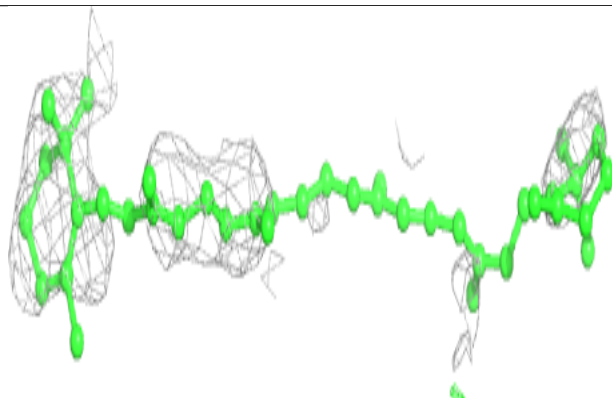
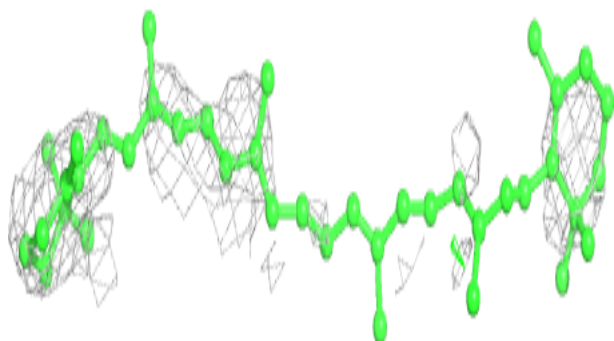
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCR k 4001:

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

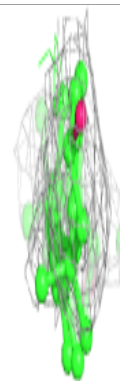
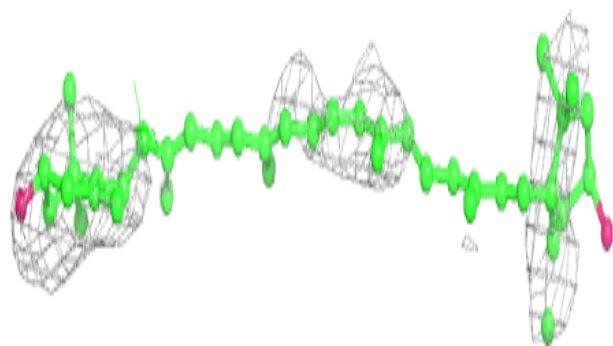
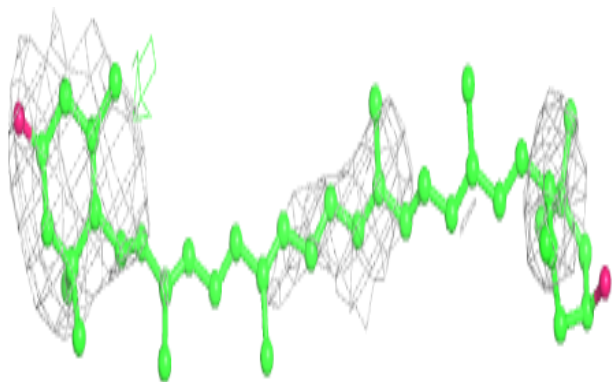
**Electron density around BCR 8 4001:**

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

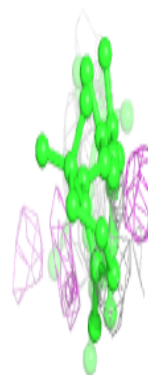
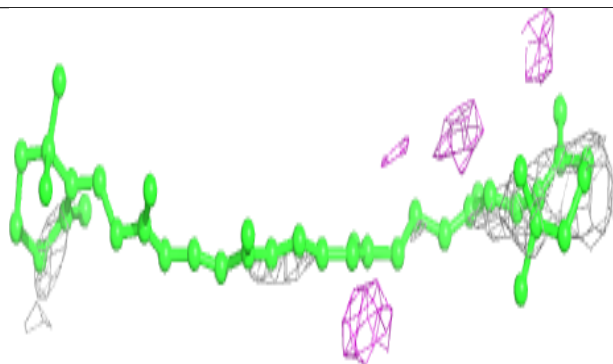
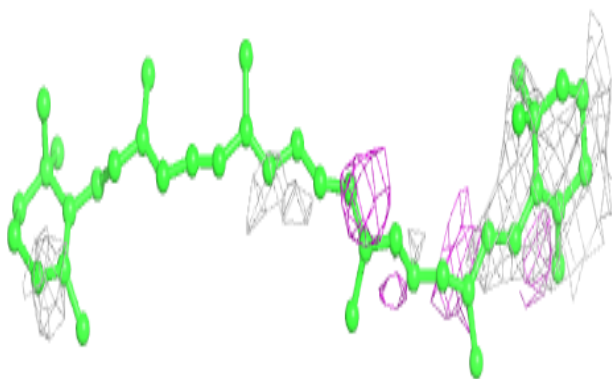


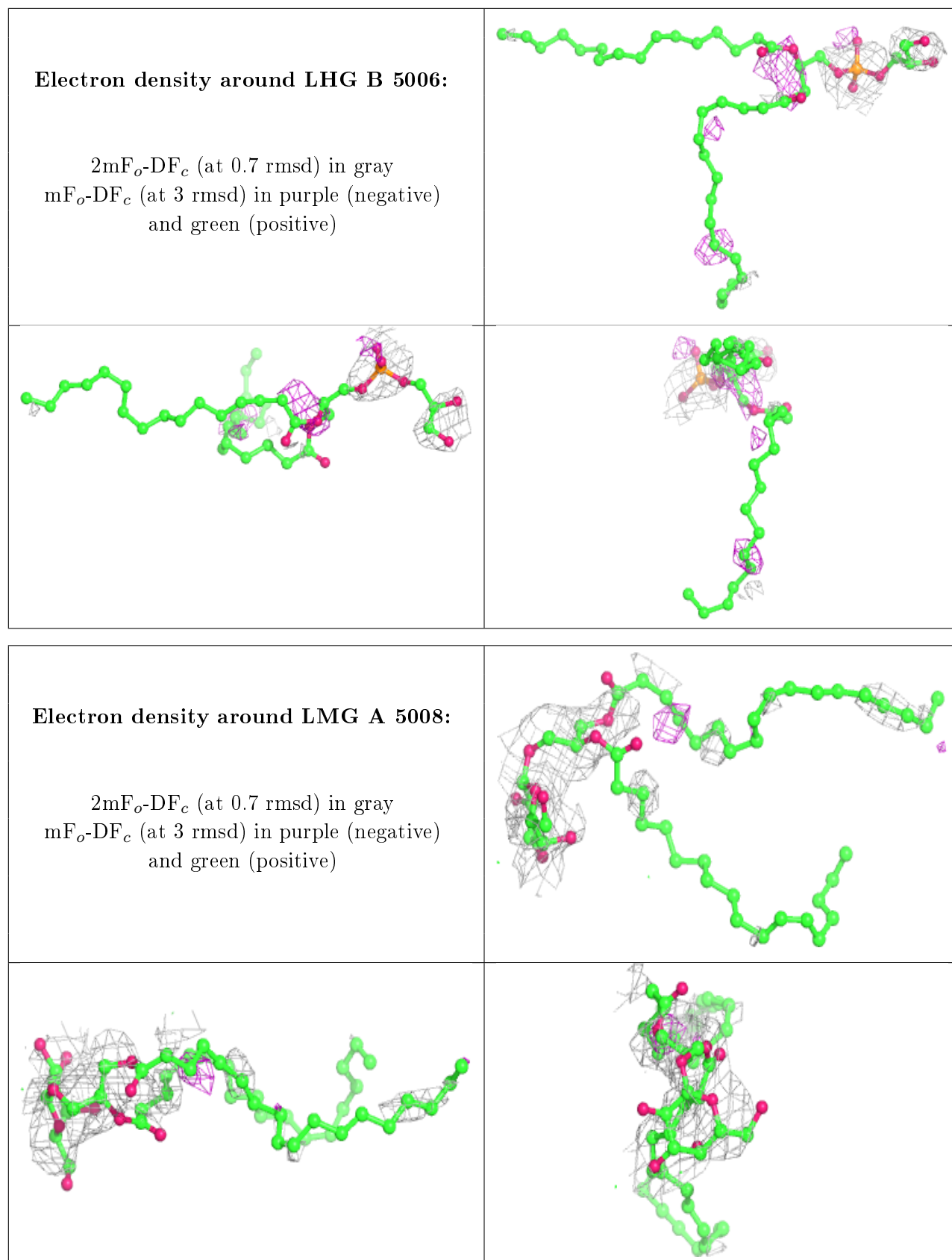
Electron density around ZEX 7 4015:

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

**Electron density around BCR 2 4004:**

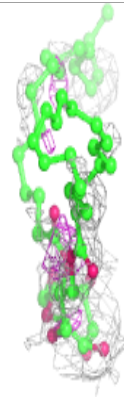
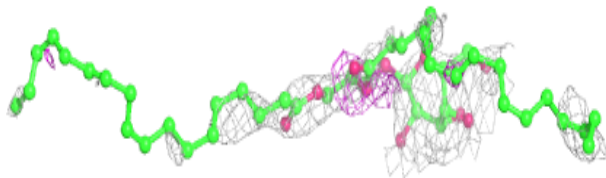
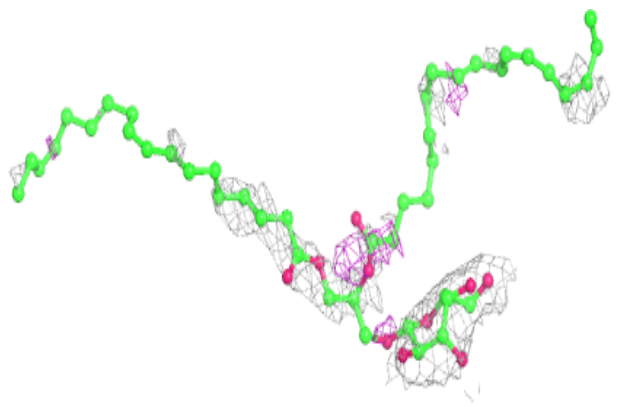
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



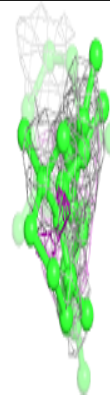
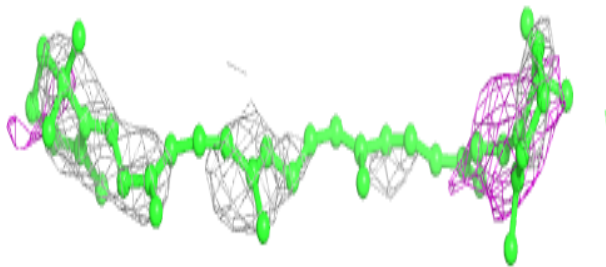
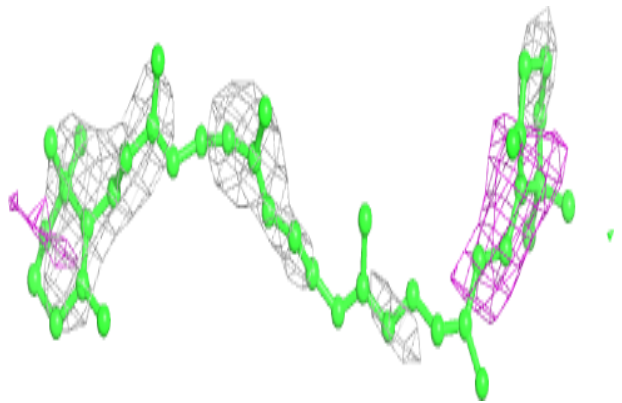


Electron density around LMG b 5007:

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

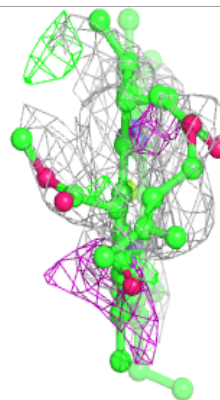
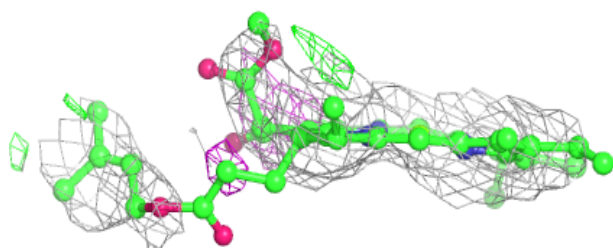
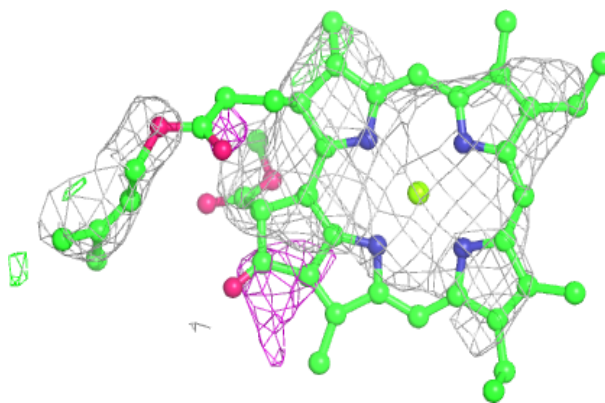
**Electron density around BCR B 4018:**

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

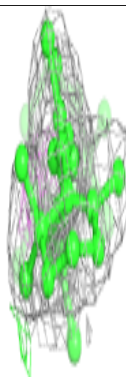
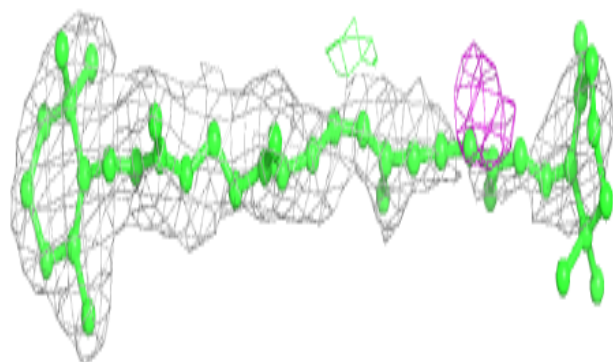
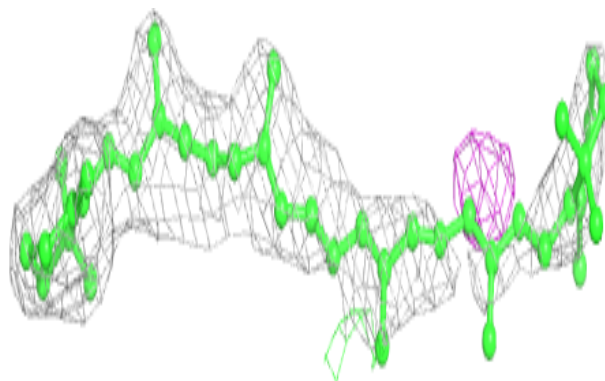


Electron density around CLA a 1113:

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

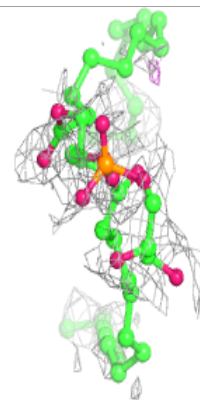
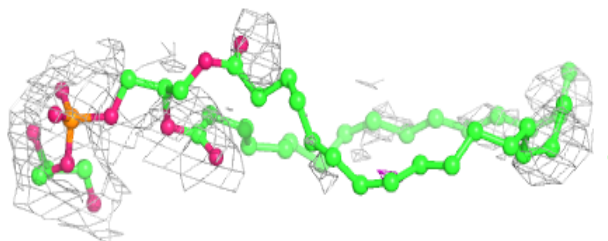
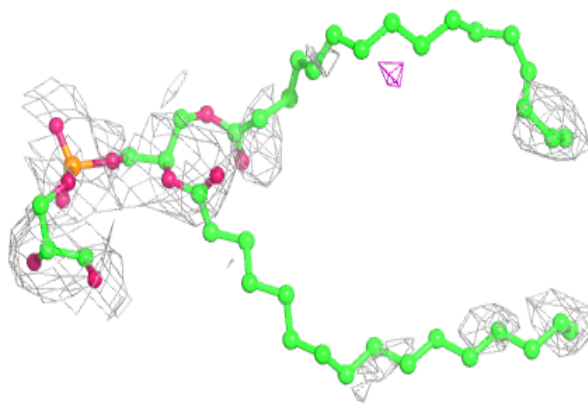
**Electron density around BCR K 4001:**

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

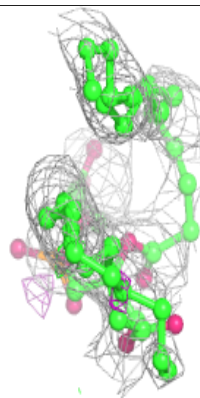
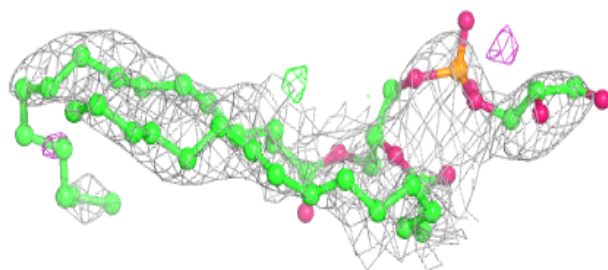
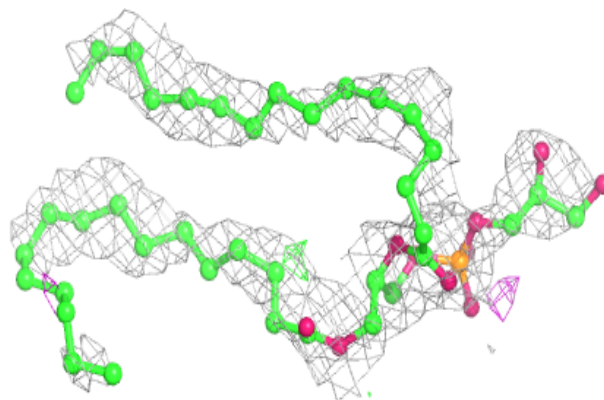


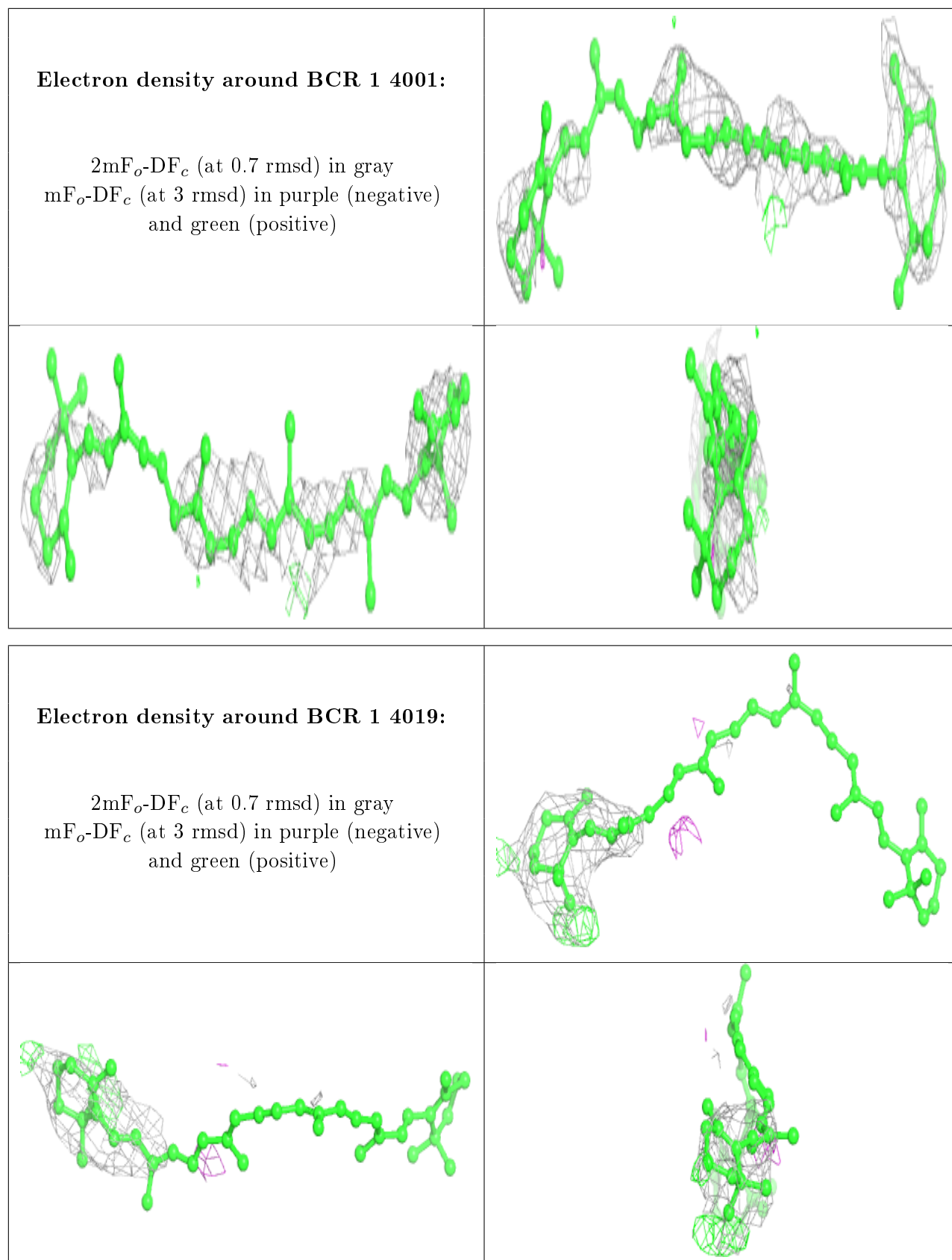
Electron density around LHG 1 5005:

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

**Electron density around LHG F 5002:**

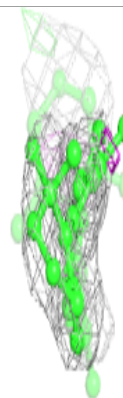
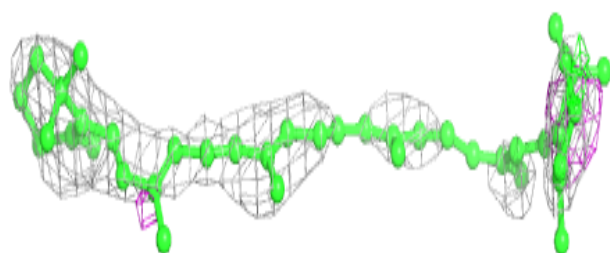
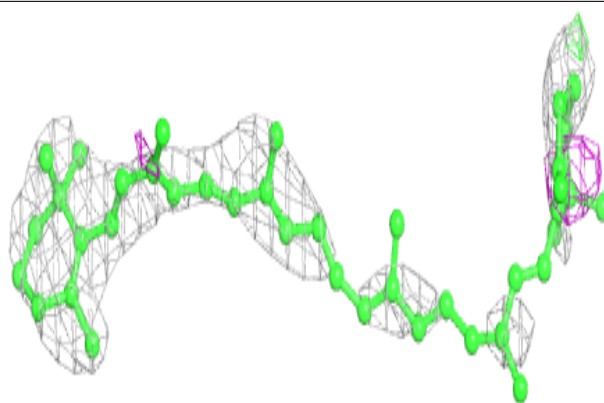
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



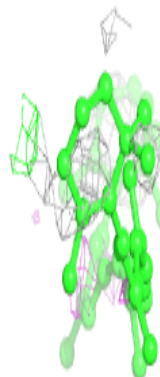
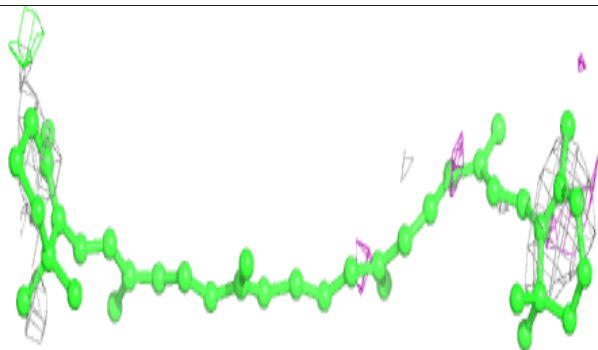
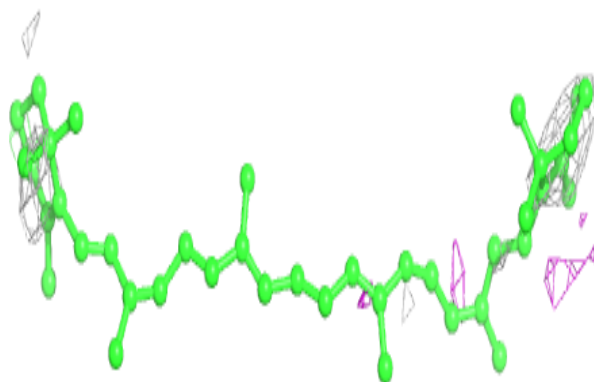


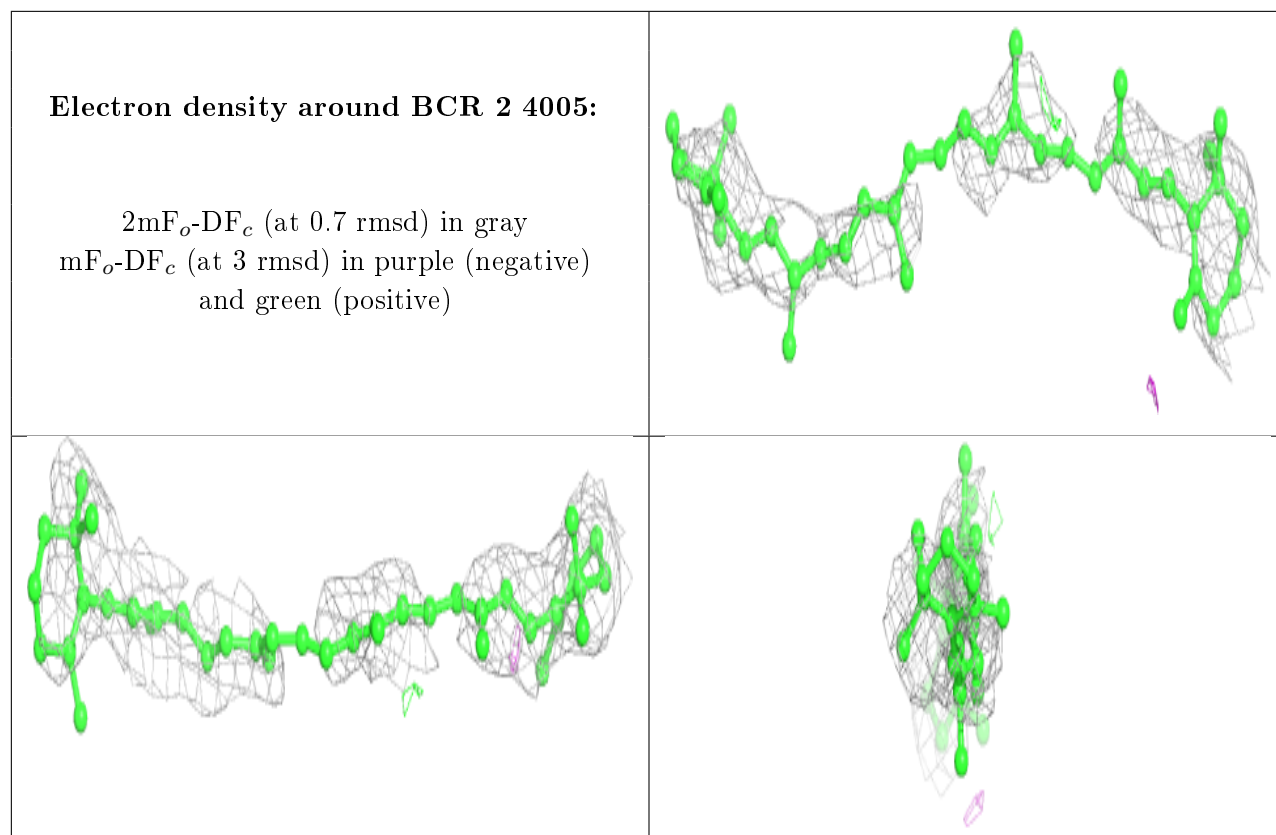
Electron density around BCR b 4018:

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

**Electron density around BCR 2 4018:**

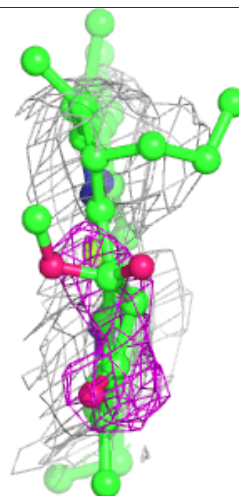
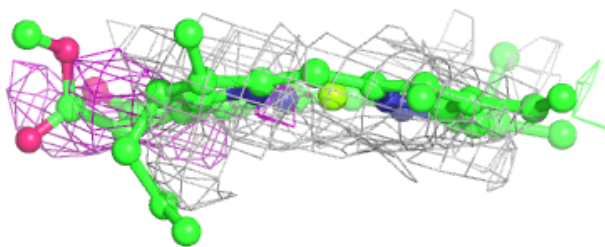
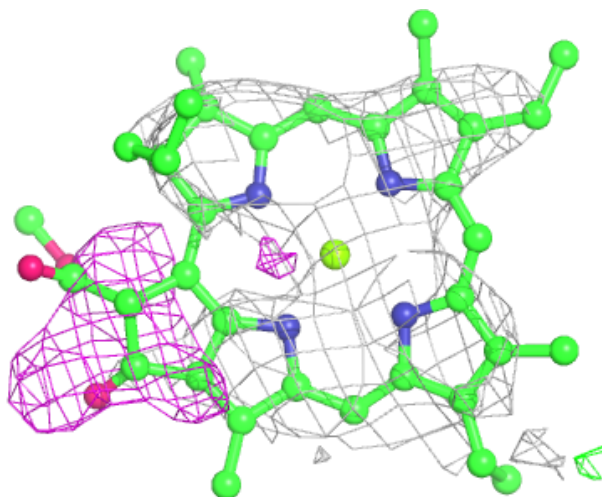
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





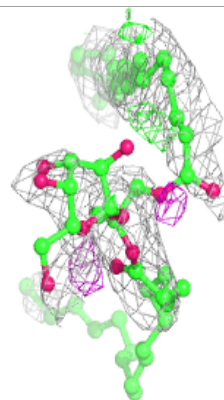
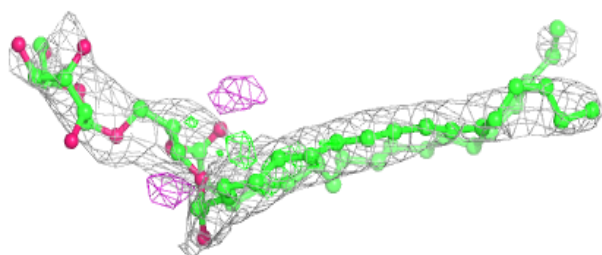
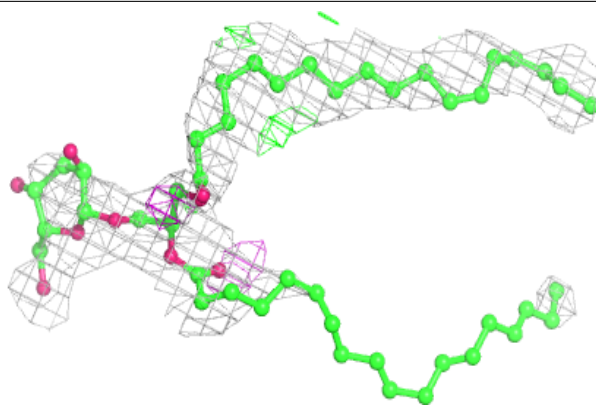
Electron density around CLA 6 1302:

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

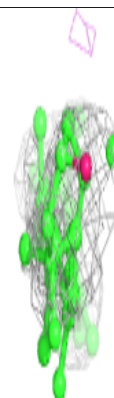
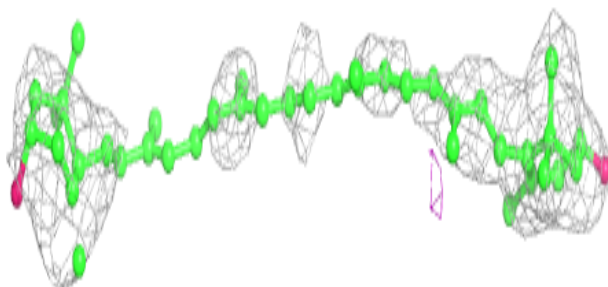
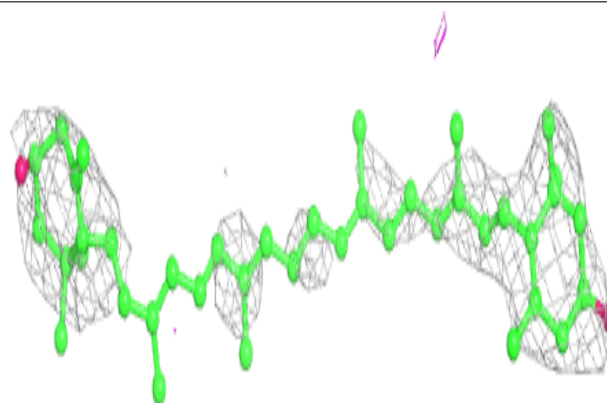


Electron density around LMG B 5005:

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

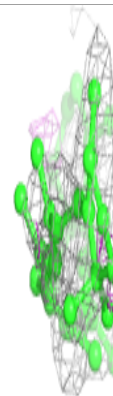
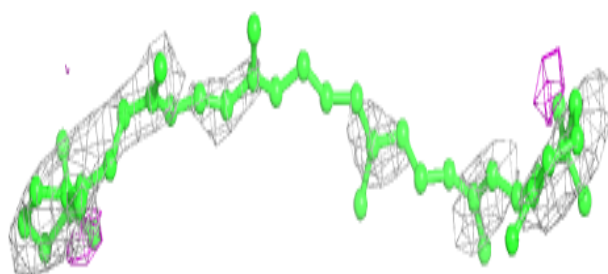
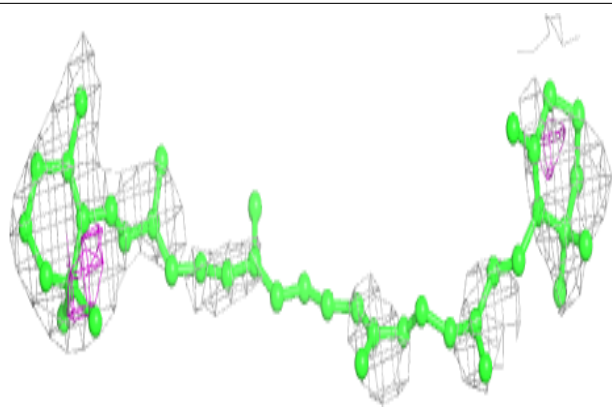
**Electron density around ZEX j 4015:**

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

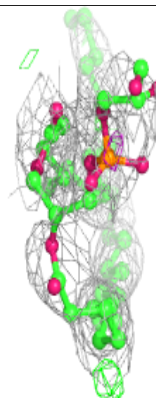
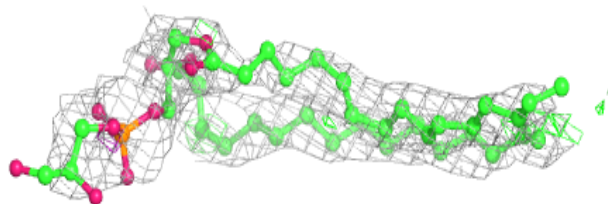
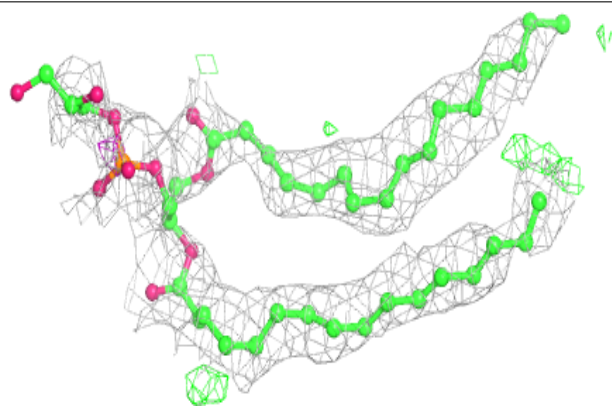


Electron density around BCR 7 4013:

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

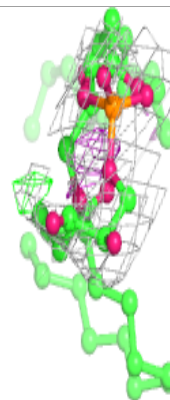
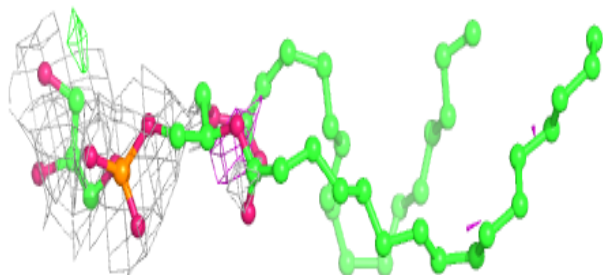
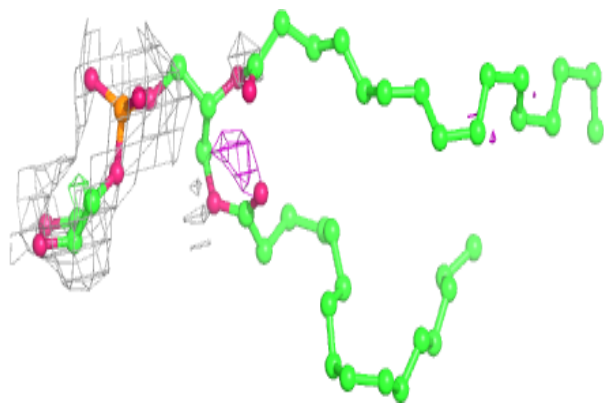
**Electron density around LHG 1 5004:**

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

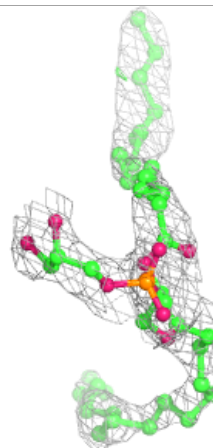
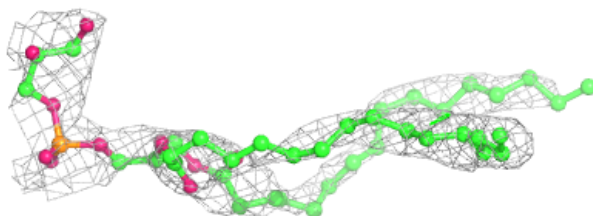
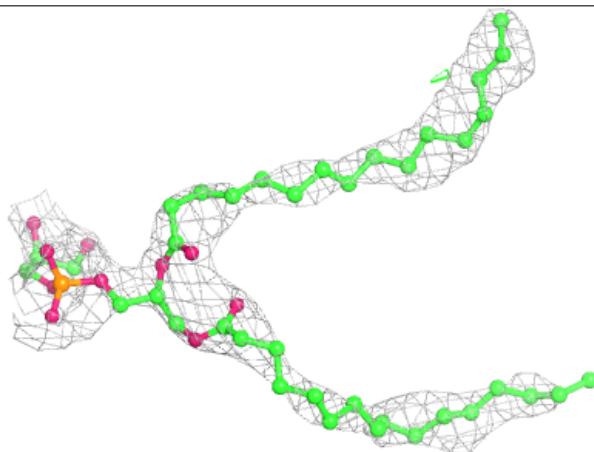


Electron density around LHG a 5007:

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

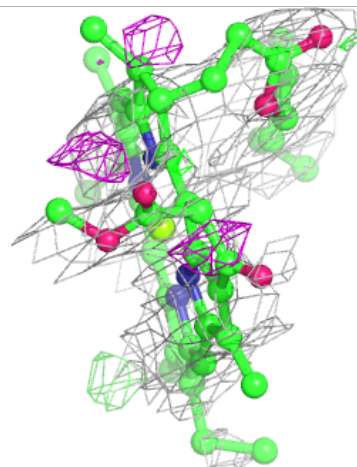
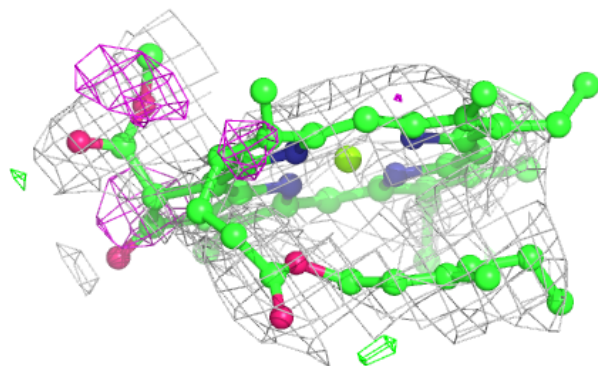
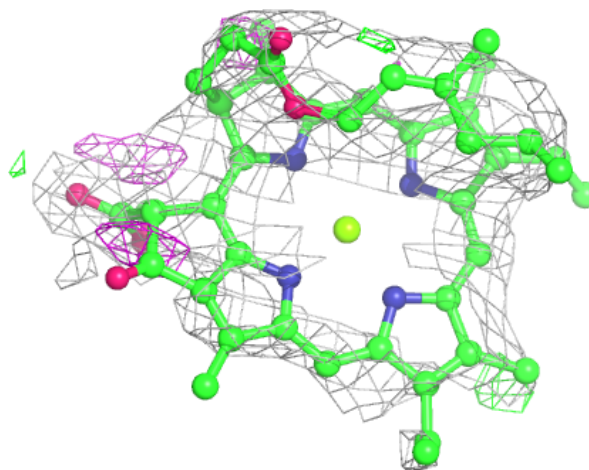
**Electron density around LHG 1 5002:**

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



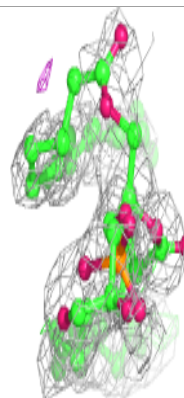
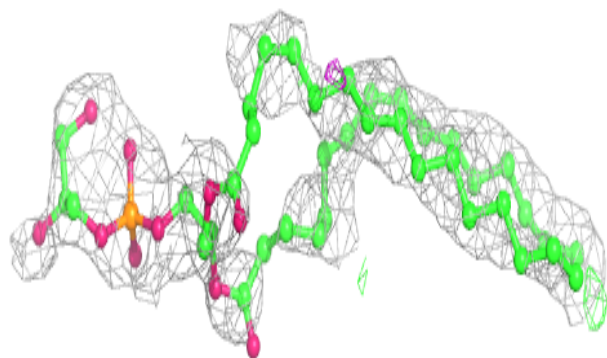
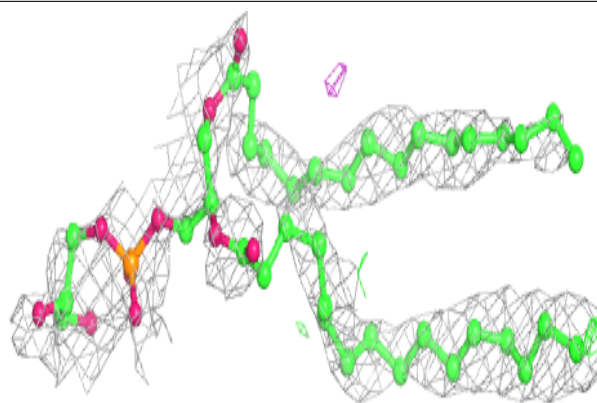
Electron density around CLA 2 1217:

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

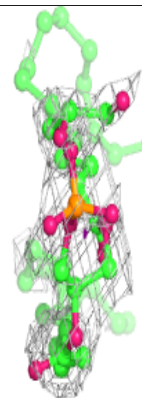
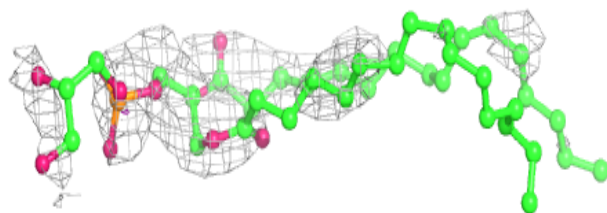
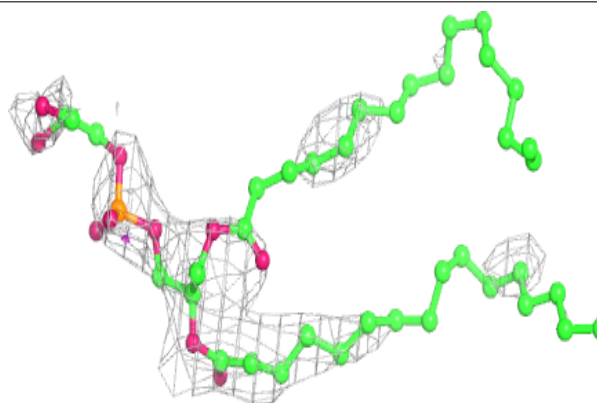


Electron density around LHG a 5005:

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

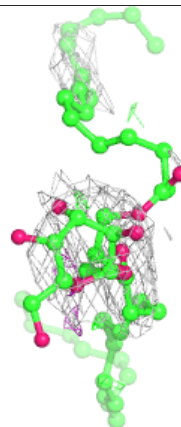
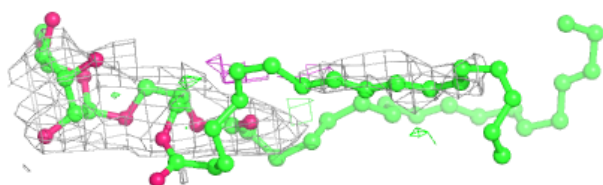
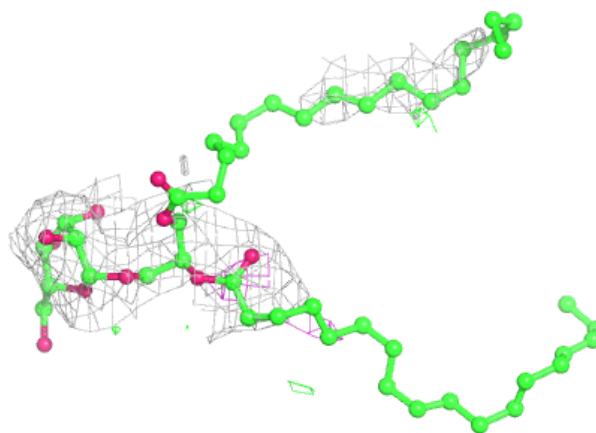
**Electron density around LHG 1 5007:**

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

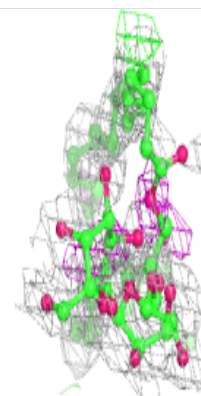
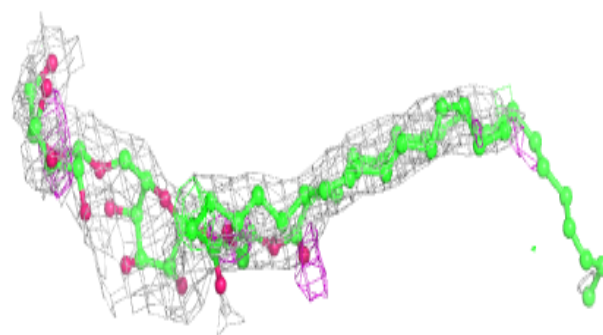
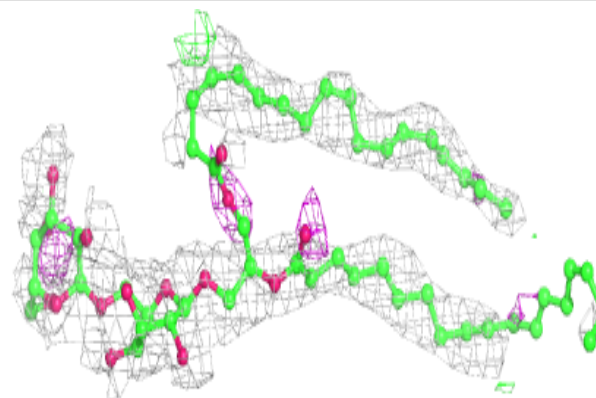


Electron density around LMG 2 5005:

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

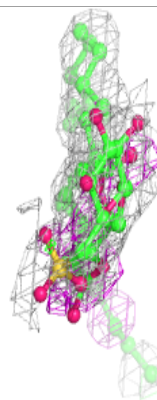
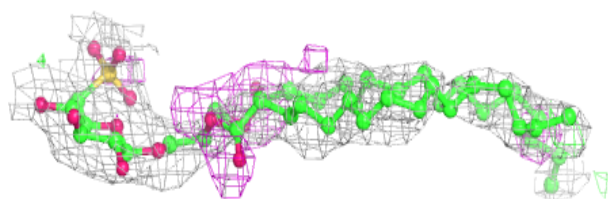
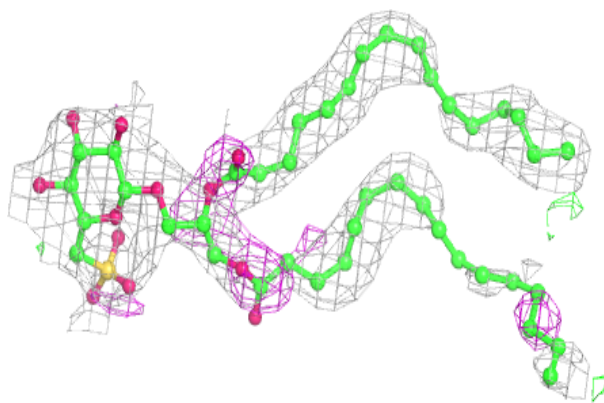
**Electron density around DGD L 5004:**

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

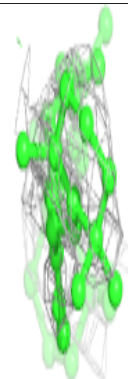
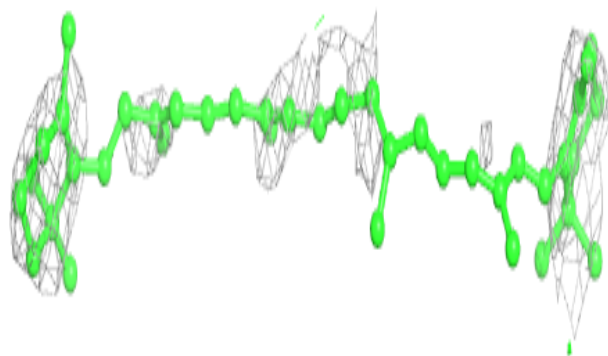
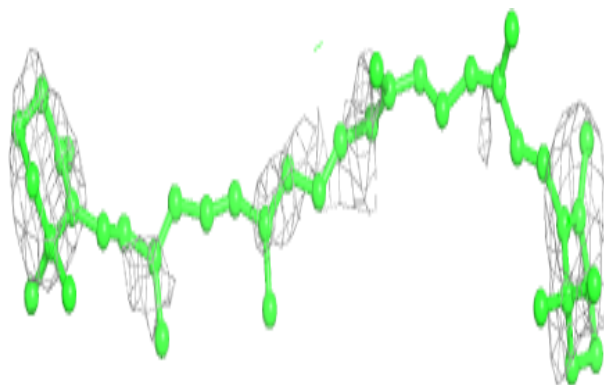


Electron density around SQD b 5006:

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

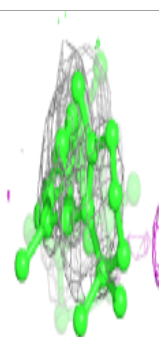
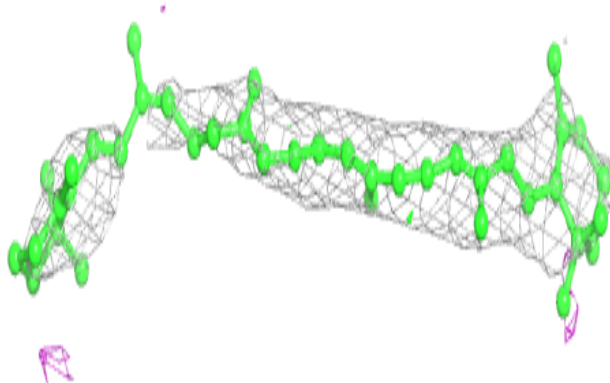
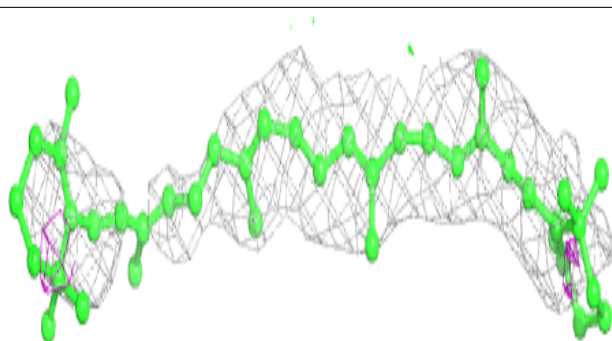
**Electron density around BCR a 4003:**

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

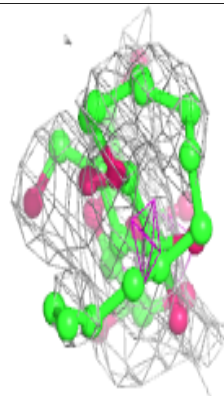
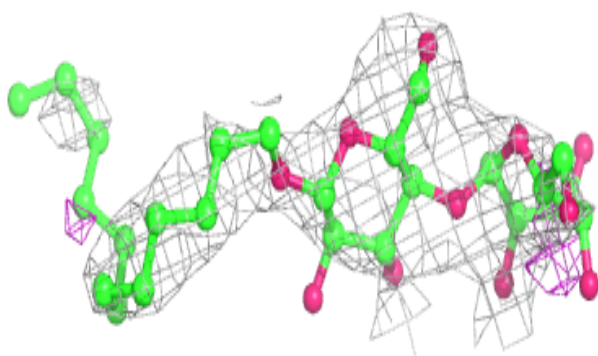
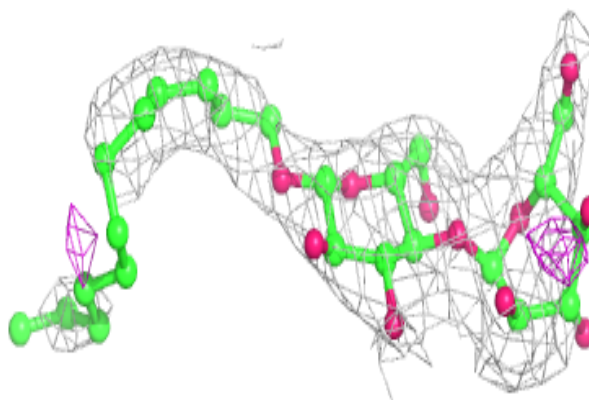


Electron density around BCR a 4001:

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

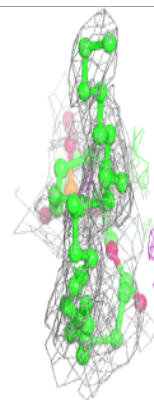
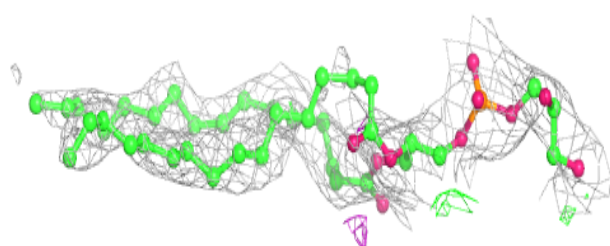
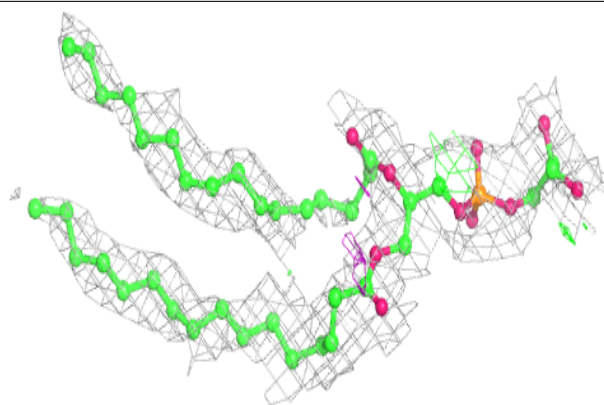
**Electron density around LMT 1 6001:**

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

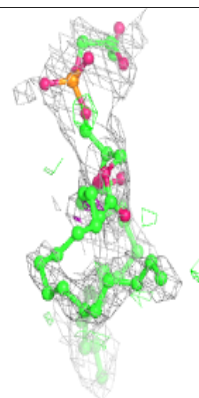
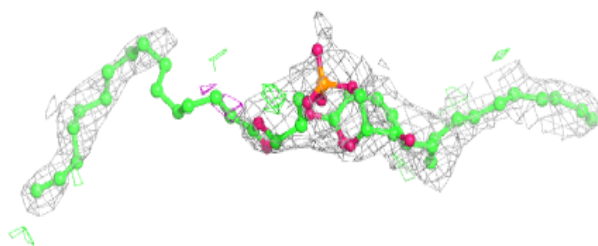
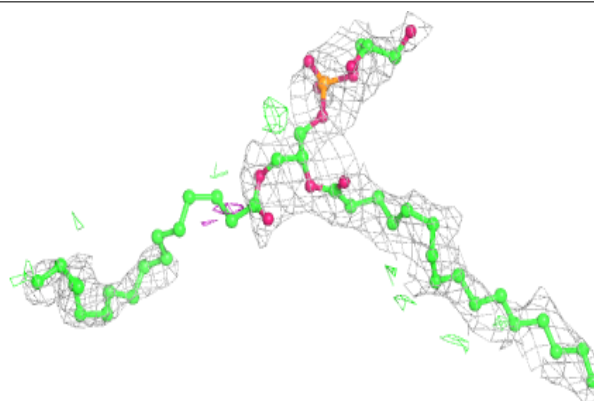


Electron density around LHG M 5001:

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

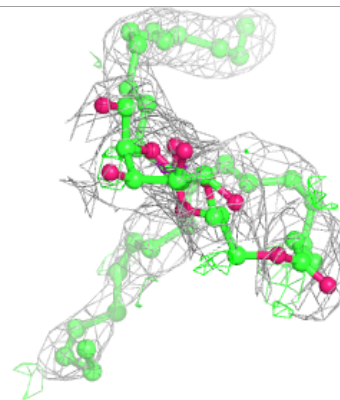
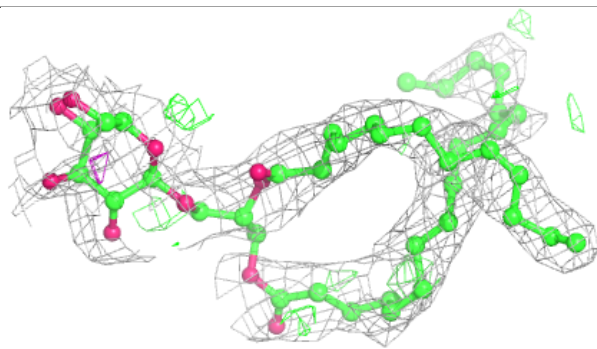
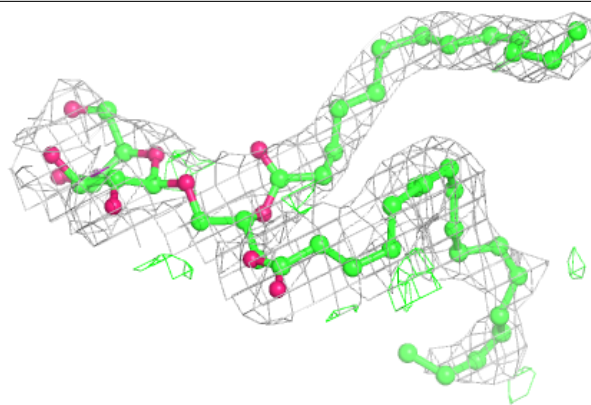
**Electron density around LHG 0 5004:**

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

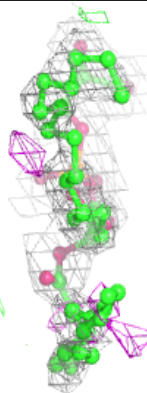
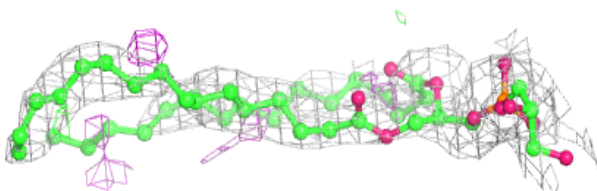
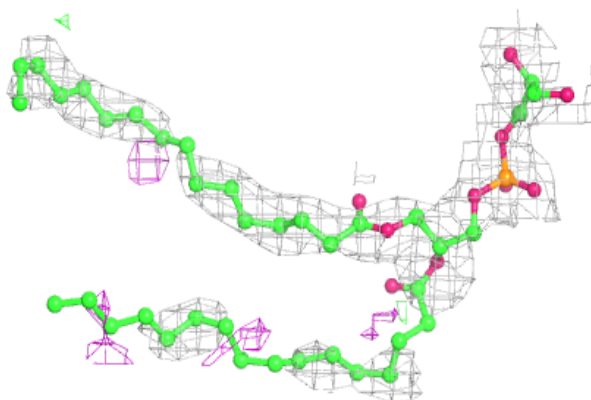


Electron density around LMG a 5002:

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

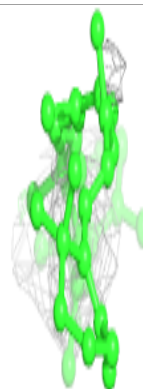
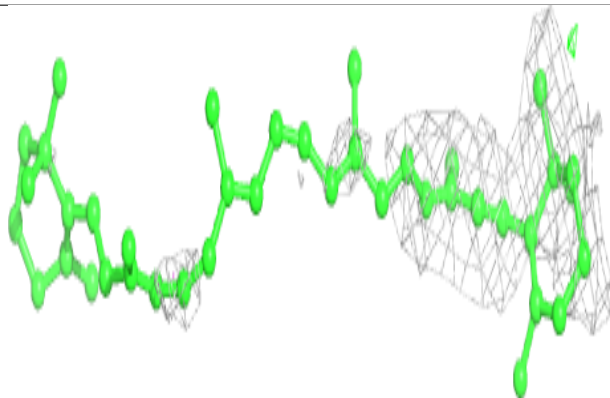
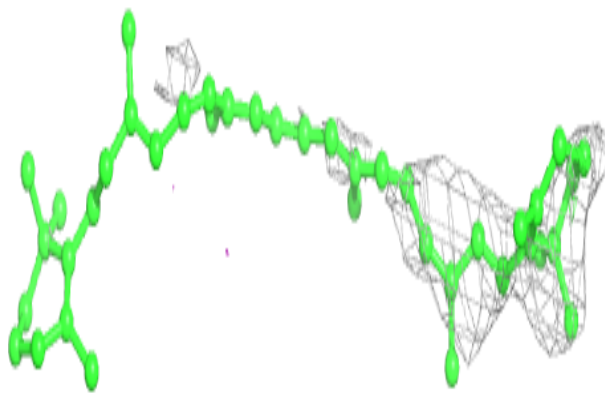
**Electron density around LHG A 5006:**

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

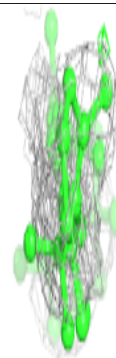
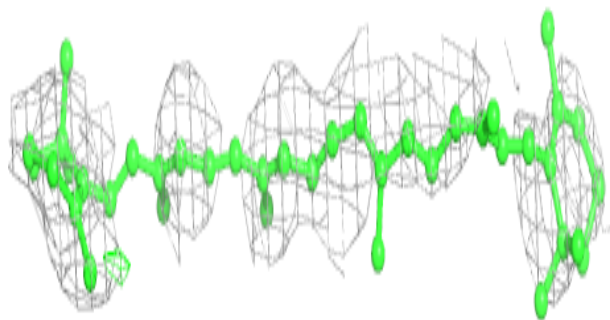
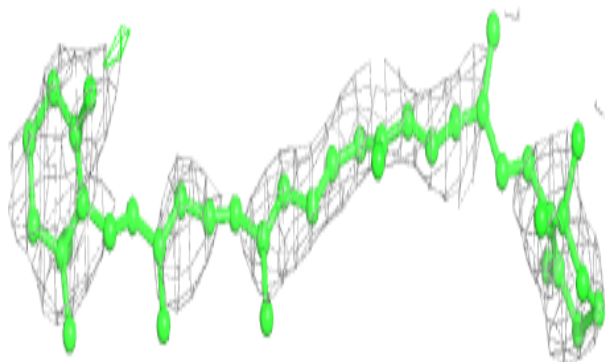


Electron density around BCR a 4019:

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

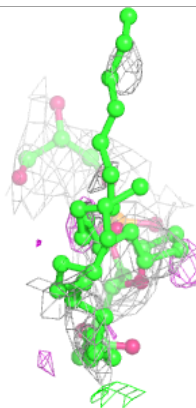
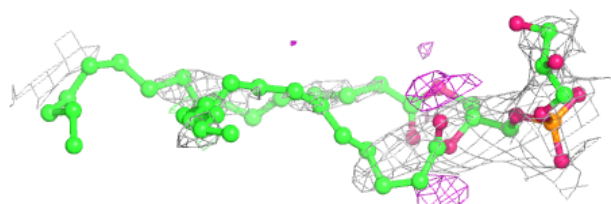
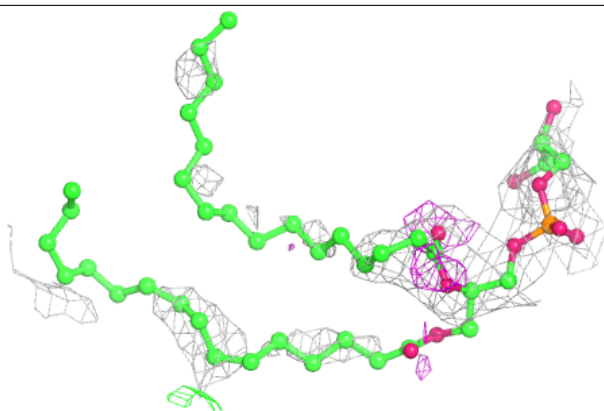
**Electron density around BCR a 4002:**

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

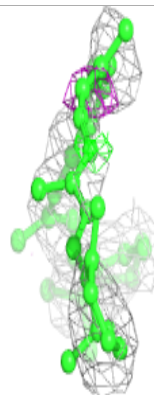
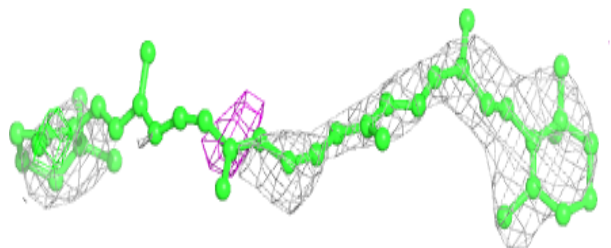
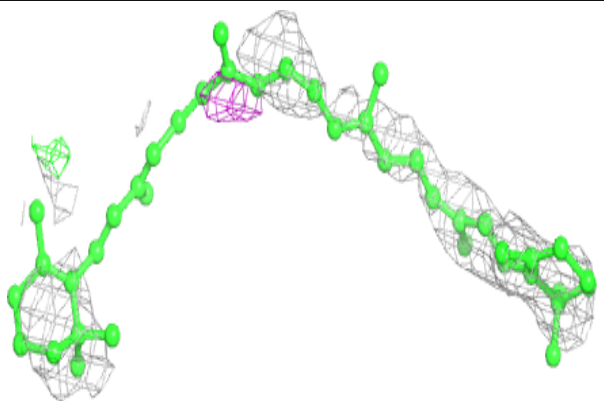


Electron density around LHG 2 5004:

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

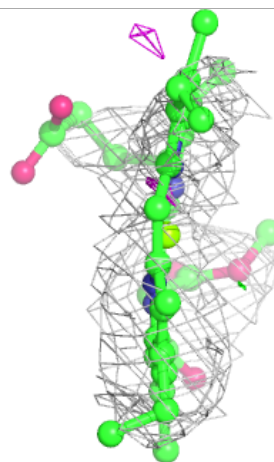
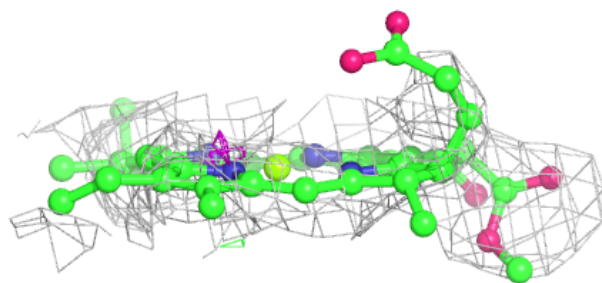
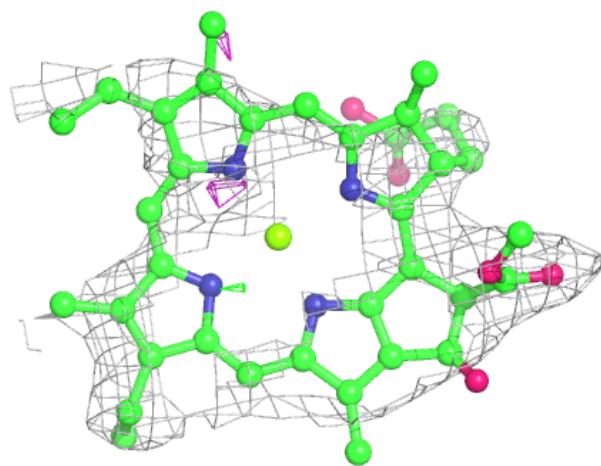
**Electron density around BCR A 4019:**

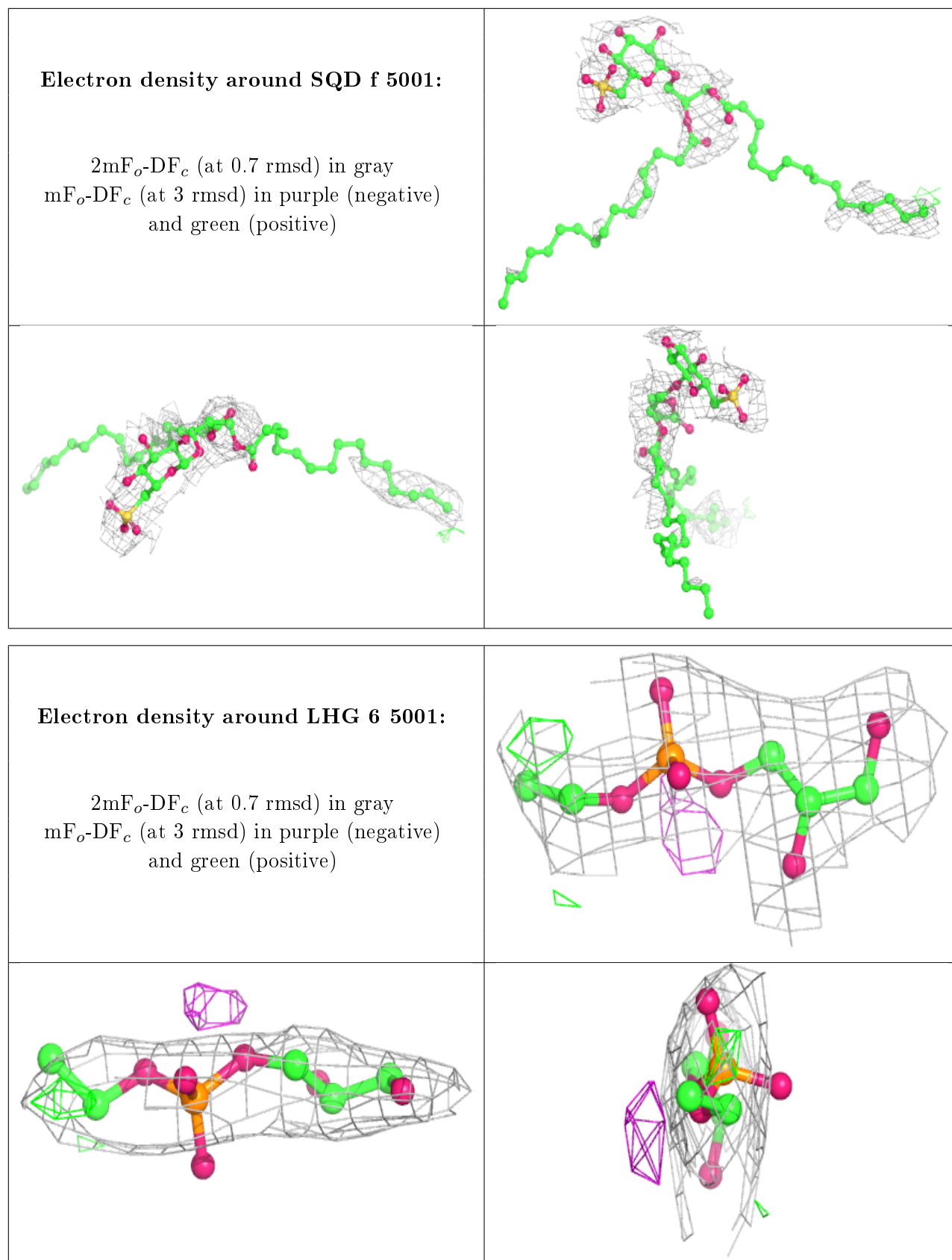
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1209:

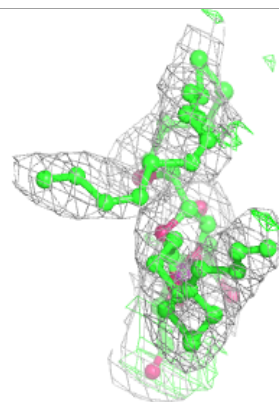
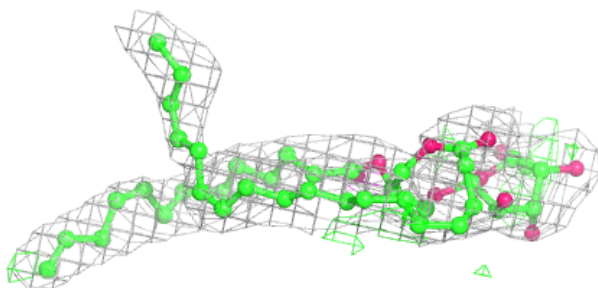
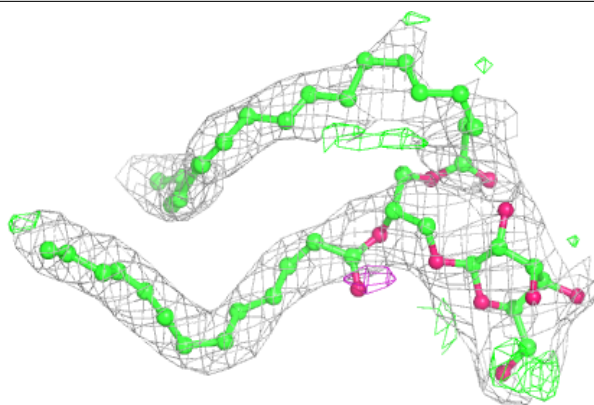
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



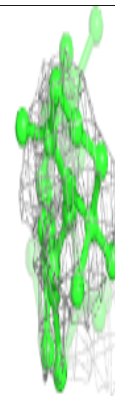
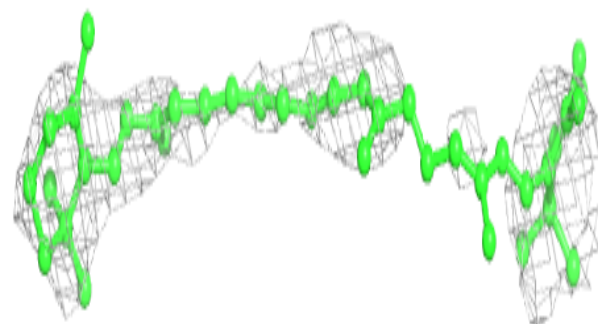
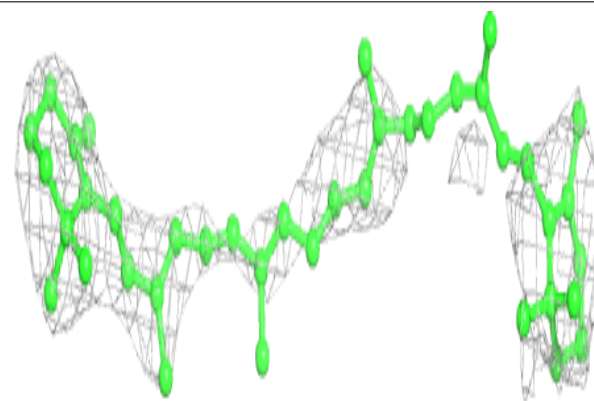


Electron density around LMG A 5002:

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

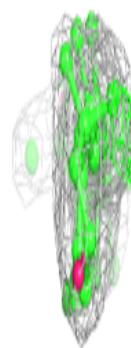
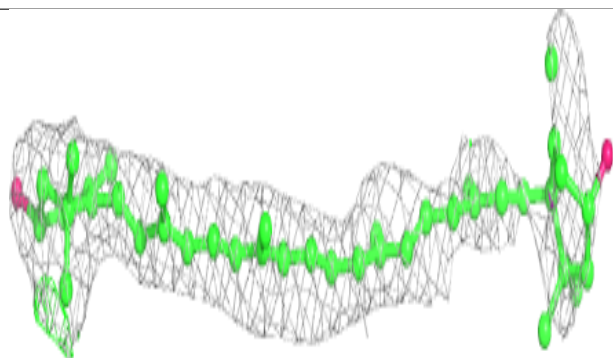
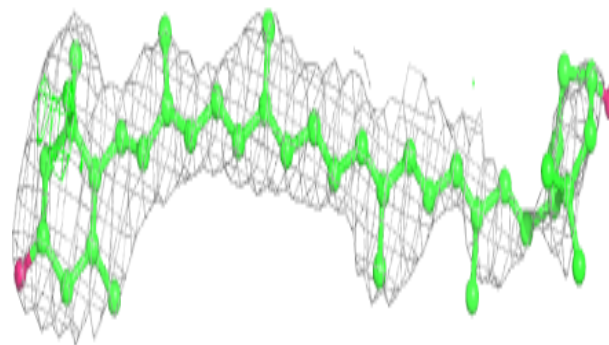
**Electron density around BCR 1 4003:**

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

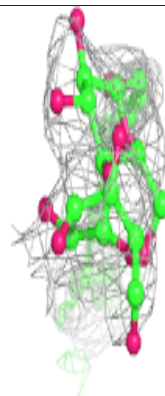
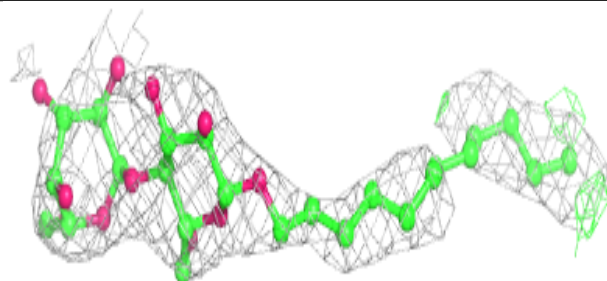
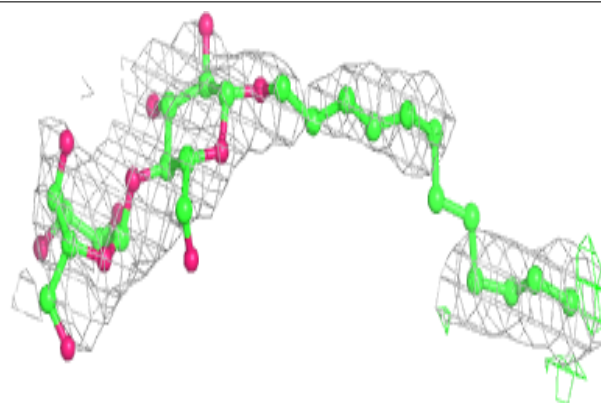


Electron density around ZEX J 4015:

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

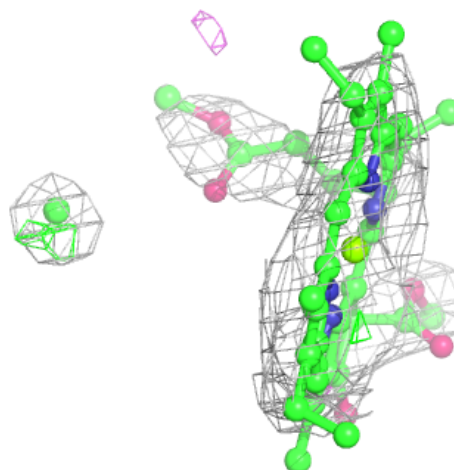
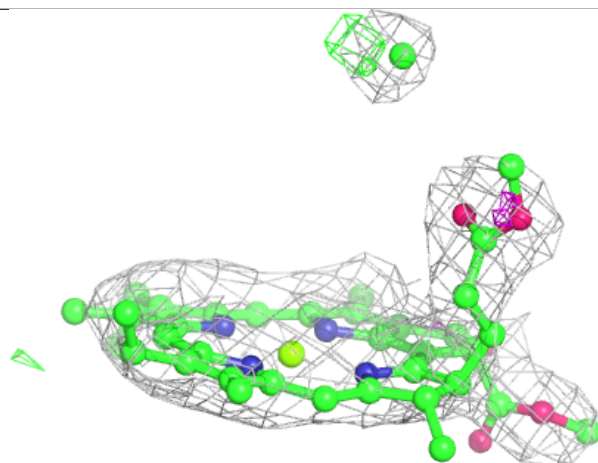
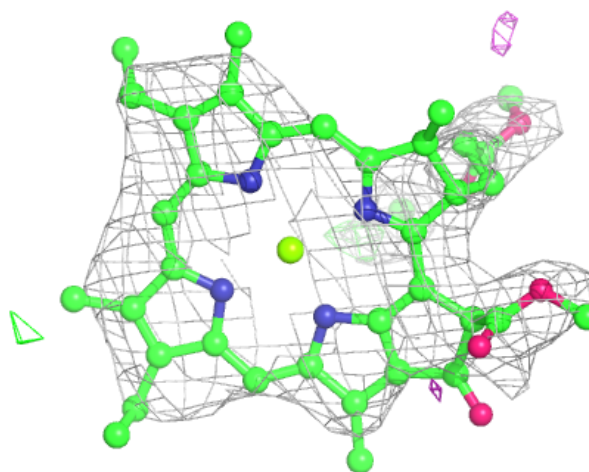
**Electron density around LMT 1 6001:**

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



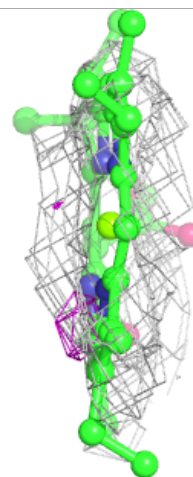
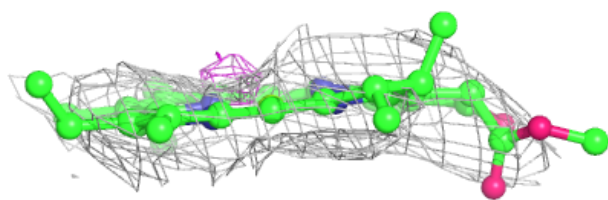
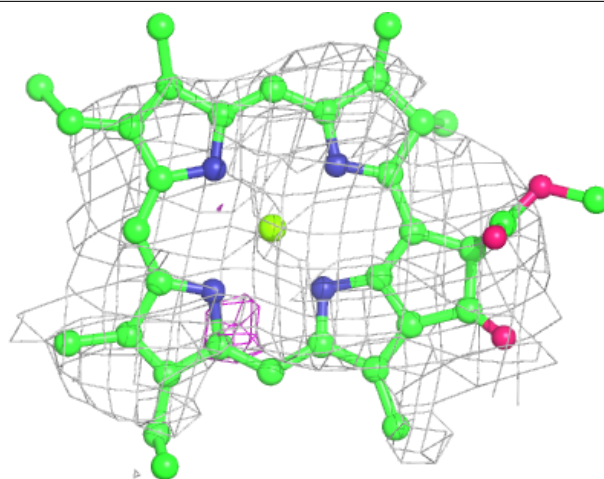
Electron density around CLA 1 1108:

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



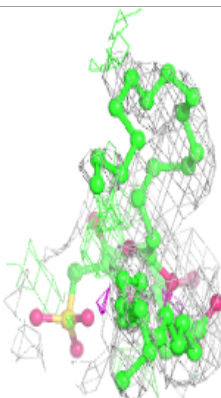
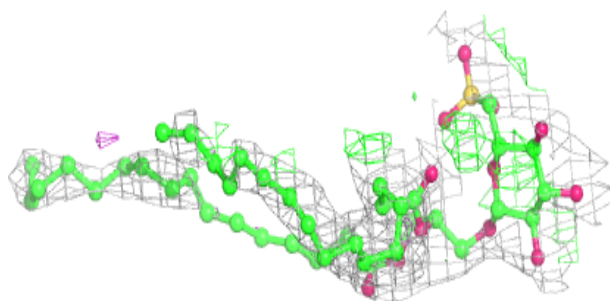
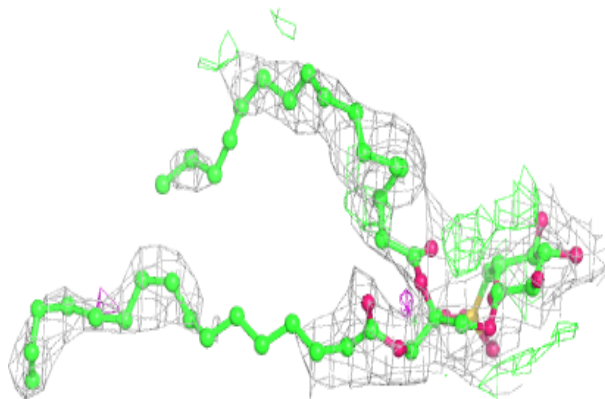
Electron density around CLA 2 1240:

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

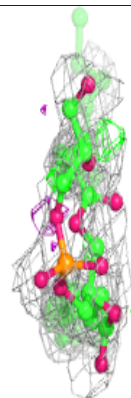
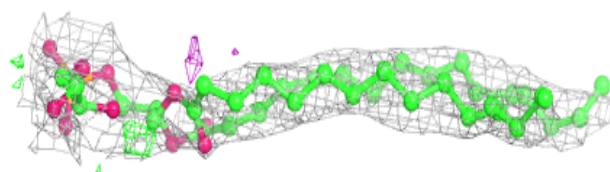
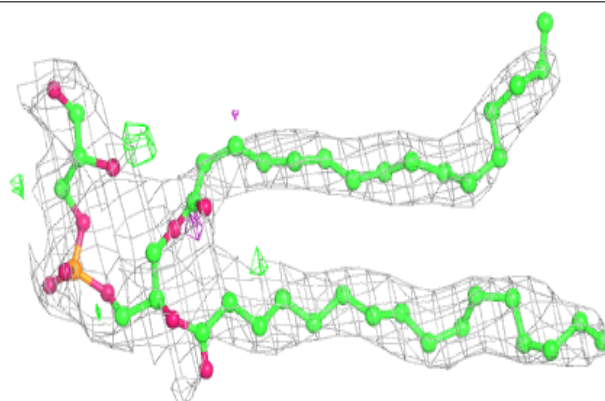


Electron density around SQD 0 5005:

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

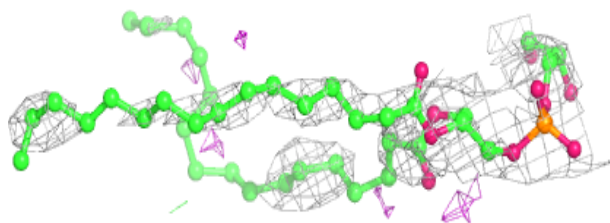
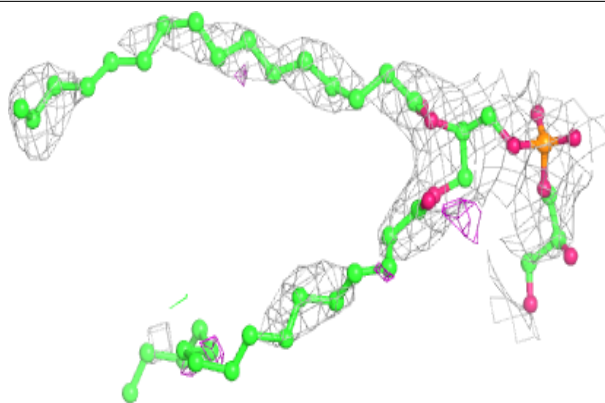
**Electron density around LHG A 5005:**

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

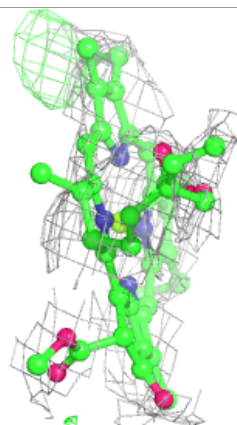
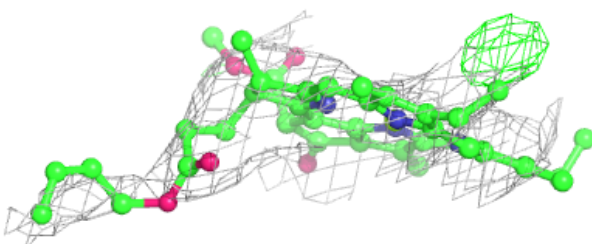
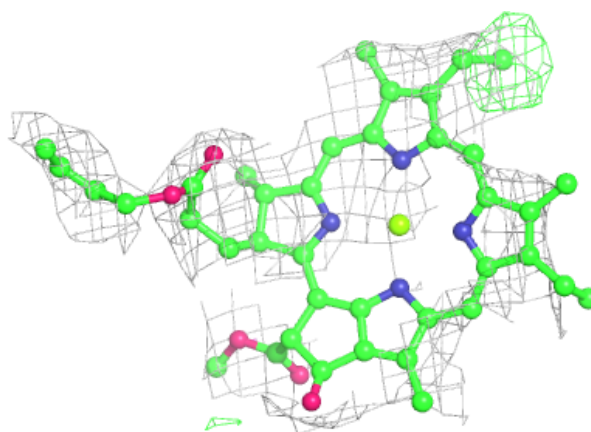


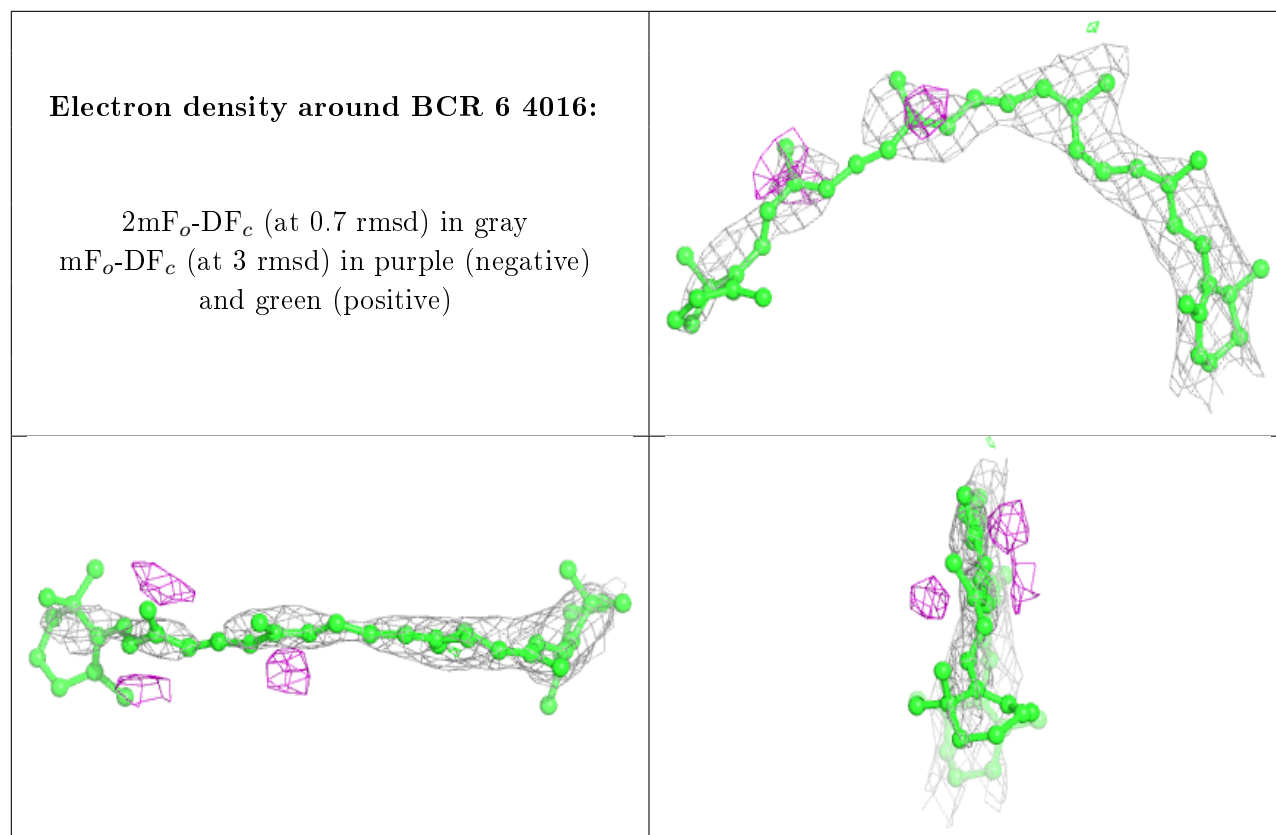
Electron density around LHG 1 5001:

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

**Electron density around CLA k 1402:**

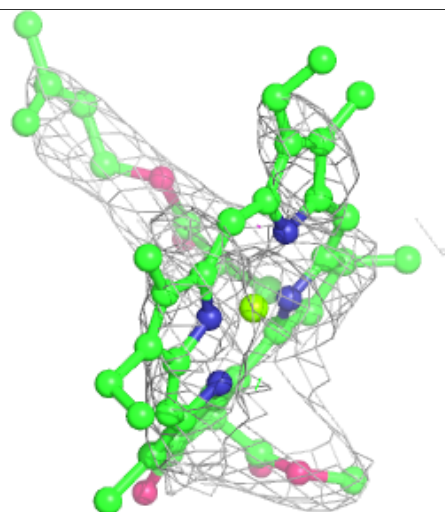
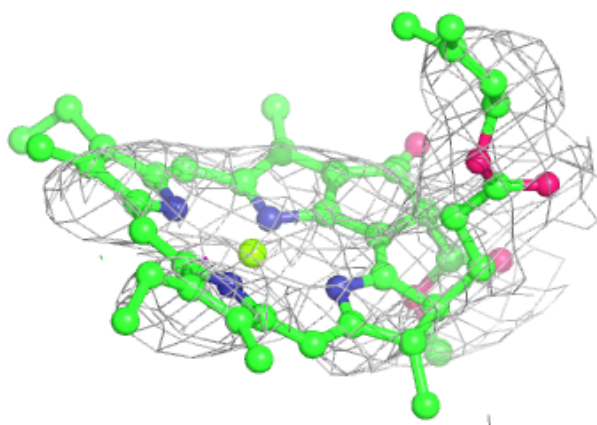
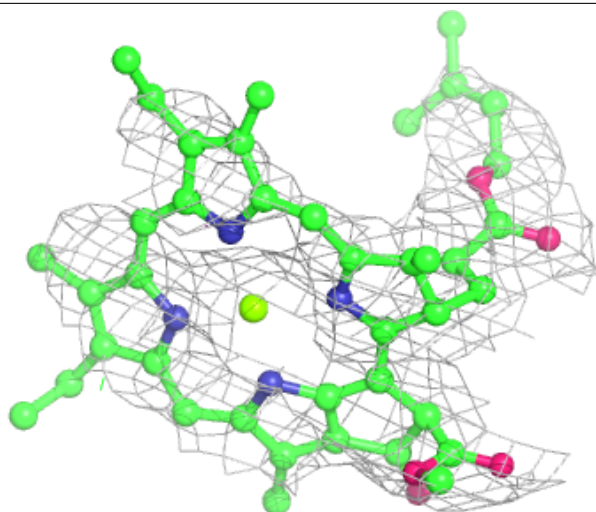
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

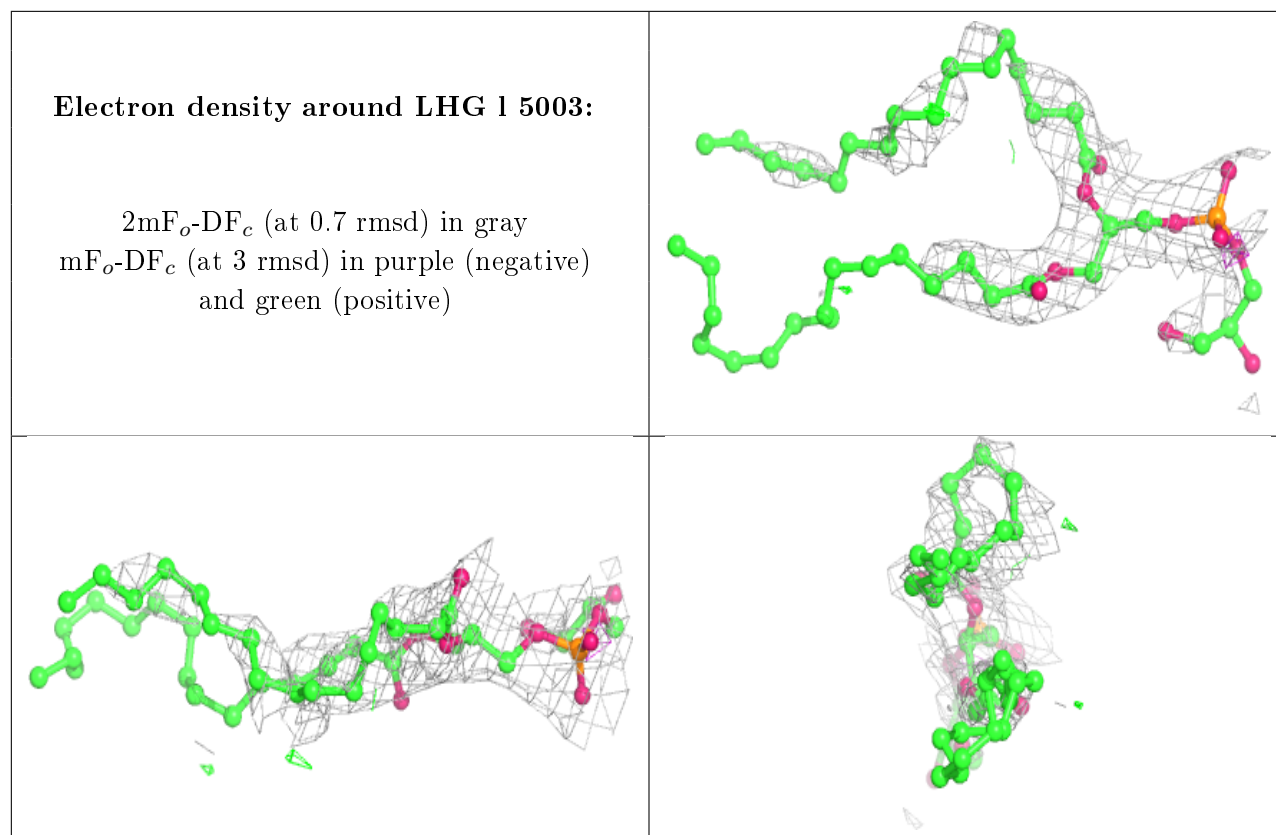




Electron density around CLA 2 1216:

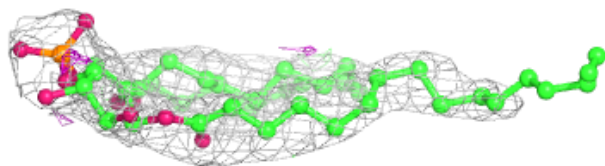
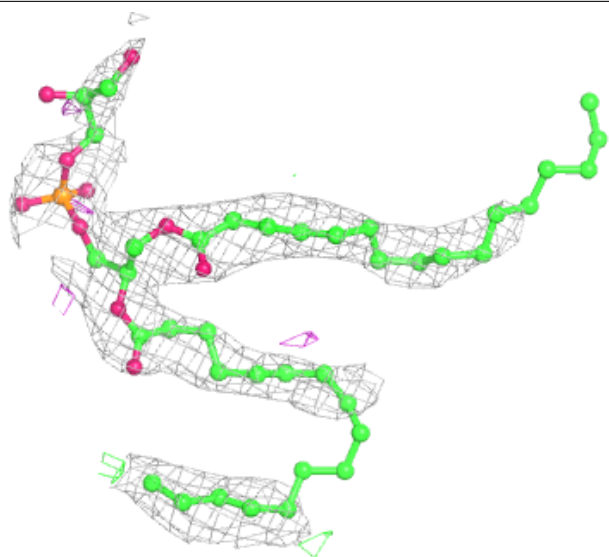
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





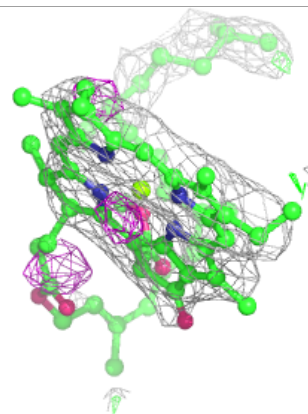
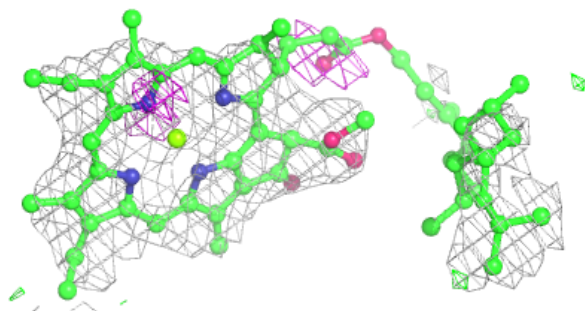
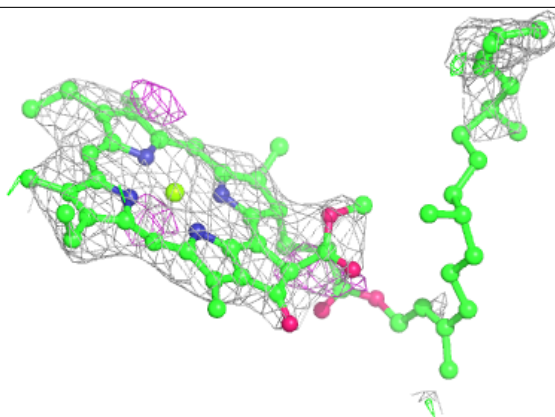
Electron density around LHG A 5007:

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

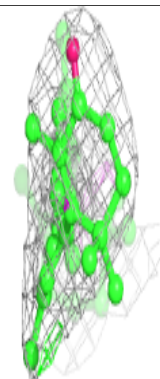
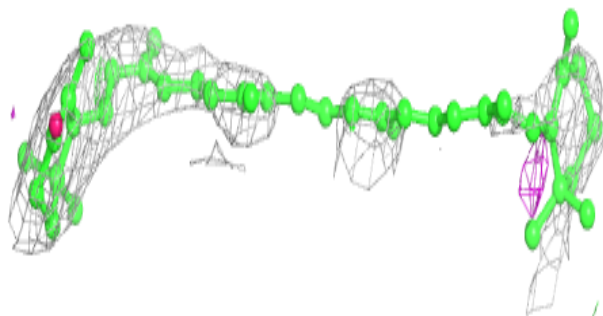
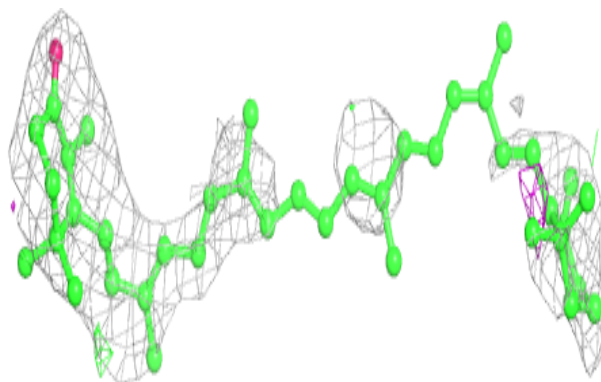


Electron density around CLA B 1240:

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

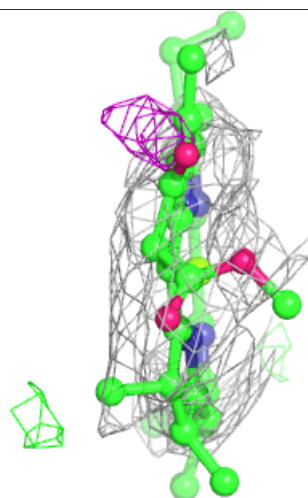
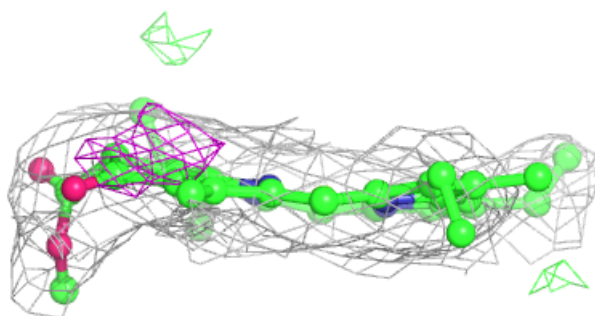
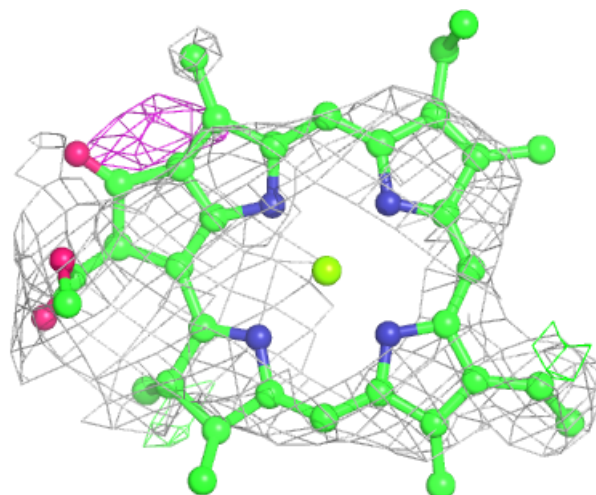
**Electron density around ECH 2 4006:**

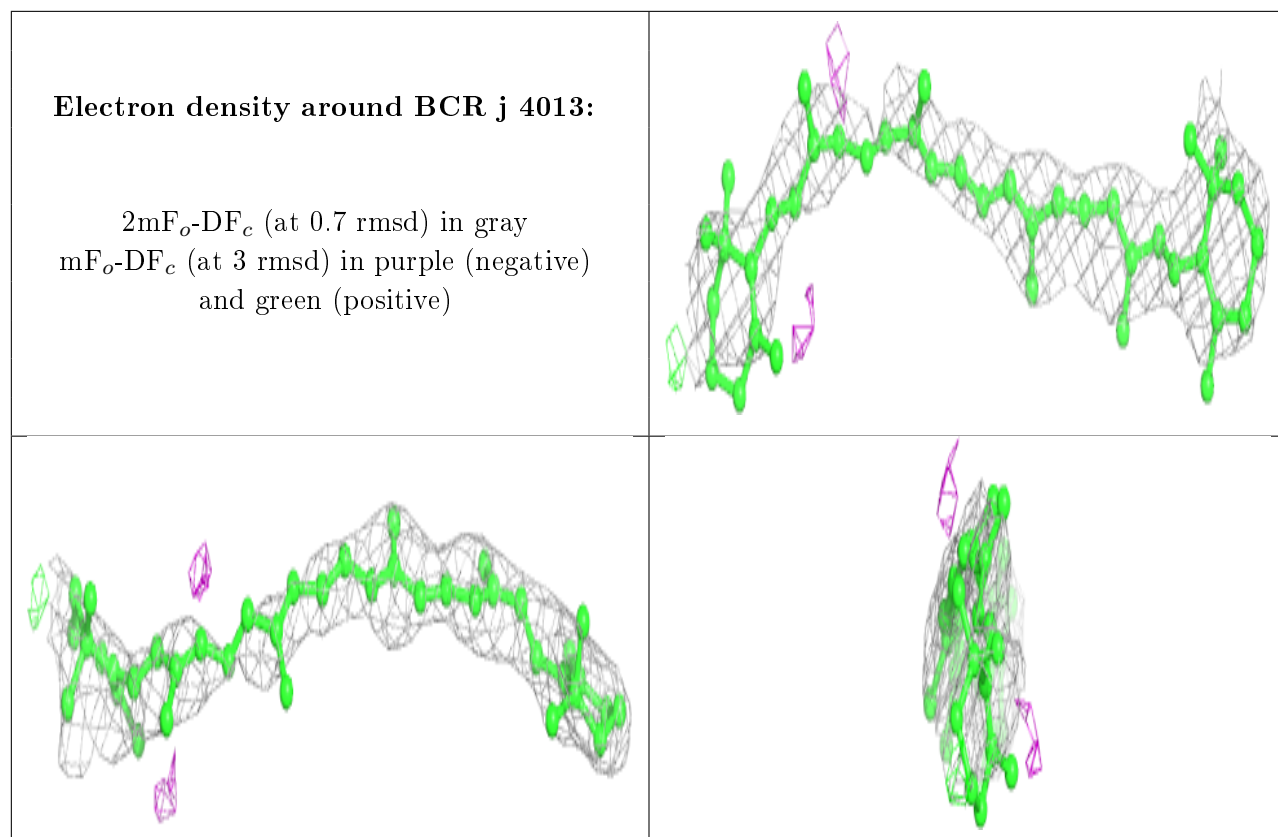
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 1212:

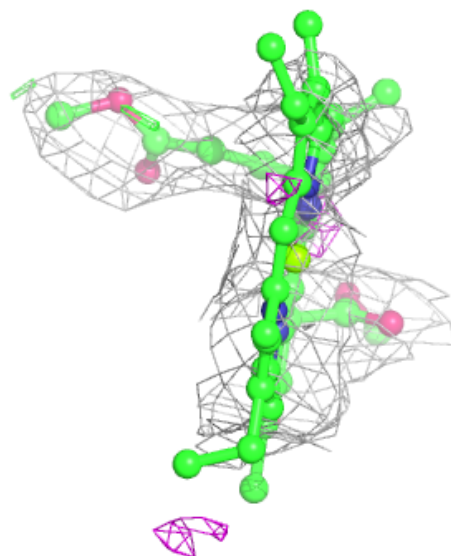
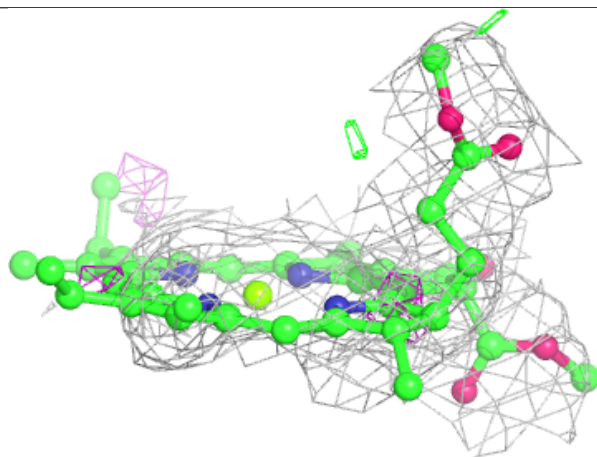
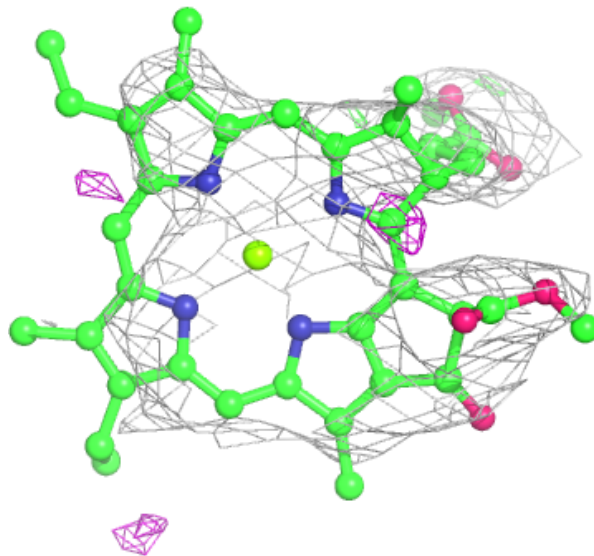
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





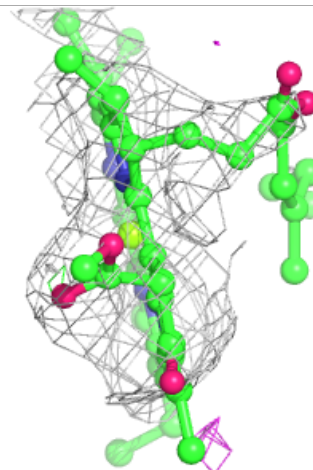
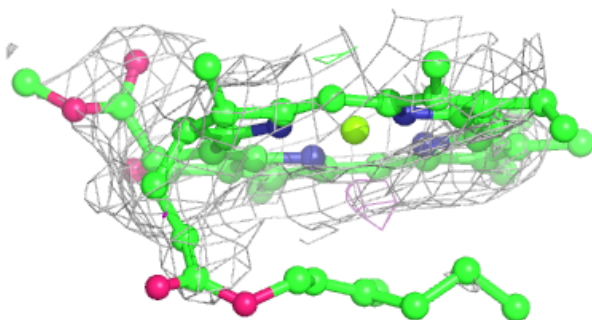
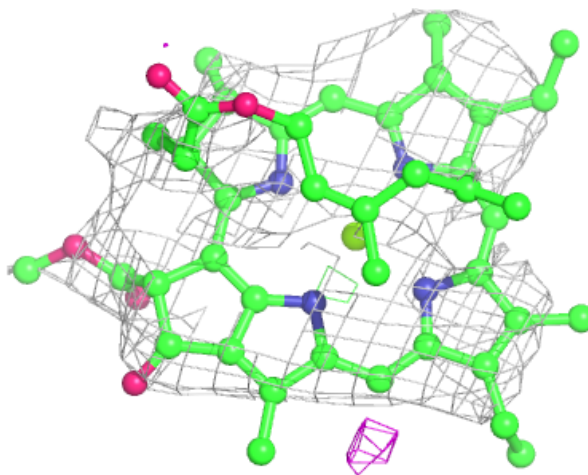
Electron density around CLA 2 1231:

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



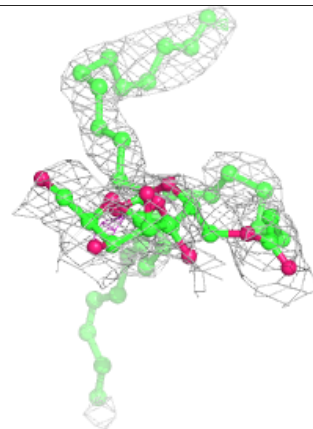
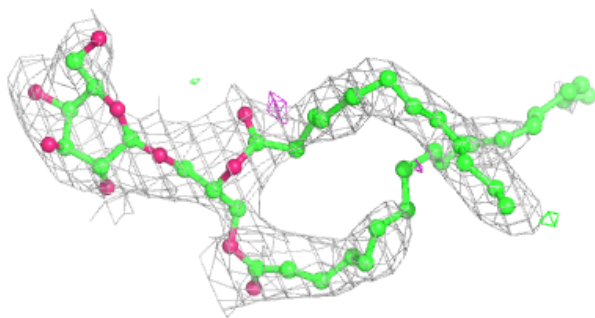
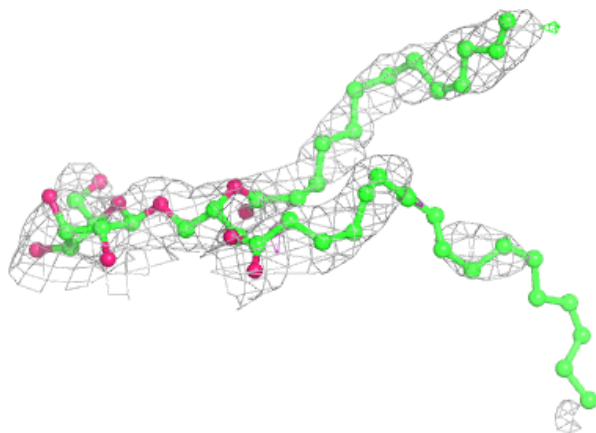
Electron density around CLA a 1114:

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

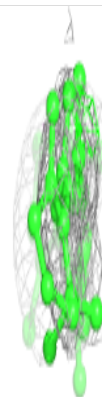
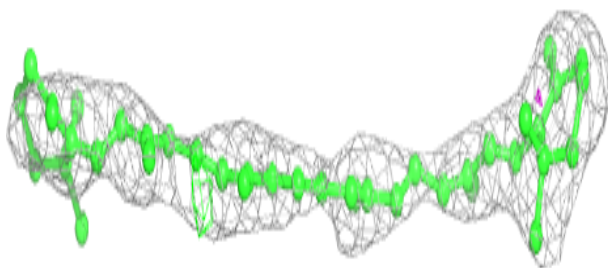
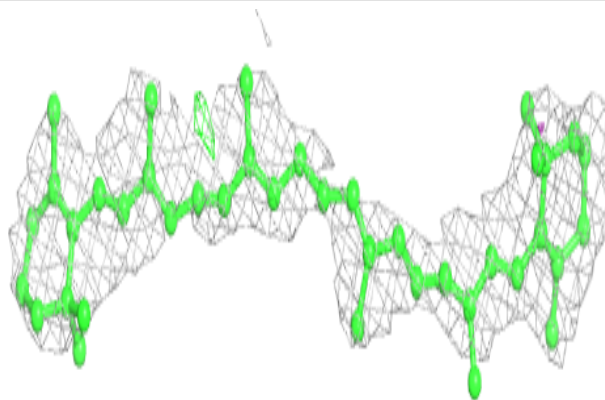


Electron density around LMG 1 5002:

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

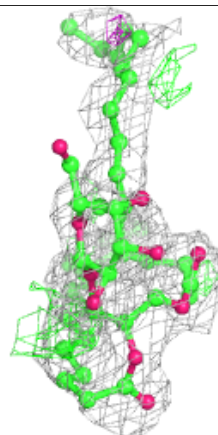
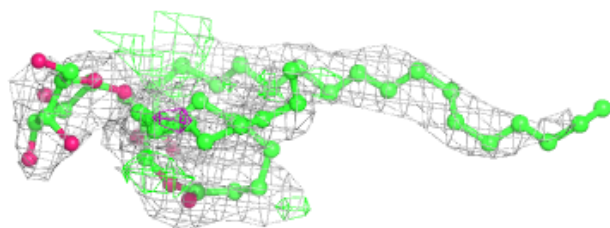
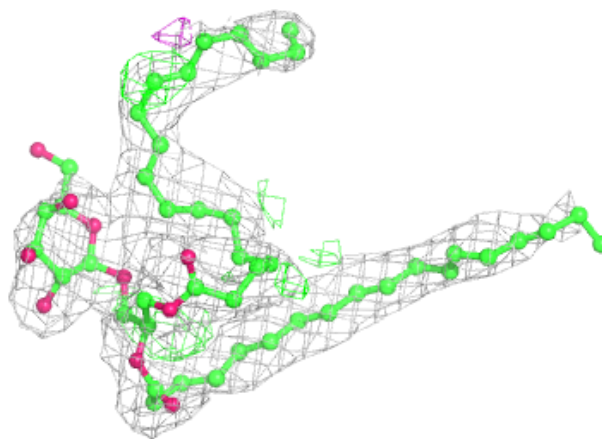
**Electron density around BCR B 4004:**

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

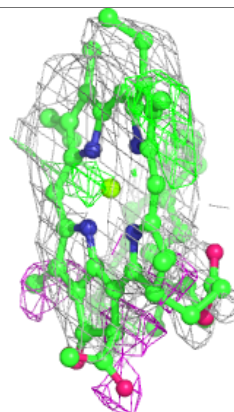
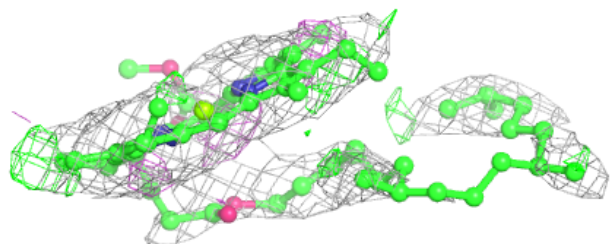
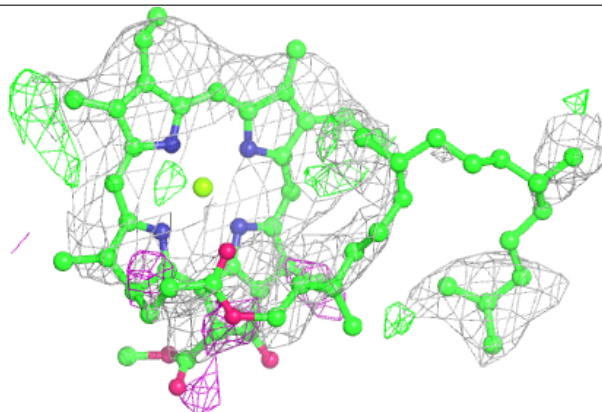


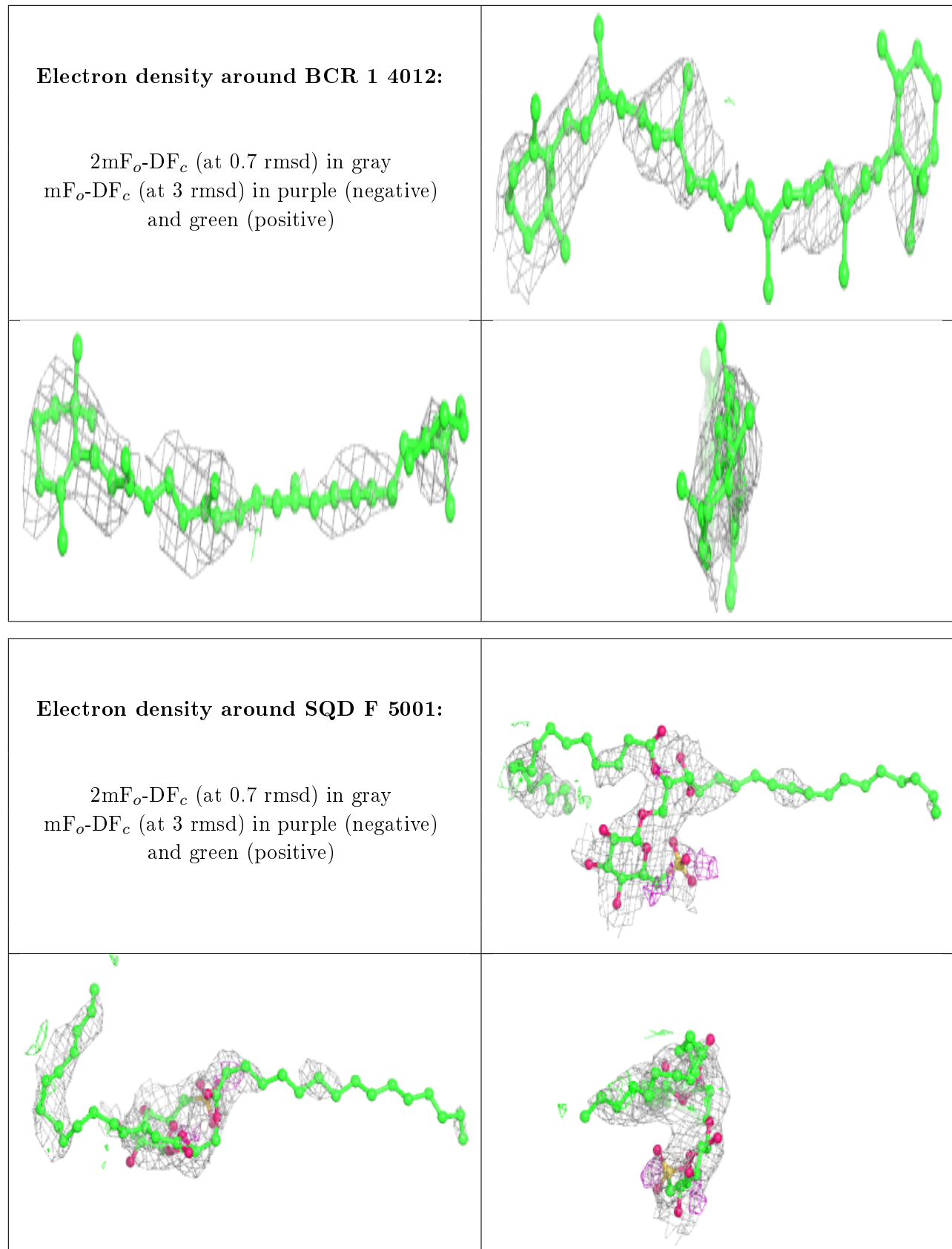
Electron density around LMG K 5009:

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

**Electron density around CLA J 1302:**

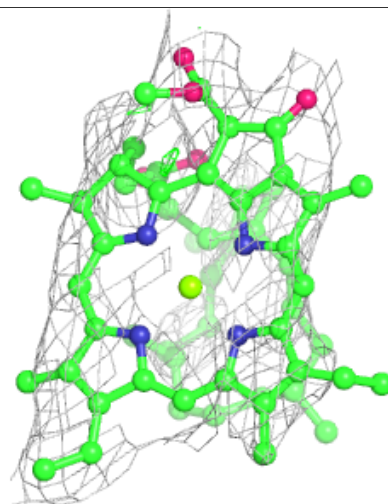
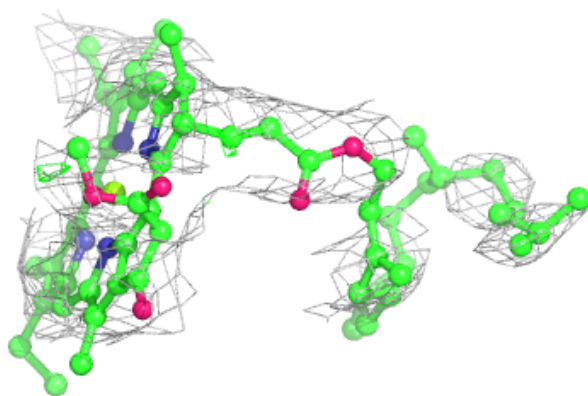
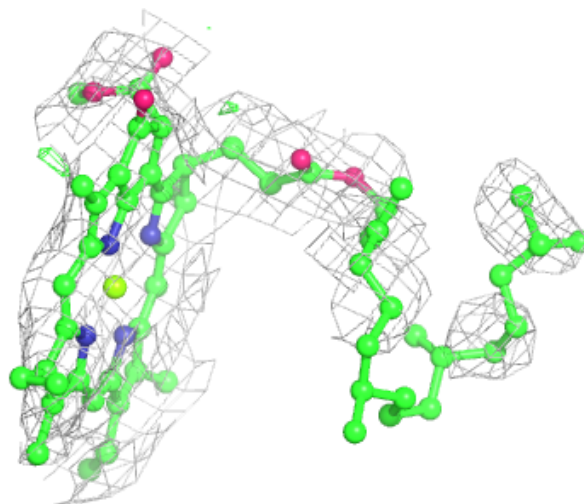
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

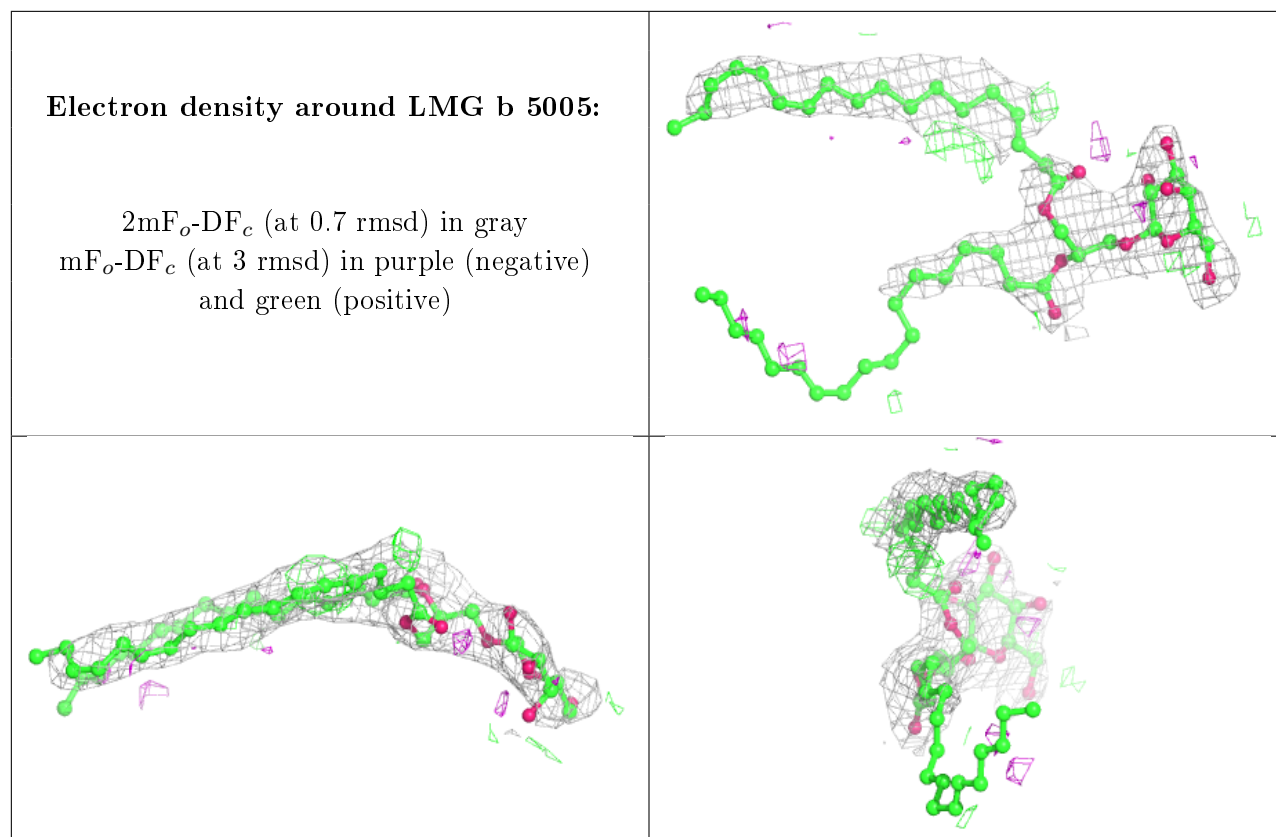




Electron density around CLA a 1112:

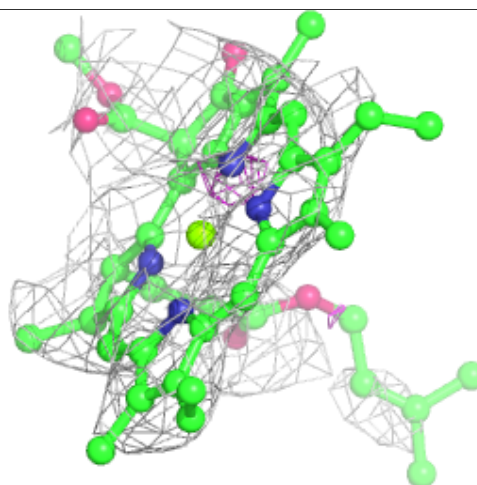
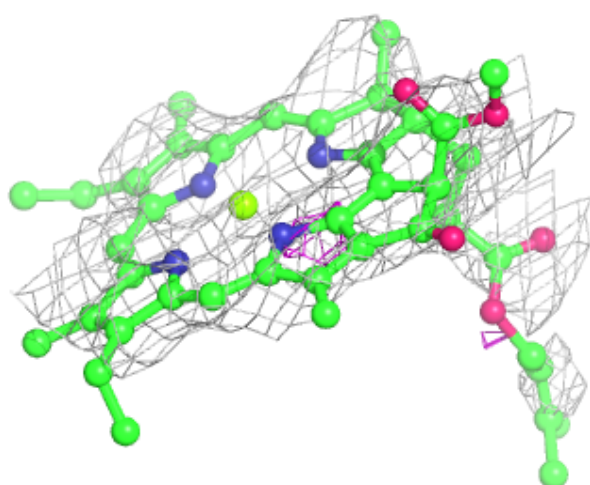
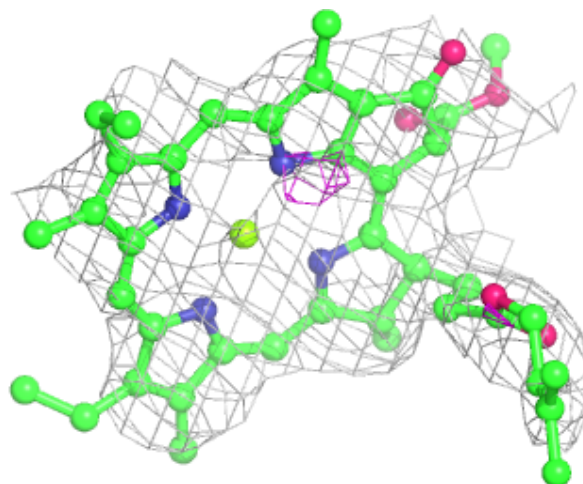
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





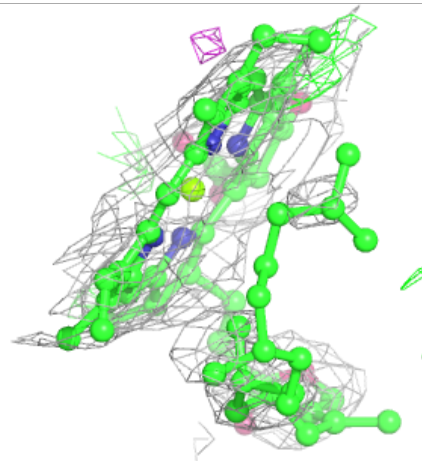
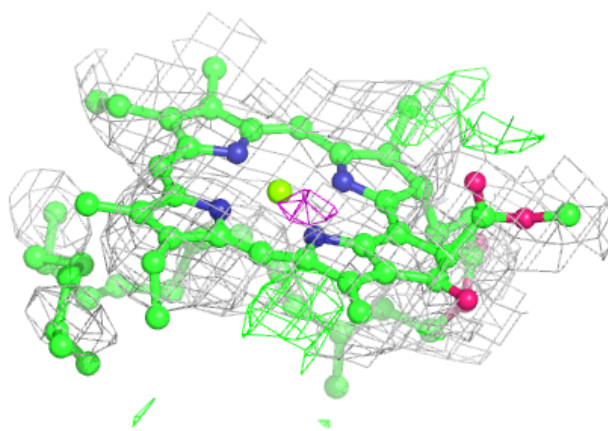
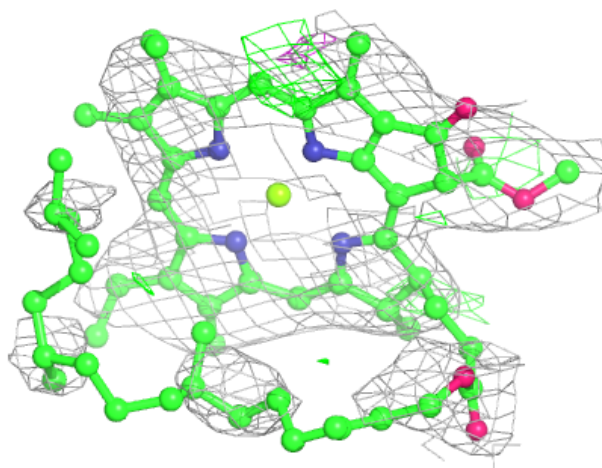
Electron density around CLA 1 1105:

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



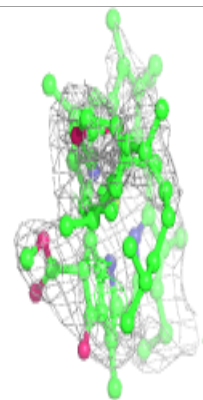
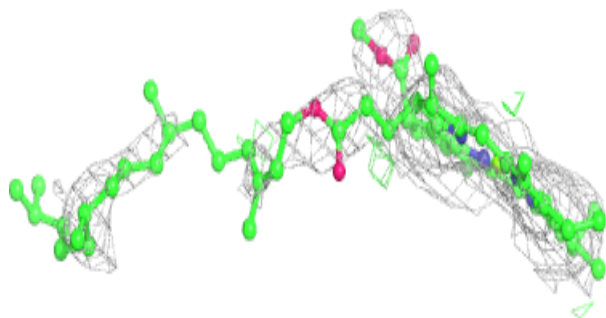
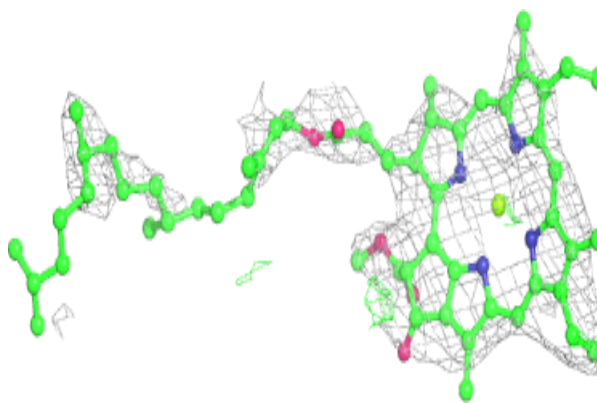
Electron density around CLA a 1118:

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

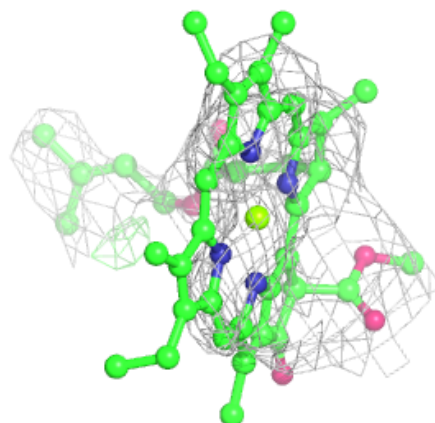
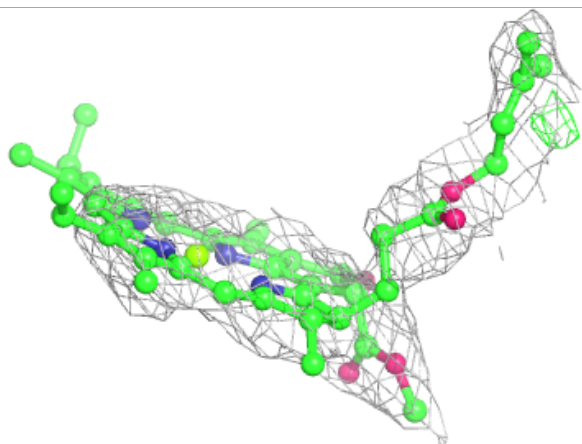
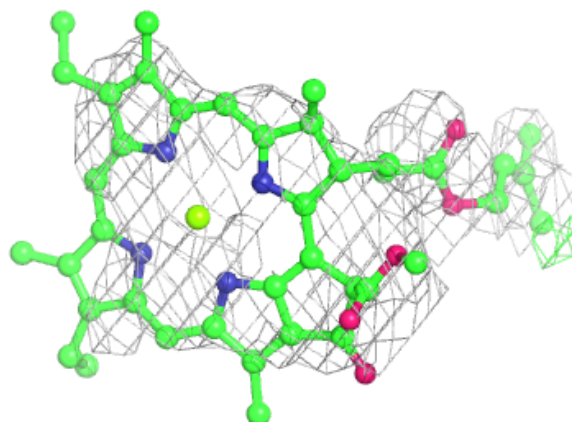


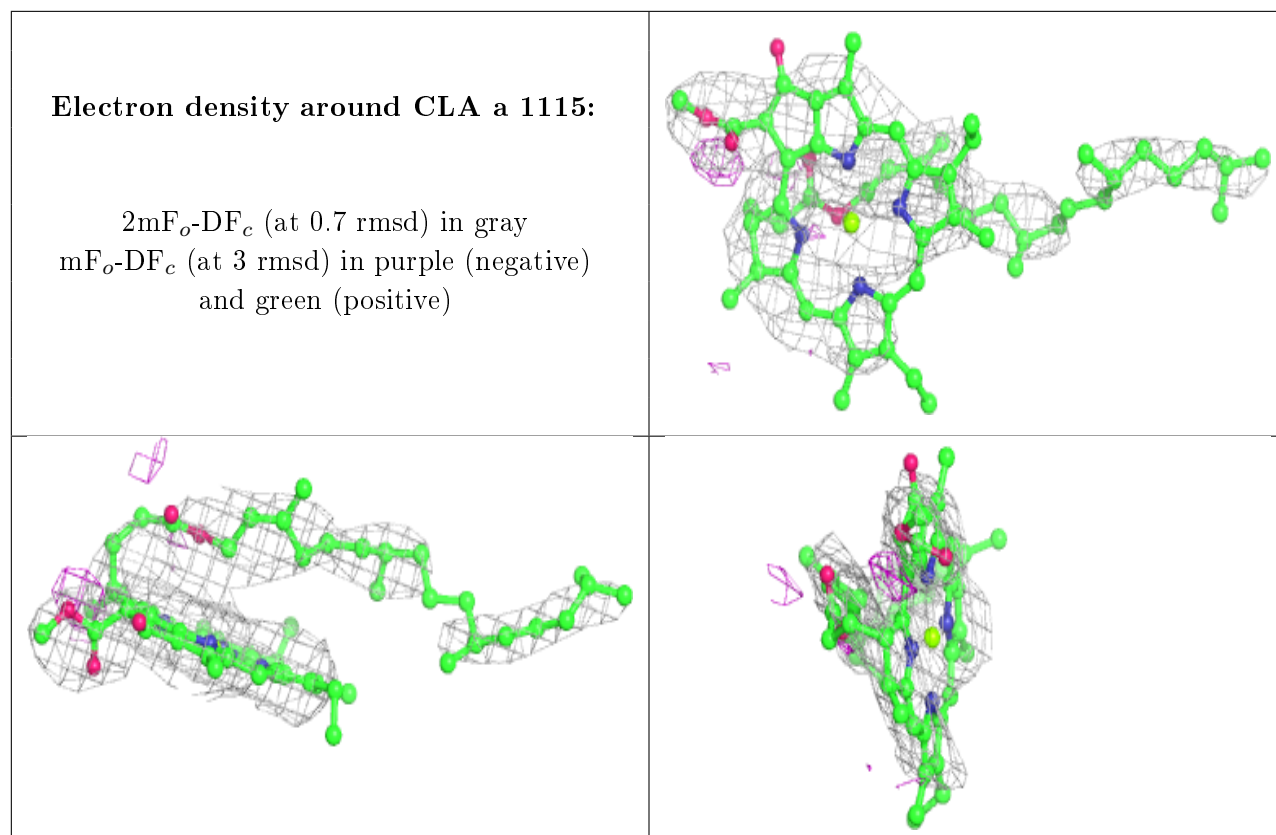
Electron density around CLA 1 1139:

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

**Electron density around CLA k 1401:**

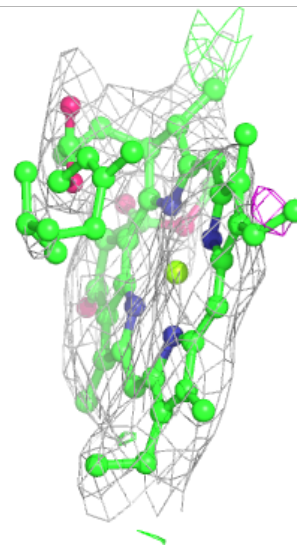
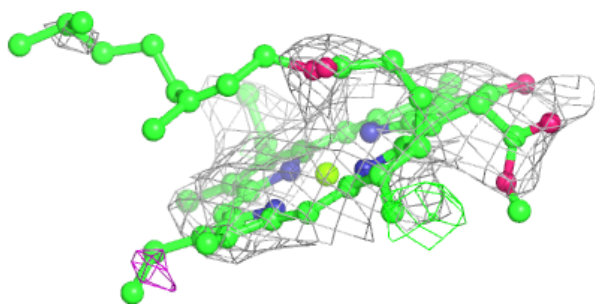
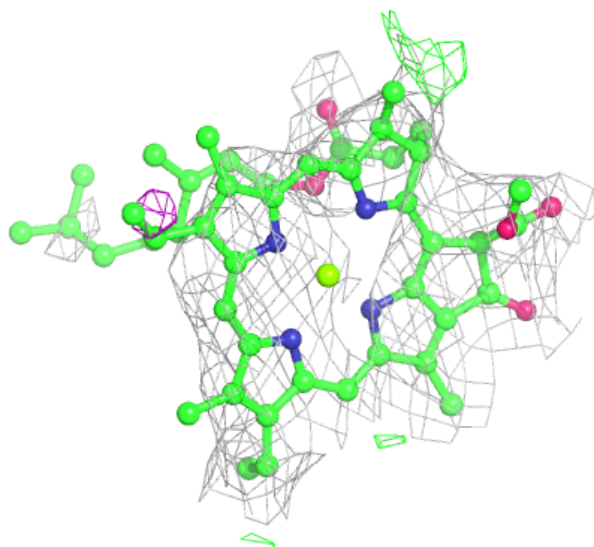
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





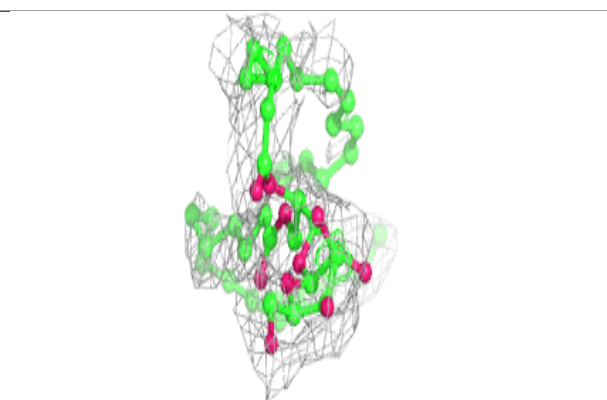
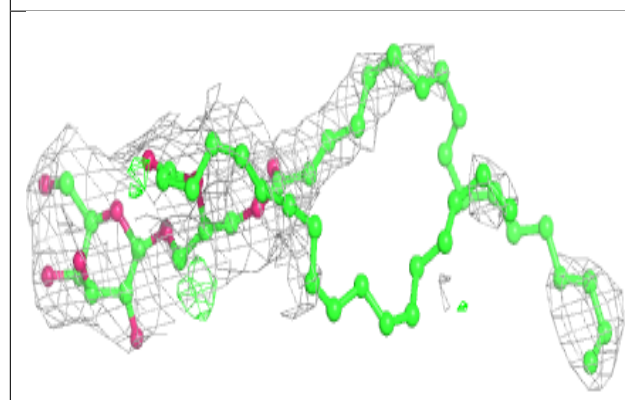
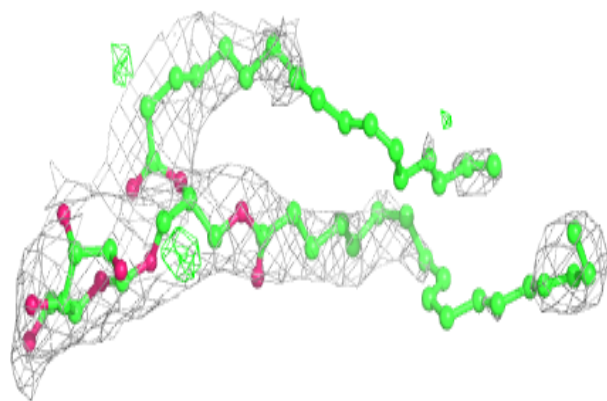
Electron density around CLA a 1120:

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

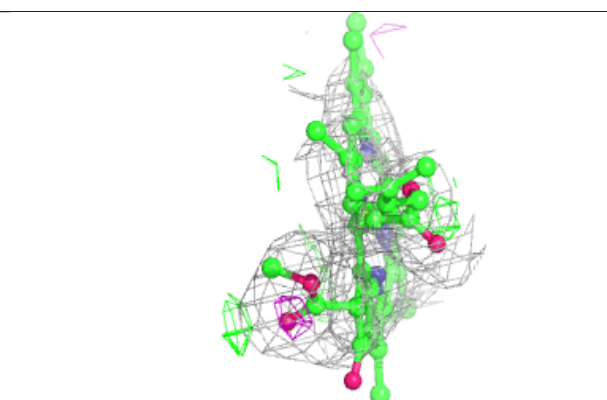
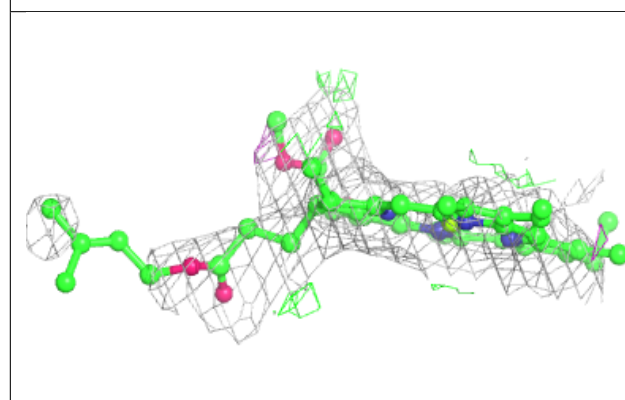
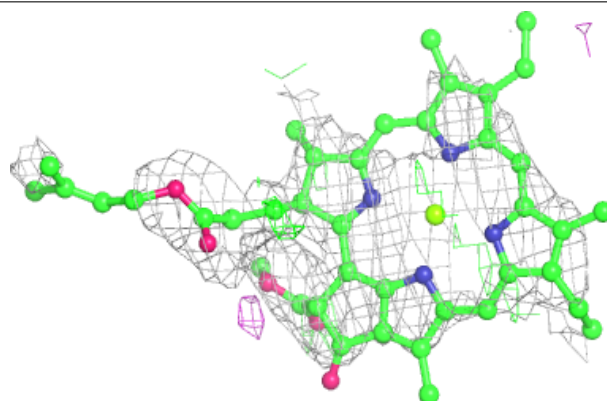


Electron density around LMG a 5004:

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

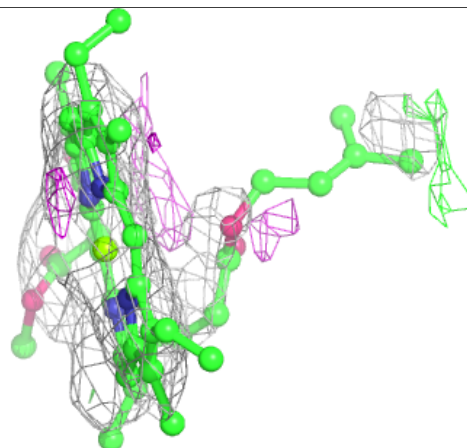
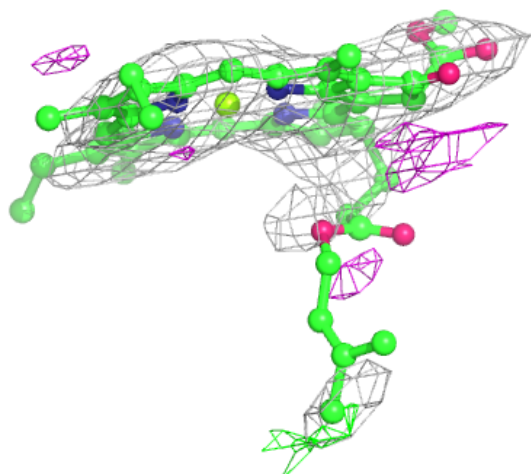
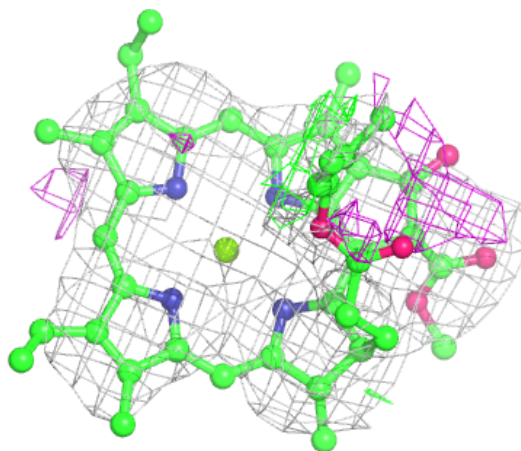
**Electron density around CLA 2 1234:**

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



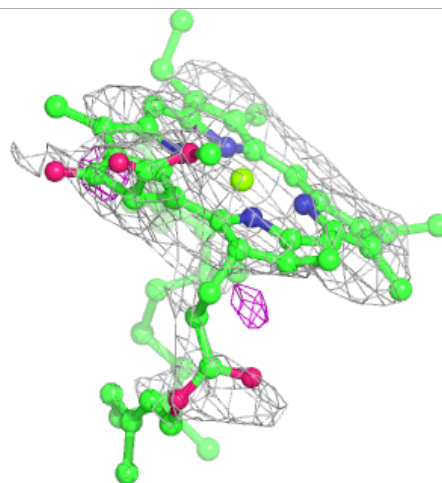
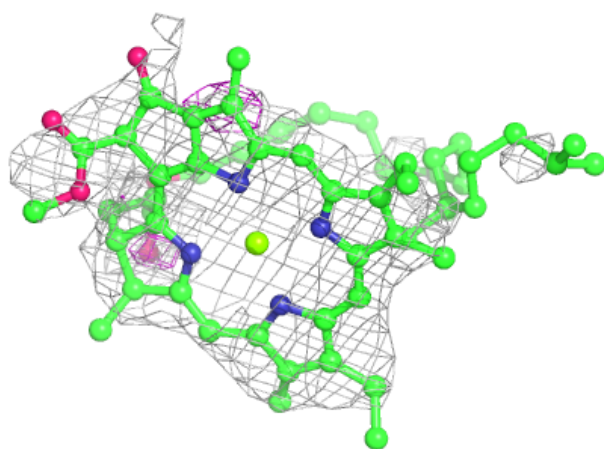
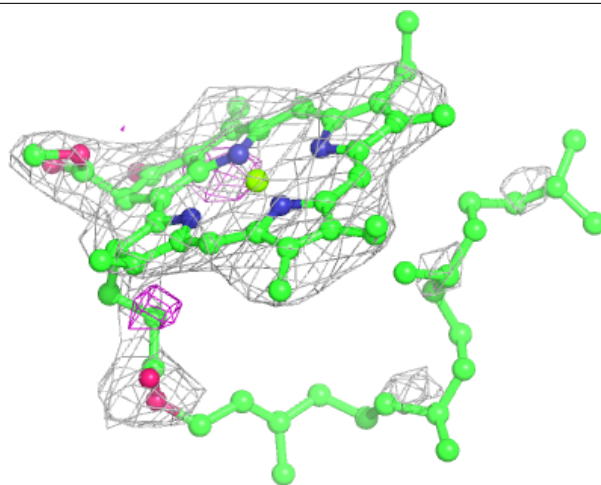
Electron density around CLA 2 1213:

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



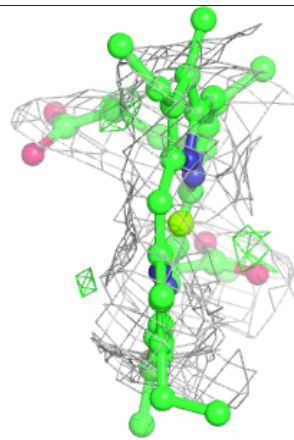
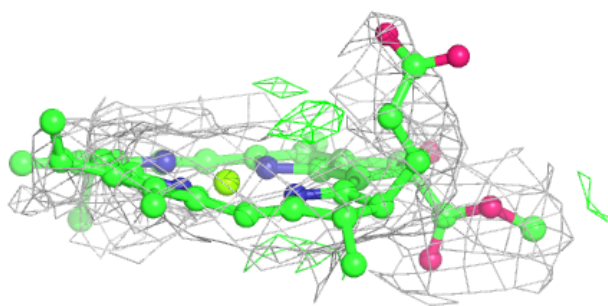
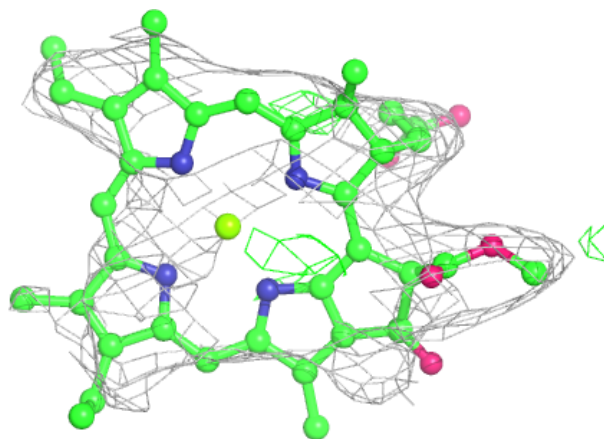
Electron density around CLA J 1303:

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

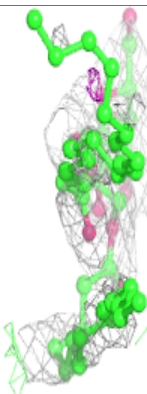
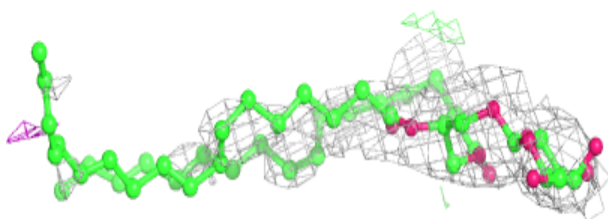
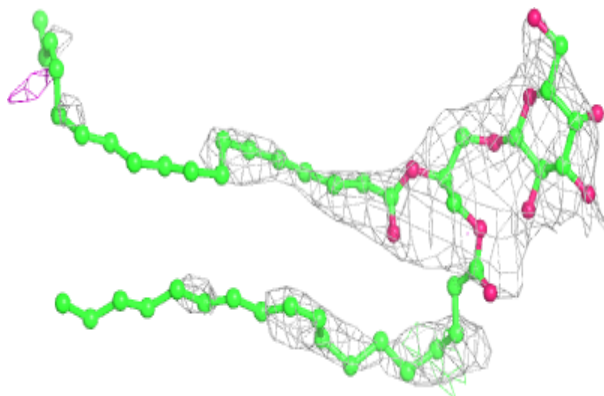


Electron density around CLA 2 1232:

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

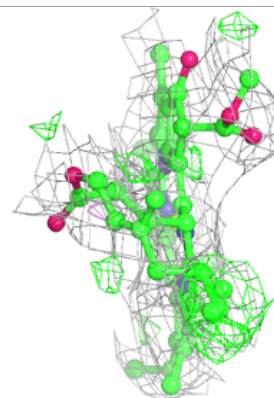
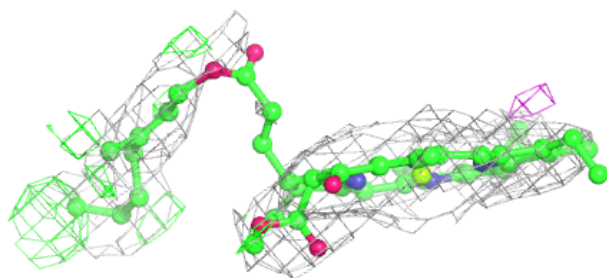
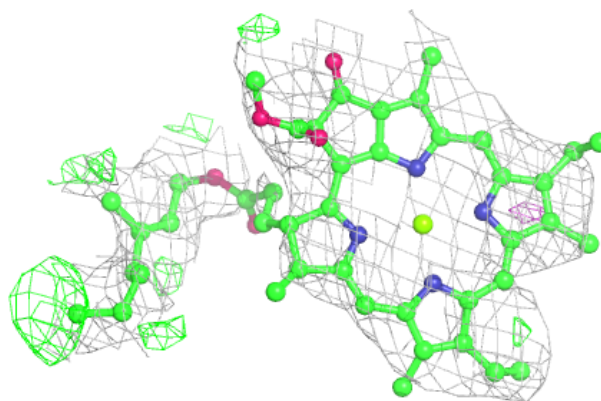
**Electron density around LMG 1 5004:**

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

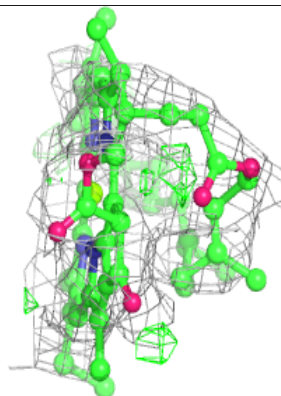
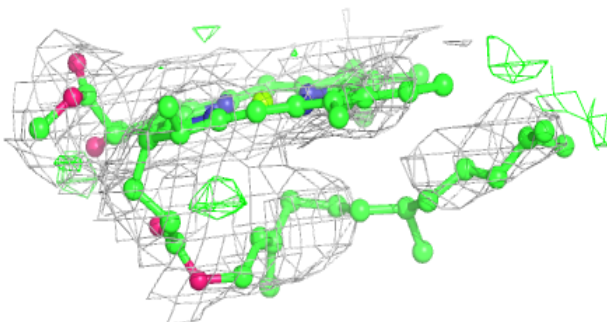
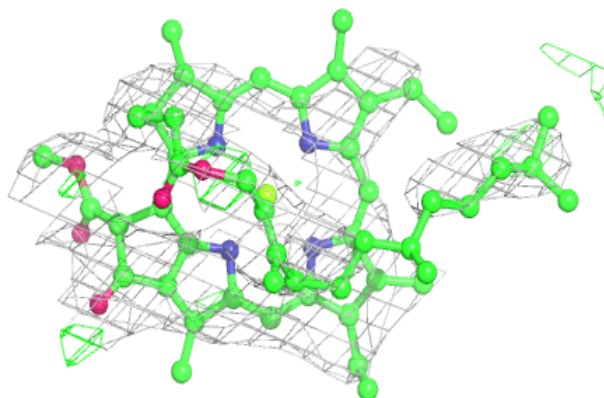


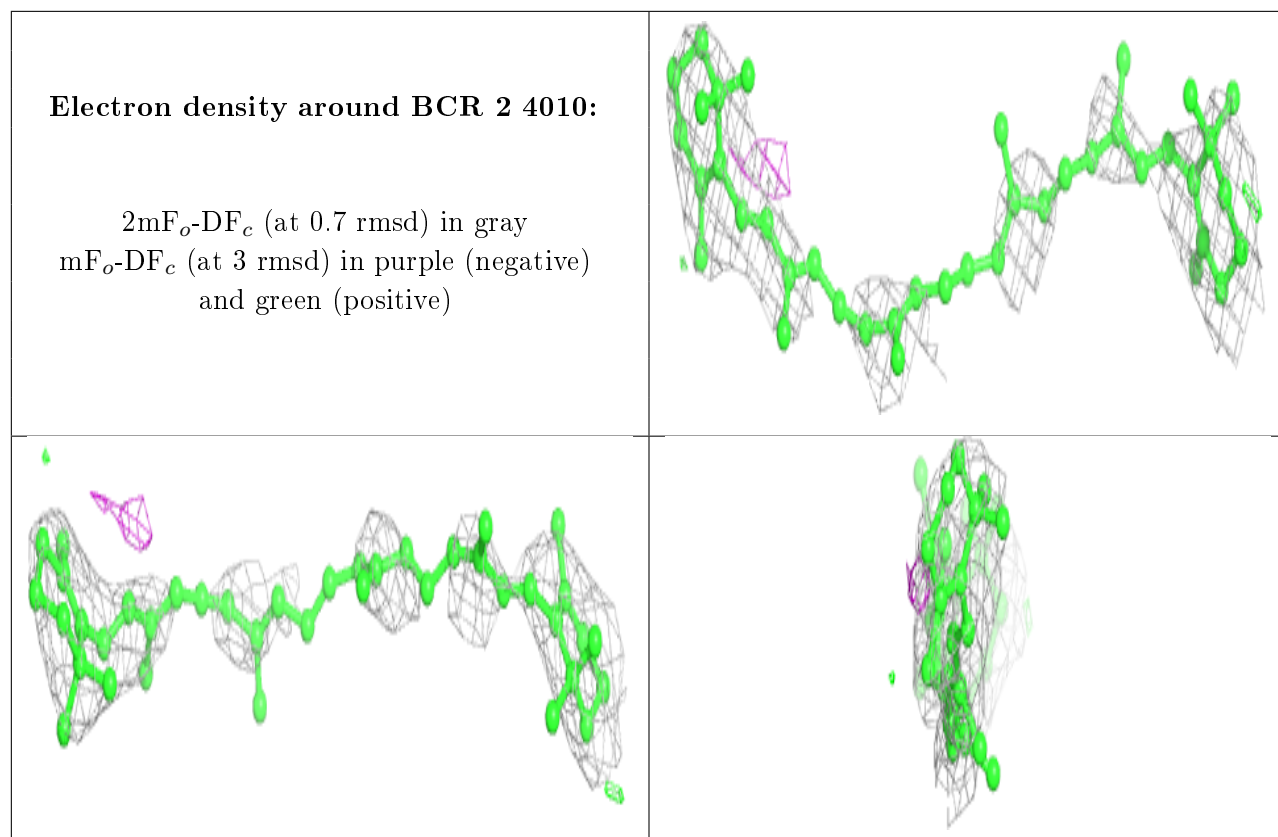
Electron density around CLA 2 1219:

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

**Electron density around CLA 1 1138:**

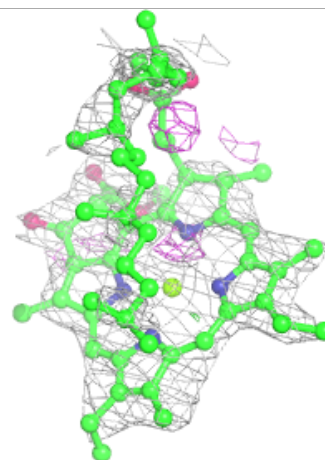
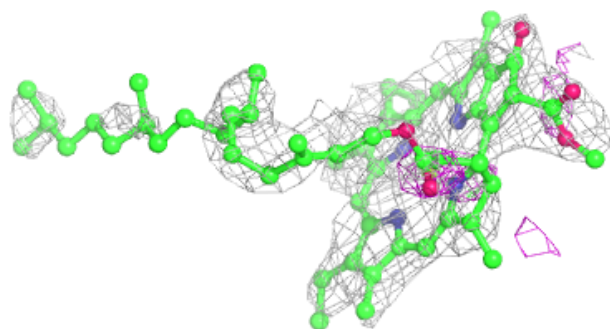
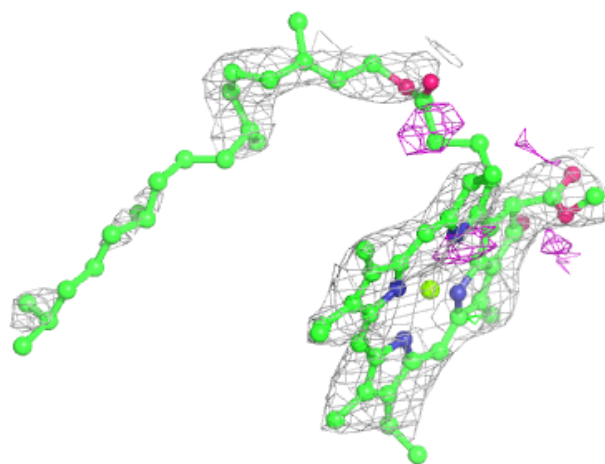
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





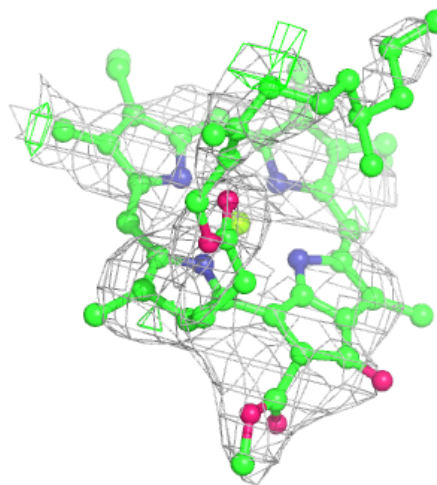
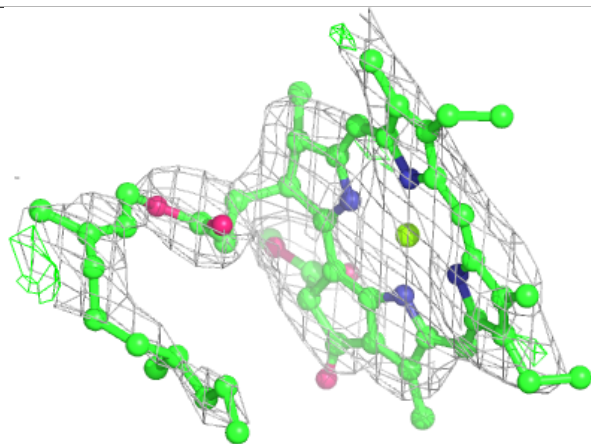
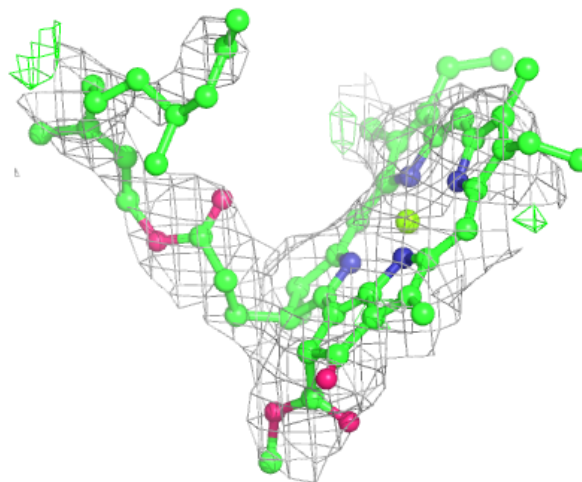
Electron density around CLA a 1102:

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



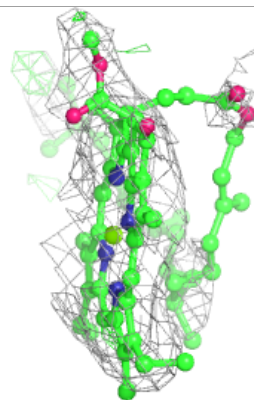
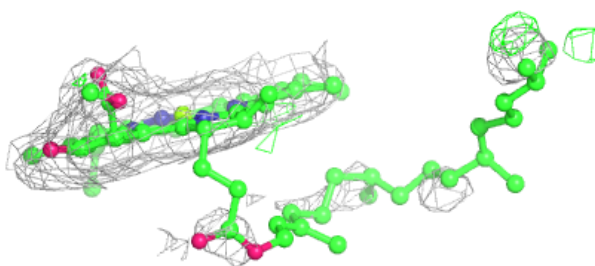
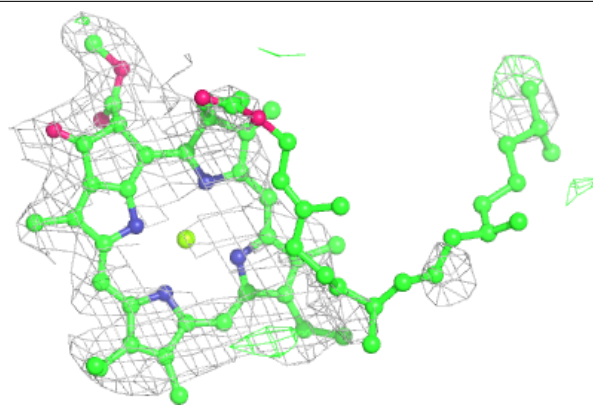
Electron density around CLA a 1108:

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

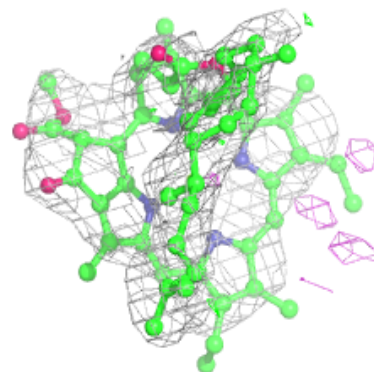
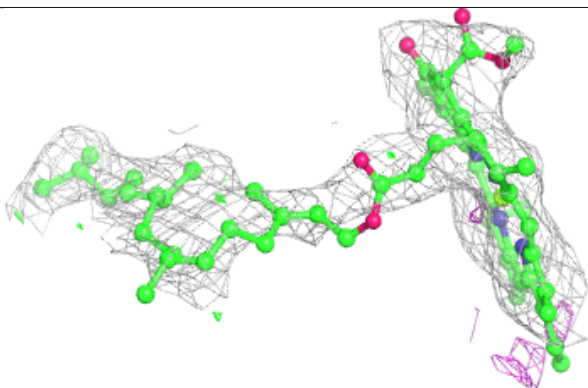
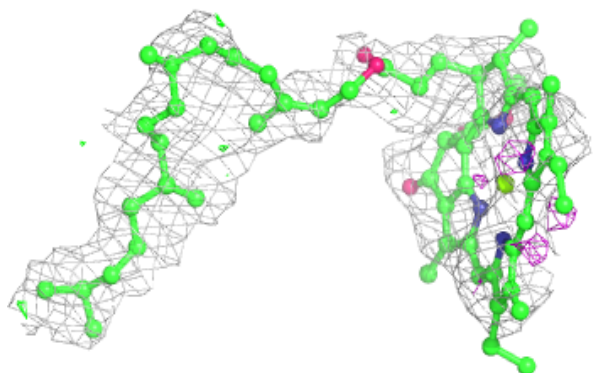


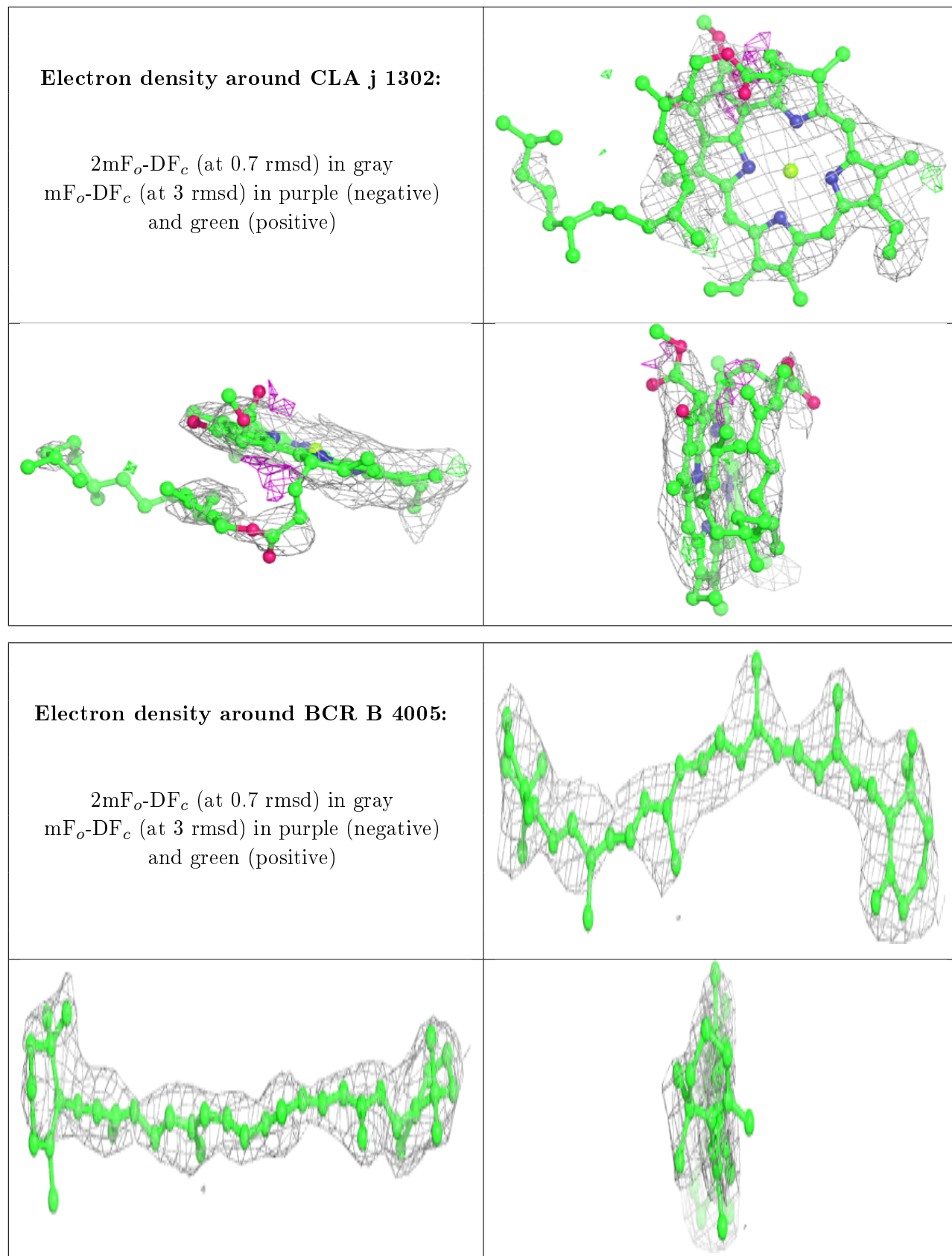
Electron density around CLA 2 1218:

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

**Electron density around CLA 1 1134:**

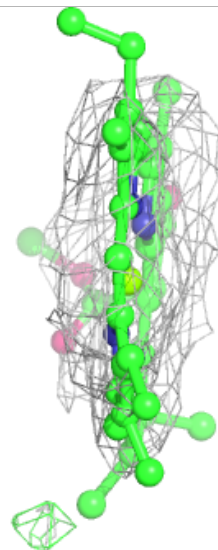
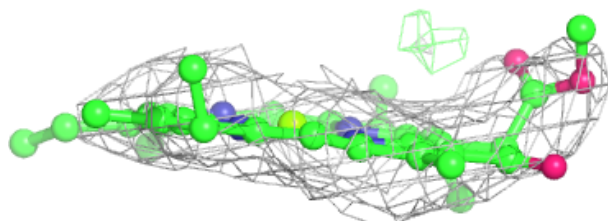
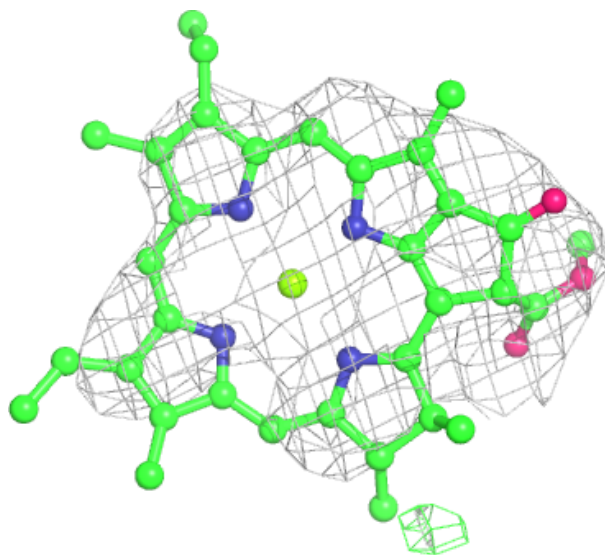
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





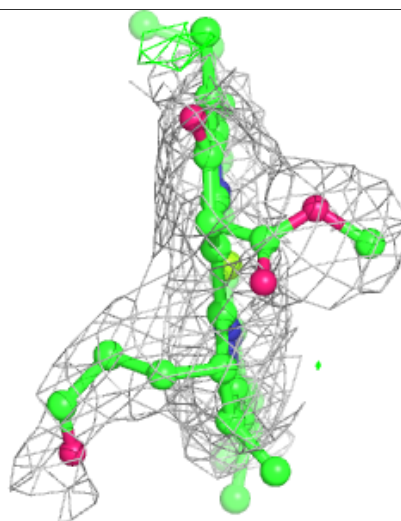
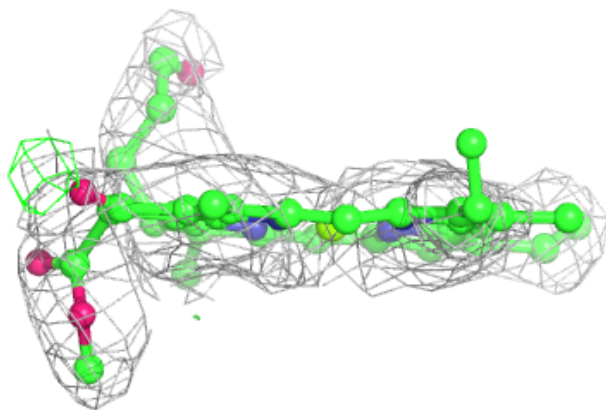
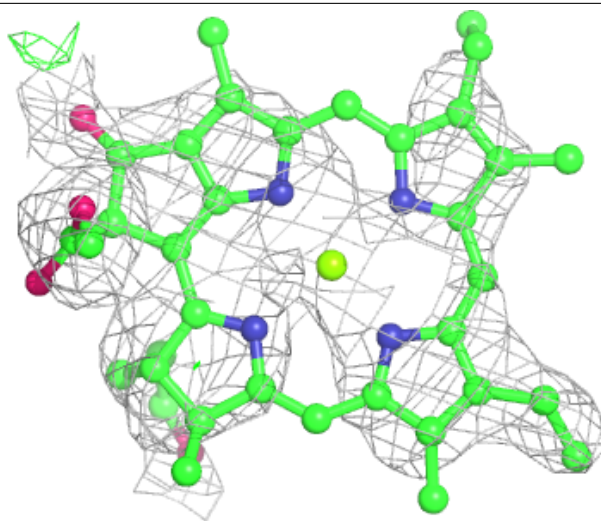
Electron density around CLA 7 1303:

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



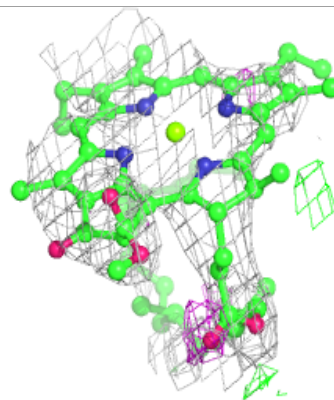
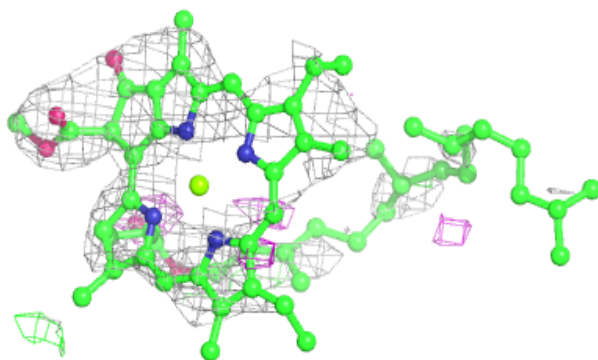
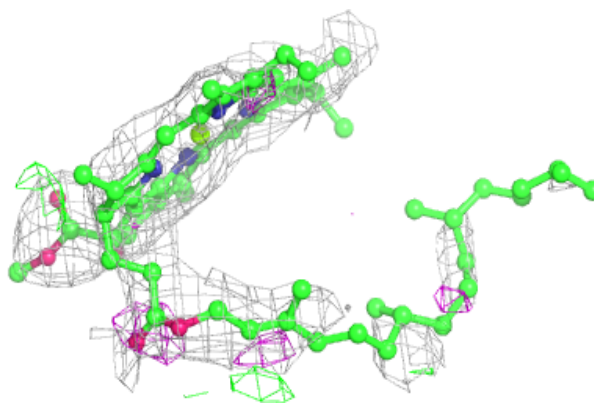
Electron density around CLA 1 1113:

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

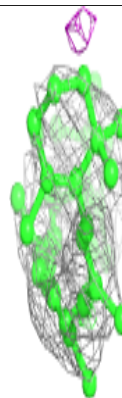
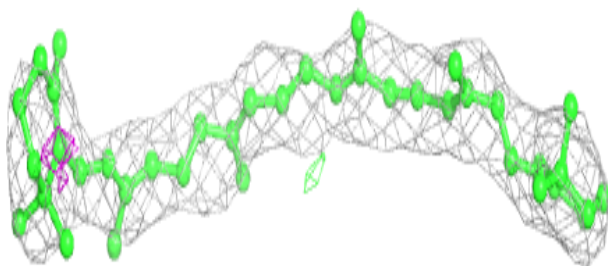
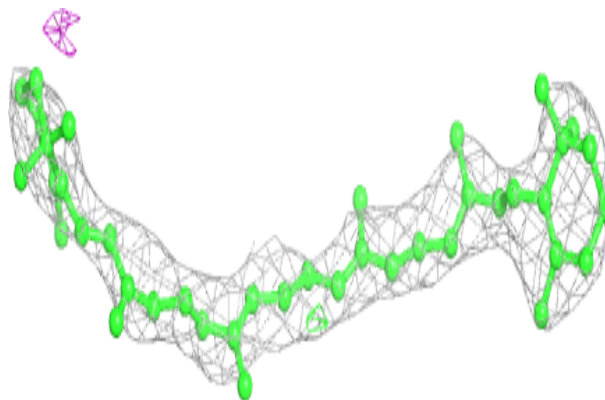


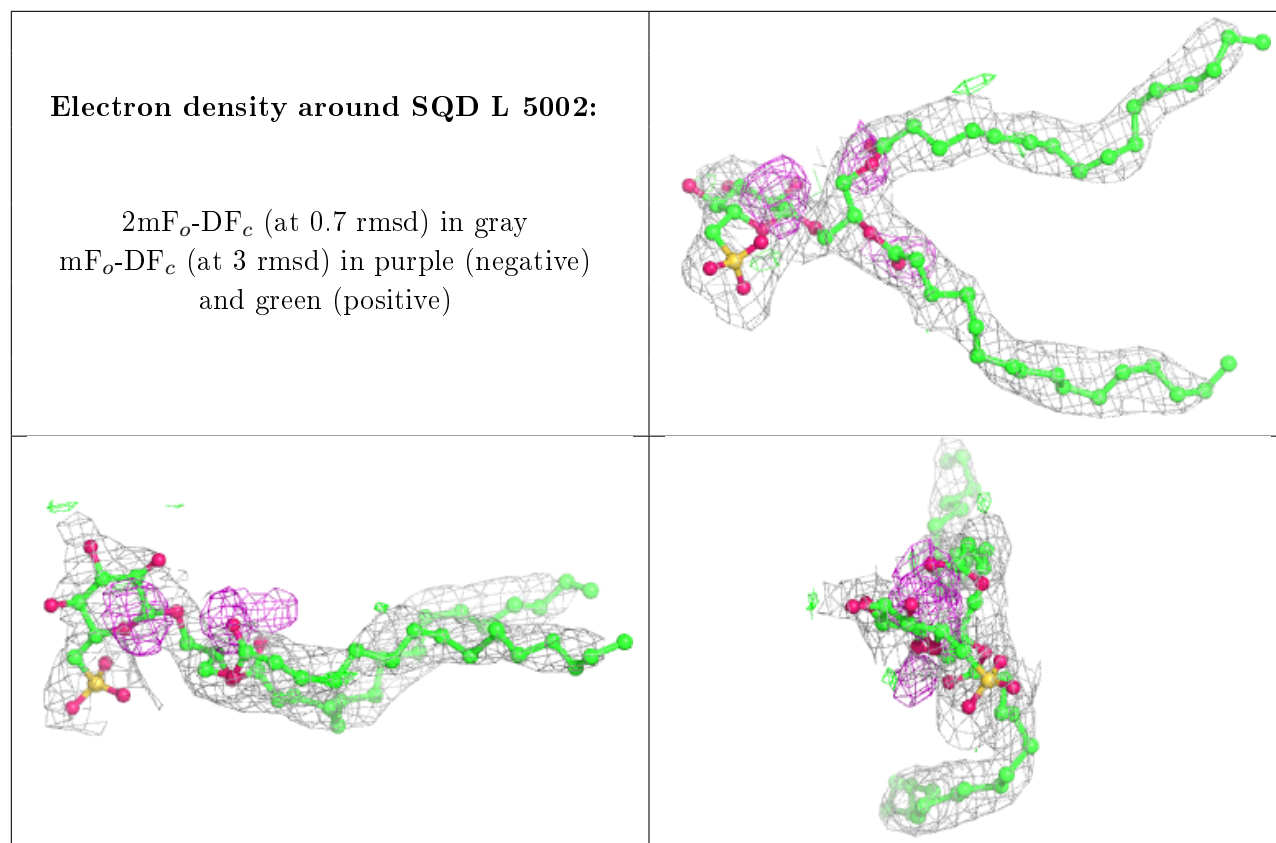
Electron density around CLA 1 1109:

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

**Electron density around BCR b 4014:**

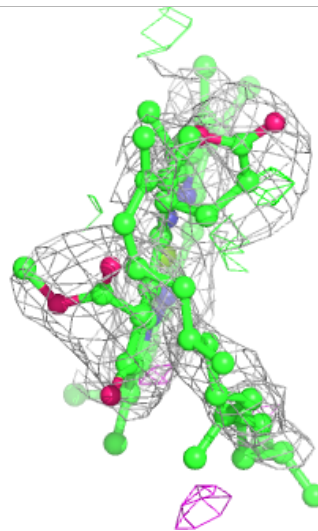
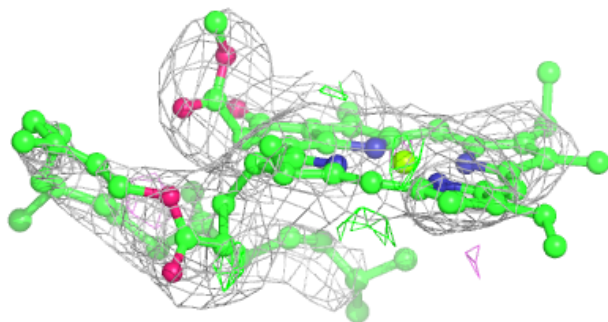
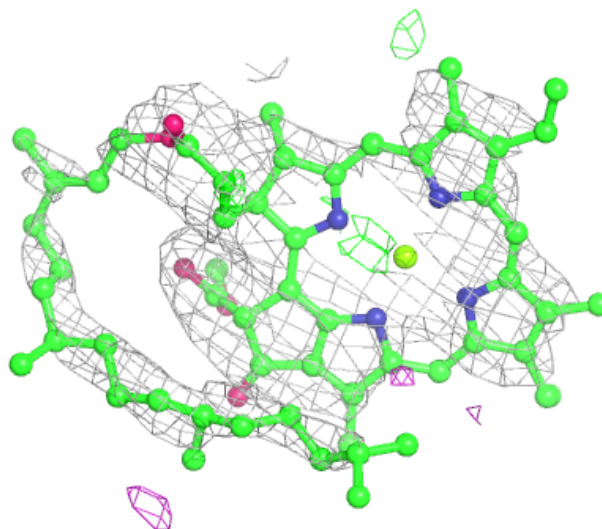
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





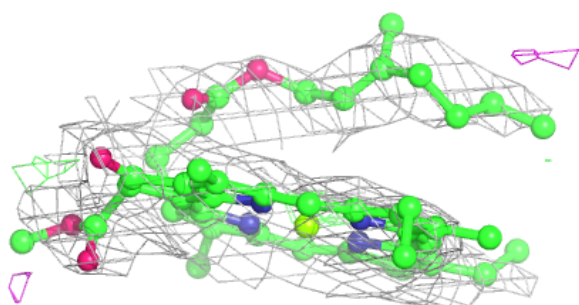
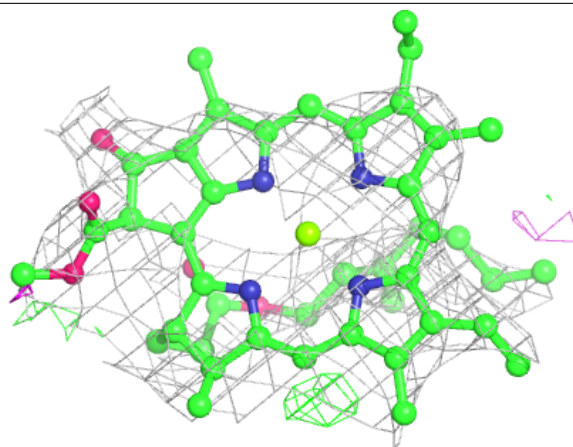
Electron density around CLA 2 1202:

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



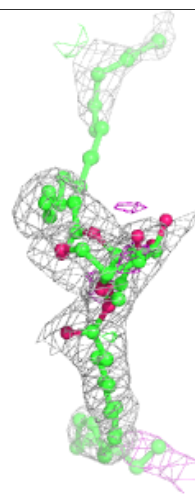
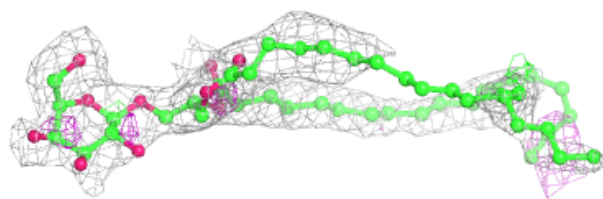
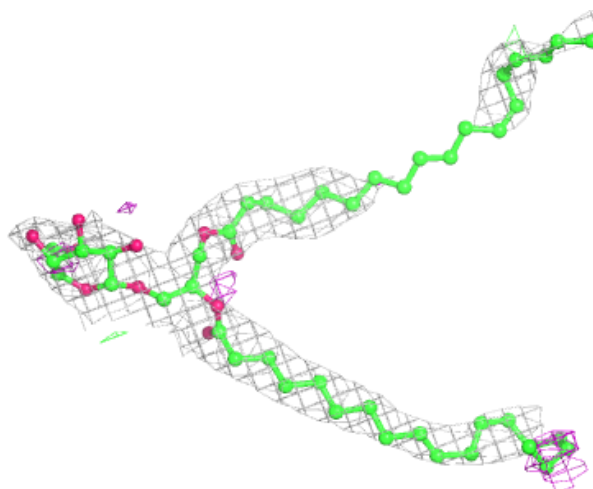
Electron density around CLA 2 1235:

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



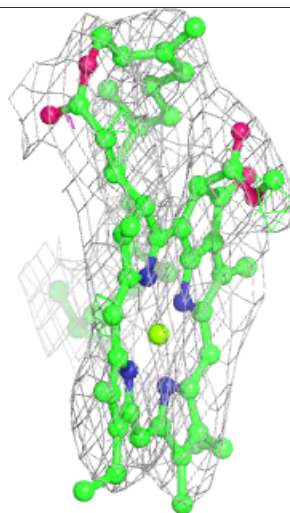
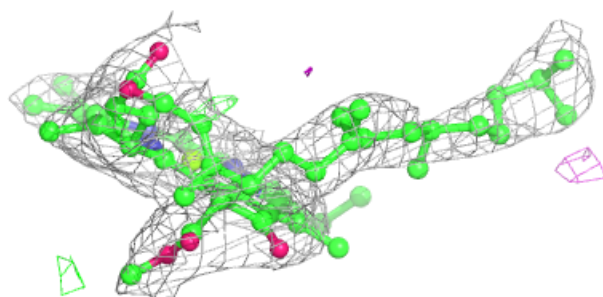
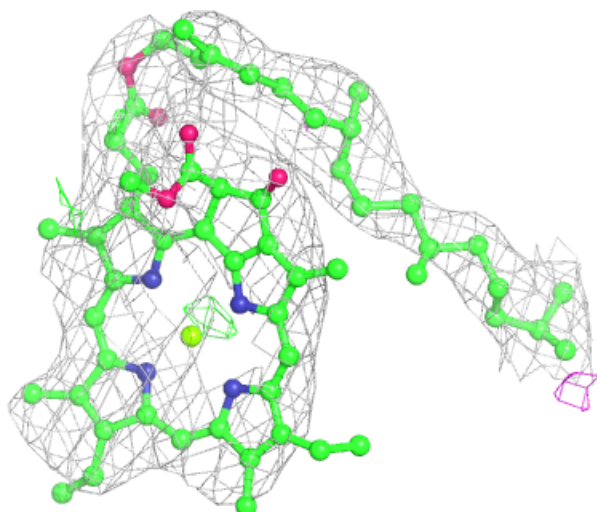
Electron density around LMG 0 5001:

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



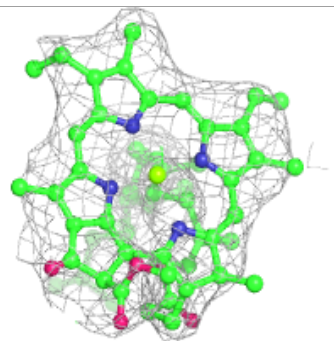
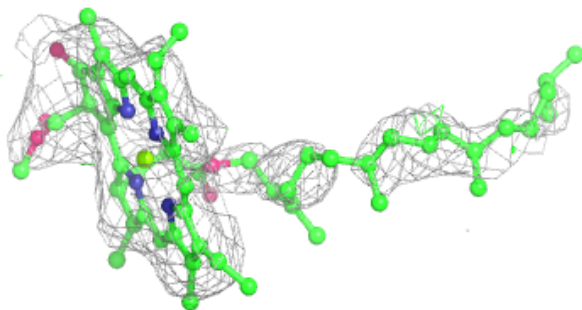
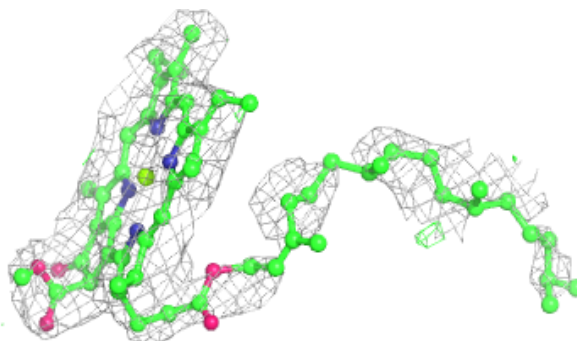
Electron density around CLA a 1123:

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

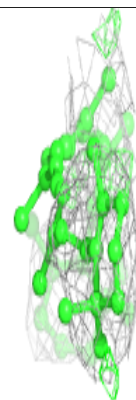
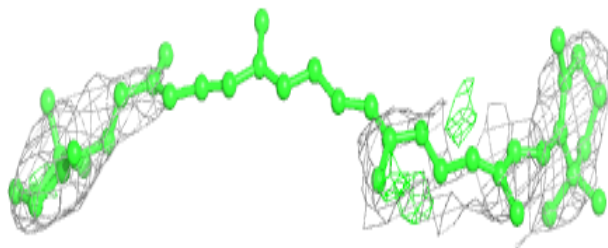
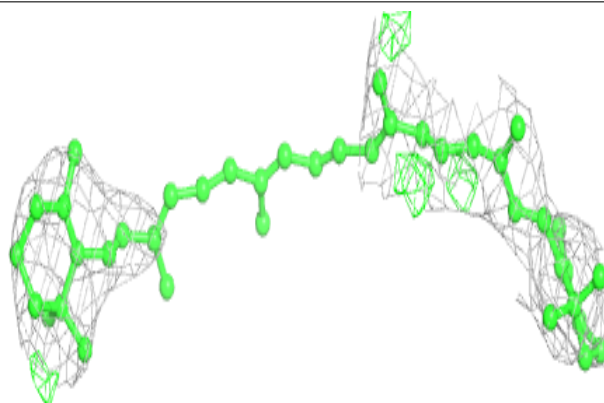


Electron density around CLA 1 1120:

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

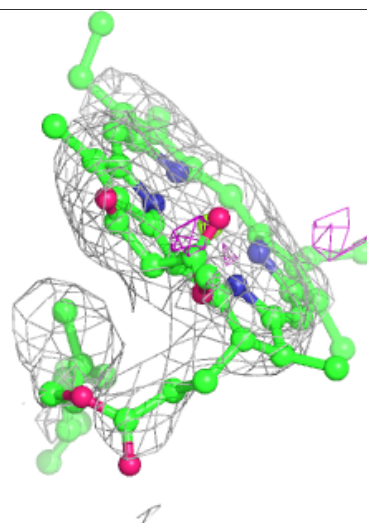
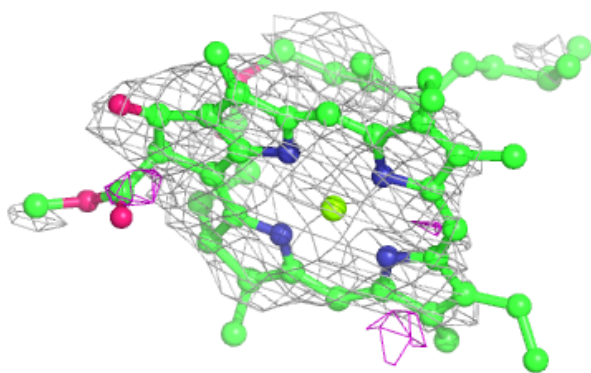
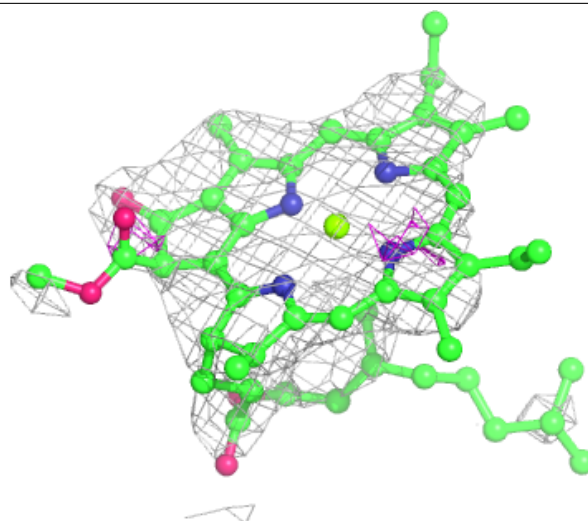
**Electron density around BCR 2 4014:**

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



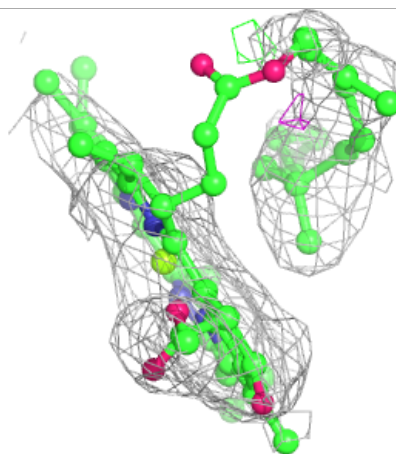
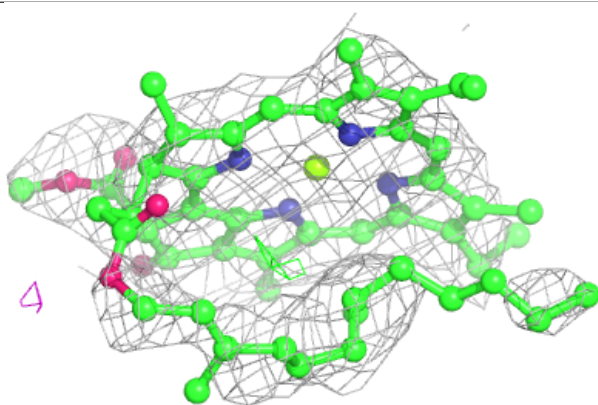
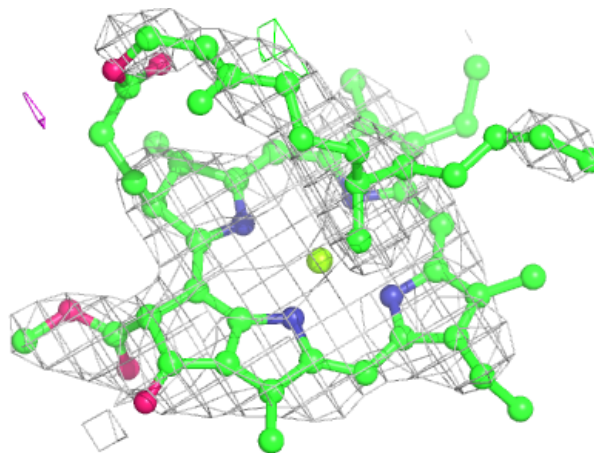
Electron density around CLA j 1303:

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



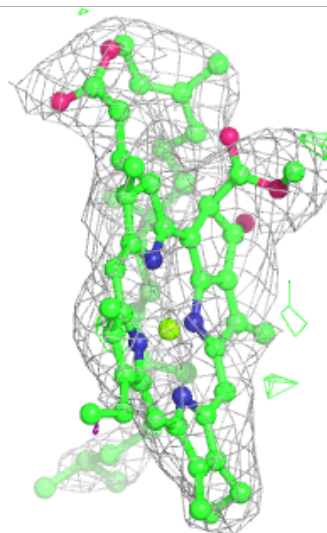
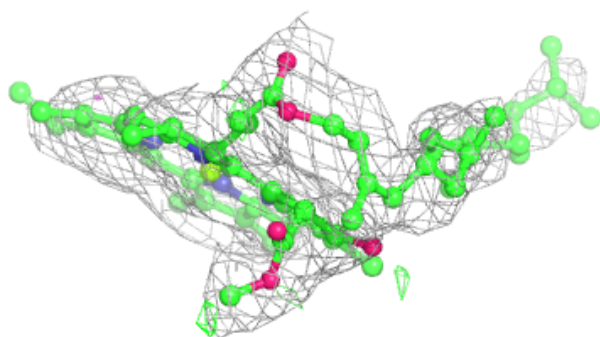
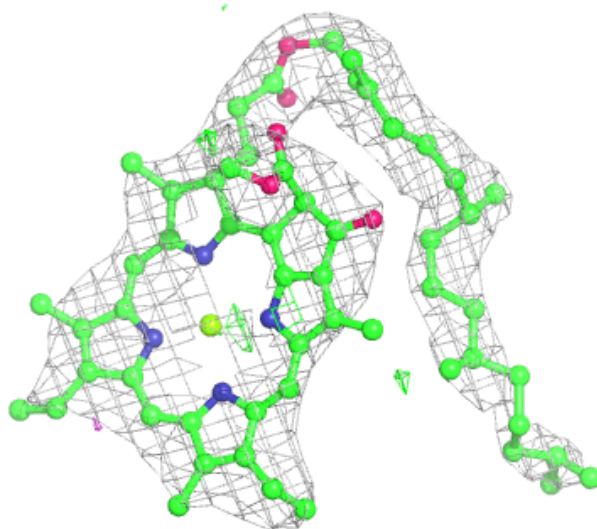
Electron density around CLA 2 1214:

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



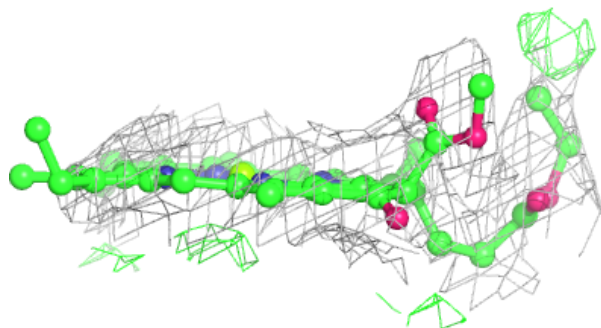
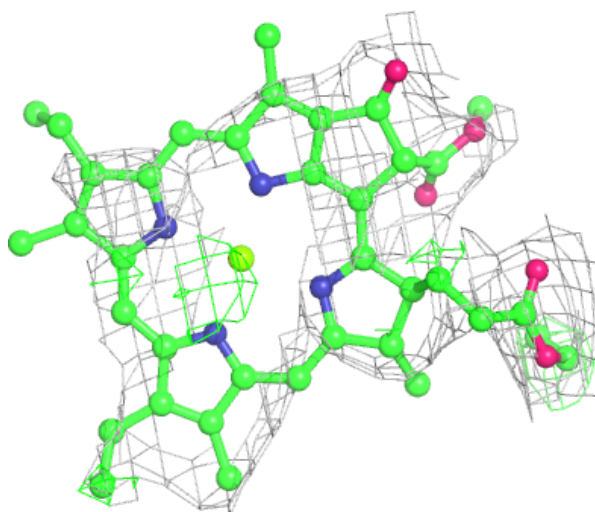
Electron density around CLA 1 1123:

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



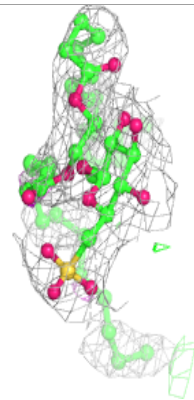
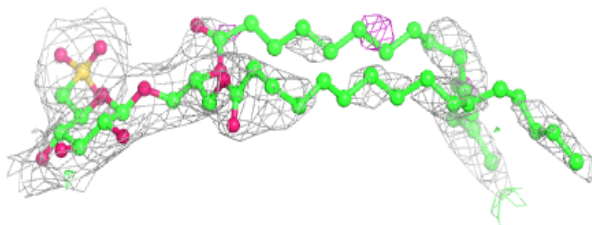
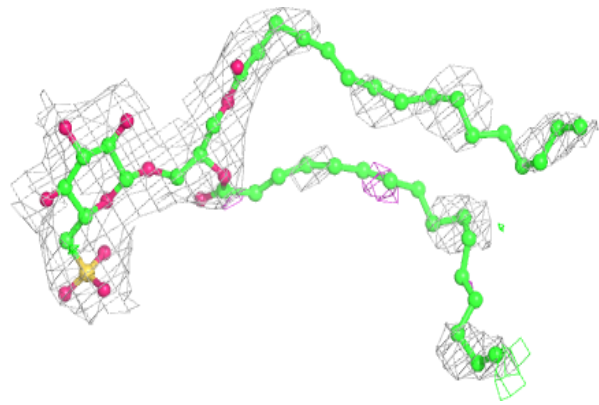
Electron density around CLA 6 1301:

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

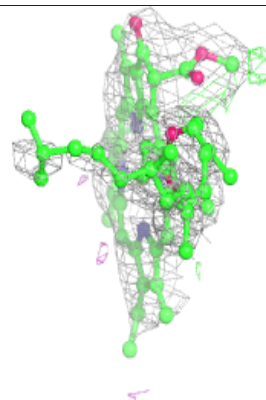
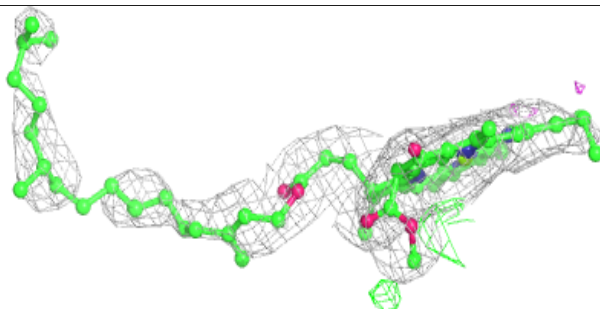
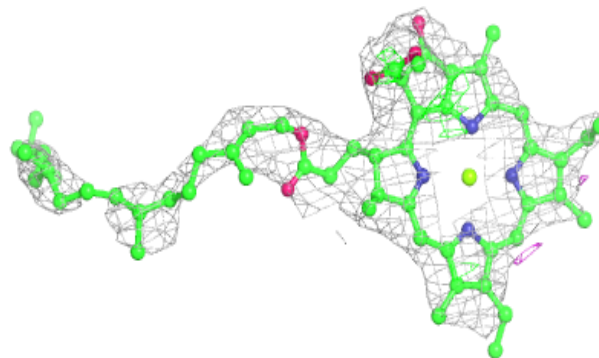


Electron density around SQD B 5008:

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

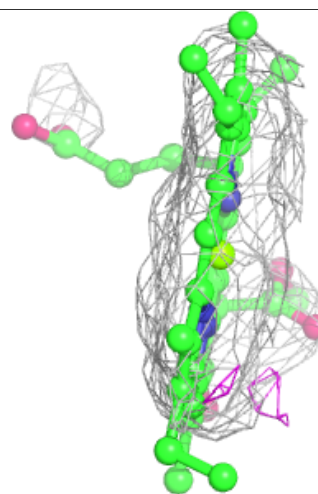
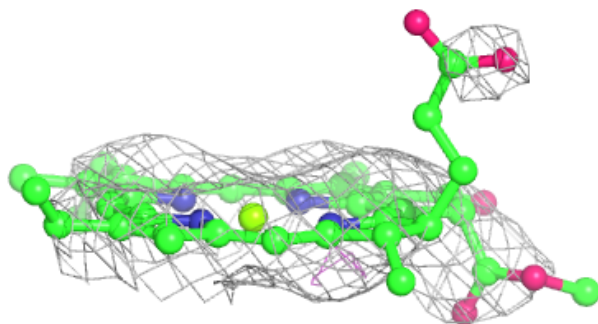
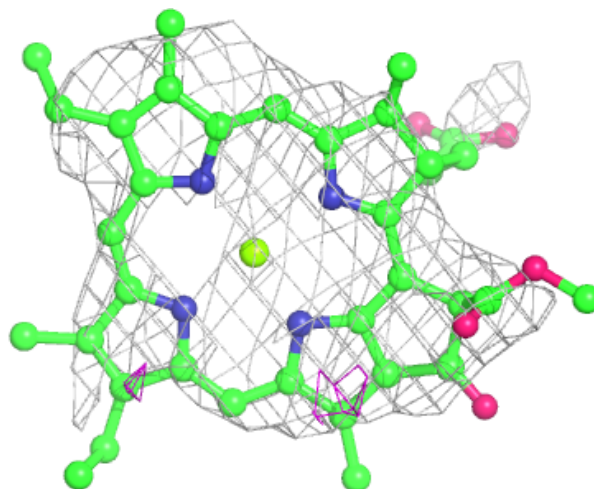
**Electron density around CLA 1 1103:**

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



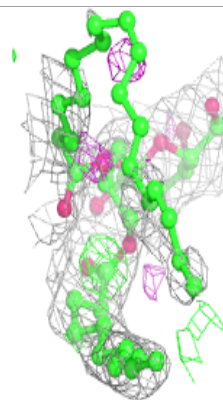
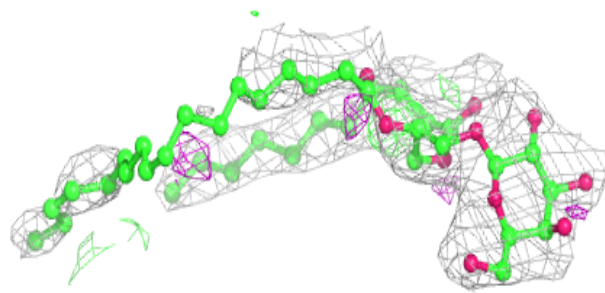
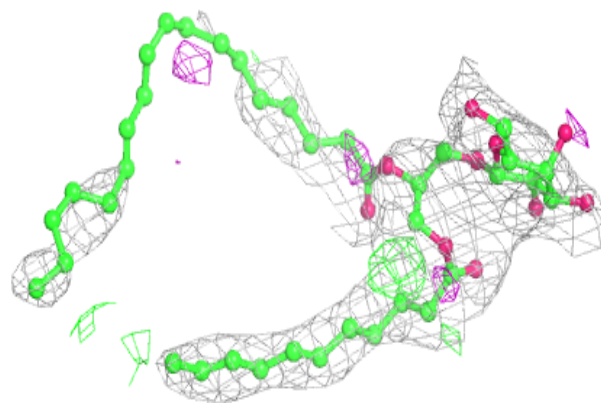
Electron density around CLA 1 1114:

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



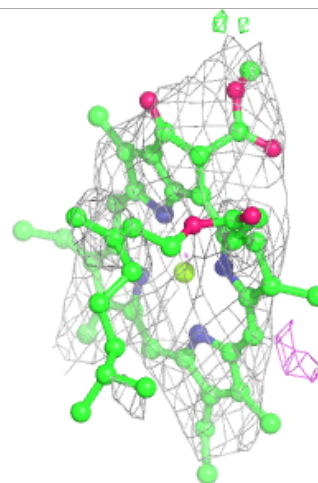
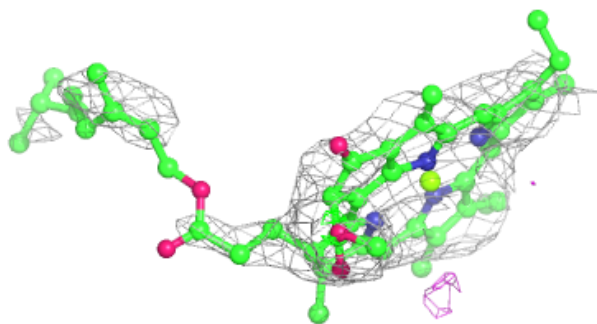
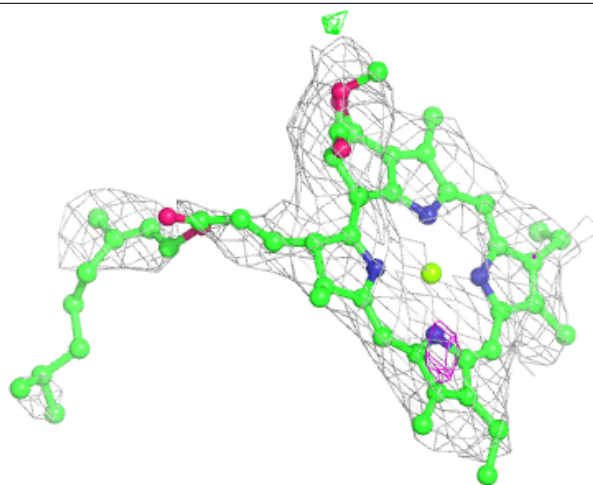
Electron density around LMG A 5004:

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



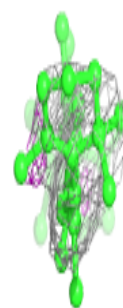
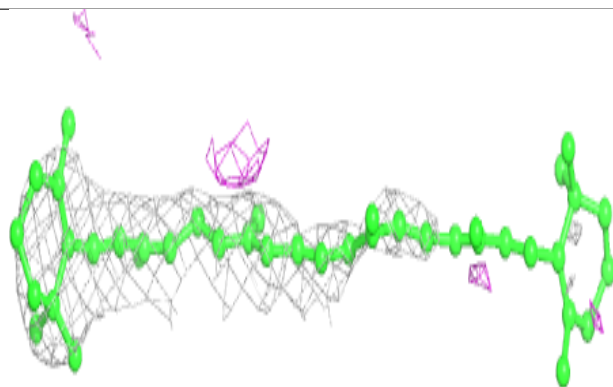
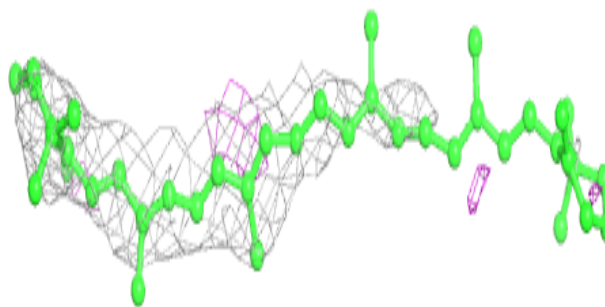
Electron density around CLA a 1801:

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

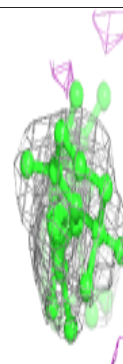
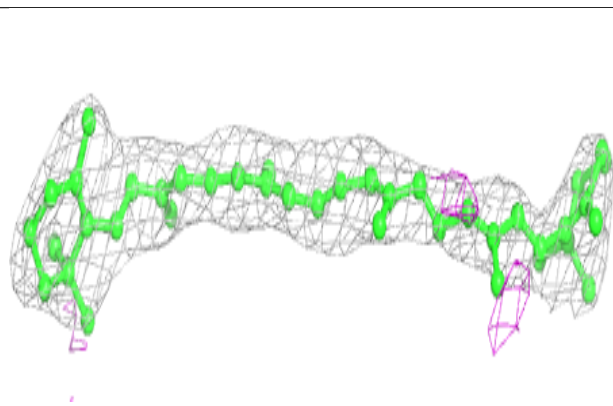
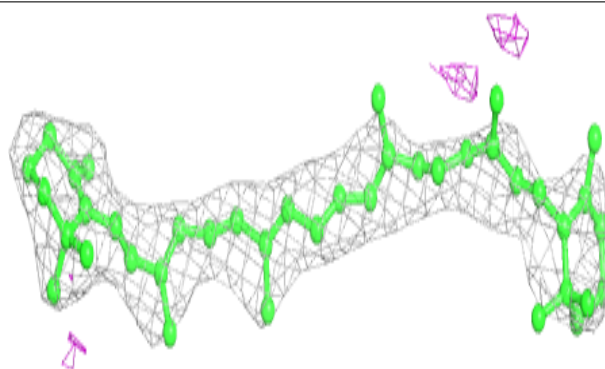


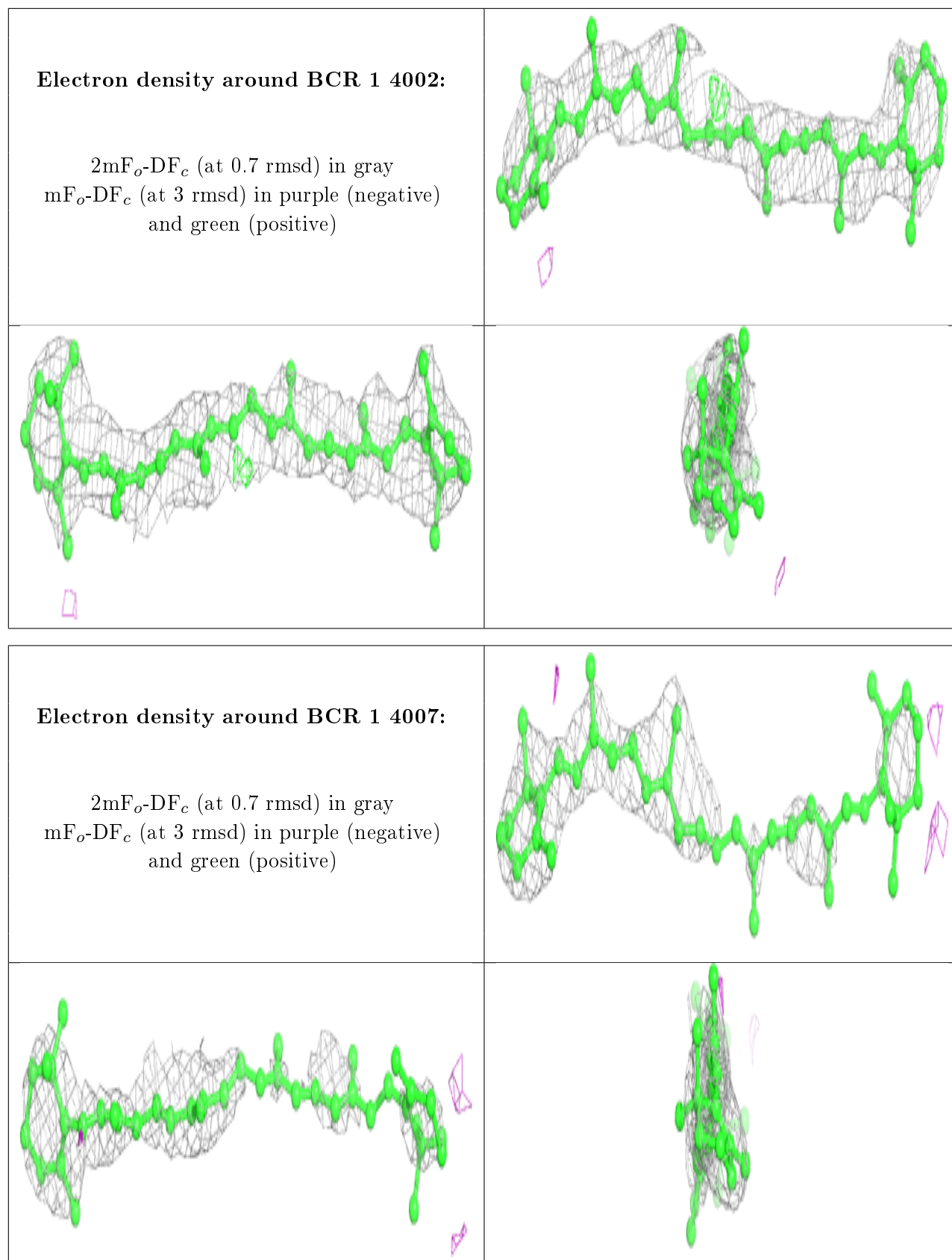
Electron density around BCR a 4007:

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

**Electron density around BCR A 4003:**

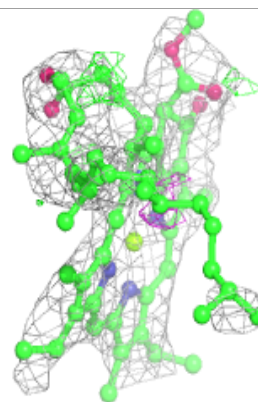
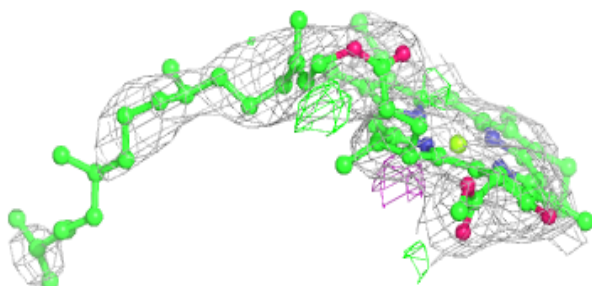
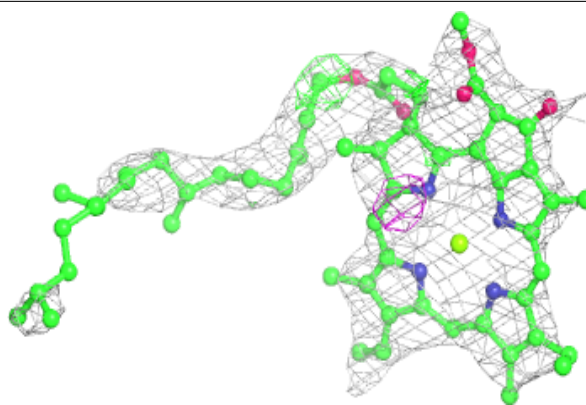
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



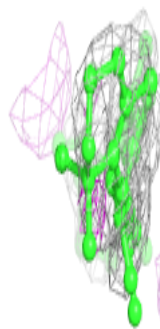
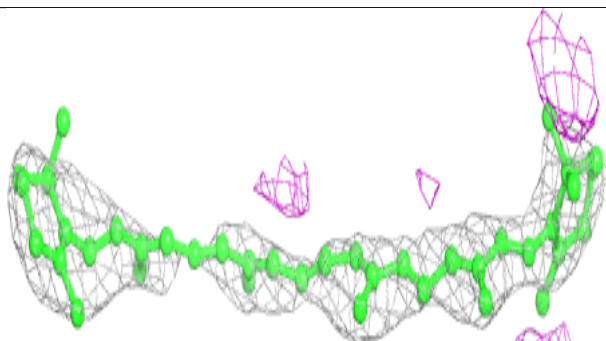
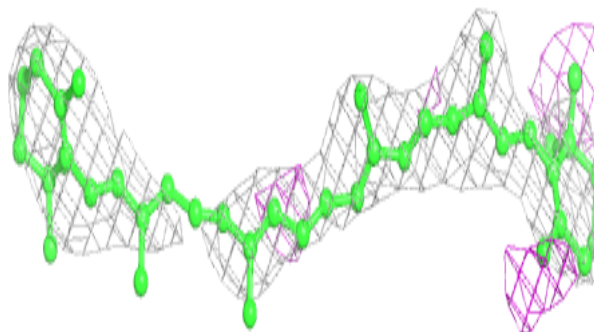


Electron density around CLA 1 1013:

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

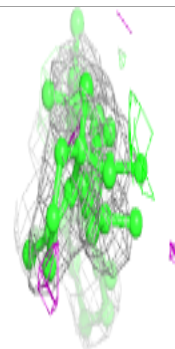
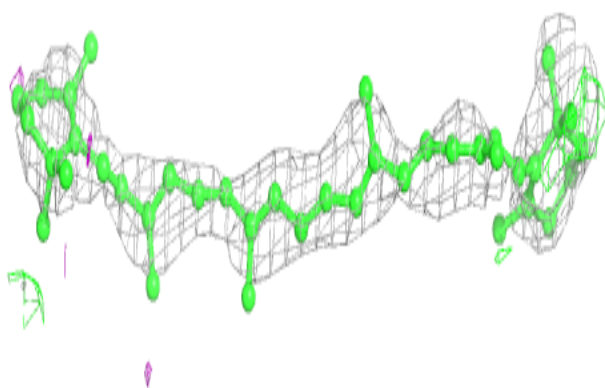
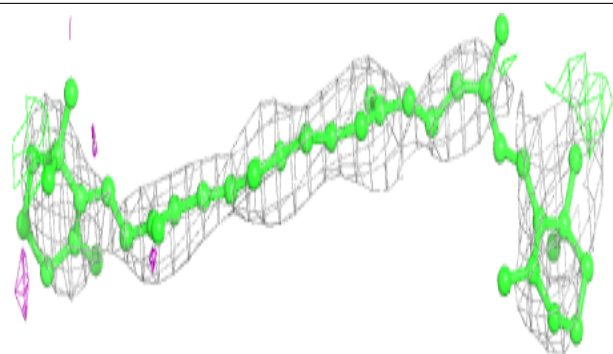
**Electron density around BCR a 4008:**

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

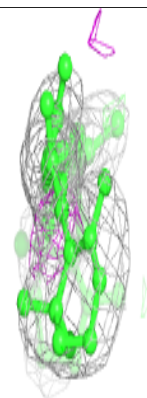
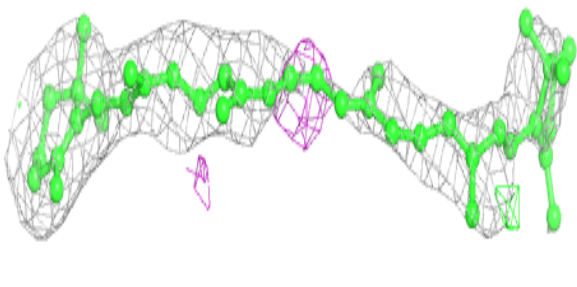
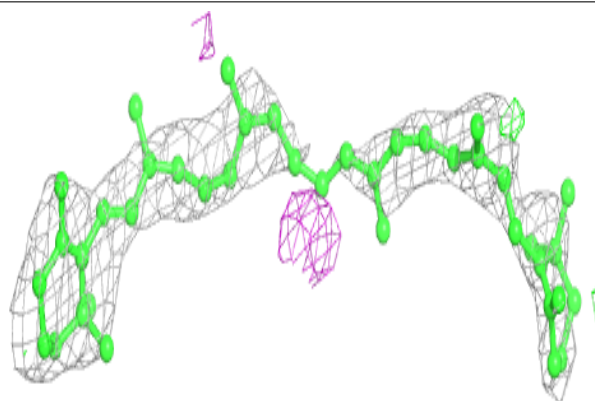


Electron density around BCR 1 4022:

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

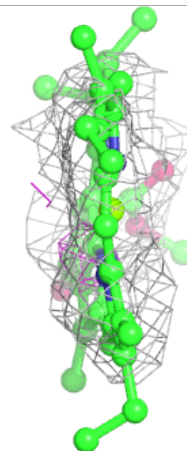
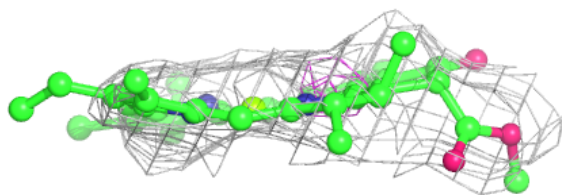
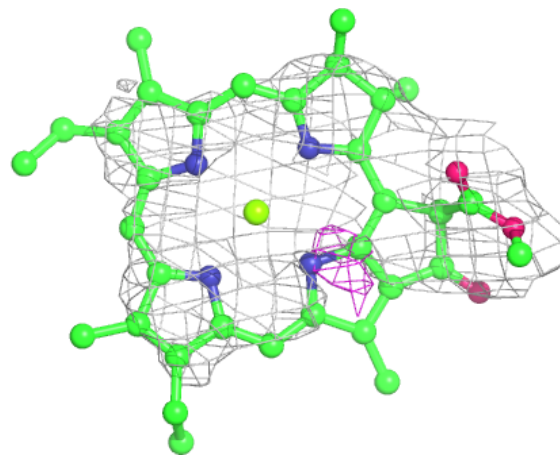
**Electron density around BCR 9 4021:**

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



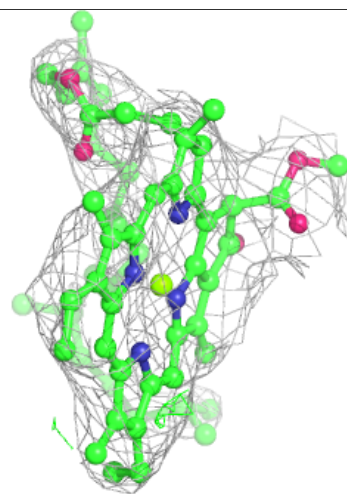
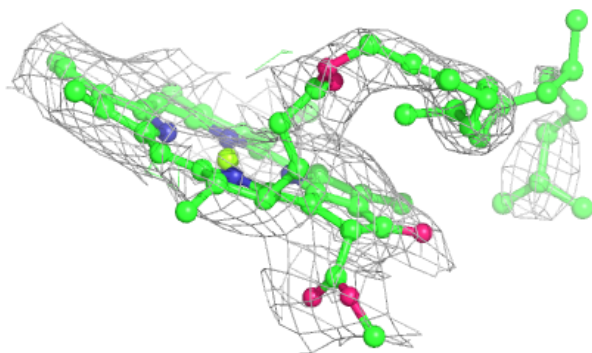
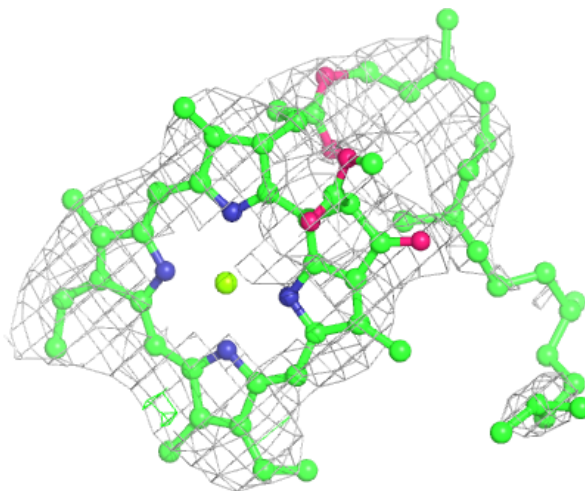
Electron density around CLA 7 1302:

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



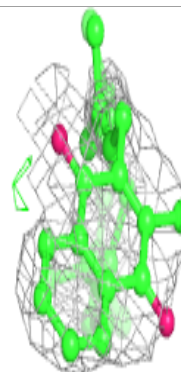
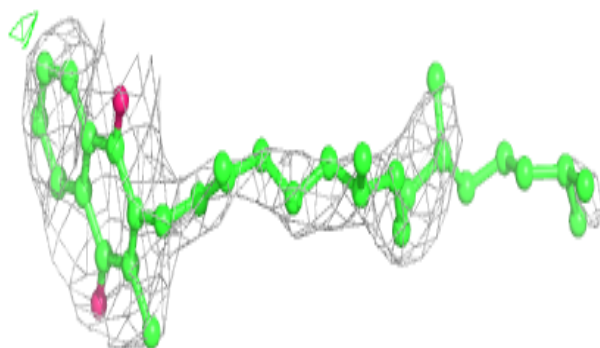
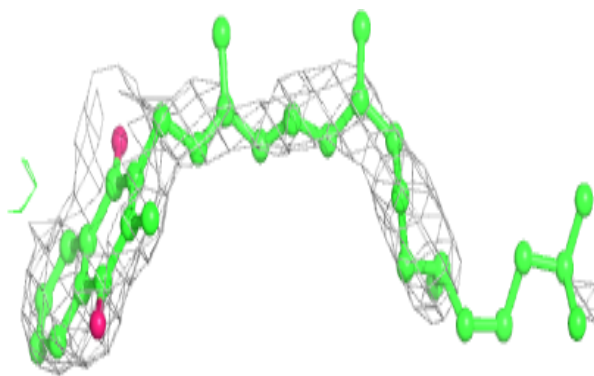
Electron density around CLA 2 1229:

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

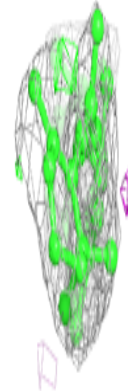
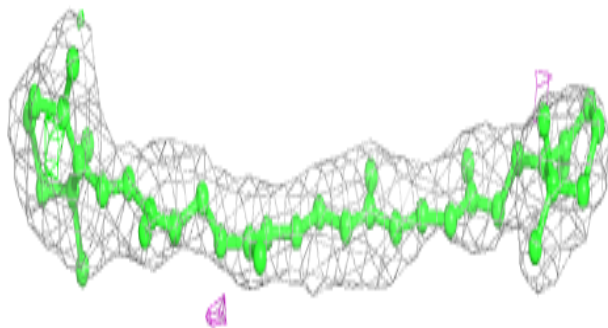
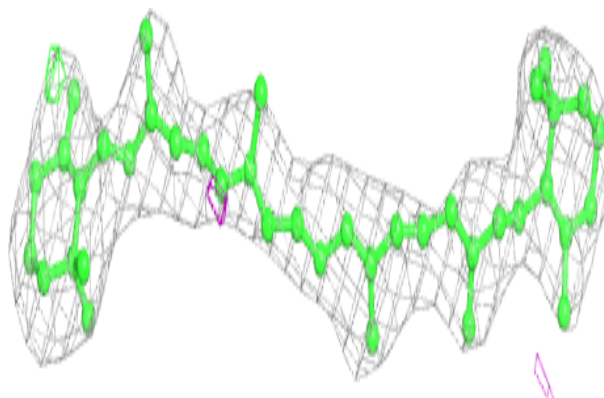


Electron density around PQN 1 2001:

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

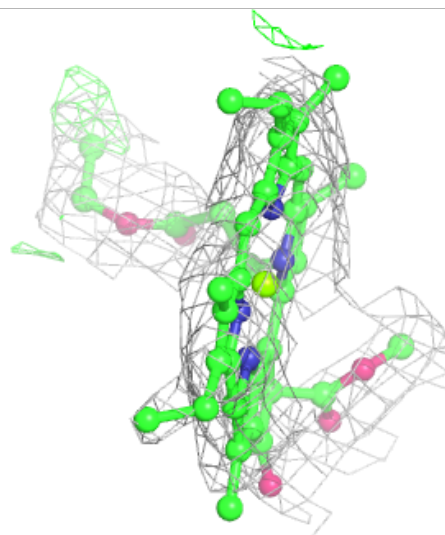
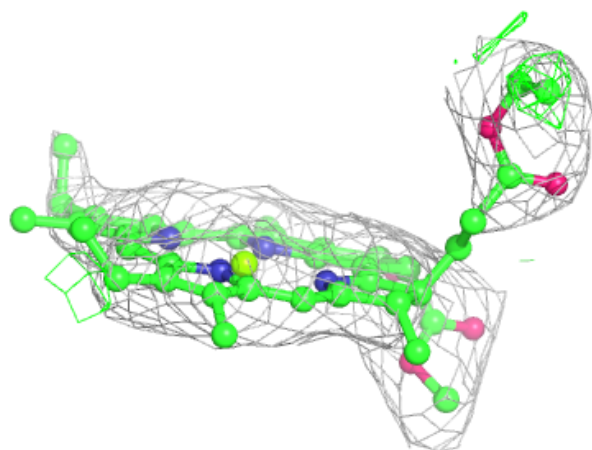
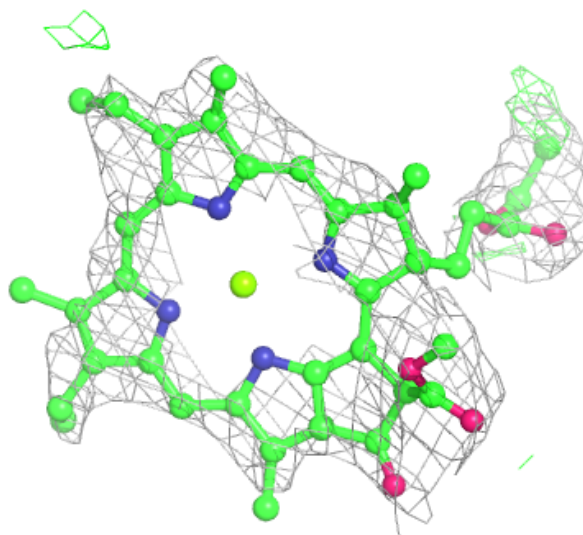
**Electron density around BCR b 4004:**

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



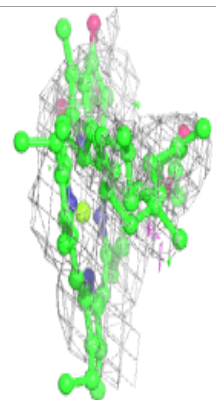
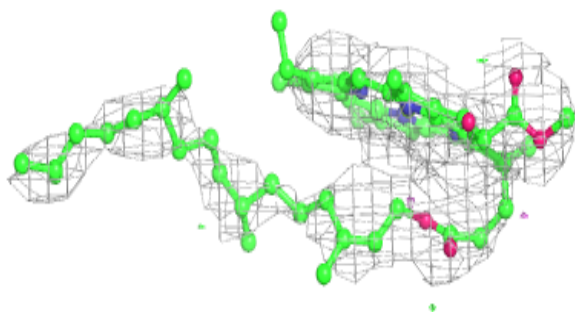
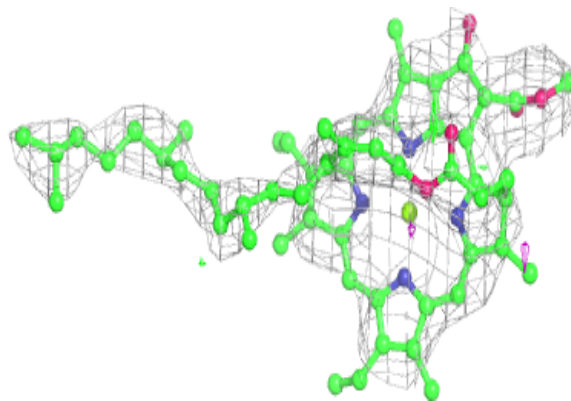
Electron density around CLA 2 1230:

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

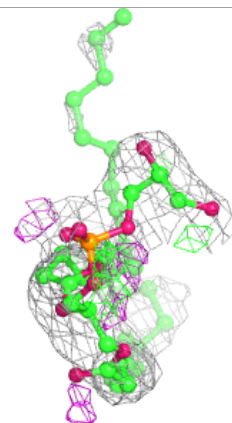
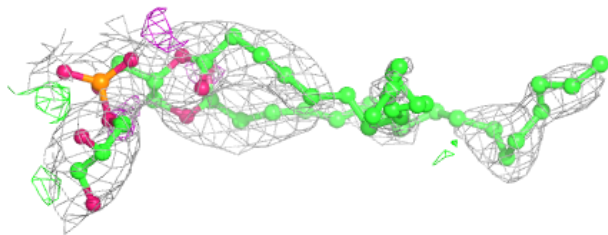
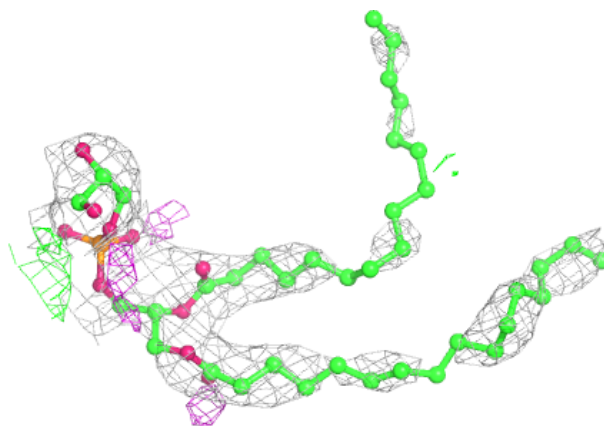


Electron density around CLA 1 1115:

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

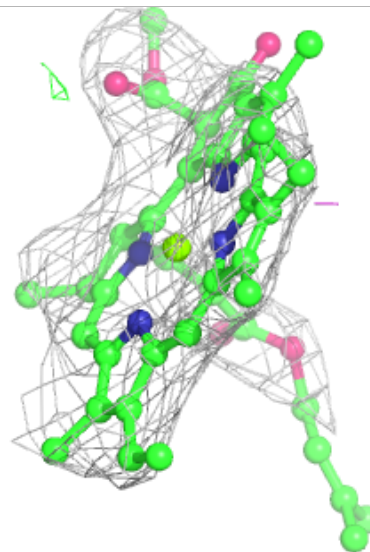
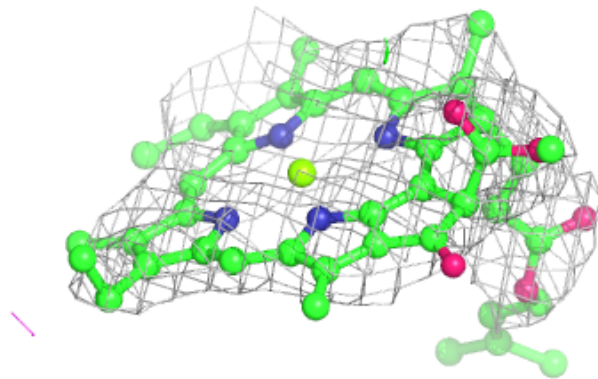
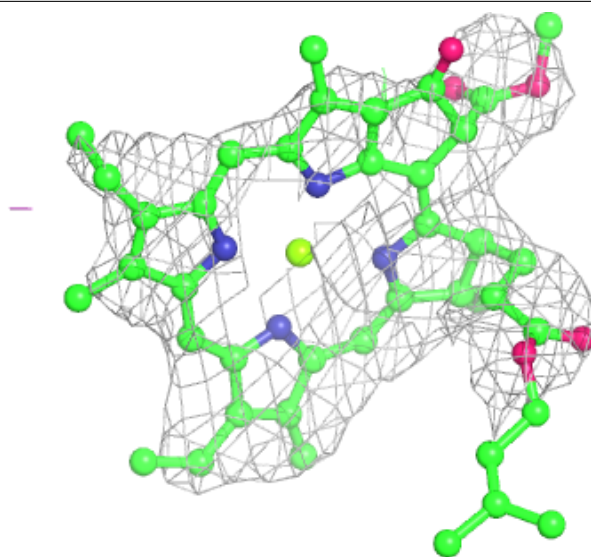
**Electron density around LHG B 5004:**

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



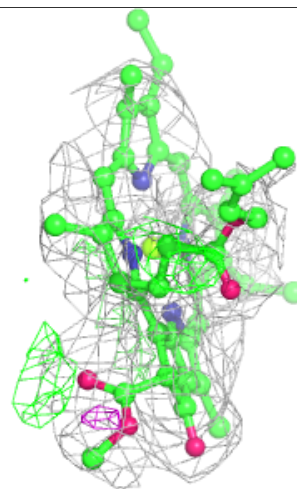
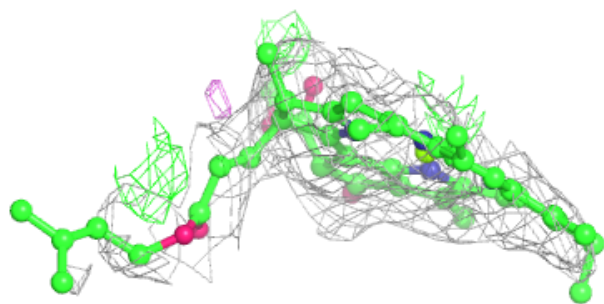
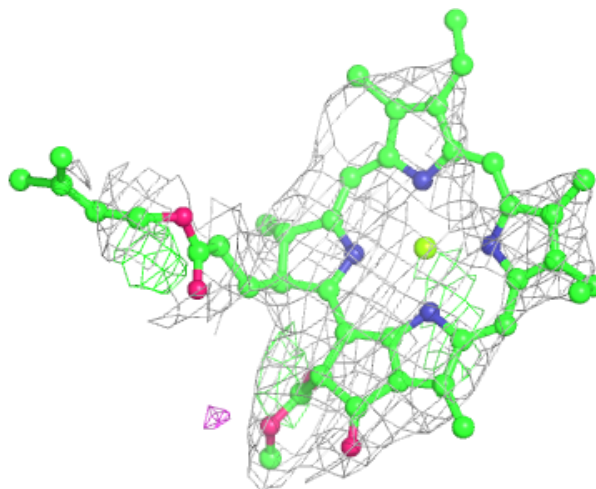
Electron density around CLA B 1232:

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



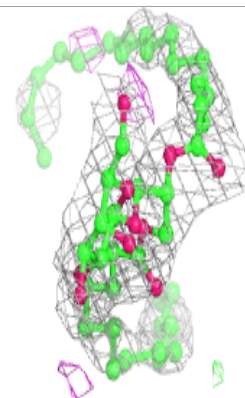
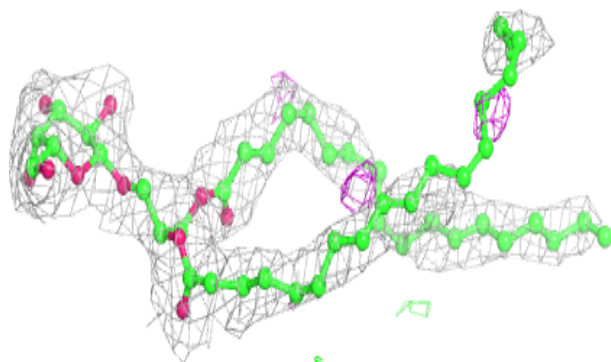
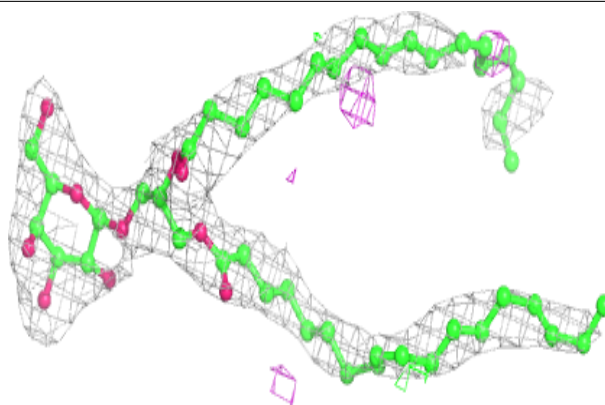
Electron density around CLA 2 1222:

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

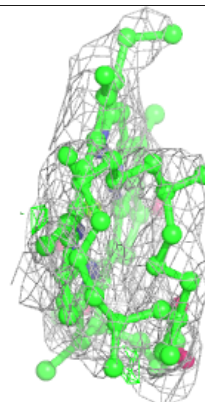
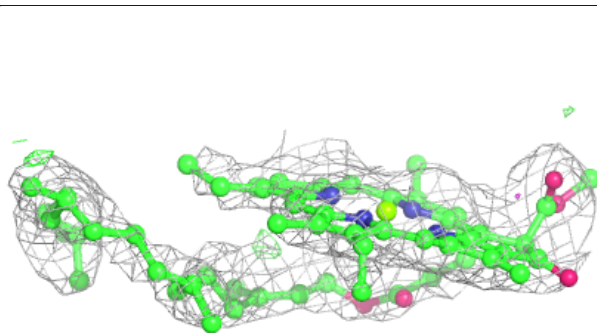
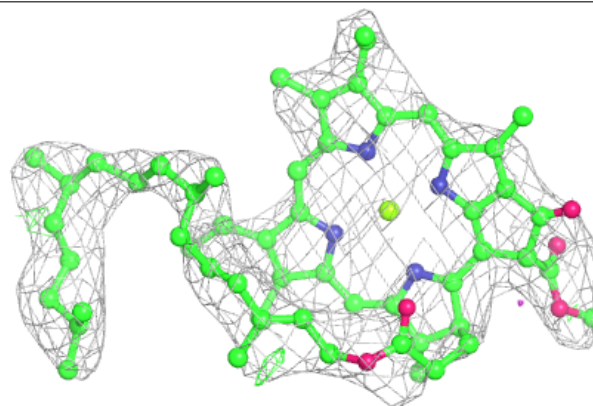


Electron density around LMG 2 5002:

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

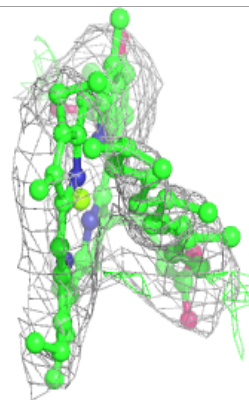
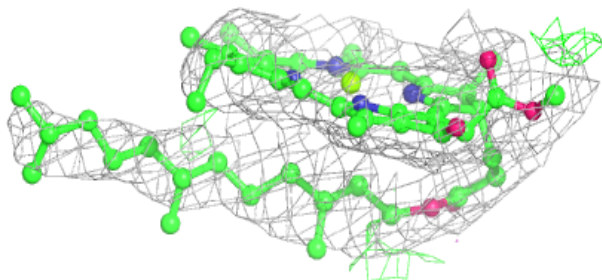
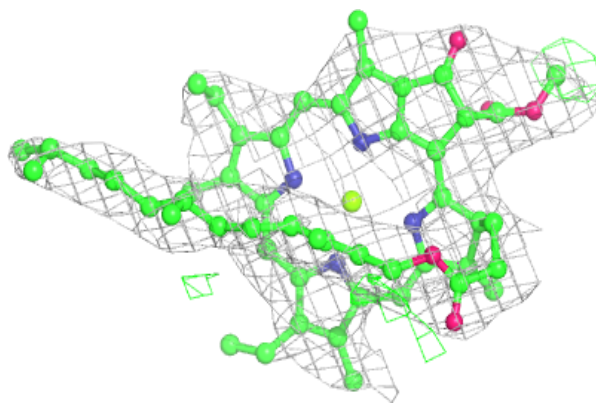
**Electron density around CLA 1 1117:**

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

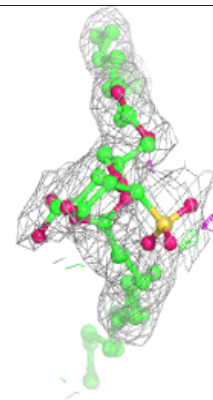
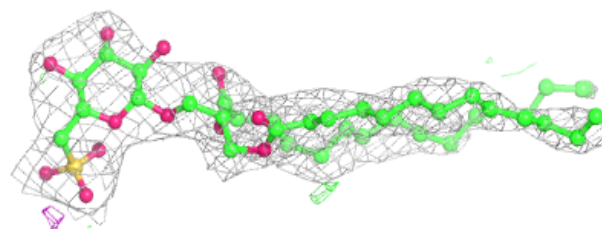
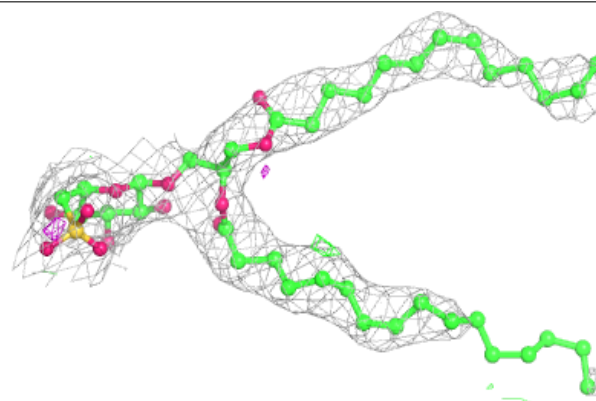


Electron density around CLA a 1116:

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

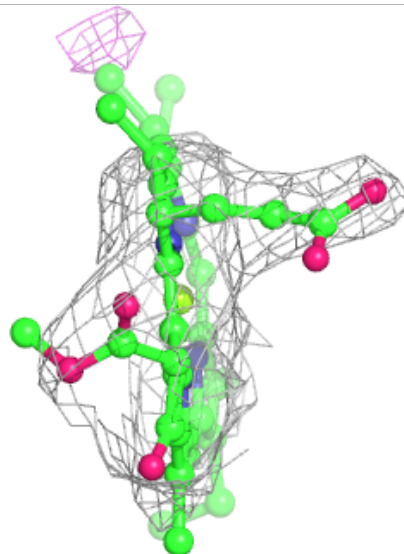
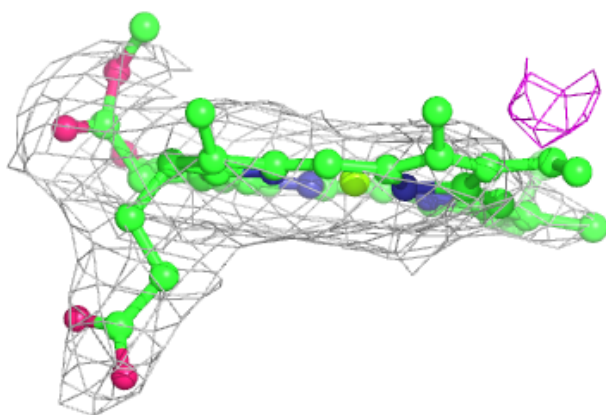
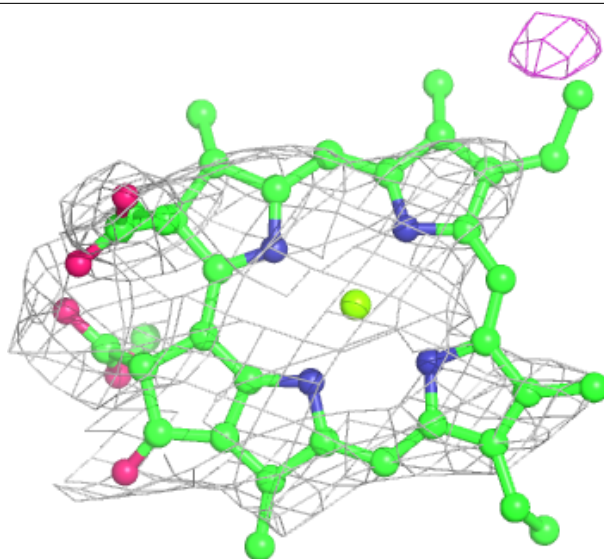
**Electron density around SQD L 5001:**

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



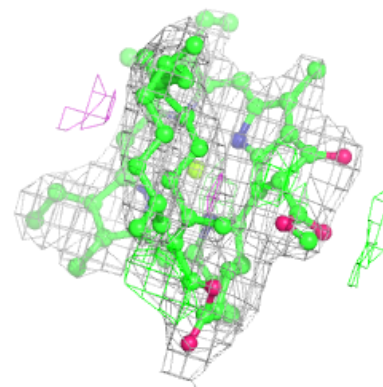
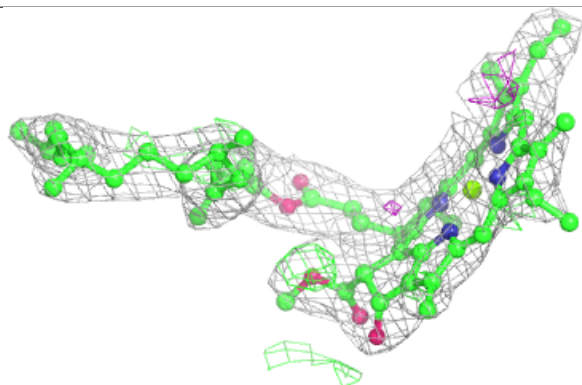
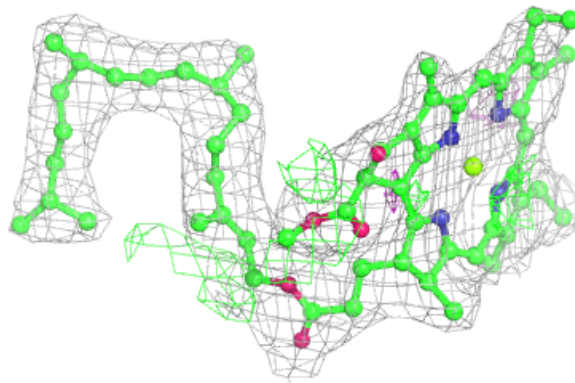
Electron density around CLA 2 1220:

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

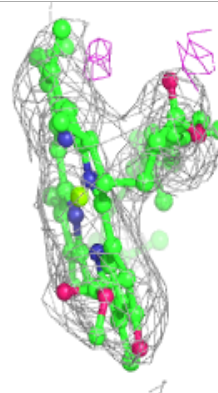
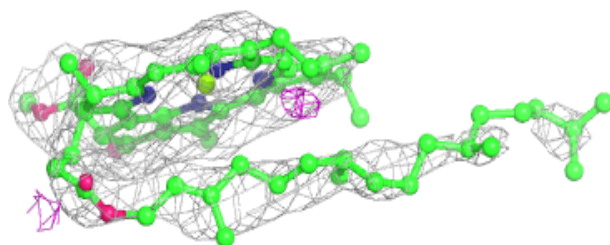
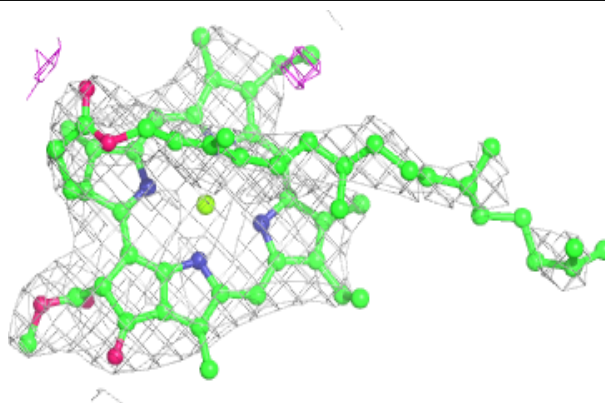


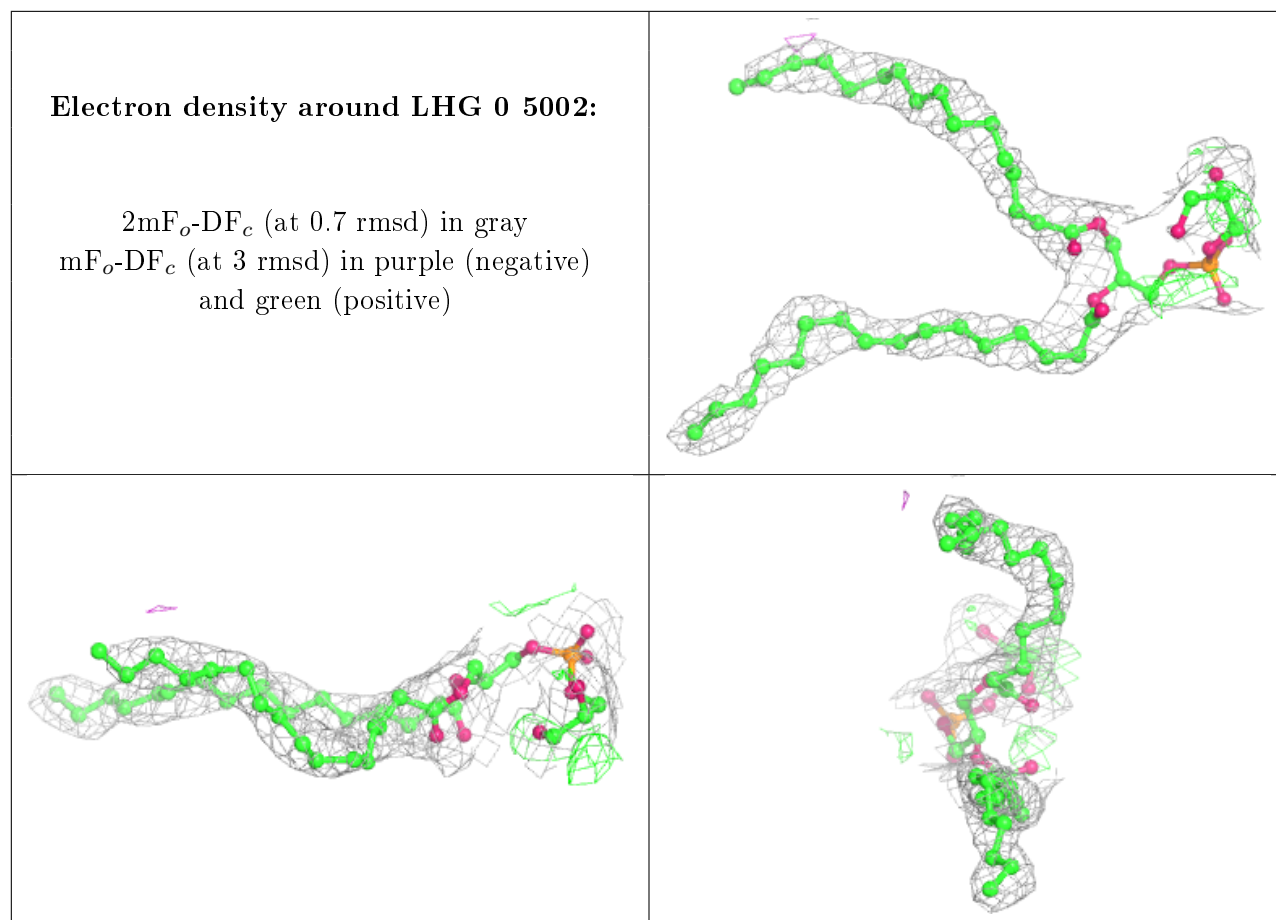
Electron density around CLA a 1011:

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

**Electron density around CLA 1 1116:**

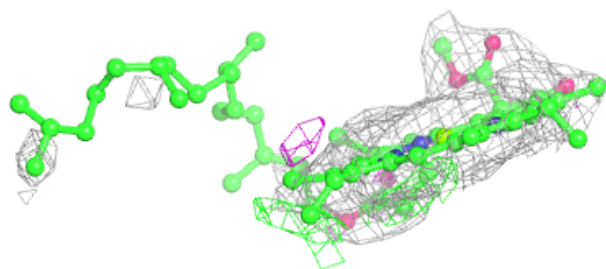
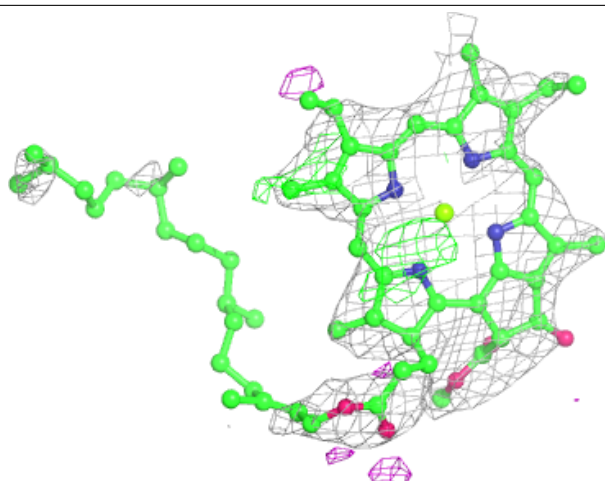
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





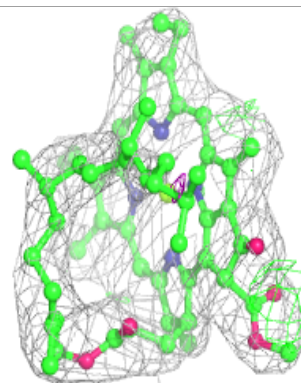
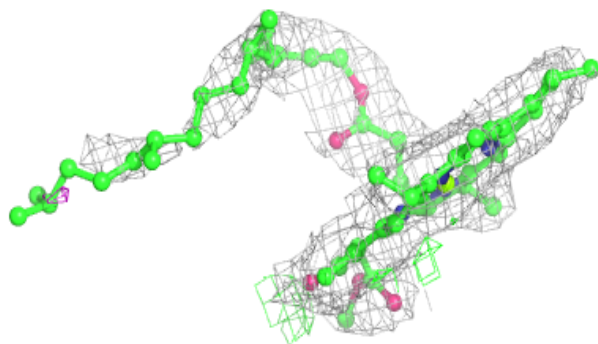
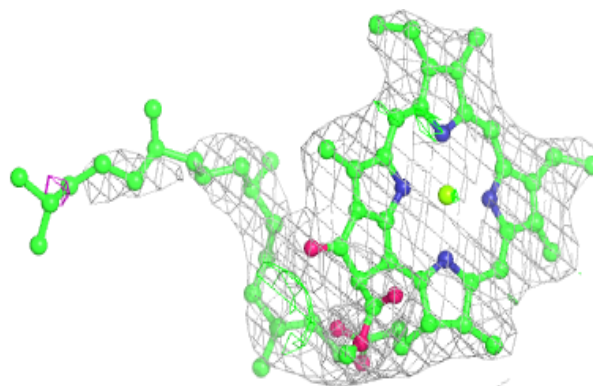
Electron density around CLA a 1111:

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

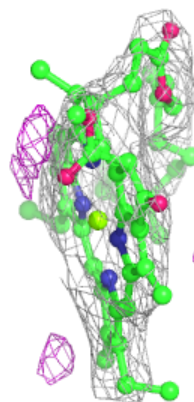
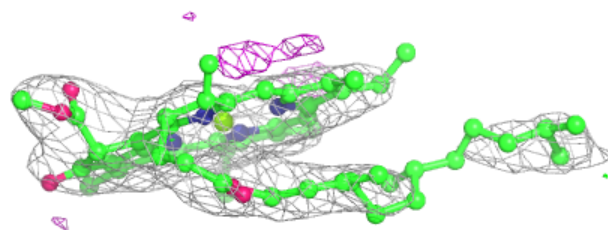
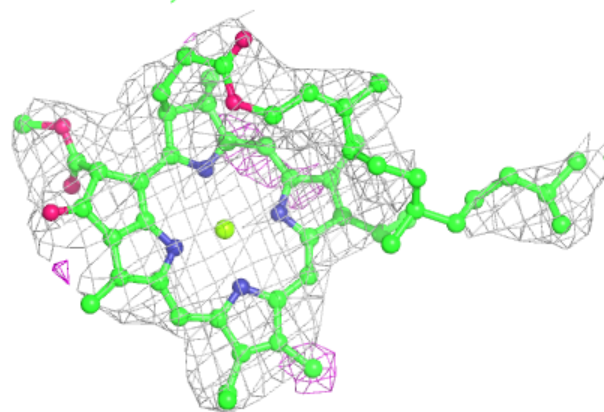


Electron density around CLA b 1231:

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

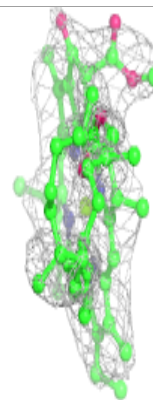
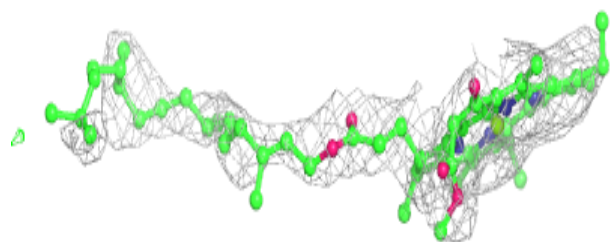
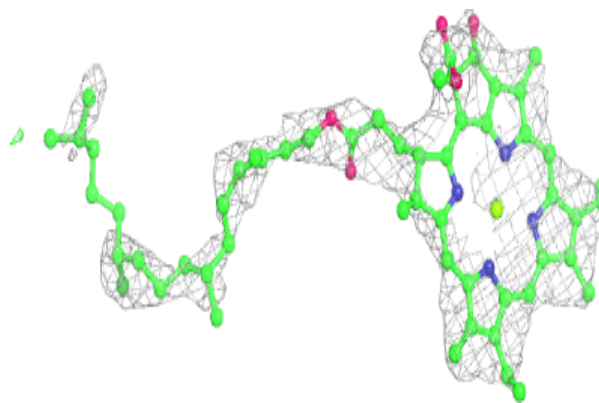
**Electron density around CLA 2 1215:**

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

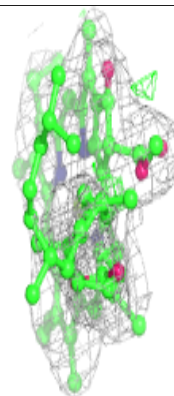
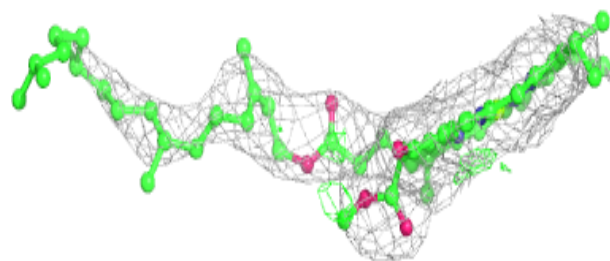
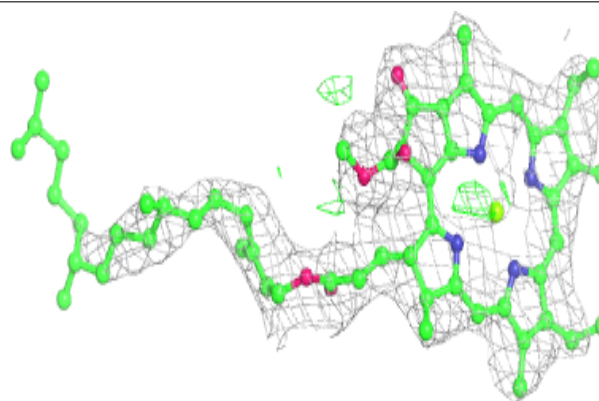


Electron density around CLA F 1302:

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

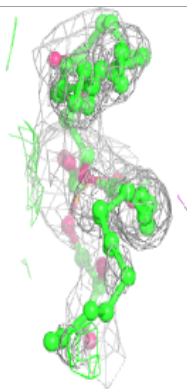
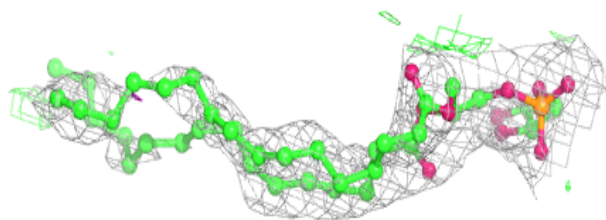
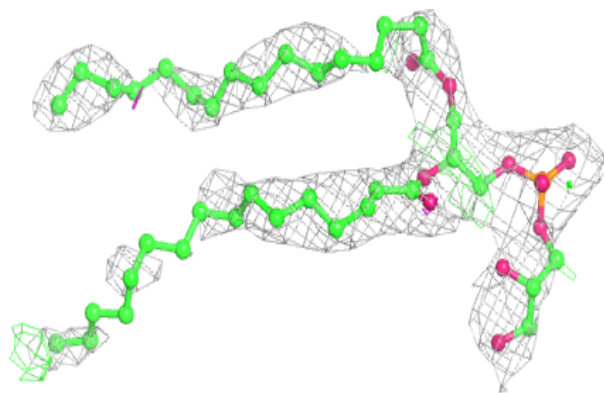
**Electron density around CLA a 1139:**

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

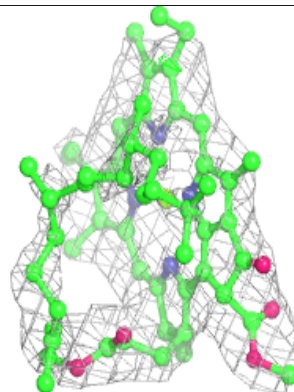
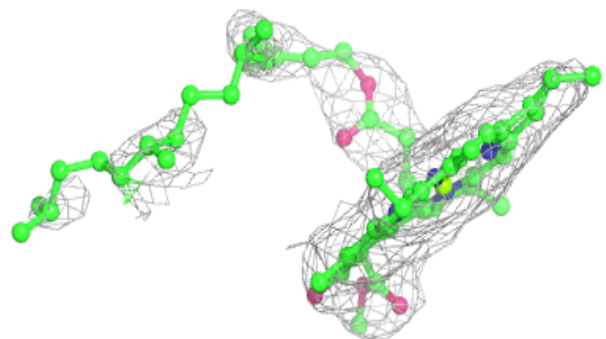
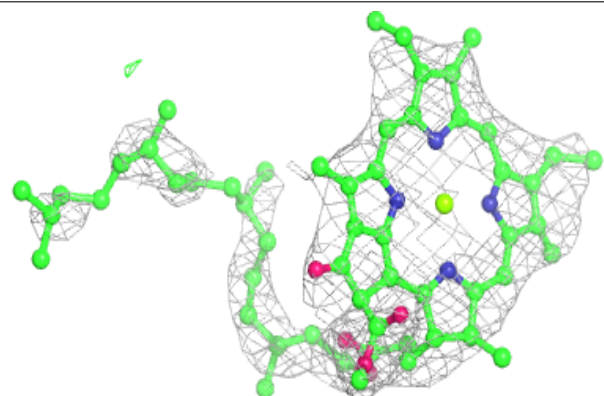


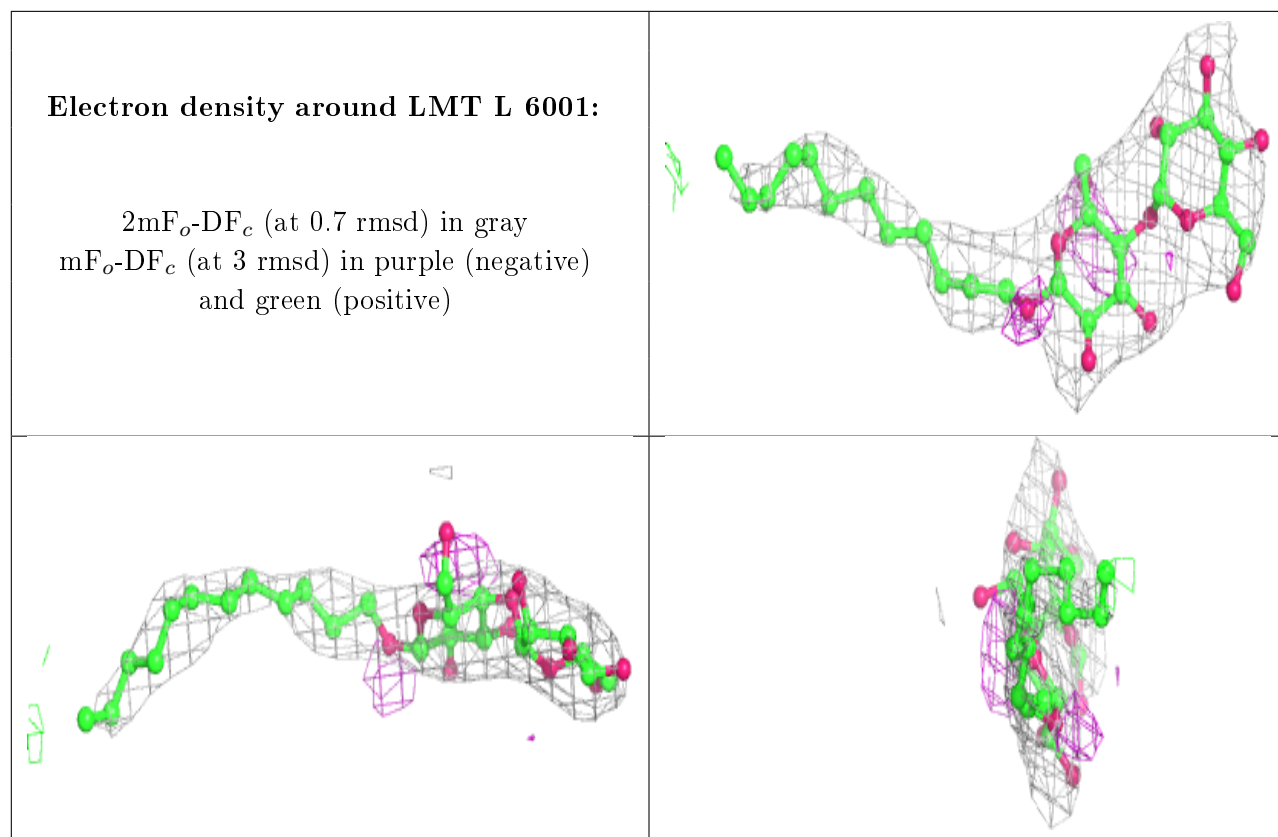
Electron density around LHG L 5005:

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

**Electron density around CLA B 1231:**

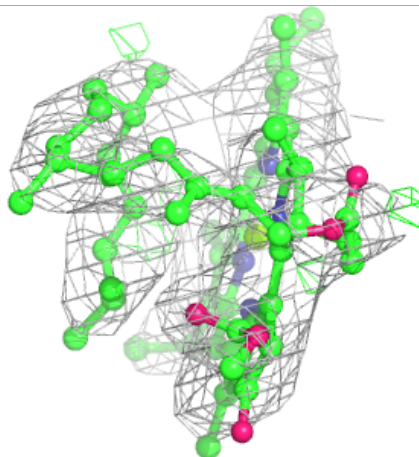
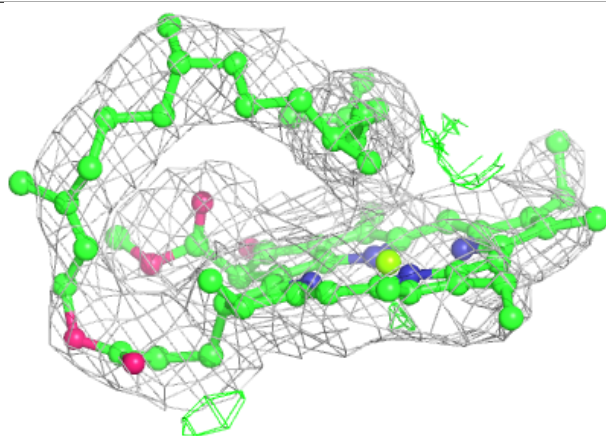
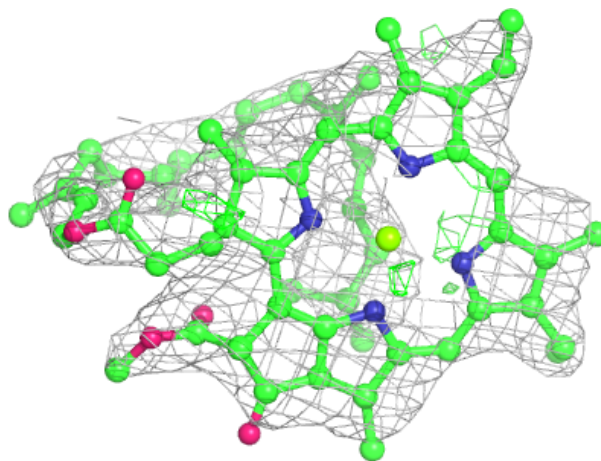
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





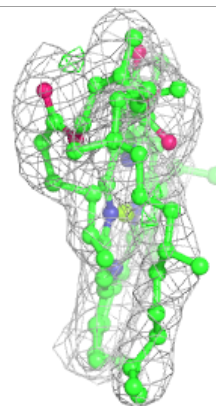
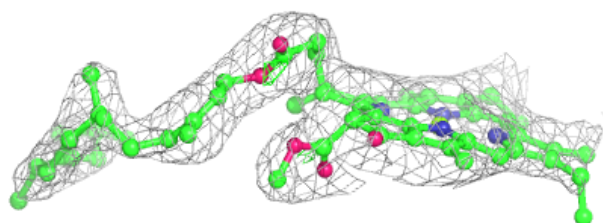
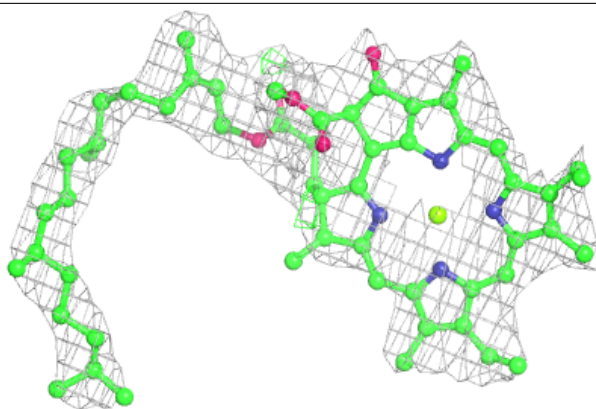
Electron density around CLA 1 1104:

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

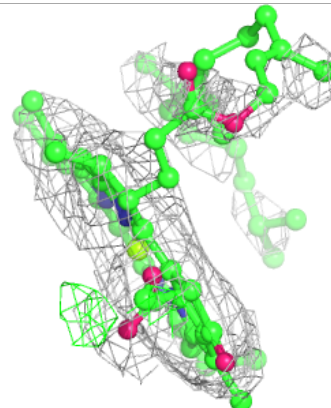
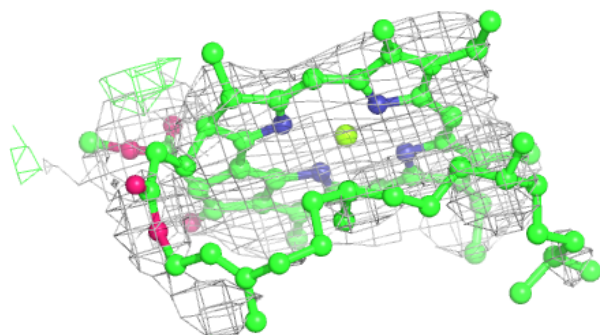
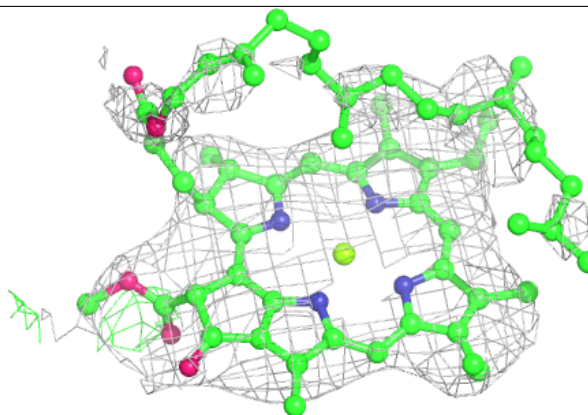


Electron density around CLA a 1101:

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

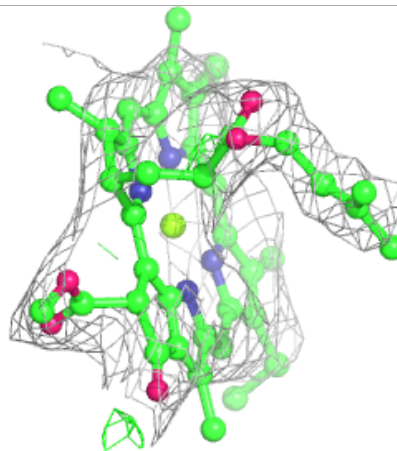
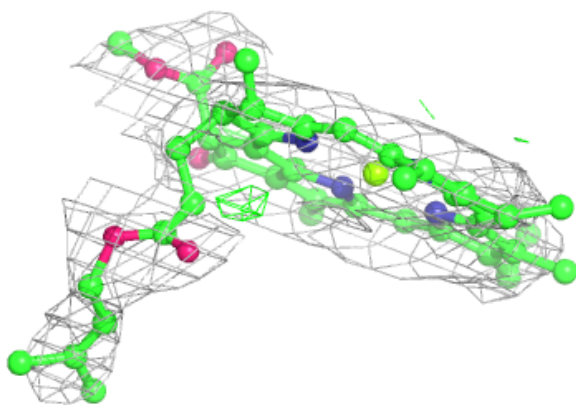
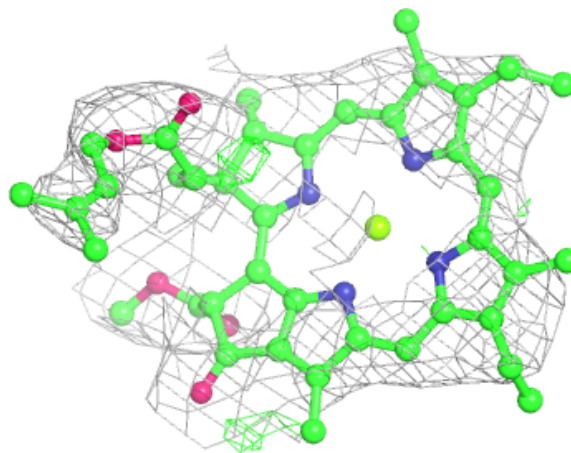
**Electron density around CLA 1 1118:**

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



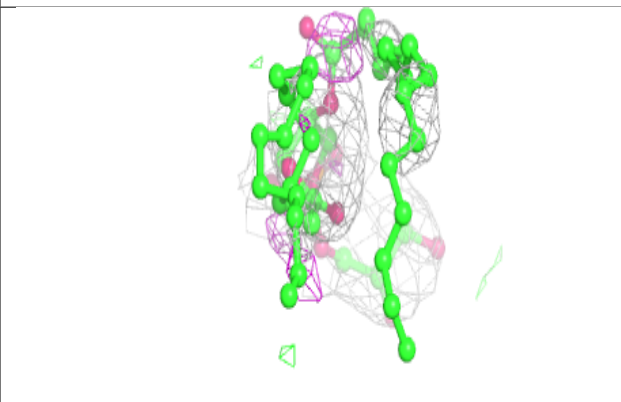
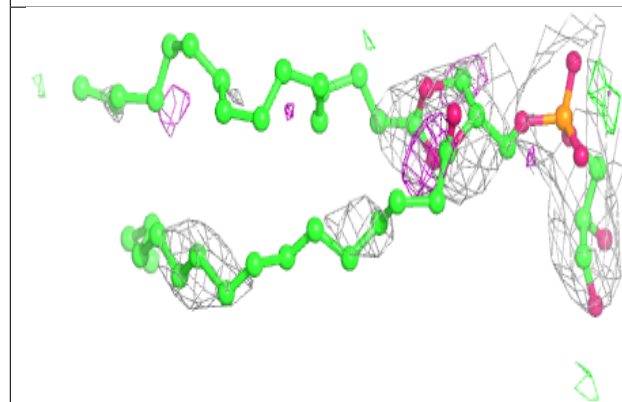
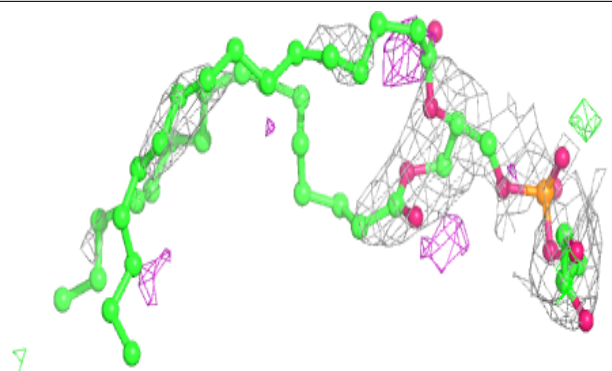
Electron density around CLA 2 1236:

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

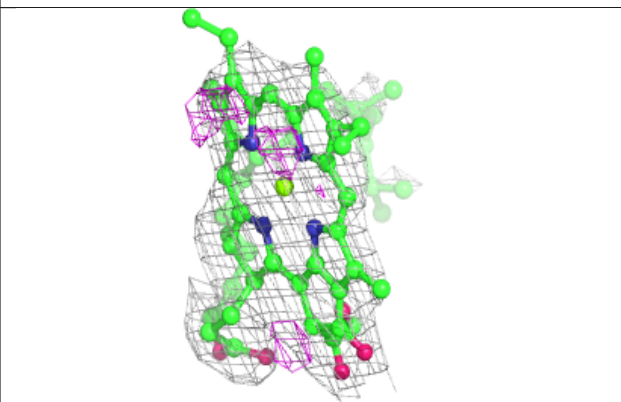
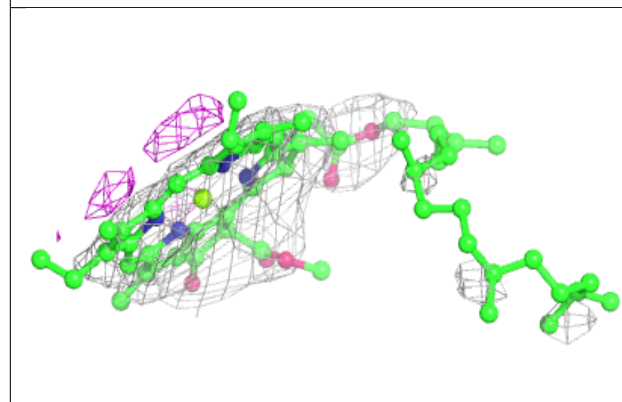
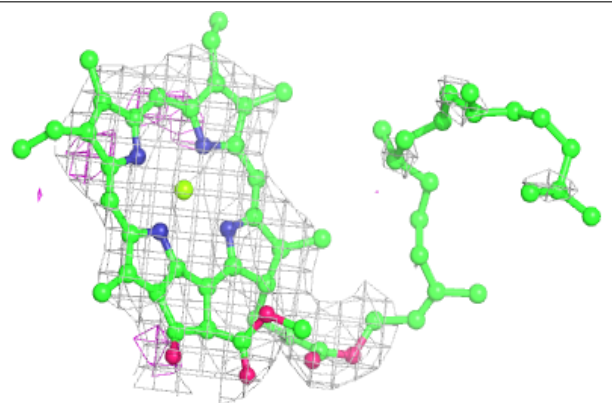


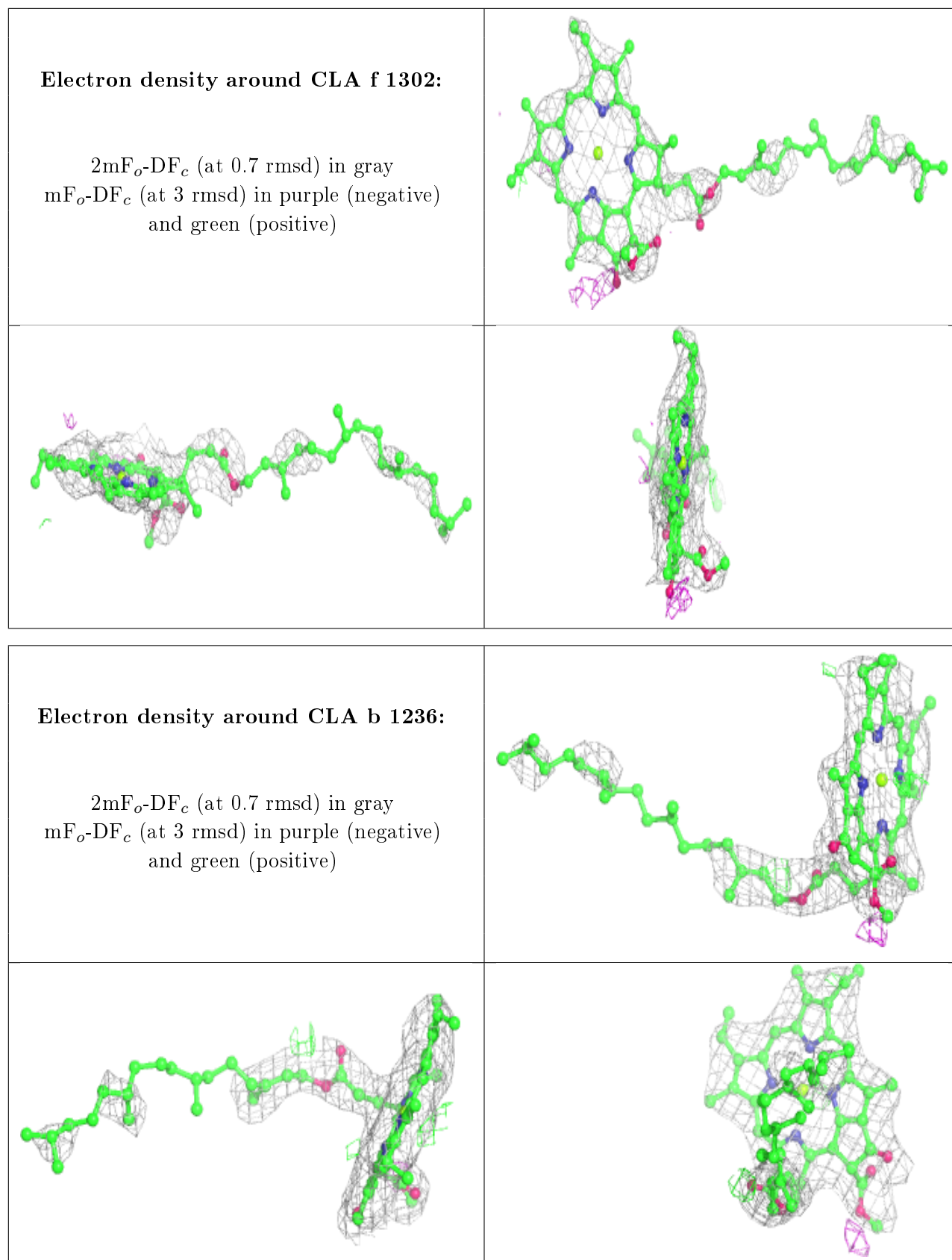
Electron density around LHG a 5003:

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

**Electron density around CLA 2 1221:**

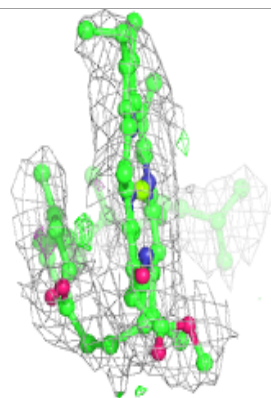
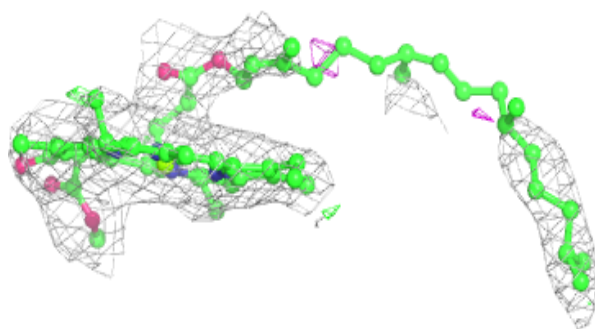
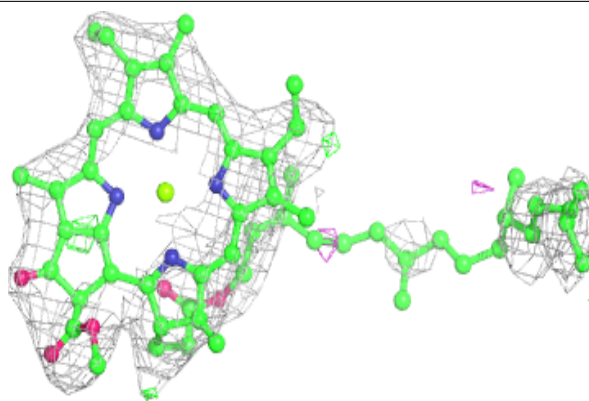
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



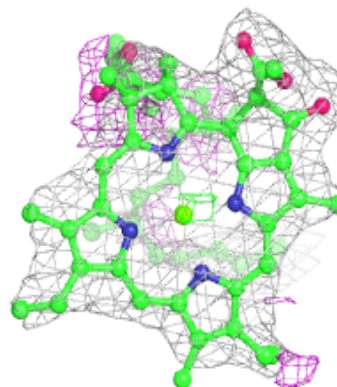
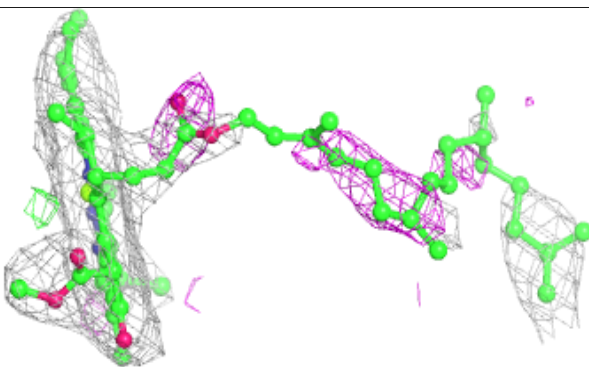
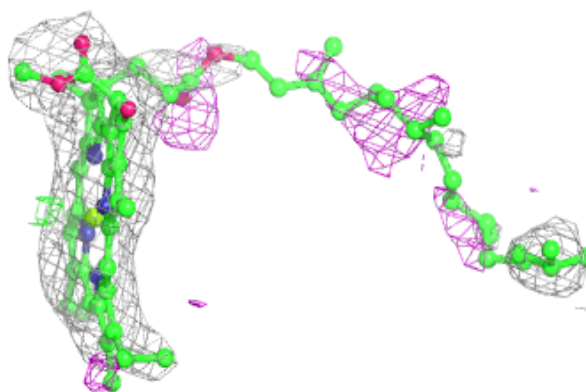


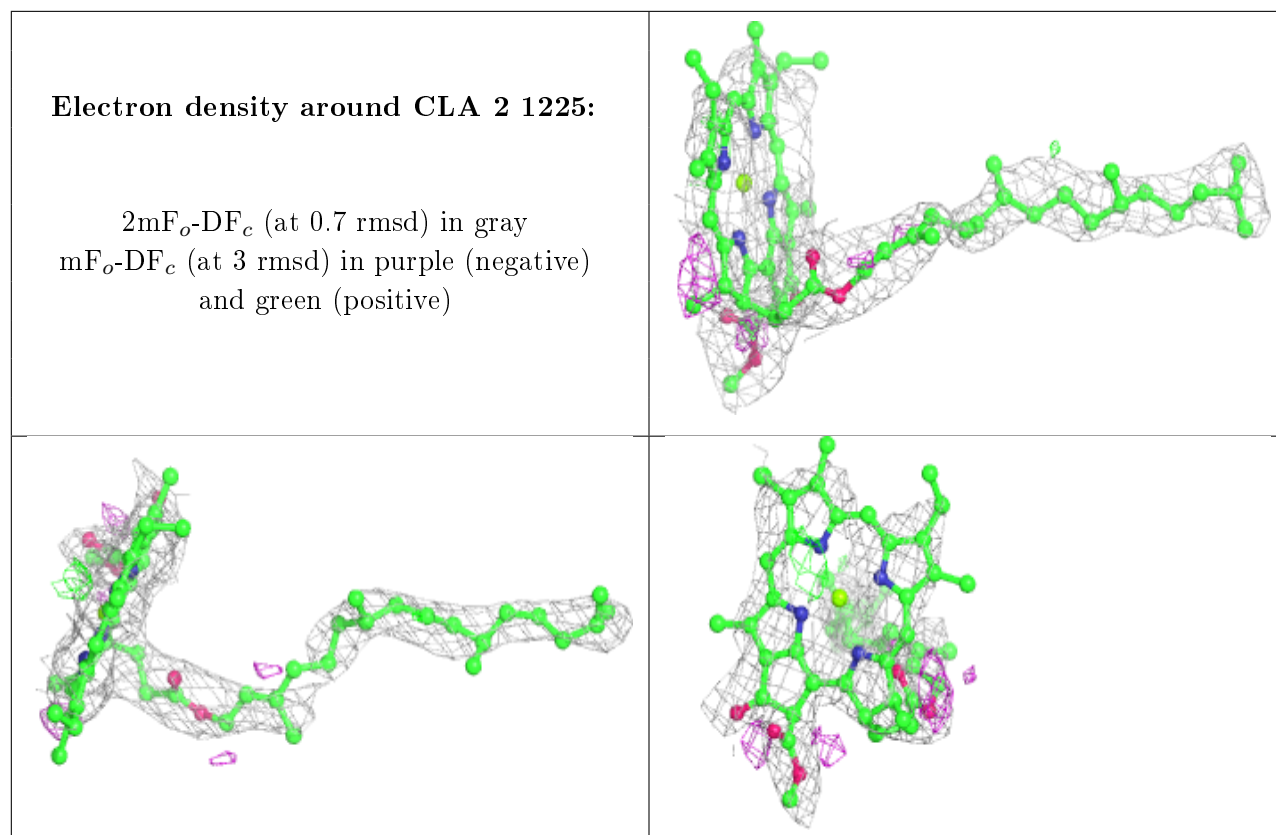
Electron density around CLA B 1209:

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

**Electron density around CLA A 1113:**

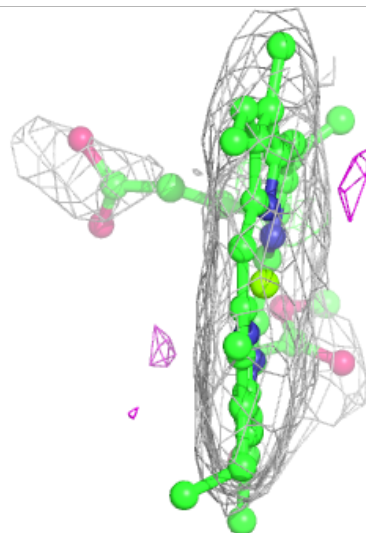
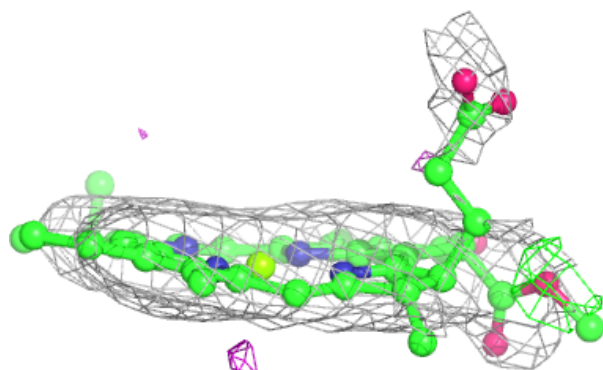
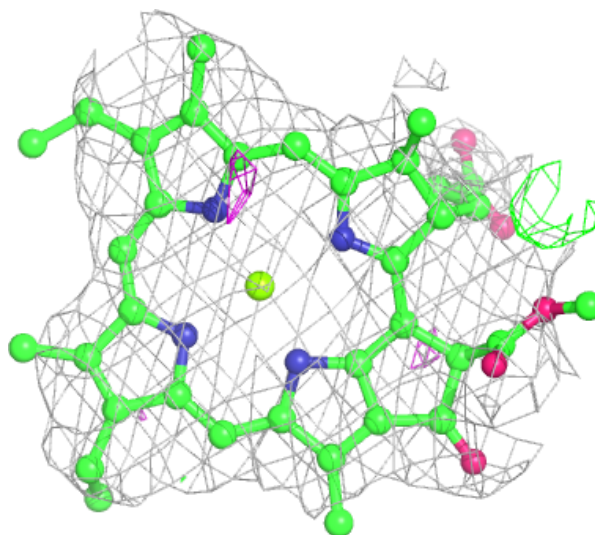
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





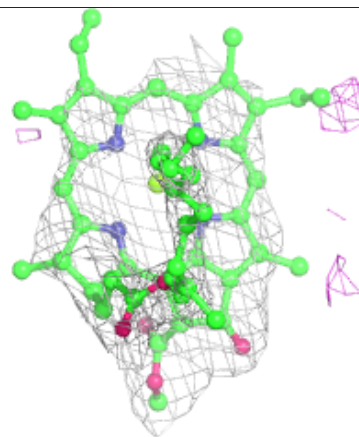
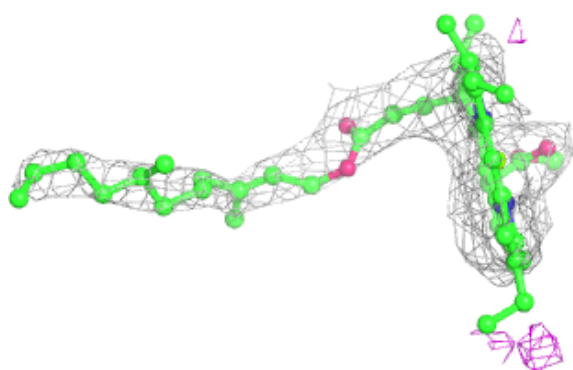
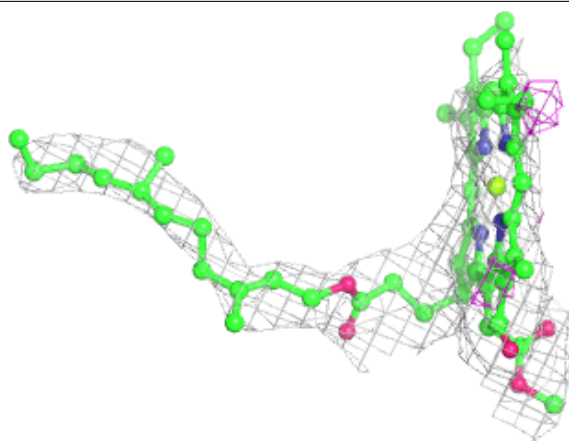
Electron density around CLA 2 1227:

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

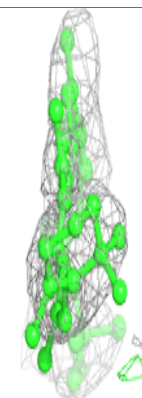
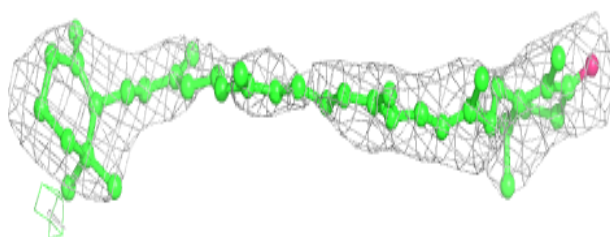
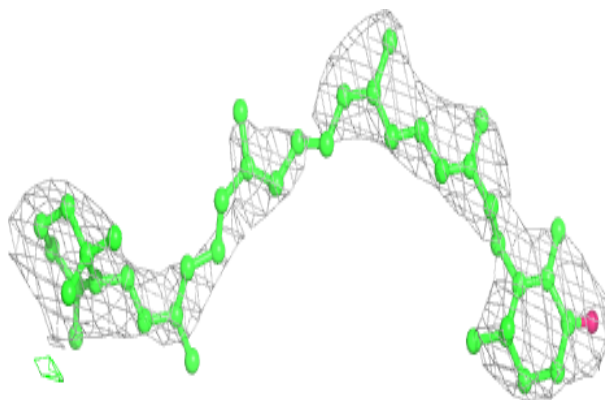


Electron density around CLA a 1105:

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

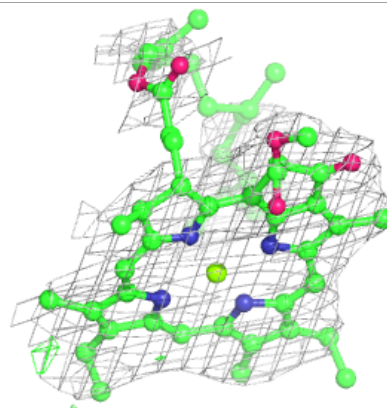
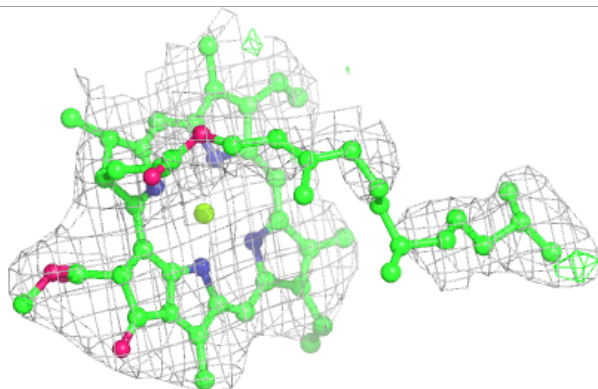
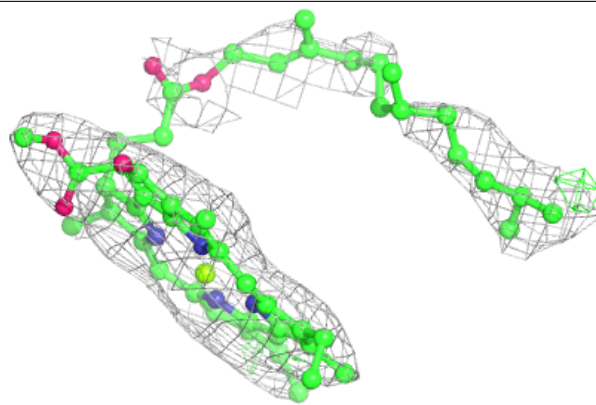
**Electron density around ECH b 4011:**

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

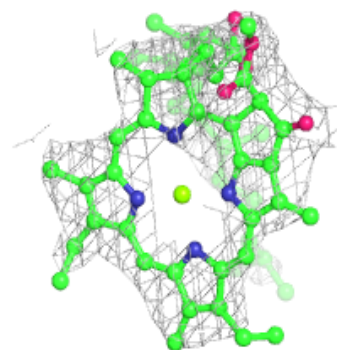
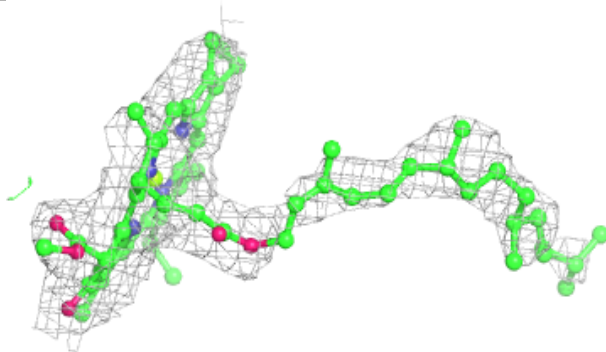
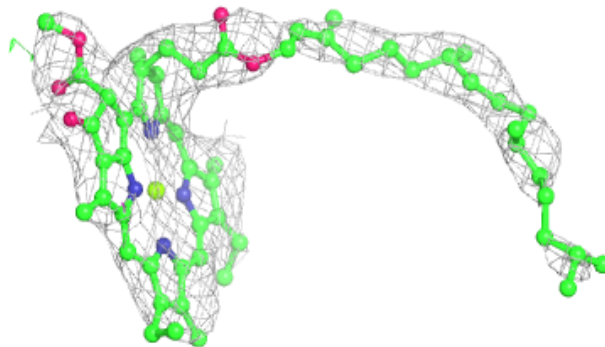


Electron density around CLA 2 1208:

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

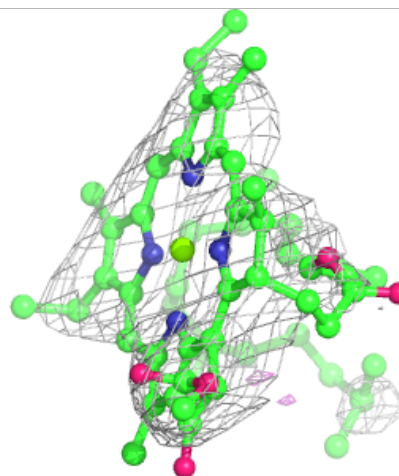
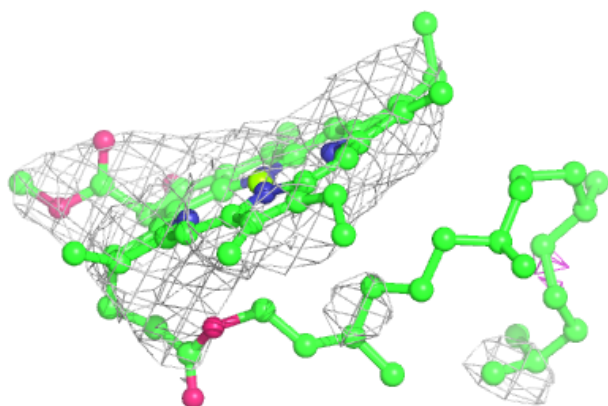
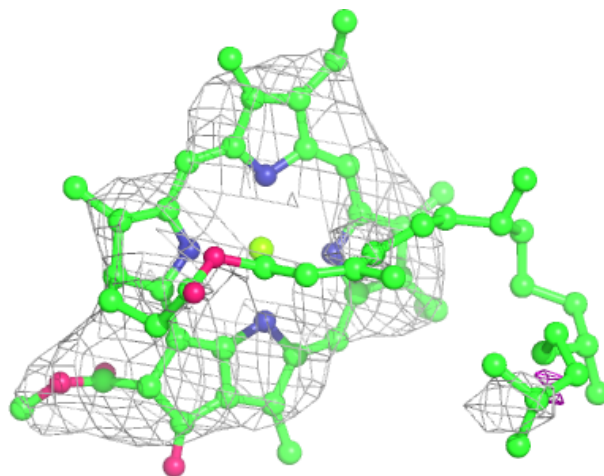
**Electron density around CLA 1 1133:**

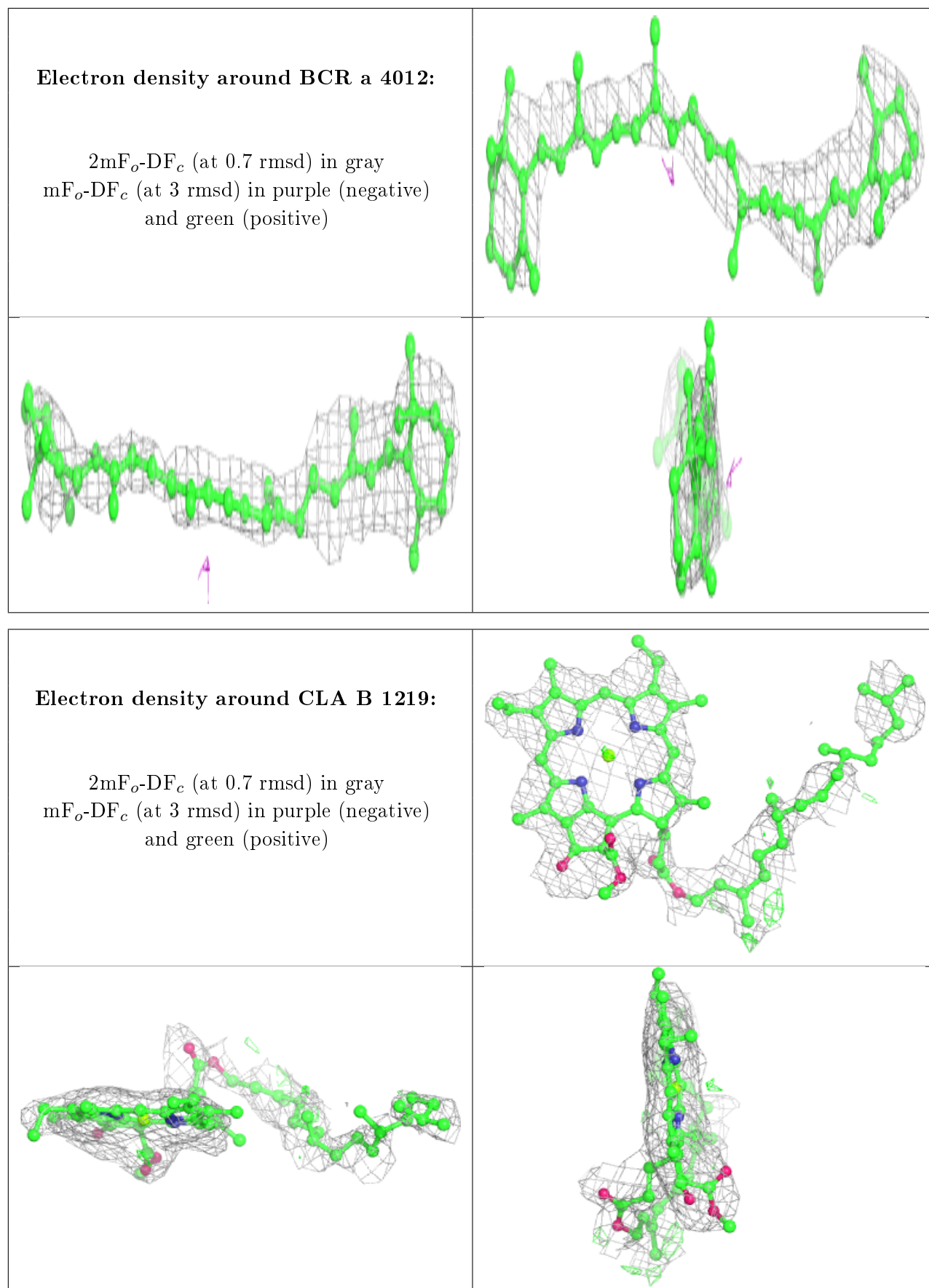
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 1121:

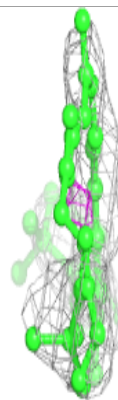
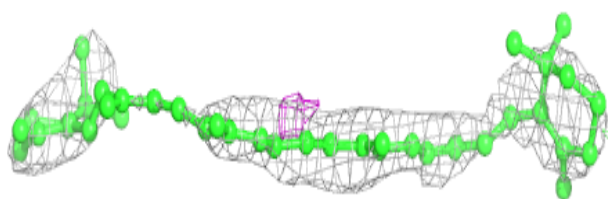
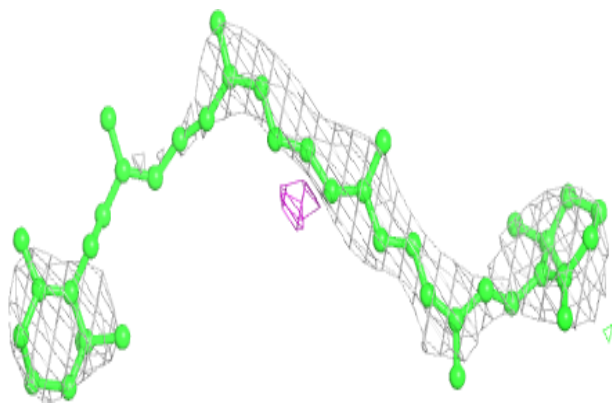
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



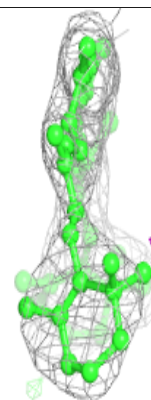
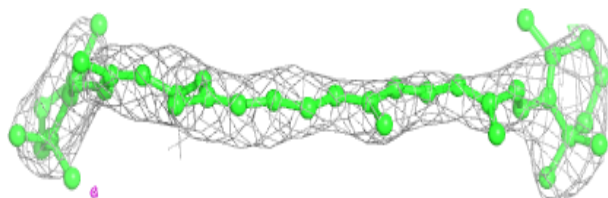
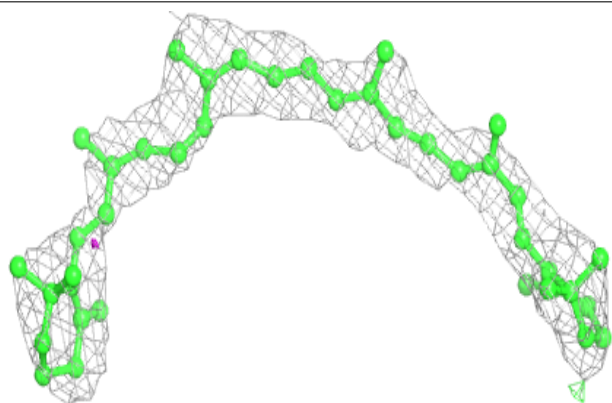


Electron density around BCR 2 4011:

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

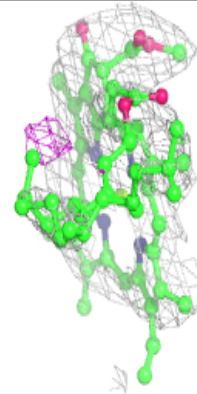
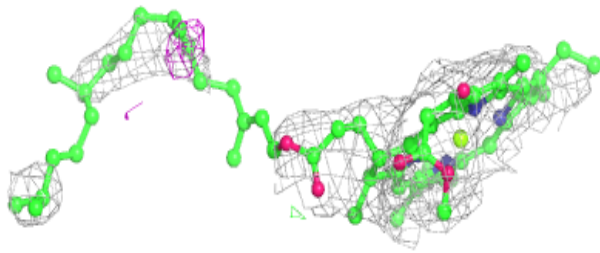
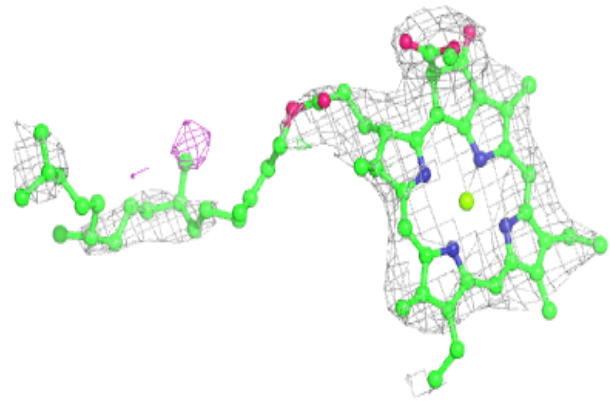
**Electron density around BCR f 4016:**

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

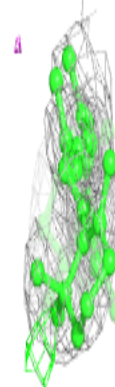
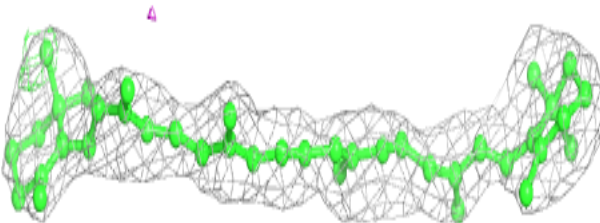
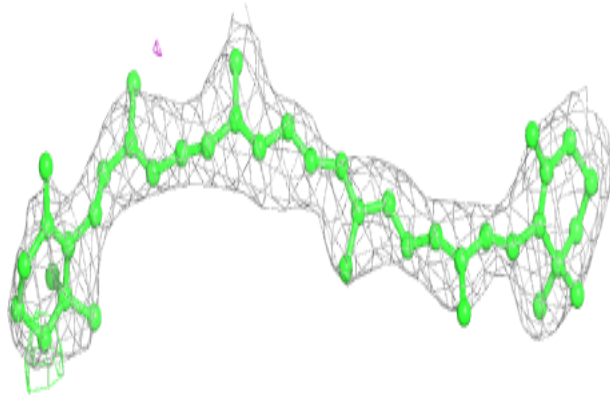


Electron density around CLA 2 1210:

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

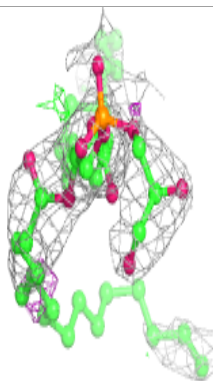
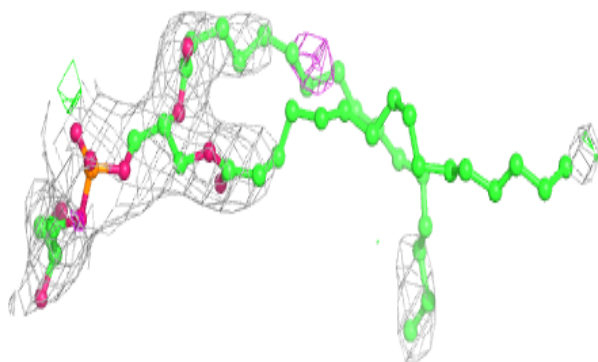
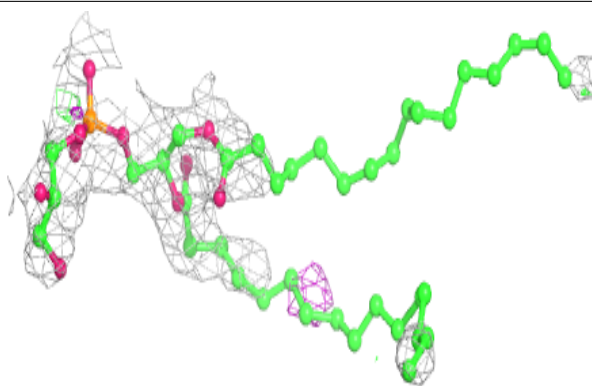
**Electron density around BCR B 4010:**

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

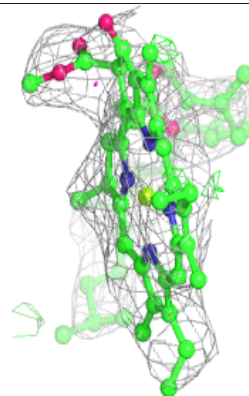
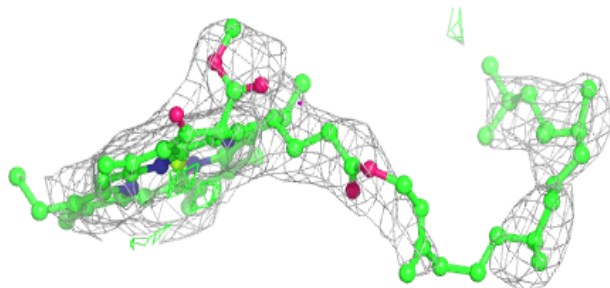
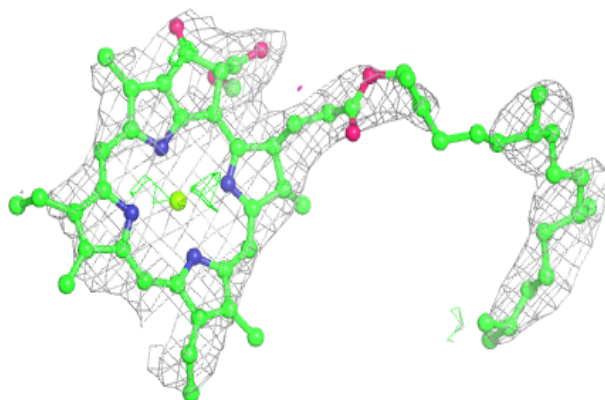


Electron density around LHG 1 5003:

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

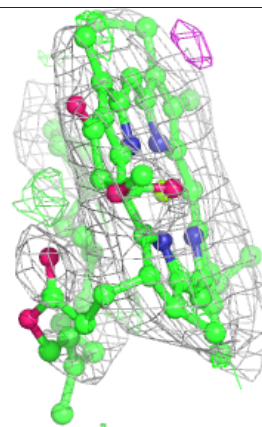
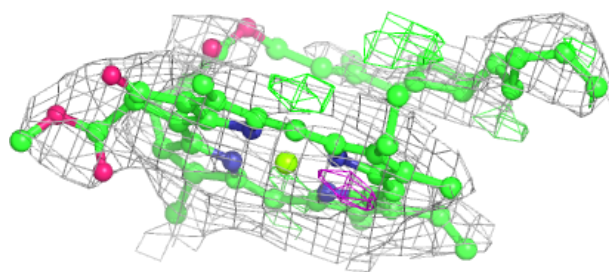
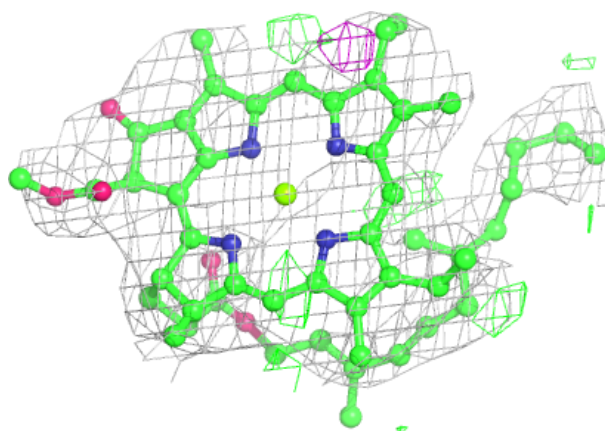
**Electron density around CLA a 1125:**

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



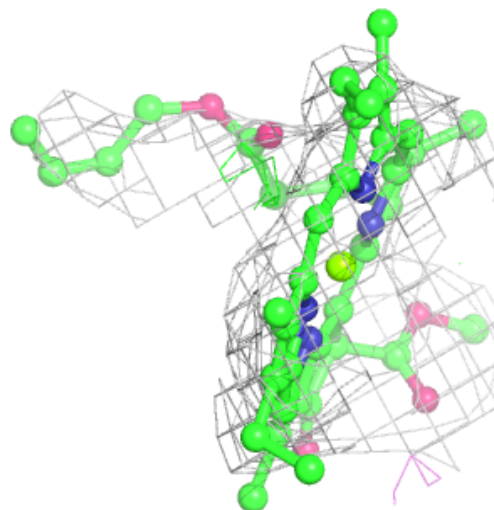
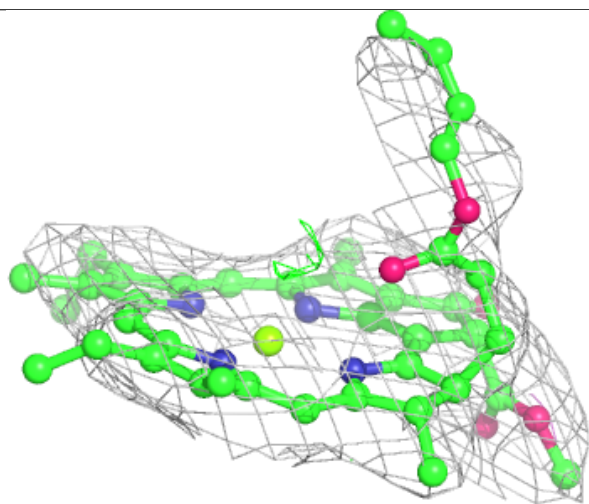
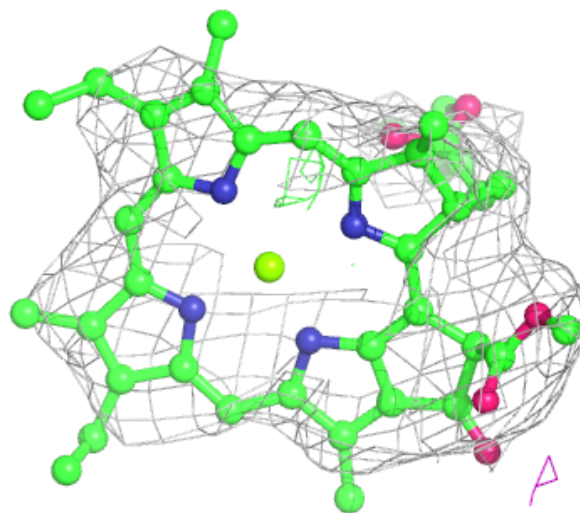
Electron density around CLA a 1110:

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



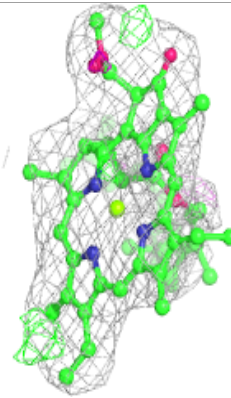
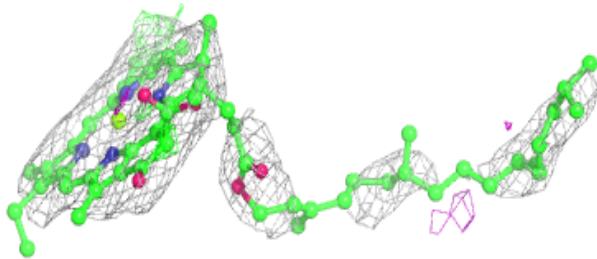
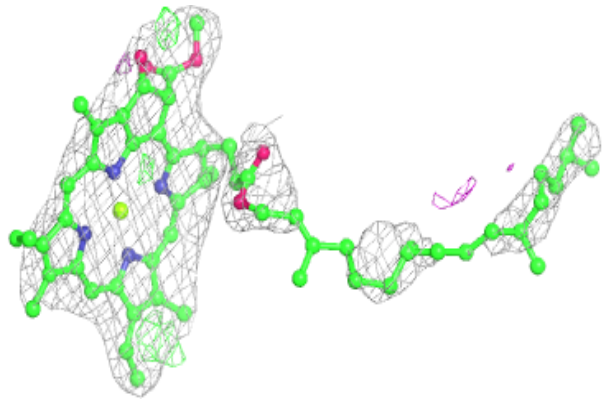
Electron density around CLA a 1134:

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

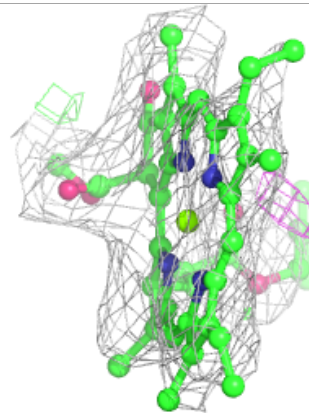
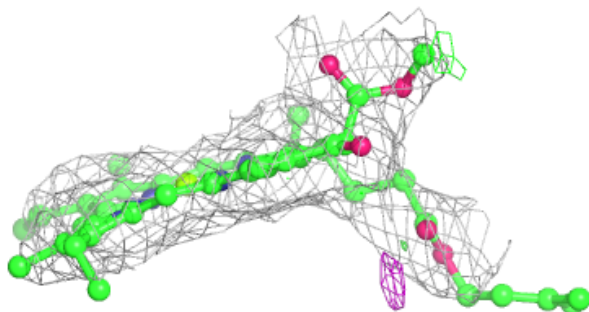
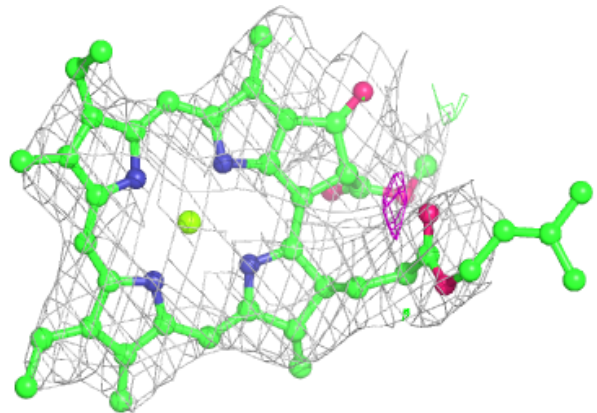


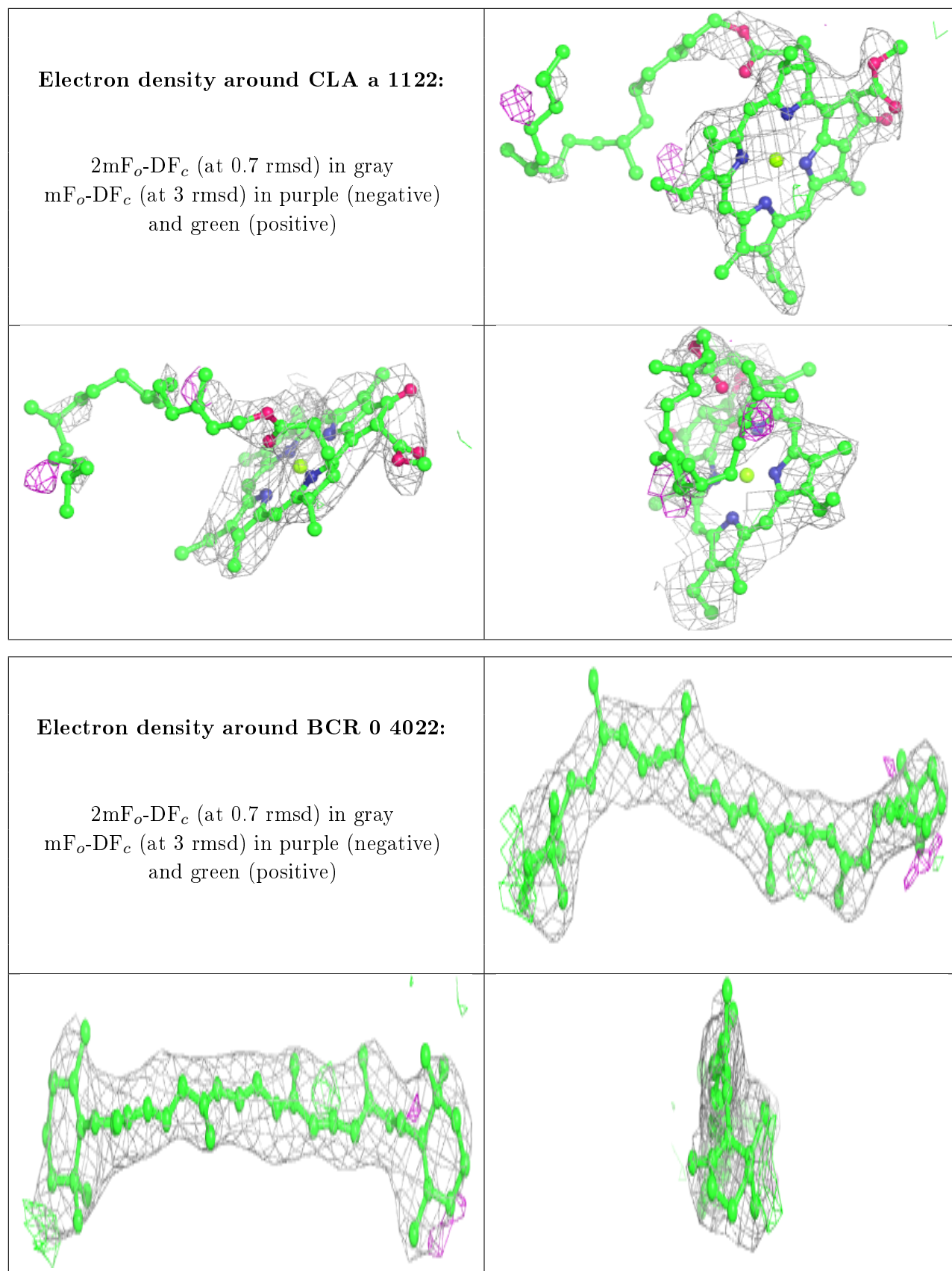
Electron density around CLA a 1119:

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

**Electron density around CLA a 1107:**

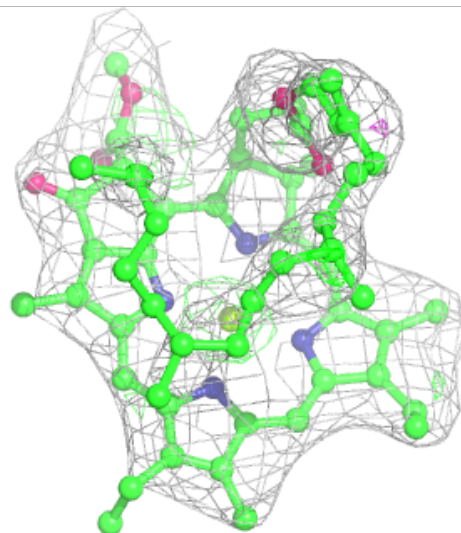
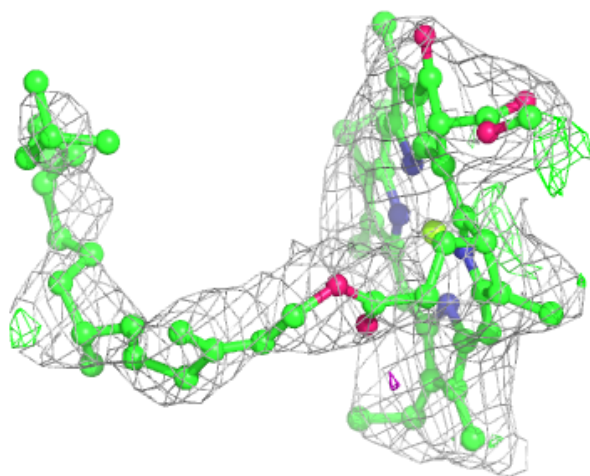
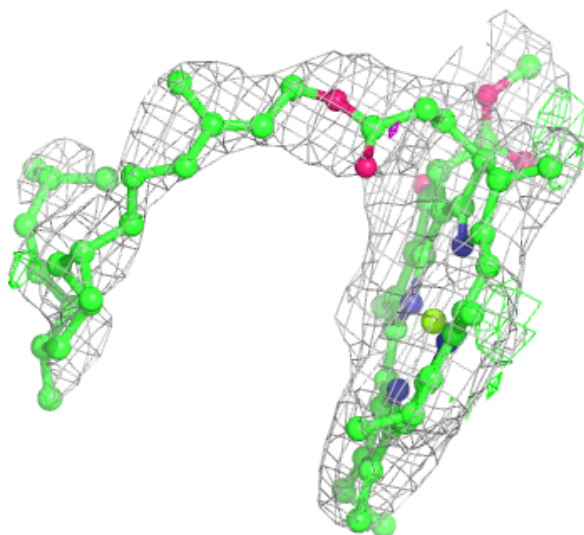
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





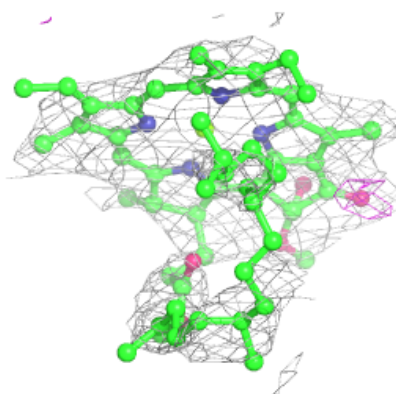
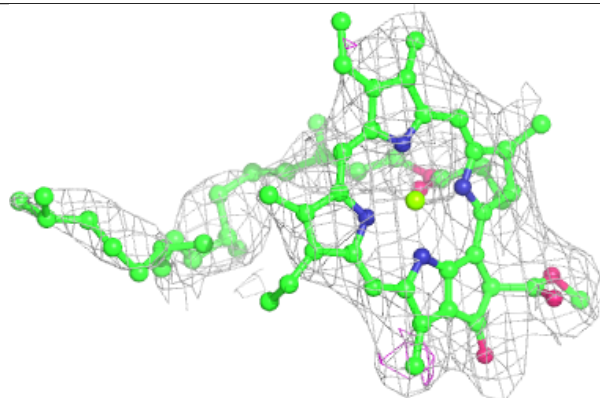
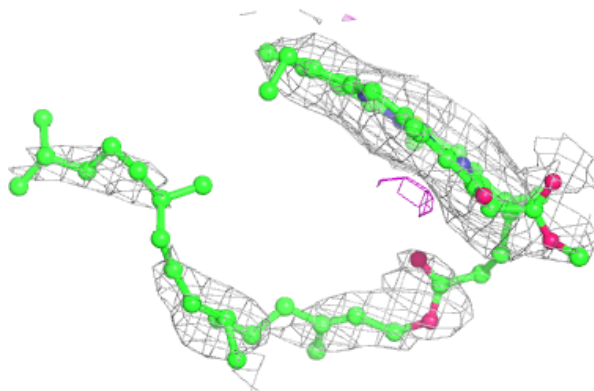
Electron density around CLA B 1216:

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

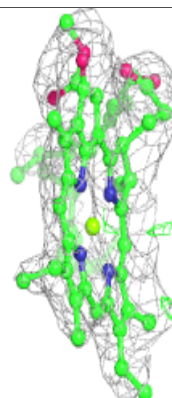
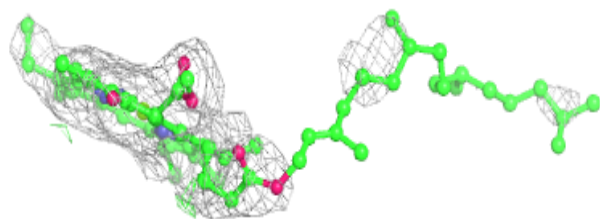
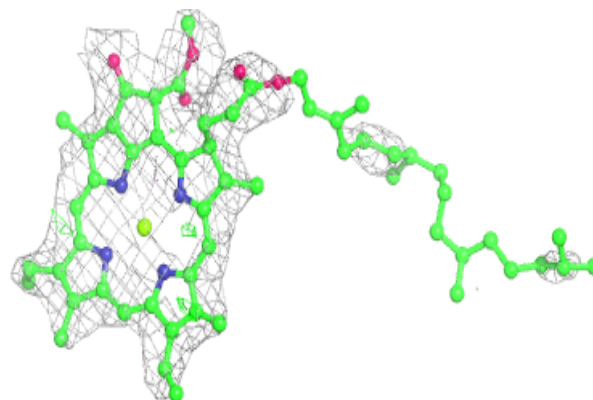


Electron density around CLA a 1109:

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

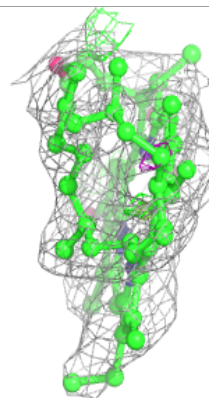
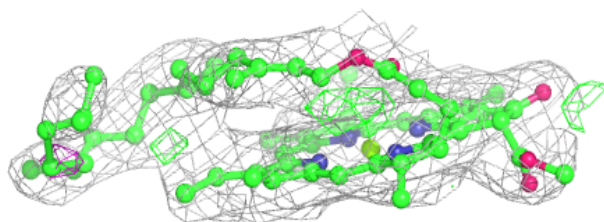
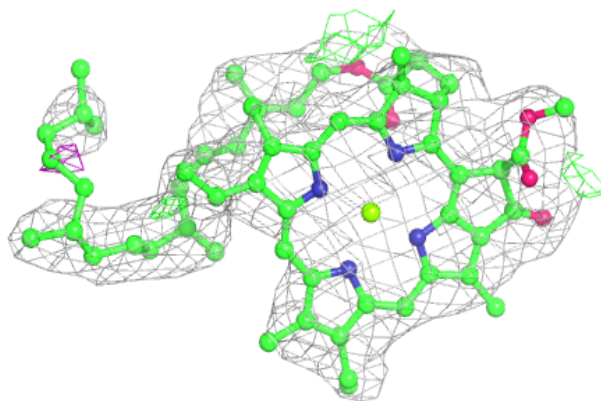
**Electron density around CLA F 1301:**

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

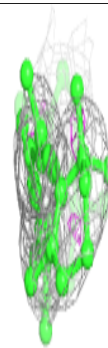
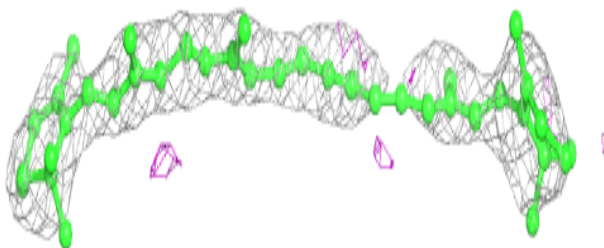
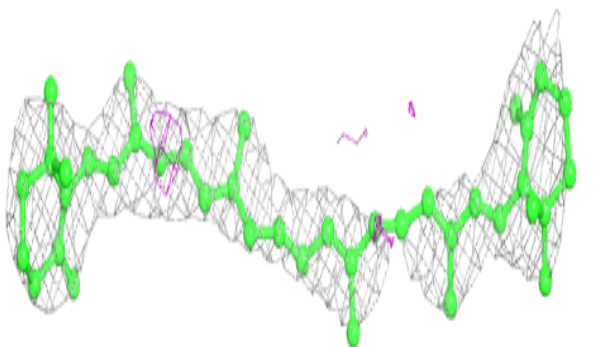


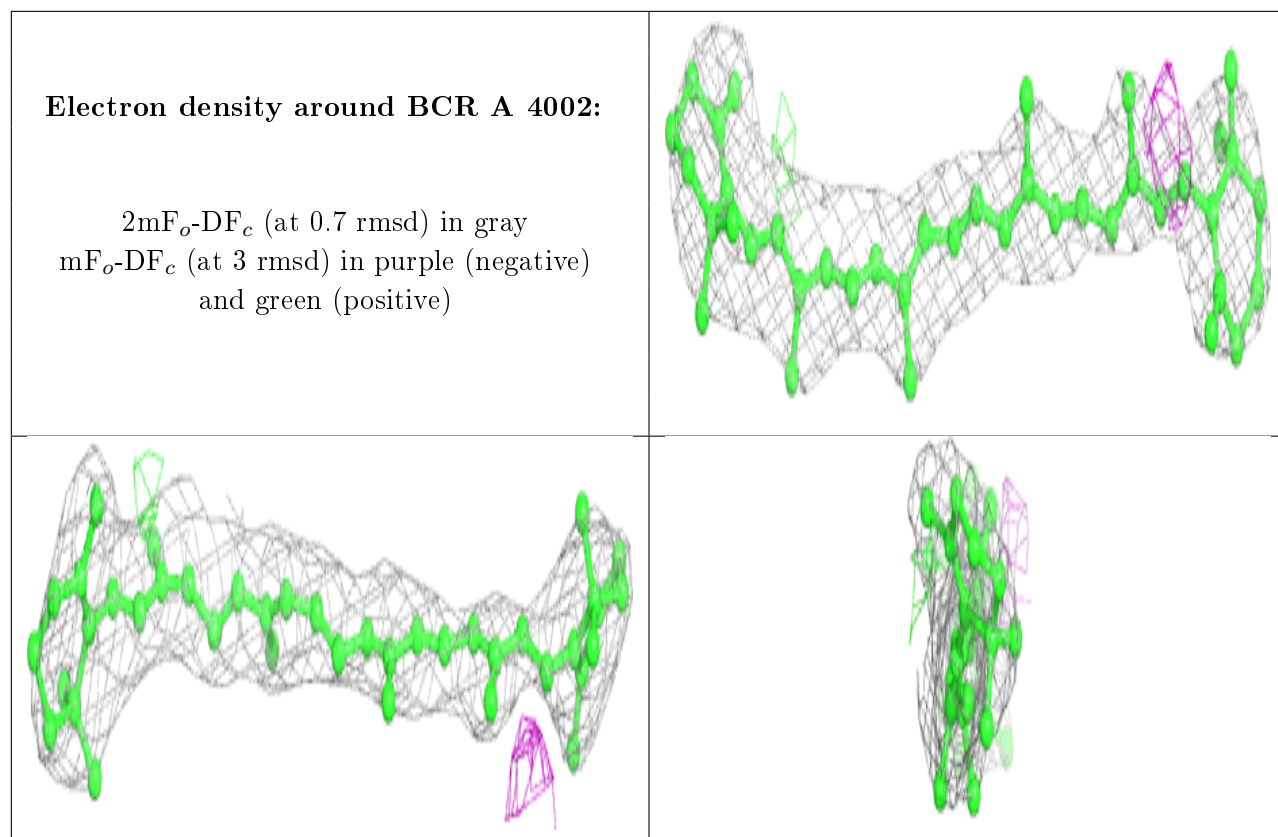
Electron density around CLA a 1117:

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

**Electron density around BCR 1 4008:**

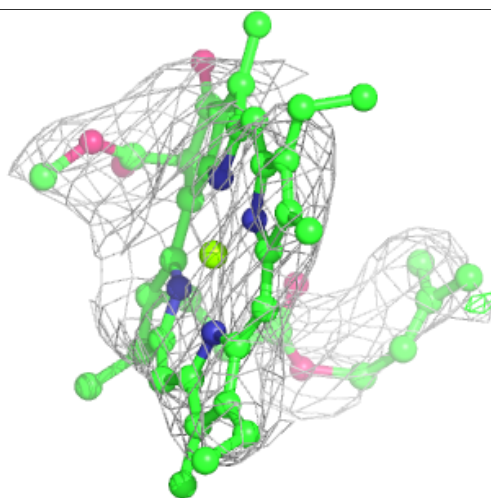
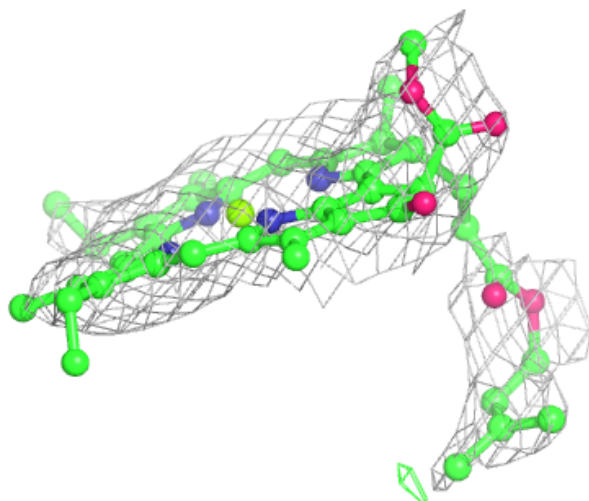
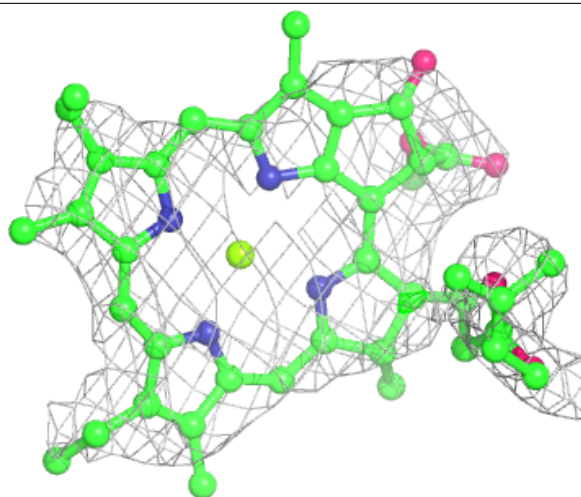
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





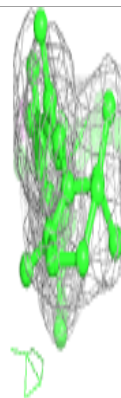
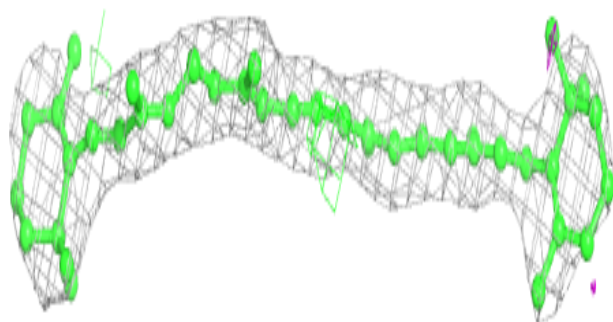
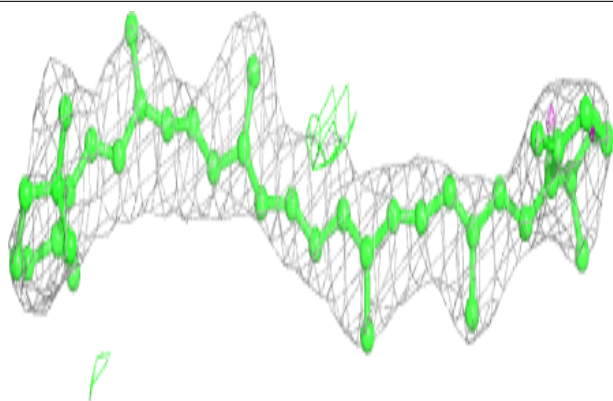
Electron density around CLA 1 1112:

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

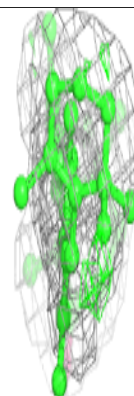
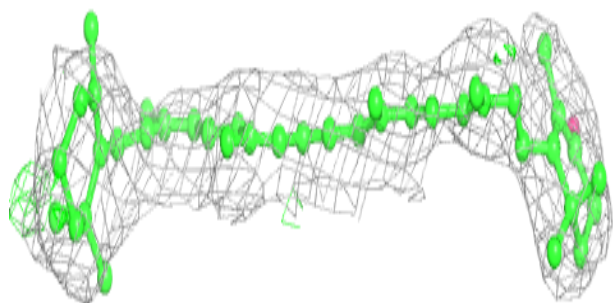
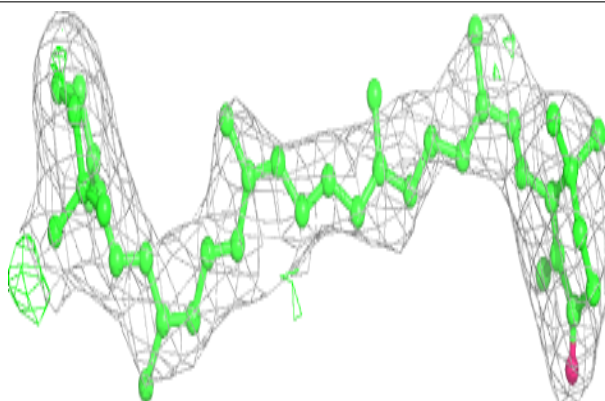


Electron density around BCR L 4022:

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

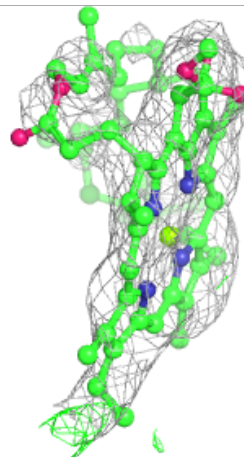
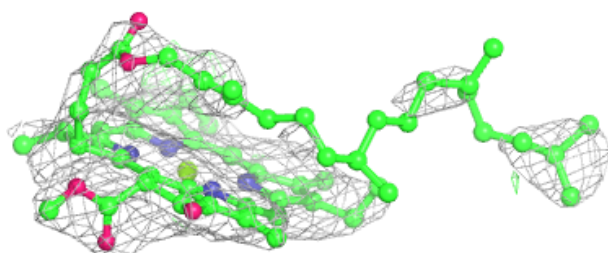
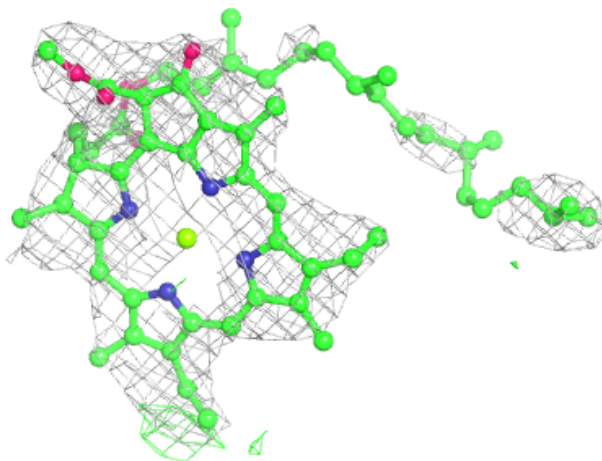
**Electron density around ECH B 4006:**

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



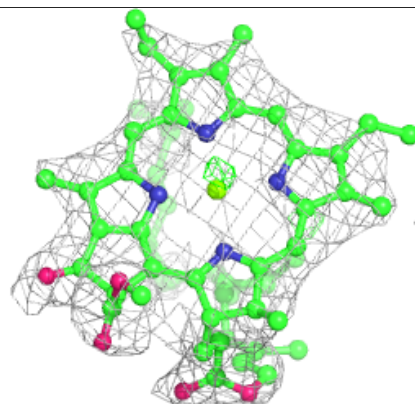
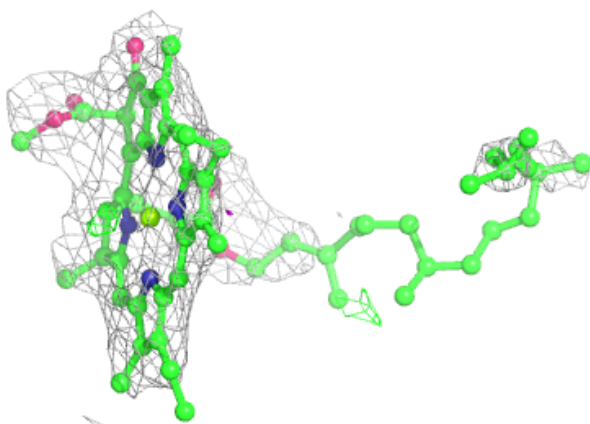
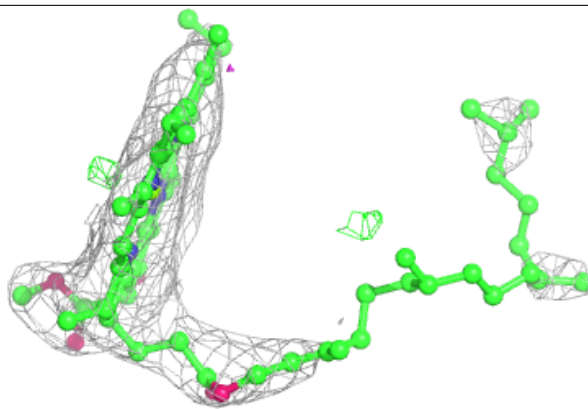
Electron density around CLA 1 1127:

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

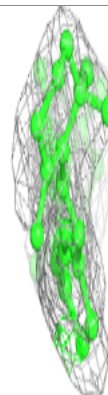
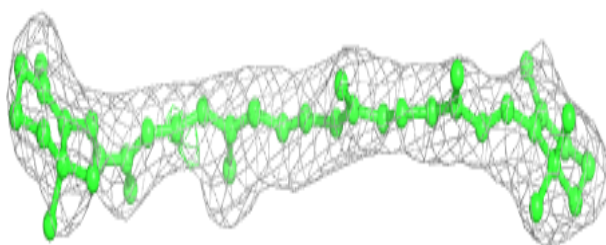
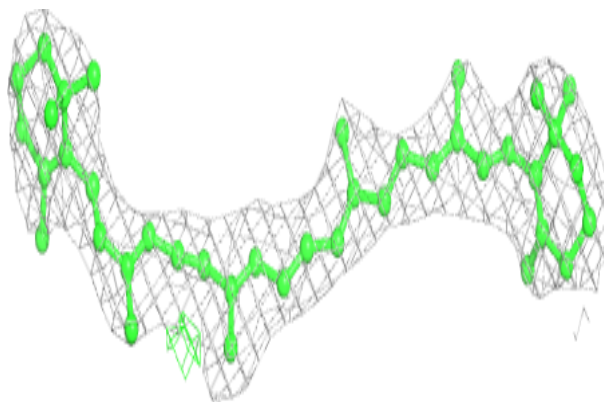


Electron density around CLA b 1227:

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

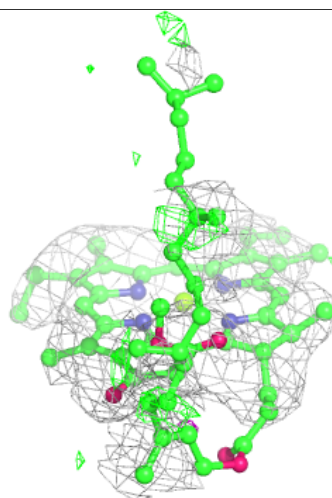
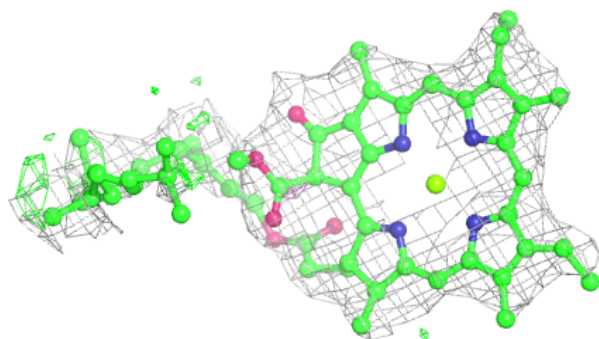
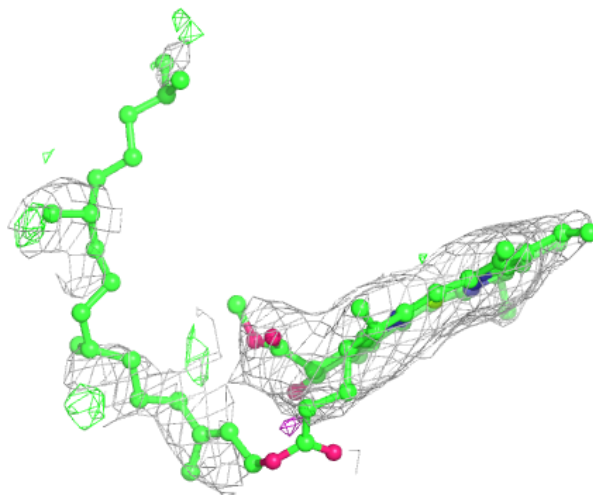
**Electron density around BCR b 4010:**

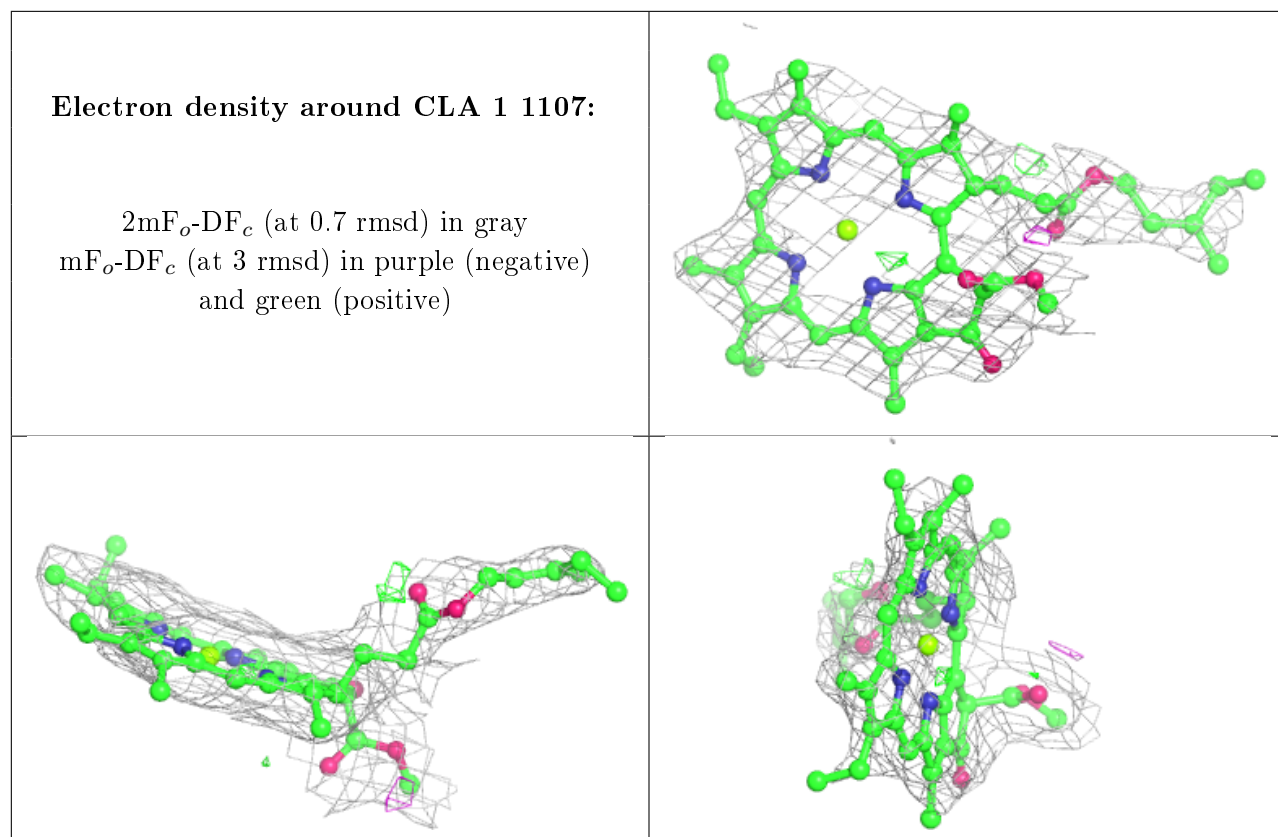
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1240:

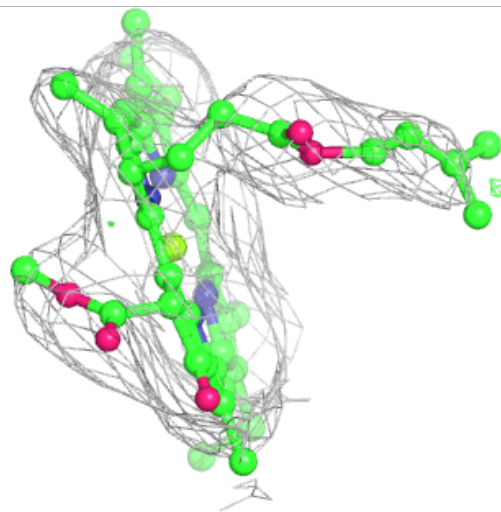
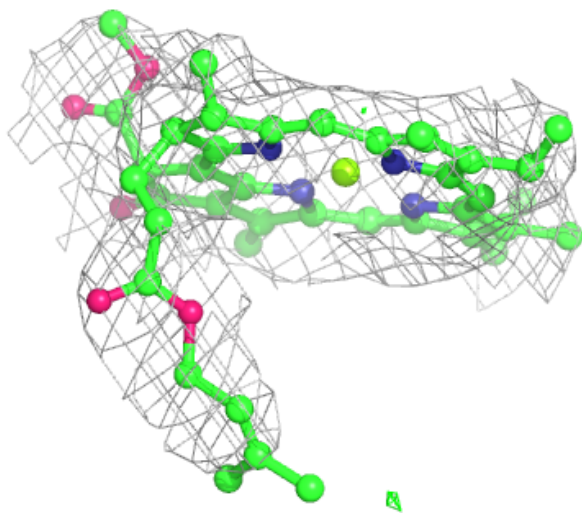
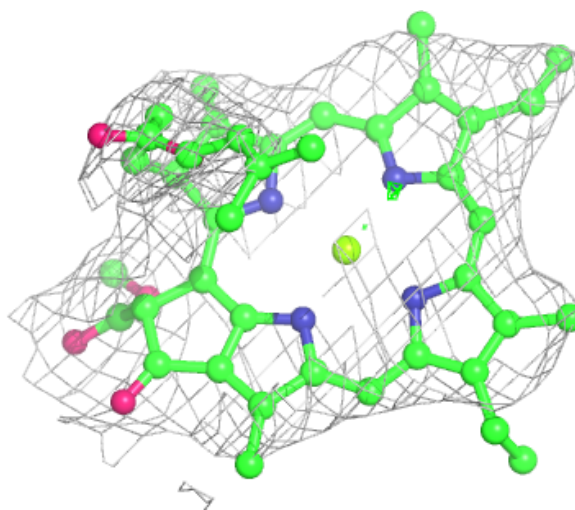
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





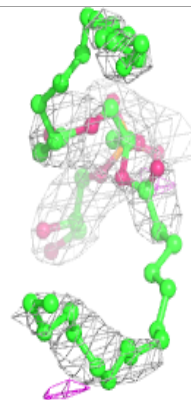
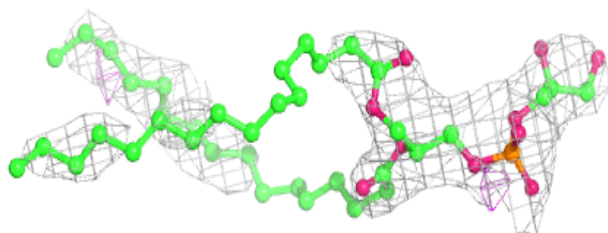
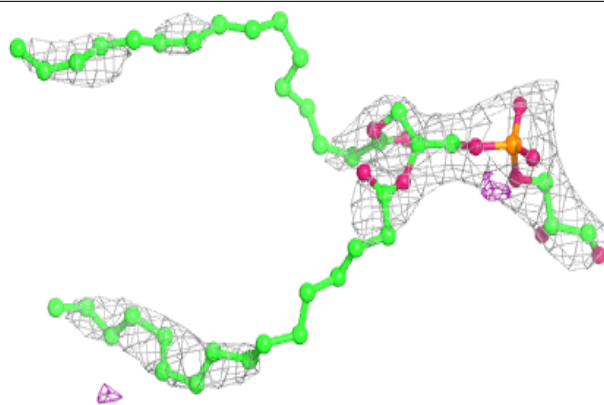
Electron density around CLA 2 1211:

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

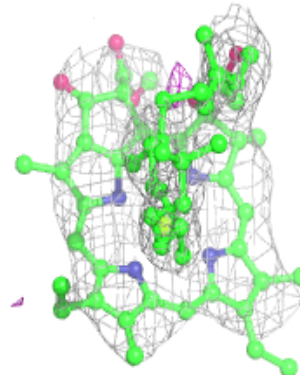
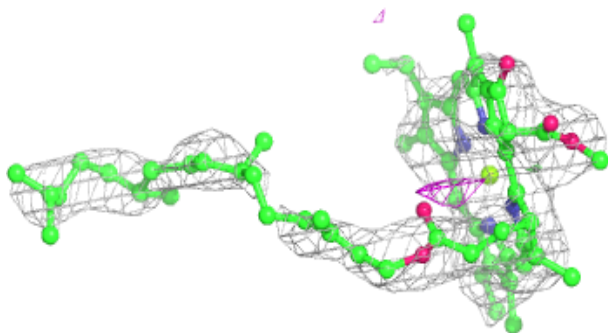
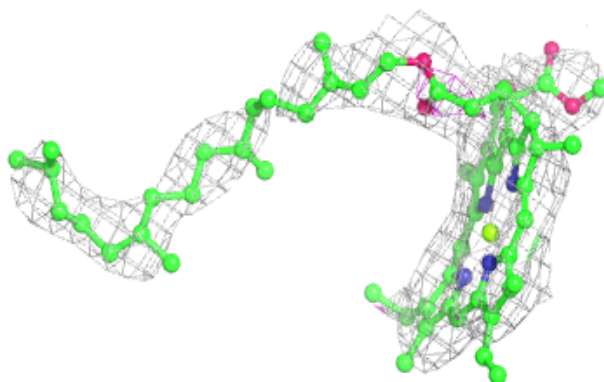


Electron density around LHG 1 5001:

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

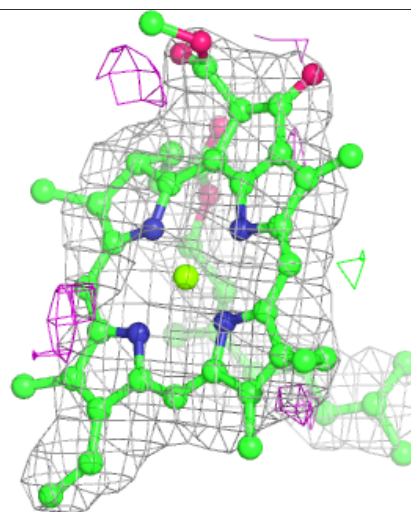
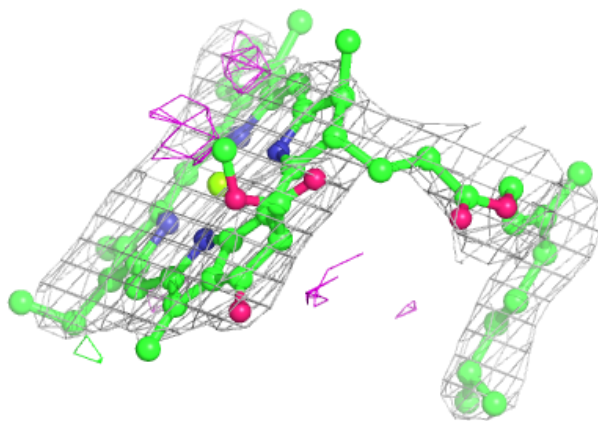
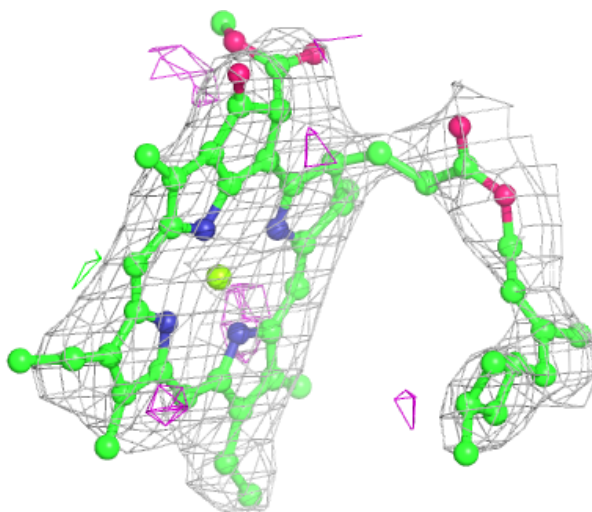
**Electron density around CLA a 1128:**

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



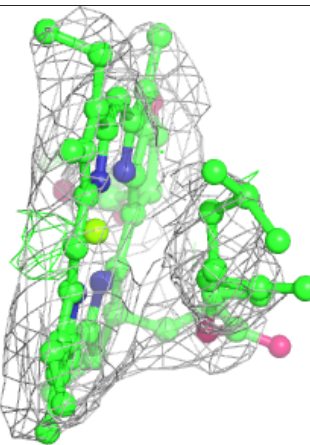
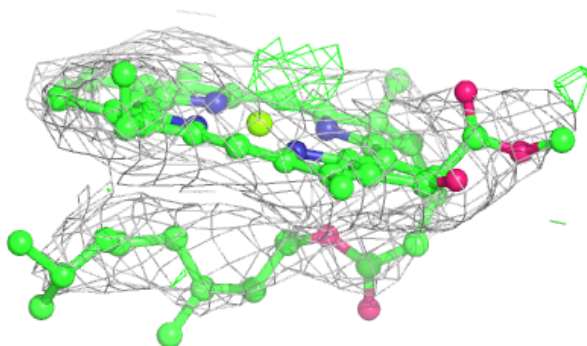
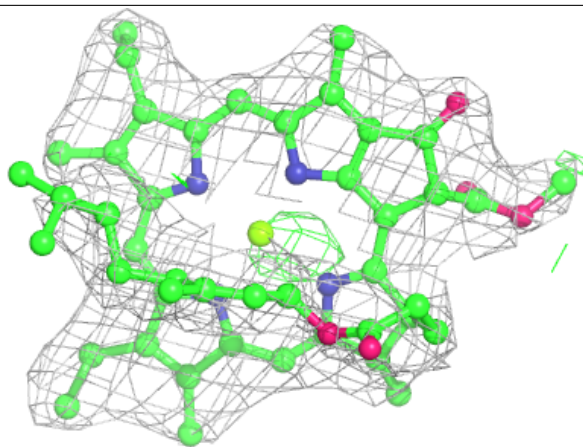
Electron density around CLA 1 1102:

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

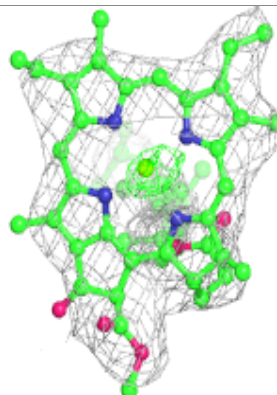
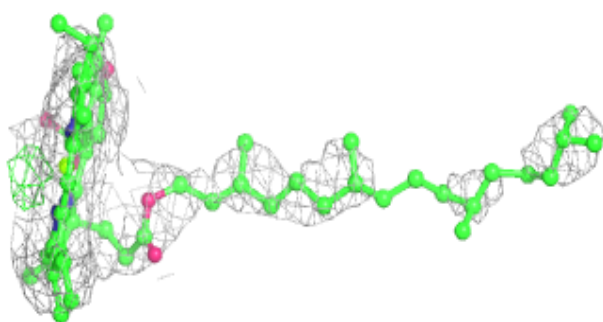
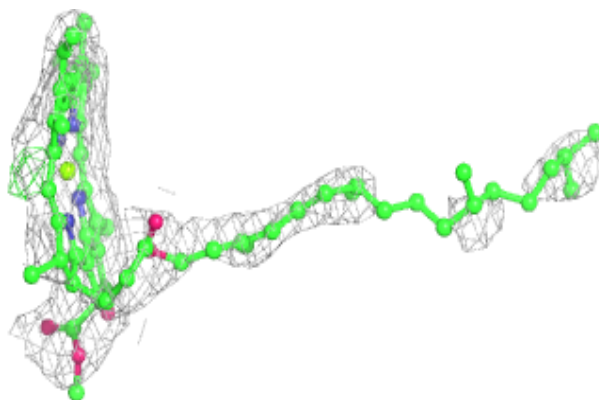


Electron density around CLA 1 1121:

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

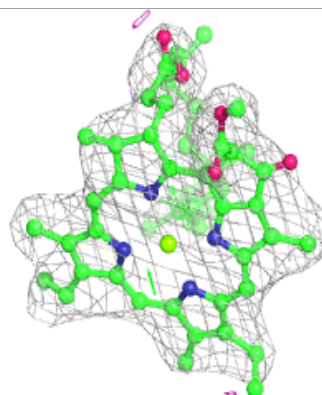
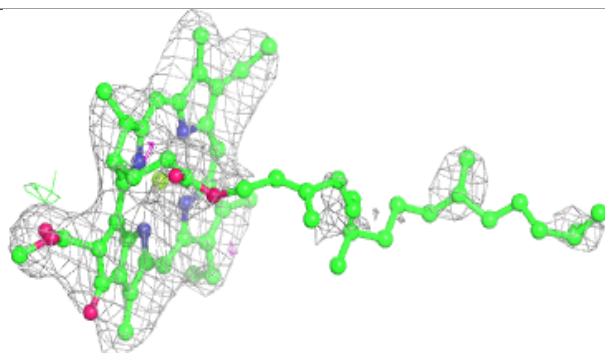
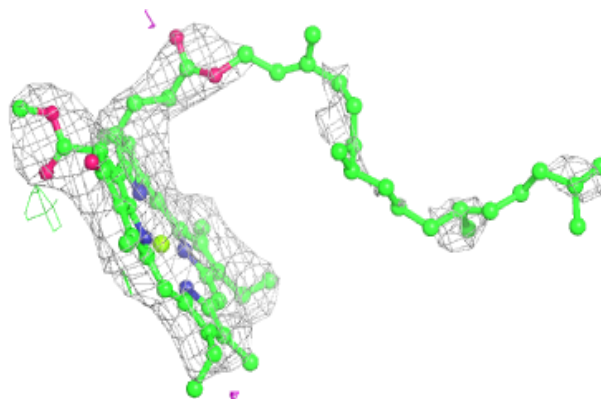
**Electron density around CLA 1 1126:**

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

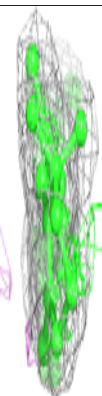
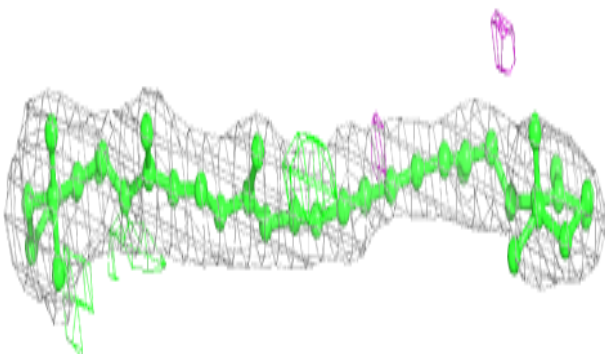
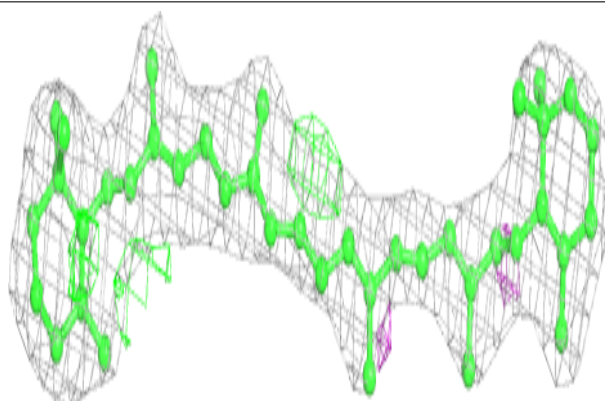


Electron density around CLA b 1232:

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

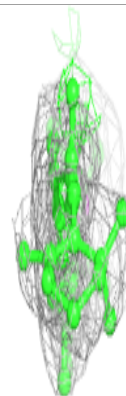
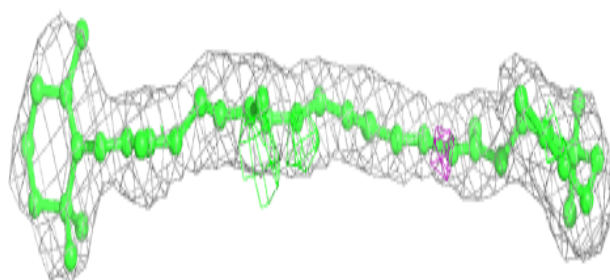
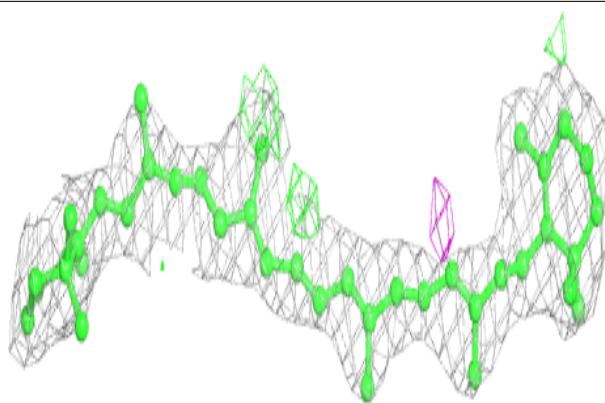
**Electron density around BCR 1 4019:**

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

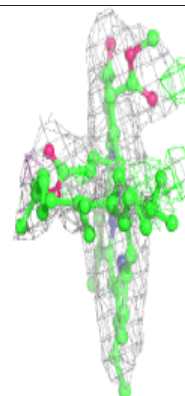
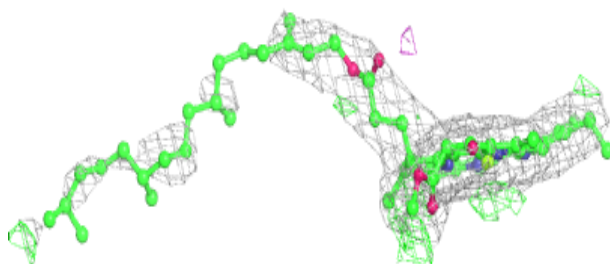
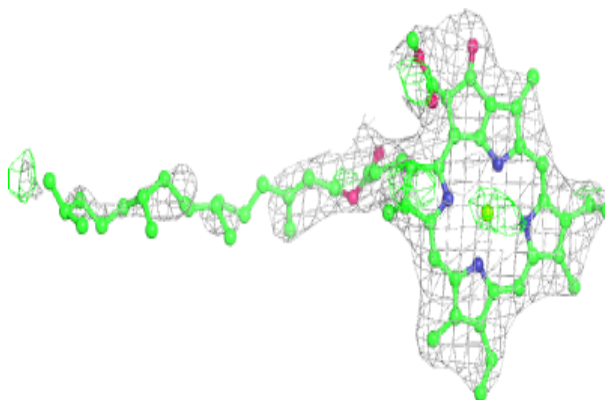


Electron density around BCR b 4005:

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

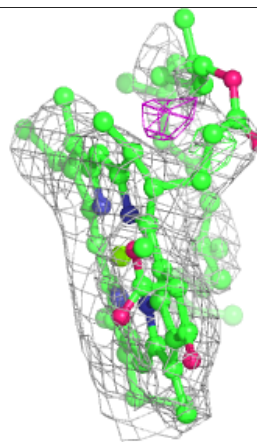
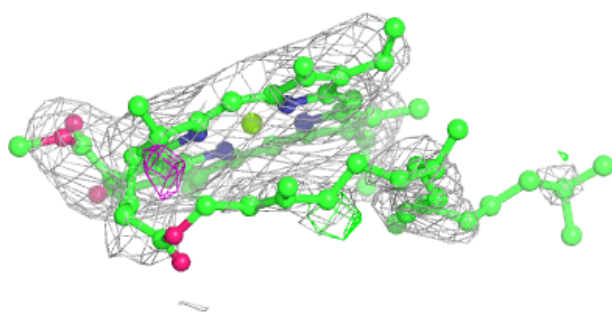
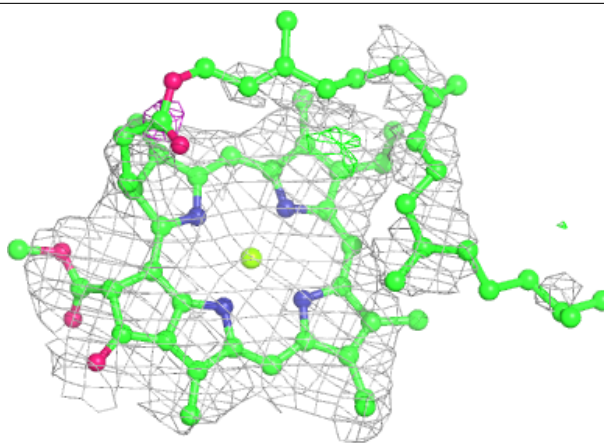
**Electron density around CLA b 1222:**

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

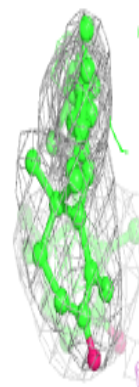
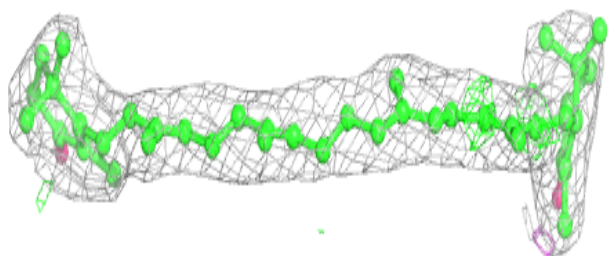
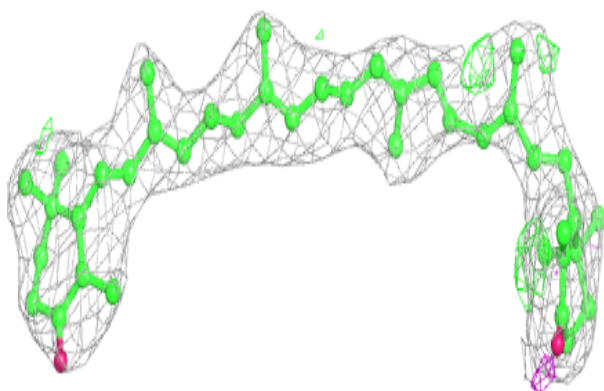


Electron density around CLA B 1218:

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

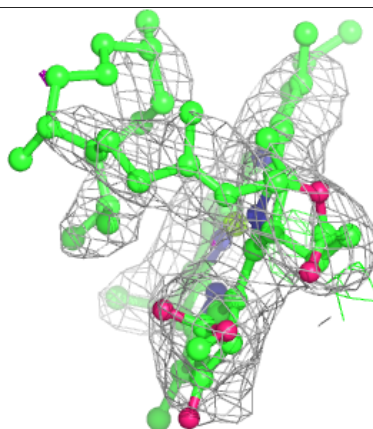
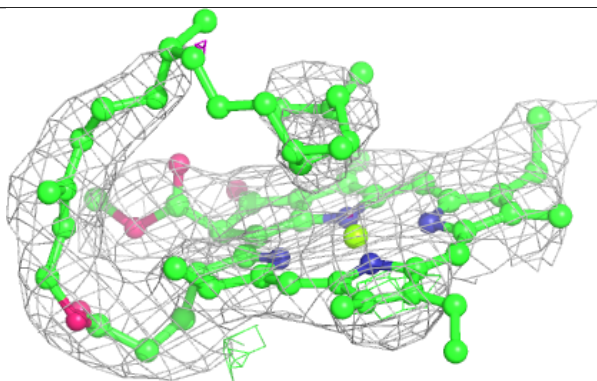
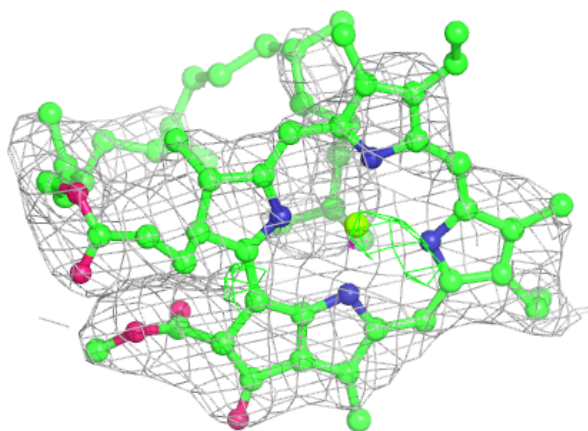
**Electron density around 45D h 4020:**

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

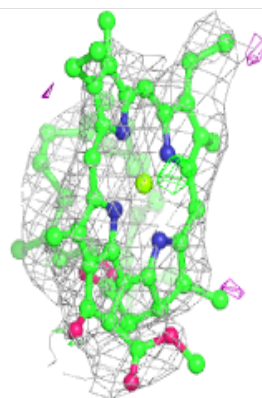
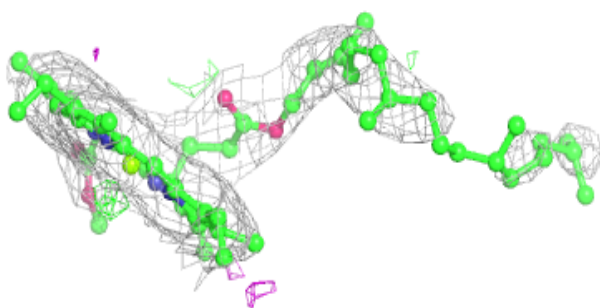
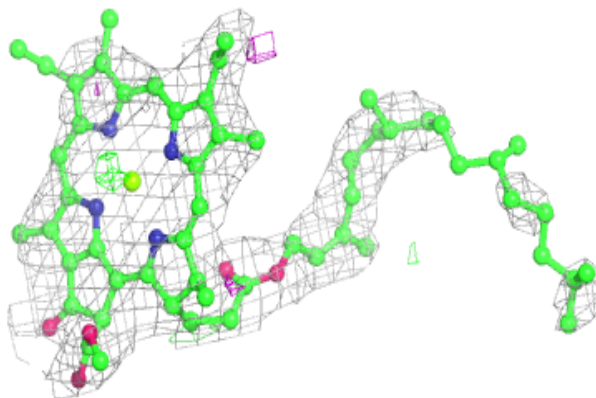


Electron density around CLA 2 1203:

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

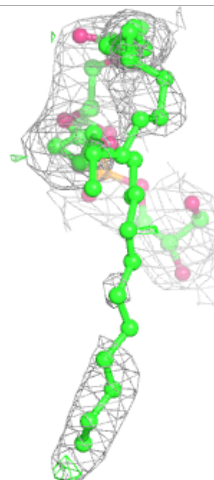
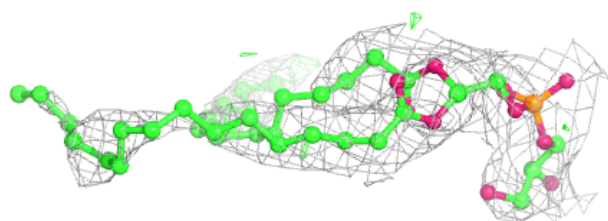
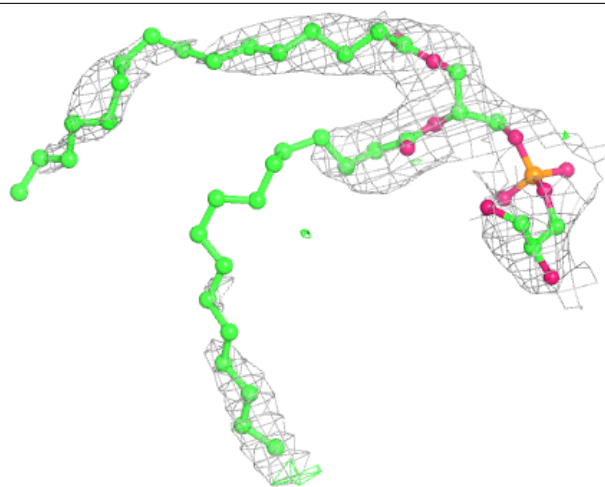
**Electron density around CLA a 1106:**

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



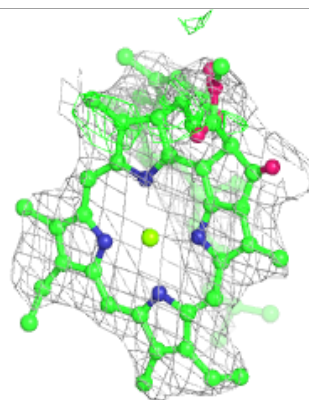
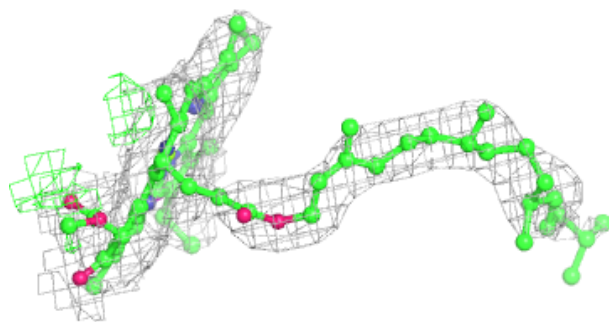
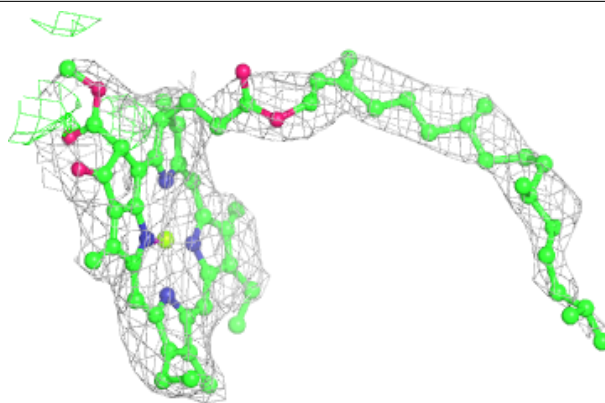
Electron density around LHG b 5004:

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

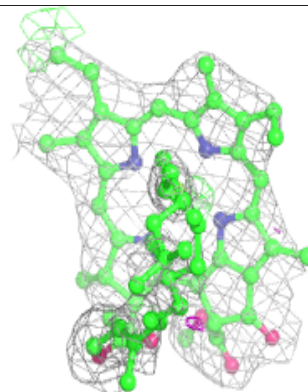
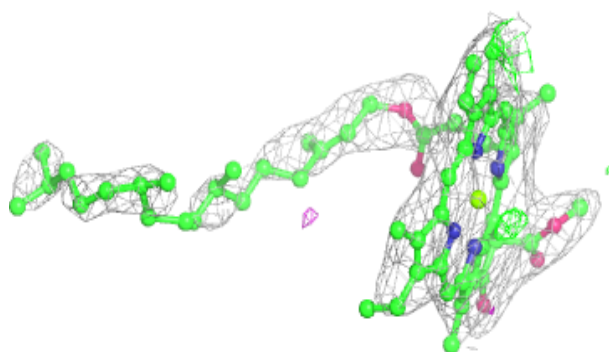
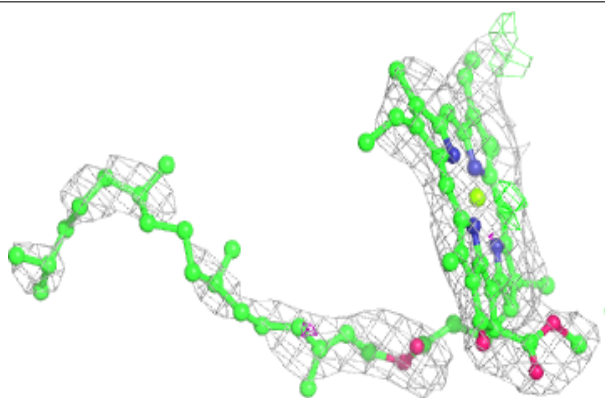


Electron density around CLA a 1133:

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

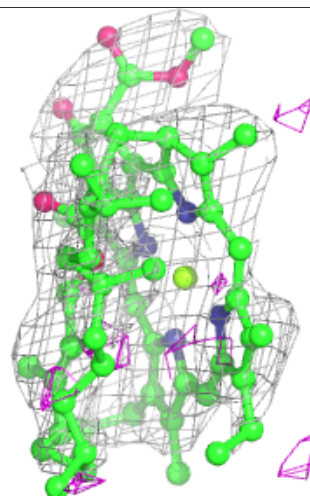
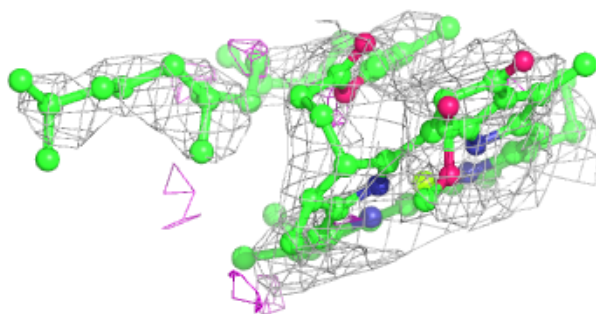
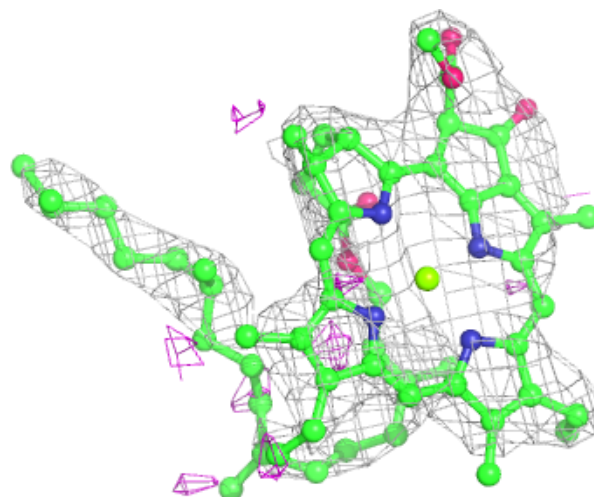
**Electron density around CLA 1 1128:**

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



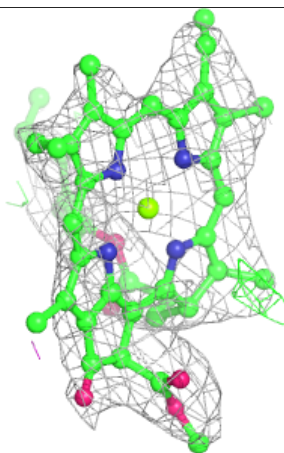
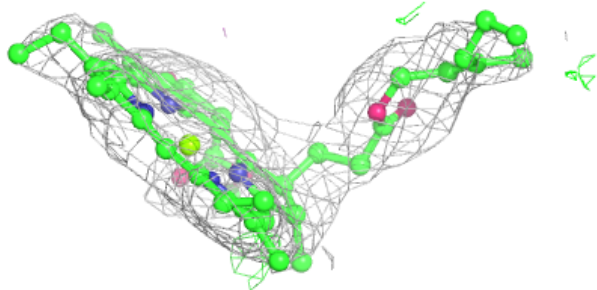
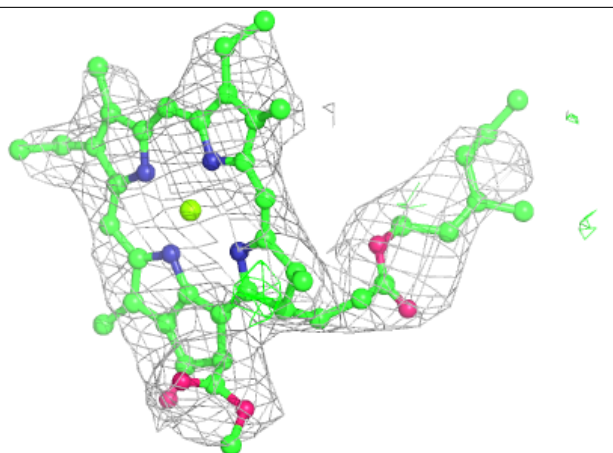
Electron density around CLA 2 1205:

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

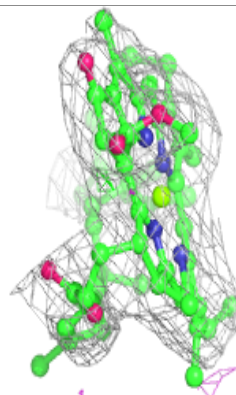
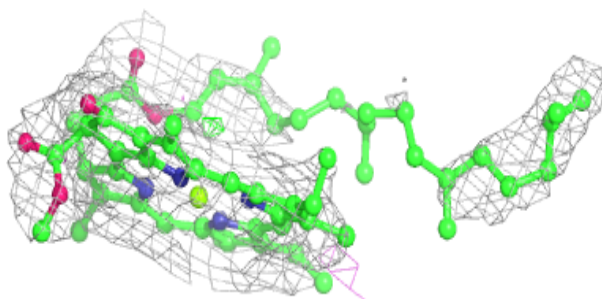
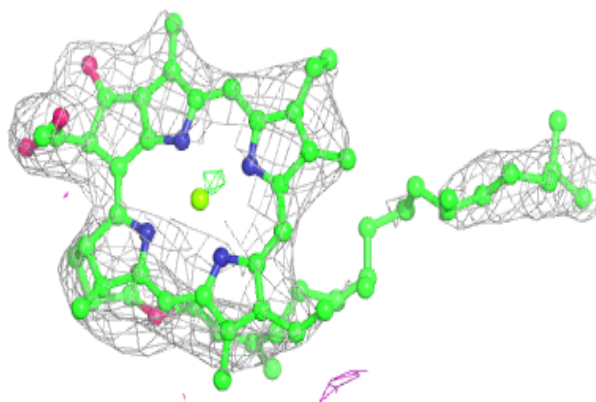


Electron density around CLA a 1129:

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

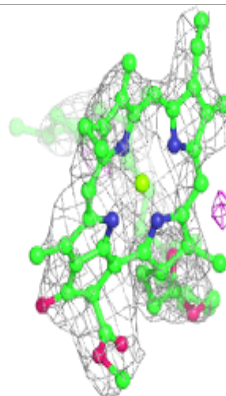
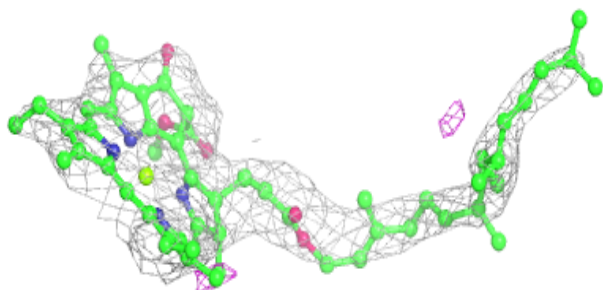
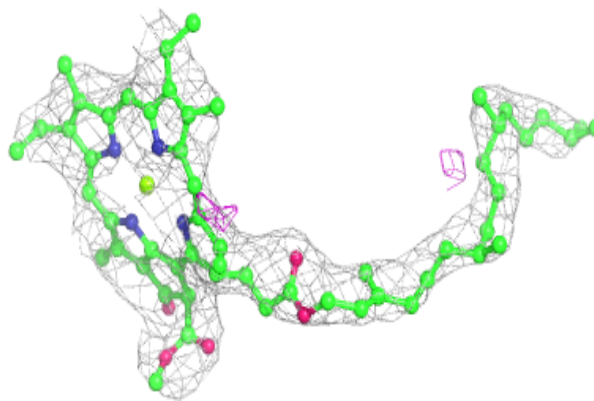
**Electron density around CLA B 1217:**

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

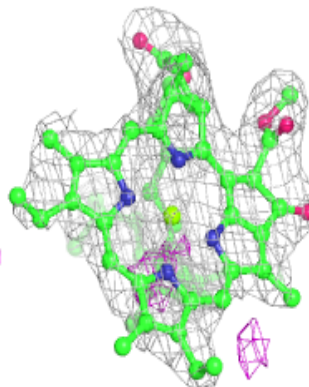
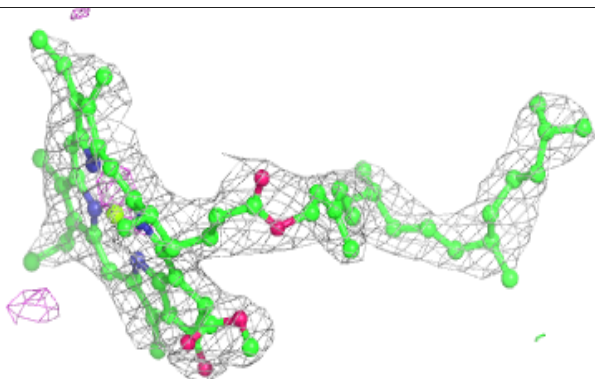
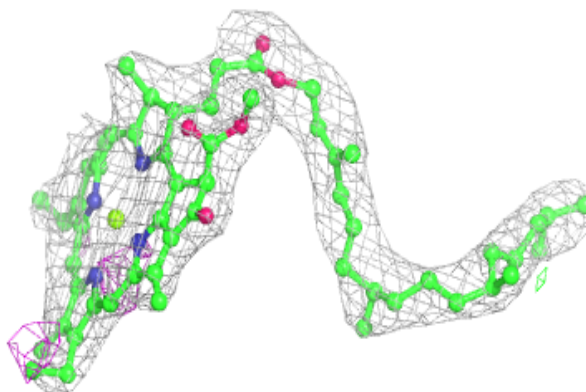


Electron density around CLA 1 1012:

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

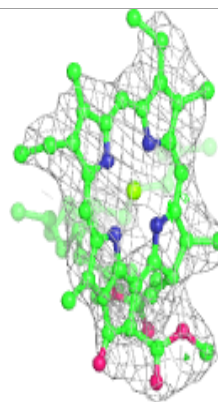
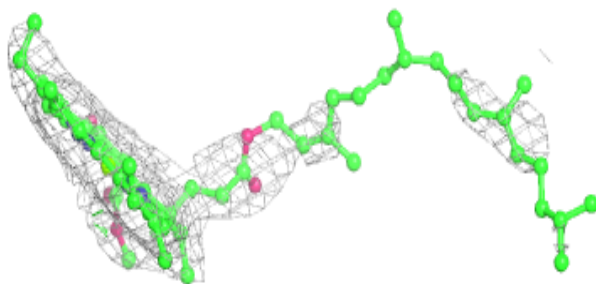
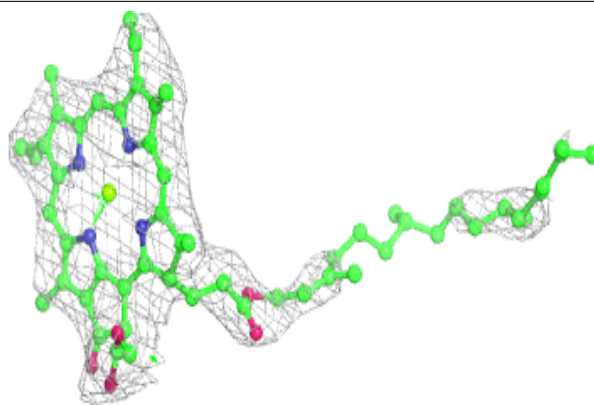
**Electron density around CLA b 1021:**

