



Full wwPDB EM Validation Report ⓘ

Jul 2, 2026 – 02:22 pm BST

PDB ID : 9SK3 / pdb_00009sk3
EMDB ID : EMD-54956
Title : Trimeric photosystem I of Acaryochloris marina NIES-2412
Authors : Leong, H.F.; Consoli, G.
Deposited on : 2025-09-01
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

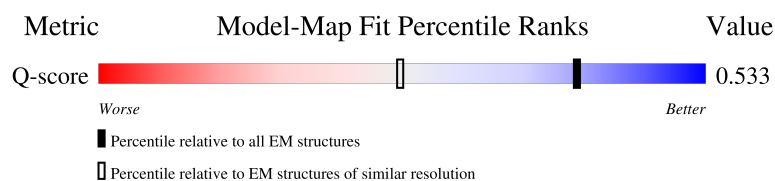
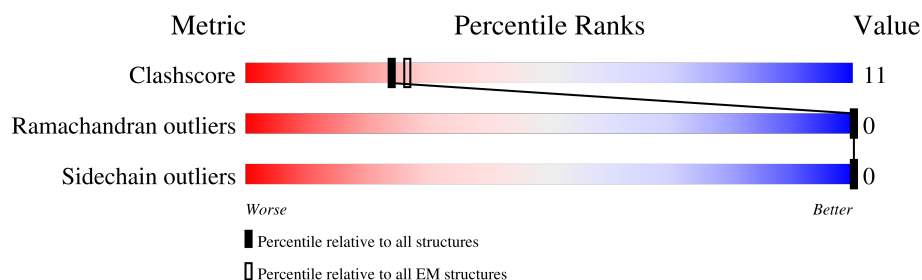
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.63 Å.

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



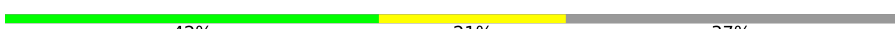
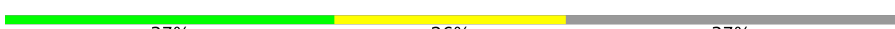
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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

Mol	Chain	Length	Quality of chain
1	aA	753	 76% 22% .
1	bA	753	 76% 22% .
1	cA	753	 75% 23% .
2	aB	733	 76% 24%

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Mol	Chain	Length	Quality of chain
2	bB	733	 77% 23%
2	cB	733	 77% 23%
3	aC	81	 77% 22% .
3	bC	81	 77% 22% .
3	cC	81	 84% 15% .
4	aD	139	 71% 27% .
4	bD	139	 79% 19% .
4	cD	139	 77% 21% .
5	aE	86	 70% 8% 22%
5	bE	86	 65% 13% 22%
5	cE	86	 71% 7% 22%
6	aF	167	 74% 11% 14%
6	bF	167	 70% 16% 14%
6	cF	167	 71% 14% 14%
7	aI	34	 79% 18% .
7	bI	34	 76% 21% .
7	cI	34	 82% 15% .
8	aJ	47	 60% 15% 26%
8	bJ	47	 68% 6% 26%
8	cJ	47	 62% 13% 26%
9	aK	86	 42% 21% 37%
9	bK	86	 44% 19% 37%
9	cK	86	 37% 26% 37%
10	aL	153	 81% 16% .
10	bL	153	 80% 16% .

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Mol	Chain	Length	Quality of chain
10	cL	153	
11	aM	31	
11	bM	31	
11	cM	31	
12	aX	27	
12	bX	27	
12	cX	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	G9R	aA	1011	X	-	-	-
13	G9R	bA	1011	X	-	-	-
13	G9R	cA	1011	X	-	-	-
15	CL7	aA	1022	X	-	-	-
15	CL7	aA	1101	X	-	-	-
15	CL7	aA	1102	X	-	-	-
15	CL7	aA	1103	X	-	-	-
15	CL7	aA	1104	X	-	-	-
15	CL7	aA	1105	X	-	-	-
15	CL7	aA	1106	X	-	-	-
15	CL7	aA	1107	X	-	-	-
15	CL7	aA	1108	X	-	-	-
15	CL7	aA	1109	X	-	-	-
15	CL7	aA	1110	X	-	-	-
15	CL7	aA	1111	X	-	-	-
15	CL7	aA	1112	X	-	-	-
15	CL7	aA	1113	X	-	-	-
15	CL7	aA	1114	X	-	-	-
15	CL7	aA	1115	X	-	-	-
15	CL7	aA	1116	X	-	-	-
15	CL7	aA	1117	X	-	-	-
15	CL7	aA	1118	X	-	-	-
15	CL7	aA	1119	X	-	-	-
15	CL7	aA	1120	X	-	-	-
15	CL7	aA	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	aA	1122	X	-	-	-
15	CL7	aA	1123	X	-	-	-
15	CL7	aA	1124	X	-	-	-
15	CL7	aA	1125	X	-	-	-
15	CL7	aA	1126	X	-	-	-
15	CL7	aA	1127	X	-	-	-
15	CL7	aA	1128	X	-	-	-
15	CL7	aA	1129	X	-	-	-
15	CL7	aA	1130	X	-	-	-
15	CL7	aA	1131	X	-	-	-
15	CL7	aA	1132	X	-	-	-
15	CL7	aA	1133	X	-	-	-
15	CL7	aA	1134	X	-	-	-
15	CL7	aA	1135	X	-	-	-
15	CL7	aA	1136	X	-	-	-
15	CL7	aA	1137	X	-	-	-
15	CL7	aA	1138	X	-	-	-
15	CL7	aA	1139	X	-	-	-
15	CL7	aA	1140	X	-	-	-
15	CL7	aA	1801	X	-	-	-
15	CL7	aB	1012	X	-	-	-
15	CL7	aB	1021	X	-	-	-
15	CL7	aB	1201	X	-	-	-
15	CL7	aB	1202	X	-	-	-
15	CL7	aB	1203	X	-	-	-
15	CL7	aB	1204	X	-	-	-
15	CL7	aB	1205	X	-	-	-
15	CL7	aB	1206	X	-	-	-
15	CL7	aB	1207	X	-	-	-
15	CL7	aB	1208	X	-	-	-
15	CL7	aB	1209	X	-	-	-
15	CL7	aB	1210	X	-	-	-
15	CL7	aB	1211	X	-	-	-
15	CL7	aB	1212	X	-	-	-
15	CL7	aB	1213	X	-	-	-
15	CL7	aB	1214	X	-	-	-
15	CL7	aB	1215	X	-	-	-
15	CL7	aB	1216	X	-	-	-
15	CL7	aB	1217	X	-	-	-
15	CL7	aB	1218	X	-	-	-
15	CL7	aB	1219	X	-	-	-
15	CL7	aB	1220	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	aB	1221	X	-	-	-
15	CL7	aB	1222	X	-	-	-
15	CL7	aB	1223	X	-	-	-
15	CL7	aB	1224	X	-	-	-
15	CL7	aB	1225	X	-	-	-
15	CL7	aB	1226	X	-	-	-
15	CL7	aB	1227	X	-	-	-
15	CL7	aB	1228	X	-	-	-
15	CL7	aB	1229	X	-	-	-
15	CL7	aB	1230	X	-	-	-
15	CL7	aB	1231	X	-	-	-
15	CL7	aB	1232	X	-	-	-
15	CL7	aB	1233	X	-	-	-
15	CL7	aB	1234	X	-	-	-
15	CL7	aB	1235	X	-	-	-
15	CL7	aB	1236	X	-	-	-
15	CL7	aB	1237	X	-	-	-
15	CL7	aB	1238	X	-	-	-
15	CL7	aB	1239	X	-	-	-
15	CL7	aB	1241	X	-	-	-
15	CL7	aF	1701	X	-	-	-
15	CL7	aI	1601	X	-	-	-
15	CL7	aJ	1301	X	-	-	-
15	CL7	aJ	1302	X	-	-	-
15	CL7	aK	1401	X	-	-	-
15	CL7	aK	1402	X	-	-	-
15	CL7	aL	1501	X	-	-	-
15	CL7	aL	1502	X	-	-	-
15	CL7	aL	1503	X	-	-	-
15	CL7	bA	1022	X	-	-	-
15	CL7	bA	1101	X	-	-	-
15	CL7	bA	1102	X	-	-	-
15	CL7	bA	1103	X	-	-	-
15	CL7	bA	1104	X	-	-	-
15	CL7	bA	1105	X	-	-	-
15	CL7	bA	1106	X	-	-	-
15	CL7	bA	1107	X	-	-	-
15	CL7	bA	1108	X	-	-	-
15	CL7	bA	1109	X	-	-	-
15	CL7	bA	1110	X	-	-	-
15	CL7	bA	1111	X	-	-	-
15	CL7	bA	1112	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	bA	1113	X	-	-	-
15	CL7	bA	1114	X	-	-	-
15	CL7	bA	1115	X	-	-	-
15	CL7	bA	1116	X	-	-	-
15	CL7	bA	1117	X	-	-	-
15	CL7	bA	1118	X	-	-	-
15	CL7	bA	1119	X	-	-	-
15	CL7	bA	1120	X	-	-	-
15	CL7	bA	1121	X	-	-	-
15	CL7	bA	1122	X	-	-	-
15	CL7	bA	1123	X	-	-	-
15	CL7	bA	1124	X	-	-	-
15	CL7	bA	1125	X	-	-	-
15	CL7	bA	1126	X	-	-	-
15	CL7	bA	1127	X	-	-	-
15	CL7	bA	1128	X	-	-	-
15	CL7	bA	1129	X	-	-	-
15	CL7	bA	1130	X	-	-	-
15	CL7	bA	1131	X	-	-	-
15	CL7	bA	1132	X	-	-	-
15	CL7	bA	1133	X	-	-	-
15	CL7	bA	1134	X	-	-	-
15	CL7	bA	1135	X	-	-	-
15	CL7	bA	1136	X	-	-	-
15	CL7	bA	1137	X	-	-	-
15	CL7	bA	1138	X	-	-	-
15	CL7	bA	1139	X	-	-	-
15	CL7	bA	1140	X	-	-	-
15	CL7	bA	1801	X	-	-	-
15	CL7	bB	1012	X	-	-	-
15	CL7	bB	1021	X	-	-	-
15	CL7	bB	1201	X	-	-	-
15	CL7	bB	1202	X	-	-	-
15	CL7	bB	1203	X	-	-	-
15	CL7	bB	1204	X	-	-	-
15	CL7	bB	1205	X	-	-	-
15	CL7	bB	1206	X	-	-	-
15	CL7	bB	1207	X	-	-	-
15	CL7	bB	1208	X	-	-	-
15	CL7	bB	1209	X	-	-	-
15	CL7	bB	1210	X	-	-	-
15	CL7	bB	1211	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	bB	1212	X	-	-	-
15	CL7	bB	1213	X	-	-	-
15	CL7	bB	1214	X	-	-	-
15	CL7	bB	1215	X	-	-	-
15	CL7	bB	1216	X	-	-	-
15	CL7	bB	1217	X	-	-	-
15	CL7	bB	1218	X	-	-	-
15	CL7	bB	1219	X	-	-	-
15	CL7	bB	1220	X	-	-	-
15	CL7	bB	1221	X	-	-	-
15	CL7	bB	1222	X	-	-	-
15	CL7	bB	1223	X	-	-	-
15	CL7	bB	1224	X	-	-	-
15	CL7	bB	1225	X	-	-	-
15	CL7	bB	1226	X	-	-	-
15	CL7	bB	1227	X	-	-	-
15	CL7	bB	1228	X	-	-	-
15	CL7	bB	1229	X	-	-	-
15	CL7	bB	1230	X	-	-	-
15	CL7	bB	1231	X	-	-	-
15	CL7	bB	1232	X	-	-	-
15	CL7	bB	1233	X	-	-	-
15	CL7	bB	1234	X	-	-	-
15	CL7	bB	1235	X	-	-	-
15	CL7	bB	1236	X	-	-	-
15	CL7	bB	1237	X	-	-	-
15	CL7	bB	1238	X	-	-	-
15	CL7	bB	1239	X	-	-	-
15	CL7	bB	1241	X	-	-	-
15	CL7	bF	1701	X	-	-	-
15	CL7	bI	1601	X	-	-	-
15	CL7	bJ	1301	X	-	-	-
15	CL7	bJ	1302	X	-	-	-
15	CL7	bK	1401	X	-	-	-
15	CL7	bK	1402	X	-	-	-
15	CL7	bL	1501	X	-	-	-
15	CL7	bL	1502	X	-	-	-
15	CL7	bL	1503	X	-	-	-
15	CL7	cA	1022	X	-	-	-
15	CL7	cA	1101	X	-	-	-
15	CL7	cA	1102	X	-	-	-
15	CL7	cA	1103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cA	1104	X	-	-	-
15	CL7	cA	1105	X	-	-	-
15	CL7	cA	1106	X	-	-	-
15	CL7	cA	1107	X	-	-	-
15	CL7	cA	1108	X	-	-	-
15	CL7	cA	1109	X	-	-	-
15	CL7	cA	1110	X	-	-	-
15	CL7	cA	1111	X	-	-	-
15	CL7	cA	1112	X	-	-	-
15	CL7	cA	1113	X	-	-	-
15	CL7	cA	1114	X	-	-	-
15	CL7	cA	1115	X	-	-	-
15	CL7	cA	1116	X	-	-	-
15	CL7	cA	1117	X	-	-	-
15	CL7	cA	1118	X	-	-	-
15	CL7	cA	1119	X	-	-	-
15	CL7	cA	1120	X	-	-	-
15	CL7	cA	1121	X	-	-	-
15	CL7	cA	1122	X	-	-	-
15	CL7	cA	1123	X	-	-	-
15	CL7	cA	1124	X	-	-	-
15	CL7	cA	1125	X	-	-	-
15	CL7	cA	1126	X	-	-	-
15	CL7	cA	1127	X	-	-	-
15	CL7	cA	1128	X	-	-	-
15	CL7	cA	1129	X	-	-	-
15	CL7	cA	1130	X	-	-	-
15	CL7	cA	1131	X	-	-	-
15	CL7	cA	1132	X	-	-	-
15	CL7	cA	1133	X	-	-	-
15	CL7	cA	1134	X	-	-	-
15	CL7	cA	1135	X	-	-	-
15	CL7	cA	1136	X	-	-	-
15	CL7	cA	1137	X	-	-	-
15	CL7	cA	1138	X	-	-	-
15	CL7	cA	1139	X	-	-	-
15	CL7	cA	1140	X	-	-	-
15	CL7	cA	1801	X	-	-	-
15	CL7	cB	1012	X	-	-	-
15	CL7	cB	1021	X	-	-	-
15	CL7	cB	1201	X	-	-	-
15	CL7	cB	1202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cB	1203	X	-	-	-
15	CL7	cB	1204	X	-	-	-
15	CL7	cB	1205	X	-	-	-
15	CL7	cB	1206	X	-	-	-
15	CL7	cB	1207	X	-	-	-
15	CL7	cB	1208	X	-	-	-
15	CL7	cB	1209	X	-	-	-
15	CL7	cB	1210	X	-	-	-
15	CL7	cB	1211	X	-	-	-
15	CL7	cB	1212	X	-	-	-
15	CL7	cB	1213	X	-	-	-
15	CL7	cB	1214	X	-	-	-
15	CL7	cB	1215	X	-	-	-
15	CL7	cB	1216	X	-	-	-
15	CL7	cB	1217	X	-	-	-
15	CL7	cB	1218	X	-	-	-
15	CL7	cB	1219	X	-	-	-
15	CL7	cB	1220	X	-	-	-
15	CL7	cB	1221	X	-	-	-
15	CL7	cB	1222	X	-	-	-
15	CL7	cB	1223	X	-	-	-
15	CL7	cB	1224	X	-	-	-
15	CL7	cB	1225	X	-	-	-
15	CL7	cB	1226	X	-	-	-
15	CL7	cB	1227	X	-	-	-
15	CL7	cB	1228	X	-	-	-
15	CL7	cB	1229	X	-	-	-
15	CL7	cB	1230	X	-	-	-
15	CL7	cB	1231	X	-	-	-
15	CL7	cB	1232	X	-	-	-
15	CL7	cB	1233	X	-	-	-
15	CL7	cB	1234	X	-	-	-
15	CL7	cB	1235	X	-	-	-
15	CL7	cB	1236	X	-	-	-
15	CL7	cB	1237	X	-	-	-
15	CL7	cB	1238	X	-	-	-
15	CL7	cB	1239	X	-	-	-
15	CL7	cB	1241	X	-	-	-
15	CL7	cF	1701	X	-	-	-
15	CL7	cI	1601	X	-	-	-
15	CL7	cJ	1301	X	-	-	-
15	CL7	cJ	1302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL7	cK	1401	X	-	-	-
15	CL7	cK	1402	X	-	-	-
15	CL7	cL	1501	X	-	-	-
15	CL7	cL	1502	X	-	-	-
15	CL7	cL	1503	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 70575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I protein PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		
1	bA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		
1	cA	737	Total	C	N	O	S	0	0
			5797	3785	989	991	32		

- Molecule 2 is a protein called Photosystem I protein PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		
2	bB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		
2	cB	731	Total	C	N	O	S	0	0
			5814	3821	966	1006	21		

- Molecule 3 is a protein called Photosystem I protein PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	bC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	cC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

- Molecule 4 is a protein called Photosystem I protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		
4	cD	136	Total	C	N	O	S	0	0
			1039	653	180	202	4		

- Molecule 5 is a protein called Photosystem I protein PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		
5	bE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		
5	cE	67	Total	C	N	O	S	0	0
			526	332	94	99	1		

- Molecule 6 is a protein called Photosystem I protein PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		
6	bF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		
6	cF	143	Total	C	N	O	S	0	0
			1056	666	185	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		
7	bI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		
7	cI	33	Total	C	N	O	S	0	0
			250	167	36	44	3		

- Molecule 8 is a protein called Photosystem I protein PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	35	Total	C	N	O	0	0
			291	207	40	44		
8	bJ	35	Total	C	N	O	0	0
			291	207	40	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	cJ	35	Total	C	N	O	0	0
			291	207	40	44		

- Molecule 9 is a protein called Photosystem I protein PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	54	Total	C	N	O	S	0	0
			397	264	63	68	2		
9	bK	54	Total	C	N	O	S	0	0
			397	264	63	68	2		
9	cK	54	Total	C	N	O	S	0	0
			397	264	63	68	2		

- Molecule 10 is a protein called Photosystem I protein PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	148	Total	C	N	O	S	0	0
			1059	680	176	196	7		
10	bL	148	Total	C	N	O	S	0	0
			1059	680	176	196	7		
10	cL	148	Total	C	N	O	S	0	0
			1059	680	176	196	7		

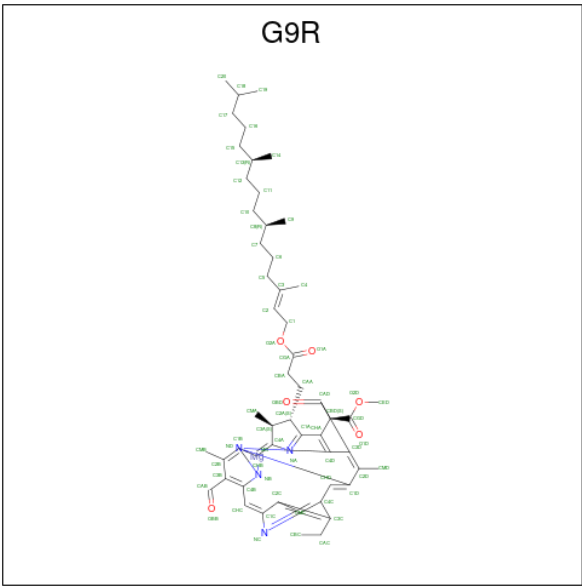
- Molecule 11 is a protein called Photosystem I protein PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			223	148	34	40	1		
11	bM	31	Total	C	N	O	S	0	0
			223	148	34	40	1		
11	cM	31	Total	C	N	O	S	0	0
			223	148	34	40	1		

- Molecule 12 is a protein called Photosystem I protein PsaX2.

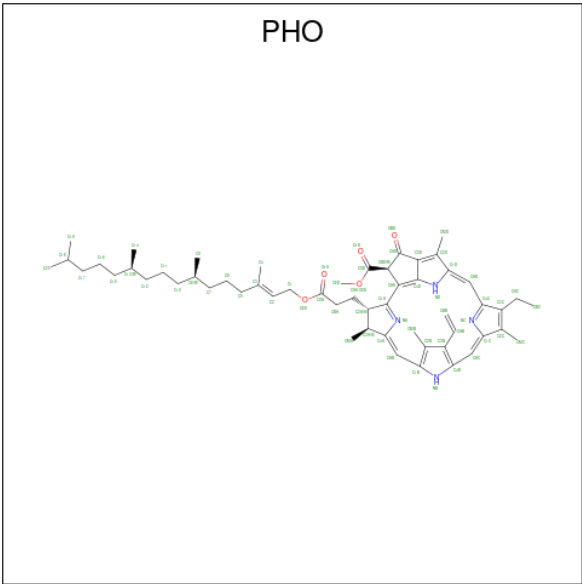
Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	24	Total	C	N	O	0	0
			187	131	28	28		
12	bX	24	Total	C	N	O	0	0
			187	131	28	28		
12	cX	24	Total	C	N	O	0	0
			187	131	28	28		

- Molecule 13 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: C₅₄H₇₀MgN₄O₆).



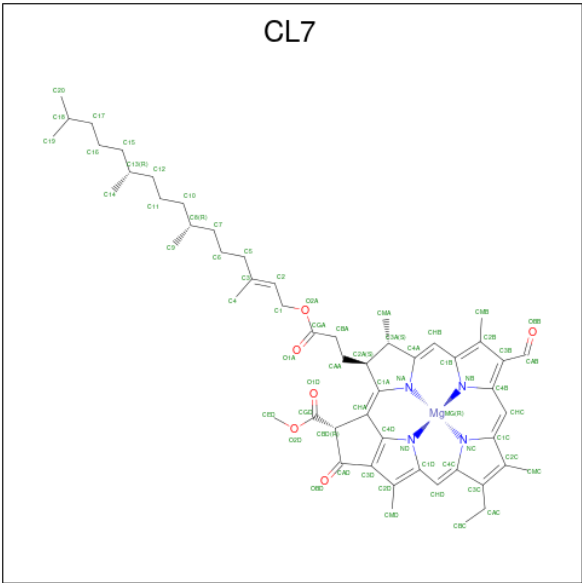
Mol	Chain	Residues	Atoms					AltConf
13	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	N	O	0
			64	55	4	5	
14	aB	1	Total	C	N	O	0
			64	55	4	5	
14	bA	1	Total	C	N	O	0
			64	55	4	5	
14	bB	1	Total	C	N	O	0
			64	55	4	5	
14	cA	1	Total	C	N	O	0
			64	55	4	5	
14	cB	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is CHLOROPHYLL D (CCD ID: CL7) (formula: C₅₄H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
15	aA	1	Total 52	C 41	Mg 1	N 4	O 6	0
15	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	aF	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aI	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aJ	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	aJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
15	aK	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	aK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
15	aL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	aL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	aL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bA	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	bA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	bB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	bB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total 45	C 34	Mg 1	N 4	O 6	0
15	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	bB	1	Total 45	C 34	Mg 1	N 4	O 6	0
15	bF	1	Total 41	C 32	Mg 1	N 4	O 4	0
15	bI	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	bJ	1	Total 41	C 32	Mg 1	N 4	O 4	0
15	bJ	1	Total 42	C 33	Mg 1	N 4	O 4	0
15	bK	1	Total 45	C 34	Mg 1	N 4	O 6	0
15	bK	1	Total 37	C 30	Mg 1	N 4	O 2	0
15	bL	1	Total 60	C 49	Mg 1	N 4	O 6	0
15	bL	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	bL	1	Total 60	C 49	Mg 1	N 4	O 6	0
15	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	cA	1	Total 41	C 32	Mg 1	N 4	O 4	0
15	cA	1	Total 52	C 41	Mg 1	N 4	O 6	0
15	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	cA	1	Total 45	C 34	Mg 1	N 4	O 6	0
15	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
15	cA	1	Total 45	C 34	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cA	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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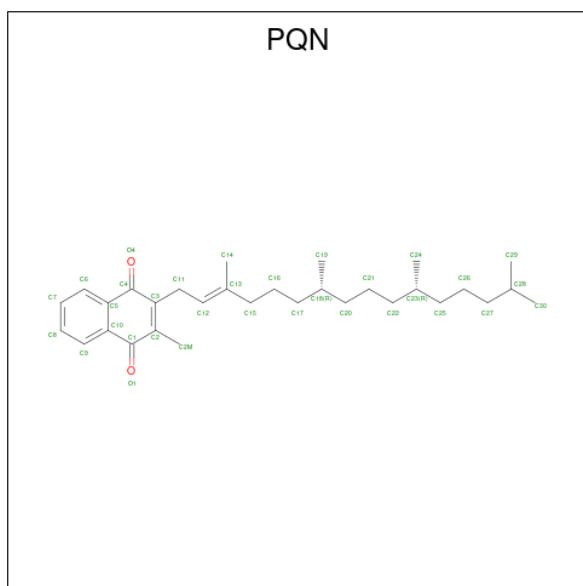
Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cB	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cB	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cF	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cI	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
15	cJ	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
15	cJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
15	cK	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
15	cK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
15	cL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
15	cL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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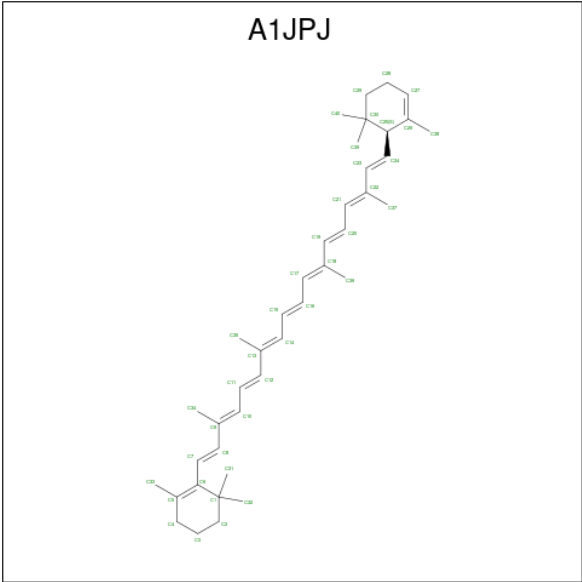
Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

- Molecule 17 is (6'S)-beta,epsilon-carotene (CCD ID: A1JPJ) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aF	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	aI	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bI	1	Total C 40 40	0

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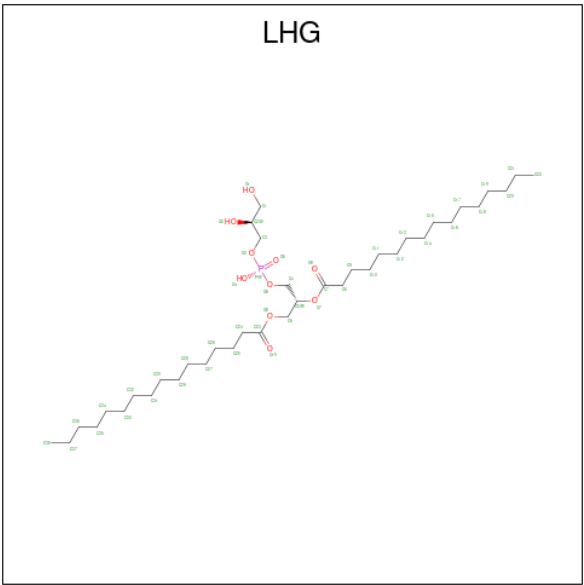
Mol	Chain	Residues	Atoms	AltConf
17	bJ	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cL	1	Total C 40 40	0

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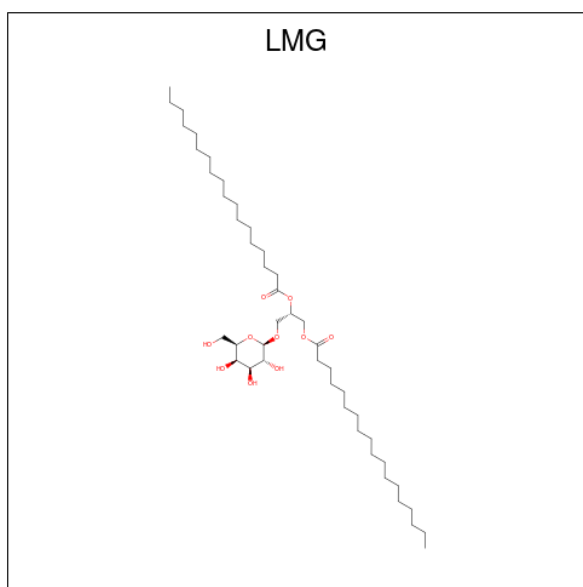
Mol	Chain	Residues	Atoms	AltConf
17	cL	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



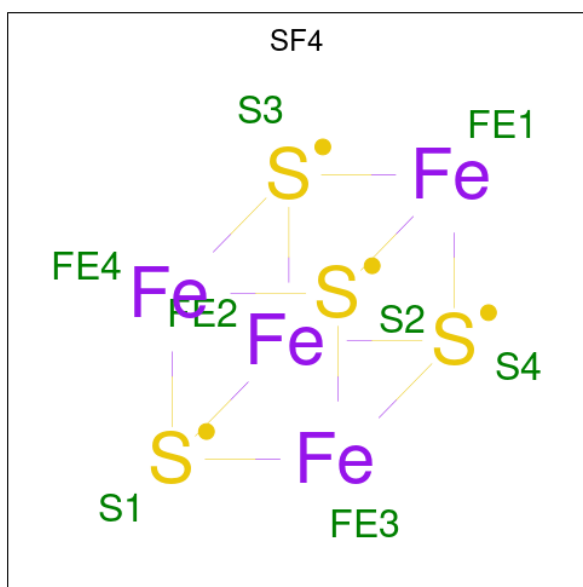
Mol	Chain	Residues	Atoms	AltConf
18	aA	1	Total C O P 49 38 10 1	0
18	aA	1	Total C O P 38 27 10 1	0
18	bA	1	Total C O P 49 38 10 1	0
18	bA	1	Total C O P 38 27 10 1	0
18	cA	1	Total C O P 49 38 10 1	0
18	cA	1	Total C O P 38 27 10 1	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
19	aB	1	Total	C	O	0
			53	43	10	
19	bB	1	Total	C	O	0
			53	43	10	
19	cB	1	Total	C	O	0
			53	43	10	

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
20	aB	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
20	aC	1	Total 8	Fe 4	S 4	0
20	aC	1	Total 8	Fe 4	S 4	0
20	bB	1	Total 8	Fe 4	S 4	0
20	bC	1	Total 8	Fe 4	S 4	0
20	bC	1	Total 8	Fe 4	S 4	0
20	cB	1	Total 8	Fe 4	S 4	0
20	cC	1	Total 8	Fe 4	S 4	0
20	cC	1	Total 8	Fe 4	S 4	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	aA	21	Total 21	O 21	0
21	aB	6	Total 6	O 6	0
21	aI	1	Total 1	O 1	0
21	aJ	1	Total 1	O 1	0
21	aL	2	Total 2	O 2	0
21	bA	21	Total 21	O 21	0
21	bB	6	Total 6	O 6	0
21	bI	1	Total 1	O 1	0
21	bJ	1	Total 1	O 1	0
21	bL	2	Total 2	O 2	0
21	cA	21	Total 21	O 21	0

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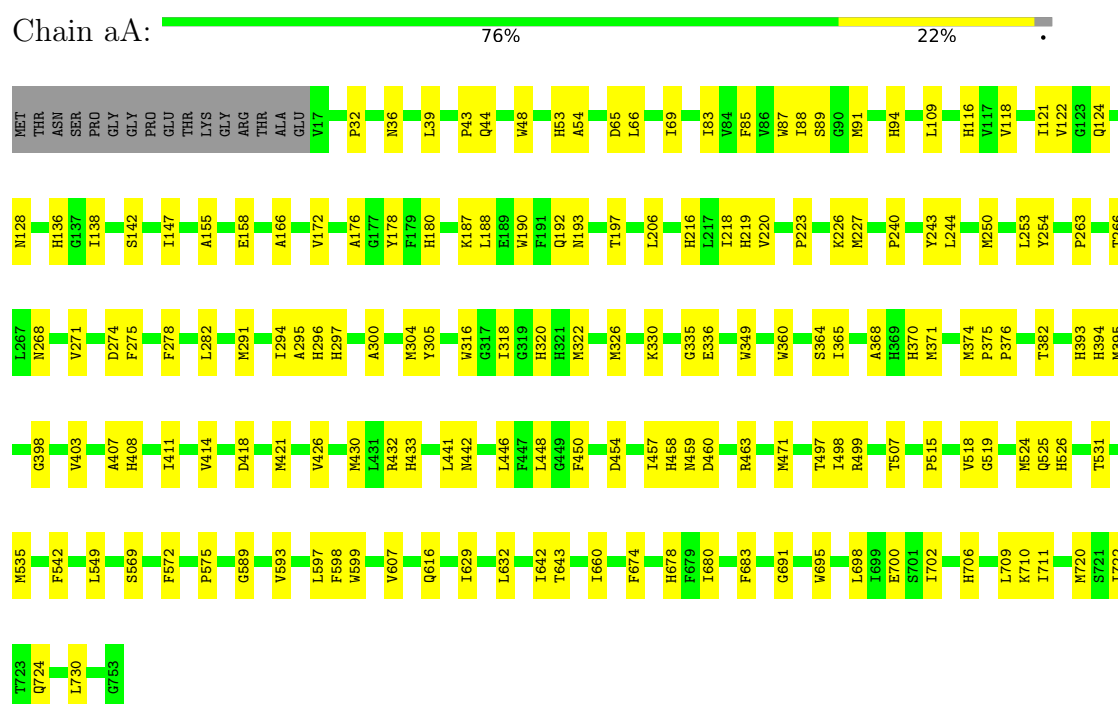
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Mol	Chain	Residues	Atoms		AltConf
21	cB	6	Total 6	O 6	0
21	cI	1	Total 1	O 1	0
21	cJ	1	Total 1	O 1	0
21	cL	2	Total 2	O 2	0

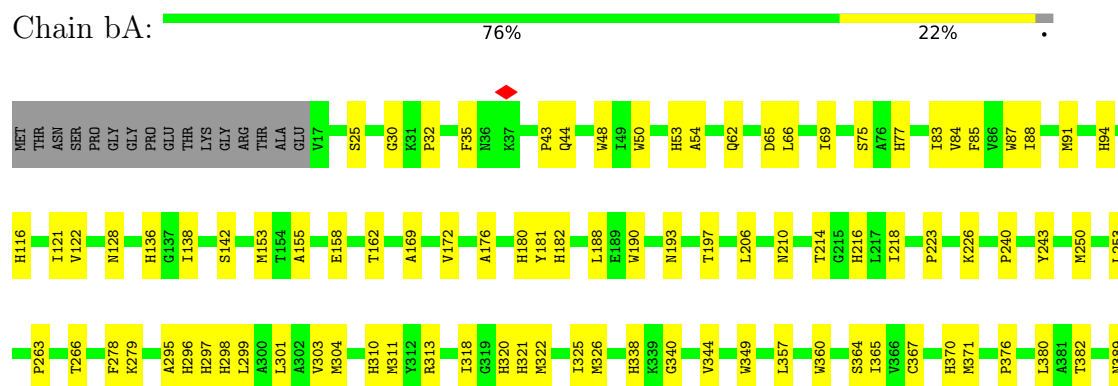
3 Residue-property plots

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

• Molecule 1: Photosystem I protein PsaA



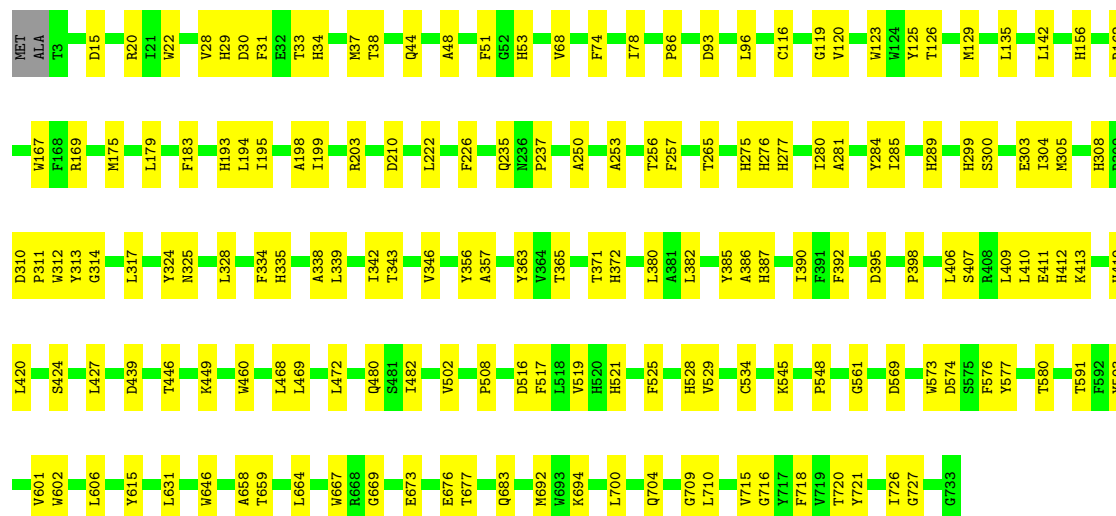
• Molecule 1: Photosystem I protein PsaA





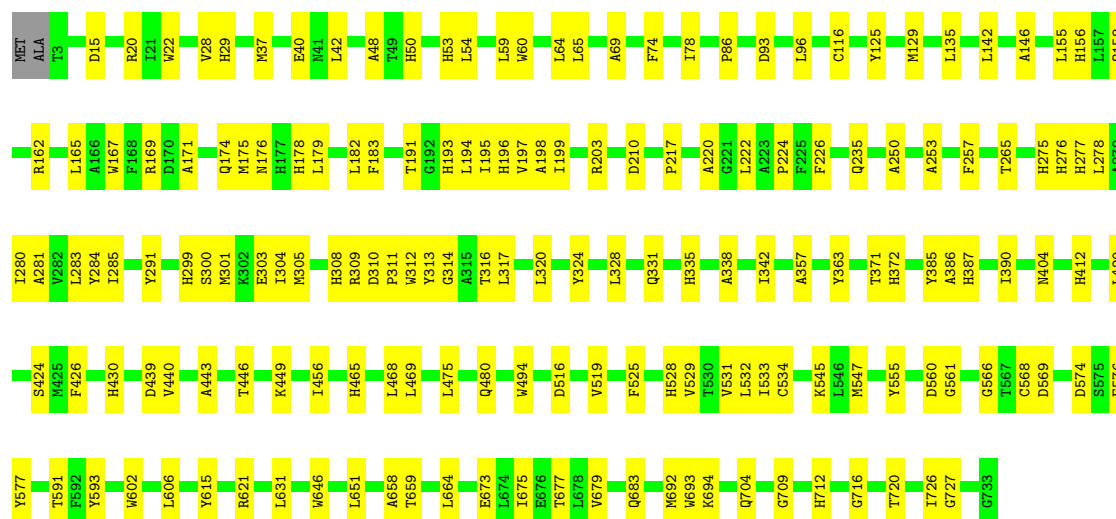
• Molecule 2: Photosystem I protein PsaB

Chain bB: 77% 23%



• Molecule 2: Photosystem I protein PsaB

Chain cB: 77% 23%



• Molecule 3: Photosystem I protein PsaC

Chain aC: 77% 22%



• Molecule 3: Photosystem I protein PsaC

Chain bC:  77% 22%



- Molecule 3: Photosystem I protein PsaC

Chain cC:  84% 15%



- Molecule 4: Photosystem I protein PsaD

Chain aD:  71% 27%



- Molecule 4: Photosystem I protein PsaD

Chain bD:  79% 19%



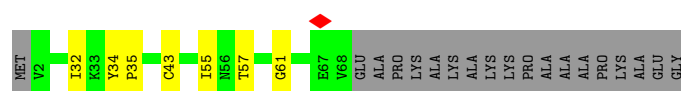
- Molecule 4: Photosystem I protein PsaD

Chain cD:  77% 21%



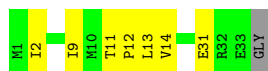
- Molecule 5: Photosystem I protein PsaE

Chain aE:  70% 8% 22%



- Molecule 5: Photosystem I protein PsaE

Chain bE:  65% 13% 22%



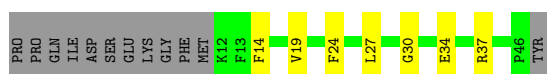
• Molecule 7: Photosystem I protein PsaI

Chain cI: 82% 15% .



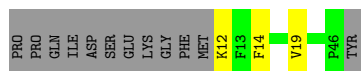
• Molecule 8: Photosystem I protein PsaJ

Chain aJ: 60% 15% 26%



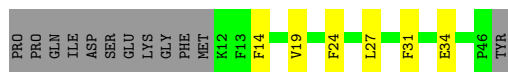
• Molecule 8: Photosystem I protein PsaJ

Chain bJ: 68% 6% 26%



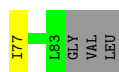
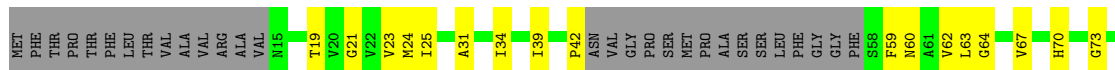
• Molecule 8: Photosystem I protein PsaJ

Chain cJ: 62% 13% 26%



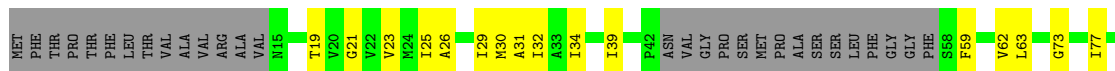
• Molecule 9: Photosystem I protein PsaK

Chain aK: 42% 21% 37%



• Molecule 9: Photosystem I protein PsaK

Chain bK: 44% 19% 37%

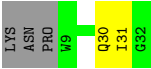
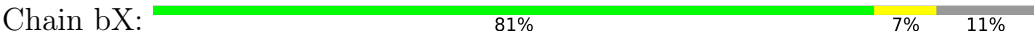




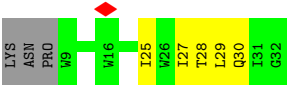
• Molecule 12: Photosystem I protein PsaX2



• Molecule 12: Photosystem I protein PsaX2



• Molecule 12: Photosystem I protein PsaX2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.435	Depositor
Minimum map value	-0.455	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	634.8, 634.8, 634.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMG, G9R, PHO, CL7, A1JPJ, LHG, SF4

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	aA	0.18	0/5993	0.36	0/8165
1	bA	0.18	0/5993	0.36	0/8165
1	cA	0.18	0/5993	0.36	0/8165
2	aB	0.17	0/6030	0.35	0/8249
2	bB	0.17	0/6030	0.36	0/8249
2	cB	0.18	0/6030	0.36	0/8249
3	aC	0.16	0/609	0.36	0/825
3	bC	0.15	0/609	0.35	0/825
3	cC	0.14	0/609	0.33	0/825
4	aD	0.15	0/1058	0.39	0/1428
4	bD	0.15	0/1058	0.36	0/1428
4	cD	0.15	0/1058	0.38	0/1428
5	aE	0.11	0/536	0.31	0/725
5	bE	0.12	0/536	0.31	0/725
5	cE	0.12	0/536	0.31	0/725
6	aF	0.13	0/1078	0.33	0/1464
6	bF	0.14	0/1078	0.36	0/1464
6	cF	0.14	0/1078	0.36	0/1464
7	aI	0.18	0/255	0.34	0/346
7	bI	0.19	0/255	0.37	0/346
7	cI	0.17	0/255	0.38	0/346
8	aJ	0.13	0/303	0.36	0/412
8	bJ	0.12	0/303	0.31	0/412
8	cJ	0.13	0/303	0.32	0/412
9	aK	0.16	0/405	0.38	0/553
9	bK	0.13	0/405	0.30	0/553
9	cK	0.15	0/405	0.40	0/553
10	aL	0.20	0/1084	0.35	0/1475
10	bL	0.20	0/1084	0.41	2/1475 (0.1%)
10	cL	0.18	0/1084	0.32	0/1475
11	aM	0.20	0/223	0.42	0/304
11	bM	0.21	0/223	0.45	0/304

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	cM	0.16	0/223	0.31	0/304
12	aX	0.13	0/194	0.33	0/269
12	bX	0.14	0/194	0.32	0/269
12	cX	0.14	0/194	0.33	0/269
All	All	0.17	0/53304	0.36	2/72645 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	104	PRO	CA-C-N	-5.35	112.96	123.56
10	bL	104	PRO	C-N-CA	-5.35	112.96	123.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5797	0	5622	155	0
1	bA	5797	0	5623	148	0
1	cA	5797	0	5623	155	0
2	aB	5814	0	5544	153	0
2	bB	5814	0	5545	149	0
2	cB	5814	0	5545	154	0
3	aC	599	0	577	12	0
3	bC	599	0	577	16	0
3	cC	599	0	577	9	0
4	aD	1039	0	1043	26	0
4	bD	1039	0	1043	25	0
4	cD	1039	0	1043	21	0
5	aE	526	0	518	4	0
5	bE	526	0	518	7	0
5	cE	526	0	518	4	0
6	aF	1056	0	1063	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1056	0	1063	23	0
6	cF	1056	0	1063	16	0
7	aI	250	0	260	7	0
7	bI	250	0	260	5	0
7	cI	250	0	260	4	0
8	aJ	291	0	289	5	0
8	bJ	291	0	289	2	0
8	cJ	291	0	289	6	0
9	aK	397	0	410	14	0
9	bK	397	0	410	11	0
9	cK	397	0	410	17	0
10	aL	1059	0	1067	20	0
10	bL	1059	0	1067	18	0
10	cL	1059	0	1067	16	0
11	aM	223	0	259	8	0
11	bM	223	0	259	4	0
11	cM	223	0	259	3	0
12	aX	187	0	199	5	0
12	bX	187	0	199	2	0
12	cX	187	0	199	4	0
13	aA	65	0	0	0	0
13	bA	65	0	0	0	0
13	cA	65	0	0	0	0
14	aA	64	0	74	3	0
14	aB	64	0	74	7	0
14	bA	64	0	74	1	0
14	bB	64	0	74	6	0
14	cA	64	0	74	1	0
14	cB	64	0	74	7	0
15	aA	2346	0	2154	119	0
15	aB	2271	0	2037	100	0
15	aF	41	0	27	0	0
15	aI	65	0	70	6	0
15	aJ	83	0	55	2	0
15	aK	82	0	54	2	0
15	aL	185	0	184	7	0
15	bA	2346	0	2154	121	0
15	bB	2271	0	2037	102	0
15	bF	41	0	27	0	0
15	bI	65	0	70	2	0
15	bJ	83	0	55	1	0
15	bK	82	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	bL	185	0	184	6	0
15	cA	2346	0	2154	101	0
15	cB	2271	0	2037	119	0
15	cF	41	0	27	0	0
15	cI	65	0	70	4	0
15	cJ	83	0	55	4	0
15	cK	82	0	54	0	0
15	cL	185	0	184	7	0
16	aA	33	0	46	1	0
16	aB	33	0	46	0	0
16	bA	33	0	46	2	0
16	bB	33	0	46	0	0
16	cA	33	0	46	0	0
16	cB	33	0	46	0	0
17	aA	240	0	0	0	0
17	aB	280	0	0	1	0
17	aF	40	0	0	0	0
17	aI	80	0	0	0	0
17	aJ	40	0	0	0	0
17	aL	80	0	0	1	0
17	bA	240	0	0	1	0
17	bB	280	0	0	0	0
17	bF	40	0	0	0	0
17	bI	80	0	0	0	0
17	bJ	40	0	0	0	0
17	bL	80	0	0	1	0
17	cA	240	0	0	0	0
17	cB	280	0	0	1	0
17	cF	40	0	0	0	0
17	cI	80	0	0	0	0
17	cJ	40	0	0	0	0
17	cL	80	0	0	0	0
18	aA	87	0	123	5	0
18	bA	87	0	123	4	0
18	cA	87	0	123	8	0
19	aB	53	0	79	3	0
19	bB	53	0	79	3	0
19	cB	53	0	79	1	0
20	aB	8	0	0	0	0
20	aC	16	0	0	0	0
20	bB	8	0	0	0	0
20	bC	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cB	8	0	0	0	0
20	cC	16	0	0	0	0
21	aA	21	0	0	0	0
21	aB	6	0	0	0	0
21	aI	1	0	0	0	0
21	aJ	1	0	0	0	0
21	aL	2	0	0	0	0
21	bA	21	0	0	0	0
21	bB	6	0	0	0	0
21	bI	1	0	0	0	0
21	bJ	1	0	0	0	0
21	bL	2	0	0	0	0
21	cA	21	0	0	1	0
21	cB	6	0	0	0	0
21	cI	1	0	0	0	0
21	cJ	1	0	0	0	0
21	cL	2	0	0	0	0
All	All	70575	0	65626	1464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:296:HIS:HE1	15:aA:1115:CL7:NB	1.62	0.95
2:cB:193:HIS:CE1	15:cB:1211:CL7:NA	2.42	0.87
2:aB:244:PHE:H	2:aB:264:GLN:HE22	1.29	0.80
1:bA:720:MET:HE3	1:bA:724:GLN:HG2	1.64	0.79
2:aB:335:HIS:CD2	15:aB:1221:CL7:HAA2	2.18	0.79
1:aA:116:HIS:HB3	1:aA:138:ILE:HB	1.66	0.78
2:aB:48:ALA:HB2	2:aB:157:LEU:HD21	1.65	0.78
2:aB:59:LEU:HD12	15:aB:1204:CL7:H91C	1.66	0.78
1:aA:316:TRP:HE3	9:aK:60:ASN:HD21	1.31	0.77
1:aA:320:HIS:NE2	15:aA:1120:CL7:ND	2.31	0.77
1:cA:709:LEU:HD21	15:cB:1228:CL7:H3A	1.66	0.77
1:aA:709:LEU:HD21	15:aB:1228:CL7:H3A	1.67	0.77
15:aB:1210:CL7:HED2	15:aB:1210:CL7:H2A	1.65	0.76
10:cL:38:ARG:HB3	10:cL:41:MET:HE2	1.65	0.76
2:bB:335:HIS:CD2	15:bB:1221:CL7:HAA2	2.21	0.76
2:cB:59:LEU:HD12	15:cB:1204:CL7:H91C	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:291:TYR:HE1	2:aB:301:MET:HE3	1.51	0.75
2:cB:191:THR:HG21	2:cB:278:LEU:HB2	1.68	0.75
2:cB:299:HIS:HB3	2:cB:304:ILE:HD11	1.69	0.74
4:bD:32:THR:O	4:bD:82:TYR:HA	1.88	0.74
3:cC:63:LEU:HD11	3:cC:66:ARG:HH11	1.53	0.73
1:bA:83:ILE:HD11	15:bA:1109:CL7:H141	1.69	0.73
4:cD:32:THR:O	4:cD:82:TYR:HA	1.89	0.73
15:aA:1122:CL7:H3A	15:aA:1133:CL7:H193	1.71	0.72
2:cB:335:HIS:CD2	15:cB:1221:CL7:HAA2	2.24	0.72
1:aA:709:LEU:HD11	15:aB:1228:CL7:HHB	1.72	0.72
2:bB:169:ARG:HH21	2:bB:325:ASN:HD22	1.37	0.72
1:cA:515:PRO:HB3	1:cA:629:ILE:HD11	1.73	0.71
2:aB:299:HIS:HB3	2:aB:304:ILE:HD11	1.73	0.71
2:aB:427:LEU:HB3	2:aB:525:PHE:HB2	1.71	0.70
9:cK:59:PHE:HA	9:cK:62:VAL:HG12	1.72	0.70
2:aB:281:ALA:O	2:aB:285:ILE:HD12	1.92	0.69
2:bB:427:LEU:HB3	2:bB:525:PHE:HB2	1.73	0.69
1:aA:296:HIS:CE1	15:aA:1115:CL7:NB	2.54	0.69
2:cB:129:MET:HE3	15:cB:1211:CL7:HMA2	1.74	0.69
15:cA:1122:CL7:H3A	15:cA:1133:CL7:H193	1.74	0.69
2:cB:420:LEU:HD23	2:cB:532:LEU:HA	1.75	0.69
1:cA:352:GLN:HG2	15:cA:1123:CL7:H112	1.74	0.69
2:aB:291:TYR:CE1	2:aB:301:MET:HE3	2.28	0.69
1:bA:360:TRP:HE1	15:bA:1104:CL7:HAB	1.57	0.68
2:aB:15:ASP:HB3	2:aB:20:ARG:HB2	1.76	0.68
1:bA:365:ILE:HG13	1:bA:398:GLY:HA3	1.76	0.68
11:cM:13:VAL:HA	11:cM:16:LEU:HD23	1.76	0.68
1:bA:720:MET:HE2	1:bA:725:GLY:HA2	1.75	0.68
1:bA:226:LYS:HD2	1:bA:253:LEU:HD13	1.76	0.68
9:aK:59:PHE:HA	9:aK:62:VAL:HG12	1.74	0.68
2:bB:299:HIS:NE2	15:bB:1218:CL7:ND	2.41	0.68
1:cA:218:ILE:HA	1:cA:222:LEU:HD12	1.74	0.68
2:cB:15:ASP:HB3	2:cB:20:ARG:HB2	1.74	0.68
15:bA:1122:CL7:H3A	15:bA:1133:CL7:H193	1.75	0.67
15:bB:1222:CL7:HED2	15:bB:1222:CL7:H2A	1.75	0.67
2:cB:317:LEU:HD11	15:cB:1241:CL7:HAB	1.76	0.67
1:bA:488:GLN:HA	1:bA:511:TRP:HE3	1.59	0.67
15:aA:1125:CL7:HMB2	15:aA:1133:CL7:HBA2	1.76	0.67
2:cB:193:HIS:HE1	15:cB:1211:CL7:NA	1.92	0.67
1:cA:360:TRP:HE1	15:cA:1104:CL7:HAB	1.60	0.67
2:bB:419:HIS:CE1	15:bB:1228:CL7:NB	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:193:HIS:HB2	15:cB:1211:CL7:C1C	2.24	0.67
2:bB:545:LYS:HE2	6:bF:165:SER:HA	1.76	0.67
1:cA:709:LEU:HD11	15:cB:1228:CL7:HHB	1.77	0.67
2:bB:521:HIS:HE1	15:bB:1235:CL7:NC	1.92	0.66
1:bA:430:MET:HG3	15:bA:1122:CL7:H192	1.77	0.66
2:cB:277:HIS:HA	2:cB:280:ILE:HG12	1.76	0.66
11:aM:13:VAL:HA	11:aM:16:LEU:HD13	1.76	0.66
2:bB:468:LEU:HD12	2:bB:469:LEU:HG	1.77	0.66
15:bB:1229:CL7:H201	15:bB:1235:CL7:H121	1.78	0.66
1:cA:116:HIS:HB3	1:cA:138:ILE:HB	1.77	0.66
1:bA:53:HIS:HE1	15:bA:1101:CL7:ND	1.93	0.66
2:aB:51:PHE:HD2	2:aB:153:GLY:HA2	1.59	0.65
15:cB:1222:CL7:H2A	15:cB:1222:CL7:HED2	1.77	0.65
1:cA:320:HIS:NE2	15:cA:1120:CL7:ND	2.45	0.65
4:cD:125:PRO:HG2	4:cD:130:ILE:HD11	1.79	0.65
1:cA:316:TRP:HB3	9:cK:60:ASN:HD21	1.61	0.65
1:cA:318:ILE:HG13	15:cA:1118:CL7:HED1	1.78	0.65
1:aA:360:TRP:HE1	15:aA:1104:CL7:HAB	1.63	0.64
15:aB:1235:CL7:H121	15:aB:1229:CL7:H201	1.80	0.64
1:aA:318:ILE:HG13	15:aA:1118:CL7:HED1	1.79	0.64
15:aB:1222:CL7:H2A	15:aB:1222:CL7:HED2	1.78	0.64
1:aA:430:MET:HE1	15:aA:1129:CL7:CHD	2.28	0.64
1:bA:448:LEU:HB3	1:bA:542:PHE:HB2	1.79	0.64
2:aB:29:HIS:CE1	15:aB:1201:CL7:NB	2.66	0.64
1:cA:148:LEU:HD22	1:cA:153:MET:HG3	1.80	0.64
2:aB:156:HIS:CE1	15:aB:1208:CL7:NA	2.65	0.63
6:aF:125:ILE:HG13	6:aF:126:ILE:HG12	1.81	0.63
2:bB:15:ASP:HB3	2:bB:20:ARG:HB2	1.80	0.63
8:cJ:34:GLU:HG3	15:cJ:1302:CL7:NB	2.13	0.63
1:aA:320:HIS:CE1	15:aA:1120:CL7:NA	2.66	0.63
4:aD:32:THR:O	4:aD:82:TYR:HA	1.98	0.63
2:bB:310:ASP:HB3	2:bB:314:GLY:H	1.64	0.62
1:aA:430:MET:HG3	15:aA:1122:CL7:H192	1.81	0.62
1:bA:66:LEU:HD23	1:bA:188:LEU:HD11	1.81	0.62
1:bA:320:HIS:CE1	15:bA:1120:CL7:NA	2.68	0.62
2:cB:468:LEU:HD12	2:cB:469:LEU:HG	1.80	0.62
2:cB:574:ASP:HA	2:cB:577:TYR:HB3	1.79	0.62
2:aB:547:MET:HE2	2:aB:550:LYS:HA	1.81	0.62
2:bB:574:ASP:HA	2:bB:577:TYR:HB3	1.80	0.62
2:aB:156:HIS:HE1	15:aB:1208:CL7:NA	1.97	0.62
1:bA:430:MET:HE1	15:bA:1129:CL7:CHD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:296:HIS:HB3	15:cA:1116:CL7:HMB2	1.82	0.62
2:aB:574:ASP:HA	2:aB:577:TYR:HB3	1.81	0.62
10:bL:144:LEU:HD21	15:cB:1207:CL7:H161	1.81	0.62
2:cB:313:TYR:HE2	15:cB:1227:CL7:HBA1	1.65	0.62
15:aA:1128:CL7:H193	15:aA:1140:CL7:H3A	1.82	0.62
2:cB:59:LEU:HD22	2:cB:146:ALA:HB1	1.82	0.62
1:bA:77:HIS:CD2	15:bA:1103:CL7:NA	2.67	0.61
2:bB:382:LEU:HG	2:bB:576:PHE:CE1	2.36	0.61
9:bK:59:PHE:HA	9:bK:62:VAL:HG12	1.81	0.61
2:cB:308:HIS:NE2	15:cB:1219:CL7:NB	2.48	0.61
1:aA:296:HIS:HB3	15:aA:1116:CL7:HMB2	1.82	0.61
2:aB:193:HIS:CE1	15:aB:1211:CL7:NA	2.68	0.61
2:bB:480:GLN:HG3	12:bX:30:GLN:HE22	1.65	0.61
2:cB:299:HIS:NE2	15:cB:1218:CL7:ND	2.48	0.61
15:bA:1125:CL7:HMB2	15:bA:1133:CL7:HBA2	1.83	0.61
2:cB:257:PHE:HE2	2:cB:494:TRP:HE3	1.49	0.61
1:cA:83:ILE:HD11	15:cA:1109:CL7:H141	1.82	0.60
2:cB:528:HIS:NE2	15:cB:1236:CL7:NA	2.48	0.60
15:cB:1204:CL7:HAA2	15:cB:1206:CL7:HED1	1.82	0.60
2:cB:465:HIS:CE1	15:cB:1231:CL7:NA	2.69	0.60
1:bA:433:HIS:NE2	15:bA:1129:CL7:ND	2.50	0.60
1:aA:188:LEU:O	1:aA:192:GLN:HG2	2.01	0.60
1:cA:226:LYS:HD2	1:cA:253:LEU:HD22	1.84	0.60
1:aA:322:MET:O	1:aA:326:MET:HG3	2.01	0.60
2:cB:156:HIS:CE1	15:cB:1208:CL7:NA	2.70	0.60
3:cC:62:PHE:HD2	4:cD:121:ILE:HG21	1.67	0.60
1:aA:121:ILE:HG23	1:aA:122:VAL:HG22	1.84	0.60
1:aA:291:MET:HA	1:aA:294:ILE:HG22	1.84	0.60
1:bA:441:LEU:HD13	1:bA:549:LEU:HA	1.82	0.60
1:aA:83:ILE:HD11	15:aA:1109:CL7:H141	1.84	0.60
2:bB:398:PRO:HD2	4:bD:126:ASN:ND2	2.16	0.60
4:aD:11:LEU:HB2	4:aD:50:VAL:HB	1.84	0.59
1:bA:182:HIS:NE2	15:bA:1109:CL7:NC	2.49	0.59
15:bB:1238:CL7:H201	10:bL:54:HIS:HD2	1.66	0.59
2:cB:281:ALA:O	2:cB:285:ILE:HG13	2.02	0.59
2:cB:305:MET:HE1	15:cB:1220:CL7:CGD	2.32	0.59
15:bB:1204:CL7:H12C	7:bI:14:VAL:HG21	1.83	0.59
2:aB:300:SER:HB2	2:aB:303:GLU:HG2	1.85	0.59
2:cB:277:HIS:HD1	2:cB:280:ILE:HD11	1.68	0.59
2:cB:420:LEU:HD21	2:cB:531:VAL:HG12	1.83	0.59
1:aA:250:MET:HG3	15:aA:1113:CL7:HED1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:301:LEU:HA	1:bA:304:MET:HE2	1.84	0.59
2:bB:22:TRP:CG	2:bB:704:GLN:HE22	2.21	0.59
2:bB:317:LEU:HD11	15:bB:1241:CL7:HAB	1.84	0.59
2:cB:178:HIS:NE2	15:cB:1210:CL7:NB	2.51	0.59
4:aD:71:LEU:HD23	4:aD:75:ARG:HE	1.67	0.59
1:bA:322:MET:O	1:bA:326:MET:HG3	2.03	0.59
1:cA:408:HIS:HE1	15:cA:1128:CL7:NA	2.00	0.59
2:aB:299:HIS:NE2	15:aB:1218:CL7:C4D	2.59	0.59
2:aB:301:MET:SD	15:aB:1216:CL7:HED2	2.42	0.59
5:cE:60:PHE:HB3	5:cE:65:LEU:HD11	1.84	0.59
1:aA:448:LEU:HB3	1:aA:542:PHE:HB2	1.83	0.58
2:aB:59:LEU:HD22	2:aB:146:ALA:HB1	1.85	0.58
2:aB:301:MET:HB3	2:aB:305:MET:HE2	1.85	0.58
1:cA:430:MET:HE2	15:cA:1122:CL7:H171	1.85	0.58
10:cL:57:TYR:HE1	15:cL:1503:CL7:C2C	2.16	0.58
10:bL:57:TYR:HE1	15:bL:1503:CL7:C2C	2.15	0.58
2:cB:631:LEU:HD13	2:cB:727:GLY:HA3	1.84	0.58
9:cK:73:GLY:O	9:cK:77:ILE:HG12	2.04	0.58
2:aB:257:PHE:HE2	2:aB:494:TRP:HE3	1.51	0.58
1:bA:408:HIS:HE1	15:bA:1128:CL7:NA	2.01	0.58
11:bM:5:ASP:O	11:bM:9:VAL:HG23	2.02	0.58
11:bM:13:VAL:HA	11:bM:16:LEU:HD13	1.83	0.58
15:cB:1204:CL7:HHB	15:cB:1205:CL7:HMB3	1.85	0.58
2:cB:475:LEU:HD21	12:cX:27:ILE:HD11	1.85	0.58
11:aM:6:LEU:O	11:aM:10:ILE:HD12	2.03	0.58
11:bM:6:LEU:O	11:bM:10:ILE:HD12	2.03	0.58
1:cA:216:HIS:CE1	15:cA:1112:CL7:NA	2.71	0.58
9:aK:21:GLY:O	9:aK:25:ILE:HG12	2.02	0.58
6:aF:52:GLU:HB2	6:aF:56:LYS:HZ2	1.68	0.58
1:bA:318:ILE:HG13	15:bA:1118:CL7:HED1	1.84	0.58
4:bD:63:LYS:HE2	4:bD:67:LEU:HD11	1.86	0.58
15:cA:1128:CL7:H193	15:cA:1140:CL7:H3A	1.84	0.58
9:bK:73:GLY:O	9:bK:77:ILE:HG12	2.04	0.58
1:aA:172:VAL:HG11	15:aA:1111:CL7:H142	1.86	0.58
2:aB:74:PHE:O	2:aB:78:ILE:HG12	2.04	0.58
2:bB:74:PHE:O	2:bB:78:ILE:HG12	2.04	0.58
1:aA:297:HIS:HB2	15:aA:1116:CL7:CHB	2.34	0.58
4:aD:125:PRO:HG2	4:aD:130:ILE:HD11	1.85	0.58
2:bB:313:TYR:HE2	15:bB:1227:CL7:HBA1	1.67	0.58
2:aB:169:ARG:HH12	2:aB:325:ASN:HD22	1.50	0.57
2:bB:545:LYS:HE3	6:bF:163:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:433:HIS:NE2	15:cA:1129:CL7:ND	2.51	0.57
1:aA:403:VAL:HG11	1:aA:597:LEU:HG	1.86	0.57
1:aA:531:THR:HG22	1:aA:535:MET:HE2	1.85	0.57
2:aB:317:LEU:HG	2:aB:320:LEU:HD12	1.85	0.57
10:aL:57:TYR:HE1	15:aL:1503:CL7:C2C	2.16	0.57
5:cE:32:ILE:HG22	5:cE:34:TYR:H	1.68	0.57
14:aB:1023:PHO:HED3	14:aB:1023:PHO:HBA2	1.86	0.57
15:bA:1126:CL7:HBC1	15:bA:1128:CL7:H141	1.85	0.57
6:bF:103:ASN:HD22	6:bF:142:TRP:HB2	1.68	0.57
15:bB:1202:CL7:H101	15:bB:1210:CL7:HAA2	1.85	0.57
2:aB:38:THR:HA	4:aD:132:TYR:CE1	2.40	0.57
15:cB:1202:CL7:H101	15:cB:1210:CL7:HAA2	1.86	0.57
1:aA:53:HIS:HE1	15:aA:1101:CL7:ND	2.02	0.57
2:aB:480:GLN:HG3	12:aX:30:GLN:HE22	1.69	0.57
1:aA:296:HIS:HE1	15:aA:1115:CL7:C1B	2.16	0.57
15:aB:1238:CL7:H201	10:aL:54:HIS:HD2	1.68	0.57
1:bA:497:THR:HG23	1:bA:499:ARG:H	1.69	0.57
1:cA:301:LEU:HA	1:cA:304:MET:HE2	1.86	0.57
15:bB:1204:CL7:HBA2	15:bB:1204:CL7:HBD	1.86	0.57
10:cL:35:PRO:HA	10:cL:41:MET:HE1	1.87	0.57
9:aK:39:ILE:HG23	9:aK:42:PRO:HG3	1.87	0.57
1:bA:216:HIS:CE1	15:bA:1112:CL7:NA	2.73	0.57
2:bB:275:HIS:CE1	15:bB:1213:CL7:NA	2.72	0.57
4:bD:125:PRO:HG2	4:bD:130:ILE:HD11	1.85	0.57
2:cB:78:ILE:HD12	2:cB:125:TYR:CD1	2.40	0.57
7:cI:24:THR:HG23	10:cL:95:LEU:HD21	1.86	0.57
1:aA:155:ALA:HB3	1:aA:158:GLU:HG3	1.86	0.56
1:bA:304:MET:HE1	15:bA:1116:CL7:HBC2	1.87	0.56
15:cA:1119:CL7:H43C	15:cA:1133:CL7:H121	1.87	0.56
2:cB:529:VAL:O	2:cB:533:ILE:HG12	2.05	0.56
2:cB:265:THR:HB	2:cB:357:ALA:HA	1.88	0.56
1:aA:499:ARG:O	15:aA:1134:CL7:ND	2.38	0.56
2:aB:136:TYR:CZ	2:aB:140:ILE:HD11	2.39	0.56
15:aB:1204:CL7:HBA2	15:aB:1204:CL7:HBD	1.87	0.56
2:bB:193:HIS:CE1	15:bB:1211:CL7:NA	2.73	0.56
2:bB:460:TRP:CE3	2:bB:472:LEU:HD23	2.40	0.56
2:bB:658:ALA:CB	14:bB:1023:PHO:HBB2	2.36	0.56
1:cA:483:PHE:O	1:cA:487:VAL:HG23	2.05	0.56
2:bB:78:ILE:HD12	2:bB:125:TYR:CD1	2.40	0.56
1:cA:448:LEU:HB3	1:cA:542:PHE:HB2	1.87	0.56
1:aA:263:PRO:HB3	1:aA:268:ASN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:126:THR:HG21	2:aB:356:TYR:HD1	1.71	0.56
2:aB:529:VAL:O	2:aB:533:ILE:HG12	2.05	0.56
7:aI:6:LEU:HD21	11:aM:12:LEU:HD11	1.88	0.56
1:bA:155:ALA:HB3	1:bA:158:GLU:HG3	1.86	0.56
1:cA:85:PHE:HE1	15:cA:1103:CL7:H142	1.71	0.56
1:cA:210:ASN:O	1:cA:214:THR:HG23	2.05	0.56
1:bA:455:LEU:HB3	1:bA:535:MET:HE3	1.86	0.56
2:cB:74:PHE:O	2:cB:78:ILE:HG12	2.05	0.56
2:aB:308:HIS:NE2	15:aB:1219:CL7:NA	2.54	0.56
15:cB:1229:CL7:H201	15:cB:1235:CL7:H121	1.86	0.56
1:aA:216:HIS:CE1	15:aA:1112:CL7:NA	2.74	0.56
9:bK:31:ALA:HA	9:bK:34:ILE:HG22	1.88	0.56
2:cB:300:SER:HB2	2:cB:303:GLU:OE2	2.06	0.56
4:cD:136:GLN:HG3	4:cD:137:ALA:H	1.71	0.56
1:bA:403:VAL:HG11	1:bA:597:LEU:HG	1.88	0.55
1:cA:88:ILE:HG23	15:cA:1127:CL7:H52C	1.88	0.55
6:cF:52:GLU:OE2	6:cF:56:LYS:HE3	2.06	0.55
1:bA:394:HIS:NE2	15:bA:1127:CL7:ND	2.53	0.55
5:aE:32:ILE:HG22	5:aE:34:TYR:H	1.71	0.55
9:aK:73:GLY:O	9:aK:77:ILE:HG12	2.06	0.55
1:bA:408:HIS:CE1	15:bA:1128:CL7:NA	2.75	0.55
1:cA:53:HIS:HE1	15:cA:1101:CL7:ND	2.04	0.55
2:cB:412:HIS:NE2	15:cB:1227:CL7:ND	2.55	0.55
1:aA:395:MET:HE2	1:aA:607:VAL:HG11	1.88	0.55
1:cA:35:PHE:HD2	1:cA:62:GLN:HG2	1.70	0.55
15:aA:1119:CL7:H43C	15:aA:1133:CL7:H121	1.89	0.55
15:bA:1119:CL7:H8	15:bA:1119:CL7:HBC3	1.87	0.55
2:bB:387:HIS:NE2	15:bB:1226:CL7:NB	2.53	0.55
2:cB:86:PRO:HB2	2:cB:116:CYS:HB3	1.89	0.55
2:aB:658:ALA:CB	14:aB:1023:PHO:HBB2	2.36	0.55
1:cA:54:ALA:HB2	18:cA:5001:LHG:HC82	1.89	0.55
1:cA:408:HIS:CE1	15:cA:1128:CL7:NA	2.74	0.55
14:cB:1023:PHO:HED3	14:cB:1023:PHO:HBA2	1.88	0.55
15:aA:1120:CL7:HMB1	15:aA:1121:CL7:H2	1.88	0.55
1:cA:121:ILE:HG23	1:cA:122:VAL:HG22	1.89	0.55
1:cA:320:HIS:CE1	15:cA:1120:CL7:NA	2.75	0.55
4:aD:52:ASN:HB2	4:aD:56:ASN:HD21	1.72	0.55
2:bB:519:VAL:HG21	2:bB:593:TYR:HB2	1.88	0.55
6:bF:97:ILE:O	6:bF:101:ILE:HG12	2.06	0.55
2:aB:78:ILE:HD12	2:aB:125:TYR:CD1	2.41	0.55
1:aA:116:HIS:NE2	15:aA:1106:CL7:NA	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:502:LEU:HD11	15:bA:1115:CL7:OBD	2.07	0.54
1:bA:522:VAL:HG21	1:bA:629:ILE:HD13	1.89	0.54
1:cA:708:LYS:HD2	6:cF:162:VAL:HG21	1.89	0.54
15:aA:1128:CL7:H62C	18:aA:5001:LHG:H111	1.88	0.54
1:bA:515:PRO:HB3	1:bA:629:ILE:HD11	1.87	0.54
2:bB:29:HIS:CE1	15:bB:1201:CL7:NB	2.75	0.54
6:bF:66:CYS:HB3	6:bF:73:PRO:HA	1.88	0.54
15:cB:1204:CL7:HBD	15:cB:1204:CL7:HBA2	1.90	0.54
1:aA:433:HIS:CD2	15:aA:1129:CL7:NA	2.75	0.54
2:bB:277:HIS:HD1	2:bB:280:ILE:HD11	1.72	0.54
1:cA:304:MET:HE1	15:cA:1116:CL7:HBC2	1.89	0.54
1:cA:172:VAL:HG11	15:cA:1111:CL7:H142	1.90	0.54
1:cA:278:PHE:HZ	15:cA:1116:CL7:H43C	1.71	0.54
2:cB:658:ALA:CB	14:cB:1023:PHO:HBB2	2.38	0.54
1:aA:226:LYS:HD2	1:aA:253:LEU:HD22	1.89	0.54
1:bA:75:SER:HB3	1:bA:181:TYR:HB2	1.89	0.54
2:bB:339:LEU:HB3	2:bB:380:LEU:HD13	1.88	0.54
3:bC:23:THR:HG23	3:bC:25:VAL:HG23	1.90	0.54
2:bB:424:SER:HB3	2:bB:529:VAL:HG22	1.89	0.54
9:bK:21:GLY:O	9:bK:25:ILE:HG12	2.08	0.54
1:cA:32:PRO:HB2	1:cA:48:TRP:HH2	1.73	0.54
2:cB:338:ALA:O	2:cB:342:ILE:HG12	2.07	0.54
2:bB:299:HIS:HE1	15:bB:1218:CL7:NA	2.06	0.54
2:bB:342:ILE:O	2:bB:346:VAL:HG23	2.08	0.54
4:bD:30:ALA:HA	4:bD:58:LEU:O	2.08	0.54
1:aA:515:PRO:HB3	1:aA:629:ILE:HD11	1.89	0.54
2:aB:386:ALA:O	2:aB:390:ILE:HG13	2.08	0.54
15:aB:1204:CL7:HHB	15:aB:1205:CL7:HMB3	1.88	0.54
1:cA:181:TYR:HD2	1:cA:182:HIS:CD2	2.26	0.54
1:cA:722:ILE:HG12	2:cB:568:CYS:SG	2.48	0.54
2:cB:29:HIS:CE1	15:cB:1201:CL7:NB	2.76	0.54
2:aB:659:THR:HA	14:aB:1023:PHO:HAB	1.90	0.54
1:bA:142:SER:HB3	15:bA:1126:CL7:HAA1	1.90	0.54
2:bB:237:PRO:HB3	2:bB:256:THR:HG21	1.89	0.54
4:cD:19:LEU:H	10:cL:14:VAL:HA	1.72	0.54
1:cA:403:VAL:HG11	1:cA:597:LEU:HG	1.90	0.53
4:cD:7:GLY:HA2	4:cD:55:GLU:OE2	2.08	0.53
1:aA:278:PHE:HZ	15:aA:1116:CL7:H43C	1.73	0.53
3:aC:23:THR:HG23	3:aC:25:VAL:HG23	1.90	0.53
2:bB:338:ALA:O	2:bB:342:ILE:HG12	2.08	0.53
2:cB:299:HIS:HE1	15:cB:1218:CL7:NA	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:bF:125:ILE:HG13	6:bF:126:ILE:HG12	1.91	0.53
3:cC:23:THR:HG23	3:cC:25:VAL:HG23	1.90	0.53
1:bA:490:LEU:O	1:bA:494:VAL:HB	2.08	0.53
2:cB:308:HIS:NE2	15:cB:1219:CL7:NC	2.57	0.53
2:cB:519:VAL:HG21	2:cB:593:TYR:HB2	1.90	0.53
1:bA:426:VAL:HG23	15:bA:1122:CL7:HBC2	1.90	0.53
1:cA:282:LEU:HB2	1:cA:516:MET:HE1	1.89	0.53
1:cA:297:HIS:HB2	15:cA:1116:CL7:CHB	2.39	0.53
3:cC:44:ARG:NH1	4:cD:99:LYS:HZ1	2.06	0.53
1:bA:370:HIS:NE2	15:bA:1125:CL7:NC	2.57	0.53
8:cJ:34:GLU:OE1	15:cJ:1302:CL7:NA	2.42	0.53
2:aB:371:THR:HG22	15:aB:1224:CL7:HAB	1.89	0.53
2:aB:387:HIS:NE2	15:aB:1226:CL7:NB	2.57	0.53
9:aK:19:THR:O	9:aK:23:VAL:HG22	2.09	0.53
1:cA:92:ILE:HG21	1:cA:162:THR:HG23	1.89	0.53
1:cA:217:LEU:HA	1:cA:221:SER:HB2	1.90	0.53
1:cA:468:PRO:HA	1:cA:471:MET:HG3	1.91	0.53
1:bA:488:GLN:HA	1:bA:511:TRP:CE3	2.42	0.53
4:bD:19:LEU:H	10:bL:14:VAL:HA	1.74	0.53
1:cA:75:SER:HB2	1:cA:181:TYR:HB2	1.91	0.53
1:cA:414:VAL:HG11	1:cA:572:PHE:N	2.23	0.53
2:cB:385:TYR:CG	2:cB:534:CYS:HB3	2.43	0.53
15:aB:1230:CL7:O2D	15:aB:1230:CL7:H2A	2.08	0.53
1:bA:172:VAL:HG11	15:bA:1111:CL7:H142	1.91	0.53
2:bB:659:THR:HA	14:bB:1023:PHO:HAB	1.91	0.53
2:cB:446:THR:HB	2:cB:449:LYS:HG3	1.90	0.53
1:aA:85:PHE:HE1	15:aA:1103:CL7:H142	1.74	0.52
1:bA:94:HIS:CE1	15:bA:1105:CL7:NA	2.77	0.52
1:cA:153:MET:HB3	1:cA:159:LEU:HD11	1.90	0.52
1:cA:462:MET:HB2	1:cA:471:MET:HG2	1.91	0.52
2:aB:528:HIS:NE2	15:aB:1236:CL7:NA	2.57	0.52
1:bA:87:TRP:HH2	15:bA:1127:CL7:HBA1	1.73	0.52
1:bA:708:LYS:HD2	6:bF:162:VAL:HG21	1.91	0.52
2:bB:385:TYR:CG	2:bB:534:CYS:HB3	2.45	0.52
4:cD:11:LEU:HB2	4:cD:50:VAL:HB	1.92	0.52
4:cD:30:ALA:HA	4:cD:58:LEU:O	2.10	0.52
15:aB:1204:CL7:HAA2	15:aB:1206:CL7:HED1	1.92	0.52
1:bA:433:HIS:CD2	15:bA:1129:CL7:NA	2.77	0.52
1:cA:441:LEU:HD13	1:cA:549:LEU:HA	1.90	0.52
15:aA:1119:CL7:H8	15:aA:1119:CL7:HBC3	1.90	0.52
6:aF:97:ILE:O	6:aF:101:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:704:TRP:HE1	6:bF:164:VAL:HG22	1.74	0.52
15:cA:1128:CL7:H62C	18:cA:5001:LHG:H111	1.91	0.52
15:cB:1238:CL7:H201	10:cL:54:HIS:HD2	1.74	0.52
2:aB:28:VAL:HG13	2:aB:29:HIS:CD2	2.44	0.52
2:aB:658:ALA:HB1	14:aB:1023:PHO:HBB2	1.91	0.52
4:aD:59:TYR:HE1	4:aD:87:VAL:HG21	1.74	0.52
1:bA:599:TRP:HE1	14:bB:1023:PHO:C1D	2.23	0.52
2:bB:398:PRO:HD2	4:bD:126:ASN:HD22	1.75	0.52
1:cA:371:MET:HE1	15:cA:1127:CL7:CAD	2.40	0.52
15:cA:1120:CL7:HMB1	15:cA:1121:CL7:H2	1.91	0.52
6:cF:111:ALA:HB1	6:cF:131:LEU:HD11	1.90	0.52
2:aB:277:HIS:HA	2:aB:280:ILE:HG12	1.91	0.52
2:bB:119:GLY:HA3	2:bB:365:THR:HG21	1.91	0.52
2:bB:502:VAL:HA	2:bB:508:PRO:HD2	1.91	0.52
2:aB:385:TYR:CG	2:aB:534:CYS:HB3	2.43	0.52
15:aL:1501:CL7:H43C	15:bI:1601:CL7:H42C	1.91	0.52
1:cA:44:GLN:NE2	5:cE:43:CYS:HB3	2.25	0.52
1:cA:298:HIS:HA	1:cA:301:LEU:HD12	1.91	0.52
2:cB:222:LEU:HB3	2:cB:226:PHE:CE1	2.45	0.52
2:cB:679:VAL:HG13	2:cB:693:TRP:CH2	2.45	0.52
1:aA:180:HIS:CE1	15:aA:1108:CL7:NA	2.77	0.52
4:aD:7:GLY:HA3	4:aD:57:LEU:HD22	1.91	0.52
1:cA:393:HIS:HB2	15:cA:1126:CL7:C1B	2.40	0.52
9:cK:24:MET:HE1	9:cK:70:HIS:HA	1.91	0.52
1:aA:371:MET:HE1	15:aA:1127:CL7:CAD	2.40	0.52
4:aD:121:ILE:HD12	4:aD:121:ILE:H	1.75	0.52
15:bA:1128:CL7:H193	15:bA:1140:CL7:H3A	1.91	0.52
2:bB:38:THR:HA	4:bD:132:TYR:CE1	2.45	0.52
1:cA:490:LEU:O	1:cA:494:VAL:HB	2.10	0.52
6:cF:97:ILE:O	6:cF:101:ILE:HG12	2.09	0.52
2:aB:311:PRO:HG2	2:aB:312:TRP:CE3	2.45	0.52
2:bB:300:SER:HB2	2:bB:303:GLU:HG2	1.91	0.52
1:cA:382:THR:HG21	1:cA:518:VAL:HB	1.91	0.52
4:aD:30:ALA:HA	4:aD:58:LEU:O	2.10	0.51
2:cB:439:ASP:OD1	2:cB:615:TYR:HB2	2.10	0.51
1:aA:418:ASP:HB3	1:aA:421:MET:HB3	1.92	0.51
5:bE:19:ARG:NH2	6:bF:164:VAL:HB	2.25	0.51
1:cA:412:PHE:CD2	1:cA:413:MET:HE2	2.44	0.51
2:cB:309:ARG:HG2	2:cB:316:THR:HG22	1.92	0.51
2:aB:31:PHE:HA	2:aB:34:HIS:CD2	2.46	0.51
1:bA:121:ILE:HG23	1:bA:122:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:210:ASN:O	1:bA:214:THR:HG23	2.11	0.51
1:bA:278:PHE:HZ	15:bA:1116:CL7:H43C	1.74	0.51
1:bA:297:HIS:HB2	15:bA:1116:CL7:CHB	2.41	0.51
5:bE:32:ILE:HG22	5:bE:34:TYR:H	1.75	0.51
15:bL:1501:CL7:H43C	15:cI:1601:CL7:H42C	1.92	0.51
1:aA:376:PRO:HB2	15:aA:1117:CL7:HAA1	1.93	0.51
3:bC:14:CYS:SG	3:bC:16:GLN:HG2	2.51	0.51
15:bI:1601:CL7:CGA	15:bI:1601:CL7:H3A	2.40	0.51
15:aA:1136:CL7:H91C	15:aL:1502:CL7:H191	1.92	0.51
2:aB:191:THR:HG21	2:aB:278:LEU:HB2	1.91	0.51
1:bA:450:PHE:O	1:bA:454:ASP:HB2	2.10	0.51
2:bB:289:HIS:HE1	15:bB:1217:CL7:NC	2.07	0.51
7:bI:9:ILE:O	7:bI:13:LEU:HD23	2.10	0.51
1:cA:182:HIS:NE2	15:cA:1109:CL7:ND	2.58	0.51
1:bA:414:VAL:HG11	1:bA:572:PHE:N	2.26	0.51
15:bA:1119:CL7:H43C	15:bA:1133:CL7:H121	1.93	0.51
2:bB:658:ALA:HB1	14:bB:1023:PHO:HBB2	1.92	0.51
15:cA:1139:CL7:HBA2	15:cA:1139:CL7:HED3	1.93	0.51
2:cB:53:HIS:HD1	15:cB:1202:CL7:HHB	1.75	0.51
1:bA:461:GLU:HG3	15:bA:1132:CL7:HAC2	1.91	0.51
2:cB:480:GLN:HG3	12:cX:30:GLN:HE22	1.76	0.51
10:cL:48:LEU:O	10:cL:52:MET:HG3	2.10	0.51
1:aA:88:ILE:HG23	15:aA:1127:CL7:H52C	1.91	0.51
15:bA:1120:CL7:HMB3	15:bA:1121:CL7:H2	1.92	0.51
2:bB:700:LEU:HB3	2:bB:704:GLN:HG2	1.92	0.51
2:bB:86:PRO:HB2	2:bB:116:CYS:HB3	1.91	0.51
2:bB:419:HIS:HD2	15:bB:1227:CL7:HMB2	1.76	0.51
1:cA:94:HIS:CE1	15:cA:1105:CL7:NA	2.79	0.51
2:aB:276:HIS:HB2	15:aB:1214:CL7:C1B	2.41	0.51
2:bB:175:MET:HE3	15:bB:1221:CL7:C2D	2.40	0.51
2:bB:419:HIS:HD2	15:bB:1227:CL7:CMB	2.23	0.51
1:bA:732:HIS:NE2	15:bA:1140:CL7:NA	2.59	0.50
2:bB:289:HIS:NE2	15:bB:1217:CL7:NA	2.59	0.50
2:bB:449:LYS:HD3	6:bF:57:ARG:HD2	1.94	0.50
2:bB:683:GLN:HG2	2:bB:692:MET:HE1	1.93	0.50
15:cB:1218:CL7:H2A	15:cB:1218:CL7:HED2	1.93	0.50
1:aA:408:HIS:HE1	15:aA:1128:CL7:NA	2.09	0.50
2:aB:576:PHE:CZ	15:aB:1226:CL7:HAC2	2.47	0.50
2:aB:683:GLN:HG2	2:aB:692:MET:HE1	1.93	0.50
2:bB:222:LEU:HB3	2:bB:226:PHE:CE2	2.46	0.50
15:cA:1123:CL7:C1C	21:cA:5010:HOH:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:382:THR:HG21	1:aA:518:VAL:HB	1.92	0.50
1:aA:599:TRP:HE1	14:aB:1023:PHO:C1D	2.25	0.50
2:aB:176:ASN:ND2	2:aB:291:TYR:HB2	2.27	0.50
11:aM:10:ILE:HA	11:aM:13:VAL:HG22	1.93	0.50
2:cB:193:HIS:CD2	2:cB:197:VAL:HB	2.46	0.50
2:cB:387:HIS:NE2	15:cB:1226:CL7:NB	2.60	0.50
1:aA:142:SER:HB3	15:aA:1126:CL7:HAA1	1.92	0.50
1:aA:458:HIS:O	1:aA:459:ASN:C	2.54	0.50
2:aB:69:ALA:HB2	2:aB:135:LEU:HB2	1.93	0.50
4:aD:42:GLU:H	4:aD:73:GLN:NE2	2.09	0.50
1:bA:301:LEU:HD23	1:bA:304:MET:HE2	1.92	0.50
1:cA:599:TRP:HE1	14:cB:1023:PHO:C1D	2.25	0.50
1:aA:433:HIS:NE2	15:aA:1129:CL7:ND	2.60	0.50
15:aI:1601:CL7:H42C	15:cL:1501:CL7:H43C	1.93	0.50
1:bA:298:HIS:HA	1:bA:301:LEU:HD12	1.93	0.50
2:bB:235:GLN:O	2:bB:253:ALA:HB2	2.12	0.50
1:cA:87:TRP:HH2	15:cA:1127:CL7:HBA1	1.77	0.50
1:cA:142:SER:HB3	15:cA:1126:CL7:HAA1	1.92	0.50
1:cA:180:HIS:HE1	15:cA:1108:CL7:NB	2.09	0.50
11:cM:6:LEU:O	11:cM:10:ILE:HG12	2.11	0.50
1:aA:193:ASN:HB3	15:aA:1111:CL7:HBC1	1.94	0.50
2:aB:516:ASP:HA	2:aB:519:VAL:HG12	1.94	0.50
8:aJ:34:GLU:OE1	15:aJ:1302:CL7:NA	2.45	0.50
1:bA:376:PRO:HD2	1:bA:380:LEU:HD23	1.94	0.50
14:bB:1023:PHO:HBA2	14:bB:1023:PHO:HED3	1.93	0.50
4:bD:10:PRO:HG2	4:bD:58:LEU:HD13	1.93	0.50
2:aB:716:GLY:O	2:aB:720:THR:HG22	2.12	0.50
10:aL:6:VAL:HA	10:aL:18:ALA:O	2.11	0.50
1:bA:714:ALA:HB2	6:bF:113:ARG:HH12	1.77	0.50
2:bB:446:THR:HB	2:bB:449:LYS:HG3	1.94	0.50
1:bA:299:LEU:O	1:bA:303:VAL:HG22	2.12	0.50
2:bB:328:LEU:HD21	15:bB:1202:CL7:H192	1.94	0.50
2:bB:676:GLU:HG2	3:bC:81:TYR:HE2	1.77	0.50
1:cA:36:ASN:HB3	1:cA:39:LEU:HB2	1.93	0.50
2:cB:280:ILE:HA	2:cB:283:LEU:HG	1.93	0.50
2:cB:683:GLN:HG2	2:cB:692:MET:HE1	1.93	0.50
1:aA:218:ILE:HD11	1:aA:295:ALA:HB1	1.94	0.50
1:aA:454:ASP:HB3	15:aA:1132:CL7:HHC	1.92	0.50
1:bA:310:HIS:NE2	15:bA:1118:CL7:NA	2.60	0.50
15:bA:1118:CL7:H3A	9:bK:63:LEU:HD11	1.93	0.50
2:bB:569:ASP:HA	2:bB:574:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:311:PRO:HG2	2:cB:312:TRP:CE3	2.47	0.50
15:cB:1230:CL7:CED	15:cB:1230:CL7:H2A	2.41	0.50
2:aB:519:VAL:HG21	2:aB:593:TYR:HB2	1.94	0.49
1:bA:193:ASN:HB3	15:bA:1111:CL7:HBC1	1.94	0.49
2:bB:53:HIS:HD1	15:bB:1202:CL7:HHB	1.77	0.49
2:bB:439:ASP:OD1	2:bB:615:TYR:HB2	2.11	0.49
1:cA:660:ILE:HD12	2:cB:621:ARG:HG3	1.94	0.49
2:aB:439:ASP:OD1	2:aB:615:TYR:HB2	2.12	0.49
1:bA:180:HIS:CE1	15:bA:1108:CL7:NA	2.79	0.49
1:bA:488:GLN:HE22	1:bA:529:LEU:HG	1.77	0.49
15:bB:1223:CL7:H171	15:bB:1227:CL7:HAC1	1.95	0.49
2:cB:576:PHE:HZ	19:cB:5002:LMG:H362	1.78	0.49
1:aA:44:GLN:NE2	5:aE:43:CYS:HB3	2.28	0.49
1:aA:320:HIS:HE1	15:aA:1120:CL7:NA	2.09	0.49
2:aB:308:HIS:NE2	15:aB:1219:CL7:ND	2.60	0.49
2:bB:576:PHE:CZ	15:bB:1226:CL7:HAC2	2.47	0.49
10:cL:43:ALA:HB1	10:cL:126:ILE:HG13	1.93	0.49
2:aB:409:LEU:HA	2:aB:412:HIS:CE1	2.47	0.49
9:bK:19:THR:O	9:bK:23:VAL:HG22	2.12	0.49
1:aA:87:TRP:HH2	15:aA:1127:CL7:HBA1	1.77	0.49
1:aA:318:ILE:HG22	9:aK:39:ILE:HD11	1.93	0.49
2:aB:387:HIS:HE1	15:aB:1226:CL7:NA	2.09	0.49
15:bA:1104:CL7:H92C	18:bA:5001:LHG:H341	1.94	0.49
1:aA:426:VAL:HG23	15:aA:1122:CL7:HBC2	1.94	0.49
15:aA:1138:CL7:HMB2	15:aB:1229:CL7:H41C	1.93	0.49
2:aB:29:HIS:HE1	15:aB:1201:CL7:C4B	2.24	0.49
2:aB:30:ASP:O	2:aB:33:THR:HG22	2.12	0.49
1:bA:218:ILE:HD11	1:bA:295:ALA:HB1	1.94	0.49
1:bA:318:ILE:HG22	9:bK:39:ILE:HD11	1.95	0.49
1:cA:223:PRO:O	1:cA:227:MET:HG2	2.13	0.49
15:cA:1136:CL7:H91C	15:cL:1502:CL7:H191	1.94	0.49
9:cK:21:GLY:O	9:cK:25:ILE:HG12	2.12	0.49
1:aA:66:LEU:HD23	1:aA:188:LEU:HD11	1.95	0.49
1:aA:244:LEU:HD23	15:aA:1114:CL7:HBC2	1.93	0.49
15:bB:1237:CL7:HMC1	15:bB:1238:CL7:H2	1.93	0.49
1:cA:578:GLY:HA2	2:cB:561:GLY:HA2	1.95	0.49
1:cA:598:PHE:CE1	1:cA:730:LEU:HD13	2.47	0.49
15:cB:1237:CL7:HMC1	15:cB:1238:CL7:H2	1.93	0.49
1:aA:54:ALA:HB2	18:aA:5001:LHG:HC82	1.95	0.49
2:aB:631:LEU:HD13	2:aB:727:GLY:HA3	1.93	0.49
1:cA:301:LEU:HD23	1:cA:304:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:53:HIS:CE1	15:cB:1202:CL7:HMA1	2.48	0.49
1:aA:223:PRO:O	1:aA:227:MET:HG2	2.12	0.49
1:aA:263:PRO:HA	1:aA:266:THR:HG22	1.94	0.49
2:aB:169:ARG:NH1	2:aB:325:ASN:HD22	2.11	0.49
15:aB:1203:CL7:H162	15:aB:1203:CL7:H122	1.52	0.49
15:aI:1601:CL7:C2	15:aI:1601:CL7:H3A	2.42	0.49
1:bA:50:TRP:CG	1:bA:724:GLN:HE22	2.31	0.49
1:bA:53:HIS:CE1	15:bA:1101:CL7:ND	2.79	0.49
1:bA:296:HIS:ND1	15:bA:1116:CL7:HAB	2.28	0.49
6:bF:103:ASN:ND2	6:bF:142:TRP:HB2	2.27	0.49
1:cA:43:PRO:HB3	1:cA:48:TRP:CE3	2.47	0.49
1:cA:426:VAL:HG23	15:cA:1122:CL7:HBC2	1.94	0.49
1:cA:459:ASN:HD21	1:cA:535:MET:HE1	1.77	0.49
2:cB:195:ILE:HA	2:cB:199:ILE:HD12	1.95	0.49
2:aB:419:HIS:NE2	15:aB:1228:CL7:NB	2.60	0.49
2:aB:676:GLU:HG2	3:aC:81:TYR:HE2	1.78	0.49
2:bB:156:HIS:CE1	15:bB:1208:CL7:NA	2.81	0.49
3:bC:62:PHE:HD2	4:bD:121:ILE:HG21	1.78	0.49
1:cA:155:ALA:HB3	1:cA:158:GLU:HG3	1.93	0.49
1:bA:116:HIS:CE1	15:bA:1106:CL7:NA	2.81	0.48
1:bA:674:PHE:CZ	1:bA:678:HIS:HE1	2.31	0.48
2:bB:427:LEU:HD11	15:bB:1235:CL7:HMB2	1.95	0.48
1:cA:597:LEU:HD23	1:cA:600:MET:HE3	1.95	0.48
15:cA:1119:CL7:HBC3	15:cA:1119:CL7:H8	1.94	0.48
6:aF:111:ALA:HB1	6:aF:131:LEU:HD11	1.95	0.48
12:aX:25:ILE:O	12:aX:29:LEU:HG	2.13	0.48
1:bA:311:MET:HB2	15:bA:1120:CL7:HAC2	1.94	0.48
10:bL:71:THR:HG22	10:bL:73:MET:H	1.78	0.48
1:cA:458:HIS:O	1:cA:459:ASN:C	2.56	0.48
2:cB:167:TRP:CZ2	15:cB:1208:CL7:H3A	2.48	0.48
2:cB:569:ASP:HA	2:cB:574:ASP:OD1	2.14	0.48
15:aA:1022:CL7:H151	15:aB:1207:CL7:HBC3	1.95	0.48
7:aI:24:THR:HG23	10:aL:95:LEU:HD21	1.95	0.48
1:bA:43:PRO:HG3	6:bF:125:ILE:HD13	1.96	0.48
1:bA:382:THR:HG21	1:bA:518:VAL:HB	1.95	0.48
2:bB:308:HIS:NE2	15:bB:1219:CL7:ND	2.61	0.48
2:bB:419:HIS:HE1	15:bB:1228:CL7:C1B	2.26	0.48
15:bB:1216:CL7:HMB2	15:bB:1221:CL7:HMA3	1.94	0.48
1:aA:275:PHE:CE2	15:aA:1113:CL7:HAC2	2.48	0.48
2:aB:408:ARG:O	2:aB:411:GLU:HG2	2.13	0.48
7:aI:13:LEU:HD11	15:cL:1503:CL7:H13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aI:1601:CL7:H3A	15:aI:1601:CL7:CGA	2.43	0.48
1:bA:35:PHE:HD2	1:bA:62:GLN:HG2	1.77	0.48
15:bA:1102:CL7:H43C	15:bA:1109:CL7:H122	1.93	0.48
2:bB:28:VAL:HG21	15:bB:1201:CL7:C3D	2.43	0.48
2:bB:720:THR:HG23	15:bB:1021:CL7:O1D	2.14	0.48
15:cA:1118:CL7:H3A	9:cK:63:LEU:HD11	1.94	0.48
1:aA:254:TYR:CD1	1:aA:275:PHE:HB3	2.48	0.48
2:aB:387:HIS:CE1	15:aB:1226:CL7:NA	2.82	0.48
2:aB:413:LYS:HB2	2:aB:539:LEU:HD13	1.96	0.48
6:aF:52:GLU:HB2	6:aF:56:LYS:NZ	2.28	0.48
2:bB:573:TRP:O	2:bB:576:PHE:HB3	2.13	0.48
3:bC:72:GLU:OE1	3:bC:77:MET:HE2	2.14	0.48
1:cA:374:MET:CE	15:cA:1116:CL7:HBD	2.43	0.48
2:cB:53:HIS:HE1	15:cB:1203:CL7:NB	2.12	0.48
2:cB:456:ILE:HD11	6:cF:78:GLY:H	1.78	0.48
1:aA:43:PRO:HB3	1:aA:48:TRP:CE3	2.48	0.48
1:aA:240:PRO:HA	1:aA:243:TYR:CE2	2.48	0.48
2:aB:120:VAL:HG23	2:aB:123:TRP:HE3	1.78	0.48
2:bB:275:HIS:HB3	15:bB:1214:CL7:HMB2	1.95	0.48
2:cB:547:MET:HE1	2:cB:560:ASP:HB2	1.94	0.48
15:aB:1238:CL7:H2	15:aB:1237:CL7:HMC1	1.94	0.48
2:bB:277:HIS:HA	2:bB:280:ILE:HG12	1.94	0.48
2:bB:386:ALA:HB2	2:bB:576:PHE:CE1	2.49	0.48
15:bB:1205:CL7:H62C	15:bB:1205:CL7:H102	1.53	0.48
1:cA:374:MET:HE1	15:cA:1116:CL7:HBD	1.96	0.48
2:cB:386:ALA:O	2:cB:390:ILE:HG13	2.14	0.48
1:aA:254:TYR:CE1	1:aA:275:PHE:HB3	2.48	0.48
15:aA:1137:CL7:H3A	15:aA:1137:CL7:HBA2	1.62	0.48
1:bA:320:HIS:HE1	15:bA:1120:CL7:NA	2.11	0.48
15:bA:1103:CL7:H143	15:bA:1103:CL7:H161	1.68	0.48
2:bB:407:SER:O	2:bB:411:GLU:OE1	2.32	0.48
2:bB:694:LYS:HD2	7:bI:31:GLU:OE2	2.14	0.48
4:bD:59:TYR:HE2	4:bD:87:VAL:HG21	1.79	0.48
15:cB:1238:CL7:H41C	15:cB:1238:CL7:H62C	1.62	0.48
10:cL:101:VAL:HG11	10:cL:123:TRP:CD1	2.49	0.48
1:aA:94:HIS:CE1	15:aA:1105:CL7:NA	2.82	0.48
2:aB:167:TRP:CZ2	15:aB:1208:CL7:H3A	2.49	0.48
2:aB:265:THR:HB	2:aB:357:ALA:HA	1.96	0.48
1:bA:263:PRO:HA	1:bA:266:THR:HG22	1.94	0.48
1:bA:376:PRO:HB2	15:bA:1117:CL7:HAA1	1.94	0.48
1:bA:567:LYS:HA	1:bA:570:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:cA:5001:LHG:H281	18:cA:5001:LHG:H251	1.77	0.48
1:aA:89:SER:HB2	1:aA:166:ALA:HB3	1.95	0.48
1:aA:368:ALA:HB2	1:aA:394:HIS:HB2	1.96	0.48
1:aA:408:HIS:CE1	15:aA:1128:CL7:NA	2.80	0.48
15:aA:1138:CL7:H142	16:aA:2001:PQN:H28	1.96	0.48
4:aD:7:GLY:HA2	4:aD:55:GLU:OE2	2.13	0.48
2:bB:631:LEU:HD13	2:bB:727:GLY:HA3	1.95	0.48
15:bB:1237:CL7:H41C	15:bB:1237:CL7:H61C	1.59	0.48
15:cB:1222:CL7:HBA2	15:cB:1222:CL7:H3A	1.44	0.48
2:aB:193:HIS:HE1	15:aB:1211:CL7:NA	2.09	0.47
2:aB:310:ASP:HB3	2:aB:314:GLY:H	1.79	0.47
4:aD:42:GLU:H	4:aD:73:GLN:HE22	1.62	0.47
2:bB:311:PRO:HG2	2:bB:312:TRP:CE3	2.49	0.47
15:bB:1220:CL7:H3A	15:bB:1220:CL7:HBA1	1.35	0.47
2:cB:308:HIS:HE1	15:cB:1219:CL7:ND	2.12	0.47
15:cB:1210:CL7:H3A	15:cB:1210:CL7:HBA2	1.35	0.47
4:cD:24:GLU:O	4:cD:89:PRO:HB3	2.14	0.47
1:aA:187:LYS:HG3	1:aA:190:TRP:H	1.79	0.47
1:aA:393:HIS:HB2	15:aA:1126:CL7:C1B	2.44	0.47
1:aA:674:PHE:CZ	1:aA:678:HIS:HE1	2.33	0.47
1:bA:320:HIS:HB3	1:bA:325:ILE:HD11	1.95	0.47
1:bA:720:MET:HE1	1:bA:728:VAL:HG21	1.96	0.47
15:cA:1110:CL7:HBA1	15:cA:1110:CL7:H3A	1.44	0.47
2:aB:126:THR:HG21	2:aB:356:TYR:CD1	2.49	0.47
2:bB:38:THR:HA	4:bD:132:TYR:HE1	1.79	0.47
6:bF:31:CYS:HA	6:bF:34:SER:HB3	1.96	0.47
15:cA:1126:CL7:HBA1	15:cA:1126:CL7:H3A	1.56	0.47
2:cB:28:VAL:HG21	15:cB:1201:CL7:C3D	2.44	0.47
2:aB:155:LEU:HD21	15:aB:1208:CL7:HBC3	1.96	0.47
2:aB:475:LEU:HD21	12:aX:27:ILE:HD11	1.95	0.47
15:aB:1209:CL7:HBA1	15:aB:1209:CL7:H3A	1.50	0.47
15:bB:1212:CL7:H2A	15:bB:1212:CL7:HED2	1.97	0.47
1:cA:722:ILE:HD11	2:cB:566:GLY:HA3	1.97	0.47
15:cA:1121:CL7:HBA1	15:cA:1121:CL7:H3A	1.54	0.47
2:cB:69:ALA:HB2	2:cB:135:LEU:HB2	1.95	0.47
2:cB:424:SER:HB3	2:cB:529:VAL:HG22	1.97	0.47
2:aB:449:LYS:NZ	6:aF:47:THR:HG21	2.29	0.47
15:bB:1226:CL7:H143	15:bB:1226:CL7:H161	1.76	0.47
4:bD:24:GLU:O	4:bD:89:PRO:HB3	2.15	0.47
2:cB:324:TYR:CE2	2:cB:331:GLN:HG2	2.49	0.47
3:cC:6:LYS:HE2	4:cD:138:TYR:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:cD:80:MET:HE3	4:cD:103:PHE:HE2	1.80	0.47
15:aA:1104:CL7:H92C	18:aA:5001:LHG:H341	1.97	0.47
2:aB:420:LEU:HD21	2:aB:531:VAL:HG12	1.96	0.47
1:bA:53:HIS:NE2	15:bA:1101:CL7:NB	2.62	0.47
1:bA:197:THR:OG1	15:bA:1111:CL7:HBC2	2.14	0.47
15:bA:1127:CL7:H41C	15:bA:1127:CL7:H62C	1.66	0.47
15:cI:1601:CL7:C2	15:cI:1601:CL7:H3A	2.44	0.47
1:aA:589:GLY:O	1:aA:593:VAL:HG23	2.14	0.47
7:aI:5:ILE:HG13	7:aI:9:ILE:HG12	1.97	0.47
9:aK:31:ALA:HA	9:aK:34:ILE:HG22	1.96	0.47
10:aL:144:LEU:HD21	15:bB:1207:CL7:H161	1.97	0.47
1:bA:735:LEU:HD22	15:bA:1140:CL7:HMA1	1.96	0.47
15:bA:1103:CL7:H3A	15:bA:1103:CL7:HBA2	1.40	0.47
2:bB:281:ALA:O	2:bB:285:ILE:HG13	2.14	0.47
1:cA:77:HIS:CD2	15:cA:1103:CL7:NA	2.83	0.47
1:cA:433:HIS:CD2	15:cA:1129:CL7:NA	2.82	0.47
1:cA:454:ASP:HB3	15:cA:1132:CL7:HHC	1.96	0.47
15:cA:1102:CL7:H3A	15:cA:1102:CL7:HBA2	1.75	0.47
15:cA:1109:CL7:H143	15:cA:1109:CL7:H112	1.64	0.47
15:cA:1130:CL7:OBD	10:cL:19:THR:HG21	2.15	0.47
2:cB:22:TRP:CG	2:cB:704:GLN:HE22	2.33	0.47
2:cB:167:TRP:CH2	15:cB:1208:CL7:HHB	2.50	0.47
2:aB:339:LEU:O	2:aB:343:THR:HG22	2.15	0.47
15:aJ:1302:CL7:H3A	15:aJ:1302:CL7:HBA2	1.62	0.47
10:aL:33:ASN:HB3	15:aL:1501:CL7:HAC1	1.97	0.47
10:aL:97:SER:O	10:aL:120:LYS:HG2	2.15	0.47
15:bB:1210:CL7:H3A	15:bB:1210:CL7:HBA2	1.40	0.47
15:cA:1104:CL7:H92C	18:cA:5001:LHG:H341	1.96	0.47
6:cF:66:CYS:HB3	6:cF:73:PRO:HA	1.97	0.47
9:cK:24:MET:HE2	9:cK:70:HIS:HD1	1.80	0.47
2:aB:502:VAL:HA	2:aB:508:PRO:HD2	1.97	0.47
10:aL:101:VAL:HG11	10:aL:123:TRP:CD1	2.50	0.47
1:bA:116:HIS:HB3	1:bA:138:ILE:HB	1.97	0.47
1:bA:240:PRO:HA	1:bA:243:TYR:CE2	2.50	0.47
15:bA:1138:CL7:H141	15:bA:1138:CL7:H162	1.68	0.47
1:cA:497:THR:HG23	1:cA:499:ARG:H	1.80	0.47
2:cB:465:HIS:HE1	15:cB:1231:CL7:NB	2.13	0.47
2:cB:516:ASP:HA	2:cB:519:VAL:HG12	1.97	0.47
4:cD:85:TYR:HA	4:cD:94:THR:O	2.15	0.47
1:aA:206:LEU:HB3	1:aA:305:TYR:CD2	2.50	0.47
1:aA:291:MET:O	1:aA:294:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aA:1118:CL7:H3A	9:aK:63:LEU:HD11	1.96	0.47
2:aB:372:HIS:CE1	15:aB:1224:CL7:ND	2.83	0.47
4:aD:43:MET:HE1	4:aD:58:LEU:HD11	1.95	0.47
1:bA:720:MET:HG2	16:bA:2001:PQN:O4	2.14	0.47
1:bA:742:TRP:HD1	15:bA:1126:CL7:HMB2	1.81	0.47
15:bL:1501:CL7:HBA1	15:bL:1501:CL7:H3A	1.38	0.47
1:cA:43:PRO:HG3	6:cF:125:ILE:HD13	1.97	0.47
1:aA:316:TRP:CD1	15:aA:1118:CL7:HBD	2.49	0.46
15:aA:1126:CL7:HBA1	15:aA:1126:CL7:H3A	1.57	0.46
2:aB:48:ALA:HB3	11:aM:29:LEU:HD21	1.97	0.46
2:aB:53:HIS:CE1	15:aB:1202:CL7:HMA1	2.50	0.46
2:aB:720:THR:HG23	15:aB:1021:CL7:O1D	2.15	0.46
9:cK:64:GLY:HA2	9:cK:67:VAL:HG12	1.96	0.46
15:aB:1205:CL7:O1A	15:aB:1224:CL7:HBD	2.15	0.46
9:aK:64:GLY:HA2	9:aK:67:VAL:HG12	1.98	0.46
1:bA:458:HIS:CE1	15:bA:1132:CL7:NA	2.83	0.46
2:bB:716:GLY:O	2:bB:720:THR:HG22	2.16	0.46
6:bF:122:MET:HE3	6:bF:126:ILE:HG13	1.97	0.46
1:cA:53:HIS:HE1	15:cA:1101:CL7:C4D	2.29	0.46
15:cA:1130:CL7:H2	15:cL:1502:CL7:H43C	1.98	0.46
10:cL:33:ASN:HB3	15:cL:1501:CL7:HAC1	1.96	0.46
2:aB:182:LEU:HD13	15:aB:1210:CL7:HHB	1.97	0.46
15:aI:1601:CL7:H3A	15:aI:1601:CL7:H2	1.96	0.46
15:bB:1230:CL7:H2A	15:bB:1230:CL7:O2D	2.15	0.46
15:cA:1138:CL7:H162	15:cA:1138:CL7:H141	1.75	0.46
2:cB:167:TRP:CZ2	15:cB:1208:CL7:HHB	2.50	0.46
2:cB:328:LEU:HD21	15:cB:1202:CL7:H192	1.98	0.46
12:cX:25:ILE:O	12:cX:29:LEU:HG	2.15	0.46
4:aD:75:ARG:NH1	4:aD:80:MET:HE1	2.31	0.46
15:bA:1123:CL7:HBA2	15:bA:1123:CL7:H11C	1.66	0.46
15:bB:1230:CL7:H2A	15:bB:1230:CL7:CED	2.45	0.46
15:cA:1127:CL7:H142	15:cA:1127:CL7:H111	1.69	0.46
1:aA:432:ARG:HG2	4:aD:15:SER:HB3	1.97	0.46
15:aA:1130:CL7:H2	15:aL:1502:CL7:H43C	1.97	0.46
15:aB:1218:CL7:H2A	15:aB:1218:CL7:HED2	1.98	0.46
1:cA:142:SER:HA	15:cA:1126:CL7:HMA2	1.98	0.46
1:cA:240:PRO:HA	1:cA:243:TYR:CE2	2.50	0.46
15:cA:1111:CL7:H61C	15:cA:1111:CL7:H2	1.73	0.46
2:cB:40:GLU:OE2	2:cB:165:LEU:HB2	2.16	0.46
15:cB:1213:CL7:HBA1	15:cB:1213:CL7:H3A	1.45	0.46
9:cK:19:THR:O	9:cK:23:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:91:MET:SD	15:aA:1106:CL7:HAA1	2.56	0.46
1:aA:300:ALA:O	1:aA:304:MET:HG3	2.16	0.46
1:aA:365:ILE:HG13	1:aA:398:GLY:HA3	1.98	0.46
1:aA:393:HIS:CE1	15:aA:1126:CL7:ND	2.83	0.46
1:aA:660:ILE:HD12	2:aB:621:ARG:HG3	1.97	0.46
9:aK:70:HIS:HE1	15:aK:1402:CL7:C4D	2.25	0.46
2:bB:129:MET:HE3	15:bB:1211:CL7:HMA2	1.97	0.46
1:cA:441:LEU:HB3	1:cA:549:LEU:HD13	1.97	0.46
2:cB:165:LEU:O	2:cB:169:ARG:HG2	2.16	0.46
2:cB:193:HIS:HD2	2:cB:197:VAL:HB	1.80	0.46
10:cL:146:TYR:CZ	10:cL:150:ILE:HD11	2.51	0.46
2:aB:222:LEU:HB3	2:aB:226:PHE:CE1	2.50	0.46
2:aB:324:TYR:CE1	2:aB:331:GLN:HG2	2.50	0.46
2:aB:569:ASP:HA	2:aB:574:ASP:OD1	2.15	0.46
15:aB:1210:CL7:H3A	15:aB:1210:CL7:HBA2	1.41	0.46
15:aB:1216:CL7:HMB2	15:aB:1221:CL7:HMA3	1.97	0.46
15:bA:1126:CL7:HBC2	15:bA:1126:CL7:HHD	1.98	0.46
2:bB:521:HIS:CE1	15:bB:1235:CL7:NC	2.79	0.46
10:bL:146:TYR:CZ	10:bL:150:ILE:HD11	2.51	0.46
1:cA:432:ARG:HG2	4:cD:15:SER:HB3	1.97	0.46
1:aA:43:PRO:HG3	6:aF:125:ILE:HD13	1.97	0.46
1:aA:142:SER:HA	15:aA:1126:CL7:HMA2	1.98	0.46
1:aA:525:GLN:HG2	1:aA:526:HIS:H	1.81	0.46
2:aB:53:HIS:HE1	15:aB:1203:CL7:NB	2.13	0.46
15:aB:1220:CL7:HBA1	15:aB:1220:CL7:H3A	1.36	0.46
15:bB:1203:CL7:H162	15:bB:1203:CL7:H122	1.52	0.46
15:bB:1211:CL7:H2	15:bB:1211:CL7:H61C	1.72	0.46
3:bC:62:PHE:CD2	4:bD:121:ILE:HG21	2.50	0.46
5:bE:39:ARG:HD2	5:bE:57:THR:HG22	1.97	0.46
1:cA:668:SER:HB2	2:cB:443:ALA:HB1	1.97	0.46
2:cB:175:MET:O	2:cB:179:LEU:HB2	2.15	0.46
2:cB:372:HIS:CE1	15:cB:1224:CL7:ND	2.83	0.46
2:bB:265:THR:HB	2:bB:357:ALA:HA	1.97	0.46
2:bB:299:HIS:CE1	15:bB:1218:CL7:NA	2.84	0.46
2:bB:387:HIS:HE1	15:bB:1226:CL7:NA	2.13	0.46
2:bB:460:TRP:HE3	2:bB:472:LEU:HD23	1.81	0.46
2:bB:482:ILE:HD11	12:bX:31:ILE:H	1.81	0.46
3:cC:61:ASP:HA	3:cC:62:PHE:HA	1.78	0.46
1:aA:374:MET:HE3	1:aA:507:THR:O	2.16	0.46
2:aB:129:MET:HE3	15:aB:1211:CL7:HMA2	1.98	0.46
2:aB:280:ILE:HA	2:aB:283:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:746:LEU:HD23	1:bA:746:LEU:HA	1.77	0.46
2:bB:183:PHE:HB3	2:bB:284:TYR:CD2	2.51	0.46
1:cA:704:TRP:HE1	6:cF:164:VAL:HG22	1.81	0.46
1:aA:700:GLU:CD	2:aB:545:LYS:HB2	2.41	0.45
1:aA:710:LYS:HE2	6:aF:106:ARG:HH21	1.80	0.45
15:aA:1127:CL7:H62C	15:aA:1127:CL7:H41C	1.75	0.45
2:bB:339:LEU:O	2:bB:343:THR:HG22	2.16	0.45
2:bB:387:HIS:CE1	15:bB:1226:CL7:NA	2.83	0.45
15:bB:1219:CL7:HAB	15:bB:1241:CL7:HAC2	1.99	0.45
15:bB:1221:CL7:H93C	15:bB:1221:CL7:H61C	1.71	0.45
1:cA:74:PHE:CE2	1:cA:78:PHE:HE2	2.34	0.45
1:cA:263:PRO:HA	1:cA:266:THR:HG22	1.97	0.45
1:cA:589:GLY:O	1:cA:593:VAL:HG23	2.16	0.45
1:cA:662:SER:HB2	1:cA:667:LEU:HB2	1.97	0.45
15:cA:1104:CL7:H161	15:cA:1104:CL7:H202	1.76	0.45
15:cA:1137:CL7:HBA2	15:cA:1137:CL7:H3A	1.63	0.45
2:cB:176:ASN:HD21	2:cB:291:TYR:H	1.63	0.45
15:cB:1230:CL7:H2A	15:cB:1230:CL7:O2D	2.16	0.45
1:aA:296:HIS:CD2	15:aA:1116:CL7:HAB	2.52	0.45
15:aA:1123:CL7:H11C	15:aA:1123:CL7:HBA2	1.75	0.45
2:aB:28:VAL:HG21	15:aB:1201:CL7:C3D	2.46	0.45
15:aB:1235:CL7:H61C	15:aB:1235:CL7:H41C	1.64	0.45
10:aL:43:ALA:HB1	10:aL:126:ILE:HG13	1.98	0.45
1:cA:349:TRP:HB3	15:cA:1103:CL7:HAC1	1.98	0.45
2:cB:694:LYS:HD2	7:cI:31:GLU:OE1	2.16	0.45
6:cF:122:MET:HE3	6:cF:126:ILE:HG13	1.99	0.45
9:cK:31:ALA:HA	9:cK:34:ILE:HG22	1.98	0.45
1:aA:219:HIS:NE2	15:aA:1113:CL7:NB	2.65	0.45
15:aA:1102:CL7:H12C	15:aA:1109:CL7:H111	1.99	0.45
15:aA:1110:CL7:H2A	15:aA:1110:CL7:CED	2.47	0.45
1:bA:77:HIS:NE2	15:bA:1103:CL7:ND	2.64	0.45
15:bA:1139:CL7:HED3	15:bA:1139:CL7:HBA2	1.97	0.45
2:bB:31:PHE:HA	2:bB:34:HIS:CD2	2.51	0.45
2:bB:299:HIS:HB3	2:bB:304:ILE:HD11	1.99	0.45
15:aL:1501:CL7:HBA1	15:aL:1501:CL7:H3A	1.36	0.45
15:bA:1127:CL7:H3A	15:bA:1127:CL7:HBA2	1.41	0.45
2:bB:721:TYR:HB2	15:bB:1021:CL7:HED3	1.98	0.45
3:bC:7:ILE:HD12	3:bC:40:ALA:HB3	1.98	0.45
6:bF:81:TRP:O	6:bF:84:ALA:HB2	2.17	0.45
1:cA:53:HIS:CE1	15:cA:1101:CL7:ND	2.85	0.45
2:cB:299:HIS:CE1	15:cB:1218:CL7:NA	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:720:THR:HG23	15:cB:1021:CL7:O1D	2.16	0.45
15:cB:1211:CL7:H61C	15:cB:1211:CL7:H2	1.63	0.45
1:aA:441:LEU:HB3	1:aA:549:LEU:HD13	1.99	0.45
2:aB:156:HIS:HE1	15:aB:1208:CL7:C1A	2.29	0.45
2:aB:194:LEU:HA	2:aB:198:ALA:HB3	1.98	0.45
15:aB:1238:CL7:H201	10:aL:54:HIS:CD2	2.50	0.45
15:aB:1222:CL7:HBA2	15:aB:1222:CL7:H3A	1.44	0.45
1:bA:43:PRO:HB3	1:bA:48:TRP:CE3	2.51	0.45
1:bA:54:ALA:HB2	18:bA:5001:LHG:HC82	1.98	0.45
1:bA:498:ILE:HD13	2:cB:210:ASP:HA	1.97	0.45
2:bB:222:LEU:HB3	2:bB:226:PHE:HE2	1.81	0.45
2:bB:409:LEU:HA	2:bB:412:HIS:CE1	2.51	0.45
1:cA:91:MET:SD	15:cA:1106:CL7:HAA1	2.57	0.45
1:cA:316:TRP:HB3	9:cK:60:ASN:ND2	2.29	0.45
15:cA:1104:CL7:H111	15:cA:1104:CL7:H152	1.77	0.45
2:cB:659:THR:HA	14:cB:1023:PHO:HAB	1.97	0.45
15:cB:1209:CL7:HBA1	15:cB:1209:CL7:H3A	1.46	0.45
15:cB:1222:CL7:HAA1	15:cB:1223:CL7:OBD	2.17	0.45
1:aA:53:HIS:NE2	15:aA:1101:CL7:NB	2.64	0.45
1:aA:706:HIS:HD2	1:aA:711:ILE:HG23	1.82	0.45
2:aB:244:PHE:H	2:aB:264:GLN:NE2	2.05	0.45
1:bA:25:SER:H	15:bA:1109:CL7:HMA3	1.81	0.45
15:bA:1126:CL7:HBA1	15:bA:1126:CL7:H3A	1.61	0.45
2:bB:93:ASP:HB3	2:bB:96:LEU:HG	1.99	0.45
15:bB:1213:CL7:HBA1	15:bB:1213:CL7:H3A	1.36	0.45
3:bC:6:LYS:HE2	4:bD:138:TYR:HD2	1.82	0.45
15:cB:1216:CL7:HMB2	15:cB:1221:CL7:HMA3	1.98	0.45
8:cJ:34:GLU:HG3	15:cJ:1302:CL7:C4B	2.46	0.45
2:aB:382:LEU:HG	2:aB:576:PHE:CE1	2.52	0.45
15:bA:1116:CL7:H11C	15:bA:1116:CL7:H51C	1.78	0.45
1:cA:318:ILE:HG22	9:cK:39:ILE:HD11	1.99	0.45
15:cA:1132:CL7:CED	15:cA:1132:CL7:H2A	2.46	0.45
15:cB:1227:CL7:HMC1	15:cB:1236:CL7:HAB	1.97	0.45
9:cK:32:ILE:HD11	9:cK:66:GLN:HE22	1.82	0.45
1:aA:53:HIS:CE1	15:aA:1101:CL7:ND	2.85	0.45
1:aA:498:ILE:HG21	2:bB:210:ASP:HA	1.99	0.45
1:aA:597:LEU:HD13	1:aA:730:LEU:HD21	1.98	0.45
15:aA:1110:CL7:HBA1	15:aA:1110:CL7:H3A	1.45	0.45
2:aB:53:HIS:HD1	15:aB:1202:CL7:HMA1	1.81	0.45
2:aB:145:VAL:O	2:aB:149:MET:HG2	2.16	0.45
2:aB:257:PHE:HE2	2:aB:494:TRP:CE3	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:700:GLU:CD	2:bB:545:LYS:HB2	2.42	0.45
8:bJ:14:PHE:HA	8:bJ:19:VAL:HG11	1.98	0.45
1:cA:254:TYR:CD1	1:cA:275:PHE:HB3	2.51	0.45
15:cA:1123:CL7:H141	15:cA:1123:CL7:H161	1.81	0.45
15:cB:1223:CL7:H202	15:cB:1223:CL7:H161	1.75	0.45
15:cB:1239:CL7:H101	15:cB:1239:CL7:H62C	1.71	0.45
15:aA:1119:CL7:H52C	15:aA:1119:CL7:H12C	1.82	0.45
2:aB:560:ASP:HA	3:aC:52:LYS:HE2	1.99	0.45
1:bA:91:MET:SD	15:bA:1106:CL7:HAA1	2.57	0.45
1:bA:600:MET:HG2	15:bA:1124:CL7:HBC1	1.98	0.45
15:bA:1119:CL7:H62C	15:bA:1119:CL7:H41C	1.66	0.45
15:bA:1138:CL7:H202	6:bF:105:SER:HA	1.99	0.45
2:bB:516:ASP:HA	2:bB:519:VAL:HG12	1.99	0.45
4:bD:42:GLU:H	4:bD:73:GLN:NE2	2.14	0.45
4:bD:58:LEU:HD12	4:bD:58:LEU:HA	1.79	0.45
1:cA:698:LEU:O	1:cA:702:ILE:HG12	2.17	0.45
2:cB:193:HIS:ND1	15:cB:1211:CL7:NB	2.64	0.45
2:cB:545:LYS:HE2	6:cF:163:THR:HG22	1.99	0.45
15:cB:1229:CL7:H2	15:cB:1229:CL7:H92C	1.98	0.45
15:cB:1241:CL7:HBA2	15:cB:1241:CL7:H3A	1.76	0.45
2:aB:364:VAL:HG21	2:aB:730:ALA:HA	1.99	0.45
8:aJ:24:PHE:O	8:aJ:27:LEU:HG	2.17	0.45
1:bA:65:ASP:O	1:bA:69:ILE:HG12	2.17	0.45
1:bA:714:ALA:HB2	6:bF:113:ARG:NH1	2.31	0.45
6:bF:139:ALA:O	6:bF:142:TRP:HB3	2.17	0.45
1:cA:525:GLN:HG2	1:cA:526:HIS:H	1.82	0.45
2:cB:646:TRP:CE2	2:cB:726:ILE:HG21	2.51	0.45
4:cD:136:GLN:HG2	4:cD:138:TYR:CE2	2.51	0.45
15:aB:1205:CL7:H62C	15:aB:1205:CL7:H102	1.54	0.44
15:aB:1223:CL7:H202	15:aB:1223:CL7:H161	1.71	0.44
1:bA:297:HIS:HB2	15:bA:1116:CL7:C1B	2.47	0.44
15:bA:1110:CL7:CED	15:bA:1110:CL7:H2A	2.47	0.44
1:cA:65:ASP:O	1:cA:69:ILE:HG12	2.17	0.44
2:cB:275:HIS:CE1	15:cB:1213:CL7:NA	2.85	0.44
2:cB:342:ILE:HG23	15:cB:1215:CL7:H71C	1.99	0.44
2:cB:673:GLU:O	2:cB:677:THR:HG23	2.17	0.44
15:aA:1106:CL7:H151	15:aA:1106:CL7:H111	1.70	0.44
3:bC:55:GLU:HB3	3:bC:63:LEU:HD11	1.98	0.44
7:bI:11:THR:HB	7:bI:12:PRO:HD3	1.98	0.44
1:cA:418:ASP:HB3	1:cA:421:MET:HB3	1.99	0.44
1:cA:724:GLN:HG3	18:cA:5001:LHG:HC81	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:cA:1106:CL7:H92C	15:cA:1106:CL7:H62C	1.81	0.44
2:cB:59:LEU:HD22	2:cB:146:ALA:CB	2.48	0.44
1:aA:710:LYS:HZ2	6:aF:157:VAL:HG13	1.82	0.44
15:aA:1130:CL7:OBD	10:aL:19:THR:HG21	2.18	0.44
2:aB:60:TRP:O	2:aB:64:LEU:HG	2.17	0.44
2:aB:95:HIS:CE1	15:aB:1207:CL7:NB	2.85	0.44
4:aD:83:LYS:HG2	4:aD:98:PRO:HD2	1.99	0.44
1:bA:30:GLY:HA3	8:bJ:12:LYS:HB2	1.99	0.44
15:bA:1137:CL7:H3A	15:bA:1137:CL7:HBA2	1.71	0.44
10:bL:101:VAL:HG11	10:bL:123:TRP:CD1	2.53	0.44
2:cB:59:LEU:HD12	15:cB:1204:CL7:C9	2.42	0.44
15:cB:1222:CL7:CHB	15:cB:1236:CL7:HAA1	2.47	0.44
1:aA:240:PRO:O	1:aA:244:LEU:HB2	2.17	0.44
1:aA:457:ILE:O	1:aA:460:ASP:HB2	2.17	0.44
15:aA:1119:CL7:HBA2	15:aA:1123:CL7:CAB	2.48	0.44
2:aB:284:TYR:HE2	15:aB:1215:CL7:HMC2	1.82	0.44
10:aL:93:MET:HE1	10:aL:130:PHE:CG	2.51	0.44
15:bA:1106:CL7:H41C	15:bA:1106:CL7:H62C	1.47	0.44
15:bA:1109:CL7:H112	15:bA:1109:CL7:H143	1.63	0.44
2:bB:48:ALA:HA	2:bB:51:PHE:HD2	1.81	0.44
2:bB:482:ILE:HD12	2:bB:482:ILE:H	1.82	0.44
1:cA:178:TYR:HB2	15:cA:1109:CL7:CMC	2.47	0.44
1:cA:746:LEU:HD23	1:cA:746:LEU:HA	1.79	0.44
2:cB:658:ALA:HB1	14:cB:1023:PHO:HBB2	1.98	0.44
1:aA:691:GLY:HA3	2:aB:569:ASP:HB2	1.99	0.44
1:aA:724:GLN:HG3	18:aA:5001:LHG:HC81	1.99	0.44
2:aB:424:SER:HB3	2:aB:529:VAL:HG22	1.98	0.44
2:aB:430:HIS:CE1	15:aB:1229:CL7:ND	2.86	0.44
2:aB:673:GLU:O	2:aB:677:THR:HG23	2.18	0.44
6:aF:66:CYS:HA	6:aF:74:ARG:HG2	2.00	0.44
15:bA:1127:CL7:H62C	15:bA:1127:CL7:H102	1.77	0.44
2:bB:34:HIS:O	2:bB:37:MET:HE3	2.18	0.44
19:bB:5002:LMG:H372	19:bB:5002:LMG:H401	1.71	0.44
1:cA:128:ASN:HB3	1:cA:136:HIS:HB3	1.99	0.44
1:aA:116:HIS:CD2	15:aA:1106:CL7:NA	2.86	0.44
1:aA:282:LEU:HD21	1:aA:375:PRO:HD2	1.99	0.44
2:aB:53:HIS:HD1	15:aB:1202:CL7:HBB	1.82	0.44
2:aB:118:SER:HA	15:aB:1224:CL7:HMA2	1.98	0.44
2:aB:386:ALA:HB2	2:aB:576:PHE:CE1	2.53	0.44
1:bA:206:LEU:HD21	15:bA:1117:CL7:H172	2.00	0.44
1:bA:338:HIS:CE1	18:bA:5003:LHG:HC12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:bA:1102:CL7:HBA2	15:bA:1102:CL7:H3A	1.70	0.44
15:bA:1127:CL7:H142	15:bA:1127:CL7:H111	1.69	0.44
2:bB:183:PHE:HE1	15:bB:1210:CL7:H61C	1.83	0.44
6:bF:111:ALA:HB1	6:bF:131:LEU:HD11	2.00	0.44
1:cA:297:HIS:NE2	1:cA:301:LEU:HD11	2.33	0.44
2:cB:158:GLN:O	2:cB:162:ARG:HG2	2.18	0.44
8:cJ:24:PHE:O	8:cJ:27:LEU:HG	2.17	0.44
1:bA:320:HIS:HE1	15:bA:1120:CL7:C4A	2.30	0.44
15:bA:1116:CL7:H3A	15:bA:1116:CL7:HBA1	1.27	0.44
2:bB:194:LEU:HA	2:bB:198:ALA:HB3	1.99	0.44
3:bC:16:GLN:HB2	20:bC:3003:SF4:S4	2.58	0.44
4:bD:11:LEU:HB2	4:bD:50:VAL:HB	2.00	0.44
1:cA:53:HIS:NE2	15:cA:1101:CL7:NB	2.66	0.44
1:cA:393:HIS:CE1	15:cA:1126:CL7:ND	2.86	0.44
15:cA:1127:CL7:H3A	15:cA:1127:CL7:HBA2	1.34	0.44
15:cB:1205:CL7:O1A	15:cB:1224:CL7:HBD	2.18	0.44
15:aB:1241:CL7:HBA2	15:aB:1241:CL7:H3A	1.66	0.44
19:aB:5002:LMG:H301	19:aB:5002:LMG:H332	1.92	0.44
3:aC:17:CYS:HB2	3:aC:54:CYS:HB2	1.99	0.44
1:bA:585:CYS:HB2	2:bB:667:TRP:HB3	2.00	0.44
2:bB:395:ASP:HA	4:bD:131:LYS:HD2	2.00	0.44
10:bL:93:MET:HE1	10:bL:130:PHE:CG	2.53	0.44
15:cA:1119:CL7:HBA2	15:cA:1123:CL7:CAB	2.47	0.44
15:cB:1220:CL7:HBA1	15:cB:1220:CL7:H3A	1.38	0.44
15:aA:1133:CL7:H41C	15:aA:1133:CL7:H61C	1.81	0.44
2:aB:53:HIS:ND1	15:aB:1202:CL7:HMA1	2.33	0.44
2:aB:154:TRP:CD1	11:aM:24:ASN:HB3	2.53	0.44
2:aB:167:TRP:CH2	15:aB:1208:CL7:HHB	2.53	0.44
2:aB:553:PHE:HZ	3:aC:66:ARG:HD2	1.82	0.44
3:aC:55:GLU:HG3	3:aC:63:LEU:HD22	2.00	0.44
15:bA:1104:CL7:H202	15:bA:1104:CL7:H161	1.78	0.44
2:bB:167:TRP:CZ2	15:bB:1208:CL7:H3A	2.52	0.44
15:cA:1122:CL7:H111	15:cA:1122:CL7:H152	1.89	0.44
2:cB:257:PHE:CE2	2:cB:494:TRP:HE3	2.34	0.44
2:cB:465:HIS:CE1	15:cB:1231:CL7:NB	2.85	0.44
1:aA:407:ALA:O	1:aA:411:ILE:HG13	2.18	0.43
2:aB:183:PHE:HE2	15:aB:1210:CL7:H61C	1.83	0.43
10:aL:48:LEU:HD21	10:bL:131:LEU:HD23	2.00	0.43
1:bA:84:VAL:O	1:bA:88:ILE:HG13	2.18	0.43
1:bA:533:ASP:HA	1:bA:536:ILE:HG22	2.00	0.43
2:bB:126:THR:HG21	2:bB:356:TYR:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:bB:1222:CL7:H3A	15:bB:1222:CL7:HBA2	1.45	0.43
15:bB:1222:CL7:HAA1	15:bB:1223:CL7:OBD	2.18	0.43
15:bB:1226:CL7:H192	15:bB:1239:CL7:H3A	2.00	0.43
15:cI:1601:CL7:H3A	15:cI:1601:CL7:H2	1.99	0.43
1:aA:336:GLU:OE1	1:aA:336:GLU:N	2.50	0.43
15:aA:1121:CL7:HBA1	15:aA:1121:CL7:H3A	1.53	0.43
2:aB:338:ALA:O	2:aB:342:ILE:HG12	2.18	0.43
8:aJ:34:GLU:HA	8:aJ:37:ARG:HG2	2.00	0.43
1:bA:53:HIS:HE1	15:bA:1101:CL7:C4D	2.31	0.43
1:bA:525:GLN:HG2	1:bA:526:HIS:H	1.82	0.43
1:bA:720:MET:HG2	16:bA:2001:PQN:C4	2.49	0.43
15:bA:1106:CL7:H62C	15:bA:1106:CL7:H92C	1.81	0.43
15:bB:1205:CL7:O1A	15:bB:1224:CL7:HBD	2.18	0.43
15:bB:1229:CL7:HMC3	6:bF:91:GLY:HA2	2.01	0.43
15:bB:1239:CL7:H101	15:bB:1239:CL7:H62C	1.64	0.43
2:cB:155:LEU:HD21	15:cB:1208:CL7:HBC3	2.00	0.43
1:aA:178:TYR:HB2	15:aA:1109:CL7:CMC	2.48	0.43
1:aA:190:TRP:CZ2	15:aA:1108:CL7:HMA1	2.53	0.43
15:aA:1119:CL7:H62C	15:aA:1119:CL7:H41C	1.68	0.43
2:aB:430:HIS:HE1	15:aB:1229:CL7:ND	2.16	0.43
2:aB:576:PHE:HZ	15:aB:1226:CL7:HAC2	1.82	0.43
15:aB:1238:CL7:H41C	15:aB:1238:CL7:H62C	1.59	0.43
15:aB:1222:CL7:HAA1	15:aB:1223:CL7:OBD	2.17	0.43
15:aB:1223:CL7:H91C	15:aB:1223:CL7:H111	1.80	0.43
2:bB:257:PHE:HD1	15:bB:1214:CL7:HMB3	1.82	0.43
15:bB:1241:CL7:HBA2	15:bB:1241:CL7:H3A	1.78	0.43
15:bJ:1302:CL7:H3A	15:bJ:1302:CL7:HBA2	1.64	0.43
2:cB:156:HIS:HE1	15:cB:1208:CL7:NA	2.15	0.43
2:cB:276:HIS:CE1	15:cB:1214:CL7:ND	2.86	0.43
2:cB:284:TYR:HE2	15:cB:1215:CL7:HMC2	1.84	0.43
1:aA:450:PHE:HB3	15:aA:1131:CL7:HMA3	2.01	0.43
15:aA:1103:CL7:H143	15:aA:1103:CL7:H161	1.82	0.43
15:aA:1104:CL7:H18	15:aA:1106:CL7:H42C	2.01	0.43
2:aB:50:HIS:HB3	15:aB:1210:CL7:O1D	2.18	0.43
15:aB:1223:CL7:H171	15:aB:1227:CL7:HAC1	1.99	0.43
2:bB:580:THR:HB	2:bB:710:LEU:HD11	2.01	0.43
15:bB:1223:CL7:H202	15:bB:1223:CL7:H161	1.76	0.43
1:cA:176:ALA:HB2	15:cA:1108:CL7:HBC2	2.00	0.43
15:cA:1102:CL7:H12C	15:cA:1109:CL7:H111	2.01	0.43
2:cB:679:VAL:HG13	2:cB:693:TRP:CZ2	2.53	0.43
15:cB:1207:CL7:H3A	15:cB:1207:CL7:HBA2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:cB:1223:CL7:H91C	15:cB:1223:CL7:H111	1.69	0.43
1:aA:147:ILE:CD1	15:aA:1127:CL7:HAA1	2.49	0.43
15:aA:1109:CL7:H62C	15:aA:1109:CL7:H41C	1.86	0.43
2:aB:390:ILE:HG12	2:aB:555:TYR:CD2	2.54	0.43
3:aC:43:PRO:HG2	3:aC:44:ARG:HD3	2.00	0.43
7:aI:27:PHE:CE2	10:aL:95:LEU:HB3	2.54	0.43
1:bA:153:MET:HE1	1:bA:162:THR:HG21	2.00	0.43
1:cA:531:THR:O	1:cA:535:MET:HG3	2.19	0.43
15:cA:1133:CL7:H202	15:cA:1133:CL7:H162	1.78	0.43
1:aA:442:ASN:ND2	2:aB:678:LEU:HD21	2.34	0.43
1:aA:598:PHE:CE2	1:aA:730:LEU:HD13	2.54	0.43
15:aA:1132:CL7:CED	15:aA:1132:CL7:H2A	2.49	0.43
15:aB:1239:CL7:H143	15:aB:1239:CL7:H161	1.70	0.43
15:bA:1130:CL7:H2	15:bL:1502:CL7:H43C	2.00	0.43
15:bA:1130:CL7:OBD	10:bL:19:THR:HG21	2.18	0.43
2:bB:419:HIS:CE1	15:bB:1228:CL7:C1B	3.02	0.43
3:bC:30:PRO:HG3	4:bD:109:GLU:OE2	2.19	0.43
2:cB:37:MET:HE3	2:cB:42:LEU:HA	1.99	0.43
2:cB:324:TYR:CZ	15:cB:1221:CL7:NC	2.87	0.43
1:aA:36:ASN:HD22	1:aA:39:LEU:HD12	1.83	0.43
2:aB:53:HIS:NE2	15:aB:1203:CL7:ND	2.66	0.43
2:aB:244:PHE:N	2:aB:264:GLN:HE22	2.06	0.43
15:aB:1221:CL7:H61C	15:aB:1221:CL7:H93C	1.68	0.43
1:bA:223:PRO:HA	1:bA:226:LYS:HG2	2.00	0.43
15:bA:1133:CL7:H41C	15:bA:1133:CL7:H61C	1.81	0.43
2:bB:120:VAL:HG23	2:bB:123:TRP:HE3	1.83	0.43
2:bB:324:TYR:HE2	2:bB:334:PHE:HD2	1.67	0.43
10:bL:52:MET:HE3	15:bL:1501:CL7:HMA3	2.01	0.43
2:cB:171:ALA:O	2:cB:174:GLN:HB3	2.19	0.43
15:cB:1226:CL7:H92C	15:cB:1226:CL7:H62C	1.87	0.43
1:aA:53:HIS:HE1	15:aA:1101:CL7:C4D	2.31	0.43
1:aA:65:ASP:O	1:aA:69:ILE:HG12	2.19	0.43
1:aA:118:VAL:HB	1:aA:124:GLN:HE21	1.83	0.43
15:aA:1127:CL7:H3A	15:aA:1127:CL7:HBA2	1.33	0.43
1:bA:364:SER:HB2	15:bA:1127:CL7:HMC2	2.01	0.43
1:bA:738:ILE:HG21	15:bA:1126:CL7:HMC2	2.00	0.43
2:bB:276:HIS:CE1	15:bB:1214:CL7:ND	2.86	0.43
2:bB:601:VAL:HG22	2:bB:606:LEU:HD21	2.01	0.43
15:cA:1118:CL7:H92C	15:cA:1118:CL7:H62C	1.77	0.43
2:cB:60:TRP:O	2:cB:64:LEU:HG	2.19	0.43
15:cB:1021:CL7:H142	15:cB:1021:CL7:H112	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:cB:1234:CL7:H3A	15:cB:1235:CL7:HAA2	2.01	0.43
15:aA:1103:CL7:HBA2	15:aA:1103:CL7:H3A	1.38	0.43
15:aA:1138:CL7:H122	15:aA:1138:CL7:H8	1.91	0.43
2:aB:324:TYR:CZ	15:aB:1221:CL7:NC	2.87	0.43
2:aB:391:PHE:HE2	2:aB:406:LEU:HD11	1.82	0.43
3:aC:30:PRO:HG3	4:aD:109:GLU:OE2	2.19	0.43
1:bA:128:ASN:HB3	1:bA:136:HIS:HB3	2.00	0.43
1:bA:216:HIS:HB2	15:bA:1112:CL7:CHC	2.49	0.43
1:bA:250:MET:HG3	15:bA:1113:CL7:HED1	2.01	0.43
2:bB:576:PHE:HZ	15:bB:1226:CL7:HAC2	1.83	0.43
1:cA:47:THR:HG22	1:cA:51:ASN:ND2	2.34	0.43
1:cA:197:THR:OG1	15:cA:1111:CL7:HBC2	2.18	0.43
15:cA:1106:CL7:H62C	15:cA:1106:CL7:H41C	1.48	0.43
15:cA:1127:CL7:H41C	15:cA:1127:CL7:H62C	1.73	0.43
15:cA:1137:CL7:O2D	15:cA:1137:CL7:H2A	2.18	0.43
2:cB:182:LEU:HD13	15:cB:1210:CL7:HHB	2.01	0.43
15:cB:1210:CL7:H12C	17:cB:4005:A1JPJ:C21	2.49	0.43
15:cB:1212:CL7:CED	15:cB:1212:CL7:H2A	2.49	0.43
15:cB:1226:CL7:H162	15:cB:1226:CL7:H192	1.72	0.43
4:cD:7:GLY:HA3	4:cD:57:LEU:HD22	2.00	0.43
1:aA:297:HIS:HE2	15:aA:1117:CL7:C2B	2.32	0.43
2:aB:264:GLN:HG3	2:aB:265:THR:HG23	2.00	0.43
17:aB:4005:A1JPJ:C21	15:aB:1210:CL7:H12C	2.49	0.43
15:aB:1205:CL7:CGA	15:aB:1205:CL7:C1A	2.97	0.43
10:aL:48:LEU:O	10:aL:52:MET:HG3	2.18	0.43
15:bA:1110:CL7:HBA1	15:bA:1110:CL7:H3A	1.45	0.43
2:bB:548:PRO:HD2	3:bC:62:PHE:CE1	2.54	0.43
2:bB:664:LEU:HD12	2:bB:709:GLY:HA3	2.00	0.43
15:bB:1207:CL7:H51C	10:bL:77:SER:HA	2.01	0.43
15:bB:1238:CL7:H41C	15:bB:1238:CL7:H62C	1.60	0.43
1:cA:77:HIS:NE2	15:cA:1103:CL7:ND	2.67	0.43
1:cA:338:HIS:CE1	18:cA:5003:LHG:HC12	2.54	0.43
2:cB:606:LEU:HD12	2:cB:606:LEU:HA	1.87	0.43
8:cJ:14:PHE:HA	8:cJ:19:VAL:HG11	2.01	0.43
2:aB:371:THR:HG23	2:aB:591:THR:HG21	2.01	0.42
15:aB:1207:CL7:H3A	15:aB:1207:CL7:HBA2	1.81	0.42
6:aF:50:ASP:HB3	6:aF:53:SER:HB3	2.01	0.42
7:aI:24:THR:HG23	10:aL:95:LEU:HD11	2.01	0.42
15:bA:1119:CL7:HBA2	15:bA:1123:CL7:CAB	2.49	0.42
1:cA:467:ARG:NH2	10:cL:67:PRO:HB3	2.34	0.42
18:cA:5001:LHG:HC92	18:cA:5001:LHG:H121	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:257:PHE:HE2	2:cB:494:TRP:CE3	2.33	0.42
2:cB:313:TYR:CE2	15:cB:1227:CL7:HBA1	2.50	0.42
2:cB:387:HIS:CE1	15:cB:1226:CL7:NA	2.87	0.42
2:cB:658:ALA:HB3	14:cB:1023:PHO:HBB2	2.02	0.42
15:cB:1201:CL7:HHC	15:cB:1203:CL7:OBD	2.18	0.42
15:cB:1216:CL7:OBD	15:cB:1220:CL7:HED1	2.19	0.42
1:aA:220:VAL:C	1:aA:223:PRO:HD2	2.44	0.42
1:aA:720:MET:HE3	1:aA:720:MET:HB2	1.92	0.42
6:aF:66:CYS:HB3	6:aF:73:PRO:HA	2.00	0.42
1:bA:176:ALA:HB2	15:bA:1108:CL7:HBC2	2.01	0.42
15:bA:1122:CL7:HBA2	15:bA:1133:CL7:H172	2.00	0.42
18:bA:5001:LHG:H281	18:bA:5001:LHG:H251	1.77	0.42
2:bB:313:TYR:CE2	15:bB:1227:CL7:HBA1	2.52	0.42
2:bB:371:THR:HG23	2:bB:591:THR:HG21	2.01	0.42
1:cA:368:ALA:HB2	1:cA:394:HIS:HB2	2.01	0.42
1:cA:407:ALA:O	1:cA:411:ILE:HG13	2.19	0.42
2:cB:275:HIS:HB3	15:cB:1214:CL7:HMB2	2.00	0.42
2:cB:276:HIS:HE1	15:cB:1214:CL7:ND	2.17	0.42
2:cB:440:VAL:HG21	15:cB:1230:CL7:HAC2	2.00	0.42
15:cB:1206:CL7:HBA1	15:cB:1206:CL7:H3A	1.85	0.42
1:aA:32:PRO:HB2	1:aA:48:TRP:HH2	1.83	0.42
15:aB:1212:CL7:CED	15:aB:1212:CL7:H2A	2.49	0.42
15:bA:1123:CL7:H161	15:bA:1123:CL7:H141	1.83	0.42
2:bB:195:ILE:HA	2:bB:199:ILE:HD12	2.00	0.42
2:bB:646:TRP:CE2	2:bB:726:ILE:HG21	2.54	0.42
1:cA:533:ASP:HA	1:cA:536:ILE:HG22	2.01	0.42
1:cA:710:LYS:HZ2	6:cF:157:VAL:HG13	1.85	0.42
2:cB:53:HIS:HD1	15:cB:1202:CL7:HMA1	1.84	0.42
2:cB:53:HIS:ND1	15:cB:1202:CL7:HMA1	2.34	0.42
2:cB:183:PHE:HE1	15:cB:1210:CL7:H61C	1.84	0.42
2:cB:220:ALA:HB1	2:cB:224:PRO:HG2	2.01	0.42
2:cB:675:ILE:O	2:cB:679:VAL:HG23	2.19	0.42
15:cB:1235:CL7:H41C	15:cB:1235:CL7:H61C	1.69	0.42
1:aA:575:PRO:HB3	1:aA:722:ILE:HB	2.00	0.42
15:aA:1129:CL7:NC	18:aA:5003:LHG:H111	2.35	0.42
4:aD:41:PHE:CD1	4:aD:51:MET:HB2	2.54	0.42
7:aI:5:ILE:HD11	15:aI:1601:CL7:HMD3	2.02	0.42
1:bA:190:TRP:CZ2	15:bA:1108:CL7:HMA1	2.54	0.42
1:bA:616:GLN:HB2	1:bA:632:LEU:HD12	2.02	0.42
3:bC:5:VAL:HG22	3:bC:67:VAL:HG13	2.01	0.42
2:cB:65:LEU:HD12	2:cB:142:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:716:GLY:O	2:cB:720:THR:HG22	2.19	0.42
15:cB:1207:CL7:H51C	10:cL:77:SER:HA	2.01	0.42
15:cB:1223:CL7:H171	15:cB:1227:CL7:HAC1	2.02	0.42
1:aA:109:LEU:HD11	1:aA:519:GLY:HA3	2.02	0.42
1:aA:254:TYR:HB3	1:aA:274:ASP:OD2	2.18	0.42
15:aA:1108:CL7:HED3	15:aA:1108:CL7:HBD	1.92	0.42
15:aA:1118:CL7:H3A	9:aK:63:LEU:CD1	2.49	0.42
15:aA:1138:CL7:HAA1	15:aB:1228:CL7:HMB2	2.01	0.42
2:aB:363:TYR:HB3	2:aB:602:TRP:CE3	2.55	0.42
8:aJ:14:PHE:HA	8:aJ:19:VAL:HG11	2.01	0.42
15:bA:1138:CL7:O2D	15:bA:1138:CL7:H2A	2.20	0.42
2:bB:412:HIS:NE2	15:bB:1227:CL7:ND	2.67	0.42
2:bB:517:PHE:HE2	15:bB:1235:CL7:C2D	2.32	0.42
15:bB:1204:CL7:H3A	15:bB:1205:CL7:HMB2	2.02	0.42
10:bL:59:TYR:OH	10:bL:75:LEU:HD13	2.19	0.42
1:cA:575:PRO:HB3	1:cA:722:ILE:HB	2.02	0.42
14:cA:1013:PHO:H3A	14:cA:1013:PHO:HBA1	1.52	0.42
2:cB:712:HIS:NE2	15:cB:1239:CL7:NA	2.67	0.42
15:aA:1111:CL7:H2	15:aA:1111:CL7:H61C	1.75	0.42
15:aB:1241:CL7:O2D	15:aB:1241:CL7:H2A	2.19	0.42
11:aM:5:ASP:O	11:aM:9:VAL:HG23	2.19	0.42
15:bA:1103:CL7:H71C	15:bA:1111:CL7:H12C	2.01	0.42
15:bA:1132:CL7:H92C	15:bA:1132:CL7:H61C	1.91	0.42
2:bB:126:THR:HG21	2:bB:356:TYR:HD1	1.85	0.42
2:bB:142:LEU:HD23	2:bB:142:LEU:HA	1.87	0.42
2:bB:305:MET:HG2	15:bB:1220:CL7:O1D	2.19	0.42
2:bB:392:PHE:HE1	2:bB:406:LEU:HD21	1.84	0.42
1:cA:336:GLU:OE1	1:cA:424:ASN:HB3	2.19	0.42
1:cA:393:HIS:HB2	15:cA:1126:CL7:CHB	2.49	0.42
1:cA:656:SER:O	1:cA:660:ILE:HG12	2.19	0.42
1:cA:673:LEU:HD13	1:cA:742:TRP:HZ3	1.84	0.42
15:cA:1129:CL7:NC	18:cA:5003:LHG:H111	2.35	0.42
5:cE:19:ARG:NH2	6:cF:164:VAL:HB	2.34	0.42
15:cL:1501:CL7:H3A	15:cL:1501:CL7:HBA1	1.41	0.42
1:aA:322:MET:HG2	15:aA:1119:CL7:HED3	2.02	0.42
15:aA:1140:CL7:H92C	15:aA:1140:CL7:H61C	1.79	0.42
2:aB:86:PRO:HB2	2:aB:116:CYS:HB3	2.00	0.42
5:aE:55:ILE:HG22	5:aE:57:THR:H	1.84	0.42
2:bB:203:ARG:HB3	2:bB:250:ALA:HB1	2.01	0.42
2:bB:275:HIS:HE1	15:bB:1213:CL7:NA	2.15	0.42
2:bB:387:HIS:HA	2:bB:390:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:bE:4:ARG:HD3	5:bE:25:ALA:O	2.19	0.42
6:bF:129:VAL:CG2	6:bF:130:PRO:HD3	2.50	0.42
1:cA:208:LEU:HD11	15:cA:1118:CL7:HBC1	2.01	0.42
1:cA:330:LYS:HB2	1:cA:335:GLY:O	2.18	0.42
15:cA:1104:CL7:H18	15:cA:1106:CL7:H42C	2.01	0.42
15:cA:1110:CL7:CED	15:cA:1110:CL7:H2A	2.49	0.42
2:aB:47:PHE:HZ	15:aB:1208:CL7:HMB2	1.85	0.42
2:aB:119:GLY:HA3	2:aB:365:THR:HG21	2.01	0.42
4:aD:21:SER:HB2	10:aL:105:ARG:NH1	2.35	0.42
1:bA:407:ALA:O	1:bA:411:ILE:HG13	2.20	0.42
2:bB:673:GLU:O	2:bB:677:THR:HG23	2.20	0.42
1:cA:364:SER:HB2	15:cA:1127:CL7:HMC2	2.02	0.42
10:cL:59:TYR:OH	10:cL:75:LEU:HD13	2.20	0.42
1:aA:223:PRO:HA	1:aA:226:LYS:NZ	2.35	0.42
1:aA:349:TRP:HB3	15:aA:1103:CL7:HAC1	2.01	0.42
2:aB:203:ARG:HB3	2:aB:250:ALA:HB1	2.00	0.42
15:aB:1229:CL7:H2	15:aB:1229:CL7:H92C	2.00	0.42
15:aB:1229:CL7:H93C	15:aB:1229:CL7:CAD	2.50	0.42
10:aL:136:GLY:HA3	17:aL:4023:A1JPJ:C31	2.50	0.42
1:bA:313:ARG:NH2	1:bA:321:HIS:HB2	2.35	0.42
1:bA:397:LEU:HD12	1:bA:401:TYR:CZ	2.55	0.42
15:bA:1121:CL7:H3A	15:bA:1121:CL7:HBA1	1.58	0.42
4:bD:58:LEU:HD11	10:bL:13:PHE:CE2	2.55	0.42
1:cA:570:LEU:HD11	1:cA:577:ASP:OD2	2.19	0.42
2:cB:203:ARG:HB3	2:cB:250:ALA:HB1	2.02	0.42
2:cB:235:GLN:O	2:cB:253:ALA:HB2	2.20	0.42
2:cB:371:THR:HG23	2:cB:591:THR:HG21	2.02	0.42
15:cB:1229:CL7:CAD	15:cB:1229:CL7:H93C	2.50	0.42
7:cI:11:THR:HB	7:cI:12:PRO:HD3	2.02	0.42
1:aA:430:MET:HE1	15:aA:1129:CL7:C1D	2.50	0.42
15:aI:1601:CL7:H142	15:aI:1601:CL7:H112	1.92	0.42
1:bA:397:LEU:HD12	1:bA:401:TYR:CE2	2.55	0.42
2:bB:44:GLN:NE2	2:bB:162:ARG:HB3	2.35	0.42
2:bB:277:HIS:HD1	2:bB:280:ILE:CD1	2.33	0.42
4:bD:42:GLU:H	4:bD:73:GLN:HE22	1.68	0.42
10:bL:43:ALA:HB1	10:bL:126:ILE:HG13	2.02	0.42
1:cA:35:PHE:CD2	1:cA:62:GLN:HG2	2.54	0.42
2:cB:93:ASP:HB3	2:cB:96:LEU:HG	2.00	0.42
2:cB:196:HIS:CD2	2:cB:217:PRO:HG3	2.55	0.42
2:cB:363:TYR:HB3	2:cB:602:TRP:CZ3	2.54	0.42
2:cB:424:SER:O	2:cB:525:PHE:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:651:LEU:HD23	2:cB:651:LEU:HA	1.86	0.42
1:aA:616:GLN:HB2	1:aA:632:LEU:HD12	2.02	0.41
1:aA:642:ILE:HG13	1:aA:643:THR:HG23	2.02	0.41
15:aA:1104:CL7:H202	15:aA:1104:CL7:H161	1.73	0.41
2:aB:51:PHE:CD2	2:aB:153:GLY:HA2	2.48	0.41
15:aB:1226:CL7:H162	15:aB:1226:CL7:H192	1.73	0.41
3:aC:28:MET:HB3	4:aD:107:SER:HB3	2.01	0.41
1:bA:457:ILE:O	1:bA:461:GLU:HG2	2.20	0.41
15:bA:1106:CL7:H3A	15:bA:1106:CL7:HBA1	1.69	0.41
15:bA:1125:CL7:HED1	15:bA:1133:CL7:HAB	2.02	0.41
2:bB:669:GLY:O	2:bB:673:GLU:HG3	2.20	0.41
3:bC:79:LEU:HD22	3:bC:81:TYR:CZ	2.55	0.41
6:bF:103:ASN:HD22	6:bF:142:TRP:CB	2.33	0.41
1:cA:457:ILE:O	1:cA:460:ASP:HB2	2.20	0.41
15:cA:1116:CL7:H11C	15:cA:1116:CL7:H51C	1.81	0.41
15:cA:1117:CL7:H93C	15:cA:1117:CL7:H111	1.87	0.41
2:cB:142:LEU:HD23	2:cB:142:LEU:HA	1.87	0.41
2:cB:175:MET:HE3	15:cB:1221:CL7:C2D	2.50	0.41
2:cB:178:HIS:CD2	15:cB:1210:CL7:NB	2.88	0.41
3:cC:28:MET:HB3	4:cD:107:SER:HB3	2.01	0.41
10:cL:39:LYS:HD3	10:cL:39:LYS:HA	1.89	0.41
1:bA:389:ASN:HD22	15:bA:1126:CL7:HHB	1.85	0.41
15:bA:1123:CL7:H192	15:bA:1123:CL7:H162	1.82	0.41
15:bA:1138:CL7:H112	15:bA:1138:CL7:H151	1.76	0.41
3:bC:62:PHE:HD2	4:bD:121:ILE:HD13	1.85	0.41
1:cA:66:LEU:HD23	1:cA:188:LEU:HD11	2.01	0.41
1:cA:709:LEU:HD21	15:cB:1228:CL7:HBA2	2.02	0.41
15:cA:1126:CL7:H172	15:cA:1126:CL7:H13	1.95	0.41
2:cB:301:MET:O	2:cB:305:MET:HG2	2.20	0.41
4:cD:34:THR:HG22	4:cD:55:GLU:HB3	2.02	0.41
6:cF:118:LYS:HD2	6:cF:119:ASN:HB2	2.01	0.41
1:aA:393:HIS:HB2	15:aA:1126:CL7:CHB	2.51	0.41
2:aB:382:LEU:HD13	2:aB:583:MET:HB2	2.02	0.41
2:aB:573:TRP:O	2:aB:576:PHE:HB3	2.19	0.41
1:bA:53:HIS:NE2	15:bA:1101:CL7:NA	2.68	0.41
2:bB:175:MET:O	2:bB:179:LEU:HB2	2.20	0.41
2:bB:521:HIS:CE1	15:bB:1235:CL7:NB	2.89	0.41
14:bB:1023:PHO:HBC2	14:bB:1023:PHO:HHB	2.02	0.41
1:cA:446:LEU:HD23	14:cB:1023:PHO:O1A	2.20	0.41
15:cA:1140:CL7:H3A	15:cA:1140:CL7:HBA1	1.77	0.41
6:cF:91:GLY:O	6:cF:95:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:cF:109:GLN:O	6:cF:113:ARG:HG2	2.20	0.41
15:cI:1601:CL7:H3A	15:cI:1601:CL7:CGA	2.51	0.41
14:aA:1013:PHO:O1A	2:aB:425:MET:HG2	2.21	0.41
2:aB:715:VAL:HA	2:aB:718:PHE:CE2	2.56	0.41
1:bA:32:PRO:HB3	15:bA:1101:CL7:HAC1	2.01	0.41
2:bB:68:VAL:HG12	2:bB:135:LEU:HD13	2.02	0.41
15:bB:1235:CL7:H61C	15:bB:1235:CL7:H41C	1.63	0.41
1:cA:254:TYR:CE1	1:cA:275:PHE:HB3	2.55	0.41
1:cA:296:HIS:HE1	15:cA:1115:CL7:ND	2.19	0.41
2:cB:390:ILE:HG12	2:cB:555:TYR:CD1	2.55	0.41
1:aA:683:PHE:HA	14:aA:1013:PHO:HAB	2.02	0.41
2:aB:468:LEU:O	2:aB:469:LEU:HB2	2.21	0.41
2:aB:712:HIS:NE2	15:aB:1239:CL7:NA	2.69	0.41
1:bA:77:HIS:NE2	15:bA:1103:CL7:NA	2.69	0.41
15:bA:1119:CL7:H52C	15:bA:1119:CL7:H12C	1.84	0.41
15:bA:1136:CL7:H91C	15:bL:1502:CL7:H191	2.03	0.41
15:bB:1210:CL7:H143	15:bB:1210:CL7:H111	1.77	0.41
15:bB:1212:CL7:H2A	15:bB:1212:CL7:CED	2.50	0.41
1:cA:279:LYS:HA	1:cA:504:GLU:HG3	2.03	0.41
2:cB:53:HIS:NE2	15:cB:1203:CL7:ND	2.69	0.41
15:cB:1239:CL7:H143	15:cB:1239:CL7:H161	1.75	0.41
1:aA:176:ALA:HB2	15:aA:1108:CL7:HBC2	2.03	0.41
1:aA:275:PHE:HE2	15:aA:1113:CL7:HAC2	1.85	0.41
1:aA:463:ARG:HE	1:aA:471:MET:HE1	1.86	0.41
1:aA:497:THR:HG23	1:aA:499:ARG:H	1.86	0.41
1:aA:680:ILE:HD13	1:aA:680:ILE:HA	1.94	0.41
2:aB:275:HIS:HE1	15:aB:1213:CL7:ND	2.19	0.41
2:aB:662:LEU:HB2	14:aB:1023:PHO:CHC	2.51	0.41
15:aB:1203:CL7:H93C	15:aB:1203:CL7:H112	1.85	0.41
1:bA:340:GLY:O	1:bA:344:VAL:HG23	2.19	0.41
1:bA:578:GLY:HA2	2:bB:561:GLY:HA2	2.03	0.41
15:bA:1133:CL7:H202	15:bA:1133:CL7:H162	1.83	0.41
15:bB:1205:CL7:C1A	15:bB:1205:CL7:CGA	2.98	0.41
15:bB:1207:CL7:H91C	15:bB:1207:CL7:H111	1.83	0.41
10:bL:11:ASP:O	10:bL:14:VAL:HG22	2.20	0.41
1:cA:297:HIS:CE1	15:cA:1116:CL7:ND	2.88	0.41
1:cA:450:PHE:O	1:cA:454:ASP:HB2	2.21	0.41
15:cA:1103:CL7:H143	15:cA:1103:CL7:H161	1.77	0.41
15:cA:1104:CL7:H112	15:cA:1104:CL7:H72C	1.94	0.41
15:aA:1112:CL7:HBA2	15:aA:1112:CL7:H3A	1.93	0.41
2:aB:264:GLN:HG3	2:aB:265:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:512:ILE:HA	2:aB:516:ASP:OD2	2.21	0.41
19:aB:5002:LMG:H342	15:aB:1203:CL7:H51C	2.03	0.41
15:aB:1210:CL7:HED2	15:aB:1210:CL7:C2A	2.45	0.41
1:bA:279:LYS:HG2	1:bA:504:GLU:OE1	2.21	0.41
5:bE:9:ARG:HD3	5:bE:19:ARG:HG3	2.03	0.41
1:cA:188:LEU:O	1:cA:192:GLN:HG2	2.20	0.41
1:cA:216:HIS:HB2	15:cA:1112:CL7:CHC	2.49	0.41
1:cA:569:SER:OG	4:cD:72:ARG:HD3	2.20	0.41
2:cB:320:LEU:HG	2:cB:404:ASN:ND2	2.36	0.41
2:cB:664:LEU:HD12	2:cB:709:GLY:HA3	2.01	0.41
15:cB:1239:CL7:H142	15:cB:1239:CL7:H112	1.84	0.41
1:aA:128:ASN:HB3	1:aA:136:HIS:HB3	2.02	0.41
1:aA:216:HIS:HB2	15:aA:1112:CL7:CHC	2.50	0.41
1:aA:268:ASN:O	1:aA:271:VAL:HG22	2.21	0.41
1:aA:370:HIS:NE2	15:aA:1125:CL7:NC	2.69	0.41
15:aA:1119:CL7:H51C	15:aA:1133:CL7:H101	2.03	0.41
2:aB:363:TYR:HB3	2:aB:602:TRP:CZ3	2.56	0.41
15:aB:1239:CL7:H62C	15:aB:1239:CL7:H101	1.66	0.41
3:aC:6:LYS:HE2	4:aD:138:TYR:HD2	1.86	0.41
1:bA:296:HIS:CE1	15:bA:1116:CL7:HAB	2.55	0.41
1:bA:349:TRP:HB3	15:bA:1103:CL7:HAC1	2.03	0.41
1:bA:569:SER:OG	4:bD:72:ARG:HD3	2.21	0.41
1:bA:589:GLY:O	1:bA:593:VAL:HG23	2.20	0.41
1:bA:695:TRP:HZ3	14:bA:1013:PHO:O1D	2.04	0.41
15:bA:1104:CL7:H111	15:bA:1104:CL7:H152	1.73	0.41
2:bB:372:HIS:HB2	15:bB:1224:CL7:CHB	2.51	0.41
2:bB:528:HIS:CE1	15:bB:1236:CL7:NA	2.89	0.41
15:bB:1239:CL7:H142	15:bB:1239:CL7:H112	1.75	0.41
7:bI:2:ILE:HG12	11:bM:5:ASP:HB3	2.03	0.41
1:cA:254:TYR:HB3	1:cA:274:ASP:OD2	2.21	0.41
2:cB:50:HIS:O	2:cB:54:LEU:HD23	2.21	0.41
2:cB:194:LEU:HA	2:cB:198:ALA:HB3	2.02	0.41
15:cB:1201:CL7:HMC3	15:cB:1203:CL7:OBD	2.21	0.41
1:aA:463:ARG:HH21	1:aA:471:MET:HE1	1.86	0.41
1:aA:695:TRP:HZ3	14:aA:1013:PHO:O1D	2.04	0.41
15:aA:1133:CL7:H202	15:aA:1133:CL7:H162	1.85	0.41
2:aB:141:PHE:O	2:aB:145:VAL:HG23	2.21	0.41
2:aB:176:ASN:CG	2:aB:291:TYR:HB2	2.45	0.41
2:aB:452:LEU:HD22	2:aB:614:THR:HG21	2.03	0.41
19:aB:5002:LMG:H372	19:aB:5002:LMG:H401	1.75	0.41
3:aC:61:ASP:HA	3:aC:62:PHE:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:aK:24:MET:SD	9:aK:73:GLY:HA3	2.60	0.41
11:aM:29:LEU:HD23	11:aM:29:LEU:HA	1.90	0.41
1:bA:720:MET:CE	1:bA:724:GLN:HG2	2.43	0.41
15:bA:1127:CL7:H2A	15:bA:1127:CL7:O2D	2.20	0.41
2:bB:30:ASP:O	2:bB:33:THR:HG22	2.21	0.41
2:bB:386:ALA:O	2:bB:390:ILE:HG13	2.21	0.41
2:bB:419:HIS:NE2	15:bB:1228:CL7:NA	2.69	0.41
15:bB:1237:CL7:HMC2	15:bB:1238:CL7:ND	2.36	0.41
15:bB:1207:CL7:H102	15:bB:1207:CL7:H13	1.93	0.41
5:bE:8:VAL:HG11	5:bE:65:LEU:HD23	2.03	0.41
9:bK:21:GLY:HA2	15:bK:1402:CL7:OBD	2.21	0.41
10:bL:12:PRO:HG2	10:bL:13:PHE:CD1	2.56	0.41
1:cA:74:PHE:HE2	1:cA:180:HIS:ND1	2.19	0.41
1:cA:278:PHE:CE2	1:cA:503:ALA:HB2	2.56	0.41
1:cA:294:ILE:HG23	15:cA:1117:CL7:HMA3	2.03	0.41
1:cA:296:HIS:HE1	15:cA:1115:CL7:C4D	2.33	0.41
1:cA:316:TRP:HE3	9:cK:60:ASN:HD21	1.68	0.41
1:cA:412:PHE:CD1	1:cA:416:ASP:HB2	2.56	0.41
15:cA:1119:CL7:H92C	15:cA:1119:CL7:H41C	2.02	0.41
15:cA:1124:CL7:HBA1	15:cA:1124:CL7:H3A	1.82	0.41
2:cB:426:PHE:HA	15:cB:1229:CL7:O1D	2.21	0.41
2:cB:555:TYR:HD1	15:cB:1226:CL7:HED2	1.85	0.41
15:cB:1210:CL7:H143	15:cB:1210:CL7:H111	1.77	0.41
4:cD:51:MET:O	4:cD:51:MET:HG3	2.20	0.41
9:cK:24:MET:CE	9:cK:70:HIS:HA	2.50	0.41
9:cK:83:LEU:HD23	9:cK:83:LEU:HA	1.92	0.41
12:cX:25:ILE:HA	12:cX:28:THR:HG22	2.03	0.41
1:aA:569:SER:OG	4:aD:72:ARG:HD3	2.21	0.41
2:aB:382:LEU:HD21	2:aB:580:THR:HA	2.03	0.41
15:aB:1212:CL7:H2A	15:aB:1212:CL7:HED2	2.02	0.41
15:aB:1212:CL7:HBA1	15:aB:1212:CL7:H3A	1.27	0.41
15:aB:1216:CL7:HBA2	15:aB:1216:CL7:H3A	1.95	0.41
4:aD:29:TYR:CE2	4:aD:63:LYS:HB2	2.56	0.41
4:aD:42:GLU:N	4:aD:73:GLN:HE22	2.19	0.41
6:aF:129:VAL:CG2	6:aF:130:PRO:HD3	2.51	0.41
10:aL:32:ASN:OD1	10:aL:110:THR:HG22	2.20	0.41
10:aL:59:TYR:OH	10:aL:75:LEU:HD13	2.21	0.41
12:aX:9:TRP:HB3	12:aX:10:PRO:HD3	2.03	0.41
1:bA:85:PHE:CE1	15:bA:1103:CL7:H142	2.56	0.41
1:bA:706:HIS:CE1	15:bA:1138:CL7:ND	2.89	0.41
15:bA:1108:CL7:HED3	15:bA:1108:CL7:HBD	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:bA:1109:CL7:H62C	15:bA:1109:CL7:H41C	1.88	0.41
2:bB:385:TYR:CD1	2:bB:534:CYS:HB3	2.56	0.41
15:bB:1209:CL7:H3A	15:bB:1209:CL7:HBA1	1.48	0.41
10:bL:136:GLY:HA3	17:bL:4023:A1JPJ:C31	2.51	0.41
15:cB:1203:CL7:H162	15:cB:1203:CL7:H122	1.78	0.41
15:cB:1222:CL7:HBA1	15:cB:1236:CL7:HAA2	2.01	0.41
1:aA:326:MET:HE2	1:aA:326:MET:HB3	1.92	0.40
1:aA:446:LEU:HD23	14:aB:1023:PHO:O1A	2.21	0.40
15:aA:1124:CL7:HBA1	15:aA:1124:CL7:H3A	1.83	0.40
15:aA:1127:CL7:H2A	15:aA:1127:CL7:O2D	2.21	0.40
15:aA:1137:CL7:H2A	15:aA:1137:CL7:O2D	2.21	0.40
2:aB:93:ASP:HB3	2:aB:96:LEU:HG	2.02	0.40
15:aB:1234:CL7:H3A	15:aB:1235:CL7:HAA2	2.03	0.40
4:aD:85:TYR:HA	4:aD:94:THR:O	2.21	0.40
5:aE:35:PRO:HD2	5:aE:61:GLY:HA2	2.03	0.40
15:aL:1503:CL7:HBA1	15:aL:1503:CL7:H3A	1.84	0.40
1:bA:709:LEU:HD21	15:bB:1228:CL7:H3A	2.02	0.40
2:bB:342:ILE:HG23	15:bB:1215:CL7:H71C	2.02	0.40
2:bB:420:LEU:HD13	15:bB:1236:CL7:C3B	2.51	0.40
9:bK:26:ALA:O	9:bK:30:MET:HG2	2.21	0.40
1:cA:206:LEU:HB3	1:cA:305:TYR:CD2	2.56	0.40
1:cA:527:VAL:O	1:cA:527:VAL:HG23	2.21	0.40
2:cB:430:HIS:HE1	15:cB:1229:CL7:C4D	2.33	0.40
6:cF:64:ALA:HA	6:cF:83:ARG:HH12	1.86	0.40
1:aA:524:MET:HE3	1:aA:525:GLN:H	1.85	0.40
15:aA:1109:CL7:H3A	15:aA:1109:CL7:HBA1	1.63	0.40
15:aA:1119:CL7:H41C	15:aA:1119:CL7:H92C	2.03	0.40
15:aA:1138:CL7:H112	15:aA:1138:CL7:H151	1.84	0.40
2:aB:196:HIS:CE1	2:aB:217:PRO:HG3	2.57	0.40
3:aC:5:VAL:HG11	3:aC:26:LEU:HD21	2.03	0.40
1:bA:85:PHE:HE1	15:bA:1103:CL7:H142	1.86	0.40
1:bA:357:LEU:HD23	1:bA:357:LEU:HA	1.89	0.40
15:bA:1104:CL7:H18	15:bA:1106:CL7:H42C	2.03	0.40
2:bB:363:TYR:HB3	2:bB:602:TRP:CE3	2.56	0.40
2:bB:410:LEU:O	2:bB:413:LYS:HG2	2.21	0.40
2:bB:715:VAL:HA	2:bB:718:PHE:CE2	2.57	0.40
15:bB:1202:CL7:H71C	15:bB:1210:CL7:HBA1	2.04	0.40
19:bB:5002:LMG:H301	19:bB:5002:LMG:H332	1.93	0.40
1:cA:349:TRP:HZ3	15:cA:1123:CL7:H111	1.86	0.40
15:cB:1221:CL7:H93C	15:cB:1221:CL7:H61C	1.67	0.40
3:cC:18:VAL:HG22	3:cC:26:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:cI:6:LEU:HD12	7:cI:6:LEU:HA	1.72	0.40
8:cJ:31:PHE:HE2	15:cJ:1301:CL7:HMA1	1.86	0.40
1:aA:197:THR:OG1	15:aA:1111:CL7:HBC2	2.22	0.40
1:aA:414:VAL:HG11	1:aA:572:PHE:N	2.35	0.40
1:aA:706:HIS:CD2	1:aA:711:ILE:HG23	2.56	0.40
15:aA:1126:CL7:H172	15:aA:1126:CL7:H13	1.94	0.40
15:aA:1128:CL7:H92C	15:aA:1128:CL7:H61C	1.87	0.40
15:aA:1131:CL7:H143	15:aA:1131:CL7:H161	1.97	0.40
15:aB:1238:CL7:ND	15:aB:1237:CL7:HMC2	2.36	0.40
9:aK:24:MET:HG2	15:aK:1402:CL7:C3D	2.52	0.40
1:bA:169:ALA:HA	1:bA:172:VAL:HG12	2.04	0.40
1:bA:367:CYS:O	1:bA:371:MET:HG3	2.22	0.40
17:bA:4014:A1JPJ:C17	15:bB:1229:CL7:H3A	2.51	0.40
2:bB:276:HIS:ND1	15:bB:1214:CL7:NB	2.70	0.40
15:bB:1203:CL7:H93C	15:bB:1203:CL7:H112	1.91	0.40
15:bB:1226:CL7:H2	19:bB:5002:LMG:H311	2.02	0.40
15:bB:1229:CL7:H52C	15:bB:1229:CL7:H8	1.91	0.40
9:bK:29:ILE:HA	9:bK:32:ILE:HG22	2.04	0.40
1:cA:749:ILE:HD12	1:cA:749:ILE:HA	1.94	0.40
15:cA:1103:CL7:HBA2	15:cA:1103:CL7:H3A	1.38	0.40
2:cB:48:ALA:HB3	11:cM:29:LEU:HD21	2.03	0.40
2:cB:310:ASP:HB3	2:cB:314:GLY:H	1.86	0.40
2:cB:363:TYR:HB3	2:cB:602:TRP:CE3	2.55	0.40
15:cB:1237:CL7:HMC2	15:cB:1238:CL7:ND	2.37	0.40
15:cB:1202:CL7:H122	15:cB:1202:CL7:H161	1.92	0.40
15:cB:1212:CL7:H3A	15:cB:1212:CL7:HBA1	1.26	0.40
1:aA:330:LYS:HB2	1:aA:335:GLY:O	2.21	0.40
1:aA:698:LEU:O	1:aA:702:ILE:HG12	2.21	0.40
1:aA:709:LEU:HD21	15:aB:1228:CL7:HBA2	2.03	0.40
15:aB:1202:CL7:H92C	15:aB:1202:CL7:H62C	1.90	0.40
6:aF:95:ILE:HD13	6:aF:95:ILE:HA	1.98	0.40
1:bA:44:GLN:NE2	5:bE:43:CYS:HB3	2.36	0.40
1:bA:746:LEU:HA	1:bA:749:ILE:HG22	2.03	0.40
15:bB:1212:CL7:HBA1	15:bB:1212:CL7:H3A	1.26	0.40
3:bC:29:VAL:HG21	4:bD:113:ALA:HB2	2.03	0.40
9:bK:26:ALA:O	9:bK:29:ILE:HG22	2.21	0.40
15:cB:1237:CL7:H162	15:cB:1237:CL7:H141	1.76	0.40
15:cB:1205:CL7:CGA	15:cB:1205:CL7:C1A	2.99	0.40
15:cB:1238:CL7:H12C	15:cB:1238:CL7:H51C	1.91	0.40
3:cC:75:ARG:HD3	4:cD:86:ARG:HH12	1.85	0.40
9:cK:17:THR:HB	9:cK:20:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:180:HIS:HE1	15:aA:1108:CL7:NA	2.20	0.40
1:aA:364:SER:HB2	15:aA:1127:CL7:HMC2	2.04	0.40
1:aA:706:HIS:CE1	15:aA:1138:CL7:ND	2.89	0.40
2:aB:312:TRP:CZ3	12:aX:12:LEU:HD11	2.55	0.40
15:aB:1226:CL7:H92C	15:aB:1226:CL7:H62C	1.90	0.40
8:aJ:30:GLY:O	8:aJ:34:GLU:HG2	2.21	0.40
1:bA:296:HIS:HE1	15:bA:1115:CL7:ND	2.19	0.40
1:bA:371:MET:HE1	15:bA:1127:CL7:C3D	2.52	0.40
2:bB:193:HIS:HB2	15:bB:1211:CL7:C1C	2.52	0.40
15:bB:1238:CL7:H51C	15:bB:1238:CL7:H12C	1.92	0.40
1:cA:53:HIS:CE1	15:cA:1101:CL7:NA	2.90	0.40
1:cA:684:SER:HB2	1:cA:729:GLY:O	2.21	0.40
2:cB:193:HIS:CE1	15:cB:1211:CL7:C4A	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	735/753 (98%)	717 (98%)	18 (2%)	0	100	100
1	bA	735/753 (98%)	715 (97%)	20 (3%)	0	100	100
1	cA	735/753 (98%)	716 (97%)	19 (3%)	0	100	100
2	aB	729/733 (100%)	708 (97%)	21 (3%)	0	100	100
2	bB	729/733 (100%)	701 (96%)	28 (4%)	0	100	100
2	cB	729/733 (100%)	702 (96%)	27 (4%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	bC	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	cC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	aD	134/139 (96%)	125 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	bD	134/139 (96%)	127 (95%)	7 (5%)	0	100	100
4	cD	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
5	aE	65/86 (76%)	63 (97%)	2 (3%)	0	100	100
5	bE	65/86 (76%)	61 (94%)	4 (6%)	0	100	100
5	cE	65/86 (76%)	62 (95%)	3 (5%)	0	100	100
6	aF	141/167 (84%)	137 (97%)	4 (3%)	0	100	100
6	bF	141/167 (84%)	136 (96%)	5 (4%)	0	100	100
6	cF	141/167 (84%)	136 (96%)	5 (4%)	0	100	100
7	aI	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
7	bI	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
7	cI	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
8	aJ	33/47 (70%)	33 (100%)	0	0	100	100
8	bJ	33/47 (70%)	33 (100%)	0	0	100	100
8	cJ	33/47 (70%)	33 (100%)	0	0	100	100
9	aK	50/86 (58%)	50 (100%)	0	0	100	100
9	bK	50/86 (58%)	50 (100%)	0	0	100	100
9	cK	50/86 (58%)	50 (100%)	0	0	100	100
10	aL	146/153 (95%)	142 (97%)	4 (3%)	0	100	100
10	bL	146/153 (95%)	140 (96%)	6 (4%)	0	100	100
10	cL	146/153 (95%)	141 (97%)	5 (3%)	0	100	100
11	aM	29/31 (94%)	29 (100%)	0	0	100	100
11	bM	29/31 (94%)	29 (100%)	0	0	100	100
11	cM	29/31 (94%)	29 (100%)	0	0	100	100
12	aX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
12	bX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
12	cX	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	6579/7011 (94%)	6372 (97%)	207 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	590/602 (98%)	590 (100%)	0	100	100
1	bA	590/602 (98%)	590 (100%)	0	100	100
1	cA	590/602 (98%)	590 (100%)	0	100	100
2	aB	592/593 (100%)	592 (100%)	0	100	100
2	bB	592/593 (100%)	592 (100%)	0	100	100
2	cB	592/593 (100%)	592 (100%)	0	100	100
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	110/112 (98%)	110 (100%)	0	100	100
4	bD	110/112 (98%)	110 (100%)	0	100	100
4	cD	110/112 (98%)	110 (100%)	0	100	100
5	aE	57/68 (84%)	57 (100%)	0	100	100
5	bE	57/68 (84%)	57 (100%)	0	100	100
5	cE	57/68 (84%)	57 (100%)	0	100	100
6	aF	111/131 (85%)	111 (100%)	0	100	100
6	bF	111/131 (85%)	111 (100%)	0	100	100
6	cF	111/131 (85%)	111 (100%)	0	100	100
7	aI	26/26 (100%)	26 (100%)	0	100	100
7	bI	26/26 (100%)	26 (100%)	0	100	100
7	cI	26/26 (100%)	26 (100%)	0	100	100
8	aJ	31/42 (74%)	31 (100%)	0	100	100
8	bJ	31/42 (74%)	31 (100%)	0	100	100
8	cJ	31/42 (74%)	31 (100%)	0	100	100
9	aK	40/65 (62%)	40 (100%)	0	100	100
9	bK	40/65 (62%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	cK	40/65 (62%)	40 (100%)	0	100	100
10	aL	110/113 (97%)	110 (100%)	0	100	100
10	bL	110/113 (97%)	110 (100%)	0	100	100
10	cL	110/113 (97%)	110 (100%)	0	100	100
11	aM	25/25 (100%)	25 (100%)	0	100	100
11	bM	25/25 (100%)	25 (100%)	0	100	100
11	cM	25/25 (100%)	25 (100%)	0	100	100
12	aX	19/22 (86%)	19 (100%)	0	100	100
12	bX	19/22 (86%)	19 (100%)	0	100	100
12	cX	19/22 (86%)	19 (100%)	0	100	100
All	All	5337/5604 (95%)	5337 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	36	ASN
1	aA	62	GLN
1	aA	136	HIS
1	aA	192	GLN
1	aA	210	ASN
1	aA	296	HIS
1	aA	321	HIS
1	aA	369	HIS
1	aA	408	HIS
1	aA	458	HIS
1	aA	480	GLN
1	aA	493	ASN
1	aA	525	GLN
1	aA	608	ASN
2	aB	196	HIS
2	aB	264	GLN
3	aC	16	GLN
4	aD	73	GLN
4	aD	93	ASN
4	aD	136	GLN
6	aF	109	GLN

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Mol	Chain	Res	Type
9	aK	60	ASN
9	aK	70	HIS
10	aL	33	ASN
1	bA	36	ASN
1	bA	62	GLN
1	bA	116	HIS
1	bA	136	HIS
1	bA	320	HIS
1	bA	369	HIS
1	bA	458	HIS
1	bA	488	GLN
1	bA	493	ASN
1	bA	608	ASN
2	bB	29	HIS
2	bB	156	HIS
2	bB	325	ASN
2	bB	419	HIS
2	bB	462	GLN
2	bB	465	HIS
4	bD	73	GLN
4	bD	93	ASN
4	bD	126	ASN
6	bF	103	ASN
8	bJ	36	ASN
12	bX	30	GLN
1	cA	62	GLN
1	cA	136	HIS
1	cA	192	GLN
1	cA	210	ASN
1	cA	296	HIS
1	cA	369	HIS
1	cA	458	HIS
1	cA	478	GLN
1	cA	480	GLN
1	cA	525	GLN
1	cA	526	HIS
1	cA	543	GLN
1	cA	608	ASN
2	cB	29	HIS
2	cB	156	HIS
2	cB	176	ASN
2	cB	193	HIS

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Mol	Chain	Res	Type
2	cB	277	HIS
2	cB	465	HIS
2	cB	704	GLN
3	cC	16	GLN
4	cD	93	ASN
6	cF	46	ASN
9	cK	60	ASN
9	cK	66	GLN
12	cX	30	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

369 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	CL7	bA	1102	15	58,60,73	1.47	9 (15%)	64,97,113	1.39	8 (12%)
15	CL7	aA	1129	1	56,58,73	1.49	10 (17%)	62,95,113	1.37	9 (14%)
15	CL7	aB	1233	-	47,49,73	1.61	9 (19%)	51,84,113	1.47	7 (13%)
15	CL7	aB	1216	21	51,53,73	1.59	10 (19%)	56,89,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	cB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	aI	1601	21	71,73,73	1.33	12 (16%)	80,113,113	1.24	6 (7%)
17	A1JPJ	cA	4014	-	40,41,41	1.82	8 (20%)	50,56,56	2.07	12 (24%)
15	CL7	cA	1103	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	bB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	aA	1115	1	47,49,73	1.60	11 (23%)	51,84,113	1.49	5 (9%)
15	CL7	cB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	aA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.24	6 (7%)
17	A1JPJ	cB	4010	-	40,41,41	1.70	8 (20%)	50,56,56	1.77	11 (22%)
15	CL7	cB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	6 (7%)
15	CL7	aA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
15	CL7	aB	1202	2	71,73,73	1.32	11 (15%)	80,113,113	1.21	5 (6%)
15	CL7	cA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
15	CL7	cB	1226	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	cA	1135	1	56,58,73	1.48	11 (19%)	62,95,113	1.44	9 (14%)
15	CL7	bF	1701	6	47,49,73	1.58	11 (23%)	51,84,113	1.46	7 (13%)
18	LHG	cA	5001	-	48,48,48	0.51	0	51,54,54	0.52	0
15	CL7	bB	1220	-	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	bA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.30	7 (10%)
15	CL7	cA	1122	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
15	CL7	bB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.39	6 (10%)
19	LMG	cB	5002	-	53,53,55	0.51	0	61,61,63	0.65	1 (1%)
15	CL7	cA	1138	-	71,73,73	1.31	11 (15%)	80,113,113	1.29	10 (12%)
15	CL7	bA	1022	21	71,73,73	1.32	12 (16%)	80,113,113	1.19	5 (6%)
15	CL7	bL	1503	21	66,68,73	1.37	11 (16%)	74,107,113	1.26	6 (8%)
15	CL7	aB	1226	2	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)
15	CL7	bB	1021	2	71,73,73	1.30	11 (15%)	80,113,113	1.17	6 (7%)
15	CL7	cB	1233	-	47,49,73	1.60	8 (17%)	51,84,113	1.45	6 (11%)
15	CL7	cB	1218	2	47,49,73	1.60	9 (19%)	51,84,113	1.48	6 (11%)
15	CL7	cB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)
15	CL7	aA	1022	21	71,73,73	1.32	12 (16%)	80,113,113	1.21	5 (6%)
15	CL7	cB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	8 (15%)
15	CL7	bA	1134	1	49,52,73	1.56	10 (20%)	56,87,113	1.43	5 (8%)
17	A1JPJ	aF	4016	-	40,41,41	1.77	8 (20%)	50,56,56	1.90	15 (30%)
17	A1JPJ	aB	4010	-	40,41,41	1.70	8 (20%)	50,56,56	1.75	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	aB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	cA	1131	1	71,73,73	1.33	12 (16%)	80,113,113	1.22	5 (6%)
15	CL7	bB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.24	6 (7%)
15	CL7	cL	1502	10	71,73,73	1.31	11 (15%)	80,113,113	1.32	8 (10%)
15	CL7	bB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.28	8 (10%)
15	CL7	bB	1201	2	60,62,73	1.44	11 (18%)	66,99,113	1.35	6 (9%)
15	CL7	bA	1117	1	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)
15	CL7	cA	1140	1	66,68,73	1.38	11 (16%)	74,107,113	1.24	6 (8%)
17	A1JPJ	bL	4023	-	40,41,41	1.66	8 (20%)	50,56,56	1.59	11 (22%)
17	A1JPJ	aB	4004	-	40,41,41	1.72	7 (17%)	50,56,56	1.79	10 (20%)
15	CL7	aB	1227	2	51,53,73	1.58	11 (21%)	56,89,113	1.36	5 (8%)
15	CL7	aB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	4 (7%)
15	CL7	bA	1127	1	71,73,73	1.30	12 (16%)	80,113,113	1.17	5 (6%)
15	CL7	aA	1123	21	71,73,73	1.35	12 (16%)	80,113,113	1.27	7 (8%)
15	CL7	cJ	1301	21	47,49,73	1.63	10 (21%)	51,84,113	1.46	7 (13%)
15	CL7	cB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	5 (8%)
15	CL7	aB	1224	2	62,64,73	1.41	11 (17%)	69,102,113	1.29	6 (8%)
17	A1JPJ	aB	4005	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	11 (22%)
15	CL7	cB	1236	2	51,53,73	1.55	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bB	1211	2	61,63,73	1.43	10 (16%)	68,101,113	1.32	7 (10%)
15	CL7	aB	1219	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
17	A1JPJ	cI	4018	-	40,41,41	1.63	8 (20%)	50,56,56	1.66	12 (24%)
15	CL7	aB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.38	8 (12%)
17	A1JPJ	cB	4006	-	40,41,41	1.79	8 (20%)	50,56,56	2.15	13 (26%)
17	A1JPJ	cA	4008	-	40,41,41	1.62	8 (20%)	50,56,56	1.63	11 (22%)
15	CL7	bA	1123	21	71,73,73	1.34	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	bB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.20	8 (10%)
20	SF4	aC	3002	3	0,12,12	-	-	-	-	-
15	CL7	cL	1503	21	66,68,73	1.38	11 (16%)	74,107,113	1.27	6 (8%)
15	CL7	cA	1117	1	71,73,73	1.33	11 (15%)	80,113,113	1.28	9 (11%)
14	PHO	bB	1023	-	58,69,69	1.96	12 (20%)	56,99,99	1.71	9 (16%)
17	A1JPJ	cF	4016	-	40,41,41	1.67	8 (20%)	50,56,56	1.70	10 (20%)
15	CL7	aB	1228	2	51,53,73	1.57	11 (21%)	56,89,113	1.37	5 (8%)
15	CL7	bA	1114	21	51,53,73	1.58	10 (19%)	56,89,113	1.38	5 (8%)
15	CL7	cA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	bB	1226	2	71,73,73	1.33	11 (15%)	80,113,113	1.27	9 (11%)
15	CL7	bJ	1302	8	47,50,73	1.63	9 (19%)	51,85,113	1.35	4 (7%)
15	CL7	bB	1204	2	71,73,73	1.33	10 (14%)	80,113,113	1.28	7 (8%)
15	CL7	bA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	bA	1135	1	56,58,73	1.49	11 (19%)	62,95,113	1.40	8 (12%)
17	A1JPJ	bA	4007	-	40,41,41	1.68	8 (20%)	50,56,56	1.61	11 (22%)
18	LHG	bA	5001	-	48,48,48	0.51	0	51,54,54	0.51	0
15	CL7	aA	1103	1	71,73,73	1.32	11 (15%)	80,113,113	1.25	6 (7%)
15	CL7	bA	1113	1	51,53,73	1.57	10 (19%)	56,89,113	1.39	5 (8%)
15	CL7	cB	1213	2	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
17	A1JPJ	cL	4023	-	40,41,41	1.66	8 (20%)	50,56,56	1.59	11 (22%)
20	SF4	aB	3001	2,1	0,12,12	-	-	-	-	-
15	CL7	aA	1112	1	71,73,73	1.33	11 (15%)	80,113,113	1.32	7 (8%)
15	CL7	cA	1106	1	71,73,73	1.31	12 (16%)	80,113,113	1.29	9 (11%)
15	CL7	bA	1109	15,1	71,73,73	1.34	10 (14%)	80,113,113	1.25	6 (7%)
15	CL7	aA	1121	1	61,63,73	1.42	11 (18%)	68,101,113	1.26	5 (7%)
15	CL7	aA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	6 (7%)
15	CL7	aB	1220	-	51,53,73	1.57	12 (23%)	56,89,113	1.40	5 (8%)
15	CL7	aA	1127	1	71,73,73	1.31	11 (15%)	80,113,113	1.18	5 (6%)
15	CL7	cA	1128	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	6 (7%)
17	A1JPJ	aA	4011	-	40,41,41	1.64	8 (20%)	50,56,56	1.63	9 (18%)
15	CL7	cA	1101	1	47,49,73	1.60	10 (21%)	51,84,113	1.50	8 (15%)
15	CL7	cB	1219	2	47,49,73	1.61	8 (17%)	51,84,113	1.49	6 (11%)
15	CL7	cB	1021	2	71,73,73	1.31	11 (15%)	80,113,113	1.16	5 (6%)
15	CL7	cA	1125	1	56,58,73	1.50	11 (19%)	62,95,113	1.38	8 (12%)
17	A1JPJ	aB	4006	-	40,41,41	1.78	8 (20%)	50,56,56	2.12	14 (28%)
16	PQN	bA	2001	-	34,34,34	0.35	0	42,45,45	0.66	1 (2%)
15	CL7	bB	1212	2	51,53,73	1.57	10 (19%)	56,89,113	1.43	7 (12%)
15	CL7	cB	1239	2	71,73,73	1.32	12 (16%)	80,113,113	1.27	7 (8%)
17	A1JPJ	aA	4003	-	40,41,41	1.65	8 (20%)	50,56,56	1.59	10 (20%)
15	CL7	aA	1134	1	49,52,73	1.56	10 (20%)	56,87,113	1.44	7 (12%)
15	CL7	bB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.31	6 (8%)
15	CL7	bB	1239	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	cB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.19	8 (10%)
15	CL7	aK	1401	-	51,53,73	1.59	11 (21%)	56,89,113	1.44	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	A1JPJ	aA	4008	-	40,41,41	1.63	8 (20%)	50,56,56	1.61	12 (24%)
15	CL7	aA	1135	1	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
16	PQN	aA	2001	-	34,34,34	0.36	0	42,45,45	0.65	2 (4%)
18	LHG	aA	5001	-	48,48,48	0.51	0	51,54,54	0.51	0
15	CL7	cB	1229	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	bA	1119	21	61,63,73	1.44	11 (18%)	68,101,113	1.33	8 (11%)
15	CL7	aA	1126	1	71,73,73	1.32	11 (15%)	80,113,113	1.21	5 (6%)
15	CL7	aF	1701	6	47,49,73	1.59	10 (21%)	51,84,113	1.46	8 (15%)
15	CL7	aB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.29	9 (11%)
15	CL7	cA	1121	1	61,63,73	1.41	10 (16%)	68,101,113	1.26	6 (8%)
15	CL7	aB	1221	2	66,68,73	1.41	12 (18%)	74,107,113	1.29	7 (9%)
15	CL7	cB	1241	2	51,53,73	1.56	10 (19%)	56,89,113	1.35	6 (10%)
15	CL7	aB	1236	2	51,53,73	1.56	11 (21%)	56,89,113	1.40	5 (8%)
15	CL7	cA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.40	6 (10%)
15	CL7	bA	1122	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
15	CL7	bA	1130	1	57,59,73	1.47	11 (19%)	63,96,113	1.39	7 (11%)
17	A1JPJ	aJ	4012	-	40,41,41	1.66	8 (20%)	50,56,56	1.88	13 (26%)
15	CL7	bB	1213	2	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
15	CL7	cA	1119	21	61,63,73	1.44	11 (18%)	68,101,113	1.32	7 (10%)
15	CL7	bB	1216	21	51,53,73	1.59	11 (21%)	56,89,113	1.39	5 (8%)
15	CL7	bA	1124	21	56,58,73	1.47	11 (19%)	62,95,113	1.42	7 (11%)
15	CL7	bA	1801	18	47,49,73	1.58	11 (23%)	51,84,113	1.46	6 (11%)
15	CL7	cB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.32	6 (8%)
15	CL7	aA	1131	1	71,73,73	1.33	11 (15%)	80,113,113	1.21	6 (7%)
15	CL7	bB	1206	2	56,58,73	1.48	10 (17%)	62,95,113	1.38	8 (12%)
20	SF4	bC	3002	3	0,12,12	-	-	-	-	-
15	CL7	aA	1139	21	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	cI	1601	21	71,73,73	1.33	10 (14%)	80,113,113	1.24	5 (6%)
15	CL7	bB	1219	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	aA	1105	1	51,53,73	1.55	11 (21%)	56,89,113	1.41	5 (8%)
15	CL7	bB	1214	2	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
15	CL7	aA	1110	21	51,53,73	1.57	9 (17%)	56,89,113	1.44	6 (10%)
15	CL7	bA	1136	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	6 (7%)
15	CL7	aB	1209	2	51,53,73	1.58	9 (17%)	56,89,113	1.42	5 (8%)
15	CL7	aB	1208	2	71,73,73	1.33	10 (14%)	80,113,113	1.20	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	bJ	1301	21	47,49,73	1.61	9 (19%)	51,84,113	1.46	6 (11%)
15	CL7	bA	1129	1	56,58,73	1.49	10 (17%)	62,95,113	1.34	8 (12%)
15	CL7	cB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	cF	1701	6	47,49,73	1.58	10 (21%)	51,84,113	1.47	9 (17%)
15	CL7	aB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.28	7 (8%)
15	CL7	bB	1207	2	71,73,73	1.32	11 (15%)	80,113,113	1.27	8 (10%)
15	CL7	cA	1107	1	51,53,73	1.56	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bA	1131	1	71,73,73	1.32	12 (16%)	80,113,113	1.21	5 (6%)
15	CL7	aA	1102	15,1	58,60,73	1.47	10 (17%)	64,97,113	1.37	8 (12%)
15	CL7	bA	1110	21	51,53,73	1.57	10 (19%)	56,89,113	1.45	6 (10%)
15	CL7	bB	1234	2	56,58,73	1.50	12 (21%)	62,95,113	1.39	8 (12%)
15	CL7	aB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.39	6 (10%)
16	PQN	cA	2001	-	34,34,34	0.35	0	42,45,45	0.61	1 (2%)
14	PHO	aA	1013	-	58,69,69	1.99	12 (20%)	56,99,99	1.72	8 (14%)
15	CL7	aA	1117	1	71,73,73	1.33	10 (14%)	80,113,113	1.31	8 (10%)
17	A1JPJ	aI	4018	-	40,41,41	1.63	8 (20%)	50,56,56	1.65	12 (24%)
15	CL7	aA	1111	1	71,73,73	1.33	10 (14%)	80,113,113	1.25	7 (8%)
15	CL7	aB	1210	2	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
15	CL7	cA	1110	21	51,53,73	1.56	11 (21%)	56,89,113	1.44	6 (10%)
15	CL7	cA	1115	1	47,49,73	1.60	11 (23%)	51,84,113	1.52	6 (11%)
17	A1JPJ	bA	4003	-	40,41,41	1.65	8 (20%)	50,56,56	1.60	10 (20%)
15	CL7	bB	1238	21	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
15	CL7	bA	1103	1	71,73,73	1.33	11 (15%)	80,113,113	1.24	7 (8%)
17	A1JPJ	cB	4017	-	40,41,41	1.67	8 (20%)	50,56,56	1.74	10 (20%)
15	CL7	bA	1118	1	61,63,73	1.44	10 (16%)	68,101,113	1.31	8 (11%)
15	CL7	aA	1104	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	6 (7%)
15	CL7	aB	1215	2	61,63,73	1.43	12 (19%)	68,101,113	1.31	6 (8%)
17	A1JPJ	aL	4023	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	12 (24%)
17	A1JPJ	aA	4014	-	40,41,41	1.85	8 (20%)	50,56,56	2.10	12 (24%)
15	CL7	aA	1109	15,1	71,73,73	1.34	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	cA	1139	21	51,53,73	1.57	11 (21%)	56,89,113	1.39	5 (8%)
17	A1JPJ	bA	4002	-	40,41,41	1.70	8 (20%)	50,56,56	1.63	10 (20%)
15	CL7	bA	1104	1	71,73,73	1.34	10 (14%)	80,113,113	1.23	6 (7%)
15	CL7	cA	1129	1	56,58,73	1.49	11 (19%)	62,95,113	1.37	7 (11%)
19	LMG	bB	5002	-	53,53,55	0.51	0	61,61,63	0.65	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	aB	1213	2	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bB	1227	2	51,53,73	1.59	10 (19%)	56,89,113	1.41	7 (12%)
15	CL7	aB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	6 (7%)
15	CL7	cB	1222	21	51,53,73	1.55	11 (21%)	56,89,113	1.40	6 (10%)
17	A1JPJ	aB	4015	-	40,41,41	1.67	8 (20%)	50,56,56	1.98	15 (30%)
15	CL7	bB	1209	2	51,53,73	1.58	9 (17%)	56,89,113	1.41	5 (8%)
15	CL7	cB	1202	2	71,73,73	1.33	12 (16%)	80,113,113	1.22	5 (6%)
15	CL7	aB	1211	2	61,63,73	1.42	10 (16%)	68,101,113	1.32	6 (8%)
17	A1JPJ	aA	4002	-	40,41,41	1.70	8 (20%)	50,56,56	1.64	10 (20%)
16	PQN	aB	2002	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
15	CL7	cB	1208	2	71,73,73	1.32	10 (14%)	80,113,113	1.20	4 (5%)
15	CL7	bA	1106	1	71,73,73	1.32	12 (16%)	80,113,113	1.27	7 (8%)
15	CL7	bB	1236	2	51,53,73	1.56	11 (21%)	56,89,113	1.39	5 (8%)
17	A1JPJ	cB	4005	-	40,41,41	1.70	8 (20%)	50,56,56	1.77	12 (24%)
17	A1JPJ	cA	4002	-	40,41,41	1.68	8 (20%)	50,56,56	1.62	9 (18%)
15	CL7	cB	1210	2	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	bB	1208	2	71,73,73	1.32	10 (14%)	80,113,113	1.21	6 (7%)
15	CL7	aK	1402	9	45,45,73	1.61	11 (24%)	49,78,113	1.41	7 (14%)
20	SF4	bB	3001	2,1	0,12,12	-	-	-	-	-
15	CL7	aB	1204	2	71,73,73	1.33	11 (15%)	80,113,113	1.29	7 (8%)
15	CL7	bA	1105	1	51,53,73	1.55	11 (21%)	56,89,113	1.41	5 (8%)
13	G9R	bA	1011	1	54,71,71	2.34	10 (18%)	54,104,104	1.33	9 (16%)
15	CL7	bA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bA	1111	1	71,73,73	1.34	11 (15%)	80,113,113	1.25	8 (10%)
15	CL7	cB	1215	2	61,63,73	1.41	9 (14%)	68,101,113	1.27	10 (14%)
15	CL7	aJ	1302	8	47,50,73	1.63	8 (17%)	51,85,113	1.38	4 (7%)
17	A1JPJ	bB	4005	-	40,41,41	1.69	8 (20%)	50,56,56	1.77	12 (24%)
15	CL7	bB	1210	2	71,73,73	1.34	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	cB	1206	2	56,58,73	1.48	11 (19%)	62,95,113	1.38	7 (11%)
15	CL7	aA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.30	7 (10%)
15	CL7	cB	1224	2	62,64,73	1.42	11 (17%)	69,102,113	1.23	4 (5%)
17	A1JPJ	bB	4017	-	40,41,41	1.67	8 (20%)	50,56,56	1.76	10 (20%)
15	CL7	aA	1132	1	71,73,73	1.39	13 (18%)	80,113,113	1.25	11 (13%)
15	CL7	cA	1137	1	61,63,73	1.43	11 (18%)	68,101,113	1.32	7 (10%)
13	G9R	aA	1011	1	54,71,71	2.32	10 (18%)	54,104,104	1.33	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	aB	1232	21	47,49,73	1.60	10 (21%)	51,84,113	1.42	6 (11%)
15	CL7	bL	1501	10	66,68,73	1.37	10 (15%)	74,107,113	1.31	6 (8%)
15	CL7	cB	1211	2	61,63,73	1.43	10 (16%)	68,101,113	1.30	5 (7%)
17	A1JPJ	aI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.56	9 (18%)
14	PHO	cA	1013	-	58,69,69	1.98	11 (18%)	56,99,99	1.76	9 (16%)
15	CL7	bA	1101	1	47,49,73	1.59	12 (25%)	51,84,113	1.50	8 (15%)
18	LHG	cA	5003	15	37,37,48	0.56	0	40,43,54	0.55	0
15	CL7	cB	1205	2	71,73,73	1.30	12 (16%)	80,113,113	1.28	8 (10%)
17	A1JPJ	aL	4020	-	40,41,41	1.64	8 (20%)	50,56,56	1.65	10 (20%)
15	CL7	aB	1203	2	71,73,73	1.32	11 (15%)	80,113,113	1.24	5 (6%)
17	A1JPJ	bB	4010	-	40,41,41	1.69	8 (20%)	50,56,56	1.76	12 (24%)
15	CL7	aB	1235	2	66,68,73	1.37	11 (16%)	74,107,113	1.31	6 (8%)
15	CL7	cB	1221	2	66,68,73	1.42	11 (16%)	74,107,113	1.29	8 (10%)
15	CL7	aB	1218	2	47,49,73	1.60	9 (19%)	51,84,113	1.48	6 (11%)
15	CL7	bB	1237	21	71,73,73	1.32	12 (16%)	80,113,113	1.23	5 (6%)
15	CL7	aA	1106	1	71,73,73	1.31	12 (16%)	80,113,113	1.29	8 (10%)
15	CL7	bA	1126	1	71,73,73	1.41	11 (15%)	80,113,113	1.23	6 (7%)
15	CL7	aA	1138	1	71,73,73	1.31	11 (15%)	80,113,113	1.28	7 (8%)
15	CL7	bA	1132	1	71,73,73	1.31	12 (16%)	80,113,113	1.31	9 (11%)
17	A1JPJ	bB	4015	-	40,41,41	1.68	8 (20%)	50,56,56	1.91	16 (32%)
15	CL7	aB	1212	2	51,53,73	1.57	11 (21%)	56,89,113	1.44	7 (12%)
15	CL7	cA	1134	1	49,52,73	1.56	11 (22%)	56,87,113	1.42	5 (8%)
17	A1JPJ	aB	4021	-	40,41,41	1.65	8 (20%)	50,56,56	1.55	10 (20%)
15	CL7	cB	1204	2	71,73,73	1.34	13 (18%)	80,113,113	1.30	7 (8%)
15	CL7	bK	1401	-	51,53,73	1.59	9 (17%)	56,89,113	1.43	6 (10%)
17	A1JPJ	bL	4020	-	40,41,41	1.64	8 (20%)	50,56,56	1.62	10 (20%)
17	A1JPJ	cJ	4012	-	40,41,41	1.66	8 (20%)	50,56,56	1.88	12 (24%)
20	SF4	aC	3003	3	0,12,12	-	-	-	-	-
15	CL7	aA	1120	1	51,53,73	1.59	11 (21%)	56,89,113	1.41	6 (10%)
15	CL7	bB	1229	2	71,73,73	1.33	10 (14%)	80,113,113	1.23	6 (7%)
15	CL7	cA	1112	1	71,73,73	1.33	11 (15%)	80,113,113	1.34	10 (12%)
17	A1JPJ	bB	4004	-	40,41,41	1.73	7 (17%)	50,56,56	1.79	10 (20%)
15	CL7	cA	1133	1	71,73,73	1.33	10 (14%)	80,113,113	1.26	7 (8%)
15	CL7	cA	1126	1	71,73,73	1.32	11 (15%)	80,113,113	1.20	4 (5%)
15	CL7	cB	1232	21	47,49,73	1.61	9 (19%)	51,84,113	1.44	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	cA	1801	18	47,49,73	1.58	11 (23%)	51,84,113	1.48	7 (13%)
15	CL7	cB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.48	6 (11%)
15	CL7	bI	1601	21	71,73,73	1.32	12 (16%)	80,113,113	1.22	4 (5%)
15	CL7	bB	1233	-	47,49,73	1.61	8 (17%)	51,84,113	1.43	5 (9%)
15	CL7	cB	1220	-	51,53,73	1.58	11 (21%)	56,89,113	1.43	6 (10%)
15	CL7	bB	1224	2	62,64,73	1.42	11 (17%)	69,102,113	1.25	5 (7%)
15	CL7	bA	1140	1	66,68,73	1.38	11 (16%)	74,107,113	1.24	6 (8%)
14	PHO	aB	1023	-	58,69,69	1.95	12 (20%)	56,99,99	1.66	8 (14%)
15	CL7	aA	1101	1	47,49,73	1.59	9 (19%)	51,84,113	1.49	8 (15%)
15	CL7	bA	1107	1	51,53,73	1.56	11 (21%)	56,89,113	1.40	6 (10%)
17	A1JPJ	cA	4003	-	40,41,41	1.64	8 (20%)	50,56,56	1.59	10 (20%)
15	CL7	aB	1206	2	56,58,73	1.48	12 (21%)	62,95,113	1.39	7 (11%)
15	CL7	aB	1012	21	71,73,73	1.32	12 (16%)	80,113,113	1.20	7 (8%)
15	CL7	aA	1118	1	61,63,73	1.44	11 (18%)	68,101,113	1.31	7 (10%)
15	CL7	aA	1130	1	57,59,73	1.47	11 (19%)	63,96,113	1.37	6 (9%)
17	A1JPJ	bI	4018	-	40,41,41	1.64	8 (20%)	50,56,56	1.66	12 (24%)
15	CL7	aA	1124	21	56,58,73	1.48	11 (19%)	62,95,113	1.40	7 (11%)
15	CL7	bB	1228	2	51,53,73	1.57	10 (19%)	56,89,113	1.35	3 (5%)
15	CL7	aB	1241	2	51,53,73	1.56	9 (17%)	56,89,113	1.38	6 (10%)
15	CL7	bA	1115	1	47,49,73	1.61	11 (23%)	51,84,113	1.48	8 (15%)
20	SF4	cB	3001	2,1	0,12,12	-	-	-	-	-
15	CL7	cB	1223	2	71,73,73	1.34	11 (15%)	80,113,113	1.24	6 (7%)
15	CL7	cK	1402	9	45,45,73	1.64	10 (22%)	49,78,113	1.45	6 (12%)
15	CL7	cA	1124	21	56,58,73	1.48	11 (19%)	62,95,113	1.41	7 (11%)
17	A1JPJ	cL	4020	-	40,41,41	1.65	8 (20%)	50,56,56	1.64	10 (20%)
20	SF4	bC	3003	3	0,12,12	-	-	-	-	-
15	CL7	bB	1218	2	47,49,73	1.61	11 (23%)	51,84,113	1.48	6 (11%)
20	SF4	cC	3003	3	0,12,12	-	-	-	-	-
15	CL7	bA	1139	21	51,53,73	1.57	10 (19%)	56,89,113	1.40	5 (8%)
15	CL7	bB	1215	2	61,63,73	1.42	12 (19%)	68,101,113	1.30	6 (8%)
15	CL7	cB	1234	2	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
16	PQN	cB	2002	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
17	A1JPJ	bB	4006	-	40,41,41	1.78	8 (20%)	50,56,56	2.10	12 (24%)
15	CL7	aB	1021	2	71,73,73	1.30	10 (14%)	80,113,113	1.16	5 (6%)
15	CL7	cB	1228	2	51,53,73	1.58	11 (21%)	56,89,113	1.38	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PHO	cB	1023	-	58,69,69	1.95	12 (20%)	56,99,99	1.63	8 (14%)
15	CL7	bB	1232	21	47,49,73	1.62	11 (23%)	51,84,113	1.43	7 (13%)
15	CL7	aL	1502	10	71,73,73	1.30	11 (15%)	80,113,113	1.32	9 (11%)
15	CL7	cA	1118	1	61,63,73	1.43	10 (16%)	68,101,113	1.32	7 (10%)
15	CL7	cA	1130	1	57,59,73	1.46	11 (19%)	63,96,113	1.37	7 (11%)
15	CL7	aA	1801	18	47,49,73	1.58	10 (21%)	51,84,113	1.45	6 (11%)
15	CL7	bB	1225	2	71,73,73	1.32	12 (16%)	80,113,113	1.19	7 (8%)
15	CL7	cA	1104	1	71,73,73	1.33	11 (15%)	80,113,113	1.25	6 (7%)
17	A1JPJ	cB	4015	-	40,41,41	1.68	8 (20%)	50,56,56	1.92	15 (30%)
15	CL7	cA	1111	1	71,73,73	1.33	11 (15%)	80,113,113	1.24	8 (10%)
15	CL7	cK	1401	-	51,53,73	1.59	9 (17%)	56,89,113	1.43	5 (8%)
17	A1JPJ	bA	4008	-	40,41,41	1.62	8 (20%)	50,56,56	1.63	10 (20%)
15	CL7	bA	1112	1	71,73,73	1.34	11 (15%)	80,113,113	1.30	8 (10%)
15	CL7	bB	1223	2	71,73,73	1.34	12 (16%)	80,113,113	1.24	6 (7%)
15	CL7	aB	1229	2	71,73,73	1.34	11 (15%)	80,113,113	1.23	7 (8%)
15	CL7	cB	1209	2	51,53,73	1.58	8 (15%)	56,89,113	1.40	6 (10%)
14	PHO	bA	1013	-	58,69,69	1.97	12 (20%)	56,99,99	1.73	8 (14%)
15	CL7	bA	1116	1	66,68,73	1.38	11 (16%)	74,107,113	1.29	7 (9%)
17	A1JPJ	cA	4011	-	40,41,41	1.64	8 (20%)	50,56,56	1.66	9 (18%)
17	A1JPJ	bA	4011	-	40,41,41	1.63	8 (20%)	50,56,56	1.64	8 (16%)
15	CL7	cL	1501	10	66,68,73	1.38	11 (16%)	74,107,113	1.31	7 (9%)
15	CL7	aB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	10 (19%)
15	CL7	cB	1216	21	51,53,73	1.58	11 (21%)	56,89,113	1.42	6 (10%)
15	CL7	bB	1241	2	51,53,73	1.57	10 (19%)	56,89,113	1.35	5 (8%)
20	SF4	cC	3002	3	0,12,12	-	-	-	-	-
17	A1JPJ	cI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.55	9 (18%)
15	CL7	aA	1116	1	66,68,73	1.39	11 (16%)	74,107,113	1.29	6 (8%)
18	LHG	aA	5003	15	37,37,48	0.57	0	40,43,54	0.57	0
15	CL7	aA	1125	1	56,58,73	1.51	11 (19%)	62,95,113	1.40	8 (12%)
17	A1JPJ	bF	4016	-	40,41,41	1.68	8 (20%)	50,56,56	1.85	14 (28%)
15	CL7	aL	1501	10	66,68,73	1.38	11 (16%)	74,107,113	1.33	7 (9%)
15	CL7	aA	1128	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	5 (6%)
17	A1JPJ	bA	4014	-	40,41,41	1.85	8 (20%)	50,56,56	2.11	12 (24%)
15	CL7	cJ	1302	8	47,50,73	1.64	8 (17%)	51,85,113	1.36	4 (7%)
15	CL7	cA	1116	1	66,68,73	1.39	12 (18%)	74,107,113	1.30	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	A1JPJ	bJ	4012	-	40,41,41	1.68	8 (20%)	50,56,56	1.89	13 (26%)
17	A1JPJ	cB	4021	-	40,41,41	1.66	8 (20%)	50,56,56	1.55	10 (20%)
13	G9R	cA	1011	1	54,71,71	2.34	10 (18%)	54,104,104	1.32	9 (16%)
15	CL7	cA	1022	21	71,73,73	1.33	11 (15%)	80,113,113	1.20	6 (7%)
15	CL7	aB	1201	2	60,62,73	1.44	12 (20%)	66,99,113	1.34	6 (9%)
15	CL7	aB	1225	2	71,73,73	1.31	11 (15%)	80,113,113	1.17	7 (8%)
15	CL7	bA	1108	1	57,59,73	1.48	10 (17%)	63,96,113	1.31	5 (7%)
15	CL7	bA	1128	1	71,73,73	1.32	11 (15%)	80,113,113	1.23	5 (6%)
17	A1JPJ	aA	4007	-	40,41,41	1.68	8 (20%)	50,56,56	1.60	11 (22%)
15	CL7	bA	1125	1	56,58,73	1.49	12 (21%)	62,95,113	1.40	8 (12%)
15	CL7	aB	1223	2	71,73,73	1.33	12 (16%)	80,113,113	1.25	7 (8%)
15	CL7	bB	1202	2	71,73,73	1.33	12 (16%)	80,113,113	1.22	6 (7%)
15	CL7	cA	1109	15,1	71,73,73	1.33	9 (12%)	80,113,113	1.25	5 (6%)
15	CL7	bK	1402	9	45,45,73	1.64	9 (20%)	49,78,113	1.42	5 (10%)
15	CL7	aB	1217	2	47,49,73	1.60	8 (17%)	51,84,113	1.46	6 (11%)
15	CL7	aL	1503	21	66,68,73	1.38	11 (16%)	74,107,113	1.27	6 (8%)
17	A1JPJ	aB	4017	-	40,41,41	1.68	8 (20%)	50,56,56	1.77	10 (20%)
15	CL7	cB	1212	2	51,53,73	1.56	10 (19%)	56,89,113	1.43	7 (12%)
15	CL7	cB	1227	2	51,53,73	1.57	11 (21%)	56,89,113	1.39	6 (10%)
15	CL7	aB	1234	2	56,58,73	1.50	11 (19%)	62,95,113	1.39	8 (12%)
15	CL7	cA	1123	21	71,73,73	1.35	12 (16%)	80,113,113	1.29	6 (7%)
15	CL7	cA	1105	1	51,53,73	1.56	11 (21%)	56,89,113	1.40	5 (8%)
15	CL7	cA	1102	15,1	58,60,73	1.48	9 (15%)	64,97,113	1.39	7 (10%)
15	CL7	aA	1140	1	66,68,73	1.37	11 (16%)	74,107,113	1.23	6 (8%)
15	CL7	bL	1502	10	71,73,73	1.30	11 (15%)	80,113,113	1.32	8 (10%)
17	A1JPJ	cA	4007	-	40,41,41	1.69	8 (20%)	50,56,56	1.62	11 (22%)
15	CL7	cA	1132	1	71,73,73	1.39	14 (19%)	80,113,113	1.26	11 (13%)
15	CL7	aB	1239	2	71,73,73	1.32	11 (15%)	80,113,113	1.26	7 (8%)
15	CL7	aA	1113	1	51,53,73	1.56	10 (19%)	56,89,113	1.42	6 (10%)
15	CL7	bB	1230	2	47,49,73	1.57	11 (23%)	51,84,113	1.62	10 (19%)
18	LHG	bA	5003	15	37,37,48	0.57	0	40,43,54	0.56	0
15	CL7	cA	1113	1	51,53,73	1.56	9 (17%)	56,89,113	1.42	6 (10%)
15	CL7	aA	1119	21	61,63,73	1.44	12 (19%)	68,101,113	1.33	7 (10%)
15	CL7	aJ	1301	21	47,49,73	1.62	10 (21%)	51,84,113	1.46	7 (13%)
15	CL7	cB	1201	2	60,62,73	1.44	12 (20%)	66,99,113	1.33	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CL7	cB	1225	2	71,73,73	1.32	11 (15%)	80,113,113	1.18	5 (6%)
15	CL7	bA	1138	1	71,73,73	1.31	11 (15%)	80,113,113	1.29	6 (7%)
17	A1JPJ	bI	4019	-	40,41,41	1.66	8 (20%)	50,56,56	1.56	9 (18%)
15	CL7	bB	1221	2	66,68,73	1.41	10 (15%)	74,107,113	1.28	8 (10%)
15	CL7	aA	1108	1	57,59,73	1.50	10 (17%)	63,96,113	1.31	4 (6%)
17	A1JPJ	bB	4021	-	40,41,41	1.66	8 (20%)	50,56,56	1.54	10 (20%)
15	CL7	bA	1121	1	61,63,73	1.43	10 (16%)	68,101,113	1.27	5 (7%)
15	CL7	cA	1108	1	57,59,73	1.49	10 (17%)	63,96,113	1.32	4 (6%)
15	CL7	aA	1107	1	51,53,73	1.57	11 (21%)	56,89,113	1.40	6 (10%)
17	A1JPJ	cB	4004	-	40,41,41	1.73	7 (17%)	50,56,56	1.80	10 (20%)
15	CL7	cA	1127	1	71,73,73	1.31	11 (15%)	80,113,113	1.19	5 (6%)
16	PQN	bB	2002	-	34,34,34	0.36	0	42,45,45	0.54	1 (2%)
19	LMG	aB	5002	-	53,53,55	0.51	0	61,61,63	0.71	1 (1%)
15	CL7	bB	1231	2	51,53,73	1.57	11 (21%)	56,89,113	1.36	4 (7%)
15	CL7	aA	1122	1	71,73,73	1.34	12 (16%)	80,113,113	1.23	5 (6%)

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
15	CL7	bA	1102	15	2/2/12/20	8/24/100/115	-
15	CL7	aA	1129	1	2/2/12/20	7/21/97/115	-
15	CL7	aB	1233	-	2/2/10/20	2/10/86/115	-
15	CL7	aB	1216	21	2/2/11/20	5/15/91/115	-
15	CL7	cB	1214	2	2/2/12/20	3/21/97/115	-
15	CL7	aI	1601	21	2/2/15/20	13/39/115/115	-
17	A1JPJ	cA	4014	-	-	8/29/63/63	0/2/2/2
15	CL7	cA	1103	1	2/2/15/20	16/39/115/115	-
15	CL7	bB	1217	2	2/2/10/20	1/10/86/115	-
15	CL7	aA	1115	1	2/2/10/20	4/10/86/115	-
15	CL7	cB	1207	2	2/2/15/20	11/39/115/115	-
15	CL7	aA	1136	1	2/2/15/20	19/39/115/115	-
17	A1JPJ	cB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	cB	1237	21	2/2/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	aA	1114	21	2/2/11/20	2/15/91/115	-
15	CL7	aB	1202	2	2/2/15/20	23/39/115/115	-
15	CL7	cA	1114	21	2/2/11/20	4/15/91/115	-
15	CL7	cB	1226	2	2/2/15/20	13/39/115/115	-
15	CL7	cA	1135	1	2/2/12/20	12/21/97/115	-
15	CL7	bF	1701	6	2/2/10/20	4/10/86/115	-
18	LHG	cA	5001	-	-	18/53/53/53	-
15	CL7	bB	1220	-	2/2/11/20	11/15/91/115	-
15	CL7	bA	1137	1	2/2/13/20	10/27/103/115	-
15	CL7	cA	1122	1	2/2/15/20	9/39/115/115	-
15	CL7	bB	1222	21	2/2/11/20	11/15/91/115	-
19	LMG	cB	5002	-	-	15/48/68/70	0/1/1/1
15	CL7	cA	1138	-	2/2/15/20	10/39/115/115	-
15	CL7	bA	1022	21	2/2/15/20	5/39/115/115	-
15	CL7	bL	1503	21	2/2/14/20	12/33/109/115	-
15	CL7	aB	1226	2	2/2/15/20	13/39/115/115	-
15	CL7	bB	1021	2	2/2/15/20	10/39/115/115	-
15	CL7	cB	1233	-	2/2/10/20	2/10/86/115	-
15	CL7	cB	1218	2	2/2/10/20	4/10/86/115	-
15	CL7	cB	1203	2	2/2/15/20	13/39/115/115	-
15	CL7	aA	1022	21	2/2/15/20	10/39/115/115	-
15	CL7	cB	1230	2	2/2/10/20	6/10/86/115	-
15	CL7	bA	1134	1	2/2/10/20	7/15/87/115	-
17	A1JPJ	aF	4016	-	-	9/29/63/63	0/2/2/2
17	A1JPJ	aB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	aB	1238	21	2/2/15/20	10/39/115/115	-
15	CL7	cA	1131	1	2/2/15/20	9/39/115/115	-
15	CL7	bB	1203	2	2/2/15/20	12/39/115/115	-
15	CL7	cL	1502	10	2/2/15/20	19/39/115/115	-
15	CL7	bB	1205	2	2/2/15/20	11/39/115/115	-
15	CL7	bB	1201	2	2/2/12/20	13/26/102/115	-
15	CL7	bA	1117	1	2/2/15/20	16/39/115/115	-
15	CL7	cA	1140	1	2/2/14/20	14/33/109/115	-
17	A1JPJ	bL	4023	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	A1JPJ	aB	4004	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	aB	1231	2	2/2/11/20	0/15/91/115	-
15	CL7	bA	1127	1	2/2/15/20	20/39/115/115	-
15	CL7	aA	1123	21	2/2/15/20	15/39/115/115	-
15	CL7	cJ	1301	21	2/2/10/20	5/10/86/115	-
15	CL7	cB	1231	2	2/2/11/20	2/15/91/115	-
15	CL7	aB	1224	2	2/2/13/20	13/29/105/115	-
17	A1JPJ	aB	4005	-	-	6/29/63/63	0/2/2/2
15	CL7	cB	1236	2	2/2/11/20	8/15/91/115	-
15	CL7	bB	1211	2	2/2/13/20	7/27/103/115	-
15	CL7	aB	1219	2	2/2/10/20	4/10/86/115	-
17	A1JPJ	cI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1214	2	2/2/12/20	6/21/97/115	-
17	A1JPJ	cB	4006	-	-	6/29/63/63	0/2/2/2
17	A1JPJ	cA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	bA	1123	21	2/2/15/20	13/39/115/115	-
15	CL7	bB	1012	21	2/2/15/20	13/39/115/115	-
20	SF4	aC	3002	3	-	-	0/6/5/5
15	CL7	cL	1503	21	2/2/14/20	12/33/109/115	-
15	CL7	cA	1117	1	2/2/15/20	16/39/115/115	-
14	PHO	bB	1023	-	-	13/37/103/103	0/5/6/6
17	A1JPJ	cF	4016	-	-	6/29/63/63	0/2/2/2
15	CL7	aB	1228	2	2/2/11/20	10/15/91/115	-
15	CL7	bA	1114	21	2/2/11/20	2/15/91/115	-
15	CL7	cA	1136	1	2/2/15/20	21/39/115/115	-
15	CL7	bB	1226	2	2/2/15/20	13/39/115/115	-
15	CL7	bJ	1302	8	2/2/10/20	4/9/85/115	-
15	CL7	bB	1204	2	2/2/15/20	7/39/115/115	-
15	CL7	bA	1133	1	2/2/15/20	11/39/115/115	-
15	CL7	bA	1135	1	2/2/12/20	13/21/97/115	-
17	A1JPJ	bA	4007	-	-	2/29/63/63	0/2/2/2
18	LHG	bA	5001	-	-	15/53/53/53	-
15	CL7	aA	1103	1	2/2/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bA	1113	1	2/2/11/20	10/15/91/115	-
15	CL7	cB	1213	2	2/2/11/20	9/15/91/115	-
17	A1JPJ	cL	4023	-	-	1/29/63/63	0/2/2/2
20	SF4	aB	3001	2,1	-	-	0/6/5/5
15	CL7	aA	1112	1	2/2/15/20	13/39/115/115	-
15	CL7	cA	1106	1	2/2/15/20	19/39/115/115	-
15	CL7	bA	1109	15,1	2/2/15/20	24/39/115/115	-
15	CL7	aA	1121	1	2/2/13/20	9/27/103/115	-
15	CL7	aA	1133	1	2/2/15/20	10/39/115/115	-
15	CL7	aB	1220	-	2/2/11/20	11/15/91/115	-
15	CL7	aA	1127	1	2/2/15/20	15/39/115/115	-
15	CL7	cA	1128	1	2/2/15/20	6/39/115/115	-
17	A1JPJ	aA	4011	-	-	6/29/63/63	0/2/2/2
15	CL7	cA	1101	1	2/2/10/20	2/10/86/115	-
15	CL7	cB	1219	2	2/2/10/20	3/10/86/115	-
15	CL7	cB	1021	2	2/2/15/20	8/39/115/115	-
15	CL7	cA	1125	1	2/2/12/20	2/21/97/115	-
17	A1JPJ	aB	4006	-	-	6/29/63/63	0/2/2/2
16	PQN	bA	2001	-	-	4/23/43/43	0/2/2/2
15	CL7	bB	1212	2	2/2/11/20	10/15/91/115	-
15	CL7	cB	1239	2	2/2/15/20	10/39/115/115	-
17	A1JPJ	aA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1134	1	2/2/10/20	7/15/87/115	-
15	CL7	bB	1235	2	2/2/14/20	12/33/109/115	-
15	CL7	bB	1239	2	2/2/15/20	13/39/115/115	-
15	CL7	cB	1012	21	2/2/15/20	15/39/115/115	-
15	CL7	aK	1401	-	2/2/11/20	7/15/91/115	-
17	A1JPJ	aA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	aA	1135	1	2/2/12/20	12/21/97/115	-
16	PQN	aA	2001	-	-	4/23/43/43	0/2/2/2
18	LHG	aA	5001	-	-	14/53/53/53	-
15	CL7	cB	1229	2	2/2/15/20	13/39/115/115	-
15	CL7	bA	1119	21	2/2/13/20	15/27/103/115	-
15	CL7	aA	1126	1	2/2/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	aF	1701	6	2/2/10/20	1/10/86/115	-
15	CL7	aB	1205	2	2/2/15/20	12/39/115/115	-
15	CL7	cA	1121	1	2/2/13/20	10/27/103/115	-
15	CL7	aB	1221	2	2/2/14/20	14/33/109/115	-
15	CL7	cB	1241	2	2/2/11/20	10/15/91/115	-
15	CL7	aB	1236	2	2/2/11/20	7/15/91/115	-
15	CL7	cA	1120	1	2/2/11/20	7/15/91/115	-
15	CL7	bA	1122	1	2/2/15/20	6/39/115/115	-
15	CL7	bA	1130	1	2/2/12/20	7/23/99/115	-
17	A1JPJ	aJ	4012	-	-	2/29/63/63	0/2/2/2
15	CL7	bB	1213	2	2/2/11/20	9/15/91/115	-
15	CL7	cA	1119	21	2/2/13/20	13/27/103/115	-
15	CL7	bB	1216	21	2/2/11/20	4/15/91/115	-
15	CL7	bA	1124	21	2/2/12/20	3/21/97/115	-
15	CL7	bA	1801	18	2/2/10/20	7/10/86/115	-
15	CL7	cB	1235	2	2/2/14/20	12/33/109/115	-
15	CL7	aA	1131	1	2/2/15/20	5/39/115/115	-
15	CL7	bB	1206	2	2/2/12/20	6/21/97/115	-
20	SF4	bC	3002	3	-	-	0/6/5/5
15	CL7	aA	1139	21	2/2/11/20	10/15/91/115	-
15	CL7	cI	1601	21	2/2/15/20	13/39/115/115	-
15	CL7	bB	1219	2	2/2/10/20	4/10/86/115	-
15	CL7	aA	1105	1	2/2/11/20	5/15/91/115	-
15	CL7	bB	1214	2	2/2/12/20	6/21/97/115	-
15	CL7	aA	1110	21	2/2/11/20	11/15/91/115	-
15	CL7	bA	1136	1	2/2/15/20	17/39/115/115	-
15	CL7	aB	1209	2	2/2/11/20	7/15/91/115	-
15	CL7	aB	1208	2	2/2/15/20	13/39/115/115	-
15	CL7	bJ	1301	21	2/2/10/20	5/10/86/115	-
15	CL7	bA	1129	1	2/2/12/20	4/21/97/115	-
15	CL7	cB	1238	21	2/2/15/20	9/39/115/115	-
15	CL7	cF	1701	6	2/2/10/20	1/10/86/115	-
15	CL7	aB	1207	2	2/2/15/20	15/39/115/115	-
15	CL7	bB	1207	2	2/2/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	cA	1107	1	2/2/11/20	4/15/91/115	-
15	CL7	bA	1131	1	2/2/15/20	7/39/115/115	-
15	CL7	aA	1102	15,1	2/2/12/20	8/24/100/115	-
15	CL7	bA	1110	21	2/2/11/20	11/15/91/115	-
15	CL7	bB	1234	2	2/2/12/20	8/21/97/115	-
15	CL7	aB	1222	21	2/2/11/20	11/15/91/115	-
16	PQN	cA	2001	-	-	4/23/43/43	0/2/2/2
14	PHO	aA	1013	-	-	6/37/103/103	0/5/6/6
15	CL7	aA	1117	1	2/2/15/20	15/39/115/115	-
17	A1JPJ	aI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1111	1	2/2/15/20	14/39/115/115	-
15	CL7	aB	1210	2	2/2/15/20	19/39/115/115	-
15	CL7	cA	1110	21	2/2/11/20	11/15/91/115	-
15	CL7	cA	1115	1	2/2/10/20	4/10/86/115	-
17	A1JPJ	bA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	bB	1238	21	2/2/15/20	7/39/115/115	-
15	CL7	bA	1103	1	2/2/15/20	20/39/115/115	-
17	A1JPJ	cB	4017	-	-	4/29/63/63	0/2/2/2
15	CL7	bA	1118	1	2/2/13/20	9/27/103/115	-
15	CL7	aA	1104	1	2/2/15/20	17/39/115/115	-
15	CL7	aB	1215	2	2/2/13/20	11/27/103/115	-
17	A1JPJ	aL	4023	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	aA	4014	-	-	7/29/63/63	0/2/2/2
15	CL7	aA	1109	15,1	2/2/15/20	24/39/115/115	-
15	CL7	cA	1139	21	2/2/11/20	10/15/91/115	-
17	A1JPJ	bA	4002	-	-	2/29/63/63	0/2/2/2
15	CL7	bA	1104	1	2/2/15/20	19/39/115/115	-
15	CL7	cA	1129	1	2/2/12/20	7/21/97/115	-
19	LMG	bB	5002	-	-	14/48/68/70	0/1/1/1
15	CL7	aB	1213	2	2/2/11/20	11/15/91/115	-
15	CL7	bB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	aB	1237	21	2/2/15/20	14/39/115/115	-
15	CL7	cB	1222	21	2/2/11/20	9/15/91/115	-
17	A1JPJ	aB	4015	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bB	1209	2	2/2/11/20	8/15/91/115	-
15	CL7	cB	1202	2	2/2/15/20	22/39/115/115	-
15	CL7	aB	1211	2	2/2/13/20	6/27/103/115	-
17	A1JPJ	aA	4002	-	-	2/29/63/63	0/2/2/2
16	PQN	aB	2002	-	-	6/23/43/43	0/2/2/2
15	CL7	cB	1208	2	2/2/15/20	11/39/115/115	-
15	CL7	bA	1106	1	2/2/15/20	19/39/115/115	-
15	CL7	bB	1236	2	2/2/11/20	8/15/91/115	-
17	A1JPJ	cB	4005	-	-	6/29/63/63	0/2/2/2
17	A1JPJ	cA	4002	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1210	2	2/2/15/20	14/39/115/115	-
15	CL7	bB	1208	2	2/2/15/20	10/39/115/115	-
15	CL7	aK	1402	9	2/2/8/20	0/4/76/115	-
20	SF4	bB	3001	2,1	-	-	0/6/5/5
15	CL7	aB	1204	2	2/2/15/20	5/39/115/115	-
15	CL7	bA	1105	1	2/2/11/20	5/15/91/115	-
13	G9R	bA	1011	1	1/1/17/22	11/37/107/107	-
15	CL7	bA	1120	1	2/2/11/20	6/15/91/115	-
15	CL7	bA	1111	1	2/2/15/20	11/39/115/115	-
15	CL7	cB	1215	2	2/2/13/20	7/27/103/115	-
15	CL7	aJ	1302	8	2/2/10/20	4/9/85/115	-
17	A1JPJ	bB	4005	-	-	6/29/63/63	0/2/2/2
15	CL7	bB	1210	2	2/2/15/20	16/39/115/115	-
15	CL7	cB	1206	2	2/2/12/20	7/21/97/115	-
15	CL7	aA	1137	1	2/2/13/20	8/27/103/115	-
15	CL7	cB	1224	2	2/2/13/20	12/29/105/115	-
17	A1JPJ	bB	4017	-	-	4/29/63/63	0/2/2/2
15	CL7	aA	1132	1	2/2/15/20	12/39/115/115	-
15	CL7	cA	1137	1	2/2/13/20	9/27/103/115	-
13	G9R	aA	1011	1	1/1/17/22	12/37/107/107	-
15	CL7	aB	1232	21	2/2/10/20	4/10/86/115	-
15	CL7	bL	1501	10	2/2/14/20	14/33/109/115	-
15	CL7	cB	1211	2	2/2/13/20	8/27/103/115	-
17	A1JPJ	aI	4019	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PHO	cA	1013	-	-	10/37/103/103	0/5/6/6
15	CL7	bA	1101	1	2/2/10/20	2/10/86/115	-
18	LHG	cA	5003	15	-	11/42/42/53	-
15	CL7	cB	1205	2	2/2/15/20	11/39/115/115	-
17	A1JPJ	aL	4020	-	-	5/29/63/63	0/2/2/2
15	CL7	aB	1203	2	2/2/15/20	12/39/115/115	-
17	A1JPJ	bB	4010	-	-	7/29/63/63	0/2/2/2
15	CL7	aB	1235	2	2/2/14/20	13/33/109/115	-
15	CL7	cB	1221	2	2/2/14/20	14/33/109/115	-
15	CL7	aB	1218	2	2/2/10/20	2/10/86/115	-
15	CL7	bB	1237	21	2/2/15/20	19/39/115/115	-
15	CL7	aA	1106	1	2/2/15/20	19/39/115/115	-
15	CL7	bA	1126	1	2/2/15/20	9/39/115/115	-
15	CL7	aA	1138	1	2/2/15/20	10/39/115/115	-
15	CL7	bA	1132	1	2/2/15/20	14/39/115/115	-
17	A1JPJ	bB	4015	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1212	2	2/2/11/20	11/15/91/115	-
15	CL7	cA	1134	1	2/2/10/20	7/15/87/115	-
17	A1JPJ	aB	4021	-	-	2/29/63/63	0/2/2/2
15	CL7	cB	1204	2	2/2/15/20	6/39/115/115	-
15	CL7	bK	1401	-	2/2/11/20	7/15/91/115	-
17	A1JPJ	bL	4020	-	-	5/29/63/63	0/2/2/2
17	A1JPJ	cJ	4012	-	-	2/29/63/63	0/2/2/2
20	SF4	aC	3003	3	-	-	0/6/5/5
15	CL7	aA	1120	1	2/2/11/20	5/15/91/115	-
15	CL7	bB	1229	2	2/2/15/20	10/39/115/115	-
15	CL7	cA	1112	1	2/2/15/20	15/39/115/115	-
17	A1JPJ	bB	4004	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1133	1	2/2/15/20	9/39/115/115	-
15	CL7	cA	1126	1	2/2/15/20	10/39/115/115	-
15	CL7	cB	1232	21	2/2/10/20	3/10/86/115	-
15	CL7	cA	1801	18	2/2/10/20	7/10/86/115	-
15	CL7	cB	1217	2	2/2/10/20	0/10/86/115	-
15	CL7	bI	1601	21	2/2/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bB	1233	-	2/2/10/20	2/10/86/115	-
15	CL7	cB	1220	-	2/2/11/20	8/15/91/115	-
15	CL7	bB	1224	2	2/2/13/20	11/29/105/115	-
15	CL7	bA	1140	1	2/2/14/20	15/33/109/115	-
14	PHO	aB	1023	-	-	12/37/103/103	0/5/6/6
15	CL7	aA	1101	1	2/2/10/20	2/10/86/115	-
15	CL7	bA	1107	1	2/2/11/20	4/15/91/115	-
17	A1JPJ	cA	4003	-	-	2/29/63/63	0/2/2/2
15	CL7	aB	1206	2	2/2/12/20	7/21/97/115	-
15	CL7	aB	1012	21	2/2/15/20	15/39/115/115	-
15	CL7	aA	1118	1	2/2/13/20	11/27/103/115	-
15	CL7	aA	1130	1	2/2/12/20	7/23/99/115	-
17	A1JPJ	bI	4018	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1124	21	2/2/12/20	4/21/97/115	-
15	CL7	bB	1228	2	2/2/11/20	8/15/91/115	-
15	CL7	aB	1241	2	2/2/11/20	6/15/91/115	-
15	CL7	bA	1115	1	2/2/10/20	4/10/86/115	-
20	SF4	cB	3001	2,1	-	-	0/6/5/5
15	CL7	cB	1223	2	2/2/15/20	17/39/115/115	-
15	CL7	cK	1402	9	2/2/8/20	2/4/76/115	-
15	CL7	cA	1124	21	2/2/12/20	4/21/97/115	-
17	A1JPJ	cL	4020	-	-	5/29/63/63	0/2/2/2
20	SF4	bC	3003	3	-	-	0/6/5/5
15	CL7	bB	1218	2	2/2/10/20	4/10/86/115	-
20	SF4	cC	3003	3	-	-	0/6/5/5
15	CL7	bA	1139	21	2/2/11/20	10/15/91/115	-
15	CL7	bB	1215	2	2/2/13/20	7/27/103/115	-
15	CL7	cB	1234	2	2/2/12/20	8/21/97/115	-
16	PQN	cB	2002	-	-	6/23/43/43	0/2/2/2
17	A1JPJ	bB	4006	-	-	6/29/63/63	0/2/2/2
15	CL7	aB	1021	2	2/2/15/20	10/39/115/115	-
15	CL7	cB	1228	2	2/2/11/20	8/15/91/115	-
14	PHO	cB	1023	-	-	13/37/103/103	0/5/6/6
15	CL7	bB	1232	21	2/2/10/20	4/10/86/115	-
15	CL7	aL	1502	10	2/2/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	cA	1118	1	2/2/13/20	12/27/103/115	-
15	CL7	cA	1130	1	2/2/12/20	7/23/99/115	-
15	CL7	aA	1801	18	2/2/10/20	7/10/86/115	-
15	CL7	bB	1225	2	2/2/15/20	11/39/115/115	-
15	CL7	cA	1104	1	2/2/15/20	18/39/115/115	-
17	A1JPJ	cB	4015	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1111	1	2/2/15/20	13/39/115/115	-
15	CL7	cK	1401	-	2/2/11/20	6/15/91/115	-
17	A1JPJ	bA	4008	-	-	3/29/63/63	0/2/2/2
15	CL7	bA	1112	1	2/2/15/20	14/39/115/115	-
15	CL7	bB	1223	2	2/2/15/20	16/39/115/115	-
15	CL7	aB	1229	2	2/2/15/20	11/39/115/115	-
15	CL7	cB	1209	2	2/2/11/20	10/15/91/115	-
14	PHO	bA	1013	-	-	11/37/103/103	0/5/6/6
15	CL7	bA	1116	1	2/2/14/20	14/33/109/115	-
17	A1JPJ	cA	4011	-	-	6/29/63/63	0/2/2/2
17	A1JPJ	bA	4011	-	-	6/29/63/63	0/2/2/2
15	CL7	cL	1501	10	2/2/14/20	17/33/109/115	-
15	CL7	aB	1230	2	2/2/10/20	6/10/86/115	-
15	CL7	cB	1216	21	2/2/11/20	3/15/91/115	-
15	CL7	bB	1241	2	2/2/11/20	10/15/91/115	-
20	SF4	cC	3002	3	-	-	0/6/5/5
17	A1JPJ	cI	4019	-	-	2/29/63/63	0/2/2/2
15	CL7	aA	1116	1	2/2/14/20	11/33/109/115	-
18	LHG	aA	5003	15	-	12/42/42/53	-
15	CL7	aA	1125	1	2/2/12/20	1/21/97/115	-
17	A1JPJ	bF	4016	-	-	8/29/63/63	0/2/2/2
15	CL7	aL	1501	10	2/2/14/20	15/33/109/115	-
15	CL7	aA	1128	1	2/2/15/20	7/39/115/115	-
17	A1JPJ	bA	4014	-	-	7/29/63/63	0/2/2/2
15	CL7	cJ	1302	8	2/2/10/20	0/9/85/115	-
15	CL7	cA	1116	1	2/2/14/20	13/33/109/115	-
17	A1JPJ	bJ	4012	-	-	2/29/63/63	0/2/2/2
17	A1JPJ	cB	4021	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	G9R	cA	1011	1	1/1/17/22	11/37/107/107	-
15	CL7	cA	1022	21	2/2/15/20	11/39/115/115	-
15	CL7	aB	1201	2	2/2/12/20	9/26/102/115	-
15	CL7	aB	1225	2	2/2/15/20	14/39/115/115	-
15	CL7	bA	1108	1	2/2/12/20	8/23/99/115	-
15	CL7	bA	1128	1	2/2/15/20	6/39/115/115	-
17	A1JPJ	aA	4007	-	-	2/29/63/63	0/2/2/2
15	CL7	bA	1125	1	2/2/12/20	2/21/97/115	-
15	CL7	aB	1223	2	2/2/15/20	17/39/115/115	-
15	CL7	bB	1202	2	2/2/15/20	22/39/115/115	-
15	CL7	cA	1109	15,1	2/2/15/20	25/39/115/115	-
15	CL7	bK	1402	9	2/2/8/20	2/4/76/115	-
15	CL7	aB	1217	2	2/2/10/20	2/10/86/115	-
15	CL7	aL	1503	21	2/2/14/20	12/33/109/115	-
17	A1JPJ	aB	4017	-	-	4/29/63/63	0/2/2/2
15	CL7	cB	1212	2	2/2/11/20	11/15/91/115	-
15	CL7	cB	1227	2	2/2/11/20	5/15/91/115	-
15	CL7	aB	1234	2	2/2/12/20	7/21/97/115	-
15	CL7	cA	1123	21	2/2/15/20	18/39/115/115	-
15	CL7	cA	1105	1	2/2/11/20	6/15/91/115	-
15	CL7	cA	1102	15,1	2/2/12/20	7/24/100/115	-
15	CL7	aA	1140	1	2/2/14/20	14/33/109/115	-
15	CL7	bL	1502	10	2/2/15/20	18/39/115/115	-
17	A1JPJ	cA	4007	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1132	1	2/2/15/20	12/39/115/115	-
15	CL7	aB	1239	2	2/2/15/20	6/39/115/115	-
15	CL7	aA	1113	1	2/2/11/20	11/15/91/115	-
15	CL7	bB	1230	2	2/2/10/20	5/10/86/115	-
18	LHG	bA	5003	15	-	10/42/42/53	-
15	CL7	cA	1113	1	2/2/11/20	6/15/91/115	-
15	CL7	aA	1119	21	2/2/13/20	11/27/103/115	-
15	CL7	aJ	1301	21	2/2/10/20	5/10/86/115	-
15	CL7	cB	1201	2	2/2/12/20	10/26/102/115	-
15	CL7	cB	1225	2	2/2/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL7	bA	1138	1	2/2/15/20	10/39/115/115	-
17	A1JPJ	bI	4019	-	-	2/29/63/63	0/2/2/2
15	CL7	bB	1221	2	2/2/14/20	14/33/109/115	-
15	CL7	aA	1108	1	2/2/12/20	9/23/99/115	-
17	A1JPJ	bB	4021	-	-	2/29/63/63	0/2/2/2
15	CL7	bA	1121	1	2/2/13/20	10/27/103/115	-
15	CL7	cA	1108	1	2/2/12/20	9/23/99/115	-
15	CL7	aA	1107	1	2/2/11/20	4/15/91/115	-
17	A1JPJ	cB	4004	-	-	2/29/63/63	0/2/2/2
15	CL7	cA	1127	1	2/2/15/20	16/39/115/115	-
16	PQN	bB	2002	-	-	6/23/43/43	0/2/2/2
19	LMG	aB	5002	-	-	15/48/68/70	0/1/1/1
15	CL7	bB	1231	2	2/2/11/20	4/15/91/115	-
15	CL7	aA	1122	1	2/2/15/20	6/39/115/115	-