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

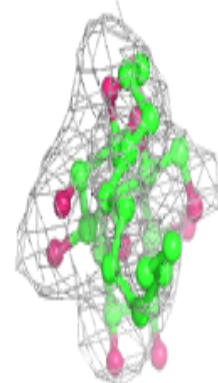
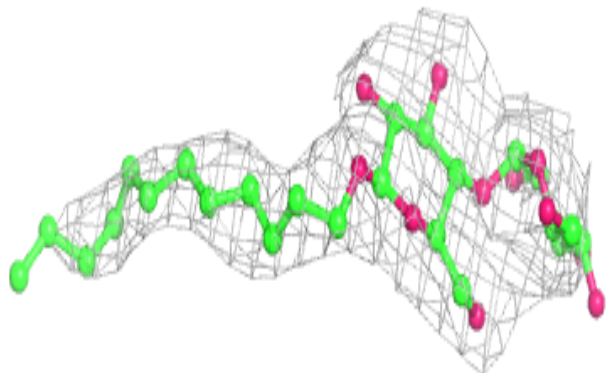
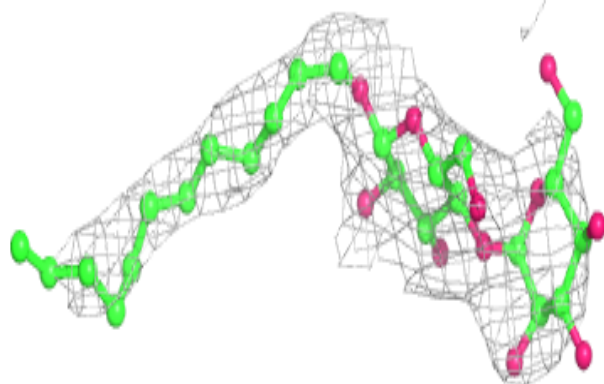


Electron density around CLA b 1230:

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

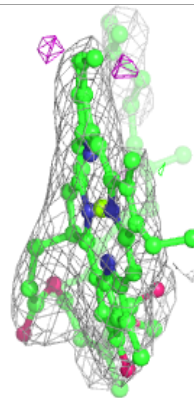
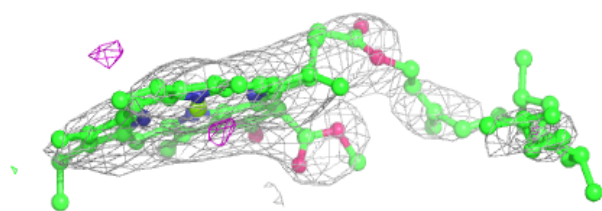
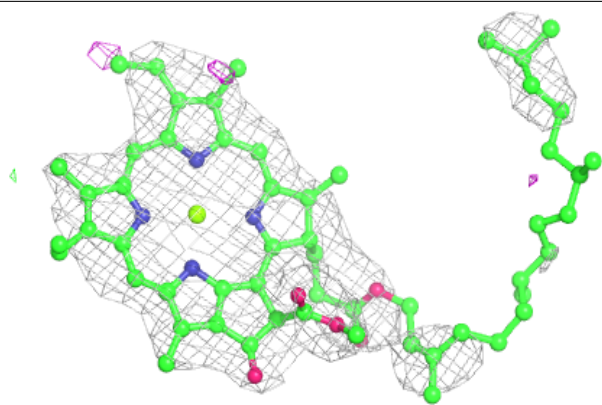
**Electron density around LMT F 6001:**

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

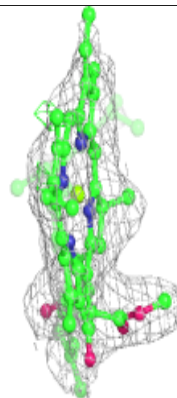
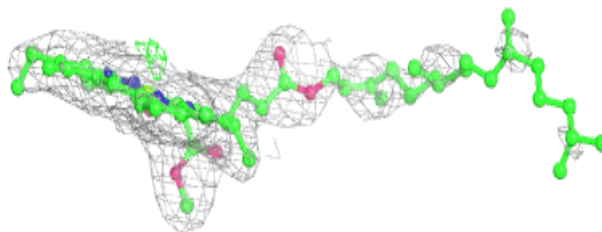
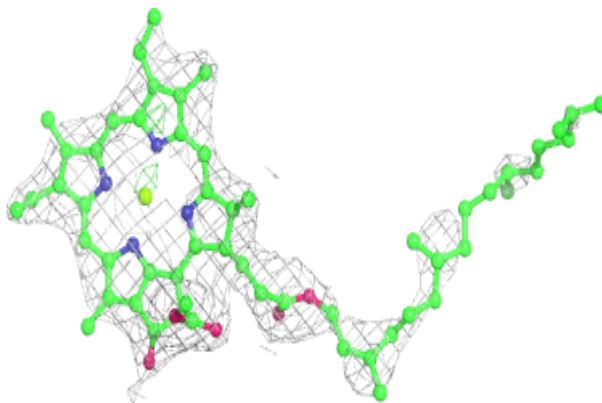


Electron density around CLA 1 1101:

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

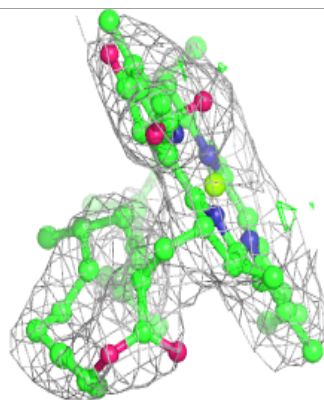
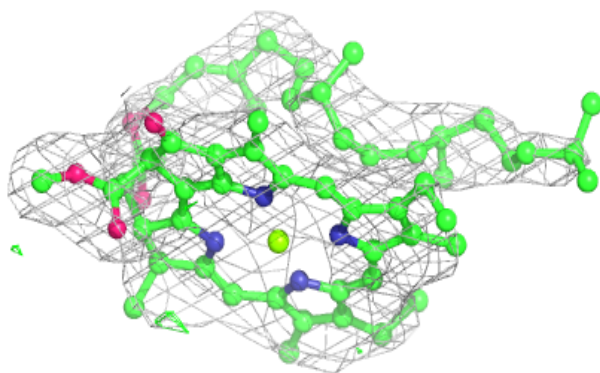
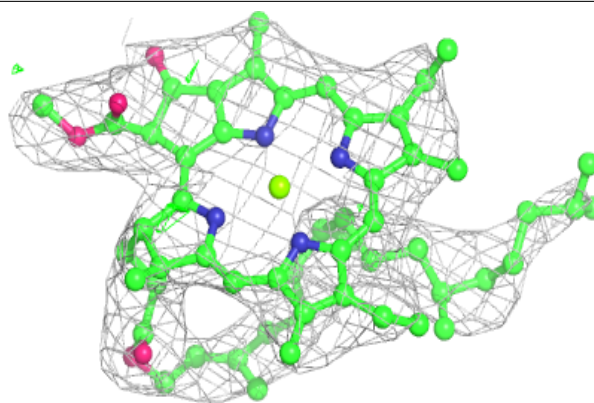
**Electron density around CLA B 1234:**

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

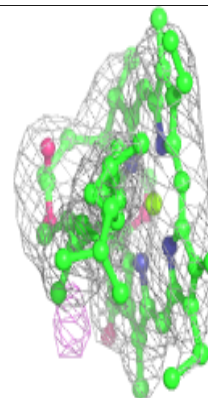
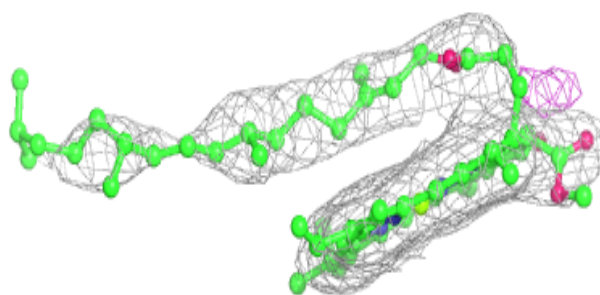
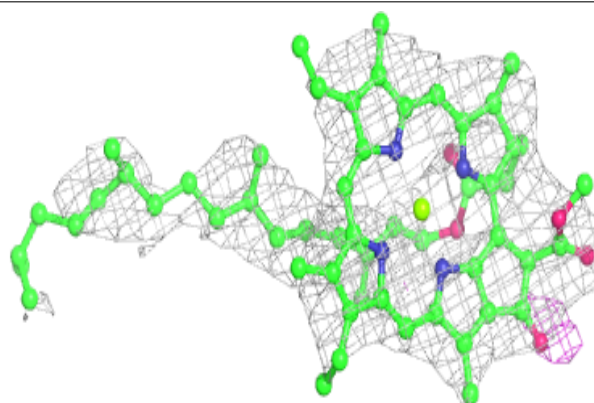


Electron density around CLA B 1214:

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

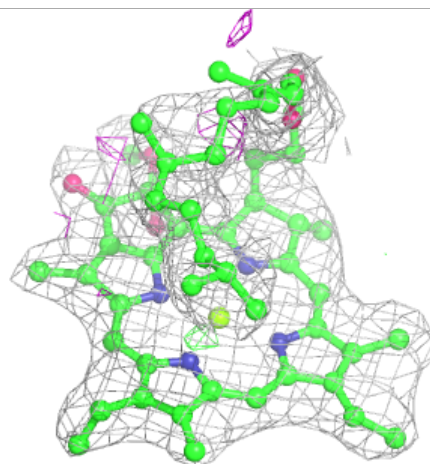
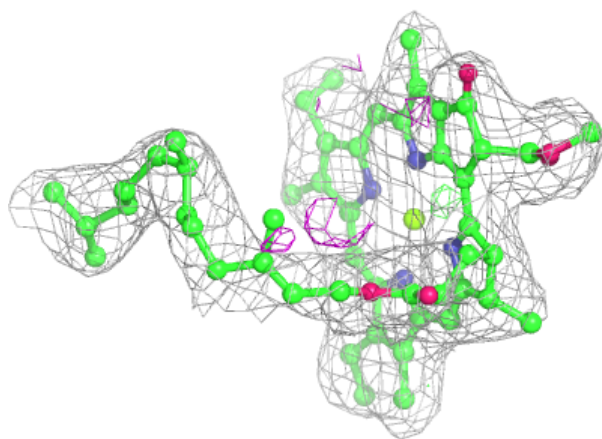
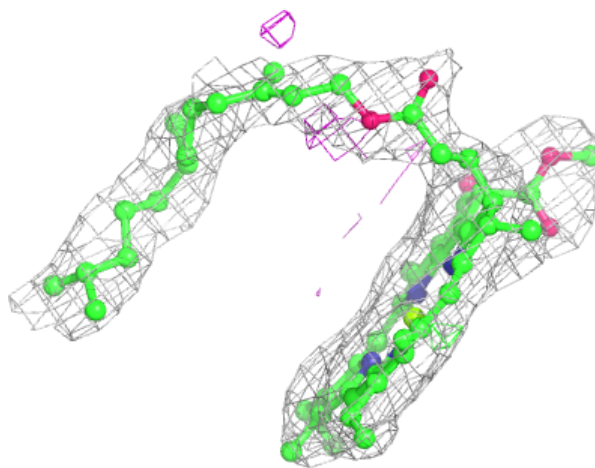
**Electron density around CLA B 1213:**

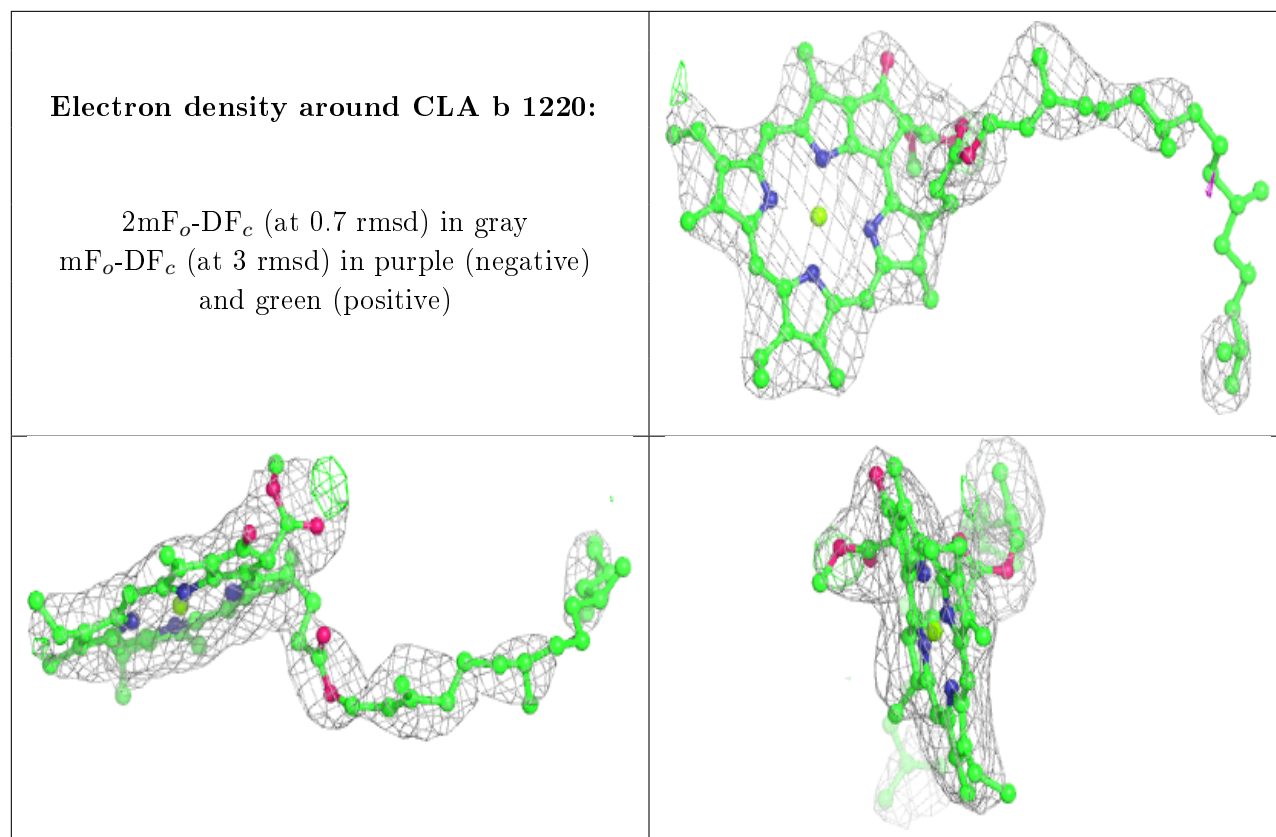
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

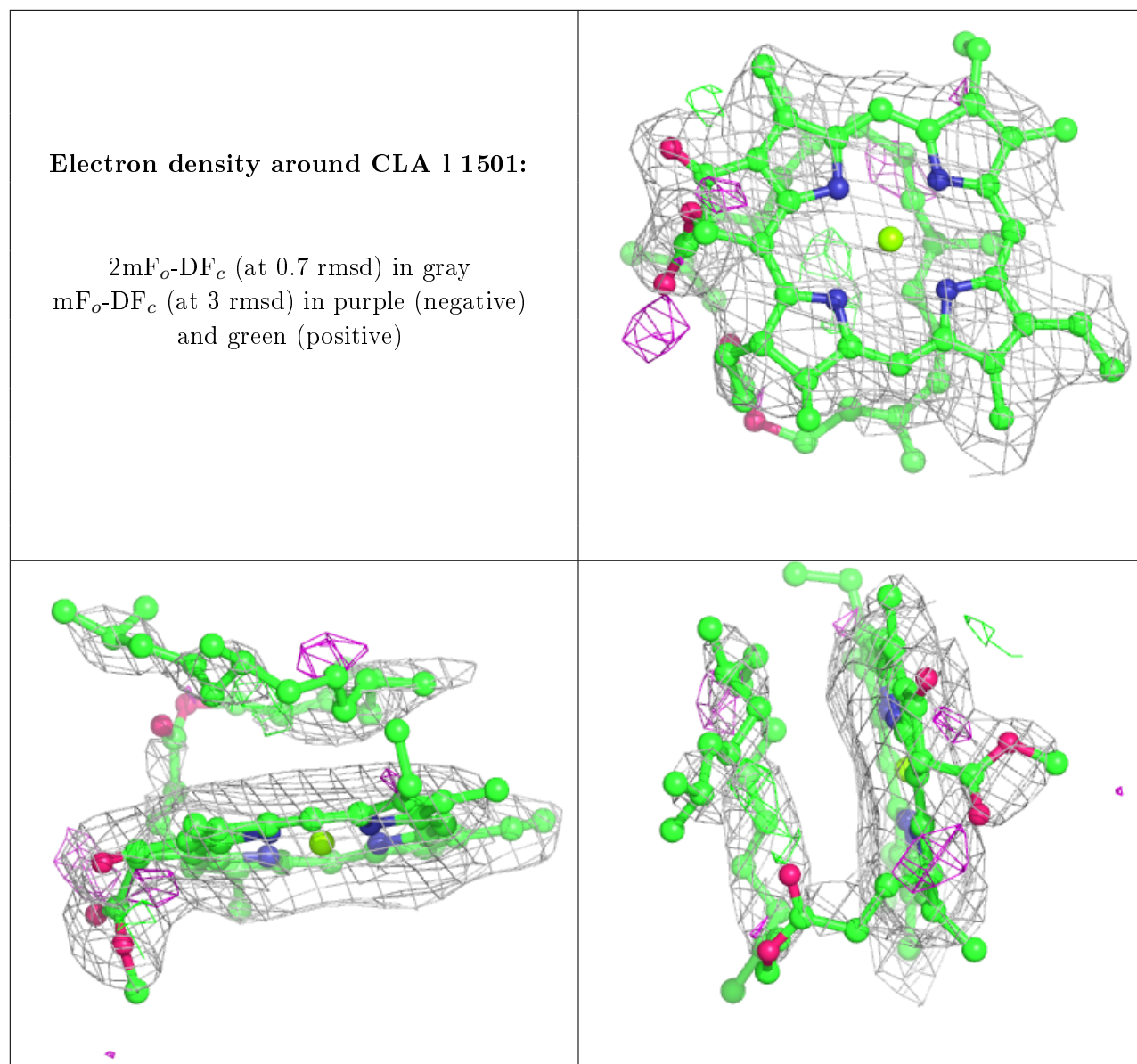


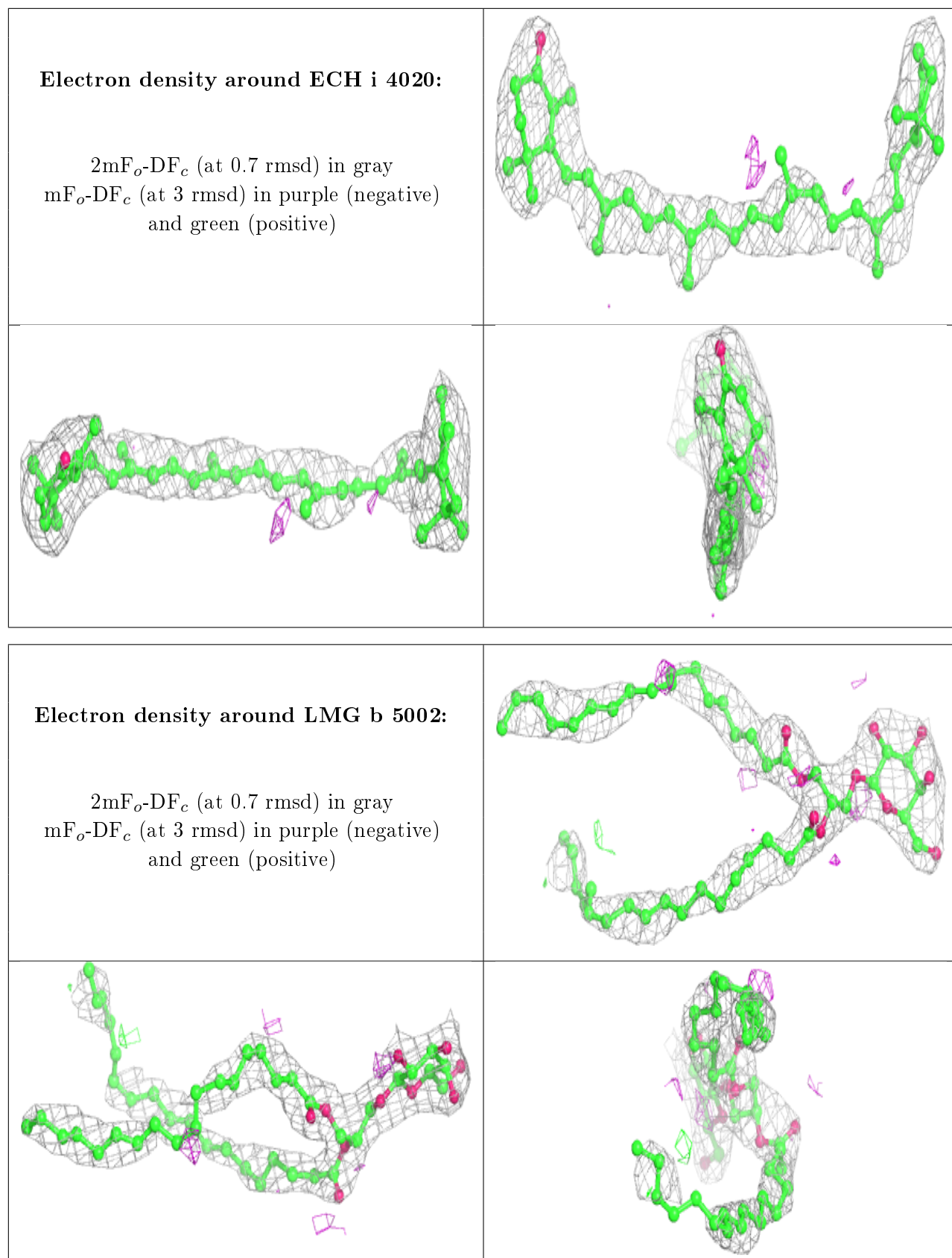
Electron density around CLA b 1208:

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



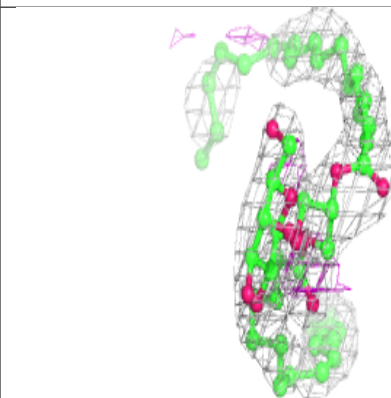
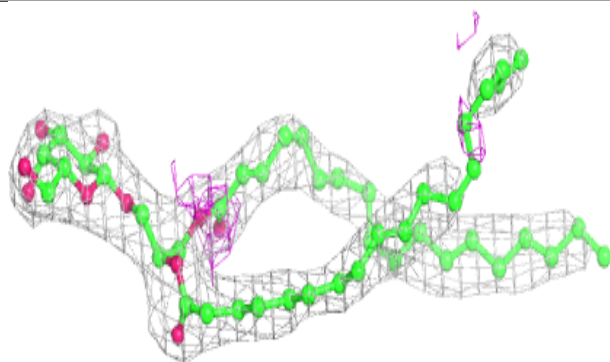
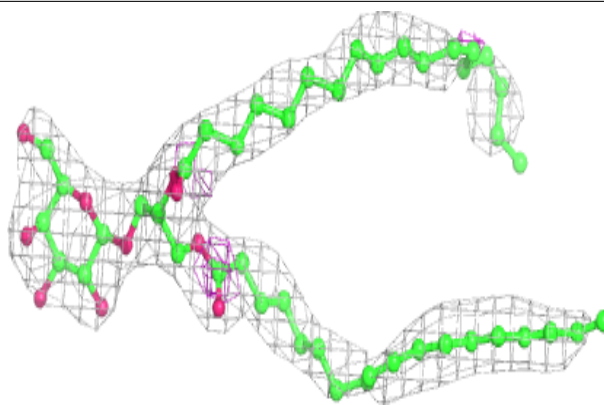




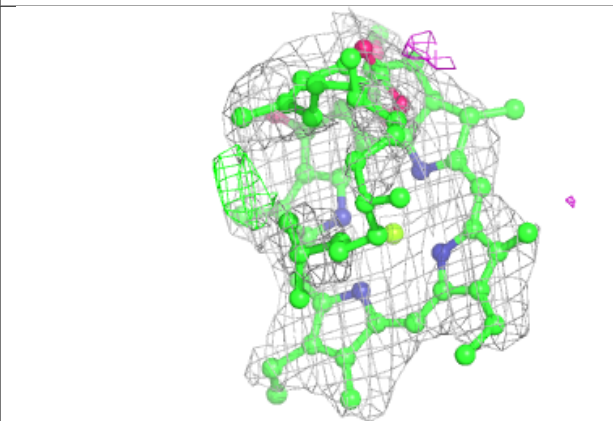
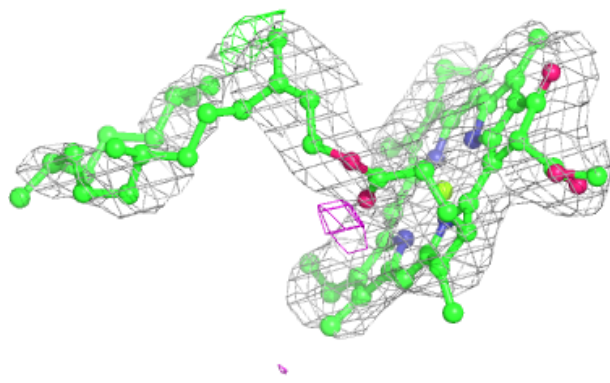
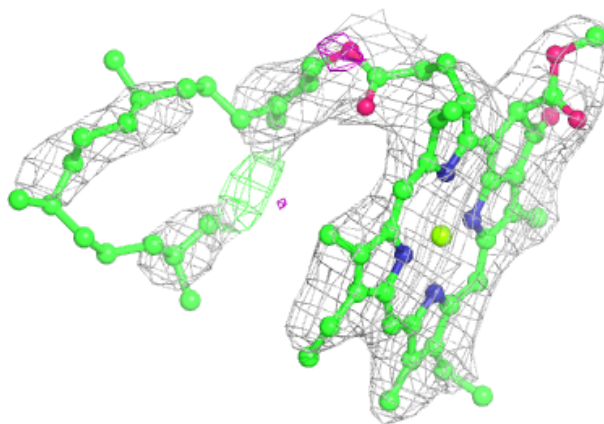


Electron density around LMG B 5002:

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

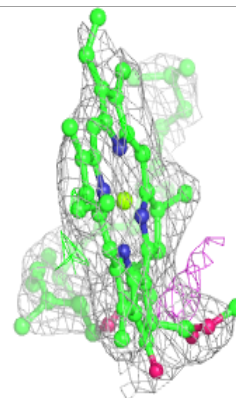
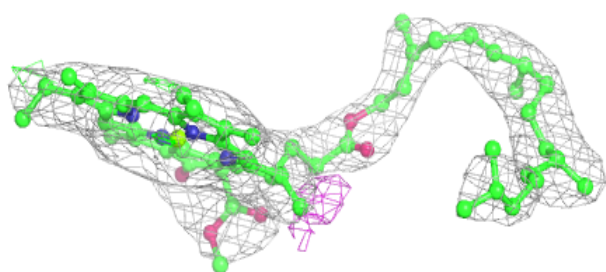
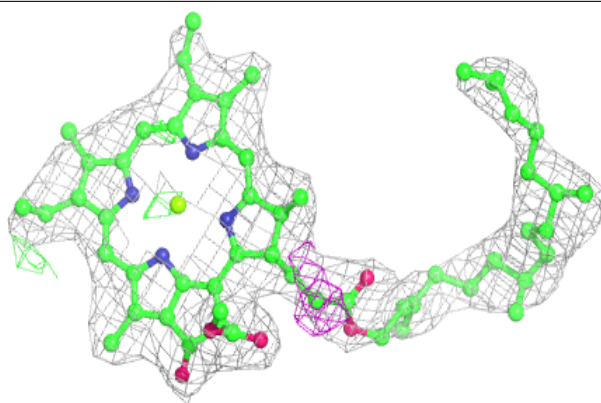
**Electron density around CLA b 1228:**

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

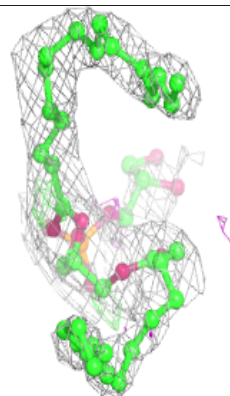
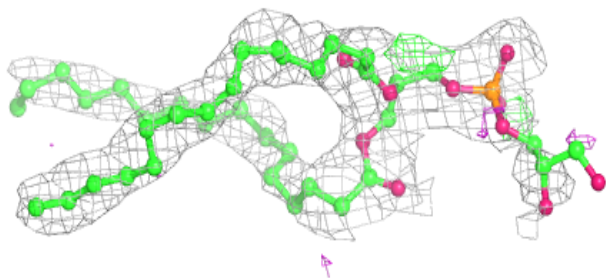
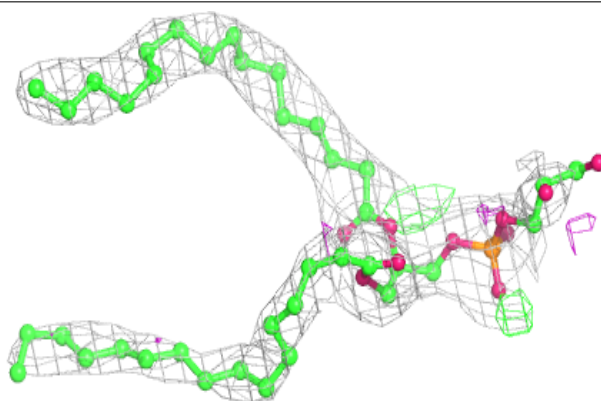


Electron density around CLA 1 1125:

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

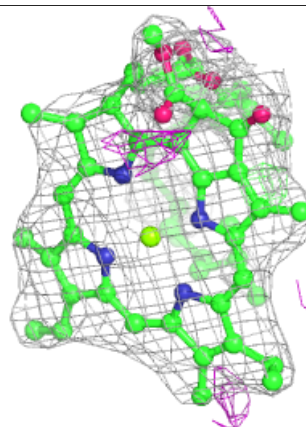
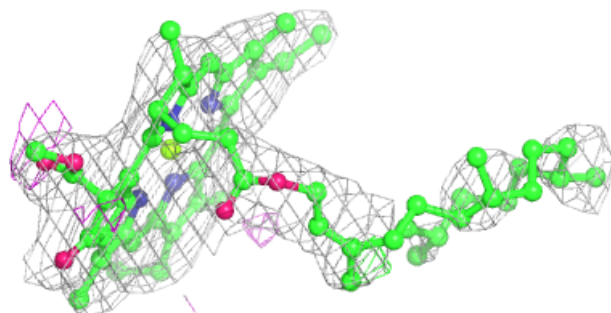
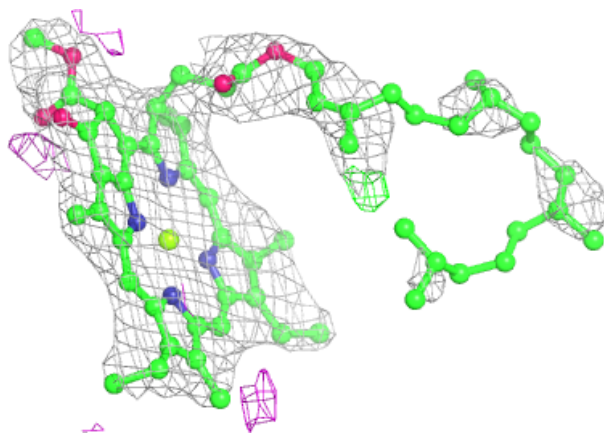
**Electron density around LHG a 5001:**

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

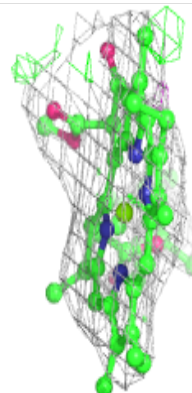
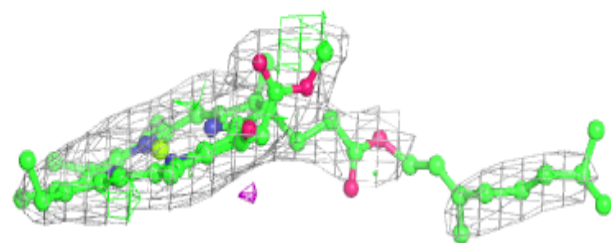
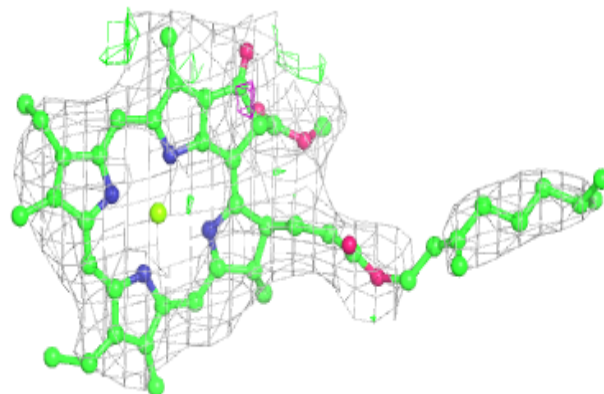


Electron density around CLA B 1228:

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

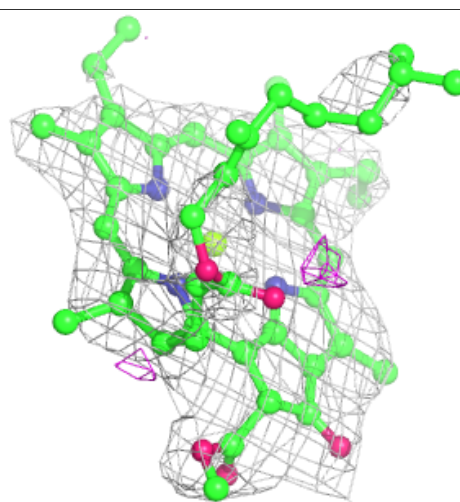
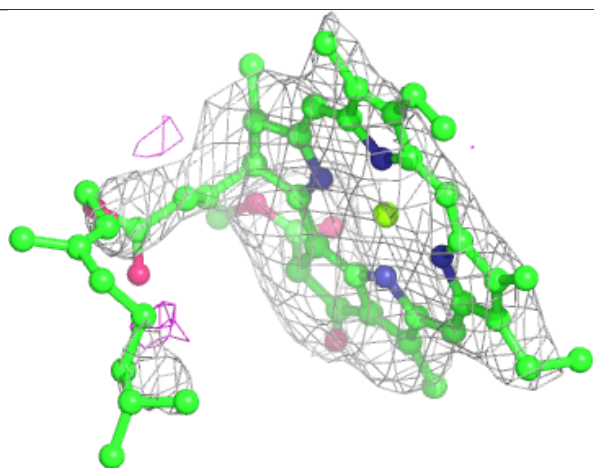
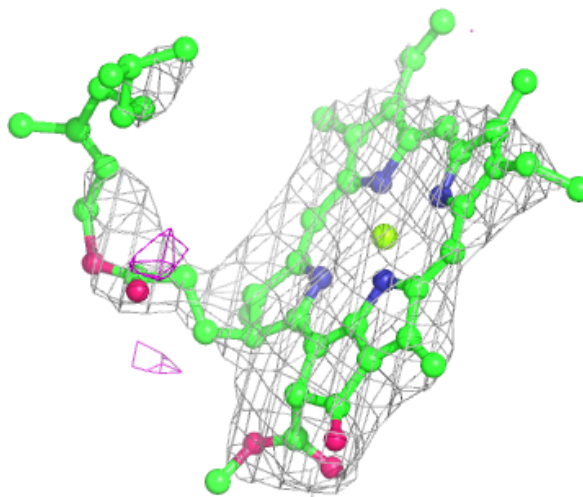
**Electron density around CLA 2 1223:**

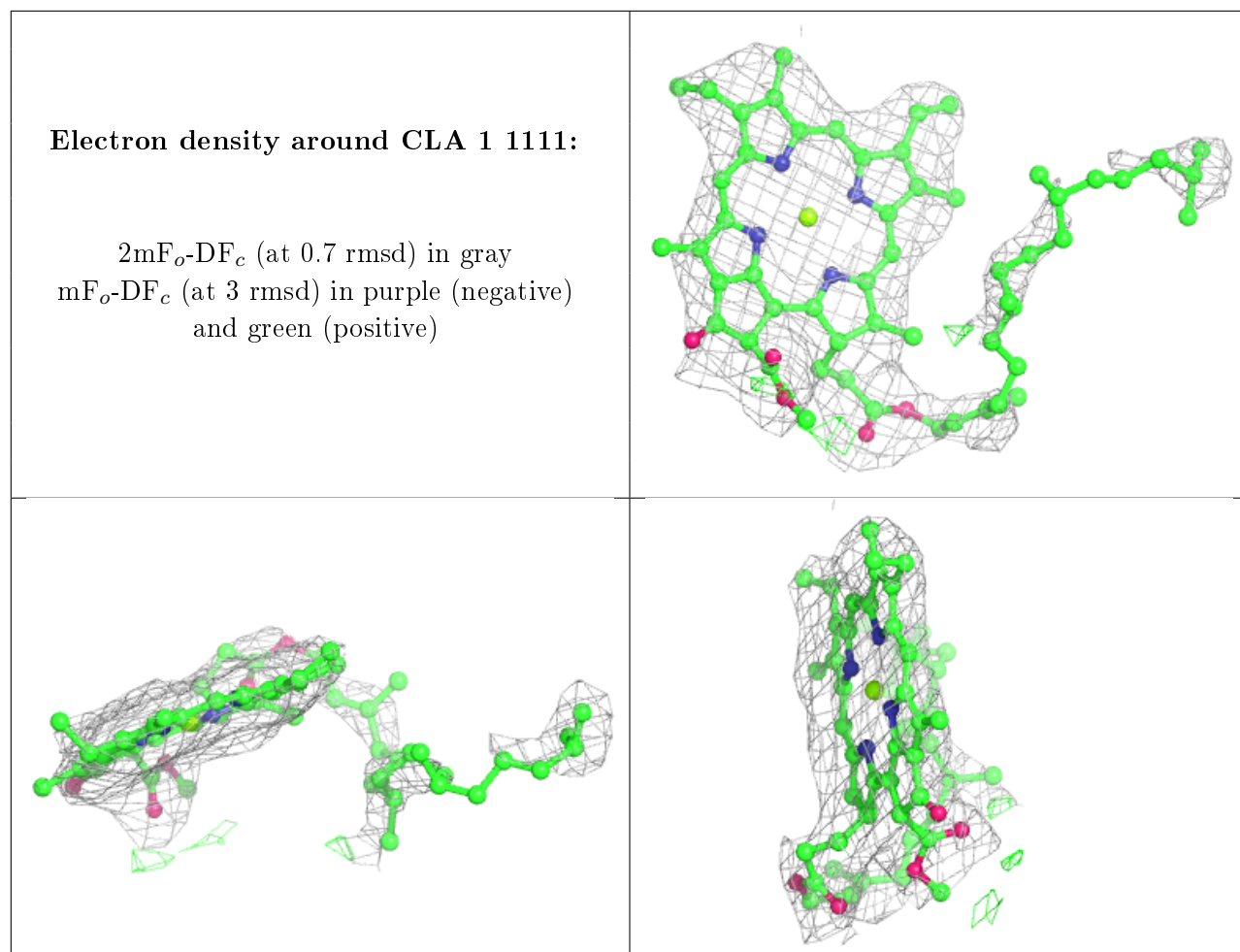
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

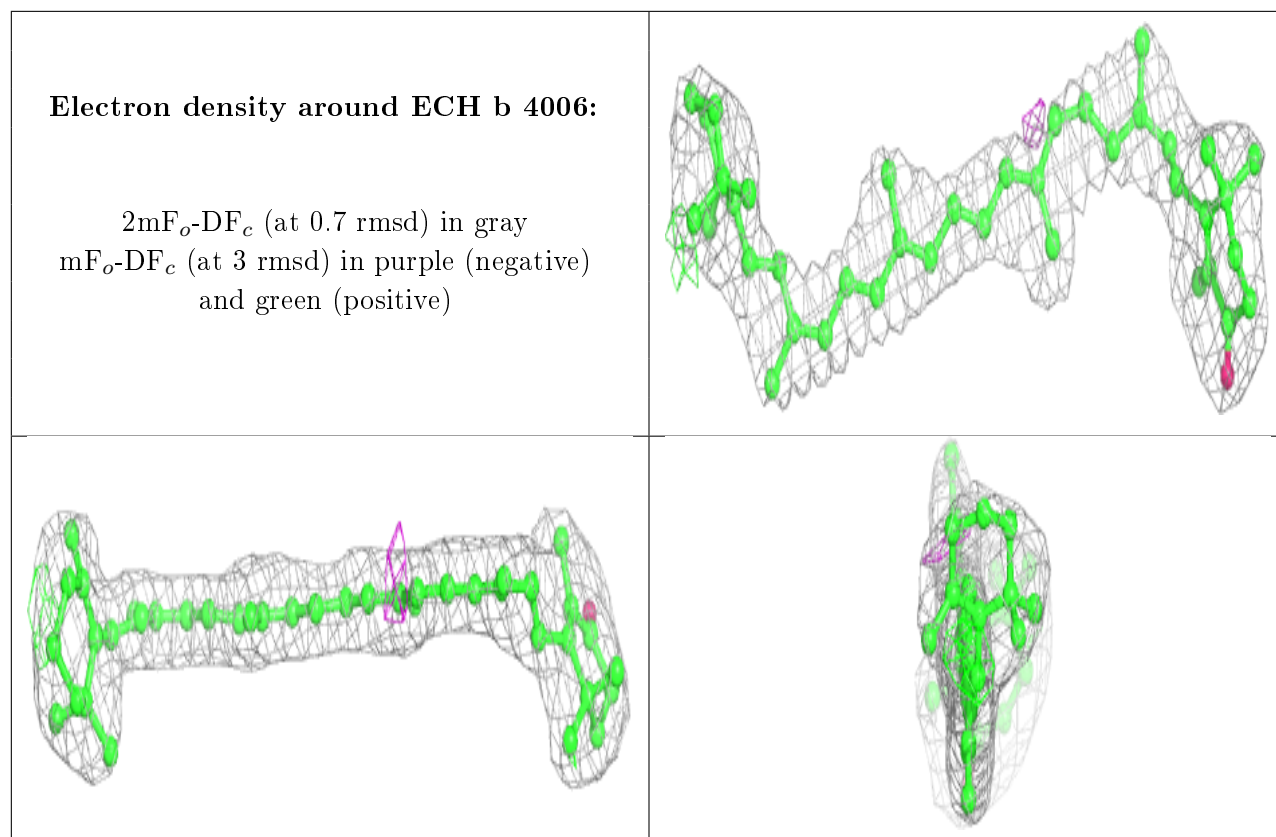


Electron density around CLA B 1227:

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

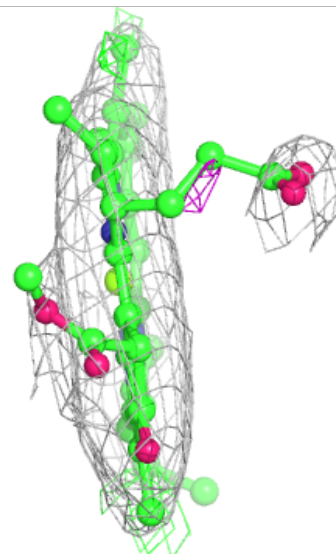
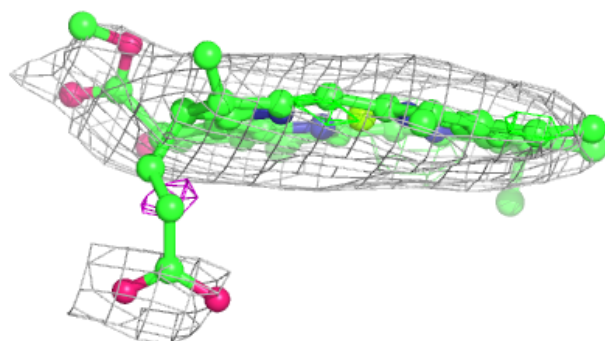
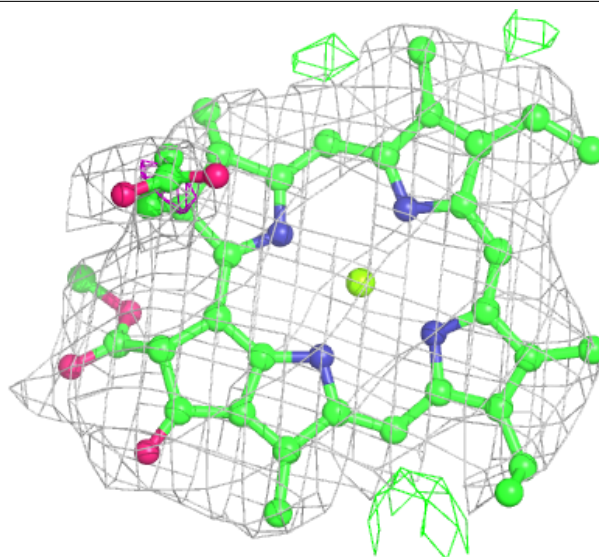






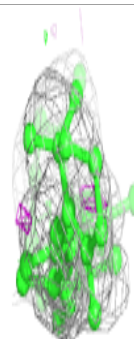
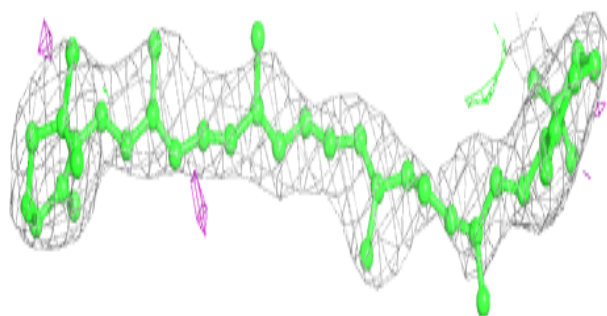
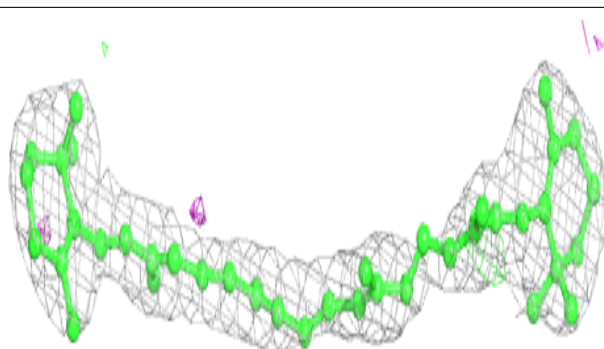
Electron density around CLA 2 1228:

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

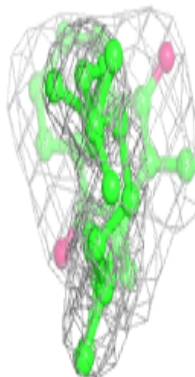
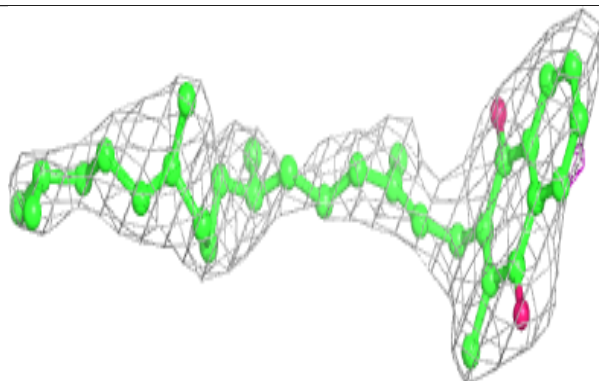
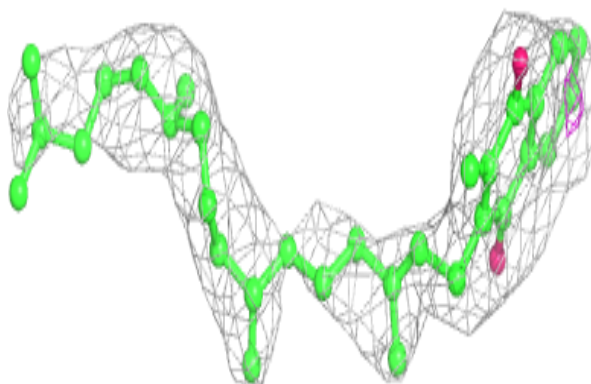


Electron density around BCR J 4013:

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

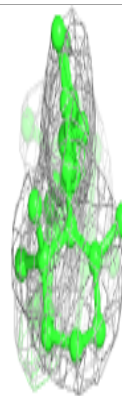
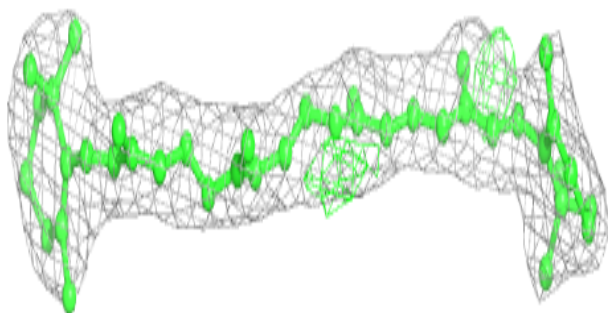
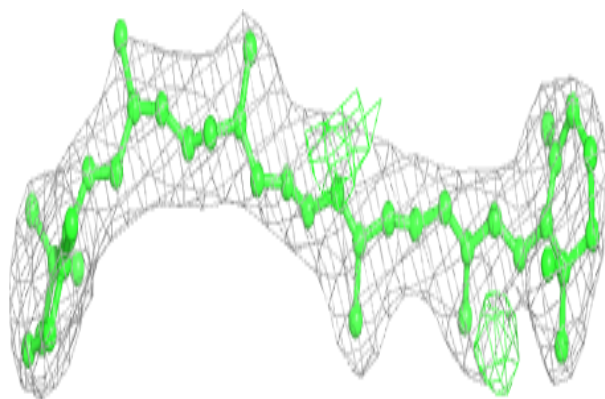
**Electron density around PQN a 2001:**

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

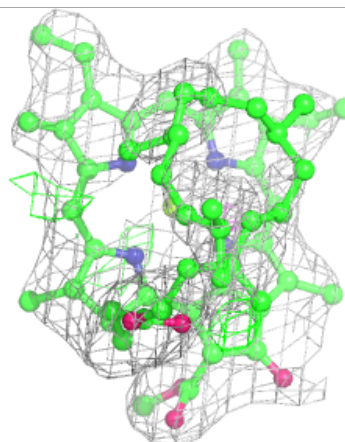
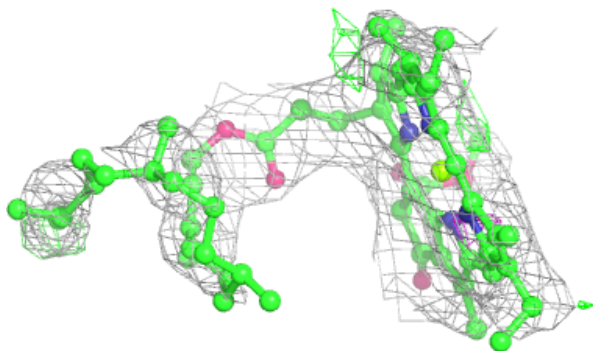
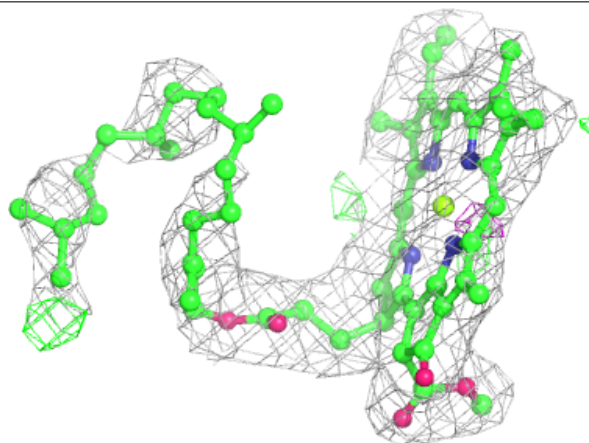


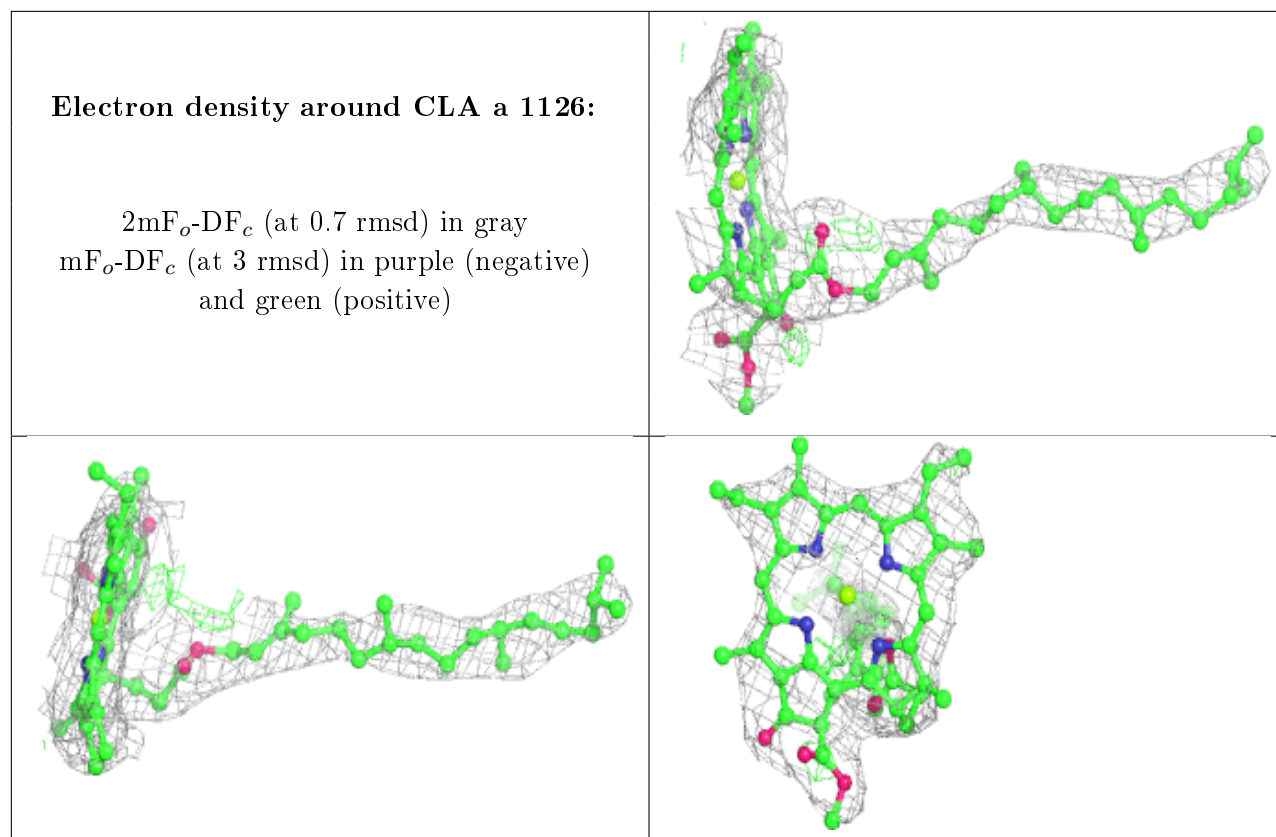
Electron density around BCR B 4017:

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

**Electron density around CLA A 1112:**

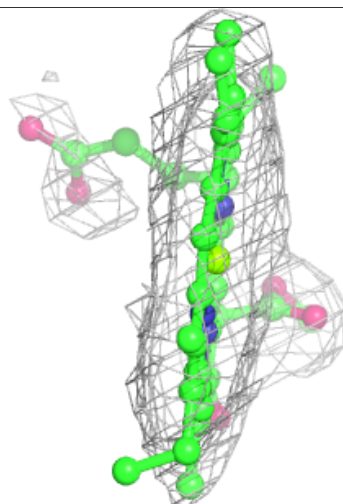
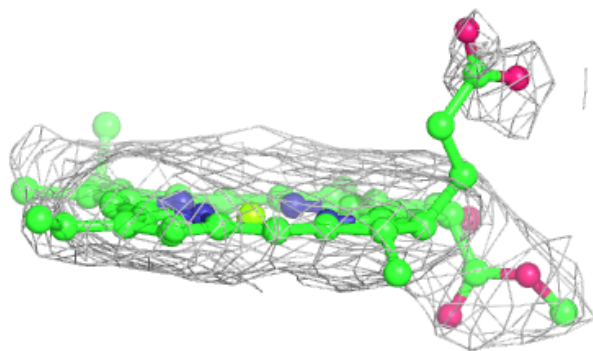
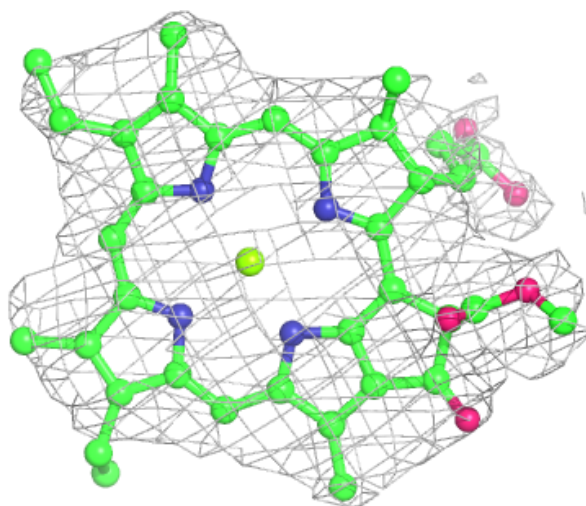
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





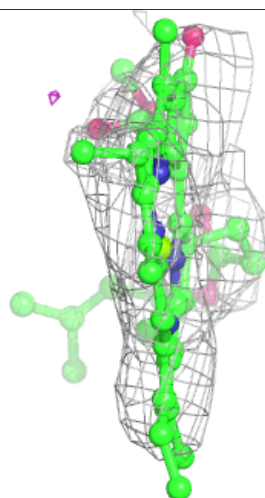
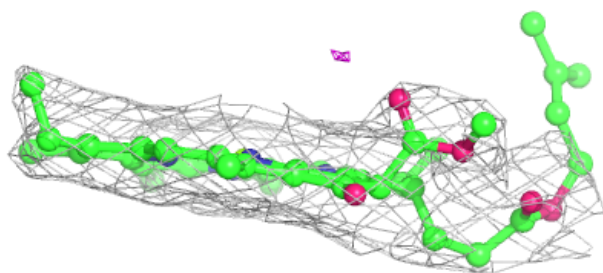
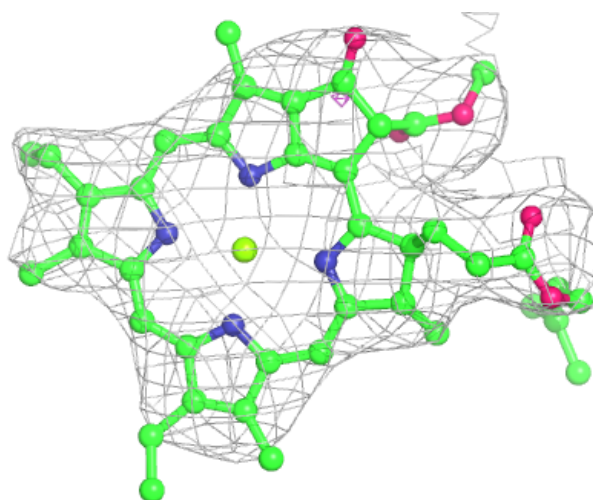
Electron density around CLA 8 1401:

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



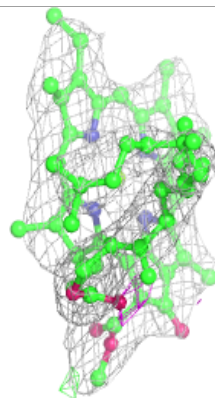
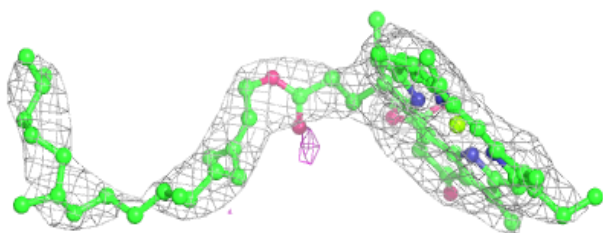
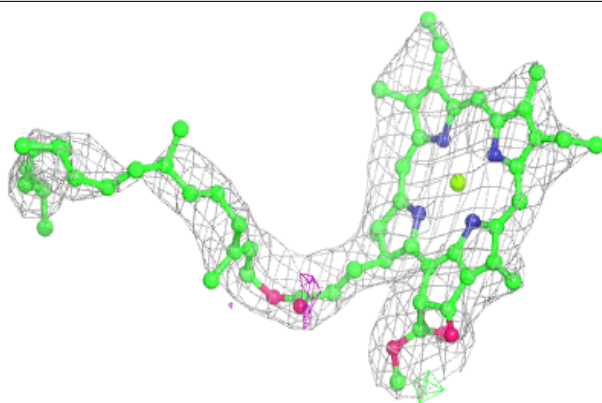
Electron density around CLA f 1301:

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

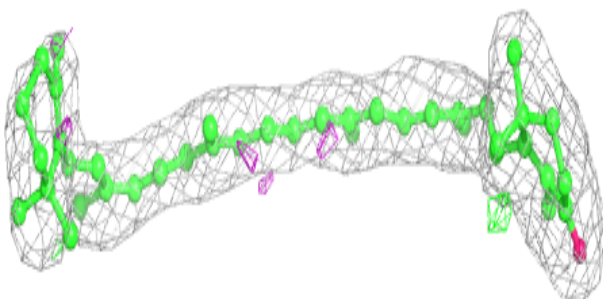
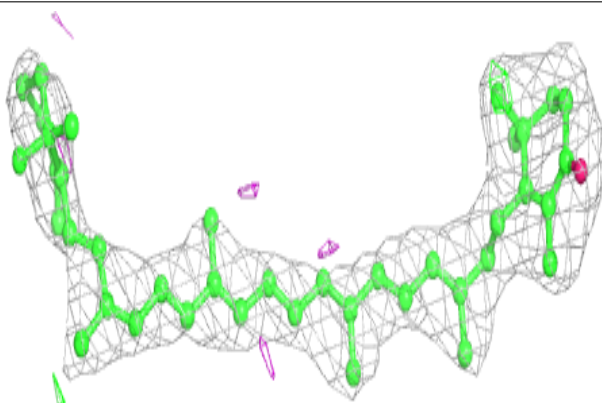


Electron density around CLA 2 1206:

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

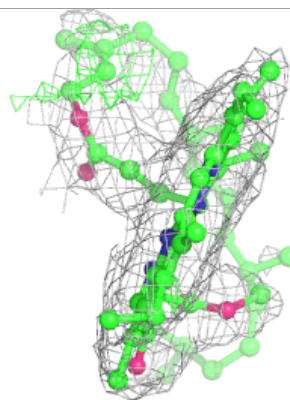
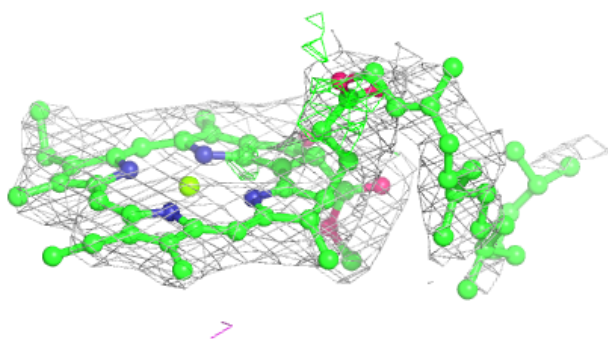
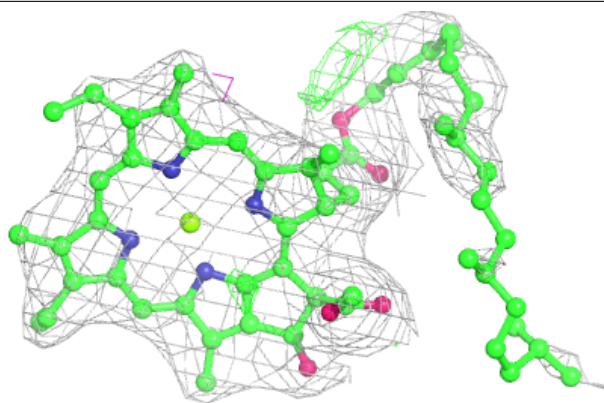
**Electron density around ECH m 4021:**

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

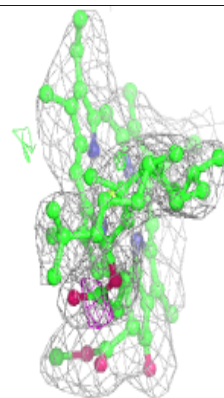
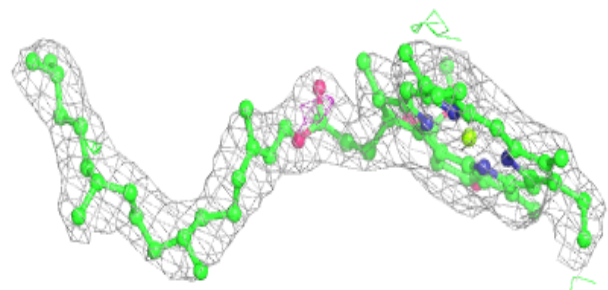
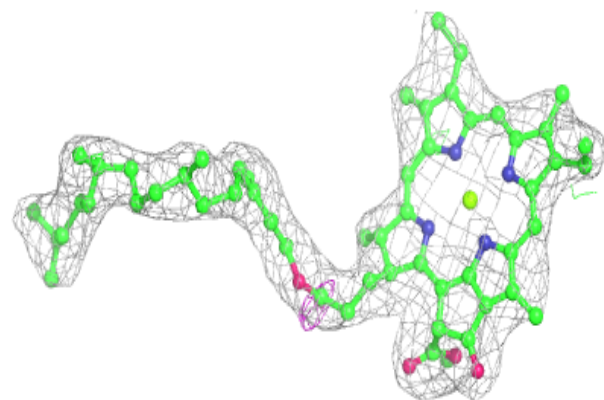


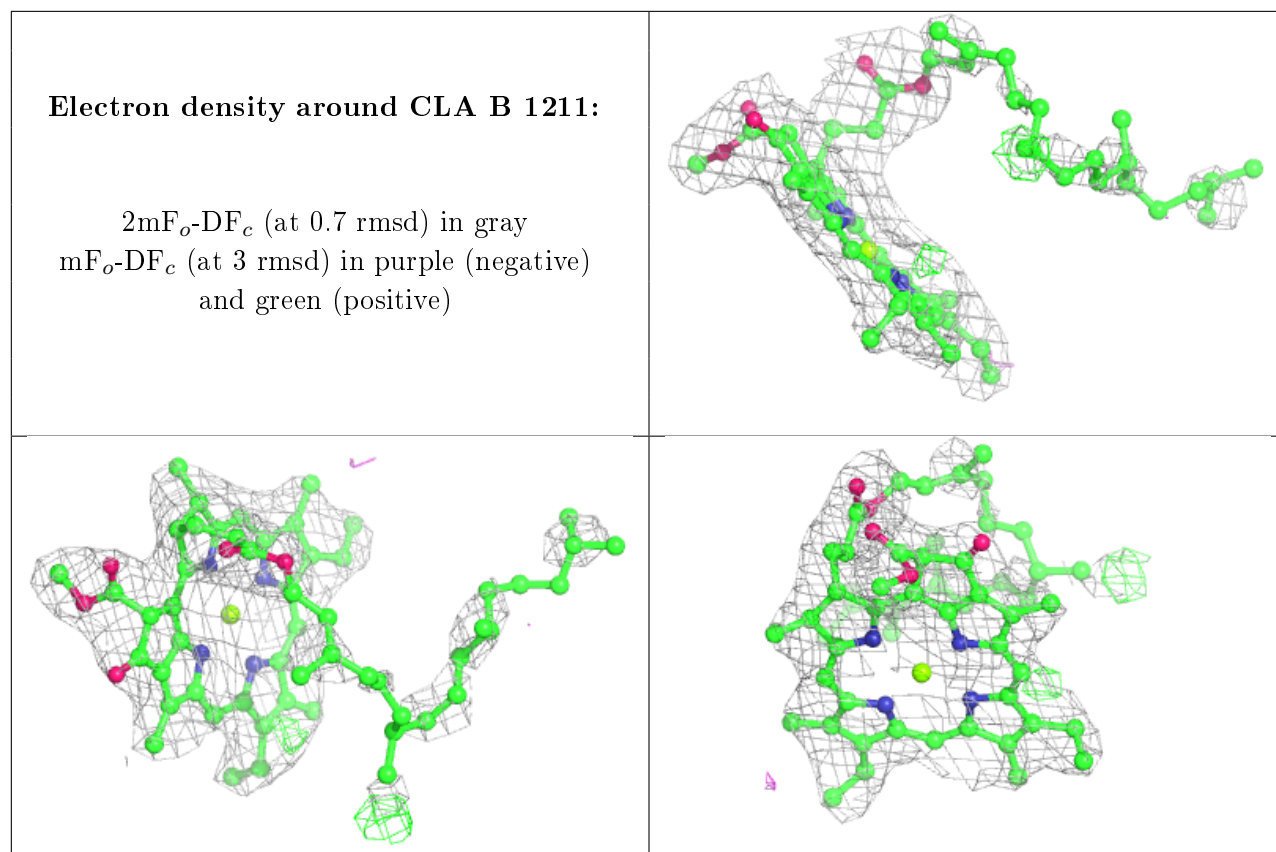
Electron density around CLA K 1402:

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

**Electron density around CLA B 1210:**

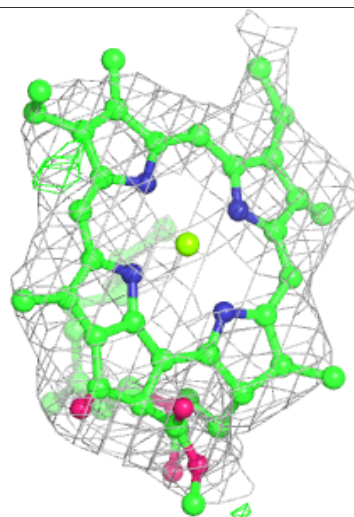
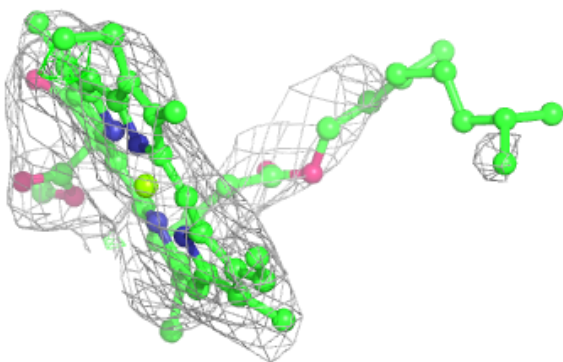
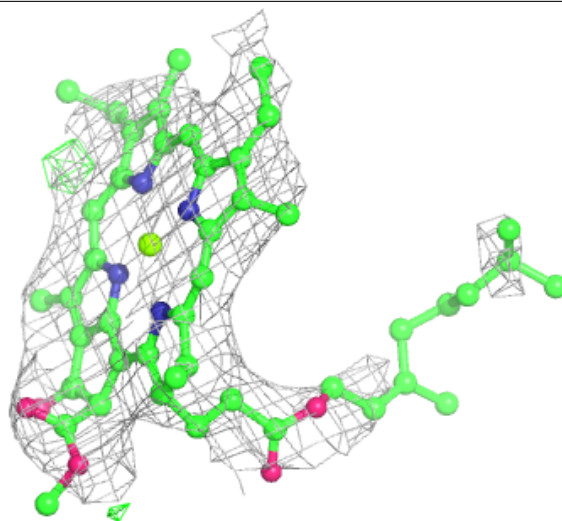
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

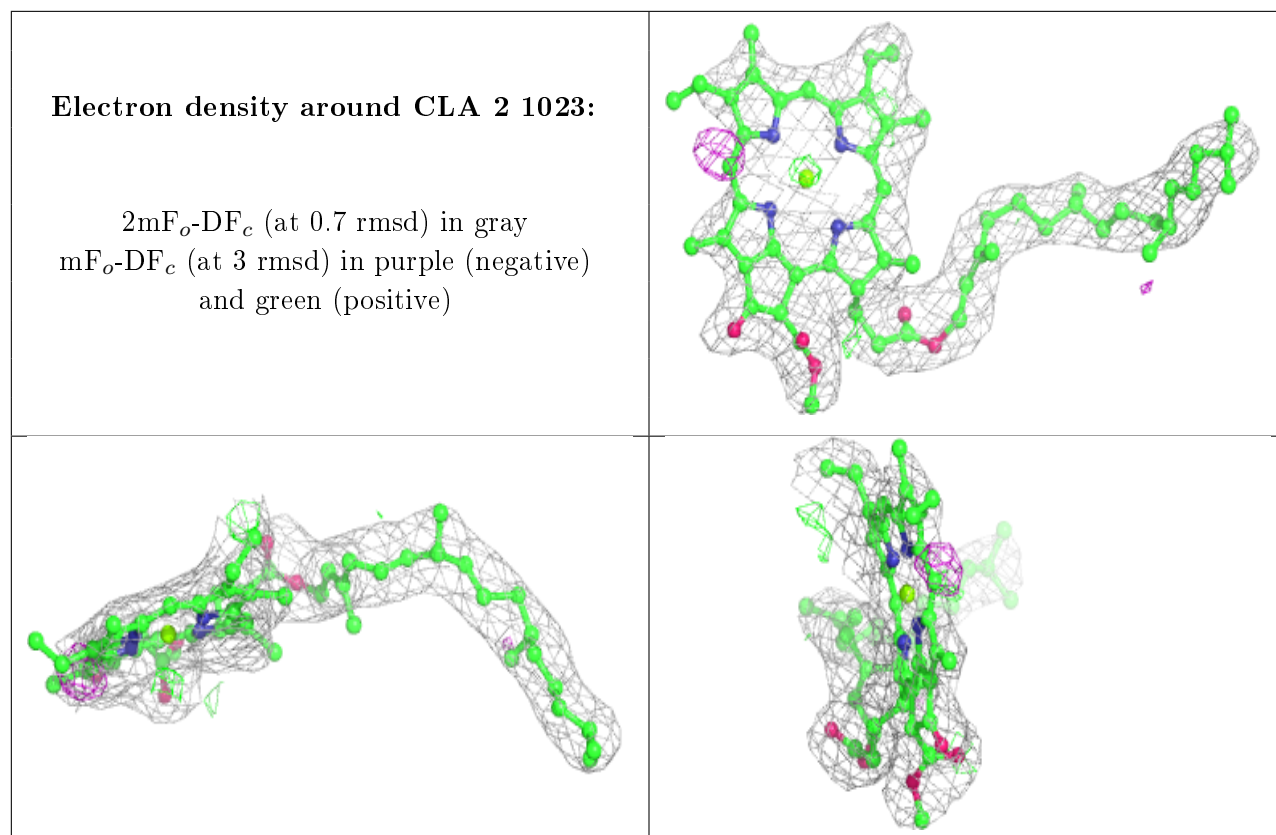




Electron density around CLA B 1212:

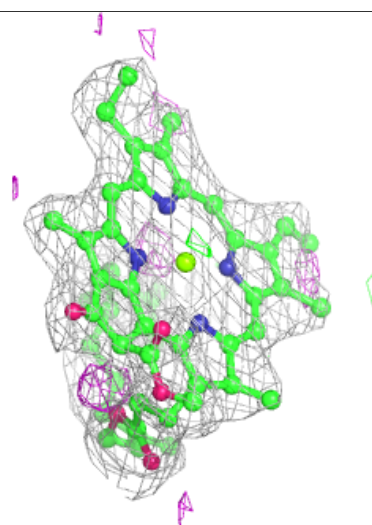
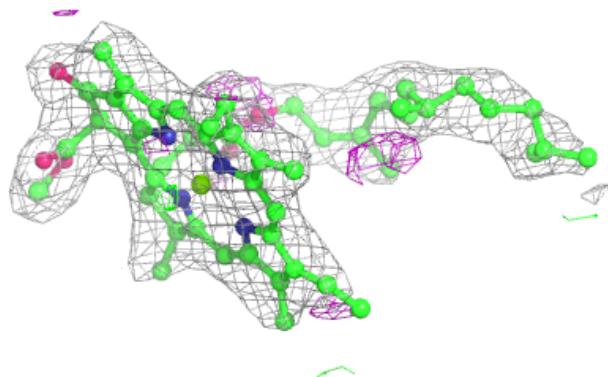
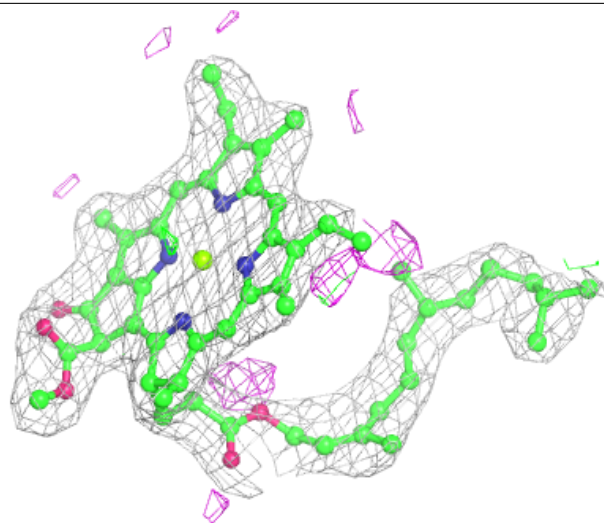
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





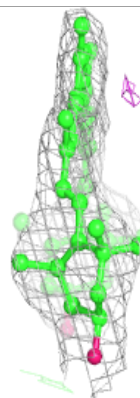
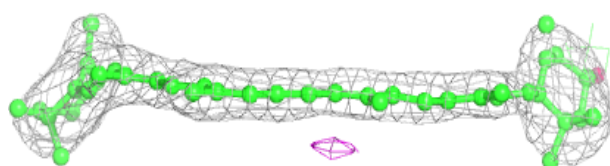
Electron density around CLA A 1122:

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

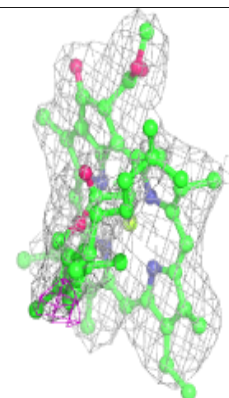
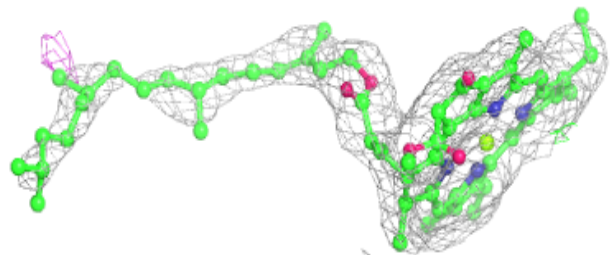
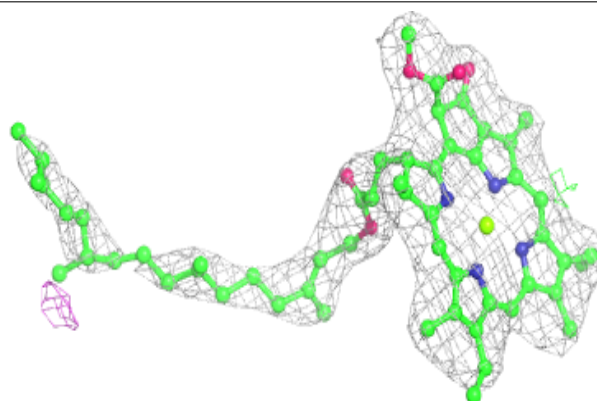


Electron density around ZEX F 4016:

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

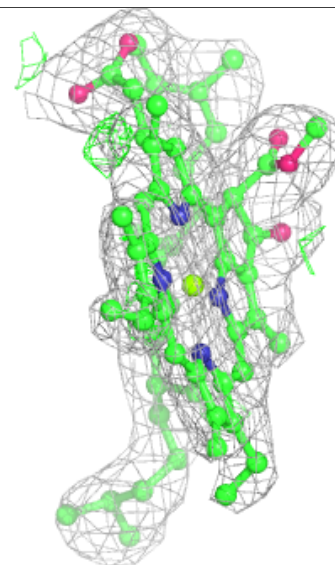
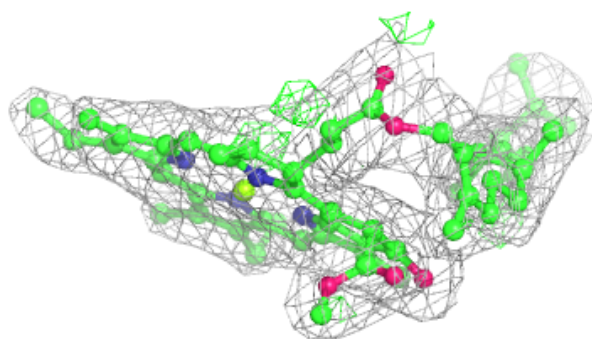
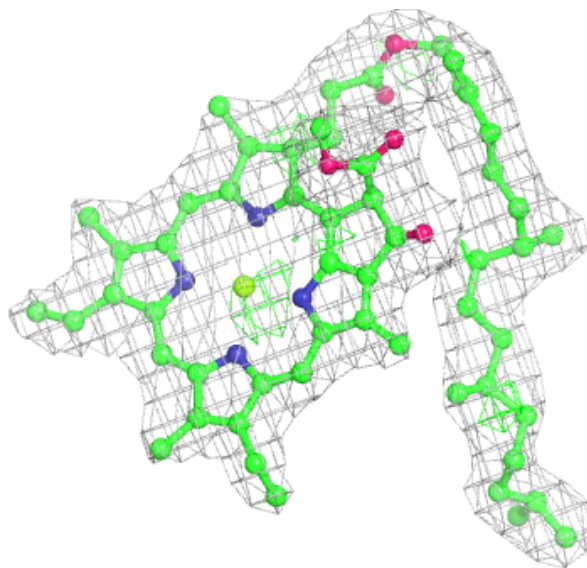
**Electron density around CLA 1 1119:**

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



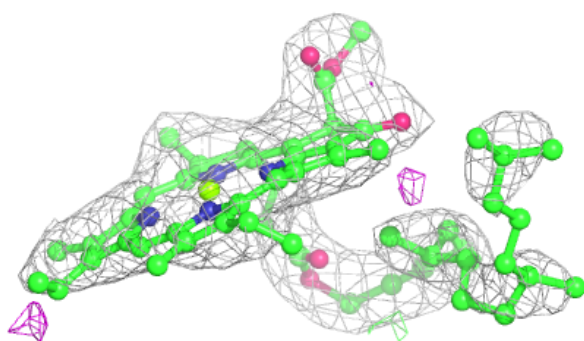
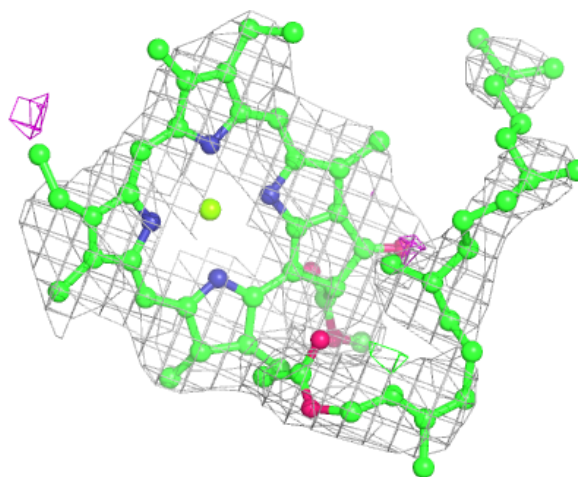
Electron density around CLA A 1123:

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



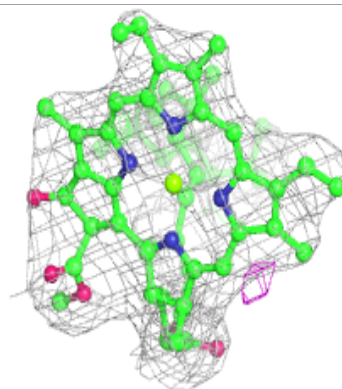
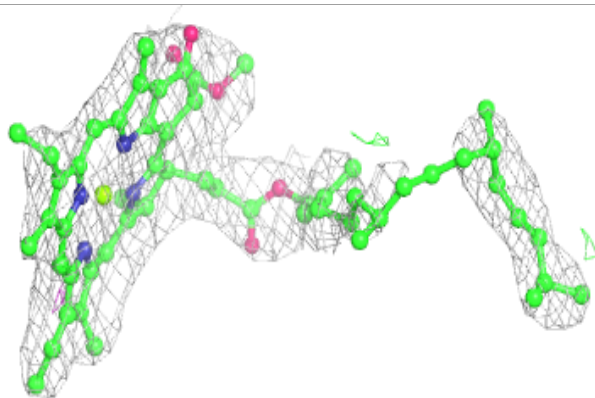
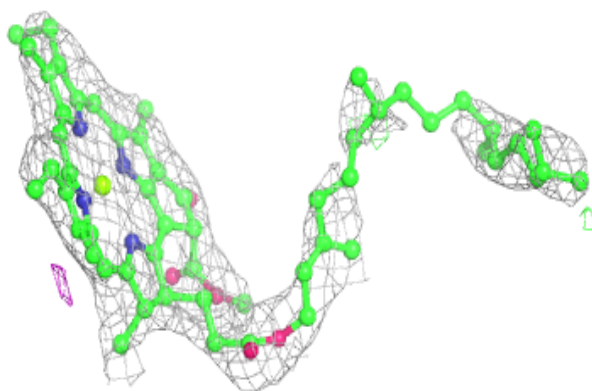
Electron density around CLA b 1229:

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

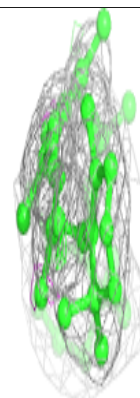
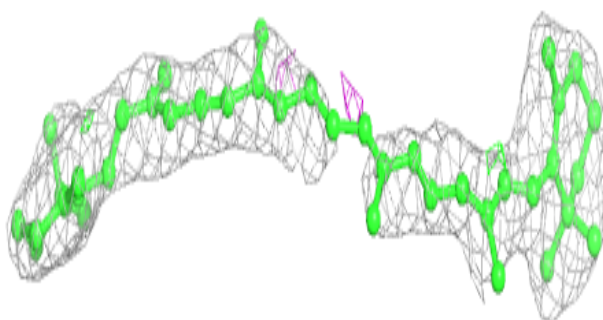
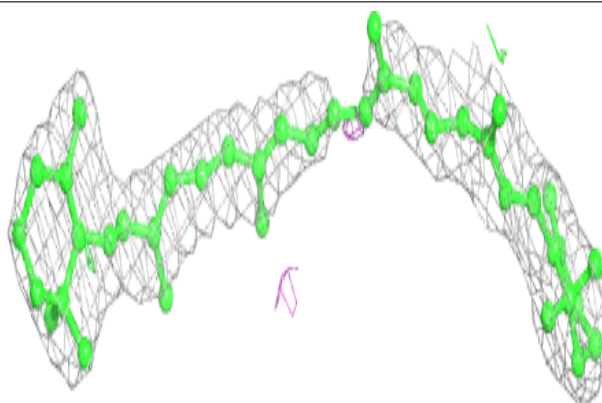


Electron density around CLA 2 1021:

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

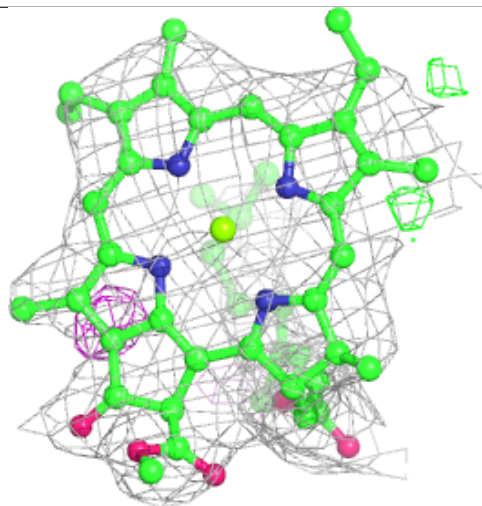
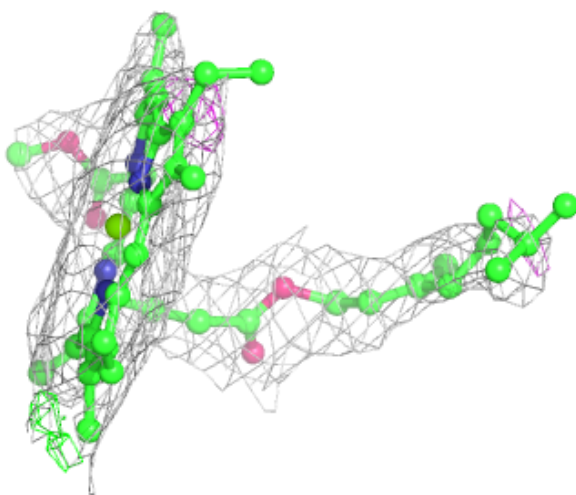
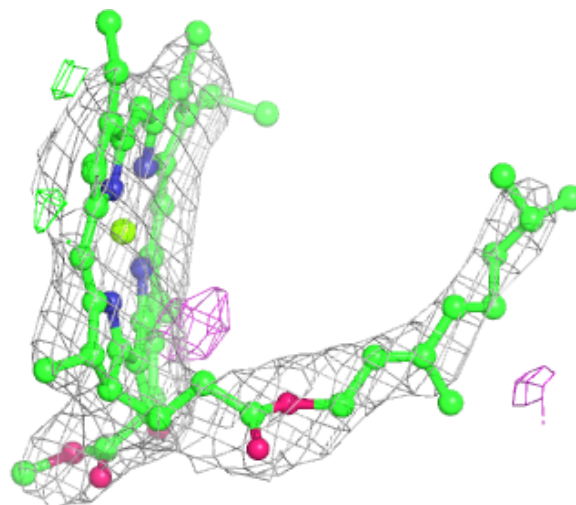
**Electron density around BCR B 4014:**

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



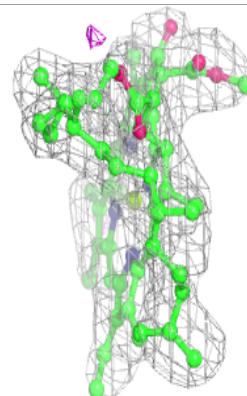
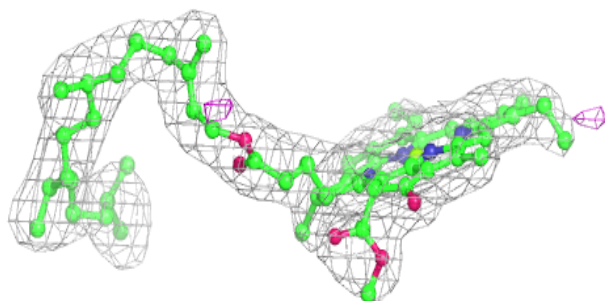
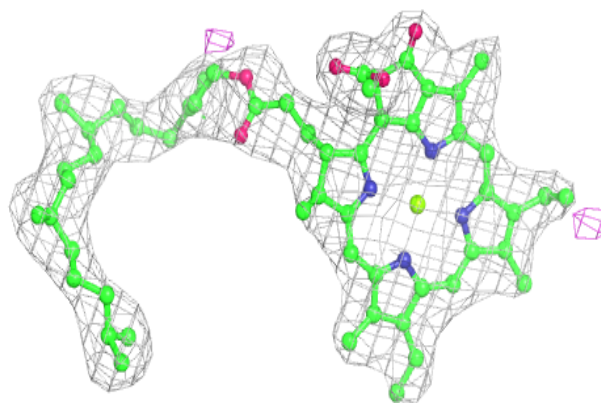
Electron density around CLA 2 1226:

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

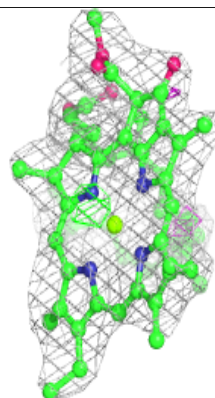
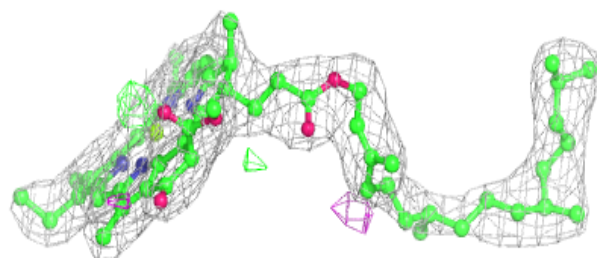
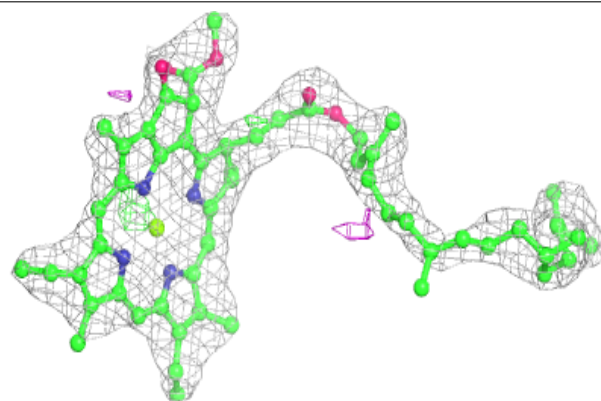


Electron density around CLA A 1125:

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

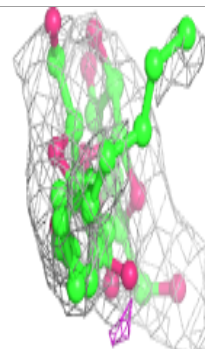
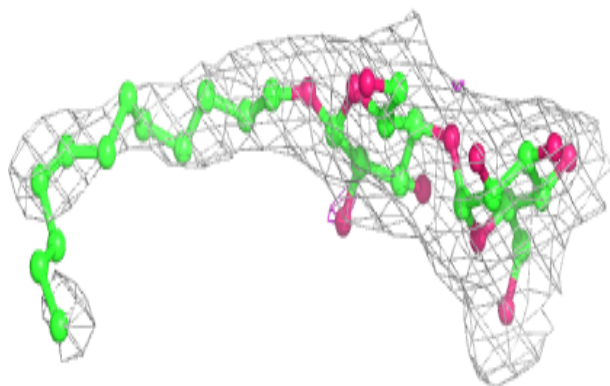
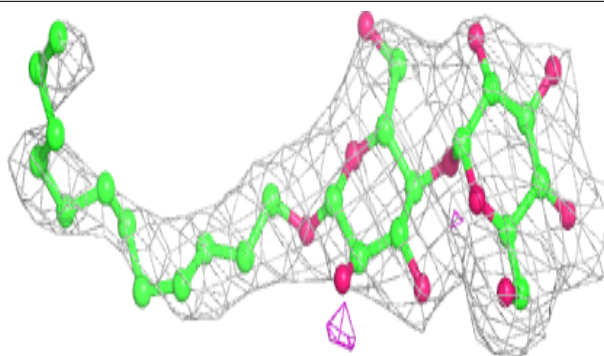
**Electron density around CLA b 1206:**

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

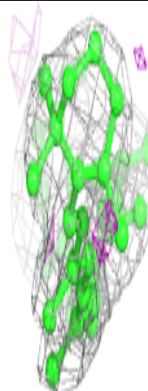
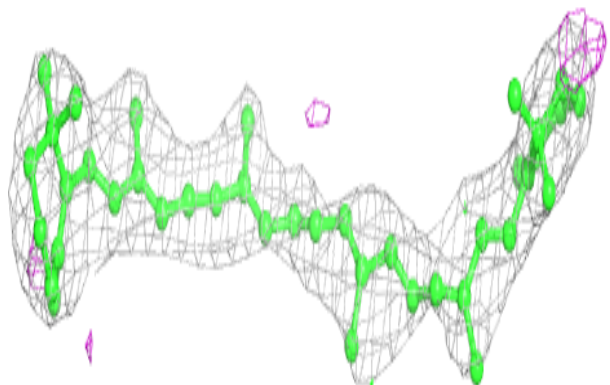
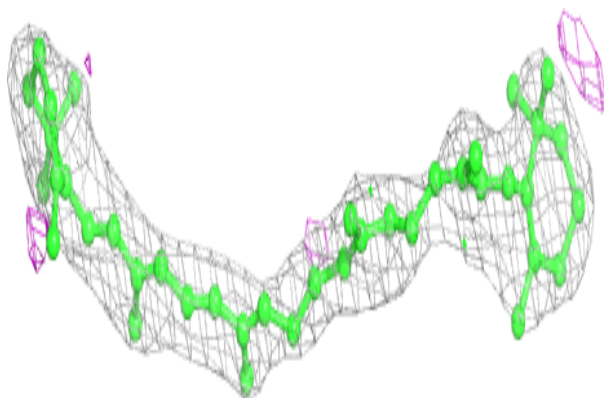


Electron density around LMT 0 6001:

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

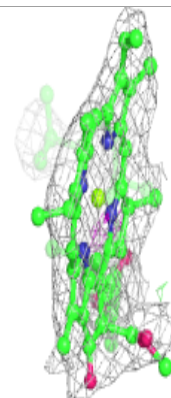
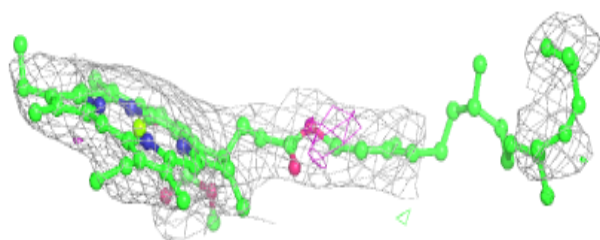
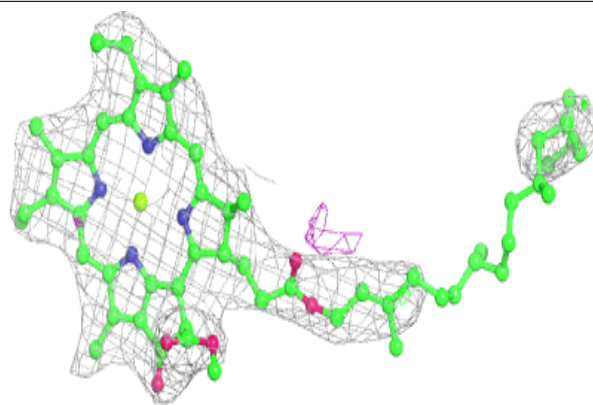
**Electron density around BCR h 4018:**

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

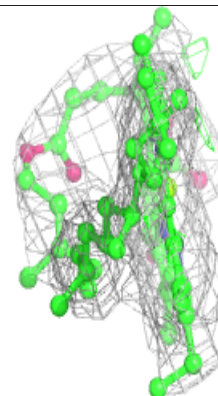
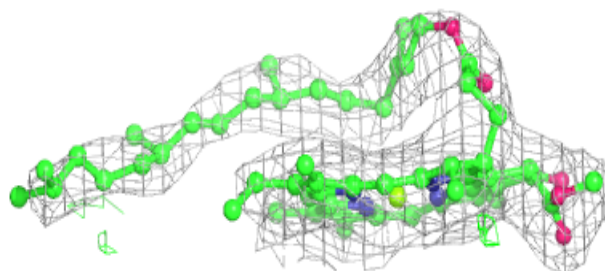
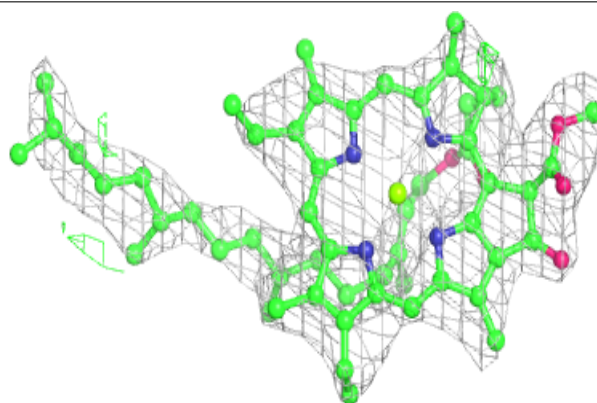


Electron density around CLA a 1135:

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

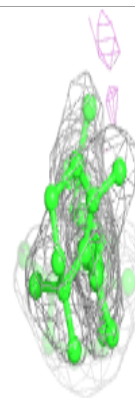
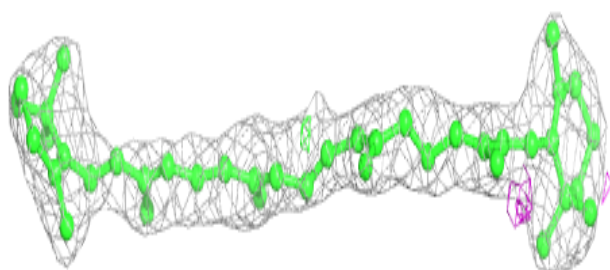
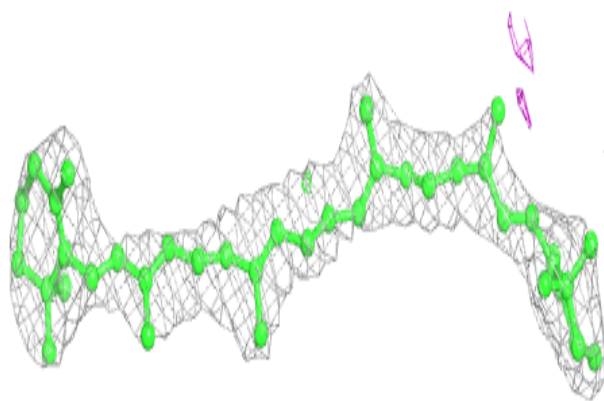
**Electron density around CLA a 1138:**