All (3541) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bA	1011	G9R	C3B-C4B	10.30	1.49	1.41
13	cA	1011	G9R	C3B-C4B	10.19	1.49	1.41
13	aA	1011	G9R	C3B-C4B	10.08	1.49	1.41
14	aA	1013	PHO	C1B-C2B	8.92	1.49	1.39
14	cA	1013	PHO	C1B-C2B	8.87	1.49	1.39
14	bA	1013	PHO	C1B-C2B	8.75	1.49	1.39
14	bB	1023	PHO	C1B-C2B	8.59	1.49	1.39
14	cB	1023	PHO	C1B-C2B	8.53	1.49	1.39
14	aB	1023	PHO	C1B-C2B	8.48	1.49	1.39
13	cA	1011	G9R	C1B-C2B	8.00	1.49	1.39
13	aA	1011	G9R	C1B-C2B	7.97	1.49	1.39
13	bA	1011	G9R	C1B-C2B	7.96	1.49	1.39
14	cB	1023	PHO	C3B-C4B	7.28	1.49	1.41
14	bA	1013	PHO	C3B-C4B	7.26	1.49	1.41
14	cA	1013	PHO	C3B-C4B	7.21	1.49	1.41
14	aA	1013	PHO	C3B-C4B	7.21	1.49	1.41
14	aB	1023	PHO	C3B-C4B	7.18	1.49	1.41
14	bB	1023	PHO	C3B-C4B	7.14	1.49	1.41
13	cA	1011	G9R	C1D-C2D	7.06	1.48	1.39
13	aA	1011	G9R	C1D-C2D	7.00	1.48	1.39
13	bA	1011	G9R	C1D-C2D	6.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	aA	4014	A1JPJ	C14-C13	5.30	1.42	1.35
17	bA	4014	A1JPJ	C14-C13	5.27	1.42	1.35
17	aF	4016	A1JPJ	C21-C22	5.15	1.42	1.35
17	cA	4014	A1JPJ	C14-C13	5.08	1.42	1.35
17	aA	4014	A1JPJ	C10-C9	4.88	1.42	1.35
17	bA	4014	A1JPJ	C10-C9	4.87	1.42	1.35
17	cA	4014	A1JPJ	C10-C9	4.75	1.42	1.35
13	bA	1011	G9R	C3D-C4D	4.70	1.47	1.41
13	cA	1011	G9R	C3D-C4D	4.66	1.47	1.41
13	aA	1011	G9R	C3D-C4D	4.64	1.47	1.41
15	bA	1126	CL7	C1D-ND	4.52	1.43	1.37
15	aA	1132	CL7	C1D-ND	4.46	1.43	1.37
17	cB	4006	A1JPJ	C10-C9	4.41	1.41	1.35
17	cB	4006	A1JPJ	C14-C13	4.40	1.41	1.35
17	cA	4014	A1JPJ	C17-C18	4.39	1.41	1.35
17	aB	4006	A1JPJ	C17-C18	4.38	1.41	1.35
17	aB	4006	A1JPJ	C10-C9	4.36	1.41	1.35
15	cA	1132	CL7	C1D-ND	4.36	1.43	1.37
17	cB	4006	A1JPJ	C17-C18	4.36	1.41	1.35
17	aB	4006	A1JPJ	C14-C13	4.35	1.41	1.35
15	cA	1132	CL7	C4B-NB	4.35	1.43	1.37
17	aA	4014	A1JPJ	C17-C18	4.35	1.41	1.35
17	bB	4006	A1JPJ	C14-C13	4.34	1.41	1.35
17	bB	4006	A1JPJ	C10-C9	4.33	1.41	1.35
17	bA	4014	A1JPJ	C17-C18	4.33	1.41	1.35
15	aA	1132	CL7	C4B-NB	4.32	1.43	1.37
17	bB	4006	A1JPJ	C17-C18	4.31	1.41	1.35
17	bB	4006	A1JPJ	C21-C22	4.28	1.41	1.35
17	aB	4006	A1JPJ	C21-C22	4.28	1.41	1.35
17	cB	4006	A1JPJ	C21-C22	4.28	1.41	1.35
17	aB	4004	A1JPJ	C21-C22	4.22	1.41	1.35
17	cB	4004	A1JPJ	C21-C22	4.21	1.41	1.35
17	bB	4004	A1JPJ	C17-C18	4.19	1.41	1.35
17	bB	4004	A1JPJ	C21-C22	4.18	1.41	1.35
17	aB	4004	A1JPJ	C17-C18	4.17	1.41	1.35
17	cB	4004	A1JPJ	C17-C18	4.16	1.41	1.35
17	cB	4004	A1JPJ	C14-C13	4.14	1.41	1.35
15	bA	1126	CL7	C4B-NB	4.14	1.42	1.37
17	cB	4010	A1JPJ	C10-C9	4.14	1.41	1.35
17	bB	4004	A1JPJ	C14-C13	4.13	1.41	1.35
17	aA	4002	A1JPJ	C17-C18	4.13	1.41	1.35
17	aB	4004	A1JPJ	C14-C13	4.13	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aK	1402	CL7	C1D-ND	4.12	1.42	1.37
17	cB	4005	A1JPJ	C14-C13	4.08	1.41	1.35
17	bB	4010	A1JPJ	C10-C9	4.07	1.41	1.35
17	bB	4004	A1JPJ	C10-C9	4.07	1.41	1.35
17	bA	4002	A1JPJ	C17-C18	4.06	1.41	1.35
17	cB	4010	A1JPJ	C14-C13	4.06	1.41	1.35
17	cB	4005	A1JPJ	C10-C9	4.05	1.41	1.35
17	bB	4010	A1JPJ	C14-C13	4.05	1.41	1.35
17	aB	4010	A1JPJ	C17-C18	4.05	1.41	1.35
17	bB	4005	A1JPJ	C17-C18	4.04	1.41	1.35
17	aL	4023	A1JPJ	C21-C22	4.04	1.41	1.35
17	aB	4010	A1JPJ	C10-C9	4.04	1.41	1.35
17	aB	4005	A1JPJ	C10-C9	4.03	1.41	1.35
15	bK	1401	CL7	C1D-ND	4.03	1.42	1.37
17	aB	4005	A1JPJ	C17-C18	4.03	1.41	1.35
17	cA	4002	A1JPJ	C17-C18	4.03	1.41	1.35
17	bB	4005	A1JPJ	C10-C9	4.03	1.41	1.35
17	aB	4010	A1JPJ	C14-C13	4.02	1.41	1.35
17	bB	4005	A1JPJ	C14-C13	4.01	1.41	1.35
17	aB	4005	A1JPJ	C14-C13	4.01	1.41	1.35
15	cK	1401	CL7	C1D-ND	4.01	1.42	1.37
17	cB	4005	A1JPJ	C17-C18	4.01	1.41	1.35
17	cB	4010	A1JPJ	C17-C18	4.01	1.41	1.35
17	aB	4004	A1JPJ	C10-C9	4.00	1.41	1.35
15	aJ	1301	CL7	C1D-ND	3.99	1.42	1.37
17	cB	4015	A1JPJ	C21-C22	3.98	1.41	1.35
17	aB	4015	A1JPJ	C21-C22	3.98	1.41	1.35
17	aF	4016	A1JPJ	C14-C13	3.97	1.41	1.35
17	bB	4015	A1JPJ	C21-C22	3.97	1.41	1.35
17	aA	4002	A1JPJ	C14-C13	3.97	1.41	1.35
17	bB	4010	A1JPJ	C17-C18	3.97	1.41	1.35
17	cB	4004	A1JPJ	C10-C9	3.97	1.41	1.35
17	aF	4016	A1JPJ	C17-C18	3.97	1.41	1.35
15	cJ	1301	CL7	C1D-ND	3.97	1.42	1.37
17	aL	4023	A1JPJ	C14-C13	3.95	1.41	1.35
15	aK	1401	CL7	C1D-ND	3.95	1.42	1.37
15	bB	1232	CL7	C1D-ND	3.94	1.42	1.37
15	aJ	1302	CL7	C1D-ND	3.94	1.42	1.37
17	bF	4016	A1JPJ	C21-C22	3.93	1.41	1.35
17	bA	4002	A1JPJ	C14-C13	3.93	1.41	1.35
15	cK	1402	CL7	C1D-ND	3.93	1.42	1.37
15	aB	1241	CL7	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bJ	1301	CL7	C1D-ND	3.93	1.42	1.37
15	aB	1213	CL7	C1D-ND	3.93	1.42	1.37
17	cB	4010	A1JPJ	C21-C22	3.93	1.41	1.35
15	cB	1221	CL7	C1D-ND	3.92	1.42	1.37
15	aB	1217	CL7	C1D-ND	3.92	1.42	1.37
17	bA	4007	A1JPJ	C17-C18	3.92	1.41	1.35
17	cB	4015	A1JPJ	C17-C18	3.92	1.41	1.35
17	cA	4007	A1JPJ	C17-C18	3.91	1.41	1.35
15	aB	1233	CL7	C1D-ND	3.91	1.42	1.37
17	bJ	4012	A1JPJ	C21-C22	3.91	1.41	1.35
17	cB	4015	A1JPJ	C10-C9	3.91	1.41	1.35
17	cB	4005	A1JPJ	C21-C22	3.90	1.41	1.35
15	bK	1402	CL7	C1D-ND	3.90	1.42	1.37
17	bF	4016	A1JPJ	C14-C13	3.89	1.40	1.35
17	bJ	4012	A1JPJ	C17-C18	3.89	1.40	1.35
17	aA	4002	A1JPJ	C21-C22	3.89	1.40	1.35
17	aB	4010	A1JPJ	C21-C22	3.89	1.40	1.35
17	cB	4015	A1JPJ	C14-C13	3.89	1.40	1.35
17	cA	4002	A1JPJ	C14-C13	3.89	1.40	1.35
15	cB	1209	CL7	C1D-ND	3.89	1.42	1.37
15	cB	1217	CL7	C1D-ND	3.89	1.42	1.37
17	bJ	4012	A1JPJ	C14-C13	3.89	1.40	1.35
15	cB	1219	CL7	C1D-ND	3.89	1.42	1.37
17	cF	4016	A1JPJ	C17-C18	3.89	1.40	1.35
15	aB	1219	CL7	C1D-ND	3.88	1.42	1.37
15	bB	1219	CL7	C1D-ND	3.88	1.42	1.37
17	bA	4002	A1JPJ	C10-C9	3.88	1.40	1.35
17	bB	4015	A1JPJ	C17-C18	3.87	1.40	1.35
15	bB	1218	CL7	C1D-ND	3.87	1.42	1.37
17	aA	4002	A1JPJ	C10-C9	3.87	1.40	1.35
17	bF	4016	A1JPJ	C17-C18	3.87	1.40	1.35
15	bB	1217	CL7	C1D-ND	3.87	1.42	1.37
17	bA	4014	A1JPJ	C21-C22	3.87	1.40	1.35
15	cB	1233	CL7	C1D-ND	3.87	1.42	1.37
17	aF	4016	A1JPJ	C10-C9	3.87	1.40	1.35
17	aA	4007	A1JPJ	C17-C18	3.87	1.40	1.35
17	bJ	4012	A1JPJ	C10-C9	3.87	1.40	1.35
15	bB	1241	CL7	C1D-ND	3.86	1.42	1.37
17	cJ	4012	A1JPJ	C21-C22	3.86	1.40	1.35
15	bB	1233	CL7	C1D-ND	3.86	1.42	1.37
17	aB	4015	A1JPJ	C17-C18	3.86	1.40	1.35
15	bB	1221	CL7	C1D-ND	3.85	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cF	4016	A1JPJ	C21-C22	3.85	1.40	1.35
15	bB	1216	CL7	C1D-ND	3.85	1.42	1.37
15	cJ	1302	CL7	C1D-ND	3.85	1.42	1.37
17	bA	4002	A1JPJ	C21-C22	3.85	1.40	1.35
15	aA	1129	CL7	C1D-ND	3.85	1.42	1.37
15	aB	1216	CL7	C1D-ND	3.85	1.42	1.37
17	bB	4010	A1JPJ	C21-C22	3.85	1.40	1.35
15	bA	1109	CL7	C1D-ND	3.84	1.42	1.37
17	aA	4014	A1JPJ	C21-C22	3.84	1.40	1.35
15	cB	1241	CL7	C1D-ND	3.84	1.42	1.37
17	bB	4015	A1JPJ	C14-C13	3.84	1.40	1.35
14	aA	1013	PHO	C1D-C2D	3.84	1.43	1.39
15	aB	1221	CL7	C1D-ND	3.84	1.42	1.37
15	cB	1213	CL7	C1D-ND	3.83	1.42	1.37
15	bA	1111	CL7	C1D-ND	3.83	1.42	1.37
15	cB	1214	CL7	C1D-ND	3.83	1.42	1.37
15	aA	1134	CL7	C1D-ND	3.83	1.42	1.37
15	bB	1209	CL7	C1D-ND	3.83	1.42	1.37
15	bB	1213	CL7	C1D-ND	3.83	1.42	1.37
17	aJ	4012	A1JPJ	C17-C18	3.83	1.40	1.35
15	cB	1216	CL7	C1D-ND	3.83	1.42	1.37
17	aB	4005	A1JPJ	C21-C22	3.83	1.40	1.35
17	bB	4015	A1JPJ	C10-C9	3.83	1.40	1.35
15	bB	1220	CL7	C1D-ND	3.83	1.42	1.37
17	bB	4017	A1JPJ	C14-C13	3.83	1.40	1.35
15	aB	1218	CL7	C1D-ND	3.83	1.42	1.37
17	aB	4017	A1JPJ	C21-C22	3.83	1.40	1.35
15	bJ	1302	CL7	C1D-ND	3.83	1.42	1.37
15	bB	1212	CL7	C1D-ND	3.83	1.42	1.37
15	aA	1139	CL7	C1D-ND	3.83	1.42	1.37
15	cA	1139	CL7	C1D-ND	3.83	1.42	1.37
17	cA	4007	A1JPJ	C14-C13	3.82	1.40	1.35
15	cB	1212	CL7	C1D-ND	3.82	1.42	1.37
15	aB	1212	CL7	C1D-ND	3.82	1.42	1.37
17	bB	4005	A1JPJ	C21-C22	3.82	1.40	1.35
15	cA	1101	CL7	C1D-ND	3.82	1.42	1.37
17	cJ	4012	A1JPJ	C17-C18	3.82	1.40	1.35
17	bF	4016	A1JPJ	C10-C9	3.82	1.40	1.35
15	aB	1232	CL7	C1D-ND	3.82	1.42	1.37
15	aB	1208	CL7	C1D-ND	3.82	1.42	1.37
17	aJ	4012	A1JPJ	C10-C9	3.82	1.40	1.35
15	aB	1209	CL7	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	4017	A1JPJ	C21-C22	3.81	1.40	1.35
15	aA	1118	CL7	C1D-ND	3.81	1.42	1.37
15	aB	1214	CL7	C1D-ND	3.81	1.42	1.37
17	aL	4023	A1JPJ	C17-C18	3.81	1.40	1.35
17	aB	4015	A1JPJ	C14-C13	3.81	1.40	1.35
15	bA	1120	CL7	C1D-ND	3.81	1.42	1.37
15	bA	1129	CL7	C1D-ND	3.81	1.42	1.37
17	cA	4002	A1JPJ	C21-C22	3.81	1.40	1.35
15	aA	1123	CL7	C1D-ND	3.80	1.42	1.37
15	aB	1223	CL7	C1D-ND	3.80	1.42	1.37
15	cA	1118	CL7	C1D-ND	3.80	1.42	1.37
17	aJ	4012	A1JPJ	C21-C22	3.80	1.40	1.35
17	bA	4007	A1JPJ	C14-C13	3.80	1.40	1.35
15	aA	1122	CL7	C1D-ND	3.80	1.42	1.37
15	cB	1232	CL7	C1D-ND	3.80	1.42	1.37
17	cF	4016	A1JPJ	C14-C13	3.80	1.40	1.35
15	aA	1101	CL7	C1D-ND	3.80	1.42	1.37
15	cA	1120	CL7	C1D-ND	3.80	1.42	1.37
15	aA	1133	CL7	C1D-ND	3.79	1.42	1.37
17	cF	4016	A1JPJ	C10-C9	3.79	1.40	1.35
15	cA	1134	CL7	C1D-ND	3.79	1.42	1.37
15	cA	1113	CL7	C1D-ND	3.79	1.42	1.37
15	cA	1114	CL7	C1D-ND	3.79	1.42	1.37
17	cB	4017	A1JPJ	C21-C22	3.79	1.40	1.35
17	aJ	4012	A1JPJ	C14-C13	3.79	1.40	1.35
17	cJ	4012	A1JPJ	C10-C9	3.79	1.40	1.35
15	bA	1110	CL7	C1D-ND	3.79	1.42	1.37
15	cB	1218	CL7	C1D-ND	3.79	1.42	1.37
15	cB	1211	CL7	C1D-ND	3.78	1.42	1.37
15	bA	1139	CL7	C1D-ND	3.78	1.42	1.37
15	cB	1227	CL7	C1D-ND	3.78	1.42	1.37
15	cI	1601	CL7	C1D-ND	3.78	1.42	1.37
17	aB	4017	A1JPJ	C17-C18	3.78	1.40	1.35
15	cA	1133	CL7	C1D-ND	3.78	1.42	1.37
15	cB	1220	CL7	C1D-ND	3.78	1.42	1.37
15	bA	1134	CL7	C1D-ND	3.78	1.42	1.37
17	bB	4017	A1JPJ	C17-C18	3.78	1.40	1.35
15	aF	1701	CL7	C1D-ND	3.78	1.42	1.37
15	cB	1228	CL7	C1D-ND	3.78	1.42	1.37
15	aA	1114	CL7	C1D-ND	3.78	1.42	1.37
15	aA	1117	CL7	C1D-ND	3.78	1.42	1.37
15	bA	1104	CL7	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1223	CL7	C1D-ND	3.77	1.42	1.37
15	aA	1111	CL7	C1D-ND	3.77	1.42	1.37
15	cA	1122	CL7	C1D-ND	3.77	1.42	1.37
15	bA	1133	CL7	C1D-ND	3.77	1.42	1.37
17	bA	4003	A1JPJ	C21-C22	3.77	1.40	1.35
17	aA	4003	A1JPJ	C21-C22	3.77	1.40	1.35
15	bA	1114	CL7	C1D-ND	3.77	1.42	1.37
15	cB	1223	CL7	C1D-ND	3.77	1.42	1.37
15	bA	1113	CL7	C1D-ND	3.77	1.42	1.37
15	bA	1118	CL7	C1D-ND	3.77	1.42	1.37
15	cA	1102	CL7	C1D-ND	3.77	1.42	1.37
17	bL	4023	A1JPJ	C21-C22	3.76	1.40	1.35
15	bB	1231	CL7	C1D-ND	3.76	1.42	1.37
15	cA	1137	CL7	C1D-ND	3.76	1.42	1.37
15	cB	1208	CL7	C1D-ND	3.76	1.42	1.37
15	cB	1234	CL7	C1D-ND	3.76	1.42	1.37
17	cA	4007	A1JPJ	C21-C22	3.76	1.40	1.35
17	aB	4017	A1JPJ	C14-C13	3.76	1.40	1.35
15	aA	1113	CL7	C1D-ND	3.76	1.42	1.37
15	aA	1109	CL7	C1D-ND	3.76	1.42	1.37
15	aA	1120	CL7	C1D-ND	3.76	1.42	1.37
15	bB	1208	CL7	C1D-ND	3.76	1.42	1.37
15	cA	1111	CL7	C1D-ND	3.76	1.42	1.37
15	aA	1110	CL7	C1D-ND	3.75	1.42	1.37
15	bA	1122	CL7	C1D-ND	3.75	1.42	1.37
15	aB	1228	CL7	C1D-ND	3.75	1.42	1.37
15	aB	1227	CL7	C1D-ND	3.75	1.42	1.37
15	bA	1130	CL7	C1D-ND	3.75	1.42	1.37
17	aA	4007	A1JPJ	C21-C22	3.75	1.40	1.35
15	cA	1129	CL7	C1D-ND	3.75	1.42	1.37
17	cJ	4012	A1JPJ	C14-C13	3.75	1.40	1.35
15	cA	1112	CL7	C1D-ND	3.74	1.42	1.37
17	cL	4023	A1JPJ	C14-C13	3.74	1.40	1.35
15	bB	1228	CL7	C1D-ND	3.74	1.42	1.37
15	bA	1112	CL7	C1D-ND	3.74	1.42	1.37
17	aL	4023	A1JPJ	C10-C9	3.74	1.40	1.35
17	bA	4007	A1JPJ	C21-C22	3.74	1.40	1.35
17	cB	4021	A1JPJ	C17-C18	3.74	1.40	1.35
15	aB	1236	CL7	C1D-ND	3.74	1.42	1.37
15	bB	1234	CL7	C1D-ND	3.74	1.42	1.37
17	aA	4007	A1JPJ	C14-C13	3.74	1.40	1.35
15	bA	1101	CL7	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1239	CL7	C1D-ND	3.74	1.42	1.37
17	bL	4023	A1JPJ	C14-C13	3.74	1.40	1.35
17	aB	4021	A1JPJ	C17-C18	3.73	1.40	1.35
15	bB	1227	CL7	C1D-ND	3.73	1.42	1.37
15	aB	1220	CL7	C1D-ND	3.73	1.42	1.37
15	bB	1214	CL7	C1D-ND	3.73	1.42	1.37
15	aB	1210	CL7	C1D-ND	3.73	1.42	1.37
15	cB	1231	CL7	C1D-ND	3.73	1.42	1.37
17	cL	4023	A1JPJ	C21-C22	3.73	1.40	1.35
15	cA	1140	CL7	C1D-ND	3.73	1.42	1.37
15	aB	1234	CL7	C1D-ND	3.73	1.42	1.37
17	cA	4002	A1JPJ	C10-C9	3.73	1.40	1.35
15	cA	1125	CL7	C1D-ND	3.73	1.42	1.37
15	cA	1128	CL7	C1D-ND	3.73	1.42	1.37
17	aA	4011	A1JPJ	C14-C13	3.73	1.40	1.35
15	bA	1106	CL7	C1D-ND	3.72	1.42	1.37
17	aB	4017	A1JPJ	C10-C9	3.72	1.40	1.35
15	bF	1701	CL7	C1D-ND	3.72	1.42	1.37
15	cA	1110	CL7	C1D-ND	3.72	1.42	1.37
15	bA	1117	CL7	C1D-ND	3.72	1.42	1.37
17	cA	4014	A1JPJ	C21-C22	3.72	1.40	1.35
17	bB	4017	A1JPJ	C10-C9	3.72	1.40	1.35
17	aI	4019	A1JPJ	C14-C13	3.72	1.40	1.35
17	cB	4021	A1JPJ	C14-C13	3.72	1.40	1.35
15	bA	1125	CL7	C1D-ND	3.72	1.42	1.37
17	bI	4019	A1JPJ	C14-C13	3.71	1.40	1.35
15	cA	1109	CL7	C1D-ND	3.71	1.42	1.37
15	cA	1123	CL7	C1D-ND	3.71	1.42	1.37
15	bB	1211	CL7	C1D-ND	3.71	1.42	1.37
17	cB	4017	A1JPJ	C14-C13	3.71	1.40	1.35
15	bB	1236	CL7	C1D-ND	3.71	1.42	1.37
15	bA	1119	CL7	C1D-ND	3.71	1.42	1.37
15	cA	1126	CL7	C1D-ND	3.71	1.42	1.37
17	cI	4019	A1JPJ	C14-C13	3.71	1.40	1.35
15	aB	1211	CL7	C1D-ND	3.71	1.42	1.37
17	bA	4003	A1JPJ	C14-C13	3.71	1.40	1.35
15	aA	1116	CL7	C1D-ND	3.70	1.42	1.37
17	aB	4015	A1JPJ	C10-C9	3.70	1.40	1.35
15	aA	1107	CL7	C1D-ND	3.70	1.42	1.37
17	cB	4017	A1JPJ	C10-C9	3.70	1.40	1.35
15	aA	1801	CL7	C1D-ND	3.70	1.42	1.37
15	cA	1104	CL7	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1222	CL7	C1D-ND	3.70	1.42	1.37
17	aA	4003	A1JPJ	C17-C18	3.70	1.40	1.35
15	cA	1117	CL7	C1D-ND	3.70	1.42	1.37
15	bB	1226	CL7	C1D-ND	3.70	1.42	1.37
15	bA	1137	CL7	C1D-ND	3.70	1.42	1.37
15	cL	1501	CL7	C1D-ND	3.70	1.42	1.37
17	bB	4021	A1JPJ	C17-C18	3.69	1.40	1.35
15	aA	1106	CL7	C1D-ND	3.69	1.42	1.37
17	aB	4021	A1JPJ	C14-C13	3.69	1.40	1.35
15	aA	1125	CL7	C1D-ND	3.69	1.42	1.37
15	cA	1136	CL7	C1D-ND	3.69	1.42	1.37
17	aB	4021	A1JPJ	C21-C22	3.69	1.40	1.35
15	aA	1104	CL7	C1D-ND	3.69	1.42	1.37
15	aA	1140	CL7	C1D-ND	3.69	1.42	1.37
15	bA	1123	CL7	C1D-ND	3.69	1.42	1.37
15	cF	1701	CL7	C1D-ND	3.69	1.42	1.37
17	cA	4011	A1JPJ	C10-C9	3.69	1.40	1.35
15	cA	1116	CL7	C1D-ND	3.69	1.42	1.37
17	cA	4011	A1JPJ	C14-C13	3.69	1.40	1.35
15	aA	1112	CL7	C1D-ND	3.69	1.42	1.37
15	bB	1224	CL7	C1D-ND	3.69	1.42	1.37
15	cA	1801	CL7	C1D-ND	3.69	1.42	1.37
15	bB	1210	CL7	C1D-ND	3.68	1.42	1.37
17	bL	4023	A1JPJ	C17-C18	3.68	1.40	1.35
17	cB	4021	A1JPJ	C21-C22	3.68	1.40	1.35
17	cA	4003	A1JPJ	C21-C22	3.68	1.40	1.35
15	bA	1140	CL7	C1D-ND	3.68	1.42	1.37
15	cB	1210	CL7	C1D-ND	3.68	1.42	1.37
15	cA	1022	CL7	C1D-ND	3.68	1.42	1.37
15	cB	1224	CL7	C1D-ND	3.68	1.42	1.37
15	bA	1801	CL7	C1D-ND	3.68	1.42	1.37
15	cB	1222	CL7	C1D-ND	3.68	1.42	1.37
17	aI	4019	A1JPJ	C17-C18	3.68	1.40	1.35
17	cB	4017	A1JPJ	C17-C18	3.68	1.40	1.35
15	bI	1601	CL7	C1D-ND	3.68	1.42	1.37
17	cA	4007	A1JPJ	C10-C9	3.68	1.40	1.35
17	cL	4023	A1JPJ	C17-C18	3.68	1.40	1.35
17	bB	4021	A1JPJ	C14-C13	3.68	1.40	1.35
15	aA	1108	CL7	C1D-ND	3.67	1.42	1.37
15	bA	1102	CL7	C1D-ND	3.67	1.42	1.37
15	aA	1102	CL7	C1D-ND	3.67	1.42	1.37
15	aI	1601	CL7	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1229	CL7	C1D-ND	3.67	1.42	1.37
15	cA	1130	CL7	C1D-ND	3.67	1.42	1.37
15	bB	1215	CL7	C1D-ND	3.67	1.42	1.37
15	aA	1119	CL7	C1D-ND	3.67	1.42	1.37
15	bB	1239	CL7	C1D-ND	3.67	1.42	1.37
15	cA	1106	CL7	C1D-ND	3.67	1.42	1.37
15	cB	1205	CL7	C1D-ND	3.67	1.42	1.37
15	aB	1229	CL7	C1D-ND	3.67	1.42	1.37
15	aB	1207	CL7	C1D-ND	3.67	1.42	1.37
15	bB	1205	CL7	C1D-ND	3.67	1.42	1.37
15	cA	1124	CL7	C1D-ND	3.67	1.42	1.37
17	bB	4021	A1JPJ	C21-C22	3.67	1.40	1.35
15	aA	1137	CL7	C1D-ND	3.66	1.42	1.37
15	bB	1202	CL7	C1D-ND	3.66	1.42	1.37
15	aA	1128	CL7	C1D-ND	3.66	1.42	1.37
15	aA	1126	CL7	C1D-ND	3.66	1.42	1.37
15	aB	1012	CL7	C1D-ND	3.66	1.42	1.37
17	cA	4003	A1JPJ	C14-C13	3.66	1.40	1.35
15	bA	1132	CL7	C1D-ND	3.66	1.42	1.37
15	bB	1207	CL7	C1D-ND	3.66	1.42	1.37
15	aB	1225	CL7	C1D-ND	3.65	1.42	1.37
15	aL	1503	CL7	C1D-ND	3.65	1.42	1.37
15	cB	1207	CL7	C1D-ND	3.65	1.42	1.37
17	bA	4003	A1JPJ	C17-C18	3.65	1.40	1.35
17	aA	4011	A1JPJ	C10-C9	3.65	1.40	1.35
15	aB	1215	CL7	C1D-ND	3.65	1.42	1.37
15	bB	1225	CL7	C1D-ND	3.65	1.42	1.37
15	bB	1230	CL7	C1D-ND	3.65	1.42	1.37
17	cL	4023	A1JPJ	C10-C9	3.65	1.40	1.35
15	cB	1204	CL7	C1D-ND	3.64	1.42	1.37
15	cA	1138	CL7	C1D-ND	3.64	1.42	1.37
15	cL	1503	CL7	C1D-ND	3.64	1.42	1.37
17	bI	4019	A1JPJ	C10-C9	3.64	1.40	1.35
15	aB	1226	CL7	C1D-ND	3.64	1.42	1.37
15	aA	1124	CL7	C1D-ND	3.64	1.42	1.37
15	cA	1108	CL7	C1D-ND	3.64	1.42	1.37
15	bB	1222	CL7	C1D-ND	3.64	1.42	1.37
15	cB	1239	CL7	C1D-ND	3.64	1.42	1.37
15	aA	1138	CL7	C1D-ND	3.64	1.42	1.37
15	cA	1131	CL7	C1D-ND	3.64	1.42	1.37
15	cB	1236	CL7	C1D-ND	3.64	1.42	1.37
15	aA	1105	CL7	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1021	CL7	C1D-ND	3.64	1.42	1.37
15	cA	1105	CL7	C1D-ND	3.64	1.42	1.37
15	aA	1130	CL7	C1D-ND	3.64	1.42	1.37
15	aB	1203	CL7	C1D-ND	3.64	1.42	1.37
15	aB	1205	CL7	C1D-ND	3.64	1.42	1.37
15	bB	1232	CL7	C4B-NB	3.64	1.42	1.37
17	aA	4011	A1JPJ	C17-C18	3.64	1.40	1.35
15	cB	1226	CL7	C1D-ND	3.64	1.42	1.37
15	aB	1230	CL7	C1D-ND	3.63	1.42	1.37
15	aB	1231	CL7	C1D-ND	3.63	1.42	1.37
17	aI	4019	A1JPJ	C10-C9	3.63	1.40	1.35
17	cI	4019	A1JPJ	C10-C9	3.63	1.40	1.35
15	bA	1105	CL7	C1D-ND	3.63	1.42	1.37
15	bB	1238	CL7	C1D-ND	3.63	1.42	1.37
15	bA	1135	CL7	C1D-ND	3.63	1.42	1.37
15	bA	1136	CL7	C1D-ND	3.63	1.42	1.37
15	cB	1201	CL7	C1D-ND	3.63	1.42	1.37
15	bA	1138	CL7	C1D-ND	3.63	1.42	1.37
15	aA	1121	CL7	C1D-ND	3.63	1.42	1.37
15	bA	1115	CL7	C1D-ND	3.63	1.42	1.37
15	cB	1202	CL7	C1D-ND	3.63	1.42	1.37
15	cA	1119	CL7	C1D-ND	3.63	1.42	1.37
17	aA	4007	A1JPJ	C10-C9	3.62	1.40	1.35
17	cL	4020	A1JPJ	C17-C18	3.62	1.40	1.35
15	aA	1131	CL7	C1D-ND	3.62	1.42	1.37
15	cA	1103	CL7	C1D-ND	3.62	1.42	1.37
15	aB	1235	CL7	C1D-ND	3.62	1.42	1.37
15	aB	1224	CL7	C1D-ND	3.62	1.42	1.37
15	cB	1021	CL7	C1D-ND	3.62	1.42	1.37
15	cB	1229	CL7	C1D-ND	3.62	1.42	1.37
15	bA	1128	CL7	C1D-ND	3.62	1.42	1.37
15	cB	1235	CL7	C1D-ND	3.62	1.42	1.37
15	bB	1227	CL7	C4B-NB	3.61	1.42	1.37
15	bB	1201	CL7	C1D-ND	3.61	1.42	1.37
15	aB	1238	CL7	C1D-ND	3.61	1.42	1.37
17	aA	4003	A1JPJ	C14-C13	3.61	1.40	1.35
17	bI	4019	A1JPJ	C17-C18	3.61	1.40	1.35
15	bA	1108	CL7	C1D-ND	3.60	1.42	1.37
15	cA	1115	CL7	C1D-ND	3.60	1.42	1.37
15	aA	1115	CL7	C4B-NB	3.60	1.42	1.37
15	bA	1118	CL7	C4B-NB	3.60	1.42	1.37
17	cA	4003	A1JPJ	C17-C18	3.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bA	4007	A1JPJ	C10-C9	3.60	1.40	1.35
15	aA	1135	CL7	C1D-ND	3.60	1.42	1.37
14	bA	1013	PHO	C1D-C2D	3.60	1.43	1.39
15	aB	1202	CL7	C1D-ND	3.60	1.42	1.37
15	cB	1203	CL7	C1D-ND	3.60	1.42	1.37
17	cA	4011	A1JPJ	C17-C18	3.60	1.40	1.35
15	aA	1022	CL7	C1D-ND	3.59	1.42	1.37
15	aL	1501	CL7	C1D-ND	3.59	1.42	1.37
15	cB	1012	CL7	C1D-ND	3.59	1.42	1.37
15	bA	1116	CL7	C1D-ND	3.59	1.42	1.37
15	bB	1206	CL7	C1D-ND	3.59	1.42	1.37
15	aA	1136	CL7	C1D-ND	3.59	1.42	1.37
15	bA	1124	CL7	C1D-ND	3.59	1.42	1.37
15	bB	1233	CL7	C4B-NB	3.59	1.42	1.37
15	bA	1131	CL7	C1D-ND	3.59	1.42	1.37
15	cB	1215	CL7	C1D-ND	3.59	1.42	1.37
17	aL	4020	A1JPJ	C14-C13	3.59	1.40	1.35
15	bA	1121	CL7	C1D-ND	3.59	1.42	1.37
15	aB	1237	CL7	C1D-ND	3.58	1.42	1.37
15	cB	1238	CL7	C1D-ND	3.58	1.42	1.37
15	bB	1237	CL7	C1D-ND	3.58	1.42	1.37
15	cA	1121	CL7	C1D-ND	3.58	1.42	1.37
15	cA	1127	CL7	C1D-ND	3.58	1.42	1.37
15	cJ	1301	CL7	C4B-NB	3.58	1.42	1.37
15	bB	1235	CL7	C1D-ND	3.58	1.42	1.37
15	bB	1228	CL7	C4B-NB	3.58	1.42	1.37
15	aB	1201	CL7	C1D-ND	3.58	1.42	1.37
15	bA	1103	CL7	C1D-ND	3.57	1.42	1.37
15	bB	1012	CL7	C1D-ND	3.57	1.42	1.37
17	cI	4019	A1JPJ	C17-C18	3.57	1.40	1.35
17	cI	4019	A1JPJ	C21-C22	3.57	1.40	1.35
17	bB	4021	A1JPJ	C10-C9	3.57	1.40	1.35
15	aA	1118	CL7	C4B-NB	3.57	1.42	1.37
15	cB	1231	CL7	C4B-NB	3.57	1.42	1.37
15	bB	1203	CL7	C1D-ND	3.57	1.42	1.37
17	aI	4019	A1JPJ	C21-C22	3.57	1.40	1.35
15	aB	1241	CL7	C4B-NB	3.57	1.42	1.37
15	bB	1231	CL7	C4B-NB	3.56	1.42	1.37
15	aA	1115	CL7	C1D-ND	3.56	1.42	1.37
15	bA	1101	CL7	C4B-NB	3.56	1.42	1.37
15	cJ	1302	CL7	C4B-NB	3.56	1.42	1.37
15	bL	1503	CL7	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	aL	4020	A1JPJ	C10-C9	3.56	1.40	1.35
17	bL	4020	A1JPJ	C14-C13	3.56	1.40	1.35
15	aA	1125	CL7	C4B-NB	3.55	1.42	1.37
15	bA	1127	CL7	C1D-ND	3.55	1.42	1.37
15	aB	1021	CL7	C1D-ND	3.55	1.42	1.37
15	cL	1502	CL7	C1D-ND	3.55	1.42	1.37
17	cL	4020	A1JPJ	C10-C9	3.55	1.40	1.35
15	aA	1127	CL7	C1D-ND	3.55	1.42	1.37
15	bA	1107	CL7	C1D-ND	3.55	1.42	1.37
15	cA	1107	CL7	C1D-ND	3.55	1.42	1.37
17	bL	4020	A1JPJ	C17-C18	3.55	1.40	1.35
17	cL	4020	A1JPJ	C14-C13	3.54	1.40	1.35
15	aB	1231	CL7	C4B-NB	3.54	1.42	1.37
15	cA	1123	CL7	C4B-NB	3.54	1.42	1.37
14	bB	1023	PHO	C1D-C2D	3.54	1.43	1.39
17	bI	4018	A1JPJ	C17-C18	3.54	1.40	1.35
17	cL	4020	A1JPJ	C21-C22	3.54	1.40	1.35
17	bL	4020	A1JPJ	C10-C9	3.54	1.40	1.35
15	cA	1115	CL7	C4B-NB	3.54	1.42	1.37
15	cB	1232	CL7	C4B-NB	3.54	1.42	1.37
17	bL	4023	A1JPJ	C10-C9	3.54	1.40	1.35
15	bB	1217	CL7	C4B-NB	3.54	1.42	1.37
15	cB	1225	CL7	C1D-ND	3.54	1.42	1.37
15	cA	1114	CL7	C4B-NB	3.54	1.42	1.37
15	cB	1219	CL7	C4B-NB	3.54	1.42	1.37
17	aL	4020	A1JPJ	C17-C18	3.54	1.40	1.35
15	cB	1237	CL7	C1D-ND	3.53	1.42	1.37
15	aB	1232	CL7	C4B-NB	3.53	1.42	1.37
17	aI	4018	A1JPJ	C21-C22	3.53	1.40	1.35
15	aL	1502	CL7	C1D-ND	3.53	1.42	1.37
15	cB	1230	CL7	C1D-ND	3.53	1.42	1.37
15	aB	1217	CL7	C4B-NB	3.53	1.42	1.37
15	bA	1115	CL7	C4B-NB	3.53	1.42	1.37
15	cB	1206	CL7	C1D-ND	3.52	1.42	1.37
17	cB	4021	A1JPJ	C10-C9	3.52	1.40	1.35
17	cA	4011	A1JPJ	C21-C22	3.52	1.40	1.35
17	bA	4008	A1JPJ	C17-C18	3.52	1.40	1.35
15	bK	1402	CL7	C4B-NB	3.52	1.42	1.37
17	bL	4020	A1JPJ	C21-C22	3.51	1.40	1.35
15	bB	1229	CL7	C4B-NB	3.51	1.42	1.37
14	cB	1023	PHO	C1D-C2D	3.51	1.43	1.39
15	bL	1502	CL7	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1215	CL7	C4B-NB	3.51	1.42	1.37
15	cB	1217	CL7	C4B-NB	3.51	1.42	1.37
15	cB	1233	CL7	C4B-NB	3.51	1.42	1.37
15	aA	1103	CL7	C1D-ND	3.51	1.42	1.37
15	aA	1128	CL7	C4B-NB	3.51	1.42	1.37
15	bB	1241	CL7	C4B-NB	3.51	1.42	1.37
17	bA	4011	A1JPJ	C17-C18	3.51	1.40	1.35
15	bB	1204	CL7	C1D-ND	3.51	1.42	1.37
17	cA	4003	A1JPJ	C10-C9	3.51	1.40	1.35
17	bA	4011	A1JPJ	C14-C13	3.50	1.40	1.35
15	bJ	1302	CL7	C4B-NB	3.50	1.42	1.37
15	aB	1201	CL7	C4B-NB	3.50	1.42	1.37
15	aB	1206	CL7	C1D-ND	3.50	1.42	1.37
15	cA	1118	CL7	C4B-NB	3.50	1.42	1.37
17	aA	4003	A1JPJ	C10-C9	3.50	1.40	1.35
15	aB	1236	CL7	C4B-NB	3.50	1.42	1.37
17	aA	4011	A1JPJ	C21-C22	3.50	1.40	1.35
17	bI	4019	A1JPJ	C21-C22	3.50	1.40	1.35
15	aB	1204	CL7	C1D-ND	3.50	1.42	1.37
15	bA	1128	CL7	C4B-NB	3.50	1.42	1.37
17	bI	4018	A1JPJ	C21-C22	3.50	1.40	1.35
14	cA	1013	PHO	C1D-C2D	3.49	1.43	1.39
15	aJ	1301	CL7	C4B-NB	3.49	1.42	1.37
15	cA	1128	CL7	C4B-NB	3.49	1.42	1.37
15	bA	1022	CL7	C1D-ND	3.49	1.42	1.37
15	aB	1233	CL7	C4B-NB	3.49	1.42	1.37
17	cI	4018	A1JPJ	C21-C22	3.49	1.40	1.35
14	bB	1023	PHO	C4D-CHA	3.49	1.45	1.39
15	aB	1229	CL7	C4B-NB	3.49	1.42	1.37
14	aB	1023	PHO	C4D-CHA	3.49	1.45	1.39
15	aA	1114	CL7	C4B-NB	3.49	1.42	1.37
15	bJ	1301	CL7	C4B-NB	3.49	1.42	1.37
17	bA	4003	A1JPJ	C10-C9	3.48	1.40	1.35
15	aB	1213	CL7	C4B-NB	3.48	1.42	1.37
15	bB	1201	CL7	C4B-NB	3.48	1.42	1.37
15	bA	1114	CL7	C4B-NB	3.48	1.42	1.37
17	aA	4008	A1JPJ	C17-C18	3.48	1.40	1.35
15	aB	1209	CL7	C4B-NB	3.48	1.42	1.37
15	bB	1219	CL7	C4B-NB	3.47	1.42	1.37
15	cA	1101	CL7	C4B-NB	3.47	1.42	1.37
15	cB	1201	CL7	C4B-NB	3.47	1.42	1.37
15	aB	1227	CL7	C4B-NB	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	1013	PHO	C4D-CHA	3.47	1.45	1.39
15	bA	1123	CL7	C4B-NB	3.47	1.42	1.37
15	cB	1229	CL7	C4B-NB	3.47	1.42	1.37
17	aB	4021	A1JPJ	C10-C9	3.46	1.40	1.35
17	bA	4011	A1JPJ	C21-C22	3.46	1.40	1.35
17	bI	4018	A1JPJ	C14-C13	3.46	1.40	1.35
15	aB	1216	CL7	C4B-NB	3.46	1.42	1.37
15	aB	1212	CL7	C4B-NB	3.46	1.42	1.37
15	bK	1401	CL7	C4B-NB	3.46	1.42	1.37
15	bB	1218	CL7	C4B-NB	3.46	1.42	1.37
15	aA	1117	CL7	C4B-NB	3.46	1.42	1.37
15	bB	1209	CL7	C4B-NB	3.46	1.42	1.37
15	cB	1212	CL7	C4B-NB	3.45	1.42	1.37
15	aB	1219	CL7	C4B-NB	3.45	1.42	1.37
15	aK	1402	CL7	C4B-NB	3.45	1.42	1.37
17	aL	4020	A1JPJ	C21-C22	3.45	1.40	1.35
15	cA	1125	CL7	C4B-NB	3.45	1.42	1.37
14	aB	1023	PHO	C1D-C2D	3.45	1.43	1.39
17	aI	4018	A1JPJ	C17-C18	3.45	1.40	1.35
15	bL	1501	CL7	C1D-ND	3.44	1.42	1.37
15	cB	1209	CL7	C4B-NB	3.44	1.42	1.37
15	cA	1117	CL7	C4B-NB	3.44	1.42	1.37
15	bB	1236	CL7	C4B-NB	3.44	1.42	1.37
15	bB	1216	CL7	C4B-NB	3.44	1.42	1.37
15	aA	1105	CL7	C4B-NB	3.43	1.42	1.37
15	cB	1226	CL7	C4B-NB	3.43	1.42	1.37
15	aA	1108	CL7	C4B-NB	3.43	1.42	1.37
15	cB	1214	CL7	C4B-NB	3.43	1.42	1.37
15	aA	1110	CL7	C4B-NB	3.43	1.42	1.37
15	aB	1218	CL7	C4B-NB	3.43	1.42	1.37
15	cK	1402	CL7	C4B-NB	3.43	1.42	1.37
15	aJ	1302	CL7	C4B-NB	3.43	1.42	1.37
15	aA	1123	CL7	C4B-NB	3.43	1.42	1.37
15	bA	1110	CL7	C4B-NB	3.43	1.42	1.37
15	cA	1109	CL7	C4B-NB	3.43	1.42	1.37
15	cA	1102	CL7	C4B-NB	3.42	1.42	1.37
15	cB	1213	CL7	C4B-NB	3.42	1.42	1.37
17	aI	4018	A1JPJ	C14-C13	3.42	1.40	1.35
15	cB	1236	CL7	C4B-NB	3.42	1.42	1.37
15	aA	1103	CL7	C4B-NB	3.42	1.42	1.37
15	bA	1133	CL7	C4B-NB	3.42	1.42	1.37
15	bB	1212	CL7	C4B-NB	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cI	4018	A1JPJ	C14-C13	3.41	1.40	1.35
15	aA	1101	CL7	C4B-NB	3.41	1.42	1.37
15	cB	1218	CL7	C4B-NB	3.41	1.42	1.37
15	aB	1214	CL7	C4B-NB	3.41	1.42	1.37
15	aA	1109	CL7	C4B-NB	3.41	1.42	1.37
15	bA	1113	CL7	C4B-NB	3.41	1.42	1.37
15	cA	1116	CL7	C4B-NB	3.41	1.42	1.37
15	bB	1213	CL7	C4B-NB	3.41	1.42	1.37
15	aA	1139	CL7	C4B-NB	3.41	1.42	1.37
15	cA	1108	CL7	C4B-NB	3.41	1.42	1.37
15	cB	1224	CL7	C4B-NB	3.41	1.42	1.37
15	cA	1139	CL7	C4B-NB	3.41	1.42	1.37
15	bB	1204	CL7	C4B-NB	3.40	1.42	1.37
15	aA	1131	CL7	C4B-NB	3.40	1.42	1.37
15	bF	1701	CL7	C4B-NB	3.40	1.42	1.37
15	aK	1401	CL7	C4B-NB	3.40	1.42	1.37
15	cA	1119	CL7	C4B-NB	3.40	1.42	1.37
15	cA	1140	CL7	C4B-NB	3.40	1.42	1.37
15	cK	1401	CL7	C4B-NB	3.40	1.42	1.37
17	cI	4018	A1JPJ	C17-C18	3.40	1.40	1.35
15	bB	1215	CL7	C4B-NB	3.40	1.42	1.37
15	aB	1221	CL7	C4B-NB	3.40	1.42	1.37
15	cB	1208	CL7	C4B-NB	3.40	1.42	1.37
15	cB	1228	CL7	C4B-NB	3.40	1.42	1.37
15	cA	1105	CL7	C4B-NB	3.40	1.42	1.37
15	aA	1116	CL7	C4B-NB	3.40	1.42	1.37
15	bA	1105	CL7	C4B-NB	3.40	1.42	1.37
15	cA	1113	CL7	C4B-NB	3.40	1.42	1.37
15	bB	1221	CL7	C4B-NB	3.39	1.42	1.37
15	bB	1224	CL7	C4B-NB	3.39	1.42	1.37
15	cB	1235	CL7	C4B-NB	3.39	1.42	1.37
15	bA	1131	CL7	C4B-NB	3.39	1.42	1.37
15	aB	1215	CL7	C4B-NB	3.39	1.42	1.37
15	bA	1119	CL7	C4B-NB	3.39	1.42	1.37
15	bA	1137	CL7	C4B-NB	3.39	1.42	1.37
14	cB	1023	PHO	C4D-CHA	3.39	1.45	1.39
15	aB	1228	CL7	C4B-NB	3.39	1.42	1.37
15	aF	1701	CL7	C4B-NB	3.39	1.42	1.37
15	bA	1109	CL7	C4B-NB	3.39	1.42	1.37
17	cA	4008	A1JPJ	C17-C18	3.39	1.40	1.35
15	cB	1211	CL7	C4B-NB	3.38	1.41	1.37
15	cF	1701	CL7	C4B-NB	3.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1102	CL7	C4B-NB	3.38	1.41	1.37
15	bA	1112	CL7	C4B-NB	3.38	1.41	1.37
15	cB	1221	CL7	C4B-NB	3.38	1.41	1.37
15	aB	1208	CL7	C4B-NB	3.38	1.41	1.37
15	bA	1139	CL7	C4B-NB	3.38	1.41	1.37
14	bA	1013	PHO	C4D-CHA	3.38	1.45	1.39
15	aA	1119	CL7	C4B-NB	3.38	1.41	1.37
15	bA	1140	CL7	C4B-NB	3.38	1.41	1.37
15	cA	1131	CL7	C4B-NB	3.38	1.41	1.37
15	aA	1120	CL7	C4B-NB	3.37	1.41	1.37
15	bB	1214	CL7	C4B-NB	3.37	1.41	1.37
14	aA	1013	PHO	C4D-CHA	3.37	1.45	1.39
15	bB	1211	CL7	C4B-NB	3.37	1.41	1.37
15	cA	1133	CL7	C4B-NB	3.37	1.41	1.37
15	cB	1227	CL7	C4B-NB	3.37	1.41	1.37
15	aB	1211	CL7	C4B-NB	3.37	1.41	1.37
15	bB	1226	CL7	C4B-NB	3.37	1.41	1.37
15	aA	1102	CL7	C4B-NB	3.37	1.41	1.37
15	aA	1129	CL7	C4B-NB	3.37	1.41	1.37
15	cA	1107	CL7	C4B-NB	3.36	1.41	1.37
15	bA	1111	CL7	C4B-NB	3.36	1.41	1.37
15	bA	1117	CL7	C4B-NB	3.36	1.41	1.37
15	bB	1208	CL7	C4B-NB	3.36	1.41	1.37
15	bA	1116	CL7	C4B-NB	3.35	1.41	1.37
15	bA	1129	CL7	C4B-NB	3.35	1.41	1.37
15	cA	1129	CL7	C4B-NB	3.35	1.41	1.37
15	cA	1110	CL7	C4B-NB	3.35	1.41	1.37
15	aA	1133	CL7	C4B-NB	3.35	1.41	1.37
15	cB	1216	CL7	C4B-NB	3.35	1.41	1.37
15	cA	1103	CL7	C4B-NB	3.35	1.41	1.37
15	aB	1210	CL7	C4B-NB	3.35	1.41	1.37
15	bA	1138	CL7	C4B-NB	3.35	1.41	1.37
15	bA	1103	CL7	C4B-NB	3.35	1.41	1.37
15	aI	1601	CL7	C4B-NB	3.35	1.41	1.37
15	cA	1120	CL7	C4B-NB	3.35	1.41	1.37
15	cA	1801	CL7	C4B-NB	3.35	1.41	1.37
15	aL	1503	CL7	C4B-NB	3.35	1.41	1.37
15	bB	1235	CL7	C4B-NB	3.35	1.41	1.37
15	cL	1503	CL7	C4B-NB	3.35	1.41	1.37
15	cB	1210	CL7	C4B-NB	3.34	1.41	1.37
15	bB	1210	CL7	C4B-NB	3.34	1.41	1.37
15	cB	1241	CL7	C4B-NB	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1223	CL7	C4B-NB	3.34	1.41	1.37
15	cA	1127	CL7	C4B-NB	3.34	1.41	1.37
15	cB	1220	CL7	C4B-NB	3.34	1.41	1.37
15	aB	1223	CL7	C4B-NB	3.34	1.41	1.37
15	bA	1121	CL7	C4B-NB	3.34	1.41	1.37
17	bA	4008	A1JPJ	C21-C22	3.34	1.40	1.35
15	aA	1137	CL7	C4B-NB	3.33	1.41	1.37
17	aA	4008	A1JPJ	C21-C22	3.33	1.40	1.35
15	aA	1140	CL7	C4B-NB	3.33	1.41	1.37
15	bL	1503	CL7	C4B-NB	3.33	1.41	1.37
15	bB	1220	CL7	C4B-NB	3.33	1.41	1.37
15	aA	1113	CL7	C4B-NB	3.32	1.41	1.37
15	bA	1136	CL7	C4B-NB	3.32	1.41	1.37
15	bA	1801	CL7	C4B-NB	3.32	1.41	1.37
17	bA	4008	A1JPJ	C14-C13	3.32	1.40	1.35
15	bB	1239	CL7	C4B-NB	3.32	1.41	1.37
15	cB	1204	CL7	C4B-NB	3.32	1.41	1.37
15	cI	1601	CL7	C4B-NB	3.32	1.41	1.37
15	aB	1239	CL7	C4B-NB	3.32	1.41	1.37
15	aB	1226	CL7	C4B-NB	3.32	1.41	1.37
15	aB	1235	CL7	C4B-NB	3.32	1.41	1.37
15	cA	1121	CL7	C4B-NB	3.31	1.41	1.37
15	cB	1021	CL7	C4B-NB	3.31	1.41	1.37
17	bA	4011	A1JPJ	C10-C9	3.31	1.40	1.35
15	aB	1220	CL7	C4B-NB	3.31	1.41	1.37
15	bB	1203	CL7	C4B-NB	3.31	1.41	1.37
17	aA	4008	A1JPJ	C14-C13	3.31	1.40	1.35
15	bA	1022	CL7	C4B-NB	3.31	1.41	1.37
15	aB	1202	CL7	C4B-NB	3.31	1.41	1.37
15	bA	1108	CL7	C4B-NB	3.31	1.41	1.37
15	bB	1223	CL7	C4B-NB	3.31	1.41	1.37
15	cB	1202	CL7	C4B-NB	3.30	1.41	1.37
15	bB	1222	CL7	C4B-NB	3.30	1.41	1.37
15	aA	1104	CL7	C4B-NB	3.30	1.41	1.37
15	aB	1021	CL7	C4B-NB	3.30	1.41	1.37
15	cB	1238	CL7	C4B-NB	3.30	1.41	1.37
15	aA	1127	CL7	C4B-NB	3.30	1.41	1.37
17	cA	4008	A1JPJ	C21-C22	3.30	1.40	1.35
17	cA	4008	A1JPJ	C14-C13	3.30	1.40	1.35
15	cA	1022	CL7	C4B-NB	3.29	1.41	1.37
15	aB	1224	CL7	C4B-NB	3.29	1.41	1.37
15	aA	1122	CL7	C4B-NB	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1801	CL7	C4B-NB	3.29	1.41	1.37
15	aA	1138	CL7	C4B-NB	3.29	1.41	1.37
15	bA	1122	CL7	C4B-NB	3.29	1.41	1.37
15	bB	1225	CL7	C4B-NB	3.29	1.41	1.37
15	cA	1112	CL7	C4B-NB	3.28	1.41	1.37
15	cB	1222	CL7	C4B-NB	3.28	1.41	1.37
15	aA	1111	CL7	C4B-NB	3.28	1.41	1.37
15	aB	1203	CL7	C4B-NB	3.28	1.41	1.37
15	aA	1121	CL7	C4B-NB	3.28	1.41	1.37
15	aA	1125	CL7	C3B-C4B	3.28	1.50	1.42
17	bA	4011	A1JPJ	C8-C9	-3.27	1.38	1.45
15	aA	1112	CL7	C4B-NB	3.27	1.41	1.37
15	bA	1120	CL7	C4B-NB	3.27	1.41	1.37
15	cB	1239	CL7	C4B-NB	3.27	1.41	1.37
15	bA	1107	CL7	C4B-NB	3.27	1.41	1.37
15	bA	1127	CL7	C4B-NB	3.27	1.41	1.37
15	cA	1106	CL7	C4B-NB	3.27	1.41	1.37
15	bB	1202	CL7	C4B-NB	3.27	1.41	1.37
15	bB	1021	CL7	C4B-NB	3.27	1.41	1.37
15	bA	1125	CL7	C4B-NB	3.26	1.41	1.37
15	bA	1126	CL7	C3B-C4B	3.26	1.50	1.42
15	aB	1204	CL7	C4B-NB	3.26	1.41	1.37
15	cB	1225	CL7	C4B-NB	3.26	1.41	1.37
15	bA	1134	CL7	C4B-NB	3.26	1.41	1.37
15	cA	1137	CL7	C4B-NB	3.26	1.41	1.37
15	aA	1134	CL7	C4B-NB	3.26	1.41	1.37
15	aA	1022	CL7	C4B-NB	3.26	1.41	1.37
15	bI	1601	CL7	C4B-NB	3.26	1.41	1.37
15	aA	1107	CL7	C4B-NB	3.26	1.41	1.37
15	aA	1124	CL7	C4B-NB	3.25	1.41	1.37
15	cL	1501	CL7	C4B-NB	3.25	1.41	1.37
17	aA	4008	A1JPJ	C8-C9	-3.25	1.39	1.45
15	aB	1238	CL7	C4B-NB	3.25	1.41	1.37
15	bA	1124	CL7	C4B-NB	3.25	1.41	1.37
15	bA	1132	CL7	C4B-NB	3.25	1.41	1.37
15	aB	1206	CL7	C4B-NB	3.25	1.41	1.37
15	aL	1501	CL7	C4B-NB	3.25	1.41	1.37
15	cB	1205	CL7	C4B-NB	3.25	1.41	1.37
15	bB	1206	CL7	C4B-NB	3.25	1.41	1.37
15	cL	1502	CL7	C4D-ND	-3.24	1.33	1.37
15	cA	1134	CL7	C4B-NB	3.24	1.41	1.37
15	aB	1205	CL7	C4B-NB	3.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1238	CL7	C4B-NB	3.24	1.41	1.37
17	cI	4018	A1JPJ	C10-C9	3.24	1.40	1.35
15	bA	1130	CL7	C4B-NB	3.24	1.41	1.37
15	bB	1012	CL7	C4B-NB	3.23	1.41	1.37
15	cA	1122	CL7	C4B-NB	3.23	1.41	1.37
15	bA	1106	CL7	C4B-NB	3.23	1.41	1.37
15	cA	1136	CL7	C4B-NB	3.23	1.41	1.37
17	bI	4018	A1JPJ	C8-C9	-3.23	1.39	1.45
15	cA	1111	CL7	C4B-NB	3.23	1.41	1.37
15	cB	1206	CL7	C4B-NB	3.23	1.41	1.37
15	bA	1126	CL7	C3D-C4D	3.23	1.48	1.39
15	aB	1222	CL7	C4B-NB	3.23	1.41	1.37
15	cB	1237	CL7	C4B-NB	3.23	1.41	1.37
15	bB	1207	CL7	C4D-ND	-3.22	1.33	1.37
15	cA	1116	CL7	C3B-C4B	3.22	1.50	1.42
15	bB	1202	CL7	C4D-ND	-3.22	1.33	1.37
15	aB	1203	CL7	C4D-ND	-3.22	1.33	1.37
15	aB	1230	CL7	C4B-NB	3.22	1.41	1.37
15	bB	1237	CL7	C4B-NB	3.22	1.41	1.37
15	bL	1501	CL7	C4B-NB	3.22	1.41	1.37
15	aB	1234	CL7	C4B-NB	3.22	1.41	1.37
15	cA	1135	CL7	C1D-ND	3.22	1.41	1.37
15	aA	1106	CL7	C4B-NB	3.22	1.41	1.37
15	cA	1104	CL7	C4B-NB	3.22	1.41	1.37
17	bI	4018	A1JPJ	C10-C9	3.22	1.40	1.35
15	aB	1237	CL7	C4B-NB	3.22	1.41	1.37
17	bA	4008	A1JPJ	C8-C9	-3.22	1.39	1.45
15	bB	1230	CL7	C4B-NB	3.21	1.41	1.37
17	aI	4018	A1JPJ	C8-C9	-3.21	1.39	1.45
17	cA	4008	A1JPJ	C8-C9	-3.21	1.39	1.45
15	aA	1130	CL7	C4B-NB	3.21	1.41	1.37
15	aJ	1301	CL7	C3B-C4B	3.21	1.50	1.42
17	cI	4018	A1JPJ	C8-C9	-3.21	1.39	1.45
15	cB	1203	CL7	C4B-NB	3.21	1.41	1.37
15	aB	1221	CL7	C3D-C4D	3.21	1.48	1.39
15	cA	1126	CL7	C4B-NB	3.20	1.41	1.37
15	cB	1202	CL7	C4D-ND	-3.20	1.33	1.37
15	bB	1204	CL7	C4D-ND	-3.20	1.33	1.37
15	aA	1136	CL7	C4B-NB	3.20	1.41	1.37
15	cA	1138	CL7	C4B-NB	3.20	1.41	1.37
15	cB	1012	CL7	C4B-NB	3.20	1.41	1.37
15	aA	1122	CL7	C4D-ND	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1126	CL7	C4B-NB	3.20	1.41	1.37
15	bB	1205	CL7	C4B-NB	3.20	1.41	1.37
15	bB	1218	CL7	C3D-C4D	3.20	1.48	1.39
15	cA	1022	CL7	C4D-ND	-3.19	1.33	1.37
15	aA	1136	CL7	C4D-ND	-3.19	1.33	1.37
15	bB	1215	CL7	C4D-ND	-3.19	1.33	1.37
15	cB	1218	CL7	C3D-C4D	3.19	1.48	1.39
15	cB	1230	CL7	C4B-NB	3.19	1.41	1.37
15	aB	1204	CL7	C4D-ND	-3.19	1.33	1.37
15	aA	1135	CL7	C4B-NB	3.19	1.41	1.37
15	bL	1502	CL7	C4D-ND	-3.19	1.33	1.37
15	bA	1120	CL7	C3B-C4B	3.19	1.50	1.42
15	cJ	1301	CL7	C3B-C4B	3.19	1.50	1.42
15	aL	1502	CL7	C4D-ND	-3.19	1.33	1.37
15	aA	1131	CL7	C4D-ND	-3.18	1.33	1.37
15	aB	1225	CL7	C4B-NB	3.18	1.41	1.37
15	cB	1234	CL7	C4B-NB	3.18	1.41	1.37
15	bB	1219	CL7	C3D-C4D	3.18	1.48	1.39
15	aA	1120	CL7	C3B-C4B	3.18	1.50	1.42
15	bB	1214	CL7	C3B-C4B	3.18	1.50	1.42
15	bA	1124	CL7	C4D-ND	-3.18	1.33	1.37
15	cA	1124	CL7	C4B-NB	3.18	1.41	1.37
15	aA	1022	CL7	C4D-ND	-3.18	1.33	1.37
15	aA	1116	CL7	C3B-C4B	3.18	1.50	1.42
15	cA	1122	CL7	C4D-ND	-3.18	1.33	1.37
15	cA	1130	CL7	C4B-NB	3.18	1.41	1.37
15	bA	1116	CL7	C3B-C4B	3.18	1.50	1.42
15	bJ	1301	CL7	C3B-C4B	3.18	1.50	1.42
15	cB	1214	CL7	C3B-C4B	3.17	1.50	1.42
15	bA	1022	CL7	C4D-ND	-3.17	1.33	1.37
15	bA	1126	CL7	MG-NC	3.17	2.12	2.05
15	aB	1012	CL7	C4B-NB	3.17	1.41	1.37
15	bB	1213	CL7	C3D-C4D	3.17	1.48	1.39
15	aA	1124	CL7	C3B-C4B	3.17	1.50	1.42
15	cB	1225	CL7	C4D-ND	-3.17	1.33	1.37
15	bA	1104	CL7	C4B-NB	3.17	1.41	1.37
15	bA	1110	CL7	C3D-C4D	3.17	1.48	1.39
15	aJ	1302	CL7	C3D-C4D	3.17	1.48	1.39
15	cA	1125	CL7	C3B-C4B	3.17	1.50	1.42
15	cA	1112	CL7	C3D-C4D	3.17	1.48	1.39
15	cJ	1302	CL7	C3D-C4D	3.17	1.48	1.39
15	aB	1213	CL7	C3D-C4D	3.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1203	CL7	C4D-ND	-3.16	1.33	1.37
15	bB	1236	CL7	C4D-ND	-3.16	1.33	1.37
15	cB	1207	CL7	C4B-NB	3.16	1.41	1.37
15	cA	1116	CL7	C4D-ND	-3.16	1.33	1.37
15	aB	1218	CL7	C3D-C4D	3.16	1.48	1.39
15	bA	1135	CL7	C4B-NB	3.16	1.41	1.37
15	cA	1124	CL7	C3B-C4B	3.16	1.50	1.42
15	bA	1124	CL7	C3B-C4B	3.16	1.50	1.42
15	bA	1115	CL7	C4D-ND	-3.16	1.33	1.37
15	bB	1221	CL7	C3D-C4D	3.16	1.48	1.39
15	cL	1502	CL7	C4B-NB	3.15	1.41	1.37
15	cA	1124	CL7	C4D-ND	-3.15	1.33	1.37
15	bJ	1302	CL7	C3D-C4D	3.15	1.48	1.39
15	bA	1106	CL7	C4D-ND	-3.15	1.33	1.37
15	aB	1218	CL7	C3B-C4B	3.15	1.50	1.42
15	aA	1112	CL7	C3D-C4D	3.15	1.48	1.39
15	cK	1402	CL7	C3D-C4D	3.15	1.48	1.39
15	cB	1236	CL7	C4D-ND	-3.15	1.33	1.37
15	aB	1235	CL7	C4D-ND	-3.15	1.33	1.37
15	cB	1204	CL7	C4D-ND	-3.15	1.33	1.37
15	aL	1503	CL7	C4D-ND	-3.15	1.33	1.37
15	bB	1223	CL7	C4D-ND	-3.15	1.33	1.37
15	bL	1501	CL7	C4D-ND	-3.15	1.33	1.37
15	bL	1502	CL7	C4B-NB	3.15	1.41	1.37
15	aJ	1301	CL7	C3D-C4D	3.15	1.48	1.39
15	cB	1213	CL7	C3D-C4D	3.15	1.48	1.39
15	aB	1207	CL7	C4D-ND	-3.15	1.33	1.37
15	cJ	1301	CL7	C3D-C4D	3.14	1.48	1.39
15	cB	1219	CL7	C3D-C4D	3.14	1.48	1.39
15	cB	1233	CL7	C3D-C4D	3.14	1.48	1.39
15	cB	1212	CL7	C3D-C4D	3.14	1.48	1.39
15	aB	1215	CL7	C4D-ND	-3.14	1.33	1.37
15	cA	1136	CL7	C4D-ND	-3.14	1.33	1.37
15	aB	1238	CL7	C4D-ND	-3.14	1.33	1.37
15	bA	1136	CL7	C4D-ND	-3.14	1.33	1.37
15	aB	1220	CL7	C3D-C4D	3.14	1.48	1.39
15	cB	1229	CL7	C4D-ND	-3.14	1.33	1.37
17	aI	4018	A1JPJ	C10-C9	3.14	1.39	1.35
15	cA	1103	CL7	C4D-ND	-3.14	1.33	1.37
15	aB	1212	CL7	C3D-C4D	3.14	1.48	1.39
15	aB	1228	CL7	C3D-C4D	3.14	1.48	1.39
15	aB	1236	CL7	C4D-ND	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1235	CL7	C4D-ND	-3.14	1.33	1.37
15	bA	1122	CL7	C4D-ND	-3.14	1.33	1.37
15	aA	1110	CL7	C3D-C4D	3.13	1.48	1.39
15	aB	1219	CL7	C3D-C4D	3.13	1.48	1.39
15	cA	1102	CL7	C3D-C4D	3.13	1.48	1.39
15	cA	1120	CL7	C3B-C4B	3.13	1.50	1.42
15	cB	1203	CL7	C4D-ND	-3.13	1.33	1.37
15	bB	1220	CL7	C3D-C4D	3.13	1.48	1.39
15	cL	1501	CL7	C4D-ND	-3.13	1.33	1.37
15	bA	1125	CL7	C3B-C4B	3.13	1.50	1.42
15	cA	1110	CL7	C3D-C4D	3.13	1.48	1.39
15	aB	1233	CL7	C3D-C4D	3.13	1.48	1.39
15	cJ	1302	CL7	C3B-C4B	3.13	1.50	1.42
15	cA	1101	CL7	C3B-C4B	3.13	1.50	1.42
15	aB	1202	CL7	C4D-ND	-3.13	1.33	1.37
15	cB	1223	CL7	C4D-ND	-3.13	1.33	1.37
15	cB	1231	CL7	C3B-C4B	3.13	1.50	1.42
15	aA	1124	CL7	C4D-ND	-3.13	1.33	1.37
15	cB	1207	CL7	C4D-ND	-3.13	1.33	1.37
15	bA	1122	CL7	C3B-C4B	3.13	1.50	1.42
15	bA	1109	CL7	C3B-C4B	3.12	1.50	1.42
15	bA	1139	CL7	C3D-C4D	3.12	1.48	1.39
15	bA	1103	CL7	C4D-ND	-3.12	1.33	1.37
15	cA	1102	CL7	C3B-C4B	3.12	1.50	1.42
15	aB	1206	CL7	C4D-ND	-3.12	1.33	1.37
15	aB	1210	CL7	C3B-C4B	3.12	1.50	1.42
15	bJ	1301	CL7	C3D-C4D	3.12	1.48	1.39
15	aB	1231	CL7	C3B-C4B	3.12	1.50	1.42
15	aB	1224	CL7	C4D-ND	-3.12	1.33	1.37
15	bB	1210	CL7	C3B-C4B	3.12	1.50	1.42
15	cB	1229	CL7	C3D-C4D	3.12	1.48	1.39
15	bB	1233	CL7	C3D-C4D	3.12	1.48	1.39
15	cB	1211	CL7	C3D-C4D	3.12	1.48	1.39
15	bB	1201	CL7	C3B-C4B	3.12	1.50	1.42
15	aA	1125	CL7	C4D-ND	-3.12	1.33	1.37
15	cB	1220	CL7	C3D-C4D	3.12	1.48	1.39
15	aB	1217	CL7	C3D-C4D	3.12	1.48	1.39
15	bA	1102	CL7	C3B-C4B	3.12	1.50	1.42
15	aJ	1302	CL7	C3B-C4B	3.12	1.50	1.42
15	bA	1102	CL7	C3D-C4D	3.11	1.48	1.39
15	bB	1212	CL7	C3D-C4D	3.11	1.48	1.39
15	aA	1117	CL7	C3B-C4B	3.11	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1210	CL7	C3D-C4D	3.11	1.48	1.39
15	cA	1140	CL7	C4D-ND	-3.11	1.33	1.37
15	bB	1217	CL7	C3D-C4D	3.11	1.48	1.39
15	cK	1401	CL7	C3D-C4D	3.11	1.48	1.39
15	cB	1232	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1237	CL7	C4D-ND	-3.11	1.33	1.37
15	cB	1219	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1228	CL7	C3B-C4B	3.11	1.50	1.42
15	bA	1112	CL7	C3D-C4D	3.11	1.48	1.39
15	cA	1139	CL7	C3D-C4D	3.11	1.48	1.39
15	bB	1238	CL7	C3B-C4B	3.11	1.50	1.42
15	aB	1217	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1216	CL7	C3D-C4D	3.11	1.48	1.39
15	aB	1214	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1232	CL7	C3B-C4B	3.11	1.50	1.42
15	bA	1134	CL7	C3D-C4D	3.11	1.48	1.39
15	aA	1114	CL7	C3D-C4D	3.11	1.48	1.39
15	cA	1135	CL7	C4B-NB	3.11	1.41	1.37
15	aB	1232	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1218	CL7	C3B-C4B	3.11	1.50	1.42
15	cA	1113	CL7	C3D-C4D	3.11	1.48	1.39
15	aA	1137	CL7	C4D-ND	-3.11	1.33	1.37
15	aB	1223	CL7	C4D-ND	-3.11	1.33	1.37
15	aA	1101	CL7	C3D-C4D	3.11	1.48	1.39
15	bJ	1302	CL7	C3B-C4B	3.11	1.50	1.42
15	aA	1109	CL7	C3B-C4B	3.11	1.50	1.42
15	cB	1201	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1211	CL7	C3D-C4D	3.11	1.48	1.39
15	cA	1134	CL7	C3D-C4D	3.11	1.48	1.39
15	cA	1125	CL7	C4D-ND	-3.11	1.33	1.37
15	cB	1217	CL7	C3B-C4B	3.11	1.50	1.42
15	aA	1118	CL7	C3D-C4D	3.11	1.48	1.39
15	cB	1228	CL7	C3D-C4D	3.11	1.48	1.39
15	bA	1113	CL7	C3B-C4B	3.11	1.50	1.42
15	aB	1229	CL7	C4D-ND	-3.11	1.33	1.37
15	bA	1117	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1227	CL7	C3B-C4B	3.11	1.50	1.42
15	bB	1239	CL7	C4D-ND	-3.10	1.33	1.37
15	bB	1207	CL7	C4B-NB	3.10	1.41	1.37
15	cB	1217	CL7	C3D-C4D	3.10	1.48	1.39
15	cA	1108	CL7	C3B-C4B	3.10	1.50	1.42
15	aA	1117	CL7	C3D-C4D	3.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1234	CL7	C4B-NB	3.10	1.41	1.37
15	cB	1228	CL7	C3B-C4B	3.10	1.50	1.42
15	cA	1129	CL7	C4D-ND	-3.10	1.33	1.37
15	aF	1701	CL7	C3B-C4B	3.10	1.50	1.42
15	bB	1228	CL7	C3D-C4D	3.10	1.48	1.39
15	cA	1123	CL7	C3D-C4D	3.10	1.48	1.39
15	cB	1209	CL7	C3D-C4D	3.10	1.48	1.39
15	bB	1235	CL7	C4D-ND	-3.10	1.33	1.37
15	aL	1502	CL7	C4B-NB	3.10	1.41	1.37
15	cA	1120	CL7	C3D-C4D	3.10	1.48	1.39
15	aB	1219	CL7	C3B-C4B	3.10	1.50	1.42
15	aA	1102	CL7	C3B-C4B	3.10	1.50	1.42
15	cA	1116	CL7	C3D-C4D	3.10	1.48	1.39
15	cB	1227	CL7	C3D-C4D	3.10	1.48	1.39
15	aA	1139	CL7	C3D-C4D	3.10	1.48	1.39
15	aB	1209	CL7	C3D-C4D	3.10	1.48	1.39
15	cA	1119	CL7	C4D-ND	-3.10	1.33	1.37
15	cB	1220	CL7	C3B-C4B	3.10	1.50	1.42
15	cA	1114	CL7	C3B-C4B	3.10	1.50	1.42
15	cB	1224	CL7	C3B-C4B	3.10	1.50	1.42
15	aA	1134	CL7	C3D-C4D	3.10	1.48	1.39
15	bA	1110	CL7	C3B-C4B	3.10	1.50	1.42
15	cA	1114	CL7	C3D-C4D	3.10	1.48	1.39
15	aA	1101	CL7	C3B-C4B	3.10	1.50	1.42
15	cB	1232	CL7	C3D-C4D	3.10	1.48	1.39
15	cA	1130	CL7	C4D-ND	-3.10	1.33	1.37
15	aB	1012	CL7	C4D-ND	-3.10	1.33	1.37
15	cA	1117	CL7	C3B-C4B	3.10	1.50	1.42
15	bA	1114	CL7	C3B-C4B	3.10	1.50	1.42
15	aA	1123	CL7	C3D-C4D	3.10	1.48	1.39
15	aA	1102	CL7	C3D-C4D	3.10	1.48	1.39
15	bB	1224	CL7	C4D-ND	-3.10	1.33	1.37
15	cB	1216	CL7	C4D-ND	-3.10	1.33	1.37
15	aB	1232	CL7	C3D-C4D	3.10	1.48	1.39
15	bA	1101	CL7	C3B-C4B	3.09	1.50	1.42
15	cB	1233	CL7	C3B-C4B	3.09	1.50	1.42
15	bA	1101	CL7	C3D-C4D	3.09	1.48	1.39
15	cB	1223	CL7	C3B-C4B	3.09	1.50	1.42
15	cB	1238	CL7	C3B-C4B	3.09	1.50	1.42
15	bK	1402	CL7	C3D-C4D	3.09	1.48	1.39
15	aA	1119	CL7	C4D-ND	-3.09	1.33	1.37
15	aA	1135	CL7	C4D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1201	CL7	C3D-C4D	3.09	1.48	1.39
15	aA	1122	CL7	C3B-C4B	3.09	1.50	1.42
15	aB	1228	CL7	C3B-C4B	3.09	1.50	1.42
15	cA	1129	CL7	C3B-C4B	3.09	1.50	1.42
15	cA	1101	CL7	C3D-C4D	3.09	1.48	1.39
15	cI	1601	CL7	C3D-C4D	3.09	1.48	1.39
15	cB	1226	CL7	C4D-ND	-3.09	1.33	1.37
15	aB	1216	CL7	C3D-C4D	3.09	1.48	1.39
15	bB	1209	CL7	C3D-C4D	3.09	1.48	1.39
15	aB	1201	CL7	C3B-C4B	3.09	1.50	1.42
15	aB	1211	CL7	C3B-C4B	3.09	1.50	1.42
15	bB	1231	CL7	C3B-C4B	3.09	1.50	1.42
15	bA	1123	CL7	C3D-C4D	3.09	1.48	1.39
15	cA	1140	CL7	C3B-C4B	3.09	1.50	1.42
15	aA	1105	CL7	C3D-C4D	3.09	1.48	1.39
15	aB	1211	CL7	C3D-C4D	3.09	1.48	1.39
15	aB	1229	CL7	C3D-C4D	3.09	1.48	1.39
15	aK	1402	CL7	C3D-C4D	3.09	1.48	1.39
15	cB	1214	CL7	C3D-C4D	3.09	1.48	1.39
15	bL	1503	CL7	C4D-ND	-3.09	1.33	1.37
15	cA	1118	CL7	C3D-C4D	3.09	1.48	1.39
15	bB	1209	CL7	C3B-C4B	3.09	1.50	1.42
15	bA	1114	CL7	C3D-C4D	3.09	1.48	1.39
15	cA	1105	CL7	C3D-C4D	3.09	1.48	1.39
15	bB	1217	CL7	C3B-C4B	3.09	1.50	1.42
15	aA	1114	CL7	C3B-C4B	3.09	1.50	1.42
15	aI	1601	CL7	C3D-C4D	3.09	1.48	1.39
15	cB	1210	CL7	C3B-C4B	3.09	1.50	1.42
15	bA	1139	CL7	C3B-C4B	3.09	1.50	1.42
15	bB	1211	CL7	C3B-C4B	3.09	1.50	1.42
15	aA	1116	CL7	C3D-C4D	3.09	1.48	1.39
15	bA	1119	CL7	C4D-ND	-3.09	1.33	1.37
15	aA	1110	CL7	C3B-C4B	3.09	1.50	1.42
15	cL	1503	CL7	C4D-ND	-3.09	1.33	1.37
15	cA	1107	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1108	CL7	C3B-C4B	3.08	1.50	1.42
15	aK	1401	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1120	CL7	C3D-C4D	3.08	1.48	1.39
15	bB	1241	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1241	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1226	CL7	C3B-C4B	3.08	1.50	1.42
15	cA	1115	CL7	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1227	CL7	C3D-C4D	3.08	1.48	1.39
15	bA	1133	CL7	C3D-C4D	3.08	1.48	1.39
15	bB	1214	CL7	C3D-C4D	3.08	1.48	1.39
15	bK	1401	CL7	C3D-C4D	3.08	1.48	1.39
15	aB	1241	CL7	C3D-C4D	3.08	1.48	1.39
15	bA	1120	CL7	C3D-C4D	3.08	1.48	1.39
15	cA	1104	CL7	C4D-ND	-3.08	1.33	1.37
17	aA	4007	A1JPJ	C8-C9	-3.08	1.39	1.45
15	bA	1115	CL7	C3B-C4B	3.08	1.50	1.42
15	bF	1701	CL7	C3B-C4B	3.08	1.50	1.42
15	bA	1118	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1130	CL7	C4D-ND	-3.08	1.33	1.37
15	cB	1237	CL7	C4D-ND	-3.08	1.33	1.37
15	aA	1139	CL7	C3B-C4B	3.08	1.50	1.42
15	bA	1105	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1221	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1234	CL7	C4D-ND	-3.08	1.33	1.37
15	bB	1229	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1113	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1115	CL7	C4D-ND	-3.08	1.33	1.37
15	aA	1108	CL7	C3D-C4D	3.08	1.48	1.39
15	bA	1113	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1209	CL7	C3B-C4B	3.08	1.50	1.42
15	bB	1233	CL7	C3B-C4B	3.08	1.50	1.42
15	cA	1110	CL7	C3B-C4B	3.08	1.50	1.42
15	bA	1107	CL7	C3D-C4D	3.08	1.48	1.39
15	cF	1701	CL7	C3D-C4D	3.08	1.48	1.39
15	bB	1232	CL7	C3D-C4D	3.08	1.48	1.39
15	bA	1116	CL7	C4D-ND	-3.08	1.33	1.37
15	aB	1210	CL7	C3D-C4D	3.08	1.48	1.39
15	aA	1129	CL7	C4D-ND	-3.08	1.33	1.37
15	bB	1234	CL7	C4D-ND	-3.08	1.33	1.37
15	cB	1210	CL7	C3D-C4D	3.08	1.48	1.39
15	cB	1218	CL7	C3B-C4B	3.08	1.50	1.42
17	bB	4021	A1JPJ	C8-C9	-3.08	1.39	1.45
15	aA	1133	CL7	C3B-C4B	3.07	1.50	1.42
15	bA	1133	CL7	C3B-C4B	3.07	1.50	1.42
15	bB	1227	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1115	CL7	C3B-C4B	3.07	1.50	1.42
15	aB	1231	CL7	C3D-C4D	3.07	1.48	1.39
15	bI	1601	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1109	CL7	C3D-C4D	3.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1107	CL7	C3B-C4B	3.07	1.49	1.42
15	bA	1106	CL7	C3B-C4B	3.07	1.49	1.42
15	aB	1209	CL7	C3B-C4B	3.07	1.49	1.42
15	aB	1214	CL7	C3D-C4D	3.07	1.48	1.39
15	bA	1801	CL7	C3D-C4D	3.07	1.48	1.39
15	bB	1234	CL7	C3D-C4D	3.07	1.48	1.39
15	bB	1206	CL7	C4D-ND	-3.07	1.33	1.37
15	bB	1225	CL7	C4D-ND	-3.07	1.33	1.37
15	bF	1701	CL7	C3D-C4D	3.07	1.48	1.39
15	bB	1208	CL7	C3D-C4D	3.07	1.48	1.39
15	aA	1104	CL7	C3D-C4D	3.07	1.48	1.39
15	bA	1108	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1128	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1126	CL7	C3D-C4D	3.07	1.48	1.39
15	bL	1501	CL7	C3D-C4D	3.07	1.48	1.39
15	cB	1231	CL7	C3D-C4D	3.07	1.48	1.39
15	aB	1216	CL7	C4D-ND	-3.07	1.33	1.37
15	aB	1230	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1113	CL7	C3B-C4B	3.07	1.49	1.42
15	cB	1238	CL7	C4D-ND	-3.07	1.33	1.37
15	aB	1234	CL7	C3D-C4D	3.07	1.48	1.39
15	cA	1109	CL7	C3B-C4B	3.07	1.49	1.42
15	bB	1224	CL7	C3B-C4B	3.07	1.49	1.42
15	cA	1105	CL7	C3B-C4B	3.07	1.49	1.42
15	bA	1104	CL7	C3D-C4D	3.07	1.48	1.39
15	bB	1230	CL7	C3D-C4D	3.07	1.48	1.39
15	bA	1140	CL7	C4D-ND	-3.06	1.33	1.37
15	bA	1121	CL7	C3B-C4B	3.06	1.49	1.42
15	bA	1128	CL7	C3D-C4D	3.06	1.48	1.39
15	bA	1137	CL7	C4D-ND	-3.06	1.33	1.37
15	aL	1501	CL7	C4D-ND	-3.06	1.33	1.37
15	bA	1125	CL7	C4D-ND	-3.06	1.33	1.37
15	bB	1231	CL7	C3D-C4D	3.06	1.48	1.39
15	bA	1105	CL7	C3B-C4B	3.06	1.49	1.42
15	aA	1115	CL7	C3B-C4B	3.06	1.49	1.42
15	cA	1103	CL7	C3B-C4B	3.06	1.49	1.42
15	bA	1107	CL7	C4D-ND	-3.06	1.33	1.37
15	cB	1211	CL7	C3B-C4B	3.06	1.49	1.42
15	aB	1220	CL7	C4D-ND	-3.06	1.33	1.37
15	bA	1108	CL7	C3B-C4B	3.06	1.49	1.42
15	cB	1205	CL7	C4D-ND	-3.06	1.33	1.37
15	cA	1801	CL7	C3D-C4D	3.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1140	CL7	C3D-C4D	3.06	1.48	1.39
15	bK	1402	CL7	C3B-C4B	3.06	1.49	1.42
15	cA	1139	CL7	C3B-C4B	3.06	1.49	1.42
15	aB	1225	CL7	C4D-ND	-3.06	1.33	1.37
15	bA	1135	CL7	C4D-ND	-3.06	1.33	1.37
15	aB	1205	CL7	C3D-C4D	3.06	1.48	1.39
15	bB	1219	CL7	C3B-C4B	3.06	1.49	1.42
15	bA	1128	CL7	C3B-C4B	3.06	1.49	1.42
15	bB	1235	CL7	C3B-C4B	3.06	1.49	1.42
15	aB	1222	CL7	C3D-C4D	3.06	1.48	1.39
15	bB	1201	CL7	C3D-C4D	3.06	1.48	1.39
15	cA	1108	CL7	C3D-C4D	3.06	1.48	1.39
15	bA	1118	CL7	C3B-C4B	3.06	1.49	1.42
15	bB	1205	CL7	C3B-C4B	3.06	1.49	1.42
15	cK	1401	CL7	C3B-C4B	3.06	1.49	1.42
15	aA	1104	CL7	C4D-ND	-3.06	1.33	1.37
15	bA	1106	CL7	C3D-C4D	3.05	1.48	1.39
15	bA	1129	CL7	C3B-C4B	3.05	1.49	1.42
15	bA	1129	CL7	C4D-ND	-3.05	1.33	1.37
15	aB	1208	CL7	C3D-C4D	3.05	1.48	1.39
15	aA	1126	CL7	C3D-C4D	3.05	1.48	1.39
15	bA	1111	CL7	C3D-C4D	3.05	1.48	1.39
15	aA	1119	CL7	C3B-C4B	3.05	1.49	1.42
15	aB	1229	CL7	C3B-C4B	3.05	1.49	1.42
15	cA	1133	CL7	C3B-C4B	3.05	1.49	1.42
15	aA	1111	CL7	C3D-C4D	3.05	1.48	1.39
15	aA	1128	CL7	C3D-C4D	3.05	1.48	1.39
15	cB	1206	CL7	C4D-ND	-3.05	1.33	1.37
15	aB	1208	CL7	C3B-C4B	3.05	1.49	1.42
15	bB	1203	CL7	C3B-C4B	3.05	1.49	1.42
15	cA	1117	CL7	C3D-C4D	3.05	1.47	1.39
15	cF	1701	CL7	C3B-C4B	3.05	1.49	1.42
15	aA	1127	CL7	C4D-ND	-3.05	1.33	1.37
15	aF	1701	CL7	C3D-C4D	3.05	1.47	1.39
15	cA	1133	CL7	C3D-C4D	3.05	1.47	1.39
15	cB	1216	CL7	C3B-C4B	3.05	1.49	1.42
15	aA	1133	CL7	C3D-C4D	3.05	1.47	1.39
15	aA	1801	CL7	C3D-C4D	3.05	1.47	1.39
15	bB	1222	CL7	C3D-C4D	3.05	1.47	1.39
15	cA	1104	CL7	C3D-C4D	3.05	1.47	1.39
15	bA	1123	CL7	C3B-C4B	3.05	1.49	1.42
15	bB	1223	CL7	C3B-C4B	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1116	CL7	C3D-C4D	3.05	1.47	1.39
15	cA	1138	CL7	C3D-C4D	3.05	1.47	1.39
15	aA	1132	CL7	C3B-C4B	3.05	1.49	1.42
15	cB	1208	CL7	C3D-C4D	3.05	1.47	1.39
15	aA	1129	CL7	C3B-C4B	3.05	1.49	1.42
15	aK	1401	CL7	C3B-C4B	3.05	1.49	1.42
15	aA	1111	CL7	C3B-C4B	3.05	1.49	1.42
15	cK	1402	CL7	C3B-C4B	3.05	1.49	1.42
15	bB	1205	CL7	C3D-C4D	3.05	1.47	1.39
15	cA	1137	CL7	C4D-ND	-3.05	1.33	1.37
15	cB	1216	CL7	C3D-C4D	3.05	1.47	1.39
15	aB	1201	CL7	C3D-C4D	3.05	1.47	1.39
15	cB	1229	CL7	C3B-C4B	3.05	1.49	1.42
15	cA	1106	CL7	C4D-ND	-3.05	1.33	1.37
15	aB	1235	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1121	CL7	C4D-ND	-3.04	1.33	1.37
15	aA	1126	CL7	C4D-ND	-3.04	1.33	1.37
15	bA	1121	CL7	C4D-ND	-3.04	1.33	1.37
15	aA	1130	CL7	C3B-C4B	3.04	1.49	1.42
15	aB	1238	CL7	C3B-C4B	3.04	1.49	1.42
15	bA	1140	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1121	CL7	C3B-C4B	3.04	1.49	1.42
15	aB	1237	CL7	C4D-ND	-3.04	1.33	1.37
15	cB	1231	CL7	C4D-ND	-3.04	1.33	1.37
15	aB	1215	CL7	C3B-C4B	3.04	1.49	1.42
15	bA	1111	CL7	C3B-C4B	3.04	1.49	1.42
15	cA	1118	CL7	C3B-C4B	3.04	1.49	1.42
15	bA	1119	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1119	CL7	C3D-C4D	3.04	1.47	1.39
15	bB	1223	CL7	C3D-C4D	3.04	1.47	1.39
15	bB	1229	CL7	C3B-C4B	3.04	1.49	1.42
15	cA	1119	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1109	CL7	C3D-C4D	3.04	1.47	1.39
15	bB	1012	CL7	C4D-ND	-3.04	1.33	1.37
15	bA	1121	CL7	C3D-C4D	3.04	1.47	1.39
15	cA	1129	CL7	C3D-C4D	3.04	1.47	1.39
15	aA	1140	CL7	C3B-C4B	3.04	1.49	1.42
15	aB	1223	CL7	C3B-C4B	3.04	1.49	1.42
15	cB	1223	CL7	C3D-C4D	3.04	1.47	1.39
15	aA	1127	CL7	C3B-C4B	3.04	1.49	1.42
15	cA	1131	CL7	C4D-ND	-3.04	1.33	1.37
15	aB	1203	CL7	C3B-C4B	3.04	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1204	CL7	C3D-C4D	3.04	1.47	1.39
15	bA	1117	CL7	C3D-C4D	3.04	1.47	1.39
15	aA	1123	CL7	C4D-ND	-3.04	1.33	1.37
15	cB	1239	CL7	C4D-ND	-3.04	1.33	1.37
15	cB	1235	CL7	C3B-C4B	3.04	1.49	1.42
15	cA	1140	CL7	C3D-C4D	3.04	1.47	1.39
15	cB	1230	CL7	C3D-C4D	3.04	1.47	1.39
15	bA	1138	CL7	C3D-C4D	3.04	1.47	1.39
15	aA	1113	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1107	CL7	C3D-C4D	3.04	1.47	1.39
15	bB	1215	CL7	C3B-C4B	3.04	1.49	1.42
15	cA	1106	CL7	C3B-C4B	3.04	1.49	1.42
15	aA	1103	CL7	C3D-C4D	3.04	1.47	1.39
15	aA	1121	CL7	C3D-C4D	3.04	1.47	1.39
15	bB	1230	CL7	C4D-ND	-3.04	1.33	1.37
15	bB	1238	CL7	C4D-ND	-3.04	1.33	1.37
15	cA	1107	CL7	C3B-C4B	3.03	1.49	1.42
15	aB	1234	CL7	C4D-ND	-3.03	1.33	1.37
15	cA	1133	CL7	C4D-ND	-3.03	1.33	1.37
15	cB	1204	CL7	C3B-C4B	3.03	1.49	1.42
15	cA	1106	CL7	C3D-C4D	3.03	1.47	1.39
15	aA	1140	CL7	C4D-ND	-3.03	1.33	1.37
15	bB	1220	CL7	C3B-C4B	3.03	1.49	1.42
15	cB	1221	CL7	C3B-C4B	3.03	1.49	1.42
15	aB	1207	CL7	C4B-NB	3.03	1.41	1.37
15	bB	1208	CL7	C3B-C4B	3.03	1.49	1.42
15	aA	1106	CL7	C3D-C4D	3.03	1.47	1.39
15	cB	1230	CL7	C4D-ND	-3.03	1.33	1.37
15	cB	1213	CL7	C3B-C4B	3.03	1.49	1.42
15	cA	1119	CL7	C3D-C4D	3.03	1.47	1.39
15	bA	1140	CL7	C3D-C4D	3.03	1.47	1.39
15	cA	1111	CL7	C3B-C4B	3.03	1.49	1.42
15	cI	1601	CL7	C3B-C4B	3.03	1.49	1.42
15	aB	1239	CL7	C4D-ND	-3.03	1.33	1.37
15	aA	1137	CL7	C3D-C4D	3.03	1.47	1.39
15	bA	1119	CL7	C3D-C4D	3.03	1.47	1.39
15	bB	1222	CL7	C4D-ND	-3.03	1.33	1.37
15	bB	1226	CL7	C4D-ND	-3.03	1.33	1.37
15	bA	1104	CL7	C4D-ND	-3.03	1.33	1.37
15	bB	1210	CL7	C4D-ND	-3.03	1.33	1.37
15	bB	1229	CL7	C4D-ND	-3.03	1.33	1.37
15	aA	1105	CL7	C3B-C4B	3.03	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1138	CL7	C3D-C4D	3.03	1.47	1.39
15	bA	1107	CL7	C3B-C4B	3.03	1.49	1.42
15	cA	1128	CL7	C3B-C4B	3.03	1.49	1.42
15	aA	1106	CL7	C4D-ND	-3.03	1.33	1.37
15	bB	1225	CL7	C3B-C4B	3.02	1.49	1.42
15	aA	1118	CL7	C3B-C4B	3.02	1.49	1.42
15	aB	1227	CL7	C3B-C4B	3.02	1.49	1.42
15	cB	1208	CL7	C3B-C4B	3.02	1.49	1.42
15	cB	1234	CL7	C3D-C4D	3.02	1.47	1.39
15	aA	1107	CL7	C4D-ND	-3.02	1.33	1.37
15	cA	1138	CL7	C4D-ND	-3.02	1.33	1.37
15	cA	1111	CL7	C3D-C4D	3.02	1.47	1.39
15	cA	1132	CL7	C3B-C4B	3.02	1.49	1.42
15	cL	1501	CL7	C3D-C4D	3.02	1.47	1.39
15	aA	1111	CL7	C4D-ND	-3.02	1.33	1.37
15	aA	1103	CL7	C3B-C4B	3.02	1.49	1.42
15	aA	1106	CL7	C3B-C4B	3.02	1.49	1.42
15	aB	1205	CL7	C3B-C4B	3.02	1.49	1.42
15	bB	1216	CL7	C3B-C4B	3.02	1.49	1.42
15	cB	1222	CL7	C3D-C4D	3.02	1.47	1.39
15	bA	1113	CL7	C4D-ND	-3.02	1.33	1.37
15	bA	1127	CL7	C4D-ND	-3.02	1.33	1.37
15	bB	1012	CL7	C3D-C4D	3.02	1.47	1.39
15	aA	1133	CL7	C4D-ND	-3.02	1.33	1.37
15	aA	1134	CL7	C4D-ND	-3.02	1.33	1.37
15	cB	1012	CL7	C4D-ND	-3.02	1.33	1.37
15	aB	1206	CL7	C3D-C4D	3.02	1.47	1.39
15	aB	1226	CL7	C3D-C4D	3.02	1.47	1.39
15	bB	1239	CL7	C3D-C4D	3.02	1.47	1.39
15	cB	1205	CL7	C3D-C4D	3.02	1.47	1.39
15	aB	1210	CL7	C4D-ND	-3.02	1.33	1.37
15	bA	1130	CL7	C4D-ND	-3.02	1.33	1.37
15	bK	1401	CL7	C3B-C4B	3.02	1.49	1.42
15	bB	1236	CL7	C3D-C4D	3.02	1.47	1.39
15	bA	1131	CL7	C4D-ND	-3.02	1.33	1.37
15	bA	1132	CL7	C3D-C4D	3.02	1.47	1.39
15	aB	1238	CL7	C3D-C4D	3.02	1.47	1.39
15	cB	1204	CL7	C3D-C4D	3.02	1.47	1.39
15	aA	1126	CL7	C3B-C4B	3.02	1.49	1.42
15	aL	1501	CL7	C3D-C4D	3.01	1.47	1.39
15	cB	1205	CL7	C3B-C4B	3.01	1.49	1.42
15	cB	1210	CL7	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bA	4003	A1JPJ	C8-C9	-3.01	1.39	1.45
15	aA	1115	CL7	C3D-C4D	3.01	1.47	1.39
15	cA	1107	CL7	C4D-ND	-3.01	1.33	1.37
15	cA	1109	CL7	C4D-ND	-3.01	1.33	1.37
15	cA	1128	CL7	C4D-ND	-3.01	1.33	1.37
15	cB	1215	CL7	C3B-C4B	3.01	1.49	1.42
15	cB	1239	CL7	C3D-C4D	3.01	1.47	1.39
15	aB	1237	CL7	C3B-C4B	3.01	1.49	1.42
15	aA	1122	CL7	C3D-C4D	3.01	1.47	1.39
15	aB	1222	CL7	C3B-C4B	3.01	1.49	1.42
15	bB	1235	CL7	C3D-C4D	3.01	1.47	1.39
15	cB	1202	CL7	C3B-C4B	3.01	1.49	1.42
15	cB	1206	CL7	C3D-C4D	3.01	1.47	1.39
15	cI	1601	CL7	C4D-ND	-3.01	1.33	1.37
15	aB	1204	CL7	C3B-C4B	3.01	1.49	1.42
15	aB	1216	CL7	C3B-C4B	3.01	1.49	1.42
15	cA	1130	CL7	C3B-C4B	3.01	1.49	1.42
15	cA	1121	CL7	C4D-ND	-3.01	1.33	1.37
15	cL	1503	CL7	C3D-C4D	3.01	1.47	1.39
15	aA	1123	CL7	C3B-C4B	3.01	1.49	1.42
17	aA	4008	A1JPJ	C10-C9	3.01	1.39	1.35
15	cA	1121	CL7	C3D-C4D	3.01	1.47	1.39
15	aA	1136	CL7	C3D-C4D	3.01	1.47	1.39
15	cA	1127	CL7	C3B-C4B	3.01	1.49	1.42
17	cI	4019	A1JPJ	C8-C9	-3.01	1.39	1.45
17	aA	4003	A1JPJ	C8-C9	-3.01	1.39	1.45
15	bB	1228	CL7	C4D-ND	-3.01	1.33	1.37
15	bA	1129	CL7	C3D-C4D	3.01	1.47	1.39
15	cA	1121	CL7	C3B-C4B	3.01	1.49	1.42
15	bA	1103	CL7	C3B-C4B	3.01	1.49	1.42
15	bA	1135	CL7	C3D-C4D	3.01	1.47	1.39
15	bB	1021	CL7	C3D-C4D	3.01	1.47	1.39
15	aA	1103	CL7	C4D-ND	-3.01	1.33	1.37
15	cB	1203	CL7	C3B-C4B	3.01	1.49	1.42
15	bB	1204	CL7	C3B-C4B	3.01	1.49	1.42
15	aI	1601	CL7	C3B-C4B	3.01	1.49	1.42
15	aB	1239	CL7	C3D-C4D	3.00	1.47	1.39
15	aB	1221	CL7	C3B-C4B	3.00	1.49	1.42
15	aB	1231	CL7	C4D-ND	-3.00	1.33	1.37
15	bB	1205	CL7	C4D-ND	-3.00	1.33	1.37
15	cB	1228	CL7	C4D-ND	-3.00	1.33	1.37
15	bB	1213	CL7	C3B-C4B	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1122	CL7	C3B-C4B	3.00	1.49	1.42
15	bB	1238	CL7	C3D-C4D	3.00	1.47	1.39
15	aB	1239	CL7	C3B-C4B	3.00	1.49	1.42
15	aB	1235	CL7	C3D-C4D	3.00	1.47	1.39
15	cA	1134	CL7	C4D-ND	-3.00	1.33	1.37
15	aB	1205	CL7	C4D-ND	-3.00	1.33	1.37
15	cA	1137	CL7	C3B-C4B	3.00	1.49	1.42
15	bB	1226	CL7	C3D-C4D	3.00	1.47	1.39
15	bA	1130	CL7	C3B-C4B	3.00	1.49	1.42
15	aA	1128	CL7	C3B-C4B	3.00	1.49	1.42
15	aB	1226	CL7	C4D-ND	-3.00	1.33	1.37
15	aB	1223	CL7	C3D-C4D	3.00	1.47	1.39
15	cA	1124	CL7	C3D-C4D	3.00	1.47	1.39
15	aA	1131	CL7	C3D-C4D	3.00	1.47	1.39
15	bA	1124	CL7	C3D-C4D	3.00	1.47	1.39
15	bB	1206	CL7	C3D-C4D	3.00	1.47	1.39
15	cB	1236	CL7	C3D-C4D	3.00	1.47	1.39
15	cB	1222	CL7	C4D-ND	-3.00	1.33	1.37
15	bB	1224	CL7	C3D-C4D	3.00	1.47	1.39
15	cB	1235	CL7	C3D-C4D	3.00	1.47	1.39
15	aB	1220	CL7	C3B-C4B	3.00	1.49	1.42
15	bB	1221	CL7	C3B-C4B	3.00	1.49	1.42
15	bA	1801	CL7	C4D-ND	-3.00	1.33	1.37
15	bB	1226	CL7	C3B-C4B	3.00	1.49	1.42
17	aB	4021	A1JPJ	C8-C9	-3.00	1.39	1.45
15	cA	1105	CL7	C4D-ND	-3.00	1.33	1.37
17	aL	4020	A1JPJ	C8-C9	-3.00	1.39	1.45
15	aB	1236	CL7	C3D-C4D	3.00	1.47	1.39
15	bB	1237	CL7	C3B-C4B	3.00	1.49	1.42
15	cA	1123	CL7	C3B-C4B	3.00	1.49	1.42
15	cB	1012	CL7	C3B-C4B	3.00	1.49	1.42
15	cB	1212	CL7	C3B-C4B	3.00	1.49	1.42
15	bA	1109	CL7	C3D-C4D	3.00	1.47	1.39
17	cA	4007	A1JPJ	C8-C9	-3.00	1.39	1.45
15	cB	1226	CL7	C3D-C4D	3.00	1.47	1.39
15	cA	1122	CL7	C3D-C4D	2.99	1.47	1.39
15	cA	1117	CL7	C4D-ND	-2.99	1.33	1.37
15	cA	1136	CL7	C3B-C4B	2.99	1.49	1.42
15	cB	1237	CL7	C3B-C4B	2.99	1.49	1.42
15	cA	1126	CL7	C3B-C4B	2.99	1.49	1.42
15	aA	1124	CL7	C3D-C4D	2.99	1.47	1.39
15	bA	1136	CL7	C3D-C4D	2.99	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1241	CL7	C4D-ND	-2.99	1.33	1.37
15	aB	1224	CL7	C3D-C4D	2.99	1.47	1.39
15	cB	1238	CL7	C3D-C4D	2.99	1.47	1.39
15	bA	1132	CL7	C4D-ND	-2.99	1.33	1.37
15	bL	1503	CL7	C3D-C4D	2.99	1.47	1.39
17	bL	4020	A1JPJ	C8-C9	-2.99	1.39	1.45
17	cA	4011	A1JPJ	C8-C9	-2.99	1.39	1.45
15	aB	1225	CL7	C3B-C4B	2.99	1.49	1.42
15	aB	1021	CL7	C3D-C4D	2.99	1.47	1.39
15	aL	1503	CL7	C3D-C4D	2.99	1.47	1.39
15	bA	1109	CL7	C4D-ND	-2.99	1.33	1.37
15	cB	1224	CL7	C4D-ND	-2.99	1.33	1.37
15	bA	1122	CL7	C3D-C4D	2.99	1.47	1.39
15	bA	1133	CL7	C4D-ND	-2.99	1.33	1.37
15	bB	1202	CL7	C3B-C4B	2.99	1.49	1.42
15	aA	1129	CL7	C3D-C4D	2.99	1.47	1.39
15	bB	1215	CL7	C3D-C4D	2.99	1.47	1.39
15	aA	1104	CL7	C3B-C4B	2.99	1.49	1.42
15	cB	1224	CL7	C3D-C4D	2.99	1.47	1.39
15	cA	1103	CL7	C3D-C4D	2.99	1.47	1.39
15	bB	1214	CL7	C4D-ND	-2.99	1.33	1.37
17	cB	4021	A1JPJ	C8-C9	-2.99	1.39	1.45
15	aB	1212	CL7	C3B-C4B	2.99	1.49	1.42
15	cB	1222	CL7	C3B-C4B	2.99	1.49	1.42
15	bB	1204	CL7	C3D-C4D	2.99	1.47	1.39
15	cA	1137	CL7	C3D-C4D	2.99	1.47	1.39
15	bA	1112	CL7	C3B-C4B	2.98	1.49	1.42
15	aA	1137	CL7	C3B-C4B	2.98	1.49	1.42
15	aA	1130	CL7	C3D-C4D	2.98	1.47	1.39
15	aB	1012	CL7	C3B-C4B	2.98	1.49	1.42
15	aA	1128	CL7	C4D-ND	-2.98	1.33	1.37
17	bA	4008	A1JPJ	C10-C9	2.98	1.39	1.35
15	bB	1239	CL7	C3B-C4B	2.98	1.49	1.42
15	cB	1012	CL7	C3D-C4D	2.98	1.47	1.39
15	bB	1207	CL7	C3D-C4D	2.98	1.47	1.39
15	aA	1801	CL7	C4D-ND	-2.98	1.33	1.37
15	bA	1103	CL7	C3D-C4D	2.98	1.47	1.39
15	cA	1131	CL7	C3D-C4D	2.98	1.47	1.39
15	aB	1021	CL7	C4D-ND	-2.98	1.33	1.37
15	bA	1117	CL7	C4D-ND	-2.98	1.33	1.37
15	bA	1131	CL7	C3D-C4D	2.98	1.47	1.39
15	bA	1136	CL7	C3B-C4B	2.98	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1237	CL7	C3D-C4D	2.98	1.47	1.39
15	bA	1137	CL7	C3B-C4B	2.98	1.49	1.42
15	aB	1202	CL7	C3B-C4B	2.98	1.49	1.42
15	aA	1127	CL7	C3D-C4D	2.98	1.47	1.39
15	bA	1137	CL7	C3D-C4D	2.98	1.47	1.39
15	bI	1601	CL7	C3B-C4B	2.98	1.49	1.42
17	cL	4020	A1JPJ	C8-C9	-2.98	1.39	1.45
15	cA	1136	CL7	C3D-C4D	2.98	1.47	1.39
15	aA	1135	CL7	C3D-C4D	2.97	1.47	1.39
15	bB	1237	CL7	C3D-C4D	2.97	1.47	1.39
15	bA	1134	CL7	C4D-ND	-2.97	1.33	1.37
15	aA	1125	CL7	C3D-C4D	2.97	1.47	1.39
15	aB	1236	CL7	C3B-C4B	2.97	1.49	1.42
15	cB	1021	CL7	C3D-C4D	2.97	1.47	1.39
15	bA	1108	CL7	C4D-ND	-2.97	1.33	1.37
15	bB	1212	CL7	C3B-C4B	2.97	1.49	1.42
15	aB	1211	CL7	C4D-ND	-2.97	1.33	1.37
15	aB	1234	CL7	C3B-C4B	2.97	1.49	1.42
15	aB	1207	CL7	C3D-C4D	2.97	1.47	1.39
15	aB	1222	CL7	C4D-ND	-2.97	1.33	1.37
17	bI	4019	A1JPJ	C8-C9	-2.97	1.39	1.45
15	cB	1220	CL7	C4D-ND	-2.97	1.33	1.37
17	cA	4003	A1JPJ	C8-C9	-2.97	1.39	1.45
15	aB	1213	CL7	C3B-C4B	2.97	1.49	1.42
15	aB	1012	CL7	C3D-C4D	2.97	1.47	1.39
15	cA	1127	CL7	C4D-ND	-2.97	1.33	1.37
15	bA	1135	CL7	C3B-C4B	2.97	1.49	1.42
15	bI	1601	CL7	C4D-ND	-2.97	1.33	1.37
15	bB	1236	CL7	C3B-C4B	2.97	1.49	1.42
15	aA	1108	CL7	C4D-ND	-2.97	1.33	1.37
15	aI	1601	CL7	C4D-ND	-2.97	1.33	1.37
15	aB	1215	CL7	C3D-C4D	2.97	1.47	1.39
15	bA	1115	CL7	C3D-C4D	2.97	1.47	1.39
15	bA	1801	CL7	C3B-C4B	2.97	1.49	1.42
17	bL	4023	A1JPJ	C8-C9	-2.97	1.39	1.45
15	aA	1116	CL7	C4D-ND	-2.97	1.33	1.37
15	cA	1127	CL7	C3D-C4D	2.97	1.47	1.39
15	bB	1207	CL7	C3B-C4B	2.97	1.49	1.42
15	cA	1115	CL7	C3D-C4D	2.97	1.47	1.39
15	cL	1502	CL7	C3D-C4D	2.97	1.47	1.39
15	bB	1222	CL7	C3B-C4B	2.96	1.49	1.42
15	cA	1126	CL7	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1130	CL7	C3D-C4D	2.96	1.47	1.39
15	cA	1125	CL7	C3D-C4D	2.96	1.47	1.39
15	cA	1123	CL7	C4D-ND	-2.96	1.33	1.37
15	cB	1227	CL7	C3B-C4B	2.96	1.49	1.42
15	bA	1126	CL7	CHC-C1C	2.96	1.44	1.38
15	aA	1112	CL7	C4D-ND	-2.96	1.33	1.37
15	aA	1117	CL7	C4D-ND	-2.96	1.33	1.37
15	bB	1012	CL7	C3B-C4B	2.96	1.49	1.42
15	cB	1239	CL7	C3B-C4B	2.96	1.49	1.42
15	cA	1111	CL7	C4D-ND	-2.96	1.33	1.37
15	cF	1701	CL7	C4D-ND	-2.96	1.33	1.37
15	aB	1208	CL7	C4D-ND	-2.96	1.33	1.37
15	aB	1237	CL7	C3D-C4D	2.96	1.47	1.39
17	aI	4019	A1JPJ	C8-C9	-2.96	1.39	1.45
15	bB	1021	CL7	C4D-ND	-2.96	1.33	1.37
15	cA	1130	CL7	C3D-C4D	2.96	1.47	1.39
15	bA	1111	CL7	C4D-ND	-2.96	1.33	1.37
17	cB	4017	A1JPJ	C8-C9	-2.96	1.39	1.45
15	aA	1801	CL7	C3B-C4B	2.96	1.49	1.42
15	bL	1502	CL7	C3D-C4D	2.96	1.47	1.39
15	bB	1211	CL7	C4D-ND	-2.96	1.33	1.37
15	cB	1207	CL7	C3B-C4B	2.96	1.49	1.42
15	bA	1127	CL7	C3D-C4D	2.96	1.47	1.39
15	cA	1102	CL7	C4D-ND	-2.96	1.33	1.37
15	bA	1123	CL7	C4D-ND	-2.96	1.33	1.37
15	bB	1216	CL7	C4D-ND	-2.96	1.33	1.37
15	cA	1801	CL7	C3B-C4B	2.96	1.49	1.42
15	aB	1227	CL7	C4D-ND	-2.96	1.33	1.37
17	bA	4007	A1JPJ	C8-C9	-2.96	1.39	1.45
15	aL	1502	CL7	C3D-C4D	2.96	1.47	1.39
15	bB	1234	CL7	C3B-C4B	2.95	1.49	1.42
15	aB	1203	CL7	C3D-C4D	2.95	1.47	1.39
15	aA	1132	CL7	C3D-C4D	2.95	1.47	1.39
15	bB	1202	CL7	C3D-C4D	2.95	1.47	1.39
15	cA	1108	CL7	C4D-ND	-2.95	1.33	1.37
15	cB	1236	CL7	C3B-C4B	2.95	1.49	1.42
15	aB	1226	CL7	C3B-C4B	2.95	1.49	1.42
15	aB	1225	CL7	C3D-C4D	2.95	1.47	1.39
15	cA	1113	CL7	C4D-ND	-2.95	1.33	1.37
15	cA	1801	CL7	C4D-ND	-2.95	1.33	1.37
17	aA	4011	A1JPJ	C8-C9	-2.95	1.39	1.45
15	bA	1112	CL7	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1203	CL7	C3D-C4D	2.95	1.47	1.39
15	cB	1214	CL7	C4D-ND	-2.95	1.33	1.37
15	cB	1225	CL7	C3D-C4D	2.95	1.47	1.39
15	aB	1224	CL7	C3B-C4B	2.95	1.49	1.42
15	aA	1135	CL7	C3B-C4B	2.95	1.49	1.42
15	cB	1201	CL7	C4D-ND	-2.95	1.33	1.37
15	cA	1139	CL7	C4D-ND	-2.95	1.33	1.37
15	cA	1131	CL7	C3B-C4B	2.94	1.49	1.42
15	cB	1203	CL7	C3D-C4D	2.94	1.47	1.39
15	aA	1105	CL7	C4D-ND	-2.94	1.33	1.37
15	aB	1214	CL7	C4D-ND	-2.94	1.33	1.37
15	bB	1201	CL7	C4D-ND	-2.94	1.33	1.37
15	aA	1113	CL7	C4D-ND	-2.94	1.33	1.37
15	cA	1120	CL7	C4D-ND	-2.94	1.33	1.37
15	cB	1021	CL7	C4D-ND	-2.94	1.33	1.37
15	aA	1109	CL7	C4D-ND	-2.94	1.33	1.37
15	aB	1228	CL7	C4D-ND	-2.94	1.33	1.37
15	aA	1022	CL7	C3D-C4D	2.94	1.47	1.39
15	cB	1207	CL7	C3D-C4D	2.93	1.47	1.39
15	aB	1233	CL7	C3B-C4B	2.93	1.49	1.42
15	bB	1241	CL7	C3B-C4B	2.93	1.49	1.42
15	bA	1138	CL7	C4D-ND	-2.93	1.33	1.37
15	bL	1503	CL7	C3B-C4B	2.93	1.49	1.42
15	cB	1225	CL7	C3B-C4B	2.93	1.49	1.42
15	aB	1230	CL7	C3B-C4B	2.93	1.49	1.42
17	cA	4008	A1JPJ	C10-C9	2.93	1.39	1.35
17	aB	4017	A1JPJ	C8-C9	-2.93	1.39	1.45
15	cB	1234	CL7	C3B-C4B	2.93	1.49	1.42
15	aA	1101	CL7	C4D-ND	-2.93	1.33	1.37
17	cL	4023	A1JPJ	C8-C9	-2.93	1.39	1.45
15	aA	1120	CL7	C4D-ND	-2.93	1.33	1.37
15	cB	1215	CL7	C4D-ND	-2.93	1.33	1.37
15	bA	1139	CL7	C4D-ND	-2.93	1.33	1.37
15	cA	1104	CL7	C3B-C4B	2.93	1.49	1.42
15	bA	1110	CL7	C4D-ND	-2.93	1.33	1.37
15	bA	1118	CL7	C4D-ND	-2.93	1.33	1.37
15	cB	1230	CL7	C3B-C4B	2.93	1.49	1.42
15	cL	1501	CL7	C3B-C4B	2.92	1.49	1.42
15	bA	1125	CL7	C3D-C4D	2.92	1.47	1.39
15	cA	1114	CL7	C4D-ND	-2.92	1.33	1.37
15	aA	1114	CL7	C4D-ND	-2.92	1.33	1.37
15	cA	1112	CL7	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1022	CL7	C3D-C4D	2.92	1.47	1.39
15	bA	1022	CL7	C3D-C4D	2.92	1.47	1.39
15	cB	1211	CL7	C4D-ND	-2.92	1.33	1.37
15	cB	1219	CL7	C4D-ND	-2.92	1.33	1.37
15	aA	1136	CL7	C3B-C4B	2.92	1.49	1.42
15	aA	1138	CL7	C3B-C4B	2.92	1.49	1.42
15	bL	1501	CL7	C3B-C4B	2.92	1.49	1.42
15	bA	1101	CL7	C4D-ND	-2.92	1.33	1.37
15	cA	1132	CL7	C3D-C4D	2.92	1.47	1.39
15	aF	1701	CL7	C4D-ND	-2.92	1.33	1.37
15	bB	1231	CL7	C4D-ND	-2.92	1.33	1.37
15	bA	1022	CL7	C3B-C4B	2.91	1.49	1.42
15	aB	1213	CL7	C4D-ND	-2.91	1.33	1.37
15	bB	1225	CL7	C3D-C4D	2.91	1.47	1.39
15	bB	1227	CL7	C4D-ND	-2.91	1.33	1.37
15	cB	1208	CL7	C4D-ND	-2.91	1.33	1.37
15	cL	1502	CL7	C3B-C4B	2.91	1.49	1.42
15	bA	1134	CL7	C3B-C4B	2.91	1.49	1.42
17	cA	4014	A1JPJ	C8-C9	-2.91	1.39	1.45
15	aA	1022	CL7	C3B-C4B	2.91	1.49	1.42
15	aA	1134	CL7	C3B-C4B	2.91	1.49	1.42
15	aA	1138	CL7	C4D-ND	-2.91	1.33	1.37
15	bA	1102	CL7	C4D-ND	-2.91	1.33	1.37
15	bA	1105	CL7	C4D-ND	-2.91	1.33	1.37
15	bA	1104	CL7	C3B-C4B	2.91	1.49	1.42
15	cA	1135	CL7	C4D-ND	-2.91	1.33	1.37
15	aB	1241	CL7	C3B-C4B	2.91	1.49	1.42
15	bA	1128	CL7	C4D-ND	-2.91	1.33	1.37
15	cA	1118	CL7	C4D-ND	-2.91	1.33	1.37
15	bB	1233	CL7	C4D-ND	-2.91	1.33	1.37
15	cA	1134	CL7	C3B-C4B	2.90	1.49	1.42
15	cJ	1302	CL7	C4D-ND	-2.90	1.33	1.37
15	bB	1209	CL7	C4D-ND	-2.90	1.33	1.37
15	cA	1112	CL7	C3B-C4B	2.90	1.49	1.42
15	bB	1230	CL7	C3B-C4B	2.90	1.49	1.42
15	aB	1206	CL7	C3B-C4B	2.90	1.49	1.42
15	bB	1213	CL7	C4D-ND	-2.90	1.33	1.37
15	aL	1501	CL7	C3B-C4B	2.90	1.49	1.42
15	aB	1202	CL7	C3D-C4D	2.90	1.47	1.39
17	bA	4014	A1JPJ	C8-C9	-2.90	1.39	1.45
17	bB	4017	A1JPJ	C8-C9	-2.90	1.39	1.45
15	cB	1221	CL7	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aL	1503	CL7	C3B-C4B	2.90	1.49	1.42
15	aB	1233	CL7	C4D-ND	-2.90	1.33	1.37
15	aB	1201	CL7	C4D-ND	-2.90	1.33	1.37
15	bJ	1301	CL7	C4D-ND	-2.89	1.33	1.37
15	bA	1120	CL7	C4D-ND	-2.89	1.33	1.37
15	cB	1227	CL7	C4D-ND	-2.89	1.33	1.37
15	aA	1131	CL7	C3B-C4B	2.89	1.49	1.42
15	cA	1101	CL7	C4D-ND	-2.89	1.33	1.37
15	bA	1114	CL7	C4D-ND	-2.89	1.33	1.37
15	cB	1213	CL7	C4D-ND	-2.89	1.33	1.37
17	cF	4016	A1JPJ	C8-C9	-2.89	1.39	1.45
14	cB	1023	PHO	CMC-C2C	-2.89	1.45	1.50
15	aA	1139	CL7	C4D-ND	-2.89	1.33	1.37
15	bF	1701	CL7	C4D-ND	-2.89	1.33	1.37
15	cB	1202	CL7	C3D-C4D	2.89	1.47	1.39
15	bA	1131	CL7	C3B-C4B	2.89	1.49	1.42
15	aB	1207	CL7	C3B-C4B	2.89	1.49	1.42
15	bB	1206	CL7	C3B-C4B	2.89	1.49	1.42
15	bB	1208	CL7	C4D-ND	-2.89	1.33	1.37
15	cA	1110	CL7	C4D-ND	-2.89	1.33	1.37
17	cA	4002	A1JPJ	C8-C9	-2.88	1.39	1.45
15	cB	1232	CL7	C4D-ND	-2.88	1.33	1.37
15	cB	1021	CL7	C3B-C4B	2.88	1.49	1.42
15	aA	1118	CL7	C4D-ND	-2.88	1.33	1.37
15	bA	1138	CL7	C3B-C4B	2.88	1.49	1.42
15	cB	1206	CL7	C3B-C4B	2.88	1.49	1.42
17	aA	4014	A1JPJ	C8-C9	-2.88	1.39	1.45
15	bA	1127	CL7	C3B-C4B	2.88	1.49	1.42
15	aB	1209	CL7	C4D-ND	-2.88	1.33	1.37
14	bB	1023	PHO	CMC-C2C	-2.88	1.45	1.50
15	cB	1233	CL7	C4D-ND	-2.88	1.33	1.37
15	cB	1217	CL7	C4D-ND	-2.88	1.33	1.37
15	cB	1218	CL7	C4D-ND	-2.88	1.33	1.37
15	cB	1209	CL7	C4D-ND	-2.87	1.33	1.37
17	aF	4016	A1JPJ	C8-C9	-2.87	1.39	1.45
15	aB	1021	CL7	C3B-C4B	2.87	1.49	1.42
15	bK	1401	CL7	C4D-ND	-2.87	1.33	1.37
15	aB	1230	CL7	C4D-ND	-2.87	1.33	1.37
15	bB	1220	CL7	C4D-ND	-2.87	1.33	1.37
15	bJ	1302	CL7	C4D-ND	-2.87	1.33	1.37
15	aA	1102	CL7	C4D-ND	-2.87	1.33	1.37
17	bA	4002	A1JPJ	C8-C9	-2.87	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1110	CL7	C4D-ND	-2.87	1.33	1.37
15	aB	1217	CL7	C4D-ND	-2.87	1.33	1.37
15	cK	1401	CL7	C4D-ND	-2.87	1.33	1.37
15	bL	1502	CL7	C3B-C4B	2.87	1.49	1.42
15	cA	1022	CL7	C3B-C4B	2.87	1.49	1.42
15	bB	1217	CL7	C4D-ND	-2.87	1.33	1.37
17	aA	4008	A1JPJ	C12-C13	-2.86	1.39	1.45
17	cA	4008	A1JPJ	C12-C13	-2.86	1.39	1.45
15	bB	1241	CL7	C4D-ND	-2.86	1.33	1.37
15	aJ	1302	CL7	C4D-ND	-2.86	1.33	1.37
17	bF	4016	A1JPJ	C8-C9	-2.86	1.39	1.45
15	bB	1218	CL7	C4D-ND	-2.86	1.33	1.37
15	aJ	1301	CL7	C4D-ND	-2.86	1.33	1.37
15	aK	1401	CL7	C4D-ND	-2.86	1.33	1.37
15	bB	1219	CL7	C4D-ND	-2.86	1.33	1.37
15	cA	1135	CL7	C3B-C4B	2.86	1.49	1.42
15	aB	1212	CL7	C4D-ND	-2.86	1.33	1.37
15	cB	1241	CL7	C3B-C4B	2.85	1.49	1.42
15	cA	1135	CL7	C3D-C4D	2.85	1.47	1.39
15	bB	1232	CL7	C4D-ND	-2.85	1.33	1.37
15	bB	1212	CL7	C4D-ND	-2.84	1.33	1.37
15	cA	1138	CL7	C3B-C4B	2.84	1.49	1.42
15	cJ	1301	CL7	C4D-ND	-2.84	1.33	1.37
15	cB	1212	CL7	C4D-ND	-2.84	1.33	1.37
17	aA	4002	A1JPJ	C8-C9	-2.84	1.39	1.45
15	aB	1221	CL7	C4D-ND	-2.83	1.33	1.37
15	aB	1218	CL7	C4D-ND	-2.83	1.33	1.37
15	cB	1215	CL7	C3D-C4D	2.83	1.47	1.39
15	aL	1502	CL7	C3B-C4B	2.83	1.49	1.42
15	bB	1221	CL7	C2A-C1A	2.83	1.55	1.50
17	aL	4023	A1JPJ	C8-C9	-2.82	1.39	1.45
15	cL	1503	CL7	C3B-C4B	2.82	1.49	1.42
15	aB	1232	CL7	C4D-ND	-2.82	1.33	1.37
17	bB	4015	A1JPJ	C8-C9	-2.82	1.39	1.45
15	aA	1112	CL7	C3B-C4B	2.82	1.49	1.42
15	bB	1221	CL7	C4D-ND	-2.82	1.33	1.37
15	cK	1402	CL7	C4D-ND	-2.82	1.33	1.37
17	bA	4008	A1JPJ	C12-C13	-2.81	1.39	1.45
14	aB	1023	PHO	CMC-C2C	-2.81	1.46	1.50
15	bK	1402	CL7	C4D-ND	-2.81	1.33	1.37
15	aB	1241	CL7	C4D-ND	-2.81	1.33	1.37
15	bA	1132	CL7	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1021	CL7	C3B-C4B	2.79	1.49	1.42
15	aB	1219	CL7	C4D-ND	-2.79	1.33	1.37
17	aB	4015	A1JPJ	C8-C9	-2.79	1.40	1.45
15	cB	1221	CL7	C2A-C1A	2.78	1.55	1.50
17	cB	4004	A1JPJ	C8-C9	-2.78	1.40	1.45
17	aJ	4012	A1JPJ	C8-C9	-2.77	1.40	1.45
15	cA	1135	CL7	CMD-C2D	-2.76	1.44	1.50
17	aI	4018	A1JPJ	C12-C13	-2.76	1.40	1.45
17	bB	4005	A1JPJ	C8-C9	-2.76	1.40	1.45
17	cB	4015	A1JPJ	C8-C9	-2.76	1.40	1.45
17	bB	4004	A1JPJ	C8-C9	-2.76	1.40	1.45
17	aB	4004	A1JPJ	C8-C9	-2.75	1.40	1.45
17	cB	4006	A1JPJ	C8-C9	-2.74	1.40	1.45
17	aB	4005	A1JPJ	C8-C9	-2.74	1.40	1.45
15	aB	1221	CL7	C2A-C1A	2.74	1.55	1.50
17	cB	4005	A1JPJ	C8-C9	-2.74	1.40	1.45
17	aB	4006	A1JPJ	C8-C9	-2.74	1.40	1.45
17	cJ	4012	A1JPJ	C8-C9	-2.73	1.40	1.45
17	bB	4006	A1JPJ	C8-C9	-2.73	1.40	1.45
17	bI	4018	A1JPJ	C12-C13	-2.73	1.40	1.45
17	bJ	4012	A1JPJ	C8-C9	-2.72	1.40	1.45
17	cI	4018	A1JPJ	C12-C13	-2.72	1.40	1.45
15	aB	1201	CL7	CHC-C1C	2.72	1.43	1.38
17	cB	4010	A1JPJ	C8-C9	-2.72	1.40	1.45
17	cA	4008	A1JPJ	C19-C18	-2.71	1.40	1.45
15	aK	1402	CL7	C3B-C4B	2.69	1.49	1.42
15	bB	1201	CL7	CHC-C1C	2.68	1.43	1.38
15	bB	1021	CL7	C1B-C2B	2.68	1.49	1.43
17	aB	4010	A1JPJ	C8-C9	-2.68	1.40	1.45
17	aA	4008	A1JPJ	C19-C18	-2.68	1.40	1.45
13	cA	1011	G9R	CMD-C2D	-2.67	1.46	1.51
15	cJ	1301	CL7	C1B-C2B	2.67	1.49	1.43
15	cA	1132	CL7	C4D-ND	-2.67	1.34	1.37
15	aA	1132	CL7	C4D-ND	-2.67	1.34	1.37
15	cL	1503	CL7	C1B-C2B	2.67	1.49	1.43
15	bB	1233	CL7	C1B-C2B	2.66	1.49	1.43
13	aA	1011	G9R	CMD-C2D	-2.66	1.46	1.51
17	bA	4008	A1JPJ	C19-C18	-2.66	1.40	1.45
15	aB	1212	CL7	C1B-C2B	2.66	1.49	1.43
13	bA	1011	G9R	CMD-C2D	-2.65	1.46	1.51
14	aA	1013	PHO	CMC-C2C	-2.65	1.46	1.50
15	cB	1201	CL7	CHC-C1C	2.65	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	4010	A1JPJ	C8-C9	-2.64	1.40	1.45
15	aJ	1301	CL7	C1B-C2B	2.64	1.49	1.43
17	aI	4018	A1JPJ	C19-C18	-2.64	1.40	1.45
15	bA	1108	CL7	C1B-C2B	2.64	1.49	1.43
15	bB	1218	CL7	C1B-C2B	2.63	1.49	1.43
15	aA	1113	CL7	C1B-C2B	2.63	1.49	1.43
14	bA	1013	PHO	CMC-C2C	-2.62	1.46	1.50
15	aK	1402	CL7	C4D-ND	-2.62	1.34	1.37
15	cA	1108	CL7	C1B-C2B	2.62	1.49	1.43
17	cA	4008	A1JPJ	C23-C22	-2.62	1.40	1.45
14	cA	1013	PHO	CMC-C2C	-2.62	1.46	1.50
15	cB	1218	CL7	C1B-C2B	2.62	1.49	1.43
15	cB	1215	CL7	CHC-C1C	2.62	1.43	1.38
15	aJ	1302	CL7	C1B-C2B	2.62	1.49	1.43
15	aB	1218	CL7	C1B-C2B	2.62	1.49	1.43
15	bK	1402	CL7	C1B-C2B	2.62	1.49	1.43
15	cB	1233	CL7	C1B-C2B	2.62	1.49	1.43
15	bA	1126	CL7	C4D-ND	-2.62	1.34	1.37
17	bI	4018	A1JPJ	C19-C18	-2.62	1.40	1.45
15	aA	1108	CL7	C1B-C2B	2.62	1.49	1.43
15	aB	1213	CL7	C1B-C2B	2.61	1.49	1.43
15	cB	1217	CL7	C1B-C2B	2.61	1.49	1.43
15	bB	1212	CL7	C1B-C2B	2.61	1.49	1.43
15	aB	1021	CL7	C1B-C2B	2.61	1.49	1.43
15	cK	1402	CL7	C1B-C2B	2.61	1.49	1.43
15	aB	1233	CL7	C1B-C2B	2.61	1.49	1.43
15	cB	1212	CL7	C1B-C2B	2.61	1.49	1.43
17	aA	4008	A1JPJ	C23-C22	-2.61	1.40	1.45
15	aA	1121	CL7	C1B-C2B	2.61	1.49	1.43
15	cA	1101	CL7	C1B-C2B	2.61	1.49	1.43
15	aB	1217	CL7	C1B-C2B	2.60	1.49	1.43
15	cB	1219	CL7	C1B-C2B	2.60	1.49	1.43
15	bJ	1301	CL7	C1B-C2B	2.60	1.49	1.43
17	cI	4018	A1JPJ	C19-C18	-2.60	1.40	1.45
15	bB	1219	CL7	C1B-C2B	2.60	1.49	1.43
15	aB	1209	CL7	C1B-C2B	2.60	1.49	1.43
15	cB	1021	CL7	C1B-C2B	2.60	1.49	1.43
15	bJ	1302	CL7	C1B-C2B	2.59	1.49	1.43
15	cA	1109	CL7	C1B-C2B	2.59	1.49	1.43
15	aB	1219	CL7	C1B-C2B	2.59	1.49	1.43
15	bB	1217	CL7	C1B-C2B	2.59	1.49	1.43
15	cF	1701	CL7	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1101	CL7	C1B-C2B	2.59	1.49	1.43
15	bK	1401	CL7	C1B-C2B	2.59	1.49	1.43
13	aA	1011	G9R	CMB-C2B	-2.59	1.46	1.51
15	aB	1220	CL7	C1B-C2B	2.58	1.49	1.43
15	aA	1115	CL7	C1B-C2B	2.58	1.49	1.43
15	cJ	1302	CL7	C1B-C2B	2.58	1.49	1.43
17	bA	4008	A1JPJ	C23-C22	-2.58	1.40	1.45
15	bA	1113	CL7	C1B-C2B	2.58	1.49	1.43
15	cA	1113	CL7	C1B-C2B	2.58	1.49	1.43
13	bA	1011	G9R	CMB-C2B	-2.57	1.46	1.51
15	cB	1213	CL7	C1B-C2B	2.57	1.49	1.43
15	bI	1601	CL7	C1B-C2B	2.57	1.49	1.43
15	aB	1228	CL7	C1B-C2B	2.57	1.49	1.43
15	bB	1220	CL7	C1B-C2B	2.57	1.49	1.43
15	cA	1121	CL7	C1B-C2B	2.57	1.49	1.43
15	bB	1213	CL7	C1B-C2B	2.57	1.49	1.43
15	aA	1101	CL7	C1B-C2B	2.56	1.49	1.43
15	aA	1139	CL7	C1B-C2B	2.56	1.49	1.43
15	bB	1209	CL7	C1B-C2B	2.56	1.49	1.43
15	cB	1232	CL7	C1B-C2B	2.56	1.49	1.43
15	aA	1109	CL7	C1B-C2B	2.56	1.49	1.43
15	aB	1202	CL7	C1B-C2B	2.56	1.49	1.43
15	bA	1121	CL7	C1B-C2B	2.56	1.49	1.43
15	bB	1208	CL7	C1B-C2B	2.56	1.49	1.43
15	bB	1223	CL7	C1B-C2B	2.56	1.49	1.43
15	cB	1202	CL7	C1B-C2B	2.56	1.49	1.43
15	aK	1401	CL7	C1B-C2B	2.56	1.49	1.43
15	aF	1701	CL7	C1B-C2B	2.56	1.49	1.43
15	bA	1106	CL7	CHC-C1C	2.56	1.43	1.38
15	bA	1109	CL7	C1B-C2B	2.56	1.49	1.43
15	aA	1138	CL7	C1B-C2B	2.55	1.49	1.43
15	bF	1701	CL7	C1B-C2B	2.55	1.49	1.43
15	cA	1125	CL7	C1B-C2B	2.55	1.49	1.43
17	aB	4021	A1JPJ	C12-C13	-2.55	1.40	1.45
15	cA	1115	CL7	C1B-C2B	2.55	1.49	1.43
15	cI	1601	CL7	C1B-C2B	2.55	1.49	1.43
15	cB	1209	CL7	C1B-C2B	2.55	1.49	1.43
15	aL	1503	CL7	C1B-C2B	2.55	1.49	1.43
15	aB	1231	CL7	C1B-C2B	2.55	1.49	1.43
15	cB	1215	CL7	C1B-C2B	2.55	1.49	1.43
15	aI	1601	CL7	C1B-C2B	2.55	1.49	1.43
15	bA	1114	CL7	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1231	CL7	C1B-C2B	2.55	1.49	1.43
15	bA	1139	CL7	C1B-C2B	2.54	1.49	1.43
17	bA	4003	A1JPJ	C12-C13	-2.54	1.40	1.45
15	cA	1118	CL7	C1B-C2B	2.54	1.49	1.43
15	bA	1138	CL7	C1B-C2B	2.54	1.49	1.43
15	cA	1139	CL7	C1B-C2B	2.54	1.49	1.43
15	cK	1401	CL7	C1B-C2B	2.54	1.49	1.43
15	bB	1210	CL7	C1B-C2B	2.54	1.49	1.43
15	aB	1232	CL7	C1B-C2B	2.54	1.49	1.43
15	cB	1223	CL7	C1B-C2B	2.54	1.49	1.43
15	bA	1115	CL7	C1B-C2B	2.54	1.49	1.43
15	cB	1231	CL7	C1B-C2B	2.54	1.49	1.43
15	aB	1241	CL7	C1B-C2B	2.54	1.49	1.43
15	aA	1111	CL7	C1B-C2B	2.53	1.49	1.43
15	aA	1114	CL7	C1B-C2B	2.53	1.49	1.43
17	bA	4011	A1JPJ	C19-C18	-2.53	1.40	1.45
17	cB	4021	A1JPJ	C12-C13	-2.53	1.40	1.45
15	cB	1211	CL7	C1B-C2B	2.53	1.49	1.43
15	bL	1503	CL7	C1B-C2B	2.53	1.49	1.43
15	cB	1216	CL7	C1B-C2B	2.53	1.49	1.43
15	cB	1228	CL7	C1B-C2B	2.53	1.49	1.43
14	cA	1013	PHO	C3D-C4D	2.53	1.45	1.41
15	bB	1228	CL7	C1B-C2B	2.53	1.49	1.43
15	cB	1208	CL7	C1B-C2B	2.53	1.49	1.43
15	bB	1241	CL7	C1B-C2B	2.53	1.49	1.43
17	cA	4003	A1JPJ	C12-C13	-2.53	1.40	1.45
14	aA	1013	PHO	CAC-C3C	-2.53	1.47	1.51
17	bI	4019	A1JPJ	C19-C18	-2.53	1.40	1.45
15	aB	1229	CL7	C1B-C2B	2.53	1.49	1.43
15	bA	1801	CL7	C1B-C2B	2.52	1.49	1.43
15	cA	1120	CL7	C1B-C2B	2.52	1.49	1.43
15	cA	1106	CL7	CHC-C1C	2.52	1.43	1.38
15	cA	1801	CL7	C1B-C2B	2.52	1.49	1.43
15	aB	1223	CL7	C1B-C2B	2.52	1.49	1.43
15	bB	1202	CL7	C1B-C2B	2.52	1.49	1.43
15	cB	1229	CL7	C1B-C2B	2.52	1.49	1.43
15	cA	1114	CL7	C1B-C2B	2.52	1.49	1.43
15	cA	1132	CL7	CHC-C1C	2.52	1.43	1.38
17	aA	4007	A1JPJ	C12-C13	-2.52	1.40	1.45
15	bB	1232	CL7	C1B-C2B	2.52	1.49	1.43
13	cA	1011	G9R	CMB-C2B	-2.52	1.46	1.51
15	bA	1110	CL7	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1125	CL7	C1B-C2B	2.52	1.49	1.43
15	cA	1105	CL7	C1B-C2B	2.52	1.49	1.43
17	aL	4020	A1JPJ	C19-C18	-2.52	1.40	1.45
15	cB	1220	CL7	C1B-C2B	2.52	1.49	1.43
15	bA	1105	CL7	C1B-C2B	2.51	1.49	1.43
15	cB	1241	CL7	C1B-C2B	2.51	1.49	1.43
17	cA	4011	A1JPJ	C19-C18	-2.51	1.40	1.45
17	aA	4003	A1JPJ	C12-C13	-2.51	1.40	1.45
17	aA	4011	A1JPJ	C19-C18	-2.51	1.40	1.45
15	cA	1110	CL7	C1B-C2B	2.51	1.49	1.43
15	cA	1138	CL7	C1B-C2B	2.51	1.49	1.43
15	aA	1107	CL7	C1B-C2B	2.51	1.49	1.43
15	aA	1110	CL7	C1B-C2B	2.51	1.49	1.43
15	cA	1122	CL7	C1B-C2B	2.51	1.49	1.43
15	bA	1125	CL7	CHC-C1C	2.51	1.43	1.38
17	cL	4023	A1JPJ	C12-C13	-2.51	1.40	1.45
15	aA	1103	CL7	C1B-C2B	2.51	1.49	1.43
15	cB	1210	CL7	C1B-C2B	2.51	1.49	1.43
15	aA	1132	CL7	CHC-C1C	2.51	1.43	1.38
17	bB	4021	A1JPJ	C12-C13	-2.51	1.40	1.45
15	aA	1801	CL7	C1B-C2B	2.51	1.49	1.43
15	cA	1134	CL7	C1B-C2B	2.50	1.49	1.43
15	aA	1112	CL7	C1B-C2B	2.50	1.49	1.43
15	bA	1118	CL7	C1B-C2B	2.50	1.49	1.43
15	aB	1239	CL7	C1B-C2B	2.50	1.49	1.43
15	aA	1118	CL7	C1B-C2B	2.50	1.49	1.43
15	bB	1216	CL7	C1B-C2B	2.50	1.49	1.43
15	aA	1125	CL7	CHC-C1C	2.50	1.43	1.38
14	bA	1013	PHO	C3D-C4D	2.50	1.44	1.41
15	cA	1131	CL7	C1B-C2B	2.50	1.49	1.43
15	aB	1208	CL7	C1B-C2B	2.50	1.49	1.43
15	aA	1140	CL7	C1B-C2B	2.50	1.49	1.43
17	aI	4019	A1JPJ	C12-C13	-2.50	1.40	1.45
15	cB	1230	CL7	CHC-C1C	2.50	1.43	1.38
17	bA	4007	A1JPJ	C12-C13	-2.50	1.40	1.45
15	cA	1102	CL7	CHC-C1C	2.50	1.43	1.38
15	bB	1222	CL7	C1B-C2B	2.50	1.49	1.43
15	bA	1107	CL7	C1B-C2B	2.50	1.49	1.43
15	cB	1225	CL7	C1B-C2B	2.50	1.49	1.43
15	bA	1134	CL7	C1B-C2B	2.50	1.49	1.43
15	cB	1235	CL7	C1B-C2B	2.49	1.49	1.43
15	aB	1201	CL7	C1B-C2B	2.49	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cI	4018	A1JPJ	C23-C22	-2.49	1.40	1.45
17	bL	4023	A1JPJ	C12-C13	-2.49	1.40	1.45
15	cB	1227	CL7	C1B-C2B	2.49	1.49	1.43
14	aB	1023	PHO	CMD-C2D	-2.49	1.46	1.51
15	aA	1122	CL7	C1B-C2B	2.49	1.49	1.43
15	cB	1201	CL7	C1B-C2B	2.49	1.49	1.43
15	bB	1239	CL7	C1B-C2B	2.49	1.49	1.43
17	cL	4020	A1JPJ	C12-C13	-2.49	1.40	1.45
15	bA	1102	CL7	CHC-C1C	2.49	1.43	1.38
15	bB	1229	CL7	C1B-C2B	2.49	1.49	1.43
17	aB	4017	A1JPJ	C12-C13	-2.49	1.40	1.45
15	aA	1105	CL7	C1B-C2B	2.49	1.49	1.43
15	bA	1125	CL7	C1B-C2B	2.49	1.49	1.43
17	bI	4018	A1JPJ	C23-C22	-2.49	1.40	1.45
17	bI	4019	A1JPJ	C23-C22	-2.49	1.40	1.45
15	bA	1112	CL7	C1B-C2B	2.49	1.49	1.43
15	aB	1211	CL7	C1B-C2B	2.49	1.49	1.43
17	cI	4019	A1JPJ	C12-C13	-2.49	1.40	1.45
15	aA	1102	CL7	CHC-C1C	2.48	1.43	1.38
15	bA	1120	CL7	C1B-C2B	2.48	1.49	1.43
15	bA	1122	CL7	C1B-C2B	2.48	1.49	1.43
15	aA	1106	CL7	CHC-C1C	2.48	1.43	1.38
17	bL	4020	A1JPJ	C12-C13	-2.48	1.40	1.45
17	bI	4019	A1JPJ	C12-C13	-2.48	1.40	1.45
17	bL	4020	A1JPJ	C19-C18	-2.48	1.40	1.45
15	aA	1112	CL7	CHC-C1C	2.48	1.43	1.38
15	cA	1112	CL7	CHC-C1C	2.48	1.43	1.38
15	cB	1207	CL7	C1B-C2B	2.48	1.49	1.43
15	bB	1236	CL7	C1B-C2B	2.48	1.49	1.43
15	cB	1239	CL7	C1B-C2B	2.48	1.49	1.43
14	bB	1023	PHO	CMD-C2D	-2.48	1.46	1.51
17	aI	4018	A1JPJ	C23-C22	-2.48	1.40	1.45
14	cB	1023	PHO	CMD-C2D	-2.48	1.46	1.51
17	cI	4019	A1JPJ	C19-C18	-2.48	1.40	1.45
17	aI	4019	A1JPJ	C19-C18	-2.48	1.40	1.45
15	aA	1134	CL7	C1B-C2B	2.48	1.49	1.43
15	aA	1119	CL7	C1B-C2B	2.48	1.49	1.43
15	bA	1103	CL7	C1B-C2B	2.48	1.49	1.43
15	aA	1120	CL7	C1B-C2B	2.47	1.49	1.43
15	bB	1211	CL7	C1B-C2B	2.47	1.49	1.43
15	aB	1221	CL7	C1B-C2B	2.47	1.49	1.43
15	aB	1222	CL7	C1B-C2B	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1119	CL7	C1B-C2B	2.47	1.49	1.43
17	cL	4020	A1JPJ	C19-C18	-2.47	1.40	1.45
15	bA	1133	CL7	C1B-C2B	2.47	1.49	1.43
15	cA	1136	CL7	C1B-C2B	2.47	1.49	1.43
17	cA	4007	A1JPJ	C12-C13	-2.47	1.40	1.45
15	bB	1225	CL7	C1B-C2B	2.47	1.49	1.43
14	aA	1013	PHO	C3D-C4D	2.47	1.44	1.41
15	cA	1140	CL7	C1B-C2B	2.47	1.49	1.43
15	cA	1111	CL7	C1B-C2B	2.47	1.49	1.43
15	aB	1235	CL7	C1B-C2B	2.47	1.49	1.43
13	cA	1011	G9R	CMC-C2C	-2.47	1.46	1.50
15	bA	1131	CL7	C1B-C2B	2.47	1.49	1.43
15	cB	1222	CL7	C1B-C2B	2.47	1.49	1.43
15	cA	1125	CL7	CHC-C1C	2.47	1.43	1.38
14	bB	1023	PHO	CMB-C2B	-2.47	1.46	1.51
17	cB	4021	A1JPJ	C19-C18	-2.47	1.40	1.45
17	aL	4020	A1JPJ	C23-C22	-2.47	1.40	1.45
15	aB	1207	CL7	C1B-C2B	2.47	1.49	1.43
14	aB	1023	PHO	C3B-C2B	-2.47	1.36	1.40
15	aA	1131	CL7	C1B-C2B	2.46	1.49	1.43
15	cB	1204	CL7	C1B-C2B	2.46	1.49	1.43
15	aA	1126	CL7	C1B-C2B	2.46	1.49	1.43
15	bA	1140	CL7	C1B-C2B	2.46	1.49	1.43
15	bA	1136	CL7	C1B-C2B	2.46	1.49	1.43
15	cA	1107	CL7	C1B-C2B	2.46	1.49	1.43
17	cB	4017	A1JPJ	C12-C13	-2.46	1.40	1.45
17	bB	4021	A1JPJ	C19-C18	-2.46	1.40	1.45
15	cB	1205	CL7	C1B-C2B	2.46	1.49	1.43
15	bA	1126	CL7	C1B-C2B	2.46	1.49	1.43
15	aA	1137	CL7	C1B-C2B	2.46	1.49	1.43
15	cA	1133	CL7	C1B-C2B	2.46	1.49	1.43
15	aA	1123	CL7	C1B-C2B	2.46	1.49	1.43
15	bA	1112	CL7	CHC-C1C	2.46	1.43	1.38
13	bA	1011	G9R	CMC-C2C	-2.46	1.46	1.50
15	aB	1216	CL7	C1B-C2B	2.46	1.49	1.43
15	bB	1230	CL7	CHC-C1C	2.46	1.43	1.38
14	bA	1013	PHO	CAC-C3C	-2.46	1.47	1.51
15	cA	1119	CL7	C1B-C2B	2.46	1.49	1.43
15	bA	1137	CL7	C1B-C2B	2.45	1.49	1.43
15	bB	1237	CL7	C1B-C2B	2.45	1.49	1.43
17	cI	4019	A1JPJ	C23-C22	-2.45	1.40	1.45
15	cA	1126	CL7	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1237	CL7	C1B-C2B	2.45	1.49	1.43
15	cA	1116	CL7	CHC-C1C	2.45	1.43	1.38
17	bL	4020	A1JPJ	C23-C22	-2.45	1.40	1.45
17	cL	4023	A1JPJ	C19-C18	-2.45	1.40	1.45
15	bB	1201	CL7	C1B-C2B	2.45	1.49	1.43
15	aB	1230	CL7	CHC-C1C	2.45	1.43	1.38
15	aB	1225	CL7	C1B-C2B	2.45	1.49	1.43
15	aA	1104	CL7	C1B-C2B	2.45	1.49	1.43
15	bB	1205	CL7	C1B-C2B	2.45	1.49	1.43
15	aA	1129	CL7	CHC-C1C	2.45	1.43	1.38
15	bB	1221	CL7	C1B-C2B	2.45	1.49	1.43
15	aB	1237	CL7	C1B-C2B	2.45	1.49	1.43
15	aB	1210	CL7	C1B-C2B	2.45	1.49	1.43
17	aA	4007	A1JPJ	C19-C18	-2.45	1.40	1.45
15	bA	1115	CL7	CHC-C1C	2.45	1.43	1.38
17	aI	4019	A1JPJ	C23-C22	-2.45	1.40	1.45
15	aB	1227	CL7	C1B-C2B	2.45	1.49	1.43
15	bA	1111	CL7	C1B-C2B	2.45	1.49	1.43
17	cA	4014	A1JPJ	C12-C13	-2.45	1.40	1.45
15	aB	1204	CL7	C1B-C2B	2.45	1.49	1.43
15	aA	1133	CL7	C1B-C2B	2.44	1.49	1.43
15	aB	1236	CL7	C1B-C2B	2.44	1.49	1.43
15	cA	1123	CL7	C1B-C2B	2.44	1.49	1.43
15	cB	1203	CL7	C1B-C2B	2.44	1.49	1.43
15	aB	1226	CL7	CMB-C2B	-2.44	1.45	1.50
14	aA	1013	PHO	CMB-C2B	-2.44	1.46	1.51
15	aB	1012	CL7	CHC-C1C	2.44	1.43	1.38
15	aB	1224	CL7	CHC-C1C	2.44	1.43	1.38
15	bB	1234	CL7	C1B-C2B	2.44	1.49	1.43
15	cA	1129	CL7	CHC-C1C	2.44	1.43	1.38
15	cB	1227	CL7	CHC-C1C	2.44	1.43	1.38
14	cA	1013	PHO	CMD-C2D	-2.44	1.46	1.51
15	aB	1205	CL7	C1B-C2B	2.44	1.49	1.43
13	aA	1011	G9R	CMC-C2C	-2.44	1.46	1.50
17	cL	4020	A1JPJ	C23-C22	-2.44	1.40	1.45
15	cA	1129	CL7	C1B-C2B	2.44	1.49	1.43
15	bB	1207	CL7	C1B-C2B	2.44	1.49	1.43
14	aA	1013	PHO	CMD-C2D	-2.44	1.46	1.51
15	aA	1102	CL7	C1B-C2B	2.44	1.49	1.43
15	cA	1104	CL7	C1B-C2B	2.44	1.49	1.43
15	cA	1123	CL7	CHC-C1C	2.43	1.43	1.38
17	aL	4020	A1JPJ	C12-C13	-2.43	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1124	CL7	C1B-C2B	2.43	1.49	1.43
15	bA	1123	CL7	C1B-C2B	2.43	1.49	1.43
14	cB	1023	PHO	CMB-C2B	-2.43	1.46	1.51
15	bA	1129	CL7	CHC-C1C	2.43	1.43	1.38
15	bB	1227	CL7	CMB-C2B	-2.43	1.45	1.50
15	cA	1112	CL7	C1B-C2B	2.43	1.49	1.43
14	bA	1013	PHO	CMD-C2D	-2.43	1.46	1.51
15	cA	1119	CL7	CHC-C1C	2.43	1.43	1.38
14	aB	1023	PHO	CMB-C2B	-2.43	1.46	1.51
17	bA	4011	A1JPJ	C12-C13	-2.43	1.40	1.45
15	aA	1119	CL7	CHC-C1C	2.43	1.43	1.38
17	bA	4007	A1JPJ	C19-C18	-2.43	1.40	1.45
15	bA	1129	CL7	C1B-C2B	2.43	1.49	1.43
15	bB	1203	CL7	C1B-C2B	2.43	1.49	1.43
15	cB	1211	CL7	CHC-C1C	2.43	1.43	1.38
15	aA	1108	CL7	CHC-C1C	2.43	1.43	1.38
17	aB	4021	A1JPJ	C19-C18	-2.43	1.40	1.45
17	bB	4017	A1JPJ	C12-C13	-2.42	1.40	1.45
15	cA	1124	CL7	C1B-C2B	2.42	1.49	1.43
15	bB	1204	CL7	C1B-C2B	2.42	1.49	1.43
17	bA	4011	A1JPJ	C23-C22	-2.42	1.40	1.45
15	aB	1215	CL7	C1B-C2B	2.42	1.49	1.43
15	bA	1116	CL7	CHC-C1C	2.42	1.43	1.38
15	cA	1115	CL7	CHC-C1C	2.42	1.43	1.38
15	aA	1126	CL7	CHC-C1C	2.42	1.43	1.38
17	aL	4023	A1JPJ	C12-C13	-2.42	1.40	1.45
15	cB	1236	CL7	C1B-C2B	2.42	1.48	1.43
15	bA	1106	CL7	C1B-C2B	2.42	1.48	1.43
15	aB	1234	CL7	C1B-C2B	2.42	1.48	1.43
15	aB	1224	CL7	C1B-C2B	2.42	1.48	1.43
15	aA	1115	CL7	CHC-C1C	2.42	1.43	1.38
15	bA	1124	CL7	C1B-C2B	2.42	1.48	1.43
15	cB	1221	CL7	C1B-C2B	2.42	1.48	1.43
17	cA	4003	A1JPJ	C19-C18	-2.42	1.40	1.45
14	bA	1013	PHO	CMB-C2B	-2.42	1.46	1.51
15	aA	1116	CL7	CHC-C1C	2.42	1.43	1.38
15	aA	1136	CL7	C1B-C2B	2.42	1.48	1.43
17	cA	4007	A1JPJ	C19-C18	-2.41	1.40	1.45
15	cA	1108	CL7	CHC-C1C	2.41	1.43	1.38
15	bB	1210	CL7	CHC-C1C	2.41	1.43	1.38
15	aA	1110	CL7	CHC-C1C	2.41	1.43	1.38
15	aA	1129	CL7	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1139	CL7	CHC-C1C	2.41	1.43	1.38
17	aA	4014	A1JPJ	C12-C13	-2.41	1.40	1.45
15	cB	1238	CL7	CHC-C1C	2.41	1.43	1.38
15	cB	1234	CL7	C1B-C2B	2.41	1.48	1.43
17	bA	4003	A1JPJ	C19-C18	-2.41	1.40	1.45
15	aA	1135	CL7	C1B-C2B	2.41	1.48	1.43
15	cB	1224	CL7	C1B-C2B	2.41	1.48	1.43
17	aA	4003	A1JPJ	C19-C18	-2.41	1.40	1.45
15	bB	1215	CL7	C1B-C2B	2.41	1.48	1.43
15	bB	1012	CL7	CHC-C1C	2.41	1.43	1.38
15	cJ	1301	CL7	CHC-C1C	2.40	1.43	1.38
15	bA	1104	CL7	C1B-C2B	2.40	1.48	1.43
15	bA	1116	CL7	C1B-C2B	2.40	1.48	1.43
15	cB	1214	CL7	CHC-C1C	2.40	1.43	1.38
15	cA	1102	CL7	C1B-C2B	2.40	1.48	1.43
15	cA	1103	CL7	C1B-C2B	2.40	1.48	1.43
15	aB	1203	CL7	C1B-C2B	2.40	1.48	1.43
17	aA	4011	A1JPJ	C23-C22	-2.40	1.40	1.45
15	aB	1214	CL7	C1B-C2B	2.40	1.48	1.43
15	aA	1139	CL7	CHC-C1C	2.40	1.43	1.38
17	bA	4014	A1JPJ	C12-C13	-2.40	1.40	1.45
15	bB	1224	CL7	C1B-C2B	2.40	1.48	1.43
15	bB	1235	CL7	C1B-C2B	2.40	1.48	1.43
15	aA	1128	CL7	C1B-C2B	2.40	1.48	1.43
17	bB	4017	A1JPJ	C23-C22	-2.40	1.40	1.45
17	cB	4017	A1JPJ	C23-C22	-2.39	1.40	1.45
15	cB	1209	CL7	CHC-C1C	2.39	1.43	1.38
15	cA	1137	CL7	C1B-C2B	2.39	1.48	1.43
15	aJ	1301	CL7	CHC-C1C	2.39	1.43	1.38
15	bA	1119	CL7	CHC-C1C	2.39	1.43	1.38
15	bB	1230	CL7	C1B-C2B	2.39	1.48	1.43
14	cA	1013	PHO	CMB-C2B	-2.39	1.46	1.51
15	aB	1221	CL7	CHC-C1C	2.39	1.43	1.38
15	aA	1135	CL7	CHC-C1C	2.39	1.43	1.38
15	bA	1110	CL7	CHC-C1C	2.39	1.43	1.38
15	bB	1211	CL7	CHC-C1C	2.39	1.43	1.38
14	cA	1013	PHO	CAC-C3C	-2.39	1.47	1.51
15	aA	1104	CL7	CHC-C1C	2.39	1.43	1.38
15	aA	1124	CL7	CHC-C1C	2.39	1.43	1.38
15	aK	1401	CL7	CHC-C1C	2.39	1.43	1.38
15	aA	1105	CL7	CHC-C1C	2.39	1.43	1.38
15	cB	1233	CL7	CHC-C1C	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1206	CL7	CMB-C2B	-2.39	1.45	1.50
15	cB	1226	CL7	CMB-C2B	-2.39	1.45	1.50
15	bB	1206	CL7	C1B-C2B	2.39	1.48	1.43
15	cB	1012	CL7	CHC-C1C	2.39	1.43	1.38
15	bA	1132	CL7	C1B-C2B	2.39	1.48	1.43
15	aA	1129	CL7	C1D-C2D	2.39	1.48	1.43
15	bB	1222	CL7	CHC-C1C	2.38	1.43	1.38
15	cA	1128	CL7	C1B-C2B	2.38	1.48	1.43
15	aA	1123	CL7	CHC-C1C	2.38	1.43	1.38
15	bA	1122	CL7	CHC-C1C	2.38	1.43	1.38
15	aA	1106	CL7	C1B-C2B	2.38	1.48	1.43
17	bL	4023	A1JPJ	C19-C18	-2.38	1.40	1.45
15	bA	1135	CL7	C1B-C2B	2.38	1.48	1.43
17	bA	4002	A1JPJ	C12-C13	-2.38	1.40	1.45
15	bA	1117	CL7	CMB-C2B	-2.38	1.45	1.50
15	cA	1117	CL7	CMB-C2B	-2.38	1.45	1.50
15	cB	1202	CL7	CHC-C1C	2.38	1.43	1.38
17	cA	4011	A1JPJ	C12-C13	-2.38	1.40	1.45
15	bB	1238	CL7	CHC-C1C	2.38	1.43	1.38
15	bB	1012	CL7	C1B-C2B	2.38	1.48	1.43
15	aB	1238	CL7	CHC-C1C	2.38	1.43	1.38
15	bB	1214	CL7	CHC-C1C	2.38	1.43	1.38
15	cA	1120	CL7	CHC-C1C	2.38	1.43	1.38
15	cK	1401	CL7	CHC-C1C	2.38	1.43	1.38
15	bB	1226	CL7	C1B-C2B	2.38	1.48	1.43
13	bA	1011	G9R	CAC-C3C	-2.38	1.47	1.51
17	cJ	4012	A1JPJ	C12-C13	-2.37	1.40	1.45
15	cB	1214	CL7	C1B-C2B	2.37	1.48	1.43
17	aB	4017	A1JPJ	C23-C22	-2.37	1.40	1.45
15	bB	1206	CL7	CMB-C2B	-2.37	1.45	1.50
15	cA	1106	CL7	C1B-C2B	2.37	1.48	1.43
15	cA	1135	CL7	MG-NB	-2.37	2.01	2.05
15	cA	1130	CL7	CHC-C1C	2.37	1.43	1.38
15	cA	1139	CL7	CHC-C1C	2.37	1.43	1.38
15	bA	1120	CL7	CHC-C1C	2.37	1.43	1.38
15	aB	1215	CL7	CHC-C1C	2.37	1.43	1.38
15	bB	1208	CL7	CHC-C1C	2.37	1.43	1.38
17	cA	4003	A1JPJ	C23-C22	-2.37	1.40	1.45
15	cB	1210	CL7	CHC-C1C	2.37	1.43	1.38
15	bA	1128	CL7	C1B-C2B	2.37	1.48	1.43
15	aB	1214	CL7	CHC-C1C	2.37	1.43	1.38
15	aB	1206	CL7	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1230	CL7	C1B-C2B	2.37	1.48	1.43
15	cA	1105	CL7	CHC-C1C	2.37	1.43	1.38
17	aA	4011	A1JPJ	C12-C13	-2.37	1.40	1.45
15	cB	1206	CL7	C1B-C2B	2.37	1.48	1.43
13	cA	1011	G9R	CAC-C3C	-2.36	1.47	1.51
15	aA	1127	CL7	C1B-C2B	2.36	1.48	1.43
15	aB	1233	CL7	CHC-C1C	2.36	1.43	1.38
15	bB	1227	CL7	CHC-C1C	2.36	1.43	1.38
15	aL	1502	CL7	C1B-C2B	2.36	1.48	1.43
15	aB	1012	CL7	C1B-C2B	2.36	1.48	1.43
15	aB	1227	CL7	CHC-C1C	2.36	1.43	1.38
17	bA	4003	A1JPJ	C23-C22	-2.36	1.40	1.45
17	cJ	4012	A1JPJ	C19-C18	-2.36	1.40	1.45
15	cA	1127	CL7	C1B-C2B	2.36	1.48	1.43
15	aB	1222	CL7	CHC-C1C	2.36	1.43	1.38
15	bA	1123	CL7	CHC-C1C	2.36	1.43	1.38
17	cA	4002	A1JPJ	C12-C13	-2.36	1.40	1.45
15	cB	1224	CL7	CHC-C1C	2.36	1.43	1.38
15	cB	1228	CL7	CHC-C1C	2.36	1.43	1.38
17	aB	4015	A1JPJ	C19-C18	-2.36	1.40	1.45
15	aB	1211	CL7	CHC-C1C	2.36	1.43	1.38
15	cB	1231	CL7	CHC-C1C	2.36	1.43	1.38
15	bA	1105	CL7	CHC-C1C	2.36	1.43	1.38
15	bA	1102	CL7	C1B-C2B	2.36	1.48	1.43
15	cB	1220	CL7	CHC-C1C	2.36	1.43	1.38
17	bB	4015	A1JPJ	C19-C18	-2.36	1.40	1.45
15	bA	1108	CL7	CHC-C1C	2.36	1.43	1.38
15	cA	1103	CL7	CHC-C1C	2.36	1.43	1.38
15	cJ	1302	CL7	CHC-C1C	2.35	1.43	1.38
15	aA	1130	CL7	CHC-C1C	2.35	1.43	1.38
15	aB	1220	CL7	CHC-C1C	2.35	1.43	1.38
15	aB	1226	CL7	C1B-C2B	2.35	1.48	1.43
15	cL	1501	CL7	C1B-C2B	2.35	1.48	1.43
15	cK	1402	CL7	CHC-C1C	2.35	1.43	1.38
17	bB	4010	A1JPJ	C19-C18	-2.35	1.40	1.45
15	bA	1130	CL7	CHC-C1C	2.35	1.43	1.38
15	bJ	1301	CL7	CHC-C1C	2.35	1.43	1.38
15	aB	1218	CL7	CHC-C1C	2.35	1.43	1.38
15	bB	1232	CL7	CHC-C1C	2.35	1.43	1.38
15	bK	1401	CL7	CHC-C1C	2.35	1.43	1.38
15	aA	1120	CL7	CHC-C1C	2.35	1.42	1.38
15	aB	1228	CL7	CHC-C1C	2.35	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cL	1502	CL7	C1B-C2B	2.35	1.48	1.43
17	cB	4015	A1JPJ	C19-C18	-2.35	1.40	1.45
15	cB	1203	CL7	CHC-C1C	2.35	1.42	1.38
15	cB	1216	CL7	CHC-C1C	2.35	1.42	1.38
17	cA	4011	A1JPJ	C23-C22	-2.35	1.40	1.45
15	cA	1114	CL7	CHC-C1C	2.35	1.42	1.38
15	cA	1801	CL7	CHC-C1C	2.35	1.42	1.38
15	bA	1104	CL7	CHC-C1C	2.35	1.42	1.38
15	bK	1402	CL7	CHC-C1C	2.35	1.42	1.38
13	aA	1011	G9R	CAC-C3C	-2.35	1.47	1.51
15	bL	1501	CL7	C1B-C2B	2.35	1.48	1.43
14	bB	1023	PHO	C3B-C2B	-2.35	1.37	1.40
15	bB	1228	CL7	CHC-C1C	2.35	1.42	1.38
15	aA	1133	CL7	CHC-C1C	2.35	1.42	1.38
15	cA	1117	CL7	CHC-C1C	2.35	1.42	1.38
17	aJ	4012	A1JPJ	C19-C18	-2.35	1.40	1.45
15	bB	1226	CL7	CMB-C2B	-2.35	1.45	1.50
15	aA	1114	CL7	CHC-C1C	2.34	1.42	1.38
15	cB	1222	CL7	CHC-C1C	2.34	1.42	1.38
15	aB	1210	CL7	CHC-C1C	2.34	1.42	1.38
15	bL	1502	CL7	C1B-C2B	2.34	1.48	1.43
17	bJ	4012	A1JPJ	C12-C13	-2.34	1.40	1.45
17	cJ	4012	A1JPJ	C23-C22	-2.34	1.40	1.45
15	bA	1113	CL7	CHC-C1C	2.34	1.42	1.38
15	aA	1117	CL7	CMB-C2B	-2.34	1.45	1.50
15	bA	1129	CL7	C1D-C2D	2.34	1.48	1.43
17	cL	4023	A1JPJ	C23-C22	-2.34	1.40	1.45
15	aF	1701	CL7	CHC-C1C	2.34	1.42	1.38
15	bB	1207	CL7	CHC-C1C	2.34	1.42	1.38
15	cA	1128	CL7	CMB-C2B	-2.34	1.45	1.50
15	aB	1206	CL7	C1B-C2B	2.34	1.48	1.43
15	bA	1135	CL7	CHC-C1C	2.34	1.42	1.38
15	cB	1226	CL7	C1B-C2B	2.34	1.48	1.43
15	aB	1209	CL7	CHC-C1C	2.34	1.42	1.38
15	cA	1104	CL7	CHC-C1C	2.34	1.42	1.38
15	cA	1126	CL7	CHC-C1C	2.34	1.42	1.38
15	cA	1135	CL7	C1B-C2B	2.34	1.48	1.43
17	bB	4017	A1JPJ	C19-C18	-2.34	1.40	1.45
17	bJ	4012	A1JPJ	C19-C18	-2.34	1.40	1.45
15	aA	1132	CL7	C1B-C2B	2.34	1.48	1.43
15	bA	1127	CL7	C1B-C2B	2.34	1.48	1.43
17	aA	4003	A1JPJ	C23-C22	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1117	CL7	CHC-C1C	2.34	1.42	1.38
15	bB	1224	CL7	CHC-C1C	2.34	1.42	1.38
15	aA	1103	CL7	CHC-C1C	2.34	1.42	1.38
15	bA	1132	CL7	CHC-C1C	2.34	1.42	1.38
15	bA	1022	CL7	C1B-C2B	2.34	1.48	1.43
15	aB	1208	CL7	CHC-C1C	2.34	1.42	1.38
17	aJ	4012	A1JPJ	C12-C13	-2.34	1.40	1.45
15	aJ	1302	CL7	CHC-C1C	2.34	1.42	1.38
15	cA	1133	CL7	CHC-C1C	2.33	1.42	1.38
15	aL	1501	CL7	C1B-C2B	2.33	1.48	1.43
17	aB	4021	A1JPJ	C23-C22	-2.33	1.40	1.45
15	bB	1218	CL7	CHC-C1C	2.33	1.42	1.38
15	cB	1012	CL7	C1B-C2B	2.33	1.48	1.43
15	aB	1231	CL7	CHC-C1C	2.33	1.42	1.38
15	cA	1022	CL7	CHC-C1C	2.33	1.42	1.38
15	bA	1130	CL7	C1B-C2B	2.33	1.48	1.43
15	bA	1133	CL7	CHC-C1C	2.33	1.42	1.38
15	bJ	1302	CL7	CHC-C1C	2.33	1.42	1.38
15	cA	1110	CL7	CHC-C1C	2.33	1.42	1.38
17	aA	4007	A1JPJ	C23-C22	-2.33	1.40	1.45
14	bB	1023	PHO	CAC-C3C	-2.33	1.47	1.51
15	cB	1238	CL7	C1B-C2B	2.33	1.48	1.43
15	bB	1208	CL7	C1D-C2D	2.33	1.48	1.43
17	cF	4016	A1JPJ	C12-C13	-2.33	1.40	1.45
17	cF	4016	A1JPJ	C19-C18	-2.33	1.40	1.45
15	cL	1502	CL7	CHC-C1C	2.33	1.42	1.38
15	bA	1022	CL7	CHC-C1C	2.33	1.42	1.38
15	cA	1116	CL7	C1B-C2B	2.33	1.48	1.43
15	cF	1701	CL7	CHC-C1C	2.33	1.42	1.38
15	aA	1122	CL7	CHC-C1C	2.33	1.42	1.38
15	bB	1202	CL7	CHC-C1C	2.33	1.42	1.38
17	aA	4002	A1JPJ	C12-C13	-2.32	1.41	1.45
15	bA	1128	CL7	CMB-C2B	-2.32	1.45	1.50
15	bA	1111	CL7	CHC-C1C	2.32	1.42	1.38
15	bB	1231	CL7	CHC-C1C	2.32	1.42	1.38
15	aK	1402	CL7	C1B-C2B	2.32	1.48	1.43
15	cB	1208	CL7	CHC-C1C	2.32	1.42	1.38
15	cA	1022	CL7	C1B-C2B	2.32	1.48	1.43
17	bL	4023	A1JPJ	C23-C22	-2.32	1.41	1.45
17	cA	4007	A1JPJ	C23-C22	-2.32	1.41	1.45
15	cB	1223	CL7	CHC-C1C	2.32	1.42	1.38
17	aJ	4012	A1JPJ	C23-C22	-2.32	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1114	CL7	CHC-C1C	2.32	1.42	1.38
13	aA	1011	G9R	C4D-CHA	2.32	1.43	1.40
15	cB	1215	CL7	CMD-C2D	-2.32	1.45	1.50
15	cA	1130	CL7	C1B-C2B	2.32	1.48	1.43
15	aA	1022	CL7	C1B-C2B	2.32	1.48	1.43
15	bB	1217	CL7	CHC-C1C	2.32	1.42	1.38
17	cA	4002	A1JPJ	C19-C18	-2.32	1.41	1.45
15	aA	1130	CL7	C1B-C2B	2.32	1.48	1.43
15	aA	1801	CL7	CHC-C1C	2.32	1.42	1.38
15	cB	1021	CL7	CHC-C1C	2.32	1.42	1.38
15	bA	1801	CL7	CHC-C1C	2.32	1.42	1.38
15	bF	1701	CL7	CHC-C1C	2.32	1.42	1.38
15	cA	1137	CL7	CHC-C1C	2.32	1.42	1.38
17	aB	4005	A1JPJ	C19-C18	-2.32	1.41	1.45
15	aL	1501	CL7	CMB-C2B	-2.32	1.45	1.50
17	aA	4002	A1JPJ	C19-C18	-2.31	1.41	1.45
17	aL	4023	A1JPJ	C23-C22	-2.31	1.41	1.45
15	cA	1140	CL7	CHC-C1C	2.31	1.42	1.38
14	cB	1023	PHO	CAC-C3C	-2.31	1.47	1.51
15	cB	1218	CL7	CHC-C1C	2.31	1.42	1.38
15	bA	1104	CL7	MG-NB	-2.31	2.01	2.05
17	bF	4016	A1JPJ	C12-C13	-2.31	1.41	1.45
15	aA	1101	CL7	CHC-C1C	2.31	1.42	1.38
15	aB	1203	CL7	CHC-C1C	2.31	1.42	1.38
15	bA	1137	CL7	CHC-C1C	2.31	1.42	1.38
17	bB	4015	A1JPJ	C12-C13	-2.31	1.41	1.45
15	bL	1502	CL7	CHC-C1C	2.31	1.42	1.38
15	aA	1116	CL7	C1B-C2B	2.31	1.48	1.43
15	bA	1101	CL7	CHC-C1C	2.31	1.42	1.38
15	cA	1124	CL7	CHC-C1C	2.31	1.42	1.38
15	cB	1217	CL7	CHC-C1C	2.31	1.42	1.38
15	bB	1223	CL7	CHC-C1C	2.31	1.42	1.38
17	bA	4002	A1JPJ	C19-C18	-2.31	1.41	1.45
15	cB	1208	CL7	C1D-C2D	2.31	1.48	1.43
17	aB	4015	A1JPJ	C12-C13	-2.31	1.41	1.45
15	aB	1232	CL7	CHC-C1C	2.31	1.42	1.38
15	cB	1206	CL7	CHC-C1C	2.31	1.42	1.38
17	aB	4010	A1JPJ	C19-C18	-2.31	1.41	1.45
17	cA	4014	A1JPJ	C19-C18	-2.31	1.41	1.45
17	cB	4017	A1JPJ	C19-C18	-2.31	1.41	1.45
15	cB	1230	CL7	C1B-C2B	2.31	1.48	1.43
15	bA	1140	CL7	CHC-C1C	2.31	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1209	CL7	CHC-C1C	2.31	1.42	1.38
15	bB	1214	CL7	C1B-C2B	2.31	1.48	1.43
17	cB	4010	A1JPJ	C19-C18	-2.31	1.41	1.45
15	aB	1241	CL7	CHC-C1C	2.31	1.42	1.38
15	aA	1132	CL7	C4C-NC	2.31	1.40	1.37
15	bA	1109	CL7	CHC-C1C	2.30	1.42	1.38
15	bA	1115	CL7	CMC-C2C	-2.30	1.45	1.50
15	bB	1241	CL7	C1D-C2D	2.30	1.48	1.43
15	aB	1208	CL7	C1D-C2D	2.30	1.48	1.43
15	bB	1238	CL7	C1B-C2B	2.30	1.48	1.43
15	cA	1115	CL7	CMC-C2C	-2.30	1.45	1.50
15	cB	1221	CL7	CHC-C1C	2.30	1.42	1.38
15	cB	1232	CL7	CHC-C1C	2.30	1.42	1.38
15	cA	1101	CL7	CHC-C1C	2.30	1.42	1.38
15	aB	1238	CL7	C1B-C2B	2.30	1.48	1.43
15	aA	1117	CL7	CHC-C1C	2.30	1.42	1.38
15	cB	1226	CL7	CHC-C1C	2.30	1.42	1.38
14	aB	1023	PHO	CAC-C3C	-2.30	1.47	1.51
17	cB	4021	A1JPJ	C23-C22	-2.30	1.41	1.45
15	cL	1503	CL7	CMB-C2B	-2.30	1.45	1.50
15	aB	1021	CL7	CHC-C1C	2.30	1.42	1.38
15	cL	1501	CL7	CHC-C1C	2.30	1.42	1.38
17	aF	4016	A1JPJ	C12-C13	-2.30	1.41	1.45
15	aB	1219	CL7	CHC-C1C	2.30	1.42	1.38
15	bB	1219	CL7	CHC-C1C	2.30	1.42	1.38
15	aA	1140	CL7	CHC-C1C	2.30	1.42	1.38
15	bB	1233	CL7	CHC-C1C	2.30	1.42	1.38
15	cB	1235	CL7	CHC-C1C	2.30	1.42	1.38
15	cA	1132	CL7	C1B-C2B	2.30	1.48	1.43
14	aB	1023	PHO	C3B-CAB	-2.30	1.43	1.47
15	aB	1217	CL7	CHC-C1C	2.30	1.42	1.38
17	aB	4010	A1JPJ	C23-C22	-2.30	1.41	1.45
17	bA	4007	A1JPJ	C23-C22	-2.30	1.41	1.45
15	aA	1109	CL7	CHC-C1C	2.29	1.42	1.38
15	bA	1103	CL7	CHC-C1C	2.29	1.42	1.38
15	aA	1127	CL7	CHC-C1C	2.29	1.42	1.38
15	aB	1209	CL7	C1D-C2D	2.29	1.48	1.43
15	cA	1135	CL7	CHC-C1C	2.29	1.42	1.38
17	aB	4015	A1JPJ	C23-C22	-2.29	1.41	1.45
15	cK	1402	CL7	C1D-C2D	2.29	1.48	1.43
15	bB	1241	CL7	CHC-C1C	2.29	1.42	1.38
15	bA	1136	CL7	CHC-C1C	2.29	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1221	CL7	CHC-C1C	2.29	1.42	1.38
15	cA	1113	CL7	CHC-C1C	2.29	1.42	1.38
15	aL	1502	CL7	CHC-C1C	2.29	1.42	1.38
17	aB	4017	A1JPJ	C19-C18	-2.29	1.41	1.45
15	aB	1227	CL7	C1D-C2D	2.29	1.48	1.43
15	cB	1213	CL7	CHC-C1C	2.29	1.42	1.38
15	bB	1225	CL7	CHC-C1C	2.29	1.42	1.38
17	bB	4015	A1JPJ	C23-C22	-2.29	1.41	1.45
15	aB	1225	CL7	CHC-C1C	2.29	1.42	1.38
15	cA	1111	CL7	CHC-C1C	2.29	1.42	1.38
15	aB	1216	CL7	CHC-C1C	2.29	1.42	1.38
15	cB	1204	CL7	CHC-C1C	2.29	1.42	1.38
17	bF	4016	A1JPJ	C19-C18	-2.29	1.41	1.45
14	bB	1023	PHO	C3D-C4D	2.28	1.44	1.41
15	cA	1127	CL7	CHC-C1C	2.28	1.42	1.38
15	cB	1207	CL7	CHC-C1C	2.28	1.42	1.38
15	aB	1223	CL7	CHC-C1C	2.28	1.42	1.38
15	aA	1128	CL7	CMB-C2B	-2.28	1.46	1.50
15	aB	1235	CL7	CHC-C1C	2.28	1.42	1.38
15	bA	1121	CL7	CHC-C1C	2.28	1.42	1.38
17	bA	4014	A1JPJ	C19-C18	-2.28	1.41	1.45
15	aA	1131	CL7	CMB-C2B	-2.28	1.46	1.50
15	cB	1217	CL7	C1D-C2D	2.28	1.48	1.43
15	bB	1215	CL7	CHC-C1C	2.28	1.42	1.38
15	bL	1501	CL7	CHC-C1C	2.28	1.42	1.38
17	cB	4005	A1JPJ	C23-C22	-2.28	1.41	1.45
15	aB	1202	CL7	CHC-C1C	2.28	1.42	1.38
15	aA	1118	CL7	CHC-C1C	2.28	1.42	1.38
15	bB	1213	CL7	CHC-C1C	2.28	1.42	1.38
15	cB	1219	CL7	CHC-C1C	2.28	1.42	1.38
15	bA	1112	CL7	C1D-C2D	2.28	1.48	1.43
15	cJ	1302	CL7	C1D-C2D	2.28	1.48	1.43
15	cA	1022	CL7	CMB-C2B	-2.28	1.46	1.50
15	aB	1229	CL7	CHC-C1C	2.28	1.42	1.38
15	bB	1220	CL7	CHC-C1C	2.28	1.42	1.38
15	bA	1117	CL7	C1B-C2B	2.28	1.48	1.43
15	bB	1209	CL7	C1D-C2D	2.28	1.48	1.43
15	aA	1022	CL7	CHC-C1C	2.28	1.42	1.38
17	bB	4021	A1JPJ	C23-C22	-2.28	1.41	1.45
15	aB	1239	CL7	CHC-C1C	2.27	1.42	1.38
15	bB	1204	CL7	CHC-C1C	2.27	1.42	1.38
15	cB	1225	CL7	CHC-C1C	2.27	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	1023	PHO	C3B-CAB	-2.27	1.43	1.47
15	cA	1102	CL7	C1D-C2D	2.27	1.48	1.43
14	cB	1023	PHO	C3B-C2B	-2.27	1.37	1.40
15	cA	1132	CL7	MG-NC	2.27	2.10	2.05
17	cB	4015	A1JPJ	C12-C13	-2.27	1.41	1.45
15	aB	1213	CL7	CHC-C1C	2.27	1.42	1.38
15	bB	1021	CL7	CHC-C1C	2.27	1.42	1.38
15	cA	1122	CL7	CHC-C1C	2.27	1.42	1.38
15	cB	1234	CL7	CHC-C1C	2.27	1.42	1.38
17	bA	4002	A1JPJ	C23-C22	-2.27	1.41	1.45
17	bJ	4012	A1JPJ	C23-C22	-2.27	1.41	1.45
17	cB	4015	A1JPJ	C23-C22	-2.27	1.41	1.45
15	bA	1131	CL7	CMB-C2B	-2.27	1.46	1.50
15	cA	1134	CL7	CHC-C1C	2.27	1.42	1.38
15	cB	1229	CL7	CHC-C1C	2.27	1.42	1.38
15	bA	1127	CL7	CHC-C1C	2.27	1.42	1.38
15	cB	1231	CL7	C1D-C2D	2.27	1.48	1.43
15	bA	1102	CL7	C1D-C2D	2.27	1.48	1.43
15	aA	1121	CL7	CHC-C1C	2.27	1.42	1.38
15	aB	1204	CL7	CHC-C1C	2.27	1.42	1.38
15	bA	1107	CL7	CHC-C1C	2.27	1.42	1.38
17	bB	4010	A1JPJ	C23-C22	-2.27	1.41	1.45
15	aB	1234	CL7	CHC-C1C	2.27	1.42	1.38
15	aI	1601	CL7	CHC-C1C	2.27	1.42	1.38
15	aK	1402	CL7	CMB-C2B	-2.27	1.46	1.50
15	cA	1132	CL7	C4C-NC	2.27	1.40	1.37
15	aA	1137	CL7	CHC-C1C	2.27	1.42	1.38
15	aB	1206	CL7	CHC-C1C	2.26	1.42	1.38
15	aL	1501	CL7	CHC-C1C	2.26	1.42	1.38
15	aA	1111	CL7	CHC-C1C	2.26	1.42	1.38
15	bB	1216	CL7	CHC-C1C	2.26	1.42	1.38
15	cB	1237	CL7	CHC-C1C	2.26	1.42	1.38
17	bF	4016	A1JPJ	C23-C22	-2.26	1.41	1.45
15	cA	1136	CL7	CHC-C1C	2.26	1.42	1.38
15	cB	1241	CL7	C1D-C2D	2.26	1.48	1.43
15	bA	1022	CL7	MG-NB	-2.26	2.01	2.05
15	aA	1102	CL7	C1D-C2D	2.26	1.48	1.43
15	bA	1022	CL7	CMB-C2B	-2.26	1.46	1.50
15	cB	1209	CL7	C1D-C2D	2.26	1.48	1.43
17	aF	4016	A1JPJ	C19-C18	-2.26	1.41	1.45
15	bB	1236	CL7	CHC-C1C	2.26	1.42	1.38
15	cB	1239	CL7	CHC-C1C	2.26	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1206	CL7	MG-NB	-2.26	2.01	2.05
15	aA	1022	CL7	CMB-C2B	-2.26	1.46	1.50
15	aB	1207	CL7	CHC-C1C	2.26	1.42	1.38
14	cB	1023	PHO	C3D-C4D	2.26	1.44	1.41
15	bB	1203	CL7	CHC-C1C	2.26	1.42	1.38
15	cB	1206	CL7	MG-NB	-2.26	2.01	2.05
15	bB	1232	CL7	C1D-C2D	2.26	1.48	1.43
14	aB	1023	PHO	C3D-C4D	2.26	1.44	1.41
15	aB	1232	CL7	C1D-C2D	2.26	1.48	1.43
15	cA	1022	CL7	MG-NB	-2.26	2.01	2.05
15	bB	1235	CL7	CHC-C1C	2.26	1.42	1.38
15	bL	1501	CL7	MG-NB	-2.26	2.01	2.05
15	bB	1206	CL7	CHC-C1C	2.25	1.42	1.38
15	cA	1121	CL7	CHC-C1C	2.25	1.42	1.38
15	cB	1219	CL7	C1D-C2D	2.25	1.48	1.43
15	bA	1124	CL7	CHC-C1C	2.25	1.42	1.38
14	bB	1023	PHO	C4D-ND	-2.25	1.35	1.38
15	cI	1601	CL7	CHC-C1C	2.25	1.42	1.38
15	cA	1117	CL7	C1B-C2B	2.25	1.48	1.43
15	cB	1207	CL7	MG-NB	-2.25	2.01	2.05
15	bB	1237	CL7	CHC-C1C	2.25	1.42	1.38
15	aK	1402	CL7	MG-NB	-2.25	2.01	2.05
17	aA	4002	A1JPJ	C23-C22	-2.25	1.41	1.45
15	bB	1233	CL7	C1D-C2D	2.25	1.48	1.43
15	aA	1134	CL7	CHC-C1C	2.25	1.42	1.38
17	aF	4016	A1JPJ	C23-C22	-2.25	1.41	1.45
17	cB	4005	A1JPJ	C19-C18	-2.25	1.41	1.45
15	aL	1503	CL7	CHC-C1C	2.25	1.42	1.38
15	aB	1236	CL7	CHC-C1C	2.25	1.42	1.38
13	bA	1011	G9R	C4D-CHA	2.25	1.43	1.40
17	cA	4002	A1JPJ	C23-C22	-2.25	1.41	1.45
15	cB	1236	CL7	CHC-C1C	2.25	1.42	1.38
15	bJ	1302	CL7	C1D-C2D	2.25	1.48	1.43
17	cB	4004	A1JPJ	C12-C13	-2.25	1.41	1.45
15	aA	1136	CL7	MG-NB	-2.25	2.01	2.05
15	aB	1219	CL7	C1D-C2D	2.25	1.48	1.43
17	aB	4005	A1JPJ	C23-C22	-2.25	1.41	1.45
15	aA	1135	CL7	MG-NB	-2.25	2.01	2.05
15	aA	1136	CL7	CHC-C1C	2.25	1.42	1.38
15	cA	1109	CL7	CHC-C1C	2.25	1.42	1.38
17	cF	4016	A1JPJ	C23-C22	-2.25	1.41	1.45
15	cB	1214	CL7	C1D-C2D	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1128	CL7	CHC-C1C	2.25	1.42	1.38
15	cB	1232	CL7	C1D-C2D	2.24	1.48	1.43
15	bB	1204	CL7	CMD-C2D	-2.24	1.46	1.50
15	bB	1234	CL7	CHC-C1C	2.24	1.42	1.38
15	aA	1119	CL7	C1D-C2D	2.24	1.48	1.43
15	aB	1205	CL7	CHC-C1C	2.24	1.42	1.38
15	cB	1241	CL7	CHC-C1C	2.24	1.42	1.38
15	aA	1127	CL7	MG-NB	-2.24	2.01	2.05
15	cA	1119	CL7	C1D-C2D	2.24	1.48	1.43
17	aA	4014	A1JPJ	C19-C18	-2.24	1.41	1.45
15	cL	1501	CL7	CMB-C2B	-2.24	1.46	1.50
15	bB	1227	CL7	MG-NB	-2.24	2.01	2.05
15	cA	1107	CL7	CHC-C1C	2.24	1.42	1.38
15	bB	1219	CL7	C1D-C2D	2.24	1.48	1.43
15	aA	1117	CL7	C1B-C2B	2.24	1.48	1.43
15	cB	1226	CL7	CMD-C2D	-2.24	1.46	1.50
17	aB	4006	A1JPJ	C23-C22	-2.24	1.41	1.45
15	bL	1501	CL7	CMB-C2B	-2.24	1.46	1.50
15	bB	1229	CL7	CHC-C1C	2.24	1.42	1.38
15	cA	1138	CL7	MG-NB	-2.24	2.01	2.05
15	bA	1118	CL7	CHC-C1C	2.24	1.42	1.38
15	aB	1214	CL7	C1D-C2D	2.24	1.48	1.43
15	aB	1212	CL7	CHC-C1C	2.23	1.42	1.38
15	aA	1022	CL7	MG-NB	-2.23	2.01	2.05
15	bB	1210	CL7	C1D-C2D	2.23	1.48	1.43
15	bA	1134	CL7	CHC-C1C	2.23	1.42	1.38
15	bI	1601	CL7	CHC-C1C	2.23	1.42	1.38
15	aB	1237	CL7	CHC-C1C	2.23	1.42	1.38
15	aB	1217	CL7	C1D-C2D	2.23	1.48	1.43
17	aB	4005	A1JPJ	C12-C13	-2.23	1.41	1.45
17	cB	4005	A1JPJ	C12-C13	-2.23	1.41	1.45
15	aA	1113	CL7	CHC-C1C	2.23	1.42	1.38
17	bB	4005	A1JPJ	C12-C13	-2.23	1.41	1.45
15	bB	1227	CL7	C1D-C2D	2.23	1.48	1.43
15	aA	1115	CL7	CMC-C2C	-2.23	1.46	1.50
15	bK	1402	CL7	C1D-C2D	2.23	1.48	1.43
15	cB	1210	CL7	C1D-C2D	2.23	1.48	1.43
15	bL	1503	CL7	CHC-C1C	2.23	1.42	1.38
15	cB	1227	CL7	C1D-C2D	2.23	1.48	1.43
15	cL	1502	CL7	CMB-C2B	-2.23	1.46	1.50
17	cA	4014	A1JPJ	C23-C22	-2.23	1.41	1.45
15	cA	1122	CL7	C1D-C2D	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	1212	CL7	CHC-C1C	2.23	1.42	1.38
17	bB	4005	A1JPJ	C19-C18	-2.23	1.41	1.45
17	bB	4005	A1JPJ	C23-C22	-2.23	1.41	1.45
15	bB	1228	CL7	C1D-C2D	2.23	1.48	1.43
15	cA	1139	CL7	C1D-C2D	2.23	1.48	1.43
17	cB	4010	A1JPJ	C23-C22	-2.23	1.41	1.45
15	bB	1217	CL7	C1D-C2D	2.23	1.48	1.43
15	bB	1206	CL7	MG-NB	-2.22	2.01	2.05
15	aB	1211	CL7	C1D-C2D	2.22	1.48	1.43
15	cB	1233	CL7	C1D-C2D	2.22	1.48	1.43
15	cA	1118	CL7	CHC-C1C	2.22	1.42	1.38
15	aA	1114	CL7	C1D-C2D	2.22	1.48	1.43
15	aA	1133	CL7	C1D-C2D	2.22	1.48	1.43
15	bA	1111	CL7	C1D-C2D	2.22	1.48	1.43
15	bB	1214	CL7	CMB-C2B	-2.22	1.46	1.50
15	aB	1241	CL7	C1D-C2D	2.22	1.48	1.43
15	cF	1701	CL7	C1D-C2D	2.22	1.48	1.43
15	cA	1105	CL7	C1D-C2D	2.22	1.48	1.43
15	aL	1502	CL7	MG-NB	-2.22	2.01	2.05
15	aB	1210	CL7	C1D-C2D	2.22	1.48	1.43
15	cA	1123	CL7	CMB-C2B	-2.22	1.46	1.50
15	cL	1502	CL7	MG-NB	-2.22	2.01	2.05
13	cA	1011	G9R	C4D-CHA	2.22	1.43	1.40
15	bA	1103	CL7	CMB-C2B	-2.22	1.46	1.50
15	cB	1220	CL7	C1D-C2D	2.22	1.48	1.43
15	bB	1231	CL7	C1D-C2D	2.22	1.48	1.43
15	aA	1107	CL7	CHC-C1C	2.22	1.42	1.38
15	bA	1113	CL7	C1D-C2D	2.22	1.48	1.43
15	aK	1402	CL7	C1D-C2D	2.22	1.48	1.43
15	bA	1122	CL7	C1D-C2D	2.21	1.48	1.43
17	cB	4004	A1JPJ	C19-C18	-2.21	1.41	1.45
15	bB	1212	CL7	CHC-C1C	2.21	1.42	1.38
15	aA	1136	CL7	CMB-C2B	-2.21	1.46	1.50
15	cK	1401	CL7	C1D-C2D	2.21	1.48	1.43
17	aL	4023	A1JPJ	C19-C18	-2.21	1.41	1.45
15	cA	1114	CL7	C1D-C2D	2.21	1.48	1.43
15	aB	1233	CL7	C1D-C2D	2.21	1.48	1.43
15	aB	1231	CL7	C1D-C2D	2.21	1.48	1.43
15	cA	1131	CL7	CMB-C2B	-2.21	1.46	1.50
15	cA	1133	CL7	C1D-C2D	2.21	1.48	1.43
17	bA	4014	A1JPJ	C23-C22	-2.21	1.41	1.45
15	cB	1230	CL7	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1115	CL7	CMD-C2D	-2.21	1.46	1.50
15	cA	1115	CL7	CMD-C2D	-2.21	1.46	1.50
17	bB	4004	A1JPJ	C12-C13	-2.21	1.41	1.45
15	bB	1205	CL7	CHC-C1C	2.21	1.42	1.38
15	cB	1205	CL7	CHC-C1C	2.21	1.42	1.38
14	cB	1023	PHO	C4D-ND	-2.21	1.35	1.38
15	aB	1230	CL7	MG-NB	-2.21	2.01	2.05
15	bA	1133	CL7	C1D-C2D	2.21	1.48	1.43
15	bA	1115	CL7	MG-NB	-2.21	2.01	2.05
15	bB	1216	CL7	CMB-C2B	-2.21	1.46	1.50
15	cA	1131	CL7	CHC-C1C	2.21	1.42	1.38
15	aK	1401	CL7	C1D-C2D	2.20	1.48	1.43
15	cI	1601	CL7	C1D-C2D	2.20	1.48	1.43
15	bB	1239	CL7	CHC-C1C	2.20	1.42	1.38
15	bA	1119	CL7	C1D-C2D	2.20	1.48	1.43
15	bA	1107	CL7	CMD-C2D	-2.20	1.46	1.50
15	bA	1114	CL7	C1D-C2D	2.20	1.48	1.43
15	aL	1501	CL7	MG-NB	-2.20	2.01	2.05
15	bB	1234	CL7	MG-NB	-2.20	2.01	2.05
15	cB	1234	CL7	MG-NB	-2.20	2.01	2.05
15	bA	1135	CL7	MG-NB	-2.20	2.01	2.05
15	bB	1214	CL7	C1D-C2D	2.20	1.48	1.43
14	cA	1013	PHO	C4D-ND	-2.20	1.35	1.38
15	cA	1104	CL7	MG-NB	-2.20	2.01	2.05
15	aB	1215	CL7	MG-NB	-2.20	2.01	2.05
15	aF	1701	CL7	C1D-C2D	2.20	1.48	1.43
15	aJ	1301	CL7	C1D-C2D	2.20	1.48	1.43
15	cA	1108	CL7	C1D-C2D	2.20	1.48	1.43
15	bB	1207	CL7	MG-NB	-2.20	2.01	2.05
17	cB	4006	A1JPJ	C23-C22	-2.20	1.41	1.45
15	aA	1120	CL7	C1D-C2D	2.20	1.48	1.43
15	bB	1211	CL7	C1D-C2D	2.20	1.48	1.43
15	aA	1128	CL7	CHC-C1C	2.20	1.42	1.38
17	bB	4006	A1JPJ	C23-C22	-2.20	1.41	1.45
15	aA	1113	CL7	C1D-C2D	2.19	1.48	1.43
15	aA	1122	CL7	C1D-C2D	2.19	1.48	1.43
15	bA	1105	CL7	C1D-C2D	2.19	1.48	1.43
15	cA	1117	CL7	C1D-C2D	2.19	1.48	1.43
15	cA	1107	CL7	CMD-C2D	-2.19	1.46	1.50
15	cB	1226	CL7	MG-NB	-2.19	2.01	2.05
15	bB	1220	CL7	C1D-C2D	2.19	1.48	1.43
15	bL	1503	CL7	CMB-C2B	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1127	CL7	MG-NB	-2.19	2.01	2.05
15	bA	1108	CL7	C1D-C2D	2.19	1.48	1.43
15	bA	1139	CL7	C1D-C2D	2.19	1.48	1.43
15	bJ	1301	CL7	C1D-C2D	2.19	1.48	1.43
15	bB	1230	CL7	MG-NB	-2.19	2.01	2.05
15	bA	1120	CL7	C1D-C2D	2.19	1.48	1.43
15	cL	1501	CL7	MG-NB	-2.19	2.01	2.05
14	bA	1013	PHO	C4D-ND	-2.19	1.35	1.38
15	cA	1111	CL7	C1D-C2D	2.19	1.48	1.43
15	aA	1115	CL7	CMD-C2D	-2.19	1.46	1.50
15	aJ	1302	CL7	C1D-C2D	2.19	1.48	1.43
15	bA	1109	CL7	CMD-C2D	-2.19	1.46	1.50
14	aB	1023	PHO	C4D-ND	-2.19	1.35	1.38
15	bK	1401	CL7	C1D-C2D	2.19	1.48	1.43
15	cA	1136	CL7	MG-NB	-2.19	2.01	2.05
15	aA	1111	CL7	C1D-C2D	2.19	1.48	1.43
15	bF	1701	CL7	C1D-C2D	2.19	1.48	1.43
15	cB	1229	CL7	C1D-C2D	2.19	1.48	1.43
15	cJ	1301	CL7	C1D-C2D	2.19	1.48	1.43
15	bA	1130	CL7	MG-NB	-2.19	2.01	2.05
15	aB	1226	CL7	CMD-C2D	-2.19	1.46	1.50
15	bB	1216	CL7	C1D-C2D	2.18	1.48	1.43
17	cB	4006	A1JPJ	C19-C18	-2.18	1.41	1.45
15	bB	1226	CL7	C1D-C2D	2.18	1.48	1.43
15	bA	1104	CL7	CMB-C2B	-2.18	1.46	1.50
15	cB	1225	CL7	CMD-C2D	-2.18	1.46	1.50
15	bA	1801	CL7	C1D-C2D	2.18	1.48	1.43
15	aA	1120	CL7	MG-NB	-2.18	2.01	2.05
15	bA	1137	CL7	MG-NB	-2.18	2.01	2.05
15	cA	1128	CL7	CHC-C1C	2.18	1.42	1.38
15	aA	1138	CL7	MG-NB	-2.18	2.01	2.05
15	bB	1203	CL7	MG-NB	-2.18	2.01	2.05
15	cB	1228	CL7	C1D-C2D	2.18	1.48	1.43
15	bB	1012	CL7	MG-NB	-2.18	2.01	2.05
15	aB	1237	CL7	CMB-C2B	-2.18	1.46	1.50
17	aB	4006	A1JPJ	C19-C18	-2.18	1.41	1.45
15	bI	1601	CL7	CMC-C2C	-2.18	1.46	1.50
15	bA	1109	CL7	C1D-C2D	2.18	1.48	1.43
15	aB	1226	CL7	MG-NB	-2.18	2.01	2.05
15	cB	1230	CL7	C1D-C2D	2.18	1.48	1.43
15	bA	1136	CL7	MG-NB	-2.18	2.01	2.05
15	aA	1116	CL7	C1D-C2D	2.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aL	1502	CL7	CMB-C2B	-2.18	1.46	1.50
15	bL	1502	CL7	CMB-C2B	-2.18	1.46	1.50
15	aA	1130	CL7	C1D-C2D	2.18	1.48	1.43
15	bL	1502	CL7	MG-NB	-2.18	2.01	2.05
15	cB	1211	CL7	C1D-C2D	2.18	1.48	1.43
15	cA	1130	CL7	CMB-C2B	-2.18	1.46	1.50
17	bB	4010	A1JPJ	C11-C12	2.18	1.40	1.34
15	aA	1104	CL7	C1D-C2D	2.18	1.48	1.43
15	aA	1132	CL7	MG-NC	2.18	2.10	2.05
15	bB	1237	CL7	CMB-C2B	-2.18	1.46	1.50
15	aB	1234	CL7	MG-NB	-2.17	2.01	2.05
15	bA	1130	CL7	CMB-C2B	-2.17	1.46	1.50
15	cB	1237	CL7	CMB-C2B	-2.17	1.46	1.50
15	bB	1204	CL7	MG-NB	-2.17	2.01	2.05
15	cL	1503	CL7	CHC-C1C	2.17	1.42	1.38
15	bA	1140	CL7	C1D-C2D	2.17	1.48	1.43
15	bA	1119	CL7	MG-NB	-2.17	2.01	2.05
15	aA	1107	CL7	CMD-C2D	-2.17	1.46	1.50
15	cA	1113	CL7	C1D-C2D	2.17	1.48	1.43
15	aB	1238	CL7	CMD-C2D	-2.17	1.46	1.50
15	aB	1021	CL7	CMD-C2D	-2.17	1.46	1.50
15	cB	1218	CL7	C1D-C2D	2.17	1.48	1.43
15	cA	1104	CL7	C1D-C2D	2.17	1.48	1.43
15	aA	1109	CL7	C1D-C2D	2.17	1.48	1.43
15	bB	1021	CL7	CMC-C2C	-2.17	1.46	1.50
15	cB	1238	CL7	CMD-C2D	-2.17	1.46	1.50
15	bL	1502	CL7	C1D-C2D	2.17	1.48	1.43
14	aA	1013	PHO	C3B-C2B	-2.17	1.37	1.40
15	cB	1216	CL7	C1D-C2D	2.17	1.48	1.43
17	aA	4014	A1JPJ	C23-C22	-2.17	1.41	1.45
15	bA	1127	CL7	MG-NB	-2.17	2.01	2.05
15	aB	1228	CL7	C1D-C2D	2.17	1.48	1.43
15	cA	1118	CL7	C1D-C2D	2.17	1.48	1.43
15	aB	1207	CL7	MG-NB	-2.17	2.01	2.05
15	bB	1226	CL7	CHC-C1C	2.17	1.42	1.38
15	cA	1801	CL7	C1D-C2D	2.17	1.48	1.43
15	aA	1112	CL7	MG-NB	-2.17	2.01	2.05
15	aA	1801	CL7	MG-NB	-2.17	2.01	2.05
15	aA	1112	CL7	C1D-C2D	2.17	1.48	1.43
15	aB	1226	CL7	C1D-C2D	2.17	1.48	1.43
15	aL	1502	CL7	C1D-C2D	2.17	1.48	1.43
14	aA	1013	PHO	C4D-ND	-2.17	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1135	CL7	CMB-C2B	-2.17	1.46	1.50
15	cA	1103	CL7	CMB-C2B	-2.16	1.46	1.50
15	bB	1229	CL7	C1D-C2D	2.16	1.48	1.43
15	aA	1801	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1202	CL7	C1D-C2D	2.16	1.48	1.43
17	aB	4004	A1JPJ	C19-C18	-2.16	1.41	1.45
15	aA	1133	CL7	CMB-C2B	-2.16	1.46	1.50
15	aB	1204	CL7	CMD-C2D	-2.16	1.46	1.50
15	aA	1104	CL7	MG-NB	-2.16	2.01	2.05
15	aA	1106	CL7	MG-NB	-2.16	2.01	2.05
15	cA	1130	CL7	MG-NB	-2.16	2.01	2.05
15	aB	1214	CL7	CMB-C2B	-2.16	1.46	1.50
15	bB	1021	CL7	CMD-C2D	-2.16	1.46	1.50
15	bB	1237	CL7	MG-NB	-2.16	2.01	2.05
15	cA	1106	CL7	MG-NB	-2.16	2.01	2.05
15	aA	1108	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1216	CL7	C1D-C2D	2.16	1.48	1.43
17	aB	4004	A1JPJ	C12-C13	-2.16	1.41	1.45
15	bA	1132	CL7	MG-NB	-2.16	2.01	2.05
15	cB	1021	CL7	CMD-C2D	-2.16	1.46	1.50
15	bA	1117	CL7	MG-NB	-2.16	2.01	2.05
15	cB	1012	CL7	MG-NB	-2.16	2.01	2.05
17	bB	4006	A1JPJ	C19-C18	-2.16	1.41	1.45
15	aA	1121	CL7	C1D-C2D	2.16	1.48	1.43
15	cA	1101	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1236	CL7	MG-NB	-2.16	2.01	2.05
15	aA	1130	CL7	MG-NB	-2.16	2.01	2.05
15	aA	1130	CL7	CMB-C2B	-2.16	1.46	1.50
15	cA	1134	CL7	C1D-C2D	2.16	1.48	1.43
15	cA	1117	CL7	MG-NB	-2.16	2.01	2.05
15	bA	1118	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1203	CL7	MG-NB	-2.16	2.01	2.05
15	aA	1139	CL7	C1D-C2D	2.16	1.48	1.43
15	bA	1134	CL7	C1D-C2D	2.16	1.48	1.43
15	aA	1123	CL7	CMB-C2B	-2.16	1.46	1.50
15	cL	1502	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1226	CL7	CHC-C1C	2.16	1.42	1.38
15	cA	1124	CL7	C1D-C2D	2.16	1.48	1.43
15	aB	1012	CL7	MG-NB	-2.16	2.01	2.05
15	cB	1235	CL7	MG-NB	-2.16	2.01	2.05
15	aB	1231	CL7	CMB-C2B	-2.16	1.46	1.50
15	aA	1101	CL7	C1D-C2D	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1137	CL7	MG-NB	-2.16	2.01	2.05
15	bB	1226	CL7	MG-NB	-2.16	2.01	2.05
15	bA	1132	CL7	C1D-C2D	2.16	1.48	1.43
15	aA	1119	CL7	MG-NB	-2.15	2.01	2.05
15	bB	1202	CL7	MG-NB	-2.15	2.01	2.05
15	cA	1123	CL7	C1D-C2D	2.15	1.48	1.43
15	aB	1021	CL7	CMC-C2C	-2.15	1.46	1.50
15	bA	1136	CL7	C1D-C2D	2.15	1.48	1.43
15	aB	1234	CL7	C1D-C2D	2.15	1.48	1.43
15	cB	1203	CL7	MG-NB	-2.15	2.01	2.05
15	aB	1235	CL7	C1D-C2D	2.15	1.48	1.43
15	aA	1127	CL7	CMD-C2D	-2.15	1.46	1.50
15	aL	1503	CL7	CMB-C2B	-2.15	1.46	1.50
15	aB	1229	CL7	C1D-C2D	2.15	1.48	1.43
14	cA	1013	PHO	C3B-C2B	-2.15	1.37	1.40
15	bA	1121	CL7	C1D-C2D	2.15	1.48	1.43
15	cA	1130	CL7	C1D-C2D	2.15	1.48	1.43
15	bA	1131	CL7	CHC-C1C	2.15	1.42	1.38
15	bA	1127	CL7	CMB-C2B	-2.15	1.46	1.50
15	aA	1131	CL7	CHC-C1C	2.15	1.42	1.38
15	aA	1103	CL7	CMD-C2D	-2.15	1.46	1.50
15	aA	1125	CL7	CMC-C2C	-2.15	1.46	1.50
15	aB	1218	CL7	C1D-C2D	2.15	1.48	1.43
15	aA	1135	CL7	CMD-C2D	-2.15	1.46	1.50
15	bA	1117	CL7	C1D-C2D	2.15	1.48	1.43
15	aA	1119	CL7	CMB-C2B	-2.15	1.46	1.50
15	aB	1230	CL7	C1D-C2D	2.15	1.48	1.43
15	bA	1134	CL7	MG-NB	-2.15	2.01	2.05
15	bB	1234	CL7	C1D-C2D	2.15	1.48	1.43
15	cA	1112	CL7	C1D-C2D	2.15	1.48	1.43
15	cA	1127	CL7	CMB-C2B	-2.15	1.46	1.50
15	aA	1105	CL7	C1D-C2D	2.15	1.48	1.43
15	bA	1104	CL7	C1D-C2D	2.15	1.48	1.43
15	cA	1133	CL7	CMB-C2B	-2.15	1.46	1.50
15	cB	1202	CL7	C1D-C2D	2.15	1.48	1.43
15	cB	1213	CL7	C1D-C2D	2.15	1.48	1.43
15	bA	1123	CL7	C1D-C2D	2.15	1.48	1.43
15	cL	1503	CL7	MG-NB	-2.15	2.01	2.05
15	cA	1801	CL7	CMC-C2C	-2.15	1.46	1.50
15	bB	1225	CL7	C1D-C2D	2.14	1.48	1.43
15	cA	1123	CL7	MG-NB	-2.14	2.01	2.05
15	cA	1137	CL7	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1230	CL7	C1D-C2D	2.14	1.48	1.43
15	aA	1114	CL7	CMB-C2B	-2.14	1.46	1.50
15	cJ	1301	CL7	CMD-C2D	-2.14	1.46	1.50
15	cB	1021	CL7	CMC-C2C	-2.14	1.46	1.50
15	bA	1124	CL7	MG-NB	-2.14	2.01	2.05
17	bB	4004	A1JPJ	C19-C18	-2.14	1.41	1.45
15	aA	1118	CL7	C1D-C2D	2.14	1.48	1.43
15	bL	1503	CL7	C1D-C2D	2.14	1.48	1.43
15	cB	1238	CL7	C1D-C2D	2.14	1.48	1.43
15	bA	1135	CL7	CMD-C2D	-2.14	1.46	1.50
15	aB	1216	CL7	CMB-C2B	-2.14	1.46	1.50
15	aA	1134	CL7	C1D-C2D	2.14	1.48	1.43
15	cA	1120	CL7	C1D-C2D	2.14	1.48	1.43
15	bA	1103	CL7	MG-NB	-2.14	2.01	2.05
15	cA	1119	CL7	MG-NB	-2.14	2.01	2.05
15	cB	1222	CL7	MG-NB	-2.14	2.01	2.05
15	bA	1130	CL7	C1D-C2D	2.14	1.48	1.43
15	cA	1121	CL7	C1D-C2D	2.14	1.48	1.43
15	bB	1222	CL7	MG-NB	-2.14	2.01	2.05
15	cA	1112	CL7	MG-NB	-2.14	2.01	2.05
15	aB	1227	CL7	CMB-C2B	-2.14	1.46	1.50
15	aB	1212	CL7	C1D-C2D	2.14	1.48	1.43
17	aB	4010	A1JPJ	C11-C12	2.14	1.40	1.34
15	cB	1237	CL7	MG-NB	-2.14	2.01	2.05
15	aB	1201	CL7	C1D-C2D	2.14	1.48	1.43
15	aI	1601	CL7	CMC-C2C	-2.14	1.46	1.50
15	cA	1125	CL7	CMD-C2D	-2.14	1.46	1.50
15	aL	1503	CL7	MG-NB	-2.14	2.01	2.05
15	cA	1129	CL7	C1D-C2D	2.14	1.48	1.43
15	cA	1131	CL7	C1D-C2D	2.14	1.48	1.43
15	aB	1230	CL7	CMB-C2B	-2.14	1.46	1.50
15	aA	1124	CL7	C1D-C2D	2.14	1.48	1.43
15	aA	1138	CL7	C1D-C2D	2.14	1.48	1.43
15	aA	1140	CL7	C1D-C2D	2.14	1.48	1.43
15	aA	1117	CL7	MG-NB	-2.14	2.01	2.05
15	cB	1236	CL7	C1D-C2D	2.14	1.48	1.43
15	aB	1207	CL7	C1D-C2D	2.14	1.48	1.43
15	bA	1124	CL7	C1D-C2D	2.14	1.48	1.43
15	cB	1215	CL7	C4C-NC	2.14	1.40	1.37
15	aB	1205	CL7	CMD-C2D	-2.13	1.46	1.50
15	cA	1136	CL7	CMB-C2B	-2.13	1.46	1.50
15	bB	1212	CL7	C1D-C2D	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1237	CL7	MG-NB	-2.13	2.01	2.05
15	aB	1012	CL7	CMD-C2D	-2.13	1.46	1.50
15	bA	1132	CL7	CMB-C2B	-2.13	1.46	1.50
15	cB	1225	CL7	MG-NB	-2.13	2.01	2.05
15	cB	1236	CL7	MG-NB	-2.13	2.01	2.05
15	aB	1012	CL7	CMB-C2B	-2.13	1.46	1.50
15	bB	1239	CL7	MG-NB	-2.13	2.01	2.05
15	cB	1216	CL7	MG-NB	-2.13	2.01	2.05
15	aA	1122	CL7	CMC-C2C	-2.13	1.46	1.50
17	bB	4006	A1JPJ	C12-C13	-2.13	1.41	1.45
15	cB	1239	CL7	C1D-C2D	2.13	1.48	1.43
15	cA	1801	CL7	MG-NB	-2.13	2.01	2.05
15	bB	1234	CL7	CMB-C2B	-2.13	1.46	1.50
15	aA	1124	CL7	MG-NB	-2.13	2.01	2.05
15	cF	1701	CL7	CMD-C2D	-2.13	1.46	1.50
15	cB	1237	CL7	C1D-C2D	2.13	1.48	1.43
15	aB	1238	CL7	C1D-C2D	2.13	1.48	1.43
15	cB	1239	CL7	MG-NB	-2.13	2.01	2.05
15	cA	1138	CL7	CMB-C2B	-2.13	1.46	1.50
17	aB	4006	A1JPJ	C12-C13	-2.13	1.41	1.45
15	cB	1222	CL7	C1D-C2D	2.13	1.48	1.43
15	bB	1231	CL7	CMB-C2B	-2.13	1.46	1.50
15	cA	1140	CL7	C1D-C2D	2.13	1.48	1.43
15	aA	1123	CL7	CMD-C2D	-2.13	1.46	1.50
15	cA	1022	CL7	C1D-C2D	2.13	1.48	1.43
15	bB	1238	CL7	CMD-C2D	-2.13	1.46	1.50
15	cA	1124	CL7	MG-NB	-2.13	2.01	2.05
15	cA	1127	CL7	CMD-C2D	-2.13	1.46	1.50
15	aB	1215	CL7	C1D-C2D	2.13	1.48	1.43
15	aB	1222	CL7	C1D-C2D	2.13	1.48	1.43
15	aA	1123	CL7	MG-NB	-2.13	2.01	2.05
15	bA	1123	CL7	CMB-C2B	-2.13	1.46	1.50
15	bB	1205	CL7	CMD-C2D	-2.13	1.46	1.50
15	aB	1224	CL7	C1D-C2D	2.13	1.48	1.43
15	cA	1103	CL7	C1D-C2D	2.13	1.48	1.43
15	aA	1131	CL7	MG-NB	-2.13	2.01	2.05
14	cB	1023	PHO	C3B-CAB	-2.13	1.43	1.47
15	bA	1138	CL7	C1D-C2D	2.13	1.48	1.43
15	bB	1226	CL7	CMD-C2D	-2.13	1.46	1.50
15	bL	1502	CL7	CMD-C2D	-2.13	1.46	1.50
15	bA	1107	CL7	MG-NB	-2.13	2.01	2.05
15	bB	1215	CL7	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1107	CL7	MG-NB	-2.13	2.01	2.05
15	cA	1103	CL7	CMD-C2D	-2.12	1.46	1.50
15	bB	1218	CL7	C1D-C2D	2.12	1.48	1.43
15	cB	1205	CL7	CMC-C2C	-2.12	1.46	1.50
15	aA	1136	CL7	C1D-C2D	2.12	1.48	1.43
15	bA	1125	CL7	CMD-C2D	-2.12	1.46	1.50
15	bB	1237	CL7	C1D-C2D	2.12	1.48	1.43
15	cB	1227	CL7	MG-NB	-2.12	2.01	2.05
15	bA	1136	CL7	CMB-C2B	-2.12	1.46	1.50
15	cA	1136	CL7	C1D-C2D	2.12	1.48	1.43
15	bA	1106	CL7	C1D-C2D	2.12	1.48	1.43
15	cL	1502	CL7	CMD-C2D	-2.12	1.46	1.50
15	bA	1126	CL7	C4C-NC	2.12	1.40	1.37
15	bA	1123	CL7	MG-NB	-2.12	2.01	2.05
15	cA	1138	CL7	C1D-C2D	2.12	1.48	1.43
15	bA	1119	CL7	CMB-C2B	-2.12	1.46	1.50
15	bB	1237	CL7	CMD-C2D	-2.12	1.46	1.50
15	bL	1503	CL7	MG-NB	-2.12	2.01	2.05
15	bB	1225	CL7	CMB-C2B	-2.12	1.46	1.50
15	cA	1125	CL7	CMC-C2C	-2.12	1.46	1.50
15	cB	1237	CL7	CMD-C2D	-2.12	1.46	1.50
15	cB	1012	CL7	CMD-C2D	-2.12	1.46	1.50
15	cB	1021	CL7	CMB-C2B	-2.12	1.46	1.50
15	bA	1138	CL7	MG-NB	-2.12	2.01	2.05
15	bA	1801	CL7	MG-NB	-2.12	2.01	2.05
15	bB	1213	CL7	MG-NB	-2.12	2.01	2.05
15	bA	1103	CL7	CMD-C2D	-2.12	1.46	1.50
15	cA	1103	CL7	MG-NB	-2.12	2.01	2.05
15	aB	1238	CL7	MG-NB	-2.12	2.01	2.05
15	bB	1235	CL7	MG-NB	-2.12	2.01	2.05
15	cA	1140	CL7	MG-NB	-2.12	2.01	2.05
15	cB	1238	CL7	MG-NB	-2.12	2.01	2.05
15	aB	1225	CL7	MG-NB	-2.12	2.01	2.05
15	aA	1117	CL7	C1D-C2D	2.12	1.48	1.43
15	aB	1213	CL7	C1D-C2D	2.12	1.48	1.43
15	cB	1224	CL7	CMD-C2D	-2.12	1.46	1.50
17	cB	4010	A1JPJ	C11-C12	2.12	1.40	1.34
15	cA	1120	CL7	MG-NB	-2.12	2.01	2.05
15	cB	1202	CL7	MG-NB	-2.12	2.01	2.05
15	cB	1207	CL7	C1D-C2D	2.12	1.48	1.43
15	aA	1129	CL7	CMB-C2B	-2.12	1.46	1.50
15	cB	1214	CL7	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1131	CL7	MG-NB	-2.12	2.01	2.05
15	aB	1237	CL7	C1D-C2D	2.12	1.48	1.43
15	bA	1137	CL7	CMB-C2B	-2.12	1.46	1.50
15	bA	1131	CL7	C1D-C2D	2.12	1.48	1.43
15	cI	1601	CL7	CMC-C2C	-2.12	1.46	1.50
15	cA	1106	CL7	C1D-C2D	2.11	1.48	1.43
15	cB	1212	CL7	C1D-C2D	2.11	1.48	1.43
15	bB	1225	CL7	CMD-C2D	-2.11	1.46	1.50
15	bB	1235	CL7	C1D-C2D	2.11	1.48	1.43
15	bA	1133	CL7	CMB-C2B	-2.11	1.46	1.50
15	bA	1131	CL7	MG-NB	-2.11	2.01	2.05
15	bB	1214	CL7	MG-NB	-2.11	2.01	2.05
15	cB	1213	CL7	MG-NB	-2.11	2.01	2.05
15	aA	1022	CL7	C1D-C2D	2.11	1.48	1.43
15	cB	1205	CL7	C1D-C2D	2.11	1.48	1.43
15	bA	1106	CL7	MG-NB	-2.11	2.01	2.05
15	aB	1236	CL7	C1D-C2D	2.11	1.48	1.43
15	cA	1109	CL7	C1D-C2D	2.11	1.48	1.43
15	bL	1503	CL7	CMD-C2D	-2.11	1.46	1.50
15	cB	1012	CL7	CMB-C2B	-2.11	1.46	1.50
15	bB	1201	CL7	C1D-C2D	2.11	1.48	1.43
15	aB	1207	CL7	CMD-C2D	-2.11	1.46	1.50
15	cB	1207	CL7	CMD-C2D	-2.11	1.46	1.50
15	aA	1130	CL7	CMD-C2D	-2.11	1.46	1.50
15	bB	1213	CL7	C1D-C2D	2.11	1.48	1.43
15	aA	1124	CL7	CMD-C2D	-2.11	1.46	1.50
15	bB	1012	CL7	CMD-C2D	-2.11	1.46	1.50
15	bB	1222	CL7	C1D-C2D	2.11	1.48	1.43
15	cA	1129	CL7	MG-NB	-2.11	2.01	2.05
15	cB	1216	CL7	CMB-C2B	-2.11	1.46	1.50
15	cB	1230	CL7	CMD-C2D	-2.11	1.46	1.50
15	bA	1137	CL7	C1D-C2D	2.11	1.48	1.43
15	bB	1207	CL7	C1D-C2D	2.11	1.48	1.43
15	cB	1201	CL7	C1D-C2D	2.11	1.48	1.43
15	cA	1128	CL7	C1D-C2D	2.11	1.48	1.43
15	aB	1216	CL7	MG-NB	-2.11	2.01	2.05
15	cB	1214	CL7	MG-NB	-2.11	2.01	2.05
15	bB	1224	CL7	MG-NB	-2.11	2.01	2.05
15	aL	1502	CL7	CMD-C2D	-2.11	1.46	1.50
15	bA	1129	CL7	CMB-C2B	-2.11	1.46	1.50
15	bB	1236	CL7	MG-NB	-2.11	2.01	2.05
15	bA	1103	CL7	C1D-C2D	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1213	CL7	MG-NB	-2.11	2.01	2.05
15	bB	1205	CL7	C1D-C2D	2.11	1.48	1.43
15	bA	1801	CL7	CMC-C2C	-2.11	1.46	1.50
15	cA	1119	CL7	CMB-C2B	-2.11	1.46	1.50
15	aA	1124	CL7	CMB-C2B	-2.11	1.46	1.50
15	bB	1215	CL7	C1D-C2D	2.11	1.48	1.43
15	bA	1128	CL7	C1D-C2D	2.10	1.48	1.43
15	aA	1103	CL7	CMB-C2B	-2.10	1.46	1.50
15	aB	1205	CL7	CMC-C2C	-2.10	1.46	1.50
15	cB	1211	CL7	MG-NB	-2.10	2.01	2.05
15	bB	1238	CL7	C1D-C2D	2.10	1.48	1.43
14	bA	1013	PHO	C3B-C2B	-2.10	1.37	1.40
15	aB	1225	CL7	CMD-C2D	-2.10	1.46	1.50
15	cA	1137	CL7	C1D-C2D	2.10	1.48	1.43
15	bB	1207	CL7	CMB-C2B	-2.10	1.46	1.50
15	cA	1111	CL7	CMD-C2D	-2.10	1.46	1.50
15	bB	1238	CL7	MG-NB	-2.10	2.01	2.05
15	bB	1238	CL7	CMB-C2B	-2.10	1.46	1.50
15	aL	1503	CL7	C1D-C2D	2.10	1.48	1.43
15	aA	1022	CL7	CMD-C2D	-2.10	1.46	1.50
15	bA	1140	CL7	CMB-C2B	-2.10	1.46	1.50
15	cA	1116	CL7	CMB-C2B	-2.10	1.46	1.50
15	aB	1239	CL7	C1D-C2D	2.10	1.48	1.43
15	cB	1223	CL7	MG-NB	-2.10	2.01	2.05
15	bB	1221	CL7	CMB-C2B	-2.10	1.46	1.50
15	bB	1203	CL7	C1D-C2D	2.10	1.48	1.43
15	cA	1126	CL7	C1D-C2D	2.10	1.48	1.43
15	aA	1109	CL7	CMD-C2D	-2.10	1.46	1.50
15	aA	1116	CL7	CMB-C2B	-2.10	1.46	1.50
15	aB	1205	CL7	C1D-C2D	2.10	1.48	1.43
15	bA	1112	CL7	CMD-C2D	-2.10	1.46	1.50
15	bB	1230	CL7	CMB-C2B	-2.10	1.46	1.50
15	cB	1241	CL7	MG-NB	-2.10	2.01	2.05
15	aA	1106	CL7	C1D-C2D	2.10	1.48	1.43
15	aA	1128	CL7	C1D-C2D	2.10	1.48	1.43
15	bB	1207	CL7	CMD-C2D	-2.10	1.46	1.50
15	aB	1237	CL7	CMD-C2D	-2.10	1.46	1.50
15	cA	1112	CL7	CMD-C2D	-2.10	1.46	1.50
15	cB	1202	CL7	CMB-C2B	-2.10	1.46	1.50
15	bA	1114	CL7	CMB-C2B	-2.10	1.46	1.50
15	cA	1132	CL7	CMB-C2B	-2.10	1.46	1.50
15	cB	1225	CL7	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1107	CL7	MG-NB	-2.10	2.01	2.05
15	bA	1102	CL7	MG-NB	-2.10	2.01	2.05
15	cA	1132	CL7	C1D-C2D	2.10	1.48	1.43
15	aA	1134	CL7	MG-NB	-2.10	2.01	2.05
15	bB	1205	CL7	CMC-C2C	-2.10	1.46	1.50
15	aB	1207	CL7	CMB-C2B	-2.10	1.46	1.50
15	aB	1210	CL7	MG-NB	-2.10	2.01	2.05
15	cA	1127	CL7	C1D-C2D	2.10	1.48	1.43
15	bB	1202	CL7	C1D-C2D	2.09	1.48	1.43
15	aA	1126	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1235	CL7	MG-NB	-2.09	2.01	2.05
15	aA	1106	CL7	CMC-C2C	-2.09	1.46	1.50
15	bA	1123	CL7	CMD-C2D	-2.09	1.46	1.50
15	aA	1135	CL7	C1D-C2D	2.09	1.48	1.43
15	bB	1221	CL7	C1D-C2D	2.09	1.48	1.43
15	cB	1201	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1220	CL7	CMC-C2C	-2.09	1.46	1.50
15	aB	1224	CL7	CMB-C2B	-2.09	1.46	1.50
15	cA	1138	CL7	CMD-C2D	-2.09	1.46	1.50
15	cB	1238	CL7	CMB-C2B	-2.09	1.46	1.50
15	cB	1225	CL7	C1D-C2D	2.09	1.48	1.43
15	aA	1125	CL7	MG-NB	-2.09	2.01	2.05
15	aA	1138	CL7	CMB-C2B	-2.09	1.46	1.50
15	aJ	1301	CL7	CMD-C2D	-2.09	1.46	1.50
15	bF	1701	CL7	CMD-C2D	-2.09	1.46	1.50
15	aA	1125	CL7	CMD-C2D	-2.09	1.46	1.50
15	bA	1120	CL7	MG-NB	-2.09	2.01	2.05
15	bA	1138	CL7	CMB-C2B	-2.09	1.46	1.50
15	aB	1239	CL7	CMD-C2D	-2.09	1.46	1.50
15	aL	1503	CL7	CMD-C2D	-2.09	1.46	1.50
17	cB	4006	A1JPJ	C12-C13	-2.09	1.41	1.45
15	bB	1225	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1203	CL7	C1D-C2D	2.09	1.48	1.43
15	aA	1126	CL7	CMB-C2B	-2.09	1.46	1.50
15	aA	1127	CL7	CMB-C2B	-2.09	1.46	1.50
15	aB	1224	CL7	MG-NB	-2.09	2.01	2.05
15	aA	1126	CL7	C1D-C2D	2.09	1.48	1.43
15	aA	1103	CL7	MG-NB	-2.09	2.01	2.05
15	aA	1121	CL7	MG-NB	-2.09	2.01	2.05
15	cA	1022	CL7	CMD-C2D	-2.09	1.46	1.50
15	aB	1202	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1202	CL7	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cL	1503	CL7	CMD-C2D	-2.09	1.46	1.50
15	bB	1012	CL7	CMB-C2B	-2.09	1.46	1.50
15	cB	1207	CL7	CMB-C2B	-2.09	1.46	1.50
15	aA	1107	CL7	C1D-C2D	2.09	1.48	1.43
15	aB	1221	CL7	C1D-C2D	2.09	1.48	1.43
15	cL	1501	CL7	C1D-C2D	2.09	1.48	1.43
15	cB	1234	CL7	C1D-C2D	2.09	1.48	1.43
15	cK	1402	CL7	CBD-CAD	2.09	1.56	1.51
15	aB	1239	CL7	MG-NB	-2.09	2.01	2.05
15	bA	1112	CL7	MG-NB	-2.09	2.01	2.05
15	cA	1114	CL7	CMB-C2B	-2.09	1.46	1.50
15	cA	1110	CL7	C1D-C2D	2.09	1.48	1.43
15	bA	1122	CL7	CMC-C2C	-2.09	1.46	1.50
15	cA	1123	CL7	CMD-C2D	-2.09	1.46	1.50
15	aB	1220	CL7	MG-NB	-2.09	2.01	2.05
15	cA	1136	CL7	CMD-C2D	-2.09	1.46	1.50
15	cB	1224	CL7	C1D-C2D	2.09	1.48	1.43
15	aA	1128	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1201	CL7	CMC-C2C	-2.09	1.46	1.50
15	cA	1104	CL7	CMB-C2B	-2.09	1.46	1.50
15	cA	1128	CL7	MG-NB	-2.09	2.01	2.05
15	aB	1234	CL7	CMB-C2B	-2.08	1.46	1.50
15	cA	1112	CL7	CMB-C2B	-2.08	1.46	1.50
15	cA	1115	CL7	MG-NB	-2.08	2.01	2.05
15	bB	1224	CL7	C1D-C2D	2.08	1.48	1.43
15	cB	1235	CL7	C1D-C2D	2.08	1.48	1.43
15	aB	1238	CL7	CMB-C2B	-2.08	1.46	1.50
15	bA	1106	CL7	CMC-C2C	-2.08	1.46	1.50
15	bB	1211	CL7	CMB-C2B	-2.08	1.46	1.50
15	bA	1111	CL7	MG-NB	-2.08	2.01	2.05
15	bB	1216	CL7	MG-NB	-2.08	2.01	2.05
15	cA	1134	CL7	MG-NB	-2.08	2.01	2.05
15	aA	1127	CL7	C1D-C2D	2.08	1.48	1.43
15	aB	1225	CL7	C1D-C2D	2.08	1.48	1.43
15	cA	1132	CL7	CMD-C2D	-2.08	1.46	1.50
15	cB	1205	CL7	CMD-C2D	-2.08	1.46	1.50
15	cB	1221	CL7	CMB-C2B	-2.08	1.46	1.50
15	aK	1402	CL7	CHC-C1C	2.08	1.42	1.38
15	aA	1132	CL7	CMB-C2B	-2.08	1.46	1.50
15	aA	1133	CL7	MG-NB	-2.08	2.01	2.05
15	aB	1227	CL7	MG-NB	-2.08	2.01	2.05
15	cA	1105	CL7	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1106	CL7	CMD-C2D	-2.08	1.46	1.50
15	bB	1021	CL7	CMB-C2B	-2.08	1.46	1.50
15	aA	1129	CL7	MG-NB	-2.08	2.01	2.05
15	cA	1116	CL7	MG-NB	-2.08	2.01	2.05
15	aA	1140	CL7	MG-NB	-2.08	2.01	2.05
15	aA	1118	CL7	CMB-C2B	-2.08	1.46	1.50
15	aA	1132	CL7	CMD-C2D	-2.08	1.46	1.50
15	aA	1137	CL7	CMD-C2D	-2.08	1.46	1.50
15	aB	1232	CL7	CMB-C2B	-2.08	1.46	1.50
15	bA	1124	CL7	CMB-C2B	-2.08	1.46	1.50
15	aA	1123	CL7	C1D-C2D	2.08	1.48	1.43
15	bA	1121	CL7	MG-NB	-2.08	2.01	2.05
15	bA	1124	CL7	CMD-C2D	-2.08	1.46	1.50
15	cA	1111	CL7	MG-NB	-2.08	2.01	2.05
15	aA	1110	CL7	C1D-C2D	2.08	1.48	1.43
15	aB	1222	CL7	MG-NB	-2.08	2.01	2.05
15	aA	1132	CL7	C1D-C2D	2.08	1.48	1.43
15	aA	1112	CL7	CMB-C2B	-2.08	1.46	1.50
15	cA	1106	CL7	CMC-C2C	-2.08	1.46	1.50
15	cL	1501	CL7	CMD-C2D	-2.08	1.46	1.50
15	aB	1203	CL7	CMB-C2B	-2.08	1.46	1.50
15	cB	1211	CL7	CMB-C2B	-2.08	1.46	1.50
15	aB	1233	CL7	MG-NB	-2.08	2.01	2.05
15	cA	1124	CL7	CMB-C2B	-2.08	1.46	1.50
15	cB	1203	CL7	CMD-C2D	-2.08	1.46	1.50
15	cB	1230	CL7	CMB-C2B	-2.08	1.46	1.50
15	aA	1116	CL7	MG-NB	-2.08	2.01	2.05
15	aL	1501	CL7	C1D-C2D	2.08	1.48	1.43
15	bB	1236	CL7	C1D-C2D	2.08	1.48	1.43
15	bB	1202	CL7	CMD-C2D	-2.08	1.46	1.50
15	cB	1222	CL7	CMD-C2D	-2.08	1.46	1.50
15	aB	1220	CL7	C1D-C2D	2.08	1.48	1.43
15	aI	1601	CL7	C1D-C2D	2.08	1.48	1.43
15	aA	1107	CL7	CMB-C2B	-2.08	1.46	1.50
15	bB	1202	CL7	CMB-C2B	-2.08	1.46	1.50
15	cB	1234	CL7	CMB-C2B	-2.08	1.46	1.50
15	aB	1201	CL7	MG-NB	-2.08	2.01	2.05
15	aF	1701	CL7	CMD-C2D	-2.08	1.46	1.50
15	bB	1201	CL7	CMC-C2C	-2.08	1.46	1.50
15	cA	1131	CL7	CMD-C2D	-2.08	1.46	1.50
15	bA	1110	CL7	C1D-C2D	2.08	1.48	1.43
15	bA	1138	CL7	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aL	1501	CL7	CMD-C2D	-2.08	1.46	1.50
15	bA	1106	CL7	CMB-C2B	-2.08	1.46	1.50
15	bB	1222	CL7	CMD-C2D	-2.08	1.46	1.50
15	cA	1128	CL7	CMD-C2D	-2.08	1.46	1.50
15	aA	1137	CL7	C1D-C2D	2.08	1.48	1.43
15	aA	1132	CL7	MG-NB	-2.08	2.01	2.05
15	bB	1021	CL7	MG-NB	-2.08	2.01	2.05
15	bB	1201	CL7	MG-NB	-2.08	2.01	2.05
15	bA	1022	CL7	C1D-C2D	2.07	1.48	1.43
15	bA	1121	CL7	CMD-C2D	-2.07	1.46	1.50
15	bB	1223	CL7	MG-NB	-2.07	2.01	2.05
15	cA	1109	CL7	CMD-C2D	-2.07	1.46	1.50
15	bB	1239	CL7	C1D-C2D	2.07	1.48	1.43
15	aB	1208	CL7	MG-NB	-2.07	2.01	2.05
15	bA	1118	CL7	CMB-C2B	-2.07	1.46	1.50
15	cA	1129	CL7	CMB-C2B	-2.07	1.46	1.50
15	bA	1116	CL7	C1D-C2D	2.07	1.48	1.43
15	cA	1132	CL7	MG-NB	-2.07	2.01	2.05
15	aA	1110	CL7	MG-NB	-2.07	2.01	2.05
15	aB	1204	CL7	MG-NB	-2.07	2.01	2.05
15	cB	1204	CL7	CMB-C2B	-2.07	1.46	1.50
15	cB	1235	CL7	CMD-C2D	-2.07	1.46	1.50
15	bB	1220	CL7	MG-NB	-2.07	2.01	2.05
15	bA	1128	CL7	CMD-C2D	-2.07	1.46	1.50
15	aK	1401	CL7	MG-NB	-2.07	2.01	2.05
15	cA	1110	CL7	MG-NB	-2.07	2.01	2.05
15	cB	1220	CL7	MG-NB	-2.07	2.01	2.05
15	cB	1223	CL7	CMB-C2B	-2.07	1.46	1.50
15	cB	1235	CL7	CMB-C2B	-2.07	1.46	1.50
15	bI	1601	CL7	MG-NB	-2.07	2.01	2.05
15	cB	1208	CL7	MG-NB	-2.07	2.01	2.05
15	aB	1231	CL7	CMD-C2D	-2.07	1.46	1.50
15	cB	1231	CL7	CMB-C2B	-2.07	1.46	1.50
15	aB	1211	CL7	CMB-C2B	-2.07	1.46	1.50
15	cA	1119	CL7	CMD-C2D	-2.07	1.46	1.50
15	aB	1225	CL7	CMB-C2B	-2.07	1.46	1.50
15	bA	1138	CL7	CMD-C2D	-2.07	1.46	1.50
15	cB	1222	CL7	CMB-C2B	-2.07	1.46	1.50
15	bA	1125	CL7	MG-NB	-2.07	2.01	2.05
15	bA	1135	CL7	C1D-C2D	2.07	1.48	1.43
15	bB	1239	CL7	CMD-C2D	-2.07	1.46	1.50
15	aB	1204	CL7	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1239	CL7	CMB-C2B	-2.07	1.46	1.50
15	cB	1228	CL7	CMB-C2B	-2.07	1.46	1.50
15	cA	1126	CL7	MG-NB	-2.07	2.01	2.05
15	aA	1122	CL7	CMB-C2B	-2.07	1.46	1.50
15	aA	1136	CL7	CMD-C2D	-2.07	1.46	1.50
15	bB	1232	CL7	CMD-C2D	-2.07	1.46	1.50
15	aA	1138	CL7	CHC-C1C	2.07	1.42	1.38
15	aB	1229	CL7	MG-NB	-2.07	2.01	2.05
15	aA	1125	CL7	CMB-C2B	-2.07	1.46	1.50
15	aB	1223	CL7	C1D-C2D	2.07	1.48	1.43
15	bA	1101	CL7	C1D-C2D	2.07	1.48	1.43
15	cL	1503	CL7	C1D-C2D	2.07	1.48	1.43
15	bB	1236	CL7	CMD-C2D	-2.07	1.46	1.50
15	cA	1124	CL7	CMD-C2D	-2.07	1.46	1.50
15	cB	1227	CL7	CMB-C2B	-2.07	1.46	1.50
15	aA	1118	CL7	CMD-C2D	-2.07	1.46	1.50
15	bA	1105	CL7	CMD-C2D	-2.07	1.46	1.50
15	aA	1104	CL7	CMB-C2B	-2.07	1.46	1.50
15	aA	1120	CL7	CMB-C2B	-2.07	1.46	1.50
15	cA	1126	CL7	CMB-C2B	-2.07	1.46	1.50
15	cB	1202	CL7	CMD-C2D	-2.07	1.46	1.50
15	bA	1122	CL7	MG-NB	-2.07	2.01	2.05
15	bA	1110	CL7	MG-NB	-2.07	2.01	2.05
15	cA	1121	CL7	CMD-C2D	-2.07	1.46	1.50
15	aB	1228	CL7	MG-NB	-2.06	2.01	2.05
15	cA	1121	CL7	MG-NB	-2.06	2.01	2.05
15	aB	1229	CL7	CMB-C2B	-2.06	1.46	1.50
15	bB	1224	CL7	CMB-C2B	-2.06	1.46	1.50
15	cA	1113	CL7	CMB-C2B	-2.06	1.46	1.50
15	cA	1102	CL7	MG-NB	-2.06	2.01	2.05
15	cB	1021	CL7	MG-NB	-2.06	2.01	2.05
15	aB	1223	CL7	CMB-C2B	-2.06	1.46	1.50
15	aB	1210	CL7	CMD-C2D	-2.06	1.46	1.50
15	aB	1235	CL7	CMB-C2B	-2.06	1.46	1.50
15	bB	1215	CL7	CMB-C2B	-2.06	1.46	1.50
15	cA	1105	CL7	CMD-C2D	-2.06	1.46	1.50
15	cA	1125	CL7	CMB-C2B	-2.06	1.46	1.50
15	bA	1140	CL7	MG-NB	-2.06	2.01	2.05
15	bB	1229	CL7	CMB-C2B	-2.06	1.46	1.50
15	aA	1102	CL7	MG-NB	-2.06	2.01	2.05
15	bB	1206	CL7	CMD-C2D	-2.06	1.46	1.50
15	bB	1208	CL7	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1223	CL7	CMB-C2B	-2.06	1.46	1.50
15	bB	1223	CL7	CMD-C2D	-2.06	1.46	1.50
15	bB	1224	CL7	CMD-C2D	-2.06	1.46	1.50
15	bA	1129	CL7	MG-NB	-2.06	2.01	2.05
15	cB	1205	CL7	MG-NB	-2.06	2.01	2.05
15	bB	1214	CL7	CMD-C2D	-2.06	1.46	1.50
15	aA	1103	CL7	C1D-C2D	2.06	1.48	1.43
15	bA	1112	CL7	CMB-C2B	-2.06	1.46	1.50
15	cB	1232	CL7	CMB-C2B	-2.06	1.46	1.50
15	cA	1122	CL7	MG-NB	-2.06	2.01	2.05
15	aA	1140	CL7	CMB-C2B	-2.06	1.46	1.50
15	aB	1202	CL7	CMB-C2B	-2.06	1.46	1.50
15	bA	1131	CL7	CMD-C2D	-2.06	1.46	1.50
15	cA	1108	CL7	CMD-C2D	-2.06	1.46	1.50
15	aA	1135	CL7	CMB-C2B	-2.06	1.46	1.50
15	cA	1118	CL7	CMB-C2B	-2.06	1.46	1.50
15	aB	1222	CL7	CMD-C2D	-2.06	1.46	1.50
15	aB	1223	CL7	MG-NB	-2.06	2.01	2.05
15	aB	1208	CL7	CMB-C2B	-2.06	1.46	1.50
15	cB	1212	CL7	CMB-C2B	-2.06	1.46	1.50
15	aA	1111	CL7	MG-NB	-2.06	2.01	2.05
15	bB	1231	CL7	CMD-C2D	-2.06	1.46	1.50
15	aB	1012	CL7	C1D-C2D	2.06	1.48	1.43
15	aB	1021	CL7	CMB-C2B	-2.06	1.46	1.50
15	aB	1228	CL7	CMB-C2B	-2.06	1.46	1.50
15	bL	1501	CL7	CMD-C2D	-2.06	1.46	1.50
15	cB	1239	CL7	CMB-C2B	-2.06	1.46	1.50
15	aB	1224	CL7	CMD-C2D	-2.06	1.46	1.50
15	cA	1135	CL7	MG-ND	-2.06	2.01	2.05
15	bB	1235	CL7	CMD-C2D	-2.06	1.46	1.50
15	bK	1402	CL7	CBD-CAD	2.06	1.56	1.51
15	aA	1137	CL7	CMB-C2B	-2.06	1.46	1.50
15	bA	1116	CL7	CMB-C2B	-2.06	1.46	1.50
15	aA	1108	CL7	MG-NB	-2.06	2.01	2.05
15	cB	1228	CL7	MG-NB	-2.06	2.01	2.05
15	aB	1205	CL7	CMB-C2B	-2.06	1.46	1.50
15	cB	1205	CL7	CMB-C2B	-2.06	1.46	1.50
15	cB	1206	CL7	CMD-C2D	-2.06	1.46	1.50
15	cB	1224	CL7	CMB-C2B	-2.06	1.46	1.50
15	bA	1109	CL7	MG-NB	-2.06	2.01	2.05
15	bB	1210	CL7	CMD-C2D	-2.05	1.46	1.50
15	bB	1228	CL7	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1012	CL7	C1D-C2D	2.05	1.48	1.43
15	cB	1239	CL7	CMD-C2D	-2.05	1.46	1.50
15	bB	1241	CL7	MG-NB	-2.05	2.01	2.05
15	aB	1234	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1137	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1204	CL7	CMD-C2D	-2.05	1.46	1.50
15	aB	1235	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1111	CL7	CMB-C2B	-2.05	1.46	1.50
15	bA	1135	CL7	CMB-C2B	-2.05	1.46	1.50
15	bA	1113	CL7	CMD-C2D	-2.05	1.46	1.50
15	cA	1130	CL7	CMD-C2D	-2.05	1.46	1.50
15	aB	1206	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1107	CL7	CMB-C2B	-2.05	1.46	1.50
15	cA	1107	CL7	C1D-C2D	2.05	1.48	1.43
15	bA	1101	CL7	MG-NB	-2.05	2.01	2.05
15	cB	1204	CL7	MG-NB	-2.05	2.01	2.05
15	aB	1215	CL7	CMB-C2B	-2.05	1.46	1.50
15	cB	1201	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1236	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1101	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1108	CL7	CMD-C2D	-2.05	1.46	1.50
15	bB	1201	CL7	CMD-C2D	-2.05	1.46	1.50
15	cA	1106	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1220	CL7	CMD-C2D	-2.05	1.46	1.50
15	cA	1138	CL7	CHC-C1C	2.05	1.42	1.38
15	aA	1106	CL7	CMB-C2B	-2.05	1.46	1.50
15	cB	1229	CL7	CMB-C2B	-2.05	1.46	1.50
15	cA	1137	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1203	CL7	C1D-C2D	2.05	1.48	1.43
15	aA	1131	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1106	CL7	CMD-C2D	-2.05	1.46	1.50
15	aA	1131	CL7	C1D-C2D	2.05	1.48	1.43
15	aB	1211	CL7	MG-NB	-2.05	2.01	2.05
15	aA	1121	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1130	CL7	CMD-C2D	-2.05	1.46	1.50
15	cA	1106	CL7	CMB-C2B	-2.05	1.46	1.50
15	cA	1133	CL7	MG-NB	-2.05	2.01	2.05
15	bA	1132	CL7	CMD-C2D	-2.05	1.46	1.50
15	bB	1232	CL7	CMB-C2B	-2.05	1.46	1.50
15	bA	1107	CL7	C1D-C2D	2.05	1.48	1.43
15	aB	1213	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1127	CL7	C1D-C2D	2.05	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	1140	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1204	CL7	C2A-C1A	2.05	1.53	1.50
15	bB	1234	CL7	CMD-C2D	-2.05	1.46	1.50
15	cA	1801	CL7	CMB-C2B	-2.05	1.46	1.50
15	cA	1116	CL7	C1D-C2D	2.05	1.48	1.43
13	cA	1011	G9R	C3B-C2B	-2.05	1.37	1.40
15	bA	1136	CL7	CMD-C2D	-2.05	1.46	1.50
15	cB	1012	CL7	C1D-C2D	2.05	1.48	1.43
15	bB	1218	CL7	MG-NB	-2.05	2.01	2.05
15	bK	1401	CL7	MG-NB	-2.05	2.01	2.05
15	bA	1113	CL7	CMB-C2B	-2.05	1.46	1.50
15	bB	1230	CL7	CMD-C2D	-2.05	1.46	1.50
15	bB	1211	CL7	MG-NB	-2.05	2.01	2.05
15	aB	1239	CL7	CMB-C2B	-2.05	1.46	1.50
15	aB	1210	CL7	CMB-C2B	-2.05	1.46	1.50
15	aB	1214	CL7	CMD-C2D	-2.05	1.46	1.50
15	aA	1120	CL7	CMD-C2D	-2.05	1.46	1.50
15	bA	1134	CL7	CMB-C2B	-2.05	1.46	1.50
15	bA	1108	CL7	MG-NB	-2.04	2.01	2.05
15	cB	1204	CL7	C1D-C2D	2.04	1.48	1.43
15	cB	1226	CL7	C1D-C2D	2.04	1.48	1.43
15	bB	1227	CL7	C1B-C2B	2.04	1.48	1.43
15	aB	1214	CL7	MG-NB	-2.04	2.01	2.05
15	aB	1241	CL7	MG-NB	-2.04	2.01	2.05
15	aB	1215	CL7	CMC-C2C	-2.04	1.46	1.50
15	aB	1230	CL7	CMD-C2D	-2.04	1.46	1.50
15	bB	1205	CL7	CMB-C2B	-2.04	1.46	1.50
15	cB	1229	CL7	MG-NB	-2.04	2.01	2.05
15	aB	1212	CL7	CMD-C2D	-2.04	1.46	1.50
15	cA	1140	CL7	CMB-C2B	-2.04	1.46	1.50
15	aA	1108	CL7	CMD-C2D	-2.04	1.46	1.50
15	cB	1212	CL7	CMD-C2D	-2.04	1.46	1.50
15	bA	1127	CL7	CMD-C2D	-2.04	1.46	1.50
15	aB	1237	CL7	CMC-C2C	-2.04	1.46	1.50
15	cB	1210	CL7	CMD-C2D	-2.04	1.46	1.50
15	bB	1208	CL7	MG-NB	-2.04	2.01	2.05
15	bB	1229	CL7	MG-NB	-2.04	2.01	2.05
15	cA	1125	CL7	MG-NB	-2.04	2.01	2.05
15	cA	1134	CL7	CMB-C2B	-2.04	1.46	1.50
15	cA	1137	CL7	CMB-C2B	-2.04	1.46	1.50
15	cB	1203	CL7	CMB-C2B	-2.04	1.46	1.50
15	aB	1231	CL7	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	1133	CL7	MG-NB	-2.04	2.01	2.05
15	bA	1125	CL7	C1D-C2D	2.04	1.48	1.43
13	aA	1011	G9R	C3B-C2B	-2.04	1.37	1.40
15	aB	1236	CL7	CMB-C2B	-2.04	1.46	1.50
15	aI	1601	CL7	CMD-C2D	-2.04	1.46	1.50
15	cA	1122	CL7	CMB-C2B	-2.04	1.46	1.50
15	cB	1201	CL7	CMC-C2C	-2.04	1.46	1.50
15	cB	1223	CL7	CMD-C2D	-2.04	1.46	1.50
15	aA	1111	CL7	CMB-C2B	-2.04	1.46	1.50
15	aA	1112	CL7	CMD-C2D	-2.04	1.46	1.50
15	aA	1104	CL7	CMD-C2D	-2.04	1.46	1.50
15	bA	1128	CL7	MG-NB	-2.04	2.01	2.05
15	bA	1139	CL7	MG-NB	-2.04	2.01	2.05
15	bB	1231	CL7	MG-NB	-2.04	2.01	2.05
15	aB	1203	CL7	CMD-C2D	-2.04	1.46	1.50
15	bA	1022	CL7	CMD-C2D	-2.04	1.46	1.50
15	cA	1104	CL7	CMD-C2D	-2.04	1.46	1.50
15	cA	1110	CL7	CMB-C2B	-2.04	1.46	1.50
15	cA	1115	CL7	CMB-C2B	-2.04	1.46	1.50
15	bB	1212	CL7	MG-NB	-2.04	2.01	2.05
15	aA	1105	CL7	CMD-C2D	-2.04	1.46	1.50
15	bA	1801	CL7	CMB-C2B	-2.04	1.46	1.50
15	bA	1117	CL7	CMD-C2D	-2.04	1.46	1.50
15	bB	1223	CL7	CMC-C2C	-2.04	1.46	1.50
15	aA	1105	CL7	CMB-C2B	-2.04	1.46	1.50
15	bB	1235	CL7	CMB-C2B	-2.04	1.46	1.50
15	cA	1107	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1116	CL7	CMD-C2D	-2.03	1.46	1.50
15	cB	1223	CL7	C1D-C2D	2.03	1.48	1.43
15	cA	1114	CL7	CMD-C2D	-2.03	1.46	1.50
15	bB	1204	CL7	CMB-C2B	-2.03	1.46	1.50
15	bB	1223	CL7	C1D-C2D	2.03	1.48	1.43
15	bA	1116	CL7	CMD-C2D	-2.03	1.46	1.50
15	bA	1127	CL7	CMC-C2C	-2.03	1.46	1.50
15	bB	1215	CL7	CMD-C2D	-2.03	1.46	1.50
15	bI	1601	CL7	CMD-C2D	-2.03	1.46	1.50
15	aF	1701	CL7	MG-NB	-2.03	2.01	2.05
15	bF	1701	CL7	MG-NB	-2.03	2.01	2.05
15	aB	1212	CL7	CMB-C2B	-2.03	1.46	1.50
15	aB	1213	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1139	CL7	CMB-C2B	-2.03	1.46	1.50
15	cB	1231	CL7	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1204	CL7	C2A-C1A	2.03	1.53	1.50
15	bJ	1301	CL7	CMD-C2D	-2.03	1.46	1.50
15	aA	1109	CL7	CMB-C2B	-2.03	1.46	1.50
15	bB	1237	CL7	CMC-C2C	-2.03	1.46	1.50
14	aA	1013	PHO	C3B-CAB	-2.03	1.43	1.47
15	bA	1110	CL7	CMB-C2B	-2.03	1.46	1.50
15	bB	1209	CL7	MG-NB	-2.03	2.01	2.05
15	aA	1119	CL7	CMD-C2D	-2.03	1.46	1.50
15	aB	1215	CL7	CMD-C2D	-2.03	1.46	1.50
15	cB	1214	CL7	CMD-C2D	-2.03	1.46	1.50
15	aA	1114	CL7	CMD-C2D	-2.03	1.46	1.50
15	bB	1222	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1129	CL7	CMD-C2D	-2.03	1.46	1.50
15	cB	1201	CL7	CMB-C2B	-2.03	1.46	1.50
15	bA	1114	CL7	CMD-C2D	-2.03	1.46	1.50
15	bB	1203	CL7	CMB-C2B	-2.03	1.46	1.50
15	aA	1115	CL7	C1D-C2D	2.03	1.48	1.43
15	cB	1224	CL7	MG-NB	-2.03	2.01	2.05
15	aA	1128	CL7	CMD-C2D	-2.03	1.46	1.50
15	cA	1108	CL7	MG-NB	-2.03	2.01	2.05
15	bA	1140	CL7	CMD-C2D	-2.03	1.46	1.50
15	aA	1115	CL7	CMB-C2B	-2.03	1.46	1.50
15	aK	1401	CL7	CMB-C2B	-2.03	1.46	1.50
15	bA	1125	CL7	CMC-C2C	-2.03	1.46	1.50
15	bB	1213	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1117	CL7	CMD-C2D	-2.03	1.46	1.50
15	cA	1134	CL7	CMD-C2D	-2.03	1.46	1.50
15	cB	1208	CL7	CMB-C2B	-2.03	1.46	1.50
15	bA	1105	CL7	CMB-C2B	-2.03	1.46	1.50
15	cB	1237	CL7	CMC-C2C	-2.03	1.46	1.50
15	bB	1232	CL7	MG-NB	-2.03	2.01	2.05
15	bA	1115	CL7	CMB-C2B	-2.03	1.46	1.50
15	bB	1241	CL7	CMB-C2B	-2.03	1.46	1.50
15	cB	1221	CL7	C1D-C2D	2.03	1.48	1.43
15	aB	1220	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1111	CL7	CMB-C2B	-2.03	1.46	1.50
15	cA	1140	CL7	CMD-C2D	-2.03	1.46	1.50
15	bB	1202	CL7	CMC-C2C	-2.03	1.46	1.50
15	cA	1126	CL7	CMD-C2D	-2.02	1.46	1.50
15	cB	1216	CL7	CMD-C2D	-2.02	1.46	1.50
15	aA	1105	CL7	MG-NB	-2.02	2.01	2.05
15	aK	1402	CL7	CBD-CAD	2.02	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	1206	CL7	C1D-C2D	2.02	1.48	1.43
15	aA	1119	CL7	CMC-C2C	-2.02	1.46	1.50
15	aB	1012	CL7	CMC-C2C	-2.02	1.46	1.50
15	bB	1012	CL7	CMC-C2C	-2.02	1.46	1.50
15	bB	1218	CL7	CMD-C2D	-2.02	1.46	1.50
15	aB	1228	CL7	CMD-C2D	-2.02	1.46	1.50
15	cB	1213	CL7	CMD-C2D	-2.02	1.46	1.50
15	cA	1101	CL7	MG-NB	-2.02	2.01	2.05
15	cK	1401	CL7	MG-NB	-2.02	2.01	2.05
15	aB	1236	CL7	CMD-C2D	-2.02	1.46	1.50
15	cA	1123	CL7	CMC-C2C	-2.02	1.46	1.50
15	cB	1234	CL7	CMD-C2D	-2.02	1.46	1.50
15	aA	1122	CL7	MG-NB	-2.02	2.01	2.05
13	bA	1011	G9R	C3B-C2B	-2.02	1.37	1.40
15	aB	1218	CL7	CMD-C2D	-2.02	1.46	1.50
15	aB	1221	CL7	CMB-C2B	-2.02	1.46	1.50
15	bA	1126	CL7	CMB-C2B	-2.02	1.46	1.50
15	aA	1139	CL7	CMB-C2B	-2.02	1.46	1.50
15	bA	1111	CL7	CMD-C2D	-2.02	1.46	1.50
15	bF	1701	CL7	CMB-C2B	-2.02	1.46	1.50
15	bA	1132	CL7	CMC-C2C	-2.02	1.46	1.50
15	aI	1601	CL7	MG-NB	-2.02	2.01	2.05
15	bB	1213	CL7	CMD-C2D	-2.02	1.46	1.50
15	aB	1201	CL7	CMB-C2B	-2.02	1.46	1.50
15	cA	1139	CL7	CMD-C2D	-2.02	1.46	1.50
15	cB	1012	CL7	CMC-C2C	-2.02	1.46	1.50
15	cK	1402	CL7	CMD-C2D	-2.02	1.46	1.50
15	cI	1601	CL7	CMB-C2B	-2.02	1.46	1.50
15	aB	1209	CL7	MG-NB	-2.02	2.01	2.05
15	aA	1123	CL7	CMC-C2C	-2.02	1.46	1.50
15	aA	1801	CL7	CMB-C2B	-2.02	1.46	1.50
15	aB	1223	CL7	CMD-C2D	-2.02	1.46	1.50
15	bB	1216	CL7	CMD-C2D	-2.02	1.46	1.50
15	cA	1116	CL7	CMC-C2C	-2.02	1.46	1.50
15	cB	1221	CL7	MG-NB	-2.02	2.01	2.05
15	bA	1118	CL7	CMD-C2D	-2.02	1.46	1.50
15	cA	1105	CL7	CMB-C2B	-2.02	1.46	1.50
15	bB	1210	CL7	MG-NB	-2.02	2.01	2.05
15	aB	1220	CL7	CMD-C2D	-2.02	1.46	1.50
15	bB	1215	CL7	CMC-C2C	-2.02	1.46	1.50
15	aB	1205	CL7	MG-NB	-2.02	2.01	2.05
15	aA	1113	CL7	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	1203	CL7	CMD-C2D	-2.02	1.46	1.50
15	aK	1401	CL7	CMD-C2D	-2.02	1.46	1.50
15	bB	1228	CL7	CMD-C2D	-2.02	1.46	1.50
15	bB	1236	CL7	CMB-C2B	-2.02	1.46	1.50
15	cB	1228	CL7	CMD-C2D	-2.02	1.46	1.50
15	aB	1212	CL7	MG-NB	-2.02	2.01	2.05
15	bI	1601	CL7	C1D-C2D	2.02	1.48	1.43
15	bA	1122	CL7	CMB-C2B	-2.01	1.46	1.50
15	cF	1701	CL7	CMC-C2C	-2.01	1.46	1.50
15	aI	1601	CL7	CMB-C2B	-2.01	1.46	1.50
15	aA	1101	CL7	MG-NB	-2.01	2.01	2.05
15	bA	1139	CL7	CMD-C2D	-2.01	1.46	1.50
15	bA	1101	CL7	CMB-C2B	-2.01	1.46	1.50
15	aA	1118	CL7	MG-NB	-2.01	2.01	2.05
15	aB	1232	CL7	MG-NB	-2.01	2.01	2.05
15	bB	1205	CL7	MG-NB	-2.01	2.01	2.05
15	cA	1139	CL7	MG-NB	-2.01	2.01	2.05
15	aA	1134	CL7	CMB-C2B	-2.01	1.46	1.50
15	aA	1138	CL7	CMD-C2D	-2.01	1.46	1.50
15	aB	1222	CL7	CMB-C2B	-2.01	1.46	1.50
15	bA	1125	CL7	CMB-C2B	-2.01	1.46	1.50
15	bB	1220	CL7	CMB-C2B	-2.01	1.46	1.50
15	bA	1105	CL7	MG-NB	-2.01	2.01	2.05
15	bB	1234	CL7	CMC-C2C	-2.01	1.46	1.50
14	bA	1013	PHO	C3B-CAB	-2.01	1.43	1.47
15	bA	1120	CL7	CMD-C2D	-2.01	1.46	1.50
15	cB	1213	CL7	CMB-C2B	-2.01	1.46	1.50
15	cB	1220	CL7	CMB-C2B	-2.01	1.46	1.50
15	bA	1116	CL7	MG-NB	-2.01	2.01	2.05
15	aA	1102	CL7	CMB-C2B	-2.01	1.46	1.50
15	cA	1118	CL7	CMD-C2D	-2.01	1.46	1.50
15	cB	1204	CL7	CMC-C2C	-2.01	1.46	1.50
15	cB	1218	CL7	CMB-C2B	-2.01	1.46	1.50
15	cB	1231	CL7	MG-NB	-2.01	2.01	2.05
15	aA	1126	CL7	CMD-C2D	-2.01	1.46	1.50
15	bA	1131	CL7	CMC-C2C	-2.01	1.46	1.50
15	bB	1212	CL7	CMD-C2D	-2.01	1.46	1.50
15	aB	1201	CL7	CMD-C2D	-2.01	1.46	1.50
15	bI	1601	CL7	CMB-C2B	-2.01	1.46	1.50
15	cA	1122	CL7	CMD-C2D	-2.01	1.46	1.50
15	cB	1241	CL7	CMB-C2B	-2.01	1.46	1.50
15	bA	1119	CL7	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	1120	CL7	CMD-C2D	-2.01	1.46	1.50
15	aB	1223	CL7	CMC-C2C	-2.01	1.46	1.50
15	cA	1131	CL7	CMC-C2C	-2.01	1.46	1.50
15	aJ	1301	CL7	CMB-C2B	-2.01	1.46	1.50
15	cB	1229	CL7	CMD-C2D	-2.01	1.46	1.50
15	aB	1206	CL7	CMC-C2C	-2.01	1.46	1.50
15	cA	1120	CL7	CMB-C2B	-2.01	1.46	1.50
15	cB	1239	CL7	CMC-C2C	-2.01	1.46	1.50
15	aB	1221	CL7	MG-NB	-2.01	2.01	2.05
15	bA	1126	CL7	CMD-C2D	-2.01	1.46	1.50
15	aA	1121	CL7	CMB-C2B	-2.00	1.46	1.50
15	aA	1113	CL7	CMB-C2B	-2.00	1.46	1.50
15	aA	1122	CL7	CMD-C2D	-2.00	1.46	1.50
15	bJ	1302	CL7	MG-NB	-2.00	2.01	2.05
15	bB	1218	CL7	CMB-C2B	-2.00	1.46	1.50
15	cB	1202	CL7	CMC-C2C	-2.00	1.46	1.50
15	cJ	1301	CL7	MG-NB	-2.00	2.01	2.05
15	bA	1022	CL7	CMC-C2C	-2.00	1.46	1.50
15	bA	1101	CL7	CMC-C2C	-2.00	1.46	1.50
15	cB	1227	CL7	CMD-C2D	-2.00	1.46	1.50
15	aA	1139	CL7	MG-NB	-2.00	2.01	2.05
15	cB	1210	CL7	MG-NB	-2.00	2.01	2.05
15	aB	1227	CL7	CMD-C2D	-2.00	1.46	1.50
15	cA	1101	CL7	CMB-C2B	-2.00	1.46	1.50
15	cA	1110	CL7	CMD-C2D	-2.00	1.46	1.50
15	cB	1206	CL7	CMC-C2C	-2.00	1.46	1.50
15	aA	1022	CL7	CMC-C2C	-2.00	1.46	1.50
15	aA	1116	CL7	CMD-C2D	-2.00	1.46	1.50
15	aB	1221	CL7	CMD-C2D	-2.00	1.46	1.50
15	aB	1229	CL7	CMD-C2D	-2.00	1.46	1.50
15	bA	1120	CL7	CMB-C2B	-2.00	1.46	1.50
15	bB	1225	CL7	CMC-C2C	-2.00	1.46	1.50
15	cB	1236	CL7	CMB-C2B	-2.00	1.46	1.50
15	cA	1132	CL7	MG-NA	2.00	2.09	2.05

All (2516) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	cA	1013	PHO	C4D-CHA-CBD	-8.75	104.56	108.52
14	bB	1023	PHO	C4D-CHA-CBD	-8.57	104.64	108.52
17	bA	4014	A1JPJ	C15-C16-C17	8.48	140.85	123.47
14	bA	1013	PHO	C4D-CHA-CBD	-8.45	104.70	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aA	4014	A1JPJ	C15-C16-C17	8.41	140.70	123.47
14	aA	1013	PHO	C4D-CHA-CBD	-8.33	104.75	108.52
14	aB	1023	PHO	C4D-CHA-CBD	-8.17	104.82	108.52
17	cA	4014	A1JPJ	C15-C16-C17	8.16	140.20	123.47
14	cB	1023	PHO	C4D-CHA-CBD	-7.97	104.91	108.52
17	cB	4006	A1JPJ	C23-C22-C21	6.71	129.24	118.94
17	aB	4006	A1JPJ	C23-C22-C21	6.51	128.92	118.94
17	bB	4006	A1JPJ	C23-C22-C21	6.40	128.75	118.94
17	bA	4011	A1JPJ	C15-C16-C17	6.08	135.94	123.47
15	bA	1138	CL7	C1A-NA-C4A	5.94	109.90	106.30
15	aA	1138	CL7	C1A-NA-C4A	5.85	109.84	106.30
15	aJ	1302	CL7	C1A-NA-C4A	5.79	109.81	106.30
15	cB	1205	CL7	C1A-NA-C4A	5.77	109.80	106.30
15	aB	1205	CL7	C1A-NA-C4A	5.76	109.79	106.30
15	bB	1205	CL7	C1A-NA-C4A	5.71	109.76	106.30
15	cA	1138	CL7	C1A-NA-C4A	5.70	109.75	106.30
15	cB	1219	CL7	C1A-NA-C4A	5.68	109.74	106.30
15	cB	1212	CL7	C1A-NA-C4A	5.68	109.74	106.30
15	aB	1212	CL7	C1A-NA-C4A	5.67	109.73	106.30
15	cB	1235	CL7	C1A-NA-C4A	5.67	109.73	106.30
15	bB	1212	CL7	C1A-NA-C4A	5.66	109.73	106.30
15	cL	1503	CL7	C1A-NA-C4A	5.66	109.73	106.30
15	aA	1134	CL7	C1A-NA-C4A	5.66	109.73	106.30
15	aA	1103	CL7	C1A-NA-C4A	5.65	109.72	106.30
15	aB	1235	CL7	C1A-NA-C4A	5.65	109.72	106.30
15	bB	1213	CL7	C1A-NA-C4A	5.64	109.71	106.30
15	bB	1235	CL7	C1A-NA-C4A	5.64	109.71	106.30
15	bB	1223	CL7	C1A-NA-C4A	5.62	109.70	106.30
15	cB	1211	CL7	C1A-NA-C4A	5.62	109.70	106.30
15	bB	1211	CL7	C1A-NA-C4A	5.61	109.70	106.30
15	bI	1601	CL7	C1A-NA-C4A	5.61	109.70	106.30
15	bA	1134	CL7	C1A-NA-C4A	5.61	109.69	106.30
15	cJ	1302	CL7	C1A-NA-C4A	5.61	109.69	106.30
15	aB	1213	CL7	C1A-NA-C4A	5.60	109.69	106.30
15	cA	1134	CL7	C1A-NA-C4A	5.60	109.69	106.30
17	cA	4011	A1JPJ	C15-C16-C17	5.59	134.93	123.47
15	aA	1137	CL7	C1A-NA-C4A	5.59	109.68	106.30
15	bB	1228	CL7	C1A-NA-C4A	5.59	109.68	106.30
15	aA	1110	CL7	C1A-NA-C4A	5.58	109.68	106.30
15	cA	1137	CL7	C1A-NA-C4A	5.58	109.68	106.30
15	aB	1211	CL7	C1A-NA-C4A	5.57	109.67	106.30
15	aB	1219	CL7	C1A-NA-C4A	5.57	109.67	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1133	CL7	C1A-NA-C4A	5.57	109.67	106.30
15	cB	1236	CL7	C1A-NA-C4A	5.57	109.67	106.30
15	aI	1601	CL7	C1A-NA-C4A	5.56	109.67	106.30
15	cB	1223	CL7	C1A-NA-C4A	5.56	109.67	106.30
15	aA	1101	CL7	C1A-NA-C4A	5.56	109.67	106.30
15	aA	1113	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	cA	1110	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	aB	1218	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	aA	1118	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	cA	1115	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	bA	1101	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	bA	1137	CL7	C1A-NA-C4A	5.55	109.66	106.30
15	bB	1218	CL7	C1A-NA-C4A	5.54	109.66	106.30
15	aA	1115	CL7	C1A-NA-C4A	5.54	109.66	106.30
15	bB	1219	CL7	C1A-NA-C4A	5.54	109.65	106.30
15	cB	1229	CL7	C1A-NA-C4A	5.54	109.65	106.30
15	aA	1106	CL7	C1A-NA-C4A	5.53	109.65	106.30
15	aK	1401	CL7	C1A-NA-C4A	5.53	109.65	106.30
15	aB	1220	CL7	C1A-NA-C4A	5.53	109.65	106.30
15	cA	1121	CL7	C1A-NA-C4A	5.52	109.64	106.30
15	cK	1401	CL7	C1A-NA-C4A	5.51	109.64	106.30
15	aA	1116	CL7	C1A-NA-C4A	5.51	109.64	106.30
15	cB	1218	CL7	C1A-NA-C4A	5.51	109.64	106.30
15	bA	1110	CL7	C1A-NA-C4A	5.51	109.63	106.30
15	bA	1121	CL7	C1A-NA-C4A	5.51	109.63	106.30
15	bK	1401	CL7	C1A-NA-C4A	5.50	109.63	106.30
15	aL	1502	CL7	C1A-NA-C4A	5.50	109.63	106.30
15	cA	1101	CL7	C1A-NA-C4A	5.50	109.63	106.30
15	cK	1402	CL7	C1A-NA-C4A	5.50	109.63	106.30
17	aA	4011	A1JPJ	C15-C16-C17	5.50	134.73	123.47
15	aA	1133	CL7	C1A-NA-C4A	5.49	109.63	106.30
15	aB	1223	CL7	C1A-NA-C4A	5.49	109.63	106.30
15	bB	1220	CL7	C1A-NA-C4A	5.49	109.63	106.30
15	cL	1502	CL7	C1A-NA-C4A	5.49	109.62	106.30
15	cB	1239	CL7	C1A-NA-C4A	5.49	109.62	106.30
15	cJ	1301	CL7	C1A-NA-C4A	5.49	109.62	106.30
15	cA	1133	CL7	C1A-NA-C4A	5.48	109.62	106.30
15	aB	1236	CL7	C1A-NA-C4A	5.48	109.62	106.30
15	cA	1128	CL7	C1A-NA-C4A	5.48	109.62	106.30
15	cA	1112	CL7	C1A-NA-C4A	5.48	109.62	106.30
15	bA	1118	CL7	C1A-NA-C4A	5.47	109.61	106.30
15	bB	1231	CL7	C1A-NA-C4A	5.47	109.61	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bJ	1302	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	cA	1113	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	aA	1121	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	aJ	1301	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	bB	1215	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	bB	1229	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	bK	1402	CL7	C1A-NA-C4A	5.46	109.61	106.30
15	aB	1209	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	aL	1503	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	bB	1239	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	cB	1213	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	cA	1106	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	bA	1115	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	bA	1113	CL7	C1A-NA-C4A	5.45	109.60	106.30
15	cA	1118	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	aA	1112	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	aA	1117	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	aB	1229	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	aA	1105	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	cI	1601	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	bJ	1301	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	cA	1109	CL7	C1A-NA-C4A	5.44	109.59	106.30
15	bL	1502	CL7	C1A-NA-C4A	5.43	109.59	106.30
15	bB	1021	CL7	C1A-NA-C4A	5.43	109.59	106.30
15	bA	1132	CL7	C1A-NA-C4A	5.43	109.59	106.30
15	aA	1136	CL7	C1A-NA-C4A	5.43	109.59	106.30
15	cB	1217	CL7	C1A-NA-C4A	5.43	109.59	106.30
15	aA	1114	CL7	C1A-NA-C4A	5.42	109.58	106.30
15	bA	1128	CL7	C1A-NA-C4A	5.42	109.58	106.30
15	bA	1107	CL7	C1A-NA-C4A	5.42	109.58	106.30
15	cA	1107	CL7	C1A-NA-C4A	5.42	109.58	106.30
15	bA	1139	CL7	C1A-NA-C4A	5.42	109.58	106.30
15	aB	1239	CL7	C1A-NA-C4A	5.41	109.58	106.30
15	cA	1140	CL7	C1A-NA-C4A	5.41	109.58	106.30
15	bL	1501	CL7	C1A-NA-C4A	5.41	109.57	106.30
15	cA	1801	CL7	C1A-NA-C4A	5.41	109.57	106.30
15	aB	1217	CL7	C1A-NA-C4A	5.40	109.57	106.30
15	bA	1116	CL7	C1A-NA-C4A	5.40	109.57	106.30
15	cB	1204	CL7	C1A-NA-C4A	5.40	109.57	106.30
15	aA	1120	CL7	C1A-NA-C4A	5.39	109.57	106.30
15	bA	1114	CL7	C1A-NA-C4A	5.39	109.56	106.30
15	bA	1106	CL7	C1A-NA-C4A	5.39	109.56	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1206	CL7	C1A-NA-C4A	5.39	109.56	106.30
15	bB	1224	CL7	C1A-NA-C4A	5.38	109.56	106.30
15	aA	1107	CL7	C1A-NA-C4A	5.38	109.56	106.30
15	aA	1128	CL7	C1A-NA-C4A	5.38	109.56	106.30
15	aA	1122	CL7	C1A-NA-C4A	5.38	109.56	106.30
15	aB	1230	CL7	C1A-NA-C4A	5.38	109.56	106.30
15	aA	1126	CL7	C1A-NA-C4A	5.37	109.55	106.30
15	aL	1501	CL7	C1A-NA-C4A	5.37	109.55	106.30
15	bA	1120	CL7	C1A-NA-C4A	5.37	109.55	106.30
15	bB	1209	CL7	C1A-NA-C4A	5.37	109.55	106.30
15	aB	1238	CL7	C1A-NA-C4A	5.37	109.55	106.30
15	aA	1139	CL7	C1A-NA-C4A	5.36	109.55	106.30
15	bB	1204	CL7	C1A-NA-C4A	5.36	109.55	106.30
15	bF	1701	CL7	C1A-NA-C4A	5.36	109.55	106.30
15	cA	1114	CL7	C1A-NA-C4A	5.36	109.55	106.30
15	aB	1233	CL7	C1A-NA-C4A	5.36	109.55	106.30
15	aB	1204	CL7	C1A-NA-C4A	5.36	109.54	106.30
15	cB	1222	CL7	C1A-NA-C4A	5.36	109.54	106.30
15	aA	1131	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cA	1122	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cA	1123	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cA	1105	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	bB	1230	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cA	1136	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cB	1233	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cL	1501	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	aA	1109	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cA	1131	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	cB	1209	CL7	C1A-NA-C4A	5.35	109.54	106.30
15	aB	1221	CL7	C1A-NA-C4A	5.34	109.54	106.30
15	aB	1231	CL7	C1A-NA-C4A	5.34	109.53	106.30
15	bA	1122	CL7	C1A-NA-C4A	5.34	109.53	106.30
15	aA	1123	CL7	C1A-NA-C4A	5.34	109.53	106.30
15	cA	1125	CL7	C1A-NA-C4A	5.34	109.53	106.30
15	bA	1105	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cB	1237	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cB	1231	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	bA	1131	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	bA	1801	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cA	1135	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cA	1139	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cF	1701	CL7	C1A-NA-C4A	5.33	109.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1125	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	bB	1222	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	cA	1120	CL7	C1A-NA-C4A	5.33	109.53	106.30
15	aB	1226	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	bB	1217	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	bA	1136	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	bA	1140	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	aA	1104	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	bA	1112	CL7	C1A-NA-C4A	5.32	109.52	106.30
15	bB	1226	CL7	C1A-NA-C4A	5.31	109.52	106.30
15	cB	1228	CL7	C1A-NA-C4A	5.31	109.52	106.30
15	aB	1222	CL7	C1A-NA-C4A	5.31	109.51	106.30
15	cA	1102	CL7	C1A-NA-C4A	5.31	109.51	106.30
15	aA	1140	CL7	C1A-NA-C4A	5.30	109.51	106.30
15	cB	1226	CL7	C1A-NA-C4A	5.30	109.51	106.30
15	aA	1102	CL7	C1A-NA-C4A	5.30	109.51	106.30
15	aB	1228	CL7	C1A-NA-C4A	5.30	109.51	106.30
15	bB	1236	CL7	C1A-NA-C4A	5.29	109.51	106.30
15	cB	1220	CL7	C1A-NA-C4A	5.29	109.51	106.30
15	cB	1227	CL7	C1A-NA-C4A	5.29	109.51	106.30
15	aA	1801	CL7	C1A-NA-C4A	5.29	109.50	106.30
15	bB	1232	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	bB	1233	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	aB	1206	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	cB	1210	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	cA	1116	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	aB	1215	CL7	C1A-NA-C4A	5.28	109.50	106.30
15	aA	1108	CL7	C1A-NA-C4A	5.27	109.49	106.30
15	cB	1238	CL7	C1A-NA-C4A	5.27	109.49	106.30
15	bB	1237	CL7	C1A-NA-C4A	5.27	109.49	106.30
15	bA	1102	CL7	C1A-NA-C4A	5.27	109.49	106.30
15	bA	1103	CL7	C1A-NA-C4A	5.27	109.49	106.30
15	cB	1206	CL7	C1A-NA-C4A	5.26	109.49	106.30
15	cA	1126	CL7	C1A-NA-C4A	5.26	109.49	106.30
15	bA	1123	CL7	C1A-NA-C4A	5.26	109.49	106.30
15	bB	1201	CL7	C1A-NA-C4A	5.25	109.48	106.30
15	aF	1701	CL7	C1A-NA-C4A	5.25	109.48	106.30
15	aB	1201	CL7	C1A-NA-C4A	5.24	109.47	106.30
15	bB	1216	CL7	C1A-NA-C4A	5.24	109.47	106.30
15	aB	1021	CL7	C1A-NA-C4A	5.23	109.47	106.30
15	cB	1232	CL7	C1A-NA-C4A	5.23	109.47	106.30
15	aB	1232	CL7	C1A-NA-C4A	5.23	109.47	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cB	1230	CL7	C1A-NA-C4A	5.23	109.47	106.30
15	cB	1021	CL7	C1A-NA-C4A	5.23	109.47	106.30
15	aB	1216	CL7	C1A-NA-C4A	5.23	109.47	106.30
15	cA	1108	CL7	C1A-NA-C4A	5.22	109.46	106.30
15	bL	1503	CL7	C1A-NA-C4A	5.22	109.46	106.30
15	bB	1238	CL7	C1A-NA-C4A	5.22	109.46	106.30
15	cA	1129	CL7	C1A-NA-C4A	5.22	109.46	106.30
15	cB	1224	CL7	C1A-NA-C4A	5.22	109.46	106.30
17	aF	4016	A1JPJ	C15-C16-C17	5.21	134.15	123.47
15	cA	1104	CL7	C1A-NA-C4A	5.21	109.45	106.30
15	bA	1124	CL7	C1A-NA-C4A	5.21	109.45	106.30
17	aB	4006	A1JPJ	C16-C15-C14	5.21	134.14	123.47
15	bA	1108	CL7	C1A-NA-C4A	5.19	109.44	106.30
15	bA	1117	CL7	C1A-NA-C4A	5.19	109.44	106.30
15	aB	1224	CL7	C1A-NA-C4A	5.19	109.44	106.30
15	aB	1214	CL7	C1A-NA-C4A	5.18	109.44	106.30
15	cB	1208	CL7	C1A-NA-C4A	5.18	109.44	106.30
15	bB	1210	CL7	C1A-NA-C4A	5.17	109.43	106.30
15	cA	1124	CL7	C1A-NA-C4A	5.17	109.43	106.30
15	bA	1111	CL7	C1A-NA-C4A	5.17	109.43	106.30
15	bB	1221	CL7	C1A-NA-C4A	5.17	109.43	106.30
15	aB	1241	CL7	C1A-NA-C4A	5.17	109.43	106.30
17	cB	4006	A1JPJ	C16-C15-C14	5.16	134.05	123.47
15	aB	1208	CL7	C1A-NA-C4A	5.16	109.43	106.30
15	cB	1225	CL7	C1A-NA-C4A	5.16	109.43	106.30
15	cA	1103	CL7	C1A-NA-C4A	5.16	109.43	106.30
15	bB	1202	CL7	C1A-NA-C4A	5.16	109.42	106.30
15	bB	1207	CL7	C1A-NA-C4A	5.16	109.42	106.30
15	cB	1201	CL7	C1A-NA-C4A	5.16	109.42	106.30
15	aA	1111	CL7	C1A-NA-C4A	5.15	109.42	106.30
17	bB	4006	A1JPJ	C16-C15-C14	5.15	134.03	123.47
15	cB	1214	CL7	C1A-NA-C4A	5.15	109.42	106.30
15	aB	1237	CL7	C1A-NA-C4A	5.15	109.42	106.30
15	aB	1227	CL7	C1A-NA-C4A	5.15	109.42	106.30
15	bB	1214	CL7	C1A-NA-C4A	5.14	109.41	106.30
15	bA	1109	CL7	C1A-NA-C4A	5.14	109.41	106.30
15	bA	1135	CL7	C1A-NA-C4A	5.13	109.41	106.30
15	bB	1208	CL7	C1A-NA-C4A	5.13	109.41	106.30
15	cA	1111	CL7	C1A-NA-C4A	5.13	109.41	106.30
15	aA	1124	CL7	C1A-NA-C4A	5.13	109.40	106.30
15	aB	1207	CL7	C1A-NA-C4A	5.12	109.40	106.30
15	cB	1216	CL7	C1A-NA-C4A	5.12	109.40	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1130	CL7	C1A-NA-C4A	5.12	109.40	106.30
15	cB	1207	CL7	C1A-NA-C4A	5.12	109.40	106.30
15	cA	1130	CL7	C1A-NA-C4A	5.11	109.40	106.30
15	bB	1225	CL7	C1A-NA-C4A	5.10	109.39	106.30
15	bB	1203	CL7	C1A-NA-C4A	5.10	109.39	106.30
15	aB	1202	CL7	C1A-NA-C4A	5.09	109.38	106.30
15	aB	1210	CL7	C1A-NA-C4A	5.09	109.38	106.30
15	aB	1225	CL7	C1A-NA-C4A	5.09	109.38	106.30
15	bA	1129	CL7	C1A-NA-C4A	5.09	109.38	106.30
15	bA	1119	CL7	C1A-NA-C4A	5.08	109.38	106.30
15	bA	1104	CL7	C1A-NA-C4A	5.07	109.37	106.30
15	cB	1221	CL7	C1A-NA-C4A	5.05	109.36	106.30
15	cA	1117	CL7	C1A-NA-C4A	5.03	109.35	106.30
15	cB	1241	CL7	C1A-NA-C4A	5.03	109.34	106.30
15	bB	1241	CL7	C1A-NA-C4A	5.02	109.34	106.30
15	cB	1203	CL7	C1A-NA-C4A	5.02	109.34	106.30
15	aA	1130	CL7	C1A-NA-C4A	5.01	109.34	106.30
15	cB	1202	CL7	C1A-NA-C4A	5.00	109.33	106.30
15	aA	1135	CL7	C1A-NA-C4A	4.99	109.32	106.30
15	aA	1119	CL7	C1A-NA-C4A	4.99	109.32	106.30
17	cB	4006	A1JPJ	C37-C22-C21	-4.97	115.96	122.92
15	bA	1125	CL7	C1A-NA-C4A	4.96	109.30	106.30
15	aB	1203	CL7	C1A-NA-C4A	4.95	109.30	106.30
15	bA	1127	CL7	C1A-NA-C4A	4.95	109.30	106.30
15	cA	1119	CL7	C1A-NA-C4A	4.94	109.29	106.30
15	aA	1022	CL7	C1A-NA-C4A	4.93	109.28	106.30
15	aA	1129	CL7	C1A-NA-C4A	4.91	109.27	106.30
17	aB	4006	A1JPJ	C37-C22-C21	-4.91	116.05	122.92
15	bB	1234	CL7	C1A-NA-C4A	4.90	109.27	106.30
15	cB	1012	CL7	C1A-NA-C4A	4.90	109.27	106.30
17	bB	4006	A1JPJ	C37-C22-C21	-4.90	116.06	122.92
15	bB	1012	CL7	C1A-NA-C4A	4.89	109.26	106.30
15	cB	1234	CL7	C1A-NA-C4A	4.87	109.25	106.30
15	cB	1215	CL7	C1A-NA-C4A	4.85	109.24	106.30
15	aB	1012	CL7	C1A-NA-C4A	4.84	109.23	106.30
15	aK	1402	CL7	C1A-NA-C4A	4.83	109.23	106.30
15	cA	1127	CL7	C1A-NA-C4A	4.83	109.22	106.30
15	bA	1022	CL7	C1A-NA-C4A	4.79	109.20	106.30
15	cA	1022	CL7	C1A-NA-C4A	4.78	109.19	106.30
17	aB	4015	A1JPJ	C34-C9-C10	-4.78	116.23	122.92
15	aA	1127	CL7	C1A-NA-C4A	4.77	109.19	106.30
15	aB	1234	CL7	C1A-NA-C4A	4.77	109.19	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aJ	4012	A1JPJ	C16-C15-C14	4.71	133.12	123.47
17	cB	4005	A1JPJ	C16-C15-C14	4.70	133.10	123.47
17	cB	4004	A1JPJ	C37-C22-C21	-4.66	116.40	122.92
17	aB	4004	A1JPJ	C37-C22-C21	-4.65	116.40	122.92
17	bB	4005	A1JPJ	C16-C15-C14	4.64	132.99	123.47
17	bB	4004	A1JPJ	C37-C22-C21	-4.63	116.43	122.92
17	aB	4005	A1JPJ	C16-C15-C14	4.60	132.89	123.47
17	cJ	4012	A1JPJ	C16-C15-C14	4.60	132.89	123.47
17	bJ	4012	A1JPJ	C16-C15-C14	4.55	132.79	123.47
15	bB	1227	CL7	C1A-NA-C4A	4.51	109.03	106.30
17	bB	4017	A1JPJ	C37-C22-C21	-4.51	116.61	122.92
17	aB	4017	A1JPJ	C37-C22-C21	-4.50	116.62	122.92
17	cB	4017	A1JPJ	C37-C22-C21	-4.49	116.63	122.92
17	bB	4015	A1JPJ	C34-C9-C10	-4.43	116.71	122.92
17	cB	4015	A1JPJ	C34-C9-C10	-4.42	116.73	122.92
17	cB	4010	A1JPJ	C16-C15-C14	4.41	132.52	123.47
17	aL	4023	A1JPJ	C37-C22-C21	-4.41	116.75	122.92
17	bB	4010	A1JPJ	C16-C15-C14	4.39	132.47	123.47
17	aL	4023	A1JPJ	C15-C16-C17	4.38	132.45	123.47
17	bA	4014	A1JPJ	C16-C15-C14	4.38	132.44	123.47
17	bJ	4012	A1JPJ	C34-C9-C10	-4.38	116.79	122.92
17	aB	4010	A1JPJ	C16-C15-C14	4.37	132.42	123.47
17	aJ	4012	A1JPJ	C34-C9-C10	-4.36	116.82	122.92
17	cB	4010	A1JPJ	C34-C9-C10	-4.36	116.82	122.92
17	bA	4002	A1JPJ	C15-C16-C17	4.35	132.38	123.47
17	cJ	4012	A1JPJ	C34-C9-C10	-4.33	116.86	122.92
17	aA	4014	A1JPJ	C16-C15-C14	4.33	132.34	123.47
17	cL	4020	A1JPJ	C37-C22-C21	-4.32	116.87	122.92
17	cA	4011	A1JPJ	C37-C22-C21	-4.32	116.88	122.92
17	cB	4006	A1JPJ	C34-C9-C10	-4.32	116.88	122.92
17	bB	4010	A1JPJ	C34-C9-C10	-4.31	116.89	122.92
17	cB	4004	A1JPJ	C15-C16-C17	4.30	132.29	123.47
17	aB	4010	A1JPJ	C34-C9-C10	-4.30	116.90	122.92
17	cA	4002	A1JPJ	C15-C16-C17	4.30	132.27	123.47
17	aA	4002	A1JPJ	C15-C16-C17	4.30	132.27	123.47
17	cA	4014	A1JPJ	C16-C15-C14	4.28	132.25	123.47
17	aL	4020	A1JPJ	C37-C22-C21	-4.28	116.92	122.92
17	bB	4006	A1JPJ	C34-C9-C10	-4.28	116.93	122.92
17	bA	4011	A1JPJ	C37-C22-C21	-4.27	116.94	122.92
17	aB	4006	A1JPJ	C34-C9-C10	-4.27	116.94	122.92
17	bB	4004	A1JPJ	C15-C16-C17	4.25	132.18	123.47
17	aB	4004	A1JPJ	C15-C16-C17	4.24	132.17	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	bL	4020	A1JPJ	C37-C22-C21	-4.24	116.98	122.92
17	cF	4016	A1JPJ	C37-C22-C21	-4.24	116.98	122.92
17	aF	4016	A1JPJ	C34-C9-C10	-4.24	116.99	122.92
17	bB	4004	A1JPJ	C34-C9-C10	-4.23	117.00	122.92
17	cB	4004	A1JPJ	C34-C9-C10	-4.22	117.00	122.92
17	aB	4004	A1JPJ	C34-C9-C10	-4.22	117.02	122.92
17	aA	4002	A1JPJ	C37-C22-C21	-4.19	117.06	122.92
17	bF	4016	A1JPJ	C37-C22-C21	-4.18	117.07	122.92
17	bF	4016	A1JPJ	C34-C9-C10	-4.18	117.07	122.92
17	cA	4002	A1JPJ	C37-C22-C21	-4.17	117.08	122.92
17	cF	4016	A1JPJ	C34-C9-C10	-4.15	117.11	122.92
17	bI	4019	A1JPJ	C16-C15-C14	4.15	131.97	123.47
15	bA	1126	CL7	C1D-ND-C4D	-4.15	103.39	106.33
17	aI	4019	A1JPJ	C16-C15-C14	4.15	131.97	123.47
17	bA	4002	A1JPJ	C37-C22-C21	-4.12	117.16	122.92
17	aA	4011	A1JPJ	C37-C22-C21	-4.11	117.16	122.92
17	bA	4014	A1JPJ	C16-C17-C18	4.11	133.18	127.31
17	aB	4017	A1JPJ	C15-C16-C17	4.10	131.87	123.47
17	aB	4017	A1JPJ	C23-C22-C21	4.10	125.23	118.94
17	cA	4003	A1JPJ	C34-C9-C10	-4.08	117.21	122.92
17	aA	4002	A1JPJ	C34-C9-C10	-4.08	117.21	122.92
17	aJ	4012	A1JPJ	C37-C22-C21	-4.08	117.21	122.92
17	bA	4003	A1JPJ	C34-C9-C10	-4.08	117.21	122.92
17	cA	4003	A1JPJ	C37-C22-C21	-4.07	117.22	122.92
17	cA	4011	A1JPJ	C34-C9-C10	-4.07	117.22	122.92
17	aA	4014	A1JPJ	C16-C17-C18	4.07	133.12	127.31
17	bB	4017	A1JPJ	C15-C16-C17	4.07	131.80	123.47
17	aA	4003	A1JPJ	C34-C9-C10	-4.06	117.23	122.92
17	aL	4023	A1JPJ	C23-C22-C21	4.06	125.17	118.94
17	bL	4023	A1JPJ	C37-C22-C21	-4.06	117.24	122.92
17	bB	4017	A1JPJ	C34-C9-C10	-4.06	117.24	122.92
17	bJ	4012	A1JPJ	C37-C22-C21	-4.06	117.24	122.92
17	aA	4008	A1JPJ	C34-C9-C10	-4.05	117.25	122.92
17	cI	4019	A1JPJ	C16-C15-C14	4.05	131.77	123.47
17	bJ	4012	A1JPJ	C25-C26-C27	-4.05	116.49	121.47
17	bA	4002	A1JPJ	C34-C9-C10	-4.05	117.25	122.92
17	cA	4008	A1JPJ	C34-C9-C10	-4.04	117.26	122.92
17	cJ	4012	A1JPJ	C37-C22-C21	-4.04	117.26	122.92
17	cL	4023	A1JPJ	C34-C9-C10	-4.04	117.27	122.92
17	bA	4003	A1JPJ	C37-C22-C21	-4.04	117.27	122.92
17	aB	4005	A1JPJ	C34-C9-C10	-4.03	117.27	122.92
17	cL	4023	A1JPJ	C37-C22-C21	-4.03	117.27	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aA	4003	A1JPJ	C37-C22-C21	-4.03	117.28	122.92
17	cB	4017	A1JPJ	C34-C9-C10	-4.03	117.28	122.92
17	bB	4015	A1JPJ	C16-C15-C14	4.02	131.72	123.47
17	cB	4017	A1JPJ	C15-C16-C17	4.02	131.71	123.47
17	cB	4015	A1JPJ	C16-C15-C14	4.02	131.71	123.47
17	aA	4011	A1JPJ	C34-C9-C10	-4.02	117.29	122.92
17	aB	4015	A1JPJ	C37-C22-C21	-4.02	117.29	122.92
17	aL	4023	A1JPJ	C34-C9-C10	-4.02	117.30	122.92
17	aB	4010	A1JPJ	C37-C22-C21	-4.02	117.30	122.92
17	bA	4008	A1JPJ	C34-C9-C10	-4.01	117.30	122.92
17	aI	4018	A1JPJ	C25-C26-C27	-4.01	116.53	121.47
17	bB	4005	A1JPJ	C34-C9-C10	-4.01	117.31	122.92
17	aB	4017	A1JPJ	C34-C9-C10	-4.00	117.31	122.92
17	cI	4018	A1JPJ	C28-C27-C26	-4.00	121.01	124.85
17	cI	4019	A1JPJ	C34-C9-C10	-3.99	117.33	122.92
17	bF	4016	A1JPJ	C16-C15-C14	3.99	131.65	123.47
17	cB	4005	A1JPJ	C34-C9-C10	-3.99	117.34	122.92
17	bL	4023	A1JPJ	C34-C9-C10	-3.99	117.34	122.92
17	cB	4017	A1JPJ	C23-C22-C21	3.98	125.05	118.94
17	cB	4010	A1JPJ	C37-C22-C21	-3.98	117.35	122.92
17	cB	4015	A1JPJ	C37-C22-C21	-3.97	117.36	122.92
17	aA	4007	A1JPJ	C37-C22-C21	-3.97	117.36	122.92
17	bB	4015	A1JPJ	C37-C22-C21	-3.97	117.36	122.92
17	cL	4020	A1JPJ	C34-C9-C10	-3.96	117.37	122.92
17	cA	4002	A1JPJ	C34-C9-C10	-3.96	117.37	122.92
17	cA	4007	A1JPJ	C37-C22-C21	-3.96	117.37	122.92
17	bI	4019	A1JPJ	C34-C9-C10	-3.96	117.37	122.92
15	aA	1132	CL7	C1A-NA-C4A	3.96	108.70	106.30
17	bB	4017	A1JPJ	C23-C22-C21	3.95	125.01	118.94
17	aL	4020	A1JPJ	C34-C9-C10	-3.95	117.39	122.92
17	cA	4014	A1JPJ	C16-C17-C18	3.95	132.95	127.31
17	aI	4019	A1JPJ	C37-C22-C21	-3.95	117.39	122.92
17	aI	4019	A1JPJ	C34-C9-C10	-3.95	117.39	122.92
17	cF	4016	A1JPJ	C16-C15-C14	3.94	131.54	123.47
17	aJ	4012	A1JPJ	C25-C26-C27	-3.94	116.62	121.47
17	bI	4018	A1JPJ	C25-C26-C27	-3.93	116.63	121.47
17	cI	4018	A1JPJ	C25-C26-C27	-3.93	116.63	121.47
17	bI	4019	A1JPJ	C37-C22-C21	-3.93	117.42	122.92
17	bL	4020	A1JPJ	C34-C9-C10	-3.92	117.43	122.92
17	bI	4018	A1JPJ	C28-C27-C26	-3.92	121.09	124.85
17	cB	4006	A1JPJ	C8-C9-C10	3.91	124.95	118.94
17	bB	4010	A1JPJ	C37-C22-C21	-3.91	117.44	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	cJ	4012	A1JPJ	C25-C26-C27	-3.91	116.65	121.47
15	cA	1132	CL7	C1A-NA-C4A	3.91	108.67	106.30
17	bA	4007	A1JPJ	C37-C22-C21	-3.90	117.46	122.92
17	cI	4019	A1JPJ	C37-C22-C21	-3.89	117.47	122.92
17	aB	4015	A1JPJ	C8-C9-C10	3.88	124.89	118.94
17	bA	4007	A1JPJ	C15-C16-C17	3.87	131.41	123.47
17	cI	4018	A1JPJ	C34-C9-C10	-3.87	117.50	122.92
17	cB	4021	A1JPJ	C37-C22-C21	-3.87	117.50	122.92
17	aI	4018	A1JPJ	C28-C27-C26	-3.87	121.14	124.85
17	cA	4007	A1JPJ	C15-C16-C17	3.87	131.39	123.47
17	bB	4005	A1JPJ	C37-C22-C21	-3.86	117.52	122.92
17	bB	4015	A1JPJ	C25-C26-C27	-3.85	116.72	121.47
17	aB	4015	A1JPJ	C25-C26-C27	-3.85	116.73	121.47
17	aB	4021	A1JPJ	C34-C9-C10	-3.84	117.54	122.92
17	cB	4005	A1JPJ	C37-C22-C21	-3.84	117.54	122.92
17	bI	4018	A1JPJ	C34-C9-C10	-3.84	117.54	122.92
17	aB	4006	A1JPJ	C8-C9-C10	3.84	124.84	118.94
17	bB	4021	A1JPJ	C37-C22-C21	-3.84	117.54	122.92
17	aB	4021	A1JPJ	C37-C22-C21	-3.84	117.54	122.92
17	aB	4005	A1JPJ	C37-C22-C21	-3.84	117.55	122.92
17	cB	4021	A1JPJ	C34-C9-C10	-3.84	117.55	122.92
17	cA	4014	A1JPJ	C11-C10-C9	3.83	132.77	127.31
17	cA	4007	A1JPJ	C34-C9-C10	-3.83	117.56	122.92
17	cB	4004	A1JPJ	C37-C22-C23	3.82	124.10	118.08
17	cB	4010	A1JPJ	C35-C13-C14	-3.81	117.58	122.92
17	aI	4018	A1JPJ	C34-C9-C10	-3.81	117.59	122.92
17	bI	4018	A1JPJ	C37-C22-C21	-3.79	117.62	122.92
17	bB	4021	A1JPJ	C34-C9-C10	-3.78	117.62	122.92
17	aB	4004	A1JPJ	C37-C22-C23	3.78	124.04	118.08
17	bB	4015	A1JPJ	C28-C27-C26	-3.78	121.23	124.85
17	aB	4015	A1JPJ	C16-C15-C14	3.78	131.21	123.47
17	aI	4018	A1JPJ	C37-C22-C21	-3.78	117.63	122.92
17	bF	4016	A1JPJ	C28-C27-C26	-3.77	121.23	124.85
17	aL	4020	A1JPJ	C16-C15-C14	3.77	131.19	123.47
17	cI	4018	A1JPJ	C37-C22-C21	-3.76	117.65	122.92
17	cA	4014	A1JPJ	C37-C22-C21	-3.76	117.66	122.92
17	cB	4015	A1JPJ	C25-C26-C27	-3.75	116.85	121.47
14	aA	1013	PHO	O1D-CGD-CBD	3.75	130.99	124.74
17	bB	4004	A1JPJ	C37-C22-C23	3.75	123.99	118.08
17	aB	4010	A1JPJ	C35-C13-C14	-3.75	117.67	122.92
17	aB	4015	A1JPJ	C28-C27-C26	-3.75	121.25	124.85
15	bA	1126	CL7	C1A-NA-C4A	3.75	108.57	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	bB	4010	A1JPJ	C35-C13-C14	-3.75	117.67	122.92
17	aA	4007	A1JPJ	C34-C9-C10	-3.75	117.67	122.92
17	bA	4007	A1JPJ	C34-C9-C10	-3.74	117.68	122.92
17	cL	4020	A1JPJ	C16-C15-C14	3.74	131.14	123.47
17	aF	4016	A1JPJ	C36-C18-C17	-3.74	117.68	122.92
14	bA	1013	PHO	O1D-CGD-CBD	3.74	130.97	124.74
17	aA	4014	A1JPJ	C11-C10-C9	3.73	132.64	127.31
17	aA	4007	A1JPJ	C15-C16-C17	3.73	131.12	123.47
17	bA	4014	A1JPJ	C37-C22-C21	-3.73	117.70	122.92
17	bA	4014	A1JPJ	C11-C10-C9	3.73	132.63	127.31
17	aA	4014	A1JPJ	C37-C22-C21	-3.73	117.70	122.92
17	cJ	4012	A1JPJ	C28-C27-C26	-3.72	121.28	124.85
17	cB	4015	A1JPJ	C28-C27-C26	-3.70	121.31	124.85
17	cB	4021	A1JPJ	C16-C15-C14	3.69	131.03	123.47
17	aA	4003	A1JPJ	C16-C15-C14	3.68	131.01	123.47
17	aF	4016	A1JPJ	C19-C18-C17	3.68	124.58	118.94
17	aF	4016	A1JPJ	C35-C13-C14	-3.68	117.77	122.92
14	cA	1013	PHO	O1D-CGD-CBD	3.67	130.85	124.74
17	aJ	4012	A1JPJ	C35-C13-C14	-3.66	117.79	122.92
17	bB	4006	A1JPJ	C8-C9-C10	3.66	124.56	118.94
17	cA	4014	A1JPJ	C10-C11-C12	3.66	134.64	123.22
17	cJ	4012	A1JPJ	C35-C13-C14	-3.65	117.81	122.92
17	bL	4020	A1JPJ	C16-C15-C14	3.64	130.93	123.47
17	aB	4017	A1JPJ	C36-C18-C17	-3.64	117.83	122.92
17	cL	4023	A1JPJ	C15-C16-C17	3.63	130.91	123.47
17	bA	4011	A1JPJ	C34-C9-C10	-3.63	117.84	122.92
17	bJ	4012	A1JPJ	C35-C13-C14	-3.62	117.85	122.92
17	aL	4023	A1JPJ	C36-C18-C17	-3.62	117.86	122.92
17	aA	4008	A1JPJ	C37-C22-C23	3.61	123.77	118.08
17	bB	4017	A1JPJ	C36-C18-C17	-3.61	117.86	122.92
17	bA	4003	A1JPJ	C16-C15-C14	3.61	130.87	123.47
14	bB	1023	PHO	O1D-CGD-CBD	3.60	130.73	124.74
17	cA	4008	A1JPJ	C37-C22-C23	3.59	123.74	118.08
17	bA	4008	A1JPJ	C37-C22-C21	-3.59	117.89	122.92
17	bB	4021	A1JPJ	C16-C15-C14	3.59	130.83	123.47
17	cB	4006	A1JPJ	C20-C21-C22	3.59	132.43	127.31
17	cB	4017	A1JPJ	C36-C18-C17	-3.58	117.90	122.92
17	aB	4015	A1JPJ	C35-C13-C14	-3.58	117.91	122.92
17	cB	4005	A1JPJ	C35-C13-C14	-3.57	117.92	122.92
17	cA	4003	A1JPJ	C16-C15-C14	3.57	130.78	123.47
17	aB	4021	A1JPJ	C16-C15-C14	3.56	130.77	123.47
17	aA	4008	A1JPJ	C37-C22-C21	-3.56	117.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	bB	4015	A1JPJ	C35-C13-C14	-3.56	117.94	122.92
17	cA	4008	A1JPJ	C37-C22-C21	-3.56	117.94	122.92
17	aF	4016	A1JPJ	C12-C13-C14	3.55	124.39	118.94
17	bB	4005	A1JPJ	C35-C13-C14	-3.55	117.95	122.92
17	cB	4004	A1JPJ	C36-C18-C17	-3.55	117.95	122.92
17	aA	4014	A1JPJ	C10-C11-C12	3.55	134.29	123.22
17	cB	4015	A1JPJ	C35-C13-C14	-3.55	117.95	122.92
17	bL	4023	A1JPJ	C15-C16-C17	3.55	130.74	123.47
17	aB	4006	A1JPJ	C35-C13-C14	-3.54	117.97	122.92
17	cB	4006	A1JPJ	C35-C13-C14	-3.54	117.97	122.92
17	bB	4004	A1JPJ	C36-C18-C17	-3.53	117.98	122.92
17	aB	4005	A1JPJ	C35-C13-C14	-3.52	117.99	122.92
17	aB	4004	A1JPJ	C36-C18-C17	-3.52	117.99	122.92
15	bA	1110	CL7	O2D-CGD-O1D	-3.52	116.95	123.84
17	bB	4006	A1JPJ	C35-C13-C14	-3.52	118.00	122.92
17	aJ	4012	A1JPJ	C12-C13-C14	3.51	124.33	118.94
15	aB	1201	CL7	C3B-C4B-NB	-3.49	107.27	110.52
17	aB	4006	A1JPJ	C20-C21-C22	3.48	132.28	127.31
17	cB	4005	A1JPJ	C28-C27-C26	-3.48	121.52	124.85
17	cL	4020	A1JPJ	C35-C13-C14	-3.48	118.06	122.92
15	aA	1110	CL7	O2D-CGD-O1D	-3.47	117.05	123.84
14	aB	1023	PHO	O1D-CGD-CBD	3.47	130.52	124.74
17	aL	4020	A1JPJ	C35-C13-C14	-3.47	118.07	122.92
17	bJ	4012	A1JPJ	C12-C13-C14	3.46	124.25	118.94
17	bA	4014	A1JPJ	C10-C11-C12	3.46	134.02	123.22
17	aJ	4012	A1JPJ	C28-C27-C26	-3.46	121.53	124.85
17	cJ	4012	A1JPJ	C12-C13-C14	3.46	124.25	118.94
15	bB	1201	CL7	C3B-C4B-NB	-3.46	107.31	110.52
17	bB	4006	A1JPJ	C20-C21-C22	3.45	132.24	127.31
17	bA	4008	A1JPJ	C37-C22-C23	3.45	123.51	118.08
17	bJ	4012	A1JPJ	C28-C27-C26	-3.44	121.55	124.85
17	bL	4020	A1JPJ	C35-C13-C14	-3.44	118.11	122.92
17	aB	4005	A1JPJ	C28-C27-C26	-3.44	121.56	124.85
17	bB	4010	A1JPJ	C10-C11-C12	3.43	133.93	123.22
15	aA	1125	CL7	C3B-C4B-NB	-3.42	107.34	110.52
17	bA	4008	A1JPJ	C28-C27-C26	-3.42	121.57	124.85
17	cB	4010	A1JPJ	C10-C11-C12	3.41	133.87	123.22
15	bA	1126	CL7	C3B-C4B-NB	-3.41	107.35	110.52
15	cB	1201	CL7	C3B-C4B-NB	-3.40	107.36	110.52
15	cA	1132	CL7	CHB-C1B-NB	3.40	127.85	124.26
17	aB	4006	A1JPJ	C12-C13-C14	3.40	124.15	118.94
15	bA	1115	CL7	C3B-C4B-NB	-3.39	107.37	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aB	4010	A1JPJ	C10-C11-C12	3.39	133.80	123.22
17	cF	4016	A1JPJ	C36-C18-C17	-3.39	118.17	122.92
17	aA	4008	A1JPJ	C15-C16-C17	3.39	130.42	123.47
15	cA	1110	CL7	O2D-CGD-O1D	-3.39	117.22	123.84
14	cB	1023	PHO	O1D-CGD-CBD	3.38	130.36	124.74
17	aB	4015	A1JPJ	C12-C13-C14	3.37	124.12	118.94
15	cB	1230	CL7	C3B-C4B-NB	-3.37	107.39	110.52
17	aF	4016	A1JPJ	C20-C21-C22	3.37	132.12	127.31
17	cF	4016	A1JPJ	C15-C16-C17	3.36	130.37	123.47
15	bA	1134	CL7	O2D-CGD-O1D	-3.36	117.27	123.84
17	aB	4017	A1JPJ	C35-C13-C14	-3.36	118.22	122.92
17	bB	4005	A1JPJ	C12-C13-C14	3.35	124.09	118.94
17	cB	4015	A1JPJ	C12-C13-C14	3.35	124.09	118.94
17	bB	4017	A1JPJ	C19-C18-C17	3.35	124.08	118.94
17	cB	4005	A1JPJ	C12-C13-C14	3.35	124.08	118.94
17	bB	4005	A1JPJ	C28-C27-C26	-3.35	121.64	124.85
15	aA	1132	CL7	O2D-CGD-O1D	-3.35	117.30	123.84
17	bB	4015	A1JPJ	C12-C13-C14	3.34	124.07	118.94
17	cB	4004	A1JPJ	C35-C13-C14	-3.34	118.24	122.92
17	aB	4017	A1JPJ	C19-C18-C17	3.34	124.07	118.94
17	bB	4017	A1JPJ	C35-C13-C14	-3.34	118.25	122.92
17	bB	4004	A1JPJ	C35-C13-C14	-3.33	118.26	122.92
17	bA	4002	A1JPJ	C36-C18-C17	-3.33	118.26	122.92
17	cA	4008	A1JPJ	C15-C16-C17	3.32	130.27	123.47
15	cA	1132	CL7	O2D-CGD-O1D	-3.32	117.35	123.84
17	bF	4016	A1JPJ	C36-C18-C17	-3.31	118.28	122.92
15	bL	1502	CL7	O2D-CGD-O1D	-3.31	117.36	123.84
17	cB	4006	A1JPJ	C12-C13-C14	3.31	124.02	118.94
17	cA	4002	A1JPJ	C36-C18-C17	-3.31	118.28	122.92
17	bF	4016	A1JPJ	C25-C26-C27	-3.31	117.40	121.47
15	aA	1132	CL7	CHB-C1B-NB	3.31	127.76	124.26
17	aA	4002	A1JPJ	C36-C18-C17	-3.31	118.29	122.92
15	bB	1209	CL7	O2D-CGD-O1D	-3.30	117.38	123.84
15	bB	1230	CL7	C3B-C4B-NB	-3.30	107.45	110.52
17	cB	4015	A1JPJ	C8-C9-C10	3.30	124.01	118.94
17	bB	4006	A1JPJ	C12-C13-C14	3.30	124.01	118.94
15	aL	1502	CL7	O2D-CGD-O1D	-3.30	117.39	123.84
15	cB	1212	CL7	O2D-CGD-O1D	-3.30	117.39	123.84
14	cA	1013	PHO	C2B-C1B-NB	-3.30	107.25	109.53
17	aB	4005	A1JPJ	C12-C13-C14	3.29	124.00	118.94
17	bA	4008	A1JPJ	C15-C16-C17	3.29	130.22	123.47
15	aB	1241	CL7	O2D-CGD-O1D	-3.29	117.40	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	cB	4017	A1JPJ	C19-C18-C17	3.29	123.99	118.94
17	aB	4004	A1JPJ	C35-C13-C14	-3.29	118.31	122.92
17	bB	4004	A1JPJ	C16-C15-C14	3.29	130.21	123.47
15	aB	1230	CL7	O2D-CGD-O1D	-3.29	117.41	123.84
17	bI	4019	A1JPJ	C35-C13-C14	-3.28	118.32	122.92
17	aB	4015	A1JPJ	C36-C18-C17	-3.28	118.33	122.92
17	aB	4004	A1JPJ	C16-C15-C14	3.28	130.19	123.47
15	bA	1132	CL7	O2D-CGD-O1D	-3.28	117.43	123.84
15	aA	1109	CL7	O2D-CGD-O1D	-3.28	117.43	123.84
15	cB	1216	CL7	O2D-CGD-O1D	-3.28	117.43	123.84
17	cB	4017	A1JPJ	C35-C13-C14	-3.28	118.33	122.92
17	bF	4016	A1JPJ	C15-C16-C17	3.27	130.18	123.47
17	bF	4016	A1JPJ	C35-C13-C14	-3.27	118.35	122.92
17	aL	4020	A1JPJ	C36-C18-C17	-3.26	118.35	122.92
17	cB	4015	A1JPJ	C36-C18-C17	-3.26	118.36	122.92
17	cL	4020	A1JPJ	C36-C18-C17	-3.26	118.36	122.92
17	aB	4015	A1JPJ	C15-C16-C17	3.26	130.14	123.47
15	aB	1212	CL7	O2D-CGD-O1D	-3.25	117.48	123.84
17	cF	4016	A1JPJ	C35-C13-C14	-3.25	118.36	122.92
17	cA	4008	A1JPJ	C28-C27-C26	-3.25	121.73	124.85
17	bB	4010	A1JPJ	C8-C9-C10	3.25	123.93	118.94
17	bL	4020	A1JPJ	C36-C18-C17	-3.25	118.37	122.92
17	cI	4019	A1JPJ	C35-C13-C14	-3.25	118.37	122.92
15	aA	1125	CL7	C1-C2-C3	-3.25	121.50	126.75
15	cL	1502	CL7	O2D-CGD-O1D	-3.24	117.50	123.84
15	cA	1115	CL7	C3B-C4B-NB	-3.24	107.51	110.52
15	cA	1106	CL7	C3B-C4B-NB	-3.24	107.51	110.52
15	aB	1209	CL7	O2D-CGD-O1D	-3.24	117.51	123.84
17	aF	4016	A1JPJ	C21-C20-C19	3.24	133.31	123.22
17	cB	4004	A1JPJ	C19-C18-C17	3.23	123.90	118.94
17	aI	4019	A1JPJ	C35-C13-C14	-3.23	118.39	122.92
15	cB	1230	CL7	OBB-CAB-C3B	-3.23	118.38	125.69
15	aA	1134	CL7	O2D-CGD-O1D	-3.23	117.52	123.84
17	bA	4003	A1JPJ	C35-C13-C14	-3.23	118.40	122.92
17	cA	4007	A1JPJ	C36-C18-C17	-3.23	118.40	122.92
17	bA	4003	A1JPJ	C36-C18-C17	-3.23	118.40	122.92
15	bA	1106	CL7	C3B-C4B-NB	-3.23	107.52	110.52
17	cB	4010	A1JPJ	C8-C9-C10	3.22	123.89	118.94
15	bA	1125	CL7	C3B-C4B-NB	-3.22	107.53	110.52
15	bB	1213	CL7	O2D-CGD-O1D	-3.22	117.55	123.84
17	bB	4004	A1JPJ	C19-C18-C17	3.22	123.88	118.94
15	bA	1125	CL7	C1-C2-C3	-3.21	121.56	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aA	4003	A1JPJ	C36-C18-C17	-3.21	118.43	122.92
15	aK	1401	CL7	O2D-CGD-O1D	-3.21	117.57	123.84
17	aB	4004	A1JPJ	C19-C18-C17	3.20	123.86	118.94
17	cB	4004	A1JPJ	C16-C15-C14	3.20	130.04	123.47
15	bK	1401	CL7	O2D-CGD-O1D	-3.20	117.57	123.84
17	cA	4003	A1JPJ	C35-C13-C14	-3.20	118.44	122.92
17	aL	4020	A1JPJ	C12-C13-C14	3.20	123.86	118.94
15	cB	1221	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
15	bB	1212	CL7	O2D-CGD-O1D	-3.20	117.58	123.84
17	cL	4020	A1JPJ	C12-C13-C14	3.20	123.85	118.94
17	bB	4015	A1JPJ	C36-C18-C17	-3.20	118.44	122.92
17	aA	4003	A1JPJ	C35-C13-C14	-3.20	118.44	122.92
15	aB	1205	CL7	O2D-CGD-O1D	-3.20	117.59	123.84
15	aL	1501	CL7	C3B-C4B-NB	-3.19	107.55	110.52
15	cA	1112	CL7	C3B-C4B-NB	-3.19	107.55	110.52
17	bI	4018	A1JPJ	C16-C15-C14	3.19	130.00	123.47
15	aA	1106	CL7	C3B-C4B-NB	-3.19	107.56	110.52
15	cA	1135	CL7	C3B-C4B-NB	-3.19	107.56	110.52
15	cK	1401	CL7	O2D-CGD-O1D	-3.19	117.61	123.84
15	aA	1135	CL7	C3B-C4B-NB	-3.18	107.56	110.52
15	aB	1203	CL7	C3B-C4B-NB	-3.18	107.56	110.52
15	bB	1203	CL7	C3B-C4B-NB	-3.18	107.56	110.52
15	bB	1230	CL7	O2D-CGD-O1D	-3.18	117.62	123.84
17	aB	4010	A1JPJ	C8-C9-C10	3.18	123.82	118.94
17	aB	4017	A1JPJ	C16-C15-C14	3.18	129.99	123.47
15	bB	1238	CL7	C3B-C4B-NB	-3.18	107.57	110.52
17	cL	4023	A1JPJ	C36-C18-C17	-3.18	118.47	122.92
15	bB	1230	CL7	OBB-CAB-C3B	-3.18	118.50	125.69
15	cB	1209	CL7	O2D-CGD-O1D	-3.18	117.63	123.84
15	bB	1221	CL7	C3A-C4A-CHB	-3.17	118.99	123.70
15	aA	1112	CL7	C3B-C4B-NB	-3.17	107.57	110.52
15	cA	1113	CL7	O2D-CGD-O1D	-3.17	117.63	123.84
17	bA	4007	A1JPJ	C36-C18-C17	-3.17	118.48	122.92
15	bL	1501	CL7	C3B-C4B-NB	-3.17	107.57	110.52
17	bL	4023	A1JPJ	C36-C18-C17	-3.17	118.48	122.92
15	cB	1213	CL7	O2D-CGD-O1D	-3.17	117.64	123.84
15	bA	1118	CL7	O2D-CGD-O1D	-3.17	117.64	123.84
15	aB	1210	CL7	C3B-C4B-NB	-3.17	107.58	110.52
17	cA	4003	A1JPJ	C36-C18-C17	-3.16	118.49	122.92
15	aB	1221	CL7	C3A-C4A-CHB	-3.16	119.01	123.70
15	cA	1134	CL7	O2D-CGD-O1D	-3.16	117.66	123.84
15	cB	1230	CL7	O2D-CGD-O1D	-3.16	117.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1116	CL7	C3B-C4B-NB	-3.16	107.58	110.52
15	bA	1102	CL7	C3B-C4B-NB	-3.16	107.59	110.52
15	bA	1112	CL7	C3B-C4B-NB	-3.16	107.59	110.52
15	bB	1207	CL7	C3B-C4B-NB	-3.16	107.59	110.52
15	bB	1210	CL7	C3B-C4B-NB	-3.16	107.59	110.52
17	aI	4018	A1JPJ	C16-C15-C14	3.16	129.94	123.47
15	aB	1213	CL7	O2D-CGD-O1D	-3.15	117.67	123.84
17	bB	4015	A1JPJ	C8-C9-C10	3.15	123.78	118.94
15	cB	1211	CL7	C3B-C4B-NB	-3.15	107.59	110.52
14	aA	1013	PHO	C2B-C1B-NB	-3.15	107.35	109.53
15	aA	1130	CL7	C3B-C4B-NB	-3.14	107.60	110.52
15	aB	1230	CL7	C3B-C4B-NB	-3.14	107.60	110.52
15	bB	1241	CL7	O2D-CGD-O1D	-3.14	117.70	123.84
15	aB	1230	CL7	OBB-CAB-C3B	-3.14	118.59	125.69
15	cB	1202	CL7	C3B-C4B-NB	-3.13	107.61	110.52
15	cL	1502	CL7	C3B-C4B-NB	-3.13	107.61	110.52
17	bL	4020	A1JPJ	C12-C13-C14	3.13	123.74	118.94
15	bB	1205	CL7	O2D-CGD-O1D	-3.12	117.73	123.84
17	aB	4021	A1JPJ	C35-C13-C14	-3.12	118.55	122.92
17	cA	4007	A1JPJ	C35-C13-C14	-3.12	118.55	122.92
17	aA	4007	A1JPJ	C36-C18-C17	-3.12	118.55	122.92
17	bJ	4012	A1JPJ	C36-C18-C17	-3.12	118.55	122.92
15	cA	1102	CL7	C3B-C4B-NB	-3.12	107.62	110.52
15	aA	1118	CL7	O2D-CGD-O1D	-3.12	117.75	123.84
15	cA	1118	CL7	O2D-CGD-O1D	-3.12	117.75	123.84
17	bB	4021	A1JPJ	C35-C13-C14	-3.12	118.56	122.92
15	cB	1205	CL7	O2D-CGD-O1D	-3.11	117.75	123.84
15	aA	1103	CL7	O2D-CGD-O1D	-3.11	117.76	123.84
17	cI	4018	A1JPJ	C16-C15-C14	3.11	129.85	123.47
17	bA	4007	A1JPJ	C35-C13-C14	-3.11	118.57	122.92
17	bA	4003	A1JPJ	C15-C16-C17	3.11	129.84	123.47
17	bB	4017	A1JPJ	C16-C15-C14	3.11	129.84	123.47
15	aA	1102	CL7	C3B-C4B-NB	-3.11	107.63	110.52
14	bA	1013	PHO	C2B-C1B-NB	-3.10	107.38	109.53
15	cB	1219	CL7	O2D-CGD-O1D	-3.10	117.77	123.84
15	bA	1103	CL7	O2D-CGD-O1D	-3.10	117.77	123.84
15	aA	1115	CL7	C3B-C4B-NB	-3.10	107.64	110.52
15	bA	1101	CL7	O2D-CGD-O1D	-3.10	117.78	123.84
15	bA	1128	CL7	O2D-CGD-O1D	-3.10	117.78	123.84
15	cL	1501	CL7	C3B-C4B-NB	-3.10	107.64	110.52
17	cB	4017	A1JPJ	C16-C15-C14	3.10	129.81	123.47
15	cA	1112	CL7	OBB-CAB-C3B	-3.10	118.69	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1204	CL7	O2D-CGD-O1D	-3.09	117.79	123.84
13	aA	1011	G9R	O2D-CGD-O1D	-3.09	117.79	123.84
17	cB	4021	A1JPJ	C35-C13-C14	-3.09	118.59	122.92
15	bB	1208	CL7	O2D-CGD-O1D	-3.09	117.79	123.84
15	bA	1116	CL7	C3B-C4B-NB	-3.09	107.65	110.52
15	cB	1206	CL7	C3B-C4B-NB	-3.09	107.65	110.52
15	cB	1203	CL7	C3B-C4B-NB	-3.09	107.65	110.52
15	aA	1122	CL7	C3B-C4B-NB	-3.09	107.65	110.52
15	cB	1238	CL7	C3B-C4B-NB	-3.09	107.65	110.52
17	aL	4023	A1JPJ	C19-C18-C17	3.09	123.68	118.94
15	cA	1109	CL7	O2D-CGD-O1D	-3.09	117.81	123.84
15	aB	1238	CL7	C3B-C4B-NB	-3.09	107.65	110.52
15	cA	1103	CL7	O2D-CGD-O1D	-3.08	117.81	123.84
15	aB	1202	CL7	C3B-C4B-NB	-3.08	107.65	110.52
15	cA	1101	CL7	O2D-CGD-O1D	-3.08	117.81	123.84
15	aB	1206	CL7	C3B-C4B-NB	-3.08	107.66	110.52
15	cA	1104	CL7	C3B-C4B-NB	-3.08	107.66	110.52
17	aA	4011	A1JPJ	C35-C13-C14	-3.08	118.61	122.92
15	aA	1116	CL7	C3B-C4B-NB	-3.08	107.66	110.52
17	aA	4007	A1JPJ	C35-C13-C14	-3.07	118.62	122.92
15	aB	1204	CL7	O2D-CGD-O1D	-3.07	117.83	123.84
15	cA	1125	CL7	C1-C2-C3	-3.07	121.78	126.75
17	cA	4003	A1JPJ	C15-C16-C17	3.07	129.77	123.47
15	bA	1135	CL7	C3B-C4B-NB	-3.07	107.67	110.52
15	cA	1130	CL7	C3B-C4B-NB	-3.07	107.67	110.52
15	bA	1138	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
15	cA	1137	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
15	cB	1204	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
15	aA	1101	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
17	aF	4016	A1JPJ	C8-C9-C10	3.06	123.64	118.94
17	cB	4010	A1JPJ	C36-C18-C17	-3.06	118.63	122.92
15	bA	1111	CL7	C3B-C4B-NB	-3.06	107.67	110.52
15	bB	1202	CL7	C3B-C4B-NB	-3.06	107.67	110.52
15	bL	1502	CL7	C3B-C4B-NB	-3.06	107.68	110.52
17	cB	4015	A1JPJ	C15-C16-C17	3.06	129.74	123.47
15	aA	1126	CL7	C3B-C4B-NB	-3.06	107.68	110.52
15	bB	1219	CL7	O2D-CGD-O1D	-3.06	117.86	123.84
17	cJ	4012	A1JPJ	C36-C18-C17	-3.06	118.64	122.92
15	aB	1219	CL7	O2D-CGD-O1D	-3.05	117.87	123.84
15	bA	1110	CL7	C3B-C4B-NB	-3.05	107.68	110.52
15	cB	1201	CL7	O2D-CGD-O1D	-3.05	117.87	123.84
15	aB	1230	CL7	C3A-C4A-CHB	-3.05	119.17	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	cA	4011	A1JPJ	C35-C13-C14	-3.05	118.65	122.92
15	bA	1104	CL7	C3B-C4B-NB	-3.05	107.69	110.52
15	cA	1125	CL7	C3B-C4B-NB	-3.05	107.69	110.52
13	bA	1011	G9R	O2D-CGD-O1D	-3.05	117.88	123.84
15	bA	1130	CL7	C3B-C4B-NB	-3.05	107.69	110.52
15	cB	1214	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
15	cB	1220	CL7	O2D-CGD-O1D	-3.04	117.89	123.84
15	bA	1105	CL7	C3B-C4B-NB	-3.04	107.69	110.52
14	cB	1023	PHO	CMB-C2B-C3B	3.04	130.37	124.68
15	bB	1201	CL7	O2D-CGD-O1D	-3.04	117.89	123.84
17	cB	4021	A1JPJ	C36-C18-C17	-3.04	118.67	122.92
15	aA	1105	CL7	C3B-C4B-NB	-3.04	107.70	110.52
15	cA	1117	CL7	O2D-CGD-O1D	-3.04	117.90	123.84
15	cB	1207	CL7	C3B-C4B-NB	-3.04	107.70	110.52
17	aA	4003	A1JPJ	C15-C16-C17	3.04	129.69	123.47
17	aJ	4012	A1JPJ	C36-C18-C17	-3.03	118.67	122.92
15	aL	1502	CL7	C3B-C4B-NB	-3.03	107.70	110.52
15	cB	1214	CL7	C3B-C4B-NB	-3.03	107.70	110.52
15	bA	1119	CL7	C3B-C4B-NB	-3.03	107.70	110.52
15	bA	1109	CL7	O2D-CGD-O1D	-3.03	117.92	123.84
15	bB	1234	CL7	O2D-CGD-O1D	-3.03	117.92	123.84
15	cA	1136	CL7	C3B-C4B-NB	-3.03	107.71	110.52
15	cA	1126	CL7	C3B-C4B-NB	-3.03	107.71	110.52
15	aA	1128	CL7	O2D-CGD-O1D	-3.03	117.92	123.84
15	aA	1137	CL7	O2D-CGD-O1D	-3.02	117.92	123.84
15	aB	1208	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
14	bA	1013	PHO	CMB-C2B-C3B	3.02	130.34	124.68
15	aB	1226	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
15	bA	1117	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
17	cA	4002	A1JPJ	C19-C18-C17	3.02	123.58	118.94
15	bB	1239	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
15	cB	1236	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
15	aB	1215	CL7	O2D-CGD-O1D	-3.02	117.93	123.84
17	aL	4023	A1JPJ	C35-C13-C14	-3.02	118.69	122.92
15	bB	1206	CL7	C3B-C4B-NB	-3.02	107.71	110.52
15	bL	1503	CL7	C3B-C4B-NB	-3.02	107.71	110.52
15	cA	1111	CL7	C3B-C4B-NB	-3.02	107.71	110.52
17	bB	4005	A1JPJ	C36-C18-C17	-3.02	118.69	122.92
15	bB	1230	CL7	C3A-C4A-CHB	-3.02	119.22	123.70
17	aL	4020	A1JPJ	C15-C16-C17	3.02	129.66	123.47
15	aB	1236	CL7	O2D-CGD-O1D	-3.02	117.94	123.84
15	aA	1112	CL7	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1207	CL7	C3B-C4B-NB	-3.02	107.72	110.52
15	aA	1110	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	aA	1136	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	bB	1211	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	cB	1230	CL7	C3A-C4A-CHB	-3.01	119.23	123.70
15	cA	1110	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	cB	1226	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	bA	1124	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
17	bB	4010	A1JPJ	C36-C18-C17	-3.01	118.70	122.92
15	cA	1119	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	cA	1127	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
15	cA	1801	CL7	C3B-C4B-NB	-3.01	107.72	110.52
15	bB	1235	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
15	bL	1503	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
17	bI	4019	A1JPJ	C36-C18-C17	-3.01	118.71	122.92
15	bB	1214	CL7	C3B-C4B-NB	-3.01	107.73	110.52
15	bB	1236	CL7	O2D-CGD-O1D	-3.01	117.96	123.84
15	aA	1112	CL7	OBB-CAB-C3B	-3.01	118.89	125.69
17	aB	4010	A1JPJ	C36-C18-C17	-3.01	118.71	122.92
15	bA	1124	CL7	C3B-C4B-NB	-3.01	107.73	110.52
17	aA	4002	A1JPJ	C35-C13-C14	-3.00	118.71	122.92
15	bA	1137	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
15	aA	1104	CL7	C3B-C4B-NB	-3.00	107.73	110.52
15	cB	1208	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
17	bI	4018	A1JPJ	C35-C13-C14	-3.00	118.72	122.92
15	bA	1101	CL7	C3B-C4B-NB	-3.00	107.73	110.52
15	cA	1128	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
15	aB	1235	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
15	cA	1112	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
15	aA	1022	CL7	O2D-CGD-O1D	-3.00	117.98	123.84
15	aB	1211	CL7	C3B-C4B-NB	-3.00	107.73	110.52
15	cB	1220	CL7	C3B-C4B-NB	-3.00	107.74	110.52
15	cA	1135	CL7	C2D-C1D-ND	-3.00	108.22	110.23
13	cA	1011	G9R	O2D-CGD-O1D	-2.99	117.98	123.84
17	bA	4002	A1JPJ	C19-C18-C17	2.99	123.53	118.94
17	bL	4023	A1JPJ	C35-C13-C14	-2.99	118.73	122.92
15	aA	1124	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
15	cB	1239	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
15	aB	1223	CL7	C3B-C4B-NB	-2.99	107.74	110.52
14	bB	1023	PHO	C2B-C1B-NB	-2.99	107.46	109.53
15	bA	1121	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
15	bA	1122	CL7	C3B-C4B-NB	-2.99	107.74	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1124	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
17	bA	4002	A1JPJ	C35-C13-C14	-2.99	118.74	122.92
15	cA	1115	CL7	CAA-C2A-C3A	-2.99	109.13	116.10
17	aB	4021	A1JPJ	C36-C18-C17	-2.99	118.74	122.92
17	aI	4019	A1JPJ	C36-C18-C17	-2.99	118.74	122.92
17	bB	4021	A1JPJ	C36-C18-C17	-2.99	118.74	122.92
17	aB	4005	A1JPJ	C36-C18-C17	-2.99	118.74	122.92
17	cA	4002	A1JPJ	C35-C13-C14	-2.99	118.74	122.92
15	bA	1132	CL7	C3B-C4B-NB	-2.99	107.75	110.52
15	cA	1140	CL7	O2D-CGD-O1D	-2.98	118.00	123.84
17	cF	4016	A1JPJ	C19-C18-C17	2.98	123.52	118.94
15	cA	1121	CL7	O2D-CGD-O1D	-2.98	118.00	123.84
15	aL	1503	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	cB	1235	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	aA	1117	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	aA	1121	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	bB	1226	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	cB	1202	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
15	cA	1022	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
17	aA	4002	A1JPJ	C19-C18-C17	2.98	123.51	118.94
15	aA	1127	CL7	O2D-CGD-O1D	-2.98	118.01	123.84
17	aB	4017	A1JPJ	C12-C13-C14	2.98	123.51	118.94
15	cA	1138	CL7	O2D-CGD-O1D	-2.98	118.02	123.84
15	bA	1136	CL7	O2D-CGD-O1D	-2.98	118.02	123.84
15	aB	1239	CL7	O2D-CGD-O1D	-2.97	118.02	123.84
15	aB	1217	CL7	O2D-CGD-O1D	-2.97	118.02	123.84
15	bA	1136	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	cB	1210	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
15	cB	1223	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	aA	1105	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
15	bB	1211	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
15	aA	1115	CL7	CAA-C2A-C3A	-2.97	109.16	116.10
17	bL	4020	A1JPJ	C15-C16-C17	2.97	129.56	123.47
15	cA	1124	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	cB	1210	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	aB	1211	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
15	cB	1241	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
15	aA	1124	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	aA	1106	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
17	cB	4005	A1JPJ	C36-C18-C17	-2.97	118.77	122.92
15	cB	1234	CL7	O2D-CGD-O1D	-2.97	118.04	123.84
15	bB	1215	CL7	O2D-CGD-O1D	-2.97	118.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1210	CL7	O2D-CGD-O1D	-2.97	118.04	123.84
15	bA	1125	CL7	O2D-CGD-O1D	-2.97	118.04	123.84
15	cB	1228	CL7	C3B-C4B-NB	-2.97	107.76	110.52
15	bA	1130	CL7	O2D-CGD-O1D	-2.96	118.04	123.84
15	cA	1105	CL7	C3B-C4B-NB	-2.96	107.77	110.52
15	cA	1102	CL7	O2D-CGD-O1D	-2.96	118.04	123.84
17	bB	4015	A1JPJ	C15-C16-C17	2.96	129.54	123.47
15	aB	1201	CL7	O2D-CGD-O1D	-2.96	118.05	123.84
15	aB	1202	CL7	O2D-CGD-O1D	-2.96	118.05	123.84
15	aB	1012	CL7	O2D-CGD-O1D	-2.96	118.06	123.84
15	bA	1109	CL7	C3B-C4B-NB	-2.96	107.77	110.52
15	cA	1139	CL7	C3B-C4B-NB	-2.96	107.77	110.52
17	bF	4016	A1JPJ	C19-C18-C17	2.96	123.48	118.94
15	aA	1102	CL7	O2D-CGD-O1D	-2.96	118.06	123.84
15	aA	1125	CL7	O2D-CGD-O1D	-2.95	118.06	123.84
15	bA	1123	CL7	C3B-C4B-NB	-2.95	107.78	110.52
15	cA	1101	CL7	C3B-C4B-NB	-2.95	107.78	110.52
17	cI	4019	A1JPJ	C36-C18-C17	-2.95	118.79	122.92
17	bB	4017	A1JPJ	C12-C13-C14	2.95	123.47	118.94
14	aB	1023	PHO	CMB-C2B-C3B	2.95	130.19	124.68
15	aB	1234	CL7	O2D-CGD-O1D	-2.95	118.08	123.84
15	aA	1138	CL7	O2D-CGD-O1D	-2.95	118.08	123.84
15	cB	1211	CL7	O2D-CGD-O1D	-2.95	118.08	123.84
14	aA	1013	PHO	CMB-C2B-C3B	2.95	130.19	124.68
17	cI	4018	A1JPJ	C35-C13-C14	-2.95	118.80	122.92
15	aB	1223	CL7	O2D-CGD-O1D	-2.95	118.08	123.84
15	bA	1102	CL7	O2D-CGD-O1D	-2.94	118.08	123.84
15	aB	1234	CL7	C3B-C4B-NB	-2.94	107.78	110.52
15	bB	1207	CL7	O2D-CGD-O1D	-2.94	118.08	123.84
15	bB	1210	CL7	O2D-CGD-O1D	-2.94	118.08	123.84
17	cL	4023	A1JPJ	C35-C13-C14	-2.94	118.80	122.92
15	aA	1136	CL7	O2D-CGD-O1D	-2.94	118.08	123.84
15	bB	1225	CL7	O2D-CGD-O1D	-2.94	118.08	123.84
15	cB	1217	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
15	aA	1119	CL7	C3B-C4B-NB	-2.94	107.79	110.52
14	bA	1013	PHO	CMA-C3A-C4A	-2.94	107.94	114.38
15	aB	1206	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
15	cB	1238	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
15	bB	1227	CL7	CHB-C1B-NB	2.94	127.37	124.26
15	cB	1234	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	bA	1112	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
15	cA	1111	CL7	O2D-CGD-O1D	-2.94	118.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1237	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	cA	1129	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	bA	1127	CL7	O2D-CGD-O1D	-2.94	118.10	123.84
17	aB	4004	A1JPJ	C12-C13-C14	2.94	123.45	118.94
15	cA	1107	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	cA	1133	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	bB	1231	CL7	O2D-CGD-O1D	-2.94	118.10	123.84
15	bB	1237	CL7	C3B-C4B-NB	-2.94	107.79	110.52
15	bB	1229	CL7	O2D-CGD-O1D	-2.93	118.10	123.84
15	cA	1135	CL7	O2D-CGD-O1D	-2.93	118.10	123.84
15	cA	1123	CL7	C3B-C4B-NB	-2.93	107.79	110.52
17	cL	4020	A1JPJ	C15-C16-C17	2.93	129.48	123.47
17	bB	4004	A1JPJ	C12-C13-C14	2.93	123.44	118.94
14	bB	1023	PHO	CMB-C2B-C3B	2.93	130.17	124.68
15	bA	1140	CL7	O2D-CGD-O1D	-2.93	118.10	123.84
15	cA	1136	CL7	O2D-CGD-O1D	-2.93	118.10	123.84
17	aI	4018	A1JPJ	C35-C13-C14	-2.93	118.81	122.92
15	cL	1503	CL7	C3B-C4B-NB	-2.93	107.80	110.52
17	aI	4018	A1JPJ	C36-C18-C17	-2.93	118.82	122.92
17	bA	4014	A1JPJ	C37-C22-C23	2.93	122.70	118.08
15	cA	1125	CL7	O2D-CGD-O1D	-2.93	118.11	123.84
15	cB	1231	CL7	O2D-CGD-O1D	-2.93	118.11	123.84
15	bA	1102	CL7	C3A-C4A-CHB	-2.93	119.35	123.70
15	aA	1130	CL7	O2D-CGD-O1D	-2.93	118.11	123.84
15	bA	1133	CL7	C3B-C4B-NB	-2.93	107.80	110.52
15	cA	1103	CL7	C3B-C4B-NB	-2.93	107.80	110.52
14	cA	1013	PHO	CMB-C2B-C3B	2.93	130.16	124.68
17	bA	4014	A1JPJ	C20-C21-C22	2.93	131.49	127.31
15	bB	1234	CL7	C3B-C4B-NB	-2.93	107.80	110.52
15	bB	1228	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
15	cA	1106	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
15	cB	1206	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
15	bB	1225	CL7	C3B-C4B-NB	-2.92	107.80	110.52
15	bB	1217	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
15	cA	1129	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
15	cA	1131	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
17	cB	4004	A1JPJ	C12-C13-C14	2.92	123.42	118.94
15	aL	1503	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	cB	1239	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	aA	1140	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
15	aB	1232	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
15	cA	1122	CL7	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1012	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
15	aA	1111	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	aB	1228	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	aA	1129	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
15	bB	1214	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
15	aB	1215	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	bB	1206	CL7	O2D-CGD-O1D	-2.92	118.14	123.84
15	aA	1133	CL7	C3B-C4B-NB	-2.92	107.81	110.52
15	bA	1111	CL7	O2D-CGD-O1D	-2.92	118.14	123.84
15	cA	1130	CL7	O2D-CGD-O1D	-2.92	118.14	123.84
15	aA	1113	CL7	O2D-CGD-O1D	-2.91	118.14	123.84
15	aA	1123	CL7	C3B-C4B-NB	-2.91	107.81	110.52
15	cJ	1302	CL7	C3B-C4B-NB	-2.91	107.81	110.52
15	aB	1231	CL7	O2D-CGD-O1D	-2.91	118.14	123.84
15	aA	1134	CL7	C3B-C4B-NB	-2.91	107.81	110.52
15	aB	1207	CL7	O2D-CGD-O1D	-2.91	118.14	123.84
15	aB	1239	CL7	C3B-C4B-NB	-2.91	107.81	110.52
15	bA	1139	CL7	C3B-C4B-NB	-2.91	107.81	110.52
15	cB	1222	CL7	C3B-C4B-NB	-2.91	107.81	110.52
17	bI	4018	A1JPJ	C36-C18-C17	-2.91	118.84	122.92
15	cB	1207	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
15	bB	1202	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
15	bA	1106	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
15	cA	1112	CL7	C3A-C4A-CHB	-2.91	119.38	123.70
15	aB	1214	CL7	C3B-C4B-NB	-2.91	107.82	110.52
15	bB	1222	CL7	C3B-C4B-NB	-2.91	107.82	110.52
15	bB	1239	CL7	C3B-C4B-NB	-2.91	107.82	110.52
15	bA	1105	CL7	O2D-CGD-O1D	-2.91	118.16	123.84
15	cB	1223	CL7	O2D-CGD-O1D	-2.91	118.16	123.84
15	aA	1111	CL7	O2D-CGD-O1D	-2.91	118.16	123.84
15	aA	1139	CL7	C3B-C4B-NB	-2.91	107.82	110.52
15	bB	1228	CL7	C3B-C4B-NB	-2.90	107.82	110.52
15	cA	1134	CL7	C3B-C4B-NB	-2.90	107.82	110.52
15	aA	1101	CL7	C3B-C4B-NB	-2.90	107.82	110.52
15	bA	1129	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	bA	1134	CL7	C3B-C4B-NB	-2.90	107.83	110.52
15	aA	1133	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	aB	1228	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	bA	1114	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	bB	1237	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	aI	1601	CL7	C3B-C4B-NB	-2.90	107.83	110.52
17	aA	4014	A1JPJ	C15-C14-C13	2.90	131.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1214	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
15	cA	1120	CL7	O2D-CGD-O1D	-2.90	118.18	123.84
15	cA	1105	CL7	O2D-CGD-O1D	-2.90	118.18	123.84
15	aA	1129	CL7	C3B-C4B-NB	-2.90	107.83	110.52
15	cB	1237	CL7	C3B-C4B-NB	-2.90	107.83	110.52
15	bB	1227	CL7	CMB-C2B-C1B	-2.89	120.96	125.37
15	cB	1012	CL7	O2D-CGD-O1D	-2.89	118.18	123.84
15	cA	1114	CL7	O2D-CGD-O1D	-2.89	118.18	123.84
15	aB	1238	CL7	O2D-CGD-O1D	-2.89	118.18	123.84
17	cB	4017	A1JPJ	C12-C13-C14	2.89	123.38	118.94
15	bA	1133	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
15	cA	1133	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
17	aF	4016	A1JPJ	C37-C22-C21	-2.89	118.87	122.92
15	cB	1228	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
15	cB	1227	CL7	C3B-C4B-NB	-2.89	107.83	110.52
15	cA	1123	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
15	cB	1232	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
15	aA	1107	CL7	C3B-C4B-NB	-2.89	107.84	110.52
15	aA	1120	CL7	C3B-C4B-NB	-2.89	107.84	110.52
17	bL	4023	A1JPJ	C16-C15-C14	2.89	129.39	123.47
15	cA	1104	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
15	bB	1218	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
14	aA	1013	PHO	CMA-C3A-C4A	-2.88	108.06	114.38
15	bA	1801	CL7	C3B-C4B-NB	-2.88	107.84	110.52
15	cA	1108	CL7	C3B-C4B-NB	-2.88	107.84	110.52
15	bB	1216	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
15	aB	1224	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
15	bF	1701	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
15	cB	1218	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
15	aB	1220	CL7	C3B-C4B-NB	-2.88	107.84	110.52
17	bA	4011	A1JPJ	C35-C13-C14	-2.88	118.89	122.92
14	aB	1023	PHO	C2B-C1B-NB	-2.88	107.54	109.53
15	bB	1224	CL7	O2D-CGD-O1D	-2.88	118.21	123.84
15	cA	1122	CL7	C3B-C4B-NB	-2.88	107.84	110.52
15	cB	1221	CL7	O2D-CGD-O1D	-2.88	118.21	123.84
17	aA	4014	A1JPJ	C37-C22-C23	2.88	122.61	118.08
15	bB	1223	CL7	O2D-CGD-O1D	-2.88	118.21	123.84
15	bA	1107	CL7	C3B-C4B-NB	-2.87	107.85	110.52
17	aA	4007	A1JPJ	C16-C15-C14	2.87	129.36	123.47
15	aB	1218	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
15	aA	1114	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
15	aF	1701	CL7	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1123	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
15	cB	1226	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
15	aB	1235	CL7	C3B-C4B-NB	-2.87	107.85	110.52
15	bB	1012	CL7	C3B-C4B-NB	-2.87	107.85	110.52
15	cB	1224	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	cB	1237	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
17	cA	4007	A1JPJ	C16-C15-C14	2.87	129.35	123.47
15	aB	1221	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	aB	1222	CL7	C3B-C4B-NB	-2.87	107.86	110.52
17	cA	4008	A1JPJ	C36-C18-C17	-2.87	118.91	122.92
15	aA	1123	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	aB	1237	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	cI	1601	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	aA	1104	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	cL	1503	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	bI	1601	CL7	C3B-C4B-NB	-2.87	107.86	110.52
17	cI	4018	A1JPJ	C36-C18-C17	-2.86	118.91	122.92
15	bB	1233	CL7	O2D-CGD-O1D	-2.86	118.24	123.84
15	bB	1238	CL7	O2D-CGD-O1D	-2.86	118.24	123.84
15	bB	1223	CL7	C3B-C4B-NB	-2.86	107.86	110.52
17	cB	4010	A1JPJ	C15-C16-C17	2.86	129.34	123.47
15	bB	1220	CL7	C3B-C4B-NB	-2.86	107.86	110.52
15	bB	1208	CL7	C3B-C4B-NB	-2.86	107.86	110.52
15	cB	1233	CL7	O2D-CGD-O1D	-2.86	118.25	123.84
14	cB	1023	PHO	C2B-C1B-NB	-2.86	107.55	109.53
15	cB	1229	CL7	O2D-CGD-O1D	-2.86	118.25	123.84
15	aA	1801	CL7	O2D-CGD-O1D	-2.86	118.25	123.84
15	bB	1218	CL7	C3B-C4B-NB	-2.86	107.86	110.52
17	cB	4004	A1JPJ	C8-C9-C10	2.85	123.32	118.94
15	bB	1221	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
17	bL	4020	A1JPJ	C19-C18-C17	2.85	123.32	118.94
17	bA	4007	A1JPJ	C16-C15-C14	2.85	129.32	123.47
15	bA	1103	CL7	C3B-C4B-NB	-2.85	107.87	110.52
15	bA	1113	CL7	C3B-C4B-NB	-2.85	107.87	110.52
15	cA	1120	CL7	C3B-C4B-NB	-2.85	107.87	110.52
15	cB	1216	CL7	C3B-C4B-NB	-2.85	107.87	110.52
15	cB	1218	CL7	C3B-C4B-NB	-2.85	107.87	110.52
15	aB	1218	CL7	C3B-C4B-NB	-2.85	107.87	110.52
17	cL	4020	A1JPJ	C19-C18-C17	2.85	123.31	118.94
17	aA	4014	A1JPJ	C20-C21-C22	2.85	131.38	127.31
15	aA	1120	CL7	O2D-CGD-O1D	-2.85	118.27	123.84
15	bA	1022	CL7	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1115	CL7	O2D-CGD-O1D	-2.85	118.27	123.84
17	bF	4016	A1JPJ	C12-C13-C14	2.85	123.31	118.94
15	bB	1203	CL7	O2D-CGD-O1D	-2.85	118.27	123.84
15	bA	1122	CL7	O2D-CGD-O1D	-2.85	118.28	123.84
17	bA	4008	A1JPJ	C36-C18-C17	-2.84	118.94	122.92
17	bA	4014	A1JPJ	C15-C14-C13	2.84	131.37	127.31
15	aB	1229	CL7	O2D-CGD-O1D	-2.84	118.28	123.84
17	cA	4014	A1JPJ	C20-C21-C22	2.84	131.36	127.31
15	cB	1235	CL7	C3B-C4B-NB	-2.84	107.88	110.52
15	bJ	1301	CL7	C3B-C4B-NB	-2.84	107.88	110.52
15	cA	1113	CL7	C3B-C4B-NB	-2.84	107.88	110.52
15	aA	1122	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
15	aB	1233	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
15	cB	1021	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
15	aK	1402	CL7	CAA-C2A-C3A	-2.84	109.48	116.10
15	bA	1135	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
15	cA	1107	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
17	aA	4008	A1JPJ	C36-C18-C17	-2.84	118.95	122.92
15	aA	1801	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	bA	1129	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	aA	1108	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	cA	1109	CL7	C3B-C4B-NB	-2.83	107.89	110.52
17	aL	4020	A1JPJ	C19-C18-C17	2.83	123.28	118.94
15	cB	1227	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
15	aJ	1301	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	bA	1120	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
17	cA	4014	A1JPJ	C37-C22-C23	2.83	122.53	118.08
15	cL	1501	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
15	aB	1012	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	cB	1217	CL7	CAA-C2A-C3A	-2.83	109.50	116.10
15	aB	1225	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
15	cB	1225	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
15	bA	1120	CL7	C3B-C4B-NB	-2.83	107.89	110.52
15	aI	1601	CL7	O2D-CGD-O1D	-2.82	118.31	123.84
15	bJ	1302	CL7	C3B-C4B-NB	-2.82	107.89	110.52
15	cB	1209	CL7	C3B-C4B-NB	-2.82	107.89	110.52
15	aA	1134	CL7	C3A-C4A-CHB	-2.82	119.83	124.02
15	aB	1224	CL7	C3B-C4B-NB	-2.82	107.90	110.52
15	bA	1107	CL7	O2D-CGD-O1D	-2.82	118.32	123.84
15	cF	1701	CL7	O2D-CGD-O1D	-2.82	118.32	123.84
15	aJ	1302	CL7	C3B-C4B-NB	-2.82	107.90	110.52
15	aK	1401	CL7	C3B-C4B-NB	-2.82	107.90	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aL	1501	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
14	aA	1013	PHO	C1C-C2C-C3C	-2.82	106.27	108.61
17	bI	4019	A1JPJ	C12-C13-C14	2.82	123.26	118.94
15	bA	1113	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
15	cB	1225	CL7	C3B-C4B-NB	-2.82	107.90	110.52
15	bB	1235	CL7	C3B-C4B-NB	-2.81	107.91	110.52
15	cK	1401	CL7	C3B-C4B-NB	-2.81	107.91	110.52
15	bB	1227	CL7	O2D-CGD-O1D	-2.81	118.34	123.84
15	aB	1021	CL7	O2D-CGD-O1D	-2.81	118.34	123.84
15	aA	1140	CL7	C3B-C4B-NB	-2.81	107.91	110.52
17	aB	4006	A1JPJ	C36-C18-C17	-2.81	118.99	122.92
15	cB	1203	CL7	O2D-CGD-O1D	-2.81	118.35	123.84
15	cB	1012	CL7	C3B-C4B-NB	-2.81	107.91	110.52
15	cA	1102	CL7	C3A-C4A-CHB	-2.81	119.53	123.70
15	bK	1401	CL7	C3B-C4B-NB	-2.81	107.91	110.52
15	bA	1119	CL7	O2D-CGD-O1D	-2.80	118.35	123.84
15	bA	1022	CL7	C3B-C4B-NB	-2.80	107.91	110.52
15	cA	1108	CL7	O2D-CGD-O1D	-2.80	118.36	123.84
15	cB	1213	CL7	C3B-C4B-NB	-2.80	107.92	110.52
15	aB	1203	CL7	O2D-CGD-O1D	-2.80	118.36	123.84
15	cJ	1301	CL7	C3B-C4B-NB	-2.80	107.92	110.52
15	bB	1213	CL7	C3B-C4B-NB	-2.80	107.92	110.52
17	aB	4015	A1JPJ	C19-C18-C17	2.80	123.23	118.94
17	aL	4020	A1JPJ	C23-C22-C21	2.80	123.23	118.94
17	cF	4016	A1JPJ	C12-C13-C14	2.80	123.23	118.94
15	aB	1227	CL7	O2D-CGD-O1D	-2.80	118.37	123.84
15	aA	1115	CL7	O2D-CGD-O1D	-2.79	118.37	123.84
15	cA	1119	CL7	O2D-CGD-O1D	-2.79	118.37	123.84
15	aB	1204	CL7	CAA-C2A-C3A	-2.79	105.13	112.78
15	bA	1112	CL7	OBB-CAB-C3B	-2.79	119.37	125.69
15	aA	1109	CL7	C3B-C4B-NB	-2.79	107.92	110.52
15	bB	1226	CL7	C3B-C4B-NB	-2.79	107.92	110.52
15	bB	1204	CL7	C3B-C4B-NB	-2.79	107.92	110.52
15	cB	1221	CL7	C3B-C4B-NB	-2.79	107.92	110.52
15	cK	1402	CL7	CAA-C2A-C3A	-2.79	109.58	116.10
15	bI	1601	CL7	O2D-CGD-O1D	-2.79	118.38	123.84
15	aB	1221	CL7	C3B-C4B-NB	-2.79	107.92	110.52
15	aB	1208	CL7	C3B-C4B-NB	-2.79	107.93	110.52
14	cA	1013	PHO	CMA-C3A-C4A	-2.79	108.27	114.38
15	cB	1214	CL7	C3A-C4A-CHB	-2.79	119.56	123.70
17	aB	4010	A1JPJ	C15-C16-C17	2.79	129.19	123.47
15	cA	1801	CL7	O2D-CGD-O1D	-2.79	118.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1117	CL7	CHB-C1B-NB	2.79	127.21	124.26
17	cA	4007	A1JPJ	C19-C18-C17	2.79	123.22	118.94
15	bA	1131	CL7	O2D-CGD-O1D	-2.79	118.39	123.84
15	cI	1601	CL7	C3B-C4B-NB	-2.79	107.93	110.52
17	aI	4019	A1JPJ	C12-C13-C14	2.79	123.22	118.94
15	aB	1216	CL7	C3B-C4B-NB	-2.78	107.93	110.52
15	cA	1114	CL7	C3B-C4B-NB	-2.78	107.93	110.52
15	aB	1213	CL7	C3B-C4B-NB	-2.78	107.93	110.52
15	bA	1108	CL7	O2D-CGD-O1D	-2.78	118.40	123.84
15	cB	1216	CL7	O2D-CGD-CBD	2.78	116.21	111.27
15	bA	1112	CL7	C3A-C4A-CHB	-2.78	119.57	123.70
17	bB	4005	A1JPJ	C25-C26-C27	-2.78	118.04	121.47
17	aB	4021	A1JPJ	C15-C16-C17	2.78	129.17	123.47
14	bA	1013	PHO	C1C-C2C-C3C	-2.78	106.30	108.61
15	aA	1135	CL7	O2D-CGD-O1D	-2.78	118.40	123.84
15	bB	1209	CL7	C3B-C4B-NB	-2.78	107.94	110.52
15	bA	1801	CL7	O2D-CGD-O1D	-2.78	118.40	123.84
15	bA	1108	CL7	C3B-C4B-NB	-2.78	107.94	110.52
15	bF	1701	CL7	C3B-C4B-NB	-2.78	107.94	110.52
17	cA	4014	A1JPJ	C34-C9-C10	-2.78	119.03	122.92
15	aA	1108	CL7	O2D-CGD-O1D	-2.77	118.41	123.84
15	bB	1222	CL7	O2D-CGD-O1D	-2.77	118.41	123.84
15	bB	1215	CL7	C3B-C4B-NB	-2.77	107.94	110.52
15	aB	1222	CL7	O2D-CGD-O1D	-2.77	118.42	123.84
15	bB	1221	CL7	C3B-C4B-NB	-2.77	107.94	110.52
15	cB	1222	CL7	O2D-CGD-O1D	-2.77	118.42	123.84
15	bB	1021	CL7	O2D-CGD-O1D	-2.77	118.43	123.84
17	cB	4006	A1JPJ	C36-C18-C17	-2.77	119.05	122.92
15	aB	1205	CL7	C3B-C4B-NB	-2.77	107.95	110.52
17	bF	4016	A1JPJ	C8-C9-C10	2.77	123.19	118.94
15	bB	1220	CL7	O2D-CGD-O1D	-2.77	118.43	123.84
17	bB	4010	A1JPJ	C15-C16-C17	2.76	129.14	123.47
15	aA	1107	CL7	O2D-CGD-O1D	-2.76	118.43	123.84
15	aL	1501	CL7	C3A-C4A-CHB	-2.76	119.60	123.70
17	cA	4014	A1JPJ	C15-C14-C13	2.76	131.25	127.31
15	cL	1501	CL7	C3A-C4A-CHB	-2.76	119.60	123.70
15	cB	1208	CL7	C3B-C4B-NB	-2.76	107.95	110.52
15	bB	1204	CL7	CAA-C2A-C3A	-2.76	105.22	112.78
15	aA	1116	CL7	O2D-CGD-O1D	-2.76	118.44	123.84
15	bA	1135	CL7	C3A-C4A-CHB	-2.76	119.60	123.70
15	aA	1022	CL7	C3B-C4B-NB	-2.76	107.95	110.52
17	aA	4011	A1JPJ	C36-C18-C17	-2.76	119.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	cI	4019	A1JPJ	C12-C13-C14	2.76	123.17	118.94
17	bA	4014	A1JPJ	C34-C9-C10	-2.76	119.06	122.92
15	aB	1209	CL7	C3B-C4B-NB	-2.76	107.96	110.52
15	aB	1212	CL7	C3B-C4B-NB	-2.76	107.96	110.52
15	cA	1134	CL7	C3A-C4A-CHB	-2.76	119.93	124.02
15	aB	1210	CL7	C3A-C4A-CHB	-2.75	119.61	123.70
17	cA	4011	A1JPJ	C36-C18-C17	-2.75	119.06	122.92
15	aA	1119	CL7	O2D-CGD-O1D	-2.75	118.45	123.84
15	bB	1234	CL7	C3A-C4A-CHB	-2.75	119.61	123.70
17	bA	4003	A1JPJ	C12-C13-C14	2.75	123.16	118.94
15	cA	1126	CL7	O2D-CGD-O1D	-2.75	118.46	123.84
15	aA	1117	CL7	C3B-C4B-NB	-2.75	107.97	110.52
15	aB	1231	CL7	C3B-C4B-NB	-2.75	107.97	110.52
15	cK	1402	CL7	C3B-C4B-NB	-2.75	107.97	110.52
17	aB	4004	A1JPJ	C8-C9-C10	2.75	123.16	118.94
17	bB	4006	A1JPJ	C36-C18-C17	-2.75	119.08	122.92
15	cB	1204	CL7	CAA-C2A-C3A	-2.75	105.26	112.78
15	aA	1103	CL7	C3B-C4B-NB	-2.75	107.97	110.52
15	bB	1205	CL7	C3B-C4B-NB	-2.75	107.97	110.52
15	bA	1110	CL7	O2D-CGD-CBD	2.74	116.14	111.27
15	bK	1402	CL7	C3B-C4B-NB	-2.74	107.97	110.52
15	cB	1231	CL7	C3B-C4B-NB	-2.74	107.97	110.52
15	aB	1225	CL7	C3B-C4B-NB	-2.74	107.97	110.52
15	bA	1116	CL7	O2D-CGD-O1D	-2.74	118.48	123.84
17	cL	4023	A1JPJ	C16-C15-C14	2.74	129.08	123.47
17	cB	4015	A1JPJ	C19-C18-C17	2.74	123.14	118.94
15	bL	1501	CL7	O2D-CGD-O1D	-2.74	118.49	123.84
15	cJ	1301	CL7	O2D-CGD-O1D	-2.73	118.49	123.84
15	aA	1114	CL7	C3B-C4B-NB	-2.73	107.98	110.52
15	cA	1137	CL7	C3B-C4B-NB	-2.73	107.98	110.52
15	aA	1120	CL7	C3A-C4A-CHB	-2.73	119.64	123.70
15	aB	1234	CL7	C3A-C4A-CHB	-2.73	119.64	123.70
17	aB	4017	A1JPJ	C21-C20-C19	2.73	131.75	123.22
15	aA	1135	CL7	C3A-C4A-CHB	-2.73	119.64	123.70
17	aA	4008	A1JPJ	C35-C13-C14	-2.73	119.10	122.92
15	aA	1110	CL7	O2D-CGD-CBD	2.73	116.12	111.27
17	aA	4014	A1JPJ	C34-C9-C10	-2.73	119.10	122.92
17	cL	4020	A1JPJ	C23-C22-C21	2.73	123.13	118.94
17	aB	4015	A1JPJ	C10-C11-C12	2.73	131.74	123.22
15	bJ	1301	CL7	O2D-CGD-O1D	-2.73	118.50	123.84
15	aB	1220	CL7	O2D-CGD-O1D	-2.73	118.50	123.84
15	aB	1214	CL7	C3A-C4A-CHB	-2.73	119.65	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cB	1210	CL7	C3A-C4A-CHB	-2.73	119.65	123.70
15	bB	1216	CL7	C3B-C4B-NB	-2.73	107.98	110.52
15	cA	1117	CL7	C3B-C4B-NB	-2.73	107.99	110.52
15	bA	1126	CL7	O2D-CGD-O1D	-2.73	118.51	123.84
15	cB	1238	CL7	C3A-C4A-CHB	-2.72	119.66	123.70
15	bA	1140	CL7	C3B-C4B-NB	-2.72	107.99	110.52
17	aA	4003	A1JPJ	C12-C13-C14	2.72	123.12	118.94
17	bA	4008	A1JPJ	C35-C13-C14	-2.72	119.11	122.92
15	bA	1115	CL7	CAA-C2A-C3A	-2.72	109.75	116.10
15	bB	1231	CL7	C3B-C4B-NB	-2.72	107.99	110.52
15	bB	1232	CL7	O2D-CGD-O1D	-2.72	118.52	123.84
15	aA	1131	CL7	O2D-CGD-O1D	-2.72	118.53	123.84
15	bB	1235	CL7	C3A-C4A-CHB	-2.72	119.67	123.70
17	bB	4004	A1JPJ	C8-C9-C10	2.72	123.11	118.94
15	cA	1022	CL7	C3B-C4B-NB	-2.72	108.00	110.52
15	bA	1132	CL7	OBb-CAB-C3B	-2.71	119.55	125.69
15	cB	1205	CL7	C3B-C4B-NB	-2.71	108.00	110.52
13	bA	1011	G9R	O2D-CGD-CBD	2.71	114.43	111.00
15	bA	1114	CL7	C3B-C4B-NB	-2.71	108.00	110.52
15	bA	1120	CL7	C3A-C4A-CHB	-2.71	119.68	123.70
15	aB	1201	CL7	OBb-CAB-C3B	-2.71	119.56	125.69
15	aJ	1301	CL7	O2D-CGD-O1D	-2.71	118.54	123.84
15	bB	1238	CL7	C3A-C4A-CHB	-2.71	119.68	123.70
17	bA	4007	A1JPJ	C19-C18-C17	2.71	123.09	118.94
15	bA	1139	CL7	O2D-CGD-O1D	-2.71	118.55	123.84
15	bL	1501	CL7	C3A-C4A-CHB	-2.70	119.69	123.70
15	bB	1214	CL7	C3A-C4A-CHB	-2.70	119.69	123.70
15	aA	1139	CL7	O2D-CGD-O1D	-2.70	118.56	123.84
15	cA	1116	CL7	O2D-CGD-O1D	-2.70	118.56	123.84
17	bA	4003	A1JPJ	C19-C18-C17	2.70	123.08	118.94
15	bA	1117	CL7	CHB-C1B-NB	2.70	127.11	124.26
15	bA	1134	CL7	C3A-C4A-CHB	-2.70	120.02	124.02
15	aB	1226	CL7	C3B-C4B-NB	-2.70	108.01	110.52
15	bA	1137	CL7	C3B-C4B-NB	-2.70	108.01	110.52
15	bA	1117	CL7	C3B-C4B-NB	-2.70	108.01	110.52
15	bA	1104	CL7	O2D-CGD-O1D	-2.70	118.57	123.84
17	cF	4016	A1JPJ	C23-C22-C21	2.69	123.08	118.94
15	aB	1021	CL7	C3B-C4B-NB	-2.69	108.02	110.52
15	aA	1126	CL7	O2D-CGD-O1D	-2.69	118.57	123.84
13	aA	1011	G9R	C1C-C2C-C3C	-2.69	106.37	108.61
15	cB	1233	CL7	C3B-C4B-NB	-2.69	108.02	110.52
15	bB	1210	CL7	C3A-C4A-CHB	-2.69	119.71	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	aA	4007	A1JPJ	C34-C9-C8	2.69	122.31	118.08
15	aA	1102	CL7	C3A-C4A-CHB	-2.69	119.71	123.70
15	aB	1238	CL7	C3A-C4A-CHB	-2.69	119.72	123.70
17	bL	4020	A1JPJ	C23-C22-C21	2.68	123.06	118.94
15	aF	1701	CL7	C3B-C4B-NB	-2.68	108.03	110.52
15	cA	1127	CL7	C3B-C4B-NB	-2.68	108.03	110.52
15	cA	1120	CL7	C3A-C4A-CHB	-2.68	119.72	123.70
15	bA	1116	CL7	C3A-C4A-CHB	-2.68	119.72	123.70
17	cA	4008	A1JPJ	C35-C13-C14	-2.68	119.17	122.92
17	cA	4003	A1JPJ	C12-C13-C14	2.68	123.05	118.94
15	cB	1212	CL7	C3B-C4B-NB	-2.68	108.03	110.52
15	cA	1139	CL7	O2D-CGD-O1D	-2.68	118.61	123.84
15	cA	1116	CL7	C3A-C4A-CHB	-2.68	119.73	123.70
17	cB	4021	A1JPJ	C15-C16-C17	2.67	128.95	123.47
15	aA	1113	CL7	C3B-C4B-NB	-2.67	108.03	110.52
15	aA	1127	CL7	C3B-C4B-NB	-2.67	108.03	110.52
15	aB	1235	CL7	C3A-C4A-CHB	-2.67	119.73	123.70
15	bB	1218	CL7	CAA-C2A-C3A	-2.67	109.86	116.10
15	cB	1234	CL7	C3A-C4A-CHB	-2.67	119.74	123.70
15	aB	1218	CL7	CAA-C2A-C3A	-2.67	109.87	116.10
15	cB	1201	CL7	OBB-CAB-C3B	-2.67	119.66	125.69
15	bB	1212	CL7	C3B-C4B-NB	-2.67	108.04	110.52
15	bB	1214	CL7	CHB-C1B-NB	2.67	127.08	124.26
15	cA	1137	CL7	C3A-C4A-CHB	-2.67	119.74	123.70
17	bB	4021	A1JPJ	C15-C16-C17	2.67	128.94	123.47
15	cB	1217	CL7	C3B-C4B-NB	-2.66	108.04	110.52
13	aA	1011	G9R	O2D-CGD-CBD	2.66	114.37	111.00
17	cB	4017	A1JPJ	C21-C20-C19	2.66	131.53	123.22
15	bB	1224	CL7	C3B-C4B-NB	-2.66	108.05	110.52
17	bB	4017	A1JPJ	C21-C20-C19	2.66	131.53	123.22
15	bB	1201	CL7	OBB-CAB-C3B	-2.66	119.67	125.69
15	cB	1235	CL7	C3A-C4A-CHB	-2.66	119.75	123.70
15	aK	1402	CL7	CHD-C1D-ND	-2.66	121.44	124.26
15	aA	1132	CL7	O2D-CGD-CBD	2.66	115.99	111.27
14	cB	1023	PHO	CMA-C3A-C4A	-2.66	108.56	114.38
17	aA	4003	A1JPJ	C19-C18-C17	2.66	123.02	118.94
17	bB	4015	A1JPJ	C19-C18-C17	2.65	123.01	118.94
15	aB	1205	CL7	O2A-CGA-O1A	-2.65	116.89	123.59
15	cA	1140	CL7	C3B-C4B-NB	-2.65	108.06	110.52
15	cA	1117	CL7	CHB-C1B-NB	2.65	127.06	124.26
15	bB	1230	CL7	O2D-CGD-CBD	2.65	115.97	111.27
17	aB	4021	A1JPJ	C37-C22-C23	2.65	122.25	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	cF	4016	A1JPJ	C8-C9-C10	2.65	123.00	118.94
17	aB	4005	A1JPJ	C25-C26-C27	-2.65	118.21	121.47
13	aA	1011	G9R	C3D-C4D-CHA	2.65	112.56	108.54
17	aF	4016	A1JPJ	C23-C22-C21	2.65	123.00	118.94
15	aB	1226	CL7	CHB-C1B-NB	2.65	127.06	124.26
15	cB	1203	CL7	C3A-C4A-CHB	-2.65	119.77	123.70
17	cA	4007	A1JPJ	C34-C9-C8	2.65	122.25	118.08
15	aB	1217	CL7	C3B-C4B-NB	-2.64	108.06	110.52
15	cB	1204	CL7	C3B-C4B-NB	-2.64	108.06	110.52
14	aB	1023	PHO	CMA-C3A-C4A	-2.64	108.59	114.38
15	bB	1217	CL7	C3B-C4B-NB	-2.64	108.06	110.52
15	cA	1104	CL7	C3A-C4A-CHB	-2.64	119.78	123.70
15	aA	1118	CL7	C3A-C4A-CHB	-2.64	119.78	123.70
15	aB	1204	CL7	C3B-C4B-NB	-2.64	108.06	110.52
15	aK	1402	CL7	C3B-C4B-NB	-2.64	108.06	110.52
17	bA	4007	A1JPJ	C34-C9-C8	2.64	122.24	118.08
15	aB	1216	CL7	O2D-CGD-O1D	-2.64	118.68	123.84
15	cA	1101	CL7	CAA-C2A-C3A	-2.64	109.94	116.10
15	bA	1115	CL7	O2D-CGD-O1D	-2.64	118.68	123.84
15	cA	1132	CL7	C2B-C1B-NB	2.64	112.00	110.23
15	cA	1118	CL7	C3A-C4A-CHB	-2.64	119.79	123.70
15	aA	1101	CL7	CAA-C2A-C3A	-2.64	109.95	116.10
17	aA	4008	A1JPJ	C28-C27-C26	-2.63	122.32	124.85
15	cB	1230	CL7	O2D-CGD-CBD	2.63	115.95	111.27
15	bJ	1301	CL7	C3A-C4A-CHB	-2.63	119.80	123.70
13	bA	1011	G9R	CMD-C2D-C3D	2.63	129.60	124.68
15	bA	1118	CL7	C3A-C4A-CHB	-2.63	119.80	123.70
15	cA	1110	CL7	O2D-CGD-CBD	2.63	115.93	111.27
15	cB	1226	CL7	CHB-C1B-NB	2.62	127.03	124.26
15	aL	1502	CL7	OBB-CAB-C3B	-2.62	119.75	125.69
15	aJ	1302	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
15	aK	1401	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
15	bA	1110	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
17	bA	4011	A1JPJ	C36-C18-C17	-2.62	119.25	122.92
15	cL	1502	CL7	OBB-CAB-C3B	-2.62	119.76	125.69
15	cK	1402	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
15	cL	1502	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
15	aB	1203	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
17	cA	4003	A1JPJ	C19-C18-C17	2.62	122.96	118.94
15	cB	1218	CL7	CAA-C2A-C3A	-2.62	109.99	116.10
15	cA	1138	CL7	C3B-C4B-NB	-2.62	108.09	110.52
15	bJ	1302	CL7	C3A-C4A-CHB	-2.62	119.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1107	CL7	C3A-C4A-CHB	-2.62	119.82	123.70
15	aJ	1301	CL7	C3A-C4A-CHB	-2.62	119.82	123.70
15	cB	1204	CL7	C3A-C4A-CHB	-2.62	119.82	123.70
13	bA	1011	G9R	C3D-C4D-CHA	2.61	112.51	108.54
15	aL	1501	CL7	OBB-CAB-C3B	-2.61	119.78	125.69
17	aA	4014	A1JPJ	C12-C13-C14	2.61	122.95	118.94
17	bB	4021	A1JPJ	C12-C13-C14	2.61	122.95	118.94
15	aB	1227	CL7	C3B-C4B-NB	-2.61	108.09	110.52
15	aB	1209	CL7	C3A-C4A-CHB	-2.61	119.82	123.70
15	cK	1401	CL7	C3A-C4A-CHB	-2.61	119.82	123.70
17	aB	4021	A1JPJ	C12-C13-C14	2.61	122.95	118.94
13	bA	1011	G9R	C1C-C2C-C3C	-2.61	106.44	108.61
13	cA	1011	G9R	C1C-C2C-C3C	-2.61	106.44	108.61
15	bB	1230	CL7	CAA-C2A-C3A	-2.61	110.01	116.10
15	bA	1128	CL7	C3B-C4B-NB	-2.61	108.09	110.52
15	cB	1229	CL7	C3B-C4B-NB	-2.61	108.09	110.52
15	aA	1116	CL7	C3A-C4A-CHB	-2.61	119.83	123.70
15	aA	1117	CL7	C3A-C4A-CHB	-2.61	119.83	123.70
17	bJ	4012	A1JPJ	C8-C9-C10	2.61	122.94	118.94
15	aB	1230	CL7	CAA-C2A-C3A	-2.61	110.01	116.10
15	cF	1701	CL7	C3B-C4B-NB	-2.61	108.10	110.52
17	cA	4002	A1JPJ	C16-C15-C14	2.61	128.81	123.47
15	bL	1502	CL7	C3A-C4A-CHB	-2.61	119.83	123.70
15	cA	1107	CL7	C3A-C4A-CHB	-2.61	119.83	123.70
17	aA	4007	A1JPJ	C19-C18-C17	2.60	122.94	118.94
15	aB	1233	CL7	C3B-C4B-NB	-2.60	108.10	110.52
15	aA	1129	CL7	C1-C2-C3	-2.60	122.54	126.75
15	cB	1234	CL7	C1-C2-C3	-2.60	122.54	126.75
15	cB	1209	CL7	C3A-C4A-CHB	-2.60	119.84	123.70
17	aL	4023	A1JPJ	C16-C15-C14	2.60	128.80	123.47
15	bA	1101	CL7	CAA-C2A-C3A	-2.60	110.04	116.10
15	aA	1137	CL7	C3B-C4B-NB	-2.60	108.11	110.52
15	bB	1021	CL7	C3B-C4B-NB	-2.60	108.11	110.52
15	cA	1128	CL7	C3B-C4B-NB	-2.60	108.11	110.52
15	bB	1209	CL7	C3A-C4A-CHB	-2.59	119.85	123.70
15	cB	1219	CL7	C3A-C4A-CHB	-2.59	119.85	123.70
15	aA	1121	CL7	C3B-C4B-NB	-2.59	108.11	110.52
14	bB	1023	PHO	CMA-C3A-C4A	-2.59	108.70	114.38
15	aA	1128	CL7	C3B-C4B-NB	-2.59	108.11	110.52
13	aA	1011	G9R	CMD-C2D-C3D	2.59	129.52	124.68
15	aA	1130	CL7	CHB-C1B-NB	2.59	127.00	124.26
15	aA	1137	CL7	C3A-C4A-CHB	-2.59	119.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	bJ	4012	A1JPJ	C15-C16-C17	2.59	128.77	123.47
13	aA	1011	G9R	C4D-CHA-CBD	-2.59	106.22	108.89
15	cA	1130	CL7	CHB-C1B-NB	2.59	127.00	124.26
15	cB	1021	CL7	C3B-C4B-NB	-2.59	108.12	110.52
17	cA	4007	A1JPJ	C12-C13-C14	2.59	122.91	118.94
17	cB	4021	A1JPJ	C12-C13-C14	2.59	122.91	118.94
15	aA	1104	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
15	bA	1137	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
15	aA	1110	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
15	bB	1232	CL7	C3B-C4B-NB	-2.58	108.12	110.52
15	bB	1219	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
15	aA	1135	CL7	OBB-CAB-C3B	-2.58	119.85	125.69
15	aB	1236	CL7	C3B-C4B-NB	-2.58	108.12	110.52
15	cB	1219	CL7	C3B-C4B-NB	-2.58	108.12	110.52
15	bL	1502	CL7	OBB-CAB-C3B	-2.58	119.86	125.69
15	bA	1130	CL7	CHB-C1B-NB	2.58	126.99	124.26
15	cB	1230	CL7	CAA-C2A-C3A	-2.58	110.08	116.10
15	cA	1110	CL7	C3A-C4A-CHB	-2.58	119.88	123.70
15	bB	1223	CL7	C3A-C4A-CHB	-2.57	119.88	123.70
15	bA	1107	CL7	C3A-C4A-CHB	-2.57	119.88	123.70
15	cJ	1301	CL7	C3A-C4A-CHB	-2.57	119.88	123.70
15	bK	1401	CL7	C3A-C4A-CHB	-2.57	119.88	123.70
17	aA	4002	A1JPJ	C16-C15-C14	2.57	128.74	123.47
13	cA	1011	G9R	C3D-C4D-CHA	2.57	112.45	108.54
15	cB	1215	CL7	O2D-CGD-O1D	-2.57	118.81	123.84
15	aA	1138	CL7	C3B-C4B-NB	-2.57	108.13	110.52
15	cA	1131	CL7	C3B-C4B-NB	-2.57	108.13	110.52
15	cB	1224	CL7	C3B-C4B-NB	-2.57	108.14	110.52
17	bA	4014	A1JPJ	C12-C13-C14	2.56	122.88	118.94
15	bK	1402	CL7	CAA-C2A-C3A	-2.56	110.11	116.10
15	bB	1205	CL7	O2A-CGA-O1A	-2.56	117.12	123.59
15	cB	1206	CL7	CHB-C1B-NB	2.56	126.97	124.26
14	bB	1023	PHO	O2D-CGD-O1D	-2.56	118.83	123.84
17	bA	4002	A1JPJ	C16-C15-C14	2.56	128.72	123.47
15	bB	1203	CL7	C3A-C4A-CHB	-2.56	119.90	123.70
15	bA	1125	CL7	C3A-C4A-CHB	-2.56	119.90	123.70
15	bB	1207	CL7	C3A-C4A-CHB	-2.56	119.90	123.70
15	bB	1219	CL7	C3B-C4B-NB	-2.56	108.14	110.52
15	aB	1230	CL7	O2D-CGD-CBD	2.55	115.81	111.27
15	aL	1502	CL7	C3A-C4A-CHB	-2.55	119.91	123.70
15	bA	1132	CL7	C3A-C4A-CHB	-2.55	119.91	123.70
15	cA	1135	CL7	C3A-C4A-CHB	-2.55	119.91	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	aB	5002	LMG	C3-C4-C5	-2.55	105.69	110.24
17	bJ	4012	A1JPJ	C19-C18-C17	2.55	122.85	118.94
15	aB	1224	CL7	OBB-CAB-C3B	-2.55	119.93	125.69
15	bA	1106	CL7	CHB-C1B-NB	2.55	126.95	124.26
15	bB	1238	CL7	CHB-C1B-NB	2.55	126.95	124.26
15	cA	1101	CL7	C3A-C4A-CHB	-2.54	119.92	123.70
15	aB	1204	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	aB	1207	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	bA	1104	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	bB	1218	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	bB	1229	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	aB	1234	CL7	C1-C2-C3	-2.54	122.64	126.75
15	bA	1123	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
15	cB	1223	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
17	bB	4021	A1JPJ	C37-C22-C23	2.54	122.08	118.08
15	bA	1121	CL7	C3B-C4B-NB	-2.54	108.16	110.52
15	aI	1601	CL7	C3A-C4A-CHB	-2.54	119.94	123.70
15	bB	1226	CL7	CHB-C1B-NB	2.54	126.94	124.26
15	aB	1229	CL7	C3B-C4B-NB	-2.54	108.16	110.52
15	aB	1206	CL7	CHB-C1B-NB	2.53	126.94	124.26
15	aB	1217	CL7	C3A-C4A-CHB	-2.53	119.94	123.70
14	cA	1013	PHO	C1C-C2C-C3C	-2.53	106.50	108.61
15	bA	1128	CL7	CHB-C1B-NB	2.53	126.94	124.26
15	cA	1119	CL7	CHB-C1B-NB	2.53	126.94	124.26
15	cB	1214	CL7	CHB-C1B-NB	2.53	126.94	124.26
15	aB	1219	CL7	C3A-C4A-CHB	-2.53	119.94	123.70
15	aA	1119	CL7	CHB-C1B-NB	2.53	126.94	124.26
15	aA	1132	CL7	C2B-C1B-NB	2.53	111.93	110.23
15	aB	1241	CL7	O2D-CGD-CBD	2.53	115.76	111.27
17	cI	4019	A1JPJ	C15-C16-C17	2.53	128.65	123.47
15	bB	1236	CL7	C3B-C4B-NB	-2.53	108.17	110.52
15	cB	1218	CL7	C3A-C4A-CHB	-2.53	119.95	123.70
15	cB	1213	CL7	C3A-C4A-CHB	-2.53	119.95	123.70
15	cA	1132	CL7	CHB-C1B-C2B	-2.52	120.11	127.24
15	aB	1207	CL7	OBB-CAB-C3B	-2.52	119.98	125.69
15	bB	1212	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
15	bB	1213	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
15	cA	1801	CL7	CAA-C2A-C3A	-2.52	110.21	116.10
13	cA	1011	G9R	CMB-C2B-C3B	2.52	129.40	124.68
14	aB	1023	PHO	O2D-CGD-O1D	-2.52	118.91	123.84
15	cB	1205	CL7	O2A-CGA-O1A	-2.52	117.23	123.59
15	bA	1131	CL7	C3B-C4B-NB	-2.52	108.18	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1106	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
15	aB	1223	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
15	cA	1103	CL7	CHB-C1B-NB	2.52	126.92	124.26
15	aA	1118	CL7	C3B-C4B-NB	-2.52	108.18	110.52
15	aA	1101	CL7	C3A-C4A-CHB	-2.52	119.97	123.70
15	cA	1121	CL7	C3B-C4B-NB	-2.51	108.18	110.52
15	bB	1227	CL7	C3B-C4B-NB	-2.51	108.18	110.52
15	aB	1219	CL7	C3B-C4B-NB	-2.51	108.18	110.52
15	bA	1126	CL7	CHB-C1B-NB	2.51	126.92	124.26
15	aA	1112	CL7	C3A-C4A-CHB	-2.51	119.97	123.70
15	aB	1233	CL7	CAA-C2A-C3A	-2.51	110.24	116.10
17	aB	4005	A1JPJ	C37-C22-C23	2.51	122.03	118.08
15	bA	1101	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
15	cB	1230	CL7	CHB-C1B-NB	2.51	126.91	124.26
17	bA	4011	A1JPJ	C34-C9-C8	2.51	122.03	118.08
15	cB	1239	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
15	aB	1233	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
15	bA	1138	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
16	bA	2001	PQN	C11-C3-C4	-2.51	115.82	118.50
15	cA	1106	CL7	CHB-C1B-NB	2.51	126.91	124.26
15	cB	1217	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
15	aL	1501	CL7	CHB-C1B-NB	2.50	126.91	124.26
15	aA	1115	CL7	C3A-C4A-CHB	-2.50	119.99	123.70
17	cB	4010	A1JPJ	C12-C13-C14	2.50	122.78	118.94
15	bA	1125	CL7	OBB-CAB-C3B	-2.50	120.03	125.69
15	cA	1138	CL7	C3A-C4A-CHB	-2.50	119.99	123.70
15	cA	1135	CL7	OBB-CAB-C3B	-2.50	120.03	125.69
15	bB	1234	CL7	C1-C2-C3	-2.50	122.71	126.75
13	bA	1011	G9R	C4D-CHA-CBD	-2.50	106.31	108.89
17	cB	4021	A1JPJ	C37-C22-C23	2.50	122.01	118.08
15	bB	1222	CL7	C3A-C4A-CHB	-2.50	120.00	123.70
15	cA	1022	CL7	OBB-CAB-C3B	-2.50	120.05	125.69
15	bB	1236	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
15	bK	1402	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
17	cB	4005	A1JPJ	C25-C26-C27	-2.49	118.40	121.47
15	aB	1236	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
15	cA	1115	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
15	aB	1212	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
14	aA	1013	PHO	O2D-CGD-O1D	-2.49	118.97	123.84
15	cB	1212	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
17	cI	4018	A1JPJ	C37-C22-C23	2.49	122.00	118.08
17	bA	4007	A1JPJ	C12-C13-C14	2.49	122.76	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1217	CL7	C3A-C4A-CHB	-2.49	120.01	123.70
15	cA	1130	CL7	C3A-C4A-CHB	-2.49	120.01	123.70
15	cA	1118	CL7	C3B-C4B-NB	-2.48	108.21	110.52
15	cB	1222	CL7	C3A-C4A-CHB	-2.48	120.01	123.70
14	cB	1023	PHO	O2D-CGD-O1D	-2.48	118.98	123.84
15	cB	1232	CL7	C3B-C4B-NB	-2.48	108.21	110.52
15	cA	1801	CL7	C3A-C4A-CHB	-2.48	120.02	123.70
17	aJ	4012	A1JPJ	C8-C9-C10	2.48	122.75	118.94
15	aB	1218	CL7	C3A-C4A-CHB	-2.48	120.02	123.70
15	cA	1133	CL7	C3A-C4A-CHB	-2.48	120.02	123.70
15	cB	1229	CL7	C3A-C4A-CHB	-2.48	120.02	123.70
17	aA	4007	A1JPJ	C12-C13-C14	2.48	122.74	118.94
15	aA	1131	CL7	C3B-C4B-NB	-2.48	108.22	110.52
15	aB	1226	CL7	C3A-C4A-CHB	-2.48	120.03	123.70
15	bB	1204	CL7	C1-C2-C3	-2.48	121.76	126.04
15	aB	1214	CL7	CHB-C1B-NB	2.48	126.88	124.26
15	cA	1116	CL7	CHB-C1B-NB	2.48	126.88	124.26
15	aA	1133	CL7	C3A-C4A-CHB	-2.48	120.03	123.70
15	cB	1233	CL7	CAA-C2A-C3A	-2.47	110.33	116.10
15	aL	1502	CL7	O2D-CGD-CBD	2.47	115.66	111.27
15	bA	1119	CL7	CHB-C1B-NB	2.47	126.88	124.26
15	bA	1138	CL7	C3B-C4B-NB	-2.47	108.22	110.52
15	bB	1211	CL7	C3A-C4A-CHB	-2.47	120.03	123.70
15	aA	1106	CL7	CHB-C1B-NB	2.47	126.87	124.26
15	cA	1128	CL7	CHB-C1B-NB	2.47	126.87	124.26
17	bI	4018	A1JPJ	C37-C22-C23	2.47	121.97	118.08
13	bA	1011	G9R	CMA-C3A-C4A	-2.47	108.97	114.38
15	bB	1217	CL7	CAA-C2A-C3A	-2.47	110.34	116.10
17	bB	4010	A1JPJ	C12-C13-C14	2.47	122.73	118.94
15	aB	1233	CL7	OBB-CAB-C3B	-2.47	120.11	125.69
15	aA	1136	CL7	CHB-C1B-NB	2.47	126.87	124.26
15	aA	1132	CL7	CHB-C1B-C2B	-2.47	120.27	127.24
15	bA	1111	CL7	C3A-C4A-CHB	-2.47	120.04	123.70
15	aA	1128	CL7	CHB-C1B-NB	2.47	126.87	124.26
15	bB	1220	CL7	C3A-C4A-CHB	-2.47	120.04	123.70
15	aB	1213	CL7	C3A-C4A-CHB	-2.46	120.04	123.70
15	aA	1022	CL7	OBB-CAB-C3B	-2.46	120.12	125.69
15	bA	1122	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
15	bB	1229	CL7	C3B-C4B-NB	-2.46	108.23	110.52
15	cA	1106	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
15	cJ	1302	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
15	bA	1129	CL7	C1-C2-C3	-2.46	122.77	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1135	CL7	CHB-C1B-NB	2.46	126.86	124.26
15	aA	1138	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
15	bF	1701	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
17	cJ	4012	A1JPJ	C15-C16-C17	2.46	128.50	123.47
15	bB	1239	CL7	C3A-C4A-CHB	-2.46	120.06	123.70
15	bB	1206	CL7	CHB-C1B-NB	2.46	126.86	124.26
15	bA	1801	CL7	C3A-C4A-CHB	-2.45	120.06	123.70
15	aA	1123	CL7	C3A-C4A-CHB	-2.45	120.06	123.70
17	cJ	4012	A1JPJ	C19-C18-C17	2.45	122.70	118.94
15	aA	1801	CL7	CAA-C2A-C3A	-2.45	110.38	116.10
15	aA	1801	CL7	C3A-C4A-CHB	-2.45	120.06	123.70
17	bA	4011	A1JPJ	C23-C22-C21	2.45	122.70	118.94
15	bA	1801	CL7	CAA-C2A-C3A	-2.45	110.38	116.10
15	aB	1222	CL7	C3A-C4A-CHB	-2.45	120.06	123.70
15	aB	1229	CL7	C3A-C4A-CHB	-2.45	120.07	123.70
15	bA	1118	CL7	C3B-C4B-NB	-2.45	108.24	110.52
13	cA	1011	G9R	O2D-CGD-CBD	2.45	114.10	111.00
15	aJ	1301	CL7	CAA-C2A-C3A	-2.45	110.39	116.10
15	aK	1402	CL7	C3A-C4A-CHB	-2.45	120.07	123.70
17	aI	4018	A1JPJ	C37-C22-C23	2.45	121.93	118.08
17	cB	4021	A1JPJ	C34-C9-C8	2.45	121.93	118.08
15	bA	1124	CL7	C3A-C4A-CHB	-2.45	120.07	123.70
15	cA	1129	CL7	C1-C2-C3	-2.45	122.80	126.75
15	aA	1131	CL7	C1-C2-C3	-2.44	121.82	126.04
15	bB	1204	CL7	C3A-C4A-CHB	-2.44	120.07	123.70
15	cA	1123	CL7	C3A-C4A-CHB	-2.44	120.07	123.70
15	aA	1105	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
15	bA	1130	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
15	aB	1239	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
15	cB	1233	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
15	cA	1122	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
15	aB	1216	CL7	CHB-C1B-NB	2.44	126.84	124.26
15	cB	1216	CL7	CHB-C1B-NB	2.44	126.84	124.26
17	aL	4023	A1JPJ	C12-C13-C14	2.44	122.68	118.94
17	aA	4011	A1JPJ	C12-C13-C14	2.44	122.68	118.94
13	cA	1011	G9R	CMD-C2D-C3D	2.44	129.24	124.68
15	cB	1220	CL7	C3A-C4A-CHB	-2.43	120.09	123.70
15	bB	1232	CL7	C3A-C4A-CHB	-2.43	120.09	123.70
17	cB	4010	A1JPJ	C19-C18-C17	2.43	122.67	118.94
15	aB	1220	CL7	C3A-C4A-CHB	-2.43	120.09	123.70
15	cL	1502	CL7	CHB-C1B-NB	2.43	126.83	124.26
17	cA	4014	A1JPJ	C12-C13-C14	2.43	122.67	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1012	CL7	OBB-CAB-C3B	-2.43	120.20	125.69
15	aA	1113	CL7	C3A-C4A-CHB	-2.43	120.10	123.70
15	aA	1122	CL7	C3A-C4A-CHB	-2.43	120.10	123.70
17	aB	4010	A1JPJ	C12-C13-C14	2.43	122.66	118.94
17	aL	4023	A1JPJ	C21-C20-C19	2.43	130.79	123.22
15	aA	1139	CL7	C3A-C4A-CHB	-2.42	120.10	123.70
15	aL	1502	CL7	CHB-C1B-NB	2.42	126.82	124.26
15	cB	1204	CL7	C1-C2-C3	-2.42	121.85	126.04
15	bJ	1301	CL7	CAA-C2A-C3A	-2.42	110.44	116.10
15	cB	1238	CL7	CHB-C1B-NB	2.42	126.82	124.26
15	cB	1207	CL7	C3A-C4A-CHB	-2.42	120.11	123.70
15	bA	1127	CL7	C3B-C4B-NB	-2.42	108.27	110.52
15	bB	1241	CL7	C3B-C4B-NB	-2.42	108.27	110.52
15	aA	1133	CL7	CHB-C1B-NB	2.42	126.82	124.26
17	aA	4002	A1JPJ	C12-C13-C14	2.42	122.66	118.94
15	cI	1601	CL7	C3A-C4A-CHB	-2.42	120.11	123.70
17	bI	4019	A1JPJ	C15-C16-C17	2.42	128.43	123.47
15	aA	1109	CL7	C3A-C4A-CHB	-2.42	120.11	123.70
17	aA	4002	A1JPJ	C23-C22-C21	2.42	122.65	118.94
15	bB	1226	CL7	C3A-C4A-CHB	-2.42	120.11	123.70
17	aI	4019	A1JPJ	C15-C16-C17	2.42	128.42	123.47
15	bL	1502	CL7	CHB-C1B-NB	2.42	126.81	124.26
13	aA	1011	G9R	CMB-C2B-C3B	2.41	129.20	124.68
15	bA	1120	CL7	CHB-C1B-NB	2.41	126.81	124.26
15	bA	1105	CL7	C3A-C4A-CHB	-2.41	120.12	123.70
15	aB	1217	CL7	CAA-C2A-C3A	-2.41	110.47	116.10
15	bA	1116	CL7	CHB-C1B-NB	2.41	126.81	124.26
15	cA	1109	CL7	C3A-C4A-CHB	-2.41	120.12	123.70
15	cA	1105	CL7	C3A-C4A-CHB	-2.41	120.12	123.70
17	cA	4011	A1JPJ	C12-C13-C14	2.41	122.64	118.94
15	bA	1114	CL7	C3A-C4A-CHB	-2.41	120.12	123.70
15	aB	1203	CL7	CHB-C1B-NB	2.41	126.81	124.26
13	bA	1011	G9R	CMB-C2B-C3B	2.41	129.19	124.68
15	cB	1241	CL7	C3B-C4B-NB	-2.41	108.28	110.52
17	aJ	4012	A1JPJ	C19-C18-C17	2.41	122.64	118.94
15	bA	1133	CL7	C3A-C4A-CHB	-2.41	120.13	123.70
15	bA	1103	CL7	CHB-C1B-NB	2.41	126.81	124.26
15	cA	1125	CL7	O2A-CGA-O1A	-2.41	117.52	123.59
15	bA	1135	CL7	CHB-C1B-NB	2.41	126.80	124.26
15	bB	1207	CL7	OBB-CAB-C3B	-2.40	120.25	125.69
15	cA	1124	CL7	CHB-C1B-NB	2.40	126.80	124.26
15	cL	1501	CL7	CHB-C1B-NB	2.40	126.80	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1224	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
15	bA	1022	CL7	OBB-CAB-C3B	-2.40	120.25	125.69
15	aB	1215	CL7	CHB-C1B-NB	2.40	126.80	124.26
15	aA	1114	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
15	bL	1501	CL7	OBB-CAB-C3B	-2.40	120.26	125.69
15	aA	1111	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
17	cJ	4012	A1JPJ	C8-C9-C10	2.40	122.62	118.94
15	bL	1502	CL7	O2D-CGD-CBD	2.40	115.53	111.27
17	cA	4002	A1JPJ	C12-C13-C14	2.40	122.62	118.94
14	bA	1013	PHO	O2D-CGD-O1D	-2.40	119.15	123.84
15	cB	1234	CL7	CHB-C1B-NB	2.40	126.79	124.26
15	bA	1104	CL7	OBB-CAB-C3B	-2.40	120.27	125.69
15	cA	1114	CL7	C3A-C4A-CHB	-2.39	120.15	123.70
15	aA	1125	CL7	O2A-CGA-O1A	-2.39	117.55	123.59
15	aA	1103	CL7	C3A-C4A-CHB	-2.39	120.15	123.70
15	bA	1135	CL7	OBB-CAB-C3B	-2.39	120.28	125.69
15	bA	1139	CL7	C3A-C4A-CHB	-2.39	120.15	123.70
17	cI	4018	A1JPJ	C15-C16-C17	2.39	128.37	123.47
17	bA	4002	A1JPJ	C12-C13-C14	2.39	122.61	118.94
15	cB	1228	CL7	C3A-C4A-CHB	-2.39	120.16	123.70
13	cA	1011	G9R	C4D-CHA-CBD	-2.39	106.43	108.89
15	cA	1106	CL7	C1-C2-C3	-2.39	121.91	126.04
15	aF	1701	CL7	C3A-C4A-CHB	-2.39	120.16	123.70
15	aA	1125	CL7	CHD-C4C-NC	2.39	126.65	124.45
15	bA	1136	CL7	CHB-C1B-NB	2.39	126.78	124.26
15	aB	1012	CL7	OBB-CAB-C3B	-2.39	120.29	125.69
15	cA	1124	CL7	C1-C2-C3	-2.39	122.89	126.75
15	cB	1206	CL7	C3A-C4A-CHB	-2.39	120.16	123.70
17	cL	4023	A1JPJ	C19-C18-C17	2.39	122.60	118.94
17	bB	4005	A1JPJ	C15-C16-C17	2.39	128.36	123.47
15	aB	1228	CL7	C3A-C4A-CHB	-2.39	120.16	123.70
15	cJ	1301	CL7	CAA-C2A-C3A	-2.38	110.53	116.10
15	aA	1120	CL7	CHB-C1B-NB	2.38	126.78	124.26
15	bA	1124	CL7	CHB-C1B-NB	2.38	126.78	124.26
15	cA	1133	CL7	CHB-C1B-NB	2.38	126.78	124.26
15	cA	1139	CL7	C3A-C4A-CHB	-2.38	120.16	123.70
17	cB	4021	A1JPJ	C19-C18-C17	2.38	122.60	118.94
15	cB	1219	CL7	CAA-C2A-C3A	-2.38	110.54	116.10
17	cB	4005	A1JPJ	C37-C22-C23	2.38	121.83	118.08
15	cA	1111	CL7	C3A-C4A-CHB	-2.38	120.17	123.70
15	aB	1215	CL7	C3A-C4A-CHB	-2.38	120.17	123.70
15	cA	1132	CL7	O2D-CGD-CBD	2.38	115.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cL	1501	CL7	OBB-CAB-C3B	-2.37	120.32	125.69
15	aB	1234	CL7	CHB-C1B-NB	2.37	126.77	124.26
15	bA	1125	CL7	O2A-CGA-O1A	-2.37	117.60	123.59
15	bB	1201	CL7	CHB-C1B-NB	2.37	126.77	124.26
15	bL	1501	CL7	CHB-C1B-NB	2.37	126.77	124.26
15	bA	1106	CL7	C3A-C4A-CHB	-2.37	120.18	123.70
15	aB	1232	CL7	C3B-C4B-NB	-2.37	108.32	110.52
15	cB	1236	CL7	C3A-C4A-CHB	-2.37	120.18	123.70
15	aB	1238	CL7	CHB-C1B-NB	2.37	126.77	124.26
17	bI	4018	A1JPJ	C12-C13-C14	2.37	122.58	118.94
15	aA	1106	CL7	C1-C2-C3	-2.37	121.95	126.04
17	bL	4023	A1JPJ	C12-C13-C14	2.37	122.58	118.94
15	bB	1230	CL7	CHB-C1B-NB	2.37	126.76	124.26
15	cA	1120	CL7	CHB-C1B-NB	2.37	126.76	124.26
15	cA	1123	CL7	O2A-CGA-O1A	-2.37	117.62	123.59
15	bB	1233	CL7	CAA-C2A-C3A	-2.37	110.58	116.10
15	cB	1216	CL7	C3A-C4A-CHB	-2.37	120.19	123.70
15	aA	1124	CL7	CHB-C1B-NB	2.37	126.76	124.26
15	aB	1206	CL7	C3A-C4A-CHB	-2.36	120.19	123.70
17	cB	4015	A1JPJ	C10-C11-C12	2.36	130.60	123.22
17	bL	4023	A1JPJ	C19-C18-C17	2.36	122.57	118.94
15	bA	1124	CL7	C1-C2-C3	-2.36	122.93	126.75
15	bB	1203	CL7	CHB-C1B-NB	2.36	126.76	124.26
15	aB	1219	CL7	CAA-C2A-C3A	-2.36	110.59	116.10
14	cA	1013	PHO	CMD-C2D-C3D	2.36	129.09	124.68
17	bB	4010	A1JPJ	C19-C18-C17	2.36	122.56	118.94
15	aA	1124	CL7	C3A-C4A-CHB	-2.36	120.20	123.70
15	cA	1124	CL7	C3A-C4A-CHB	-2.36	120.20	123.70
15	cA	1102	CL7	CHB-C1B-NB	2.36	126.75	124.26
17	cA	4002	A1JPJ	C23-C22-C21	2.36	122.56	118.94
15	bB	1213	CL7	O2D-CGD-CBD	2.36	115.45	111.27
15	aA	1130	CL7	C3A-C4A-CHB	-2.35	120.21	123.70
15	cA	1118	CL7	C1-C2-C3	-2.35	121.97	126.04
15	aA	1122	CL7	CHB-C1B-NB	2.35	126.75	124.26
15	cA	1123	CL7	CHB-C1B-NB	2.35	126.75	124.26
15	cF	1701	CL7	CAA-C2A-C3A	-2.35	110.61	116.10
15	bA	1115	CL7	C3A-C4A-CHB	-2.35	120.21	123.70
17	cL	4023	A1JPJ	C12-C13-C14	2.35	122.55	118.94
15	aB	1210	CL7	CHB-C1B-NB	2.35	126.74	124.26
17	aJ	4012	A1JPJ	C15-C16-C17	2.35	128.29	123.47
15	bB	1234	CL7	CHB-C1B-NB	2.35	126.74	124.26
17	bF	4016	A1JPJ	C23-C22-C21	2.35	122.54	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1201	CL7	CHB-C1B-NB	2.35	126.74	124.26
15	cB	1203	CL7	CHB-C1B-NB	2.35	126.74	124.26
15	cB	1232	CL7	C3A-C4A-CHB	-2.35	120.22	123.70
15	bA	1117	CL7	C3A-C4A-CHB	-2.34	120.22	123.70
15	aB	1216	CL7	C3A-C4A-CHB	-2.34	120.22	123.70
15	aA	1121	CL7	C3A-C4A-CHB	-2.34	120.22	123.70
15	bA	1121	CL7	C3A-C4A-CHB	-2.34	120.22	123.70
16	aA	2001	PQN	C11-C3-C4	-2.34	116.00	118.50
15	bA	1113	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
15	cB	1226	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
15	bB	1219	CL7	CAA-C2A-C3A	-2.34	110.64	116.10
15	aB	1230	CL7	CHB-C1B-NB	2.34	126.73	124.26
15	aA	1112	CL7	CHB-C1B-NB	2.34	126.73	124.26
15	aA	1123	CL7	O2A-CGA-O1A	-2.34	117.70	123.59
15	bB	1215	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
17	cI	4018	A1JPJ	C12-C13-C14	2.33	122.52	118.94
15	cB	1213	CL7	CHB-C1B-NB	2.33	126.73	124.26
15	bB	1232	CL7	CAA-C2A-C3A	-2.33	110.65	116.10
15	cB	1212	CL7	O2D-CGD-CBD	2.33	115.41	111.27
17	bA	4002	A1JPJ	C23-C22-C21	2.33	122.52	118.94
17	aA	4014	A1JPJ	C35-C13-C14	-2.33	119.66	122.92
17	bI	4018	A1JPJ	C15-C16-C17	2.33	128.25	123.47
15	bB	1216	CL7	C3A-C4A-CHB	-2.33	120.24	123.70
17	aB	4021	A1JPJ	C34-C9-C8	2.33	121.75	118.08
15	bA	1117	CL7	O2A-CGA-O1A	-2.33	117.71	123.59
17	aI	4018	A1JPJ	C15-C16-C17	2.33	128.25	123.47
17	cI	4018	A1JPJ	C34-C9-C8	2.33	121.75	118.08
15	bA	1104	CL7	CHB-C1B-NB	2.33	126.72	124.26
15	cA	1140	CL7	C1-C2-C3	-2.33	122.02	126.04
15	bB	1222	CL7	OBB-CAB-C3B	-2.33	120.42	125.69
17	bB	4021	A1JPJ	C19-C18-C17	2.33	122.51	118.94
17	aB	4005	A1JPJ	C15-C16-C17	2.33	128.24	123.47
15	cA	1132	CL7	C3A-C4A-CHB	-2.33	120.25	123.70
15	bA	1123	CL7	O2A-CGA-O1A	-2.33	117.72	123.59
17	aB	4021	A1JPJ	C19-C18-C17	2.32	122.51	118.94
15	cA	1102	CL7	C1-C2-C3	-2.32	122.02	126.04
15	cA	1117	CL7	O2A-CGA-O1A	-2.32	117.73	123.59
17	bB	4005	A1JPJ	C19-C18-C17	2.32	122.50	118.94
15	aA	1102	CL7	CHB-C1B-NB	2.32	126.72	124.26
15	cA	1121	CL7	C3A-C4A-CHB	-2.32	120.25	123.70
15	cB	1012	CL7	OBB-CAB-C3B	-2.32	120.44	125.69
17	aB	4010	A1JPJ	C19-C18-C17	2.32	122.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aF	1701	CL7	CAA-C2A-C3A	-2.32	110.68	116.10
15	aA	1135	CL7	CHB-C1B-NB	2.32	126.71	124.26
15	bB	1221	CL7	CHB-C1B-NB	2.32	126.71	124.26
15	cB	1221	CL7	CHB-C1B-NB	2.32	126.71	124.26
15	cB	1232	CL7	CAA-C2A-C3A	-2.32	110.69	116.10
15	aA	1128	CL7	C3A-C4A-CHB	-2.32	120.26	123.70
15	bB	1206	CL7	C3A-C4A-CHB	-2.32	120.26	123.70
15	bA	1109	CL7	C2D-C1D-ND	-2.32	108.68	110.23
15	cL	1502	CL7	O2D-CGD-CBD	2.32	115.38	111.27
15	cA	1103	CL7	C3A-C4A-CHB	-2.31	120.27	123.70
15	cA	1112	CL7	CHB-C1B-NB	2.31	126.70	124.26
15	cA	1136	CL7	CHB-C1B-NB	2.31	126.70	124.26
17	aB	4015	A1JPJ	C1-C6-C7	2.31	122.31	115.78
15	aA	1132	CL7	C3A-C4A-CHB	-2.31	120.27	123.70
15	cA	1113	CL7	C3A-C4A-CHB	-2.31	120.27	123.70
15	cF	1701	CL7	C3A-C4A-CHB	-2.31	120.28	123.70
15	aA	1139	CL7	CHB-C1B-NB	2.31	126.70	124.26
17	bB	4015	A1JPJ	C10-C11-C12	2.31	130.41	123.22
15	cB	1201	CL7	CHB-C1B-NB	2.31	126.70	124.26
15	bA	1140	CL7	C1-C2-C3	-2.30	122.06	126.04
15	cA	1132	CL7	C2D-C1D-ND	-2.30	108.69	110.23
17	aI	4018	A1JPJ	C34-C9-C8	2.30	121.71	118.08
14	cA	1013	PHO	O2D-CGD-O1D	-2.30	119.33	123.84
15	aA	1103	CL7	CHB-C1B-NB	2.30	126.69	124.26
15	aB	1232	CL7	C3A-C4A-CHB	-2.30	120.29	123.70
15	aA	1117	CL7	O2A-CGA-O1A	-2.30	117.78	123.59
15	aB	1232	CL7	CAA-C2A-C3A	-2.30	110.73	116.10
15	bB	1233	CL7	C3B-C4B-NB	-2.30	108.38	110.52
15	aB	1207	CL7	C2D-C1D-ND	-2.30	108.69	110.23
13	bA	1011	G9R	O2A-CGA-O1A	-2.30	117.79	123.59
15	aB	1212	CL7	O2D-CGD-CBD	2.30	115.35	111.27
15	bB	1207	CL7	CHB-C1B-NB	2.30	126.69	124.26
15	bA	1138	CL7	O2A-CGA-O1A	-2.30	117.79	123.59
15	bA	1133	CL7	CHB-C1B-NB	2.30	126.69	124.26
15	aA	1111	CL7	CHB-C1B-NB	2.30	126.69	124.26
15	aB	1206	CL7	C1-C2-C3	-2.30	123.04	126.75
15	bB	1224	CL7	C3A-C4A-CHB	-2.30	120.29	123.70
15	cB	1222	CL7	OBB-CAB-C3B	-2.29	120.50	125.69
15	bA	1128	CL7	C3A-C4A-CHB	-2.29	120.30	123.70
15	aA	1116	CL7	CHB-C1B-NB	2.29	126.69	124.26
15	bA	1109	CL7	C3A-C4A-CHB	-2.29	120.30	123.70
15	bB	1216	CL7	CHB-C1B-NB	2.29	126.68	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1211	CL7	C3A-C4A-CHB	-2.29	120.31	123.70
15	bA	1102	CL7	CHB-C1B-NB	2.29	126.68	124.26
15	bA	1132	CL7	CHB-C1B-NB	2.29	126.68	124.26
17	bL	4023	A1JPJ	C34-C9-C8	2.29	121.68	118.08
15	cA	1104	CL7	CHB-C1B-NB	2.29	126.68	124.26
15	cA	1111	CL7	CHB-C1B-NB	2.29	126.68	124.26
17	aF	4016	A1JPJ	C10-C11-C12	2.29	130.35	123.22
15	bB	1233	CL7	C3A-C4A-CHB	-2.28	120.31	123.70
15	cB	1221	CL7	C2D-C1D-ND	-2.28	108.70	110.23
15	aA	1124	CL7	C1-C2-C3	-2.28	123.06	126.75
15	cB	1215	CL7	CHB-C1B-NB	2.28	126.67	124.26
15	aB	1241	CL7	OBB-CAB-C3B	-2.28	120.53	125.69
15	cB	1227	CL7	C3A-C4A-CHB	-2.28	120.31	123.70
17	aI	4018	A1JPJ	C12-C13-C14	2.28	122.44	118.94
17	cB	4005	A1JPJ	C15-C16-C17	2.28	128.14	123.47
15	bB	1215	CL7	CHB-C1B-NB	2.28	126.67	124.26
15	bA	1116	CL7	O2A-CGA-O1A	-2.28	117.84	123.59
15	bL	1503	CL7	CHB-C1B-NB	2.28	126.67	124.26
15	aK	1402	CL7	CHC-C1C-NC	2.27	126.54	124.45
16	cA	2001	PQN	C11-C3-C4	-2.27	116.07	118.50
17	cA	4011	A1JPJ	C23-C22-C21	2.27	122.43	118.94
17	bI	4018	A1JPJ	C34-C9-C8	2.27	121.66	118.08
15	cA	1132	CL7	O2A-CGA-O1A	-2.27	117.86	123.59
15	aA	1125	CL7	C3A-C4A-CHB	-2.27	120.33	123.70
17	bA	4007	A1JPJ	C37-C22-C23	2.27	121.65	118.08
15	bA	1110	CL7	CHB-C1B-NB	2.27	126.66	124.26
15	cB	1207	CL7	CHB-C1B-NB	2.27	126.66	124.26
15	cA	1125	CL7	C3A-C4A-CHB	-2.27	120.34	123.70
15	bA	1136	CL7	O2A-CGA-O1A	-2.27	117.87	123.59
13	cA	1011	G9R	CMA-C3A-C4A	-2.26	109.42	114.38
15	bB	1205	CL7	C1-C2-C3	-2.26	122.13	126.04
17	cA	4014	A1JPJ	C35-C13-C14	-2.26	119.75	122.92
15	aB	1229	CL7	CHB-C1B-NB	2.26	126.65	124.26
15	bB	1235	CL7	CHB-C1B-NB	2.26	126.65	124.26
15	bA	1111	CL7	CHB-C1B-NB	2.26	126.65	124.26
15	bA	1136	CL7	C3A-C4A-CHB	-2.26	120.35	123.70
15	aB	1222	CL7	OBB-CAB-C3B	-2.26	120.58	125.69
15	aB	1221	CL7	OBB-CAB-C3B	-2.26	120.58	125.69
15	cA	1136	CL7	O2A-CGA-O1A	-2.26	117.90	123.59
15	bA	1102	CL7	C1-C2-C3	-2.25	122.14	126.04
15	aA	1104	CL7	CHB-C1B-NB	2.25	126.64	124.26
15	aA	1132	CL7	O2A-CGA-O1A	-2.25	117.90	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1106	CL7	C1-C2-C3	-2.25	122.15	126.04
15	bB	1202	CL7	CHB-C1B-NB	2.25	126.64	124.26
15	cA	1129	CL7	C3A-C4A-CHB	-2.25	120.36	123.70
15	bK	1401	CL7	O2D-CGD-CBD	2.25	115.27	111.27
17	aB	4005	A1JPJ	C19-C18-C17	2.25	122.39	118.94
17	cB	4006	A1JPJ	C15-C16-C17	2.25	128.08	123.47
17	bB	4021	A1JPJ	C34-C9-C8	2.25	121.62	118.08
15	cB	1224	CL7	C3A-C4A-CHB	-2.25	120.36	123.70
15	bA	1117	CL7	C1-C2-C3	-2.25	122.16	126.04
17	cL	4023	A1JPJ	C34-C9-C8	2.25	121.62	118.08
15	cA	1131	CL7	C1-C2-C3	-2.25	122.16	126.04
17	cA	4007	A1JPJ	C7-C8-C9	2.25	129.63	126.23
15	cB	1229	CL7	CHB-C1B-NB	2.25	126.63	124.26
15	cA	1022	CL7	C2D-C1D-ND	-2.24	108.73	110.23
17	bB	4005	A1JPJ	C37-C22-C23	2.24	121.61	118.08
16	aB	2002	PQN	C11-C3-C4	-2.24	116.10	118.50
15	bA	1132	CL7	O2D-CGD-CBD	2.24	115.25	111.27
17	bA	4008	A1JPJ	C16-C15-C14	2.24	128.06	123.47
15	bB	1210	CL7	CHB-C1B-NB	2.24	126.63	124.26
17	cB	4005	A1JPJ	C19-C18-C17	2.24	122.38	118.94
15	cA	1110	CL7	CHB-C1B-NB	2.24	126.63	124.26
15	cK	1401	CL7	O2D-CGD-CBD	2.24	115.24	111.27
15	cB	1220	CL7	CHB-C1B-NB	2.24	126.62	124.26
15	bB	1021	CL7	C1-C2-C3	-2.24	122.18	126.04
15	aB	1235	CL7	CHB-C1B-NB	2.23	126.62	124.26
15	bB	1225	CL7	C2D-C1D-ND	-2.23	108.73	110.23
15	cA	1104	CL7	OBB-CAB-C3B	-2.23	120.64	125.69
15	aB	1226	CL7	C2D-C1D-ND	-2.23	108.73	110.23
15	aA	1136	CL7	O2A-CGA-O1A	-2.23	117.96	123.59
15	aA	1129	CL7	CHB-C1B-NB	2.23	126.62	124.26
15	aA	1125	CL7	CHB-C1B-NB	2.23	126.62	124.26
15	cA	1128	CL7	C3A-C4A-CHB	-2.23	120.39	123.70
17	bA	4014	A1JPJ	C35-C13-C14	-2.23	119.80	122.92
15	cB	1228	CL7	CHB-C1B-NB	2.23	126.62	124.26
15	aA	1138	CL7	O2A-CGA-O1A	-2.23	117.97	123.59
14	aB	1023	PHO	O2A-CGA-O1A	-2.23	117.97	123.59
15	cA	1135	CL7	C1-C2-C3	-2.23	123.15	126.75
15	bA	1123	CL7	CHB-C1B-NB	2.23	126.62	124.26
15	cA	1136	CL7	C3A-C4A-CHB	-2.23	120.39	123.70
15	cB	1215	CL7	C3A-C4A-CHB	-2.23	120.40	123.70
15	aB	1239	CL7	CHB-C1B-NB	2.23	126.61	124.26
15	cB	1235	CL7	CHB-C1B-NB	2.23	126.61	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1117	CL7	C3A-C4A-CHB	-2.23	120.40	123.70
15	cA	1109	CL7	CHB-C1B-NB	2.23	126.61	124.26
15	cA	1129	CL7	CHB-C1B-NB	2.23	126.61	124.26
15	cB	1206	CL7	OBB-CAB-C3B	-2.22	120.66	125.69
15	bA	1108	CL7	C3A-C4A-CHB	-2.22	120.40	123.70
15	bA	1139	CL7	CHB-C1B-NB	2.22	126.61	124.26
17	bB	4010	A1JPJ	C37-C22-C23	2.22	121.58	118.08
15	aA	1108	CL7	C3A-C4A-CHB	-2.22	120.40	123.70
15	cB	1213	CL7	O2D-CGD-CBD	2.22	115.22	111.27
15	aB	1220	CL7	CHB-C1B-NB	2.22	126.61	124.26
15	cA	1105	CL7	CHB-C1B-NB	2.22	126.61	124.26
15	cB	1207	CL7	C2D-C1D-ND	-2.22	108.74	110.23
15	aB	1204	CL7	C1-C2-C3	-2.22	122.20	126.04
15	aA	1126	CL7	C3A-C4A-CHB	-2.22	120.41	123.70
15	cA	1126	CL7	C3A-C4A-CHB	-2.22	120.41	123.70
15	cA	1106	CL7	OBB-CAB-C3B	-2.22	120.67	125.69
15	cB	1227	CL7	OBB-CAB-C3B	-2.22	120.67	125.69
15	bA	1118	CL7	C1-C2-C3	-2.22	122.20	126.04
17	bB	4015	A1JPJ	C1-C6-C7	2.22	122.06	115.78
16	cB	2002	PQN	C11-C3-C4	-2.22	116.13	118.50
15	cB	1215	CL7	C2D-C1D-ND	-2.22	108.75	110.23
15	aA	1129	CL7	CHD-C1D-ND	-2.22	121.91	124.26
15	aB	1213	CL7	CHB-C1B-NB	2.22	126.60	124.26
15	bA	1109	CL7	CHB-C1B-NB	2.22	126.60	124.26
17	cB	4015	A1JPJ	C1-C6-C7	2.22	122.05	115.78
15	bA	1116	CL7	C1-C2-C3	-2.22	122.21	126.04
15	aA	1136	CL7	C3A-C4A-CHB	-2.22	120.41	123.70
15	cA	1112	CL7	C1-C2-C3	-2.22	122.21	126.04
15	cA	1111	CL7	C2D-C1D-ND	-2.22	108.75	110.23
15	cA	1139	CL7	CHB-C1B-NB	2.22	126.60	124.26
15	bA	1112	CL7	CHB-C1B-NB	2.21	126.60	124.26
15	bF	1701	CL7	CAA-C2A-C3A	-2.21	110.93	116.10
15	cB	1236	CL7	CHB-C1B-NB	2.21	126.60	124.26
17	aA	4002	A1JPJ	C8-C9-C10	2.21	122.34	118.94
15	bB	1206	CL7	C1-C2-C3	-2.21	123.17	126.75
15	aA	1109	CL7	C2D-C1D-ND	-2.21	108.75	110.23
15	bB	1226	CL7	C2D-C1D-ND	-2.21	108.75	110.23
15	cA	1138	CL7	O2A-CGA-O1A	-2.21	118.01	123.59
15	aB	1012	CL7	C1-C2-C3	-2.21	122.22	126.04
15	cB	1226	CL7	O2A-CGA-O1A	-2.21	118.02	123.59
15	aK	1401	CL7	O2D-CGD-CBD	2.21	115.19	111.27
17	aF	4016	A1JPJ	C16-C15-C14	2.21	128.00	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1105	CL7	CHB-C1B-NB	2.21	126.59	124.26
15	cB	1211	CL7	CHB-C1B-NB	2.21	126.59	124.26
15	aB	1211	CL7	CHB-C1B-NB	2.20	126.59	124.26
15	aA	1118	CL7	C1-C2-C3	-2.20	122.23	126.04
15	cA	1117	CL7	C1-C2-C3	-2.20	122.23	126.04
15	cB	1229	CL7	C1-C2-C3	-2.20	122.23	126.04
15	aA	1123	CL7	CHB-C1B-NB	2.20	126.59	124.26
15	aB	1213	CL7	O2D-CGD-CBD	2.20	115.18	111.27
15	bB	1234	CL7	OBB-CAB-C3B	-2.20	120.71	125.69
15	bA	1133	CL7	C1-C2-C3	-2.20	122.24	126.04
15	aB	1241	CL7	C3B-C4B-NB	-2.20	108.47	110.52
15	aA	1135	CL7	C1-C2-C3	-2.20	123.19	126.75
15	aB	1205	CL7	C1-C2-C3	-2.20	122.25	126.04
15	cB	1205	CL7	C1-C2-C3	-2.19	122.25	126.04
15	bA	1122	CL7	CHB-C1B-NB	2.19	126.58	124.26
15	bB	1227	CL7	C3A-C4A-CHB	-2.19	120.44	123.70
15	bB	1205	CL7	CHB-C1B-NB	2.19	126.58	124.26
15	bB	1210	CL7	C1-C2-C3	-2.19	122.25	126.04
15	cB	1206	CL7	C1-C2-C3	-2.19	123.20	126.75
15	bA	1111	CL7	C2D-C1D-ND	-2.19	108.76	110.23
15	cA	1108	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
17	cA	4008	A1JPJ	C20-C21-C22	2.19	130.44	127.31
15	bA	1115	CL7	CHB-C1B-NB	2.19	126.58	124.26
15	aA	1109	CL7	CHB-C1B-NB	2.19	126.58	124.26
15	aA	1129	CL7	O2A-CGA-O1A	-2.19	118.06	123.59
15	aB	1212	CL7	CHB-C1B-NB	2.19	126.58	124.26
15	aA	1129	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
15	bA	1119	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
15	bI	1601	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
15	cA	1137	CL7	O2D-CGD-CBD	2.19	115.16	111.27
15	aB	1227	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
15	bB	1236	CL7	CHB-C1B-NB	2.19	126.57	124.26
15	aA	1111	CL7	C1-C2-C3	-2.19	122.26	126.04
17	cB	4015	A1JPJ	C2-C1-C6	2.19	113.85	110.48
15	bA	1131	CL7	C1-C2-C3	-2.19	122.26	126.04
15	cB	1021	CL7	C1-C2-C3	-2.19	122.26	126.04
15	cB	1207	CL7	OBB-CAB-C3B	-2.19	120.74	125.69
15	cB	1223	CL7	CHB-C1B-NB	2.18	126.57	124.26
15	bA	1135	CL7	C1-C2-C3	-2.18	123.22	126.75
15	aB	1207	CL7	CHB-C1B-NB	2.18	126.57	124.26
15	cA	1116	CL7	C1-C2-C3	-2.18	122.27	126.04
15	aB	1226	CL7	O2A-CGA-O1A	-2.18	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1107	CL7	CHB-C1B-NB	2.18	126.57	124.26
17	aF	4016	A1JPJ	C2-C1-C6	2.18	113.84	110.48
15	aA	1119	CL7	C1-C2-C3	-2.18	122.27	126.04
15	cI	1601	CL7	CHC-C1C-NC	2.18	126.46	124.45
15	bB	1226	CL7	O2A-CGA-O1A	-2.18	118.09	123.59
15	bL	1503	CL7	C3A-C4A-CHB	-2.18	120.47	123.70
13	cA	1011	G9R	O2A-CGA-O1A	-2.18	118.09	123.59
17	bA	4007	A1JPJ	C7-C8-C9	2.18	129.53	126.23
13	aA	1011	G9R	CMA-C3A-C4A	-2.18	109.61	114.38
17	cJ	4012	A1JPJ	C1-C6-C7	2.18	121.94	115.78
15	bB	1213	CL7	CHB-C1B-NB	2.18	126.56	124.26
15	cB	1232	CL7	CHB-C1B-NB	2.18	126.56	124.26
15	cB	1239	CL7	CHB-C1B-NB	2.18	126.56	124.26
15	aA	1107	CL7	CHB-C1B-NB	2.18	126.56	124.26
15	cA	1101	CL7	CHB-C1B-NB	2.18	126.56	124.26
17	bB	4006	A1JPJ	C1-C6-C7	2.18	121.93	115.78
15	cB	1220	CL7	O2D-CGD-CBD	2.18	115.13	111.27
15	bA	1119	CL7	C1-C2-C3	-2.17	122.28	126.04
15	bB	1201	CL7	C3A-C4A-CHB	-2.17	120.47	123.70
15	cA	1107	CL7	CHB-C1B-NB	2.17	126.56	124.26
17	bB	4006	A1JPJ	C15-C16-C17	2.17	127.92	123.47
15	cB	1234	CL7	O2A-CGA-O1A	-2.17	118.11	123.59
15	aA	1137	CL7	CHB-C1B-NB	2.17	126.56	124.26
15	cA	1119	CL7	C1-C2-C3	-2.17	122.29	126.04
15	aA	1105	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	aA	1110	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	bB	1223	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	aA	1106	CL7	OBB-CAB-C3B	-2.17	120.78	125.69
17	bJ	4012	A1JPJ	C1-C6-C7	2.17	121.91	115.78
15	bB	1206	CL7	OBB-CAB-C3B	-2.17	120.78	125.69
15	cJ	1302	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	cB	1215	CL7	C3B-C4B-NB	-2.17	108.50	110.52
15	aA	1124	CL7	O2A-CGA-O1A	-2.17	118.12	123.59
15	aB	1237	CL7	C1-C2-C3	-2.17	122.30	126.04
15	bB	1225	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	bJ	1301	CL7	CHB-C1B-NB	2.17	126.55	124.26
15	cA	1115	CL7	CHB-C1B-NB	2.17	126.55	124.26
17	aJ	4012	A1JPJ	C1-C6-C7	2.16	121.90	115.78
17	bB	4015	A1JPJ	C2-C1-C6	2.16	113.81	110.48
15	bB	1239	CL7	CHB-C1B-NB	2.16	126.55	124.26
15	cA	1134	CL7	CHB-C1B-NB	2.16	126.55	124.26
15	bB	1208	CL7	O2A-CGA-O1A	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1127	CL7	C2D-C1D-ND	-2.16	108.78	110.23
15	aA	1101	CL7	CHB-C1B-NB	2.16	126.55	124.26
13	aA	1011	G9R	O2A-CGA-O1A	-2.16	118.14	123.59
15	aL	1503	CL7	CHB-C1B-NB	2.16	126.54	124.26
15	cA	1116	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
15	aB	1234	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
15	aB	1021	CL7	C1-C2-C3	-2.16	122.31	126.04
15	cA	1125	CL7	CHD-C4C-NC	2.16	126.44	124.45
15	bB	1220	CL7	CHB-C1B-NB	2.16	126.54	124.26
15	cA	1801	CL7	CHB-C1B-NB	2.16	126.54	124.26
17	cB	4006	A1JPJ	C16-C17-C18	2.16	130.39	127.31
17	bB	4015	A1JPJ	C1-C6-C5	-2.16	119.57	122.61
15	cB	1237	CL7	C1-C2-C3	-2.16	122.31	126.04
15	aB	1237	CL7	CHB-C1B-NB	2.16	126.54	124.26
15	bB	1232	CL7	CHB-C1B-NB	2.16	126.54	124.26
15	aB	1201	CL7	C3A-C4A-CHB	-2.16	120.50	123.70
17	aB	4006	A1JPJ	C1-C6-C7	2.16	121.88	115.78
15	bB	1229	CL7	O2A-CGA-O1A	-2.16	118.15	123.59
15	cB	1208	CL7	O2A-CGA-O1A	-2.16	118.15	123.59
17	aB	4006	A1JPJ	C15-C16-C17	2.16	127.89	123.47
15	bA	1101	CL7	CHB-C1B-NB	2.16	126.54	124.26
17	cB	4006	A1JPJ	C1-C6-C7	2.16	121.88	115.78
15	bJ	1302	CL7	CHB-C1B-NB	2.16	126.54	124.26
15	bB	1239	CL7	C1-C2-C3	-2.15	122.32	126.04
15	aA	1104	CL7	OBB-CAB-C3B	-2.15	120.81	125.69
17	bI	4019	A1JPJ	C19-C18-C17	2.15	122.25	118.94
17	aA	4008	A1JPJ	C20-C21-C22	2.15	130.38	127.31
15	cA	1118	CL7	CHB-C1B-NB	2.15	126.54	124.26
15	aB	1239	CL7	C1-C2-C3	-2.15	122.32	126.04
15	cA	1129	CL7	O2A-CGA-O1A	-2.15	118.16	123.59
17	bI	4019	A1JPJ	C37-C22-C23	2.15	121.47	118.08
15	aA	1134	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	bB	1229	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	aJ	1302	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	bB	1202	CL7	C3A-C4A-CHB	-2.15	120.51	123.70
15	aB	1218	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	aB	1227	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	bA	1114	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	aB	1202	CL7	O2A-CGA-O1A	-2.15	118.17	123.59
15	cB	1234	CL7	OBB-CAB-C3B	-2.15	120.83	125.69
15	aA	1801	CL7	CHB-C1B-NB	2.15	126.53	124.26
17	aI	4019	A1JPJ	C19-C18-C17	2.15	122.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	bA	4011	A1JPJ	C12-C13-C14	2.15	122.23	118.94
15	aA	1117	CL7	C1-C2-C3	-2.15	122.33	126.04
15	aA	1132	CL7	OBB-CAB-C3B	-2.15	120.84	125.69
15	aA	1114	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	bB	1218	CL7	CHB-C1B-NB	2.15	126.53	124.26
15	aA	1022	CL7	C2D-C1D-ND	-2.15	108.79	110.23
17	bB	4006	A1JPJ	C16-C17-C18	2.14	130.37	127.31
15	cB	1239	CL7	C1-C2-C3	-2.14	122.33	126.04
15	bB	1209	CL7	CHB-C1B-NB	2.14	126.53	124.26
15	cB	1215	CL7	OBB-CAB-C3B	-2.14	120.84	125.69
15	aA	1121	CL7	O2A-CGA-O1A	-2.14	118.18	123.59
15	aB	1241	CL7	C3A-C4A-CHB	-2.14	120.52	123.70
15	cB	1201	CL7	C3A-C4A-CHB	-2.14	120.52	123.70
17	cB	4006	A1JPJ	C37-C22-C23	-2.14	114.70	118.08
15	bA	1121	CL7	O2A-CGA-O1A	-2.14	118.18	123.59
15	cB	1221	CL7	O2A-CGA-O1A	-2.14	118.18	123.59
15	cB	1235	CL7	O2A-CGA-O1A	-2.14	118.19	123.59
15	aB	1206	CL7	OBB-CAB-C3B	-2.14	120.84	125.69
15	bL	1502	CL7	O2A-CGA-O1A	-2.14	118.19	123.59
15	cA	1138	CL7	C1-C2-C3	-2.14	122.34	126.04
17	aB	4006	A1JPJ	C16-C17-C18	2.14	130.37	127.31
15	bB	1212	CL7	OBB-CAB-C3B	-2.14	120.85	125.69
15	aB	1208	CL7	O2A-CGA-O1A	-2.14	118.19	123.59
15	aL	1503	CL7	C3A-C4A-CHB	-2.14	120.53	123.70
15	cB	1218	CL7	CHB-C1B-NB	2.14	126.52	124.26
15	cB	1236	CL7	C3B-C4B-NB	-2.14	108.53	110.52
15	cA	1132	CL7	OBB-CAB-C3B	-2.14	120.85	125.69
15	bA	1126	CL7	O2A-CGA-O1A	-2.14	118.20	123.59
15	cA	1140	CL7	C3A-C4A-CHB	-2.14	120.53	123.70
15	bB	1241	CL7	OBB-CAB-C3B	-2.14	120.86	125.69
15	aB	1238	CL7	O2A-CGA-O1A	-2.14	118.20	123.59
15	cB	1214	CL7	C1-C2-C3	-2.14	123.30	126.75
15	bB	1221	CL7	O2A-CGA-O1A	-2.14	118.20	123.59
16	bB	2002	PQN	C11-C3-C4	-2.14	116.22	118.50
15	aB	1212	CL7	OBB-CAB-C3B	-2.13	120.86	125.69
15	cA	1124	CL7	O2A-CGA-O1A	-2.13	118.21	123.59
17	aB	4015	A1JPJ	C2-C1-C6	2.13	113.76	110.48
15	cA	1138	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	aI	1601	CL7	CHC-C1C-NC	2.13	126.41	124.45
15	aA	1129	CL7	OBB-CAB-C3B	-2.13	120.87	125.69
15	bA	1134	CL7	CHB-C1B-NB	2.13	126.51	124.26
17	cA	4011	A1JPJ	C8-C9-C10	2.13	122.21	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aL	1503	CL7	O2A-CGA-O1A	-2.13	118.21	123.59
17	cI	4019	A1JPJ	C37-C22-C23	2.13	121.43	118.08
15	cB	1237	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	cB	1227	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	bA	1129	CL7	O2A-CGA-O1A	-2.13	118.22	123.59
15	bB	1222	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	aB	1012	CL7	O2A-CGA-O1A	-2.13	118.22	123.59
15	bB	1012	CL7	O2A-CGA-O1A	-2.13	118.22	123.59
15	bA	1138	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	cA	1114	CL7	CHB-C1B-NB	2.13	126.51	124.26
17	aB	4015	A1JPJ	C1-C6-C5	-2.13	119.62	122.61
15	bA	1113	CL7	CHB-C1B-NB	2.13	126.51	124.26
15	bA	1103	CL7	C1-C2-C3	-2.12	122.37	126.04
15	aA	1140	CL7	C1-C2-C3	-2.12	122.37	126.04
15	aK	1402	CL7	CAD-CBD-CHA	2.12	107.53	105.14
15	aJ	1301	CL7	CHB-C1B-NB	2.12	126.50	124.26
15	aB	1205	CL7	O2D-CGD-CBD	2.12	115.04	111.27
15	aB	1226	CL7	CHC-C1C-NC	2.12	126.40	124.45
17	cB	4015	A1JPJ	C1-C6-C5	-2.12	119.62	122.61
15	aL	1502	CL7	O2A-CGA-O1A	-2.12	118.24	123.59
15	bB	1235	CL7	O2A-CGA-O1A	-2.12	118.24	123.59
15	aB	1228	CL7	CHB-C1B-NB	2.12	126.50	124.26
17	aA	4011	A1JPJ	C8-C9-C10	2.12	122.19	118.94
15	bA	1130	CL7	OBB-CAB-C3B	-2.12	120.89	125.69
15	cB	1225	CL7	CHB-C1B-NB	2.12	126.50	124.26
15	aA	1132	CL7	C2D-C1D-ND	-2.12	108.81	110.23
15	cB	1212	CL7	OBB-CAB-C3B	-2.12	120.90	125.69
15	cL	1503	CL7	O2A-CGA-O1A	-2.12	118.25	123.59
15	bB	1237	CL7	C1-C2-C3	-2.12	122.38	126.04
15	cB	1012	CL7	O2A-CGA-O1A	-2.12	118.25	123.59
15	aB	1223	CL7	CHB-C1B-NB	2.12	126.50	124.26
15	bA	1801	CL7	CHB-C1B-NB	2.12	126.50	124.26
15	cF	1701	CL7	CMA-C3A-C2A	-2.12	111.16	116.10
17	aI	4019	A1JPJ	C37-C22-C23	2.12	121.41	118.08
15	aB	1230	CL7	C3A-C2A-C1A	2.12	104.17	101.64
17	aA	4008	A1JPJ	C16-C15-C14	2.12	127.81	123.47
15	aB	1221	CL7	CHB-C1B-NB	2.11	126.50	124.26
17	cI	4019	A1JPJ	C19-C18-C17	2.11	122.19	118.94
15	aA	1134	CL7	O2D-CGD-CBD	2.11	115.02	111.27
15	bB	1232	CL7	C2D-C1D-ND	-2.11	108.81	110.23
15	bL	1503	CL7	O2A-CGA-O1A	-2.11	118.26	123.59
16	aA	2001	PQN	C12-C11-C3	-2.11	106.35	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1124	CL7	O2A-CGA-O1A	-2.11	118.26	123.59
15	aA	1118	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	aB	1205	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	bA	1140	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	aA	1102	CL7	C1-C2-C3	-2.11	122.39	126.04
15	aB	1229	CL7	C1-C2-C3	-2.11	122.39	126.04
15	bB	1211	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	aB	1229	CL7	O2A-CGA-O1A	-2.11	118.26	123.59
15	bA	1132	CL7	C2D-C1D-ND	-2.11	108.82	110.23
15	cB	1209	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	cA	1121	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	aA	1131	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	cL	1502	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	bA	1129	CL7	C3A-C4A-CHB	-2.11	120.57	123.70
15	cA	1112	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	cB	1238	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
17	cA	4008	A1JPJ	C16-C15-C14	2.11	127.79	123.47
15	cA	1117	CL7	C3C-C4C-NC	-2.11	108.65	110.18
15	aA	1140	CL7	C3A-C4A-CHB	-2.11	120.57	123.70
15	aA	1133	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	aB	1235	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
15	bB	1212	CL7	O2D-CGD-CBD	2.11	115.01	111.27
15	aA	1138	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	bB	1208	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	cB	1212	CL7	CHB-C1B-NB	2.11	126.49	124.26
15	aB	1232	CL7	CHB-C1B-NB	2.10	126.48	124.26
15	bB	1205	CL7	CHC-C1C-NC	2.10	126.39	124.45
15	aK	1401	CL7	CHB-C1B-NB	2.10	126.48	124.26
15	cA	1133	CL7	C1-C2-C3	-2.10	122.41	126.04
15	aA	1119	CL7	C3A-C4A-CHB	-2.10	120.58	123.70
15	cB	1205	CL7	CHB-C1B-NB	2.10	126.48	124.26
15	bB	1212	CL7	CHB-C1B-NB	2.10	126.48	124.26
17	bF	4016	A1JPJ	C33-C5-C6	2.10	126.89	124.53
15	bB	1225	CL7	O2A-CGA-O1A	-2.10	118.29	123.59
15	bA	1101	CL7	CMA-C3A-C2A	-2.10	111.19	116.10
15	bB	1237	CL7	CHB-C1B-NB	2.10	126.48	124.26
15	bB	1221	CL7	C2D-C1D-ND	-2.10	108.82	110.23
15	bB	1205	CL7	C3A-C4A-CHB	-2.10	120.58	123.70
15	cL	1503	CL7	C3A-C4A-CHB	-2.10	120.58	123.70
15	cA	1112	CL7	CAA-CBA-CGA	-2.10	107.12	113.25
15	bB	1214	CL7	O2A-CGA-O1A	-2.10	118.29	123.59
15	aB	1211	CL7	C1-C2-C3	-2.10	122.41	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aA	1113	CL7	CHB-C1B-NB	2.10	126.48	124.26
15	cA	1103	CL7	C1-C2-C3	-2.10	122.41	126.04
15	cB	1210	CL7	CHB-C1B-NB	2.10	126.48	124.26
17	aA	4007	A1JPJ	C37-C22-C23	2.10	121.38	118.08
17	bF	4016	A1JPJ	C2-C1-C6	2.10	113.71	110.48
15	aB	1214	CL7	O2A-CGA-O1A	-2.10	118.30	123.59
15	cF	1701	CL7	CHC-C1C-NC	2.10	126.38	124.45
15	cB	1205	CL7	C3A-C4A-CHB	-2.10	120.59	123.70
15	bB	1238	CL7	O2A-CGA-O1A	-2.10	118.30	123.59
15	cB	1225	CL7	O2A-CGA-O1A	-2.10	118.30	123.59
15	cB	1226	CL7	C2D-C1D-ND	-2.09	108.83	110.23
15	cA	1133	CL7	O2A-CGA-O1A	-2.09	118.31	123.59
15	bB	1234	CL7	O2A-CGA-O1A	-2.09	118.31	123.59
15	aB	1221	CL7	O2A-CGA-O1A	-2.09	118.31	123.59
15	bB	1214	CL7	CMB-C2B-C1B	-2.09	122.18	125.37
17	aL	4023	A1JPJ	C1-C6-C7	2.09	121.69	115.78
15	aB	1222	CL7	CHB-C1B-NB	2.09	126.47	124.26
15	cB	1205	CL7	CHC-C1C-NC	2.09	126.38	124.45
15	cK	1402	CL7	CHC-C1C-NC	2.09	126.37	124.45
15	aB	1205	CL7	C3A-C4A-CHB	-2.09	120.60	123.70
15	bB	1202	CL7	O2A-CGA-O1A	-2.09	118.32	123.59
15	bA	1118	CL7	O2A-CGA-O1A	-2.09	118.32	123.59
17	aI	4018	A1JPJ	C19-C18-C17	2.09	122.14	118.94
15	aB	1234	CL7	OBb-CAB-C3B	-2.09	120.97	125.69
15	aB	1214	CL7	C1-C2-C3	-2.09	123.37	126.75
15	aB	1225	CL7	CHB-C1B-NB	2.09	126.47	124.26
15	aB	1021	CL7	O2A-CGA-O1A	-2.09	118.32	123.59
15	aA	1132	CL7	C3C-C4C-NC	-2.09	108.66	110.18
17	aA	4011	A1JPJ	C23-C22-C21	2.09	122.14	118.94
17	aL	4023	A1JPJ	C34-C9-C8	2.09	121.36	118.08
15	cA	1119	CL7	O2A-CGA-O1A	-2.09	118.33	123.59
15	aA	1117	CL7	CHC-C1C-NC	2.09	126.37	124.45
15	bA	1112	CL7	O2A-CGA-O1A	-2.08	118.33	123.59
17	cA	4011	A1JPJ	C19-C18-C17	2.08	122.14	118.94
15	aF	1701	CL7	C2D-C1D-ND	-2.08	108.83	110.23
17	cB	4005	A1JPJ	C10-C11-C12	2.08	129.72	123.22
15	bA	1133	CL7	O2A-CGA-O1A	-2.08	118.33	123.59
15	cB	1215	CL7	O2D-CGD-CBD	2.08	114.97	111.27
17	bJ	4012	A1JPJ	C10-C11-C12	2.08	129.72	123.22
15	cB	1204	CL7	O2D-CGD-CBD	2.08	114.97	111.27
15	bA	1137	CL7	CHB-C1B-NB	2.08	126.46	124.26
15	cB	1236	CL7	OBb-CAB-C3B	-2.08	120.98	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bA	1102	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
15	bB	1219	CL7	CHB-C1B-NB	2.08	126.46	124.26
15	bK	1402	CL7	CHB-C1B-NB	2.08	126.46	124.26
15	aB	1230	CL7	C2D-C1D-ND	-2.08	108.84	110.23
15	bA	1132	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
15	aA	1113	CL7	CHC-C1C-NC	2.08	126.36	124.45
15	cB	1202	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
15	cK	1402	CL7	CHB-C1B-NB	2.08	126.46	124.26
15	cA	1102	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
15	cB	1214	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
15	cA	1132	CL7	C3C-C4C-NC	-2.08	108.67	110.18
14	bB	1023	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
17	aA	4003	A1JPJ	C33-C5-C6	2.08	126.86	124.53
15	aA	1112	CL7	CHD-C4C-NC	2.08	126.36	124.45
15	cB	1215	CL7	CHC-C1C-NC	2.08	126.36	124.45
15	cB	1222	CL7	CHB-C1B-NB	2.08	126.46	124.26
15	bB	1214	CL7	C1-C2-C3	-2.08	123.39	126.75
15	bB	1012	CL7	C1-C2-C3	-2.08	122.45	126.04
15	aB	1210	CL7	O2A-CGA-O1A	-2.08	118.35	123.59
14	bB	1023	PHO	C1C-C2C-C3C	-2.08	106.88	108.61
15	aA	1138	CL7	C1-C2-C3	-2.08	122.45	126.04
15	bA	1125	CL7	CHB-C1B-NB	2.08	126.45	124.26
15	cA	1113	CL7	CHB-C1B-NB	2.08	126.45	124.26
14	bA	1013	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
15	bA	1129	CL7	CHB-C1B-NB	2.07	126.45	124.26
15	bA	1106	CL7	OBB-CAB-C3B	-2.07	121.00	125.69
17	aA	4008	A1JPJ	C30-C25-C26	2.07	115.13	111.42
15	cA	1138	CL7	C3C-C4C-NC	-2.07	108.67	110.18
15	cB	1223	CL7	O2A-CGA-O1A	-2.07	118.36	123.59
15	cA	1137	CL7	CHB-C1B-NB	2.07	126.45	124.26
15	cA	1118	CL7	O2A-CGA-O1A	-2.07	118.36	123.59
15	bB	1226	CL7	CHC-C1C-NC	2.07	126.36	124.45
15	aA	1140	CL7	CHB-C1B-NB	2.07	126.45	124.26
15	aB	1233	CL7	CHB-C1B-NB	2.07	126.45	124.26
15	bA	1127	CL7	O2A-CGA-O1A	-2.07	118.36	123.59
15	cB	1241	CL7	C3A-C4A-CHB	-2.07	120.63	123.70
15	aB	1223	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
15	bB	1021	CL7	OBB-CAB-C3B	-2.07	121.01	125.69
19	cB	5002	LMG	C3-C4-C5	-2.07	106.55	110.24
15	bB	1223	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
15	aB	1210	CL7	C2D-C1D-ND	-2.07	108.84	110.23
15	cA	1127	CL7	C2D-C1D-ND	-2.07	108.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1225	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
15	bA	1102	CL7	OBB-CAB-C3B	-2.07	121.01	125.69
15	aA	1118	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
15	bA	1101	CL7	O2D-CGD-CBD	2.07	114.94	111.27
15	aA	1127	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
15	aA	1135	CL7	C2D-C1D-ND	-2.07	108.85	110.23
15	aB	1012	CL7	C2D-C1D-ND	-2.07	108.85	110.23
15	bA	1103	CL7	C3A-C4A-CHB	-2.07	120.64	123.70
15	aB	1236	CL7	CHB-C1B-NB	2.06	126.44	124.26
15	aI	1601	CL7	O2A-CGA-O1A	-2.06	118.38	123.59
15	aA	1111	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	aJ	1301	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	cB	1238	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	cB	1241	CL7	C2D-C1D-ND	-2.06	108.85	110.23
17	bB	4010	A1JPJ	C11-C12-C13	2.06	132.21	126.42
15	aA	1103	CL7	C1-C2-C3	-2.06	122.48	126.04
15	aA	1101	CL7	CMA-C3A-C2A	-2.06	111.29	116.10
15	bA	1131	CL7	O2A-CGA-O1A	-2.06	118.39	123.59
15	cB	1233	CL7	CHB-C1B-NB	2.06	126.44	124.26
14	cB	1023	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
15	cB	1012	CL7	C1-C2-C3	-2.06	122.48	126.04
15	cB	1221	CL7	OBB-CAB-C3B	-2.06	121.03	125.69
15	aA	1107	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	cA	1103	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	bA	1119	CL7	O2A-CGA-O1A	-2.06	118.40	123.59
17	bA	4008	A1JPJ	C20-C21-C22	2.06	130.25	127.31
17	bL	4023	A1JPJ	C1-C6-C7	2.06	121.60	115.78
15	bA	1127	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	bA	1137	CL7	O2D-CGD-CBD	2.06	114.92	111.27
15	aB	1226	CL7	C3C-C4C-NC	-2.06	108.69	110.18
15	cA	1106	CL7	CHD-C4C-NC	2.06	126.34	124.45
17	bL	4023	A1JPJ	C23-C22-C21	2.06	122.10	118.94
15	cA	1101	CL7	CMA-C3A-C2A	-2.06	111.30	116.10
15	bB	1012	CL7	C2D-C1D-ND	-2.06	108.85	110.23
15	cB	1021	CL7	O2A-CGA-O1A	-2.06	118.41	123.59
17	aB	4010	A1JPJ	C11-C12-C13	2.06	132.19	126.42
15	cA	1135	CL7	O1D-CGD-CBD	2.05	128.69	124.48
15	aB	1205	CL7	CHC-C1C-NC	2.05	126.34	124.45
17	cB	4010	A1JPJ	C11-C12-C13	2.05	132.19	126.42
15	aB	1209	CL7	CHB-C1B-NB	2.05	126.43	124.26
17	cI	4018	A1JPJ	C19-C18-C17	2.05	122.09	118.94
15	cL	1503	CL7	OBB-CAB-C3B	-2.05	121.05	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bB	1227	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	cB	1012	CL7	C3A-C4A-CHB	-2.05	120.66	123.70
17	bI	4018	A1JPJ	C19-C18-C17	2.05	122.09	118.94
15	bB	1021	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
17	aA	4008	A1JPJ	C34-C9-C8	2.05	121.31	118.08
15	cA	1128	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	aB	1238	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	aA	1119	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	cA	1130	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	cB	1229	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	cA	1140	CL7	CHB-C1B-NB	2.05	126.43	124.26
15	bB	1221	CL7	OBb-CAB-C3B	-2.05	121.06	125.69
15	aB	1215	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	bB	1210	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	bB	1207	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	cL	1501	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	cA	1106	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
15	bB	1215	CL7	O2A-CGA-O1A	-2.05	118.43	123.59
15	cA	1117	CL7	CHC-C1C-NC	2.05	126.33	124.45
15	aB	1225	CL7	C2D-C1D-ND	-2.05	108.86	110.23
17	aA	4007	A1JPJ	C7-C8-C9	2.05	129.33	126.23
17	aJ	4012	A1JPJ	C23-C22-C21	2.05	122.08	118.94
15	aA	1106	CL7	O2A-CGA-O1A	-2.05	118.43	123.59
15	bA	1137	CL7	O2A-CGA-O1A	-2.05	118.43	123.59
15	cA	1138	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	cF	1701	CL7	C2D-C1D-ND	-2.05	108.86	110.23
15	aA	1130	CL7	O2A-CGA-O1A	-2.04	118.43	123.59
15	aB	1225	CL7	C3A-C4A-CHB	-2.04	120.67	123.70
15	cB	1210	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
17	cL	4023	A1JPJ	C1-C6-C7	2.04	121.56	115.78
15	bA	1140	CL7	C3A-C4A-CHB	-2.04	120.67	123.70
17	bA	4003	A1JPJ	C23-C22-C21	2.04	122.07	118.94
15	cA	1119	CL7	C3A-C4A-CHB	-2.04	120.67	123.70
15	bA	1115	CL7	CHD-C4C-NC	2.04	126.33	124.45
19	bB	5002	LMG	C3-C4-C5	-2.04	106.60	110.24
15	bB	1211	CL7	C1-C2-C3	-2.04	122.51	126.04
15	bB	1241	CL7	C2D-C1D-ND	-2.04	108.86	110.23
17	bB	4005	A1JPJ	C10-C11-C12	2.04	129.59	123.22
17	cL	4020	A1JPJ	C10-C11-C12	2.04	129.59	123.22
15	bB	1217	CL7	CHB-C1B-NB	2.04	126.42	124.26
15	aB	1214	CL7	CHC-C1C-NC	2.04	126.33	124.45
17	aF	4016	A1JPJ	C33-C5-C6	2.04	126.82	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	1127	CL7	O2A-CGA-O1A	-2.04	118.45	123.59
15	bA	1115	CL7	OBB-CAB-C3B	-2.04	121.08	125.69
15	cB	1210	CL7	C1-C2-C3	-2.04	122.52	126.04
14	cB	1023	PHO	C1C-C2C-C3C	-2.04	106.92	108.61
15	cB	1217	CL7	CHB-C1B-NB	2.04	126.42	124.26
15	cA	1113	CL7	O2D-CGD-CBD	2.04	114.89	111.27
17	bA	4002	A1JPJ	C8-C9-C10	2.04	122.07	118.94
15	aA	1137	CL7	O2A-CGA-O1A	-2.04	118.45	123.59
14	aB	1023	PHO	C1C-C2C-C3C	-2.04	106.92	108.61
15	bA	1022	CL7	C2D-C1D-ND	-2.04	108.87	110.23
15	bA	1107	CL7	C2D-C1D-ND	-2.04	108.87	110.23
15	bA	1129	CL7	OBB-CAB-C3B	-2.04	121.08	125.69
14	aA	1013	PHO	O2A-CGA-O1A	-2.04	118.46	123.59
15	bA	1111	CL7	O2A-CGA-O1A	-2.04	118.46	123.59
15	bB	1239	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
15	aA	1137	CL7	O2D-CGD-CBD	2.03	114.88	111.27
15	aA	1102	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
15	aB	1239	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
15	aB	1224	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
15	cJ	1301	CL7	CHB-C1B-NB	2.03	126.41	124.26
15	cB	1241	CL7	CHB-C1B-NB	2.03	126.41	124.26
17	cA	4003	A1JPJ	C23-C22-C21	2.03	122.06	118.94
17	cL	4023	A1JPJ	C23-C22-C21	2.03	122.06	118.94
15	bA	1118	CL7	O2D-CGD-CBD	2.03	114.88	111.27
15	bA	1118	CL7	CHB-C1B-NB	2.03	126.41	124.26
15	cA	1122	CL7	CHB-C1B-NB	2.03	126.41	124.26
15	aF	1701	CL7	CMA-C3A-C2A	-2.03	111.36	116.10
15	aA	1109	CL7	CHC-C1C-NC	2.03	126.32	124.45
15	bB	1203	CL7	O2A-CGA-O1A	-2.03	118.47	123.59
15	cB	1231	CL7	CHB-C1B-NB	2.03	126.40	124.26
15	bA	1108	CL7	O2A-CGA-O1A	-2.03	118.47	123.59
15	cB	1012	CL7	C2D-C1D-ND	-2.03	108.87	110.23
15	bB	1224	CL7	O2A-CGA-O1A	-2.03	118.48	123.59
17	bB	4015	A1JPJ	C37-C22-C23	2.03	121.27	118.08
15	cB	1211	CL7	O2A-CGA-O1A	-2.03	118.48	123.59
15	cF	1701	CL7	CHB-C1B-NB	2.03	126.40	124.26
15	bA	1112	CL7	C1-C2-C3	-2.03	122.54	126.04
15	cA	1112	CL7	CHC-C1C-NC	2.03	126.31	124.45
15	bA	1130	CL7	C2D-C1D-ND	-2.02	108.88	110.23
15	cB	1219	CL7	CHB-C1B-NB	2.02	126.40	124.26
15	bA	1123	CL7	C1-C2-C3	-2.02	122.54	126.04
15	bB	1206	CL7	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aB	1231	CL7	O2A-CGA-O1A	-2.02	118.26	123.30
15	cA	1111	CL7	O2A-CGA-O1A	-2.02	118.49	123.59
17	cA	4008	A1JPJ	C34-C9-C8	2.02	121.26	118.08
17	cA	4003	A1JPJ	C33-C5-C6	2.02	126.80	124.53
15	cA	1107	CL7	C2D-C1D-ND	-2.02	108.88	110.23
15	cB	1203	CL7	O2A-CGA-O1A	-2.02	118.50	123.59
15	cB	1202	CL7	CHB-C1B-NB	2.02	126.39	124.26
17	bL	4020	A1JPJ	C10-C11-C12	2.02	129.52	123.22
15	aA	1131	CL7	C3A-C4A-CHB	-2.02	120.70	123.70
15	bB	1226	CL7	C3C-C4C-NC	-2.02	108.71	110.18
14	bB	1023	PHO	C1-C2-C3	-2.02	122.55	126.04
15	aB	1223	CL7	OBB-CAB-C3B	-2.02	121.12	125.69
15	aF	1701	CL7	CHC-C1C-NC	2.02	126.31	124.45
15	bB	1238	CL7	C2D-C1D-ND	-2.02	108.88	110.23
15	bA	1120	CL7	O2A-CGA-O1A	-2.02	118.27	123.30
15	bB	1207	CL7	O2A-CGA-O1A	-2.02	118.50	123.59
15	cA	1138	CL7	CHC-C1C-NC	2.02	126.31	124.45
15	cB	1214	CL7	CHC-C1C-NC	2.02	126.31	124.45
15	bB	1204	CL7	O2D-CGD-CBD	2.02	114.85	111.27
15	bF	1701	CL7	CHB-C1B-NB	2.02	126.39	124.26
15	cA	1125	CL7	CHB-C1B-NB	2.02	126.39	124.26
15	aL	1502	CL7	C3C-C4C-NC	-2.02	108.72	110.18
15	bA	1119	CL7	OBB-CAB-C3B	-2.01	121.13	125.69
15	bB	1231	CL7	O2A-CGA-O1A	-2.01	118.28	123.30
15	cA	1137	CL7	O2A-CGA-O1A	-2.01	118.51	123.59
15	aB	1202	CL7	C1-C2-C3	-2.01	122.56	126.04
17	aA	4011	A1JPJ	C19-C18-C17	2.01	122.03	118.94
15	aA	1123	CL7	C1-C2-C3	-2.01	122.56	126.04
15	bA	1111	CL7	C1-C2-C3	-2.01	122.56	126.04
15	bF	1701	CL7	C2D-C1D-ND	-2.01	108.88	110.23
15	bB	1012	CL7	C3A-C4A-CHB	-2.01	120.72	123.70
17	bA	4008	A1JPJ	C19-C18-C17	2.01	122.03	118.94
15	cJ	1301	CL7	C2D-C1D-ND	-2.01	108.89	110.23
15	cA	1131	CL7	O2A-CGA-O1A	-2.01	118.52	123.59
17	aA	4008	A1JPJ	C29-C28-C27	-2.01	108.66	112.00
15	cA	1121	CL7	CHB-C1B-NB	2.01	126.38	124.26
17	aL	4020	A1JPJ	C10-C11-C12	2.01	129.49	123.22
17	aB	4006	A1JPJ	C37-C22-C23	-2.01	114.91	118.08
15	cB	1239	CL7	O2A-CGA-O1A	-2.01	118.52	123.59
15	aA	1101	CL7	O2D-CGD-CBD	2.01	114.84	111.27
15	cA	1120	CL7	O2A-CGA-O1A	-2.01	118.29	123.30
15	cA	1101	CL7	O2D-CGD-CBD	2.01	114.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	aL	1501	CL7	C2D-C1D-ND	-2.01	108.89	110.23
15	bA	1135	CL7	C2D-C1D-ND	-2.01	108.89	110.23
15	bK	1401	CL7	CHB-C1B-NB	2.01	126.38	124.26
15	bB	1208	CL7	C3A-C4A-CHB	-2.01	120.72	123.70
14	cA	1013	PHO	O2A-CGA-O1A	-2.01	118.53	123.59
15	bB	1211	CL7	O2A-CGA-O1A	-2.01	118.53	123.59
15	cB	1209	CL7	O2A-CGA-O1A	-2.01	118.30	123.30
15	aB	1217	CL7	CHB-C1B-NB	2.01	126.38	124.26
15	bB	1225	CL7	C3A-C4A-CHB	-2.01	120.72	123.70
17	aB	4006	A1JPJ	C19-C18-C17	2.01	122.02	118.94
15	cB	1215	CL7	O2A-CGA-O1A	-2.01	118.53	123.59
17	cA	4008	A1JPJ	C19-C18-C17	2.01	122.02	118.94
15	aA	1120	CL7	O2A-CGA-O1A	-2.00	118.30	123.30
15	cA	1130	CL7	C2D-C1D-ND	-2.00	108.89	110.23
15	aA	1126	CL7	OBB-CAB-C3B	-2.00	121.15	125.69
15	aB	1237	CL7	C3A-C4A-CHB	-2.00	120.73	123.70
15	cB	1237	CL7	C3A-C4A-CHB	-2.00	120.73	123.70
17	cA	4007	A1JPJ	C37-C22-C23	2.00	121.23	118.08
15	aA	1116	CL7	C1-C2-C3	-2.00	122.58	126.04
15	bB	1230	CL7	C2D-C1D-ND	-2.00	108.89	110.23
15	cB	1231	CL7	O2A-CGA-O1A	-2.00	118.31	123.30
15	aA	1102	CL7	OBB-CAB-C3B	-2.00	121.16	125.69
15	aB	1204	CL7	O2D-CGD-CBD	2.00	114.83	111.27
15	aA	1134	CL7	O2A-CGA-O1A	-2.00	118.31	123.30
17	aA	4003	A1JPJ	C23-C22-C21	2.00	122.01	118.94
17	bA	4003	A1JPJ	C33-C5-C6	2.00	126.78	124.53
15	cA	1022	CL7	C3A-C4A-CHB	-2.00	120.73	123.70
15	bA	1117	CL7	C2D-C1D-ND	-2.00	108.89	110.23
15	bA	1117	CL7	C3C-C4C-NC	-2.00	108.73	110.18
15	aB	1219	CL7	CHB-C1B-NB	2.00	126.38	124.26
15	cA	1801	CL7	OBB-CAB-C3B	-2.00	121.16	125.69
15	bA	1103	CL7	CHC-C1C-NC	2.00	126.29	124.45
15	bB	1230	CL7	C3A-C2A-C1A	2.00	104.03	101.64
15	cA	1111	CL7	C1-C2-C3	-2.00	122.58	126.04