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

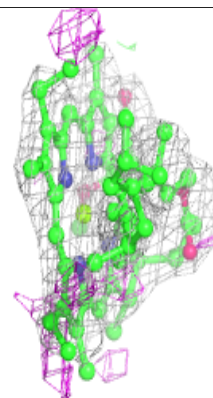
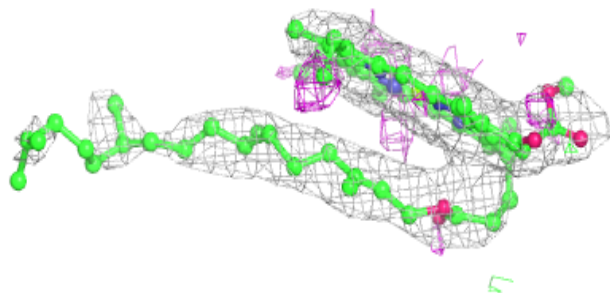
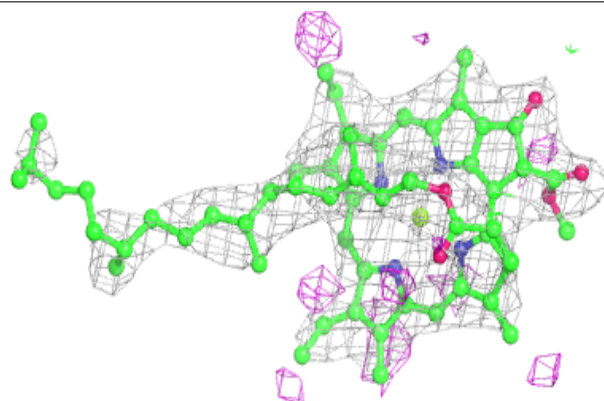


Electron density around BCR b 4017:

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

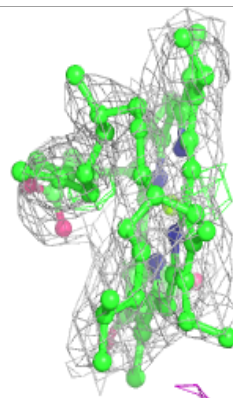
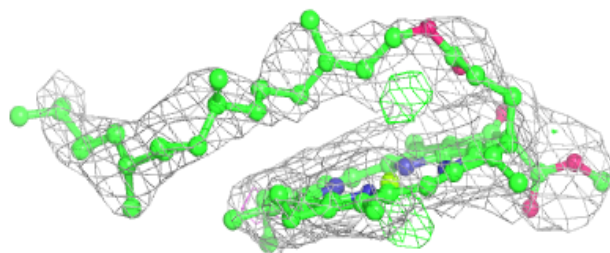
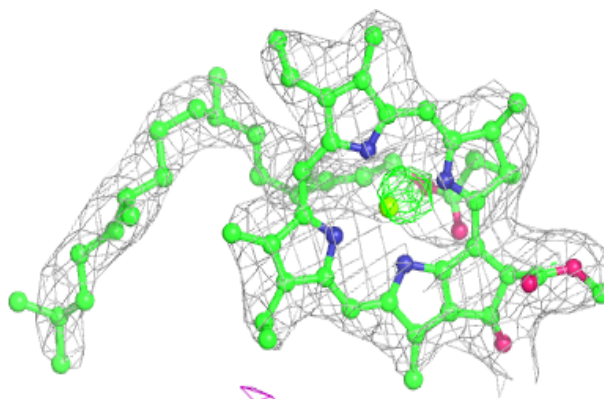
**Electron density around CLA b 1213:**

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

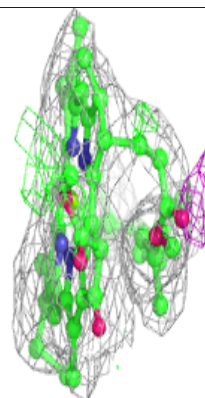
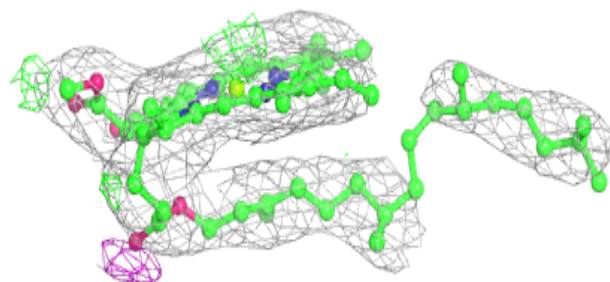
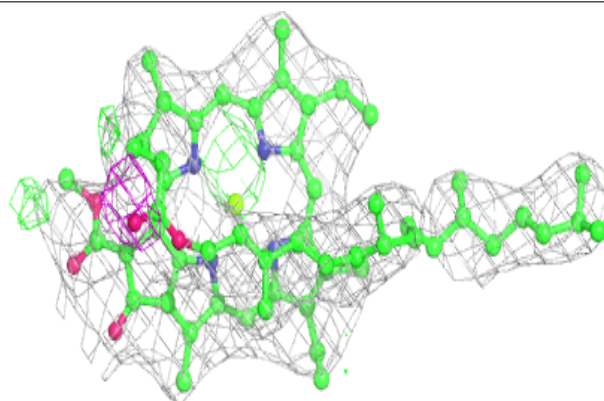


Electron density around CLA b 1235:

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

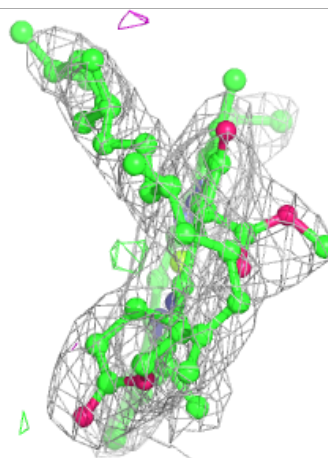
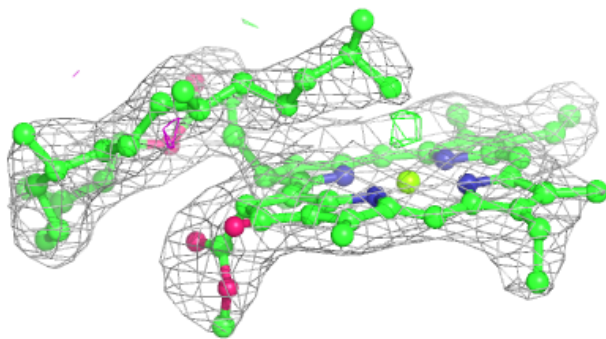
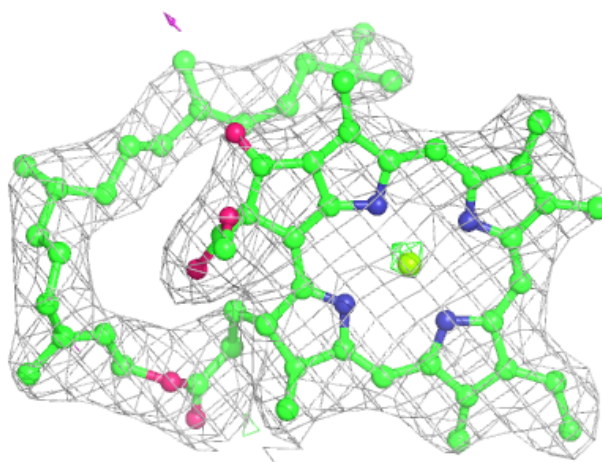
**Electron density around CLA a 1136:**

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



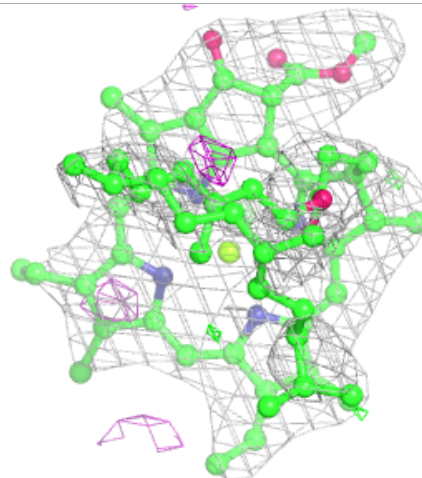
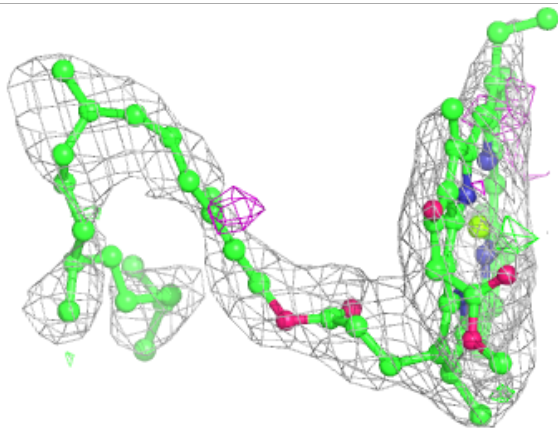
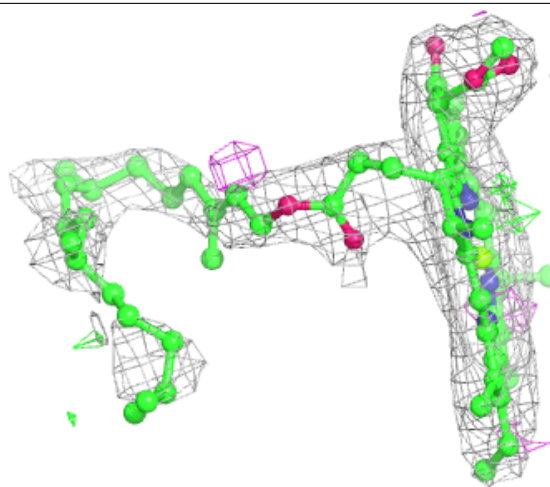
Electron density around CLA B 1202:

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



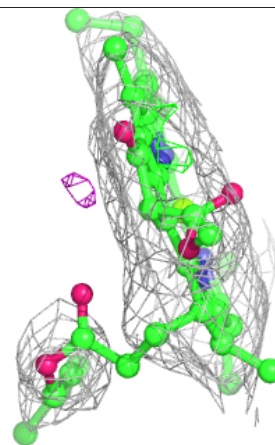
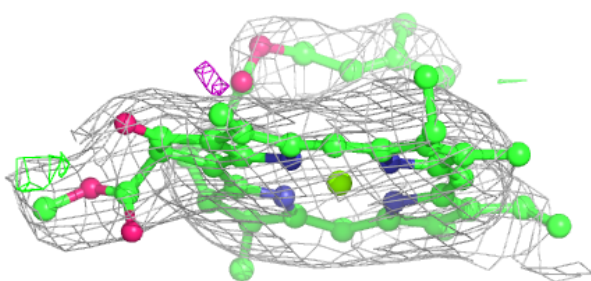
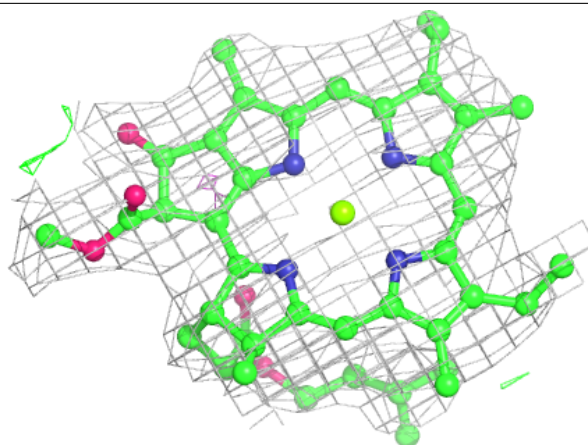
Electron density around CLA A 1134:

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

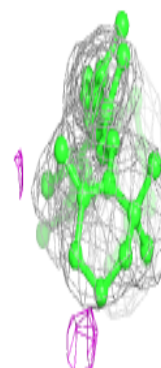
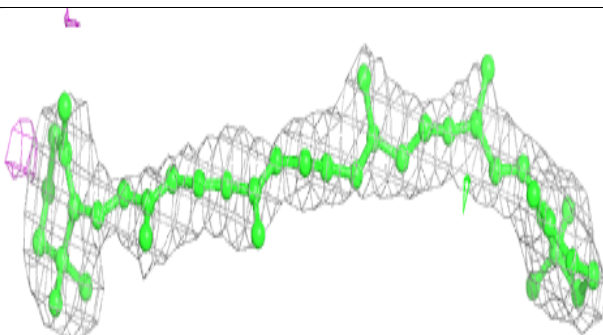
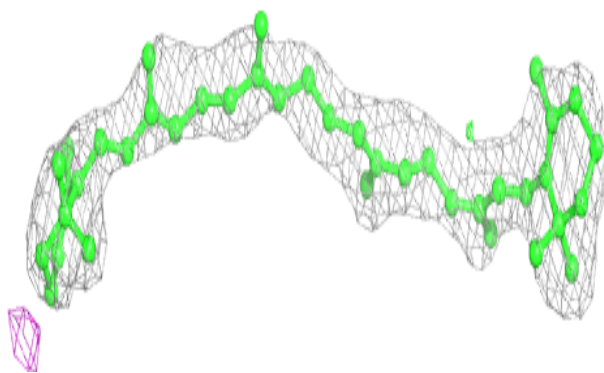


Electron density around CLA 1 1110:

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

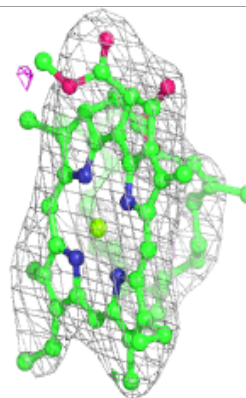
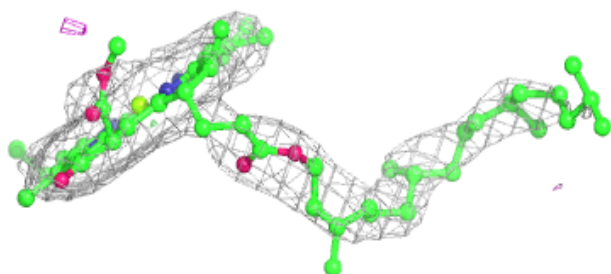
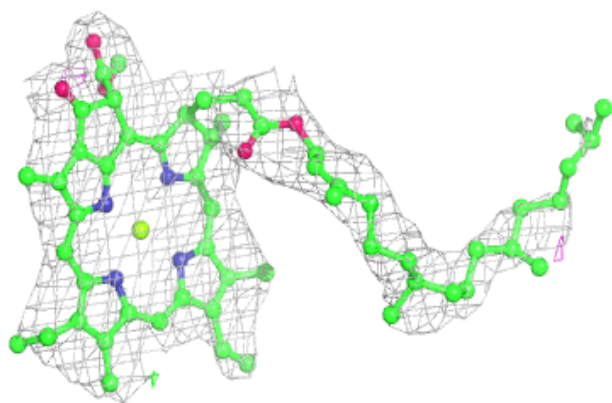
**Electron density around BCR i 4018:**

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

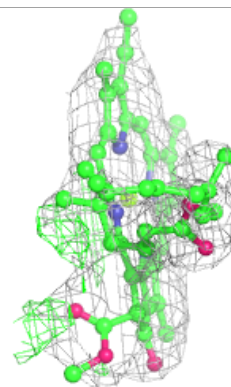
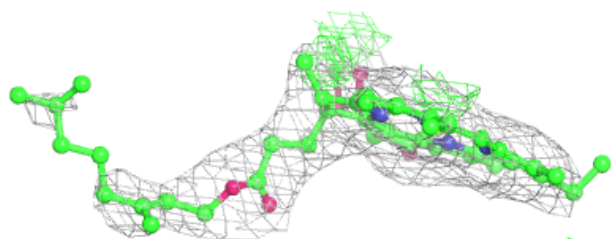
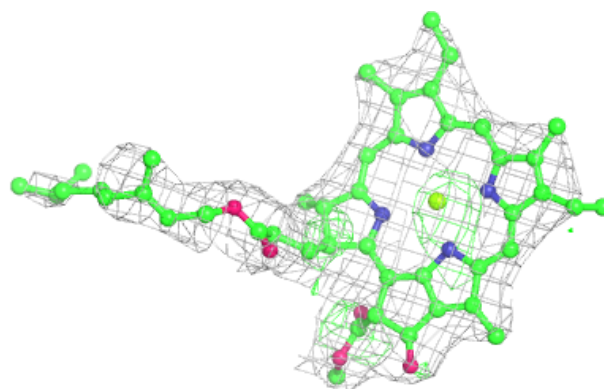


Electron density around CLA 1 1106:

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

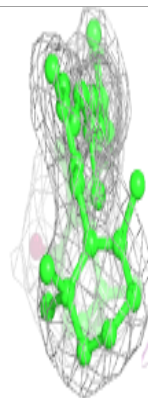
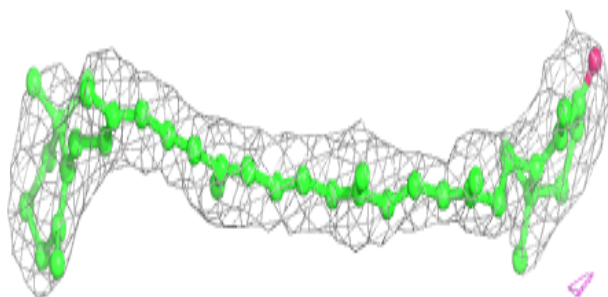
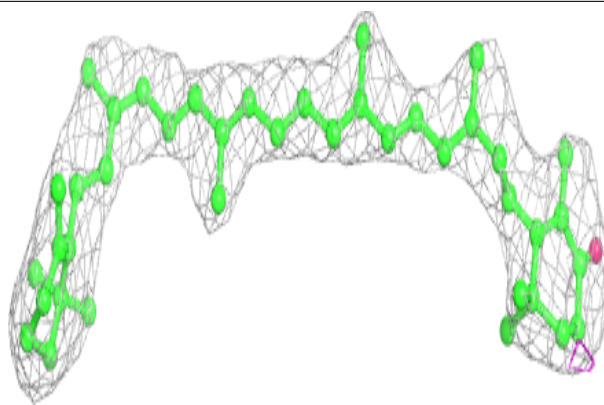
**Electron density around CLA B 1222:**

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

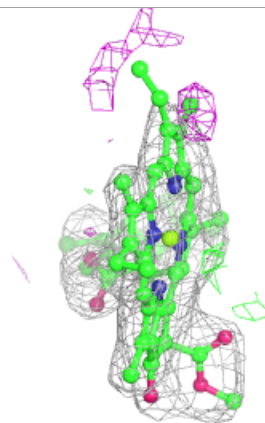
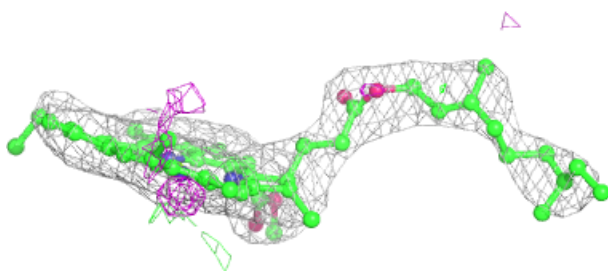
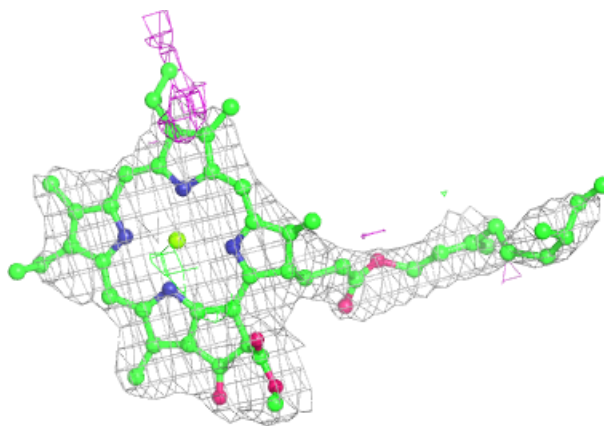


Electron density around ECH M 4021:

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

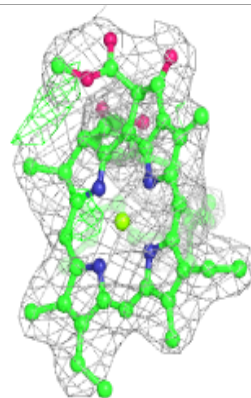
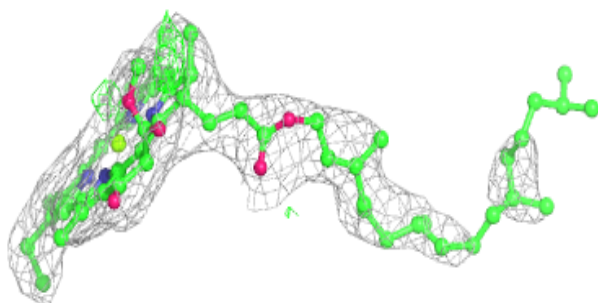
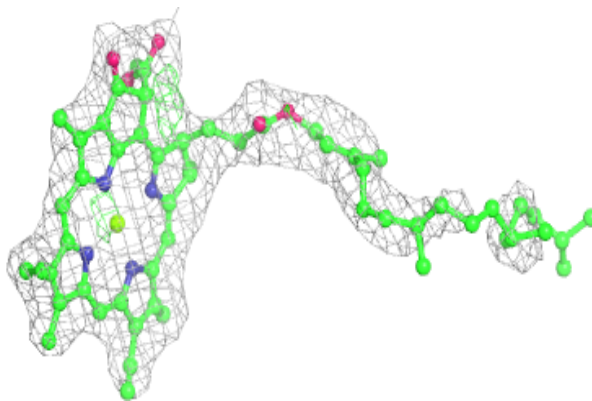
**Electron density around CLA 1 1124:**

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

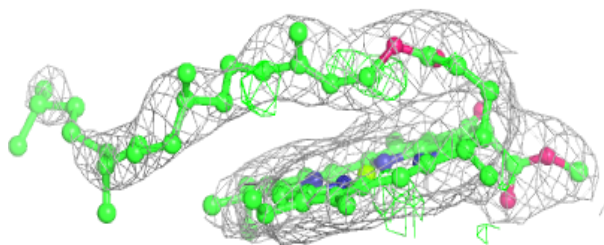
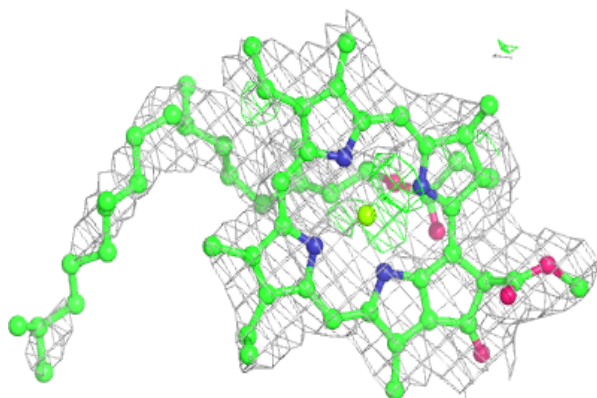


Electron density around CLA B 1230:

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

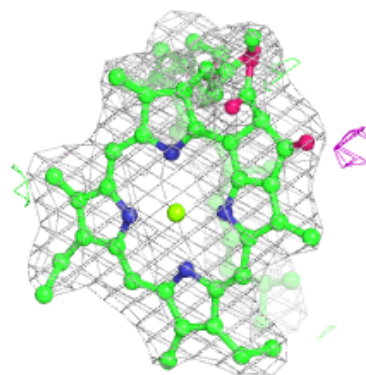
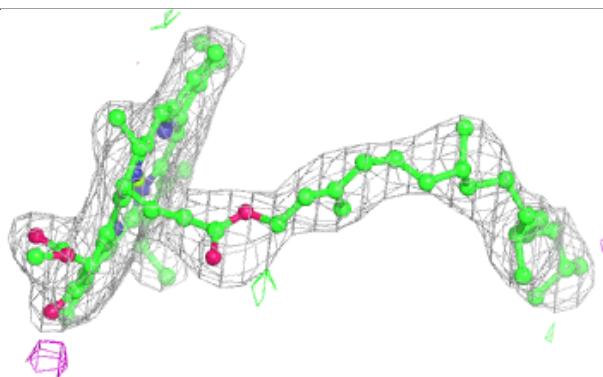
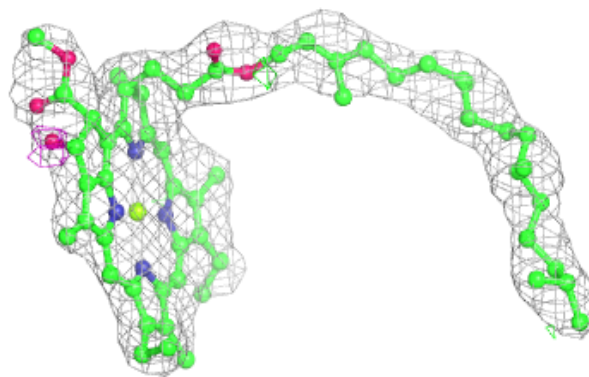
**Electron density around CLA B 1235:**

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

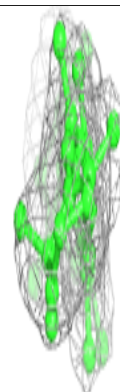
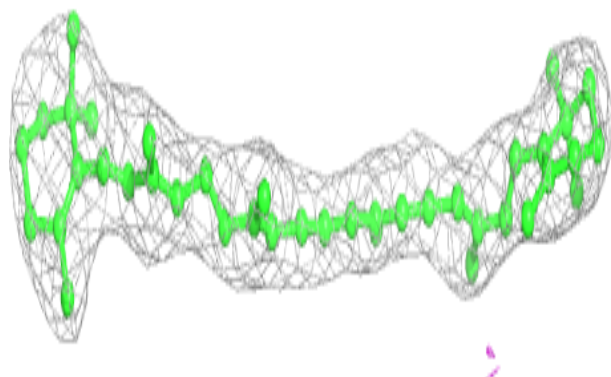
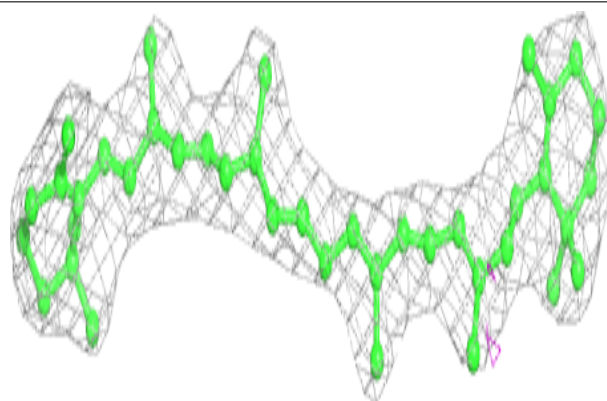


Electron density around CLA A 1133:

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

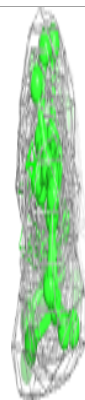
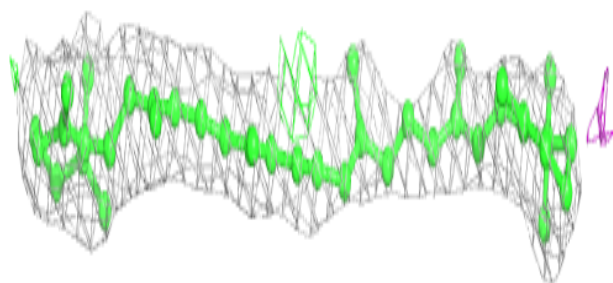
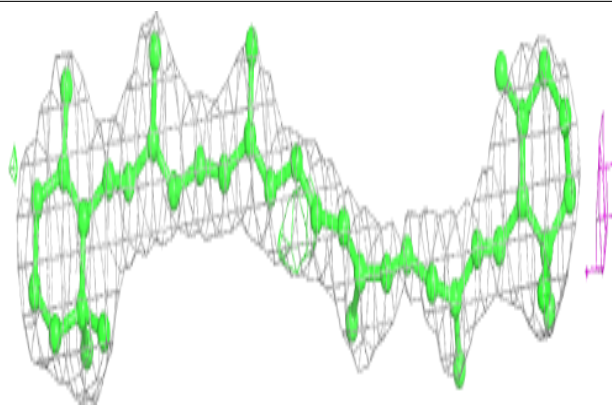
**Electron density around BCR A 4012:**

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

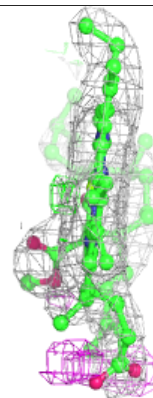
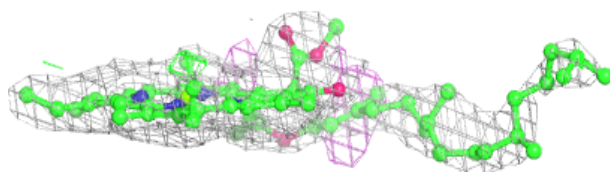
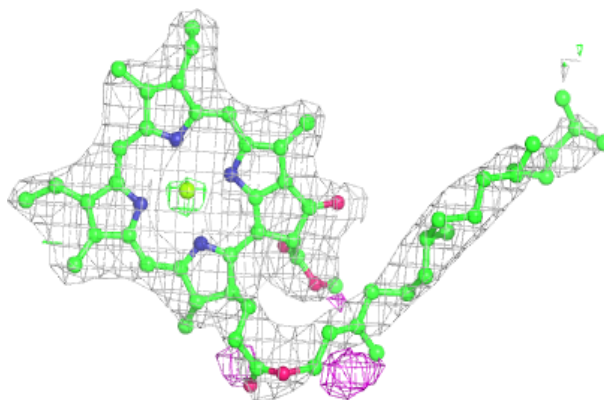


Electron density around BCR 0 4019:

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

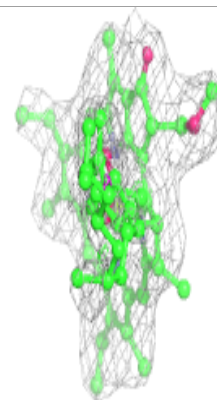
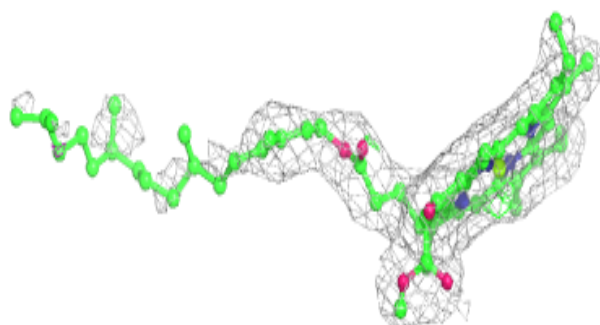
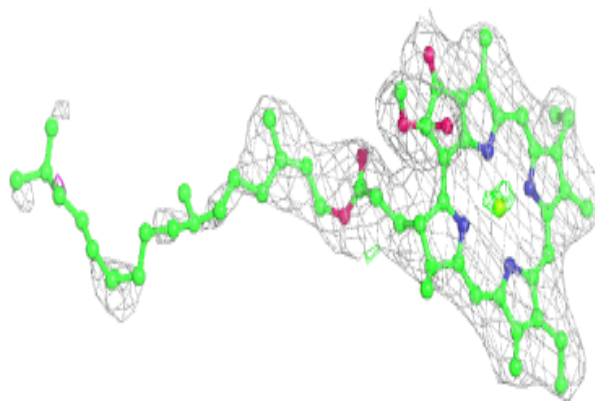
**Electron density around CLA L 1503:**

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

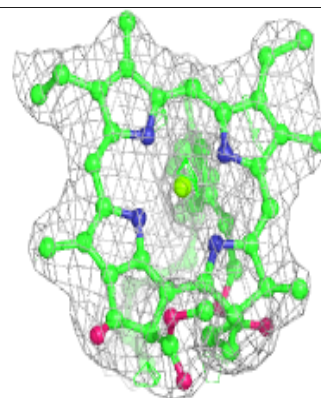
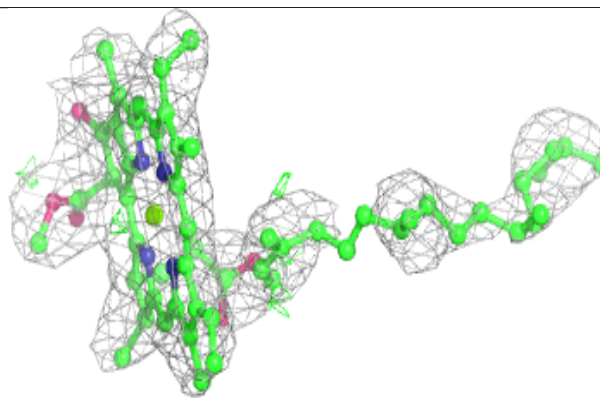
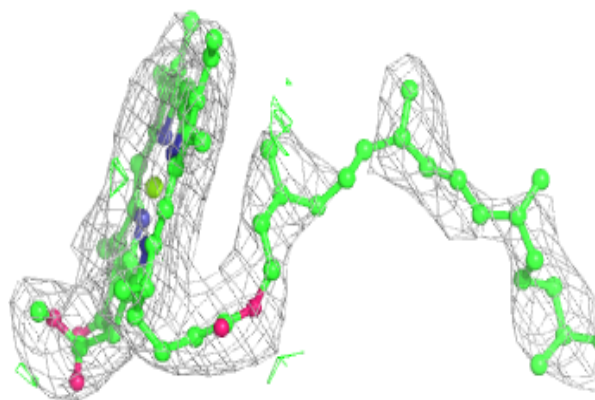


Electron density around CLA A 1107:

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

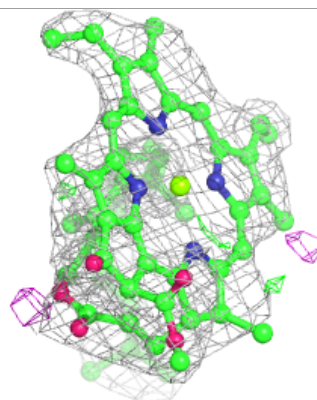
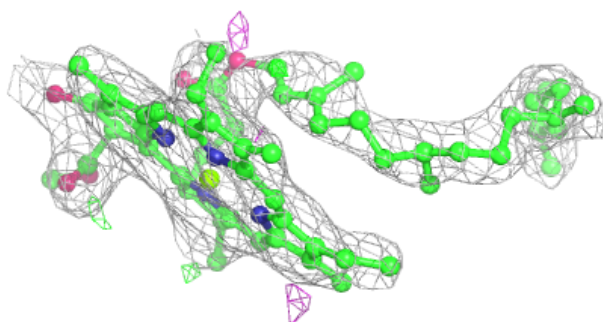
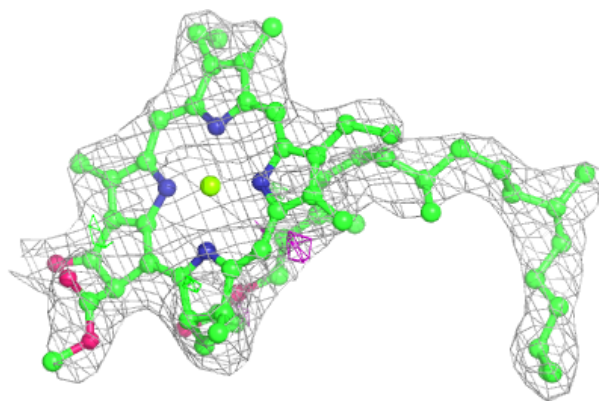
**Electron density around CLA A 1120:**

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

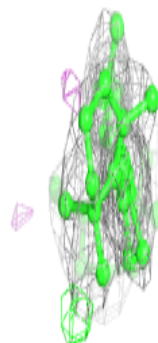
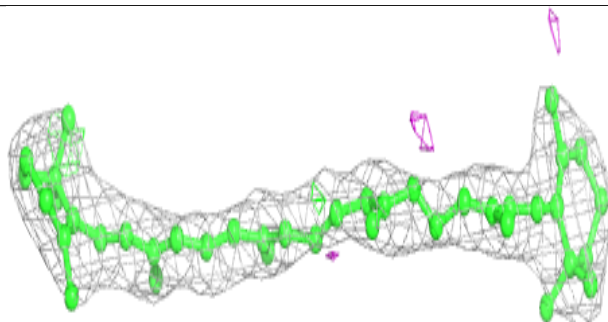
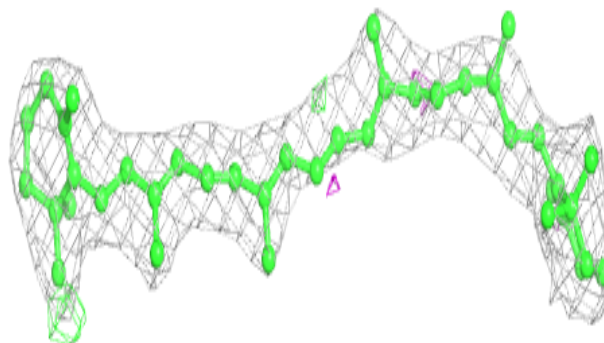


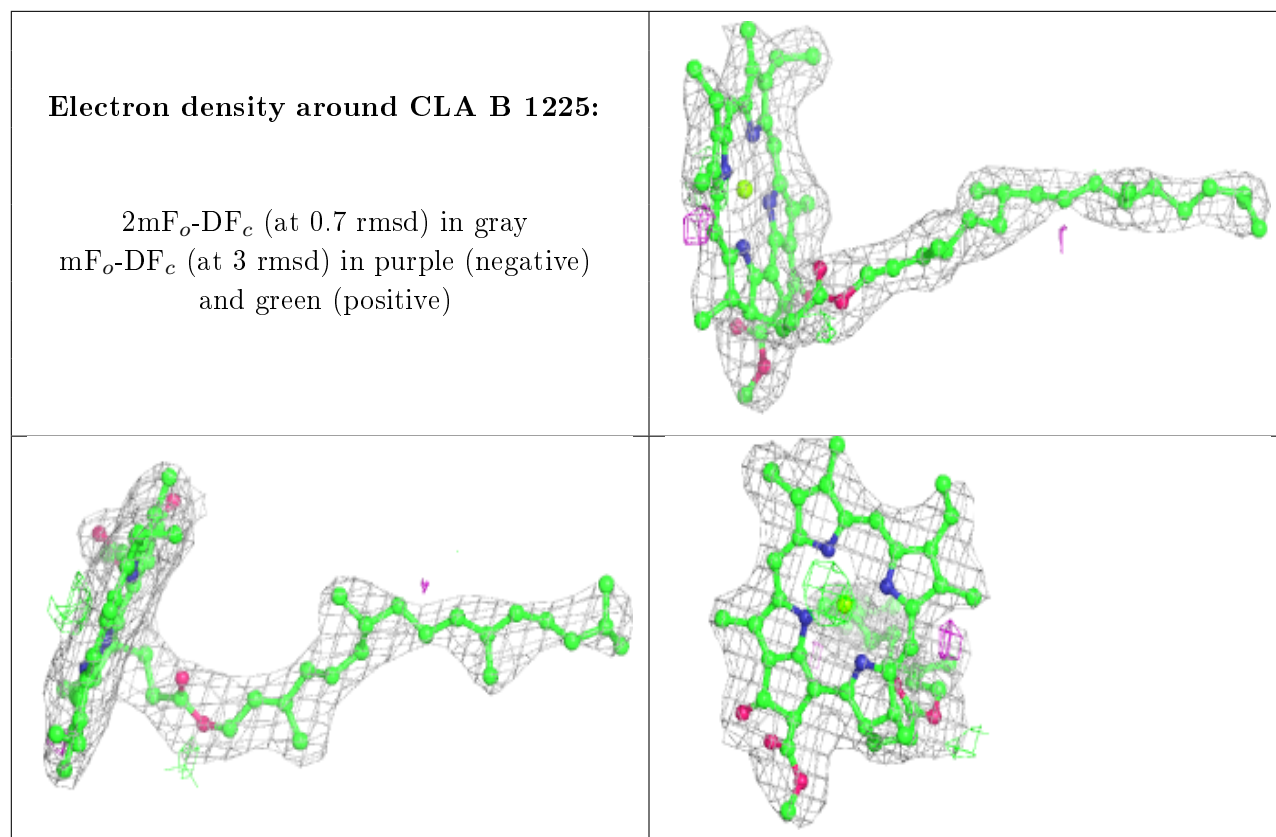
Electron density around CLA b 1237:

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

**Electron density around BCR 2 4017:**

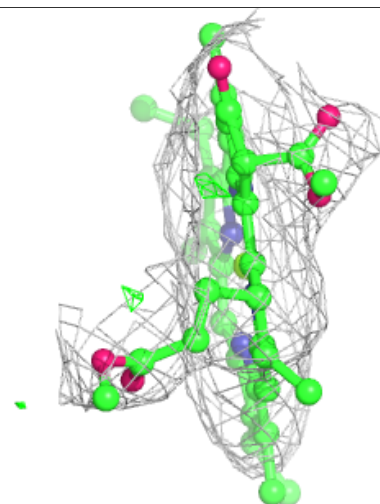
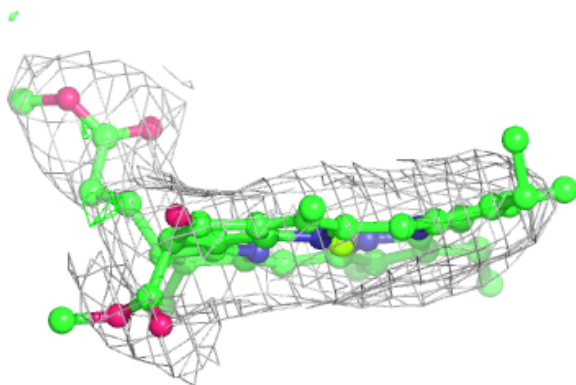
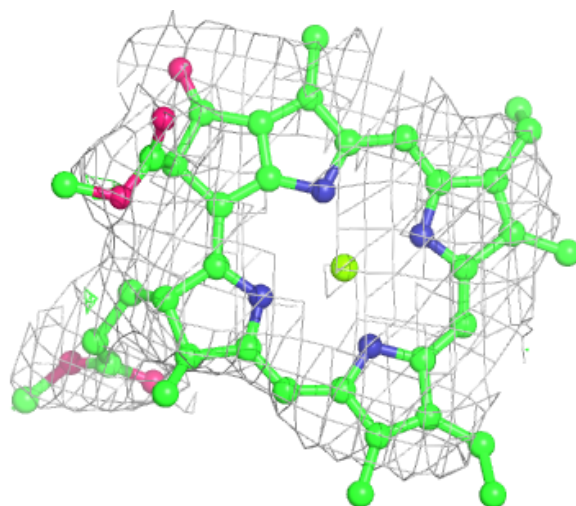
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





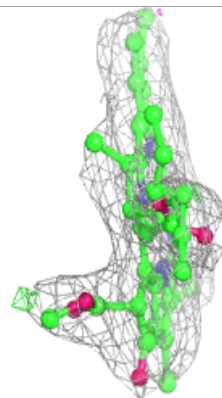
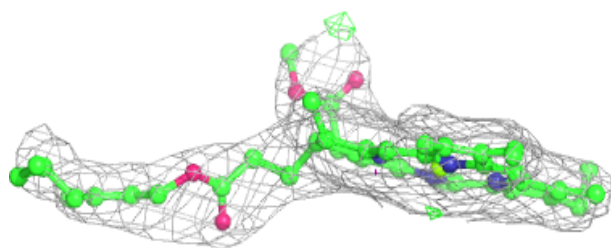
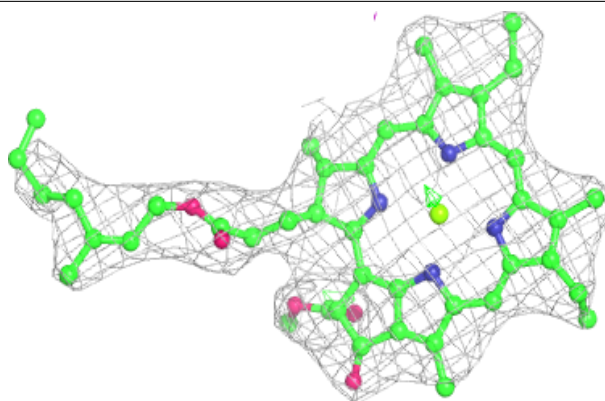
Electron density around CLA 8 1402:

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

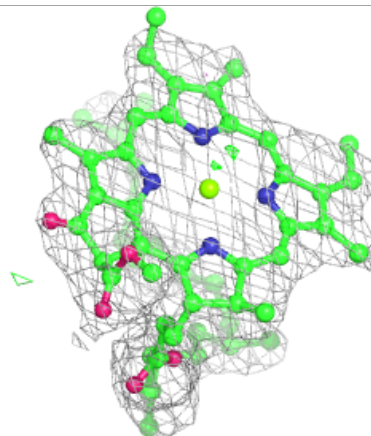
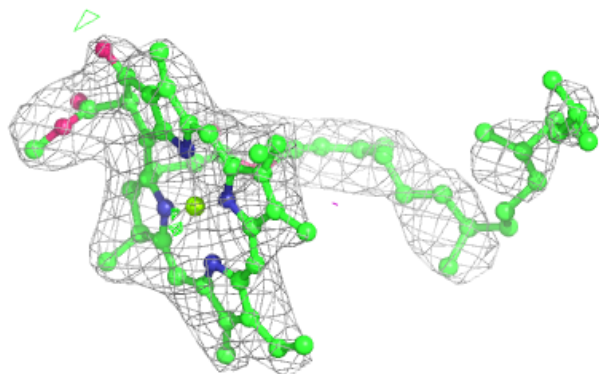
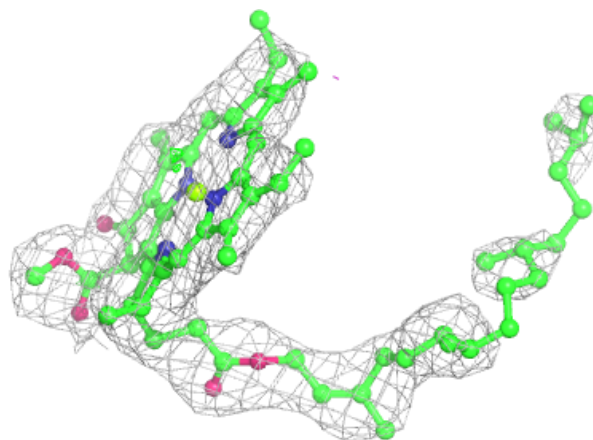


Electron density around CLA b 1234:

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

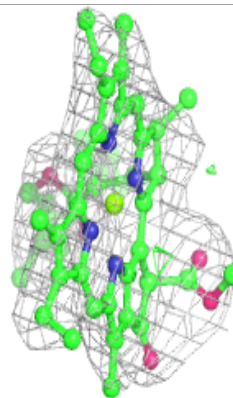
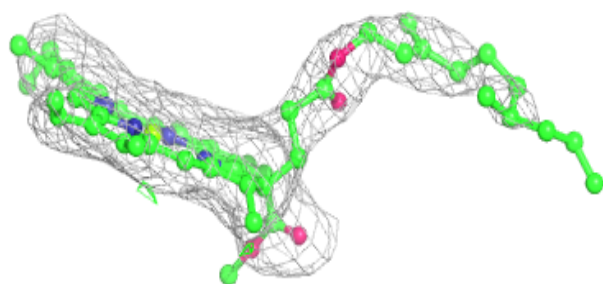
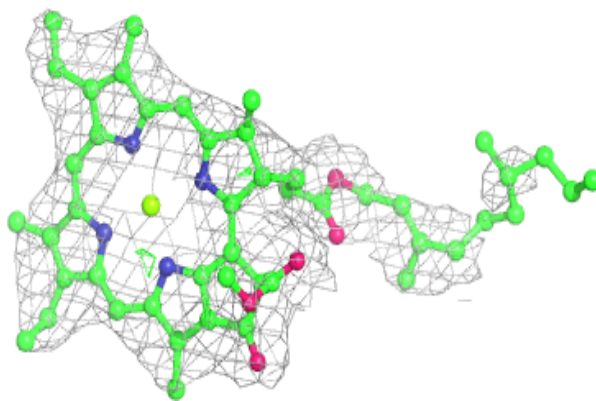
**Electron density around CLA b 1212:**

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

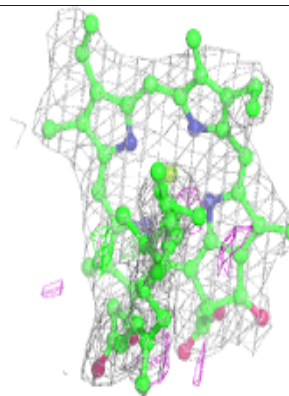
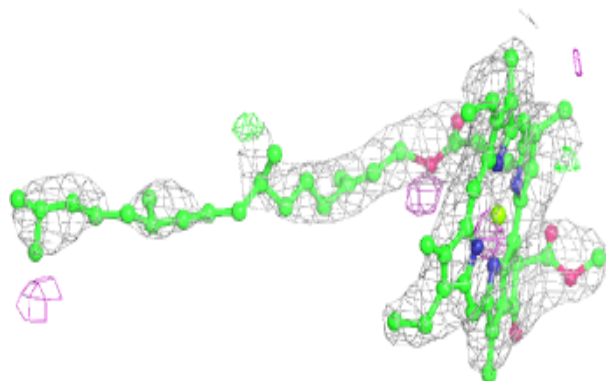
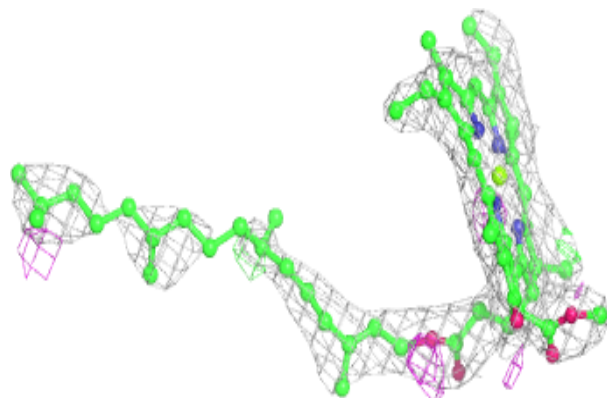


Electron density around CLA B 1220:

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

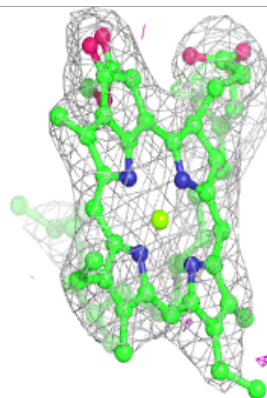
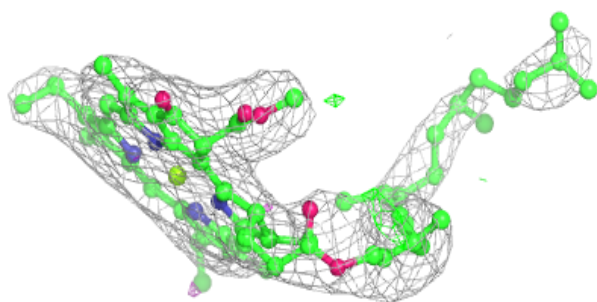
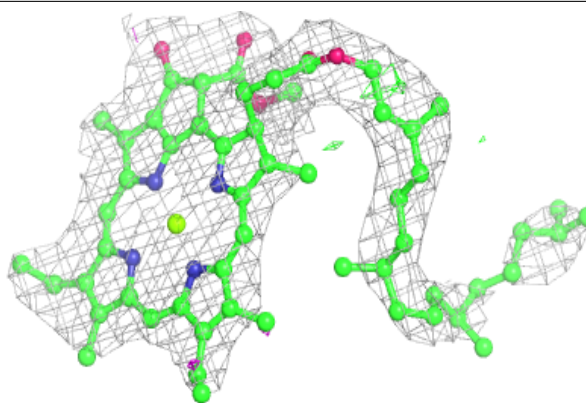
**Electron density around CLA b 1226:**

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

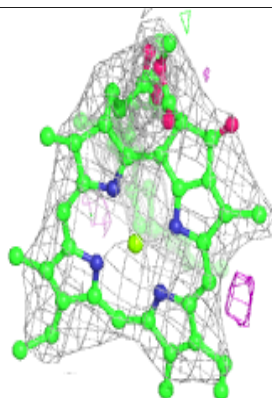
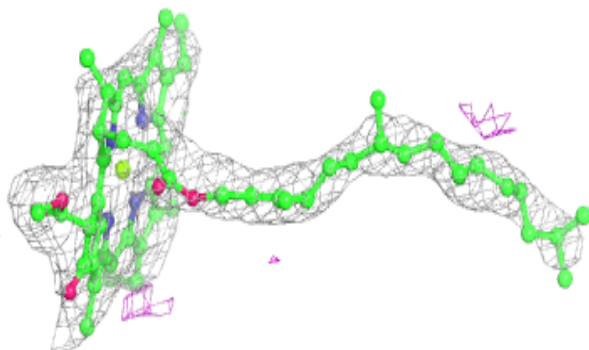
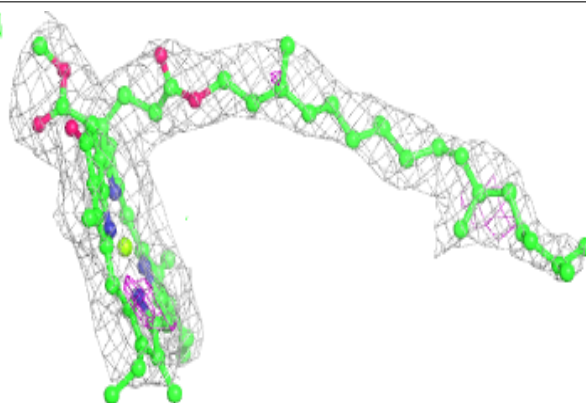


Electron density around CLA B 1221:

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

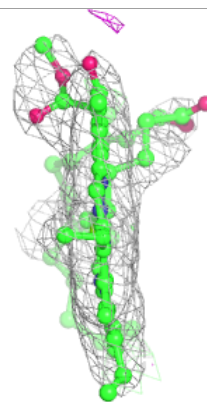
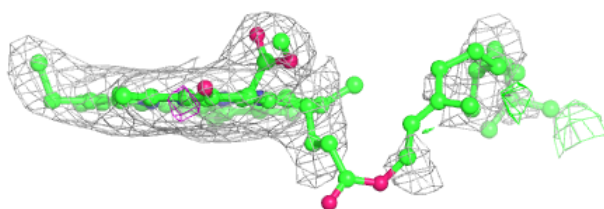
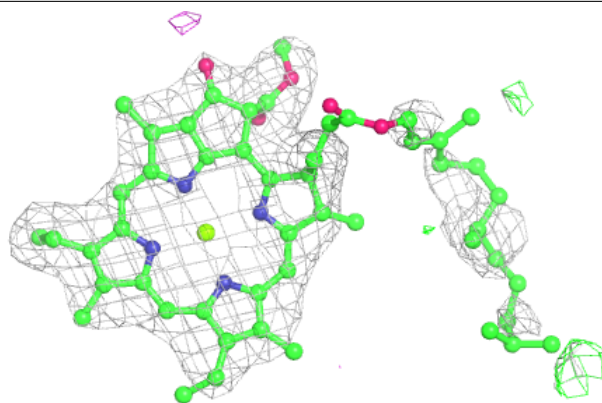
**Electron density around CLA 2 1201:**

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

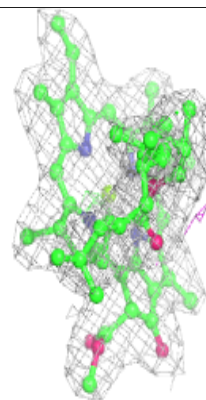
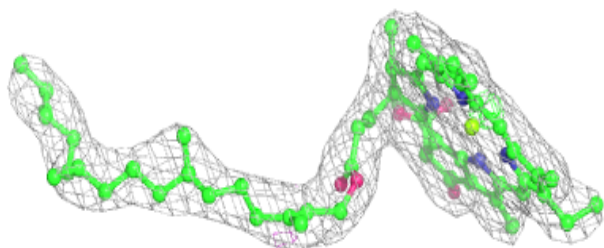
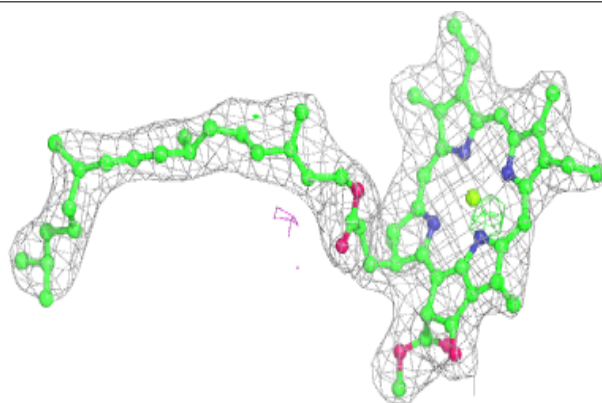


Electron density around CLA b 1219:

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

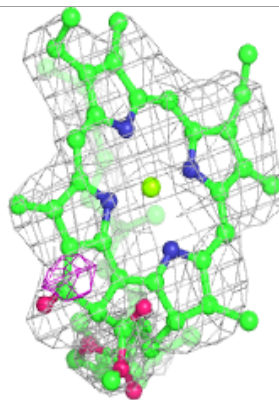
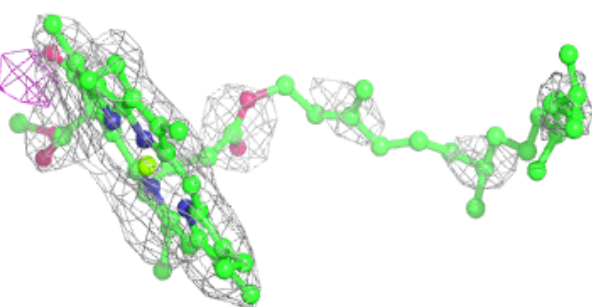
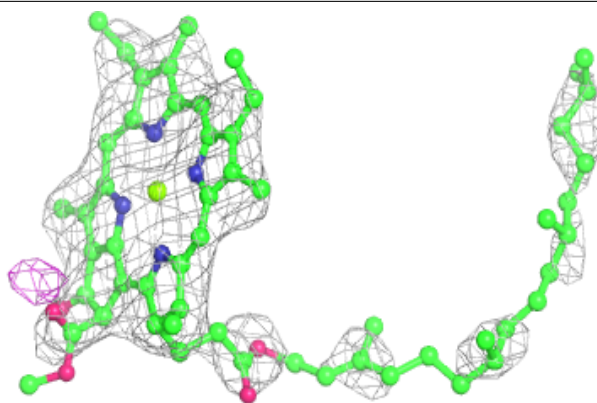
**Electron density around CLA A 1119:**

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

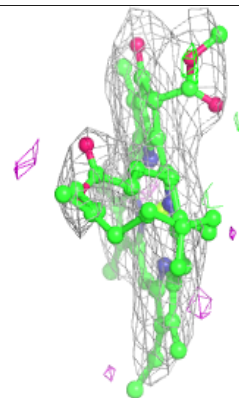
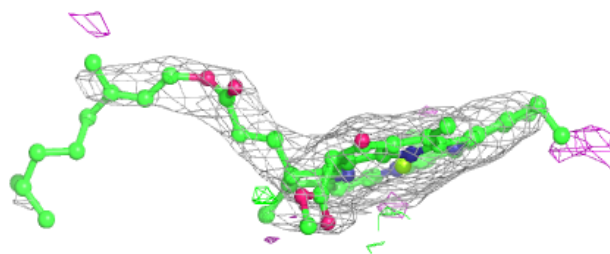
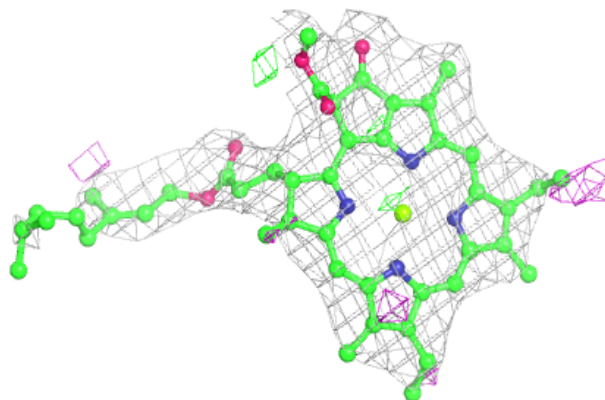


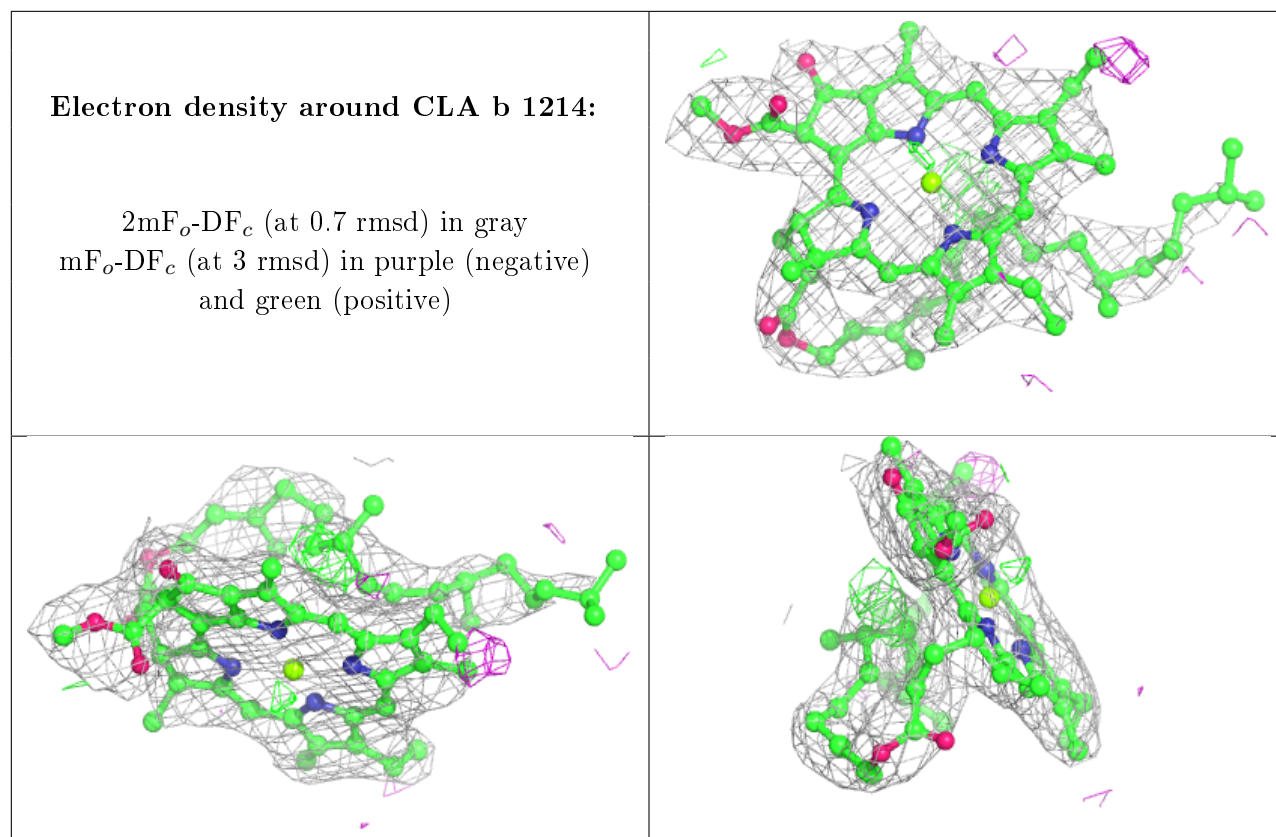
Electron density around CLA 1 1140:

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

**Electron density around CLA a 1124:**

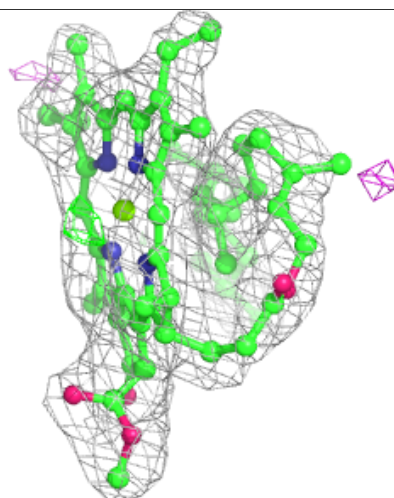
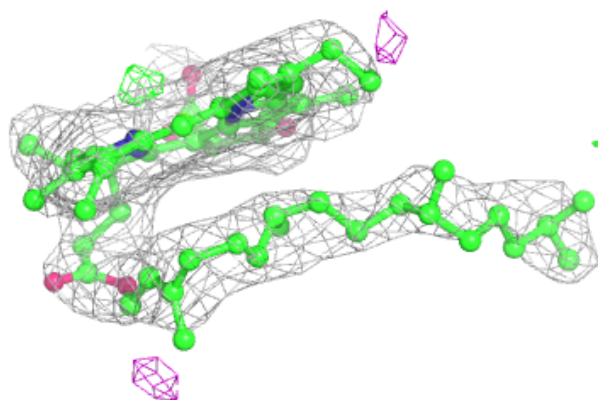
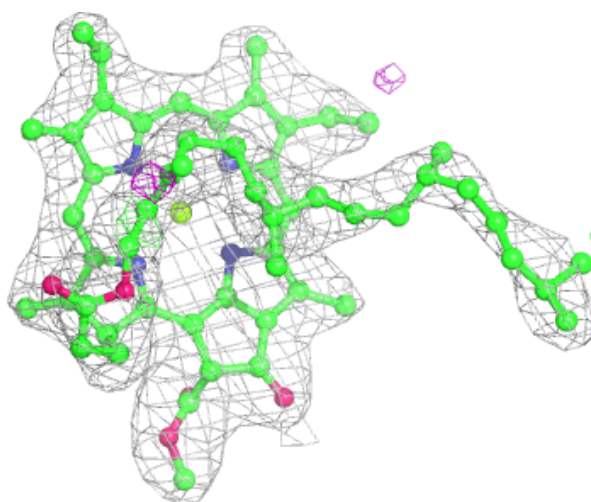
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





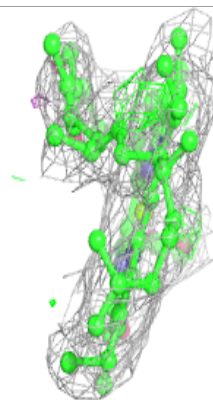
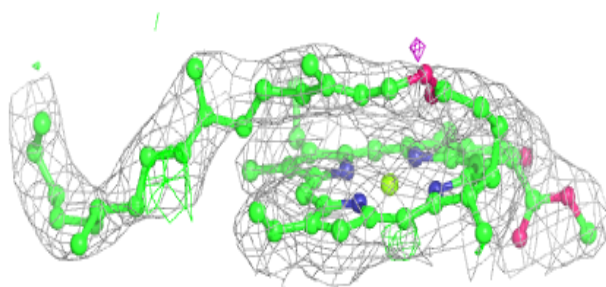
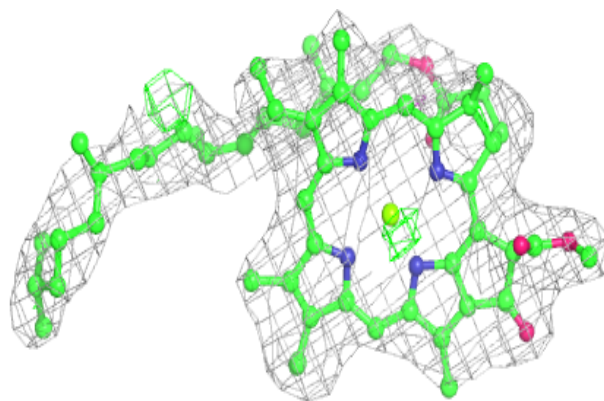
Electron density around CLA b 1224:

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



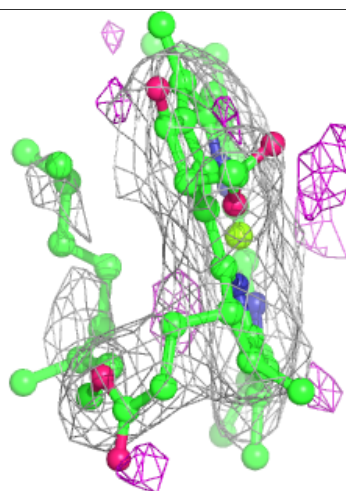
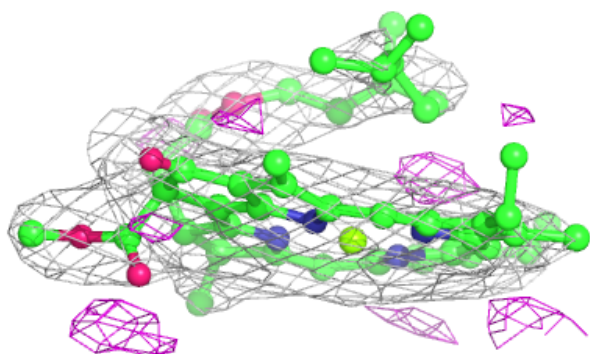
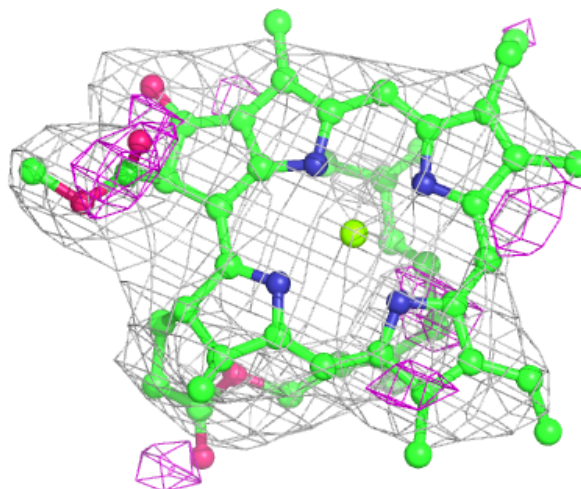
Electron density around CLA b 1209:

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



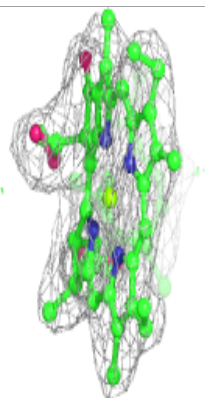
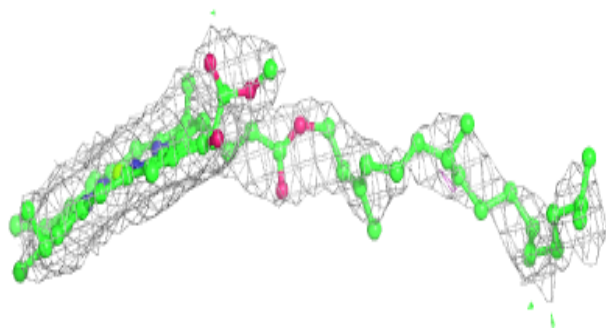
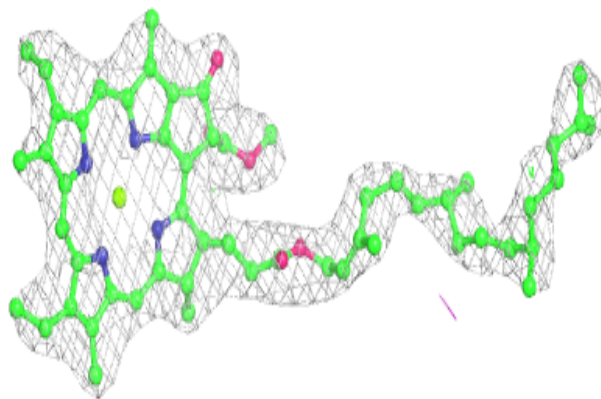
Electron density around CLA 2 1224:

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

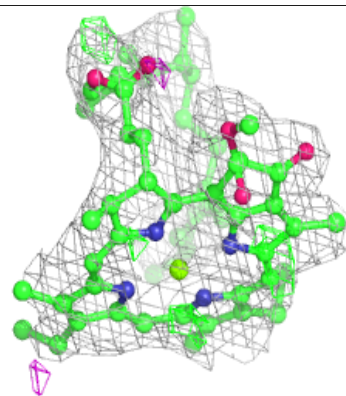
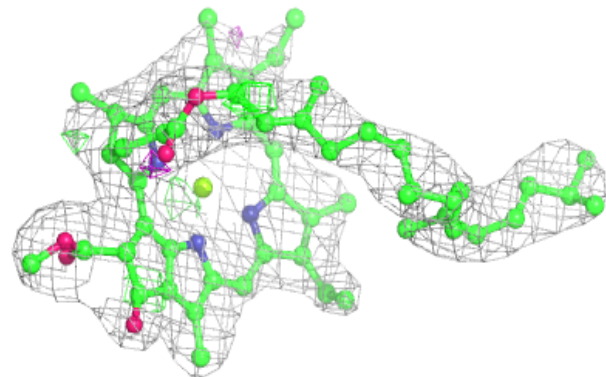
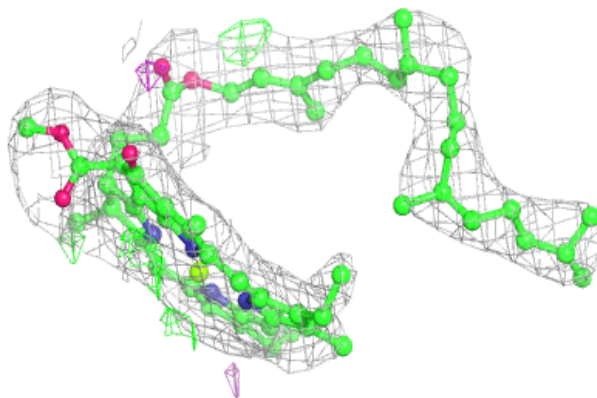


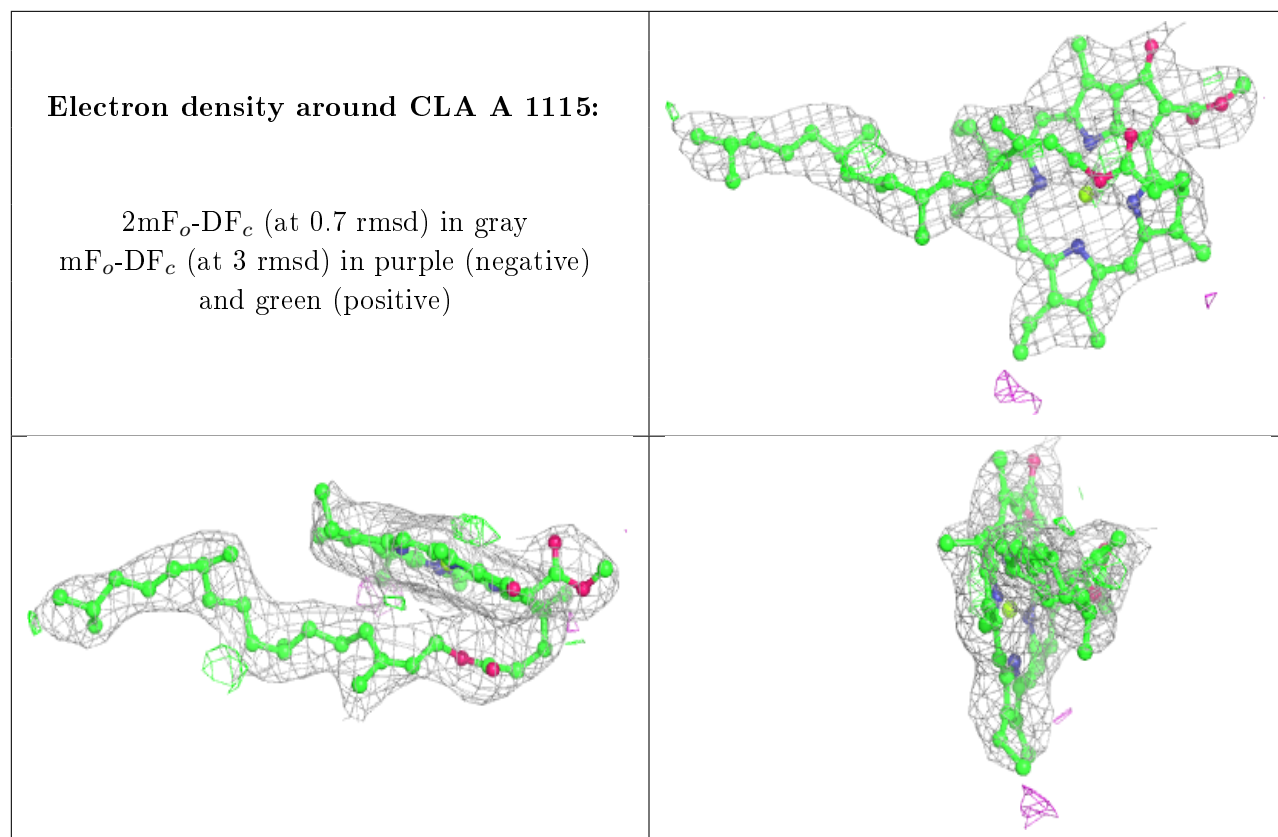
Electron density around CLA A 1139:

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

**Electron density around CLA A 1109:**

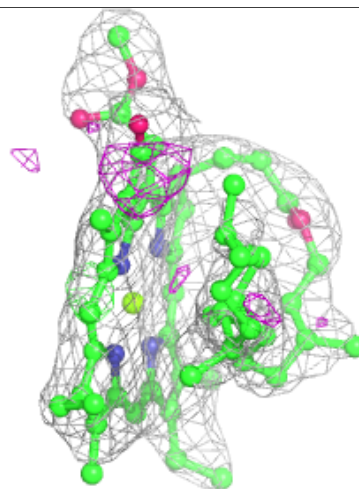
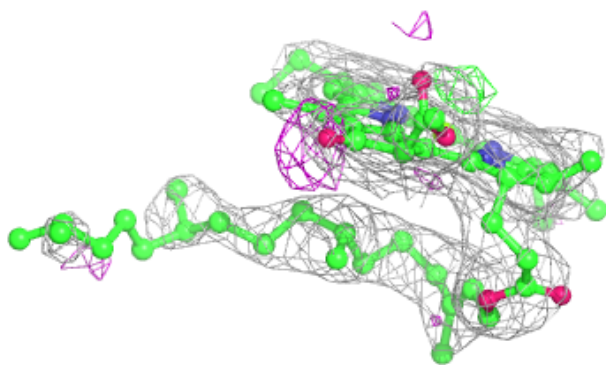
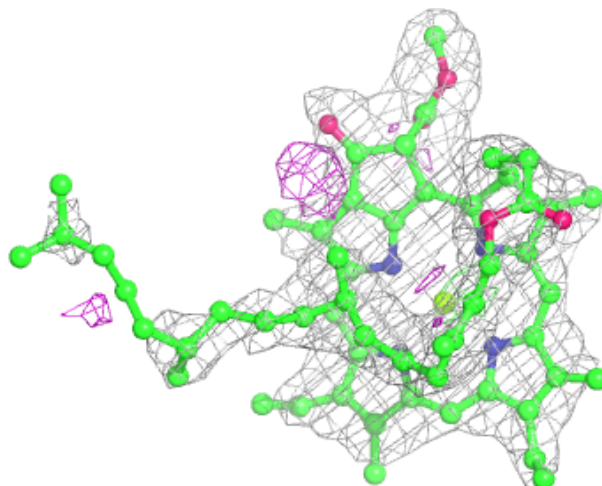
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





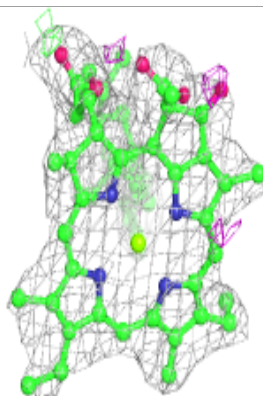
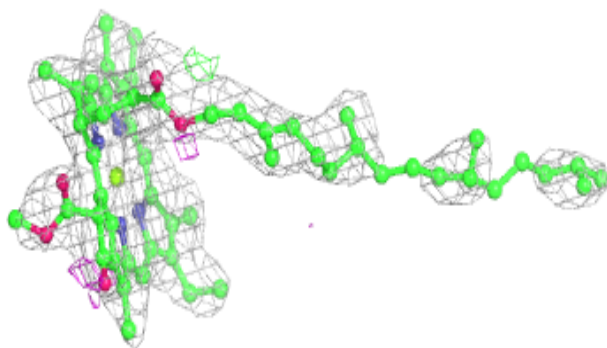
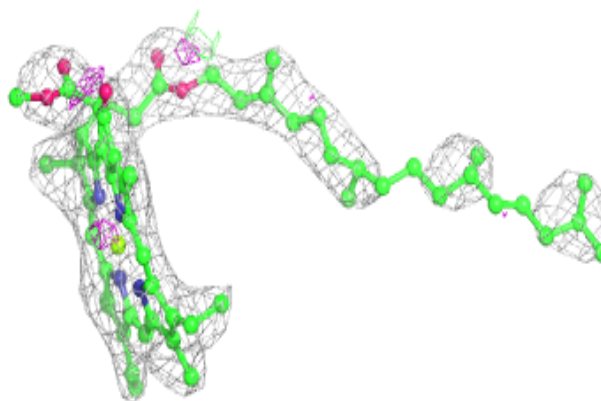
Electron density around CLA B 1224:

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

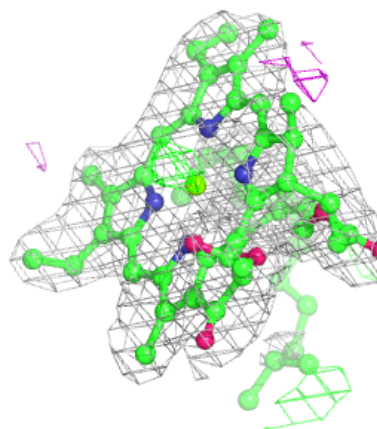
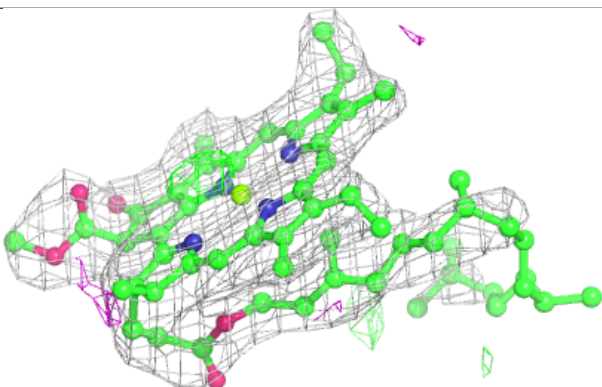
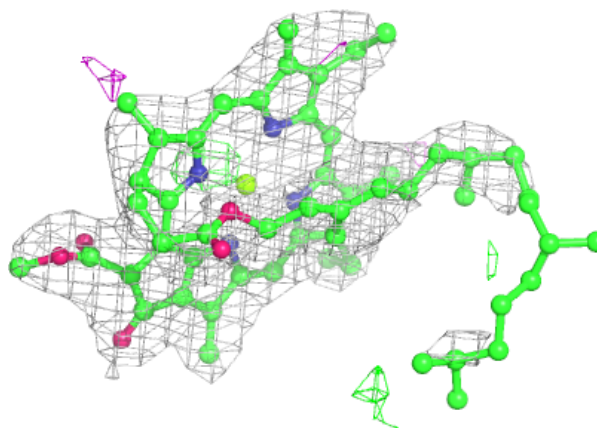


Electron density around CLA B 1226:

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

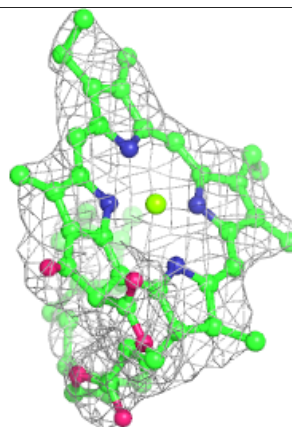
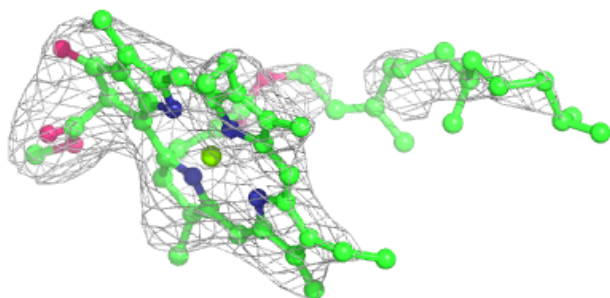
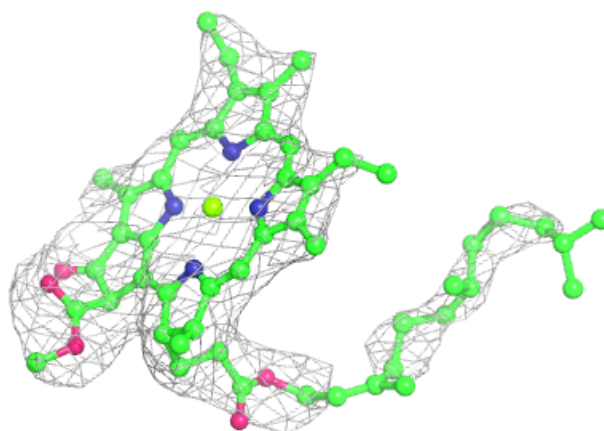
**Electron density around CLA A 1121:**

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

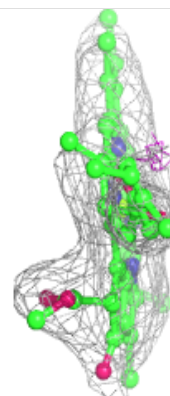
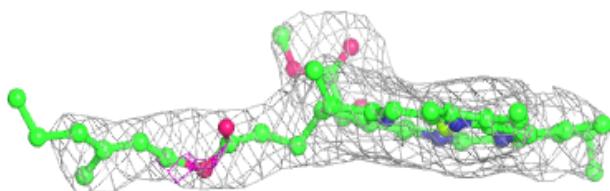
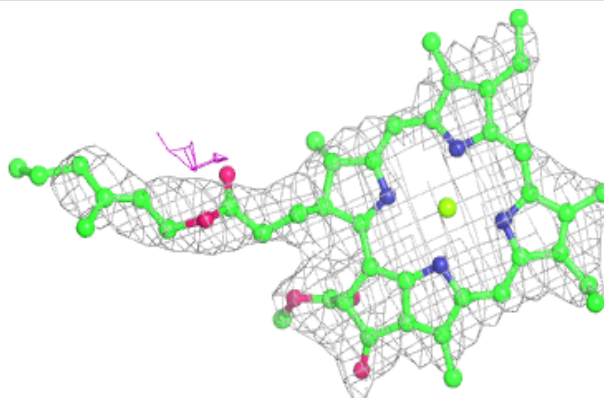


Electron density around CLA 1 1122:

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

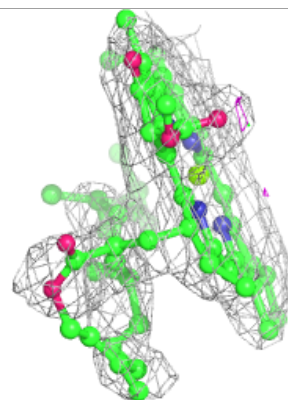
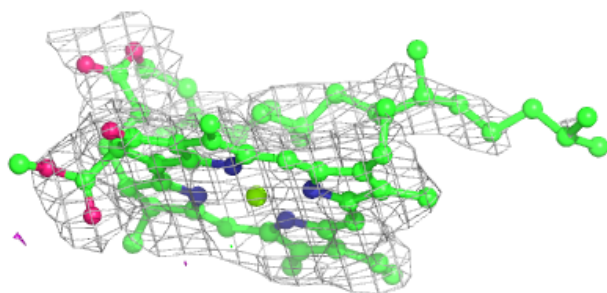
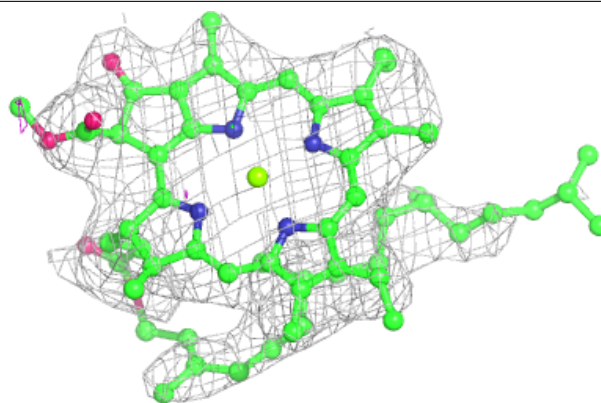
**Electron density around CLA 1 1135:**

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

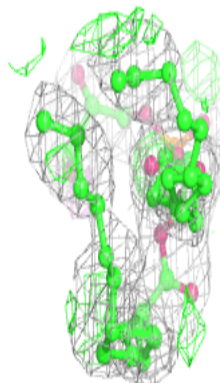
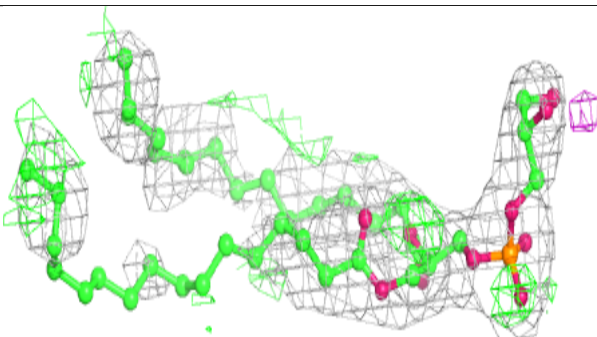
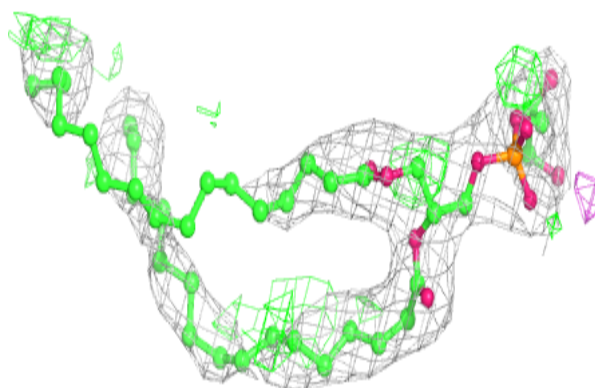


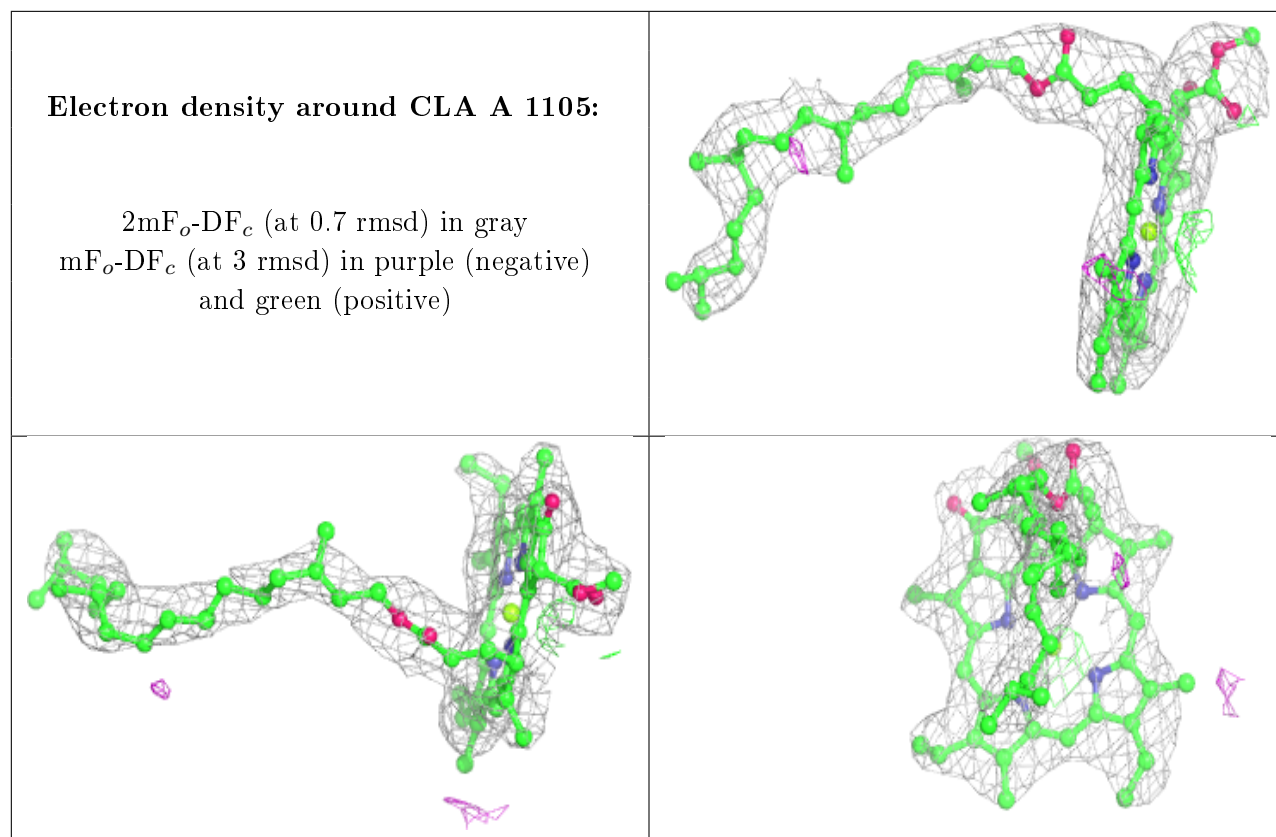
Electron density around CLA b 1218:

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

**Electron density around LHG A 5003:**

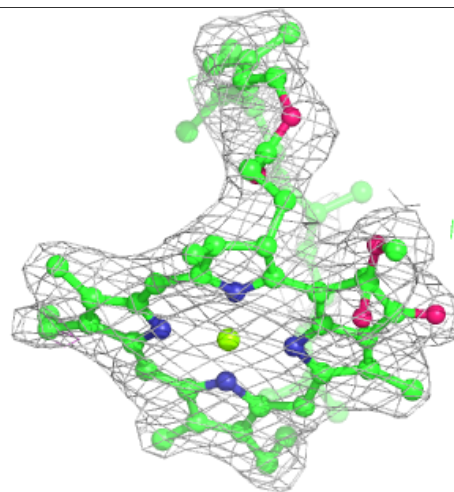
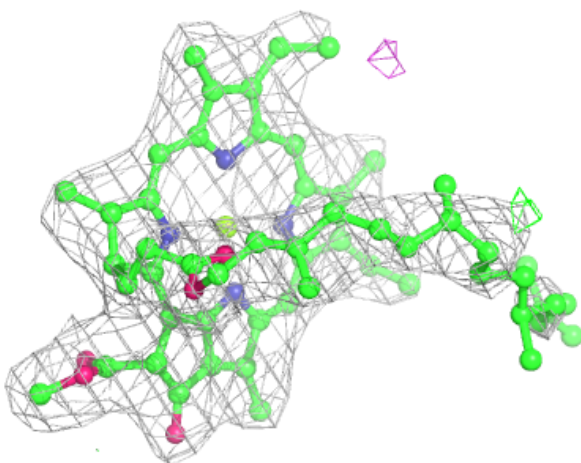
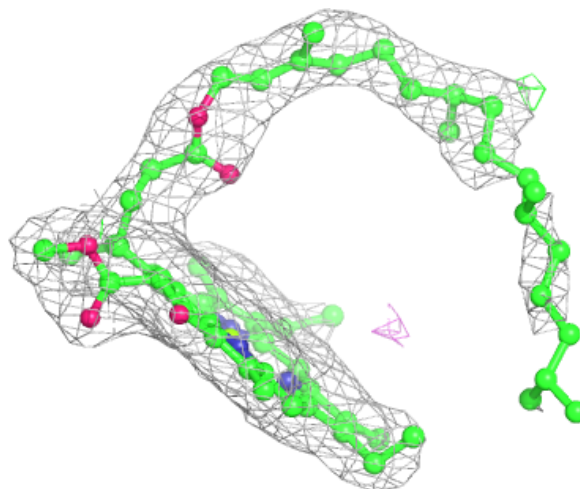
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

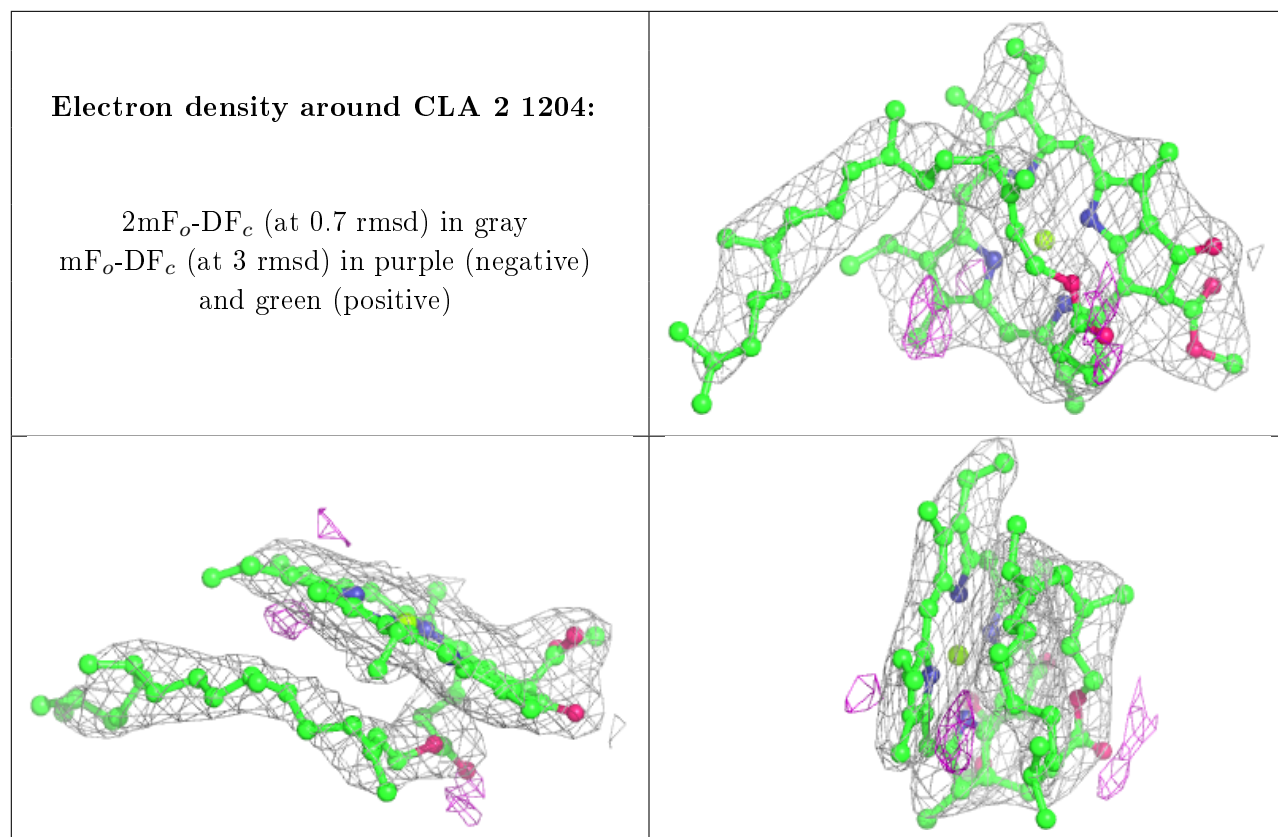




Electron density around CLA b 1216:

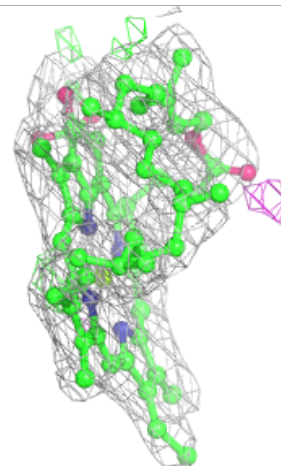
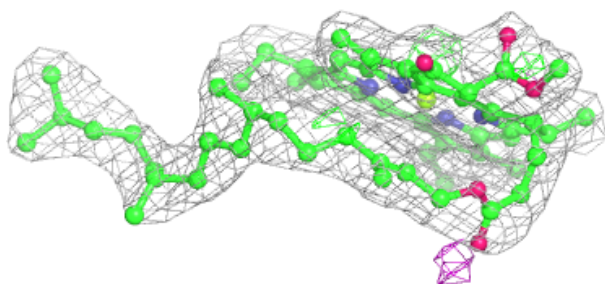
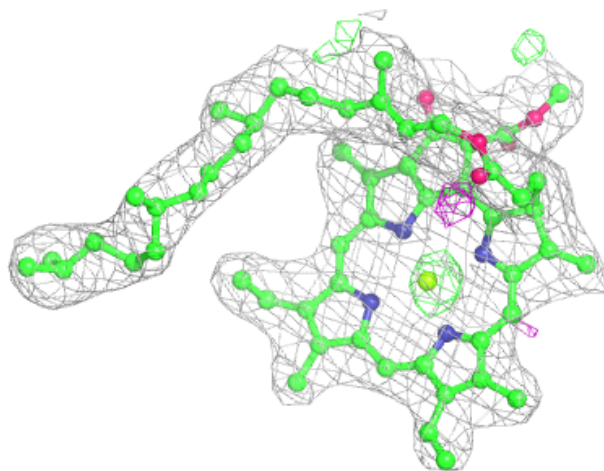
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

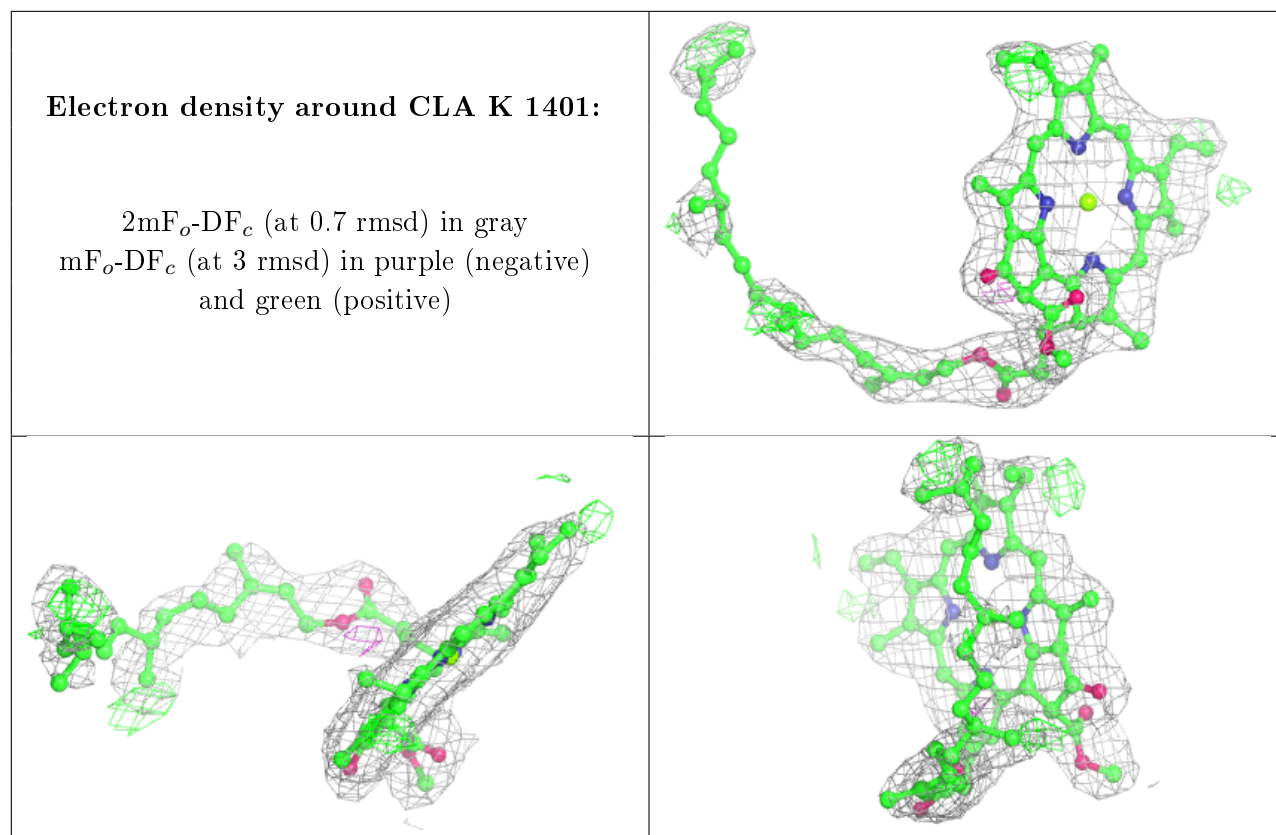




Electron density around CLA A 1127:

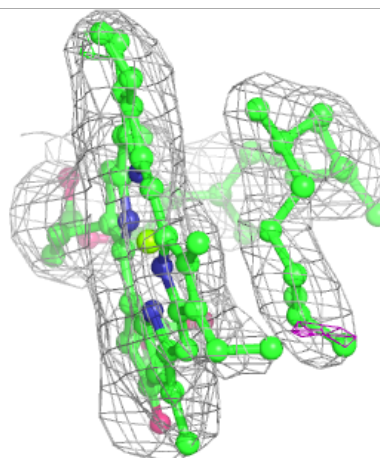
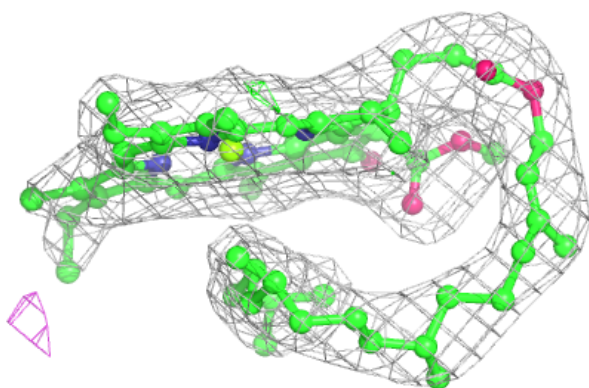
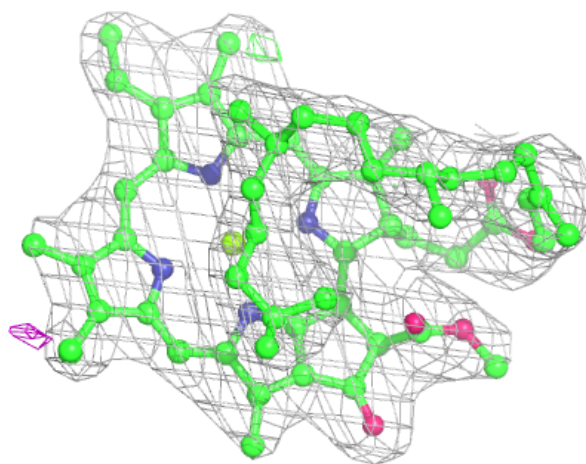
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





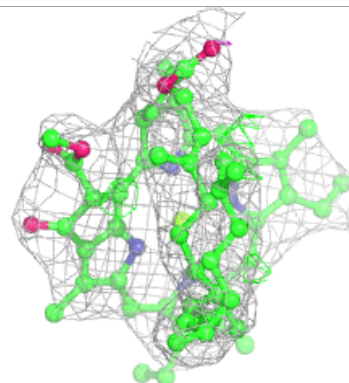
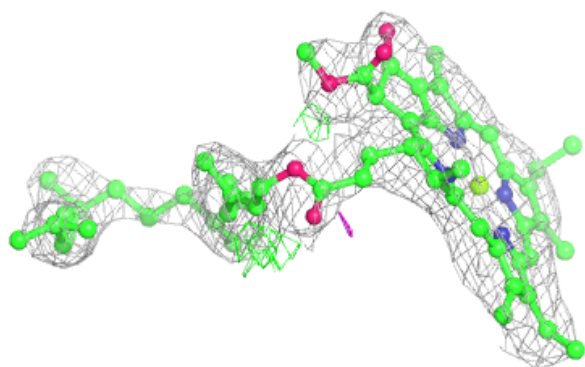
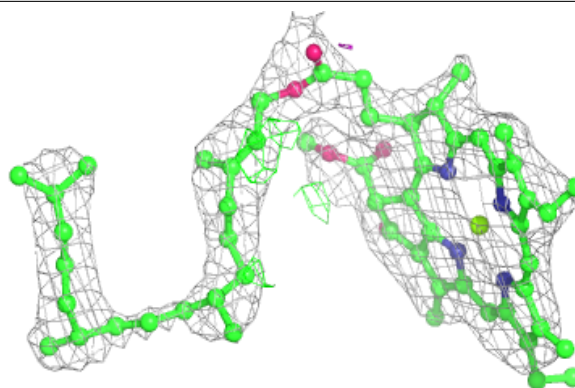
Electron density around CLA A 1104:

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

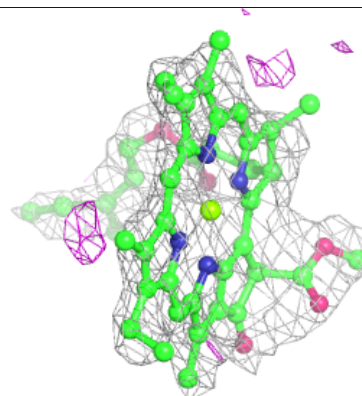
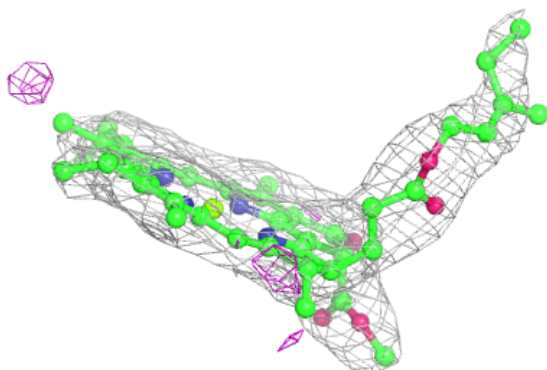
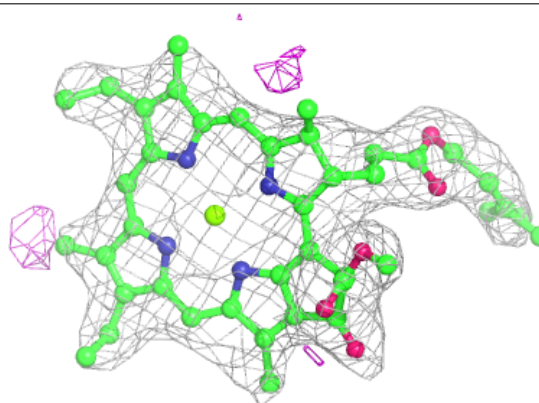


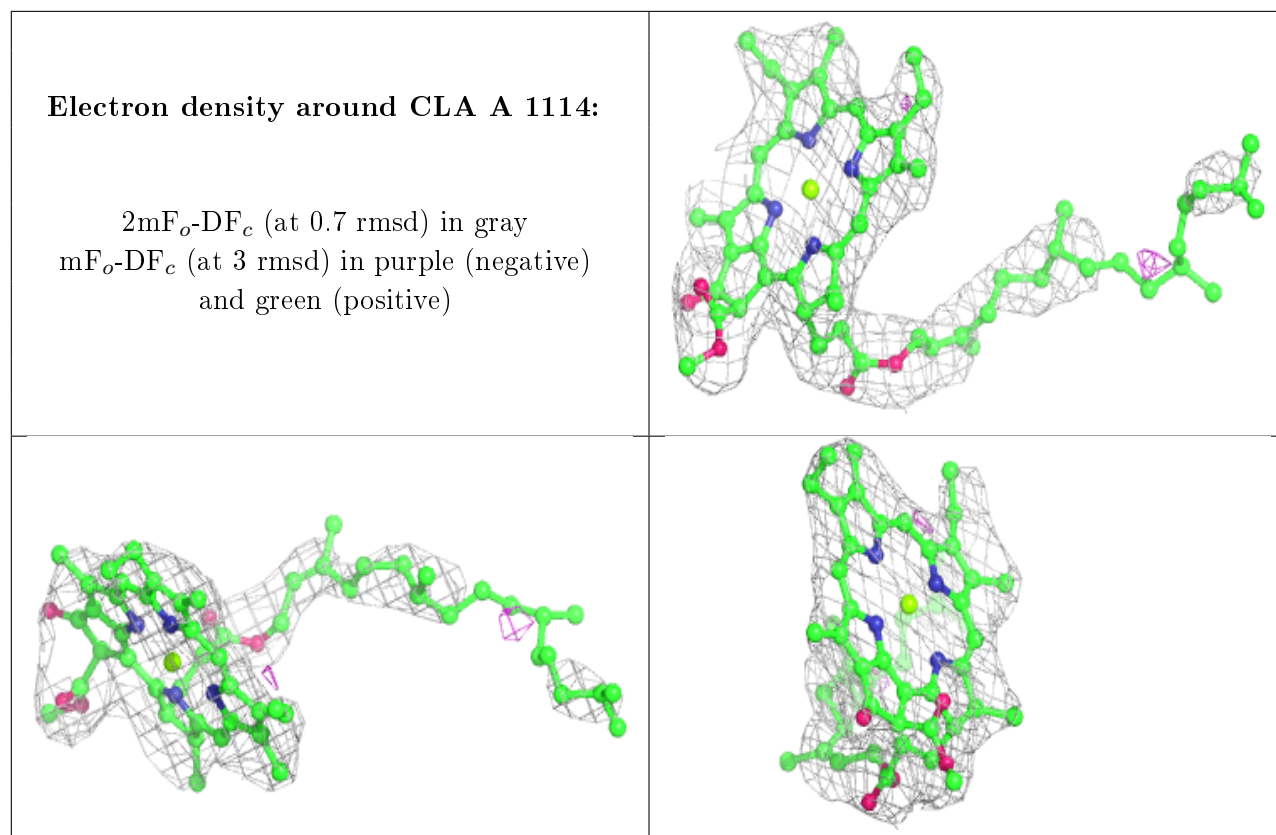
Electron density around CLA 1 1011:

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

**Electron density around CLA 1 1137:**

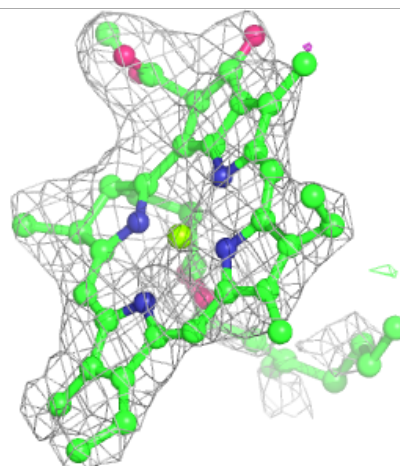
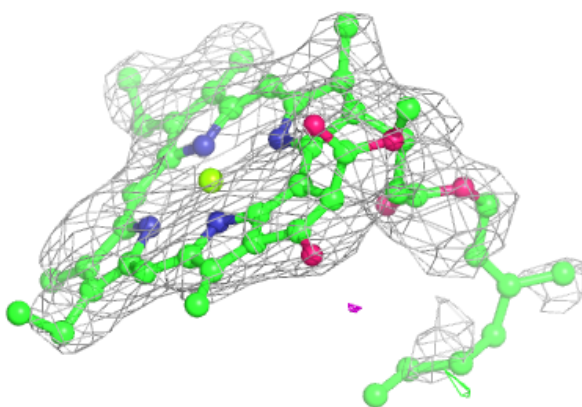
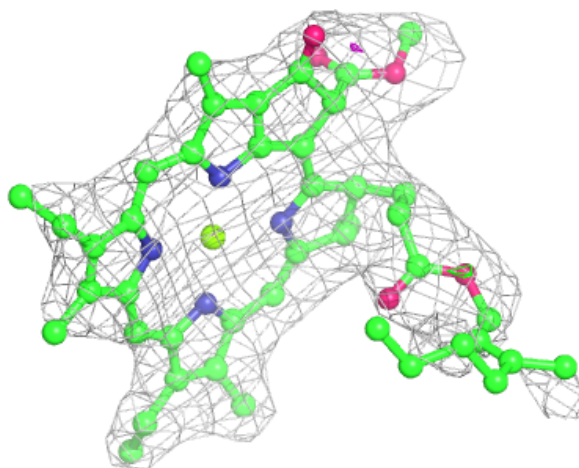
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





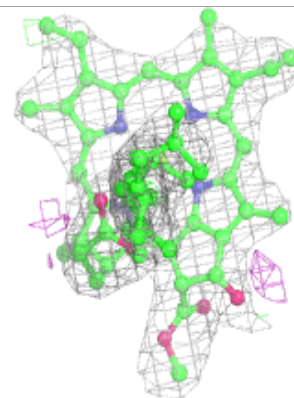
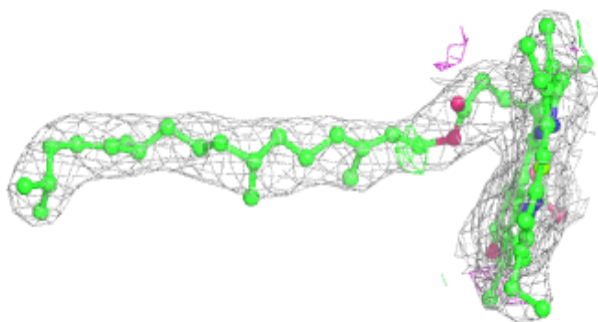
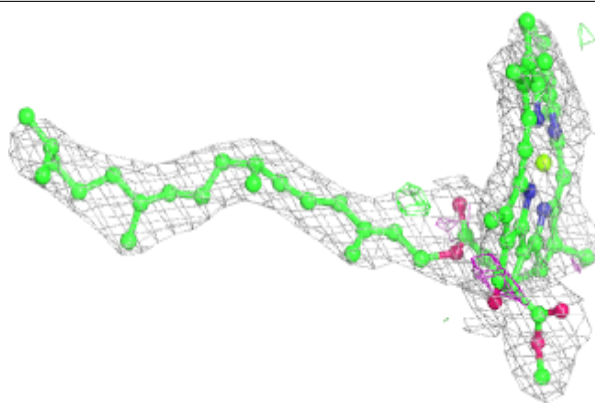
Electron density around CLA A 1108:

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

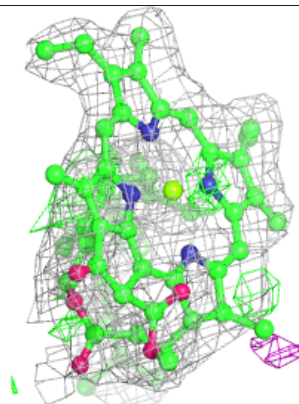
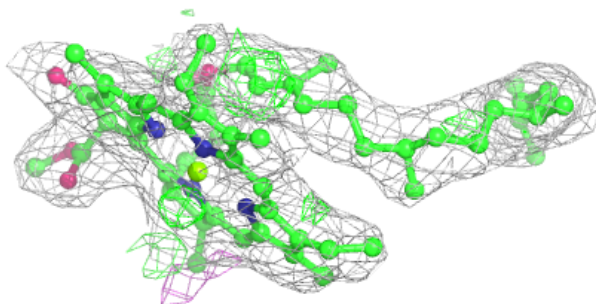
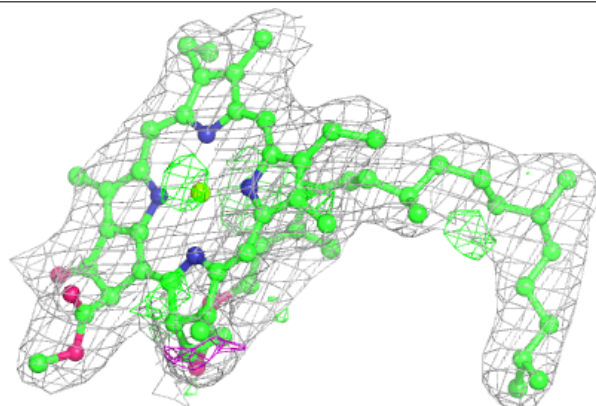


Electron density around CLA A 1126:

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

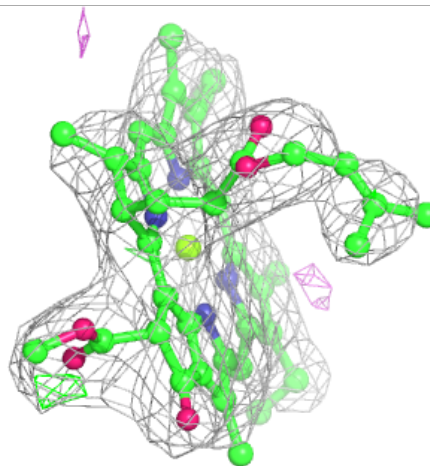
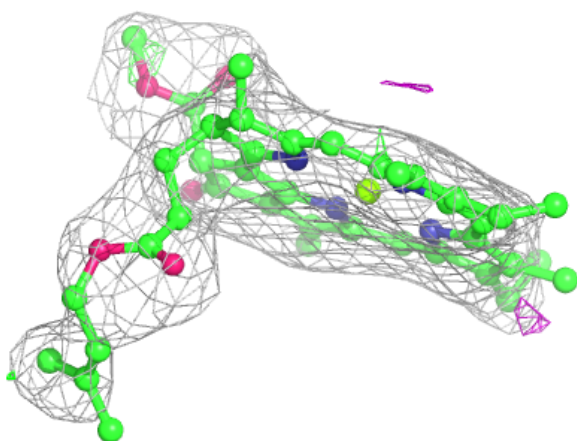
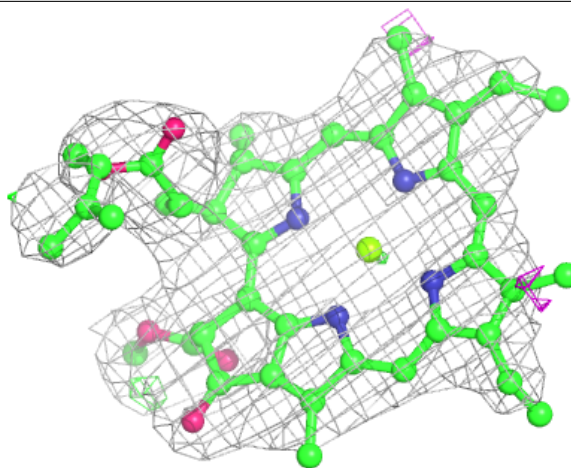
**Electron density around CLA 2 1237:**

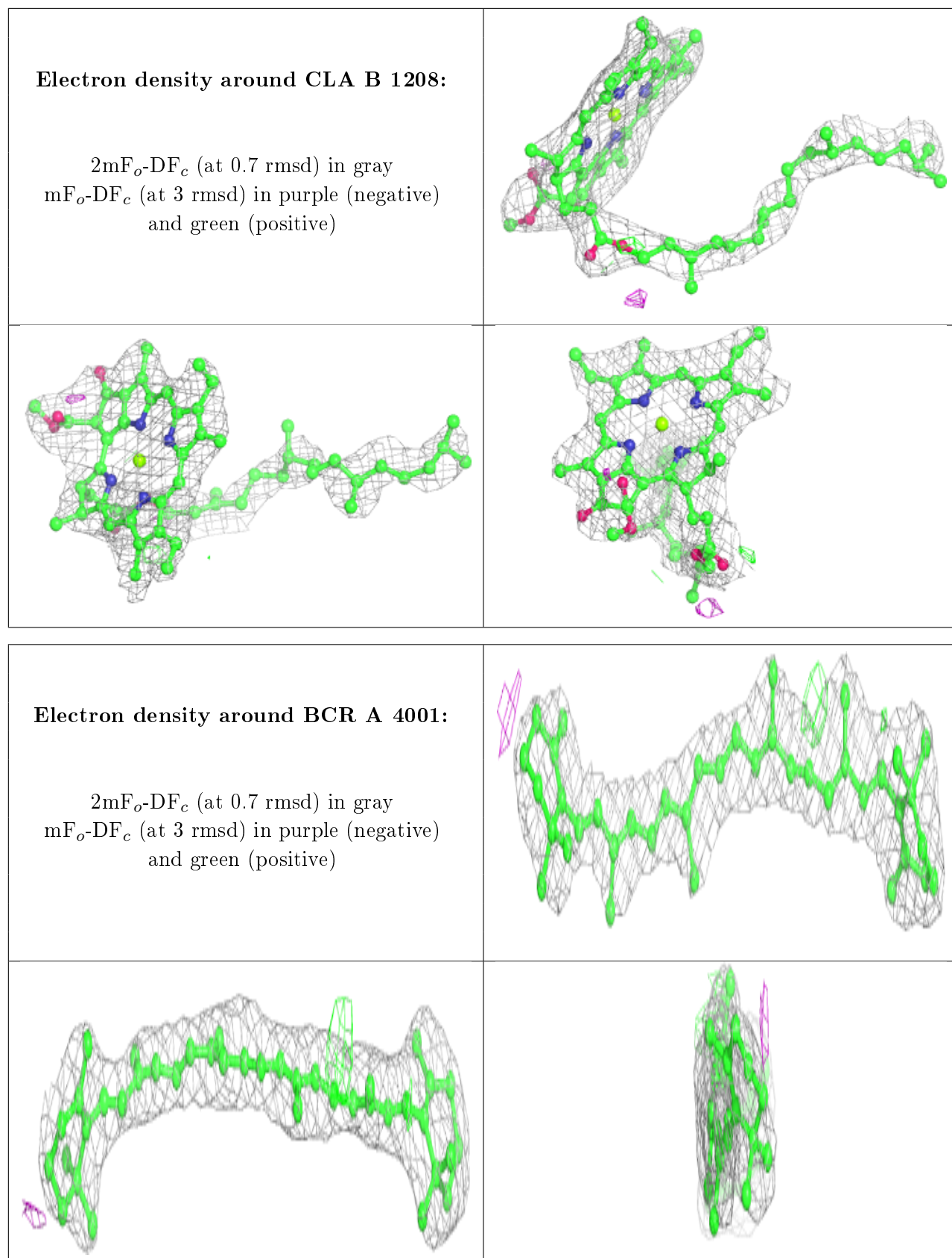
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1236:

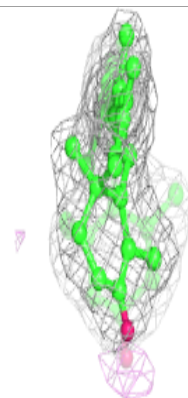
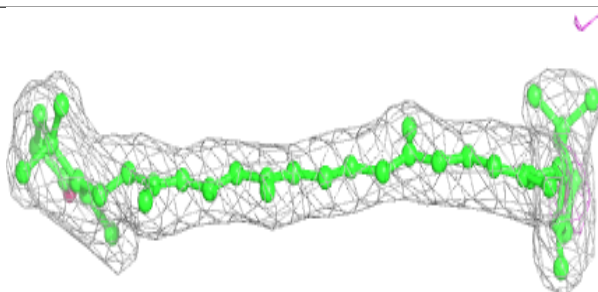
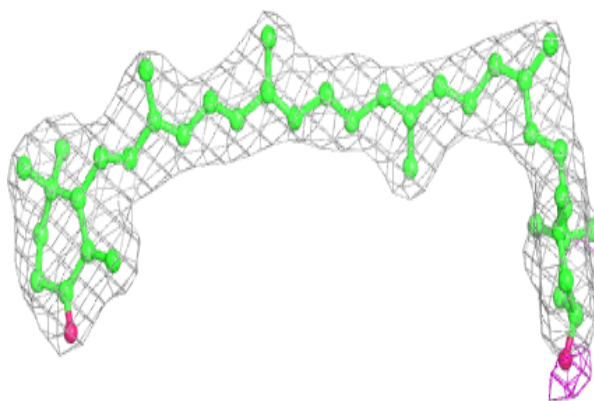
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



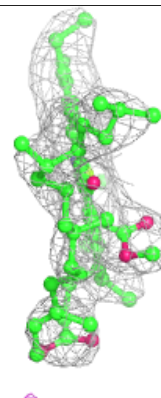
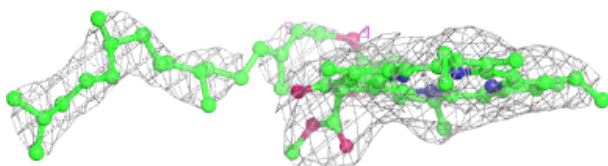
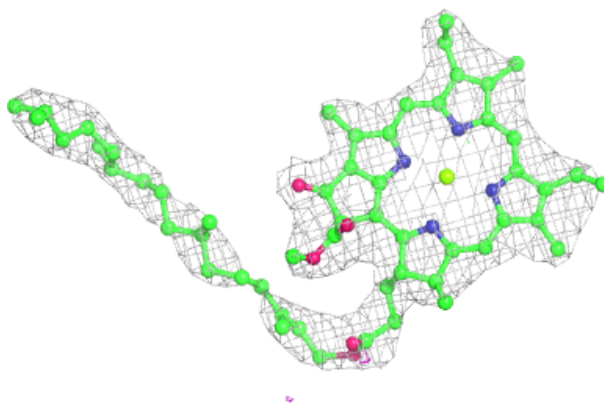


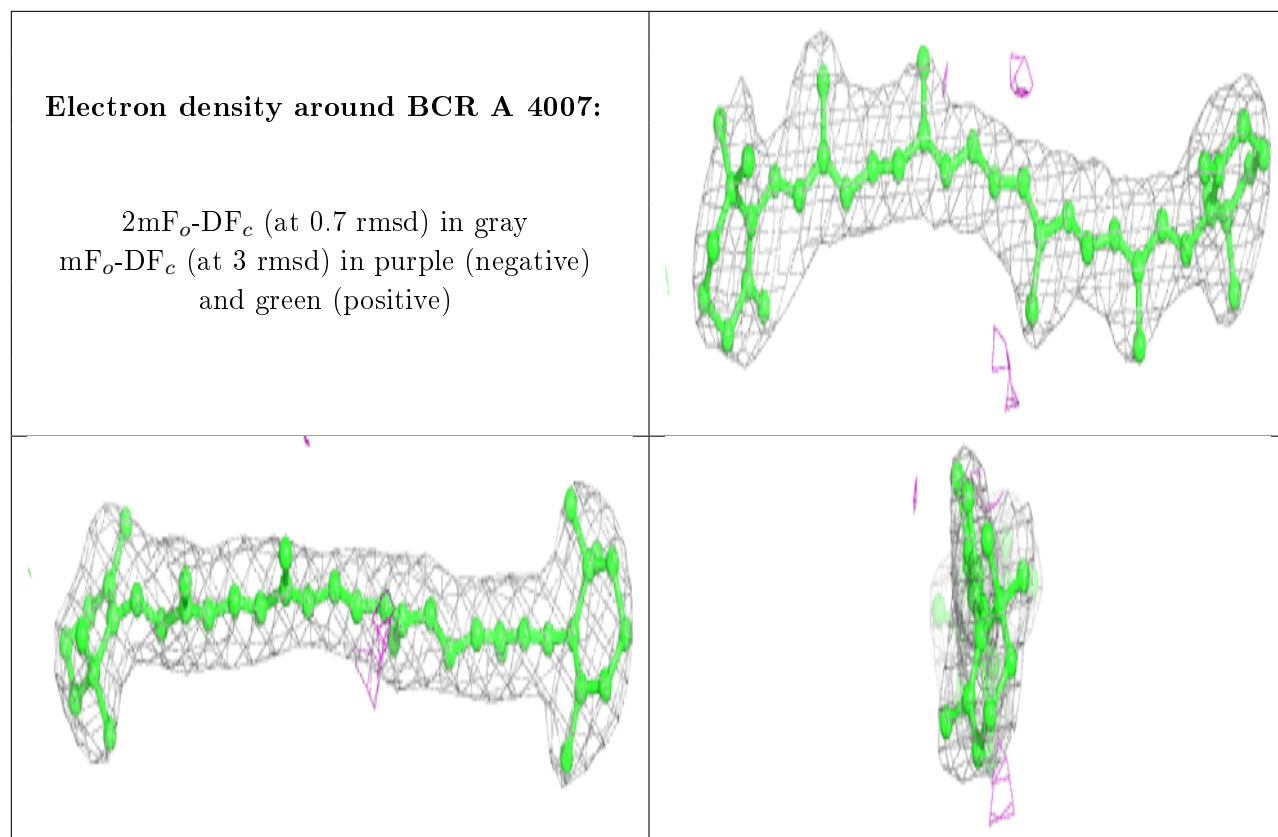
Electron density around EQ3 I 4020:

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

**Electron density around CLA 0 1503:**

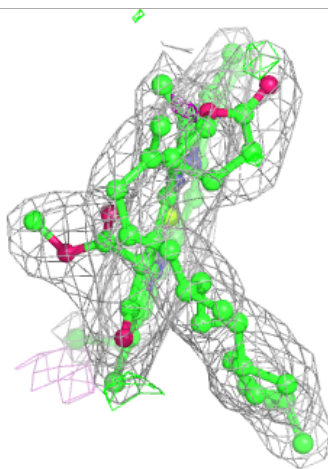
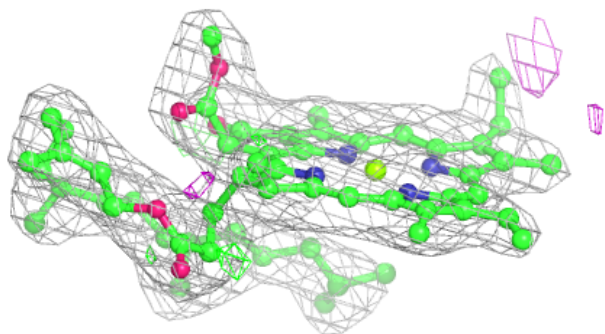
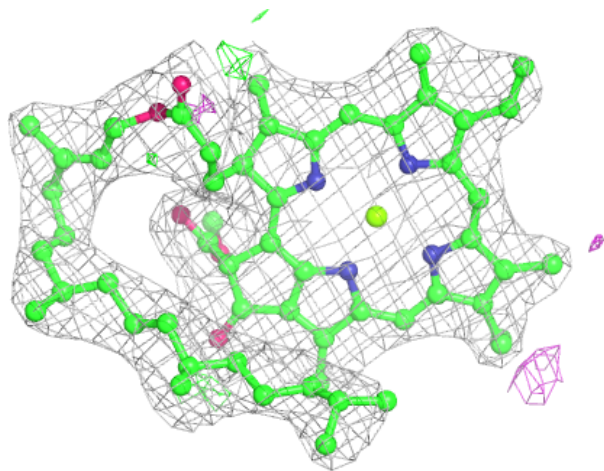
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





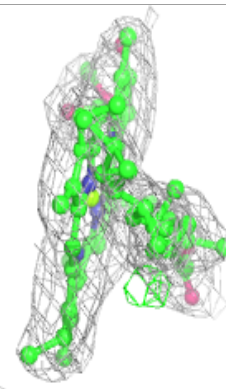
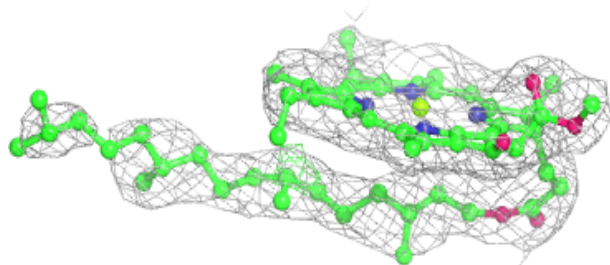
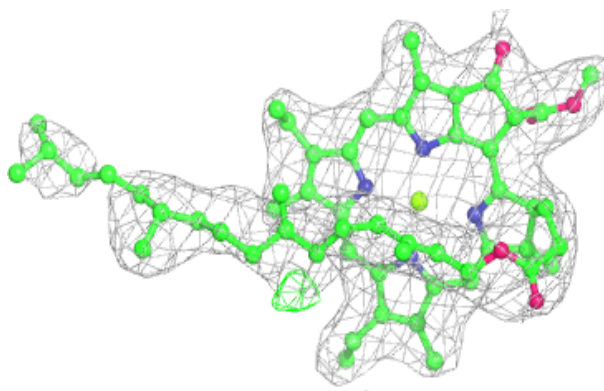
Electron density around CLA b 1202:

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

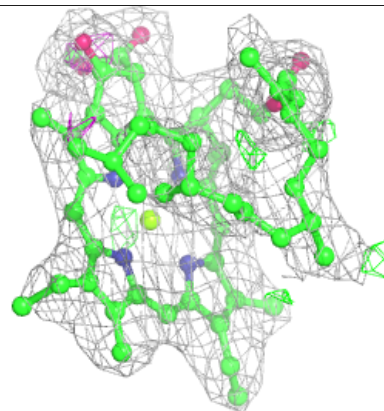
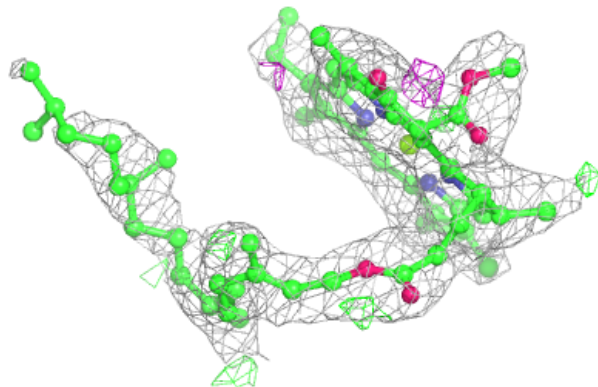
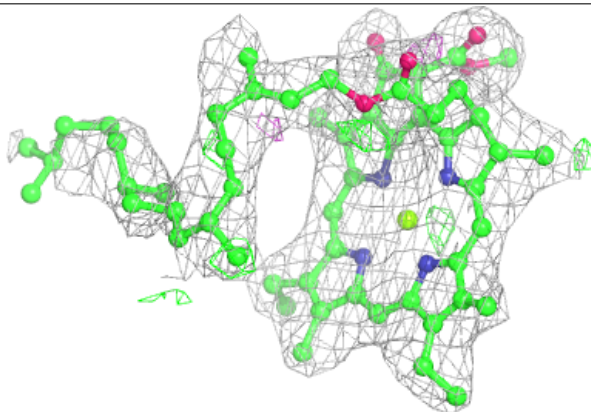


Electron density around CLA A 1116:

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

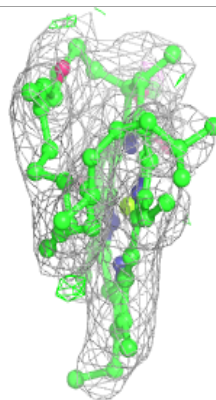
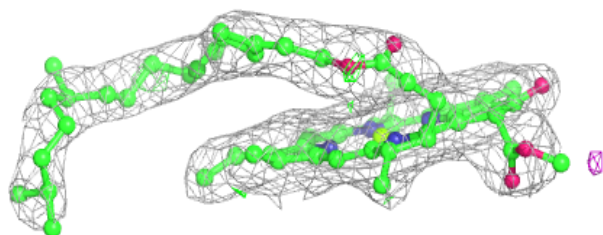
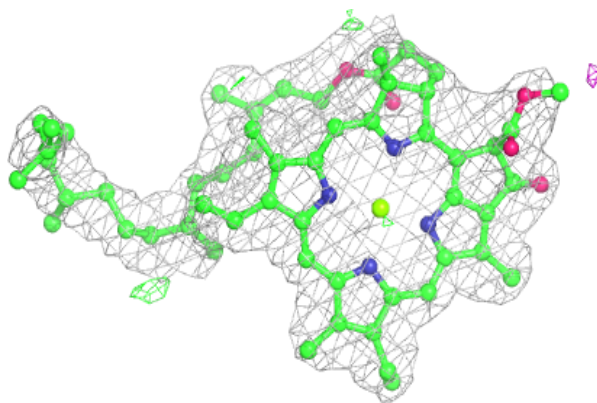
**Electron density around CLA b 1211:**

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

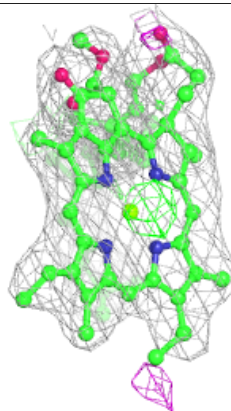
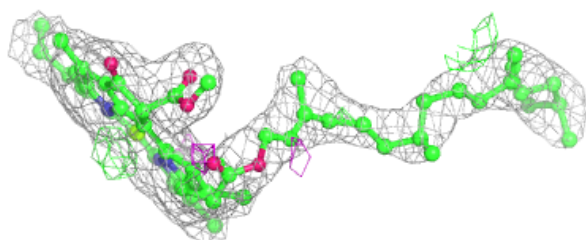
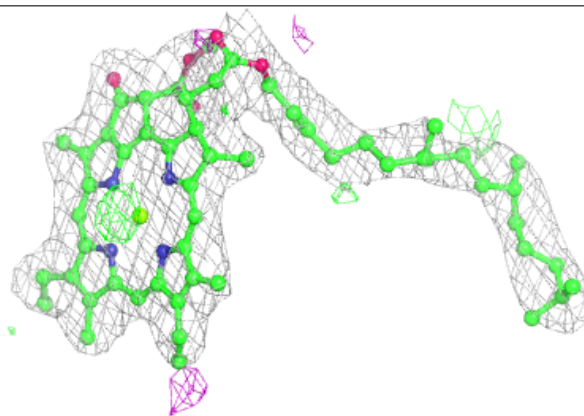


Electron density around CLA B 1215:

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

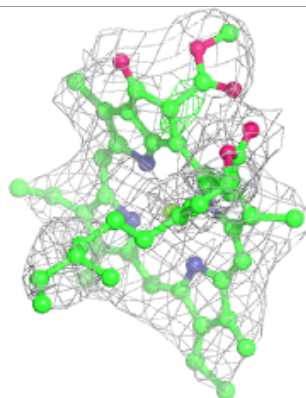
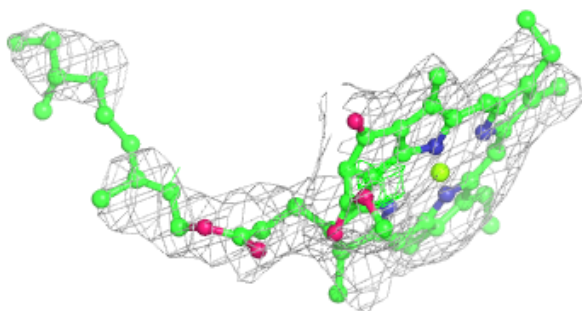
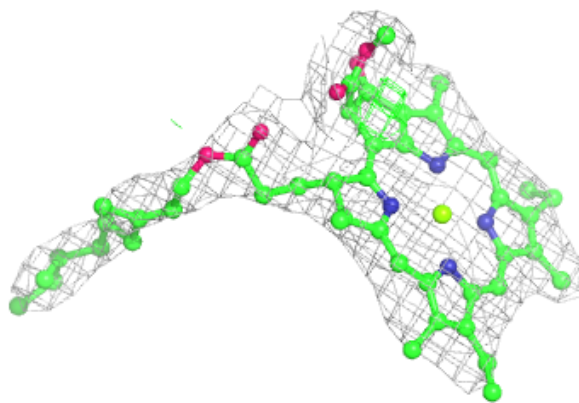
**Electron density around CLA B 1207:**

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

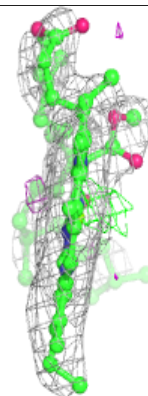
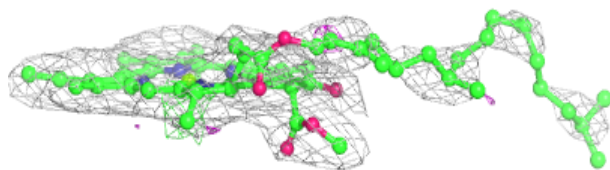
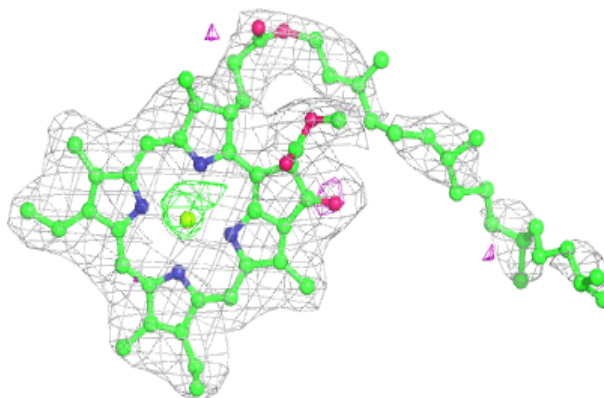


Electron density around CLA 1 1801:

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

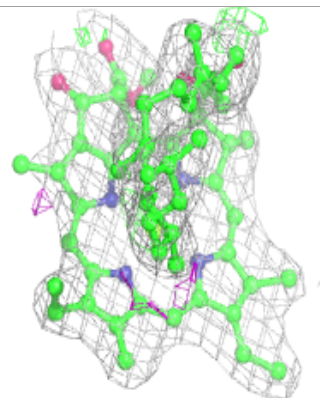
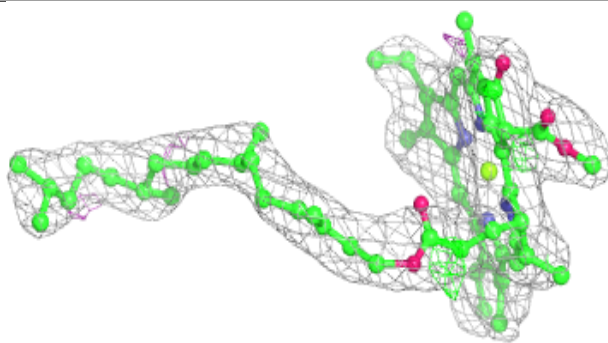
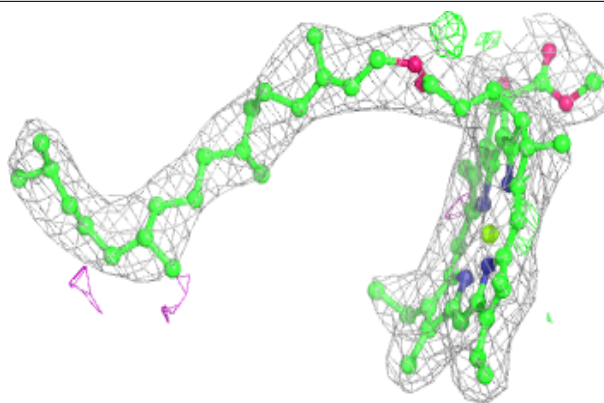
**Electron density around CLA 1 1503:**

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

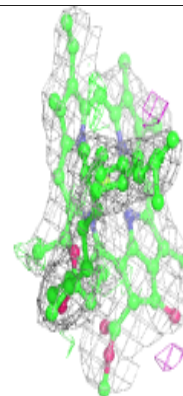
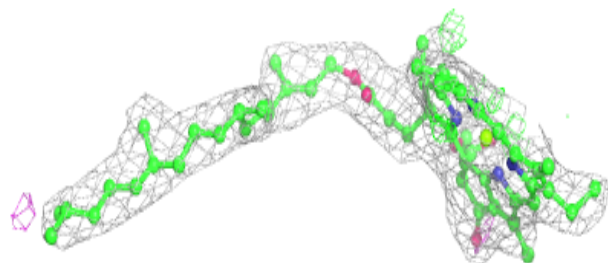
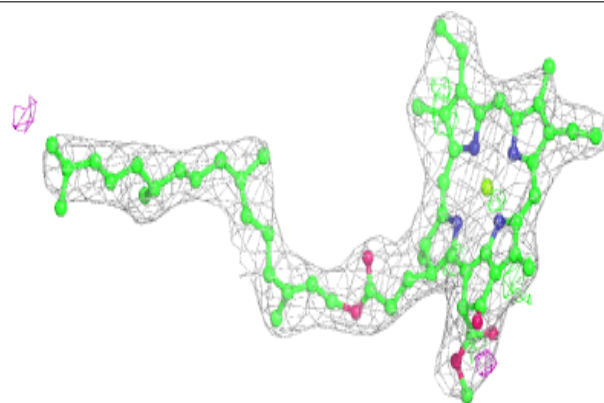


Electron density around CLA A 1128:

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

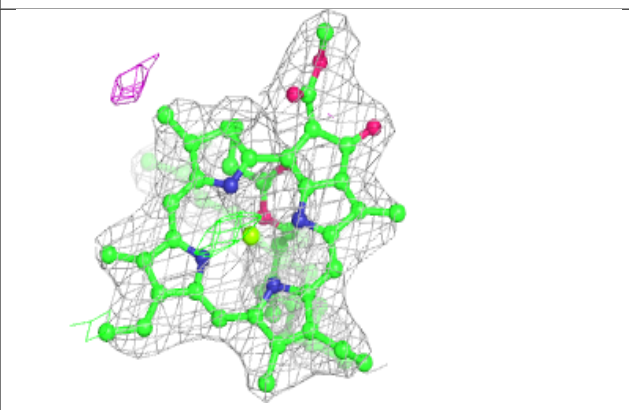
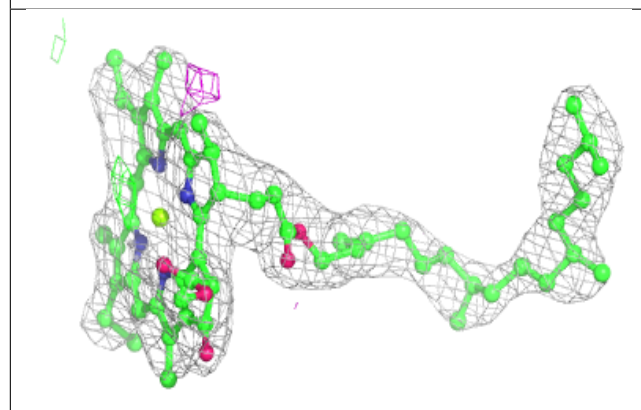
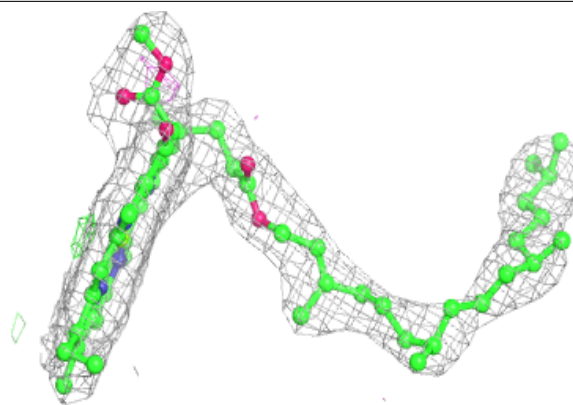
**Electron density around CLA 2 1022:**

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

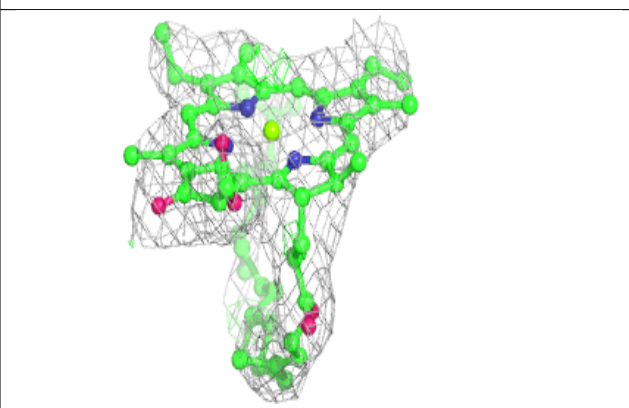
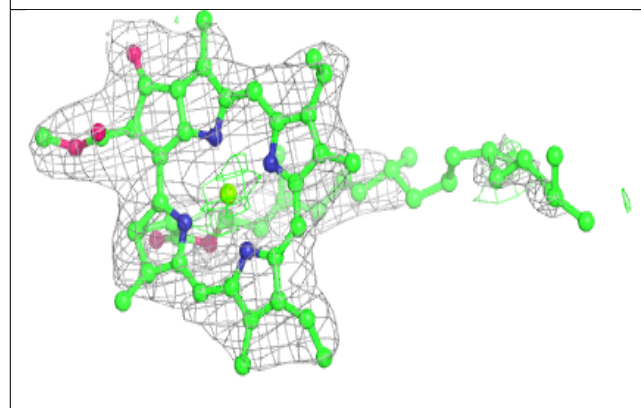
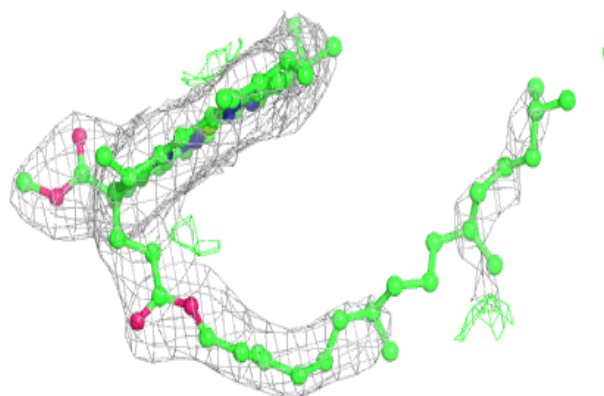


Electron density around CLA b 1238:

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

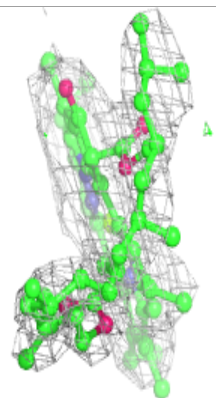
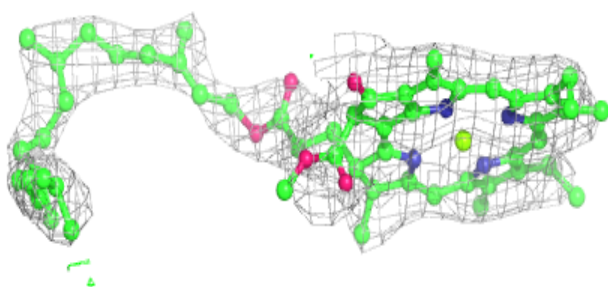
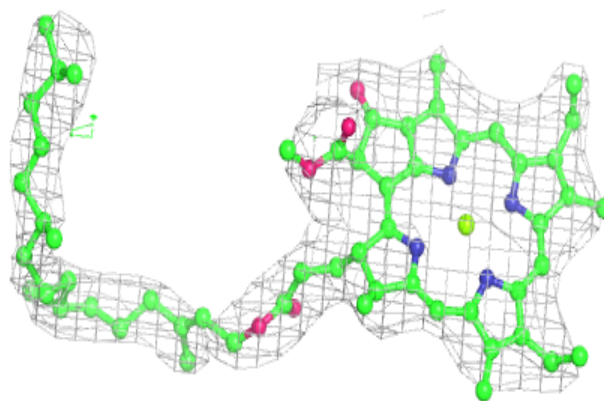
**Electron density around CLA a 1130:**

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

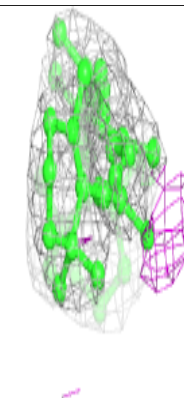
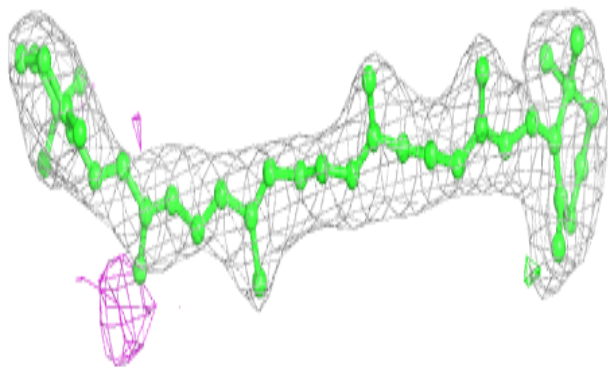
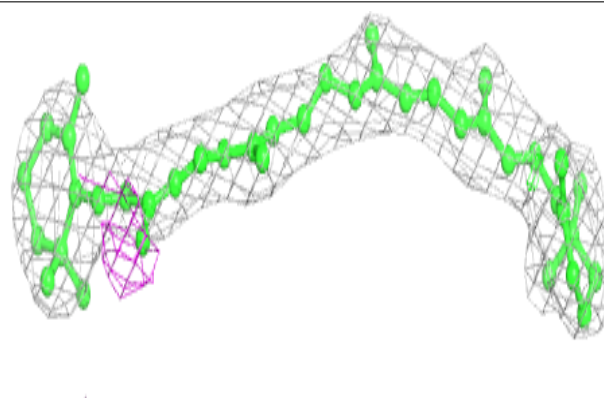


Electron density around CLA B 1223:

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

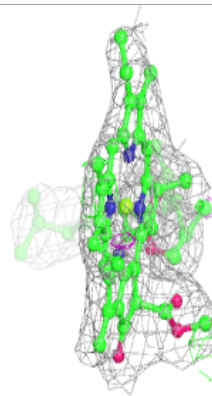
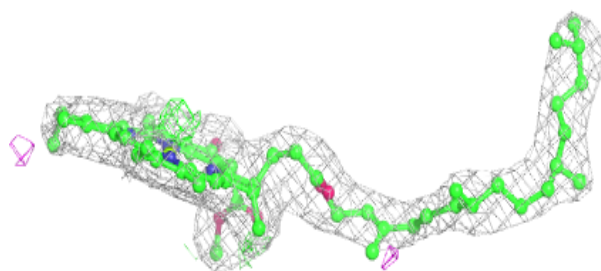
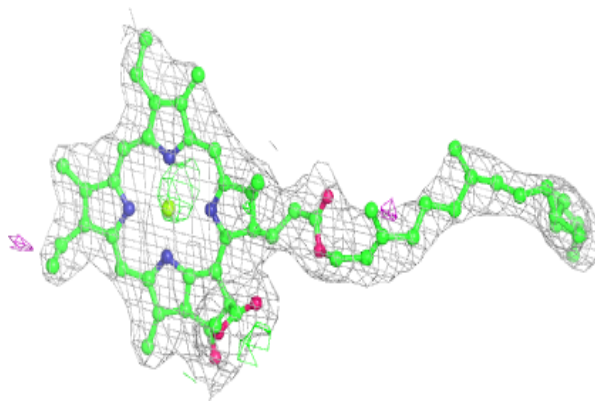
**Electron density around BCR I 4018:**

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

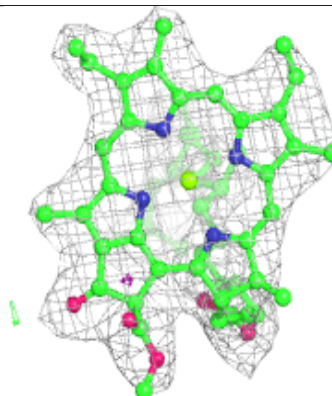
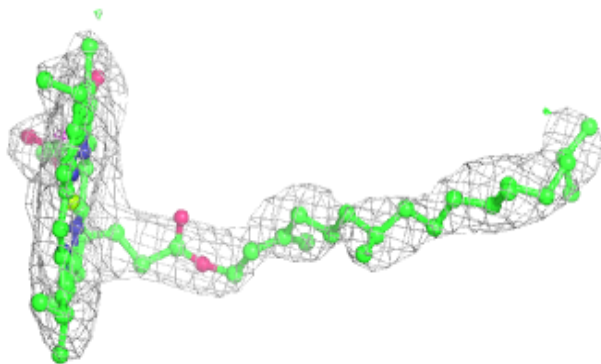
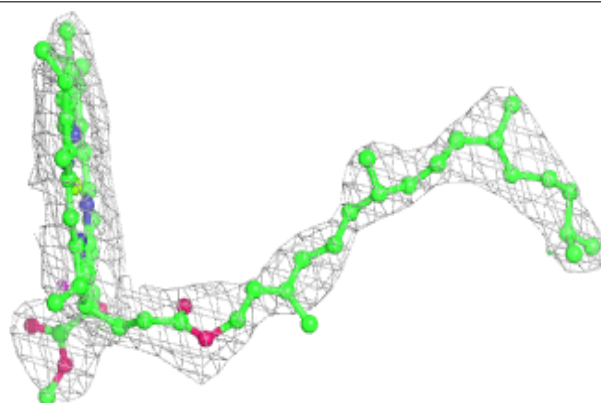


Electron density around CLA A 1103:

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

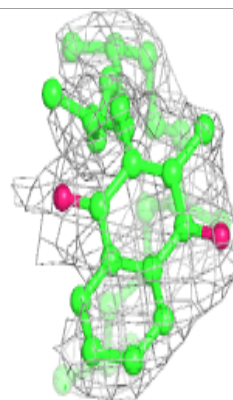
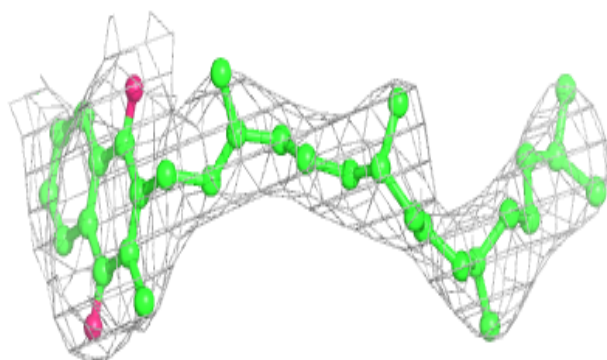
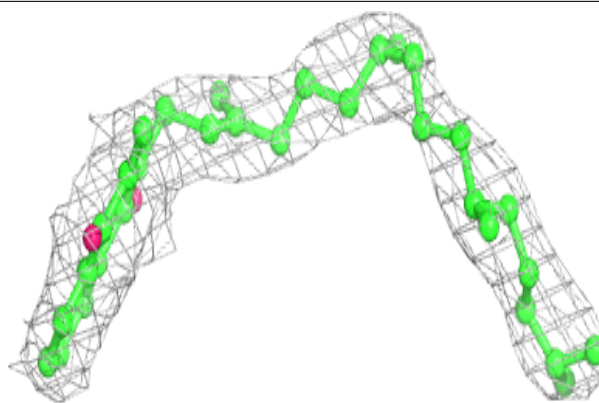
**Electron density around CLA 2 1239:**

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

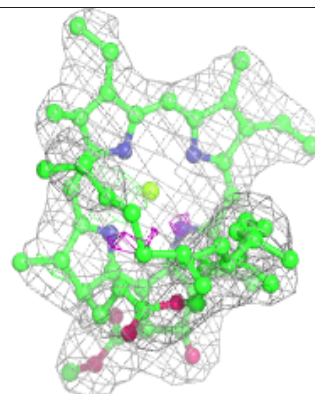
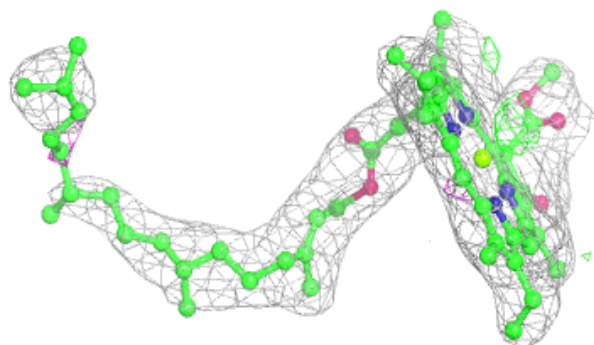
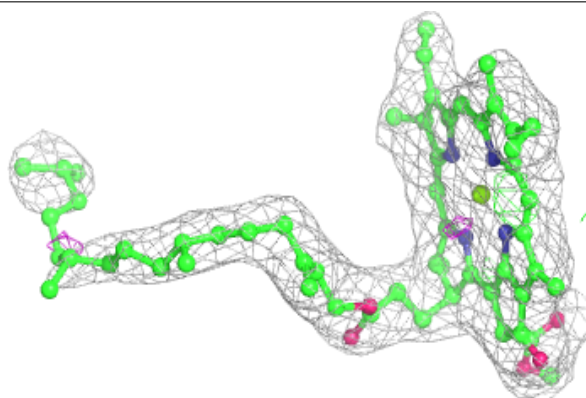


Electron density around PQN 2 2002:

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

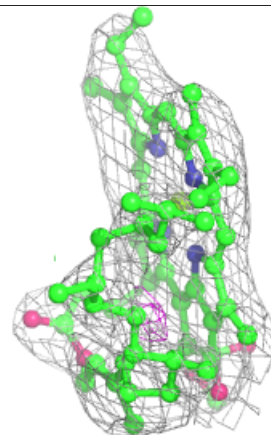
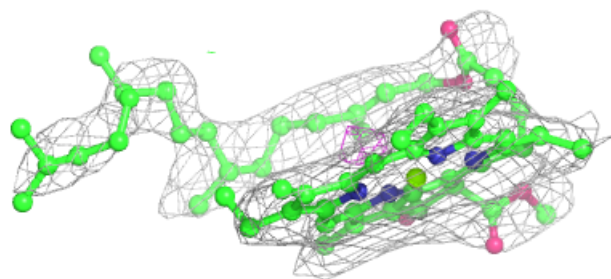
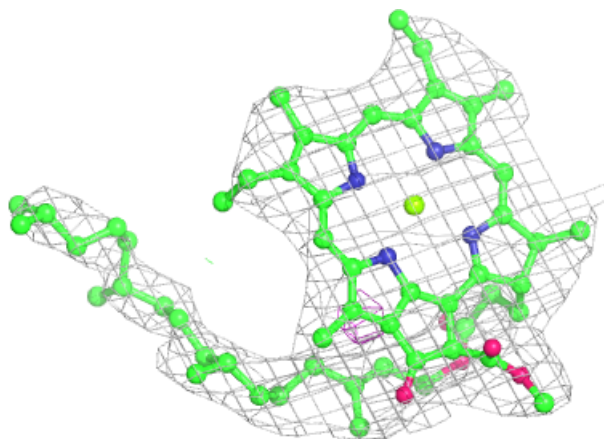
**Electron density around CLA 0 1502:**

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

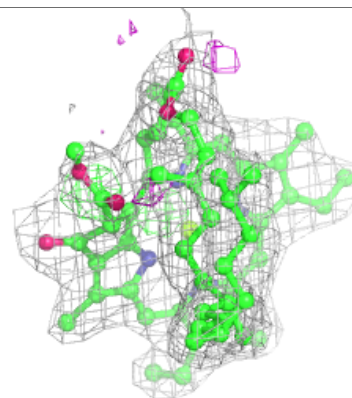
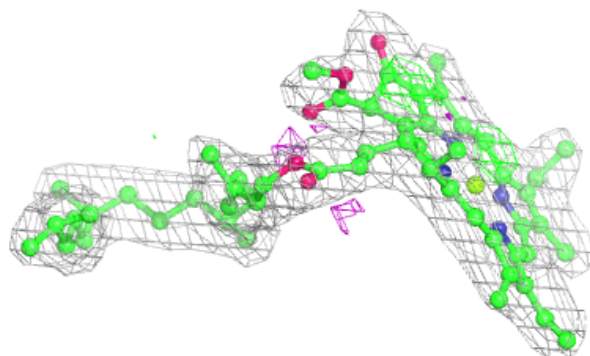
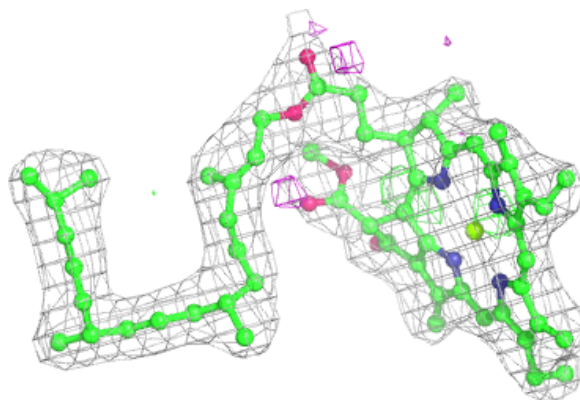


Electron density around CLA a 1127:

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

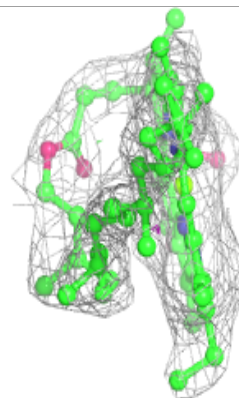
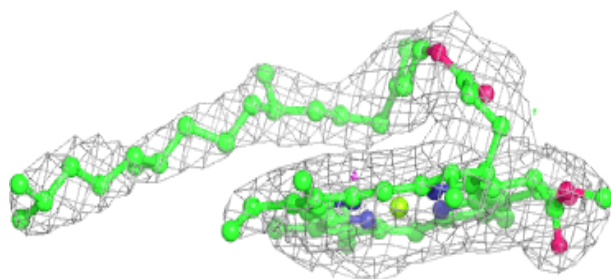
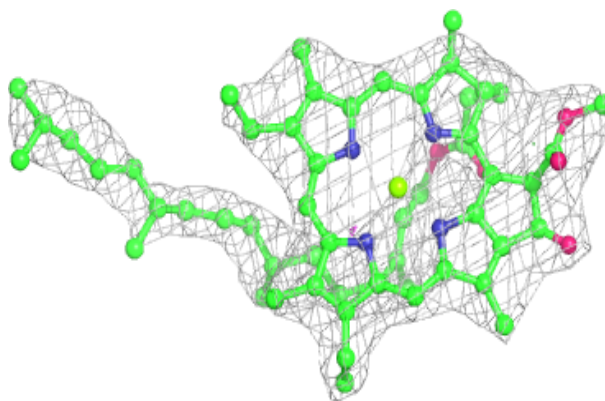
**Electron density around CLA A 1011:**

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

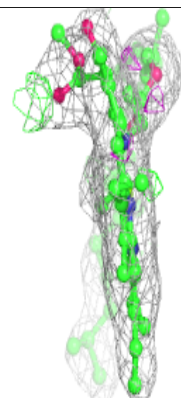
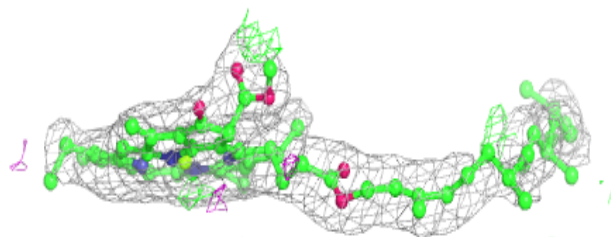
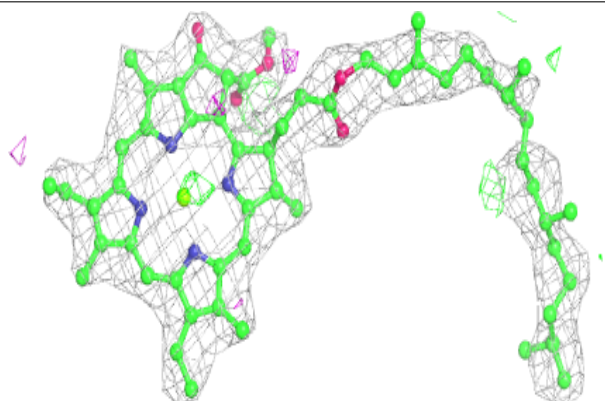


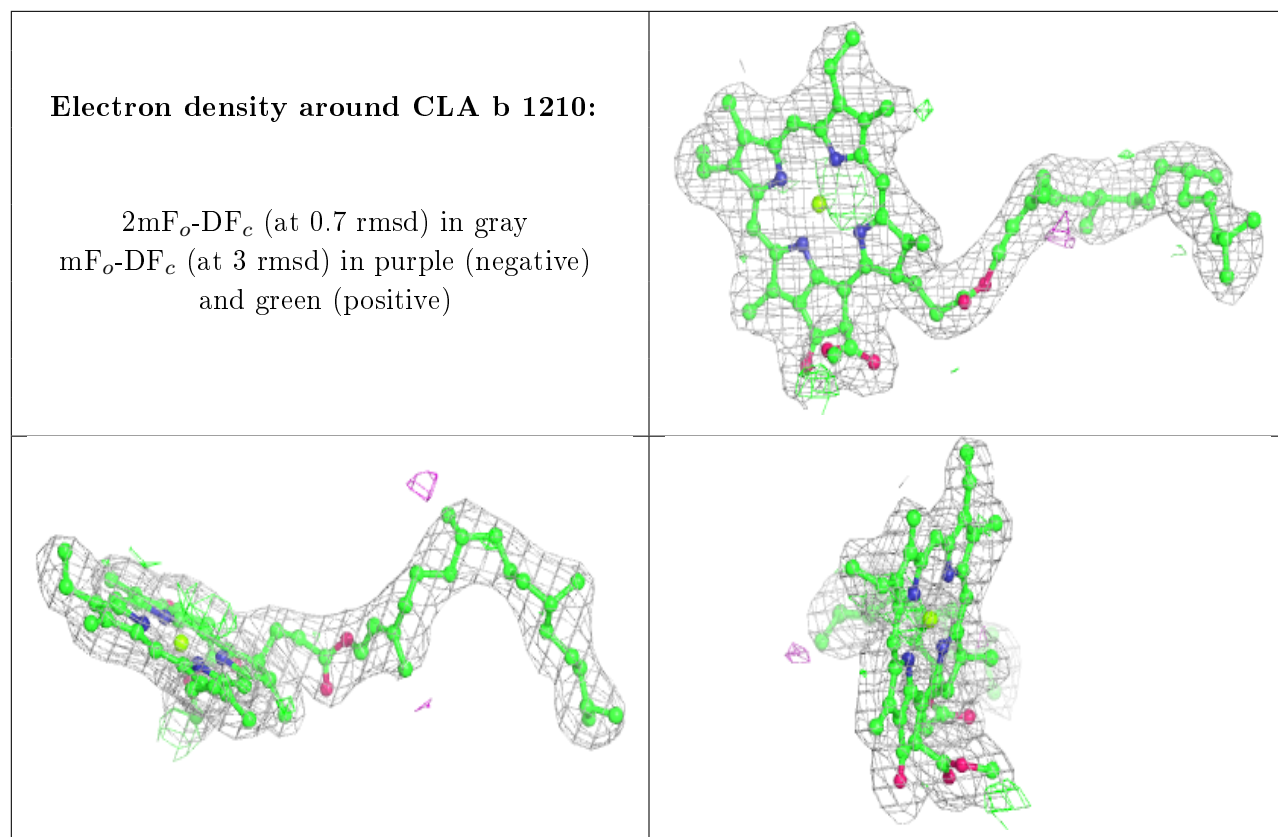
Electron density around CLA A 1138:

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

**Electron density around CLA A 1135:**

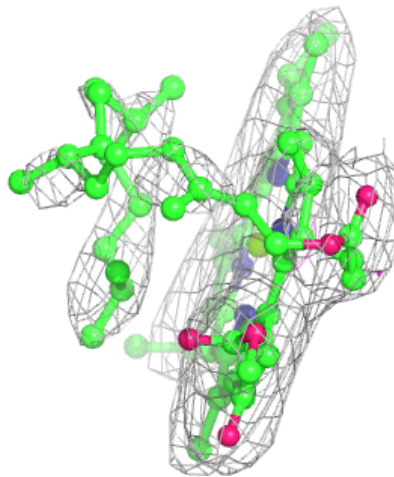
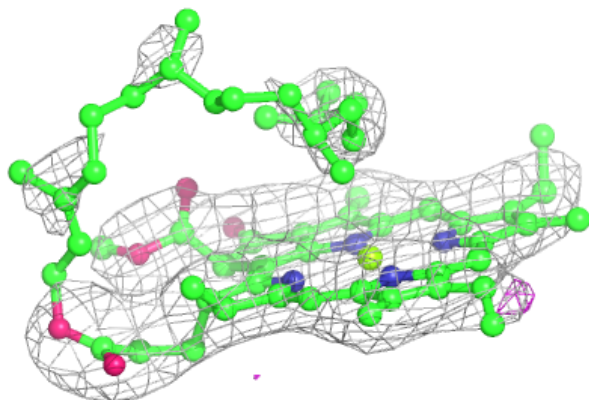
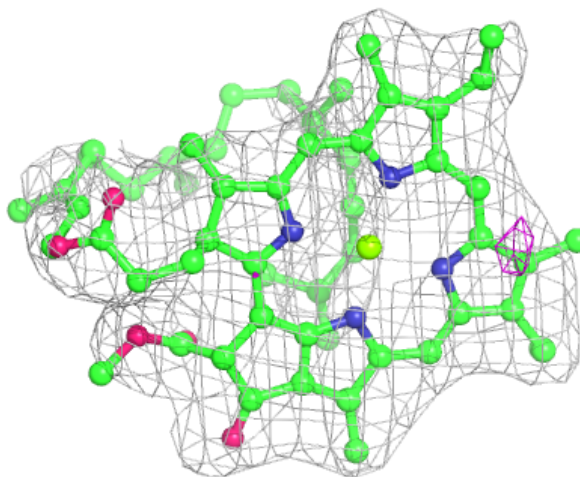
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





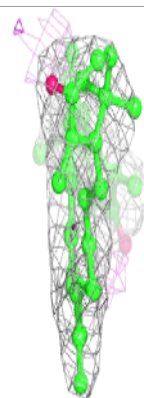
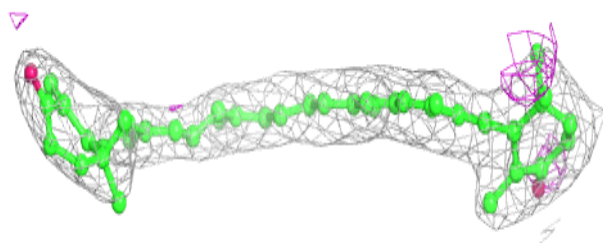
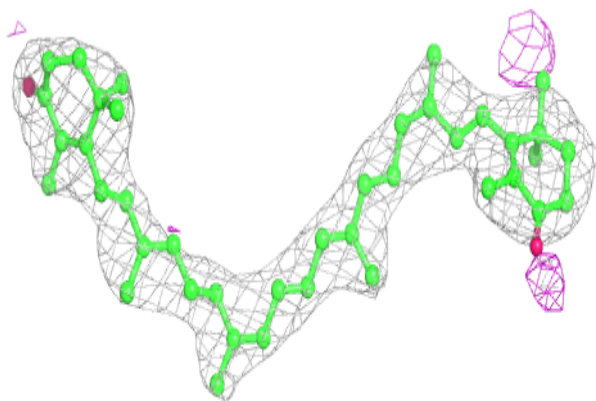
Electron density around CLA a 1104:

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

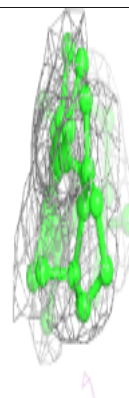
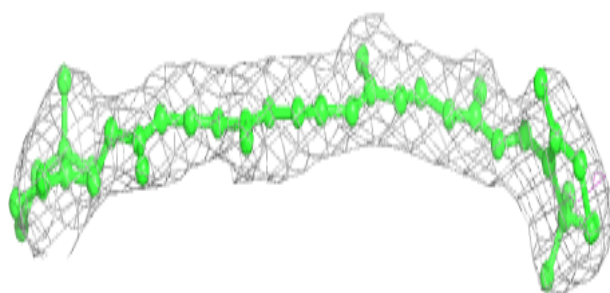
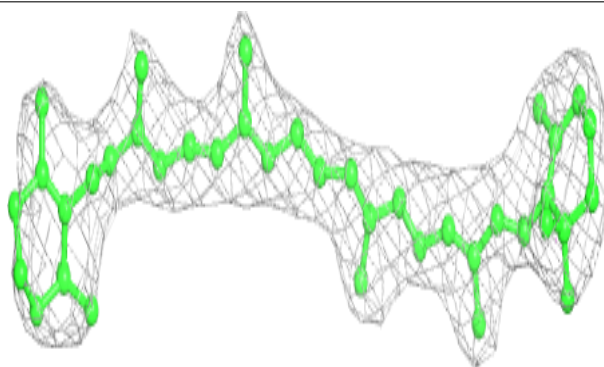


Electron density around 45D B 4011:

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

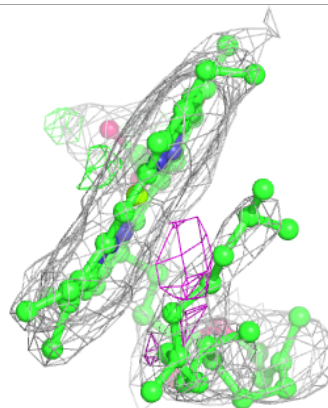
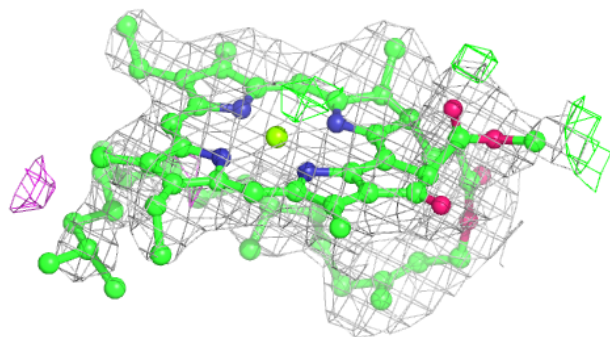
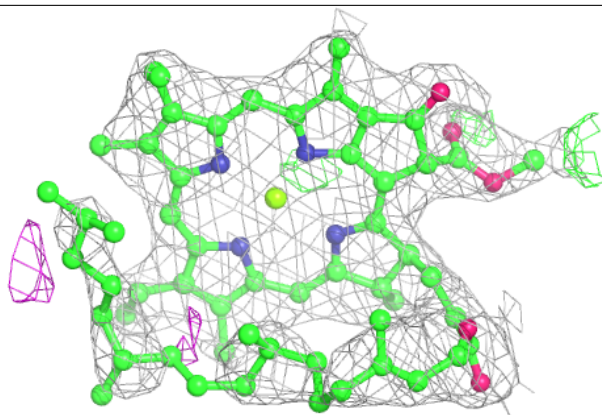
**Electron density around BCR A 4008:**

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

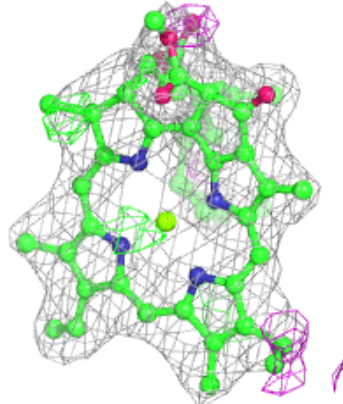
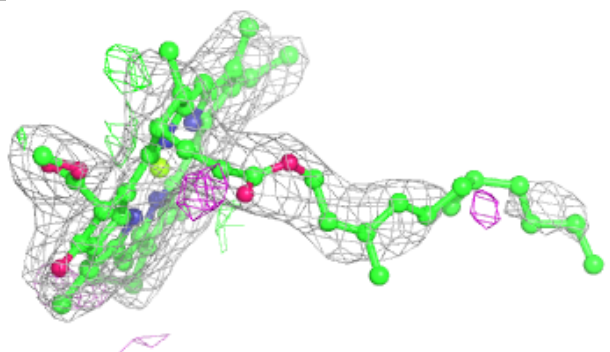
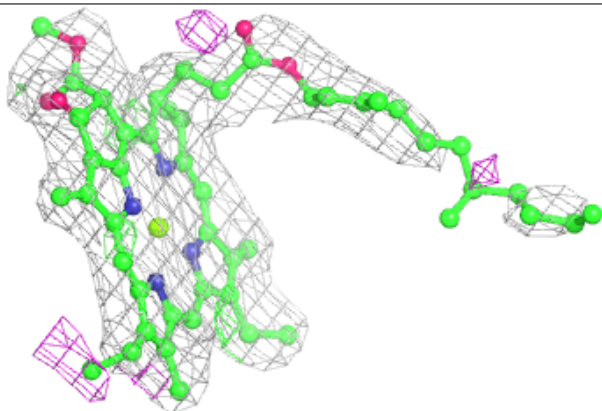


Electron density around CLA A 1118:

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

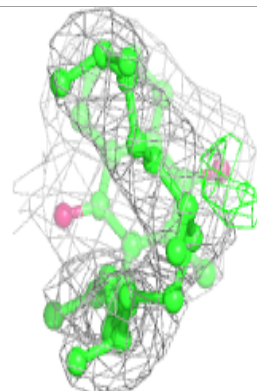
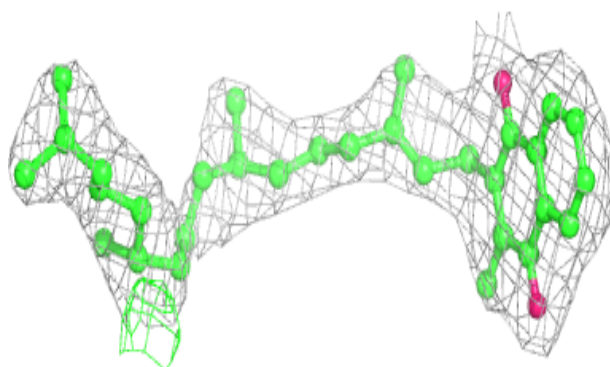
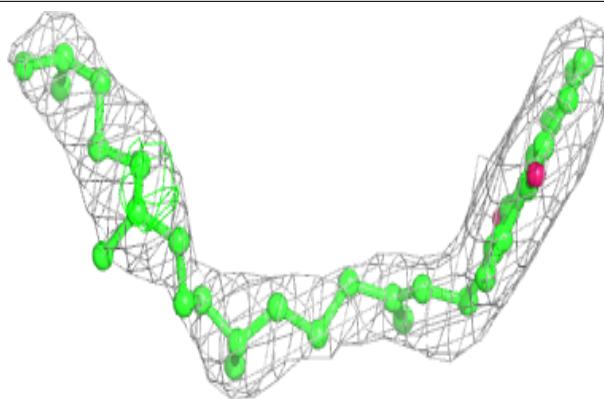
**Electron density around CLA A 1129:**

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

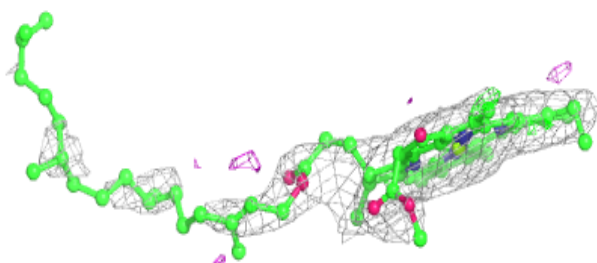
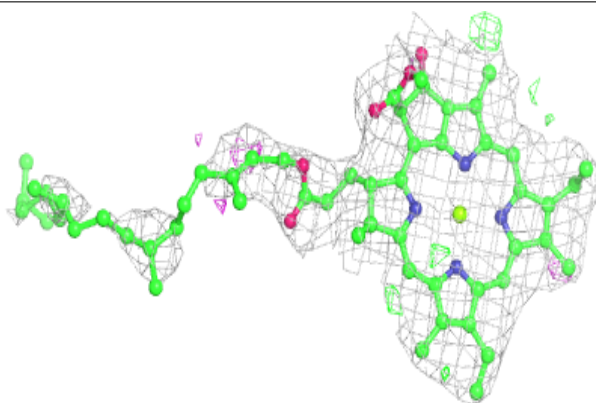


Electron density around PQN b 2002:

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

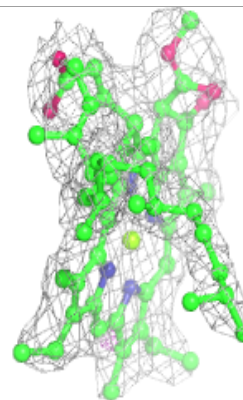
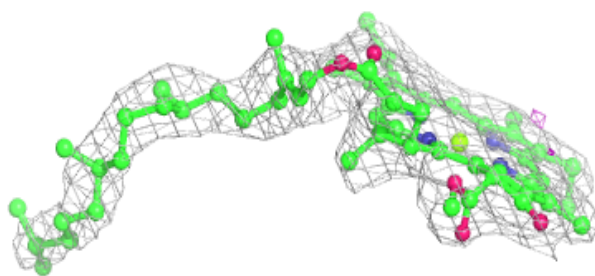
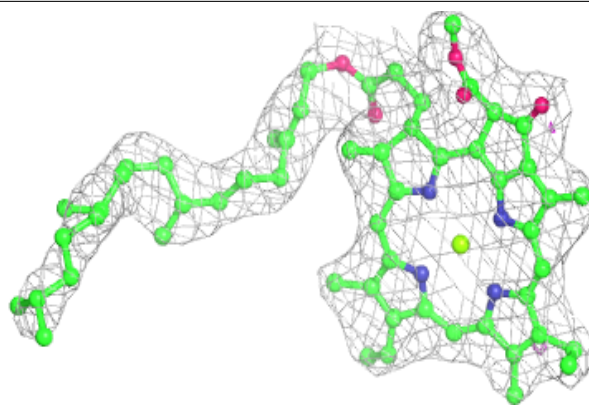
**Electron density around CLA a 1103:**

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

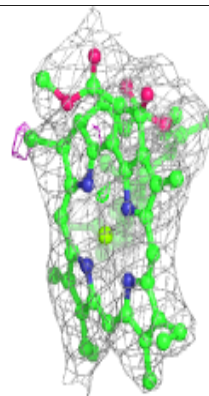
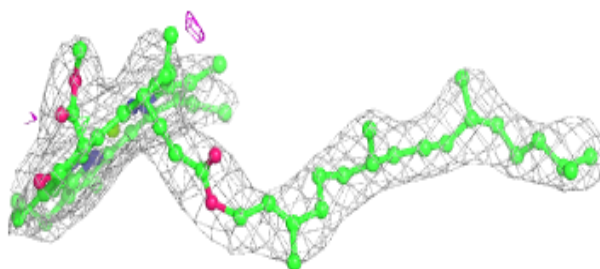
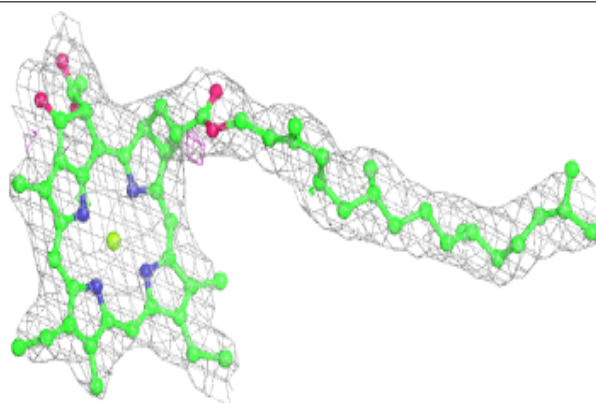


Electron density around CLA a 1013:

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

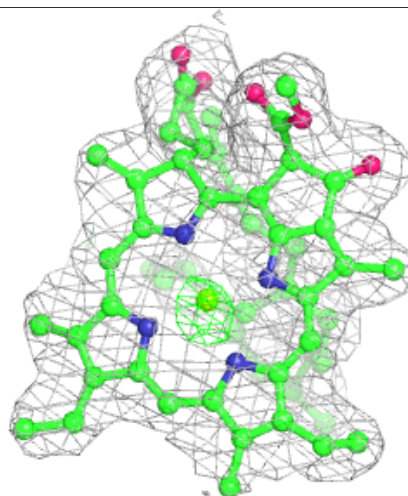
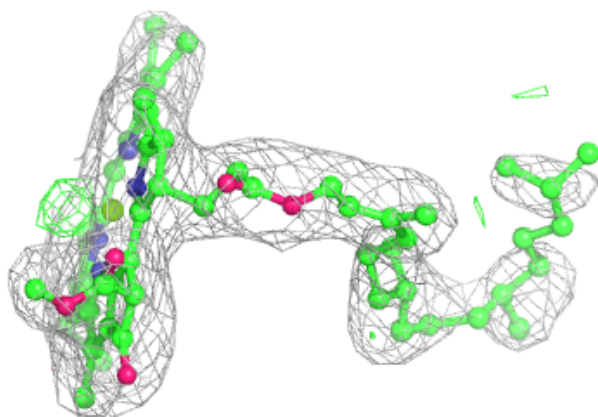
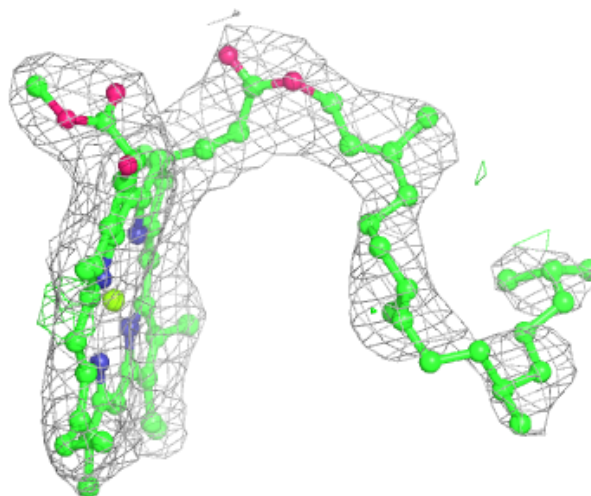
**Electron density around CLA 1 1132:**

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



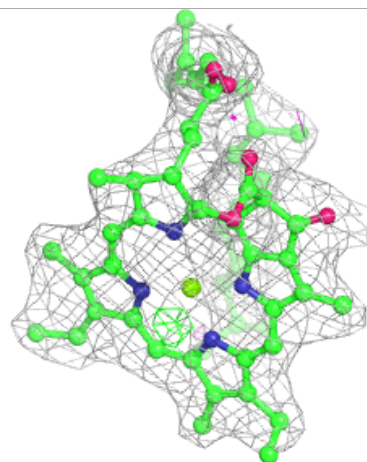
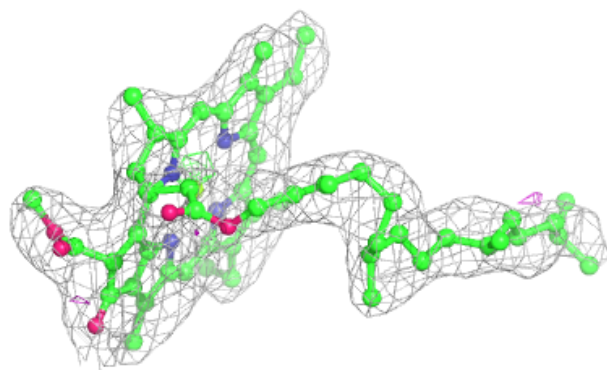
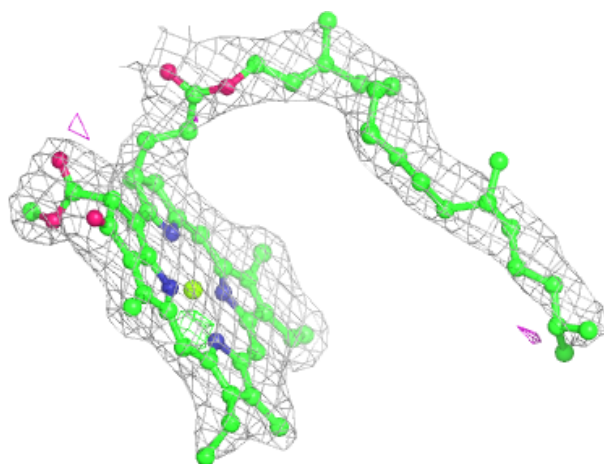
Electron density around CLA A 1801:

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



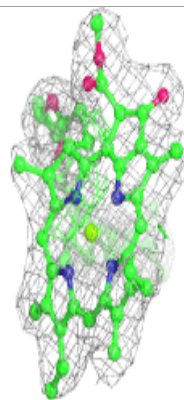
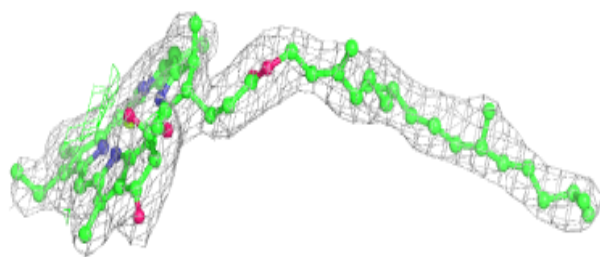
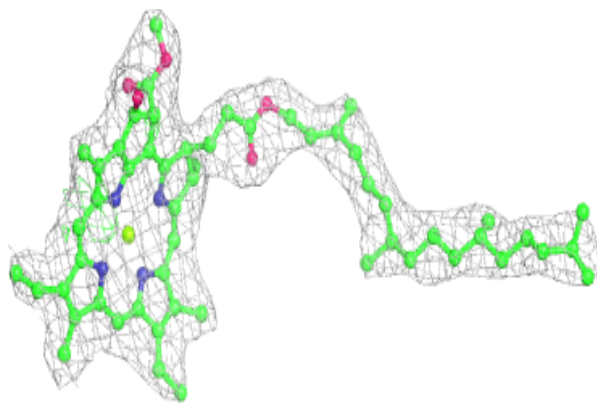
Electron density around CLA A 1102:

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

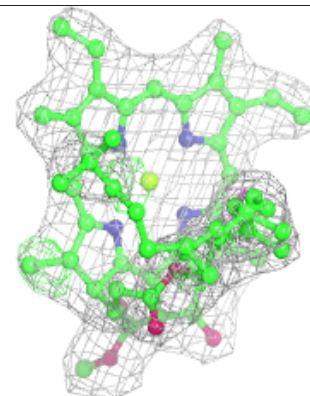
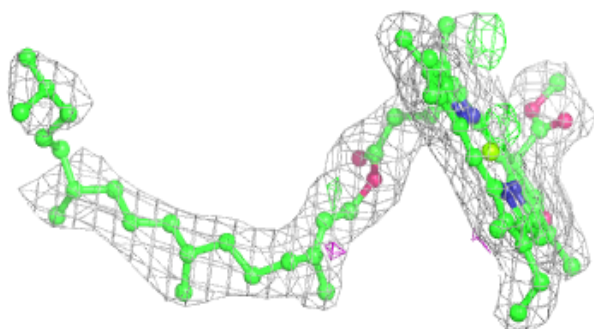
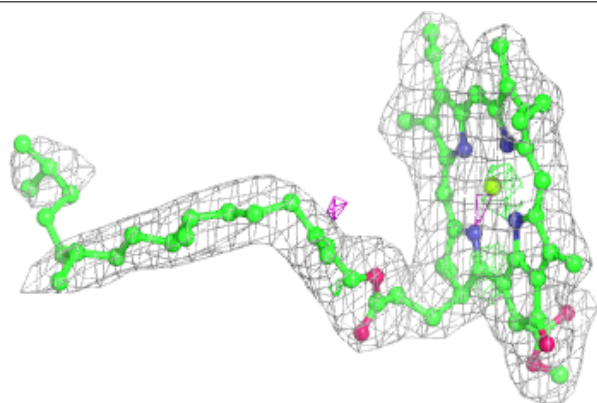


Electron density around CLA b 1022:

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

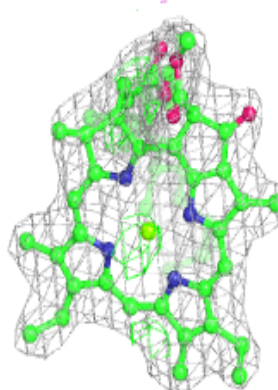
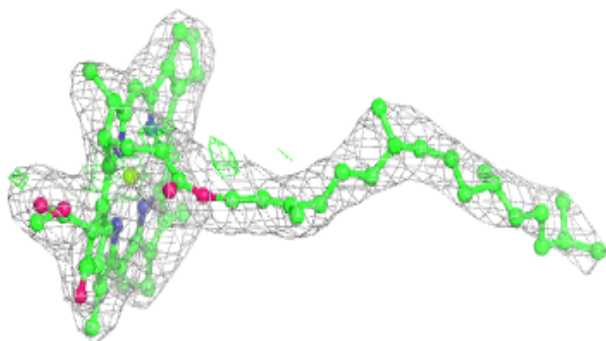
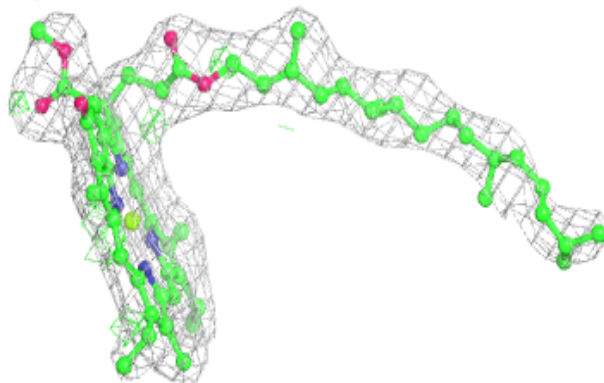
**Electron density around CLA L 1502:**

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

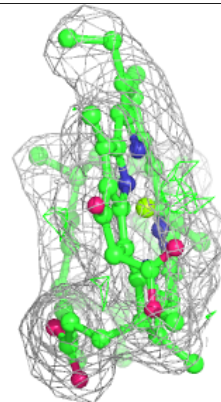
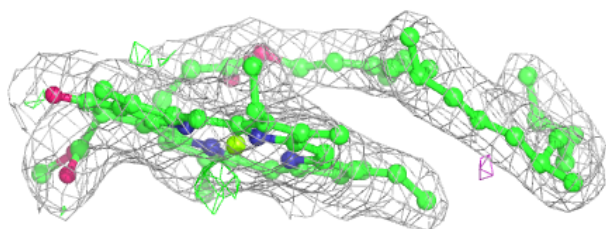
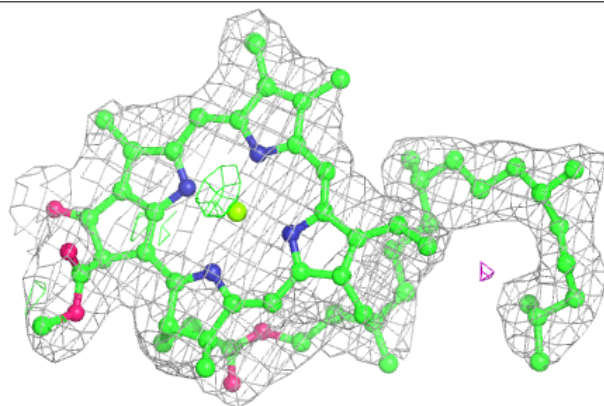


Electron density around CLA b 1201:

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

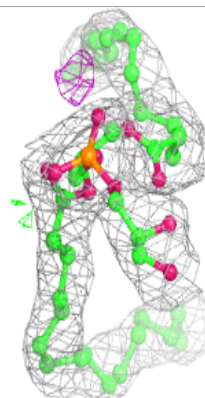
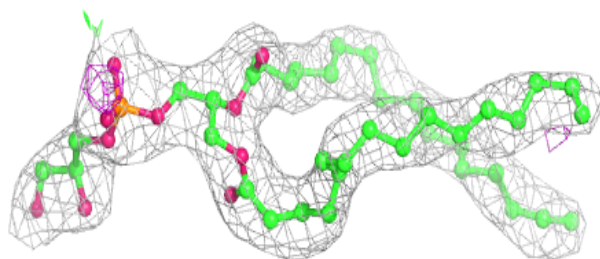
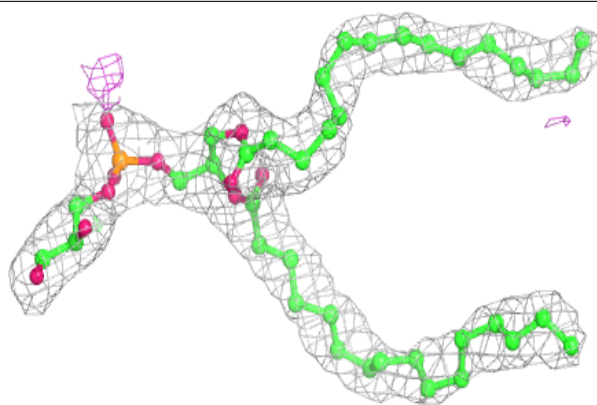
**Electron density around CLA A 1117:**

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



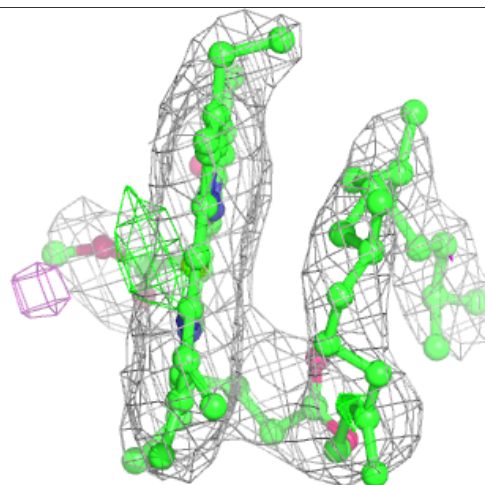
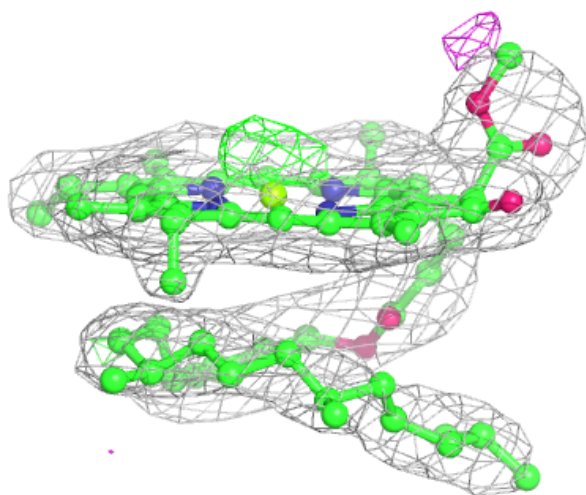
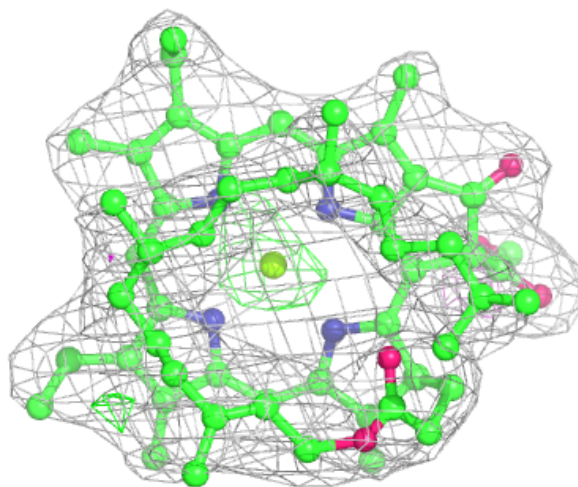
Electron density around LHG A 5001:

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



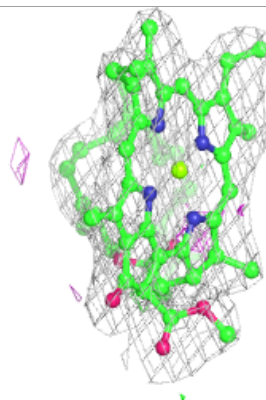
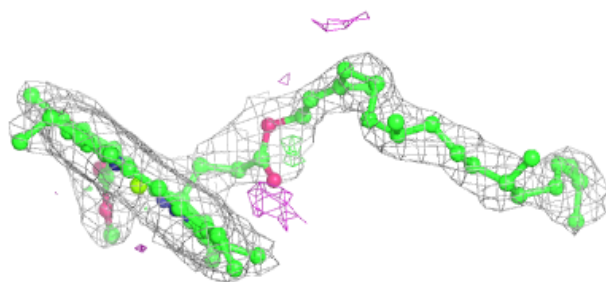
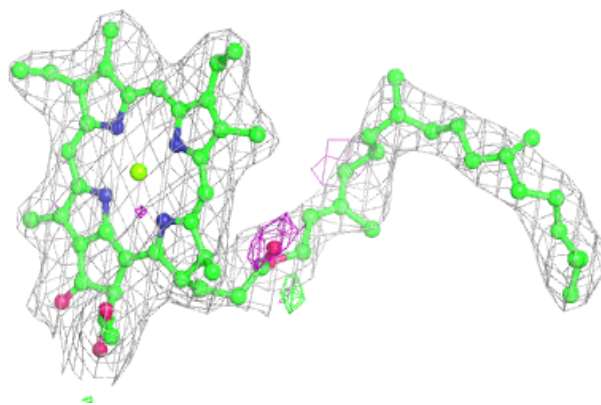
Electron density around CLA 0 1501:

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

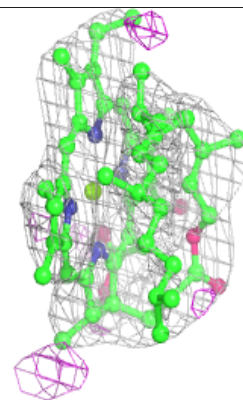
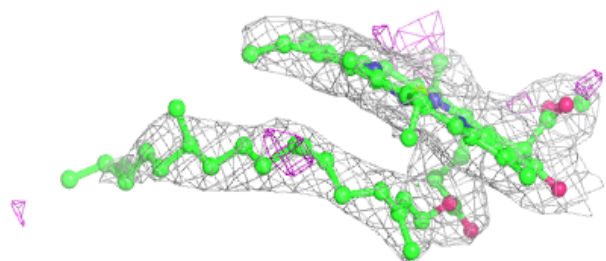
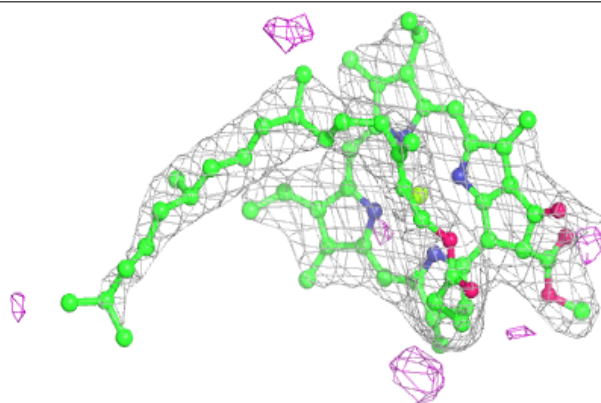


Electron density around CLA A 1106:

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

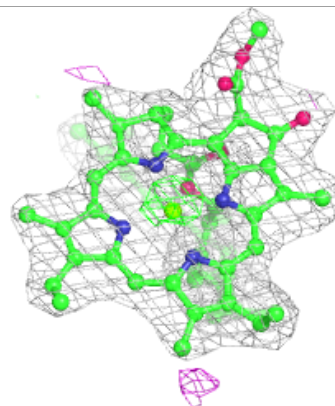
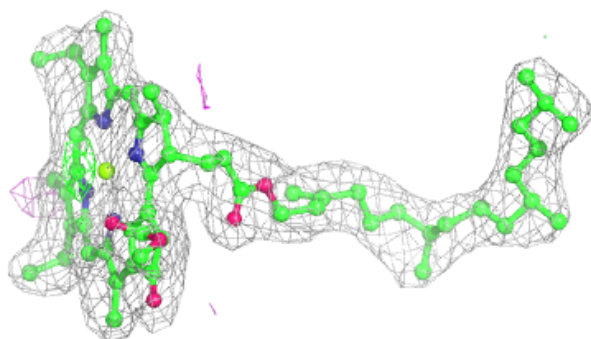
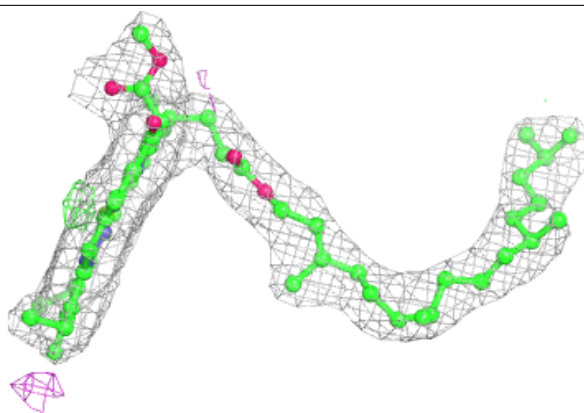
**Electron density around CLA B 1204:**

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

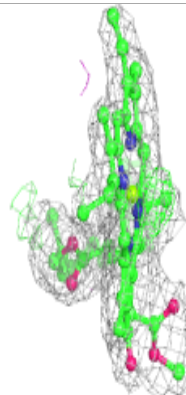
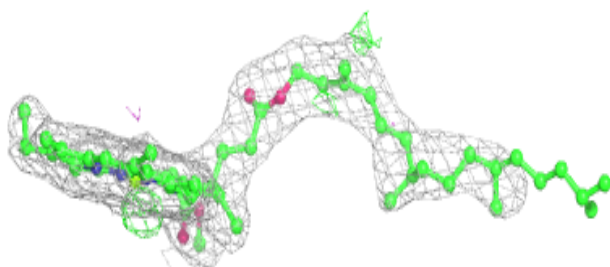
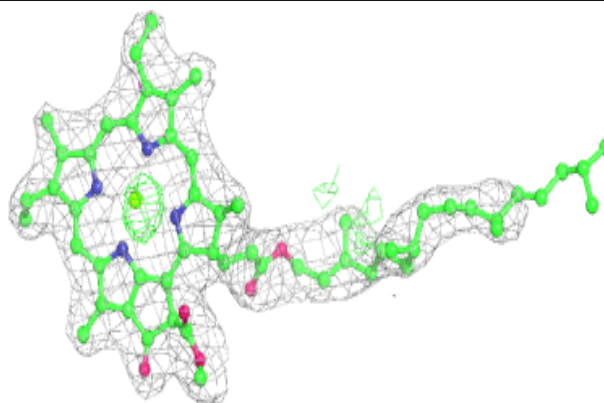


Electron density around CLA B 1238:

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

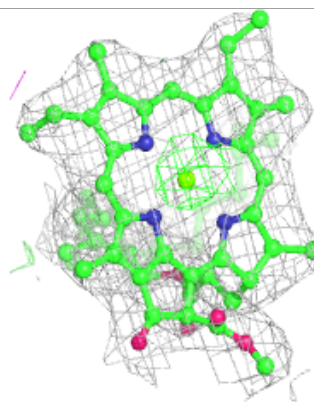
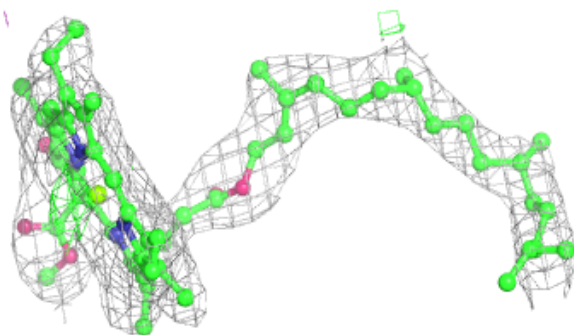
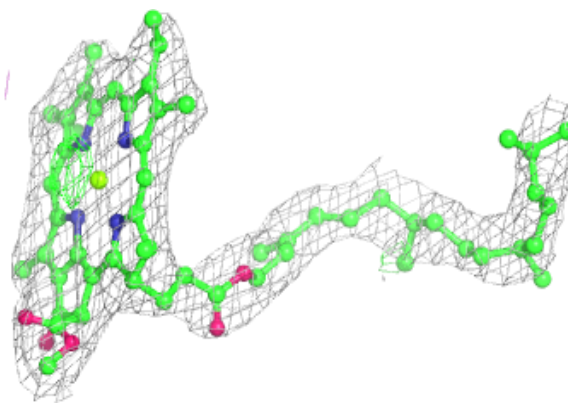
**Electron density around CLA A 1124:**

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

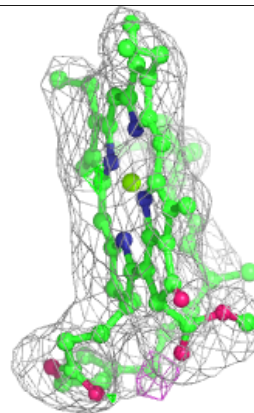
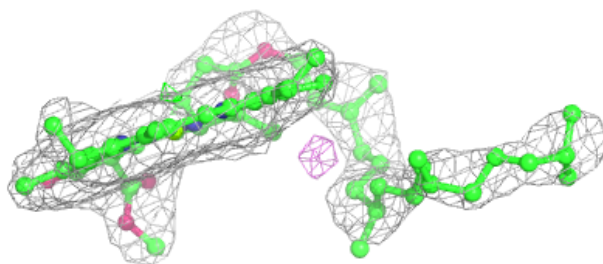
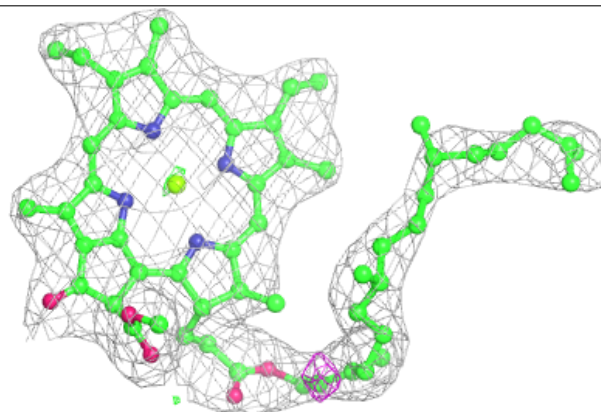


Electron density around CLA 1 1502:

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

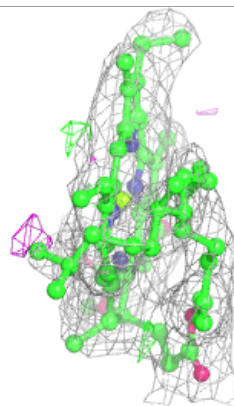
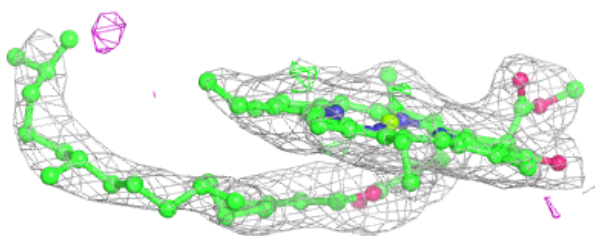
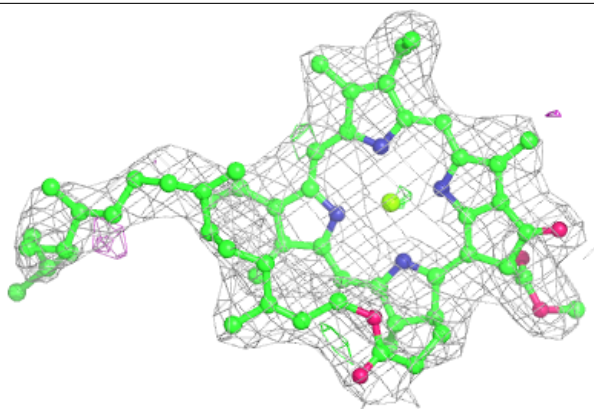
**Electron density around CLA A 1111:**

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

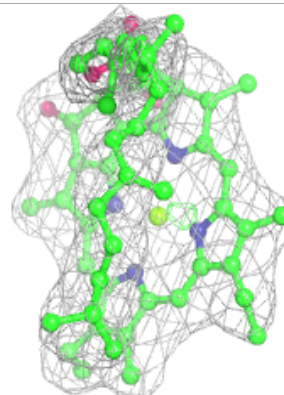
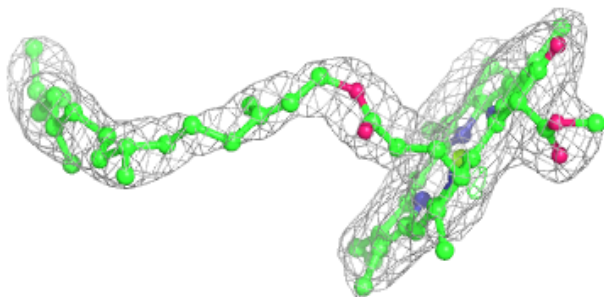
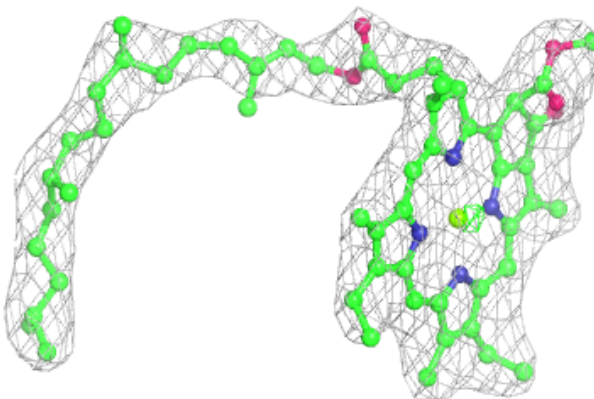


Electron density around CLA b 1215:

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

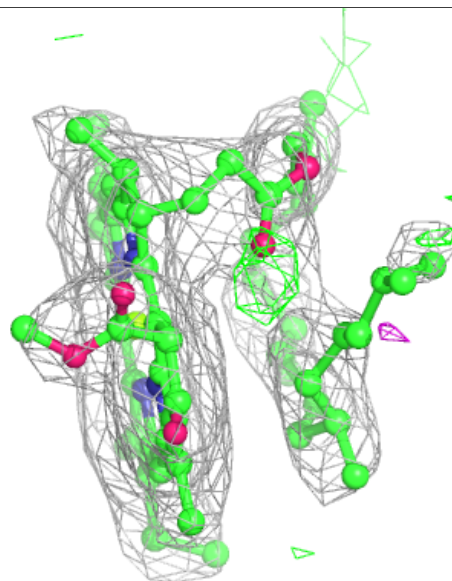
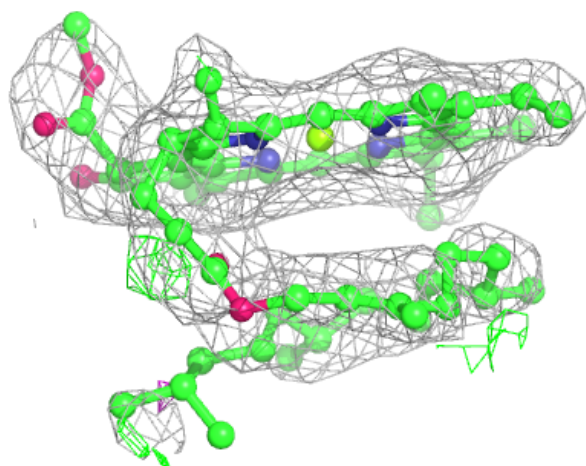
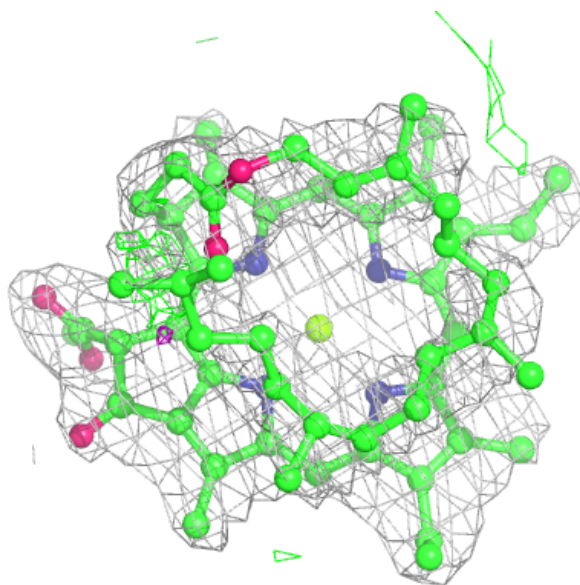
**Electron density around CLA A 1140:**

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



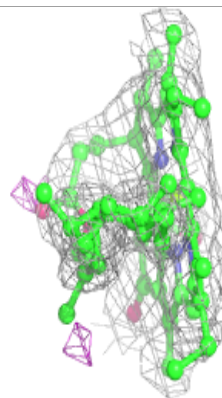
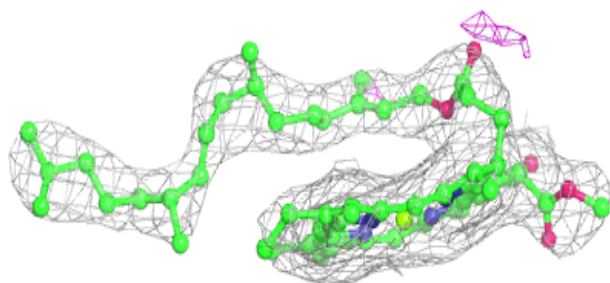
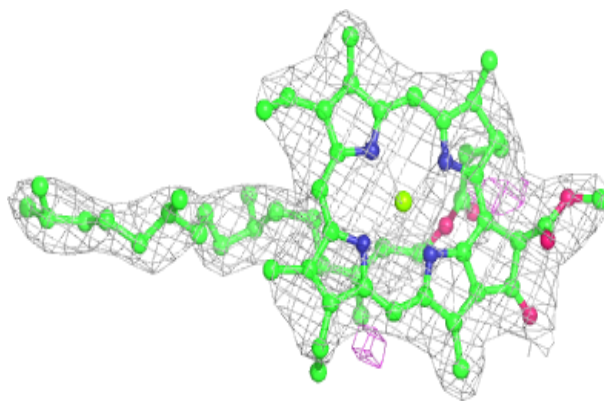
Electron density around CLA L 1501:

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

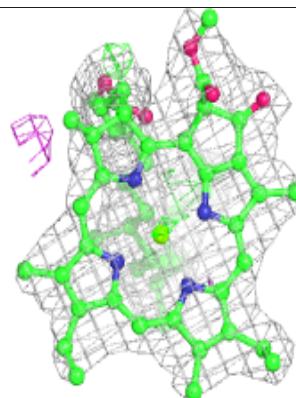
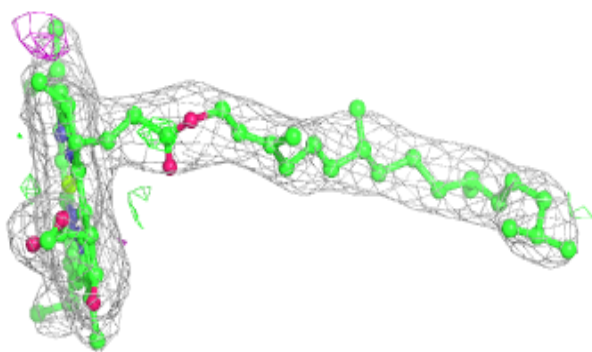
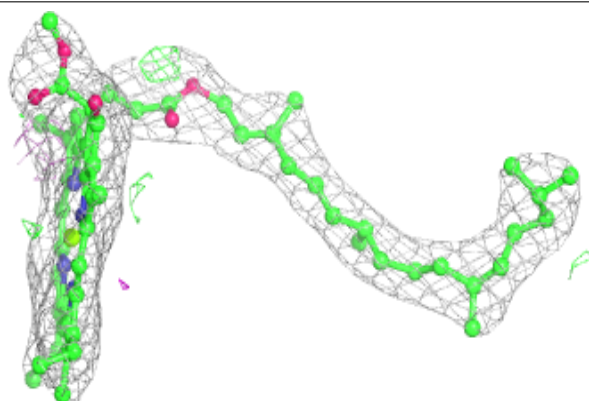


Electron density around CLA 1 1136:

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

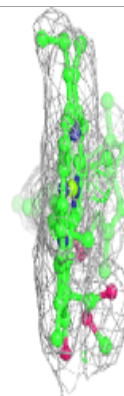
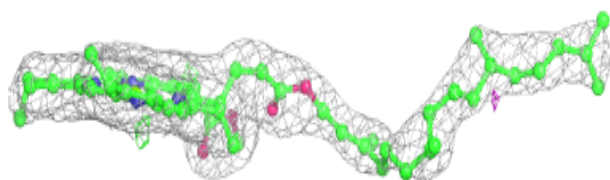
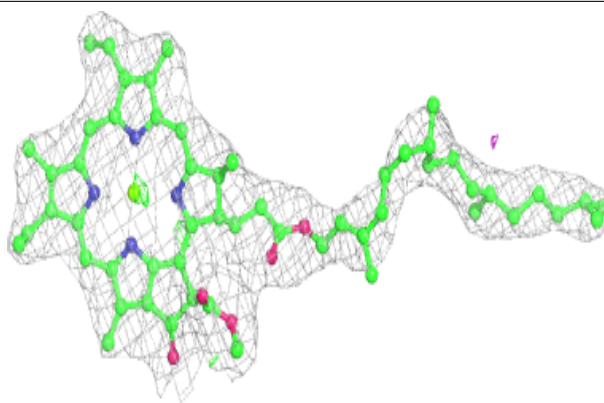
**Electron density around CLA b 1239:**

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

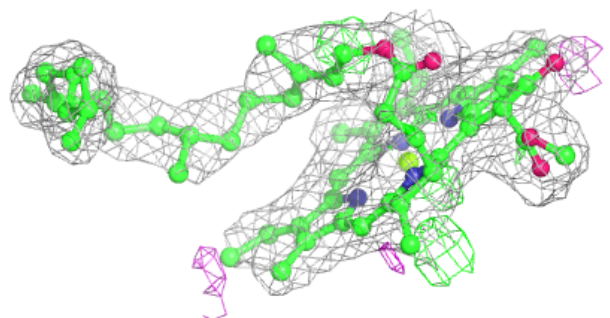
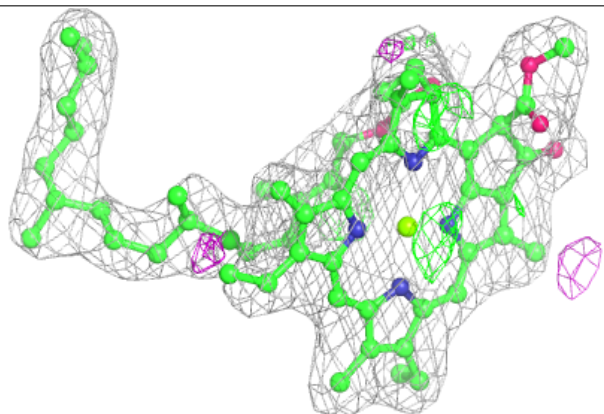


Electron density around CLA 1 1131:

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

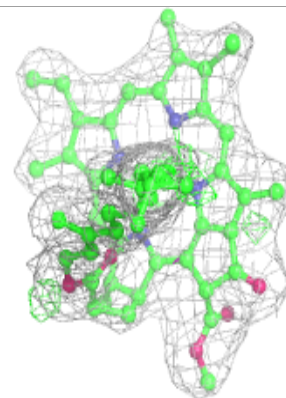
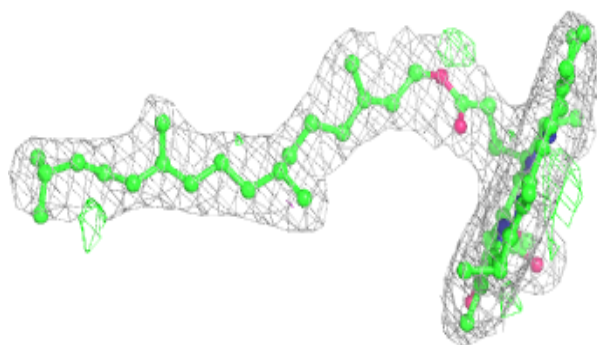
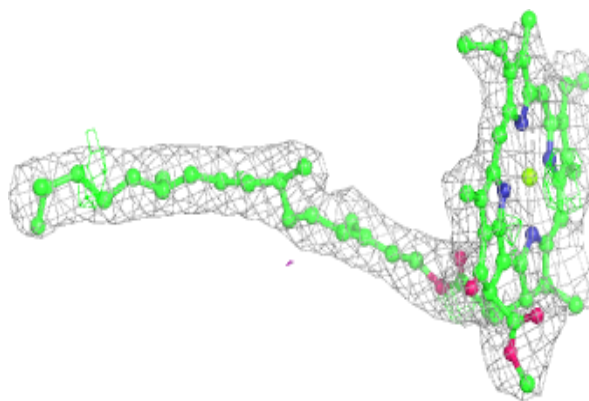
**Electron density around CLA B 1237:**

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

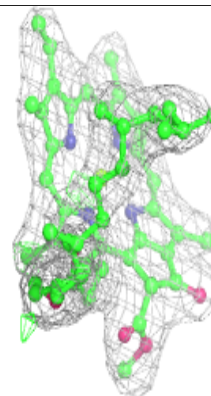
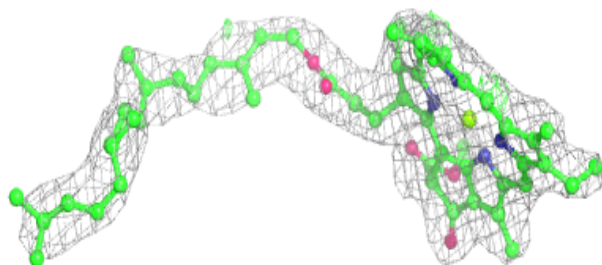
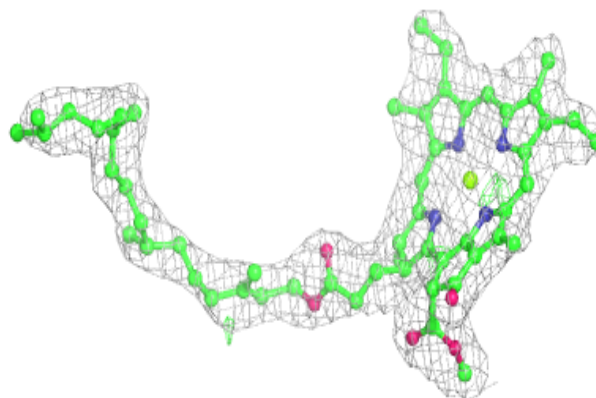


Electron density around CLA b 1225:

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

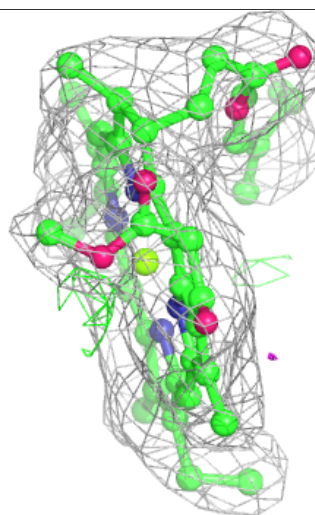
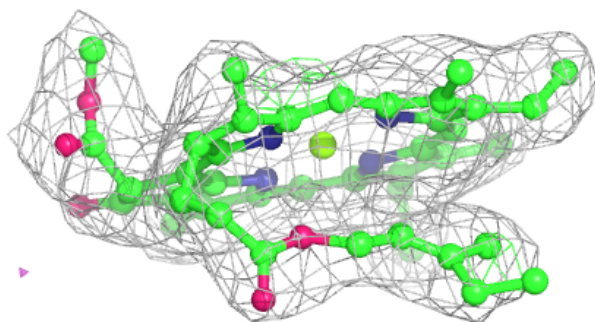
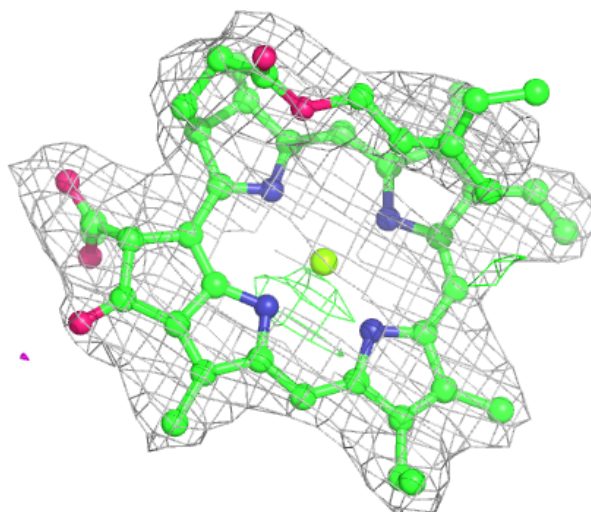
**Electron density around CLA A 1012:**

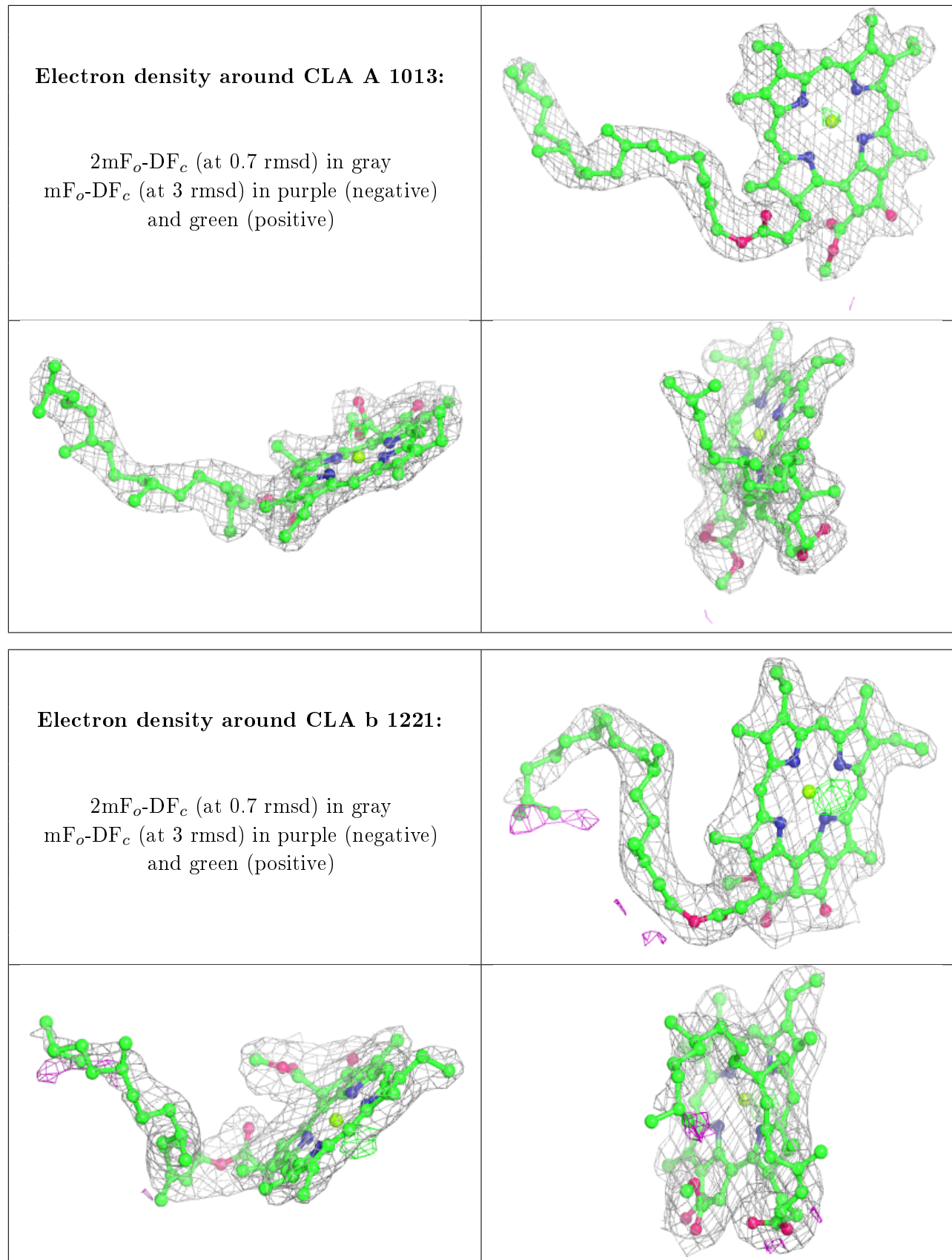
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 1217:

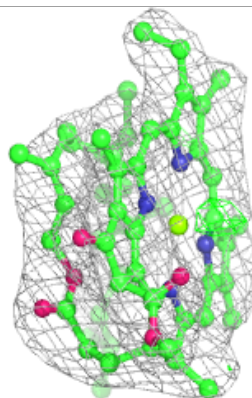
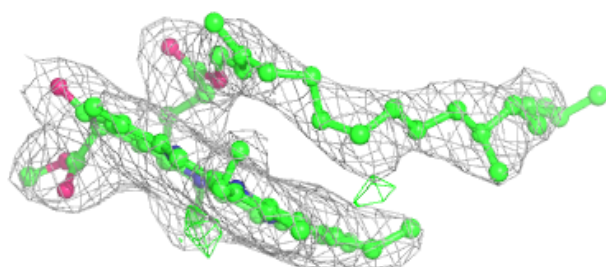
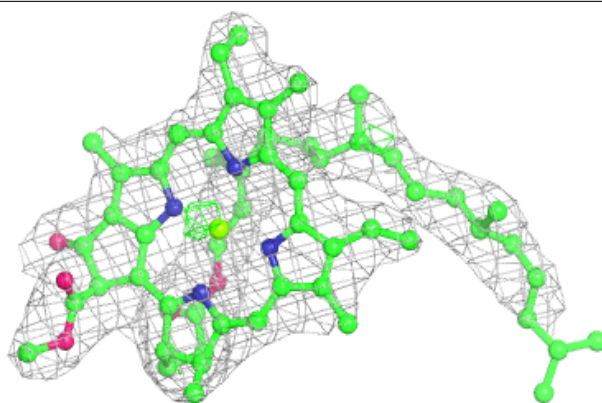
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



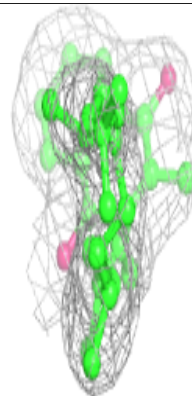
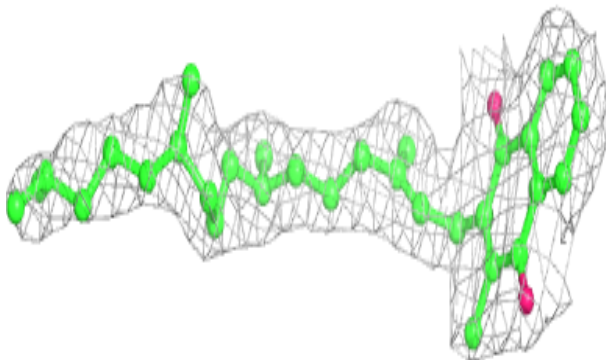
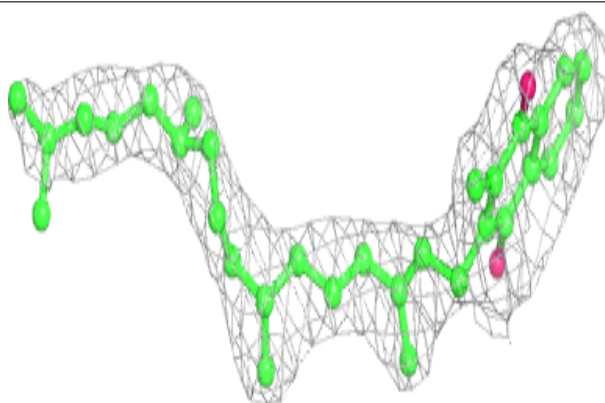


Electron density around CLA b 1204:

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

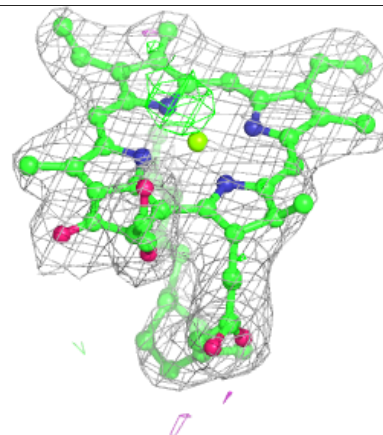
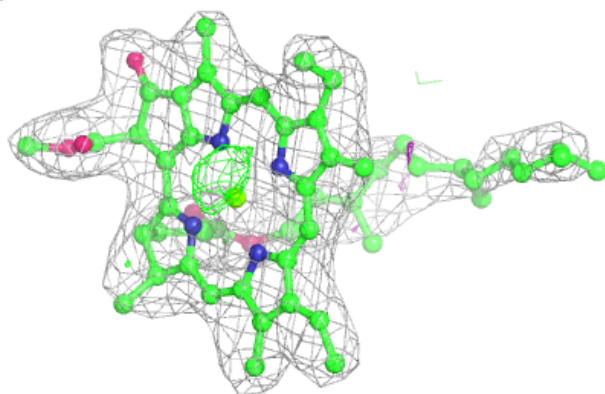
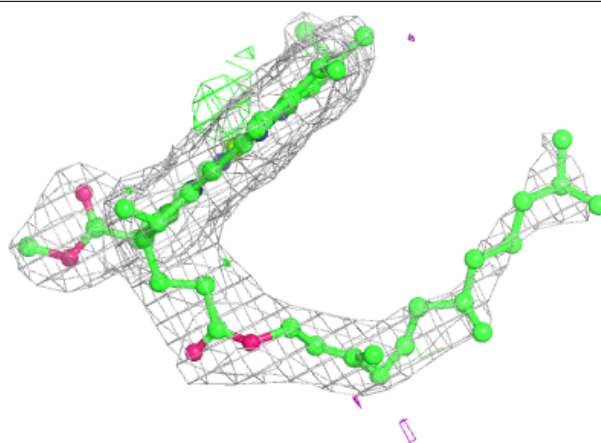
**Electron density around PQN A 2001:**

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

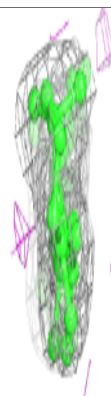
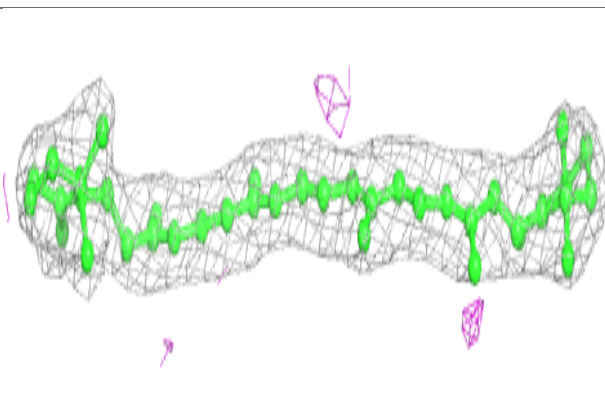
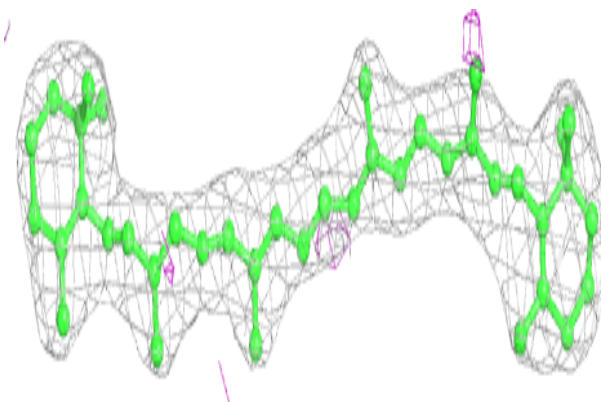


Electron density around CLA A 1130:

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

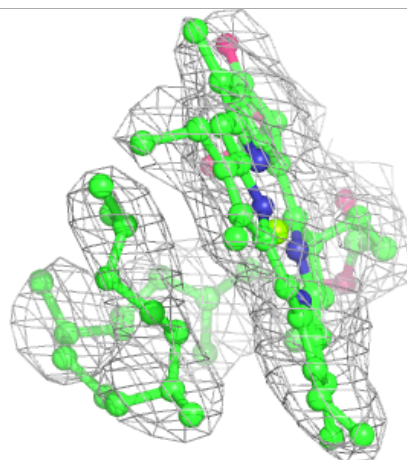
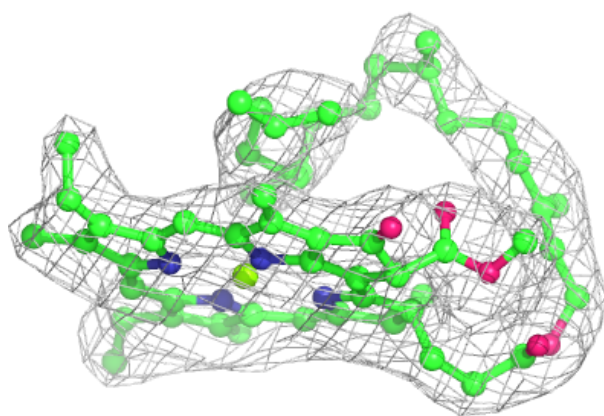
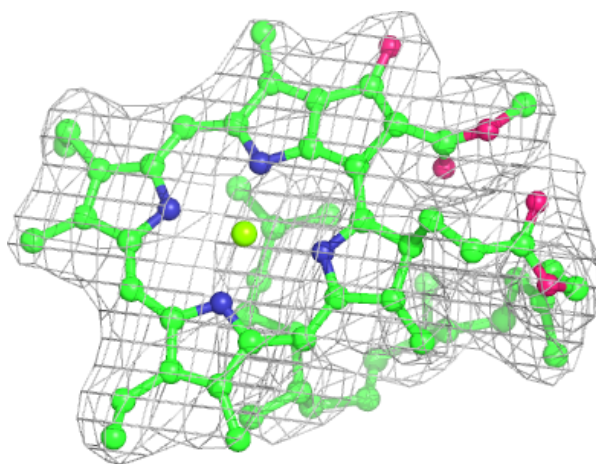
**Electron density around BCR L 4019:**

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



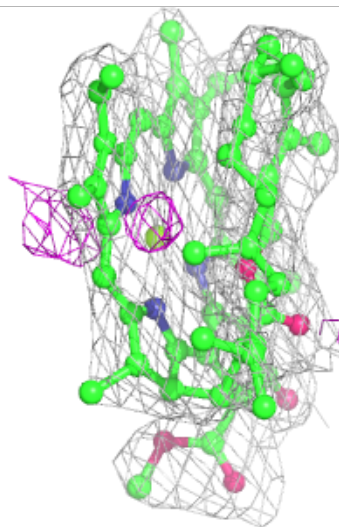
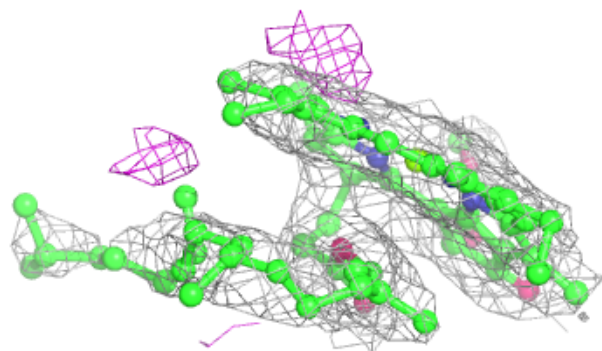
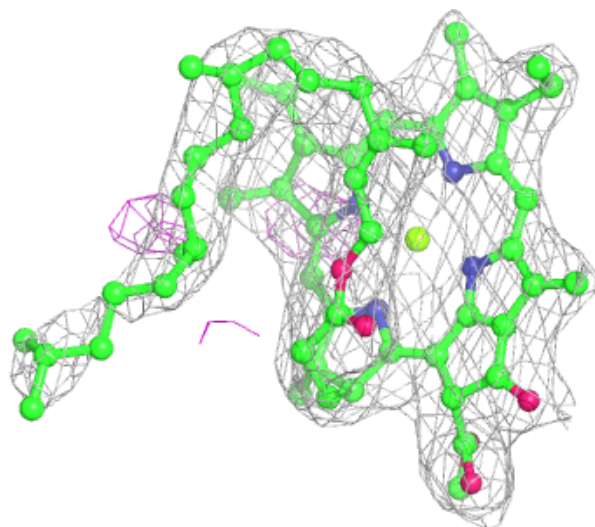
Electron density around CLA B 1203:

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



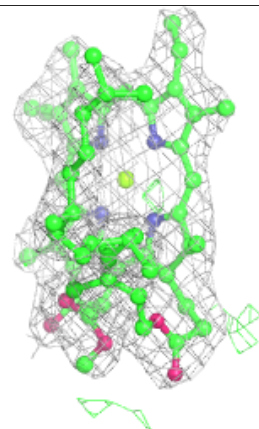
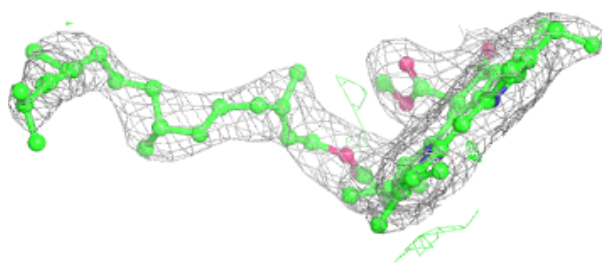
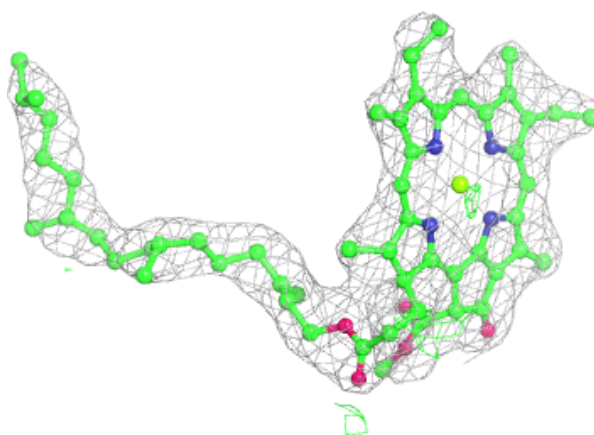
Electron density around CLA B 1205:

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

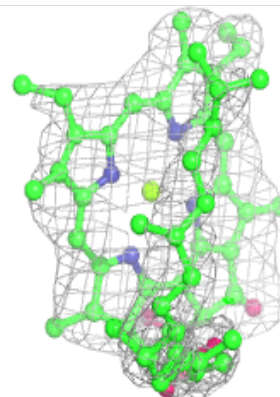
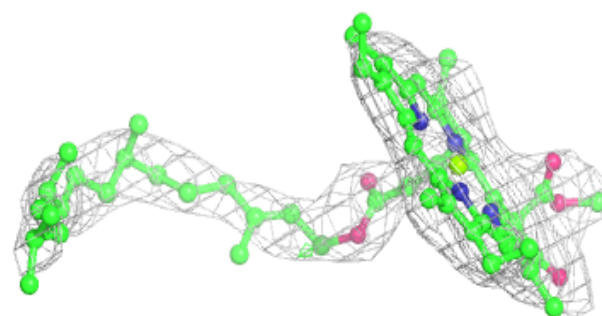
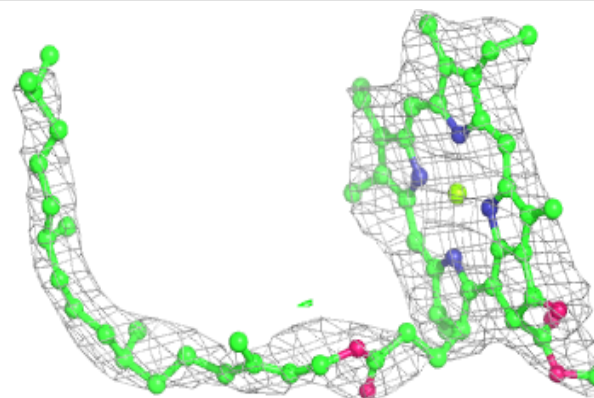


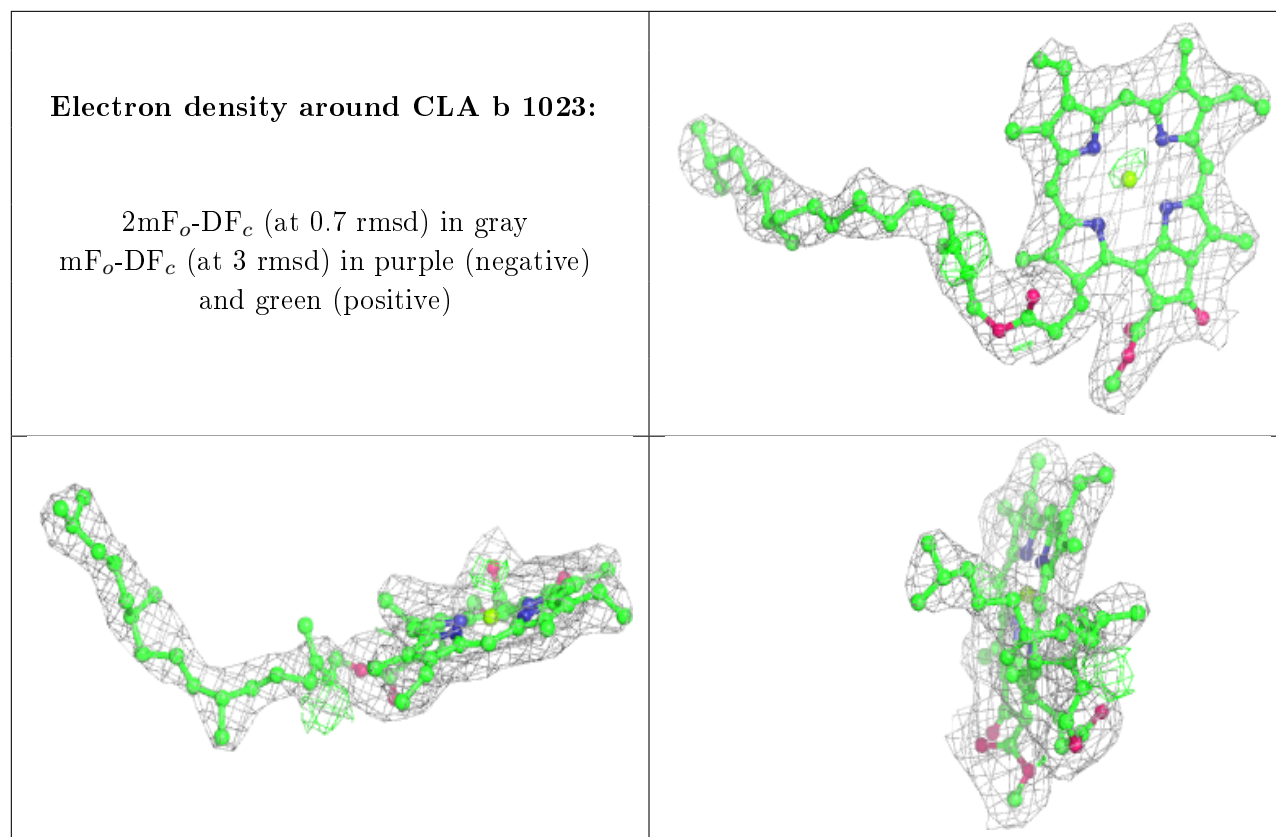
Electron density around CLA b 1207:

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

**Electron density around CLA a 1140:**

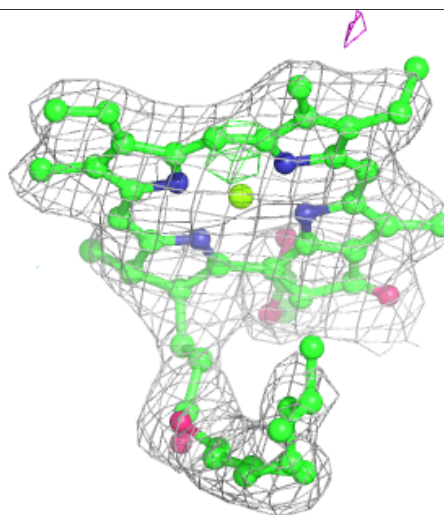
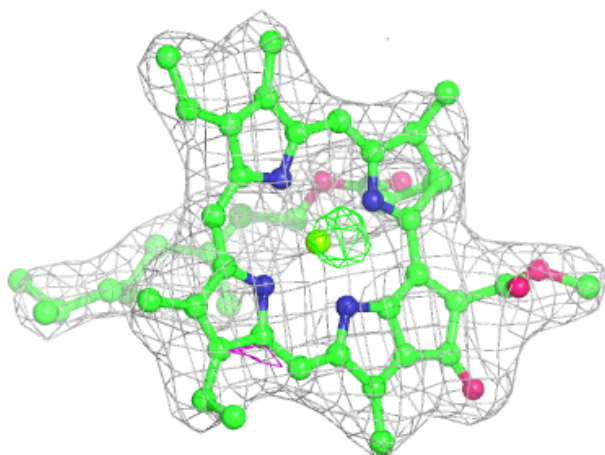
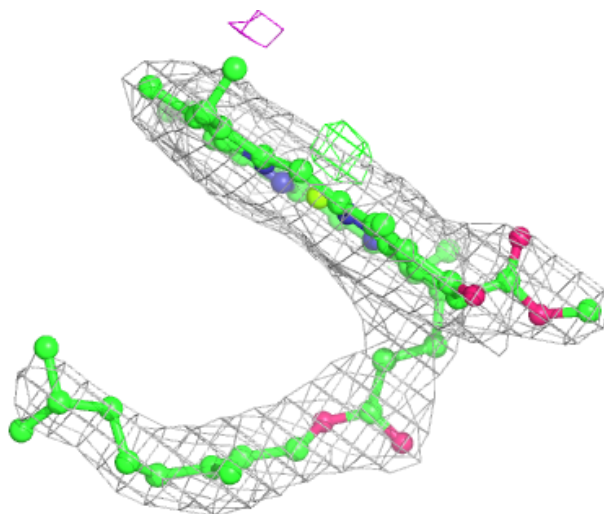
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





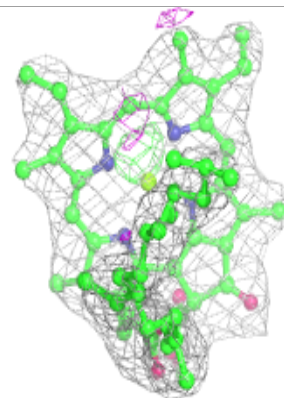
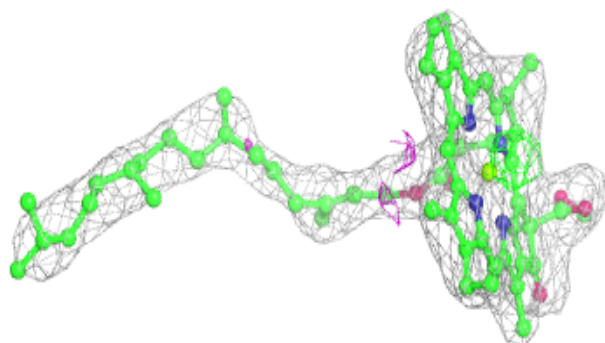
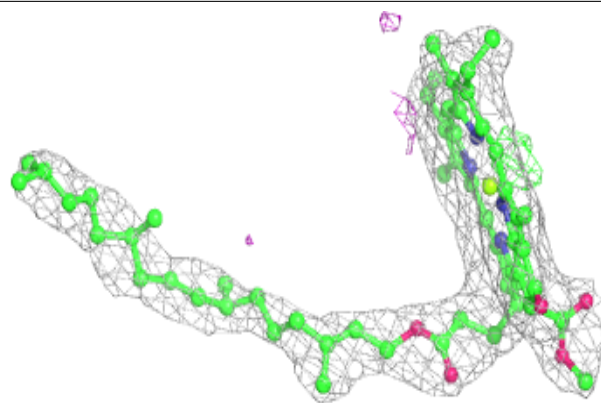
Electron density around CLA 1 1130:

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

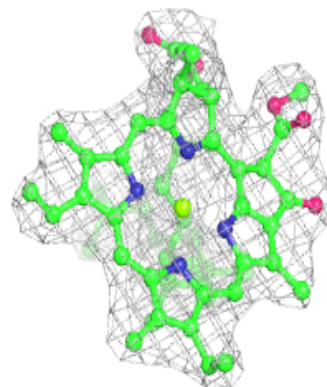
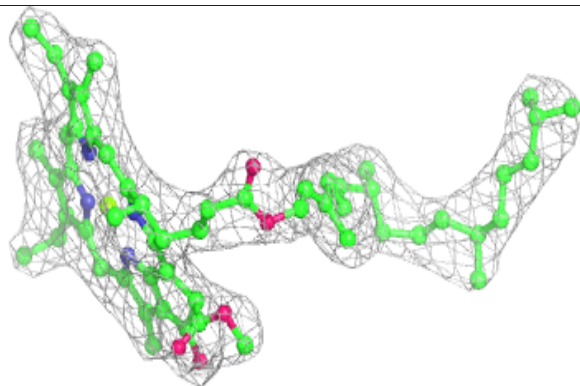
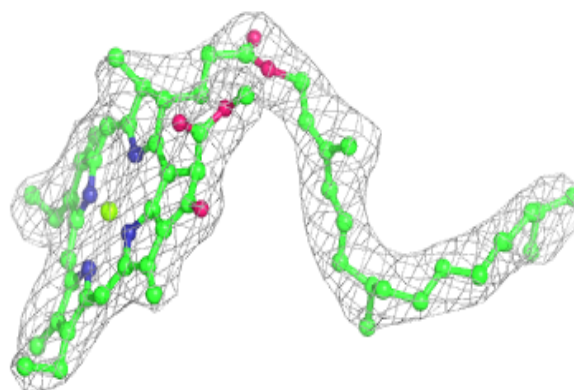


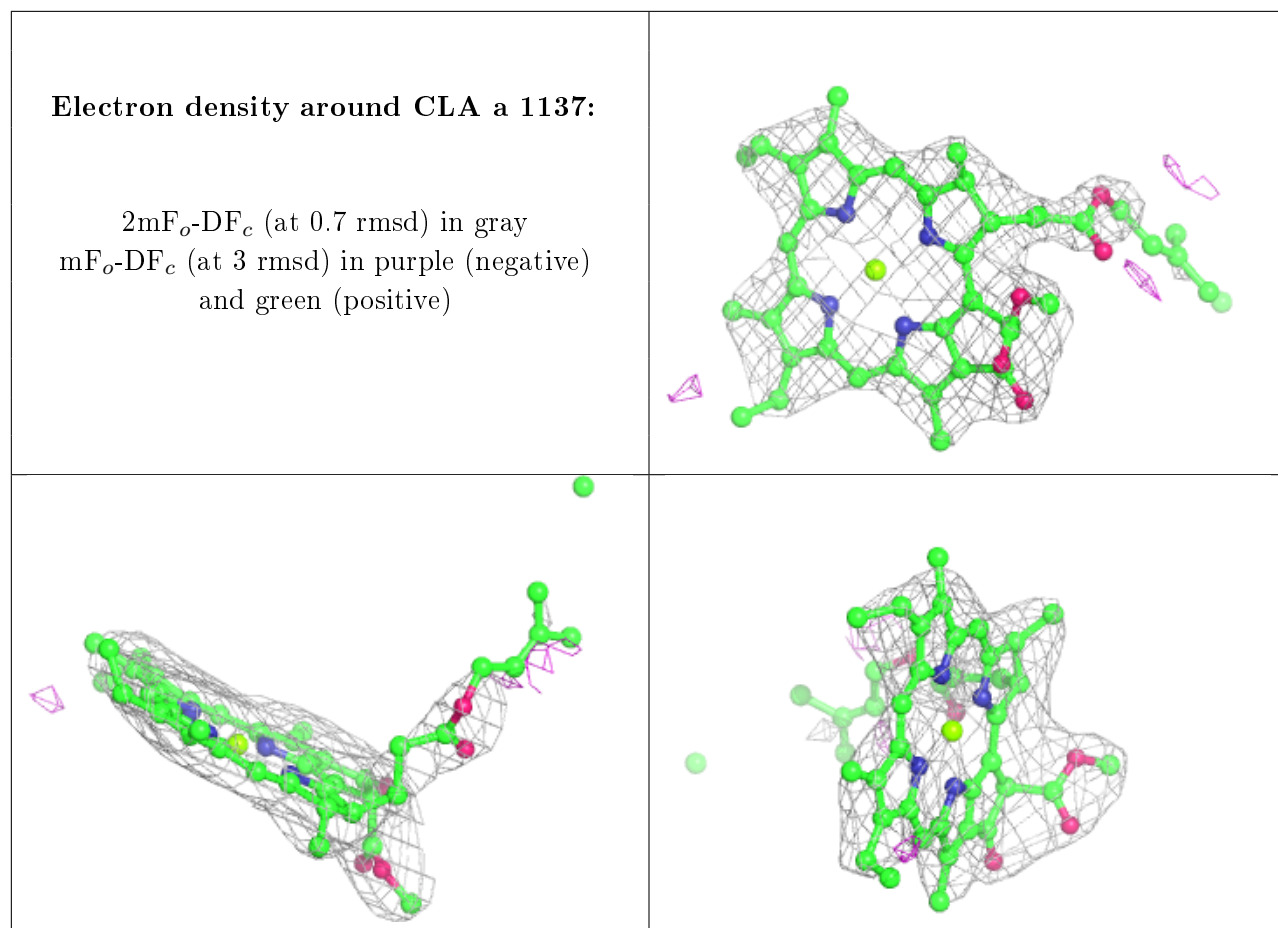
Electron density around CLA B 1201:

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

**Electron density around CLA B 1021:**

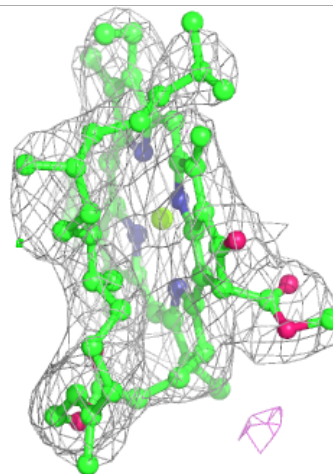
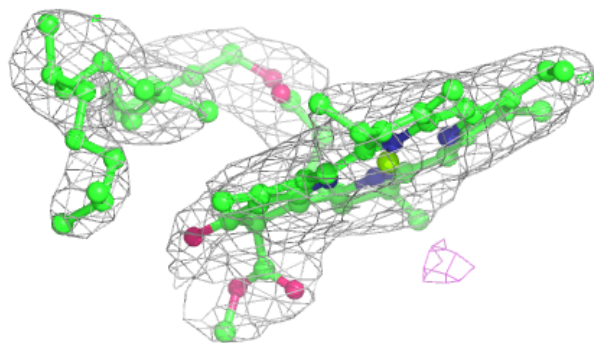
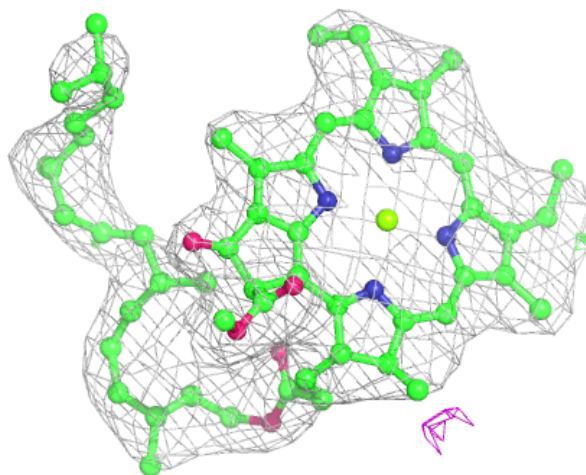
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

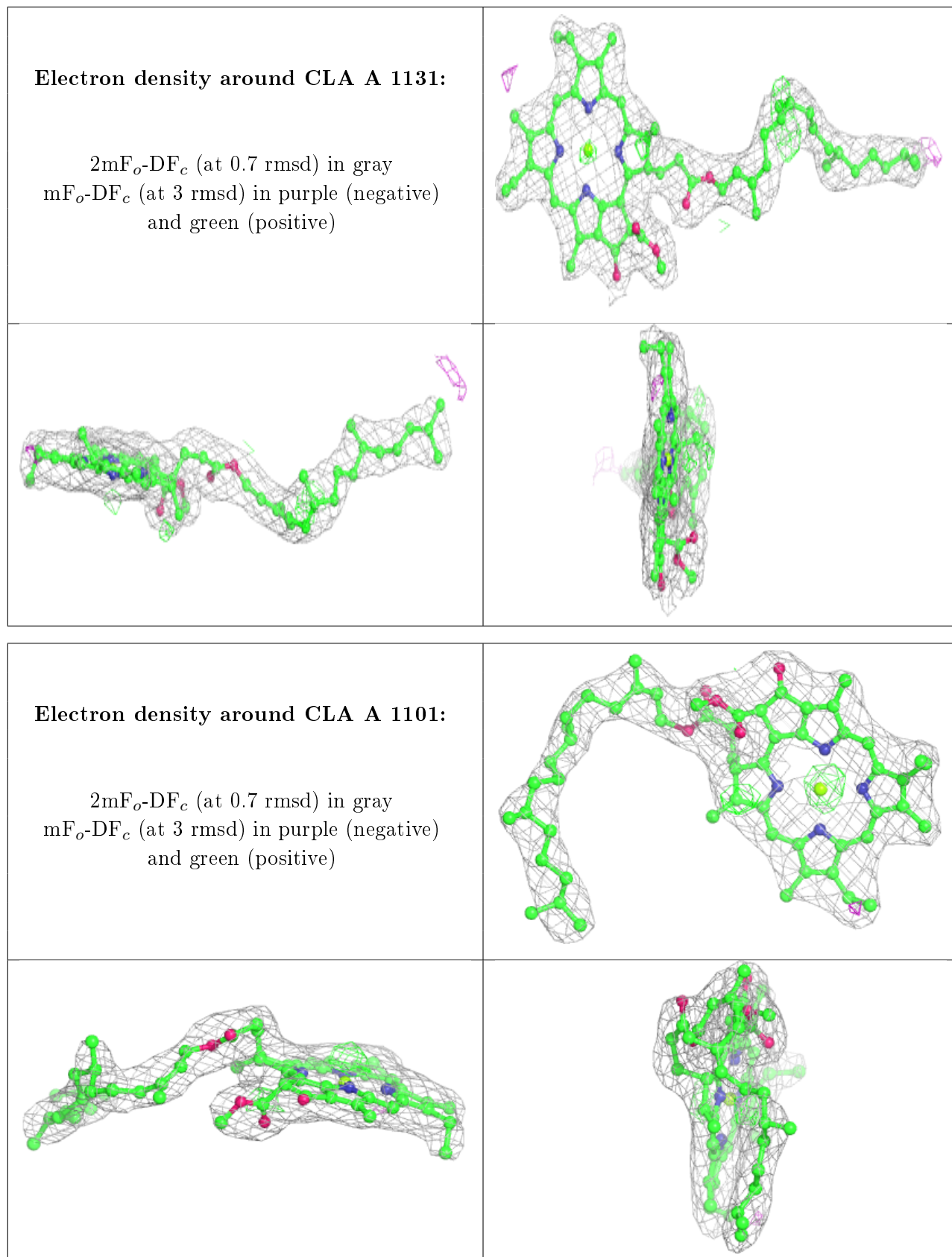




Electron density around CLA B 1229:

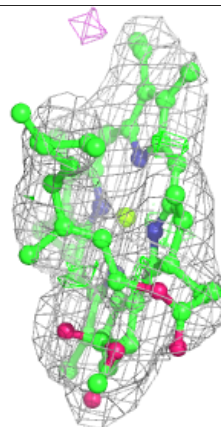
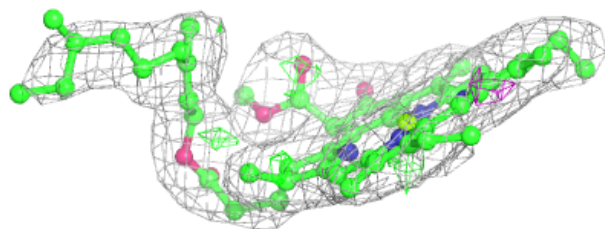
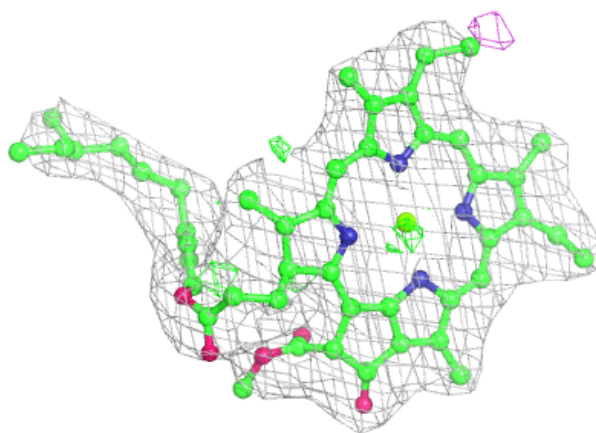
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



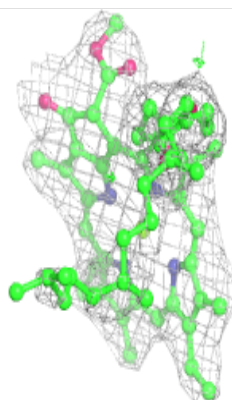
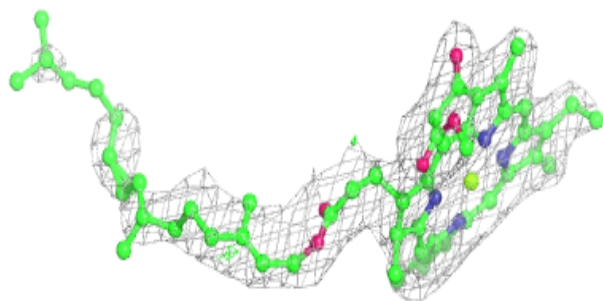
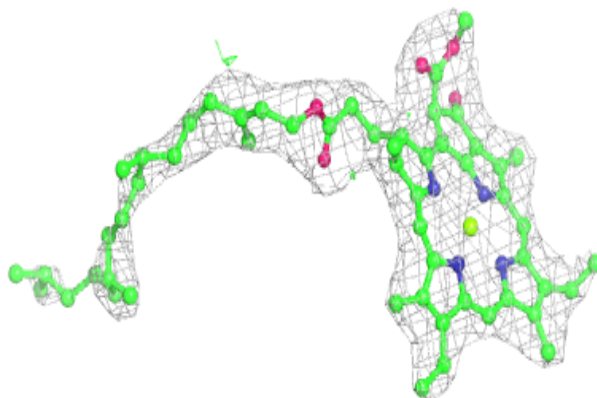


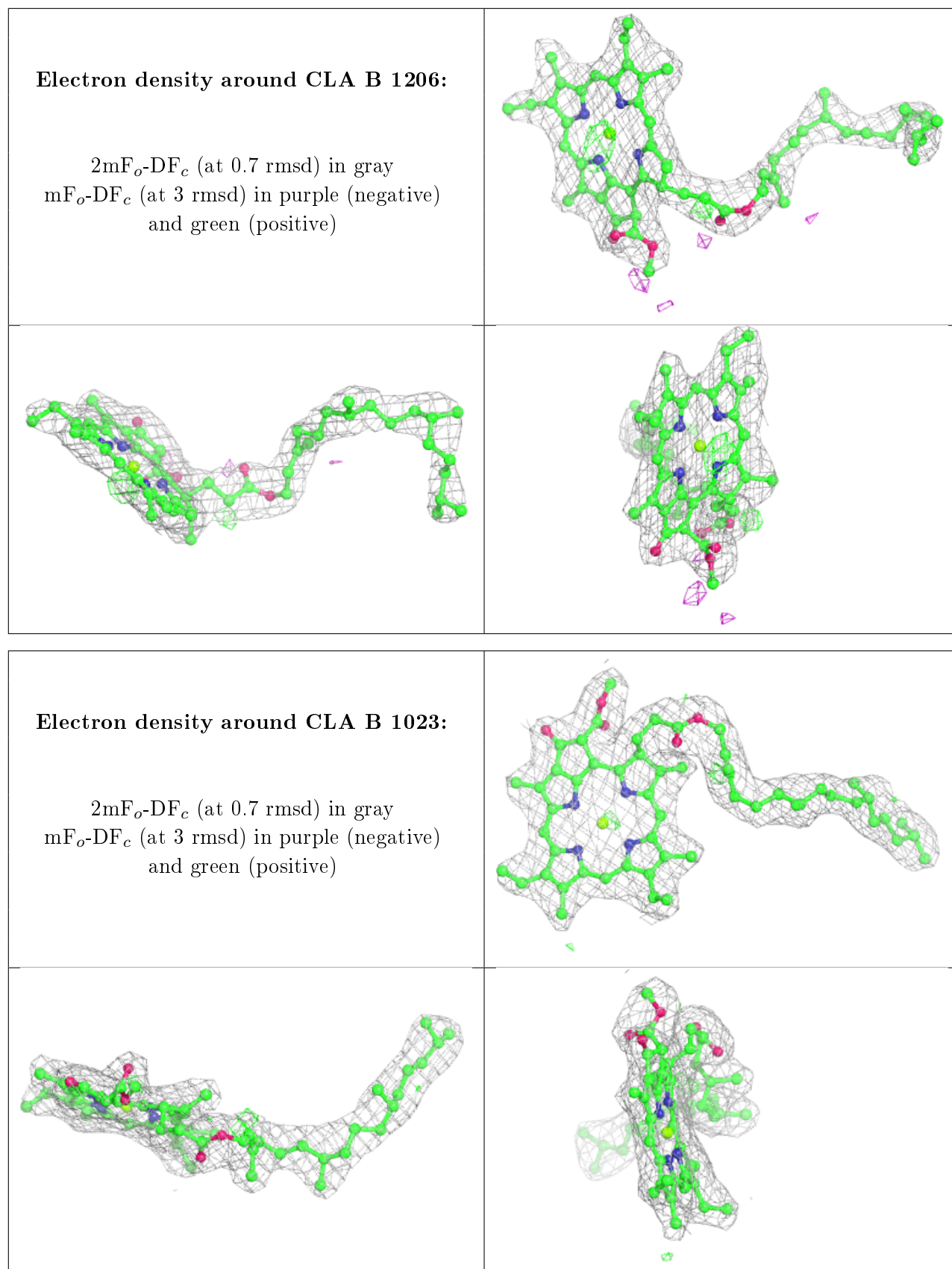
Electron density around CLA 2 1207:

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

**Electron density around CLA a 1012:**

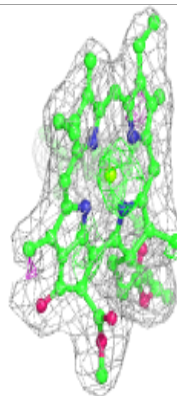
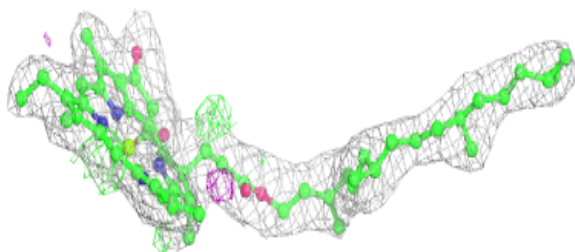
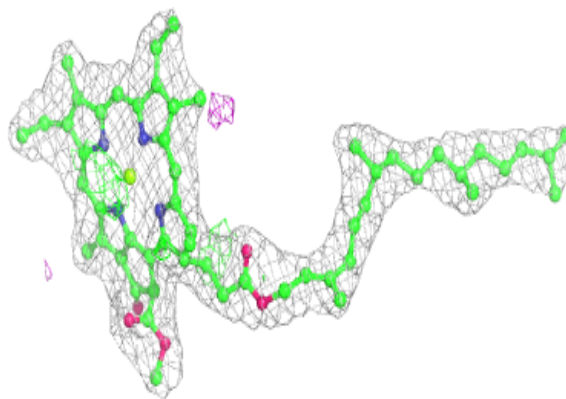
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



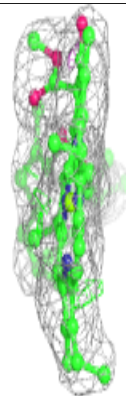
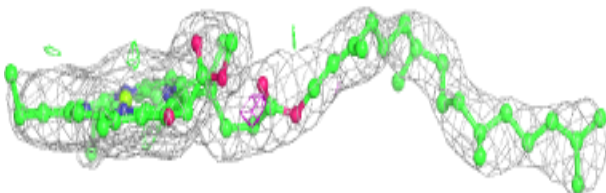
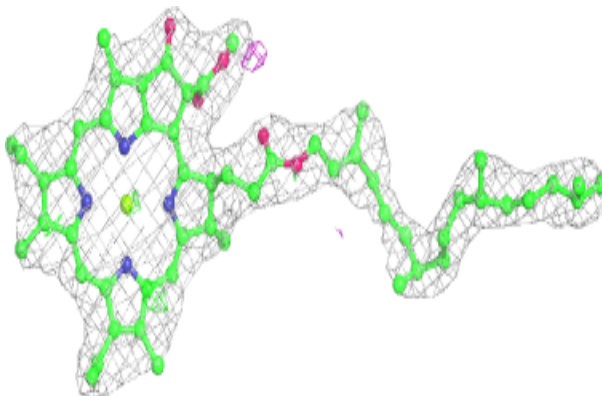


Electron density around CLA B 1022:

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

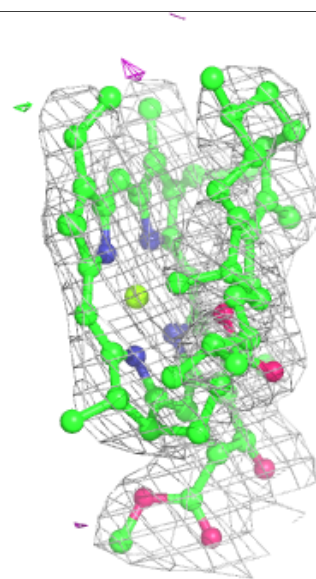
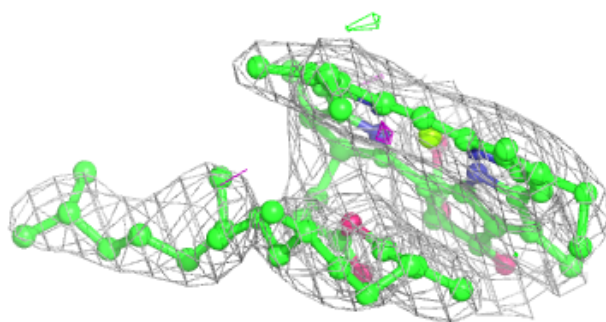
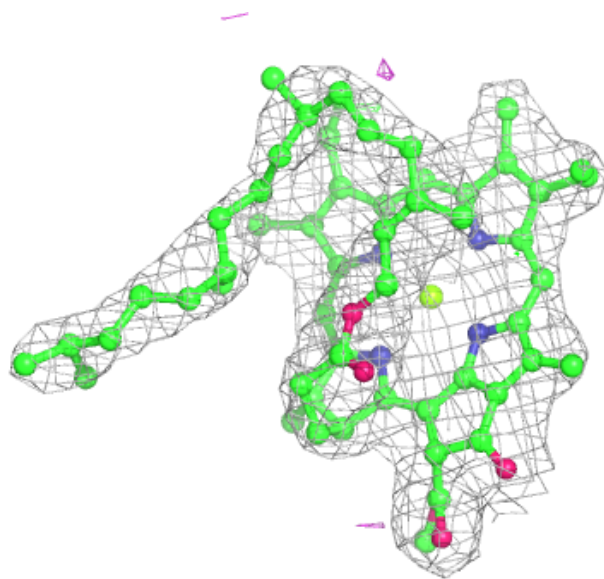
**Electron density around CLA a 1131:**

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



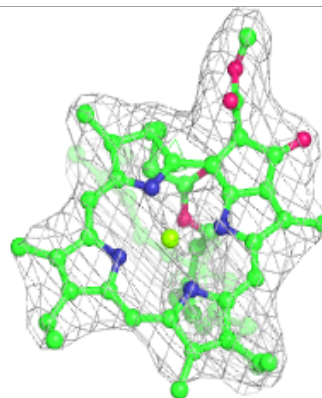
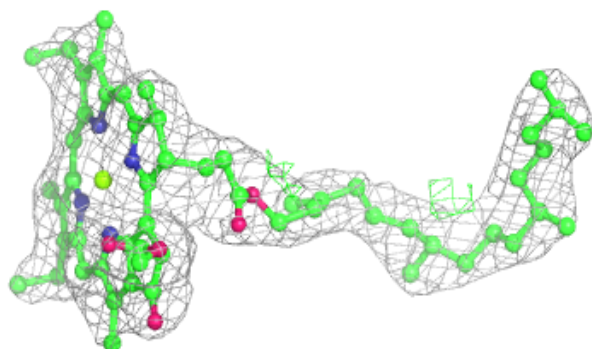
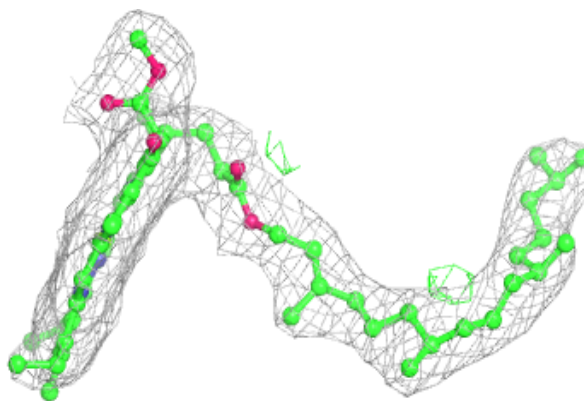
Electron density around CLA b 1205:

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

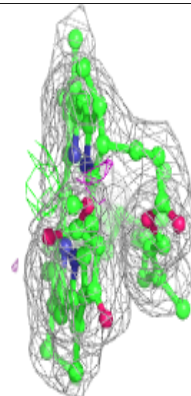
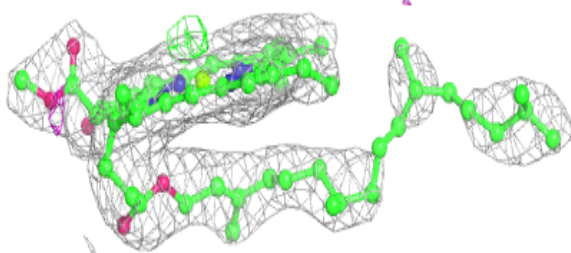
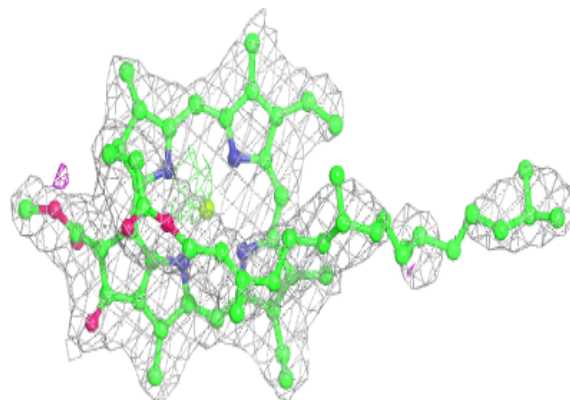


Electron density around CLA 2 1238:

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

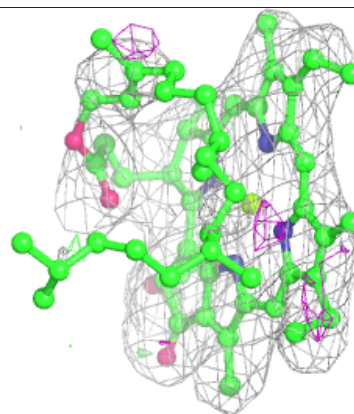
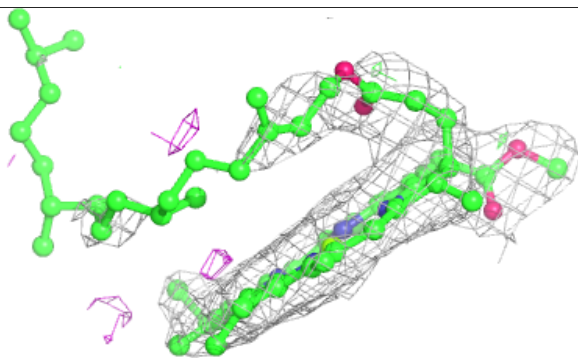
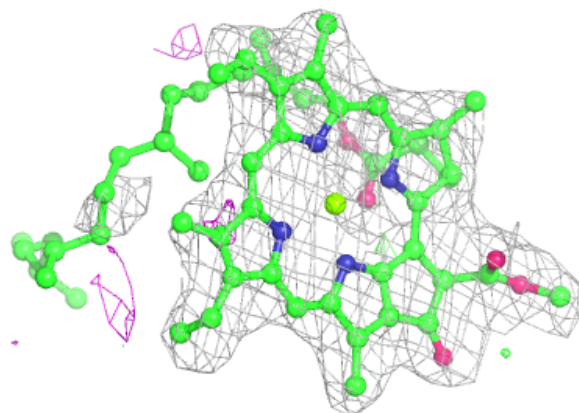
**Electron density around CLA A 1136:**

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



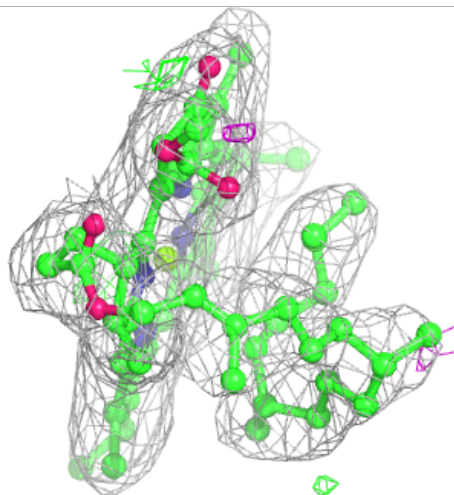
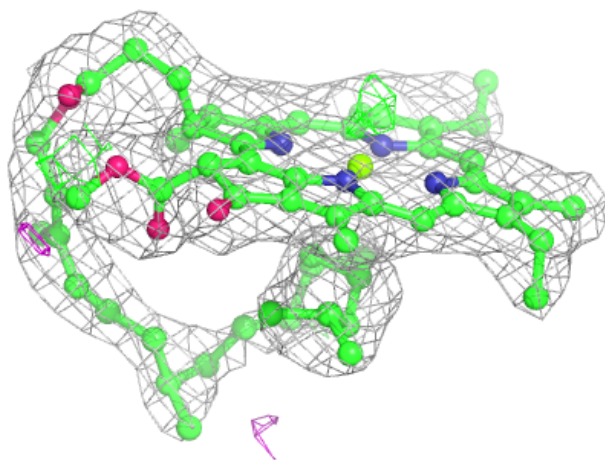
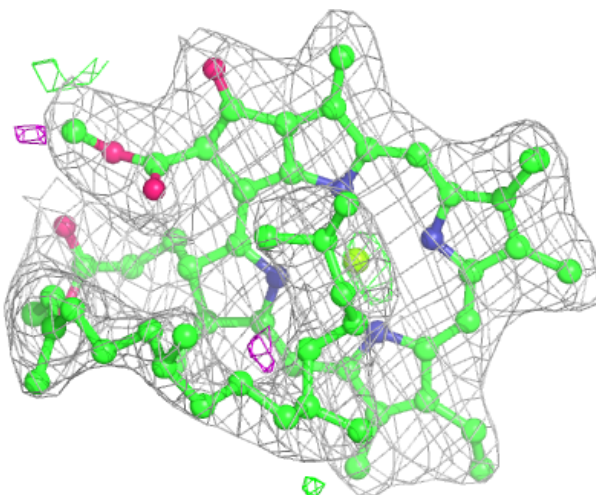
Electron density around CLA A 1110:

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



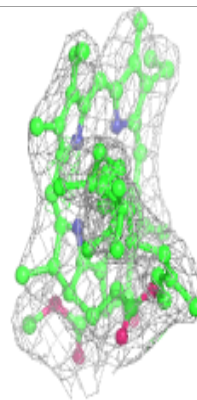
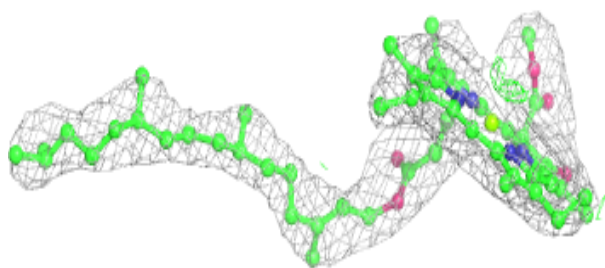
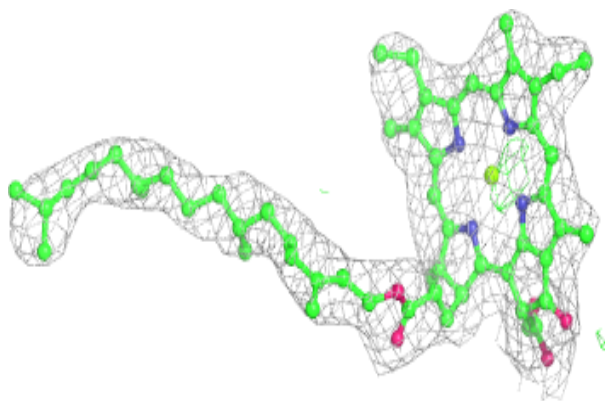
Electron density around CLA b 1203:

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

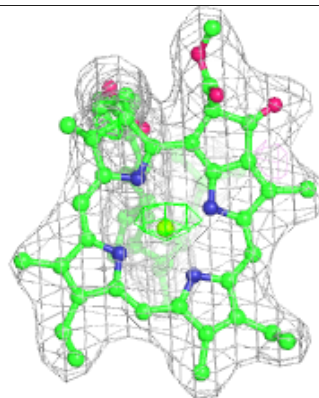
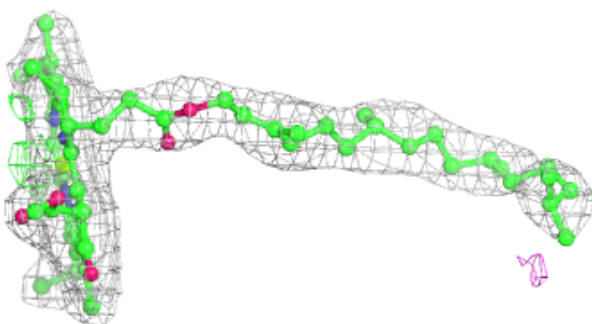
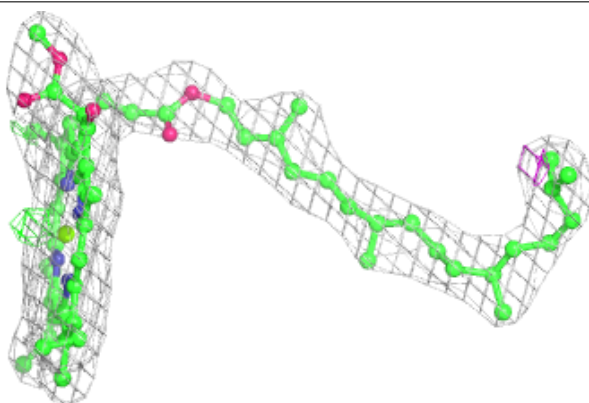


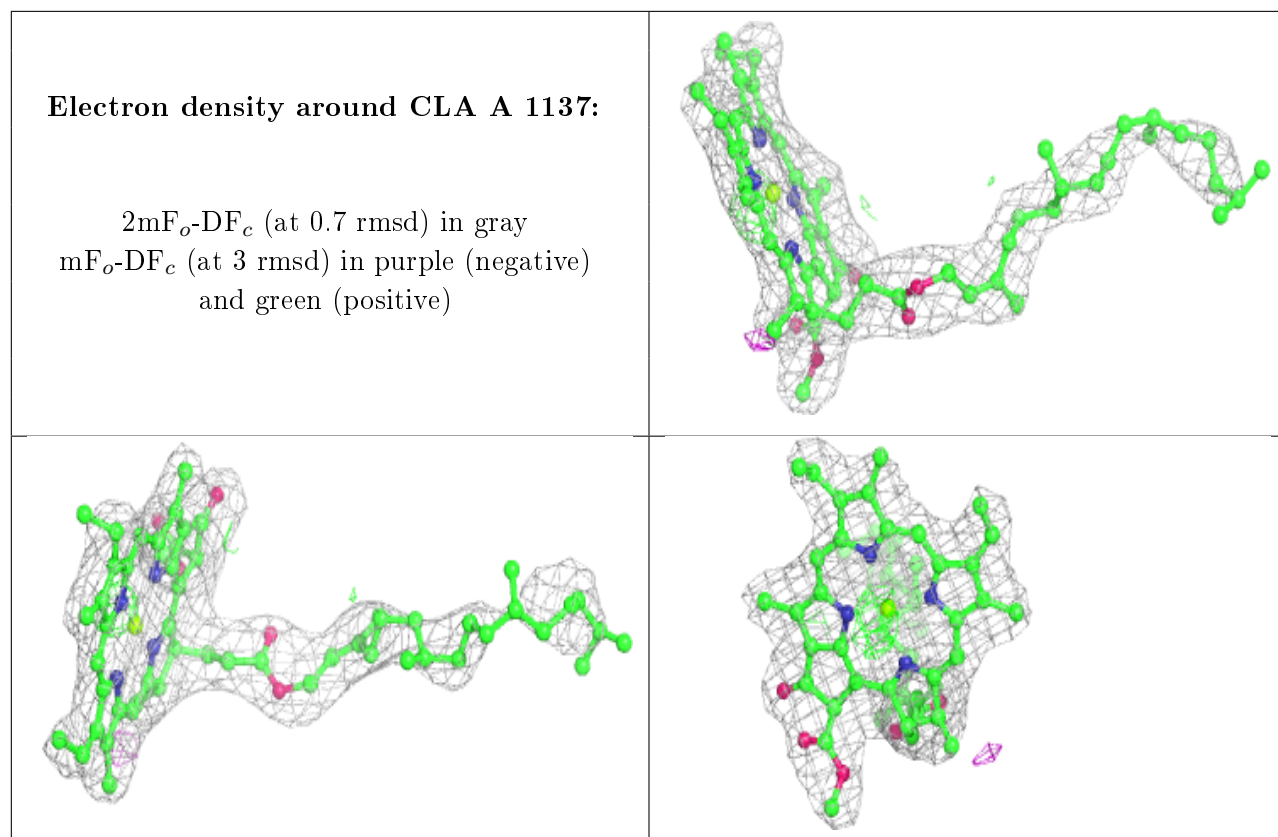
Electron density around CLA a 1132:

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

**Electron density around CLA B 1239:**

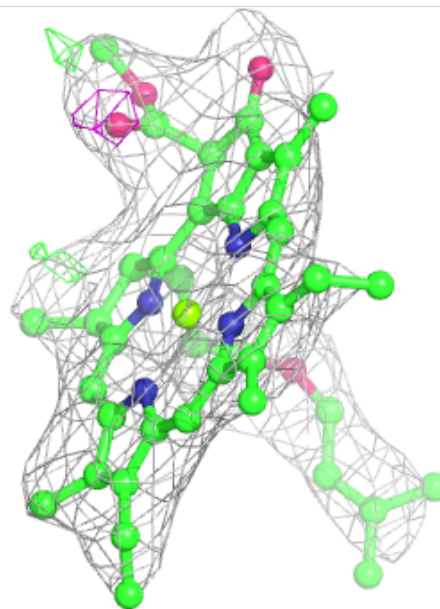
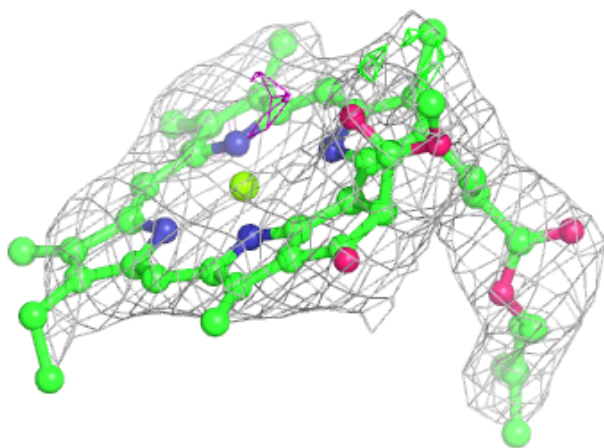
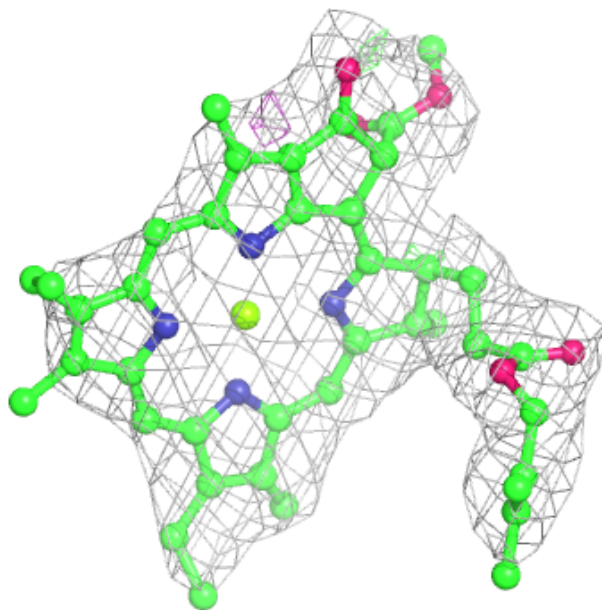
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





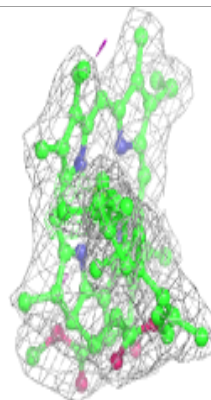
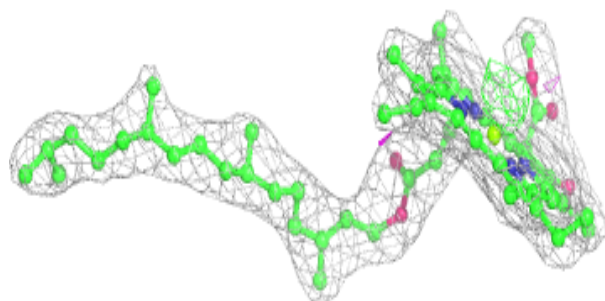
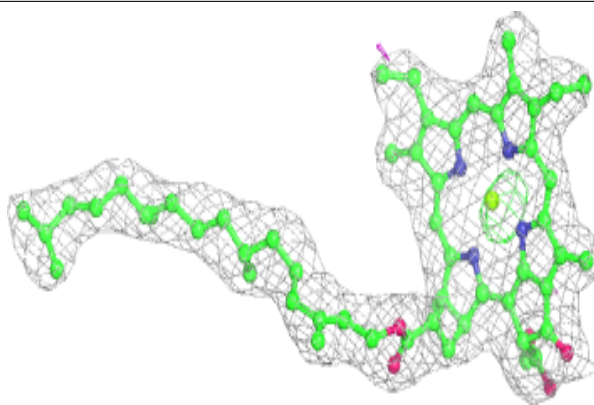
Electron density around CLA 1 1129:

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

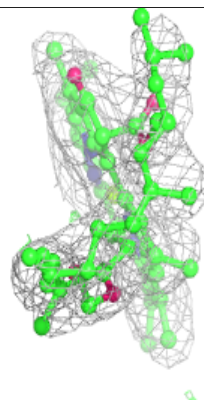
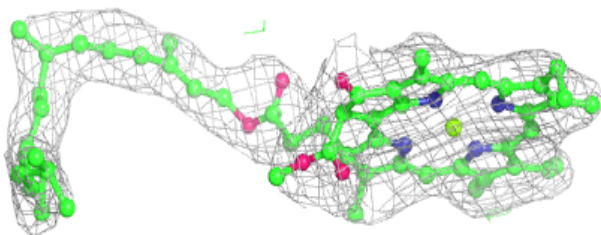
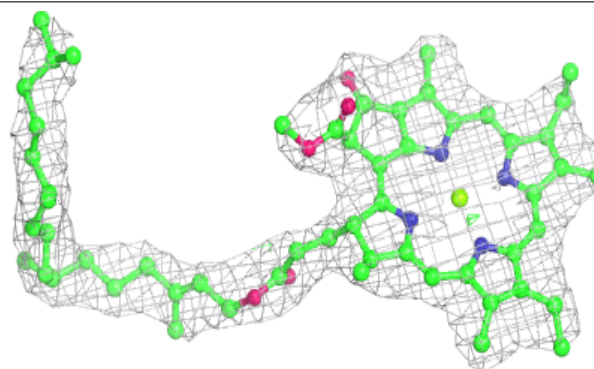


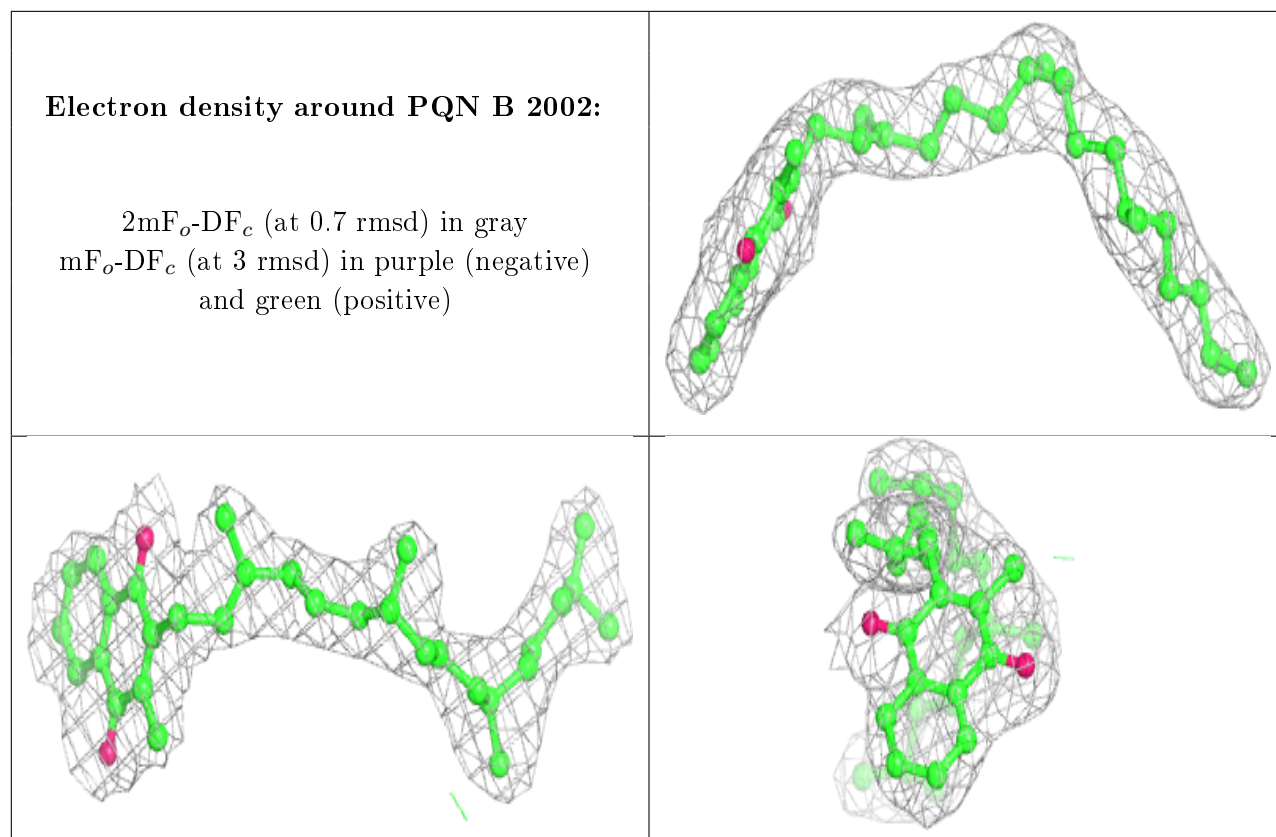
Electron density around CLA A 1132:

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

**Electron density around CLA b 1223:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.