All (561) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	aA	1011	G9R	ND
13	bA	1011	G9R	ND
13	cA	1011	G9R	ND
15	aA	1022	CL7	NC

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Mol	Chain	Res	Type	Atom
15	aA	1022	CL7	NA
15	aA	1101	CL7	NC
15	aA	1101	CL7	NA
15	aA	1102	CL7	NC
15	aA	1102	CL7	NA
15	aA	1103	CL7	NC
15	aA	1103	CL7	NA
15	aA	1104	CL7	NC
15	aA	1104	CL7	NA
15	aA	1105	CL7	NC
15	aA	1105	CL7	NA
15	aA	1106	CL7	NC
15	aA	1106	CL7	NA
15	aA	1107	CL7	NC
15	aA	1107	CL7	NA
15	aA	1108	CL7	NC
15	aA	1108	CL7	NA
15	aA	1109	CL7	NC
15	aA	1109	CL7	NA
15	aA	1110	CL7	NC
15	aA	1110	CL7	NA
15	aA	1111	CL7	NC
15	aA	1111	CL7	NA
15	aA	1112	CL7	NC
15	aA	1112	CL7	NA
15	aA	1113	CL7	NC
15	aA	1113	CL7	NA
15	aA	1114	CL7	NC
15	aA	1114	CL7	NA
15	aA	1115	CL7	NC
15	aA	1115	CL7	NA
15	aA	1116	CL7	NC
15	aA	1116	CL7	NA
15	aA	1117	CL7	NC
15	aA	1117	CL7	NA
15	aA	1118	CL7	NC
15	aA	1118	CL7	NA
15	aA	1119	CL7	NC
15	aA	1119	CL7	NA
15	aA	1120	CL7	NC
15	aA	1120	CL7	NA
15	aA	1121	CL7	NC

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Mol	Chain	Res	Type	Atom
15	aA	1121	CL7	NA
15	aA	1122	CL7	NC
15	aA	1122	CL7	NA
15	aA	1123	CL7	NC
15	aA	1123	CL7	NA
15	aA	1124	CL7	NC
15	aA	1124	CL7	NA
15	aA	1125	CL7	NC
15	aA	1125	CL7	NA
15	aA	1126	CL7	NC
15	aA	1126	CL7	NA
15	aA	1127	CL7	NC
15	aA	1127	CL7	NA
15	aA	1128	CL7	NC
15	aA	1128	CL7	NA
15	aA	1129	CL7	NC
15	aA	1129	CL7	NA
15	aA	1130	CL7	NC
15	aA	1130	CL7	NA
15	aA	1131	CL7	NC
15	aA	1131	CL7	NA
15	aA	1132	CL7	NC
15	aA	1132	CL7	NA
15	aA	1133	CL7	NC
15	aA	1133	CL7	NA
15	aA	1134	CL7	NC
15	aA	1134	CL7	NA
15	aA	1135	CL7	NC
15	aA	1135	CL7	NA
15	aA	1136	CL7	NC
15	aA	1136	CL7	NA
15	aA	1137	CL7	NC
15	aA	1137	CL7	NA
15	aA	1138	CL7	NC
15	aA	1138	CL7	NA
15	aA	1140	CL7	NC
15	aA	1140	CL7	NA
15	aA	1801	CL7	NC
15	aA	1801	CL7	NA
15	aA	1139	CL7	NC
15	aA	1139	CL7	NA
15	aB	1232	CL7	NC

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Mol	Chain	Res	Type	Atom
15	aB	1232	CL7	NA
15	aB	1233	CL7	NC
15	aB	1233	CL7	NA
15	aB	1234	CL7	NC
15	aB	1234	CL7	NA
15	aB	1235	CL7	NC
15	aB	1235	CL7	NA
15	aB	1236	CL7	NC
15	aB	1236	CL7	NA
15	aB	1238	CL7	NC
15	aB	1238	CL7	NA
15	aB	1239	CL7	NC
15	aB	1239	CL7	NA
15	aB	1241	CL7	NC
15	aB	1241	CL7	NA
15	aB	1237	CL7	NC
15	aB	1237	CL7	NA
15	aB	1203	CL7	NC
15	aB	1203	CL7	NA
15	aB	1012	CL7	NC
15	aB	1012	CL7	NA
15	aB	1021	CL7	NC
15	aB	1021	CL7	NA
15	aB	1201	CL7	NC
15	aB	1201	CL7	NA
15	aB	1202	CL7	NC
15	aB	1202	CL7	NA
15	aB	1204	CL7	NC
15	aB	1204	CL7	NA
15	aB	1205	CL7	NC
15	aB	1205	CL7	NA
15	aB	1206	CL7	NC
15	aB	1206	CL7	NA
15	aB	1207	CL7	NC
15	aB	1207	CL7	NA
15	aB	1208	CL7	NC
15	aB	1208	CL7	NA
15	aB	1209	CL7	NC
15	aB	1209	CL7	NA
15	aB	1210	CL7	NC
15	aB	1210	CL7	NA
15	aB	1211	CL7	NC

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Mol	Chain	Res	Type	Atom
15	aB	1211	CL7	NA
15	aB	1212	CL7	NC
15	aB	1212	CL7	NA
15	aB	1213	CL7	NC
15	aB	1213	CL7	NA
15	aB	1214	CL7	NC
15	aB	1214	CL7	NA
15	aB	1215	CL7	NC
15	aB	1215	CL7	NA
15	aB	1216	CL7	NC
15	aB	1216	CL7	NA
15	aB	1217	CL7	NC
15	aB	1217	CL7	NA
15	aB	1218	CL7	NC
15	aB	1218	CL7	NA
15	aB	1219	CL7	NC
15	aB	1219	CL7	NA
15	aB	1220	CL7	NC
15	aB	1220	CL7	NA
15	aB	1221	CL7	NC
15	aB	1221	CL7	NA
15	aB	1222	CL7	NC
15	aB	1222	CL7	NA
15	aB	1223	CL7	NC
15	aB	1223	CL7	NA
15	aB	1224	CL7	NC
15	aB	1224	CL7	NA
15	aB	1225	CL7	NC
15	aB	1225	CL7	NA
15	aB	1226	CL7	NC
15	aB	1226	CL7	NA
15	aB	1227	CL7	NC
15	aB	1227	CL7	NA
15	aB	1228	CL7	NC
15	aB	1228	CL7	NA
15	aB	1229	CL7	NC
15	aB	1229	CL7	NA
15	aB	1230	CL7	NC
15	aB	1230	CL7	NA
15	aB	1231	CL7	NC
15	aB	1231	CL7	NA
15	aF	1701	CL7	NC

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Mol	Chain	Res	Type	Atom
15	aF	1701	CL7	NA
15	aI	1601	CL7	NC
15	aI	1601	CL7	NA
15	aJ	1301	CL7	NC
15	aJ	1301	CL7	NA
15	aJ	1302	CL7	NC
15	aJ	1302	CL7	NA
15	aK	1401	CL7	NC
15	aK	1401	CL7	NA
15	aK	1402	CL7	NC
15	aK	1402	CL7	NA
15	aL	1501	CL7	NC
15	aL	1501	CL7	NA
15	aL	1502	CL7	NC
15	aL	1502	CL7	NA
15	aL	1503	CL7	NC
15	aL	1503	CL7	NA
15	bA	1022	CL7	NC
15	bA	1022	CL7	NA
15	bA	1101	CL7	NC
15	bA	1101	CL7	NA
15	bA	1102	CL7	NC
15	bA	1102	CL7	NA
15	bA	1103	CL7	NC
15	bA	1103	CL7	NA
15	bA	1104	CL7	NC
15	bA	1104	CL7	NA
15	bA	1105	CL7	NC
15	bA	1105	CL7	NA
15	bA	1106	CL7	NC
15	bA	1106	CL7	NA
15	bA	1107	CL7	NC
15	bA	1107	CL7	NA
15	bA	1108	CL7	NC
15	bA	1108	CL7	NA
15	bA	1109	CL7	NC
15	bA	1109	CL7	NA
15	bA	1110	CL7	NC
15	bA	1110	CL7	NA
15	bA	1111	CL7	NC
15	bA	1111	CL7	NA
15	bA	1112	CL7	NC

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Mol	Chain	Res	Type	Atom
15	bA	1112	CL7	NA
15	bA	1113	CL7	NC
15	bA	1113	CL7	NA
15	bA	1114	CL7	NC
15	bA	1114	CL7	NA
15	bA	1115	CL7	NC
15	bA	1115	CL7	NA
15	bA	1116	CL7	NC
15	bA	1116	CL7	NA
15	bA	1117	CL7	NC
15	bA	1117	CL7	NA
15	bA	1118	CL7	NC
15	bA	1118	CL7	NA
15	bA	1119	CL7	NC
15	bA	1119	CL7	NA
15	bA	1120	CL7	NC
15	bA	1120	CL7	NA
15	bA	1121	CL7	NC
15	bA	1121	CL7	NA
15	bA	1122	CL7	NC
15	bA	1122	CL7	NA
15	bA	1123	CL7	NC
15	bA	1123	CL7	NA
15	bA	1124	CL7	NC
15	bA	1124	CL7	NA
15	bA	1125	CL7	NC
15	bA	1125	CL7	NA
15	bA	1126	CL7	NC
15	bA	1126	CL7	NA
15	bA	1127	CL7	NC
15	bA	1127	CL7	NA
15	bA	1128	CL7	NC
15	bA	1128	CL7	NA
15	bA	1129	CL7	NC
15	bA	1129	CL7	NA
15	bA	1130	CL7	NC
15	bA	1130	CL7	NA
15	bA	1131	CL7	NC
15	bA	1131	CL7	NA
15	bA	1132	CL7	NC
15	bA	1132	CL7	NA
15	bA	1133	CL7	NC

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Mol	Chain	Res	Type	Atom
15	bA	1133	CL7	NA
15	bA	1134	CL7	NC
15	bA	1134	CL7	NA
15	bA	1135	CL7	NC
15	bA	1135	CL7	NA
15	bA	1136	CL7	NC
15	bA	1136	CL7	NA
15	bA	1137	CL7	NC
15	bA	1137	CL7	NA
15	bA	1138	CL7	NC
15	bA	1138	CL7	NA
15	bA	1139	CL7	NC
15	bA	1139	CL7	NA
15	bA	1140	CL7	NC
15	bA	1140	CL7	NA
15	bA	1801	CL7	NC
15	bA	1801	CL7	NA
15	bB	1237	CL7	NC
15	bB	1237	CL7	NA
15	bB	1012	CL7	NC
15	bB	1012	CL7	NA
15	bB	1021	CL7	NC
15	bB	1021	CL7	NA
15	bB	1201	CL7	NC
15	bB	1201	CL7	NA
15	bB	1202	CL7	NC
15	bB	1202	CL7	NA
15	bB	1203	CL7	NC
15	bB	1203	CL7	NA
15	bB	1204	CL7	NC
15	bB	1204	CL7	NA
15	bB	1205	CL7	NC
15	bB	1205	CL7	NA
15	bB	1206	CL7	NC
15	bB	1206	CL7	NA
15	bB	1207	CL7	NC
15	bB	1207	CL7	NA
15	bB	1208	CL7	NC
15	bB	1208	CL7	NA
15	bB	1209	CL7	NC
15	bB	1209	CL7	NA
15	bB	1210	CL7	NC

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Mol	Chain	Res	Type	Atom
15	bB	1210	CL7	NA
15	bB	1211	CL7	NC
15	bB	1211	CL7	NA
15	bB	1212	CL7	NC
15	bB	1212	CL7	NA
15	bB	1213	CL7	NC
15	bB	1213	CL7	NA
15	bB	1214	CL7	NC
15	bB	1214	CL7	NA
15	bB	1215	CL7	NC
15	bB	1215	CL7	NA
15	bB	1216	CL7	NC
15	bB	1216	CL7	NA
15	bB	1217	CL7	NC
15	bB	1217	CL7	NA
15	bB	1218	CL7	NC
15	bB	1218	CL7	NA
15	bB	1219	CL7	NC
15	bB	1219	CL7	NA
15	bB	1220	CL7	NC
15	bB	1220	CL7	NA
15	bB	1221	CL7	NC
15	bB	1221	CL7	NA
15	bB	1222	CL7	NC
15	bB	1222	CL7	NA
15	bB	1223	CL7	NC
15	bB	1223	CL7	NA
15	bB	1224	CL7	NC
15	bB	1224	CL7	NA
15	bB	1225	CL7	NC
15	bB	1225	CL7	NA
15	bB	1226	CL7	NC
15	bB	1226	CL7	NA
15	bB	1227	CL7	NC
15	bB	1227	CL7	NA
15	bB	1228	CL7	NC
15	bB	1228	CL7	NA
15	bB	1229	CL7	NC
15	bB	1229	CL7	NA
15	bB	1230	CL7	NC
15	bB	1230	CL7	NA
15	bB	1231	CL7	NC

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Mol	Chain	Res	Type	Atom
15	bB	1231	CL7	NA
15	bB	1232	CL7	NC
15	bB	1232	CL7	NA
15	bB	1233	CL7	NC
15	bB	1233	CL7	NA
15	bB	1234	CL7	NC
15	bB	1234	CL7	NA
15	bB	1235	CL7	NC
15	bB	1235	CL7	NA
15	bB	1236	CL7	NC
15	bB	1236	CL7	NA
15	bB	1238	CL7	NC
15	bB	1238	CL7	NA
15	bB	1239	CL7	NC
15	bB	1239	CL7	NA
15	bB	1241	CL7	NC
15	bB	1241	CL7	NA
15	bF	1701	CL7	NC
15	bF	1701	CL7	NA
15	bI	1601	CL7	NC
15	bI	1601	CL7	NA
15	bJ	1301	CL7	NC
15	bJ	1301	CL7	NA
15	bJ	1302	CL7	NC
15	bJ	1302	CL7	NA
15	bK	1401	CL7	NC
15	bK	1401	CL7	NA
15	bK	1402	CL7	NC
15	bK	1402	CL7	NA
15	bL	1501	CL7	NC
15	bL	1501	CL7	NA
15	bL	1502	CL7	NC
15	bL	1502	CL7	NA
15	bL	1503	CL7	NC
15	bL	1503	CL7	NA
15	cA	1022	CL7	NC
15	cA	1022	CL7	NA
15	cA	1101	CL7	NC
15	cA	1101	CL7	NA
15	cA	1102	CL7	NC
15	cA	1102	CL7	NA
15	cA	1103	CL7	NC

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Mol	Chain	Res	Type	Atom
15	cA	1103	CL7	NA
15	cA	1104	CL7	NC
15	cA	1104	CL7	NA
15	cA	1105	CL7	NC
15	cA	1105	CL7	NA
15	cA	1106	CL7	NC
15	cA	1106	CL7	NA
15	cA	1107	CL7	NC
15	cA	1107	CL7	NA
15	cA	1108	CL7	NC
15	cA	1108	CL7	NA
15	cA	1109	CL7	NC
15	cA	1109	CL7	NA
15	cA	1110	CL7	NC
15	cA	1110	CL7	NA
15	cA	1111	CL7	NC
15	cA	1111	CL7	NA
15	cA	1112	CL7	NC
15	cA	1112	CL7	NA
15	cA	1113	CL7	NC
15	cA	1113	CL7	NA
15	cA	1114	CL7	NC
15	cA	1114	CL7	NA
15	cA	1115	CL7	NC
15	cA	1115	CL7	NA
15	cA	1116	CL7	NC
15	cA	1116	CL7	NA
15	cA	1117	CL7	NC
15	cA	1117	CL7	NA
15	cA	1118	CL7	NC
15	cA	1118	CL7	NA
15	cA	1119	CL7	NC
15	cA	1119	CL7	NA
15	cA	1120	CL7	NC
15	cA	1120	CL7	NA
15	cA	1121	CL7	NC
15	cA	1121	CL7	NA
15	cA	1122	CL7	NC
15	cA	1122	CL7	NA
15	cA	1123	CL7	NC
15	cA	1123	CL7	NA
15	cA	1124	CL7	NC

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Mol	Chain	Res	Type	Atom
15	cA	1124	CL7	NA
15	cA	1125	CL7	NC
15	cA	1125	CL7	NA
15	cA	1126	CL7	NC
15	cA	1126	CL7	NA
15	cA	1127	CL7	NC
15	cA	1127	CL7	NA
15	cA	1128	CL7	NC
15	cA	1128	CL7	NA
15	cA	1129	CL7	NC
15	cA	1129	CL7	NA
15	cA	1130	CL7	NC
15	cA	1130	CL7	NA
15	cA	1131	CL7	NC
15	cA	1131	CL7	NA
15	cA	1132	CL7	NC
15	cA	1132	CL7	NA
15	cA	1133	CL7	NC
15	cA	1133	CL7	NA
15	cA	1134	CL7	NC
15	cA	1134	CL7	NA
15	cA	1135	CL7	NC
15	cA	1135	CL7	NA
15	cA	1136	CL7	NC
15	cA	1136	CL7	NA
15	cA	1137	CL7	NC
15	cA	1137	CL7	NA
15	cA	1140	CL7	NC
15	cA	1140	CL7	NA
15	cA	1801	CL7	NC
15	cA	1801	CL7	NA
15	cA	1138	CL7	NC
15	cA	1138	CL7	NA
15	cA	1139	CL7	NC
15	cA	1139	CL7	NA
15	cB	1237	CL7	NC
15	cB	1237	CL7	NA
15	cB	1012	CL7	NC
15	cB	1012	CL7	NA
15	cB	1021	CL7	NC
15	cB	1021	CL7	NA
15	cB	1201	CL7	NC

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Mol	Chain	Res	Type	Atom
15	cB	1201	CL7	NA
15	cB	1202	CL7	NC
15	cB	1202	CL7	NA
15	cB	1203	CL7	NC
15	cB	1203	CL7	NA
15	cB	1204	CL7	NC
15	cB	1204	CL7	NA
15	cB	1205	CL7	NC
15	cB	1205	CL7	NA
15	cB	1206	CL7	NC
15	cB	1206	CL7	NA
15	cB	1207	CL7	NC
15	cB	1207	CL7	NA
15	cB	1208	CL7	NC
15	cB	1208	CL7	NA
15	cB	1209	CL7	NC
15	cB	1209	CL7	NA
15	cB	1210	CL7	NC
15	cB	1210	CL7	NA
15	cB	1211	CL7	NC
15	cB	1211	CL7	NA
15	cB	1212	CL7	NC
15	cB	1212	CL7	NA
15	cB	1213	CL7	NC
15	cB	1213	CL7	NA
15	cB	1214	CL7	NC
15	cB	1214	CL7	NA
15	cB	1215	CL7	NC
15	cB	1215	CL7	NA
15	cB	1216	CL7	NC
15	cB	1216	CL7	NA
15	cB	1217	CL7	NC
15	cB	1217	CL7	NA
15	cB	1218	CL7	NC
15	cB	1218	CL7	NA
15	cB	1219	CL7	NC
15	cB	1219	CL7	NA
15	cB	1220	CL7	NC
15	cB	1220	CL7	NA
15	cB	1221	CL7	NC
15	cB	1221	CL7	NA
15	cB	1222	CL7	NC

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Mol	Chain	Res	Type	Atom
15	cB	1222	CL7	NA
15	cB	1223	CL7	NC
15	cB	1223	CL7	NA
15	cB	1224	CL7	NC
15	cB	1224	CL7	NA
15	cB	1225	CL7	NC
15	cB	1225	CL7	NA
15	cB	1226	CL7	NC
15	cB	1226	CL7	NA
15	cB	1227	CL7	NC
15	cB	1227	CL7	NA
15	cB	1228	CL7	NC
15	cB	1228	CL7	NA
15	cB	1229	CL7	NC
15	cB	1229	CL7	NA
15	cB	1230	CL7	NC
15	cB	1230	CL7	NA
15	cB	1231	CL7	NC
15	cB	1231	CL7	NA
15	cB	1232	CL7	NC
15	cB	1232	CL7	NA
15	cB	1233	CL7	NC
15	cB	1233	CL7	NA
15	cB	1234	CL7	NC
15	cB	1234	CL7	NA
15	cB	1235	CL7	NC
15	cB	1235	CL7	NA
15	cB	1236	CL7	NC
15	cB	1236	CL7	NA
15	cB	1238	CL7	NC
15	cB	1238	CL7	NA
15	cB	1239	CL7	NC
15	cB	1239	CL7	NA
15	cB	1241	CL7	NC
15	cB	1241	CL7	NA
15	cF	1701	CL7	NC
15	cF	1701	CL7	NA
15	cI	1601	CL7	NC
15	cI	1601	CL7	NA
15	cJ	1301	CL7	NC
15	cJ	1301	CL7	NA
15	cJ	1302	CL7	NC

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Mol	Chain	Res	Type	Atom
15	cJ	1302	CL7	NA
15	cK	1401	CL7	NC
15	cK	1401	CL7	NA
15	cK	1402	CL7	NC
15	cK	1402	CL7	NA
15	cL	1501	CL7	NC
15	cL	1501	CL7	NA
15	cL	1502	CL7	NC
15	cL	1502	CL7	NA
15	cL	1503	CL7	NC
15	cL	1503	CL7	NA

All (3154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	aA	1013	PHO	C1A-C2A-CAA-CBA
14	aA	1013	PHO	C3A-C2A-CAA-CBA
14	aB	1023	PHO	CBD-CGD-O2D-CED
14	bA	1013	PHO	C1A-C2A-CAA-CBA
14	bA	1013	PHO	C3A-C2A-CAA-CBA
14	bB	1023	PHO	CBD-CGD-O2D-CED
14	cA	1013	PHO	C1A-C2A-CAA-CBA
14	cA	1013	PHO	C3A-C2A-CAA-CBA
14	cB	1023	PHO	CBD-CGD-O2D-CED
15	aA	1101	CL7	CHA-CBD-CGD-O2D
15	aA	1101	CL7	CHA-CBD-CGD-O1D
15	aA	1102	CL7	C1A-C2A-CAA-CBA
15	aA	1103	CL7	C3A-C2A-CAA-CBA
15	aA	1103	CL7	CHA-CBD-CGD-O2D
15	aA	1103	CL7	CHA-CBD-CGD-O1D
15	aA	1106	CL7	C1A-C2A-CAA-CBA
15	aA	1106	CL7	C3A-C2A-CAA-CBA
15	aA	1106	CL7	C4B-C3B-CAB-OB
15	aA	1108	CL7	C1A-C2A-CAA-CBA
15	aA	1108	CL7	CBD-CGD-O2D-CED
15	aA	1109	CL7	C1A-C2A-CAA-CBA
15	aA	1109	CL7	C3A-C2A-CAA-CBA
15	aA	1109	CL7	CHA-CBD-CGD-O2D
15	aA	1109	CL7	CHA-CBD-CGD-O1D
15	aA	1109	CL7	CAD-CBD-CGD-O2D
15	aA	1109	CL7	CAD-CBD-CGD-O1D
15	aA	1110	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	aA	1110	CL7	C3A-C2A-CAA-CBA
15	aA	1110	CL7	CHA-CBD-CGD-O2D
15	aA	1110	CL7	CHA-CBD-CGD-O1D
15	aA	1112	CL7	C2B-C3B-CAB-OB
15	aA	1112	CL7	C4B-C3B-CAB-OB
15	aA	1113	CL7	C1A-C2A-CAA-CBA
15	aA	1113	CL7	C3A-C2A-CAA-CBA
15	aA	1115	CL7	CBD-CGD-O2D-CED
15	aA	1116	CL7	C3A-C2A-CAA-CBA
15	aA	1117	CL7	CHA-CBD-CGD-O2D
15	aA	1117	CL7	CHA-CBD-CGD-O1D
15	aA	1120	CL7	CHA-CBD-CGD-O2D
15	aA	1121	CL7	C1A-C2A-CAA-CBA
15	aA	1121	CL7	C3A-C2A-CAA-CBA
15	aA	1121	CL7	CHA-CBD-CGD-O2D
15	aA	1121	CL7	CHA-CBD-CGD-O1D
15	aA	1122	CL7	CHA-CBD-CGD-O2D
15	aA	1122	CL7	CHA-CBD-CGD-O1D
15	aA	1126	CL7	C1A-C2A-CAA-CBA
15	aA	1126	CL7	C3A-C2A-CAA-CBA
15	aA	1126	CL7	CBD-CGD-O2D-CED
15	aA	1127	CL7	C11-C12-C13-C14
15	aA	1127	CL7	C3A-C2A-CAA-CBA
15	aA	1129	CL7	C4B-C3B-CAB-OB
15	aA	1132	CL7	CHA-CBD-CGD-O2D
15	aA	1132	CL7	CHA-CBD-CGD-O1D
15	aA	1132	CL7	C2B-C3B-CAB-OB
15	aA	1132	CL7	C4B-C3B-CAB-OB
15	aA	1133	CL7	C2A-CAA-CBA-CGA
15	aA	1135	CL7	C2B-C3B-CAB-OB
15	aA	1135	CL7	C4B-C3B-CAB-OB
15	aA	1136	CL7	C2-C3-C5-C6
15	aA	1136	CL7	C4-C3-C5-C6
15	aA	1136	CL7	CHA-CBD-CGD-O2D
15	aA	1136	CL7	CHA-CBD-CGD-O1D
15	aA	1137	CL7	C1A-C2A-CAA-CBA
15	aA	1140	CL7	C2-C3-C5-C6
15	aA	1140	CL7	C4-C3-C5-C6
15	aA	1140	CL7	C1A-C2A-CAA-CBA
15	aA	1801	CL7	CHA-CBD-CGD-O2D
15	aA	1801	CL7	CHA-CBD-CGD-O1D
15	aA	1139	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	aA	1139	CL7	C3A-C2A-CAA-CBA
15	aB	1232	CL7	CBD-CGD-O2D-CED
15	aB	1233	CL7	C2B-C3B-CAB-OB
15	aB	1233	CL7	C4B-C3B-CAB-OB
15	aB	1234	CL7	C1A-C2A-CAA-CBA
15	aB	1235	CL7	C1A-C2A-CAA-CBA
15	aB	1236	CL7	CHA-CBD-CGD-O2D
15	aB	1236	CL7	CHA-CBD-CGD-O1D
15	aB	1238	CL7	C2-C3-C5-C6
15	aB	1238	CL7	C4-C3-C5-C6
15	aB	1241	CL7	C3A-C2A-CAA-CBA
15	aB	1241	CL7	C2B-C3B-CAB-OB
15	aB	1241	CL7	C4B-C3B-CAB-OB
15	aB	1012	CL7	CHA-CBD-CGD-O2D
15	aB	1012	CL7	CHA-CBD-CGD-O1D
15	aB	1012	CL7	CAD-CBD-CGD-O1D
15	aB	1021	CL7	CHA-CBD-CGD-O2D
15	aB	1021	CL7	CHA-CBD-CGD-O1D
15	aB	1021	CL7	CBD-CGD-O2D-CED
15	aB	1201	CL7	CHA-CBD-CGD-O2D
15	aB	1201	CL7	C2B-C3B-CAB-OB
15	aB	1201	CL7	C4B-C3B-CAB-OB
15	aB	1202	CL7	C1A-C2A-CAA-CBA
15	aB	1202	CL7	C3A-C2A-CAA-CBA
15	aB	1202	CL7	CHA-CBD-CGD-O2D
15	aB	1202	CL7	CHA-CBD-CGD-O1D
15	aB	1202	CL7	CAD-CBD-CGD-O1D
15	aB	1207	CL7	C4B-C3B-CAB-OB
15	aB	1208	CL7	CHA-CBD-CGD-O2D
15	aB	1208	CL7	CHA-CBD-CGD-O1D
15	aB	1208	CL7	CBD-CGD-O2D-CED
15	aB	1209	CL7	C1A-C2A-CAA-CBA
15	aB	1209	CL7	C3A-C2A-CAA-CBA
15	aB	1210	CL7	C3A-C2A-CAA-CBA
15	aB	1210	CL7	CBD-CGD-O2D-CED
15	aB	1212	CL7	C1A-C2A-CAA-CBA
15	aB	1212	CL7	C3A-C2A-CAA-CBA
15	aB	1212	CL7	C4B-C3B-CAB-OB
15	aB	1213	CL7	C1A-C2A-CAA-CBA
15	aB	1213	CL7	C3A-C2A-CAA-CBA
15	aB	1213	CL7	CHA-CBD-CGD-O2D
15	aB	1213	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	aB	1216	CL7	C1A-C2A-CAA-CBA
15	aB	1216	CL7	CBD-CGD-O2D-CED
15	aB	1219	CL7	CAD-CBD-CGD-O1D
15	aB	1219	CL7	CBD-CGD-O2D-CED
15	aB	1220	CL7	C1A-C2A-CAA-CBA
15	aB	1220	CL7	C3A-C2A-CAA-CBA
15	aB	1221	CL7	C4B-C3B-CAB-OBB
15	aB	1222	CL7	C3A-C2A-CAA-CBA
15	aB	1222	CL7	CBD-CGD-O2D-CED
15	aB	1223	CL7	C11-C10-C8-C9
15	aB	1223	CL7	C1A-C2A-CAA-CBA
15	aB	1223	CL7	C3A-C2A-CAA-CBA
15	aB	1224	CL7	C2B-C3B-CAB-OBB
15	aB	1224	CL7	C4B-C3B-CAB-OBB
15	aB	1230	CL7	C2B-C3B-CAB-OBB
15	aB	1230	CL7	C4B-C3B-CAB-OBB
15	aJ	1301	CL7	CHA-CBD-CGD-O2D
15	aJ	1301	CL7	CHA-CBD-CGD-O1D
15	aJ	1301	CL7	CBD-CGD-O2D-CED
15	aK	1401	CL7	CHA-CBD-CGD-O2D
15	aK	1401	CL7	CHA-CBD-CGD-O1D
15	aL	1501	CL7	C1A-C2A-CAA-CBA
15	aL	1501	CL7	C3A-C2A-CAA-CBA
15	aL	1501	CL7	C2B-C3B-CAB-OBB
15	aL	1501	CL7	C4B-C3B-CAB-OBB
15	aL	1502	CL7	CHA-CBD-CGD-O2D
15	aL	1502	CL7	CHA-CBD-CGD-O1D
15	aL	1502	CL7	C2B-C3B-CAB-OBB
15	aL	1502	CL7	C4B-C3B-CAB-OBB
15	bA	1101	CL7	CHA-CBD-CGD-O2D
15	bA	1101	CL7	CHA-CBD-CGD-O1D
15	bA	1102	CL7	C1A-C2A-CAA-CBA
15	bA	1102	CL7	C3A-C2A-CAA-CBA
15	bA	1103	CL7	C11-C10-C8-C9
15	bA	1103	CL7	C11-C12-C13-C14
15	bA	1103	CL7	C1A-C2A-CAA-CBA
15	bA	1103	CL7	C3A-C2A-CAA-CBA
15	bA	1103	CL7	CHA-CBD-CGD-O2D
15	bA	1103	CL7	CHA-CBD-CGD-O1D
15	bA	1103	CL7	CAD-CBD-CGD-O1D
15	bA	1104	CL7	C4B-C3B-CAB-OBB
15	bA	1106	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	bA	1106	CL7	C3A-C2A-CAA-CBA
15	bA	1106	CL7	C4B-C3B-CAB-OBB
15	bA	1108	CL7	C1A-C2A-CAA-CBA
15	bA	1108	CL7	CBD-CGD-O2D-CED
15	bA	1109	CL7	C11-C12-C13-C14
15	bA	1109	CL7	C1A-C2A-CAA-CBA
15	bA	1109	CL7	C3A-C2A-CAA-CBA
15	bA	1109	CL7	CHA-CBD-CGD-O2D
15	bA	1109	CL7	CHA-CBD-CGD-O1D
15	bA	1109	CL7	CAD-CBD-CGD-O1D
15	bA	1110	CL7	C1A-C2A-CAA-CBA
15	bA	1110	CL7	C3A-C2A-CAA-CBA
15	bA	1110	CL7	CHA-CBD-CGD-O2D
15	bA	1110	CL7	CHA-CBD-CGD-O1D
15	bA	1112	CL7	C1A-C2A-CAA-CBA
15	bA	1112	CL7	C2B-C3B-CAB-OBB
15	bA	1112	CL7	C4B-C3B-CAB-OBB
15	bA	1113	CL7	C1A-C2A-CAA-CBA
15	bA	1113	CL7	C3A-C2A-CAA-CBA
15	bA	1113	CL7	CBD-CGD-O2D-CED
15	bA	1115	CL7	CBD-CGD-O2D-CED
15	bA	1116	CL7	C3A-C2A-CAA-CBA
15	bA	1119	CL7	C2-C3-C5-C6
15	bA	1119	CL7	C4-C3-C5-C6
15	bA	1120	CL7	C1A-C2A-CAA-CBA
15	bA	1121	CL7	C1A-C2A-CAA-CBA
15	bA	1121	CL7	C3A-C2A-CAA-CBA
15	bA	1121	CL7	CHA-CBD-CGD-O2D
15	bA	1121	CL7	CHA-CBD-CGD-O1D
15	bA	1122	CL7	CHA-CBD-CGD-O2D
15	bA	1122	CL7	CHA-CBD-CGD-O1D
15	bA	1125	CL7	C2B-C3B-CAB-OBB
15	bA	1125	CL7	C4B-C3B-CAB-OBB
15	bA	1126	CL7	C1A-C2A-CAA-CBA
15	bA	1126	CL7	C3A-C2A-CAA-CBA
15	bA	1126	CL7	CBD-CGD-O2D-CED
15	bA	1127	CL7	C3A-C2A-CAA-CBA
15	bA	1129	CL7	C4B-C3B-CAB-OBB
15	bA	1132	CL7	CHA-CBD-CGD-O2D
15	bA	1132	CL7	CHA-CBD-CGD-O1D
15	bA	1132	CL7	C2B-C3B-CAB-OBB
15	bA	1132	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
15	bA	1135	CL7	CBD-CGD-O2D-CED
15	bA	1135	CL7	C2B-C3B-CAB-OBB
15	bA	1135	CL7	C4B-C3B-CAB-OBB
15	bA	1136	CL7	C2-C3-C5-C6
15	bA	1136	CL7	C4-C3-C5-C6
15	bA	1136	CL7	CHA-CBD-CGD-O2D
15	bA	1136	CL7	CHA-CBD-CGD-O1D
15	bA	1139	CL7	C1A-C2A-CAA-CBA
15	bA	1140	CL7	C2-C3-C5-C6
15	bA	1140	CL7	C4-C3-C5-C6
15	bA	1801	CL7	CHA-CBD-CGD-O2D
15	bA	1801	CL7	CHA-CBD-CGD-O1D
15	bB	1237	CL7	C2-C3-C5-C6
15	bB	1237	CL7	C4-C3-C5-C6
15	bB	1012	CL7	CHA-CBD-CGD-O1D
15	bB	1012	CL7	CAD-CBD-CGD-O2D
15	bB	1012	CL7	CAD-CBD-CGD-O1D
15	bB	1021	CL7	CHA-CBD-CGD-O2D
15	bB	1021	CL7	CHA-CBD-CGD-O1D
15	bB	1201	CL7	CHA-CBD-CGD-O2D
15	bB	1201	CL7	CHA-CBD-CGD-O1D
15	bB	1201	CL7	C2B-C3B-CAB-OBB
15	bB	1201	CL7	C4B-C3B-CAB-OBB
15	bB	1202	CL7	C1A-C2A-CAA-CBA
15	bB	1202	CL7	C3A-C2A-CAA-CBA
15	bB	1202	CL7	CHA-CBD-CGD-O2D
15	bB	1202	CL7	CHA-CBD-CGD-O1D
15	bB	1202	CL7	CAD-CBD-CGD-O2D
15	bB	1202	CL7	CAD-CBD-CGD-O1D
15	bB	1208	CL7	CHA-CBD-CGD-O2D
15	bB	1208	CL7	CHA-CBD-CGD-O1D
15	bB	1208	CL7	CBD-CGD-O2D-CED
15	bB	1209	CL7	C1A-C2A-CAA-CBA
15	bB	1209	CL7	C3A-C2A-CAA-CBA
15	bB	1210	CL7	C3A-C2A-CAA-CBA
15	bB	1210	CL7	CBD-CGD-O2D-CED
15	bB	1212	CL7	C1A-C2A-CAA-CBA
15	bB	1212	CL7	C3A-C2A-CAA-CBA
15	bB	1212	CL7	C4B-C3B-CAB-OBB
15	bB	1213	CL7	C1A-C2A-CAA-CBA
15	bB	1213	CL7	C3A-C2A-CAA-CBA
15	bB	1213	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	bB	1213	CL7	CHA-CBD-CGD-O1D
15	bB	1216	CL7	C1A-C2A-CAA-CBA
15	bB	1216	CL7	CBD-CGD-O2D-CED
15	bB	1219	CL7	CAD-CBD-CGD-O2D
15	bB	1219	CL7	CAD-CBD-CGD-O1D
15	bB	1219	CL7	CBD-CGD-O2D-CED
15	bB	1220	CL7	C1A-C2A-CAA-CBA
15	bB	1220	CL7	C3A-C2A-CAA-CBA
15	bB	1221	CL7	CHA-CBD-CGD-O2D
15	bB	1221	CL7	CHA-CBD-CGD-O1D
15	bB	1222	CL7	C3A-C2A-CAA-CBA
15	bB	1222	CL7	CBD-CGD-O2D-CED
15	bB	1223	CL7	C1A-C2A-CAA-CBA
15	bB	1224	CL7	CHA-CBD-CGD-O1D
15	bB	1230	CL7	C2B-C3B-CAB-OB
15	bB	1230	CL7	C4B-C3B-CAB-OB
15	bB	1232	CL7	CBD-CGD-O2D-CED
15	bB	1234	CL7	C1A-C2A-CAA-CBA
15	bB	1235	CL7	C1A-C2A-CAA-CBA
15	bB	1235	CL7	C3A-C2A-CAA-CBA
15	bB	1236	CL7	CHA-CBD-CGD-O2D
15	bB	1236	CL7	CHA-CBD-CGD-O1D
15	bB	1238	CL7	C2-C3-C5-C6
15	bB	1238	CL7	C4-C3-C5-C6
15	bB	1239	CL7	C14-C13-C15-C16
15	bB	1241	CL7	C3A-C2A-CAA-CBA
15	bB	1241	CL7	CHA-CBD-CGD-O2D
15	bB	1241	CL7	CHA-CBD-CGD-O1D
15	bB	1241	CL7	C4B-C3B-CAB-OB
15	bF	1701	CL7	CBD-CGD-O2D-CED
15	bJ	1301	CL7	CHA-CBD-CGD-O2D
15	bJ	1301	CL7	CHA-CBD-CGD-O1D
15	bJ	1301	CL7	CBD-CGD-O2D-CED
15	bK	1401	CL7	CHA-CBD-CGD-O2D
15	bK	1401	CL7	CHA-CBD-CGD-O1D
15	bL	1501	CL7	C1A-C2A-CAA-CBA
15	bL	1501	CL7	C3A-C2A-CAA-CBA
15	bL	1501	CL7	C4B-C3B-CAB-OB
15	bL	1502	CL7	C1A-C2A-CAA-CBA
15	bL	1502	CL7	CHA-CBD-CGD-O2D
15	bL	1502	CL7	CHA-CBD-CGD-O1D
15	bL	1502	CL7	C2B-C3B-CAB-OB

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Mol	Chain	Res	Type	Atoms
15	bL	1502	CL7	C4B-C3B-CAB-OBB
15	cA	1101	CL7	CHA-CBD-CGD-O2D
15	cA	1101	CL7	CHA-CBD-CGD-O1D
15	cA	1102	CL7	C1A-C2A-CAA-CBA
15	cA	1102	CL7	C3A-C2A-CAA-CBA
15	cA	1103	CL7	C1A-C2A-CAA-CBA
15	cA	1103	CL7	C3A-C2A-CAA-CBA
15	cA	1103	CL7	CHA-CBD-CGD-O2D
15	cA	1103	CL7	CHA-CBD-CGD-O1D
15	cA	1103	CL7	CAD-CBD-CGD-O1D
15	cA	1104	CL7	C4B-C3B-CAB-OBB
15	cA	1106	CL7	C1A-C2A-CAA-CBA
15	cA	1106	CL7	C3A-C2A-CAA-CBA
15	cA	1106	CL7	C2B-C3B-CAB-OBB
15	cA	1106	CL7	C4B-C3B-CAB-OBB
15	cA	1108	CL7	C1A-C2A-CAA-CBA
15	cA	1108	CL7	CBD-CGD-O2D-CED
15	cA	1109	CL7	C1A-C2A-CAA-CBA
15	cA	1109	CL7	C3A-C2A-CAA-CBA
15	cA	1109	CL7	CHA-CBD-CGD-O2D
15	cA	1109	CL7	CHA-CBD-CGD-O1D
15	cA	1109	CL7	CAD-CBD-CGD-O1D
15	cA	1110	CL7	C1A-C2A-CAA-CBA
15	cA	1110	CL7	C3A-C2A-CAA-CBA
15	cA	1110	CL7	CHA-CBD-CGD-O2D
15	cA	1110	CL7	CHA-CBD-CGD-O1D
15	cA	1112	CL7	C1A-C2A-CAA-CBA
15	cA	1112	CL7	C3A-C2A-CAA-CBA
15	cA	1112	CL7	C2B-C3B-CAB-OBB
15	cA	1112	CL7	C4B-C3B-CAB-OBB
15	cA	1113	CL7	C1A-C2A-CAA-CBA
15	cA	1113	CL7	C3A-C2A-CAA-CBA
15	cA	1115	CL7	CBD-CGD-O2D-CED
15	cA	1116	CL7	C3A-C2A-CAA-CBA
15	cA	1117	CL7	CHA-CBD-CGD-O1D
15	cA	1118	CL7	CHA-CBD-CGD-O1D
15	cA	1119	CL7	C2-C3-C5-C6
15	cA	1119	CL7	C4-C3-C5-C6
15	cA	1120	CL7	CHA-CBD-CGD-O2D
15	cA	1120	CL7	CHA-CBD-CGD-O1D
15	cA	1121	CL7	C1A-C2A-CAA-CBA
15	cA	1121	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	cA	1121	CL7	CHA-CBD-CGD-O2D
15	cA	1121	CL7	CHA-CBD-CGD-O1D
15	cA	1122	CL7	CHA-CBD-CGD-O2D
15	cA	1122	CL7	CHA-CBD-CGD-O1D
15	cA	1126	CL7	C1A-C2A-CAA-CBA
15	cA	1126	CL7	C3A-C2A-CAA-CBA
15	cA	1126	CL7	CBD-CGD-O2D-CED
15	cA	1127	CL7	C3A-C2A-CAA-CBA
15	cA	1132	CL7	CHA-CBD-CGD-O2D
15	cA	1132	CL7	CHA-CBD-CGD-O1D
15	cA	1132	CL7	C2B-C3B-CAB-OB
15	cA	1132	CL7	C4B-C3B-CAB-OB
15	cA	1133	CL7	C2A-CAA-CBA-CGA
15	cA	1133	CL7	C1A-C2A-CAA-CBA
15	cA	1135	CL7	C2B-C3B-CAB-OB
15	cA	1135	CL7	C4B-C3B-CAB-OB
15	cA	1136	CL7	C4-C3-C5-C6
15	cA	1136	CL7	CHA-CBD-CGD-O2D
15	cA	1136	CL7	CHA-CBD-CGD-O1D
15	cA	1137	CL7	C1A-C2A-CAA-CBA
15	cA	1140	CL7	C2-C3-C5-C6
15	cA	1140	CL7	C4-C3-C5-C6
15	cA	1140	CL7	C1A-C2A-CAA-CBA
15	cA	1801	CL7	CHA-CBD-CGD-O1D
15	cA	1801	CL7	CBD-CGD-O2D-CED
15	cA	1139	CL7	C1A-C2A-CAA-CBA
15	cA	1139	CL7	CBD-CGD-O2D-CED
15	cB	1012	CL7	CHA-CBD-CGD-O2D
15	cB	1012	CL7	CHA-CBD-CGD-O1D
15	cB	1012	CL7	CAD-CBD-CGD-O2D
15	cB	1012	CL7	CAD-CBD-CGD-O1D
15	cB	1021	CL7	CHA-CBD-CGD-O2D
15	cB	1021	CL7	CHA-CBD-CGD-O1D
15	cB	1021	CL7	CBD-CGD-O2D-CED
15	cB	1201	CL7	CHA-CBD-CGD-O2D
15	cB	1201	CL7	CHA-CBD-CGD-O1D
15	cB	1201	CL7	C2B-C3B-CAB-OB
15	cB	1201	CL7	C4B-C3B-CAB-OB
15	cB	1202	CL7	C1A-C2A-CAA-CBA
15	cB	1202	CL7	CHA-CBD-CGD-O2D
15	cB	1202	CL7	CHA-CBD-CGD-O1D
15	cB	1202	CL7	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	cB	1204	CL7	C1A-C2A-CAA-CBA
15	cB	1206	CL7	C4B-C3B-CAB-OBB
15	cB	1208	CL7	CHA-CBD-CGD-O1D
15	cB	1208	CL7	CBD-CGD-O2D-CED
15	cB	1209	CL7	C1A-C2A-CAA-CBA
15	cB	1209	CL7	C3A-C2A-CAA-CBA
15	cB	1210	CL7	C3A-C2A-CAA-CBA
15	cB	1212	CL7	C1A-C2A-CAA-CBA
15	cB	1212	CL7	C3A-C2A-CAA-CBA
15	cB	1212	CL7	C4B-C3B-CAB-OBB
15	cB	1213	CL7	C1A-C2A-CAA-CBA
15	cB	1213	CL7	C3A-C2A-CAA-CBA
15	cB	1213	CL7	CHA-CBD-CGD-O2D
15	cB	1213	CL7	CHA-CBD-CGD-O1D
15	cB	1216	CL7	C1A-C2A-CAA-CBA
15	cB	1219	CL7	CBD-CGD-O2D-CED
15	cB	1220	CL7	C1A-C2A-CAA-CBA
15	cB	1220	CL7	C3A-C2A-CAA-CBA
15	cB	1221	CL7	CHA-CBD-CGD-O2D
15	cB	1221	CL7	CHA-CBD-CGD-O1D
15	cB	1222	CL7	C3A-C2A-CAA-CBA
15	cB	1222	CL7	CBD-CGD-O2D-CED
15	cB	1223	CL7	C1A-C2A-CAA-CBA
15	cB	1224	CL7	CBD-CGD-O2D-CED
15	cB	1227	CL7	C4B-C3B-CAB-OBB
15	cB	1230	CL7	C2B-C3B-CAB-OBB
15	cB	1230	CL7	C4B-C3B-CAB-OBB
15	cB	1232	CL7	CBD-CGD-O2D-CED
15	cB	1234	CL7	C1A-C2A-CAA-CBA
15	cB	1235	CL7	C1A-C2A-CAA-CBA
15	cB	1235	CL7	C3A-C2A-CAA-CBA
15	cB	1235	CL7	CHA-CBD-CGD-O2D
15	cB	1235	CL7	CHA-CBD-CGD-O1D
15	cB	1236	CL7	CHA-CBD-CGD-O2D
15	cB	1236	CL7	CHA-CBD-CGD-O1D
15	cB	1236	CL7	C4B-C3B-CAB-OBB
15	cB	1238	CL7	C2-C3-C5-C6
15	cB	1238	CL7	C4-C3-C5-C6
15	cB	1241	CL7	C3A-C2A-CAA-CBA
15	cB	1241	CL7	CHA-CBD-CGD-O2D
15	cB	1241	CL7	C4B-C3B-CAB-OBB
15	cJ	1301	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	cJ	1301	CL7	CHA-CBD-CGD-O1D
15	cJ	1301	CL7	CBD-CGD-O2D-CED
15	cL	1501	CL7	C1A-C2A-CAA-CBA
15	cL	1501	CL7	C3A-C2A-CAA-CBA
15	cL	1501	CL7	C4B-C3B-CAB-OB
15	cL	1502	CL7	CHA-CBD-CGD-O2D
15	cL	1502	CL7	CHA-CBD-CGD-O1D
15	cL	1502	CL7	C2B-C3B-CAB-OB
15	cL	1502	CL7	C4B-C3B-CAB-OB
15	cL	1503	CL7	C2-C3-C5-C6
15	cL	1503	CL7	C4-C3-C5-C6
17	aA	4014	A1JPJ	C11-C12-C13-C14
17	aA	4014	A1JPJ	C11-C12-C13-C35
17	aB	4005	A1JPJ	C23-C24-C25-C26
17	aB	4005	A1JPJ	C23-C24-C25-C30
17	aB	4010	A1JPJ	C23-C24-C25-C26
17	aB	4010	A1JPJ	C23-C24-C25-C30
17	aB	4015	A1JPJ	C7-C8-C9-C10
17	aB	4015	A1JPJ	C7-C8-C9-C34
17	aB	4017	A1JPJ	C21-C22-C23-C24
17	aB	4017	A1JPJ	C37-C22-C23-C24
17	aF	4016	A1JPJ	C17-C18-C19-C20
17	aF	4016	A1JPJ	C36-C18-C19-C20
17	aF	4016	A1JPJ	C21-C22-C23-C24
17	aF	4016	A1JPJ	C37-C22-C23-C24
17	aJ	4012	A1JPJ	C7-C8-C9-C10
17	aJ	4012	A1JPJ	C7-C8-C9-C34
17	aL	4020	A1JPJ	C7-C8-C9-C34
17	aL	4020	A1JPJ	C23-C24-C25-C26
17	aL	4020	A1JPJ	C23-C24-C25-C30
17	aL	4023	A1JPJ	C37-C22-C23-C24
17	bA	4014	A1JPJ	C11-C12-C13-C14
17	bA	4014	A1JPJ	C11-C12-C13-C35
17	bB	4005	A1JPJ	C23-C24-C25-C26
17	bB	4005	A1JPJ	C23-C24-C25-C30
17	bB	4006	A1JPJ	C37-C22-C23-C24
17	bB	4010	A1JPJ	C23-C24-C25-C26
17	bB	4010	A1JPJ	C23-C24-C25-C30
17	bB	4015	A1JPJ	C7-C8-C9-C10
17	bB	4015	A1JPJ	C7-C8-C9-C34
17	bB	4017	A1JPJ	C21-C22-C23-C24
17	bB	4017	A1JPJ	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	bF	4016	A1JPJ	C21-C22-C23-C24
17	bF	4016	A1JPJ	C37-C22-C23-C24
17	bF	4016	A1JPJ	C23-C24-C25-C26
17	bF	4016	A1JPJ	C23-C24-C25-C30
17	bJ	4012	A1JPJ	C7-C8-C9-C10
17	bJ	4012	A1JPJ	C7-C8-C9-C34
17	bL	4020	A1JPJ	C23-C24-C25-C26
17	bL	4020	A1JPJ	C23-C24-C25-C30
17	cA	4014	A1JPJ	C11-C12-C13-C14
17	cB	4005	A1JPJ	C23-C24-C25-C26
17	cB	4005	A1JPJ	C23-C24-C25-C30
17	cB	4010	A1JPJ	C23-C24-C25-C26
17	cB	4010	A1JPJ	C23-C24-C25-C30
17	cB	4015	A1JPJ	C7-C8-C9-C10
17	cB	4015	A1JPJ	C7-C8-C9-C34
17	cB	4017	A1JPJ	C21-C22-C23-C24
17	cB	4017	A1JPJ	C37-C22-C23-C24
17	cF	4016	A1JPJ	C21-C22-C23-C24
17	cF	4016	A1JPJ	C37-C22-C23-C24
17	cJ	4012	A1JPJ	C7-C8-C9-C10
17	cJ	4012	A1JPJ	C7-C8-C9-C34
17	cL	4020	A1JPJ	C23-C24-C25-C26
17	cL	4020	A1JPJ	C23-C24-C25-C30
18	aA	5003	LHG	C3-O3-P-O4
18	aA	5003	LHG	C4-O6-P-O5
18	bA	5001	LHG	C3-O3-P-O6
18	bA	5003	LHG	C3-O3-P-O4
18	bA	5003	LHG	C4-O6-P-O5
18	cA	5003	LHG	C3-O3-P-O4
18	cA	5003	LHG	C4-O6-P-O5
15	aA	1108	CL7	O1D-CGD-O2D-CED
15	aB	1021	CL7	O1D-CGD-O2D-CED
15	bA	1108	CL7	O1D-CGD-O2D-CED
15	bB	1232	CL7	O1D-CGD-O2D-CED
15	cA	1108	CL7	O1D-CGD-O2D-CED
15	cA	1126	CL7	O1D-CGD-O2D-CED
15	aA	1115	CL7	O1D-CGD-O2D-CED
15	aB	1232	CL7	O1D-CGD-O2D-CED
15	aB	1208	CL7	O1D-CGD-O2D-CED
15	aJ	1301	CL7	O1D-CGD-O2D-CED
15	bB	1021	CL7	O1D-CGD-O2D-CED
15	bB	1208	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	bJ	1301	CL7	O1D-CGD-O2D-CED
15	cA	1115	CL7	O1D-CGD-O2D-CED
15	cB	1021	CL7	O1D-CGD-O2D-CED
15	cB	1208	CL7	O1D-CGD-O2D-CED
15	cB	1232	CL7	O1D-CGD-O2D-CED
15	cJ	1301	CL7	O1D-CGD-O2D-CED
15	aA	1104	CL7	CBD-CGD-O2D-CED
15	aA	1116	CL7	CBD-CGD-O2D-CED
15	aA	1121	CL7	CBD-CGD-O2D-CED
15	aA	1135	CL7	CBD-CGD-O2D-CED
15	aA	1801	CL7	CBD-CGD-O2D-CED
15	aA	1139	CL7	CBD-CGD-O2D-CED
15	aB	1218	CL7	CBD-CGD-O2D-CED
15	aB	1224	CL7	CBD-CGD-O2D-CED
15	aB	1228	CL7	CBD-CGD-O2D-CED
15	aB	1230	CL7	CBD-CGD-O2D-CED
15	bA	1117	CL7	CBD-CGD-O2D-CED
15	bA	1139	CL7	CBD-CGD-O2D-CED
15	bA	1801	CL7	CBD-CGD-O2D-CED
15	bB	1021	CL7	CBD-CGD-O2D-CED
15	bB	1224	CL7	CBD-CGD-O2D-CED
15	bB	1230	CL7	CBD-CGD-O2D-CED
15	bB	1241	CL7	CBD-CGD-O2D-CED
15	cA	1116	CL7	CBD-CGD-O2D-CED
15	cA	1135	CL7	CBD-CGD-O2D-CED
15	cB	1218	CL7	CBD-CGD-O2D-CED
15	cB	1230	CL7	CBD-CGD-O2D-CED
15	aA	1123	CL7	O1A-CGA-O2A-C1
15	bA	1102	CL7	O1A-CGA-O2A-C1
15	bA	1123	CL7	O1A-CGA-O2A-C1
15	bL	1501	CL7	O1A-CGA-O2A-C1
15	cA	1102	CL7	O1A-CGA-O2A-C1
15	cA	1123	CL7	O1A-CGA-O2A-C1
15	cL	1501	CL7	O1A-CGA-O2A-C1
18	aA	5003	LHG	O10-C23-O8-C6
18	cA	5003	LHG	O10-C23-O8-C6
15	aA	1801	CL7	O1D-CGD-O2D-CED
15	aB	1210	CL7	O1D-CGD-O2D-CED
15	aB	1222	CL7	O1D-CGD-O2D-CED
15	bB	1241	CL7	O1D-CGD-O2D-CED
15	cA	1116	CL7	O1D-CGD-O2D-CED
14	aB	1023	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	cB	1023	PHO	O1D-CGD-O2D-CED
15	aA	1126	CL7	O1D-CGD-O2D-CED
15	aB	1219	CL7	O1D-CGD-O2D-CED
15	bA	1126	CL7	O1D-CGD-O2D-CED
15	bA	1135	CL7	O1D-CGD-O2D-CED
15	bA	1139	CL7	O1D-CGD-O2D-CED
15	bB	1210	CL7	O1D-CGD-O2D-CED
15	bB	1219	CL7	O1D-CGD-O2D-CED
15	bB	1222	CL7	O1D-CGD-O2D-CED
15	bF	1701	CL7	O1D-CGD-O2D-CED
15	cA	1801	CL7	O1D-CGD-O2D-CED
15	cA	1139	CL7	O1D-CGD-O2D-CED
15	cB	1219	CL7	O1D-CGD-O2D-CED
15	cB	1222	CL7	O1D-CGD-O2D-CED
15	aA	1123	CL7	CBA-CGA-O2A-C1
15	bA	1123	CL7	CBA-CGA-O2A-C1
15	cA	1102	CL7	CBA-CGA-O2A-C1
15	cA	1123	CL7	CBA-CGA-O2A-C1
15	cL	1501	CL7	CBA-CGA-O2A-C1
18	cA	5003	LHG	C24-C23-O8-C6
15	aA	1109	CL7	CBD-CGD-O2D-CED
15	aA	1110	CL7	CBD-CGD-O2D-CED
15	aA	1117	CL7	CBD-CGD-O2D-CED
15	aA	1132	CL7	CBD-CGD-O2D-CED
15	aB	1206	CL7	CBD-CGD-O2D-CED
15	bA	1109	CL7	CBD-CGD-O2D-CED
15	bA	1110	CL7	CBD-CGD-O2D-CED
15	bA	1119	CL7	CBD-CGD-O2D-CED
15	bA	1121	CL7	CBD-CGD-O2D-CED
15	bA	1138	CL7	CBD-CGD-O2D-CED
15	bB	1206	CL7	CBD-CGD-O2D-CED
15	bB	1218	CL7	CBD-CGD-O2D-CED
15	bB	1228	CL7	CBD-CGD-O2D-CED
15	bB	1229	CL7	CBD-CGD-O2D-CED
15	cA	1022	CL7	CBD-CGD-O2D-CED
15	cA	1104	CL7	CBD-CGD-O2D-CED
15	cA	1111	CL7	CBD-CGD-O2D-CED
15	cA	1117	CL7	CBD-CGD-O2D-CED
15	cA	1121	CL7	CBD-CGD-O2D-CED
15	cA	1128	CL7	CBD-CGD-O2D-CED
15	cA	1132	CL7	CBD-CGD-O2D-CED
15	cA	1140	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	cB	1210	CL7	CBD-CGD-O2D-CED
15	cB	1220	CL7	CBD-CGD-O2D-CED
15	cB	1226	CL7	CBD-CGD-O2D-CED
15	cB	1228	CL7	CBD-CGD-O2D-CED
15	cB	1234	CL7	CBD-CGD-O2D-CED
15	cB	1236	CL7	CBD-CGD-O2D-CED
15	cL	1501	CL7	CBD-CGD-O2D-CED
14	aA	1013	PHO	O1A-CGA-O2A-C1
14	bA	1013	PHO	O1A-CGA-O2A-C1
14	cA	1013	PHO	O1A-CGA-O2A-C1
15	aA	1102	CL7	O1A-CGA-O2A-C1
15	aA	1118	CL7	O1A-CGA-O2A-C1
15	aA	1133	CL7	O1A-CGA-O2A-C1
15	aB	1237	CL7	O1A-CGA-O2A-C1
15	aL	1501	CL7	O1A-CGA-O2A-C1
15	bA	1118	CL7	O1A-CGA-O2A-C1
15	bA	1133	CL7	O1A-CGA-O2A-C1
15	bB	1237	CL7	O1A-CGA-O2A-C1
15	cA	1118	CL7	O1A-CGA-O2A-C1
15	cB	1237	CL7	O1A-CGA-O2A-C1
15	cB	1225	CL7	O1A-CGA-O2A-C1
14	bB	1023	PHO	O1D-CGD-O2D-CED
15	bA	1113	CL7	O1D-CGD-O2D-CED
15	bB	1216	CL7	O1D-CGD-O2D-CED
15	aB	1216	CL7	O1D-CGD-O2D-CED
15	bA	1115	CL7	O1D-CGD-O2D-CED
15	cA	1135	CL7	O1D-CGD-O2D-CED
15	cB	1224	CL7	O1D-CGD-O2D-CED
15	bA	1116	CL7	CBD-CGD-O2D-CED
15	bA	1132	CL7	CBD-CGD-O2D-CED
15	bB	1213	CL7	CBD-CGD-O2D-CED
15	cA	1110	CL7	CBD-CGD-O2D-CED
15	cB	1209	CL7	CBD-CGD-O2D-CED
15	cB	1213	CL7	CBD-CGD-O2D-CED
15	cI	1601	CL7	CBD-CGD-O2D-CED
15	aB	1228	CL7	O1D-CGD-O2D-CED
15	aA	1135	CL7	O1D-CGD-O2D-CED
14	aA	1013	PHO	C3-C5-C6-C7
14	bA	1013	PHO	C3-C5-C6-C7
14	cA	1013	PHO	C3-C5-C6-C7
15	aA	1118	CL7	C3-C5-C6-C7
15	aA	1119	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	aA	1140	CL7	C3-C5-C6-C7
15	aB	1205	CL7	C3-C5-C6-C7
15	aB	1207	CL7	C3-C5-C6-C7
15	aB	1221	CL7	C3-C5-C6-C7
15	aB	1229	CL7	C3-C5-C6-C7
15	aL	1501	CL7	C3-C5-C6-C7
15	bA	1112	CL7	C3-C5-C6-C7
15	bA	1118	CL7	C3-C5-C6-C7
15	bA	1119	CL7	C3-C5-C6-C7
15	bA	1127	CL7	C3-C5-C6-C7
15	bA	1140	CL7	C3-C5-C6-C7
15	bB	1237	CL7	C3-C5-C6-C7
15	bB	1201	CL7	C3-C5-C6-C7
15	bB	1221	CL7	C3-C5-C6-C7
15	bL	1501	CL7	C3-C5-C6-C7
15	bL	1502	CL7	C3-C5-C6-C7
15	cA	1112	CL7	C3-C5-C6-C7
15	cA	1118	CL7	C3-C5-C6-C7
15	cA	1119	CL7	C3-C5-C6-C7
15	cA	1122	CL7	C3-C5-C6-C7
15	cB	1237	CL7	C3-C5-C6-C7
15	cB	1221	CL7	C3-C5-C6-C7
15	cB	1229	CL7	C3-C5-C6-C7
15	cL	1501	CL7	C3-C5-C6-C7
14	aA	1013	PHO	CBA-CGA-O2A-C1
14	bA	1013	PHO	CBA-CGA-O2A-C1
14	cA	1013	PHO	CBA-CGA-O2A-C1
15	aB	1237	CL7	CBA-CGA-O2A-C1
15	bA	1102	CL7	CBA-CGA-O2A-C1
15	bA	1121	CL7	CBA-CGA-O2A-C1
15	bB	1237	CL7	CBA-CGA-O2A-C1
15	bL	1501	CL7	CBA-CGA-O2A-C1
15	cA	1118	CL7	CBA-CGA-O2A-C1
15	cB	1237	CL7	CBA-CGA-O2A-C1
18	aA	5003	LHG	C24-C23-O8-C6
18	bA	5003	LHG	C24-C23-O8-C6
15	bA	1801	CL7	O1D-CGD-O2D-CED
15	aB	1234	CL7	CBD-CGD-O2D-CED
15	aB	1012	CL7	CBD-CGD-O2D-CED
15	aB	1202	CL7	CBD-CGD-O2D-CED
15	bB	1226	CL7	CBD-CGD-O2D-CED
15	bB	1234	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	cA	1107	CL7	CBD-CGD-O2D-CED
15	cB	1202	CL7	CBD-CGD-O2D-CED
15	cA	1133	CL7	O1A-CGA-O2A-C1
15	aA	1102	CL7	C3-C5-C6-C7
15	aA	1119	CL7	C4-C3-C5-C6
15	aB	1237	CL7	C4-C3-C5-C6
15	aB	1201	CL7	C4-C3-C5-C6
15	bA	1127	CL7	C4-C3-C5-C6
15	bL	1503	CL7	C4-C3-C5-C6
15	cB	1237	CL7	C4-C3-C5-C6
15	cB	1223	CL7	C4-C3-C5-C6
15	cA	1136	CL7	C2-C3-C5-C6
15	aA	1128	CL7	CBD-CGD-O2D-CED
15	aB	1212	CL7	CBD-CGD-O2D-CED
15	bA	1128	CL7	CBD-CGD-O2D-CED
15	bB	1209	CL7	CBD-CGD-O2D-CED
15	bB	1212	CL7	CBD-CGD-O2D-CED
15	bB	1236	CL7	CBD-CGD-O2D-CED
15	cA	1138	CL7	CBD-CGD-O2D-CED
15	cB	1203	CL7	CBD-CGD-O2D-CED
15	cB	1206	CL7	CBD-CGD-O2D-CED
15	aA	1113	CL7	C2A-CAA-CBA-CGA
15	aA	1120	CL7	C2A-CAA-CBA-CGA
15	aA	1127	CL7	C2A-CAA-CBA-CGA
15	aB	1238	CL7	C2A-CAA-CBA-CGA
15	aB	1237	CL7	C2A-CAA-CBA-CGA
15	aB	1209	CL7	C2A-CAA-CBA-CGA
15	bA	1113	CL7	C2A-CAA-CBA-CGA
15	bA	1120	CL7	C2A-CAA-CBA-CGA
15	bA	1133	CL7	C2A-CAA-CBA-CGA
15	bB	1237	CL7	C2A-CAA-CBA-CGA
15	bB	1209	CL7	C2A-CAA-CBA-CGA
15	bB	1238	CL7	C2A-CAA-CBA-CGA
15	cA	1113	CL7	C2A-CAA-CBA-CGA
15	cA	1120	CL7	C2A-CAA-CBA-CGA
15	cB	1237	CL7	C2A-CAA-CBA-CGA
15	cB	1209	CL7	C2A-CAA-CBA-CGA
15	cB	1238	CL7	C2A-CAA-CBA-CGA
15	aB	1237	CL7	C3-C5-C6-C7
15	aB	1201	CL7	C3-C5-C6-C7
15	bA	1116	CL7	C3-C5-C6-C7
15	bB	1205	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	bB	1229	CL7	C3-C5-C6-C7
15	cA	1116	CL7	C3-C5-C6-C7
15	cB	1201	CL7	C3-C5-C6-C7
15	aA	1102	CL7	CBA-CGA-O2A-C1
15	aA	1118	CL7	CBA-CGA-O2A-C1
15	aA	1119	CL7	CBA-CGA-O2A-C1
15	aA	1121	CL7	CBA-CGA-O2A-C1
15	aA	1130	CL7	CBA-CGA-O2A-C1
15	aA	1133	CL7	CBA-CGA-O2A-C1
15	aA	1135	CL7	CBA-CGA-O2A-C1
15	aB	1221	CL7	CBA-CGA-O2A-C1
15	aL	1501	CL7	CBA-CGA-O2A-C1
15	bA	1118	CL7	CBA-CGA-O2A-C1
15	bA	1133	CL7	CBA-CGA-O2A-C1
15	bA	1135	CL7	CBA-CGA-O2A-C1
15	bB	1221	CL7	CBA-CGA-O2A-C1
15	cA	1119	CL7	CBA-CGA-O2A-C1
15	cA	1121	CL7	CBA-CGA-O2A-C1
15	cA	1135	CL7	CBA-CGA-O2A-C1
15	cB	1225	CL7	CBA-CGA-O2A-C1
15	aA	1116	CL7	O1D-CGD-O2D-CED
15	bB	1224	CL7	O1D-CGD-O2D-CED
15	aB	1236	CL7	CBD-CGD-O2D-CED
15	bA	1107	CL7	CBD-CGD-O2D-CED
15	bB	1203	CL7	CBD-CGD-O2D-CED
15	aB	1230	CL7	O1D-CGD-O2D-CED
15	bA	1117	CL7	O1D-CGD-O2D-CED
15	aA	1130	CL7	O1A-CGA-O2A-C1
15	aB	1225	CL7	O1A-CGA-O2A-C1
15	bA	1130	CL7	O1A-CGA-O2A-C1
15	bB	1221	CL7	O1A-CGA-O2A-C1
15	bB	1225	CL7	O1A-CGA-O2A-C1
18	bA	5003	LHG	O10-C23-O8-C6
15	aA	1139	CL7	O1D-CGD-O2D-CED
17	aA	4014	A1JPJ	C9-C10-C11-C12
17	aA	4014	A1JPJ	C13-C14-C15-C16
17	aA	4014	A1JPJ	C15-C16-C17-C18
17	aF	4016	A1JPJ	C19-C20-C21-C22
17	bA	4014	A1JPJ	C9-C10-C11-C12
17	bA	4014	A1JPJ	C13-C14-C15-C16
17	bA	4014	A1JPJ	C15-C16-C17-C18
17	cA	4014	A1JPJ	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	cA	4014	A1JPJ	C13-C14-C15-C16
17	cA	4014	A1JPJ	C15-C16-C17-C18
15	aA	1140	CL7	CBD-CGD-O2D-CED
15	aB	1203	CL7	CBD-CGD-O2D-CED
15	aB	1213	CL7	CBD-CGD-O2D-CED
15	aB	1226	CL7	CBD-CGD-O2D-CED
15	aB	1229	CL7	CBD-CGD-O2D-CED
15	aI	1601	CL7	CBD-CGD-O2D-CED
15	bB	1202	CL7	CBD-CGD-O2D-CED
15	bB	1220	CL7	CBD-CGD-O2D-CED
15	cA	1105	CL7	CBD-CGD-O2D-CED
15	cB	1211	CL7	CBD-CGD-O2D-CED
15	cB	1212	CL7	CBD-CGD-O2D-CED
15	cB	1229	CL7	CBD-CGD-O2D-CED
15	aA	1112	CL7	C3-C5-C6-C7
15	aA	1122	CL7	C3-C5-C6-C7
15	bA	1122	CL7	C3-C5-C6-C7
15	cA	1140	CL7	C3-C5-C6-C7
15	cB	1205	CL7	C3-C5-C6-C7
15	cL	1502	CL7	C3-C5-C6-C7
15	aB	1225	CL7	CBA-CGA-O2A-C1
15	bA	1119	CL7	CBA-CGA-O2A-C1
15	cA	1130	CL7	CBA-CGA-O2A-C1
15	cA	1133	CL7	CBA-CGA-O2A-C1
15	cB	1221	CL7	CBA-CGA-O2A-C1
15	aB	1221	CL7	O1A-CGA-O2A-C1
15	bA	1121	CL7	O1A-CGA-O2A-C1
15	cA	1119	CL7	O1A-CGA-O2A-C1
15	cA	1121	CL7	O1A-CGA-O2A-C1
15	cA	1130	CL7	O1A-CGA-O2A-C1
15	cB	1221	CL7	O1A-CGA-O2A-C1
14	bA	1013	PHO	CBD-CGD-O2D-CED
15	aA	1111	CL7	CBD-CGD-O2D-CED
15	aB	1215	CL7	CBD-CGD-O2D-CED
15	bA	1104	CL7	CBD-CGD-O2D-CED
15	cA	1109	CL7	CBD-CGD-O2D-CED
15	cA	1124	CL7	CBD-CGD-O2D-CED
15	cA	1127	CL7	CBD-CGD-O2D-CED
15	aA	1104	CL7	O1D-CGD-O2D-CED
15	aB	1224	CL7	O1D-CGD-O2D-CED
15	bB	1230	CL7	O1D-CGD-O2D-CED
15	bA	1119	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	aB	1220	CL7	CBD-CGD-O2D-CED
15	bA	1140	CL7	CBD-CGD-O2D-CED
15	aA	1136	CL7	CBA-CGA-O2A-C1
15	bA	1116	CL7	CBA-CGA-O2A-C1
15	bA	1130	CL7	CBA-CGA-O2A-C1
15	bB	1225	CL7	CBA-CGA-O2A-C1
15	aA	1121	CL7	O1D-CGD-O2D-CED
15	cB	1218	CL7	O1D-CGD-O2D-CED
15	aA	1121	CL7	O1A-CGA-O2A-C1
15	aA	1135	CL7	O1A-CGA-O2A-C1
15	bA	1135	CL7	O1A-CGA-O2A-C1
15	cA	1135	CL7	O1A-CGA-O2A-C1
15	aA	1106	CL7	C4-C3-C5-C6
15	bA	1106	CL7	C4-C3-C5-C6
15	cA	1106	CL7	C4-C3-C5-C6
15	aA	1106	CL7	C2-C3-C5-C6
15	aA	1119	CL7	C2-C3-C5-C6
15	bA	1106	CL7	C2-C3-C5-C6
15	cA	1106	CL7	C2-C3-C5-C6
15	bA	1105	CL7	CBD-CGD-O2D-CED
14	bB	1023	PHO	C2A-CAA-CBA-CGA
15	aA	1108	CL7	C2A-CAA-CBA-CGA
15	bA	1108	CL7	C2A-CAA-CBA-CGA
15	bB	1214	CL7	C2A-CAA-CBA-CGA
15	cB	1230	CL7	O1D-CGD-O2D-CED
15	aA	1119	CL7	O1A-CGA-O2A-C1
15	aA	1136	CL7	O1A-CGA-O2A-C1
15	bA	1116	CL7	O1A-CGA-O2A-C1
15	aA	1116	CL7	CBA-CGA-O2A-C1
15	aA	1127	CL7	CBA-CGA-O2A-C1
15	bA	1127	CL7	CBA-CGA-O2A-C1
15	bA	1136	CL7	CBA-CGA-O2A-C1
15	cA	1116	CL7	CBA-CGA-O2A-C1
15	cA	1136	CL7	CBA-CGA-O2A-C1
15	cB	1207	CL7	CBA-CGA-O2A-C1
15	cA	1131	CL7	CBD-CGD-O2D-CED
15	aB	1218	CL7	O1D-CGD-O2D-CED
15	bA	1119	CL7	O1D-CGD-O2D-CED
15	bA	1138	CL7	O1D-CGD-O2D-CED
15	cL	1501	CL7	O1D-CGD-O2D-CED
15	bA	1136	CL7	O1A-CGA-O2A-C1
15	cA	1136	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	bA	1109	CL7	O1D-CGD-O2D-CED
15	cA	1022	CL7	O1D-CGD-O2D-CED
15	cA	1128	CL7	O1D-CGD-O2D-CED
15	cA	1132	CL7	O1D-CGD-O2D-CED
15	cB	1234	CL7	O1D-CGD-O2D-CED
13	cA	1011	G9R	CBD-CGD-O2D-CED
15	aA	1138	CL7	CBD-CGD-O2D-CED
15	bA	1124	CL7	CBD-CGD-O2D-CED
15	aA	1132	CL7	O1D-CGD-O2D-CED
15	cA	1104	CL7	O1D-CGD-O2D-CED
15	aA	1116	CL7	O1A-CGA-O2A-C1
15	aA	1127	CL7	O1A-CGA-O2A-C1
15	cA	1116	CL7	O1A-CGA-O2A-C1
15	aA	1116	CL7	C3-C5-C6-C7
15	bB	1218	CL7	O1D-CGD-O2D-CED
15	cA	1111	CL7	O1D-CGD-O2D-CED
15	cB	1210	CL7	O1D-CGD-O2D-CED
15	cB	1220	CL7	O1D-CGD-O2D-CED
15	aB	1202	CL7	CBA-CGA-O2A-C1
15	aB	1207	CL7	CBA-CGA-O2A-C1
15	aB	1210	CL7	CBA-CGA-O2A-C1
15	aB	1214	CL7	CBA-CGA-O2A-C1
15	aL	1503	CL7	CBA-CGA-O2A-C1
15	bB	1202	CL7	CBA-CGA-O2A-C1
15	bB	1207	CL7	CBA-CGA-O2A-C1
15	bB	1210	CL7	CBA-CGA-O2A-C1
15	bB	1214	CL7	CBA-CGA-O2A-C1
15	bL	1503	CL7	CBA-CGA-O2A-C1
15	cA	1127	CL7	CBA-CGA-O2A-C1
15	cB	1202	CL7	CBA-CGA-O2A-C1
15	cB	1210	CL7	CBA-CGA-O2A-C1
15	cB	1214	CL7	CBA-CGA-O2A-C1
15	cL	1503	CL7	CBA-CGA-O2A-C1
15	aA	1133	CL7	CBD-CGD-O2D-CED
15	bA	1127	CL7	CBD-CGD-O2D-CED
15	bA	1133	CL7	CBD-CGD-O2D-CED
15	cL	1502	CL7	C13-C15-C16-C17
15	aA	1111	CL7	C2C-C3C-CAC-CBC
15	aA	1103	CL7	C5-C6-C7-C8
15	bB	1203	CL7	C13-C15-C16-C17
15	cA	1127	CL7	C10-C11-C12-C13
15	cB	1202	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	bB	1235	CL7	C4-C3-C5-C6
15	aB	1237	CL7	C2-C3-C5-C6
15	bA	1127	CL7	C2-C3-C5-C6
15	bL	1503	CL7	C2-C3-C5-C6
15	cB	1223	CL7	C2-C3-C5-C6
15	aA	1103	CL7	C11-C12-C13-C14
15	aA	1103	CL7	C14-C13-C15-C16
15	aA	1106	CL7	C14-C13-C15-C16
15	aA	1109	CL7	C11-C12-C13-C14
15	aA	1109	CL7	C14-C13-C15-C16
15	aA	1112	CL7	C11-C12-C13-C14
15	aB	1239	CL7	C14-C13-C15-C16
15	aB	1012	CL7	C11-C10-C8-C9
15	aB	1225	CL7	C6-C7-C8-C9
15	aB	1226	CL7	C14-C13-C15-C16
15	aL	1502	CL7	C6-C7-C8-C9
15	bA	1103	CL7	C14-C13-C15-C16
15	bA	1106	CL7	C14-C13-C15-C16
15	bA	1109	CL7	C14-C13-C15-C16
15	bA	1112	CL7	C11-C12-C13-C14
15	bB	1012	CL7	C11-C10-C8-C9
15	bB	1223	CL7	C11-C10-C8-C9
15	bB	1225	CL7	C6-C7-C8-C9
15	bB	1226	CL7	C14-C13-C15-C16
15	bL	1502	CL7	C6-C7-C8-C9
15	cA	1103	CL7	C11-C12-C13-C14
15	cA	1103	CL7	C14-C13-C15-C16
15	cA	1106	CL7	C14-C13-C15-C16
15	cA	1109	CL7	C11-C12-C13-C14
15	cA	1109	CL7	C14-C13-C15-C16
15	cA	1112	CL7	C11-C12-C13-C14
15	cA	1127	CL7	C11-C12-C13-C14
15	cB	1012	CL7	C11-C10-C8-C9
15	cB	1223	CL7	C11-C10-C8-C9
15	cB	1225	CL7	C6-C7-C8-C9
15	cB	1226	CL7	C14-C13-C15-C16
15	cB	1239	CL7	C14-C13-C15-C16
15	cL	1502	CL7	C6-C7-C8-C9
16	aA	2001	PQN	C24-C23-C25-C26
16	aB	2002	PQN	C16-C17-C18-C19
16	bA	2001	PQN	C24-C23-C25-C26
16	bB	2002	PQN	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	cA	2001	PQN	C24-C23-C25-C26
16	cB	2002	PQN	C16-C17-C18-C19
15	aA	1109	CL7	O1D-CGD-O2D-CED
15	bB	1229	CL7	O1D-CGD-O2D-CED
15	cA	1117	CL7	O1D-CGD-O2D-CED
15	cA	1121	CL7	O1D-CGD-O2D-CED
15	cB	1228	CL7	O1D-CGD-O2D-CED
14	cB	1023	PHO	C2A-CAA-CBA-CGA
15	aA	1116	CL7	C2A-CAA-CBA-CGA
15	bA	1109	CL7	C2A-CAA-CBA-CGA
15	cB	1212	CL7	C2A-CAA-CBA-CGA
17	aB	4006	A1JPJ	C37-C22-C23-C24
17	bL	4020	A1JPJ	C7-C8-C9-C34
17	cA	4014	A1JPJ	C11-C12-C13-C35
17	cB	4006	A1JPJ	C37-C22-C23-C24
17	cL	4020	A1JPJ	C7-C8-C9-C34
17	aB	4006	A1JPJ	C21-C22-C23-C24
17	aL	4023	A1JPJ	C21-C22-C23-C24
17	bB	4006	A1JPJ	C21-C22-C23-C24
17	cB	4006	A1JPJ	C21-C22-C23-C24
15	bA	1126	CL7	C2C-C3C-CAC-CBC
15	aB	1202	CL7	O1A-CGA-O2A-C1
15	aB	1207	CL7	O1A-CGA-O2A-C1
15	aL	1503	CL7	O1A-CGA-O2A-C1
15	bB	1202	CL7	O1A-CGA-O2A-C1
15	bB	1214	CL7	O1A-CGA-O2A-C1
15	bL	1503	CL7	O1A-CGA-O2A-C1
15	cA	1127	CL7	O1A-CGA-O2A-C1
15	cL	1503	CL7	O1A-CGA-O2A-C1
15	aA	1117	CL7	C15-C16-C17-C18
15	aB	1210	CL7	C8-C10-C11-C12
15	bA	1103	CL7	C13-C15-C16-C17
15	bB	1203	CL7	C8-C10-C11-C12
15	cA	1109	CL7	C5-C6-C7-C8
15	cA	1109	CL7	C10-C11-C12-C13
15	cB	1226	CL7	C13-C15-C16-C17
16	aB	2002	PQN	C18-C20-C21-C22
15	bB	1206	CL7	O1D-CGD-O2D-CED
15	cB	1226	CL7	O1D-CGD-O2D-CED
15	cB	1236	CL7	O1D-CGD-O2D-CED
15	aA	1133	CL7	C15-C16-C17-C18
15	aB	1203	CL7	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	aB	1223	CL7	C5-C6-C7-C8
15	aL	1501	CL7	C5-C6-C7-C8
15	bA	1117	CL7	C15-C16-C17-C18
15	bA	1131	CL7	C15-C16-C17-C18
15	bB	1205	CL7	C10-C11-C12-C13
15	bB	1226	CL7	C15-C16-C17-C18
15	cA	1103	CL7	C5-C6-C7-C8
15	cA	1103	CL7	C13-C15-C16-C17
15	cA	1104	CL7	C15-C16-C17-C18
15	cB	1203	CL7	C8-C10-C11-C12
15	cB	1205	CL7	C10-C11-C12-C13
16	bB	2002	PQN	C18-C20-C21-C22
15	bA	1121	CL7	O1D-CGD-O2D-CED
15	aA	1109	CL7	C5-C6-C7-C8
15	aA	1109	CL7	C10-C11-C12-C13
15	aA	1111	CL7	C5-C6-C7-C8
15	aA	1123	CL7	C15-C16-C17-C18
15	aA	1127	CL7	C10-C11-C12-C13
15	aA	1131	CL7	C15-C16-C17-C18
15	aB	1239	CL7	C15-C16-C17-C18
15	aB	1205	CL7	C10-C11-C12-C13
15	aB	1221	CL7	C5-C6-C7-C8
15	aB	1226	CL7	C13-C15-C16-C17
15	aB	1226	CL7	C15-C16-C17-C18
15	aL	1503	CL7	C8-C10-C11-C12
15	bA	1104	CL7	C15-C16-C17-C18
15	bA	1109	CL7	C5-C6-C7-C8
15	bA	1127	CL7	C10-C11-C12-C13
15	bB	1210	CL7	C8-C10-C11-C12
15	bB	1221	CL7	C5-C6-C7-C8
15	bB	1223	CL7	C5-C6-C7-C8
15	bB	1226	CL7	C13-C15-C16-C17
15	bL	1501	CL7	C5-C6-C7-C8
15	cA	1123	CL7	C15-C16-C17-C18
15	cA	1131	CL7	C15-C16-C17-C18
15	cA	1133	CL7	C15-C16-C17-C18
15	cB	1210	CL7	C8-C10-C11-C12
15	cB	1223	CL7	C5-C6-C7-C8
15	cL	1501	CL7	C5-C6-C7-C8
15	cL	1503	CL7	C8-C10-C11-C12
16	cA	2001	PQN	C20-C21-C22-C23
15	cA	1140	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	aA	1110	CL7	O1D-CGD-O2D-CED
15	bA	1110	CL7	O1D-CGD-O2D-CED
15	bA	1109	CL7	C10-C11-C12-C13
15	bA	1133	CL7	C15-C16-C17-C18
15	cB	1221	CL7	C5-C6-C7-C8
15	cB	1239	CL7	C13-C15-C16-C17
16	cB	2002	PQN	C18-C20-C21-C22
15	aA	1117	CL7	O1D-CGD-O2D-CED
19	bB	5002	LMG	C37-C38-C39-C40
15	aB	1239	CL7	C13-C15-C16-C17
15	bA	1123	CL7	C15-C16-C17-C18
15	bB	1239	CL7	C13-C15-C16-C17
15	bL	1503	CL7	C8-C10-C11-C12
15	cA	1116	CL7	C8-C10-C11-C12
15	cA	1117	CL7	C15-C16-C17-C18
15	cA	1136	CL7	C13-C15-C16-C17
15	aL	1502	CL7	C13-C15-C16-C17
15	aB	1206	CL7	O1D-CGD-O2D-CED
15	aB	1235	CL7	C11-C10-C8-C7
15	aB	1237	CL7	C6-C7-C8-C10
15	aB	1205	CL7	C6-C7-C8-C10
15	aB	1226	CL7	C12-C13-C15-C16
15	bA	1109	CL7	C11-C12-C13-C15
15	bA	1116	CL7	C11-C10-C8-C7
15	bB	1226	CL7	C12-C13-C15-C16
15	cA	1127	CL7	C12-C13-C15-C16
15	cL	1503	CL7	C6-C7-C8-C10
16	bA	2001	PQN	C22-C23-C25-C26
15	aL	1502	CL7	C3-C5-C6-C7
15	bA	1106	CL7	C3-C5-C6-C7
15	bB	1225	CL7	C3-C5-C6-C7
15	aB	1210	CL7	O1A-CGA-O2A-C1
15	aB	1214	CL7	O1A-CGA-O2A-C1
15	bB	1210	CL7	O1A-CGA-O2A-C1
15	cB	1214	CL7	O1A-CGA-O2A-C1
15	aA	1109	CL7	C2A-CAA-CBA-CGA
15	aA	1140	CL7	C2A-CAA-CBA-CGA
15	aB	1212	CL7	C2A-CAA-CBA-CGA
15	bA	1116	CL7	C2A-CAA-CBA-CGA
15	bA	1140	CL7	C2A-CAA-CBA-CGA
15	cA	1127	CL7	C2A-CAA-CBA-CGA
15	bA	1132	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	bB	1213	CL7	O1D-CGD-O2D-CED
15	bB	1228	CL7	O1D-CGD-O2D-CED
15	cB	1209	CL7	O1D-CGD-O2D-CED
15	cB	1213	CL7	O1D-CGD-O2D-CED
15	aA	1106	CL7	C13-C15-C16-C17
15	aA	1137	CL7	C5-C6-C7-C8
15	aB	1237	CL7	C10-C11-C12-C13
15	cB	1237	CL7	C10-C11-C12-C13
16	aA	2001	PQN	C20-C21-C22-C23
15	bB	1207	CL7	O1A-CGA-O2A-C1
15	cB	1210	CL7	O1A-CGA-O2A-C1
15	aA	1022	CL7	CBD-CGD-O2D-CED
15	aA	1113	CL7	CBD-CGD-O2D-CED
15	aA	1136	CL7	CBD-CGD-O2D-CED
15	aA	1104	CL7	C15-C16-C17-C18
15	aB	1210	CL7	C5-C6-C7-C8
15	bA	1137	CL7	C5-C6-C7-C8
15	bB	1239	CL7	C15-C16-C17-C18
15	cB	1012	CL7	C8-C10-C11-C12
15	cI	1601	CL7	C10-C11-C12-C13
15	cI	1601	CL7	O1D-CGD-O2D-CED
15	cB	1225	CL7	C3-C5-C6-C7
15	aA	1103	CL7	C13-C15-C16-C17
15	aI	1601	CL7	C10-C11-C12-C13
16	bA	2001	PQN	C20-C21-C22-C23
15	bA	1116	CL7	O1D-CGD-O2D-CED
15	cA	1107	CL7	O1D-CGD-O2D-CED
15	bA	1127	CL7	O1A-CGA-O2A-C1
15	cB	1207	CL7	O1A-CGA-O2A-C1
14	bB	1023	PHO	C8-C10-C11-C12
15	aA	1104	CL7	C13-C15-C16-C17
15	aA	1106	CL7	C10-C11-C12-C13
15	aA	1116	CL7	C8-C10-C11-C12
15	aB	1203	CL7	C13-C15-C16-C17
15	aL	1502	CL7	C8-C10-C11-C12
15	bB	1012	CL7	C8-C10-C11-C12
15	cA	1104	CL7	C13-C15-C16-C17
15	cL	1502	CL7	C8-C10-C11-C12
19	aB	5002	LMG	C37-C38-C39-C40
15	aB	1234	CL7	O1D-CGD-O2D-CED
15	cA	1110	CL7	O1D-CGD-O2D-CED
15	aA	1124	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	cB	5002	LMG	C30-C31-C32-C33
15	aB	1202	CL7	O1D-CGD-O2D-CED
15	aB	1012	CL7	C8-C10-C11-C12
15	aL	1503	CL7	C5-C6-C7-C8
15	bA	1106	CL7	C10-C11-C12-C13
15	bA	1112	CL7	C5-C6-C7-C8
15	cA	1112	CL7	C5-C6-C7-C8
15	cA	1137	CL7	C5-C6-C7-C8
15	cB	1239	CL7	C15-C16-C17-C18
18	aA	5003	LHG	C3-O3-P-O6
18	bA	5003	LHG	C3-O3-P-O6
18	cA	5003	LHG	C3-O3-P-O6
15	cA	1104	CL7	C3-C5-C6-C7
15	aB	1012	CL7	O1D-CGD-O2D-CED
15	aA	1132	CL7	C5-C6-C7-C8
15	cA	1106	CL7	C10-C11-C12-C13
15	cB	1202	CL7	O1D-CGD-O2D-CED
15	bB	1226	CL7	O1D-CGD-O2D-CED
15	bB	1234	CL7	O1D-CGD-O2D-CED
15	aA	1132	CL7	C4-C3-C5-C6
15	aB	1235	CL7	C4-C3-C5-C6
15	cB	1237	CL7	C2-C3-C5-C6
15	bB	1210	CL7	C10-C11-C12-C13
15	bA	1128	CL7	O1D-CGD-O2D-CED
15	bB	1209	CL7	O1D-CGD-O2D-CED
14	aB	1023	PHO	C2A-CAA-CBA-CGA
15	aA	1121	CL7	C2A-CAA-CBA-CGA
15	aB	1214	CL7	C2A-CAA-CBA-CGA
15	bA	1121	CL7	C2A-CAA-CBA-CGA
15	cA	1108	CL7	C2A-CAA-CBA-CGA
15	cA	1116	CL7	C2A-CAA-CBA-CGA
15	cA	1121	CL7	C2A-CAA-CBA-CGA
15	cB	1214	CL7	C2A-CAA-CBA-CGA
15	aA	1109	CL7	C16-C17-C18-C20
15	aL	1501	CL7	C11-C12-C13-C15
15	aA	1106	CL7	C3-C5-C6-C7
15	aB	1225	CL7	C3-C5-C6-C7
15	bA	1106	CL7	C13-C15-C16-C17
15	cA	1106	CL7	C13-C15-C16-C17
15	aA	1128	CL7	O1D-CGD-O2D-CED
15	bA	1107	CL7	O1D-CGD-O2D-CED
15	bB	1236	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	cB	1203	CL7	O1D-CGD-O2D-CED
15	aA	1111	CL7	C4C-C3C-CAC-CBC
15	cA	1138	CL7	O1D-CGD-O2D-CED
15	cA	1106	CL7	C3-C5-C6-C7
18	bA	5001	LHG	C14-C15-C16-C17
19	aB	5002	LMG	C34-C35-C36-C37
15	bB	1203	CL7	O1D-CGD-O2D-CED
15	bB	1212	CL7	O1D-CGD-O2D-CED
15	aB	1211	CL7	C6-C7-C8-C10
15	bA	1109	CL7	C16-C17-C18-C20
15	cA	1109	CL7	C16-C17-C18-C20
18	cA	5001	LHG	C12-C13-C14-C15
19	bB	5002	LMG	C30-C31-C32-C33
15	aB	1212	CL7	O1D-CGD-O2D-CED
15	cB	1206	CL7	O1D-CGD-O2D-CED
15	aB	1229	CL7	C13-C15-C16-C17
15	bA	1111	CL7	CBD-CGD-O2D-CED
18	aA	5001	LHG	C14-C15-C16-C17
18	cA	5001	LHG	C14-C15-C16-C17
18	aA	5001	LHG	C27-C28-C29-C30
15	aB	1203	CL7	O1D-CGD-O2D-CED
15	aB	1213	CL7	O1D-CGD-O2D-CED
15	cA	1111	CL7	C2C-C3C-CAC-CBC
19	bB	5002	LMG	C34-C35-C36-C37
15	aA	1140	CL7	O1D-CGD-O2D-CED
15	aB	1236	CL7	O1D-CGD-O2D-CED
15	cB	1212	CL7	O1D-CGD-O2D-CED
17	aL	4020	A1JPJ	C11-C10-C9-C8
17	bL	4020	A1JPJ	C11-C10-C9-C8
17	cL	4020	A1JPJ	C11-C10-C9-C8
15	aA	1129	CL7	CBA-CGA-O2A-C1
15	cA	1129	CL7	CBA-CGA-O2A-C1
19	cB	5002	LMG	C34-C35-C36-C37
15	aB	1215	CL7	C6-C7-C8-C10
15	bA	1128	CL7	C16-C17-C18-C20
15	bB	1215	CL7	C6-C7-C8-C10
15	bB	1221	CL7	C11-C12-C13-C15
15	cB	1211	CL7	C6-C7-C8-C10
15	cB	1215	CL7	C6-C7-C8-C10
15	aB	1229	CL7	O1D-CGD-O2D-CED
15	cB	1211	CL7	O1D-CGD-O2D-CED
15	bB	1205	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	bB	5002	LMG	C36-C37-C38-C39
15	aA	1132	CL7	C2-C3-C5-C6
13	aA	1011	G9R	C11-C12-C13-C14
15	aB	1238	CL7	C14-C13-C15-C16
15	aB	1207	CL7	C11-C12-C13-C14
15	bL	1501	CL7	C6-C7-C8-C9
15	cA	1022	CL7	C11-C10-C8-C9
15	cB	1207	CL7	C11-C12-C13-C14
15	cB	1238	CL7	C14-C13-C15-C16
15	cL	1501	CL7	C6-C7-C8-C9
18	cA	5001	LHG	C27-C28-C29-C30
18	cA	5003	LHG	C14-C15-C16-C17
14	aB	1023	PHO	C8-C10-C11-C12
15	cA	1109	CL7	C13-C15-C16-C17
15	aB	1213	CL7	C2A-CAA-CBA-CGA
15	bA	1118	CL7	C2A-CAA-CBA-CGA
15	bA	1127	CL7	C2A-CAA-CBA-CGA
15	bB	1212	CL7	C2A-CAA-CBA-CGA
15	cA	1109	CL7	C2A-CAA-CBA-CGA
15	cA	1140	CL7	C2A-CAA-CBA-CGA
19	aB	5002	LMG	C30-C31-C32-C33
19	aB	5002	LMG	C36-C37-C38-C39
19	cB	5002	LMG	C36-C37-C38-C39
15	bI	1601	CL7	C3-C5-C6-C7
15	bA	1104	CL7	C13-C15-C16-C17
15	bL	1502	CL7	C13-C15-C16-C17
19	bB	5002	LMG	C19-C20-C21-C22
15	aB	1226	CL7	O1D-CGD-O2D-CED
15	bB	1202	CL7	O1D-CGD-O2D-CED
18	aA	5001	LHG	C24-C25-C26-C27
18	bA	5001	LHG	C24-C25-C26-C27
18	bA	5001	LHG	C27-C28-C29-C30
19	aB	5002	LMG	C19-C20-C21-C22
19	cB	5002	LMG	C12-C13-C14-C15
15	bB	1211	CL7	C6-C7-C8-C10
15	bB	1211	CL7	C6-C7-C8-C9
15	cA	1109	CL7	C16-C17-C18-C19
15	aB	1223	CL7	C15-C16-C17-C18
15	cB	1210	CL7	C10-C11-C12-C13
18	cA	5001	LHG	C24-C25-C26-C27
19	cB	5002	LMG	C19-C20-C21-C22
15	aI	1601	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	bB	1220	CL7	O1D-CGD-O2D-CED
15	bA	1104	CL7	C3-C5-C6-C7
15	aB	1226	CL7	CBA-CGA-O2A-C1
15	cB	1226	CL7	CBA-CGA-O2A-C1
15	cA	1105	CL7	O1D-CGD-O2D-CED
15	aA	1104	CL7	C3A-C2A-CAA-CBA
15	aA	1108	CL7	C3A-C2A-CAA-CBA
15	aA	1120	CL7	C3A-C2A-CAA-CBA
15	aA	1135	CL7	C3A-C2A-CAA-CBA
15	aB	1234	CL7	C3A-C2A-CAA-CBA
15	aB	1235	CL7	C3A-C2A-CAA-CBA
15	aB	1204	CL7	C3A-C2A-CAA-CBA
15	bA	1104	CL7	C3A-C2A-CAA-CBA
15	bA	1108	CL7	C3A-C2A-CAA-CBA
15	bA	1120	CL7	C3A-C2A-CAA-CBA
15	bA	1123	CL7	C3A-C2A-CAA-CBA
15	bA	1135	CL7	C3A-C2A-CAA-CBA
15	bA	1139	CL7	C3A-C2A-CAA-CBA
15	bB	1204	CL7	C3A-C2A-CAA-CBA
15	bB	1223	CL7	C3A-C2A-CAA-CBA
15	bB	1234	CL7	C3A-C2A-CAA-CBA
15	cA	1104	CL7	C3A-C2A-CAA-CBA
15	cA	1108	CL7	C3A-C2A-CAA-CBA
15	cA	1120	CL7	C3A-C2A-CAA-CBA
15	cA	1135	CL7	C3A-C2A-CAA-CBA
15	cA	1139	CL7	C3A-C2A-CAA-CBA
15	cB	1202	CL7	C3A-C2A-CAA-CBA
15	cB	1204	CL7	C3A-C2A-CAA-CBA
15	cB	1223	CL7	C3A-C2A-CAA-CBA
15	cB	1234	CL7	C3A-C2A-CAA-CBA
14	cB	1023	PHO	C8-C10-C11-C12
15	bB	1202	CL7	C15-C16-C17-C18
15	cA	1133	CL7	C5-C6-C7-C8
15	cB	1226	CL7	C15-C16-C17-C18
15	cB	1229	CL7	O1D-CGD-O2D-CED
15	aA	1109	CL7	C16-C17-C18-C19
15	aB	1215	CL7	C6-C7-C8-C9
15	bA	1109	CL7	C16-C17-C18-C19
18	aA	5003	LHG	C13-C14-C15-C16
18	cA	5001	LHG	C28-C29-C30-C31
19	bB	5002	LMG	C12-C13-C14-C15
15	cB	1012	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bB	1023	PHO	C2C-C3C-CAC-CBC
15	aL	1503	CL7	C4-C3-C5-C6
15	bB	1226	CL7	CBA-CGA-O2A-C1
15	aA	1111	CL7	C2-C3-C5-C6
15	aB	1201	CL7	C2-C3-C5-C6
15	bB	1205	CL7	C2-C3-C5-C6
15	aA	1118	CL7	C2A-CAA-CBA-CGA
15	aB	1207	CL7	C2A-CAA-CBA-CGA
15	bA	1104	CL7	O1D-CGD-O2D-CED
15	cB	1202	CL7	C15-C16-C17-C18
16	aA	2001	PQN	C23-C25-C26-C27
15	bA	1137	CL7	CBD-CGD-O2D-CED
15	cB	1238	CL7	CBD-CGD-O2D-CED
18	aA	5001	LHG	C10-C11-C12-C13
15	aA	1104	CL7	C2-C1-O2A-CGA
15	bA	1104	CL7	C2-C1-O2A-CGA
15	bL	1503	CL7	C5-C6-C7-C8
15	cA	1129	CL7	O1A-CGA-O2A-C1
15	bB	1201	CL7	C5-C6-C7-C8
19	cB	5002	LMG	C37-C38-C39-C40
15	aB	1221	CL7	C11-C12-C13-C15
15	cB	1211	CL7	C6-C7-C8-C9
15	cL	1501	CL7	C11-C12-C13-C15
15	cB	1223	CL7	C3-C5-C6-C7
17	aA	4002	A1JPJ	C1-C6-C7-C8
17	aA	4002	A1JPJ	C5-C6-C7-C8
17	aA	4003	A1JPJ	C1-C6-C7-C8
17	aA	4003	A1JPJ	C5-C6-C7-C8
17	aA	4007	A1JPJ	C1-C6-C7-C8
17	aA	4007	A1JPJ	C5-C6-C7-C8
17	aA	4011	A1JPJ	C1-C6-C7-C8
17	aA	4011	A1JPJ	C5-C6-C7-C8
17	aA	4014	A1JPJ	C1-C6-C7-C8
17	aA	4014	A1JPJ	C5-C6-C7-C8
17	aB	4004	A1JPJ	C1-C6-C7-C8
17	aB	4004	A1JPJ	C5-C6-C7-C8
17	aB	4005	A1JPJ	C1-C6-C7-C8
17	aB	4010	A1JPJ	C1-C6-C7-C8
17	aB	4010	A1JPJ	C5-C6-C7-C8
17	aB	4017	A1JPJ	C1-C6-C7-C8
17	aB	4017	A1JPJ	C5-C6-C7-C8
17	aB	4021	A1JPJ	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	aB	4021	A1JPJ	C5-C6-C7-C8
17	aF	4016	A1JPJ	C1-C6-C7-C8
17	aF	4016	A1JPJ	C5-C6-C7-C8
17	aI	4018	A1JPJ	C1-C6-C7-C8
17	aI	4018	A1JPJ	C5-C6-C7-C8
17	aI	4019	A1JPJ	C1-C6-C7-C8
17	aI	4019	A1JPJ	C5-C6-C7-C8
17	bA	4002	A1JPJ	C1-C6-C7-C8
17	bA	4002	A1JPJ	C5-C6-C7-C8
17	bA	4003	A1JPJ	C1-C6-C7-C8
17	bA	4003	A1JPJ	C5-C6-C7-C8
17	bA	4007	A1JPJ	C1-C6-C7-C8
17	bA	4007	A1JPJ	C5-C6-C7-C8
17	bA	4011	A1JPJ	C1-C6-C7-C8
17	bA	4011	A1JPJ	C5-C6-C7-C8
17	bA	4014	A1JPJ	C1-C6-C7-C8
17	bA	4014	A1JPJ	C5-C6-C7-C8
17	bB	4004	A1JPJ	C1-C6-C7-C8
17	bB	4004	A1JPJ	C5-C6-C7-C8
17	bB	4005	A1JPJ	C1-C6-C7-C8
17	bB	4005	A1JPJ	C5-C6-C7-C8
17	bB	4010	A1JPJ	C1-C6-C7-C8
17	bB	4010	A1JPJ	C5-C6-C7-C8
17	bB	4017	A1JPJ	C1-C6-C7-C8
17	bB	4017	A1JPJ	C5-C6-C7-C8
17	bB	4021	A1JPJ	C1-C6-C7-C8
17	bB	4021	A1JPJ	C5-C6-C7-C8
17	bF	4016	A1JPJ	C1-C6-C7-C8
17	bF	4016	A1JPJ	C5-C6-C7-C8
17	bI	4018	A1JPJ	C1-C6-C7-C8
17	bI	4018	A1JPJ	C5-C6-C7-C8
17	bI	4019	A1JPJ	C1-C6-C7-C8
17	bI	4019	A1JPJ	C5-C6-C7-C8
17	cA	4002	A1JPJ	C1-C6-C7-C8
17	cA	4002	A1JPJ	C5-C6-C7-C8
17	cA	4003	A1JPJ	C1-C6-C7-C8
17	cA	4003	A1JPJ	C5-C6-C7-C8
17	cA	4007	A1JPJ	C1-C6-C7-C8
17	cA	4007	A1JPJ	C5-C6-C7-C8
17	cA	4011	A1JPJ	C1-C6-C7-C8
17	cA	4011	A1JPJ	C5-C6-C7-C8
17	cA	4014	A1JPJ	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	cA	4014	A1JPJ	C5-C6-C7-C8
17	cB	4004	A1JPJ	C1-C6-C7-C8
17	cB	4004	A1JPJ	C5-C6-C7-C8
17	cB	4005	A1JPJ	C1-C6-C7-C8
17	cB	4005	A1JPJ	C5-C6-C7-C8
17	cB	4010	A1JPJ	C1-C6-C7-C8
17	cB	4010	A1JPJ	C5-C6-C7-C8
17	cB	4017	A1JPJ	C1-C6-C7-C8
17	cB	4017	A1JPJ	C5-C6-C7-C8
17	cB	4021	A1JPJ	C1-C6-C7-C8
17	cB	4021	A1JPJ	C5-C6-C7-C8
17	cF	4016	A1JPJ	C1-C6-C7-C8
17	cF	4016	A1JPJ	C5-C6-C7-C8
17	cI	4018	A1JPJ	C1-C6-C7-C8
17	cI	4018	A1JPJ	C5-C6-C7-C8
17	cI	4019	A1JPJ	C1-C6-C7-C8
17	cI	4019	A1JPJ	C5-C6-C7-C8
15	cB	1201	CL7	C5-C6-C7-C8
15	bA	1103	CL7	CBA-CGA-O2A-C1
15	aA	1109	CL7	C13-C15-C16-C17
15	bA	1109	CL7	C13-C15-C16-C17
15	bA	1138	CL7	C15-C16-C17-C18
15	bB	1205	CL7	C8-C10-C11-C12
15	cB	1205	CL7	C8-C10-C11-C12
15	cB	1215	CL7	C5-C6-C7-C8
15	cB	1229	CL7	C13-C15-C16-C17
19	aB	5002	LMG	C12-C13-C14-C15
15	aB	1210	CL7	C10-C11-C12-C13
15	bB	1237	CL7	C10-C11-C12-C13
16	bB	2002	PQN	C25-C26-C27-C28
15	aB	1223	CL7	C4-C3-C5-C6
15	cB	1205	CL7	C4-C3-C5-C6
15	cA	1109	CL7	O1D-CGD-O2D-CED
13	aA	1011	G9R	C11-C12-C13-C15
13	aA	1011	G9R	C12-C13-C15-C16
14	aB	1023	PHO	C11-C10-C8-C7
14	bB	1023	PHO	C11-C10-C8-C7
14	cB	1023	PHO	C11-C10-C8-C7
15	aA	1103	CL7	C11-C12-C13-C15
15	aA	1109	CL7	C11-C12-C13-C15
15	aA	1116	CL7	C11-C10-C8-C7
15	aA	1126	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	aB	1238	CL7	C12-C13-C15-C16
15	aB	1207	CL7	C11-C12-C13-C15
15	bA	1103	CL7	C12-C13-C15-C16
15	bA	1126	CL7	C11-C10-C8-C7
15	bA	1127	CL7	C12-C13-C15-C16
15	bB	1205	CL7	C6-C7-C8-C10
15	bB	1229	CL7	C11-C12-C13-C15
15	bB	1235	CL7	C11-C10-C8-C7
15	bL	1501	CL7	C6-C7-C8-C10
15	bL	1503	CL7	C6-C7-C8-C10
15	cA	1022	CL7	C11-C10-C8-C7
15	cA	1109	CL7	C11-C12-C13-C15
15	cA	1116	CL7	C11-C10-C8-C7
15	cA	1126	CL7	C11-C10-C8-C7
15	cB	1205	CL7	C2-C3-C5-C6
15	cB	1207	CL7	C11-C12-C13-C15
15	cB	1226	CL7	C12-C13-C15-C16
15	cB	1235	CL7	C11-C10-C8-C7
15	cB	1238	CL7	C12-C13-C15-C16
15	cL	1501	CL7	C6-C7-C8-C10
16	cA	2001	PQN	C22-C23-C25-C26
15	aA	1129	CL7	O1A-CGA-O2A-C1
15	aB	1226	CL7	O1A-CGA-O2A-C1
15	bB	1226	CL7	O1A-CGA-O2A-C1
15	cB	1226	CL7	O1A-CGA-O2A-C1
15	aB	1211	CL7	C6-C7-C8-C9
15	bB	1239	CL7	C16-C17-C18-C19
14	bA	1013	PHO	O1D-CGD-O2D-CED
18	aA	5003	LHG	C23-C24-C25-C26
15	aA	1103	CL7	CBA-CGA-O2A-C1
15	bB	1224	CL7	CBA-CGA-O2A-C1
15	cA	1103	CL7	CBA-CGA-O2A-C1
15	aB	1012	CL7	C2A-CAA-CBA-CGA
15	bB	1012	CL7	C2A-CAA-CBA-CGA
15	cA	1022	CL7	C2A-CAA-CBA-CGA
15	cA	1118	CL7	C2A-CAA-CBA-CGA
15	cA	1134	CL7	C2A-CAA-CBA-CGA
15	cB	1210	CL7	C2A-CAA-CBA-CGA
15	cB	1213	CL7	C2A-CAA-CBA-CGA
15	bB	1210	CL7	C5-C6-C7-C8
15	bB	1229	CL7	C13-C15-C16-C17
15	bB	1239	CL7	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	cA	1111	CL7	C4C-C3C-CAC-CBC
18	aA	5001	LHG	C12-C13-C14-C15
15	aA	1111	CL7	O1D-CGD-O2D-CED
15	aB	1215	CL7	O1D-CGD-O2D-CED
15	aB	1205	CL7	C8-C10-C11-C12
15	bI	1601	CL7	C10-C11-C12-C13
15	cB	1225	CL7	C5-C6-C7-C8
15	bA	1140	CL7	O1D-CGD-O2D-CED
15	cA	1124	CL7	O1D-CGD-O2D-CED
14	aB	1023	PHO	C2C-C3C-CAC-CBC
15	bA	1105	CL7	O1D-CGD-O2D-CED
18	aA	5001	LHG	C28-C29-C30-C31
15	aB	1202	CL7	C15-C16-C17-C18
15	aB	1225	CL7	C5-C6-C7-C8
15	bA	1136	CL7	C13-C15-C16-C17
15	bB	1215	CL7	C6-C7-C8-C9
15	bB	1221	CL7	C11-C12-C13-C14
15	aA	1111	CL7	C4-C3-C5-C6
15	bB	1223	CL7	C4-C3-C5-C6
15	cA	1117	CL7	C4-C3-C5-C6
15	aB	1235	CL7	C2-C3-C5-C6
15	bB	1235	CL7	C2-C3-C5-C6
18	aA	5001	LHG	C25-C26-C27-C28
14	aB	1023	PHO	C11-C10-C8-C9
14	bB	1023	PHO	C11-C10-C8-C9
14	cB	1023	PHO	C11-C10-C8-C9
15	aA	1116	CL7	C11-C10-C8-C9
15	aB	1235	CL7	C11-C10-C8-C9
15	aB	1237	CL7	C6-C7-C8-C9
15	aB	1229	CL7	C11-C12-C13-C14
15	aL	1503	CL7	C6-C7-C8-C9
15	bA	1116	CL7	C11-C10-C8-C9
15	bA	1127	CL7	C14-C13-C15-C16
15	bB	1229	CL7	C11-C12-C13-C14
15	bB	1235	CL7	C11-C10-C8-C9
15	bL	1503	CL7	C6-C7-C8-C9
15	cA	1104	CL7	C6-C7-C8-C9
15	cA	1116	CL7	C11-C10-C8-C9
15	cA	1127	CL7	C14-C13-C15-C16
15	cB	1237	CL7	C6-C7-C8-C9
15	cB	1223	CL7	C11-C12-C13-C14
15	cB	1229	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	cB	1235	CL7	C11-C10-C8-C9
15	cL	1503	CL7	C6-C7-C8-C9
15	aA	1104	CL7	C3-C5-C6-C7
15	cA	1131	CL7	O1D-CGD-O2D-CED
15	aA	1022	CL7	C2A-CAA-CBA-CGA
15	aA	1106	CL7	C2A-CAA-CBA-CGA
15	aA	1134	CL7	C2A-CAA-CBA-CGA
15	bA	1117	CL7	C2A-CAA-CBA-CGA
15	bA	1134	CL7	C2A-CAA-CBA-CGA
15	bB	1207	CL7	C2A-CAA-CBA-CGA
15	bB	1210	CL7	C2A-CAA-CBA-CGA
15	cB	1207	CL7	C2A-CAA-CBA-CGA
15	cB	1211	CL7	C2A-CAA-CBA-CGA
15	cL	1501	CL7	C2A-CAA-CBA-CGA
15	aB	1220	CL7	O1D-CGD-O2D-CED
15	cB	1203	CL7	C5-C6-C7-C8
15	aA	1107	CL7	CBD-CGD-O2D-CED
15	aA	1103	CL7	O1A-CGA-O2A-C1
15	bA	1103	CL7	O1A-CGA-O2A-C1
15	cA	1127	CL7	O1D-CGD-O2D-CED
15	aA	1103	CL7	C1A-C2A-CAA-CBA
15	aA	1104	CL7	C1A-C2A-CAA-CBA
15	aA	1116	CL7	C1A-C2A-CAA-CBA
15	aA	1120	CL7	C1A-C2A-CAA-CBA
15	aA	1127	CL7	C1A-C2A-CAA-CBA
15	aA	1130	CL7	C1A-C2A-CAA-CBA
15	aA	1133	CL7	C1A-C2A-CAA-CBA
15	aA	1135	CL7	C1A-C2A-CAA-CBA
15	aB	1241	CL7	C1A-C2A-CAA-CBA
15	aB	1204	CL7	C1A-C2A-CAA-CBA
15	aB	1210	CL7	C1A-C2A-CAA-CBA
15	aB	1222	CL7	C1A-C2A-CAA-CBA
15	aB	1227	CL7	C1A-C2A-CAA-CBA
15	aJ	1302	CL7	C1A-C2A-CAA-CBA
15	bA	1104	CL7	C1A-C2A-CAA-CBA
15	bA	1116	CL7	C1A-C2A-CAA-CBA
15	bA	1127	CL7	C1A-C2A-CAA-CBA
15	bA	1130	CL7	C1A-C2A-CAA-CBA
15	bA	1135	CL7	C1A-C2A-CAA-CBA
15	bA	1137	CL7	C1A-C2A-CAA-CBA
15	bA	1140	CL7	C1A-C2A-CAA-CBA
15	bB	1204	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	bB	1210	CL7	C1A-C2A-CAA-CBA
15	bB	1222	CL7	C1A-C2A-CAA-CBA
15	bB	1227	CL7	C1A-C2A-CAA-CBA
15	bB	1241	CL7	C1A-C2A-CAA-CBA
15	cA	1104	CL7	C1A-C2A-CAA-CBA
15	cA	1116	CL7	C1A-C2A-CAA-CBA
15	cA	1120	CL7	C1A-C2A-CAA-CBA
15	cA	1127	CL7	C1A-C2A-CAA-CBA
15	cA	1130	CL7	C1A-C2A-CAA-CBA
15	cA	1135	CL7	C1A-C2A-CAA-CBA
15	cB	1210	CL7	C1A-C2A-CAA-CBA
15	cB	1222	CL7	C1A-C2A-CAA-CBA
15	cB	1227	CL7	C1A-C2A-CAA-CBA
15	cB	1241	CL7	C1A-C2A-CAA-CBA
15	cL	1502	CL7	C1A-C2A-CAA-CBA
15	aB	1221	CL7	C11-C12-C13-C14
15	bA	1128	CL7	C16-C17-C18-C19
15	bB	1239	CL7	C16-C17-C18-C20
15	cB	1215	CL7	C6-C7-C8-C9
15	cL	1501	CL7	C11-C12-C13-C14
15	bA	1111	CL7	C2C-C3C-CAC-CBC
15	aA	1136	CL7	C13-C15-C16-C17
15	bL	1502	CL7	C8-C10-C11-C12
18	bA	5001	LHG	C9-C10-C11-C12
15	bB	1225	CL7	C5-C6-C7-C8
13	cA	1011	G9R	O1D-CGD-O2D-CED
15	bA	1133	CL7	O1D-CGD-O2D-CED
19	bB	5002	LMG	C33-C34-C35-C36
15	bB	1203	CL7	C5-C6-C7-C8
15	aB	1237	CL7	C16-C17-C18-C20
15	aL	1501	CL7	C11-C12-C13-C14
15	aA	1133	CL7	O1D-CGD-O2D-CED
15	bA	1124	CL7	O1D-CGD-O2D-CED
15	aB	1201	CL7	C5-C6-C7-C8
15	aA	1112	CL7	C5-C6-C7-C8
15	cB	1203	CL7	C13-C15-C16-C17
15	cL	1503	CL7	C5-C6-C7-C8
15	bI	1601	CL7	CBD-CGD-O2D-CED
15	bA	1104	CL7	CBA-CGA-O2A-C1
15	bB	1201	CL7	C4-C3-C5-C6
19	cB	5002	LMG	C17-C18-C19-C20
15	bB	1224	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	cA	1103	CL7	O1A-CGA-O2A-C1
15	cA	1119	CL7	C2A-CAA-CBA-CGA
15	cB	1012	CL7	C2A-CAA-CBA-CGA
15	bB	1202	CL7	C16-C17-C18-C19
15	cB	1221	CL7	C11-C12-C13-C15
15	bB	1203	CL7	C3-C5-C6-C7
15	aA	1138	CL7	O1D-CGD-O2D-CED
15	bA	1127	CL7	O1D-CGD-O2D-CED
15	bA	1133	CL7	C5-C6-C7-C8
18	bA	5003	LHG	C14-C15-C16-C17
15	aA	1022	CL7	C2B-C3B-CAB-OBB
15	aA	1102	CL7	C2B-C3B-CAB-OBB
15	aA	1104	CL7	C2B-C3B-CAB-OBB
15	aA	1106	CL7	C2B-C3B-CAB-OBB
15	aA	1108	CL7	C2B-C3B-CAB-OBB
15	aA	1110	CL7	C2B-C3B-CAB-OBB
15	aA	1113	CL7	C2B-C3B-CAB-OBB
15	aA	1115	CL7	C2B-C3B-CAB-OBB
15	aA	1119	CL7	C2B-C3B-CAB-OBB
15	aA	1129	CL7	C2B-C3B-CAB-OBB
15	aA	1801	CL7	C2B-C3B-CAB-OBB
15	aA	1139	CL7	C2B-C3B-CAB-OBB
15	aB	1234	CL7	C2B-C3B-CAB-OBB
15	aB	1012	CL7	C2B-C3B-CAB-OBB
15	aB	1206	CL7	C2B-C3B-CAB-OBB
15	aB	1207	CL7	C2B-C3B-CAB-OBB
15	aB	1212	CL7	C2B-C3B-CAB-OBB
15	aB	1220	CL7	C2B-C3B-CAB-OBB
15	aB	1221	CL7	C2B-C3B-CAB-OBB
15	aB	1222	CL7	C2B-C3B-CAB-OBB
15	aB	1223	CL7	C2B-C3B-CAB-OBB
15	aK	1401	CL7	C2B-C3B-CAB-OBB
15	bA	1022	CL7	C2B-C3B-CAB-OBB
15	bA	1102	CL7	C2B-C3B-CAB-OBB
15	bA	1104	CL7	C2B-C3B-CAB-OBB
15	bA	1106	CL7	C2B-C3B-CAB-OBB
15	bA	1110	CL7	C2B-C3B-CAB-OBB
15	bA	1115	CL7	C2B-C3B-CAB-OBB
15	bA	1119	CL7	C2B-C3B-CAB-OBB
15	bA	1129	CL7	C2B-C3B-CAB-OBB
15	bA	1130	CL7	C2B-C3B-CAB-OBB
15	bA	1139	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
15	bA	1801	CL7	C2B-C3B-CAB-OBB
15	bB	1012	CL7	C2B-C3B-CAB-OBB
15	bB	1021	CL7	C2B-C3B-CAB-OBB
15	bB	1206	CL7	C2B-C3B-CAB-OBB
15	bB	1207	CL7	C2B-C3B-CAB-OBB
15	bB	1212	CL7	C2B-C3B-CAB-OBB
15	bB	1213	CL7	C2B-C3B-CAB-OBB
15	bB	1220	CL7	C2B-C3B-CAB-OBB
15	bB	1221	CL7	C2B-C3B-CAB-OBB
15	bB	1222	CL7	C2B-C3B-CAB-OBB
15	bB	1234	CL7	C2B-C3B-CAB-OBB
15	bB	1241	CL7	C2B-C3B-CAB-OBB
15	bK	1401	CL7	C2B-C3B-CAB-OBB
15	bL	1501	CL7	C2B-C3B-CAB-OBB
15	cA	1022	CL7	C2B-C3B-CAB-OBB
15	cA	1104	CL7	C2B-C3B-CAB-OBB
15	cA	1110	CL7	C2B-C3B-CAB-OBB
15	cA	1115	CL7	C2B-C3B-CAB-OBB
15	cA	1129	CL7	C2B-C3B-CAB-OBB
15	cA	1137	CL7	C2B-C3B-CAB-OBB
15	cA	1801	CL7	C2B-C3B-CAB-OBB
15	cA	1139	CL7	C2B-C3B-CAB-OBB
15	cB	1012	CL7	C2B-C3B-CAB-OBB
15	cB	1021	CL7	C2B-C3B-CAB-OBB
15	cB	1206	CL7	C2B-C3B-CAB-OBB
15	cB	1212	CL7	C2B-C3B-CAB-OBB
15	cB	1220	CL7	C2B-C3B-CAB-OBB
15	cB	1221	CL7	C2B-C3B-CAB-OBB
15	cB	1222	CL7	C2B-C3B-CAB-OBB
15	cB	1227	CL7	C2B-C3B-CAB-OBB
15	cB	1234	CL7	C2B-C3B-CAB-OBB
15	cB	1236	CL7	C2B-C3B-CAB-OBB
15	cB	1241	CL7	C2B-C3B-CAB-OBB
15	cL	1501	CL7	C2B-C3B-CAB-OBB
15	cL	1503	CL7	C2B-C3B-CAB-OBB
15	bA	1102	CL7	C4-C3-C5-C6
15	aL	1502	CL7	C16-C17-C18-C20
15	bL	1501	CL7	C11-C12-C13-C15
15	cB	1224	CL7	CBA-CGA-O2A-C1
15	bB	1239	CL7	CBD-CGD-O2D-CED
15	aA	1123	CL7	C10-C11-C12-C13
15	aB	1203	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	bA	1140	CL7	C8-C10-C11-C12
15	aA	1022	CL7	C4B-C3B-CAB-OBB
15	aB	1012	CL7	C4B-C3B-CAB-OBB
15	aB	1206	CL7	C4B-C3B-CAB-OBB
15	bA	1115	CL7	C4B-C3B-CAB-OBB
15	bB	1012	CL7	C4B-C3B-CAB-OBB
15	bB	1021	CL7	C4B-C3B-CAB-OBB
15	bB	1206	CL7	C4B-C3B-CAB-OBB
15	bB	1221	CL7	C4B-C3B-CAB-OBB
15	bB	1234	CL7	C4B-C3B-CAB-OBB
15	cA	1022	CL7	C4B-C3B-CAB-OBB
15	cA	1801	CL7	C4B-C3B-CAB-OBB
15	cB	1012	CL7	C4B-C3B-CAB-OBB
15	cB	1221	CL7	C4B-C3B-CAB-OBB
15	cL	1503	CL7	C4B-C3B-CAB-OBB
15	bA	1104	CL7	C5-C6-C7-C8
15	cI	1601	CL7	C8-C10-C11-C12
15	aA	1136	CL7	C2-C1-O2A-CGA
15	cA	1104	CL7	C2-C1-O2A-CGA
18	bA	5001	LHG	C28-C29-C30-C31
15	cB	1211	CL7	C3-C5-C6-C7
15	bA	1129	CL7	CBA-CGA-O2A-C1
15	aB	1237	CL7	C16-C17-C18-C19
15	bB	1202	CL7	C16-C17-C18-C20
15	cA	1128	CL7	C16-C17-C18-C20
19	aB	5002	LMG	C33-C34-C35-C36
15	bA	1104	CL7	O1A-CGA-O2A-C1
15	aL	1502	CL7	C10-C11-C12-C13
16	cB	2002	PQN	C25-C26-C27-C28
14	cB	1023	PHO	C2C-C3C-CAC-CBC
15	aA	1133	CL7	C5-C6-C7-C8
14	aB	1023	PHO	CHA-CBD-CGD-O1D
14	aB	1023	PHO	CHA-CBD-CGD-O2D
14	cB	1023	PHO	CHA-CBD-CGD-O1D
14	cB	1023	PHO	CHA-CBD-CGD-O2D
13	bA	1011	G9R	C12-C13-C15-C16
13	cA	1011	G9R	C12-C13-C15-C16
15	aA	1104	CL7	C6-C7-C8-C10
15	aA	1106	CL7	C11-C12-C13-C15
15	aA	1106	CL7	C12-C13-C15-C16
15	aA	1109	CL7	C12-C13-C15-C16
15	aB	1239	CL7	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	aB	1012	CL7	C11-C10-C8-C7
15	aB	1223	CL7	C11-C12-C13-C15
15	aB	1226	CL7	C11-C10-C8-C7
15	aB	1229	CL7	C11-C12-C13-C15
15	aL	1502	CL7	C6-C7-C8-C10
15	aL	1503	CL7	C2-C3-C5-C6
15	aL	1503	CL7	C6-C7-C8-C10
15	bA	1104	CL7	C6-C7-C8-C10
15	bA	1106	CL7	C12-C13-C15-C16
15	bA	1109	CL7	C12-C13-C15-C16
15	bB	1012	CL7	C11-C10-C8-C7
15	bB	1203	CL7	C12-C13-C15-C16
15	bB	1210	CL7	C12-C13-C15-C16
15	bB	1223	CL7	C11-C10-C8-C7
15	bB	1223	CL7	C11-C12-C13-C15
15	bL	1502	CL7	C6-C7-C8-C10
15	cA	1103	CL7	C11-C12-C13-C15
15	cA	1103	CL7	C12-C13-C15-C16
15	cA	1104	CL7	C6-C7-C8-C10
15	cA	1106	CL7	C11-C12-C13-C15
15	cA	1106	CL7	C12-C13-C15-C16
15	cA	1109	CL7	C12-C13-C15-C16
15	cA	1117	CL7	C6-C7-C8-C10
15	cB	1237	CL7	C6-C7-C8-C10
15	cB	1012	CL7	C11-C10-C8-C7
15	cB	1205	CL7	C6-C7-C8-C10
15	cB	1210	CL7	C12-C13-C15-C16
15	cB	1223	CL7	C11-C12-C13-C15
15	cB	1229	CL7	C11-C12-C13-C15
15	cB	1239	CL7	C12-C13-C15-C16
16	aA	2001	PQN	C22-C23-C25-C26
13	cA	1011	G9R	C3-C5-C6-C7
13	cA	1011	G9R	C11-C12-C13-C14
15	aA	1104	CL7	C6-C7-C8-C9
15	aA	1106	CL7	C11-C10-C8-C9
15	aA	1117	CL7	C11-C12-C13-C14
15	aB	1208	CL7	C14-C13-C15-C16
15	aB	1210	CL7	C14-C13-C15-C16
15	aB	1221	CL7	C6-C7-C8-C9
15	aB	1223	CL7	C11-C12-C13-C14
15	aB	1226	CL7	C11-C10-C8-C9
15	bA	1104	CL7	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	bA	1112	CL7	C6-C7-C8-C9
15	bA	1117	CL7	C11-C12-C13-C14
15	bA	1127	CL7	C11-C12-C13-C14
15	bB	1208	CL7	C14-C13-C15-C16
15	bB	1210	CL7	C14-C13-C15-C16
15	bB	1223	CL7	C11-C12-C13-C14
15	bB	1226	CL7	C11-C10-C8-C9
15	cA	1112	CL7	C6-C7-C8-C9
15	cA	1117	CL7	C11-C12-C13-C14
15	cA	1140	CL7	C6-C7-C8-C9
15	cB	1205	CL7	C11-C10-C8-C9
15	cB	1210	CL7	C14-C13-C15-C16
15	cB	1221	CL7	C6-C7-C8-C9
15	cB	1226	CL7	C11-C10-C8-C9
13	aA	1011	G9R	CBD-CGD-O2D-CED
15	bA	1109	CL7	CBA-CGA-O2A-C1
15	cA	1104	CL7	CBA-CGA-O2A-C1
15	cB	1223	CL7	C8-C10-C11-C12
15	bA	1022	CL7	C2A-CAA-CBA-CGA
18	aA	5001	LHG	C29-C30-C31-C32
18	bA	5001	LHG	C25-C26-C27-C28
19	aB	5002	LMG	C15-C16-C17-C18
15	aA	1022	CL7	O1D-CGD-O2D-CED
15	aB	1202	CL7	C16-C17-C18-C19
15	bL	1502	CL7	C16-C17-C18-C20
19	aB	5002	LMG	C20-C21-C22-C23
15	aA	1136	CL7	O1D-CGD-O2D-CED
14	aA	1013	PHO	C13-C15-C16-C17
15	aA	1119	CL7	C5-C6-C7-C8
15	cB	1210	CL7	C5-C6-C7-C8
15	aA	1104	CL7	CBA-CGA-O2A-C1
15	aA	1109	CL7	CBA-CGA-O2A-C1
15	bA	1132	CL7	CBA-CGA-O2A-C1
15	bA	1111	CL7	C4C-C3C-CAC-CBC
15	cA	1104	CL7	C5-C6-C7-C8
15	cA	1132	CL7	C5-C6-C7-C8
15	cB	1239	CL7	C10-C11-C12-C13
14	cA	1013	PHO	CBD-CGD-O2D-CED
15	aA	1105	CL7	CBD-CGD-O2D-CED
15	aB	1202	CL7	C16-C17-C18-C20
15	aB	1225	CL7	C16-C17-C18-C20
15	cB	1237	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	cB	1205	CL7	C13-C15-C16-C17
18	cA	5001	LHG	C29-C30-C31-C32
19	cB	5002	LMG	C33-C34-C35-C36
15	cB	1223	CL7	C15-C16-C17-C18
15	aA	1113	CL7	O1D-CGD-O2D-CED
15	aB	1205	CL7	C4-C3-C5-C6
15	aB	1229	CL7	C4-C3-C5-C6
15	cB	1229	CL7	C4-C3-C5-C6
15	cA	1117	CL7	C2-C3-C5-C6
15	cB	1229	CL7	C2-C3-C5-C6
15	cA	1140	CL7	C8-C10-C11-C12
15	aB	1203	CL7	C3-C5-C6-C7
15	aB	1225	CL7	C16-C17-C18-C19
15	aL	1502	CL7	C16-C17-C18-C19
18	cA	5001	LHG	C10-C11-C12-C13
15	cA	1106	CL7	C2A-CAA-CBA-CGA
15	aA	1102	CL7	C3A-C2A-CAA-CBA
15	aA	1123	CL7	C3A-C2A-CAA-CBA
15	aA	1133	CL7	C3A-C2A-CAA-CBA
15	aA	1137	CL7	C3A-C2A-CAA-CBA
15	aA	1140	CL7	C3A-C2A-CAA-CBA
15	aB	1206	CL7	C3A-C2A-CAA-CBA
15	aB	1216	CL7	C3A-C2A-CAA-CBA
15	aJ	1302	CL7	C3A-C2A-CAA-CBA
15	aL	1502	CL7	C3A-C2A-CAA-CBA
15	bA	1112	CL7	C3A-C2A-CAA-CBA
15	bA	1133	CL7	C3A-C2A-CAA-CBA
15	bA	1137	CL7	C3A-C2A-CAA-CBA
15	bA	1140	CL7	C3A-C2A-CAA-CBA
15	bB	1216	CL7	C3A-C2A-CAA-CBA
15	bJ	1302	CL7	C3A-C2A-CAA-CBA
15	bL	1502	CL7	C3A-C2A-CAA-CBA
15	cA	1123	CL7	C3A-C2A-CAA-CBA
15	cA	1133	CL7	C3A-C2A-CAA-CBA
15	cA	1137	CL7	C3A-C2A-CAA-CBA
15	cA	1140	CL7	C3A-C2A-CAA-CBA
15	cB	1216	CL7	C3A-C2A-CAA-CBA
15	cL	1502	CL7	C3A-C2A-CAA-CBA
18	bA	5003	LHG	C11-C12-C13-C14
15	cA	1118	CL7	CBD-CGD-O2D-CED
15	cL	1502	CL7	C10-C11-C12-C13
15	cB	1237	CL7	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	cB	1221	CL7	C11-C12-C13-C14
15	aB	1224	CL7	CBA-CGA-O2A-C1
15	bA	1119	CL7	C5-C6-C7-C8
15	bB	1215	CL7	C5-C6-C7-C8
15	cB	1237	CL7	C5-C6-C7-C8
15	cB	1202	CL7	C8-C10-C11-C12
16	cA	2001	PQN	C23-C25-C26-C27
15	aA	1124	CL7	O1D-CGD-O2D-CED
15	cB	1224	CL7	O1A-CGA-O2A-C1
18	cA	5001	LHG	C25-C26-C27-C28
15	aB	1235	CL7	C3-C5-C6-C7
15	aB	1211	CL7	C3-C5-C6-C7
15	bA	1111	CL7	O1D-CGD-O2D-CED
19	bB	5002	LMG	C15-C16-C17-C18
15	cB	1235	CL7	C4-C3-C5-C6
15	bL	1501	CL7	C11-C12-C13-C14
15	aB	1229	CL7	C2-C3-C5-C6
15	bL	1501	CL7	C2A-CAA-CBA-CGA
15	bA	1109	CL7	C8-C10-C11-C12
15	bB	1202	CL7	C8-C10-C11-C12
15	bA	1129	CL7	O1A-CGA-O2A-C1
15	bB	1237	CL7	C16-C17-C18-C20
15	bL	1502	CL7	C16-C17-C18-C19
15	cA	1119	CL7	C5-C6-C7-C8
15	bA	1137	CL7	O1D-CGD-O2D-CED
15	cA	1136	CL7	CBD-CGD-O2D-CED
15	cA	1104	CL7	O1A-CGA-O2A-C1
18	bA	5001	LHG	O7-C5-C6-O8
15	cA	1128	CL7	C16-C17-C18-C19
19	bB	5002	LMG	C17-C18-C19-C20
15	aA	1140	CL7	C5-C6-C7-C8
15	aI	1601	CL7	C8-C10-C11-C12
15	cB	1238	CL7	O1D-CGD-O2D-CED
15	aA	1138	CL7	C2-C1-O2A-CGA
15	aB	1225	CL7	C2-C1-O2A-CGA
15	bB	1235	CL7	C2-C1-O2A-CGA
15	cA	1136	CL7	C2-C1-O2A-CGA
15	aB	1205	CL7	C2-C3-C5-C6
15	aA	1109	CL7	C11-C10-C8-C9
15	aA	1112	CL7	C6-C7-C8-C9
15	aA	1140	CL7	C6-C7-C8-C9
15	bA	1109	CL7	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	bA	1132	CL7	C11-C10-C8-C9
15	bB	1205	CL7	C11-C10-C8-C9
15	bB	1207	CL7	C11-C12-C13-C14
15	cA	1109	CL7	C11-C10-C8-C9
15	cA	1122	CL7	C11-C10-C8-C9
15	cA	1123	CL7	C11-C12-C13-C14
15	aA	1104	CL7	C5-C6-C7-C8
15	aA	1140	CL7	C8-C10-C11-C12
15	bB	1223	CL7	C15-C16-C17-C18
15	bB	1229	CL7	C10-C11-C12-C13
15	aA	1130	CL7	C4-C3-C5-C6
15	aA	1104	CL7	O1A-CGA-O2A-C1
19	aB	5002	LMG	C31-C32-C33-C34
15	aA	1119	CL7	C2A-CAA-CBA-CGA
15	aA	1128	CL7	C16-C17-C18-C19
15	bA	1103	CL7	C3-C5-C6-C7
15	cB	1235	CL7	C3-C5-C6-C7
17	aA	4008	A1JPJ	C1-C6-C7-C8
17	aA	4008	A1JPJ	C5-C6-C7-C8
17	aB	4005	A1JPJ	C5-C6-C7-C8
17	bA	4008	A1JPJ	C1-C6-C7-C8
17	cA	4008	A1JPJ	C1-C6-C7-C8
17	cA	4008	A1JPJ	C5-C6-C7-C8
15	cB	1229	CL7	C2C-C3C-CAC-CBC
13	cA	1011	G9R	CAA-CBA-CGA-O2A
18	bA	5001	LHG	C29-C30-C31-C32
18	cA	5003	LHG	C13-C14-C15-C16
13	aA	1011	G9R	C8-C10-C11-C12
15	aA	1117	CL7	C8-C10-C11-C12
15	bA	1123	CL7	C10-C11-C12-C13
15	bB	1202	CL7	C13-C15-C16-C17
16	aB	2002	PQN	C23-C25-C26-C27
15	bB	1237	CL7	C16-C17-C18-C19
19	aB	5002	LMG	C4-C5-C6-O5
19	bB	5002	LMG	C31-C32-C33-C34
15	bA	1132	CL7	O1A-CGA-O2A-C1
13	aA	1011	G9R	CAA-CBA-CGA-O2A
13	cA	1011	G9R	C11-C12-C13-C15
15	aA	1103	CL7	C12-C13-C15-C16
15	aA	1109	CL7	C11-C10-C8-C7
15	aA	1112	CL7	C6-C7-C8-C10
15	aA	1117	CL7	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	aA	1117	CL7	C11-C12-C13-C15
15	aA	1122	CL7	C6-C7-C8-C10
15	aA	1123	CL7	C11-C12-C13-C15
15	aB	1205	CL7	C11-C10-C8-C7
15	aB	1210	CL7	C12-C13-C15-C16
15	aB	1223	CL7	C11-C10-C8-C7
15	aB	1225	CL7	C6-C7-C8-C10
15	bA	1103	CL7	C11-C10-C8-C7
15	bA	1106	CL7	C11-C12-C13-C15
15	bA	1109	CL7	C11-C10-C8-C7
15	bA	1112	CL7	C6-C7-C8-C10
15	bA	1117	CL7	C6-C7-C8-C10
15	bA	1117	CL7	C11-C12-C13-C15
15	bA	1122	CL7	C6-C7-C8-C10
15	bA	1123	CL7	C11-C12-C13-C15
15	bA	1136	CL7	C6-C7-C8-C10
15	bB	1237	CL7	C11-C10-C8-C7
15	bB	1203	CL7	C6-C7-C8-C10
15	bB	1205	CL7	C11-C10-C8-C7
15	bB	1226	CL7	C11-C10-C8-C7
15	bB	1239	CL7	C12-C13-C15-C16
15	bL	1502	CL7	C11-C10-C8-C7
15	cA	1112	CL7	C6-C7-C8-C10
15	cA	1117	CL7	C11-C12-C13-C15
15	cA	1122	CL7	C6-C7-C8-C10
15	cA	1123	CL7	C11-C12-C13-C15
15	cB	1203	CL7	C6-C7-C8-C10
15	cB	1205	CL7	C11-C10-C8-C7
15	cB	1223	CL7	C11-C10-C8-C7
15	cB	1226	CL7	C11-C10-C8-C7
15	cL	1502	CL7	C6-C7-C8-C10
15	cL	1502	CL7	C11-C10-C8-C7
15	cL	1502	CL7	C12-C13-C15-C16
15	cB	1012	CL7	O1D-CGD-O2D-CED
15	bA	1109	CL7	O1A-CGA-O2A-C1
15	bA	1117	CL7	C8-C10-C11-C12
15	bA	1135	CL7	C2A-CAA-CBA-CGA
15	bL	1502	CL7	C2A-CAA-CBA-CGA
15	cB	1223	CL7	C2A-CAA-CBA-CGA
15	cB	1203	CL7	C3-C5-C6-C7
14	cB	1023	PHO	C13-C15-C16-C17
15	bB	1239	CL7	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	aA	1109	CL7	O1A-CGA-O2A-C1
15	aA	1123	CL7	CAD-CBD-CGD-O2D
15	aA	1124	CL7	CAD-CBD-CGD-O2D
15	aA	1139	CL7	CAD-CBD-CGD-O2D
15	aB	1238	CL7	CAD-CBD-CGD-O2D
15	aB	1203	CL7	CAD-CBD-CGD-O2D
15	aB	1012	CL7	CAD-CBD-CGD-O2D
15	aB	1202	CL7	CAD-CBD-CGD-O2D
15	aB	1210	CL7	CAD-CBD-CGD-O2D
15	aB	1215	CL7	CAD-CBD-CGD-O2D
15	aB	1216	CL7	CAD-CBD-CGD-O2D
15	aB	1219	CL7	CAD-CBD-CGD-O2D
15	aB	1223	CL7	CAD-CBD-CGD-O2D
15	bA	1109	CL7	CAD-CBD-CGD-O2D
15	bA	1131	CL7	CAD-CBD-CGD-O2D
15	bA	1135	CL7	CAD-CBD-CGD-O2D
15	bA	1139	CL7	CAD-CBD-CGD-O2D
15	bB	1203	CL7	CAD-CBD-CGD-O2D
15	bB	1227	CL7	CAD-CBD-CGD-O2D
15	bB	1230	CL7	CAD-CBD-CGD-O2D
15	bB	1238	CL7	CAD-CBD-CGD-O2D
15	bB	1239	CL7	CAD-CBD-CGD-O2D
15	cA	1103	CL7	CAD-CBD-CGD-O2D
15	cA	1109	CL7	CAD-CBD-CGD-O2D
15	cA	1137	CL7	CAD-CBD-CGD-O2D
15	cB	1202	CL7	CAD-CBD-CGD-O2D
15	cB	1203	CL7	CAD-CBD-CGD-O2D
15	cB	1215	CL7	CAD-CBD-CGD-O2D
15	cB	1216	CL7	CAD-CBD-CGD-O2D
15	cB	1223	CL7	CAD-CBD-CGD-O2D
15	cB	1239	CL7	CAD-CBD-CGD-O2D
15	aB	1223	CL7	C3-C5-C6-C7
18	aA	5003	LHG	C14-C15-C16-C17
13	cA	1011	G9R	C8-C10-C11-C12
15	aB	1207	CL7	C10-C11-C12-C13
15	cB	1224	CL7	C5-C6-C7-C8
15	cB	1204	CL7	CBA-CGA-O2A-C1
15	bB	1208	CL7	C4-C3-C5-C6
15	cA	1140	CL7	C5-C6-C7-C8
16	bA	2001	PQN	C23-C25-C26-C27
15	bB	1208	CL7	C2-C3-C5-C6
15	aA	1127	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	bB	1214	CL7	CBD-CGD-O2D-CED
18	aA	5001	LHG	O6-C4-C5-O7
14	cA	1013	PHO	C13-C15-C16-C17
15	bA	1103	CL7	C5-C6-C7-C8
15	aL	1501	CL7	C2A-CAA-CBA-CGA
15	bK	1401	CL7	C2A-CAA-CBA-CGA
15	aA	1106	CL7	CHA-CBD-CGD-O2D
15	aA	1106	CL7	CHA-CBD-CGD-O1D
15	aA	1111	CL7	CHA-CBD-CGD-O2D
15	aA	1111	CL7	CHA-CBD-CGD-O1D
15	aA	1113	CL7	CHA-CBD-CGD-O1D
15	aA	1118	CL7	CHA-CBD-CGD-O2D
15	aA	1118	CL7	CHA-CBD-CGD-O1D
15	aA	1120	CL7	CHA-CBD-CGD-O1D
15	aA	1127	CL7	CHA-CBD-CGD-O2D
15	aA	1127	CL7	CHA-CBD-CGD-O1D
15	aA	1134	CL7	CHA-CBD-CGD-O1D
15	aA	1138	CL7	CHA-CBD-CGD-O2D
15	aA	1138	CL7	CHA-CBD-CGD-O1D
15	aB	1201	CL7	CHA-CBD-CGD-O1D
15	aB	1212	CL7	CHA-CBD-CGD-O2D
15	aB	1212	CL7	CHA-CBD-CGD-O1D
15	aB	1221	CL7	CHA-CBD-CGD-O2D
15	aB	1221	CL7	CHA-CBD-CGD-O1D
15	aB	1225	CL7	CHA-CBD-CGD-O1D
15	aI	1601	CL7	CHA-CBD-CGD-O2D
15	aI	1601	CL7	CHA-CBD-CGD-O1D
15	bA	1106	CL7	CHA-CBD-CGD-O2D
15	bA	1106	CL7	CHA-CBD-CGD-O1D
15	bA	1111	CL7	CHA-CBD-CGD-O2D
15	bA	1111	CL7	CHA-CBD-CGD-O1D
15	bA	1113	CL7	CHA-CBD-CGD-O2D
15	bA	1113	CL7	CHA-CBD-CGD-O1D
15	bA	1117	CL7	CHA-CBD-CGD-O2D
15	bA	1117	CL7	CHA-CBD-CGD-O1D
15	bA	1118	CL7	CHA-CBD-CGD-O2D
15	bA	1118	CL7	CHA-CBD-CGD-O1D
15	bA	1120	CL7	CHA-CBD-CGD-O2D
15	bA	1120	CL7	CHA-CBD-CGD-O1D
15	bA	1127	CL7	CHA-CBD-CGD-O2D
15	bA	1127	CL7	CHA-CBD-CGD-O1D
15	bA	1134	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	bA	1134	CL7	CHA-CBD-CGD-O1D
15	bB	1012	CL7	CHA-CBD-CGD-O2D
15	bB	1235	CL7	CHA-CBD-CGD-O1D
15	bI	1601	CL7	CHA-CBD-CGD-O2D
15	bI	1601	CL7	CHA-CBD-CGD-O1D
15	cA	1106	CL7	CHA-CBD-CGD-O2D
15	cA	1106	CL7	CHA-CBD-CGD-O1D
15	cA	1111	CL7	CHA-CBD-CGD-O1D
15	cA	1117	CL7	CHA-CBD-CGD-O2D
15	cA	1118	CL7	CHA-CBD-CGD-O2D
15	cA	1127	CL7	CHA-CBD-CGD-O2D
15	cA	1127	CL7	CHA-CBD-CGD-O1D
15	cA	1134	CL7	CHA-CBD-CGD-O2D
15	cA	1134	CL7	CHA-CBD-CGD-O1D
15	cA	1801	CL7	CHA-CBD-CGD-O2D
15	cA	1138	CL7	CHA-CBD-CGD-O2D
15	cA	1138	CL7	CHA-CBD-CGD-O1D
15	cB	1208	CL7	CHA-CBD-CGD-O2D
15	cB	1212	CL7	CHA-CBD-CGD-O2D
15	cB	1212	CL7	CHA-CBD-CGD-O1D
15	cB	1230	CL7	CHA-CBD-CGD-O1D
15	cB	1241	CL7	CHA-CBD-CGD-O1D
15	cI	1601	CL7	CHA-CBD-CGD-O2D
15	cI	1601	CL7	CHA-CBD-CGD-O1D
15	aB	1224	CL7	O1A-CGA-O2A-C1
18	aA	5001	LHG	O7-C5-C6-O8
18	cA	5001	LHG	O7-C5-C6-O8
14	bA	1013	PHO	C13-C15-C16-C17
15	aA	1107	CL7	O1D-CGD-O2D-CED
15	bA	1117	CL7	C4-C3-C5-C6
15	cA	1109	CL7	C4-C3-C5-C6
15	aB	1223	CL7	C2-C3-C5-C6
15	bA	1112	CL7	CBA-CGA-O2A-C1
15	aA	1136	CL7	C6-C7-C8-C9
15	aB	1203	CL7	C6-C7-C8-C9
15	aL	1501	CL7	C6-C7-C8-C9
15	bA	1123	CL7	C11-C12-C13-C14
15	bB	1237	CL7	C6-C7-C8-C9
15	bB	1221	CL7	C6-C7-C8-C9
15	bB	1238	CL7	C14-C13-C15-C16
15	cB	1237	CL7	C11-C10-C8-C9
15	cB	1208	CL7	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	cA	1013	PHO	O1D-CGD-O2D-CED
15	aB	1229	CL7	C2C-C3C-CAC-CBC
15	bB	1225	CL7	C16-C17-C18-C19
15	cB	1239	CL7	C16-C17-C18-C19
19	bB	5002	LMG	C22-C23-C24-C25
15	aB	1223	CL7	C2A-CAA-CBA-CGA
15	aL	1502	CL7	C2A-CAA-CBA-CGA
15	bB	1222	CL7	C2A-CAA-CBA-CGA
15	cI	1601	CL7	C2A-CAA-CBA-CGA
13	bA	1011	G9R	CBD-CGD-O2D-CED
15	cB	1204	CL7	O1A-CGA-O2A-C1
15	cA	1127	CL7	C3-C5-C6-C7
15	aA	1123	CL7	C1A-C2A-CAA-CBA
15	aB	1225	CL7	C1A-C2A-CAA-CBA
15	bA	1117	CL7	C1A-C2A-CAA-CBA
15	bA	1123	CL7	C1A-C2A-CAA-CBA
15	bB	1225	CL7	C1A-C2A-CAA-CBA
15	cA	1123	CL7	C1A-C2A-CAA-CBA
15	cB	1225	CL7	C1A-C2A-CAA-CBA
15	aB	1205	CL7	C16-C17-C18-C20
15	aB	1226	CL7	C16-C17-C18-C19
15	bB	1226	CL7	C16-C17-C18-C19
15	cB	1205	CL7	C16-C17-C18-C20
15	cB	1225	CL7	C2-C1-O2A-CGA
15	aA	1105	CL7	O1D-CGD-O2D-CED
15	bB	1239	CL7	O1D-CGD-O2D-CED
15	bB	1229	CL7	C2C-C3C-CAC-CBC
15	cB	1239	CL7	C8-C10-C11-C12
15	aB	1210	CL7	C3-C5-C6-C7
15	bI	1601	CL7	O1D-CGD-O2D-CED
18	aA	5003	LHG	C11-C12-C13-C14
18	aA	5003	LHG	C3-O3-P-O5
18	bA	5001	LHG	C3-O3-P-O4
18	bA	5003	LHG	C3-O3-P-O5
18	cA	5003	LHG	C3-O3-P-O5
15	aA	1128	CL7	C16-C17-C18-C20
15	bB	1205	CL7	C16-C17-C18-C20
15	bB	1225	CL7	C16-C17-C18-C20
15	cA	1119	CL7	C6-C7-C8-C10
15	cB	1202	CL7	C16-C17-C18-C19
15	cB	1203	CL7	C16-C17-C18-C19
15	cL	1502	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	bB	1204	CL7	CBA-CGA-O2A-C1
15	cA	1109	CL7	CBA-CGA-O2A-C1
15	bB	1215	CL7	CBD-CGD-O2D-CED
18	cA	5001	LHG	O6-C4-C5-C6
15	bA	1119	CL7	C2A-CAA-CBA-CGA
15	cA	1118	CL7	O1D-CGD-O2D-CED
18	bA	5003	LHG	C13-C14-C15-C16
18	bA	5001	LHG	C13-C14-C15-C16
15	aA	1103	CL7	CAD-CBD-CGD-O1D
15	aA	1108	CL7	C2-C3-C5-C6
15	aA	1111	CL7	CAD-CBD-CGD-O1D
15	aA	1113	CL7	CAD-CBD-CGD-O1D
15	aA	1130	CL7	C2-C3-C5-C6
15	aA	1801	CL7	CAD-CBD-CGD-O1D
15	aB	1209	CL7	CAD-CBD-CGD-O1D
15	aI	1601	CL7	CAD-CBD-CGD-O1D
15	aJ	1301	CL7	CAD-CBD-CGD-O1D
15	bA	1111	CL7	CAD-CBD-CGD-O1D
15	bA	1113	CL7	CAD-CBD-CGD-O1D
15	bA	1130	CL7	C2-C3-C5-C6
15	bA	1801	CL7	CAD-CBD-CGD-O1D
15	bB	1209	CL7	CAD-CBD-CGD-O1D
15	bI	1601	CL7	CAD-CBD-CGD-O1D
15	bJ	1301	CL7	CAD-CBD-CGD-O1D
15	cA	1130	CL7	C2-C3-C5-C6
15	cA	1801	CL7	CAD-CBD-CGD-O1D
15	cB	1209	CL7	CAD-CBD-CGD-O1D
15	cB	1219	CL7	CAD-CBD-CGD-O1D
15	cI	1601	CL7	CAD-CBD-CGD-O1D
15	cJ	1301	CL7	CAD-CBD-CGD-O1D
15	aB	1215	CL7	C5-C6-C7-C8
19	aB	5002	LMG	C17-C18-C19-C20
15	bA	1112	CL7	O1A-CGA-O2A-C1
15	bA	1116	CL7	C8-C10-C11-C12
15	cA	1117	CL7	C8-C10-C11-C12
15	aA	1132	CL7	CBA-CGA-O2A-C1
15	aB	1204	CL7	CBA-CGA-O2A-C1
18	aA	5003	LHG	C1-C2-C3-O3
15	aA	1128	CL7	C11-C10-C8-C7
15	aA	1131	CL7	C11-C12-C13-C15
15	aA	1136	CL7	C6-C7-C8-C10
15	aA	1136	CL7	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	aA	1138	CL7	C11-C10-C8-C7
15	aA	1140	CL7	C11-C10-C8-C7
15	aB	1237	CL7	C11-C10-C8-C7
15	aB	1203	CL7	C6-C7-C8-C10
15	aB	1224	CL7	C6-C7-C8-C10
15	aI	1601	CL7	C11-C10-C8-C7
15	aI	1601	CL7	C12-C13-C15-C16
15	aL	1502	CL7	C11-C10-C8-C7
15	aL	1502	CL7	C12-C13-C15-C16
15	bA	1112	CL7	C11-C12-C13-C15
15	bA	1131	CL7	C11-C12-C13-C15
15	bA	1132	CL7	C12-C13-C15-C16
15	bB	1204	CL7	C12-C13-C15-C16
15	bB	1224	CL7	C6-C7-C8-C10
15	bB	1225	CL7	C6-C7-C8-C10
15	bI	1601	CL7	C12-C13-C15-C16
15	bL	1502	CL7	C12-C13-C15-C16
15	cA	1104	CL7	C11-C12-C13-C15
15	cA	1109	CL7	C11-C10-C8-C7
15	cA	1117	CL7	C12-C13-C15-C16
15	cA	1127	CL7	C11-C12-C13-C15
15	cA	1131	CL7	C11-C12-C13-C15
15	cA	1136	CL7	C6-C7-C8-C10
15	cA	1140	CL7	C11-C10-C8-C7
15	cB	1237	CL7	C11-C10-C8-C7
15	cB	1204	CL7	C12-C13-C15-C16
15	cB	1224	CL7	C6-C7-C8-C10
15	cB	1225	CL7	C6-C7-C8-C10
15	cI	1601	CL7	C12-C13-C15-C16
17	aA	4008	A1JPJ	C23-C24-C25-C26
17	bA	4008	A1JPJ	C23-C24-C25-C26
17	bL	4023	A1JPJ	C23-C24-C25-C26
17	cA	4008	A1JPJ	C23-C24-C25-C26
17	cL	4023	A1JPJ	C23-C24-C25-C26
18	cA	5001	LHG	O6-C4-C5-O7
15	cB	1210	CL7	C3-C5-C6-C7
15	bA	1138	CL7	C13-C15-C16-C17
15	bB	1204	CL7	O1A-CGA-O2A-C1
15	aB	1204	CL7	C10-C11-C12-C13
15	aA	1135	CL7	C2A-CAA-CBA-CGA
15	aA	1136	CL7	C2A-CAA-CBA-CGA
15	aB	1211	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	bB	1213	CL7	C2A-CAA-CBA-CGA
15	cA	1136	CL7	C2A-CAA-CBA-CGA
15	cL	1502	CL7	C2A-CAA-CBA-CGA
15	cB	1226	CL7	C16-C17-C18-C19
15	aA	1127	CL7	C3-C5-C6-C7
15	bB	1210	CL7	C3-C5-C6-C7
15	cA	1123	CL7	C10-C11-C12-C13
13	aA	1011	G9R	O1D-CGD-O2D-CED
15	cL	1503	CL7	CAA-CBA-CGA-O2A
15	aB	1224	CL7	C5-C6-C7-C8
15	bB	1224	CL7	C5-C6-C7-C8
16	cB	2002	PQN	C23-C25-C26-C27
19	bB	5002	LMG	C20-C21-C22-C23
15	cA	1138	CL7	O1A-CGA-O2A-C1
15	bB	1012	CL7	C13-C15-C16-C17
15	cB	1208	CL7	C4-C3-C5-C6
15	bA	1117	CL7	C2-C3-C5-C6
15	bB	1223	CL7	C2-C3-C5-C6
13	bA	1011	G9R	CAA-CBA-CGA-O2A
15	aA	1109	CL7	C8-C10-C11-C12
13	bA	1011	G9R	C11-C12-C13-C14
15	aA	1117	CL7	C6-C7-C8-C9
15	aA	1122	CL7	C6-C7-C8-C9
15	aA	1123	CL7	C11-C12-C13-C14
15	aB	1237	CL7	C11-C10-C8-C9
15	aB	1205	CL7	C11-C10-C8-C9
15	bA	1106	CL7	C11-C10-C8-C9
15	bA	1117	CL7	C6-C7-C8-C9
15	bA	1122	CL7	C6-C7-C8-C9
15	bA	1136	CL7	C6-C7-C8-C9
15	bB	1237	CL7	C11-C10-C8-C9
15	bB	1203	CL7	C6-C7-C8-C9
15	bL	1502	CL7	C11-C10-C8-C9
15	cA	1116	CL7	C6-C7-C8-C9
15	cA	1122	CL7	C6-C7-C8-C9
15	cB	1203	CL7	C6-C7-C8-C9
15	aA	1132	CL7	O1A-CGA-O2A-C1
15	bB	1231	CL7	CBD-CGD-O2D-CED
15	cA	1109	CL7	O1A-CGA-O2A-C1
15	cA	1109	CL7	C8-C10-C11-C12
17	aB	4010	A1JPJ	C10-C11-C12-C13
17	bB	4010	A1JPJ	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	cB	4010	A1JPJ	C10-C11-C12-C13
15	aA	1123	CL7	C13-C15-C16-C17
15	aB	1204	CL7	O1A-CGA-O2A-C1
19	cB	5002	LMG	C15-C16-C17-C18
15	aA	1126	CL7	C2B-C3B-CAB-OBB
15	bA	1127	CL7	C2B-C3B-CAB-OBB
15	cA	1108	CL7	C2B-C3B-CAB-OBB
15	cA	1126	CL7	C2B-C3B-CAB-OBB
15	cB	1207	CL7	C2B-C3B-CAB-OBB
15	cB	1225	CL7	C2B-C3B-CAB-OBB
15	cB	1239	CL7	C16-C17-C18-C20
15	bB	1214	CL7	O1D-CGD-O2D-CED
15	aI	1601	CL7	CAA-CBA-CGA-O2A
15	cA	1140	CL7	CAA-CBA-CGA-O2A
15	bA	1102	CL7	C2-C3-C5-C6
15	aB	1205	CL7	C13-C15-C16-C17
15	aB	1229	CL7	C15-C16-C17-C18
15	bA	1140	CL7	C5-C6-C7-C8
16	bB	2002	PQN	C20-C21-C22-C23
16	cB	2002	PQN	C15-C16-C17-C18
15	bA	1119	CL7	C6-C7-C8-C10
15	bB	1226	CL7	C16-C17-C18-C20
15	aA	1102	CL7	C4B-C3B-CAB-OBB
15	aA	1104	CL7	C4B-C3B-CAB-OBB
15	aA	1105	CL7	C4B-C3B-CAB-OBB
15	aA	1108	CL7	C4B-C3B-CAB-OBB
15	aA	1110	CL7	C4B-C3B-CAB-OBB
15	aA	1113	CL7	C4B-C3B-CAB-OBB
15	aA	1115	CL7	C4B-C3B-CAB-OBB
15	aA	1118	CL7	C4B-C3B-CAB-OBB
15	aA	1119	CL7	C4B-C3B-CAB-OBB
15	aA	1123	CL7	C4B-C3B-CAB-OBB
15	aA	1126	CL7	C4B-C3B-CAB-OBB
15	aA	1130	CL7	C4B-C3B-CAB-OBB
15	aA	1131	CL7	C4B-C3B-CAB-OBB
15	aA	1134	CL7	C4B-C3B-CAB-OBB
15	aA	1136	CL7	C4B-C3B-CAB-OBB
15	aA	1137	CL7	C4B-C3B-CAB-OBB
15	aA	1138	CL7	C4B-C3B-CAB-OBB
15	aA	1801	CL7	C4B-C3B-CAB-OBB
15	aA	1139	CL7	C4B-C3B-CAB-OBB
15	aB	1234	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
15	aB	1236	CL7	C4B-C3B-CAB-OBB
15	aB	1238	CL7	C4B-C3B-CAB-OBB
15	aB	1021	CL7	C4B-C3B-CAB-OBB
15	aB	1202	CL7	C4B-C3B-CAB-OBB
15	aB	1213	CL7	C4B-C3B-CAB-OBB
15	aB	1215	CL7	C4B-C3B-CAB-OBB
15	aB	1220	CL7	C4B-C3B-CAB-OBB
15	aB	1222	CL7	C4B-C3B-CAB-OBB
15	aB	1223	CL7	C4B-C3B-CAB-OBB
15	aB	1227	CL7	C4B-C3B-CAB-OBB
15	aK	1401	CL7	C4B-C3B-CAB-OBB
15	aL	1503	CL7	C4B-C3B-CAB-OBB
15	bA	1022	CL7	C4B-C3B-CAB-OBB
15	bA	1102	CL7	C4B-C3B-CAB-OBB
15	bA	1105	CL7	C4B-C3B-CAB-OBB
15	bA	1108	CL7	C4B-C3B-CAB-OBB
15	bA	1110	CL7	C4B-C3B-CAB-OBB
15	bA	1113	CL7	C4B-C3B-CAB-OBB
15	bA	1118	CL7	C4B-C3B-CAB-OBB
15	bA	1119	CL7	C4B-C3B-CAB-OBB
15	bA	1127	CL7	C4B-C3B-CAB-OBB
15	bA	1130	CL7	C4B-C3B-CAB-OBB
15	bA	1131	CL7	C4B-C3B-CAB-OBB
15	bA	1134	CL7	C4B-C3B-CAB-OBB
15	bA	1137	CL7	C4B-C3B-CAB-OBB
15	bA	1138	CL7	C4B-C3B-CAB-OBB
15	bA	1139	CL7	C4B-C3B-CAB-OBB
15	bA	1801	CL7	C4B-C3B-CAB-OBB
15	bB	1207	CL7	C4B-C3B-CAB-OBB
15	bB	1213	CL7	C4B-C3B-CAB-OBB
15	bB	1220	CL7	C4B-C3B-CAB-OBB
15	bB	1222	CL7	C4B-C3B-CAB-OBB
15	bB	1223	CL7	C4B-C3B-CAB-OBB
15	bB	1233	CL7	C4B-C3B-CAB-OBB
15	bB	1236	CL7	C4B-C3B-CAB-OBB
15	bF	1701	CL7	C4B-C3B-CAB-OBB
15	bI	1601	CL7	C4B-C3B-CAB-OBB
15	bK	1401	CL7	C4B-C3B-CAB-OBB
15	bK	1402	CL7	C4B-C3B-CAB-OBB
15	bL	1503	CL7	C4B-C3B-CAB-OBB
15	cA	1102	CL7	C4B-C3B-CAB-OBB
15	cA	1108	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
15	cA	1110	CL7	C4B-C3B-CAB-OBB
15	cA	1113	CL7	C4B-C3B-CAB-OBB
15	cA	1115	CL7	C4B-C3B-CAB-OBB
15	cA	1118	CL7	C4B-C3B-CAB-OBB
15	cA	1119	CL7	C4B-C3B-CAB-OBB
15	cA	1122	CL7	C4B-C3B-CAB-OBB
15	cA	1123	CL7	C4B-C3B-CAB-OBB
15	cA	1125	CL7	C4B-C3B-CAB-OBB
15	cA	1126	CL7	C4B-C3B-CAB-OBB
15	cA	1129	CL7	C4B-C3B-CAB-OBB
15	cA	1130	CL7	C4B-C3B-CAB-OBB
15	cA	1131	CL7	C4B-C3B-CAB-OBB
15	cA	1134	CL7	C4B-C3B-CAB-OBB
15	cA	1136	CL7	C4B-C3B-CAB-OBB
15	cA	1137	CL7	C4B-C3B-CAB-OBB
15	cA	1138	CL7	C4B-C3B-CAB-OBB
15	cA	1139	CL7	C4B-C3B-CAB-OBB
15	cB	1021	CL7	C4B-C3B-CAB-OBB
15	cB	1202	CL7	C4B-C3B-CAB-OBB
15	cB	1207	CL7	C4B-C3B-CAB-OBB
15	cB	1208	CL7	C4B-C3B-CAB-OBB
15	cB	1209	CL7	C4B-C3B-CAB-OBB
15	cB	1213	CL7	C4B-C3B-CAB-OBB
15	cB	1218	CL7	C4B-C3B-CAB-OBB
15	cB	1220	CL7	C4B-C3B-CAB-OBB
15	cB	1222	CL7	C4B-C3B-CAB-OBB
15	cB	1223	CL7	C4B-C3B-CAB-OBB
15	cB	1225	CL7	C4B-C3B-CAB-OBB
15	cB	1233	CL7	C4B-C3B-CAB-OBB
15	cB	1234	CL7	C4B-C3B-CAB-OBB
15	cF	1701	CL7	C4B-C3B-CAB-OBB
15	cK	1401	CL7	C4B-C3B-CAB-OBB
15	cK	1402	CL7	C4B-C3B-CAB-OBB
15	bL	1503	CL7	CAA-CBA-CGA-O2A
16	bB	2002	PQN	C23-C25-C26-C27
15	aA	1117	CL7	C2A-CAA-CBA-CGA
15	aI	1601	CL7	C2A-CAA-CBA-CGA
15	bA	1136	CL7	C2A-CAA-CBA-CGA
15	bB	1223	CL7	C2A-CAA-CBA-CGA
15	bB	1224	CL7	C2A-CAA-CBA-CGA
15	bB	1227	CL7	C2A-CAA-CBA-CGA
15	cA	1117	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	cB	1222	CL7	C2A-CAA-CBA-CGA
15	cA	1136	CL7	O1D-CGD-O2D-CED
15	aA	1102	CL7	C2-C1-O2A-CGA
15	aA	1129	CL7	C2-C1-O2A-CGA
15	aB	1235	CL7	C2-C1-O2A-CGA
15	aL	1503	CL7	C2-C1-O2A-CGA
15	bA	1136	CL7	C2-C1-O2A-CGA
15	bB	1202	CL7	C2-C1-O2A-CGA
15	bB	1225	CL7	C2-C1-O2A-CGA
15	cA	1129	CL7	C2-C1-O2A-CGA
15	cB	1235	CL7	C2-C1-O2A-CGA
15	aA	1112	CL7	O1A-CGA-O2A-C1
15	bA	1126	CL7	O1A-CGA-O2A-C1
15	cA	1138	CL7	CBA-CGA-O2A-C1
18	bA	5001	LHG	O6-C4-C5-O7
15	aL	1503	CL7	CAA-CBA-CGA-O2A
15	aA	1118	CL7	C6-C7-C8-C9
16	cB	2002	PQN	C20-C21-C22-C23
15	bB	1215	CL7	O1D-CGD-O2D-CED
15	bB	1235	CL7	C3-C5-C6-C7
15	bB	1201	CL7	C2-C3-C5-C6
15	aA	1112	CL7	CBA-CGA-O2A-C1
15	bA	1126	CL7	CBA-CGA-O2A-C1
15	aA	1140	CL7	CAA-CBA-CGA-O2A
15	cI	1601	CL7	CAA-CBA-CGA-O2A
19	cB	5002	LMG	C31-C32-C33-C34
15	aB	1226	CL7	C16-C17-C18-C20
15	cB	1202	CL7	C16-C17-C18-C20
15	aB	1222	CL7	C2A-CAA-CBA-CGA
15	cA	1132	CL7	CBA-CGA-O2A-C1
18	aA	5001	LHG	C3-O3-P-O6
18	cA	5001	LHG	C3-O3-P-O6
15	bB	1201	CL7	C6-C7-C8-C9
13	aA	1011	G9R	CHA-CBD-CGD-O1D
13	aA	1011	G9R	CHA-CBD-CGD-O2D
13	bA	1011	G9R	CHA-CBD-CGD-O1D
13	bA	1011	G9R	CHA-CBD-CGD-O2D
13	cA	1011	G9R	CHA-CBD-CGD-O1D
13	cA	1011	G9R	CHA-CBD-CGD-O2D
14	bA	1013	PHO	CHA-CBD-CGD-O1D
14	bA	1013	PHO	CHA-CBD-CGD-O2D
14	bB	1023	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	bB	1023	PHO	CHA-CBD-CGD-O2D
14	cA	1013	PHO	CHA-CBD-CGD-O1D
14	cA	1013	PHO	CHA-CBD-CGD-O2D
15	aB	1208	CL7	C4-C3-C5-C6
19	aB	5002	LMG	C13-C14-C15-C16
15	aB	1203	CL7	C12-C13-C15-C16
15	aB	1221	CL7	C6-C7-C8-C10
15	aL	1501	CL7	C6-C7-C8-C10
15	bA	1136	CL7	C11-C12-C13-C15
15	bB	1237	CL7	C6-C7-C8-C10
15	bB	1207	CL7	C11-C12-C13-C15
15	bB	1238	CL7	C12-C13-C15-C16
15	cA	1136	CL7	C11-C12-C13-C15
15	cB	1202	CL7	C12-C13-C15-C16
15	cB	1203	CL7	C12-C13-C15-C16
15	cB	1221	CL7	C6-C7-C8-C10
15	aA	1103	CL7	C11-C10-C8-C9
15	aB	1205	CL7	C6-C7-C8-C9
15	aI	1601	CL7	C14-C13-C15-C16
15	aL	1502	CL7	C11-C10-C8-C9
15	cA	1106	CL7	C11-C10-C8-C9
15	cA	1117	CL7	C6-C7-C8-C9
15	cA	1131	CL7	C11-C12-C13-C14
15	cB	1224	CL7	C6-C7-C8-C9
15	cI	1601	CL7	C14-C13-C15-C16
15	cL	1502	CL7	C11-C10-C8-C9
15	bA	1106	CL7	C16-C17-C18-C20
15	bB	1205	CL7	C13-C15-C16-C17
19	aB	5002	LMG	O6-C5-C6-O5
15	cA	1119	CL7	C6-C7-C8-C9
15	cL	1502	CL7	C16-C17-C18-C19
15	aB	1021	CL7	C15-C16-C17-C18
15	aB	1223	CL7	C8-C10-C11-C12
13	bA	1011	G9R	O1D-CGD-O2D-CED
15	bB	1231	CL7	O1D-CGD-O2D-CED
15	bA	1140	CL7	CAA-CBA-CGA-O2A
15	cB	1235	CL7	C2-C3-C5-C6
15	cA	1132	CL7	O1A-CGA-O2A-C1
15	cA	1114	CL7	CBD-CGD-O2D-CED
15	aB	1202	CL7	C13-C15-C16-C17
15	aA	1127	CL7	O1D-CGD-O2D-CED
15	cA	1137	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	bB	1237	CL7	C8-C10-C11-C12
19	cB	5002	LMG	C20-C21-C22-C23
15	cA	1103	CL7	CAA-CBA-CGA-O2A
15	aA	1117	CL7	C4-C3-C5-C6
15	cA	1131	CL7	C4-C3-C5-C6
15	aK	1401	CL7	CAA-CBA-CGA-O2A
15	aA	1117	CL7	C2-C3-C5-C6
15	cA	1131	CL7	C2-C3-C5-C6
15	bA	1127	CL7	C8-C10-C11-C12
18	cA	5001	LHG	C32-C33-C34-C35
15	bA	1103	CL7	CAA-CBA-CGA-O2A
15	aA	1112	CL7	C2-C1-O2A-CGA
15	bB	1239	CL7	C2-C1-O2A-CGA
15	bL	1503	CL7	C2-C1-O2A-CGA
15	cL	1503	CL7	C2-C1-O2A-CGA
15	aB	1229	CL7	C10-C11-C12-C13
15	bA	1123	CL7	C13-C15-C16-C17
15	aB	1215	CL7	C2A-CAA-CBA-CGA
15	bB	1215	CL7	C2A-CAA-CBA-CGA
15	cB	1215	CL7	C2A-CAA-CBA-CGA
15	cB	1220	CL7	C2A-CAA-CBA-CGA
15	cB	1224	CL7	C2A-CAA-CBA-CGA
15	cB	1229	CL7	C10-C11-C12-C13
15	cA	1137	CL7	CBD-CGD-O2D-CED
15	aA	1022	CL7	C3A-C2A-CAA-CBA
19	bB	5002	LMG	C13-C14-C15-C16
15	aB	1202	CL7	C8-C10-C11-C12
15	bA	1107	CL7	CAA-CBA-CGA-O1A
15	cB	1241	CL7	O1D-CGD-O2D-CED
14	aB	1023	PHO	C11-C12-C13-C14
14	bB	1023	PHO	C11-C12-C13-C14
14	cB	1023	PHO	C11-C12-C13-C14
15	aA	1122	CL7	C11-C10-C8-C9
15	aA	1131	CL7	C11-C12-C13-C14
15	aB	1202	CL7	C11-C10-C8-C9
15	bA	1116	CL7	C6-C7-C8-C9
15	bA	1140	CL7	C6-C7-C8-C9
15	cA	1112	CL7	C14-C13-C15-C16
15	cA	1136	CL7	C6-C7-C8-C9
15	cB	1202	CL7	C11-C12-C13-C14
15	bA	1119	CL7	C6-C7-C8-C9
15	cA	1106	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	cB	1226	CL7	C16-C17-C18-C20
15	aA	1107	CL7	CAA-CBA-CGA-O1A
15	cA	1107	CL7	CAA-CBA-CGA-O2A
15	bA	1132	CL7	C5-C6-C7-C8
16	aB	2002	PQN	C20-C21-C22-C23
19	cB	5002	LMG	C13-C14-C15-C16
17	aA	4011	A1JPJ	C11-C10-C9-C34
17	aA	4011	A1JPJ	C16-C17-C18-C36
17	aB	4005	A1JPJ	C11-C10-C9-C34
17	aB	4006	A1JPJ	C11-C10-C9-C34
17	aB	4010	A1JPJ	C11-C10-C9-C34
17	aF	4016	A1JPJ	C35-C13-C14-C15
17	aL	4020	A1JPJ	C11-C10-C9-C34
17	bA	4011	A1JPJ	C11-C10-C9-C34
17	bA	4011	A1JPJ	C16-C17-C18-C36
17	bB	4005	A1JPJ	C11-C10-C9-C34
17	bB	4006	A1JPJ	C11-C10-C9-C34
17	bB	4010	A1JPJ	C11-C10-C9-C34
17	bF	4016	A1JPJ	C35-C13-C14-C15
17	cA	4011	A1JPJ	C11-C10-C9-C34
17	cA	4011	A1JPJ	C16-C17-C18-C36
17	cB	4005	A1JPJ	C11-C10-C9-C34
17	cB	4006	A1JPJ	C11-C10-C9-C34
17	cB	4010	A1JPJ	C11-C10-C9-C34
17	cF	4016	A1JPJ	C35-C13-C14-C15
17	cL	4020	A1JPJ	C11-C10-C9-C34
13	aA	1011	G9R	C3-C5-C6-C7
15	aA	1103	CL7	CAA-CBA-CGA-O2A
15	aB	1241	CL7	CAA-CBA-CGA-O1A
15	aA	1139	CL7	C2A-CAA-CBA-CGA
15	bA	1106	CL7	C2A-CAA-CBA-CGA
15	bB	1211	CL7	C2A-CAA-CBA-CGA
15	cA	1135	CL7	C2A-CAA-CBA-CGA
15	cA	1139	CL7	C2A-CAA-CBA-CGA
15	cB	1228	CL7	C2A-CAA-CBA-CGA
15	bA	1118	CL7	C6-C7-C8-C9
15	bK	1401	CL7	CAA-CBA-CGA-O1A
15	cA	1107	CL7	CAA-CBA-CGA-O1A
16	bB	2002	PQN	C15-C16-C17-C18
16	aB	2002	PQN	C15-C16-C17-C18
15	cA	1127	CL7	C4-C3-C5-C6
15	cA	1132	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	aA	1022	CL7	C1A-C2A-CAA-CBA
15	aA	1111	CL7	C1A-C2A-CAA-CBA
15	aA	1112	CL7	C1A-C2A-CAA-CBA
15	aB	1206	CL7	C1A-C2A-CAA-CBA
15	aB	1208	CL7	C1A-C2A-CAA-CBA
15	bA	1022	CL7	C1A-C2A-CAA-CBA
15	bA	1133	CL7	C1A-C2A-CAA-CBA
15	bB	1208	CL7	C1A-C2A-CAA-CBA
15	bJ	1302	CL7	C1A-C2A-CAA-CBA
15	cA	1022	CL7	C1A-C2A-CAA-CBA
15	cB	1208	CL7	C1A-C2A-CAA-CBA
13	bA	1011	G9R	C11-C12-C13-C15
15	aA	1104	CL7	C11-C12-C13-C15
15	aA	1117	CL7	C12-C13-C15-C16
15	aB	1207	CL7	C12-C13-C15-C16
15	aB	1208	CL7	C12-C13-C15-C16
15	aB	1210	CL7	C6-C7-C8-C10
15	bA	1104	CL7	C11-C12-C13-C15
15	bA	1133	CL7	C11-C10-C8-C7
15	bB	1208	CL7	C12-C13-C15-C16
15	bB	1210	CL7	C11-C10-C8-C7
15	cA	1112	CL7	C11-C12-C13-C15
15	cA	1138	CL7	C11-C10-C8-C7
15	cB	1012	CL7	C12-C13-C15-C16
15	cB	1208	CL7	C2-C3-C5-C6
15	cB	1239	CL7	C6-C7-C8-C10
15	cI	1601	CL7	C11-C10-C8-C7
15	cB	1241	CL7	CAA-CBA-CGA-O1A
15	bA	1107	CL7	CAA-CBA-CGA-O2A
15	bA	1110	CL7	CAA-CBA-CGA-O2A
15	bB	1236	CL7	CAA-CBA-CGA-O1A
15	bK	1401	CL7	CAA-CBA-CGA-O2A
15	cA	1116	CL7	C2C-C3C-CAC-CBC
15	cB	1225	CL7	C16-C17-C18-C19
15	aB	1224	CL7	C2A-CAA-CBA-CGA
15	aB	1012	CL7	C13-C15-C16-C17
15	cA	1111	CL7	C5-C6-C7-C8
16	aB	2002	PQN	C25-C26-C27-C28
15	bB	1241	CL7	CAA-CBA-CGA-O1A
15	cA	1139	CL7	CAA-CBA-CGA-O2A
15	cB	1236	CL7	CAA-CBA-CGA-O2A
15	bA	1127	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	aA	5001	LHG	O6-C4-C5-C6
15	cA	1114	CL7	O1D-CGD-O2D-CED
15	aB	1209	CL7	CAA-CBA-CGA-O1A
15	bA	1110	CL7	CAA-CBA-CGA-O1A
15	aB	1205	CL7	C5-C6-C7-C8
15	cB	1241	CL7	CBD-CGD-O2D-CED
15	cA	1132	CL7	C2-C3-C5-C6
15	aB	1236	CL7	CAA-CBA-CGA-O1A
15	aB	1236	CL7	CAA-CBA-CGA-O2A
15	cA	1139	CL7	CAA-CBA-CGA-O1A
15	cB	1209	CL7	CAA-CBA-CGA-O1A
15	cB	1209	CL7	CAA-CBA-CGA-O2A
15	aB	1207	CL7	C8-C10-C11-C12
15	bB	1211	CL7	CBD-CGD-O2D-CED
17	aA	4011	A1JPJ	C16-C17-C18-C19
17	aB	4005	A1JPJ	C11-C10-C9-C8
17	aB	4006	A1JPJ	C11-C10-C9-C8
17	aB	4006	A1JPJ	C20-C21-C22-C23
17	aB	4010	A1JPJ	C11-C10-C9-C8
17	aF	4016	A1JPJ	C12-C13-C14-C15
17	bA	4011	A1JPJ	C16-C17-C18-C19
17	bB	4005	A1JPJ	C11-C10-C9-C8
17	bB	4006	A1JPJ	C11-C10-C9-C8
17	bB	4006	A1JPJ	C20-C21-C22-C23
17	bB	4010	A1JPJ	C11-C10-C9-C8
17	bF	4016	A1JPJ	C12-C13-C14-C15
17	cA	4011	A1JPJ	C16-C17-C18-C19
17	cB	4005	A1JPJ	C11-C10-C9-C8
17	cB	4006	A1JPJ	C11-C10-C9-C8
17	cB	4006	A1JPJ	C20-C21-C22-C23
17	cB	4010	A1JPJ	C11-C10-C9-C8
17	cF	4016	A1JPJ	C12-C13-C14-C15
15	aA	1110	CL7	CAA-CBA-CGA-O1A
15	aA	1110	CL7	CAA-CBA-CGA-O2A
15	cB	1236	CL7	CAA-CBA-CGA-O1A
15	cB	1215	CL7	CBA-CGA-O2A-C1
19	bB	5002	LMG	C32-C33-C34-C35
15	aA	1128	CL7	C5-C6-C7-C8
15	aB	1209	CL7	CAA-CBA-CGA-O2A
15	bB	1236	CL7	CAA-CBA-CGA-O2A
15	bB	1201	CL7	O1D-CGD-O2D-CED
15	cA	1123	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	cB	1215	CL7	O1A-CGA-O2A-C1
15	aK	1401	CL7	CAA-CBA-CGA-O1A
15	bB	1209	CL7	CAA-CBA-CGA-O1A
15	cA	1110	CL7	CAA-CBA-CGA-O1A
15	cK	1401	CL7	CAA-CBA-CGA-O2A
15	aA	1137	CL7	C4-C3-C5-C6
15	aB	1210	CL7	C4-C3-C5-C6
15	cA	1102	CL7	C4-C3-C5-C6
15	cA	1137	CL7	C4-C3-C5-C6
15	aA	1111	CL7	C2-C1-O2A-CGA
15	aA	1123	CL7	C2-C1-O2A-CGA
15	aB	1224	CL7	C2-C1-O2A-CGA
15	bA	1123	CL7	C2-C1-O2A-CGA
15	cA	1123	CL7	C2-C1-O2A-CGA
15	cB	1224	CL7	C2-C1-O2A-CGA
15	cA	1123	CL7	C13-C15-C16-C17
15	aA	1107	CL7	CAA-CBA-CGA-O2A
15	aB	1241	CL7	CAA-CBA-CGA-O2A
15	cA	1105	CL7	CAA-CBA-CGA-O2A
15	aI	1601	CL7	C11-C10-C8-C9
15	bA	1122	CL7	C11-C10-C8-C9
15	cA	1103	CL7	C11-C10-C8-C9
15	bA	1139	CL7	CAA-CBA-CGA-O2A
15	cA	1110	CL7	CAA-CBA-CGA-O2A
15	cB	1241	CL7	CAA-CBA-CGA-O2A
15	bB	1021	CL7	C15-C16-C17-C18
15	bA	1130	CL7	C4-C3-C5-C6
15	cA	1130	CL7	C4-C3-C5-C6
18	cA	5001	LHG	C13-C14-C15-C16
15	aB	1239	CL7	C10-C11-C12-C13
15	aB	1210	CL7	C2A-CAA-CBA-CGA
15	aB	1220	CL7	C2A-CAA-CBA-CGA
15	aB	1228	CL7	C2A-CAA-CBA-CGA
15	bB	1220	CL7	C2A-CAA-CBA-CGA
15	cA	1114	CL7	CAA-CBA-CGA-O2A
17	bA	4008	A1JPJ	C5-C6-C7-C8
15	aA	1114	CL7	CAA-CBA-CGA-O2A
15	bB	1237	CL7	C5-C6-C7-C8
15	bB	1021	CL7	C4-C3-C5-C6
15	cB	1201	CL7	C4-C3-C5-C6
15	cB	1225	CL7	C16-C17-C18-C20
15	aA	1138	CL7	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	aB	1208	CL7	C2-C3-C5-C6
15	aB	1211	CL7	C2-C3-C5-C6
15	cB	1211	CL7	C2-C3-C5-C6
15	bA	1114	CL7	CAA-CBA-CGA-O2A
15	bB	1241	CL7	CAA-CBA-CGA-O2A
15	bA	1116	CL7	C5-C6-C7-C8
15	aA	1118	CL7	O1D-CGD-O2D-CED
15	aA	1139	CL7	CAA-CBA-CGA-O2A
15	bB	1209	CL7	CAA-CBA-CGA-O2A
15	bB	1222	CL7	CAA-CBA-CGA-O2A
15	bB	1227	CL7	CAA-CBA-CGA-O2A
15	cK	1401	CL7	CAA-CBA-CGA-O1A
15	aA	1139	CL7	CAA-CBA-CGA-O1A
15	aB	1201	CL7	C2A-CAA-CBA-CGA
15	aK	1401	CL7	C2A-CAA-CBA-CGA
15	bA	1139	CL7	C2A-CAA-CBA-CGA
15	bB	1228	CL7	C2A-CAA-CBA-CGA
15	cA	1129	CL7	C2A-CAA-CBA-CGA
15	cB	1201	CL7	C6-C7-C8-C9
15	aB	1227	CL7	CAA-CBA-CGA-O2A
15	bA	1139	CL7	CAA-CBA-CGA-O1A
15	bB	1227	CL7	CAA-CBA-CGA-O1A
15	cB	1227	CL7	CAA-CBA-CGA-O2A
15	bB	1229	CL7	C15-C16-C17-C18
15	cB	1202	CL7	C10-C11-C12-C13
18	bA	5001	LHG	O6-C4-C5-C6
15	bA	1137	CL7	C4-C3-C5-C6
15	bB	1229	CL7	C4-C3-C5-C6
15	cA	1118	CL7	C4-C3-C5-C6
15	cB	1210	CL7	C4-C3-C5-C6
15	aB	1012	CL7	C12-C13-C15-C16
15	aB	1202	CL7	C12-C13-C15-C16
15	bA	1104	CL7	C12-C13-C15-C16
15	bA	1117	CL7	C12-C13-C15-C16
15	bA	1138	CL7	C11-C10-C8-C7
15	bA	1140	CL7	C11-C10-C8-C7
15	bB	1202	CL7	C12-C13-C15-C16
15	cB	1201	CL7	CBA-CGA-O2A-C1
15	aB	1208	CL7	C10-C11-C12-C13
15	cB	1012	CL7	C13-C15-C16-C17
18	cA	5001	LHG	C34-C35-C36-C37
15	aB	1215	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	aA	1118	CL7	C2B-C3B-CAB-OBB
15	aA	1123	CL7	C2B-C3B-CAB-OBB
15	aA	1130	CL7	C2B-C3B-CAB-OBB
15	aA	1134	CL7	C2B-C3B-CAB-OBB
15	aA	1136	CL7	C2B-C3B-CAB-OBB
15	aA	1137	CL7	C2B-C3B-CAB-OBB
15	aB	1238	CL7	C2B-C3B-CAB-OBB
15	aB	1021	CL7	C2B-C3B-CAB-OBB
15	aB	1202	CL7	C2B-C3B-CAB-OBB
15	aB	1213	CL7	C2B-C3B-CAB-OBB
15	aB	1215	CL7	C2B-C3B-CAB-OBB
15	aB	1227	CL7	C2B-C3B-CAB-OBB
15	aL	1503	CL7	C2B-C3B-CAB-OBB
15	bA	1108	CL7	C2B-C3B-CAB-OBB
15	bA	1113	CL7	C2B-C3B-CAB-OBB
15	bA	1118	CL7	C2B-C3B-CAB-OBB
15	bA	1134	CL7	C2B-C3B-CAB-OBB
15	bB	1223	CL7	C2B-C3B-CAB-OBB
15	bB	1233	CL7	C2B-C3B-CAB-OBB
15	bB	1236	CL7	C2B-C3B-CAB-OBB
15	bF	1701	CL7	C2B-C3B-CAB-OBB
15	bI	1601	CL7	C2B-C3B-CAB-OBB
15	bK	1402	CL7	C2B-C3B-CAB-OBB
15	bL	1503	CL7	C2B-C3B-CAB-OBB
15	cA	1102	CL7	C2B-C3B-CAB-OBB
15	cA	1113	CL7	C2B-C3B-CAB-OBB
15	cA	1118	CL7	C2B-C3B-CAB-OBB
15	cA	1119	CL7	C2B-C3B-CAB-OBB
15	cA	1122	CL7	C2B-C3B-CAB-OBB
15	cA	1125	CL7	C2B-C3B-CAB-OBB
15	cA	1130	CL7	C2B-C3B-CAB-OBB
15	cA	1131	CL7	C2B-C3B-CAB-OBB
15	cA	1134	CL7	C2B-C3B-CAB-OBB
15	cA	1136	CL7	C2B-C3B-CAB-OBB
15	cA	1138	CL7	C2B-C3B-CAB-OBB
15	cB	1202	CL7	C2B-C3B-CAB-OBB
15	cB	1209	CL7	C2B-C3B-CAB-OBB
15	cB	1213	CL7	C2B-C3B-CAB-OBB
15	cB	1223	CL7	C2B-C3B-CAB-OBB
15	cB	1233	CL7	C2B-C3B-CAB-OBB
15	cK	1401	CL7	C2B-C3B-CAB-OBB
15	cK	1402	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
18	bA	5001	LHG	C32-C33-C34-C35
15	cA	1136	CL7	C3-C5-C6-C7
15	aB	1222	CL7	CAA-CBA-CGA-O2A
15	bA	1134	CL7	CAA-CBA-CGA-O2A
15	cB	1201	CL7	O1A-CGA-O2A-C1
15	bB	1211	CL7	O1D-CGD-O2D-CED
15	bA	1136	CL7	C8-C10-C11-C12
15	aB	1215	CL7	CBA-CGA-O2A-C1
17	aB	4006	A1JPJ	C20-C21-C22-C37
17	bB	4006	A1JPJ	C20-C21-C22-C37
17	bL	4020	A1JPJ	C11-C10-C9-C34
17	cA	4014	A1JPJ	C35-C13-C14-C15
17	cB	4006	A1JPJ	C20-C21-C22-C37
15	bA	1123	CL7	CAA-CBA-CGA-O2A
15	cA	1123	CL7	CAA-CBA-CGA-O2A
15	aA	1127	CL7	C4-C3-C5-C6
15	aA	1133	CL7	C4-C3-C5-C6
15	bA	1109	CL7	C4-C3-C5-C6
15	bB	1210	CL7	C4-C3-C5-C6
15	cB	1211	CL7	C4-C3-C5-C6
15	cA	1134	CL7	CAA-CBA-CGA-O2A
15	cA	1109	CL7	C2-C3-C5-C6
15	aA	1111	CL7	C16-C17-C18-C20
13	aA	1011	G9R	C14-C13-C15-C16
15	aA	1106	CL7	C11-C12-C13-C14
15	aA	1126	CL7	C6-C7-C8-C9
15	aA	1128	CL7	C11-C10-C8-C9
15	aA	1138	CL7	C11-C10-C8-C9
15	aA	1140	CL7	C11-C10-C8-C9
15	aB	1238	CL7	C11-C12-C13-C14
15	aB	1207	CL7	C14-C13-C15-C16
15	aB	1210	CL7	C6-C7-C8-C9
15	aB	1224	CL7	C6-C7-C8-C9
15	aL	1502	CL7	C14-C13-C15-C16
15	bA	1112	CL7	C14-C13-C15-C16
15	bA	1131	CL7	C11-C12-C13-C14
15	bA	1136	CL7	C14-C13-C15-C16
15	bA	1138	CL7	C14-C13-C15-C16
15	bB	1202	CL7	C11-C12-C13-C14
15	bB	1204	CL7	C14-C13-C15-C16
15	bB	1224	CL7	C6-C7-C8-C9
15	bI	1601	CL7	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	bL	1502	CL7	C14-C13-C15-C16
15	cA	1117	CL7	C14-C13-C15-C16
15	cA	1140	CL7	C11-C10-C8-C9
15	cB	1204	CL7	C14-C13-C15-C16
15	cL	1502	CL7	C14-C13-C15-C16
15	bA	1106	CL7	C15-C16-C17-C18
15	cA	1122	CL7	C15-C16-C17-C18
15	aB	1209	CL7	C4B-C3B-CAB-OB
15	aF	1701	CL7	C4B-C3B-CAB-OB
15	bB	1202	CL7	C4B-C3B-CAB-OB
15	bB	1224	CL7	C4B-C3B-CAB-OB
15	aA	1111	CL7	C3A-C2A-CAA-CBA
15	aA	1112	CL7	C3A-C2A-CAA-CBA
15	aB	1228	CL7	C3A-C2A-CAA-CBA
15	bA	1022	CL7	C3A-C2A-CAA-CBA
15	bB	1231	CL7	C3A-C2A-CAA-CBA
15	cB	1231	CL7	C3A-C2A-CAA-CBA
15	aA	1118	CL7	CBD-CGD-O2D-CED
15	bB	1201	CL7	CBD-CGD-O2D-CED
15	aB	1227	CL7	CAA-CBA-CGA-O1A
15	cA	1105	CL7	CAA-CBA-CGA-O1A
15	cB	1227	CL7	CAA-CBA-CGA-O1A
15	aA	1125	CL7	CAD-CBD-CGD-O2D
15	aA	1131	CL7	CAD-CBD-CGD-O2D
15	aA	1135	CL7	CAD-CBD-CGD-O2D
15	aA	1137	CL7	CAD-CBD-CGD-O2D
15	aB	1226	CL7	CAD-CBD-CGD-O2D
15	aL	1501	CL7	CAD-CBD-CGD-O2D
15	bA	1103	CL7	CAD-CBD-CGD-O2D
15	bA	1112	CL7	CAD-CBD-CGD-O2D
15	bA	1123	CL7	CAD-CBD-CGD-O2D
15	bA	1124	CL7	CAD-CBD-CGD-O2D
15	bA	1137	CL7	CAD-CBD-CGD-O2D
15	bA	1138	CL7	CAD-CBD-CGD-O2D
15	bA	1140	CL7	CAD-CBD-CGD-O2D
15	bB	1210	CL7	CAD-CBD-CGD-O2D
15	bB	1211	CL7	CAD-CBD-CGD-O2D
15	bB	1215	CL7	CAD-CBD-CGD-O2D
15	bB	1223	CL7	CAD-CBD-CGD-O2D
15	bB	1226	CL7	CAD-CBD-CGD-O2D
15	bB	1234	CL7	CAD-CBD-CGD-O2D
15	cA	1113	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	cA	1123	CL7	CAD-CBD-CGD-O2D
15	cA	1124	CL7	CAD-CBD-CGD-O2D
15	cA	1128	CL7	CAD-CBD-CGD-O2D
15	cA	1129	CL7	CAD-CBD-CGD-O2D
15	cA	1135	CL7	CAD-CBD-CGD-O2D
15	cA	1139	CL7	CAD-CBD-CGD-O2D
15	cB	1207	CL7	CAD-CBD-CGD-O2D
15	cB	1226	CL7	CAD-CBD-CGD-O2D
15	cB	1230	CL7	CAD-CBD-CGD-O2D
15	cB	1234	CL7	CAD-CBD-CGD-O2D
15	cB	1238	CL7	CAD-CBD-CGD-O2D
15	cL	1501	CL7	CAD-CBD-CGD-O2D
15	aB	1208	CL7	C3-C5-C6-C7
15	aA	1134	CL7	CAA-CBA-CGA-O2A
15	bB	1228	CL7	CAA-CBA-CGA-O2A
15	cB	1222	CL7	CAA-CBA-CGA-O2A
14	bB	1023	PHO	CAA-CBA-CGA-O2A
14	cB	1023	PHO	CAA-CBA-CGA-O2A
15	aB	1021	CL7	CAA-CBA-CGA-O2A
15	bB	1207	CL7	CAA-CBA-CGA-O2A
13	bA	1011	G9R	C8-C10-C11-C12
15	bB	1201	CL7	CBA-CGA-O2A-C1
15	aB	1211	CL7	C4-C3-C5-C6
15	cA	1133	CL7	C4-C3-C5-C6
15	aB	1212	CL7	CAA-CBA-CGA-O2A
15	aB	1228	CL7	CAA-CBA-CGA-O2A
15	bB	1222	CL7	CAA-CBA-CGA-O1A
15	cA	1114	CL7	CAA-CBA-CGA-O1A
15	aB	1210	CL7	C2-C3-C5-C6
15	cB	1203	CL7	CAA-CBA-CGA-O2A
15	aA	1114	CL7	CAA-CBA-CGA-O1A
15	bB	1204	CL7	C2C-C3C-CAC-CBC
15	aA	1136	CL7	C8-C10-C11-C12
15	aB	1223	CL7	C16-C17-C18-C20
15	bA	1114	CL7	CAA-CBA-CGA-O1A
15	cA	1123	CL7	CBD-CGD-O2D-CED
15	aA	1124	CL7	O2A-C1-C2-C3
15	aA	1126	CL7	O2A-C1-C2-C3
15	aB	1202	CL7	O2A-C1-C2-C3
15	aB	1206	CL7	O2A-C1-C2-C3
15	aB	1214	CL7	O2A-C1-C2-C3
15	bB	1202	CL7	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	bB	1206	CL7	O2A-C1-C2-C3
15	bB	1214	CL7	O2A-C1-C2-C3
15	cA	1124	CL7	O2A-C1-C2-C3
15	cA	1126	CL7	O2A-C1-C2-C3
15	aA	1110	CL7	C2A-CAA-CBA-CGA
15	cA	1110	CL7	C2A-CAA-CBA-CGA
15	aB	1221	CL7	CAA-CBA-CGA-O2A
15	bB	1203	CL7	CAA-CBA-CGA-O2A
15	bB	1221	CL7	CAA-CBA-CGA-O2A
15	bA	1138	CL7	C3-C5-C6-C7
15	aB	1222	CL7	CAA-CBA-CGA-O1A
15	bA	1134	CL7	CAA-CBA-CGA-O1A
15	bB	1237	CL7	O1D-CGD-O2D-CED
18	cA	5003	LHG	C1-C2-C3-O3
15	aA	1022	CL7	CHA-CBD-CGD-O2D
15	aA	1022	CL7	CHA-CBD-CGD-O1D
15	aA	1104	CL7	CHA-CBD-CGD-O2D
15	aA	1113	CL7	CHA-CBD-CGD-O2D
15	aA	1129	CL7	CHA-CBD-CGD-O1D
15	aA	1134	CL7	CHA-CBD-CGD-O2D
15	aA	1137	CL7	CHA-CBD-CGD-O1D
15	aB	1232	CL7	CHA-CBD-CGD-O2D
15	aB	1232	CL7	CHA-CBD-CGD-O1D
15	aB	1235	CL7	CHA-CBD-CGD-O2D
15	aB	1235	CL7	CHA-CBD-CGD-O1D
15	aB	1214	CL7	CHA-CBD-CGD-O2D
15	aB	1214	CL7	CHA-CBD-CGD-O1D
15	aB	1217	CL7	CHA-CBD-CGD-O2D
15	aB	1217	CL7	CHA-CBD-CGD-O1D
15	aB	1220	CL7	CHA-CBD-CGD-O2D
15	aB	1220	CL7	CHA-CBD-CGD-O1D
15	aB	1222	CL7	CHA-CBD-CGD-O2D
15	aB	1222	CL7	CHA-CBD-CGD-O1D
15	aB	1224	CL7	CHA-CBD-CGD-O2D
15	aB	1224	CL7	CHA-CBD-CGD-O1D
15	aB	1225	CL7	CHA-CBD-CGD-O2D
15	aB	1228	CL7	CHA-CBD-CGD-O2D
15	aB	1228	CL7	CHA-CBD-CGD-O1D
15	aB	1230	CL7	CHA-CBD-CGD-O2D
15	aB	1230	CL7	CHA-CBD-CGD-O1D
15	bA	1105	CL7	CHA-CBD-CGD-O2D
15	bA	1105	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	bA	1135	CL7	CHA-CBD-CGD-O1D
15	bA	1137	CL7	CHA-CBD-CGD-O1D
15	bB	1237	CL7	CHA-CBD-CGD-O2D
15	bB	1237	CL7	CHA-CBD-CGD-O1D
15	bB	1207	CL7	CHA-CBD-CGD-O1D
15	bB	1212	CL7	CHA-CBD-CGD-O2D
15	bB	1212	CL7	CHA-CBD-CGD-O1D
15	bB	1217	CL7	CHA-CBD-CGD-O2D
15	bB	1218	CL7	CHA-CBD-CGD-O2D
15	bB	1218	CL7	CHA-CBD-CGD-O1D
15	bB	1220	CL7	CHA-CBD-CGD-O2D
15	bB	1220	CL7	CHA-CBD-CGD-O1D
15	bB	1222	CL7	CHA-CBD-CGD-O2D
15	bB	1222	CL7	CHA-CBD-CGD-O1D
15	bB	1224	CL7	CHA-CBD-CGD-O2D
15	bB	1228	CL7	CHA-CBD-CGD-O2D
15	bB	1228	CL7	CHA-CBD-CGD-O1D
15	bB	1232	CL7	CHA-CBD-CGD-O2D
15	bB	1232	CL7	CHA-CBD-CGD-O1D
15	bB	1235	CL7	CHA-CBD-CGD-O2D
15	cA	1022	CL7	CHA-CBD-CGD-O2D
15	cA	1022	CL7	CHA-CBD-CGD-O1D
15	cA	1105	CL7	CHA-CBD-CGD-O2D
15	cA	1105	CL7	CHA-CBD-CGD-O1D
15	cA	1111	CL7	CHA-CBD-CGD-O2D
15	cA	1112	CL7	CHA-CBD-CGD-O1D
15	cA	1126	CL7	CHA-CBD-CGD-O2D
15	cA	1126	CL7	CHA-CBD-CGD-O1D
15	cB	1218	CL7	CHA-CBD-CGD-O1D
15	cB	1224	CL7	CHA-CBD-CGD-O2D
15	cB	1224	CL7	CHA-CBD-CGD-O1D
15	cB	1228	CL7	CHA-CBD-CGD-O2D
15	cB	1228	CL7	CHA-CBD-CGD-O1D
15	cB	1229	CL7	CHA-CBD-CGD-O2D
15	cB	1229	CL7	CHA-CBD-CGD-O1D
15	cB	1232	CL7	CHA-CBD-CGD-O2D
15	cK	1401	CL7	CHA-CBD-CGD-O2D
15	cK	1401	CL7	CHA-CBD-CGD-O1D
15	aA	1105	CL7	CAA-CBA-CGA-O2A
15	aB	1213	CL7	CAA-CBA-CGA-O2A
15	bJ	1302	CL7	CAA-CBA-CGA-O2A
13	bA	1011	G9R	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	aA	4011	A1JPJ	C11-C10-C9-C8
17	bA	4011	A1JPJ	C11-C10-C9-C8
17	cA	4011	A1JPJ	C11-C10-C9-C8
15	aA	1134	CL7	CAA-CBA-CGA-O1A
15	aA	1136	CL7	CAA-CBA-CGA-O2A
15	aB	1203	CL7	CAA-CBA-CGA-O2A
15	bA	1136	CL7	CAA-CBA-CGA-O2A
15	cA	1135	CL7	CAA-CBA-CGA-O2A
15	cB	1207	CL7	CAA-CBA-CGA-O2A
15	cB	1221	CL7	CAA-CBA-CGA-O2A
15	cA	1112	CL7	O1A-CGA-O2A-C1
15	bB	1201	CL7	O1A-CGA-O2A-C1
15	bA	1135	CL7	CAA-CBA-CGA-O2A
15	cA	1136	CL7	CAA-CBA-CGA-O2A
15	aJ	1302	CL7	CAA-CBA-CGA-O2A
15	cB	1228	CL7	CAA-CBA-CGA-O2A
15	cA	1136	CL7	C8-C10-C11-C12
15	aB	1238	CL7	C3-C5-C6-C7
15	aA	1123	CL7	CAA-CBA-CGA-O2A
15	aA	1135	CL7	CAA-CBA-CGA-O2A
15	bA	1119	CL7	CAA-CBA-CGA-O2A
18	cA	5001	LHG	O8-C23-C24-C25
14	bA	1013	PHO	C4-C3-C5-C6
15	bB	1208	CL7	C10-C11-C12-C13
15	bA	1103	CL7	C6-C7-C8-C10
15	bA	1137	CL7	C2-C3-C5-C6
15	bB	1012	CL7	C12-C13-C15-C16
15	cA	1111	CL7	C2-C3-C5-C6
15	cA	1123	CL7	C11-C10-C8-C7
15	cB	1208	CL7	C12-C13-C15-C16
15	aB	1207	CL7	CAA-CBA-CGA-O2A
15	bB	1228	CL7	CAA-CBA-CGA-O1A
15	aB	1208	CL7	O1A-CGA-O2A-C1
15	aB	1012	CL7	C14-C13-C15-C16
15	aB	1225	CL7	C11-C10-C8-C9
15	bA	1106	CL7	C11-C12-C13-C14
15	bA	1117	CL7	C14-C13-C15-C16
15	bA	1128	CL7	C11-C10-C8-C9
15	bA	1132	CL7	C14-C13-C15-C16
15	bA	1138	CL7	C11-C10-C8-C9
15	bA	1140	CL7	C11-C10-C8-C9
15	bB	1012	CL7	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	bB	1205	CL7	C6-C7-C8-C9
15	cA	1106	CL7	C11-C12-C13-C14
15	cA	1123	CL7	C11-C10-C8-C9
15	cA	1138	CL7	C11-C10-C8-C9
15	cI	1601	CL7	C11-C10-C8-C9
15	aB	1220	CL7	CAA-CBA-CGA-O2A
15	bB	1220	CL7	CAA-CBA-CGA-O2A
15	cA	1120	CL7	CAA-CBA-CGA-O2A
15	cA	1112	CL7	CBA-CGA-O2A-C1
14	aB	1023	PHO	CAA-CBA-CGA-O2A
15	cA	1119	CL7	CAA-CBA-CGA-O2A
13	cA	1011	G9R	CAA-CBA-CGA-O1A
15	cA	1134	CL7	CAA-CBA-CGA-O1A
15	cB	1222	CL7	CAA-CBA-CGA-O1A
15	bA	1110	CL7	C2A-CAA-CBA-CGA
15	bA	1111	CL7	C2A-CAA-CBA-CGA
15	bB	1237	CL7	CBD-CGD-O2D-CED
15	bB	1021	CL7	CAA-CBA-CGA-O2A
18	cA	5003	LHG	O7-C7-C8-C9
19	cB	5002	LMG	O7-C10-C11-C12
15	bA	1123	CL7	CAA-CBA-CGA-O1A
15	bA	1111	CL7	C16-C17-C18-C20
15	bA	1133	CL7	C4-C3-C5-C6
15	bB	1211	CL7	C2-C3-C5-C6
15	aA	1119	CL7	CAA-CBA-CGA-O2A
18	aA	5001	LHG	O8-C23-C24-C25
15	aB	1212	CL7	CAA-CBA-CGA-O1A
15	aB	1021	CL7	C1A-C2A-CAA-CBA
15	aB	1228	CL7	C1A-C2A-CAA-CBA
15	aL	1502	CL7	C1A-C2A-CAA-CBA
15	bA	1111	CL7	C1A-C2A-CAA-CBA
15	bB	1231	CL7	C1A-C2A-CAA-CBA
15	cA	1111	CL7	C1A-C2A-CAA-CBA
15	cA	1117	CL7	C1A-C2A-CAA-CBA
15	cB	1206	CL7	C1A-C2A-CAA-CBA
15	cB	1231	CL7	C1A-C2A-CAA-CBA
15	aA	1123	CL7	CAA-CBA-CGA-O1A
15	cA	1106	CL7	C15-C16-C17-C18
15	aB	1228	CL7	CAA-CBA-CGA-O1A
15	bA	1120	CL7	CAA-CBA-CGA-O2A
19	cB	5002	LMG	C32-C33-C34-C35
15	aB	1208	CL7	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	aB	1021	CL7	CAA-CBA-CGA-O1A
15	aB	1221	CL7	CAA-CBA-CGA-O1A
15	cA	1123	CL7	CAA-CBA-CGA-O1A
15	aA	1106	CL7	C16-C17-C18-C20
15	bA	1132	CL7	C16-C17-C18-C20
15	bB	1223	CL7	C16-C17-C18-C20
15	cA	1111	CL7	C16-C17-C18-C20
15	cA	1118	CL7	C6-C7-C8-C9
14	cB	1023	PHO	CAA-CBA-CGA-O1A
15	cB	1221	CL7	CAA-CBA-CGA-O1A
15	aA	1105	CL7	CAA-CBA-CGA-O1A
15	cB	1212	CL7	CAA-CBA-CGA-O2A
15	cB	1021	CL7	CAA-CBA-CGA-O2A
14	bB	1023	PHO	C13-C15-C16-C17
15	bI	1601	CL7	C8-C10-C11-C12
15	cA	1132	CL7	C13-C15-C16-C17
15	cB	1207	CL7	C8-C10-C11-C12
14	bB	1023	PHO	CAA-CBA-CGA-O1A
15	aA	1135	CL7	CAA-CBA-CGA-O1A
15	aB	1207	CL7	CAA-CBA-CGA-O1A
15	aA	1138	CL7	O1A-CGA-O2A-C1
18	aA	5003	LHG	C4-O6-P-O4
18	cA	5001	LHG	C3-O3-P-O5
14	aB	1023	PHO	CAA-CBA-CGA-O1A
15	aB	1203	CL7	CAA-CBA-CGA-O1A
15	bB	1221	CL7	CAA-CBA-CGA-O1A
15	cA	1135	CL7	CAA-CBA-CGA-O1A
15	cB	1203	CL7	CAA-CBA-CGA-O1A
15	cB	1207	CL7	CAA-CBA-CGA-O1A
15	bL	1501	CL7	CAA-CBA-CGA-O2A
15	aB	1213	CL7	CAA-CBA-CGA-O1A
15	bJ	1302	CL7	CAA-CBA-CGA-O1A
15	bB	1203	CL7	CAA-CBA-CGA-O1A
15	bA	1126	CL7	C4C-C3C-CAC-CBC
15	aJ	1302	CL7	CAA-CBA-CGA-O1A
15	cB	1223	CL7	C16-C17-C18-C20
13	aA	1011	G9R	CAA-CBA-CGA-O1A
15	bB	1207	CL7	CAA-CBA-CGA-O1A
15	aB	1202	CL7	C10-C11-C12-C13
15	bB	1202	CL7	C10-C11-C12-C13
15	cB	1228	CL7	CAA-CBA-CGA-O1A
15	aA	1109	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	aB	1220	CL7	CAA-CBA-CGA-O1A
13	bA	1011	G9R	CAD-CBD-CGD-O1D
15	aA	1022	CL7	CAD-CBD-CGD-O1D
15	aA	1112	CL7	CAD-CBD-CGD-O1D
15	aA	1129	CL7	CAD-CBD-CGD-O1D
15	aB	1235	CL7	CAD-CBD-CGD-O1D
15	aB	1228	CL7	CAD-CBD-CGD-O1D
15	bA	1132	CL7	CAD-CBD-CGD-O1D
15	bB	1207	CL7	CAD-CBD-CGD-O1D
15	bB	1228	CL7	CAD-CBD-CGD-O1D
15	cA	1111	CL7	CAD-CBD-CGD-O1D
15	cA	1112	CL7	CAD-CBD-CGD-O1D
15	cB	1237	CL7	CAD-CBD-CGD-O1D
15	cB	1224	CL7	CAD-CBD-CGD-O1D
15	cB	1228	CL7	CAD-CBD-CGD-O1D
15	aA	1136	CL7	CAA-CBA-CGA-O1A
15	bA	1136	CL7	CAA-CBA-CGA-O1A
15	cA	1136	CL7	C15-C16-C17-C18
15	cB	1202	CL7	C13-C15-C16-C17
15	aA	1117	CL7	C14-C13-C15-C16
15	aA	1127	CL7	C14-C13-C15-C16
15	bA	1103	CL7	C6-C7-C8-C9
15	bA	1104	CL7	C14-C13-C15-C16
15	bB	1225	CL7	C11-C10-C8-C9
15	cA	1104	CL7	C14-C13-C15-C16
15	cB	1012	CL7	C14-C13-C15-C16
15	cB	1202	CL7	C11-C10-C8-C9
15	cB	1205	CL7	C6-C7-C8-C9
15	cB	1238	CL7	C11-C12-C13-C14
15	bA	1116	CL7	C2C-C3C-CAC-CBC
15	bB	1220	CL7	CAA-CBA-CGA-O1A
15	aB	1225	CL7	C10-C11-C12-C13
15	cA	1108	CL7	CAA-CBA-CGA-O2A
15	cB	1206	CL7	CAA-CBA-CGA-O2A
15	bA	1136	CL7	O1D-CGD-O2D-CED
15	cA	1120	CL7	CAA-CBA-CGA-O1A
15	aA	1106	CL7	C15-C16-C17-C18
15	cA	1128	CL7	C5-C6-C7-C8
15	aA	1108	CL7	CAA-CBA-CGA-O2A
15	aB	1202	CL7	CAA-CBA-CGA-O2A
15	bA	1108	CL7	CAA-CBA-CGA-O2A
15	bB	1206	CL7	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	cB	1202	CL7	CAA-CBA-CGA-O2A
18	bA	5001	LHG	O8-C23-C24-C25
18	bA	5003	LHG	C1-C2-C3-O3
15	cA	1136	CL7	CAA-CBA-CGA-O1A
18	aA	5001	LHG	O10-C23-C24-C25
15	cA	1111	CL7	C4-C3-C5-C6
15	bB	1223	CL7	C8-C10-C11-C12
15	cB	1229	CL7	C15-C16-C17-C18
15	aA	1127	CL7	C11-C12-C13-C15
15	aB	1239	CL7	C6-C7-C8-C10
15	aB	1207	CL7	C11-C10-C8-C7
15	aB	1210	CL7	C11-C10-C8-C7
15	bA	1103	CL7	C11-C12-C13-C15
15	bA	1104	CL7	C11-C10-C8-C7
15	bA	1111	CL7	C3A-C2A-CAA-CBA
15	bA	1128	CL7	C11-C10-C8-C7
15	bB	1221	CL7	C6-C7-C8-C10
15	bB	1239	CL7	C6-C7-C8-C10
15	cA	1022	CL7	C3A-C2A-CAA-CBA
15	cA	1104	CL7	C12-C13-C15-C16
15	cA	1111	CL7	C3A-C2A-CAA-CBA
15	cA	1133	CL7	C11-C10-C8-C7
15	bA	1119	CL7	CAA-CBA-CGA-O1A
15	bA	1135	CL7	CAA-CBA-CGA-O1A
15	cA	1119	CL7	CAA-CBA-CGA-O1A
18	cA	5001	LHG	O10-C23-C24-C25
15	bB	1212	CL7	CAA-CBA-CGA-O2A
15	aB	1235	CL7	CAA-CBA-CGA-O2A
15	bB	1235	CL7	CAA-CBA-CGA-O2A
15	bB	1238	CL7	C3-C5-C6-C7
15	aA	1119	CL7	CAA-CBA-CGA-O1A
15	bB	1021	CL7	CAA-CBA-CGA-O1A
15	cB	1235	CL7	CAA-CBA-CGA-O1A
18	cA	5003	LHG	O9-C7-C8-C9
15	cB	1212	CL7	CAA-CBA-CGA-O1A
15	aL	1501	CL7	CAA-CBA-CGA-O2A
15	cB	1235	CL7	CAA-CBA-CGA-O2A
19	aB	5002	LMG	O7-C10-C11-C12
15	bA	1131	CL7	C5-C6-C7-C8
15	cA	1121	CL7	C5-C6-C7-C8
15	cB	1208	CL7	C10-C11-C12-C13
15	aB	1235	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	bB	1235	CL7	CAA-CBA-CGA-O1A
15	cB	1021	CL7	CAA-CBA-CGA-O1A
15	aA	1126	CL7	CAA-CBA-CGA-O2A
15	aA	1132	CL7	CAA-CBA-CGA-O2A
15	bB	1202	CL7	CAA-CBA-CGA-O2A
15	cL	1501	CL7	CAA-CBA-CGA-O2A
15	cA	1108	CL7	CAA-CBA-CGA-O1A
15	aB	1234	CL7	C2A-CAA-CBA-CGA
15	bB	1234	CL7	C2A-CAA-CBA-CGA
15	cB	1234	CL7	C2A-CAA-CBA-CGA
15	aA	1113	CL7	CAA-CBA-CGA-O2A
15	aB	1237	CL7	C5-C6-C7-C8
15	bA	1121	CL7	C5-C6-C7-C8
15	bA	1131	CL7	C10-C11-C12-C13
15	bB	1207	CL7	C8-C10-C11-C12
15	aB	1202	CL7	CAA-CBA-CGA-O1A
15	cB	1206	CL7	CAA-CBA-CGA-O1A
19	cB	5002	LMG	O9-C10-C11-C12
15	cB	1220	CL7	CAA-CBA-CGA-O2A

There are no ring outliers.

255 monomers are involved in 737 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	1102	CL7	2	0
15	aA	1129	CL7	5	0
15	aB	1216	CL7	3	0
15	cB	1214	CL7	3	0
15	aI	1601	CL7	6	0
15	cA	1103	CL7	6	0
15	bB	1217	CL7	2	0
15	aA	1115	CL7	3	0
15	cB	1207	CL7	3	0
15	aA	1136	CL7	1	0
15	cB	1237	CL7	3	0
15	aA	1114	CL7	1	0
15	aB	1202	CL7	5	0
15	cB	1226	CL7	5	0
18	cA	5001	LHG	6	0
15	bB	1220	CL7	2	0
15	bA	1137	CL7	1	0
15	cA	1122	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bB	1222	CL7	3	0
19	cB	5002	LMG	1	0
15	cA	1138	CL7	1	0
15	bL	1503	CL7	1	0
15	aB	1226	CL7	7	0
15	bB	1021	CL7	2	0
15	cB	1218	CL7	4	0
15	cB	1203	CL7	5	0
15	aA	1022	CL7	1	0
15	cB	1230	CL7	3	0
15	aB	1238	CL7	5	0
15	bB	1203	CL7	2	0
15	cL	1502	CL7	2	0
15	bB	1205	CL7	4	0
15	bB	1201	CL7	2	0
15	bA	1117	CL7	2	0
15	cA	1140	CL7	2	0
17	bL	4023	A1JPJ	1	0
15	aB	1227	CL7	1	0
15	bA	1127	CL7	9	0
15	aA	1123	CL7	2	0
15	cJ	1301	CL7	1	0
15	cB	1231	CL7	3	0
15	aB	1224	CL7	4	0
17	aB	4005	A1JPJ	1	0
15	cB	1236	CL7	4	0
15	bB	1211	CL7	4	0
15	aB	1219	CL7	2	0
15	aB	1214	CL7	1	0
15	bA	1123	CL7	4	0
15	cL	1503	CL7	2	0
15	cA	1117	CL7	2	0
14	bB	1023	PHO	6	0
15	aB	1228	CL7	5	0
15	cA	1136	CL7	1	0
15	bB	1226	CL7	8	0
15	bJ	1302	CL7	1	0
15	bB	1204	CL7	3	0
15	bA	1133	CL7	7	0
18	bA	5001	LHG	3	0
15	aA	1103	CL7	4	0
15	bA	1113	CL7	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cB	1213	CL7	2	0
15	aA	1112	CL7	3	0
15	cA	1106	CL7	4	0
15	bA	1109	CL7	6	0
15	aA	1121	CL7	2	0
15	aA	1133	CL7	6	0
15	aB	1220	CL7	1	0
15	aA	1127	CL7	8	0
15	cA	1128	CL7	4	0
15	cA	1101	CL7	5	0
15	cB	1219	CL7	3	0
15	cB	1021	CL7	2	0
16	bA	2001	PQN	2	0
15	bB	1212	CL7	3	0
15	cB	1239	CL7	4	0
15	aA	1134	CL7	1	0
15	bB	1235	CL7	7	0
15	bB	1239	CL7	3	0
16	aA	2001	PQN	1	0
18	aA	5001	LHG	4	0
15	cB	1229	CL7	5	0
15	bA	1119	CL7	5	0
15	aA	1126	CL7	7	0
15	aB	1205	CL7	4	0
15	cA	1121	CL7	2	0
15	aB	1221	CL7	4	0
15	cB	1241	CL7	2	0
15	aB	1236	CL7	1	0
15	cA	1120	CL7	3	0
15	bA	1122	CL7	4	0
15	bA	1130	CL7	2	0
15	bB	1213	CL7	3	0
15	cA	1119	CL7	4	0
15	bB	1216	CL7	1	0
15	bA	1124	CL7	1	0
15	cB	1235	CL7	3	0
15	aA	1131	CL7	2	0
15	cI	1601	CL7	4	0
15	bB	1219	CL7	2	0
15	aA	1105	CL7	1	0
15	bB	1214	CL7	4	0
15	aA	1110	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	1136	CL7	1	0
15	aB	1209	CL7	1	0
15	aB	1208	CL7	7	0
15	bA	1129	CL7	3	0
15	cB	1238	CL7	5	0
15	aB	1207	CL7	3	0
15	bB	1207	CL7	4	0
15	aA	1102	CL7	1	0
15	bA	1110	CL7	2	0
15	aB	1222	CL7	3	0
14	aA	1013	PHO	3	0
15	aA	1117	CL7	2	0
15	aA	1111	CL7	4	0
15	aB	1210	CL7	7	0
15	cA	1110	CL7	2	0
15	cA	1115	CL7	2	0
15	bB	1238	CL7	5	0
15	bA	1103	CL7	9	0
15	bA	1118	CL7	3	0
15	aA	1104	CL7	4	0
15	aB	1215	CL7	1	0
17	aL	4023	A1JPJ	1	0
15	aA	1109	CL7	5	0
15	cA	1139	CL7	1	0
15	bA	1104	CL7	5	0
15	cA	1129	CL7	3	0
19	bB	5002	LMG	3	0
15	aB	1213	CL7	1	0
15	bB	1227	CL7	6	0
15	aB	1237	CL7	2	0
15	cB	1222	CL7	5	0
15	bB	1209	CL7	1	0
15	cB	1202	CL7	7	0
15	aB	1211	CL7	3	0
15	cB	1208	CL7	6	0
15	bA	1106	CL7	6	0
15	bB	1236	CL7	2	0
17	cB	4005	A1JPJ	1	0
15	cB	1210	CL7	8	0
15	bB	1208	CL7	2	0
15	aK	1402	CL7	2	0
15	aB	1204	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	1105	CL7	1	0
15	bA	1120	CL7	5	0
15	bA	1111	CL7	4	0
15	cB	1215	CL7	2	0
15	aJ	1302	CL7	2	0
15	bB	1210	CL7	5	0
15	cB	1206	CL7	2	0
15	aA	1137	CL7	2	0
15	cB	1224	CL7	2	0
15	aA	1132	CL7	2	0
15	cA	1137	CL7	2	0
15	bL	1501	CL7	3	0
15	cB	1211	CL7	7	0
14	cA	1013	PHO	1	0
15	bA	1101	CL7	6	0
18	cA	5003	LHG	2	0
15	cB	1205	CL7	3	0
15	aB	1203	CL7	5	0
15	aB	1235	CL7	3	0
15	cB	1221	CL7	5	0
15	aB	1218	CL7	2	0
15	bB	1237	CL7	3	0
15	aA	1106	CL7	5	0
15	bA	1126	CL7	7	0
15	aA	1138	CL7	6	0
15	bA	1132	CL7	3	0
15	aB	1212	CL7	3	0
15	cB	1204	CL7	5	0
15	aA	1120	CL7	4	0
15	bB	1229	CL7	4	0
15	cA	1112	CL7	2	0
15	cA	1133	CL7	3	0
15	cA	1126	CL7	7	0
15	bI	1601	CL7	2	0
15	cB	1220	CL7	3	0
15	bB	1224	CL7	2	0
15	bA	1140	CL7	3	0
14	aB	1023	PHO	7	0
15	aA	1101	CL7	4	0
15	aB	1206	CL7	1	0
15	aA	1118	CL7	4	0
15	aA	1130	CL7	2	0

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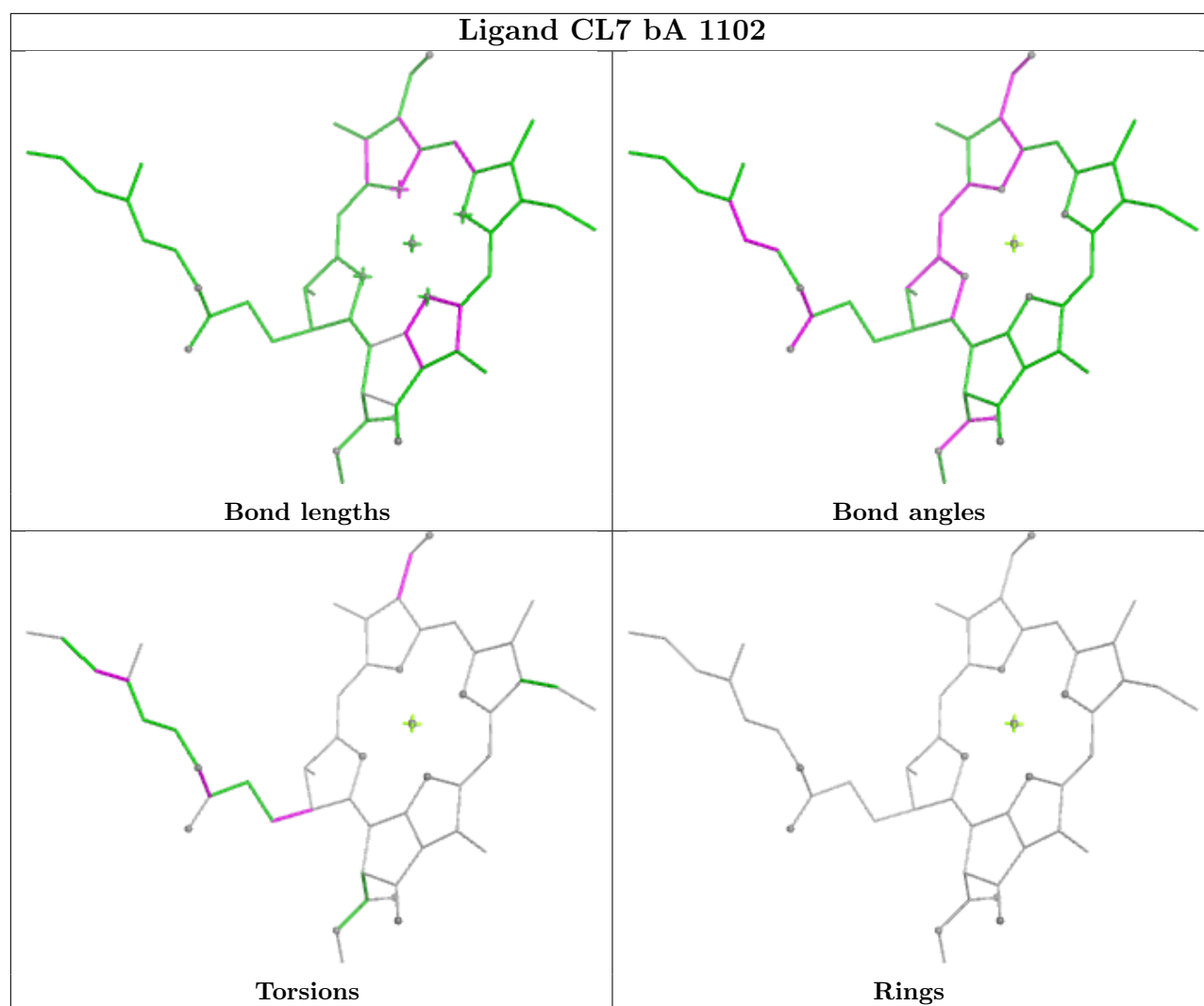
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aA	1124	CL7	1	0
15	bB	1228	CL7	5	0
15	aB	1241	CL7	2	0
15	bA	1115	CL7	2	0
15	cB	1223	CL7	4	0
15	cA	1124	CL7	1	0
20	bC	3003	SF4	1	0
15	bB	1218	CL7	3	0
15	bA	1139	CL7	1	0
15	bB	1215	CL7	1	0
15	cB	1234	CL7	1	0
15	aB	1021	CL7	1	0
15	cB	1228	CL7	3	0
14	cB	1023	PHO	7	0
15	aL	1502	CL7	2	0
15	cA	1118	CL7	4	0
15	cA	1130	CL7	2	0
15	cA	1104	CL7	6	0
15	cA	1111	CL7	3	0
15	bA	1112	CL7	2	0
15	bB	1223	CL7	3	0
15	aB	1229	CL7	6	0
15	cB	1209	CL7	1	0
14	bA	1013	PHO	1	0
15	bA	1116	CL7	8	0
15	cL	1501	CL7	3	0
15	aB	1230	CL7	1	0
15	cB	1216	CL7	2	0
15	bB	1241	CL7	3	0
15	aA	1116	CL7	4	0
18	aA	5003	LHG	1	0
15	aA	1125	CL7	2	0
15	aL	1501	CL7	3	0
15	aA	1128	CL7	5	0
17	bA	4014	A1JPJ	1	0
15	cJ	1302	CL7	3	0
15	cA	1116	CL7	8	0
15	aB	1201	CL7	3	0
15	bA	1108	CL7	4	0
15	bA	1128	CL7	4	0
15	bA	1125	CL7	3	0
15	aB	1223	CL7	4	0

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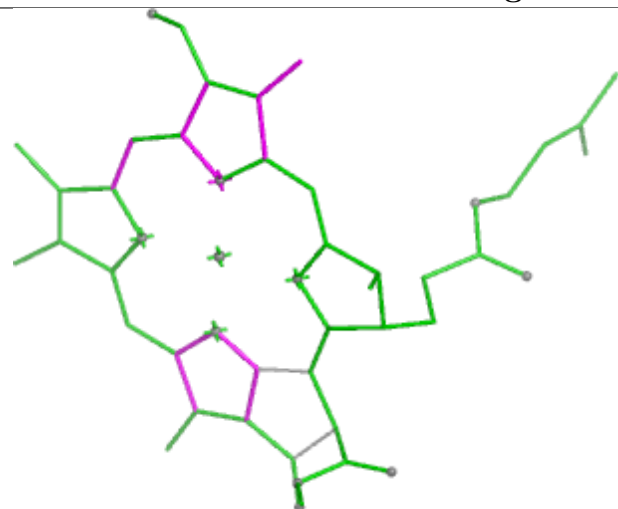
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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15	cA	1109	CL7	5	0
15	bK	1402	CL7	1	0
15	aL	1503	CL7	2	0
15	cB	1212	CL7	2	0
15	cB	1227	CL7	5	0
15	aB	1234	CL7	1	0
15	cA	1123	CL7	5	0
15	cA	1105	CL7	1	0
15	cA	1102	CL7	2	0
15	aA	1140	CL7	2	0
15	bL	1502	CL7	2	0
15	cA	1132	CL7	2	0
15	aB	1239	CL7	3	0
15	aA	1113	CL7	4	0
15	bB	1230	CL7	2	0
18	bA	5003	LHG	1	0
15	aA	1119	CL7	8	0
15	cB	1201	CL7	4	0
15	bA	1138	CL7	5	0
15	bB	1221	CL7	4	0
15	aA	1108	CL7	5	0
15	bA	1121	CL7	2	0
15	cA	1108	CL7	2	0
15	cA	1127	CL7	7	0
19	aB	5002	LMG	3	0
15	aA	1122	CL7	3	0

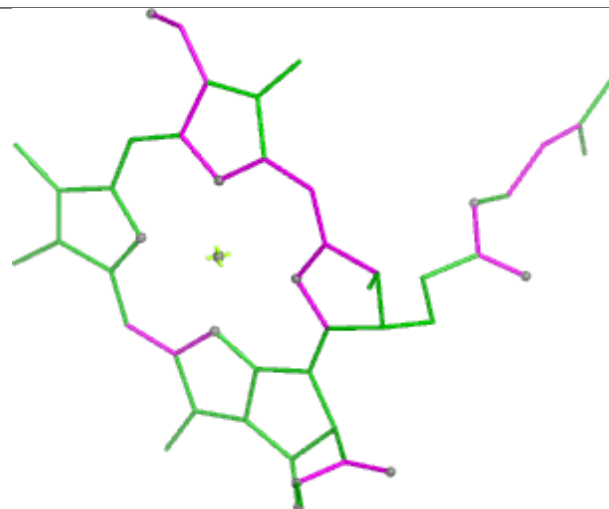
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



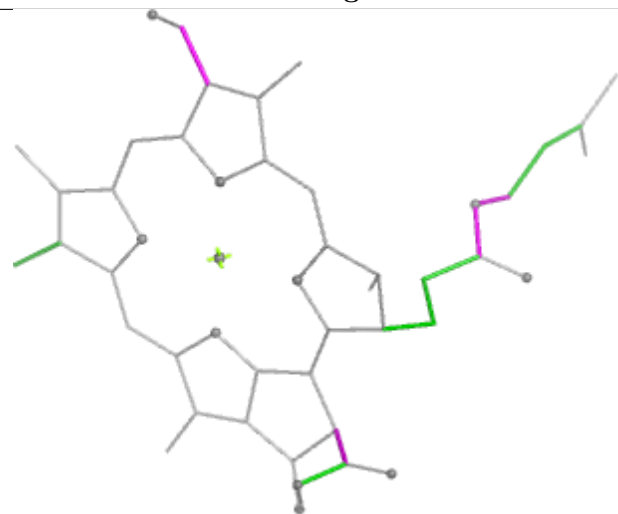
Ligand CL7 aA 1129



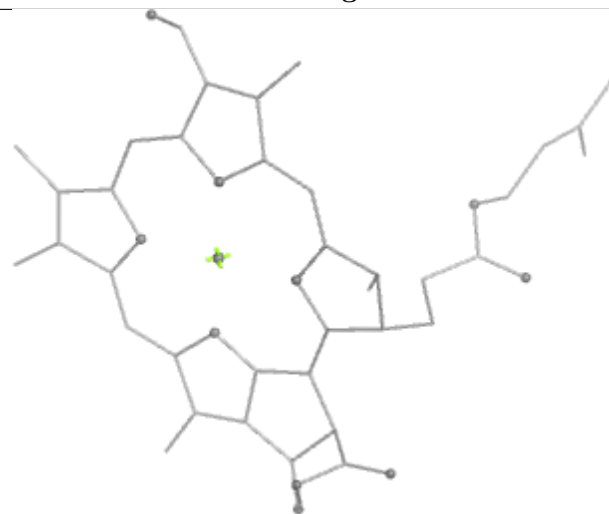
Bond lengths



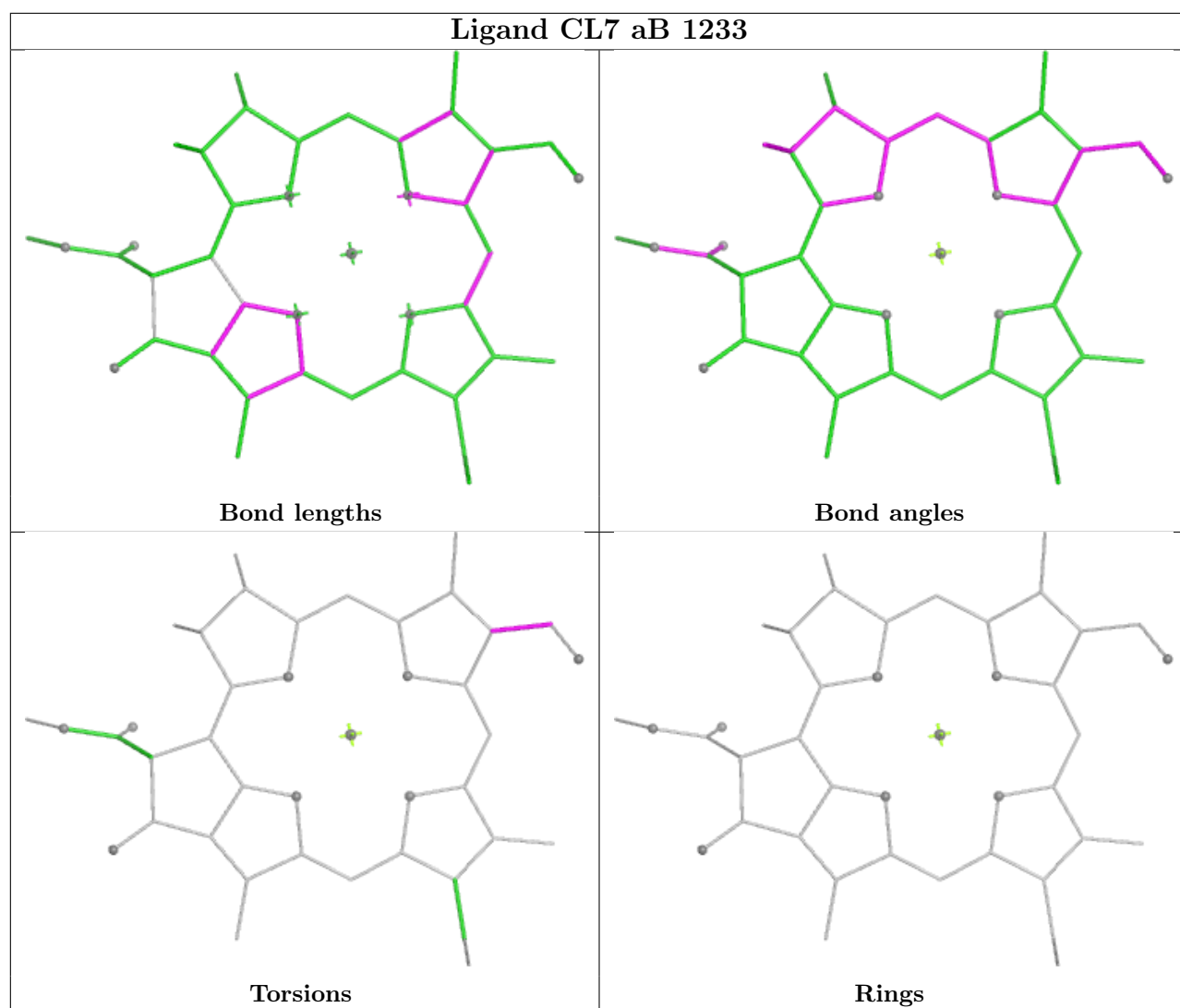
Bond angles

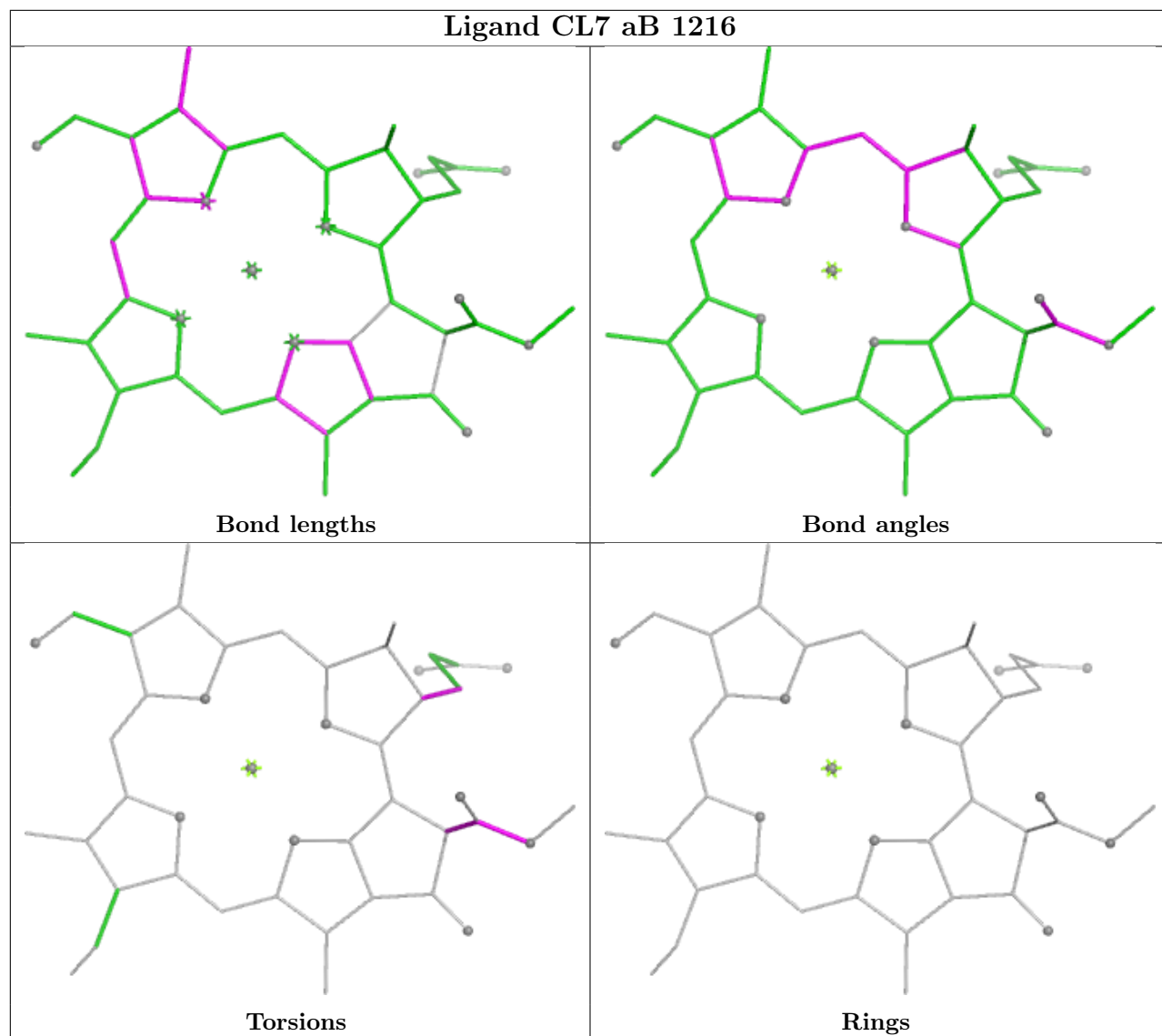


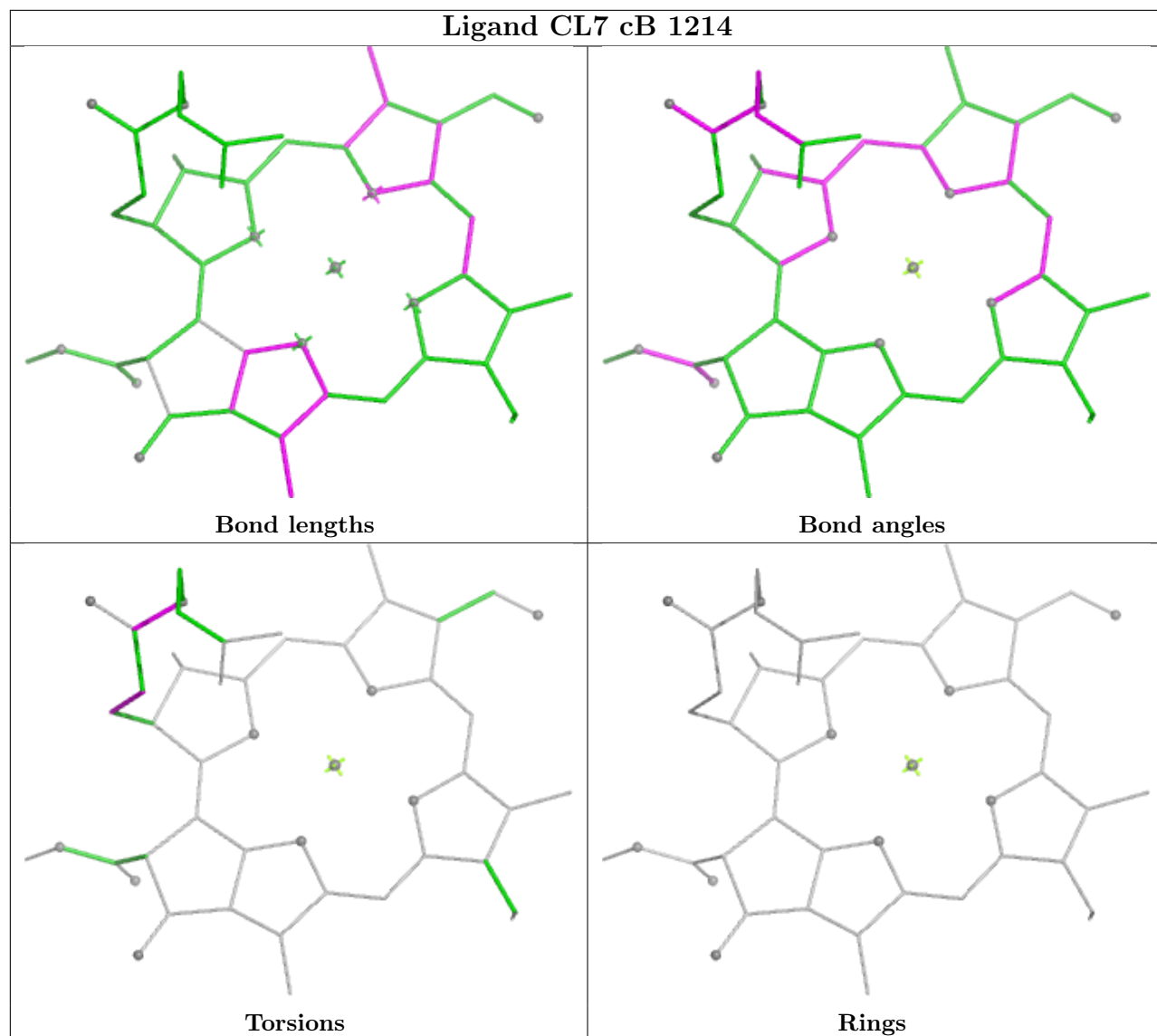
Torsions

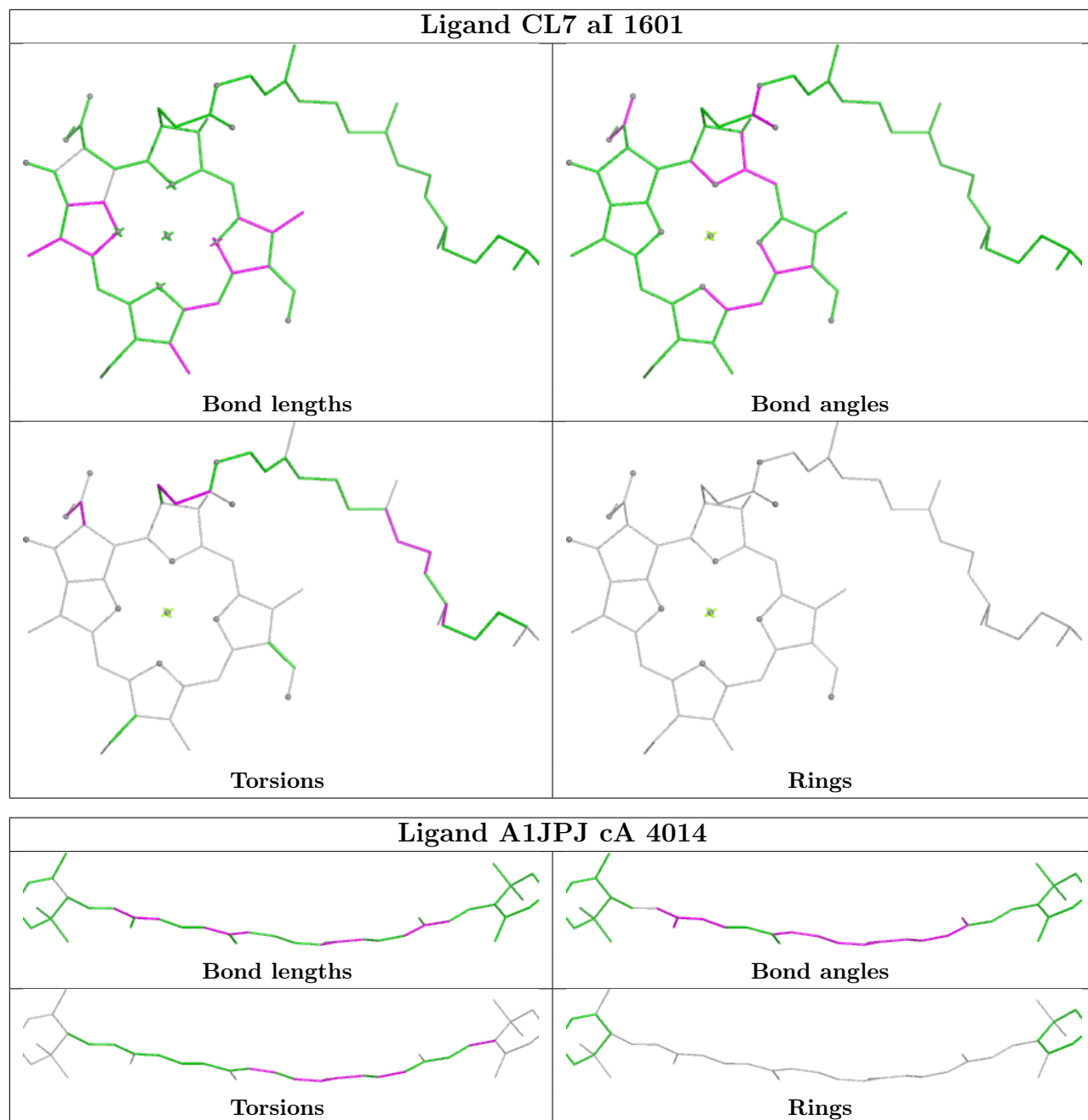


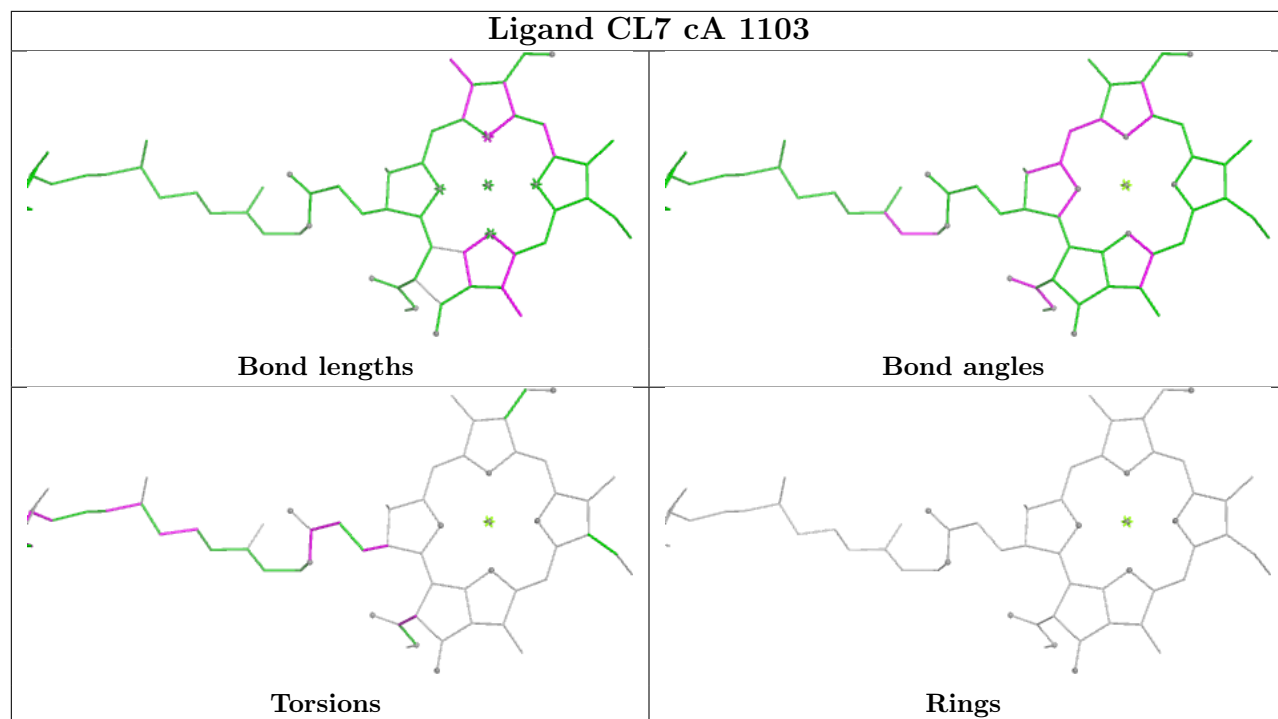
Rings

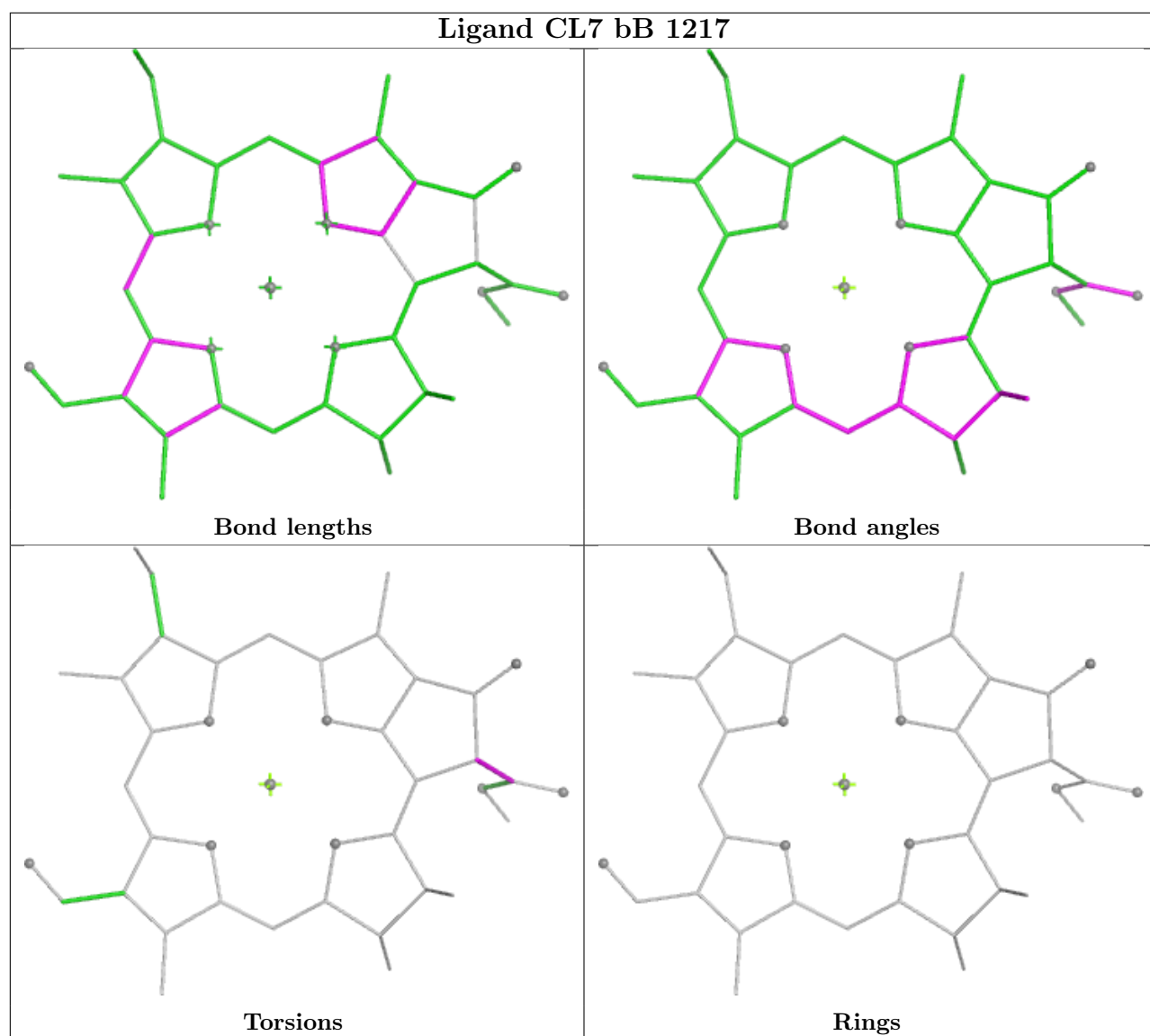




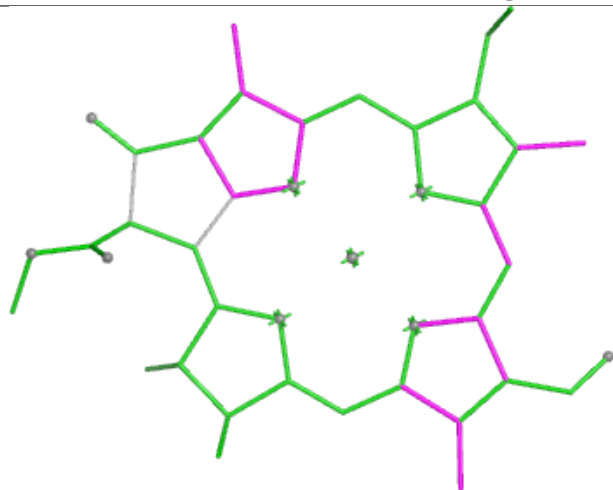




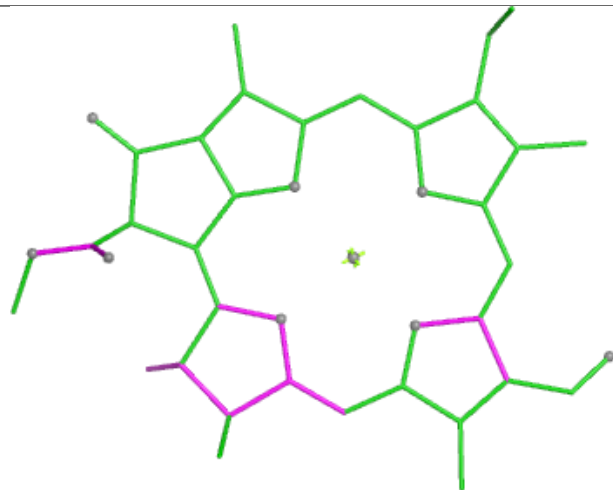




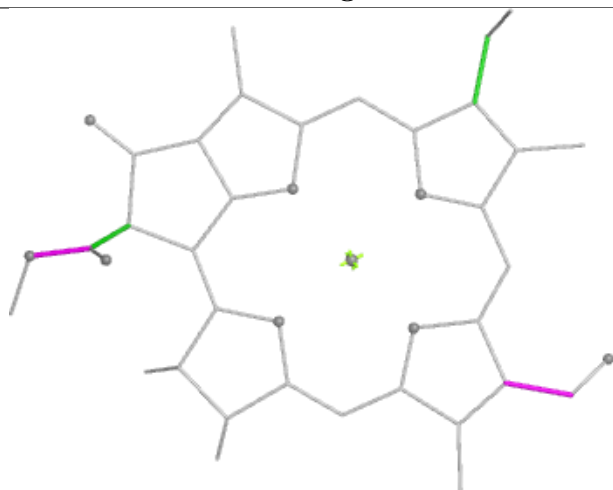
Ligand CL7 aA 1115



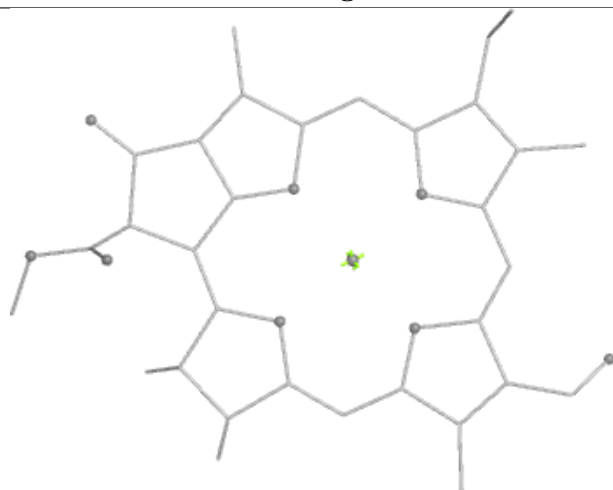
Bond lengths



Bond angles

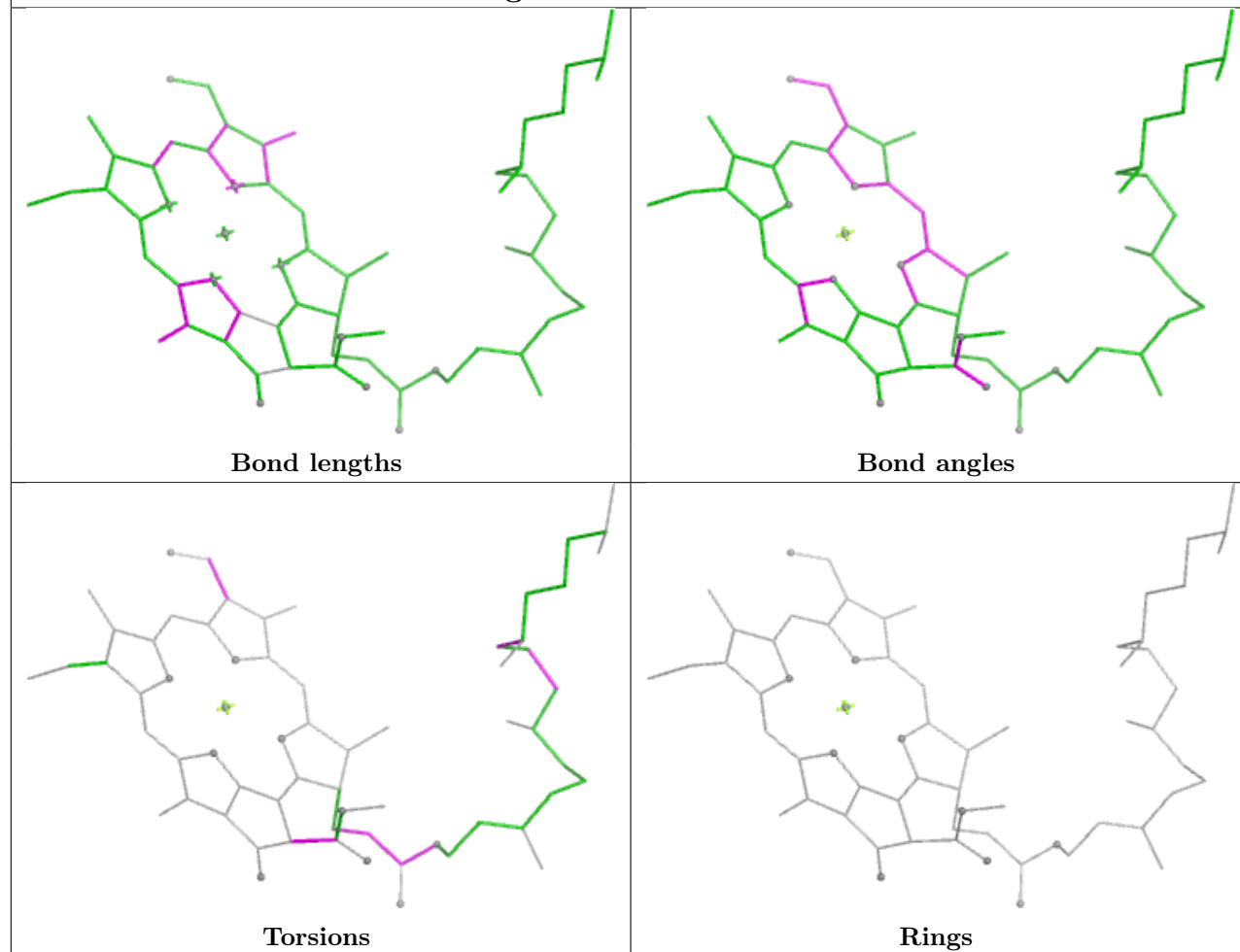


Torsions

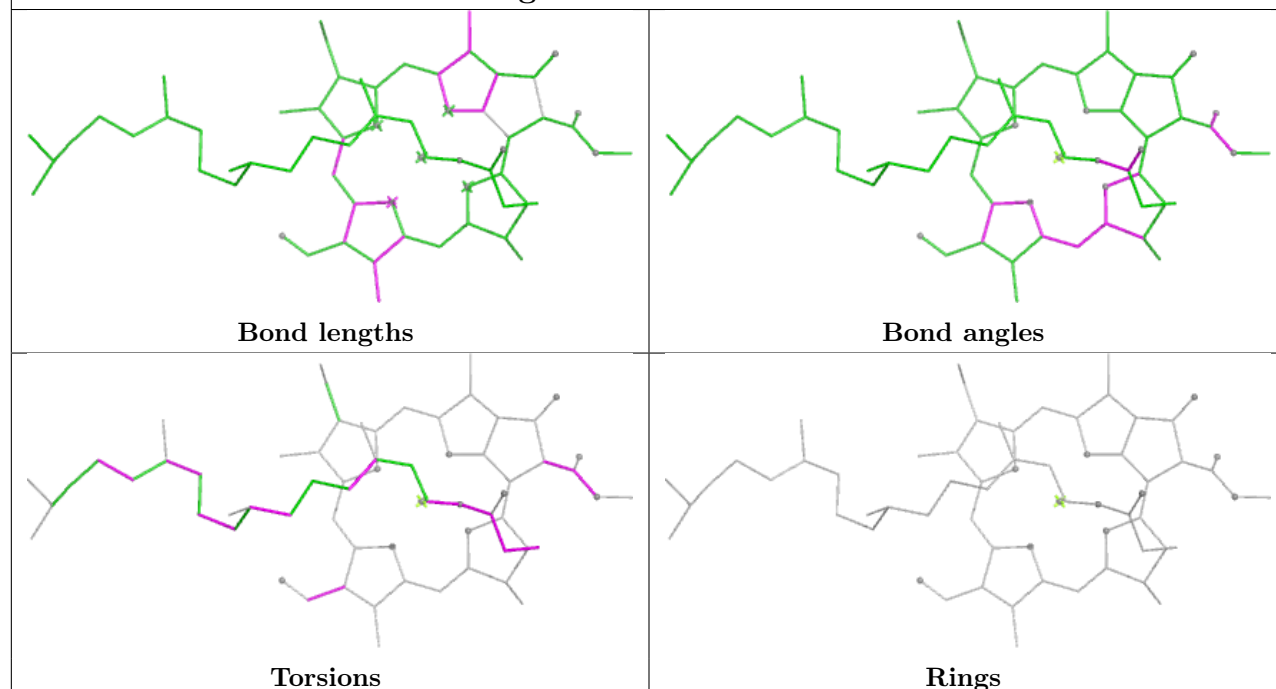


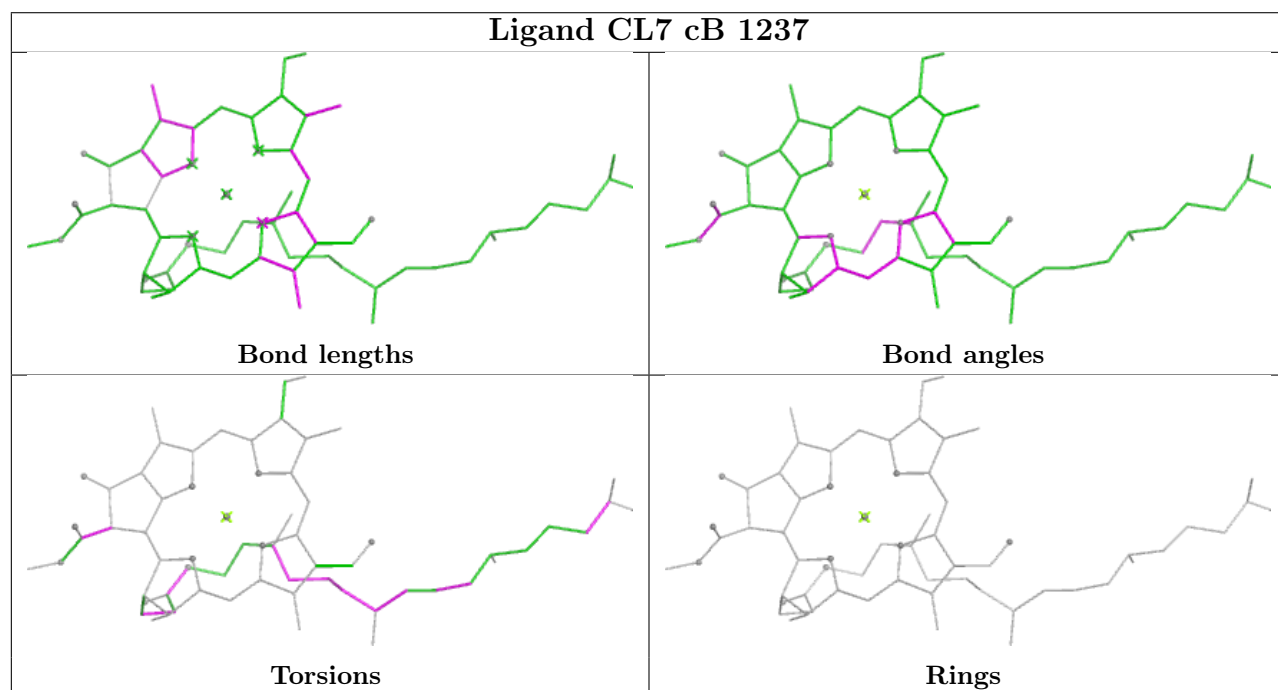
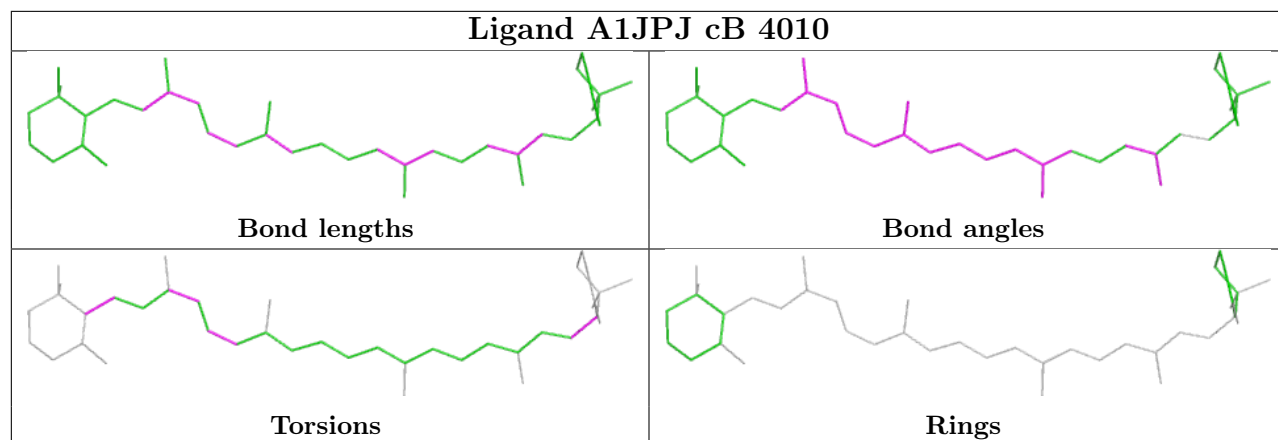
Rings

Ligand CL7 cB 1207

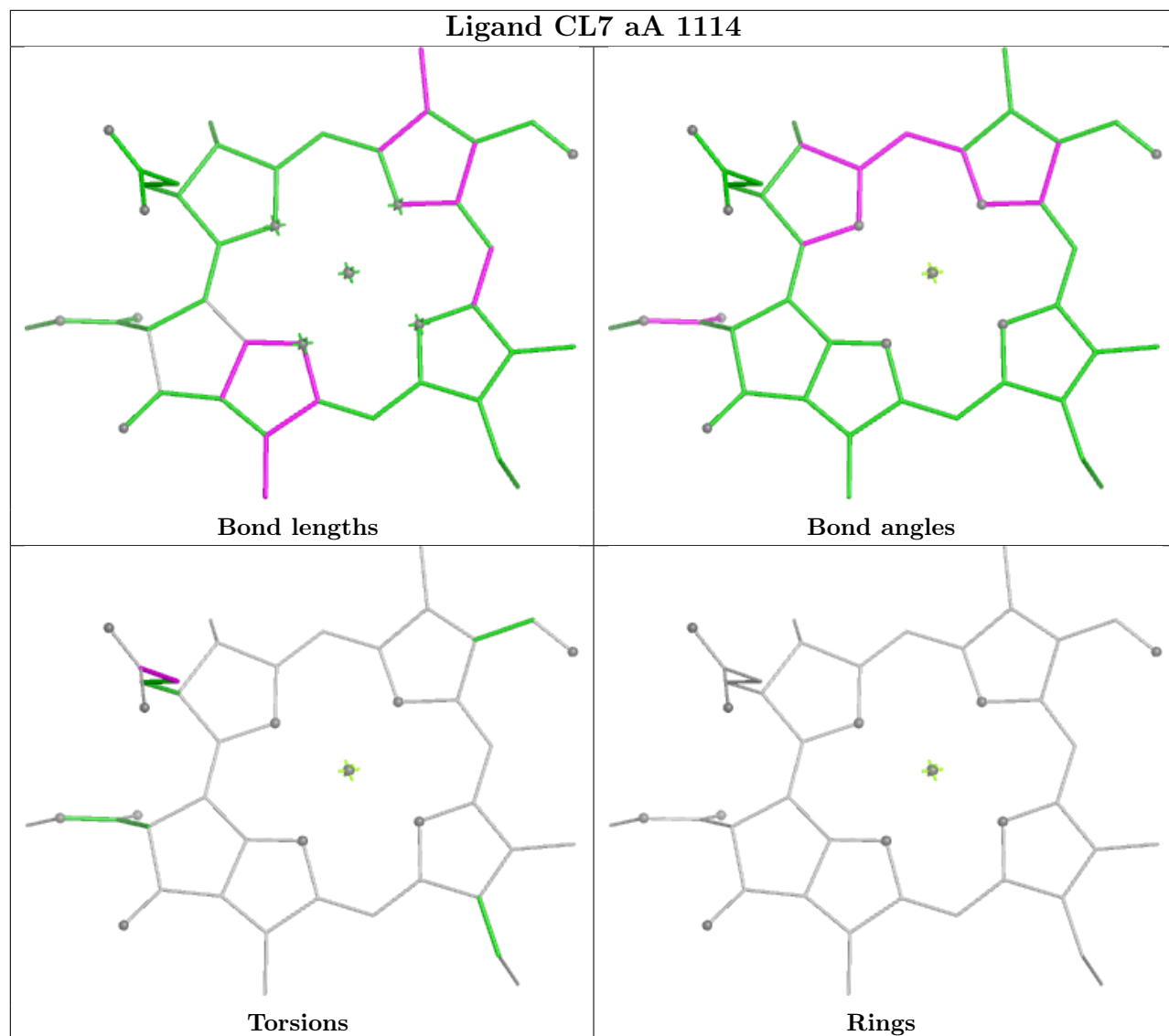


Ligand CL7 aA 1136

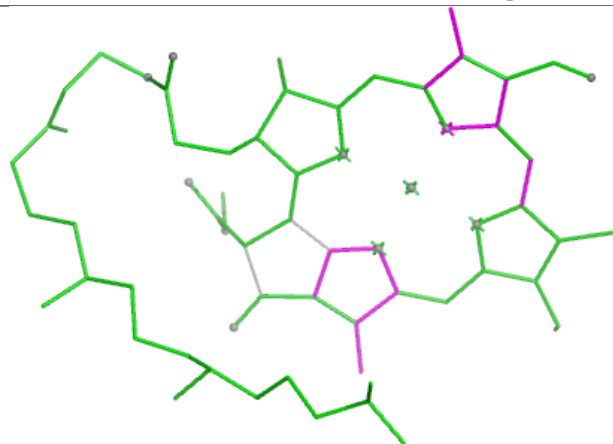




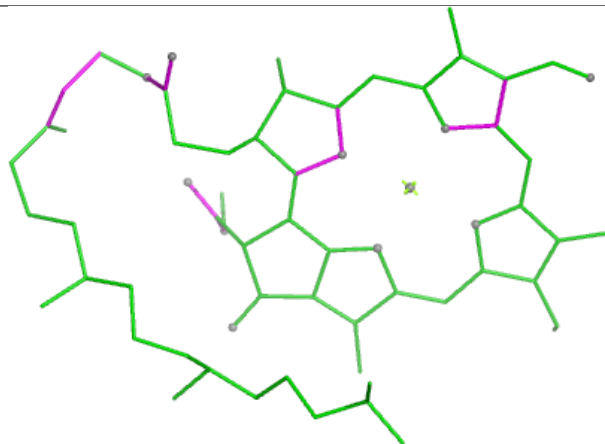
Ligand CL7 aA 1114



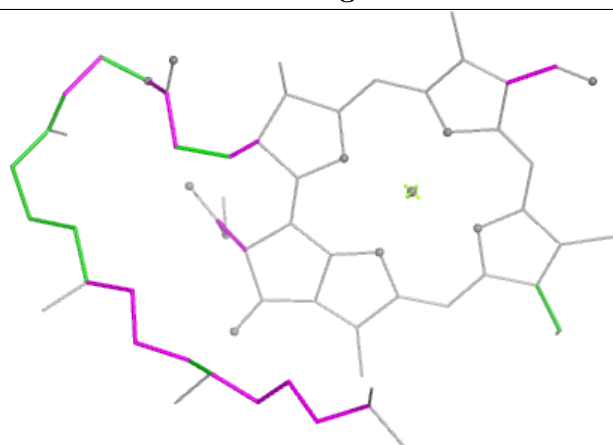
Ligand CL7 aB 1202



Bond lengths



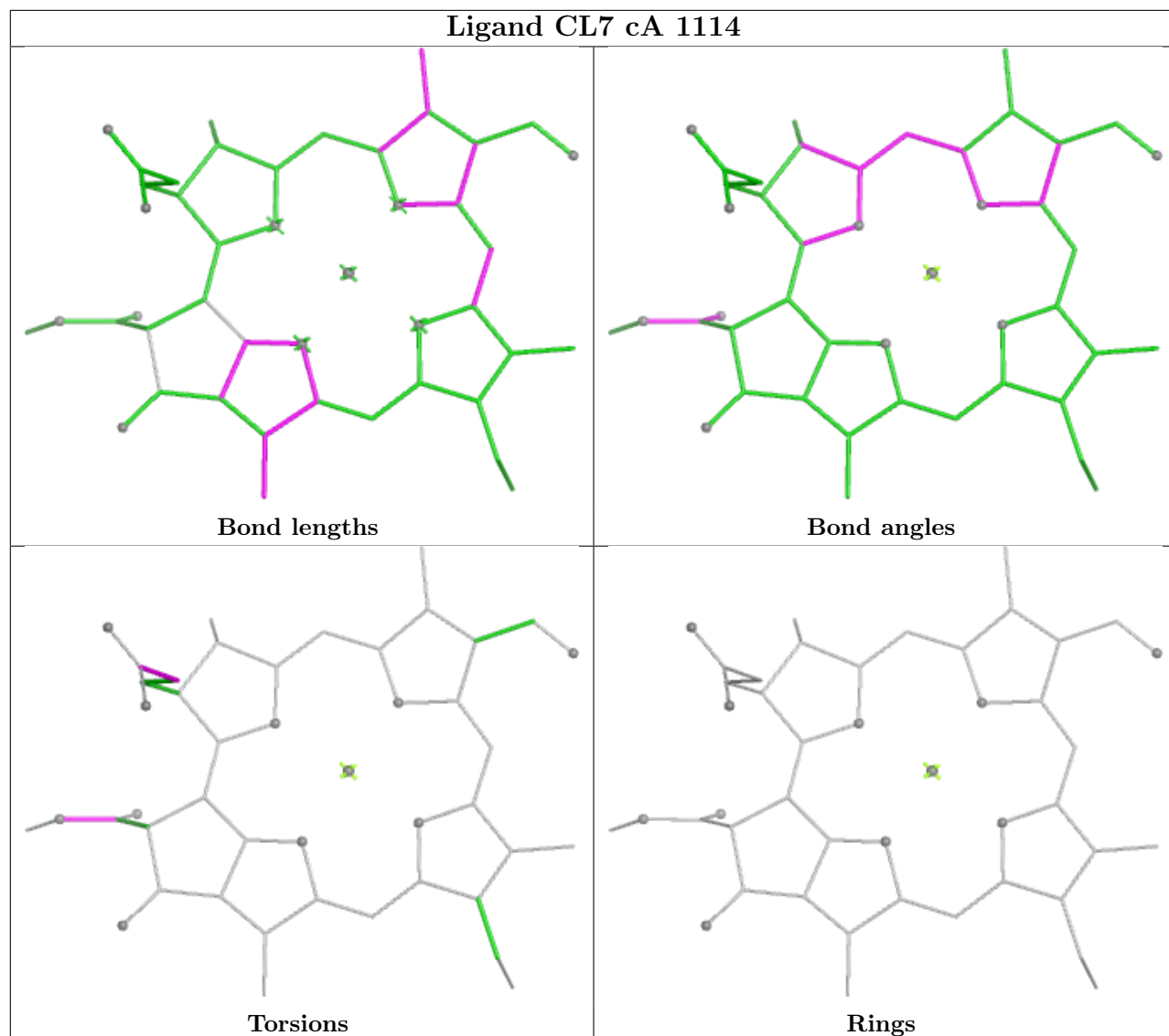
Bond angles

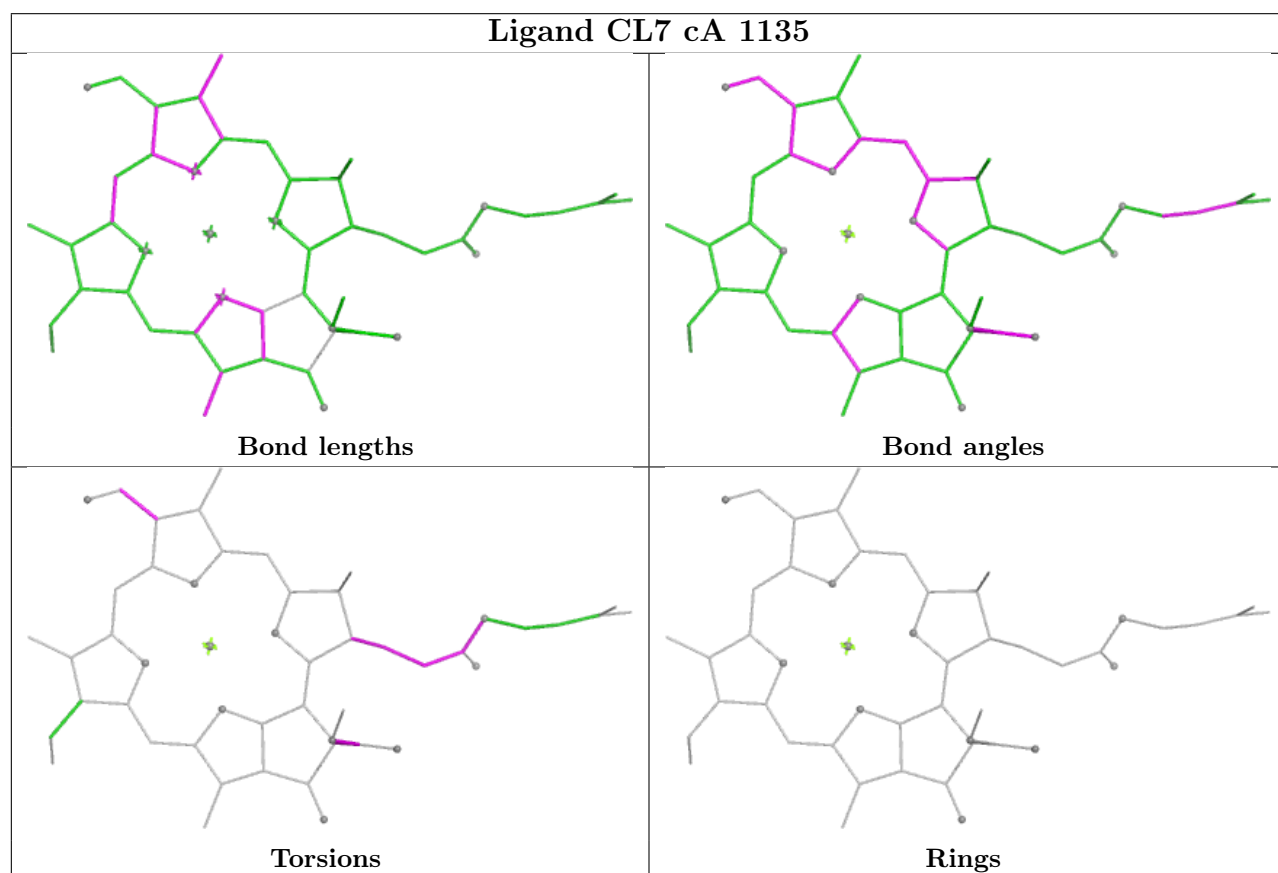
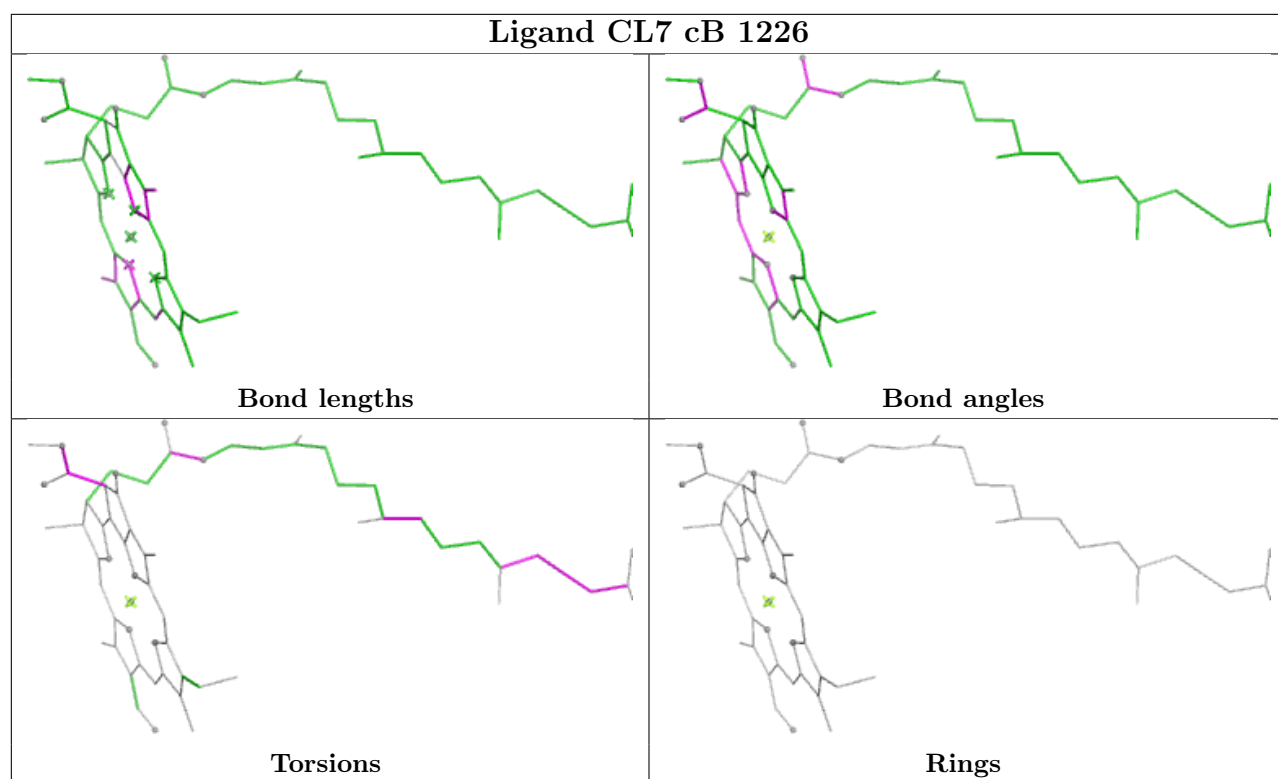


Torsions

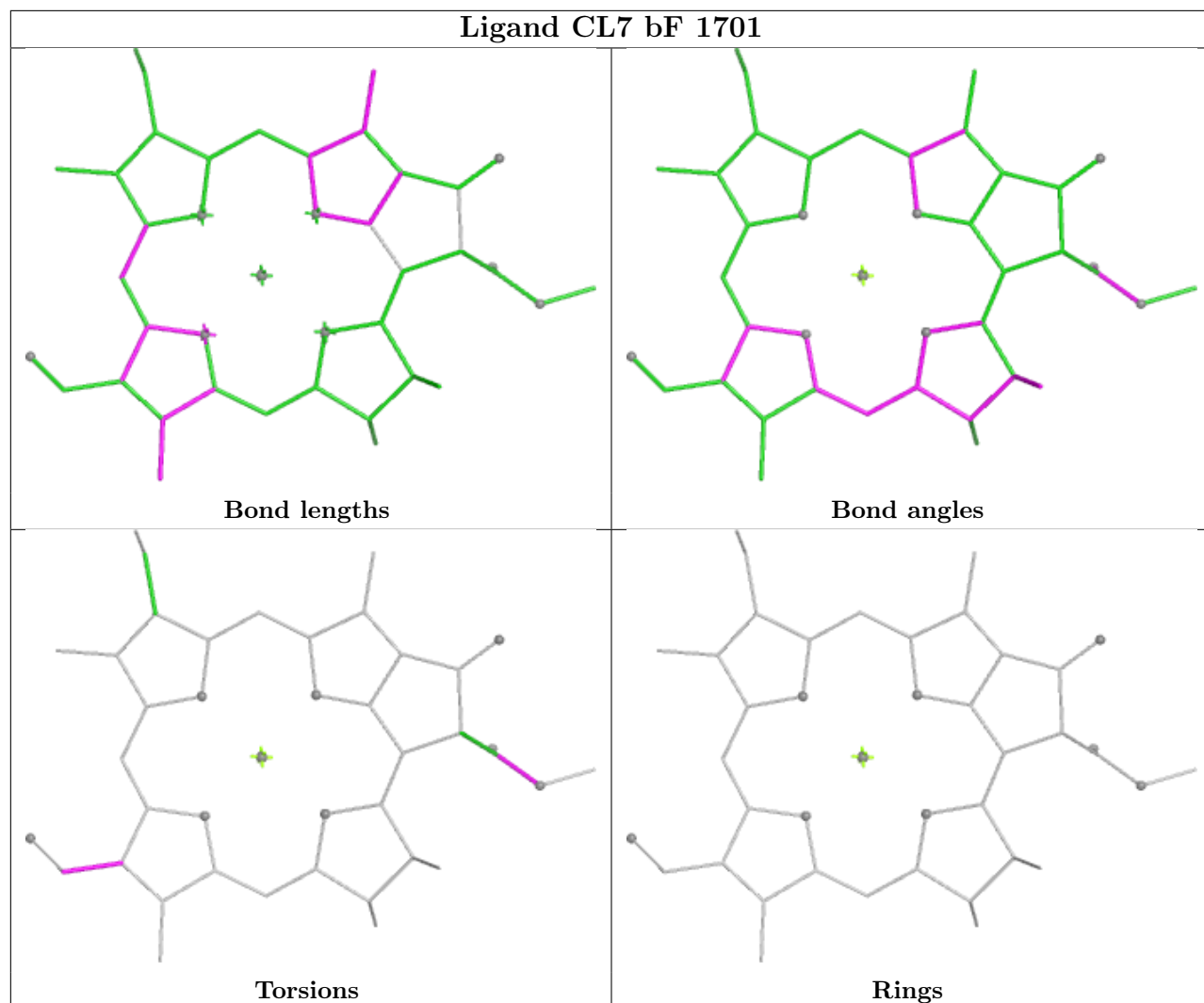


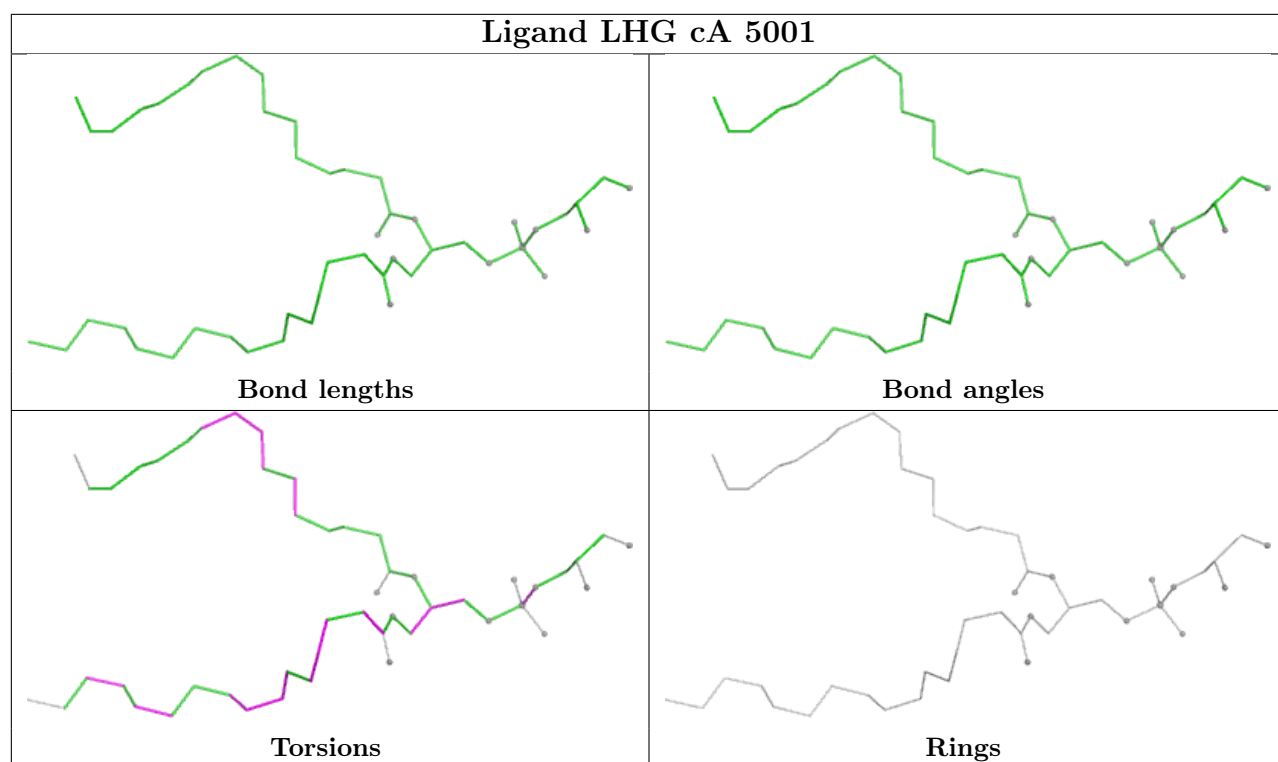
Rings



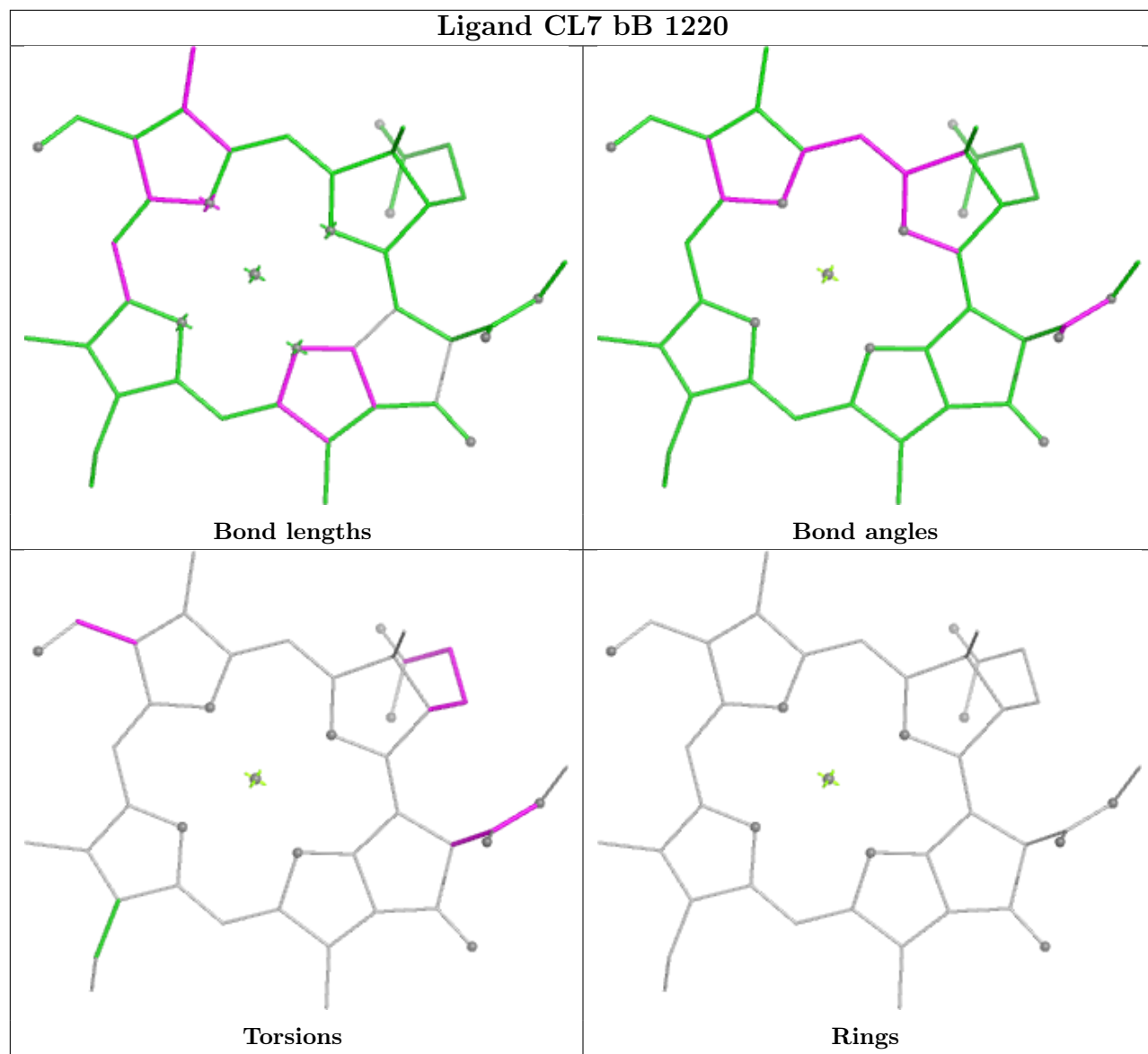


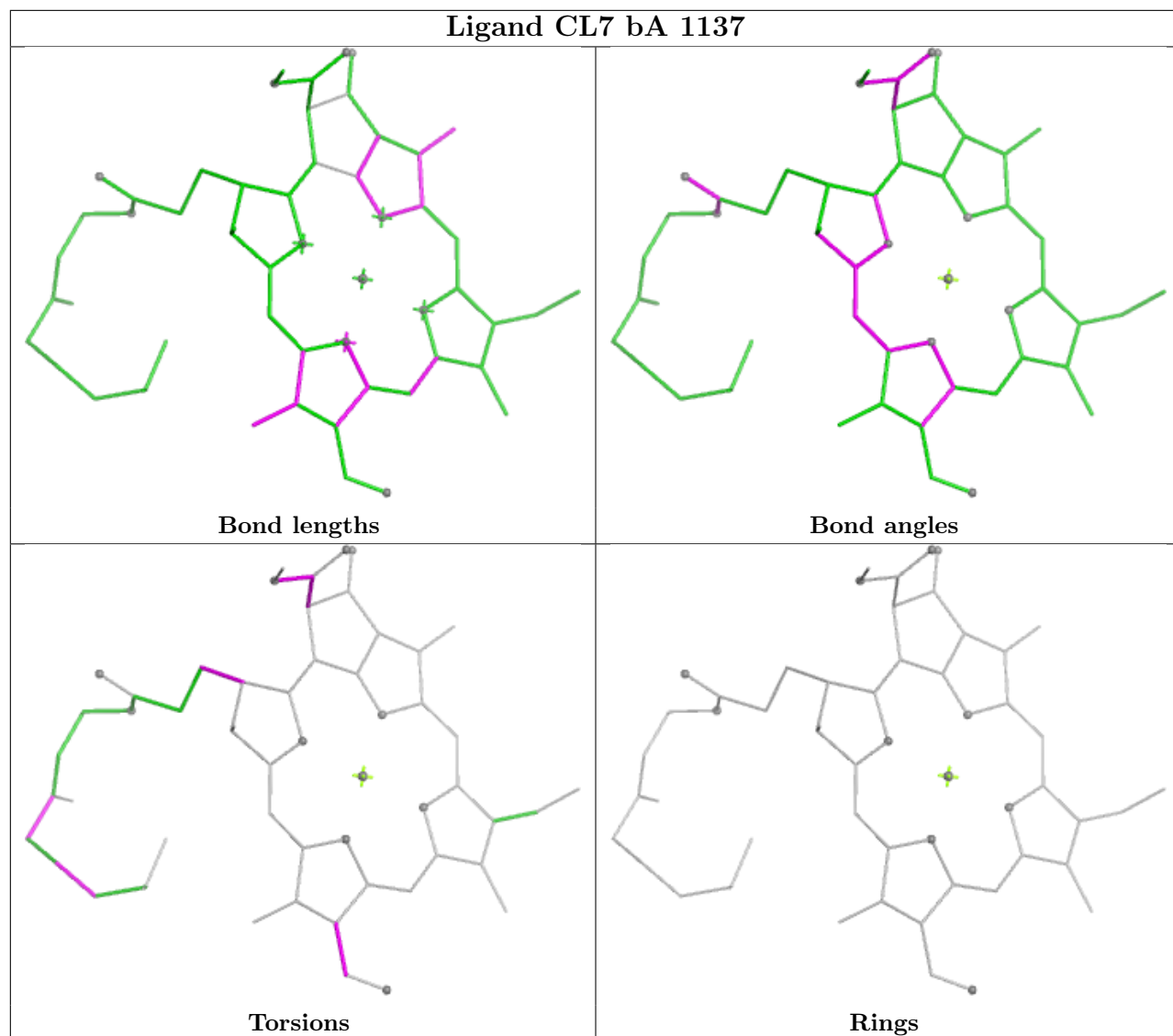
Ligand CL7 bF 1701

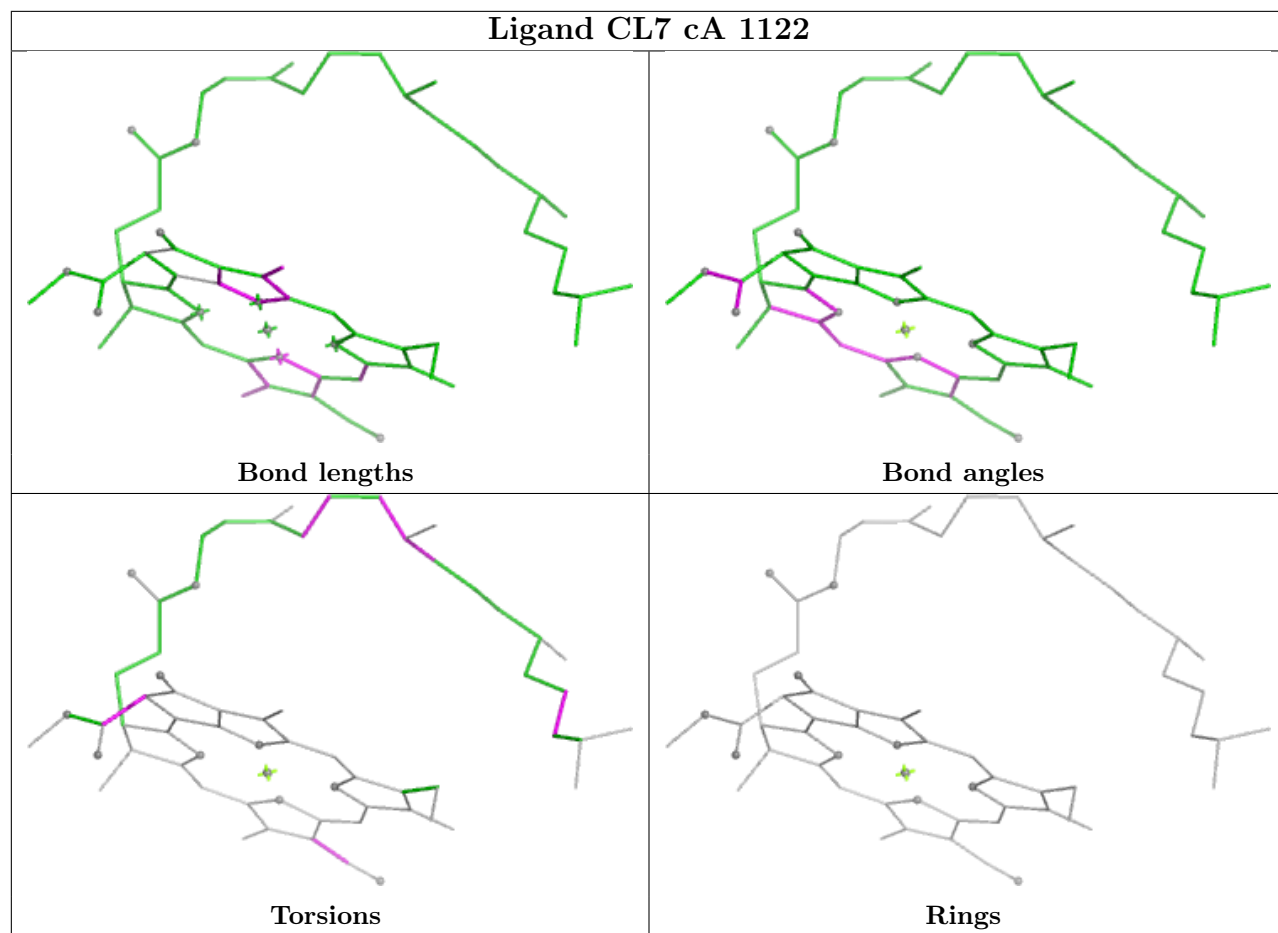


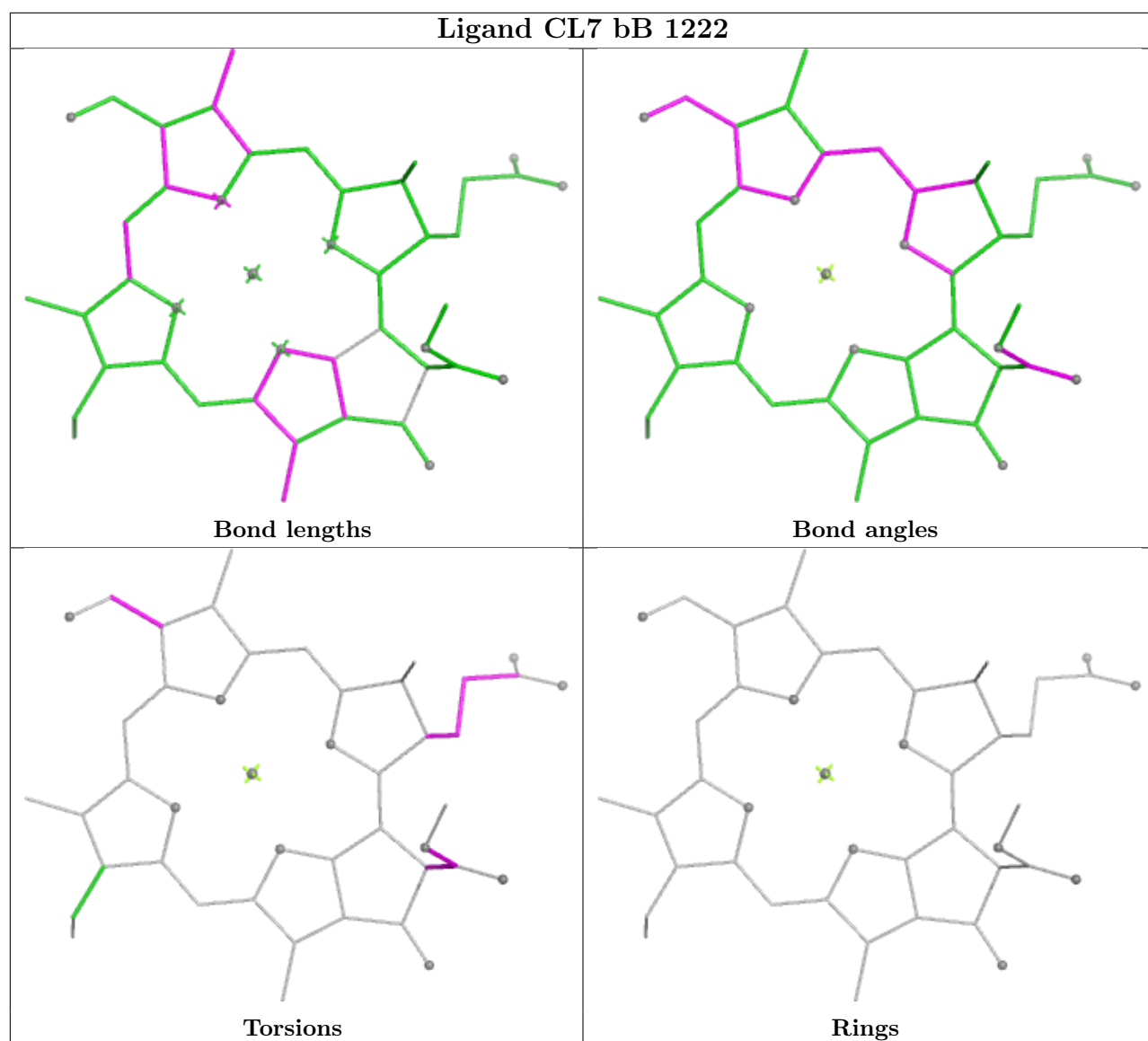


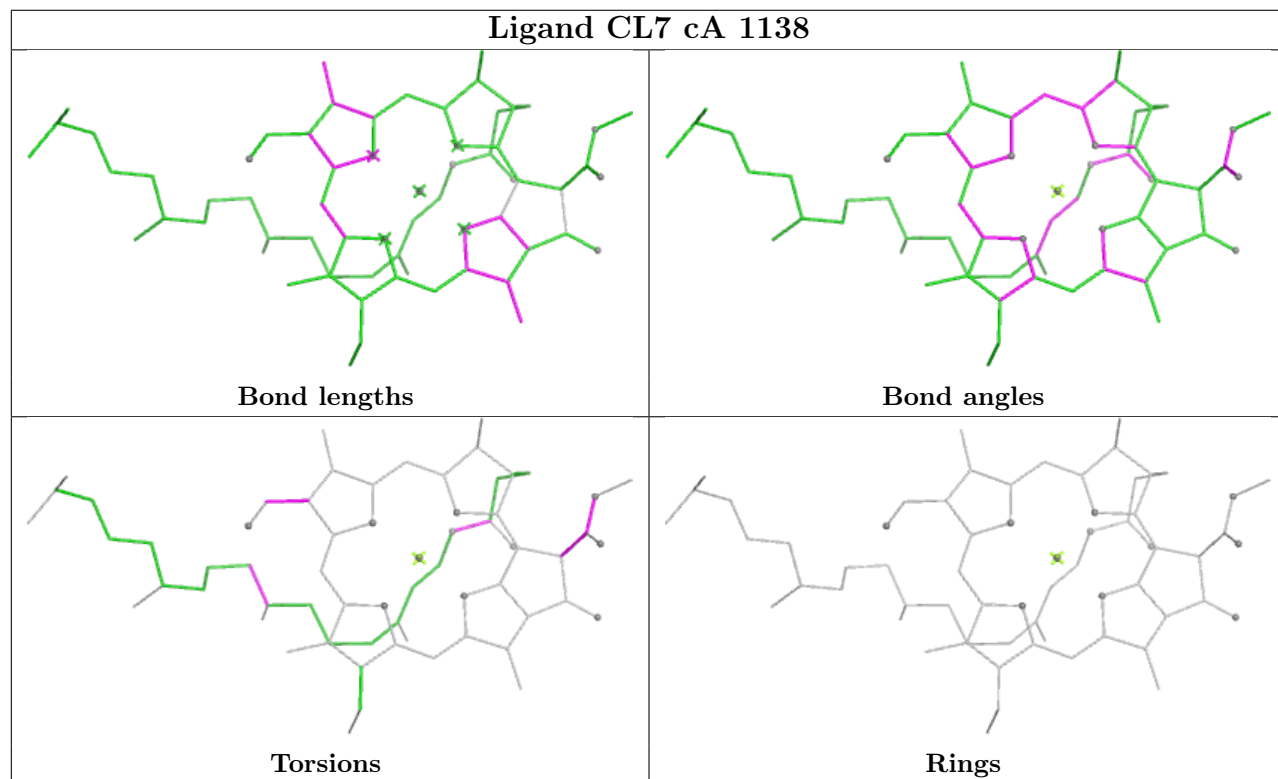
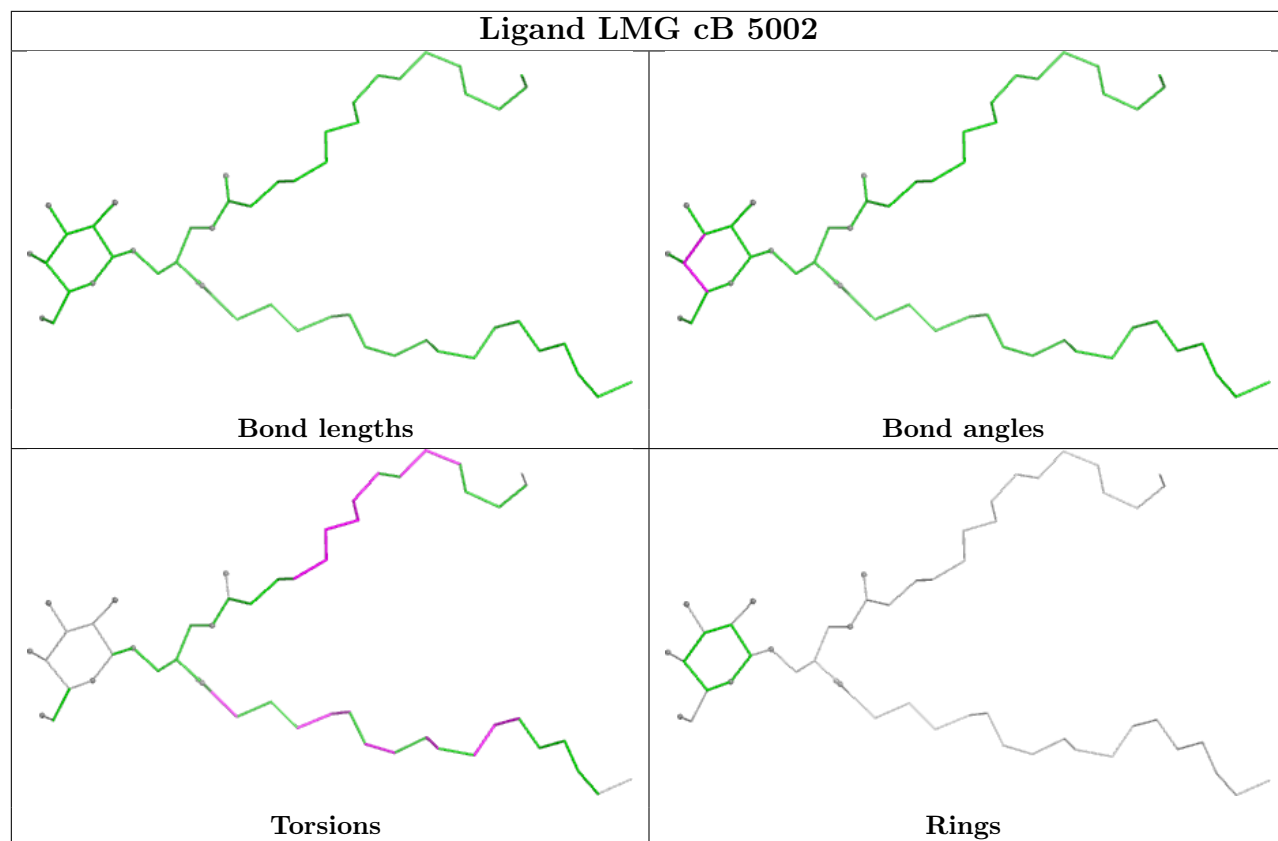
Ligand CL7 bB 1220

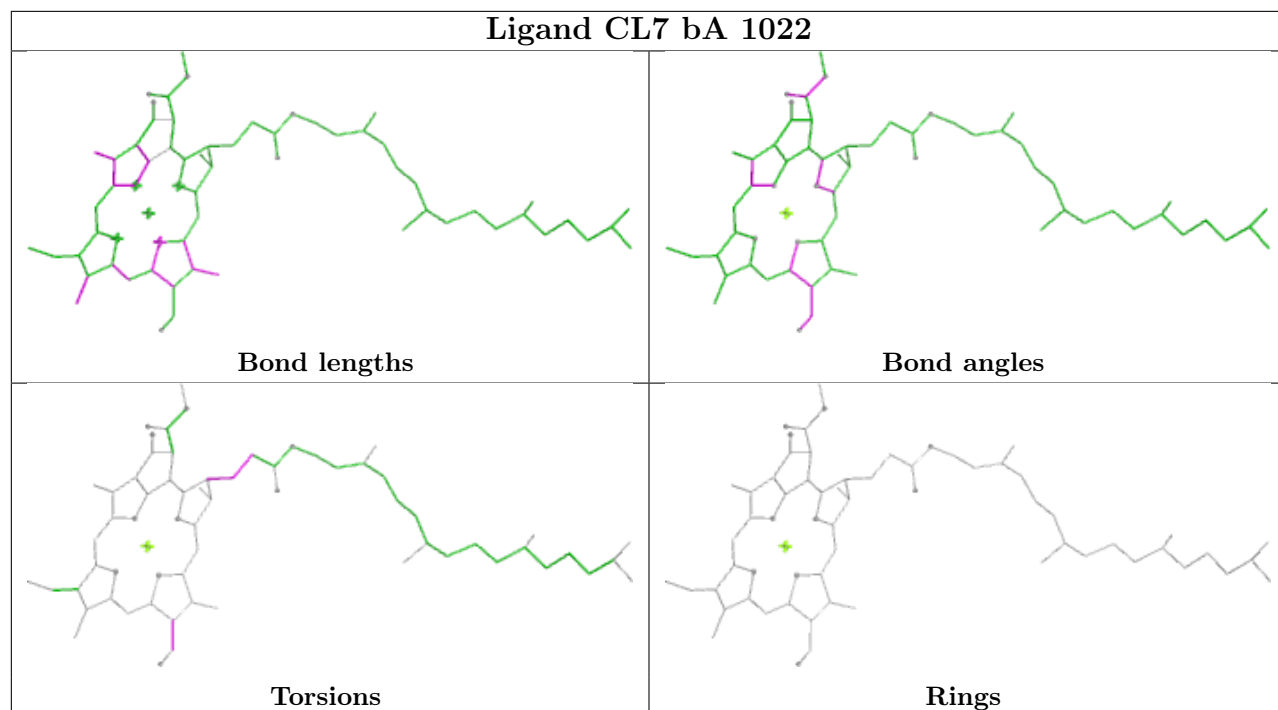




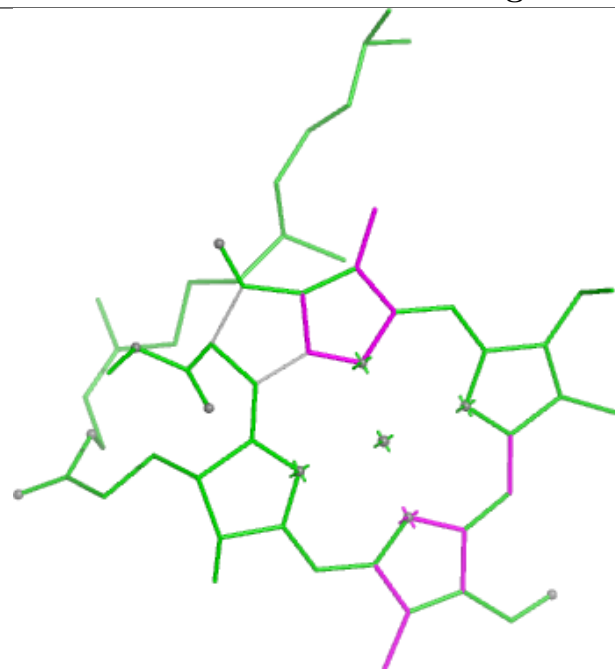




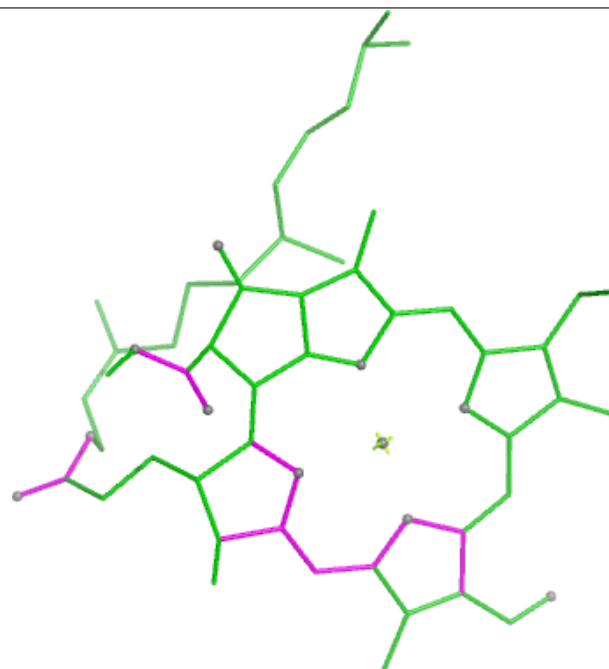




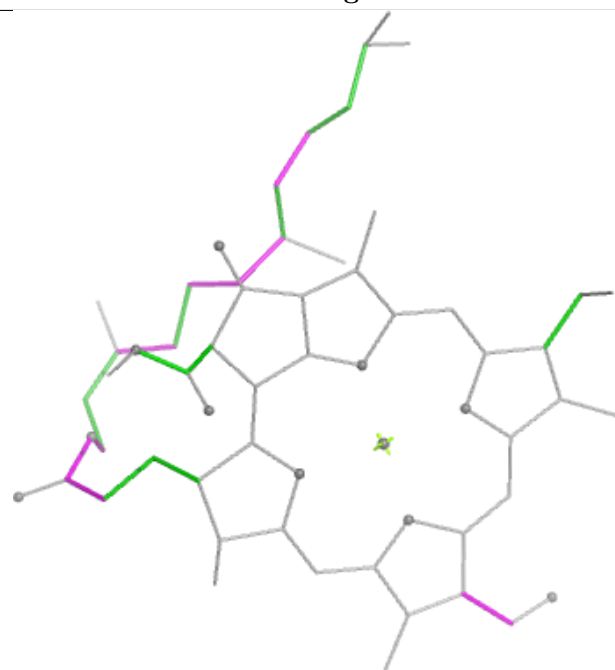
Ligand CL7 bL 1503



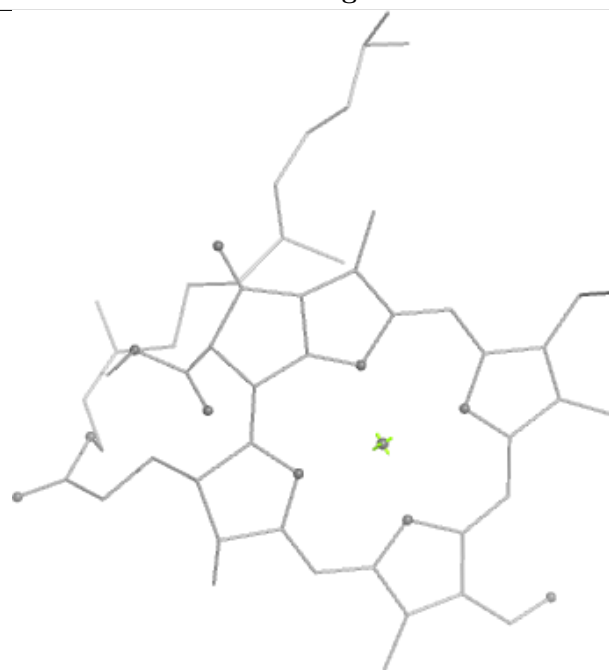
Bond lengths



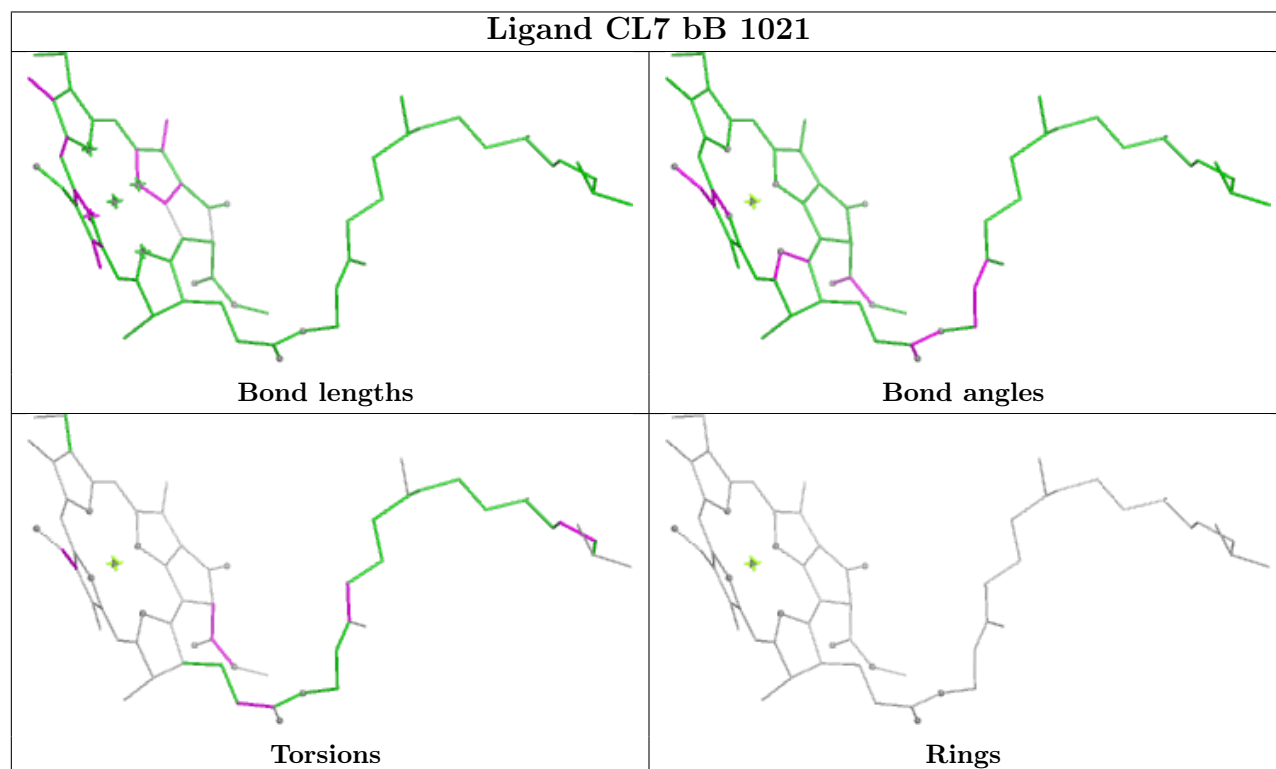
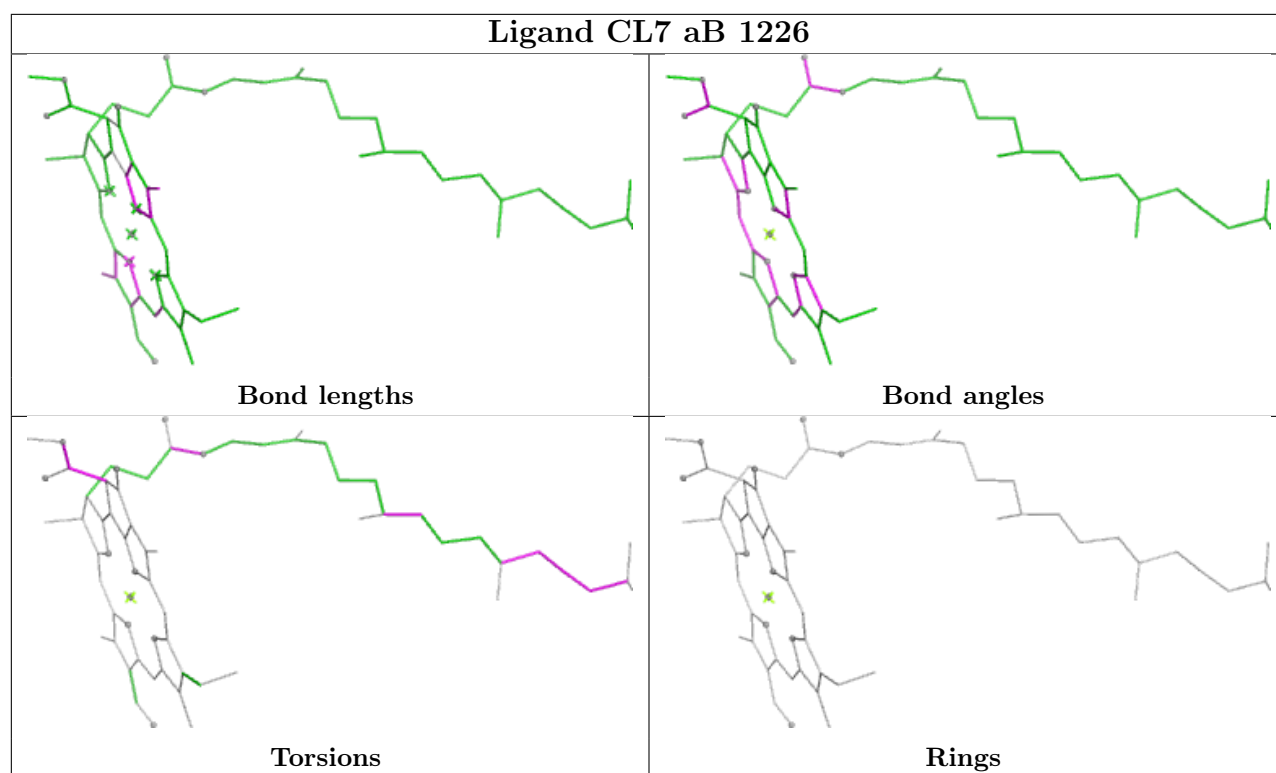
Bond angles



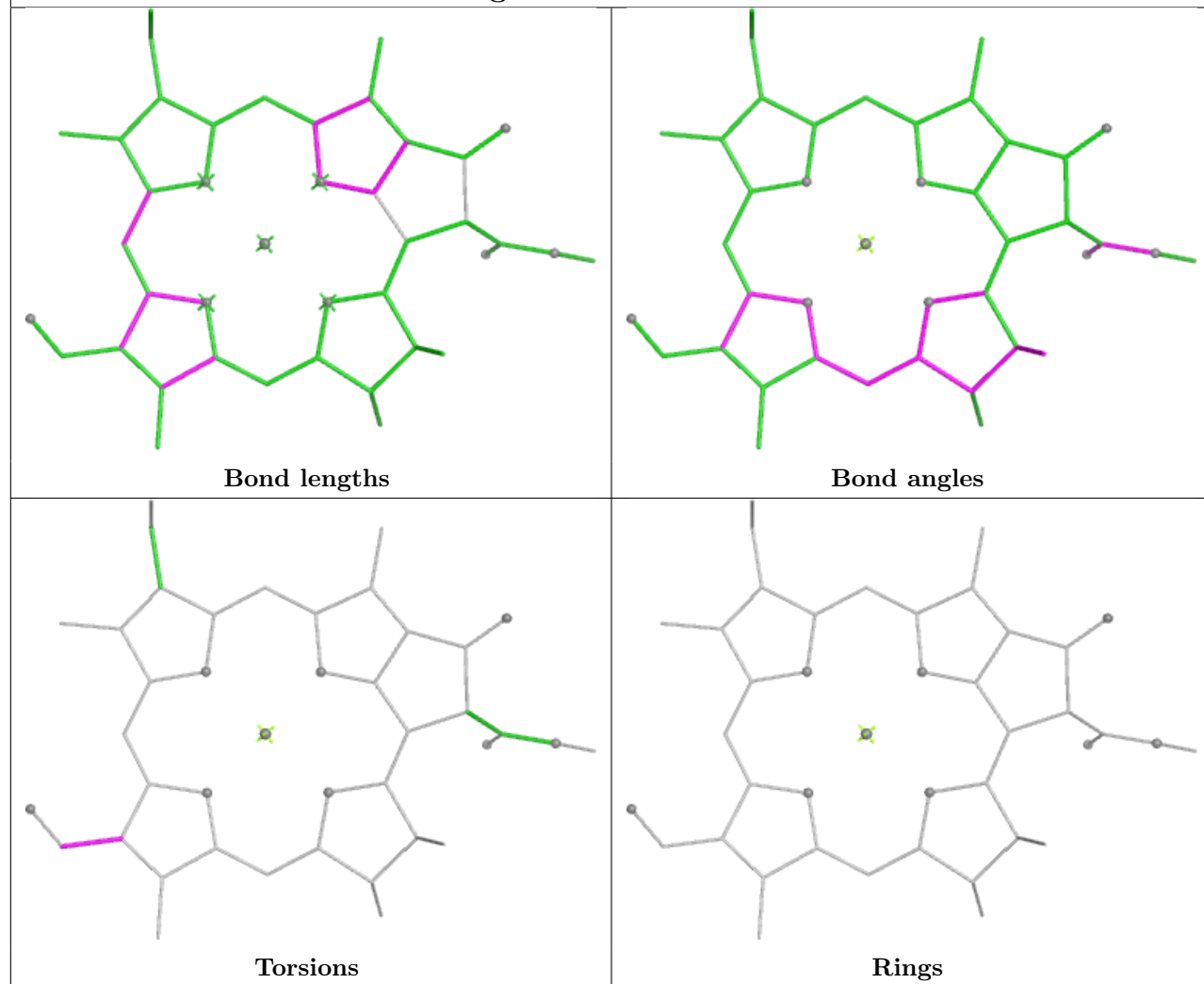
Torsions

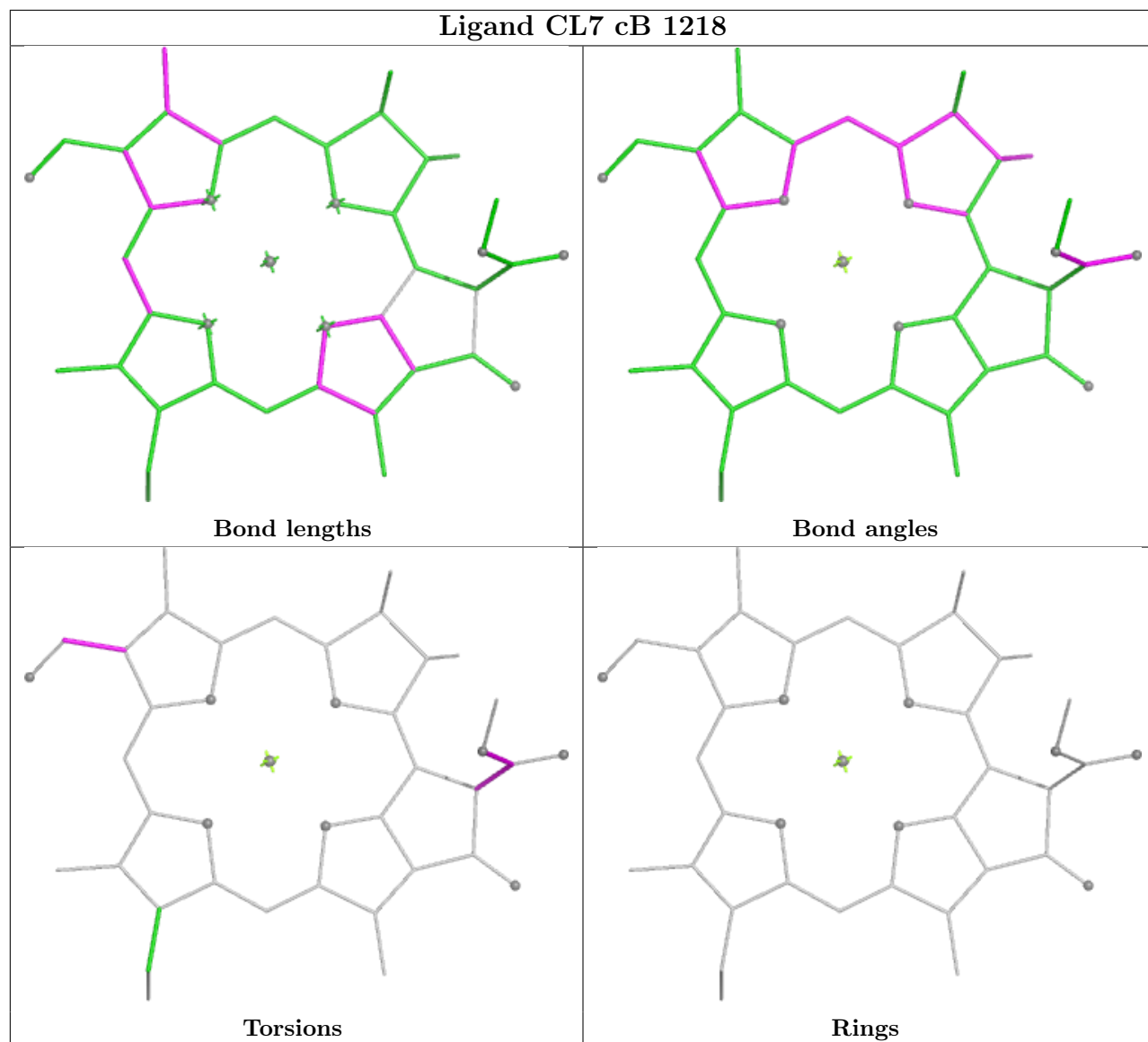


Rings

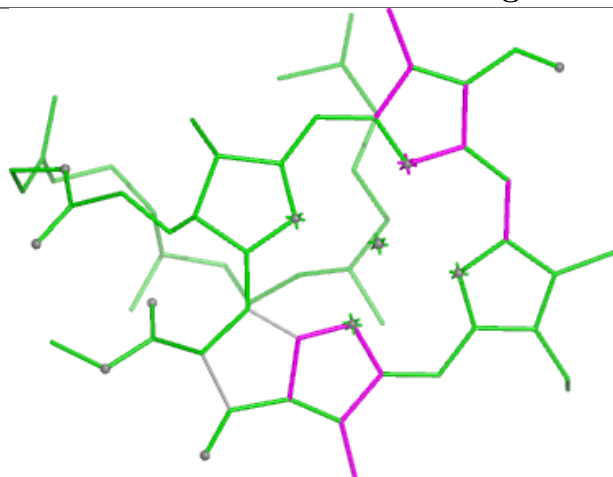


Ligand CL7 cB 1233

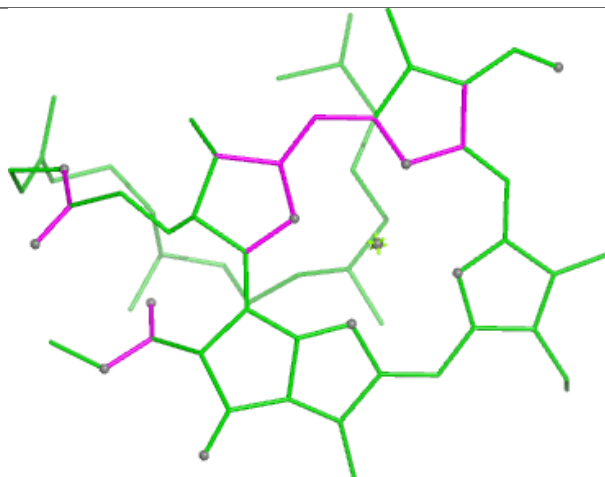




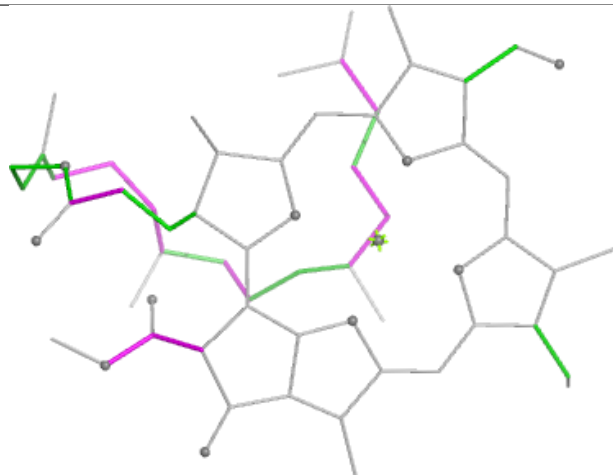
Ligand CL7 cB 1203



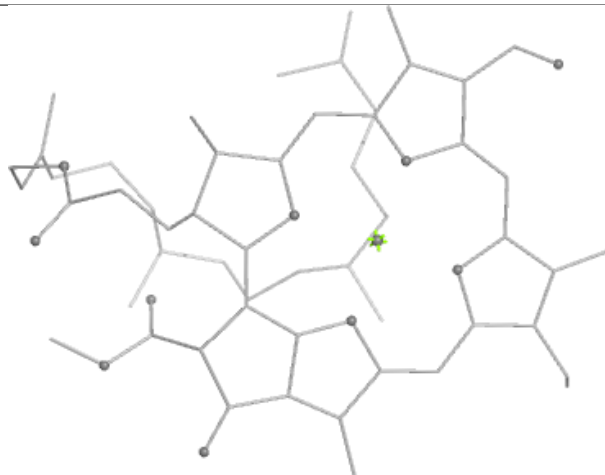
Bond lengths



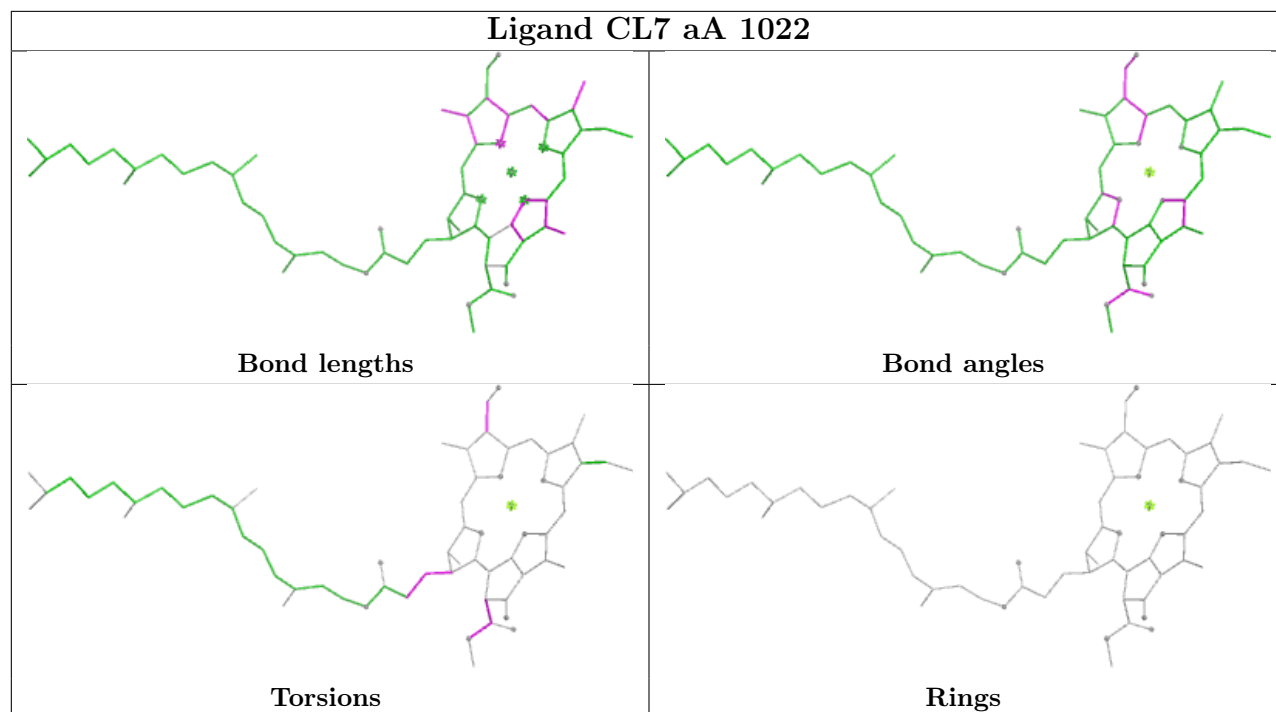
Bond angles

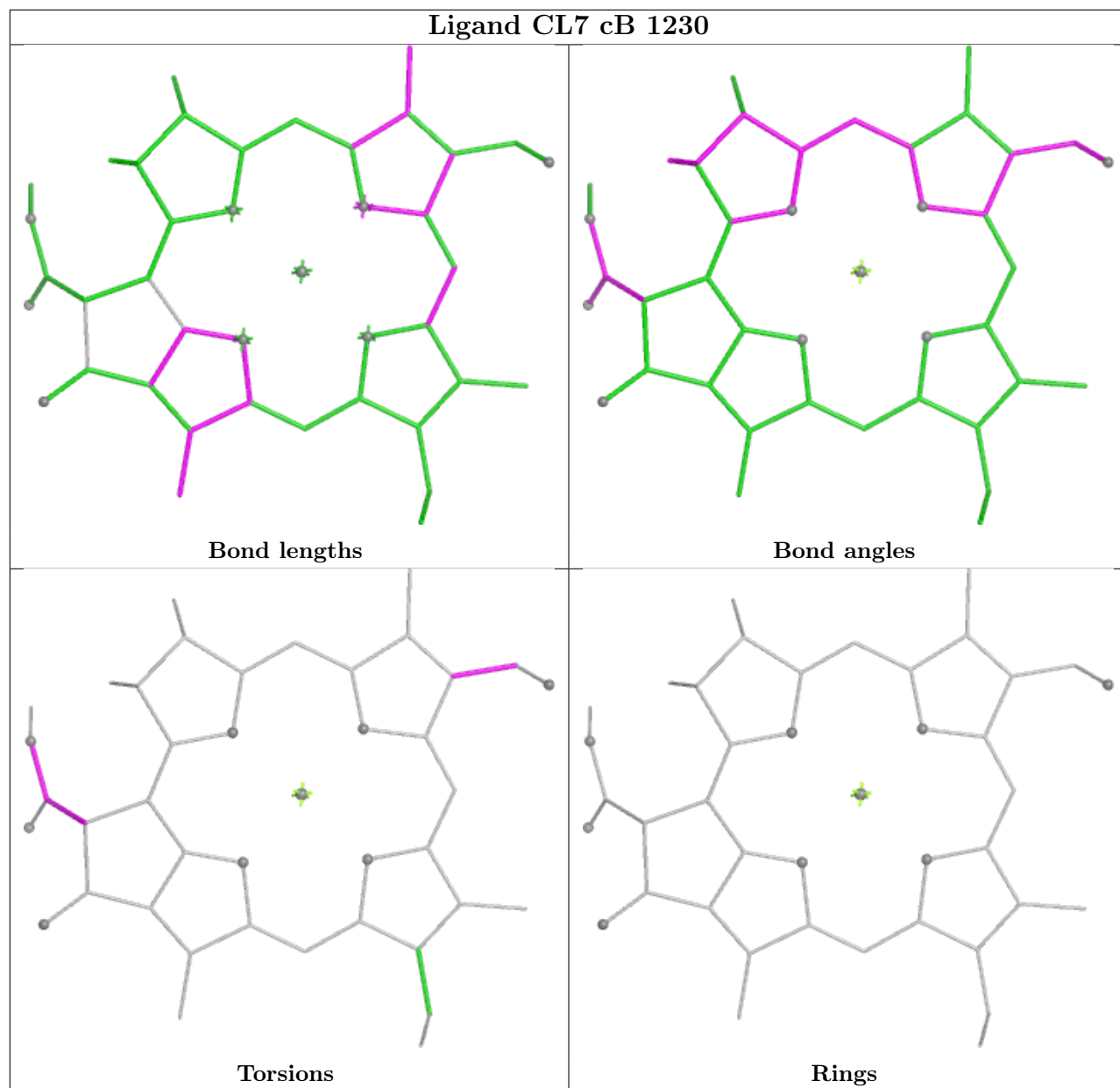


Torsions

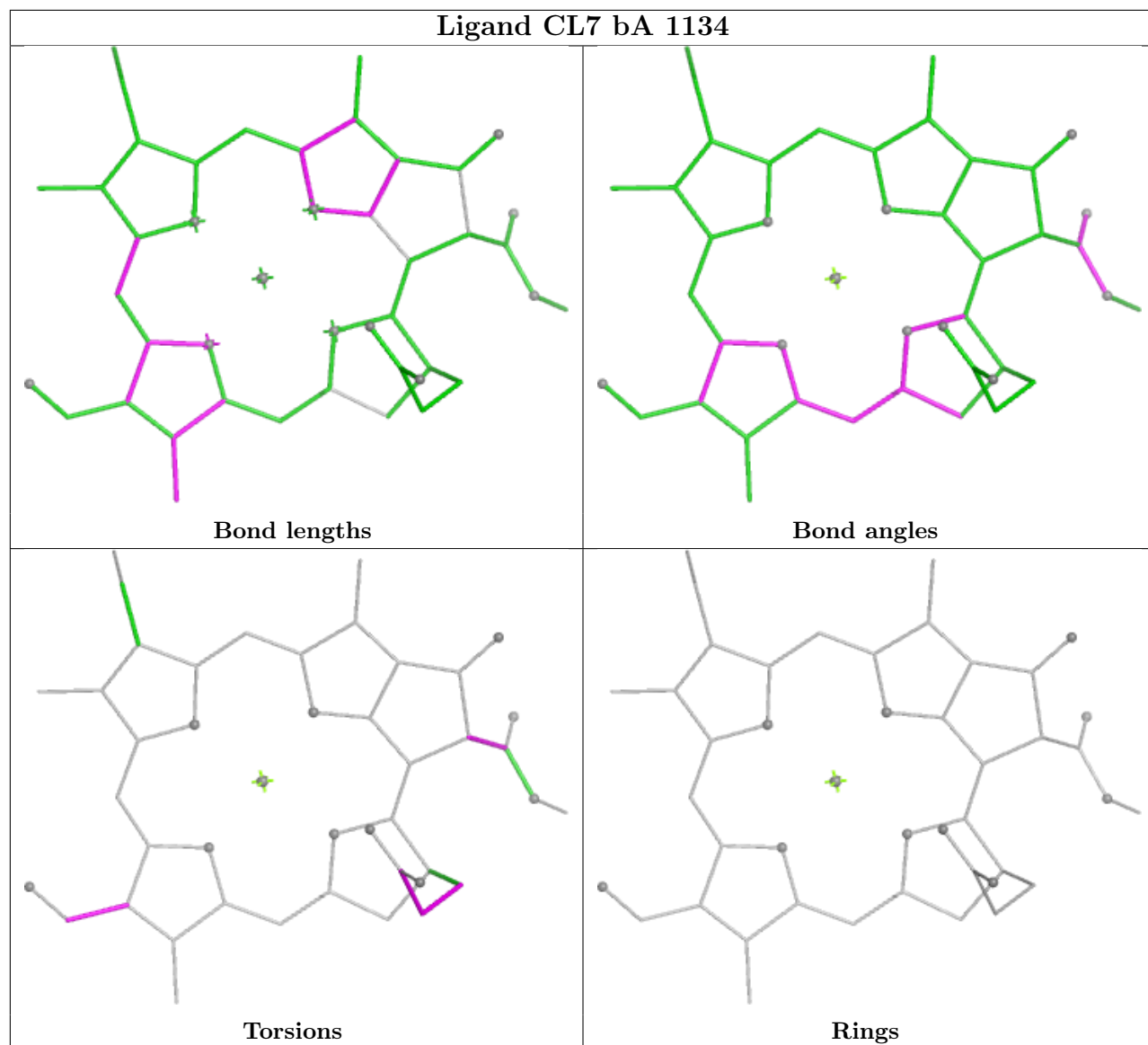


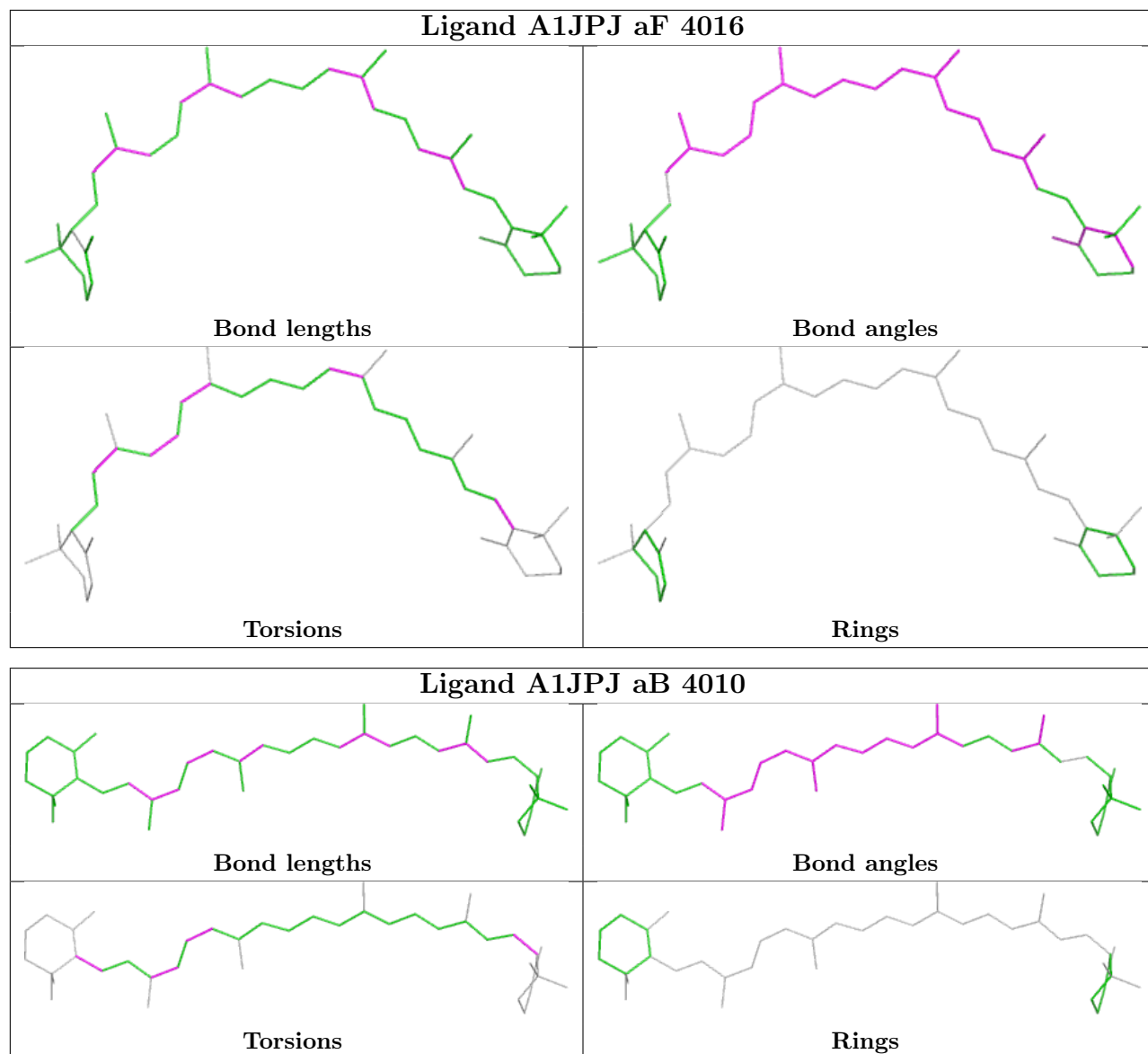
Rings

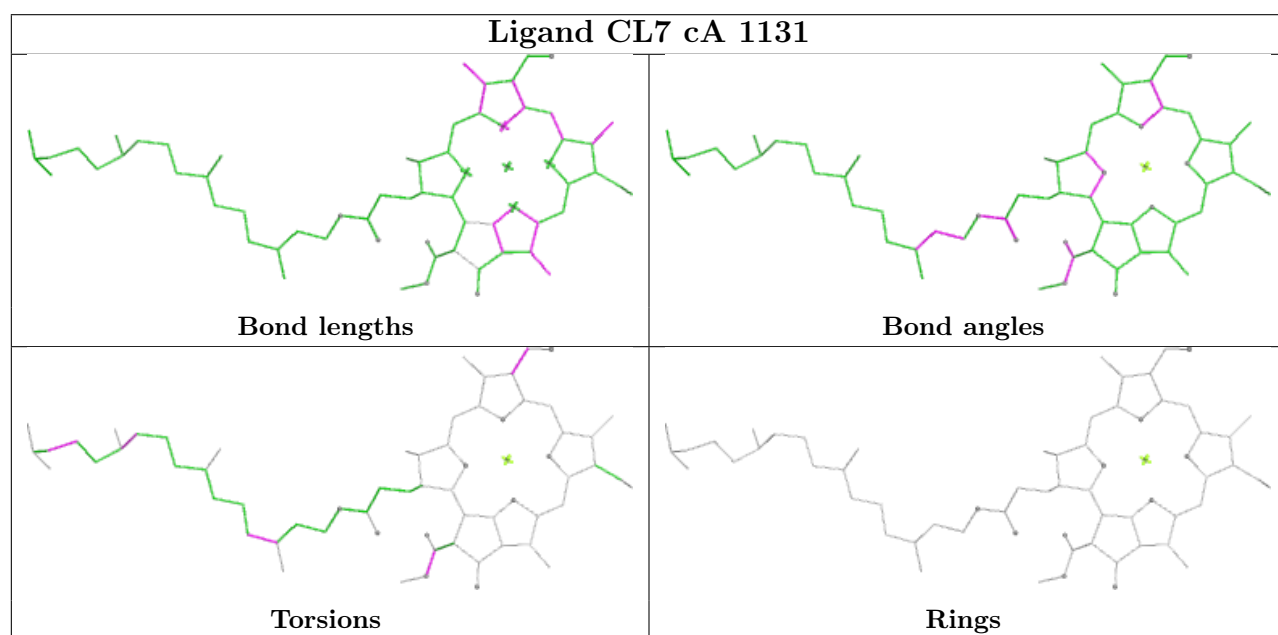
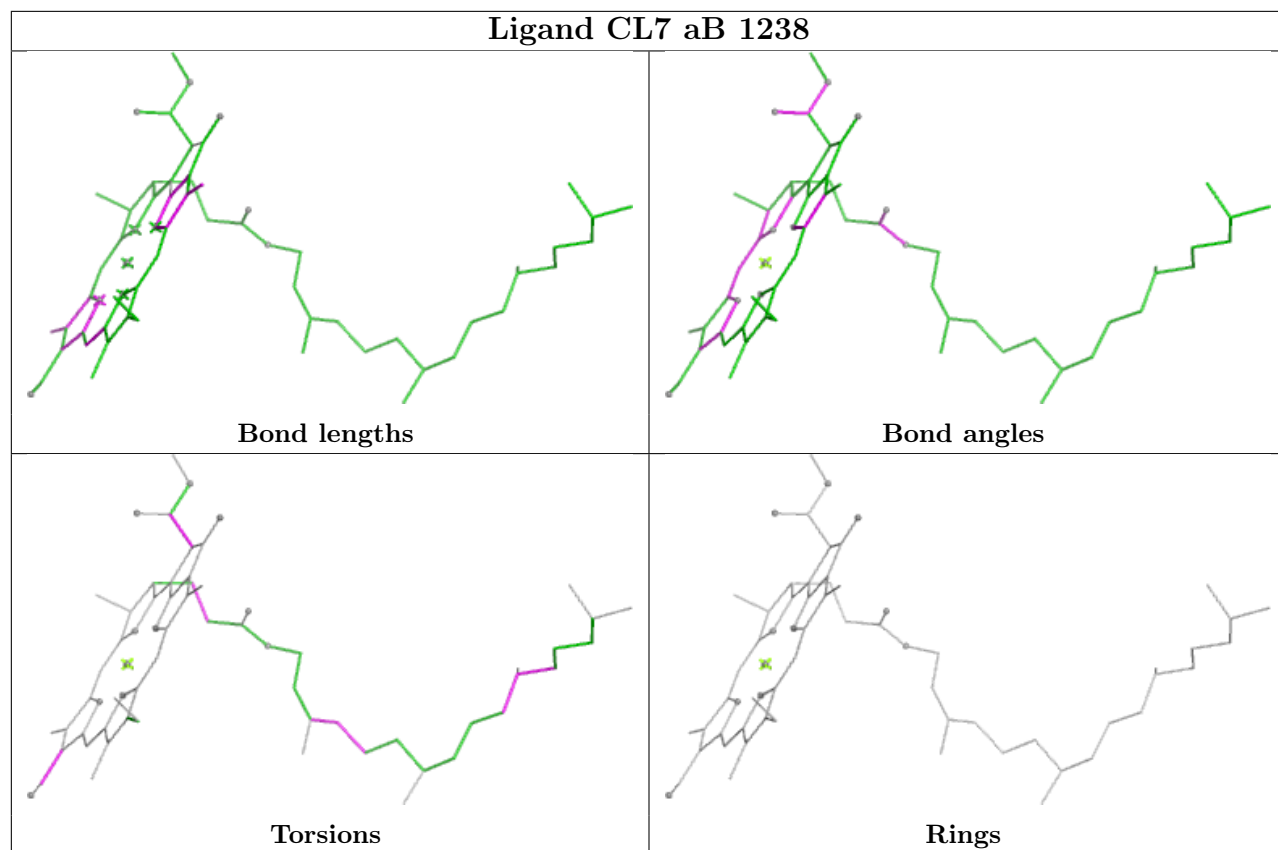




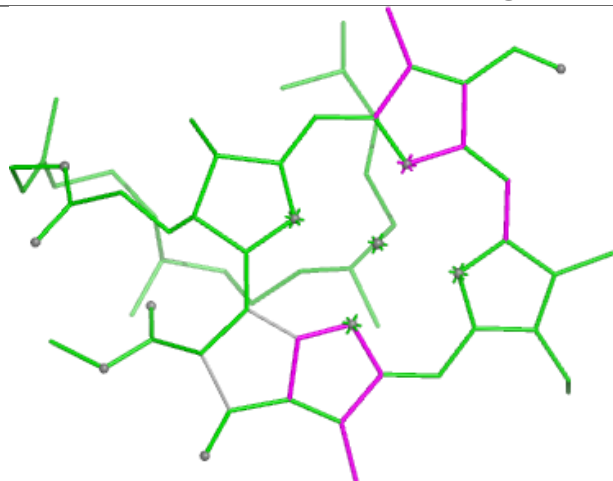
Ligand CL7 bA 1134



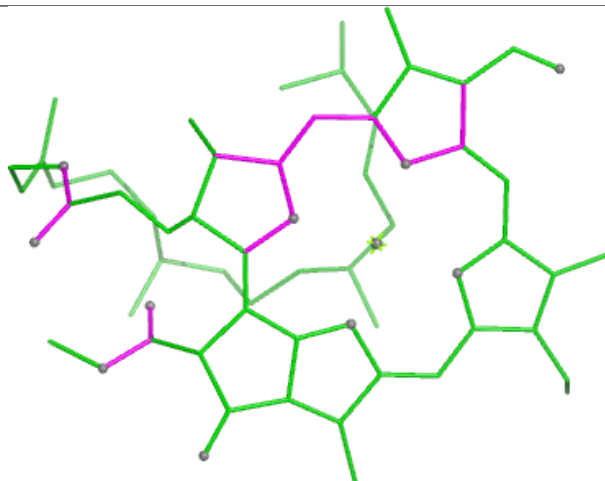




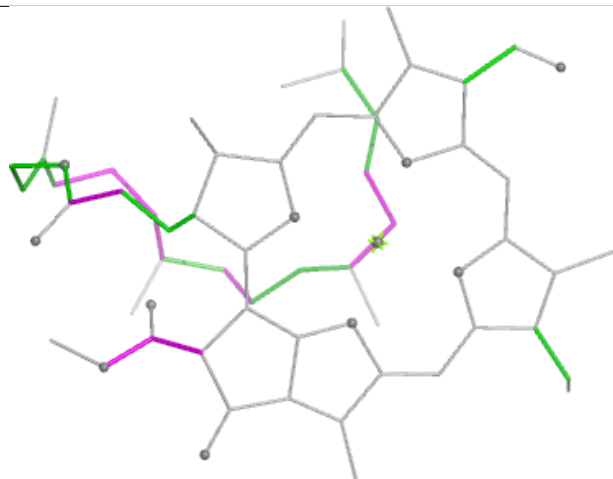
Ligand CL7 bB 1203



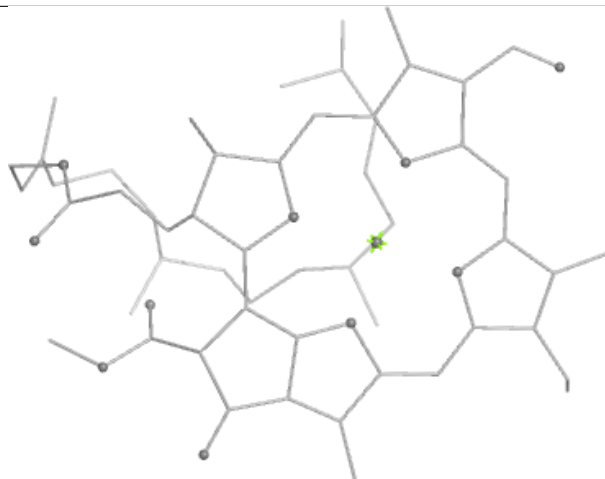
Bond lengths



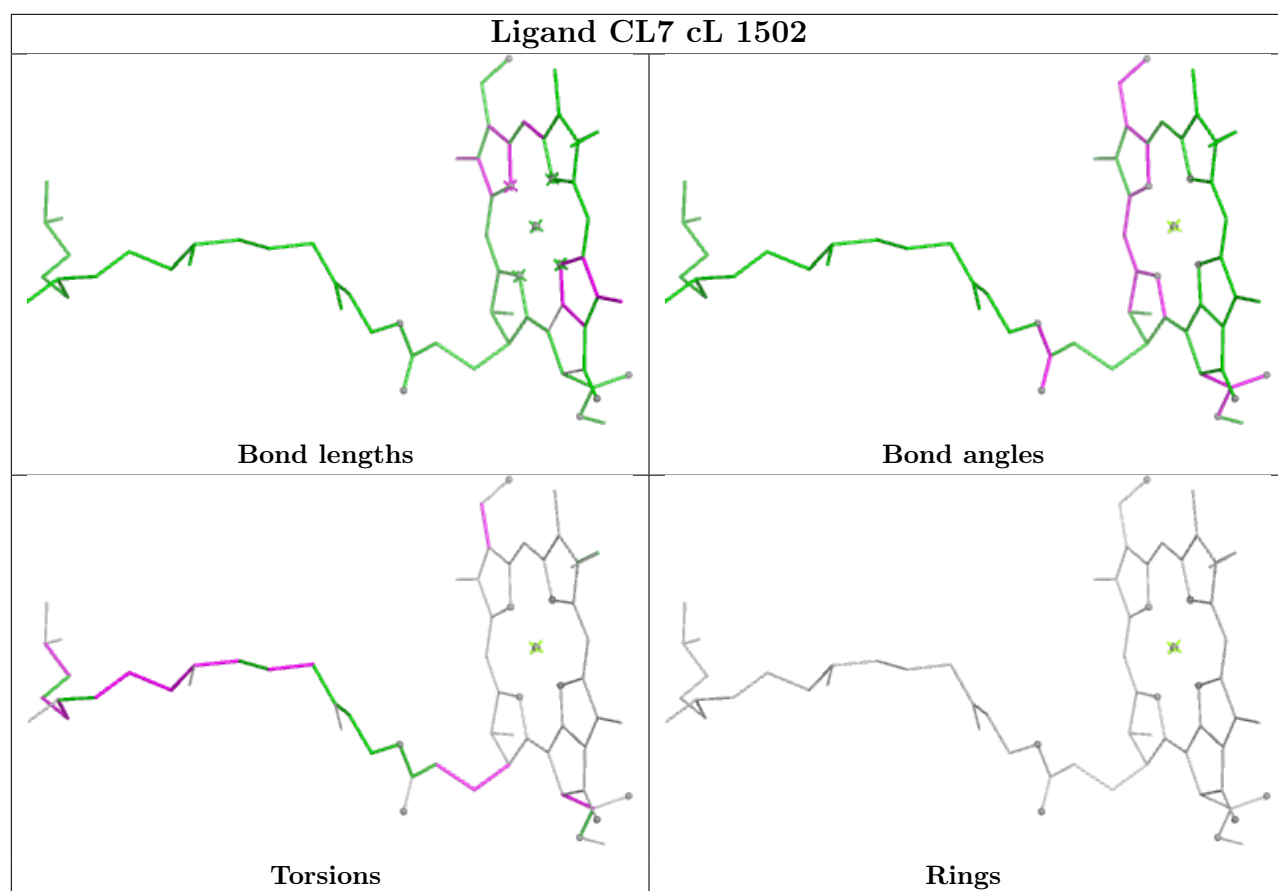
Bond angles

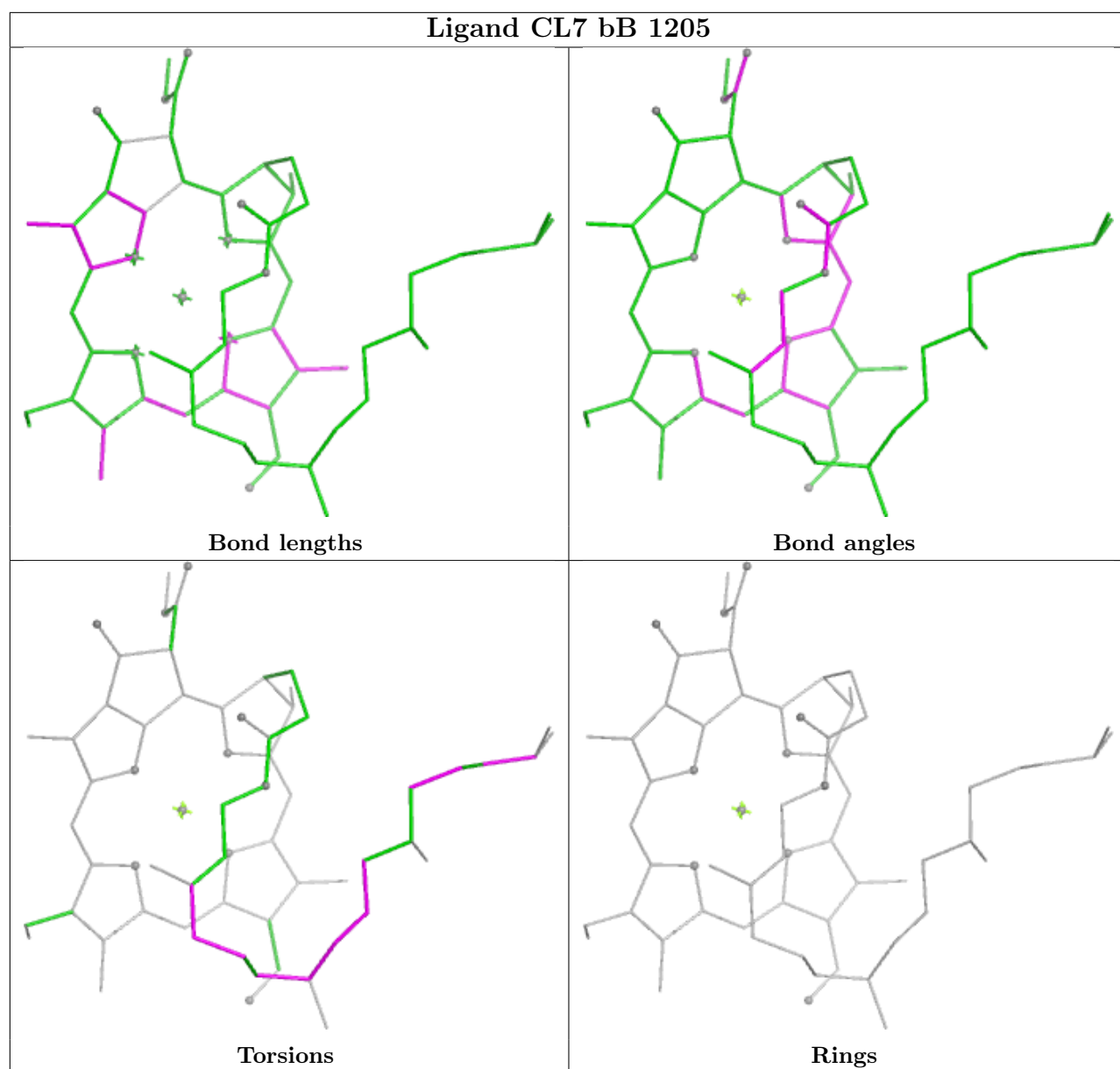


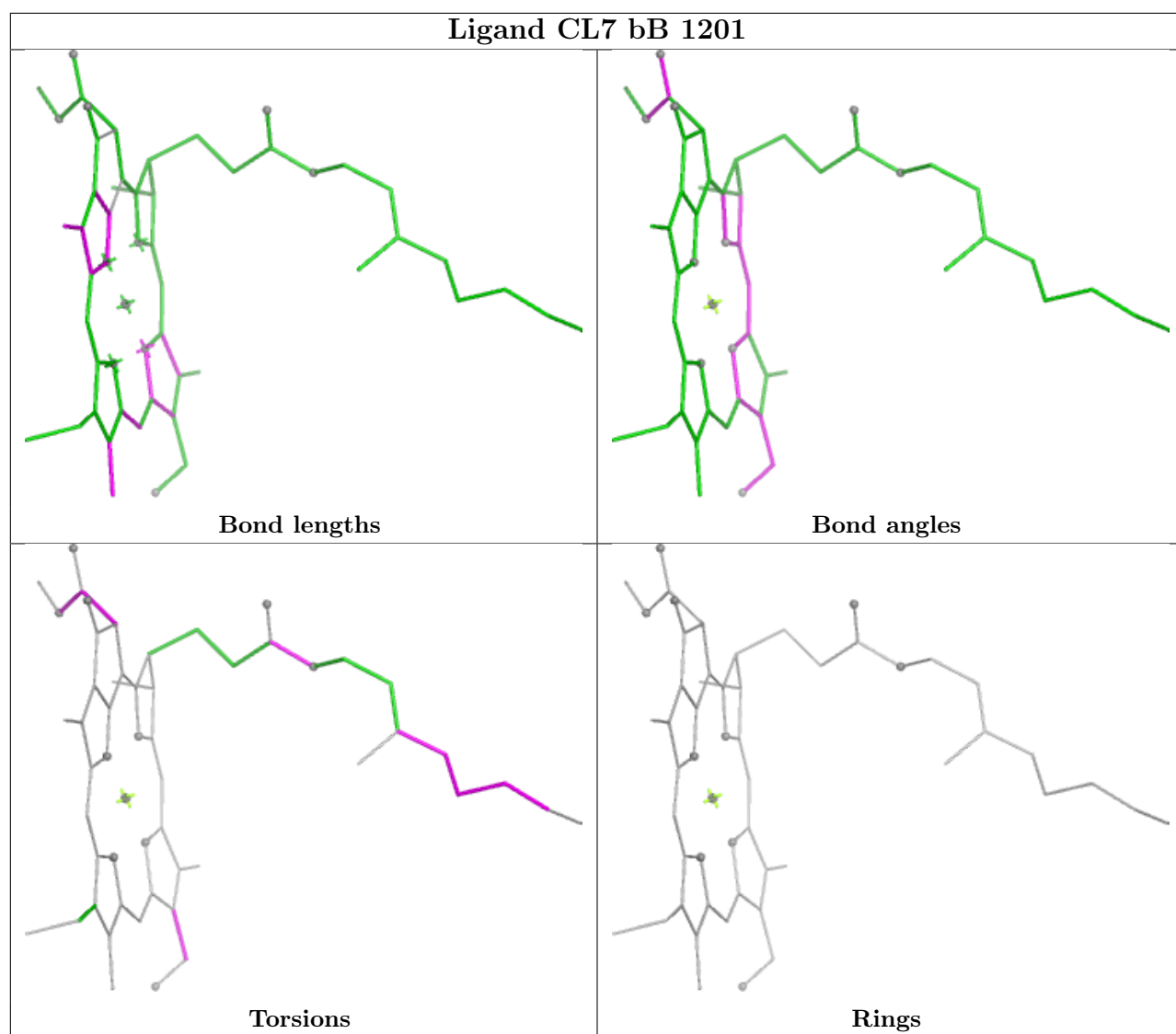
Torsions



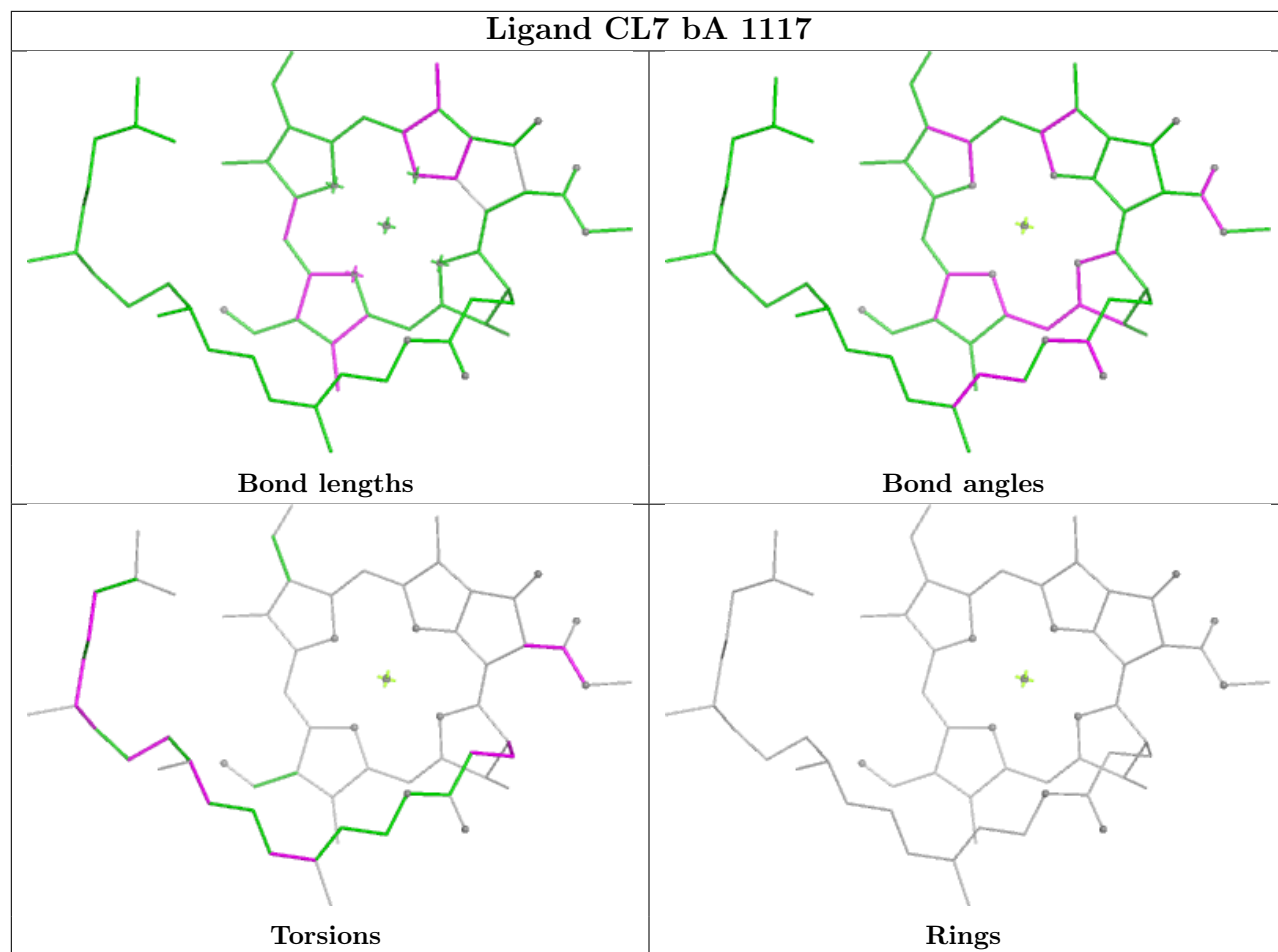
Rings

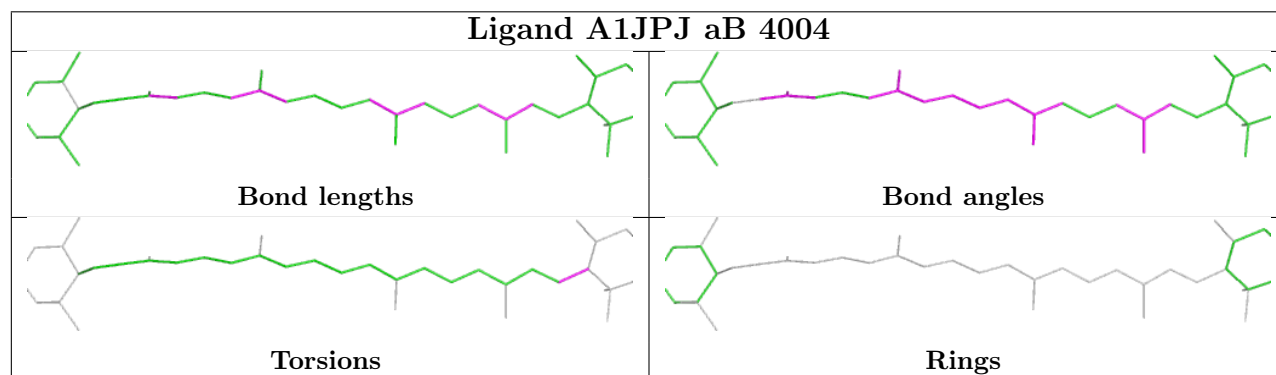
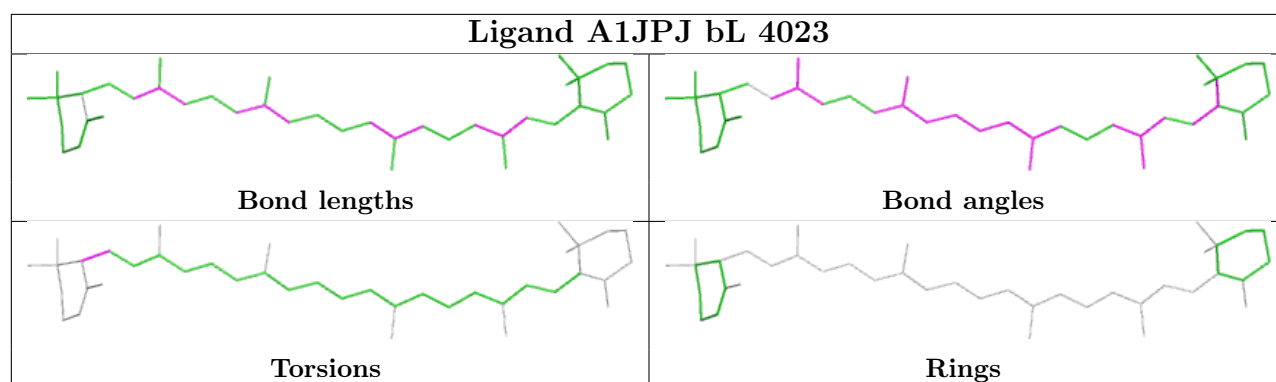
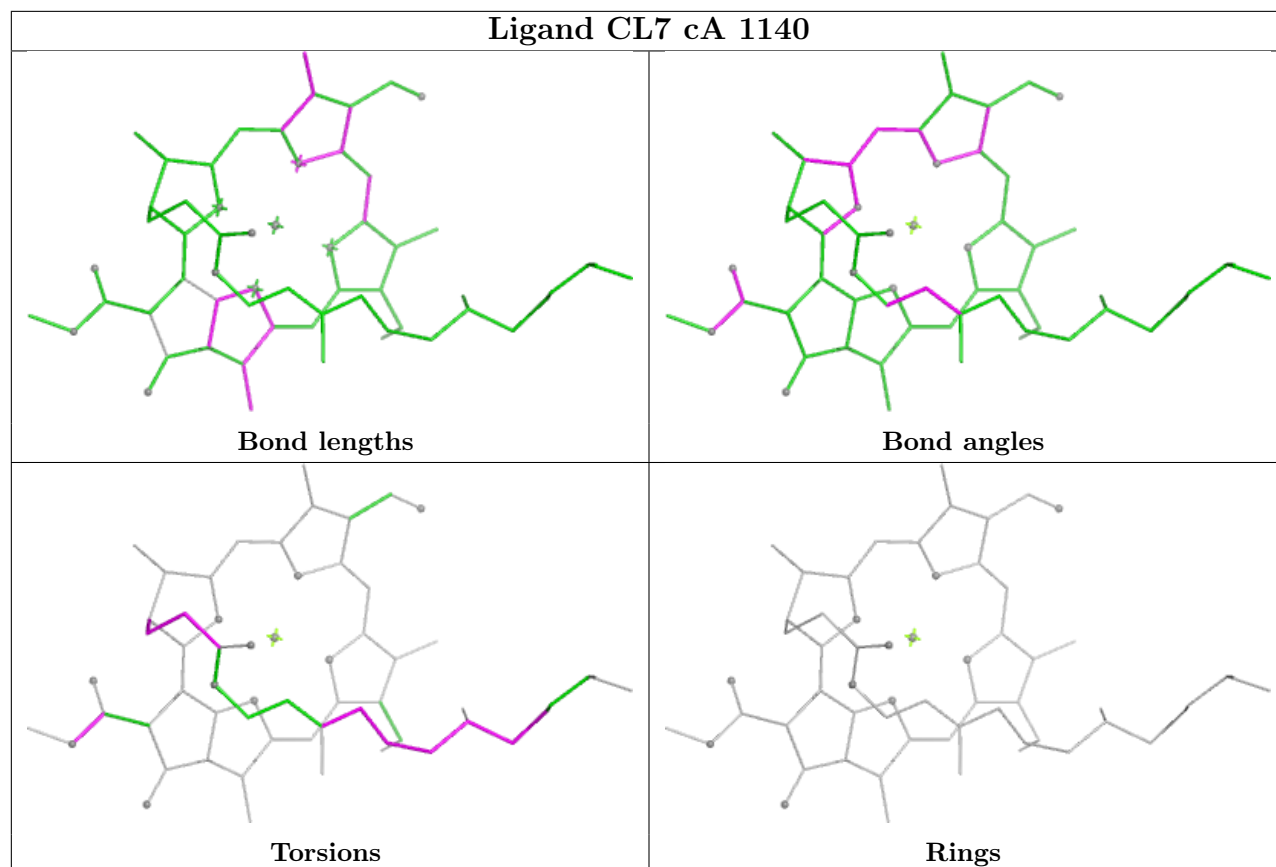


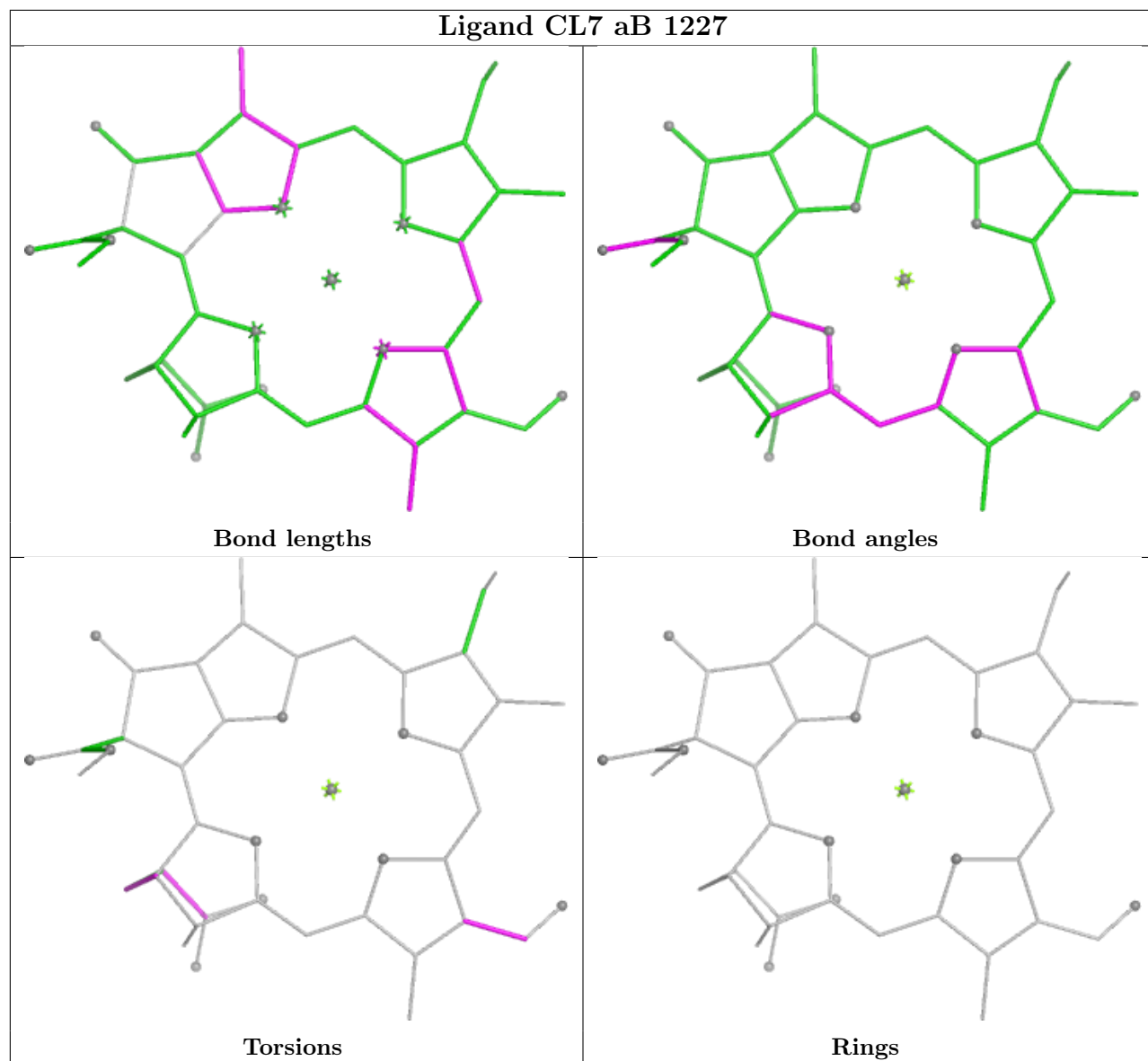


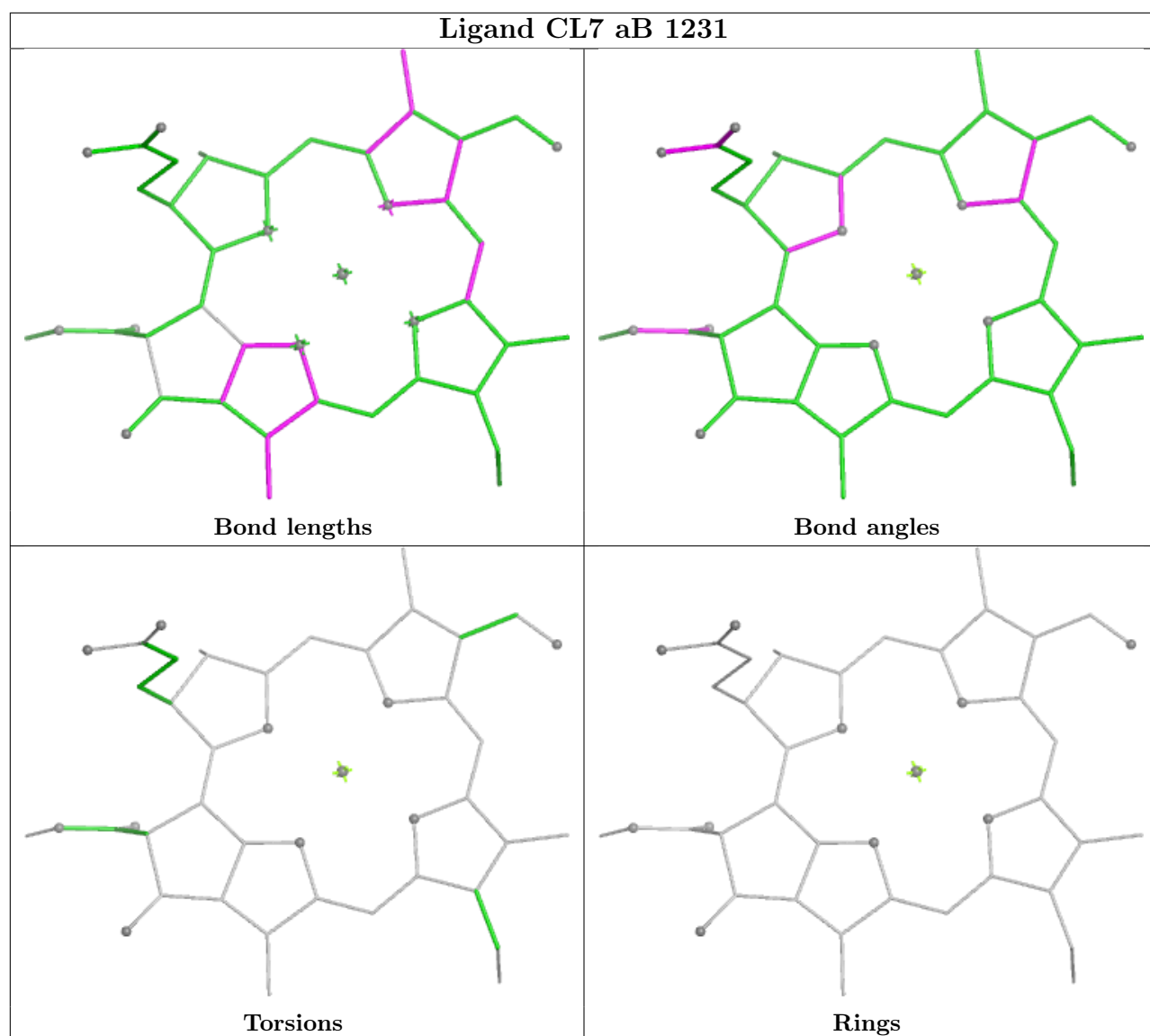


Ligand CL7 bA 1117

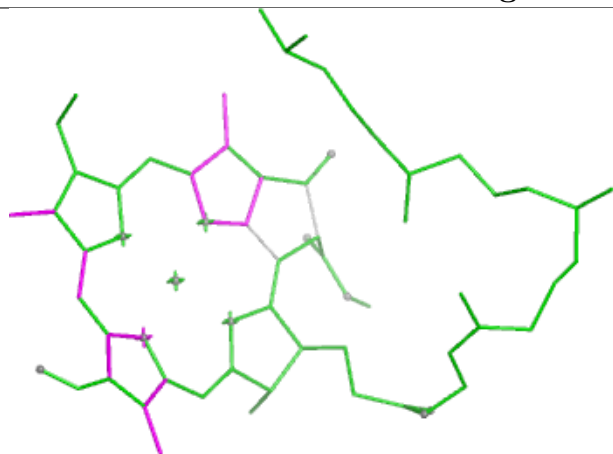




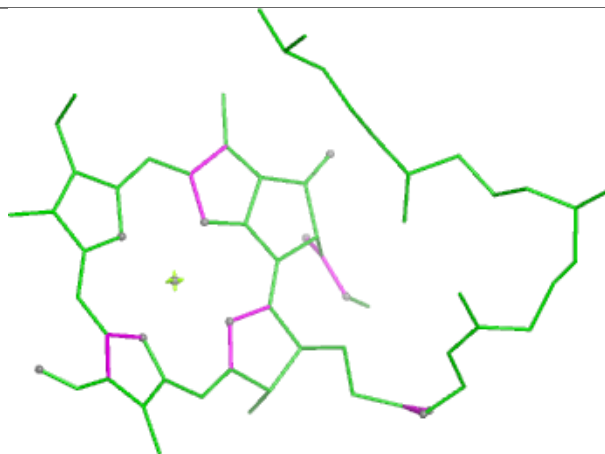




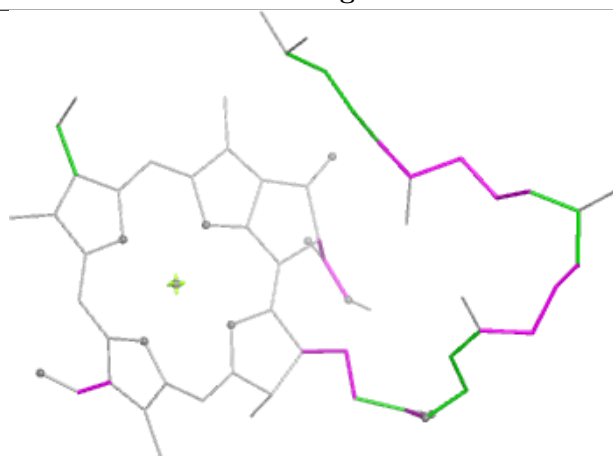
Ligand CL7 bA 1127



Bond lengths



Bond angles

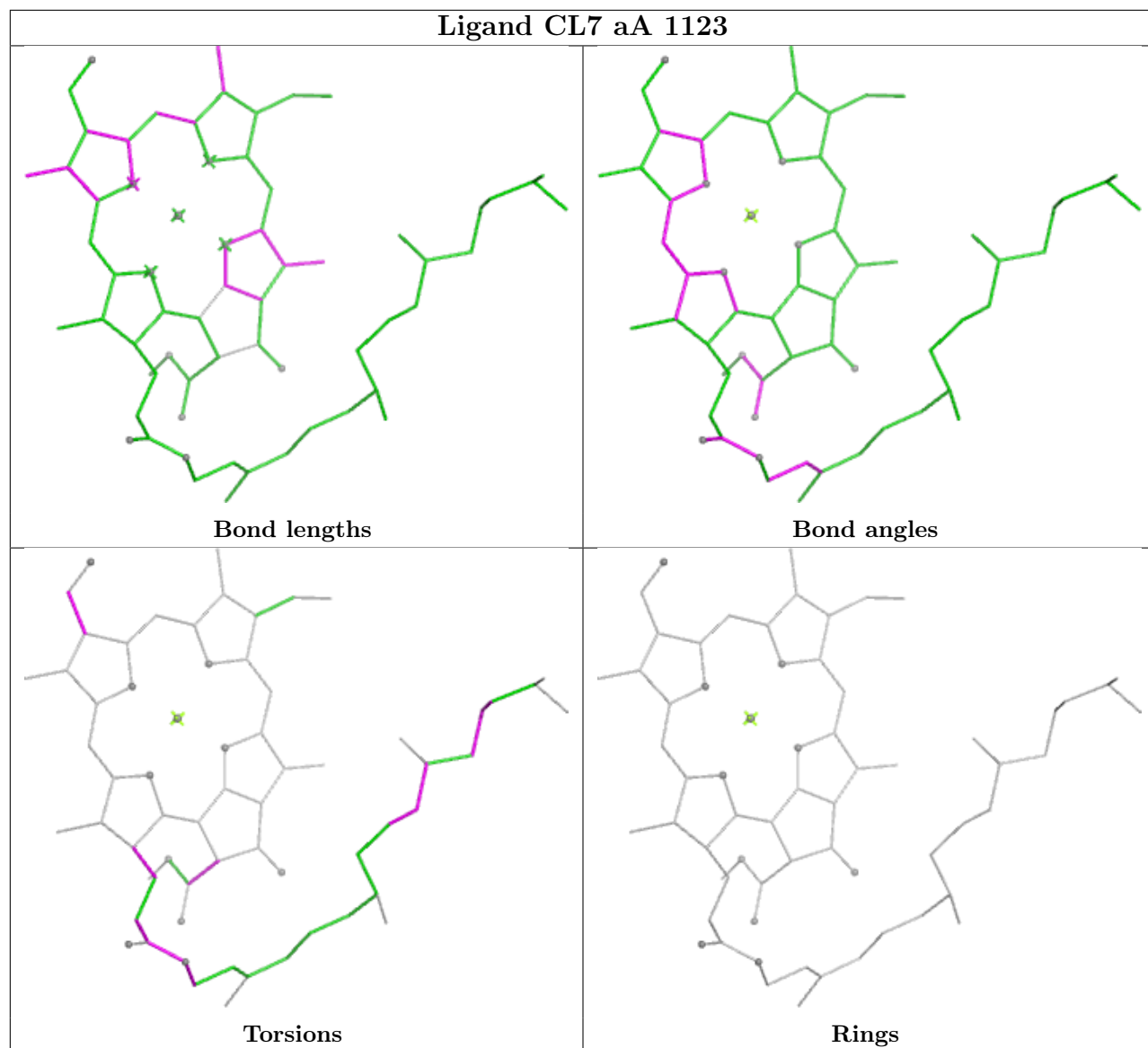


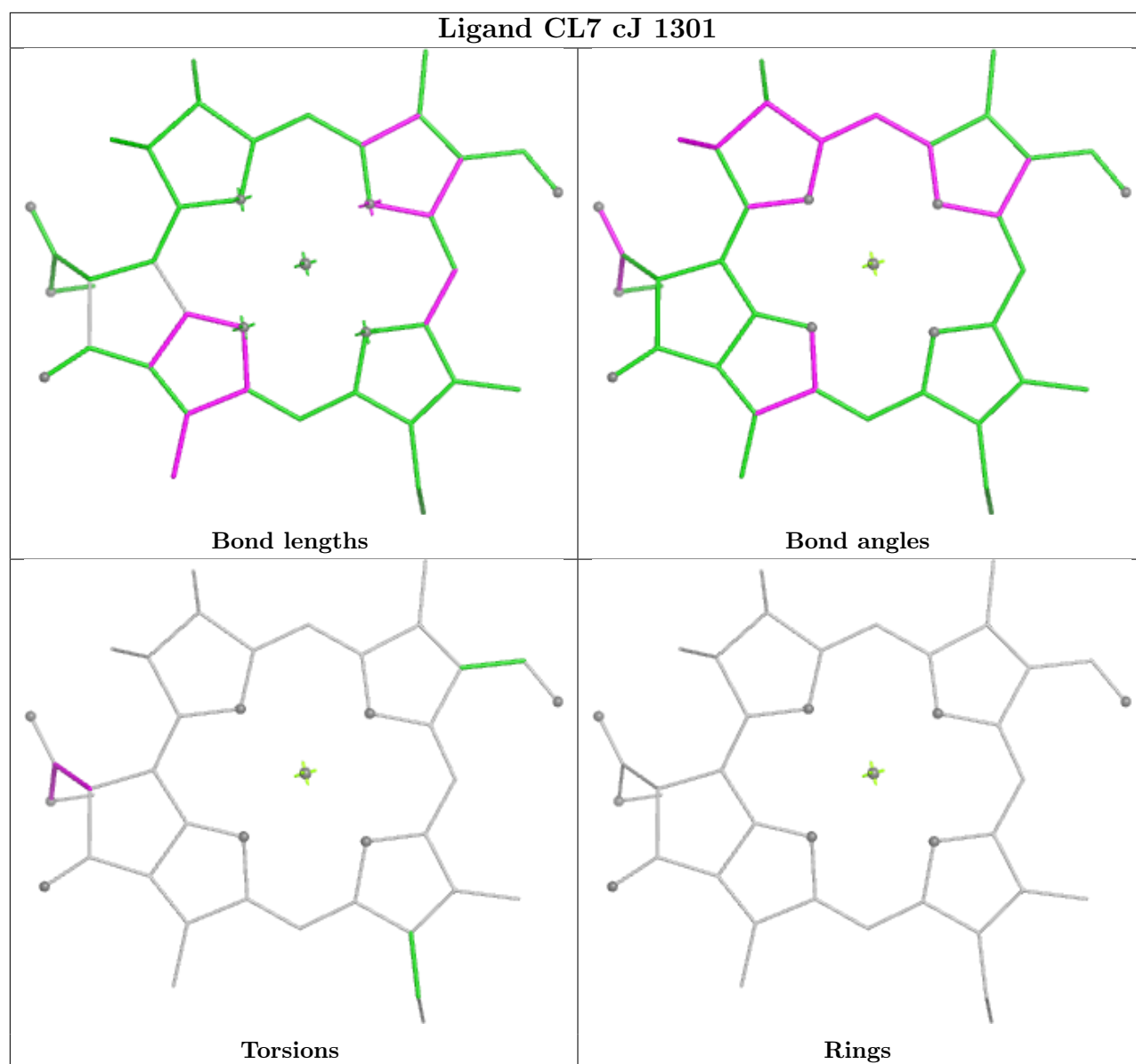
Torsions

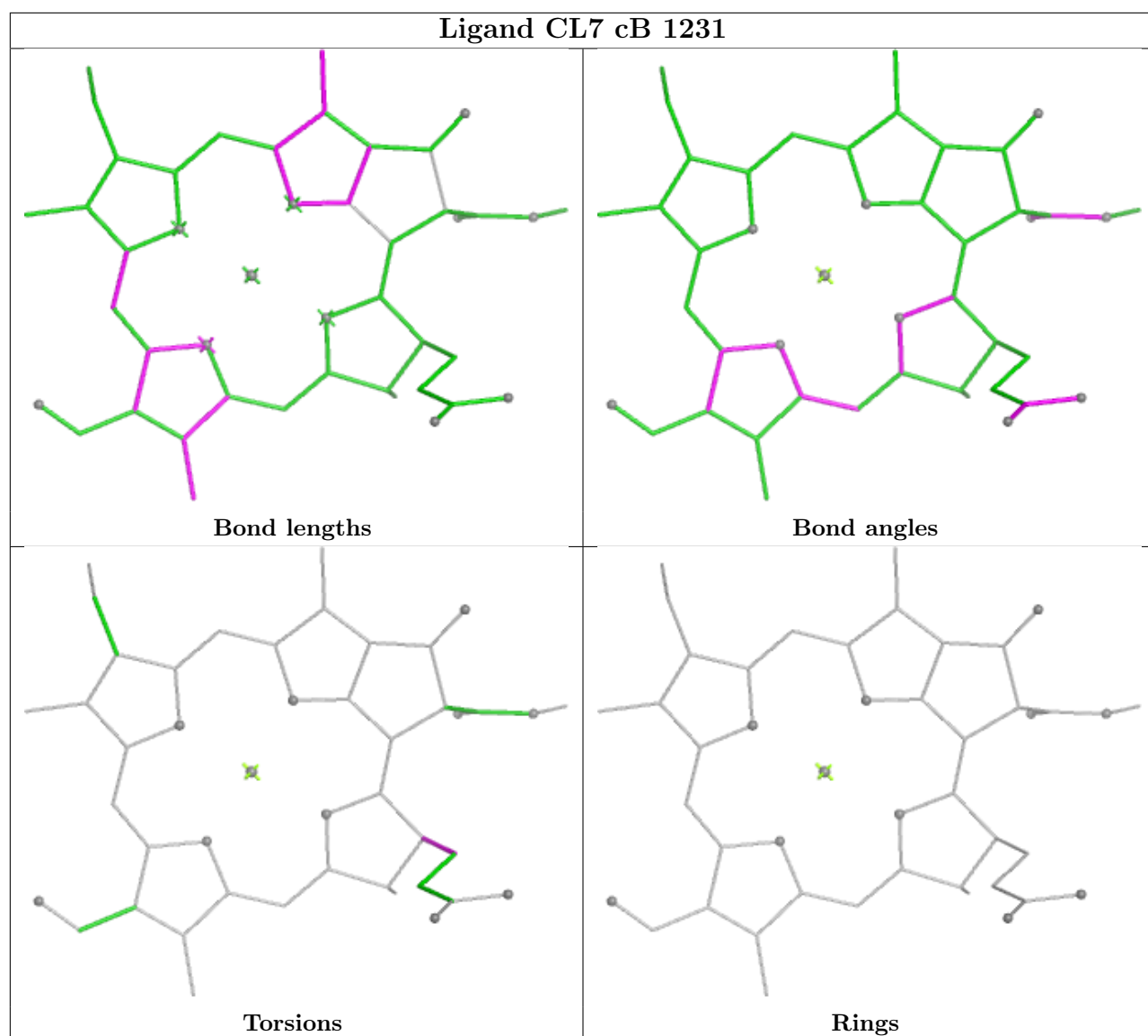


Rings

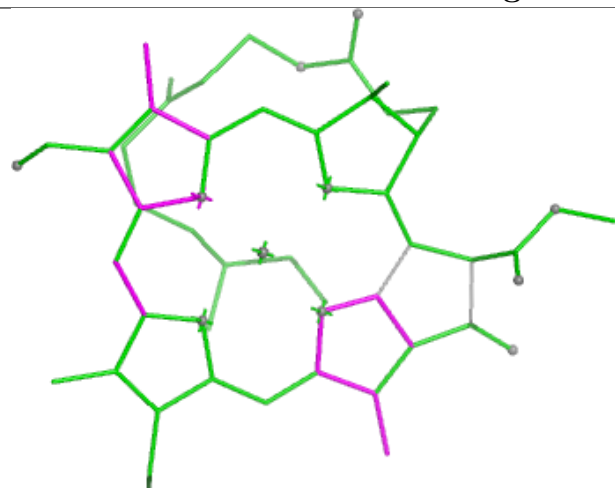
Ligand CL7 aA 1123



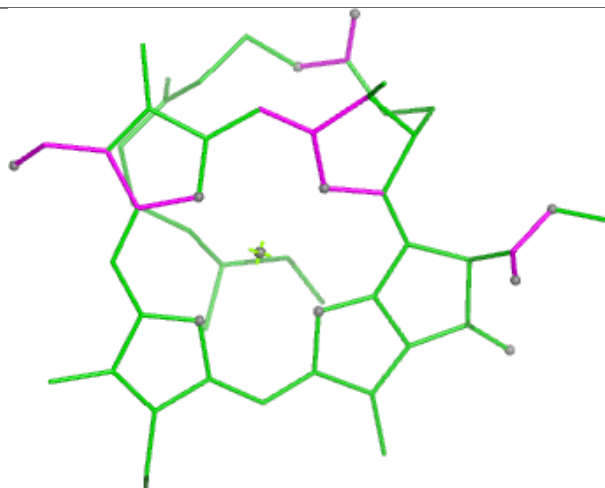




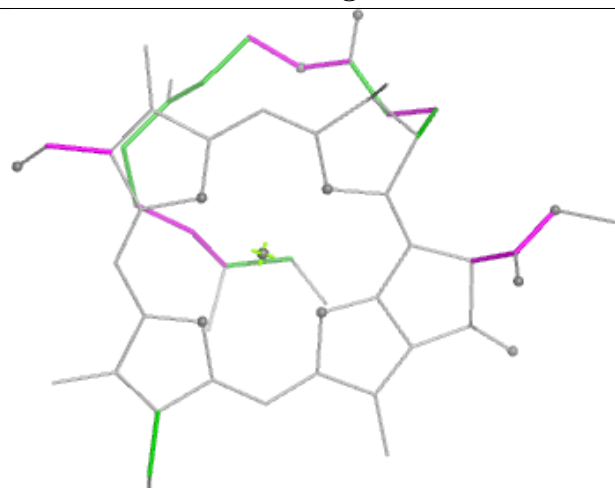
Ligand CL7 aB 1224



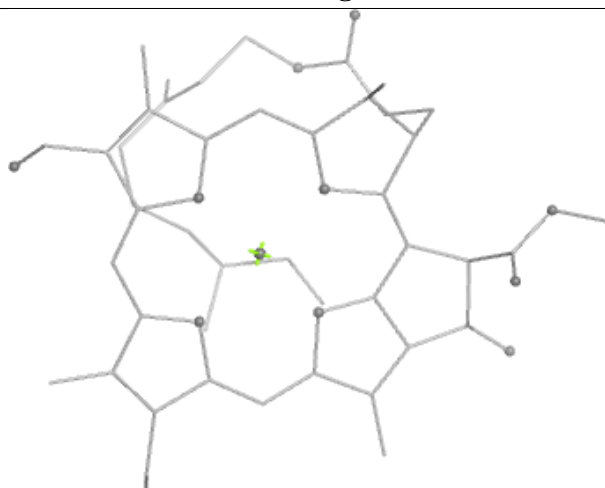
Bond lengths



Bond angles

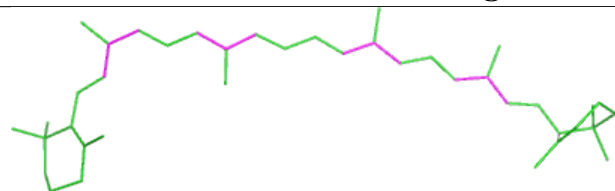


Torsions

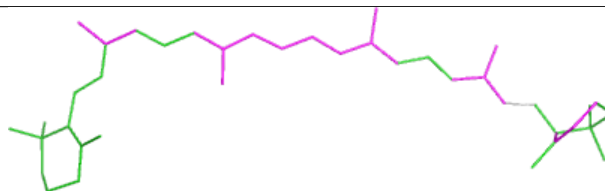


Rings

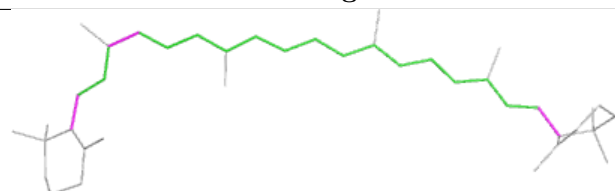
Ligand A1JPJ aB 4005



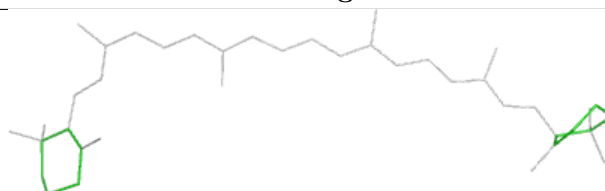
Bond lengths



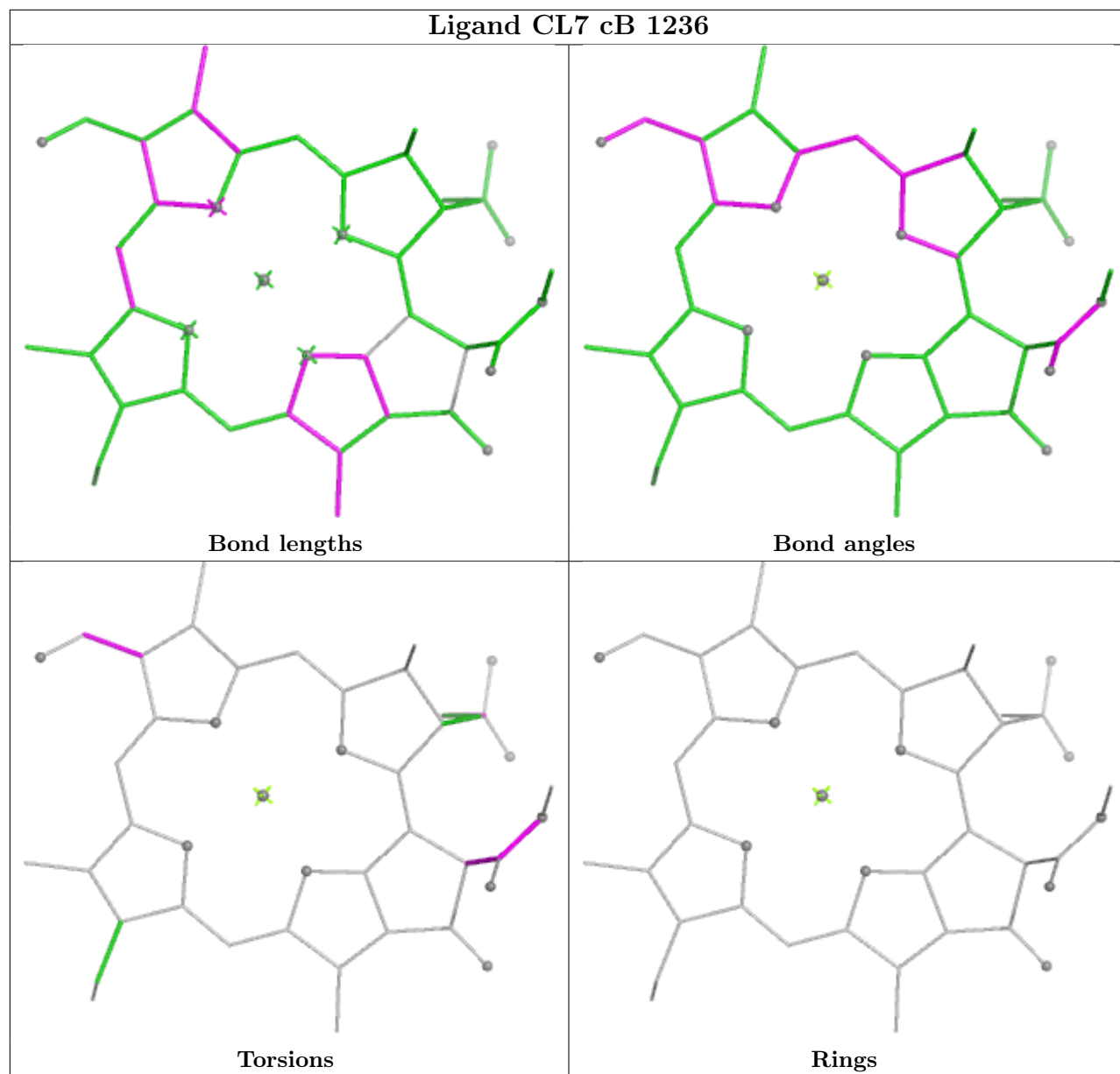
Bond angles

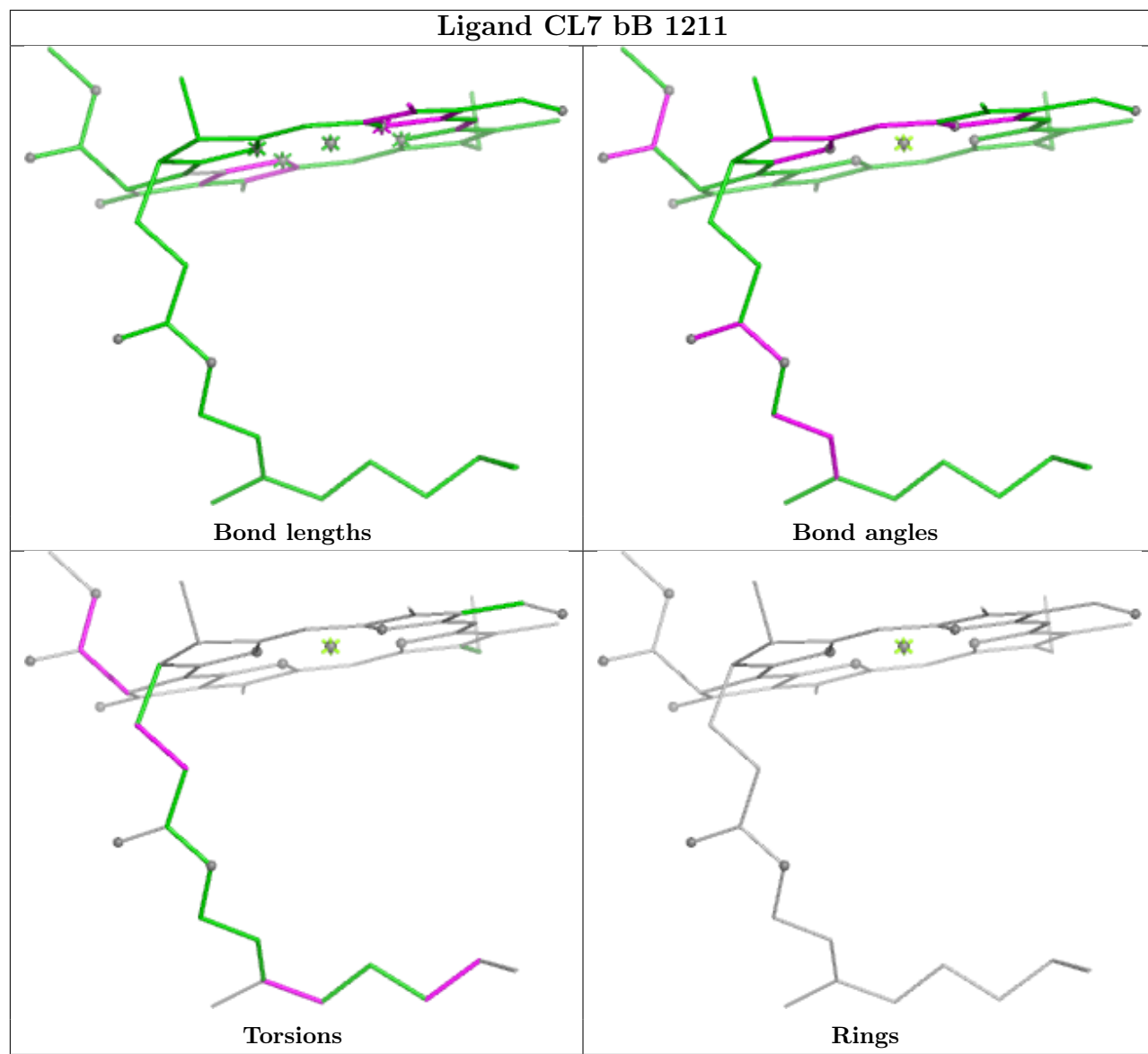


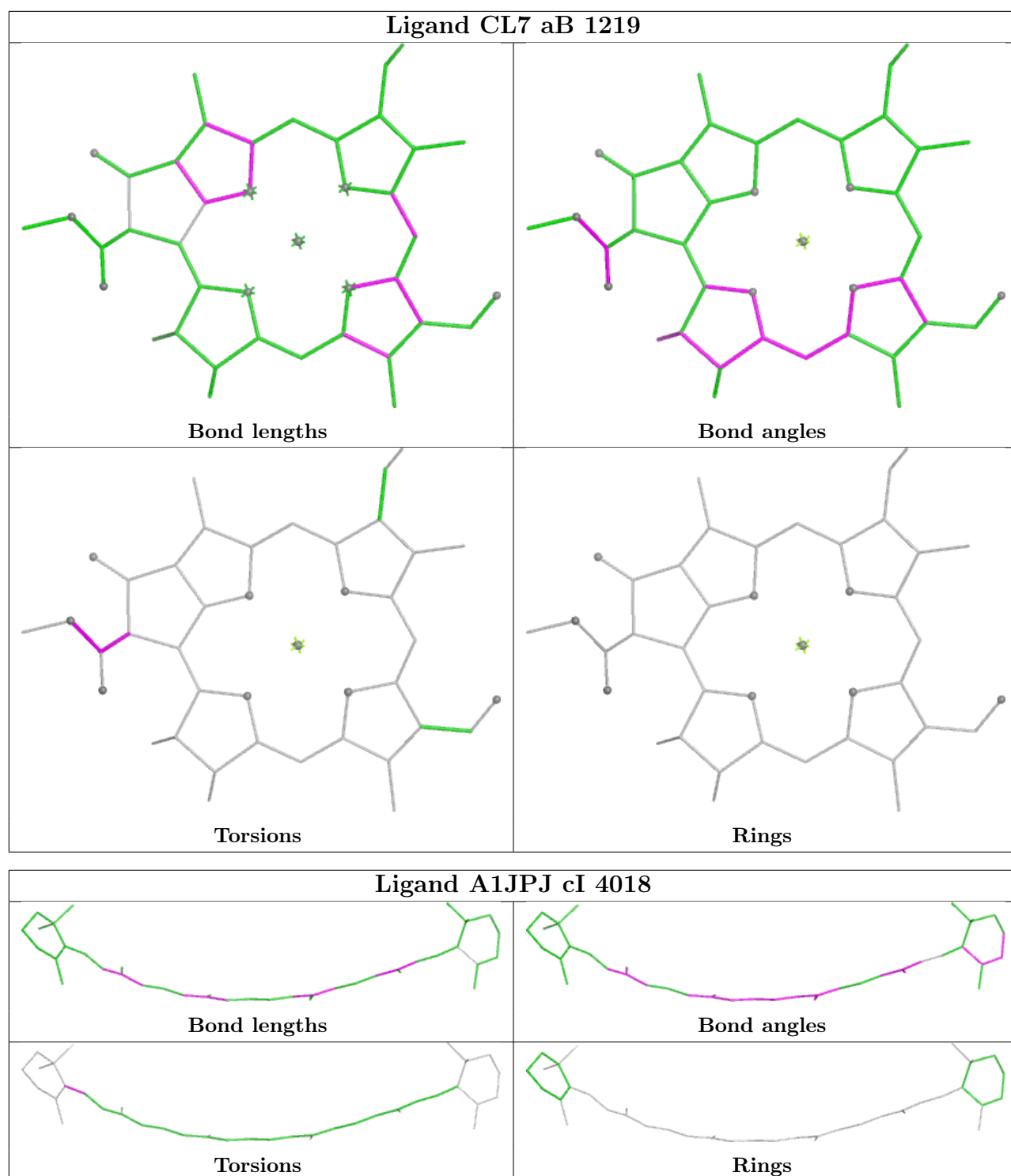
Torsions



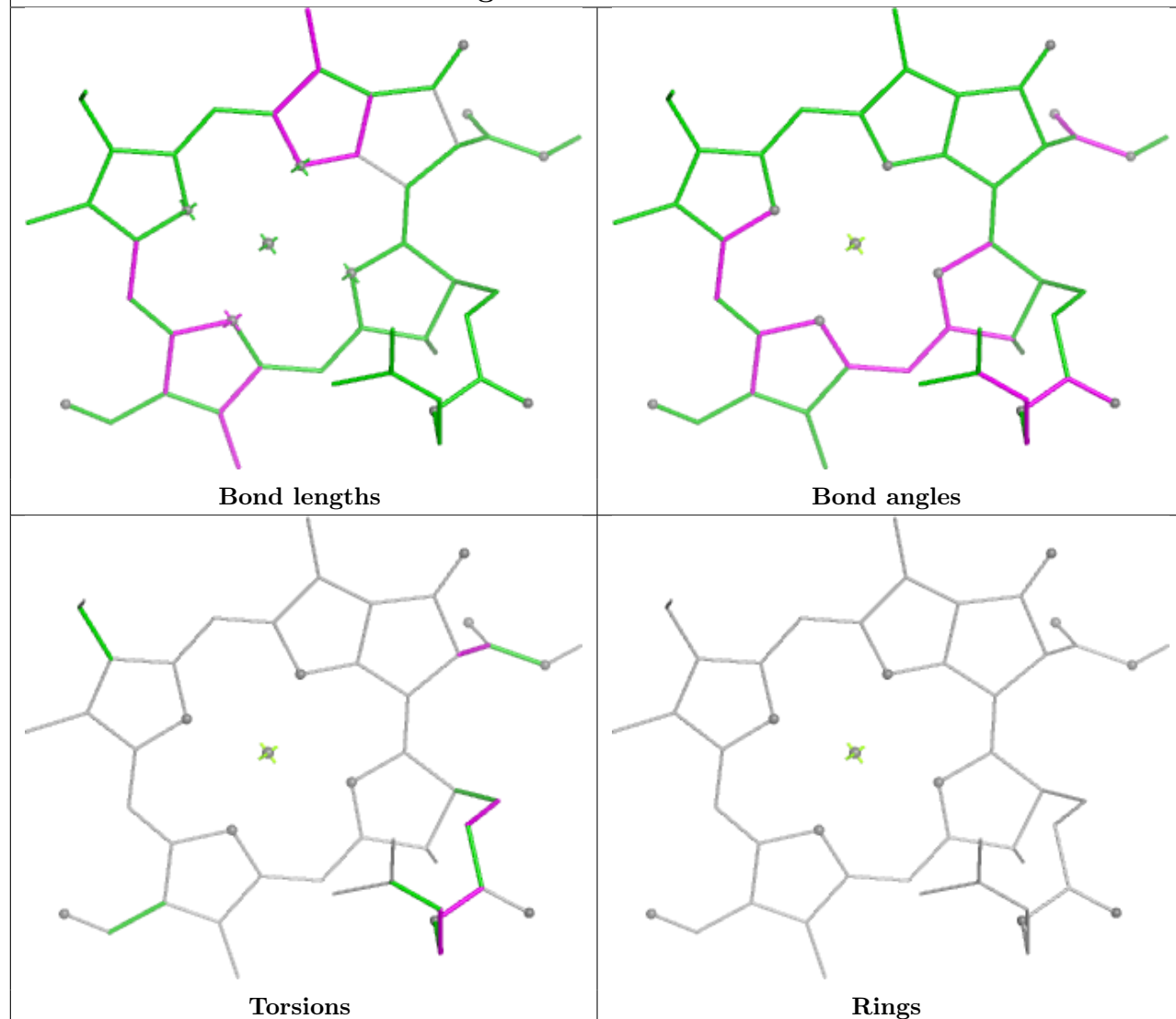
Rings



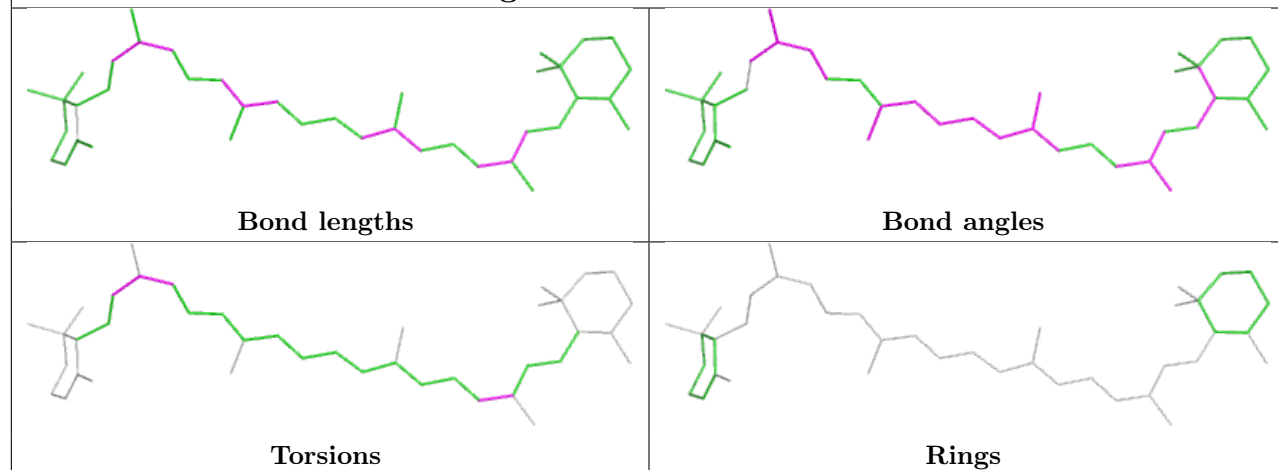


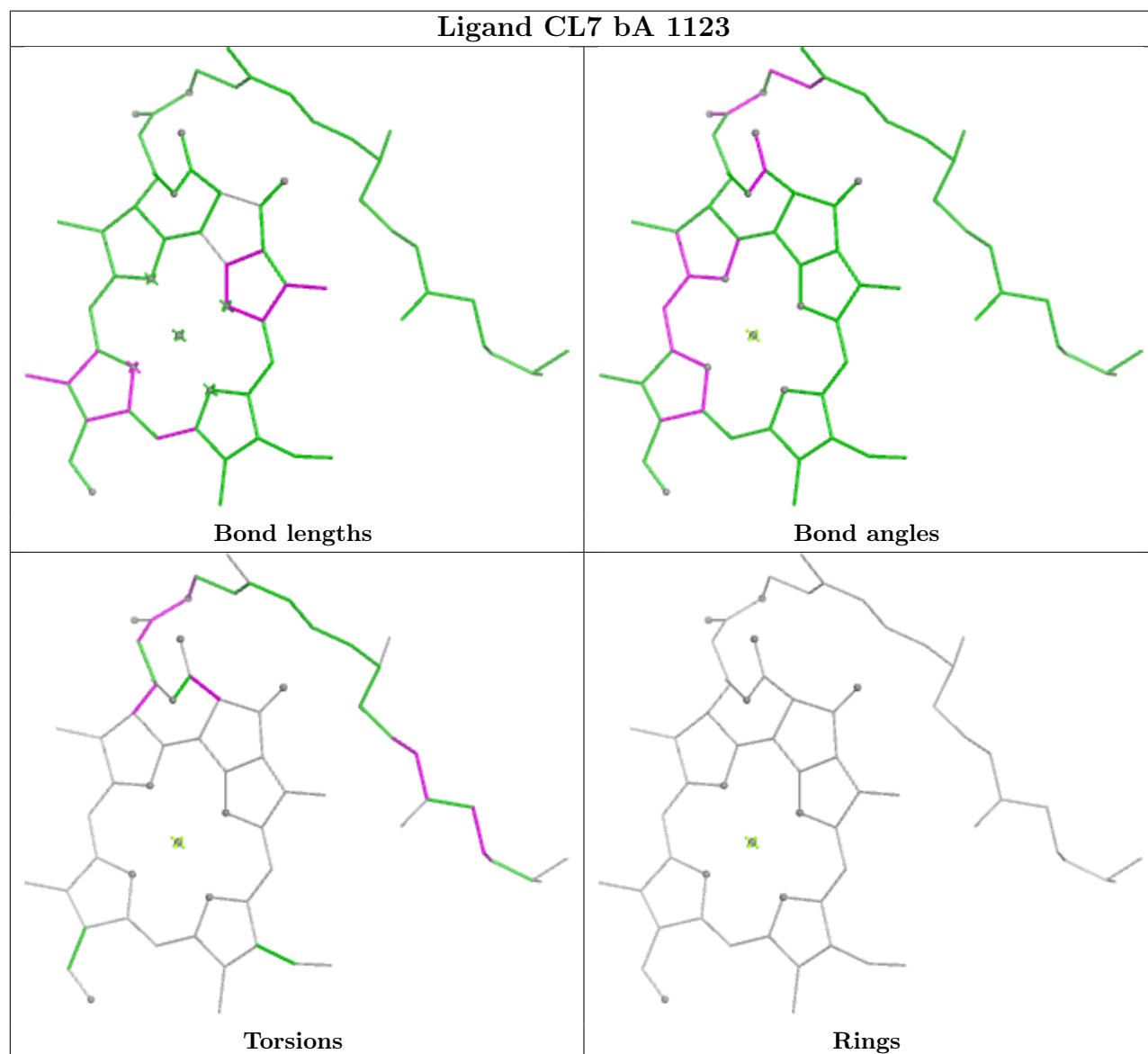
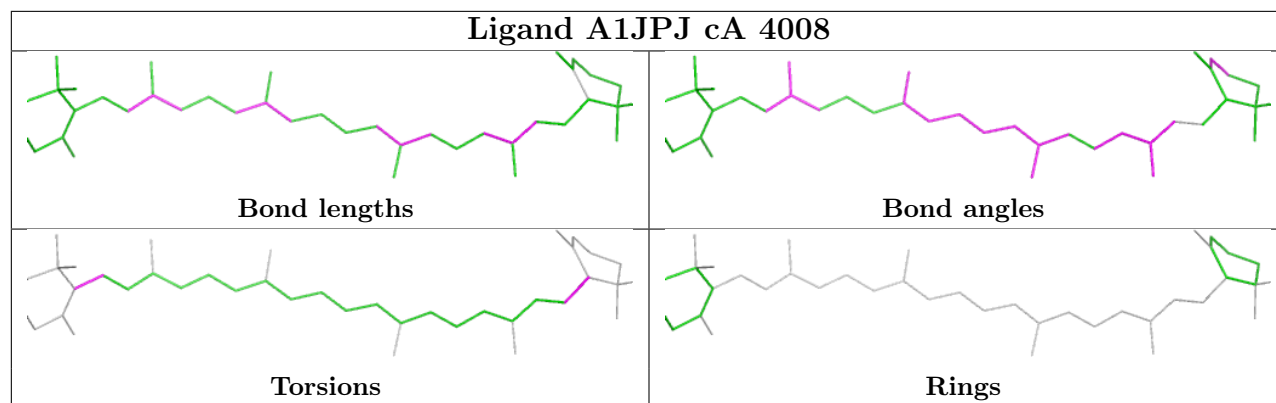


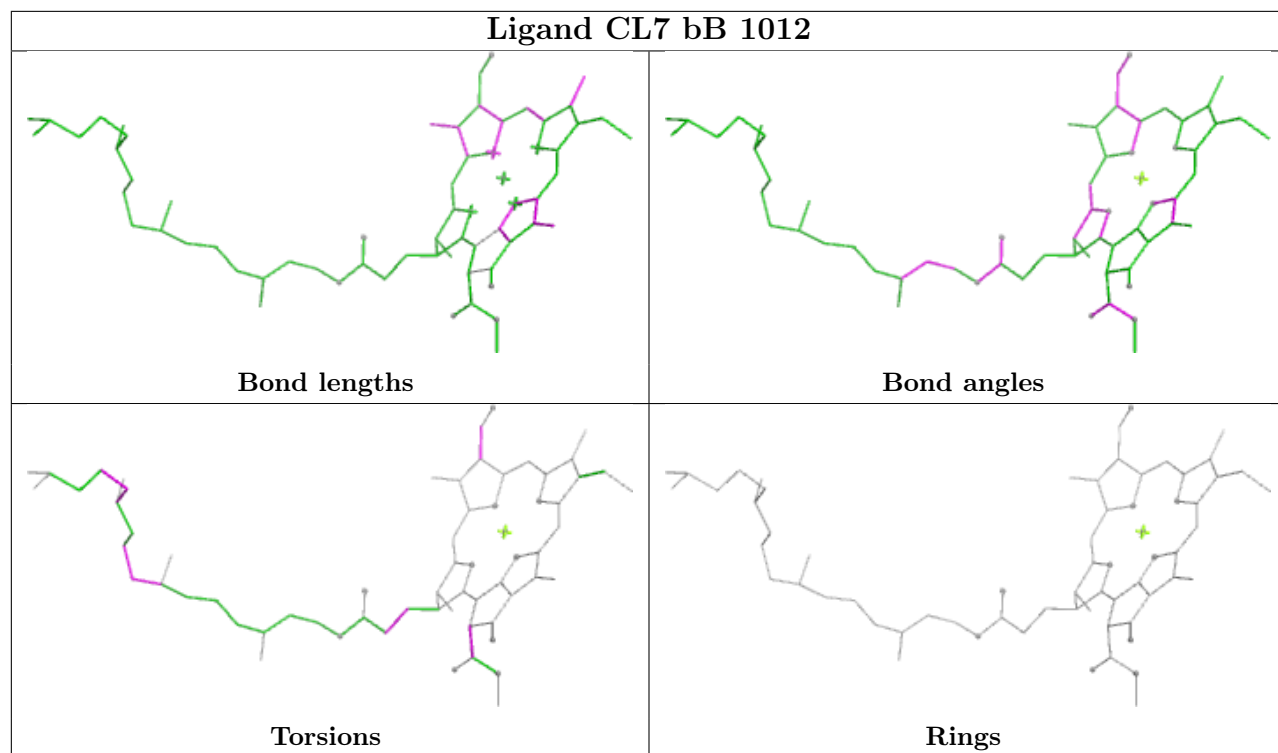
Ligand CL7 aB 1214

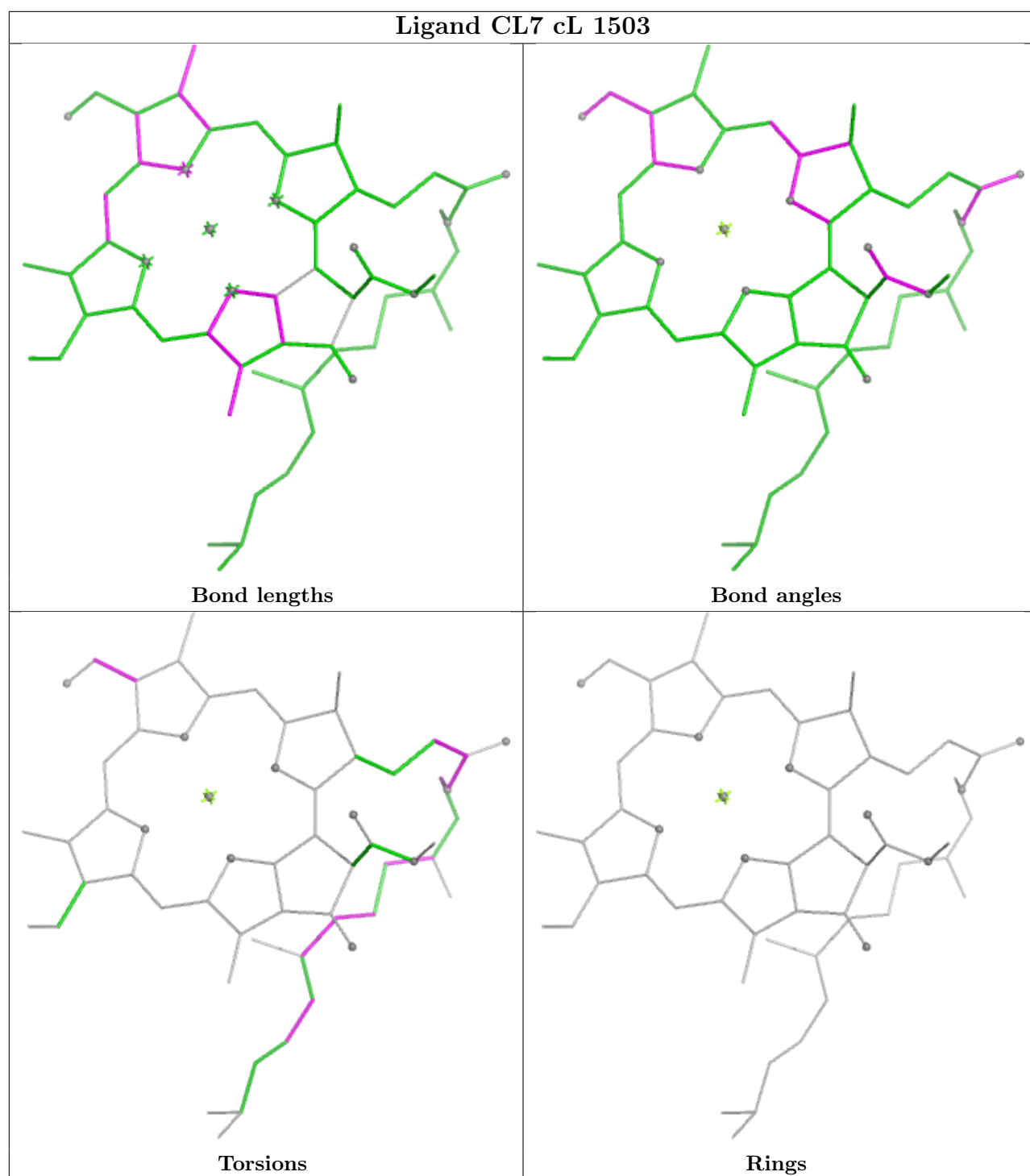


Ligand A1JPJ cB 4006

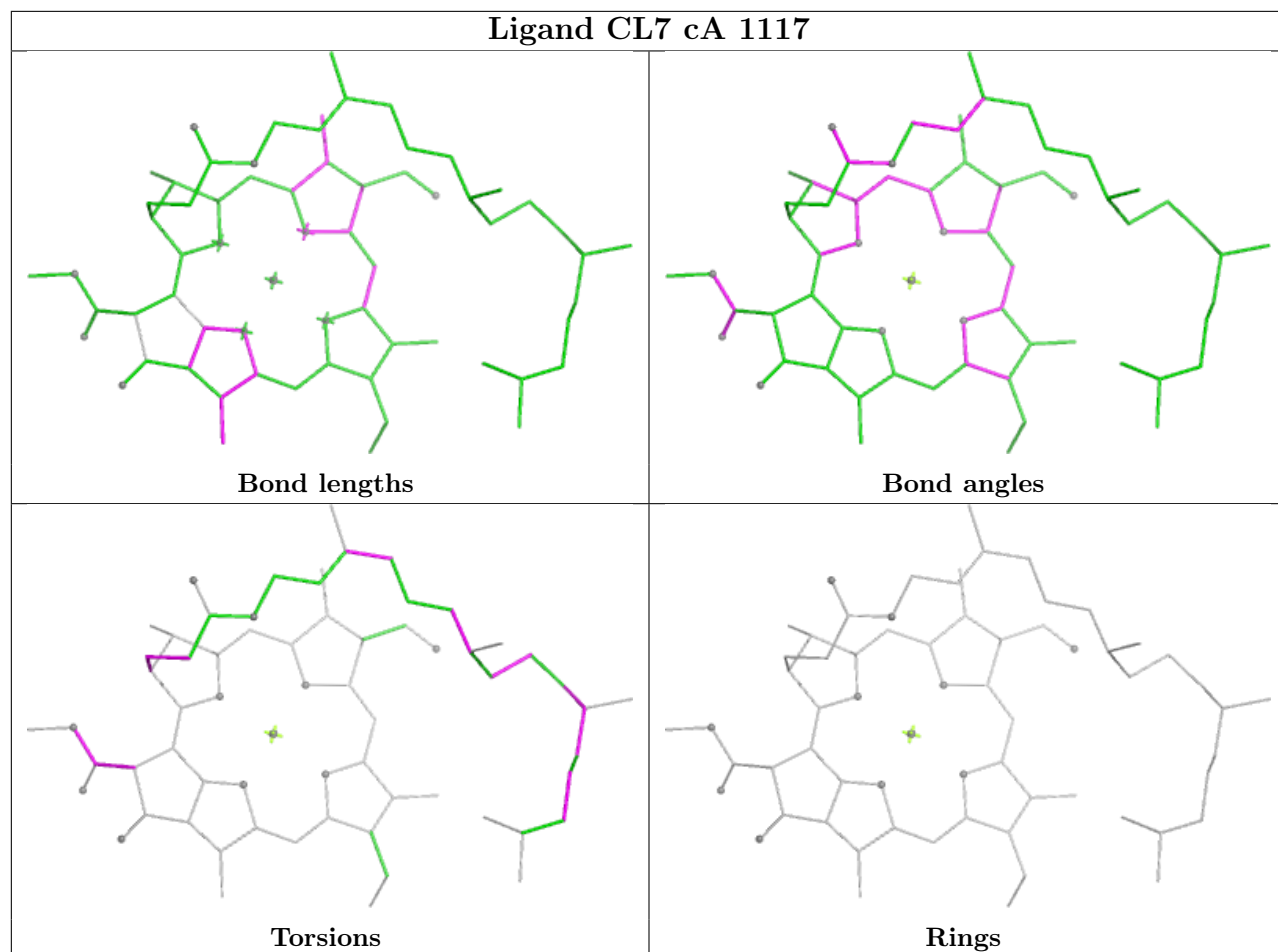




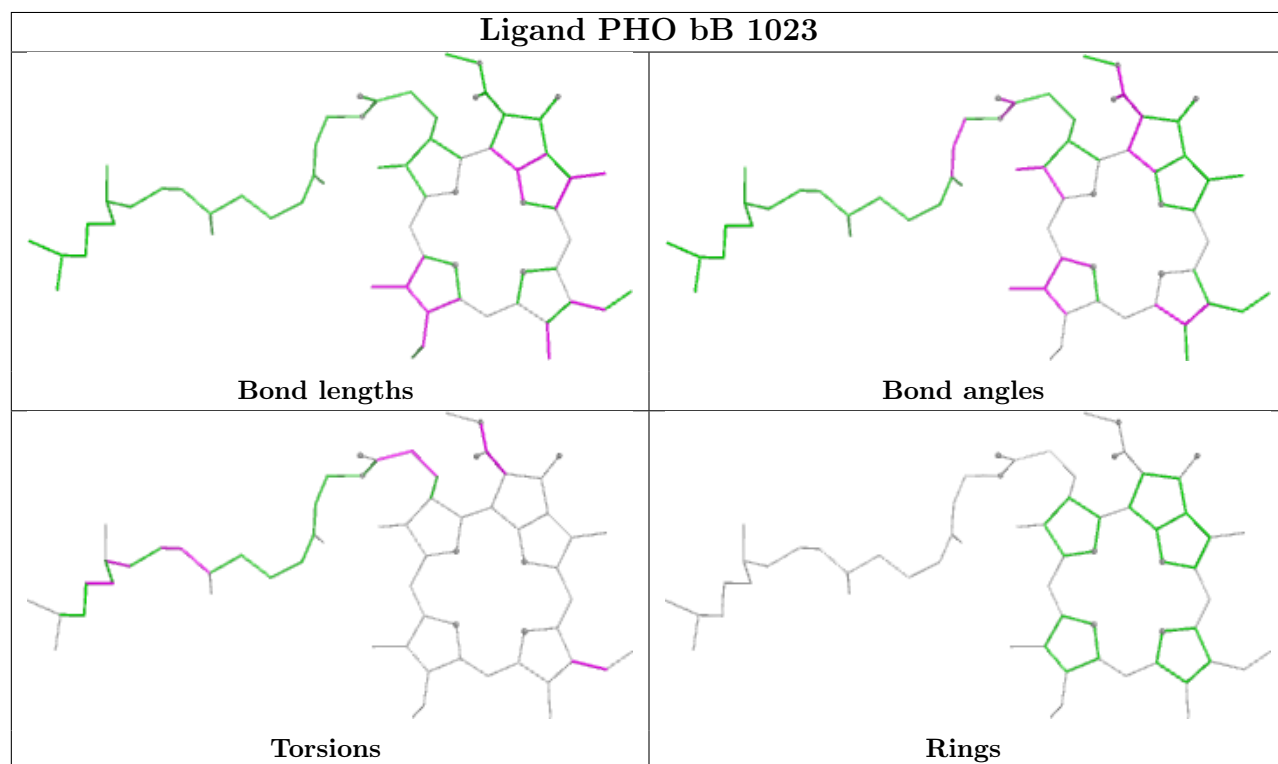


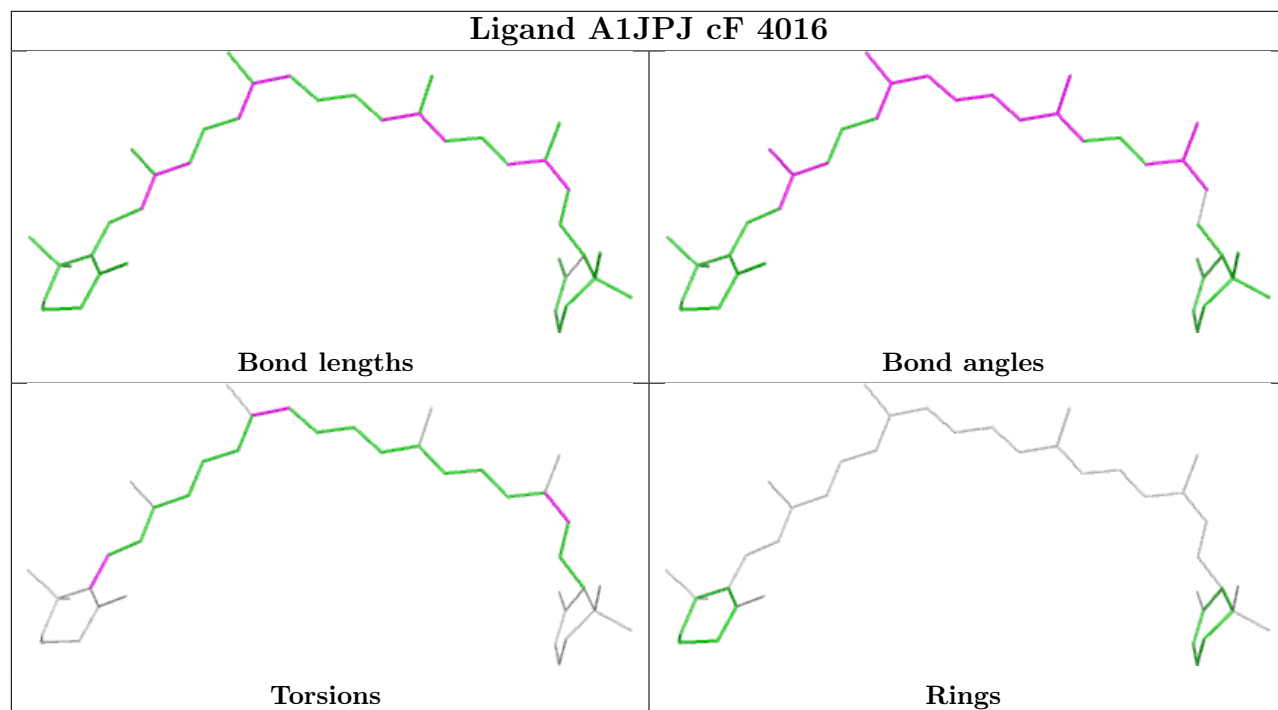


Ligand CL7 cA 1117

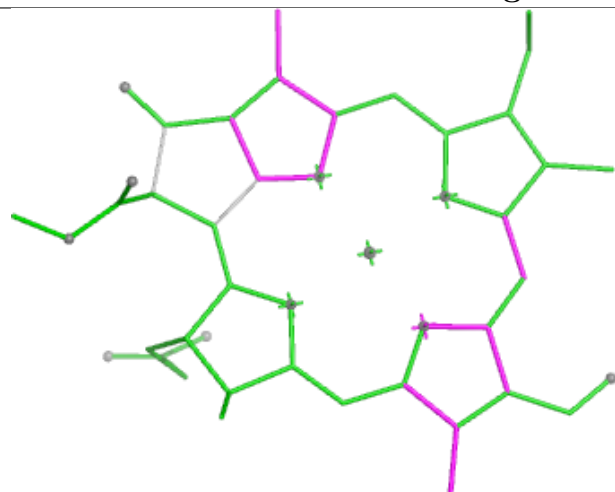


Ligand PHO bB 1023

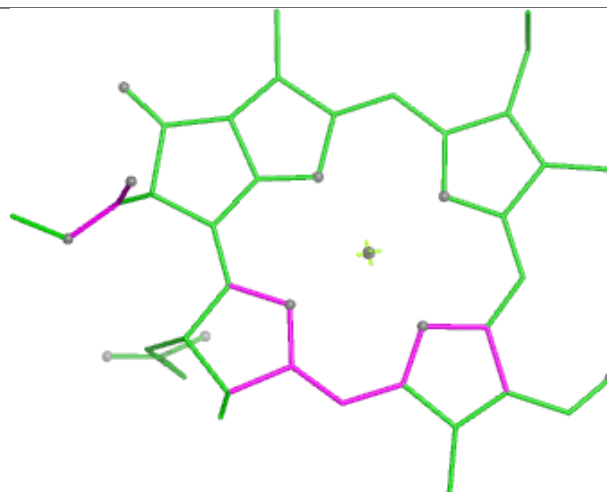




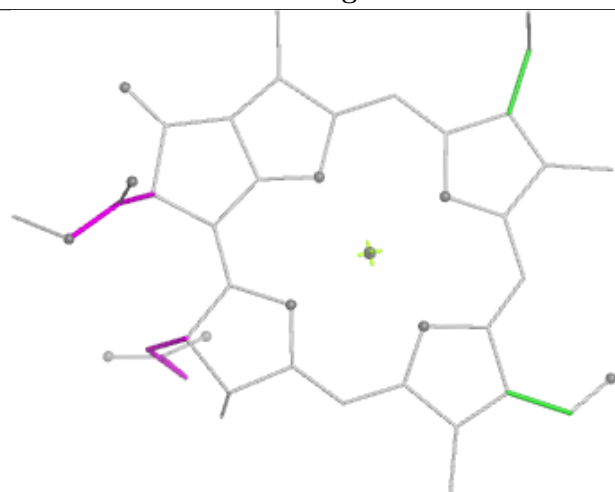
Ligand CL7 aB 1228



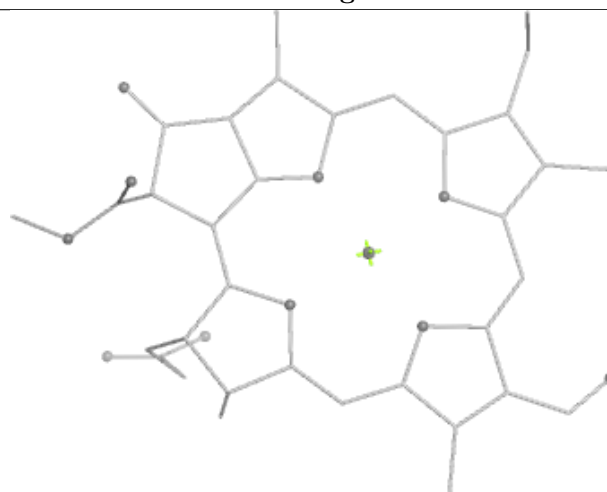
Bond lengths



Bond angles

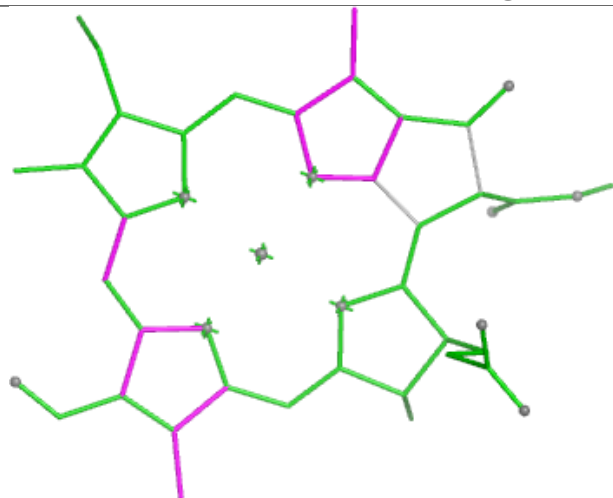


Torsions

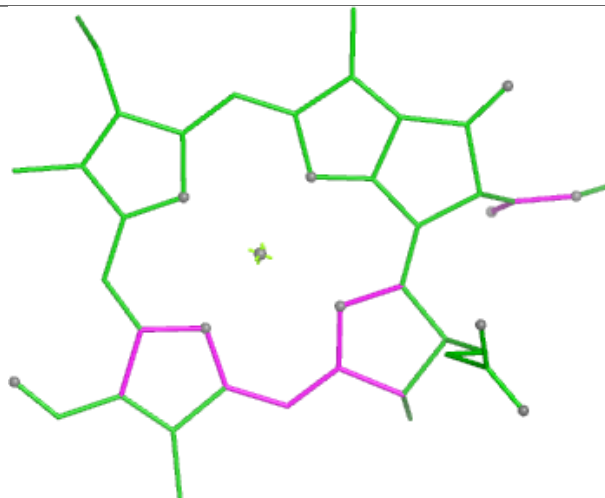


Rings

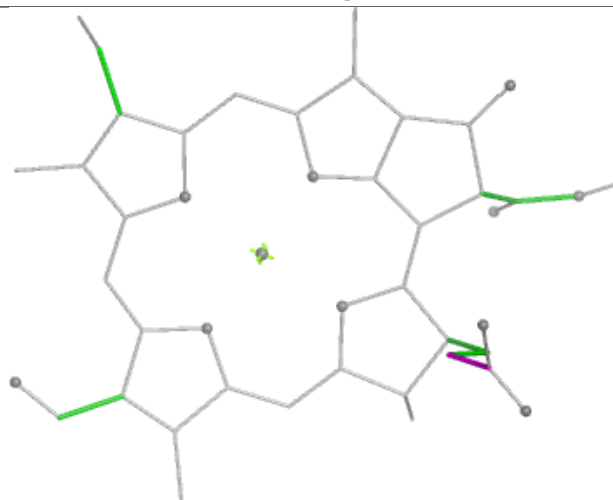
Ligand CL7 bA 1114



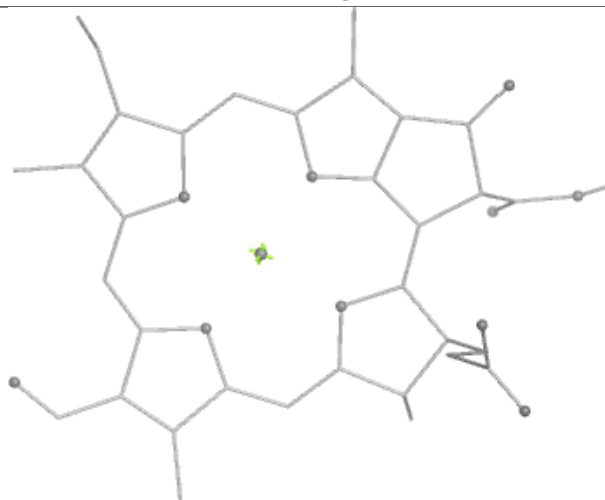
Bond lengths



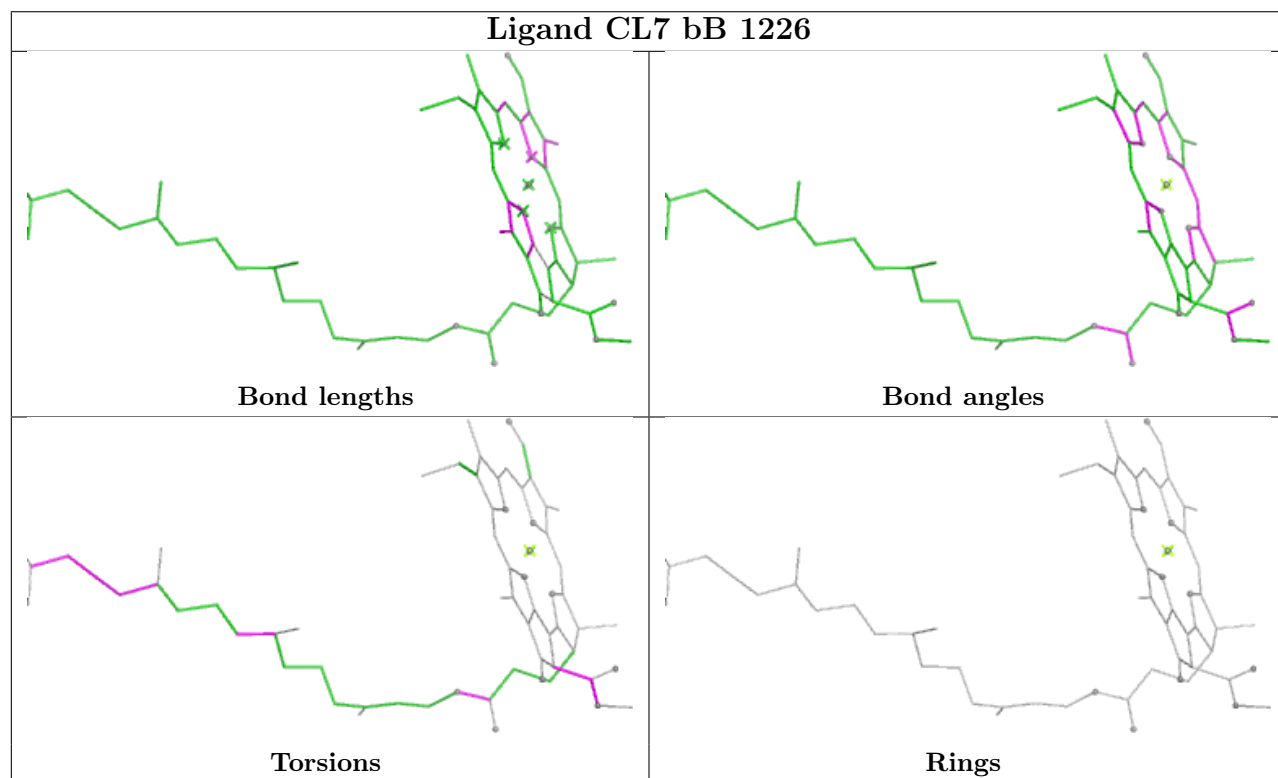
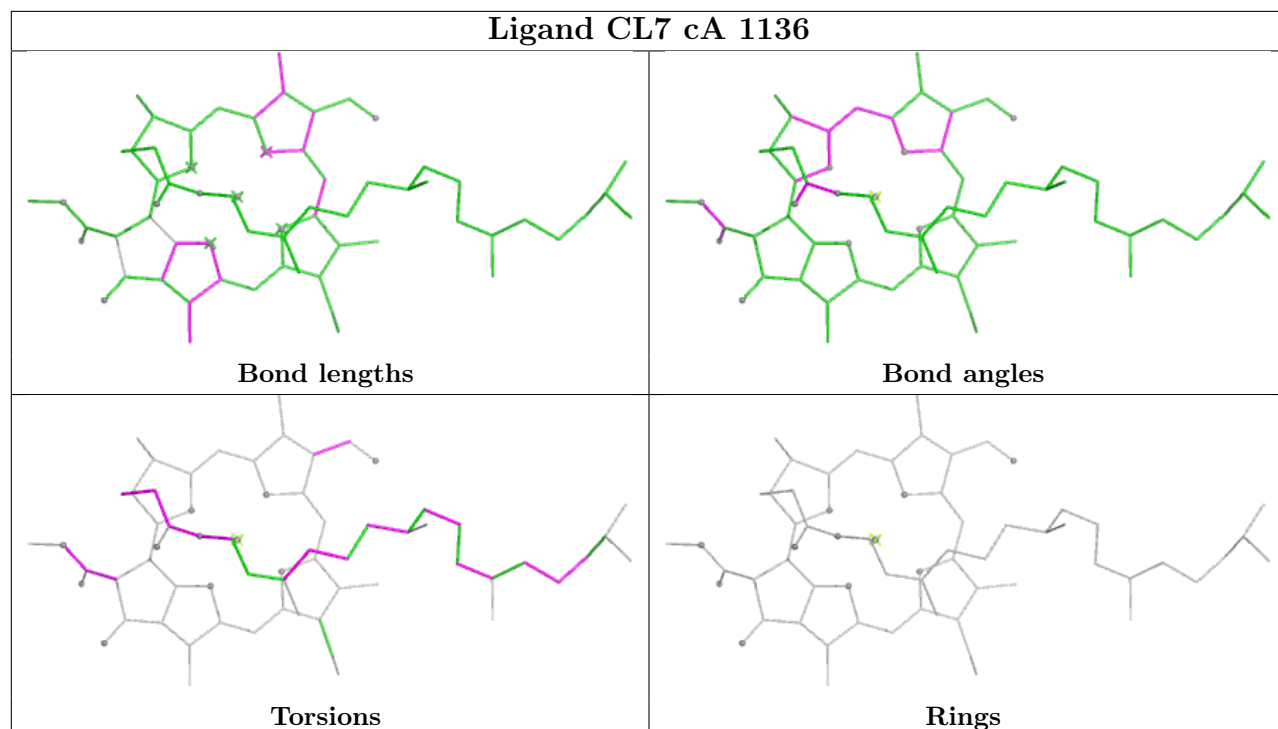
Bond angles



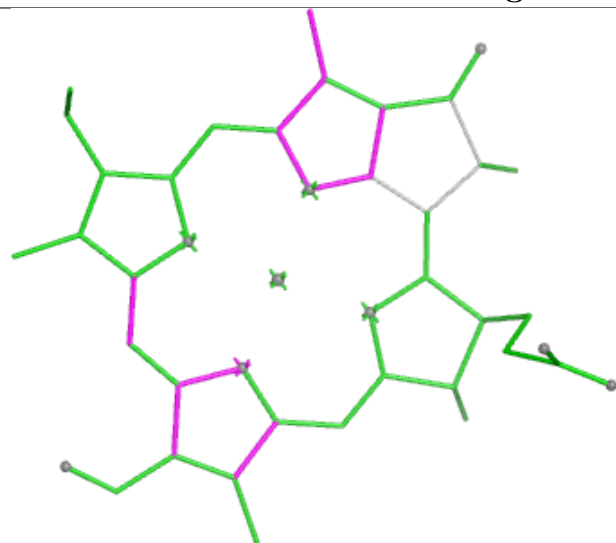
Torsions



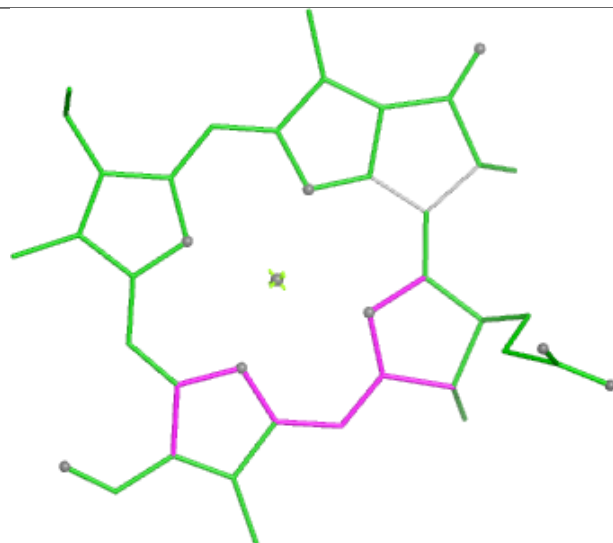
Rings



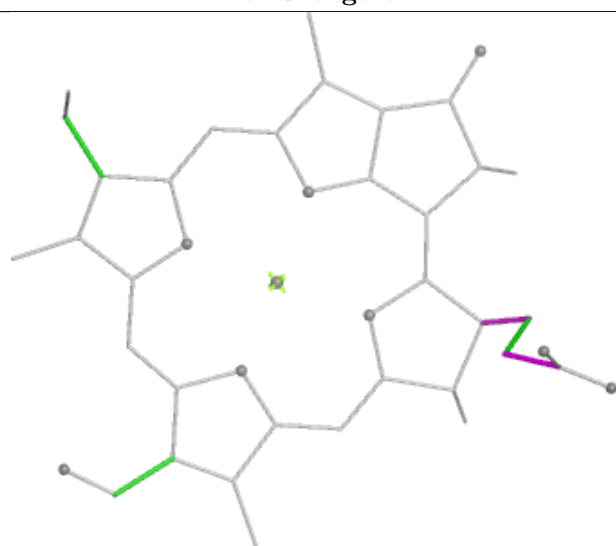
Ligand CL7 bJ 1302



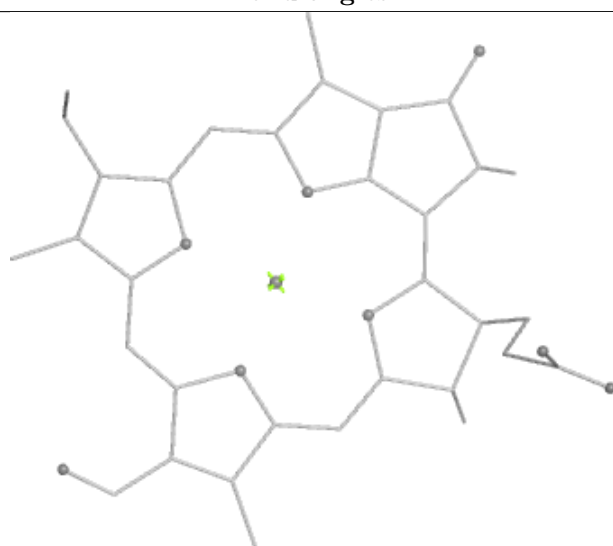
Bond lengths



Bond angles

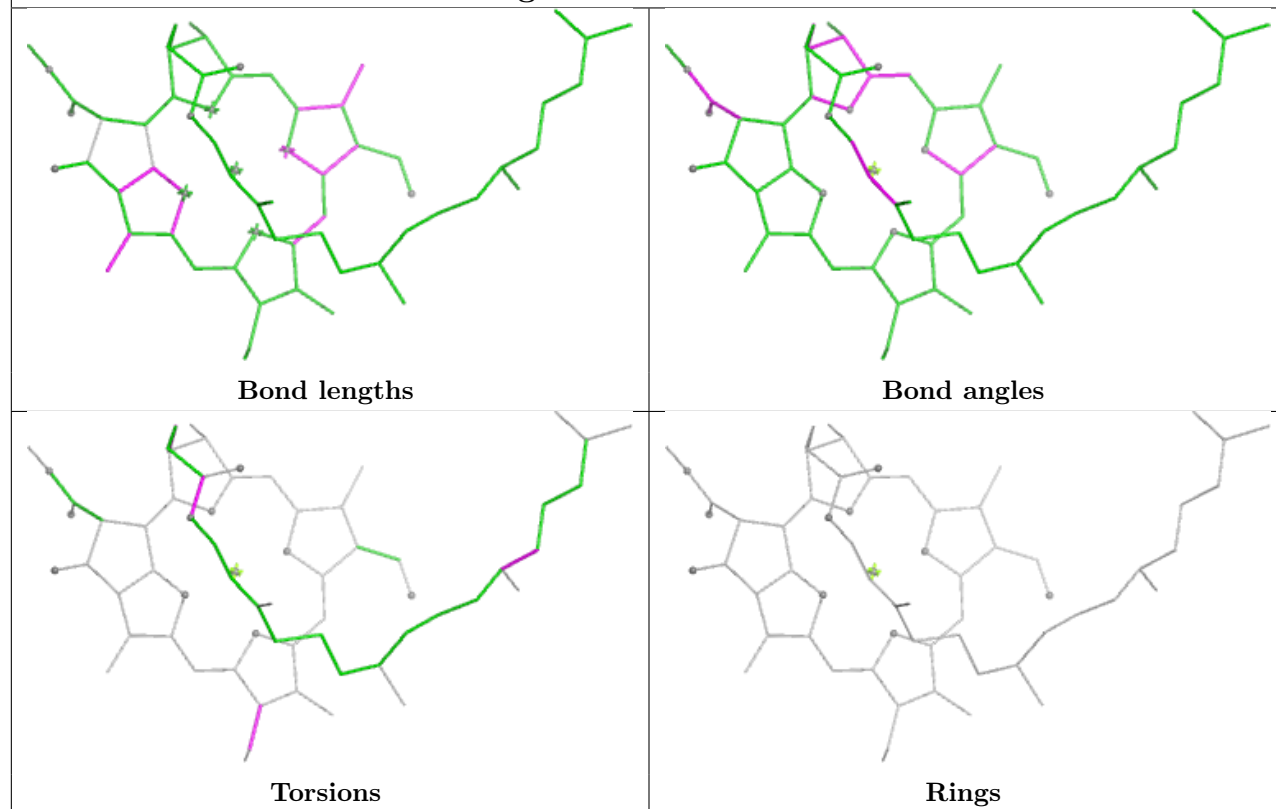


Torsions

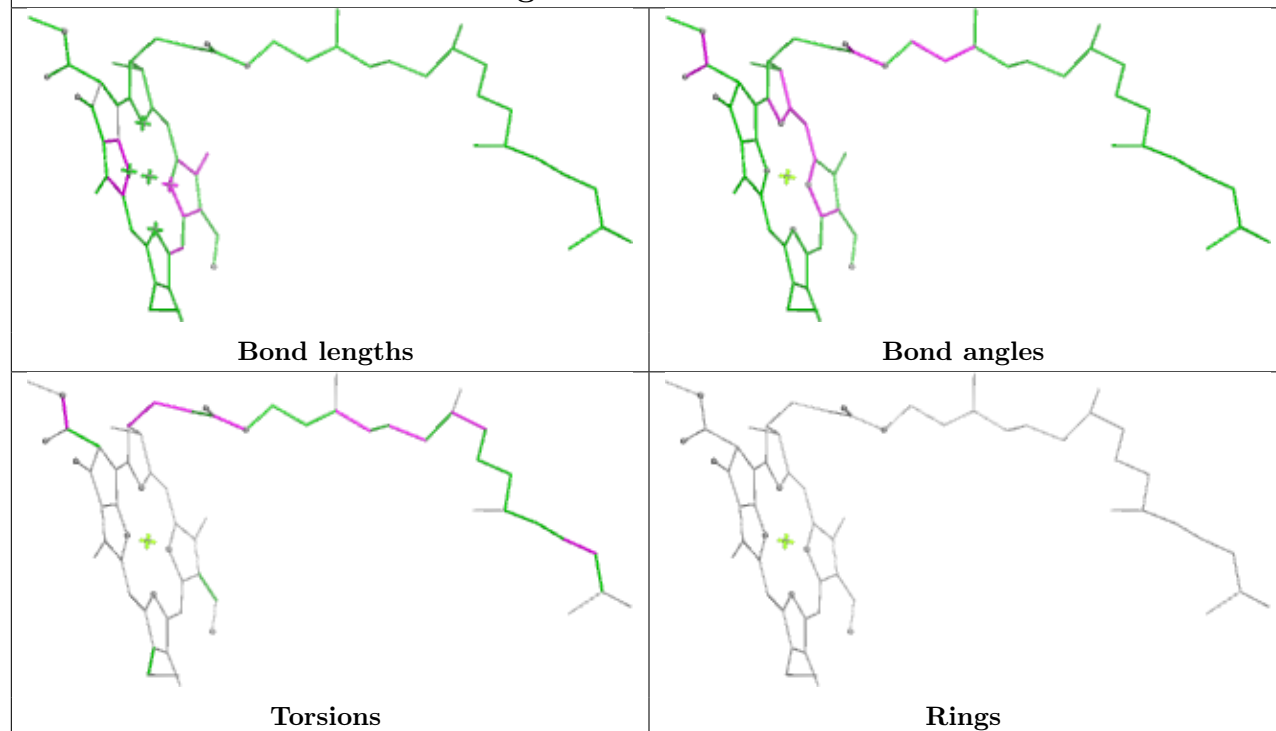


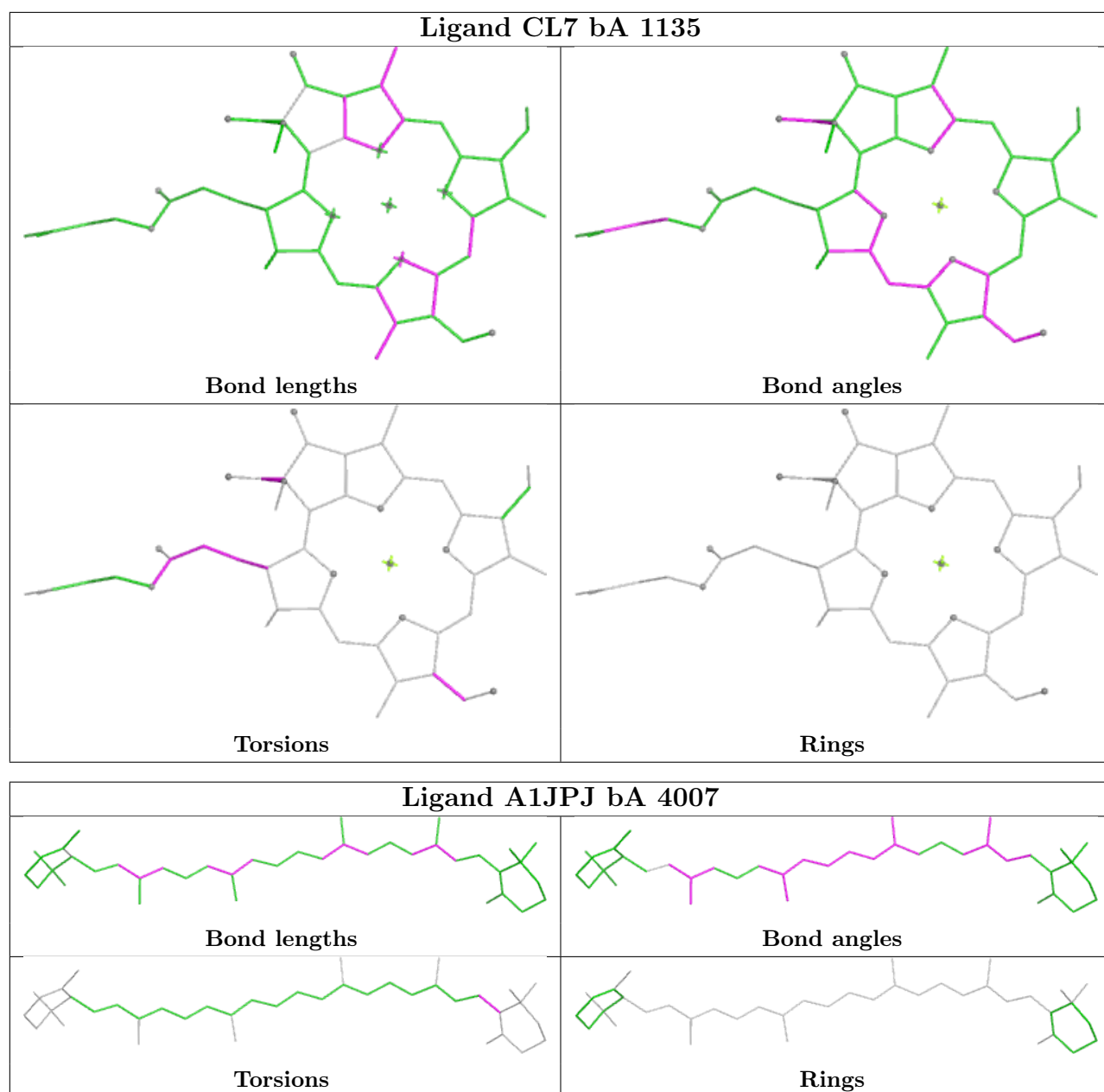
Rings

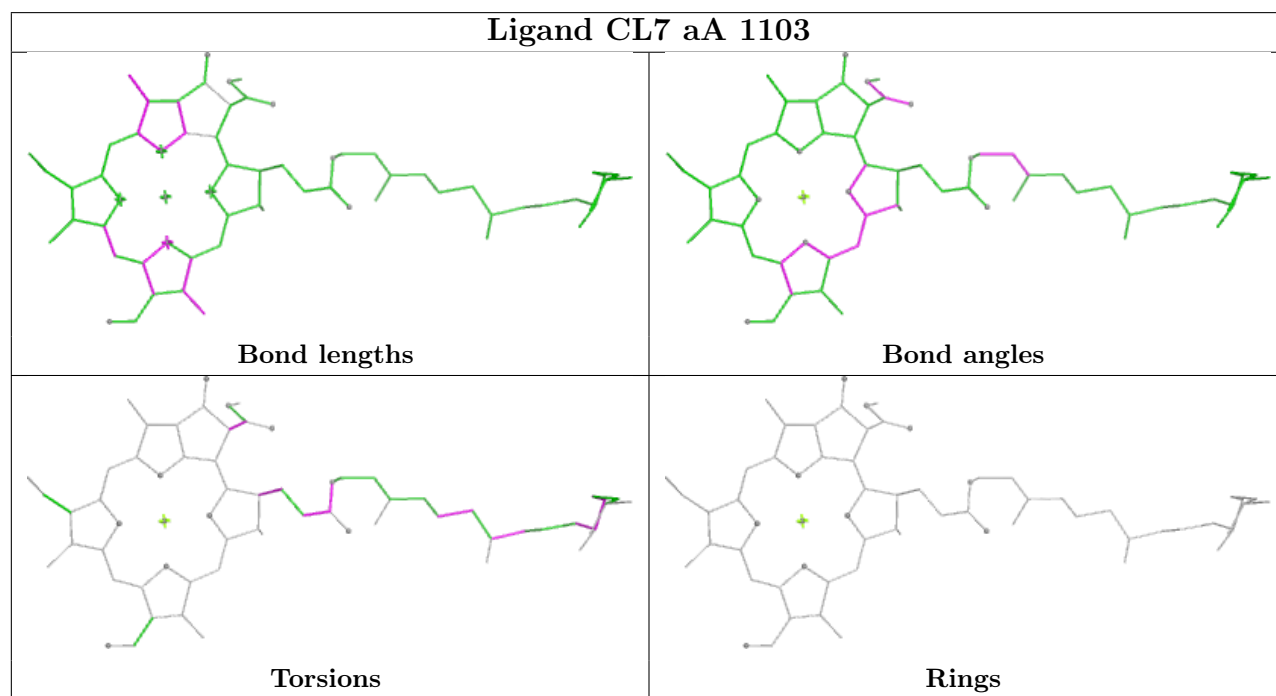
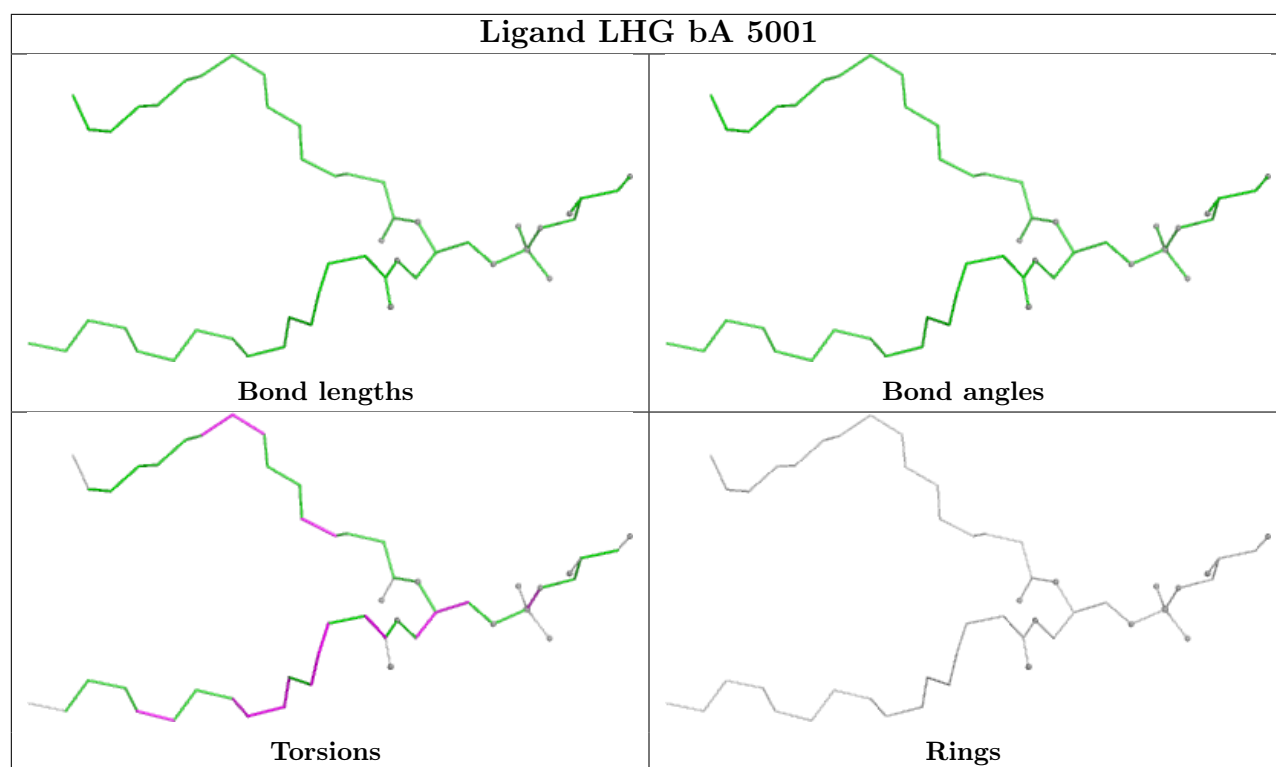
Ligand CL7 bB 1204



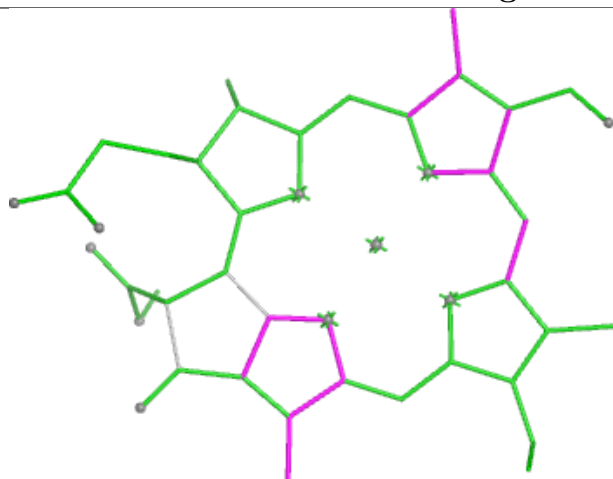
Ligand CL7 bA 1133



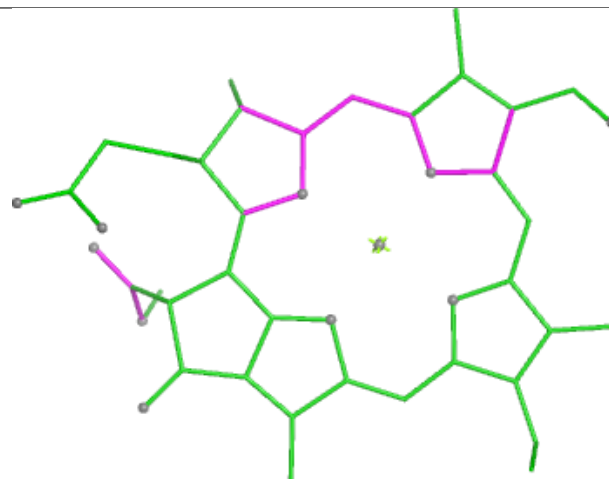




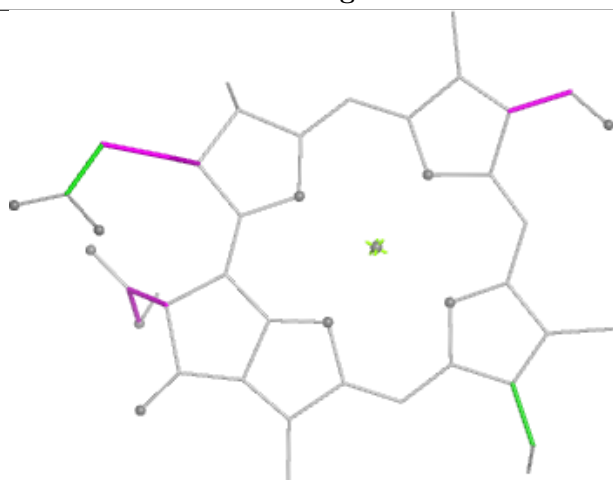
Ligand CL7 bA 1113



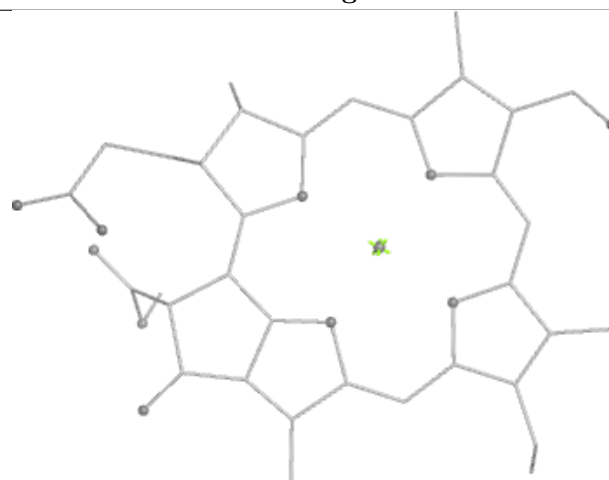
Bond lengths



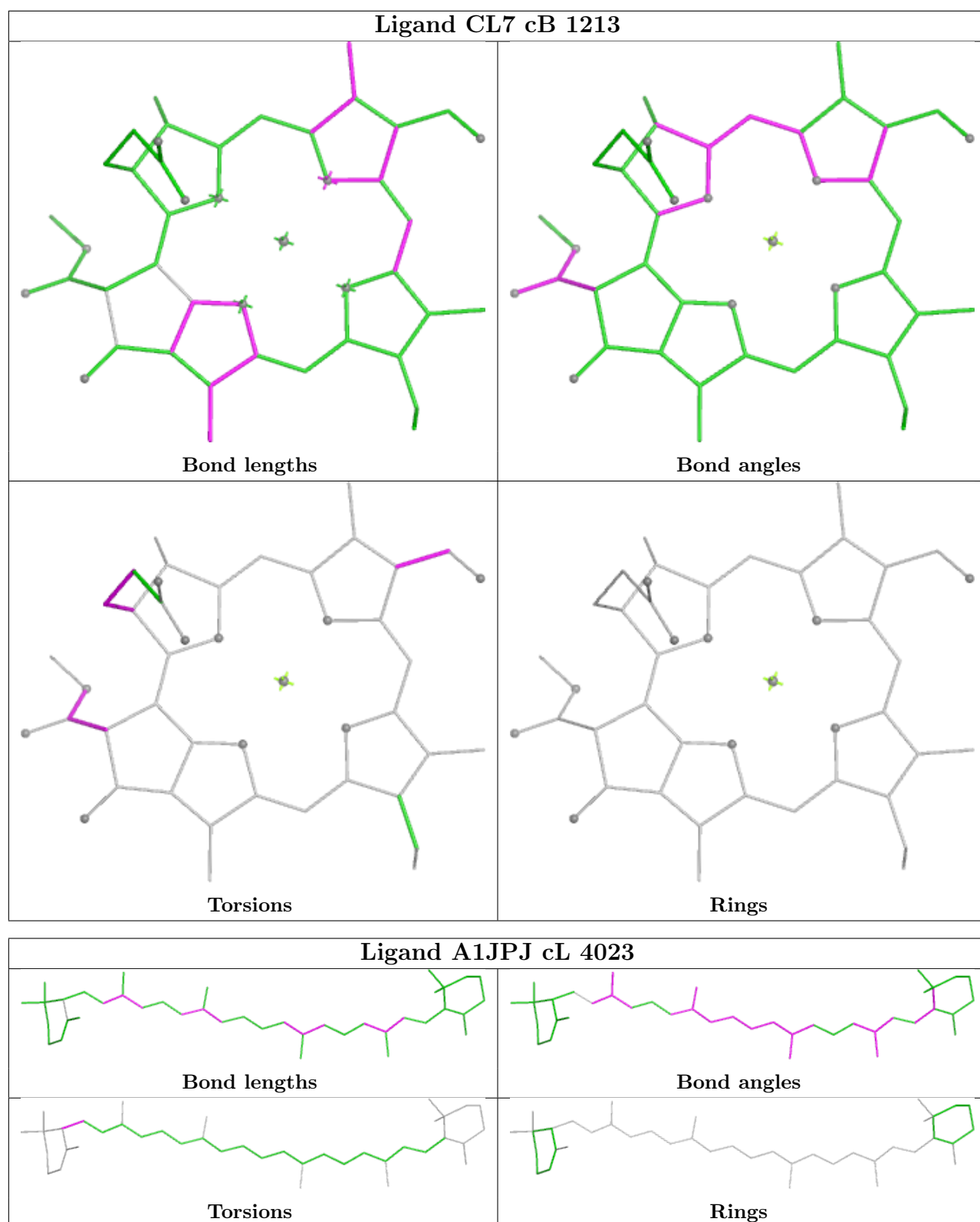
Bond angles

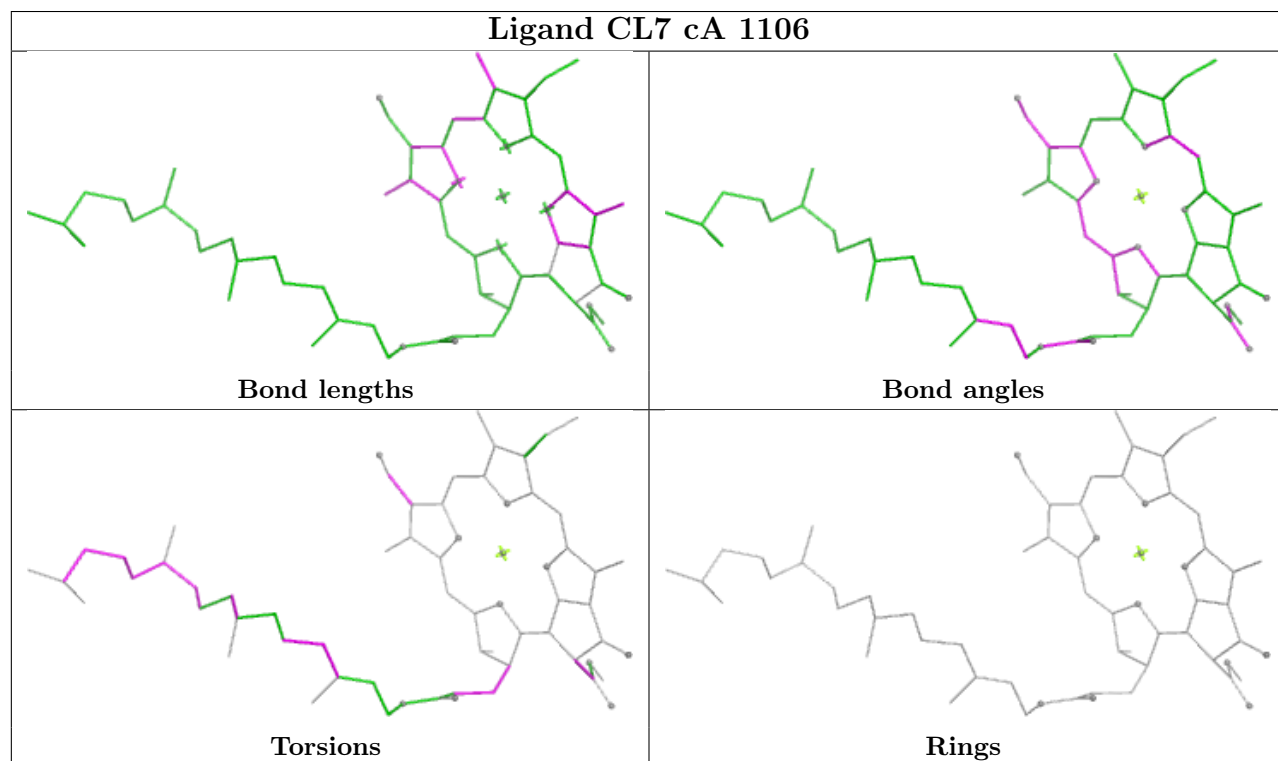
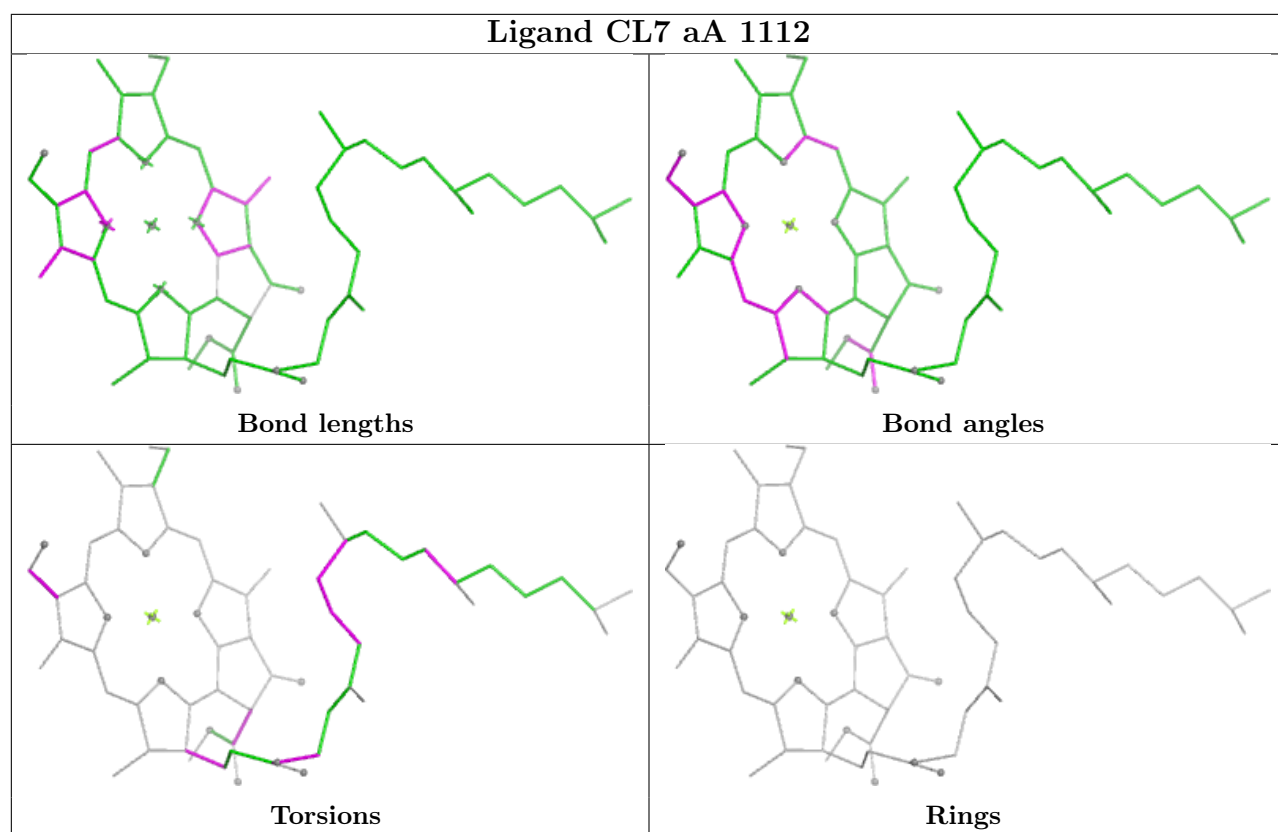


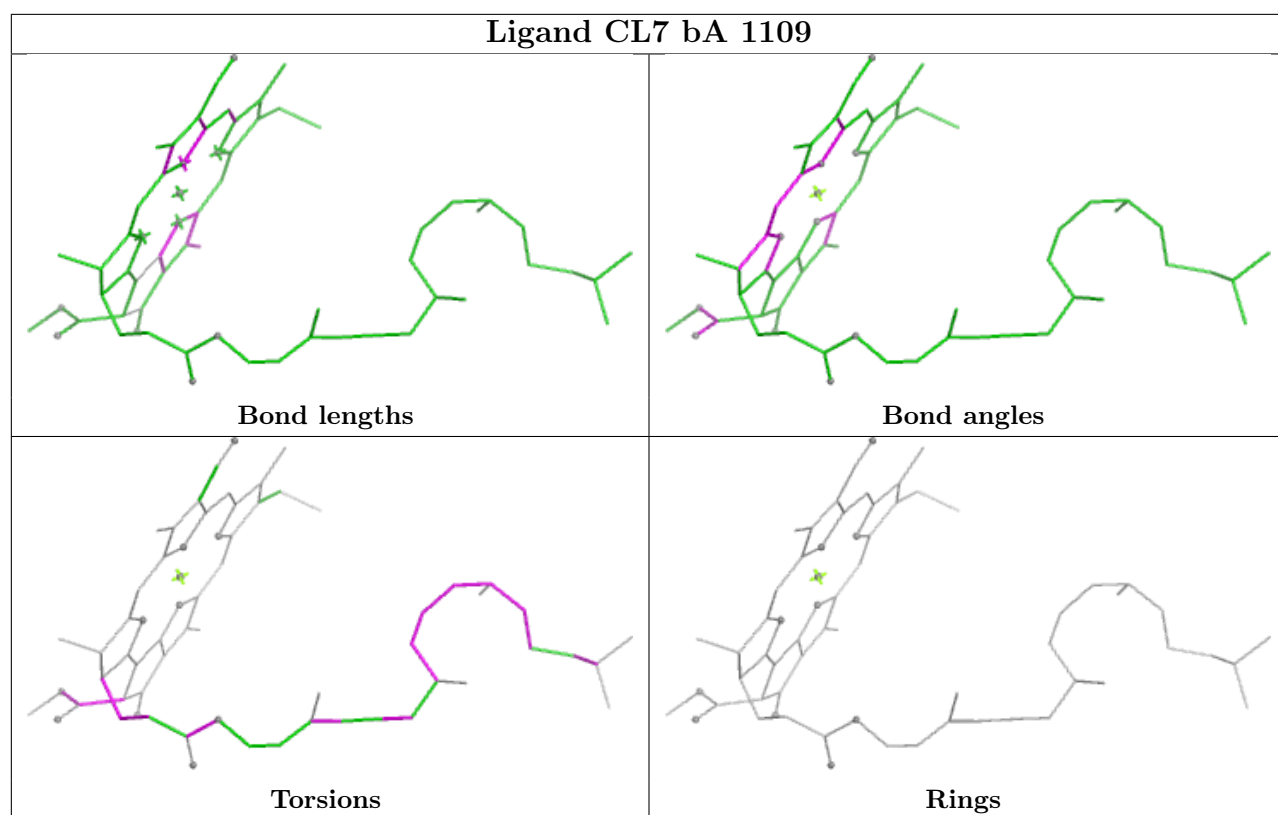
Torsions



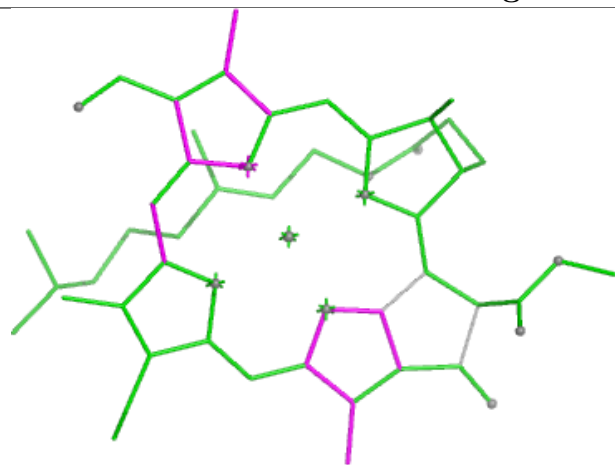
Rings



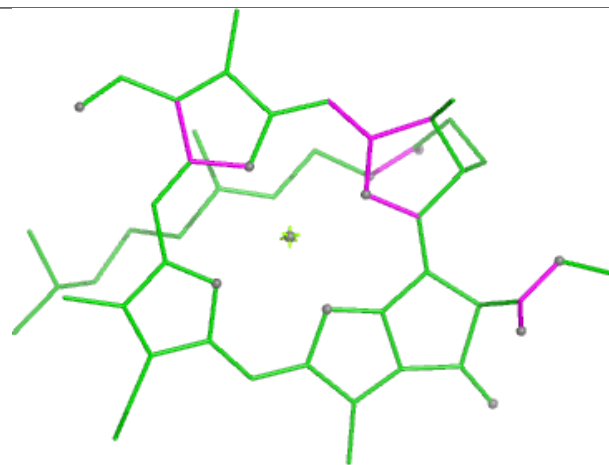




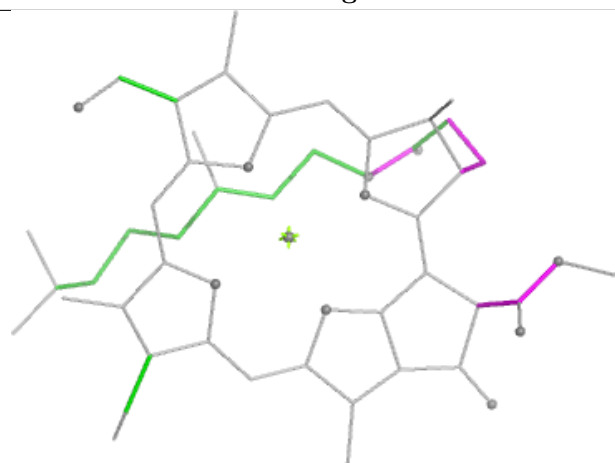
Ligand CL7 aA 1121



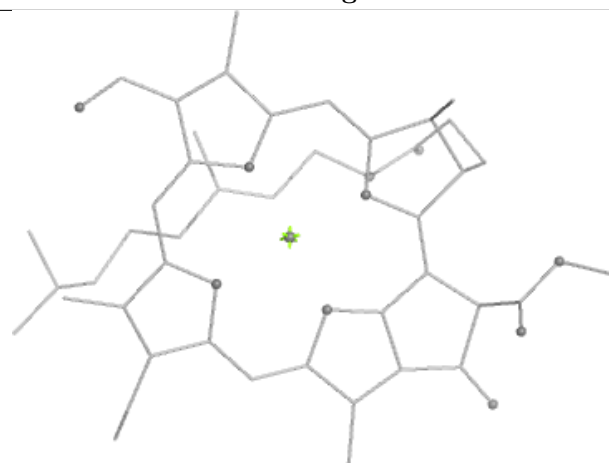
Bond lengths



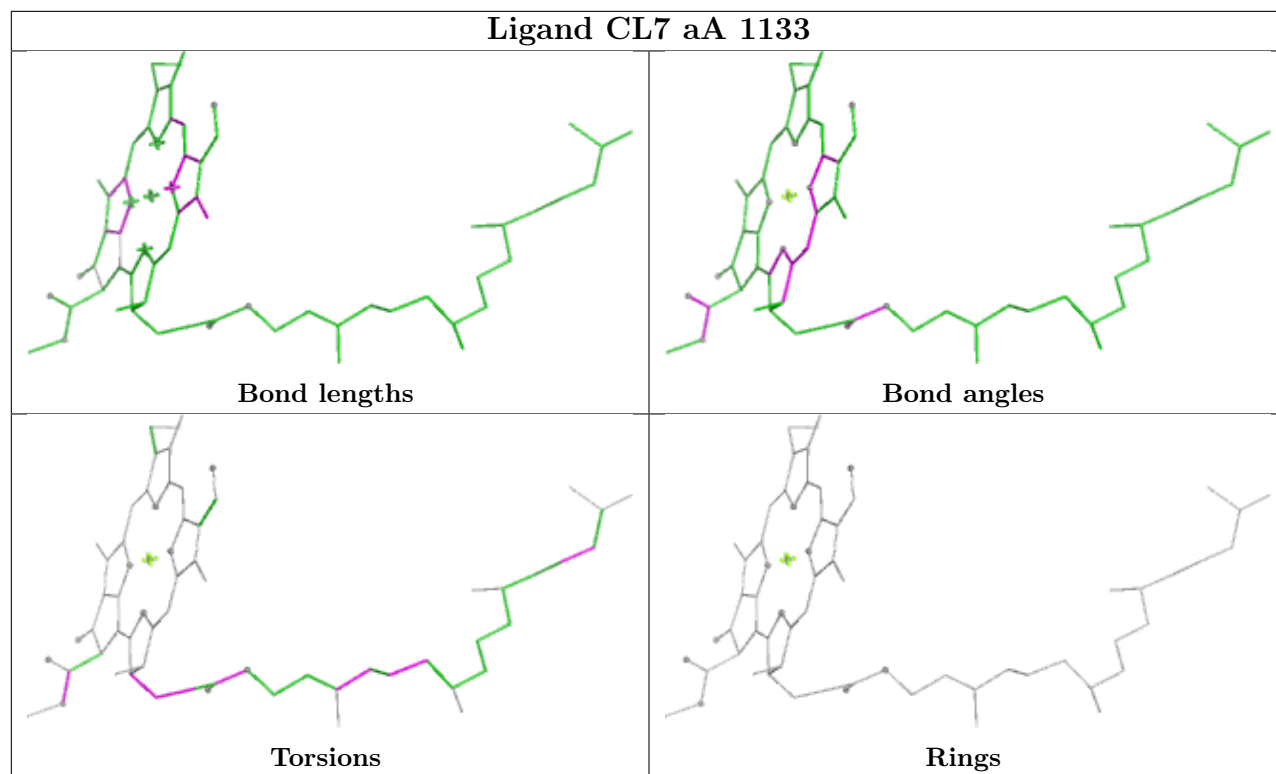
Bond angles



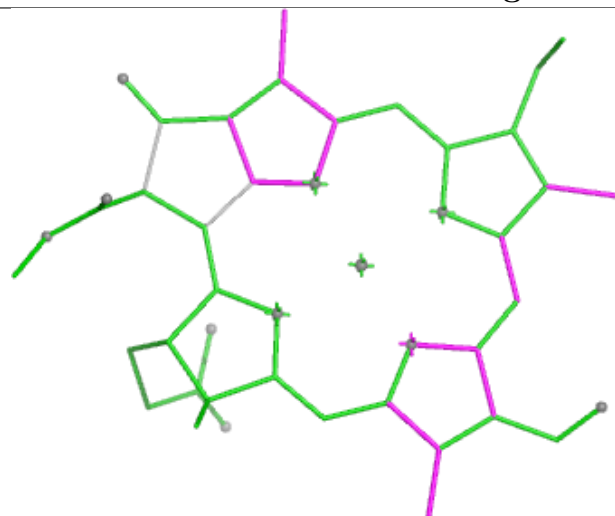
Torsions



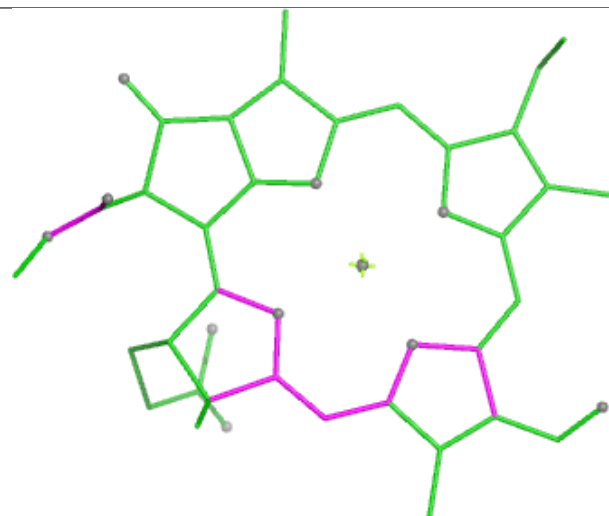
Rings



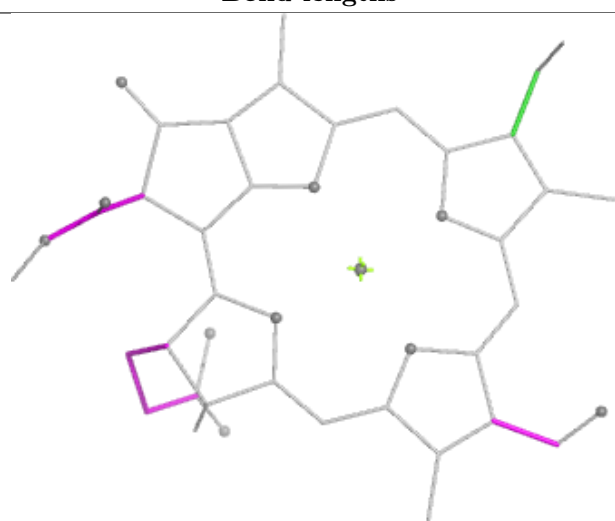
Ligand CL7 aB 1220



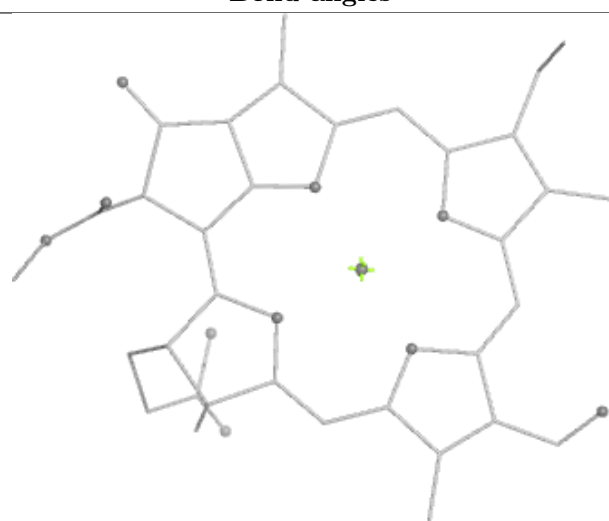
Bond lengths



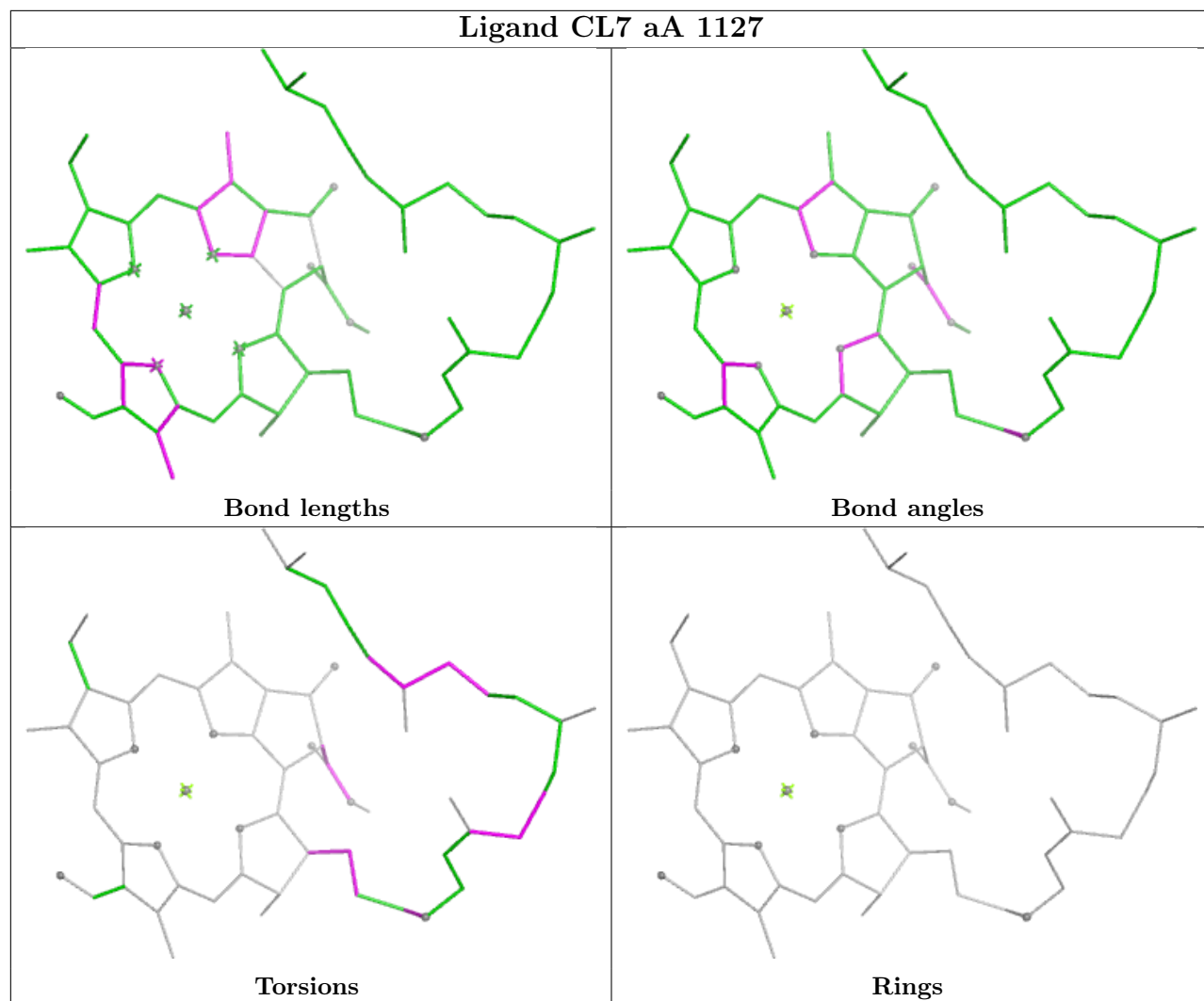
Bond angles

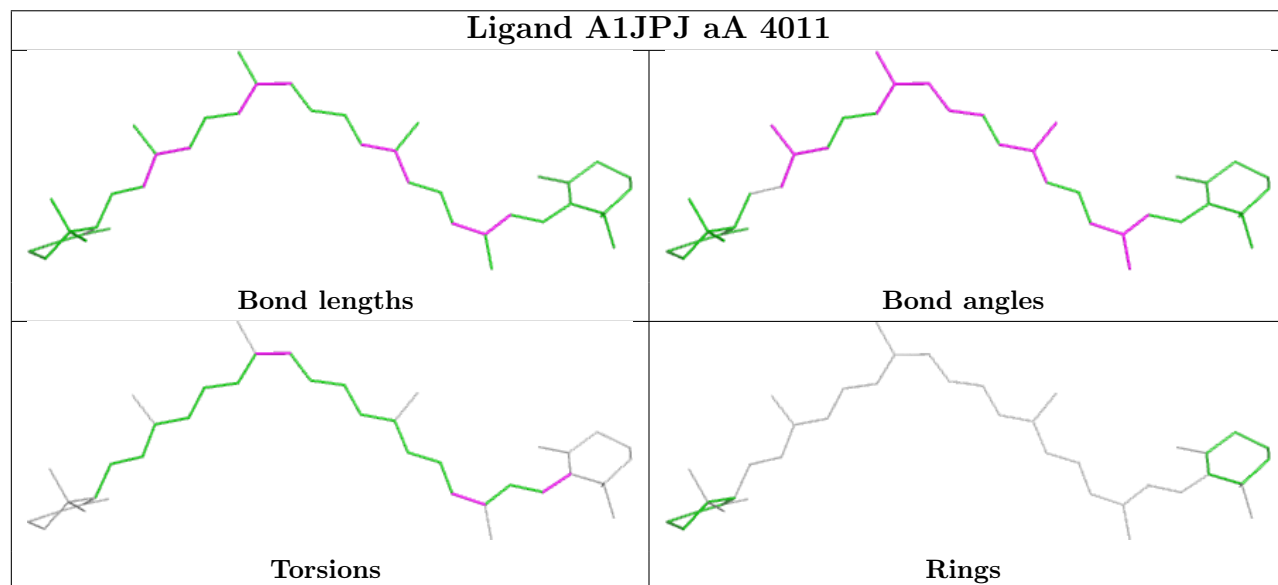
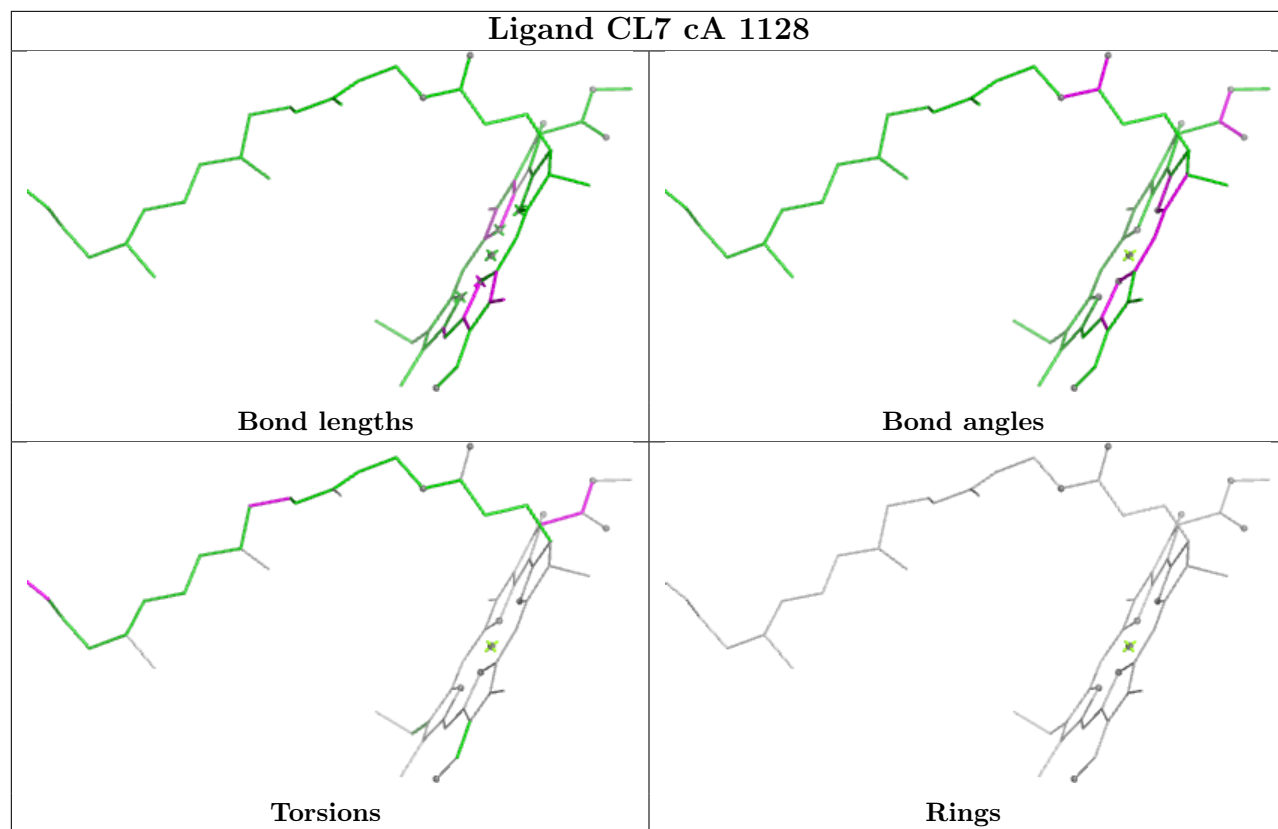


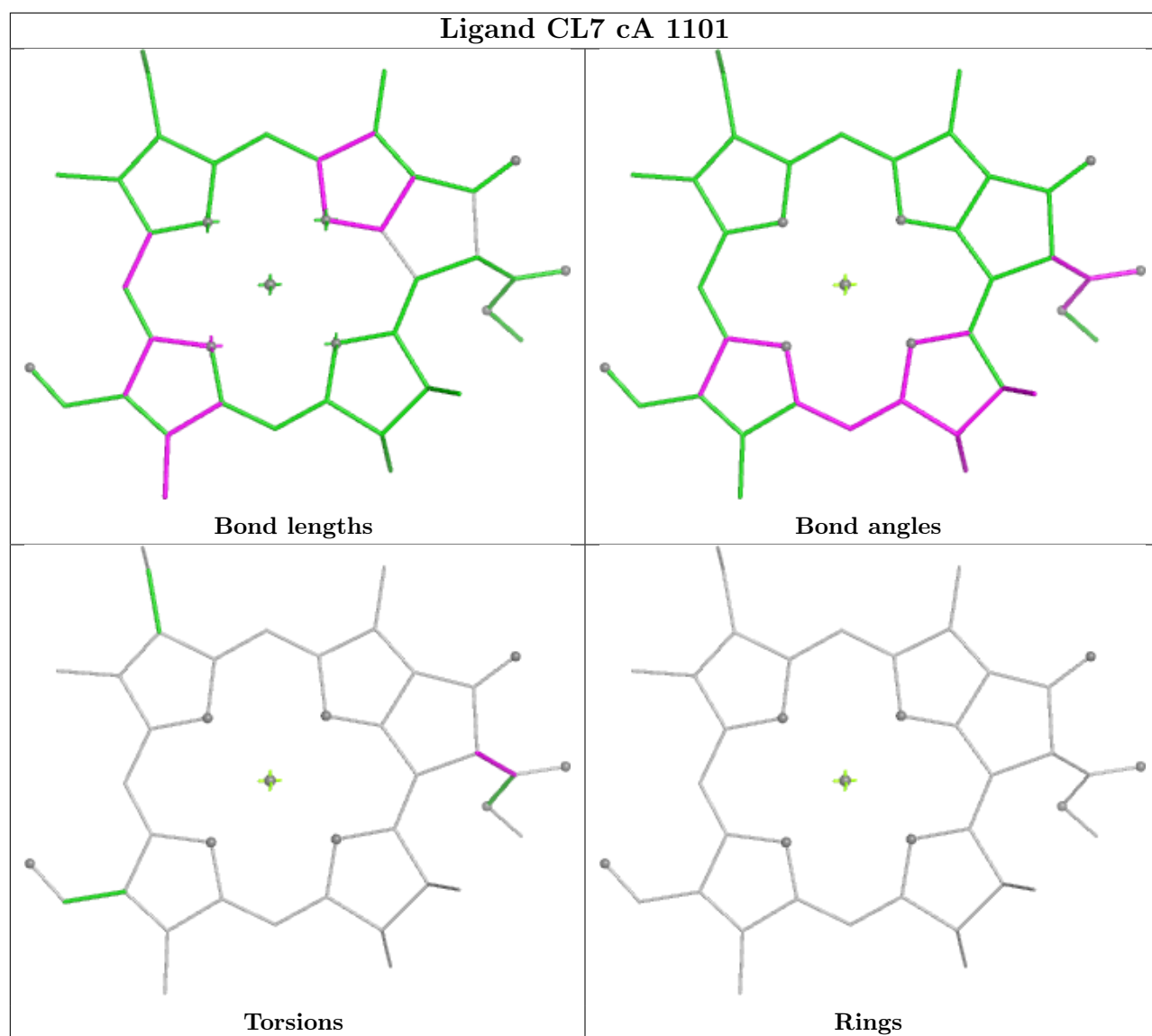
Torsions

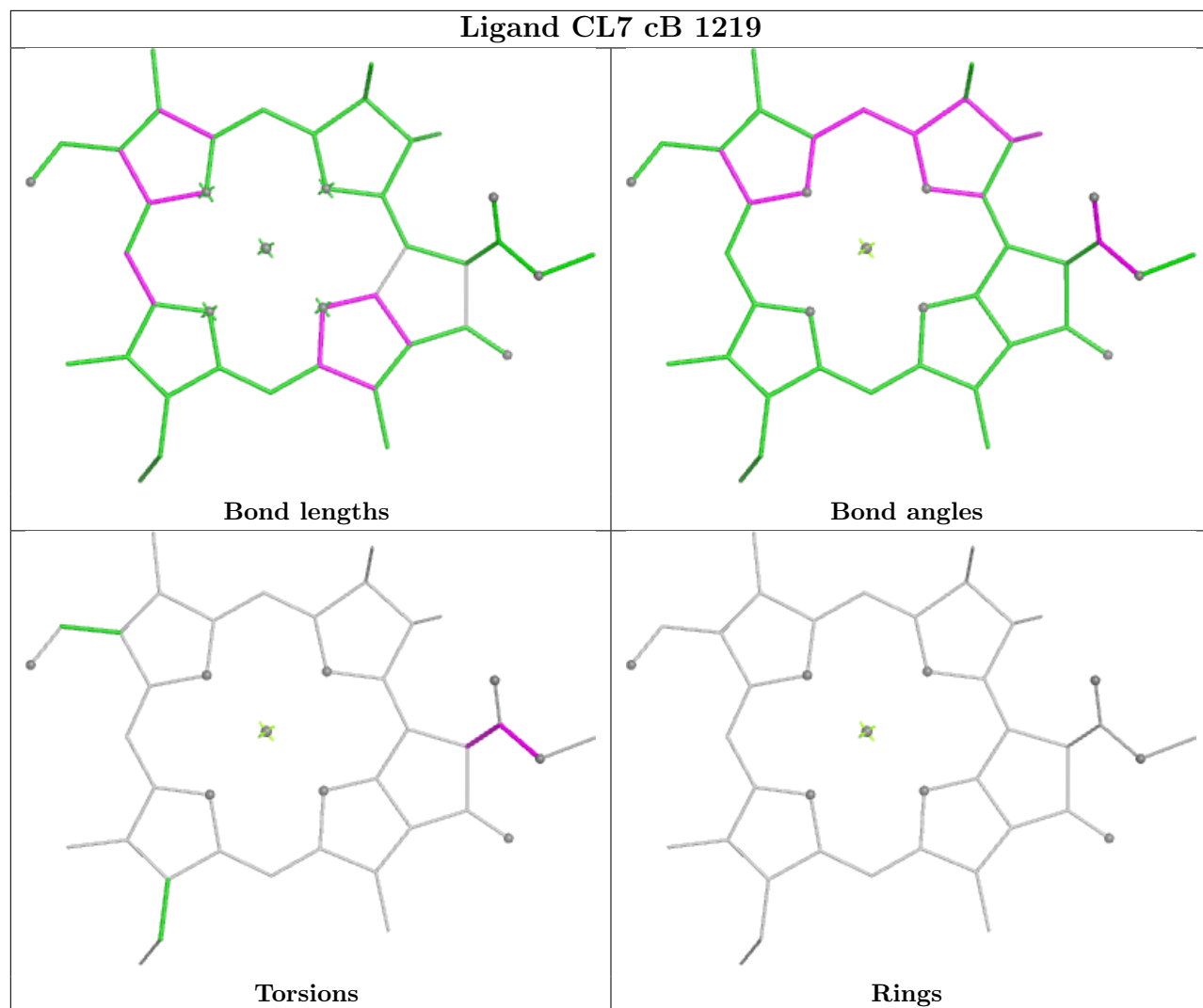


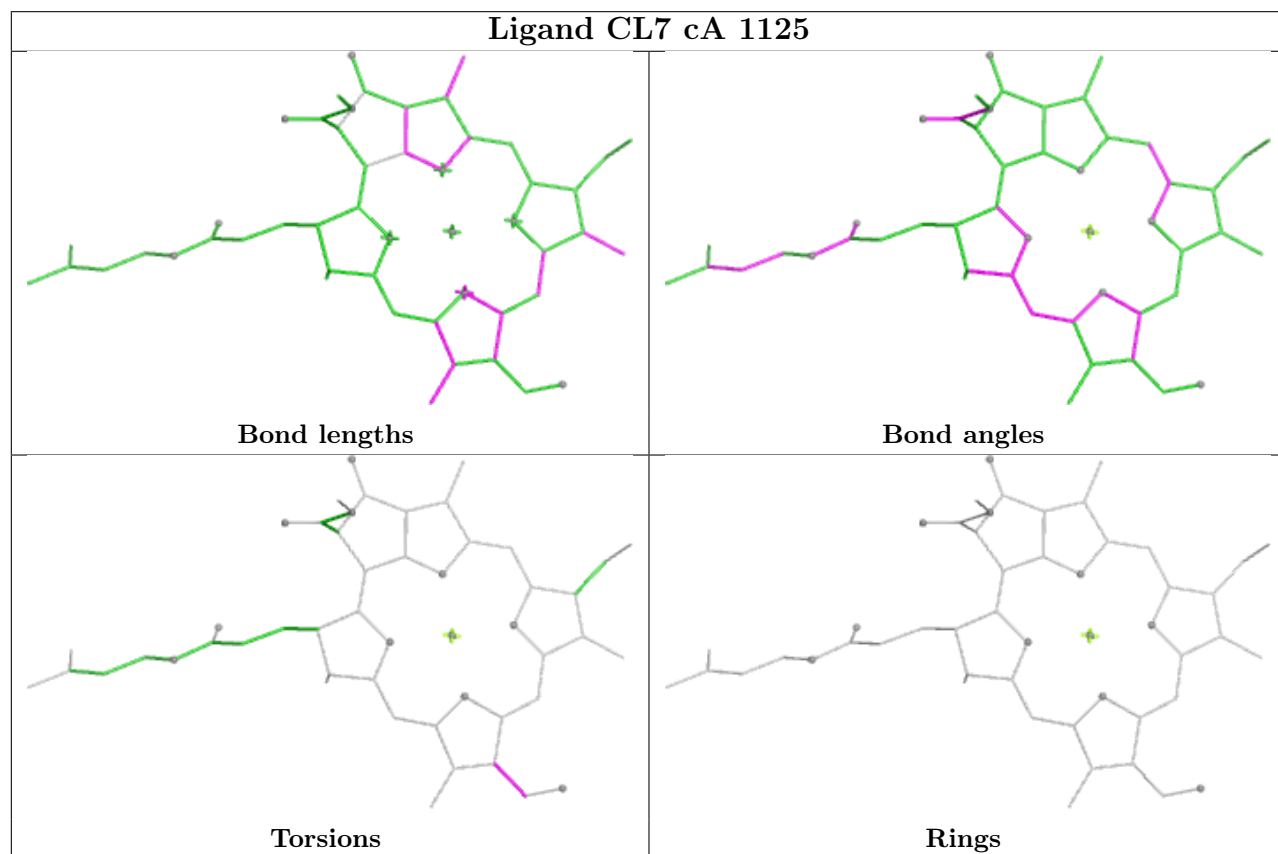
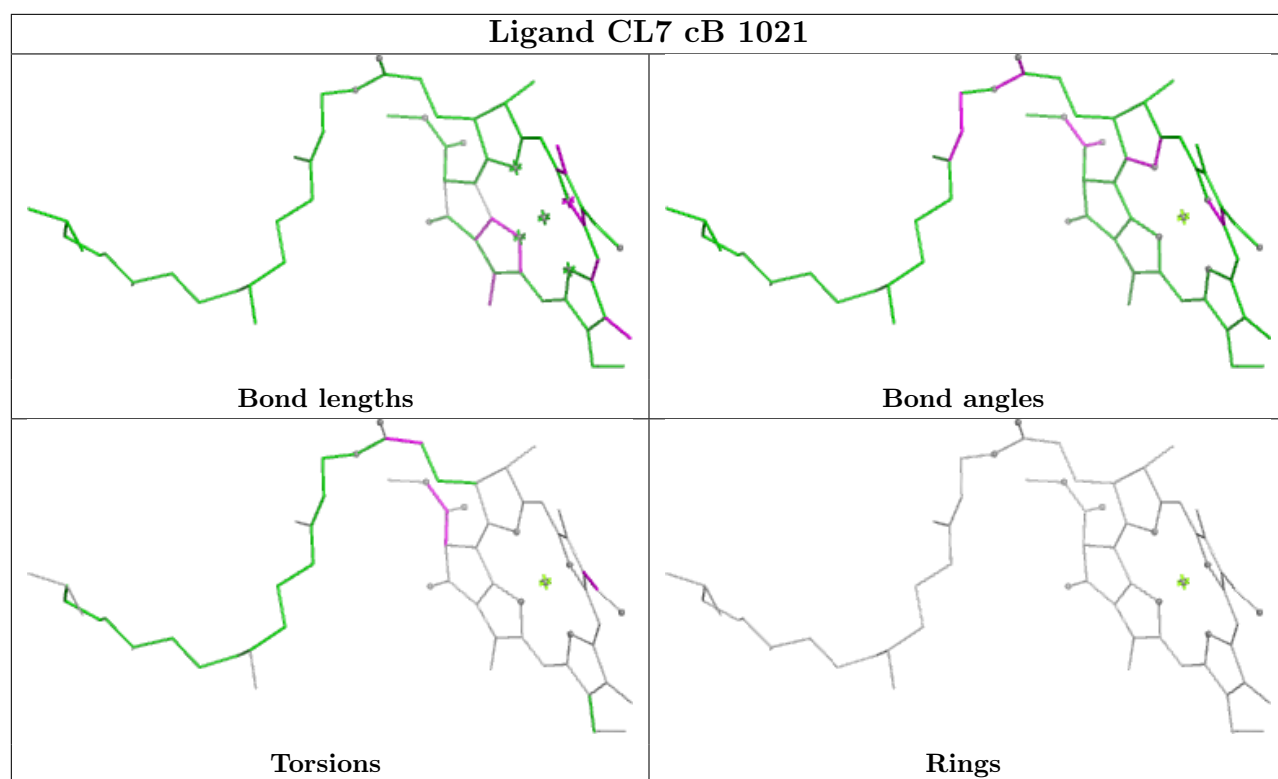
Rings

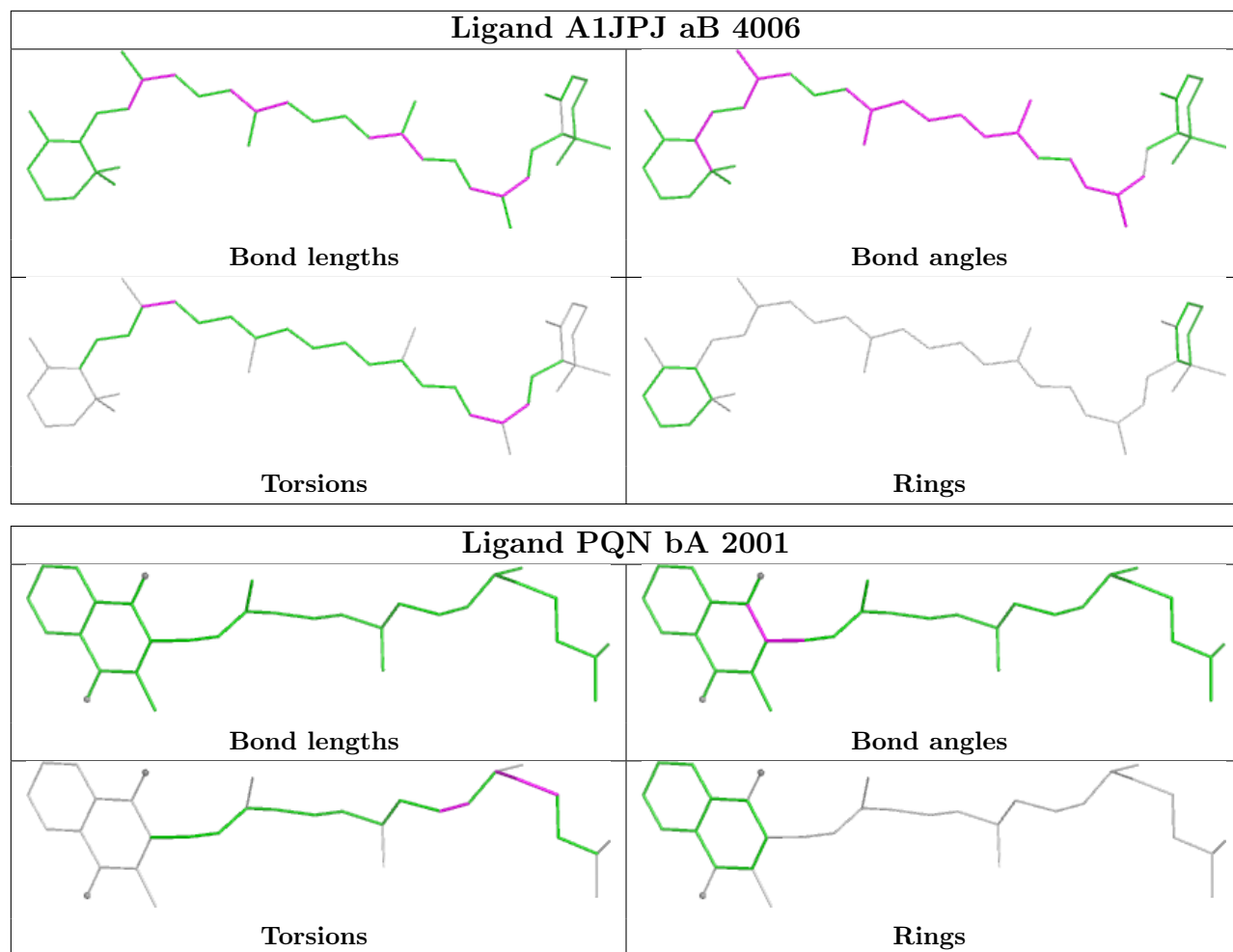




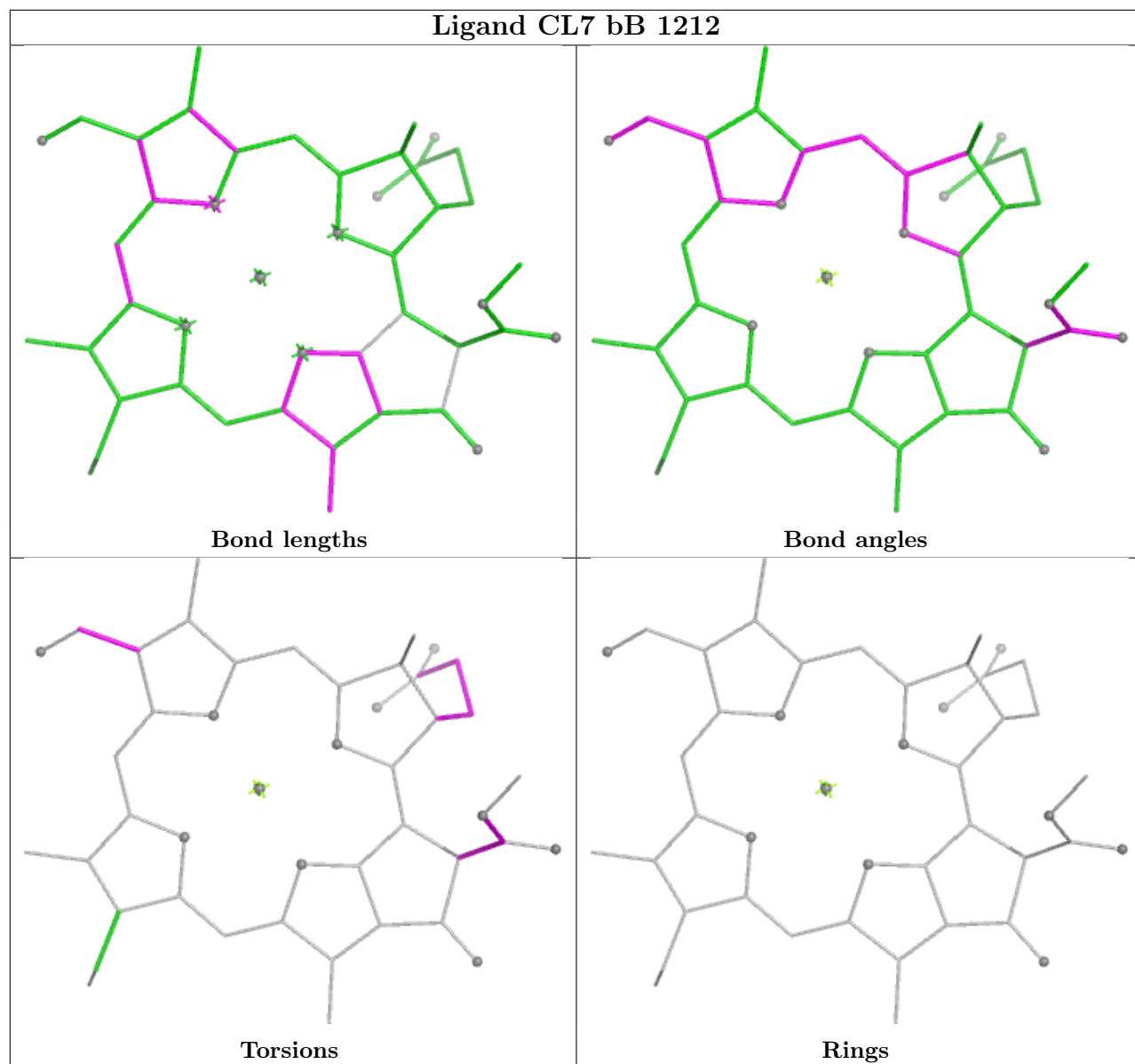


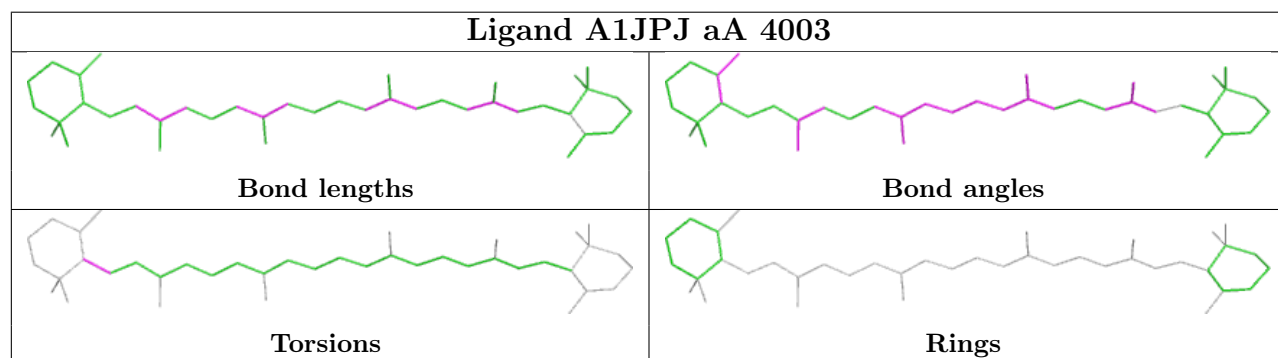
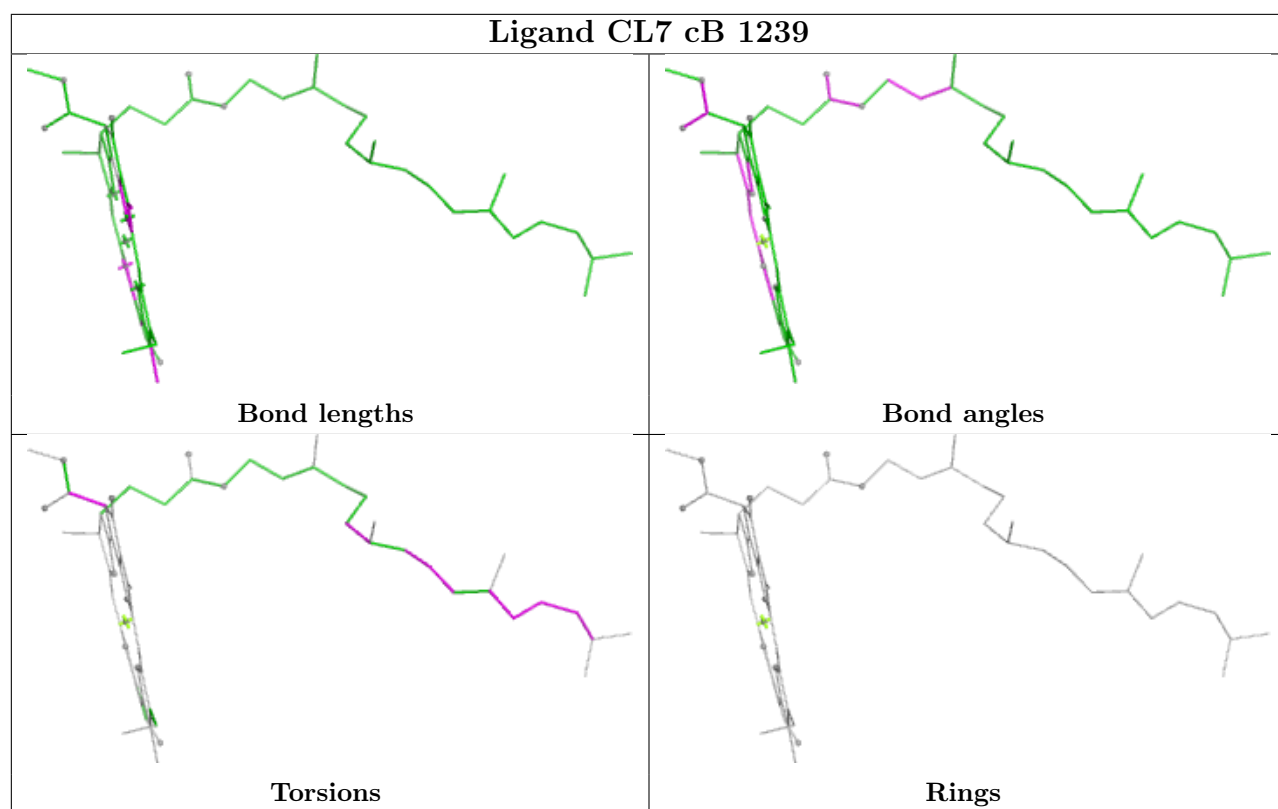


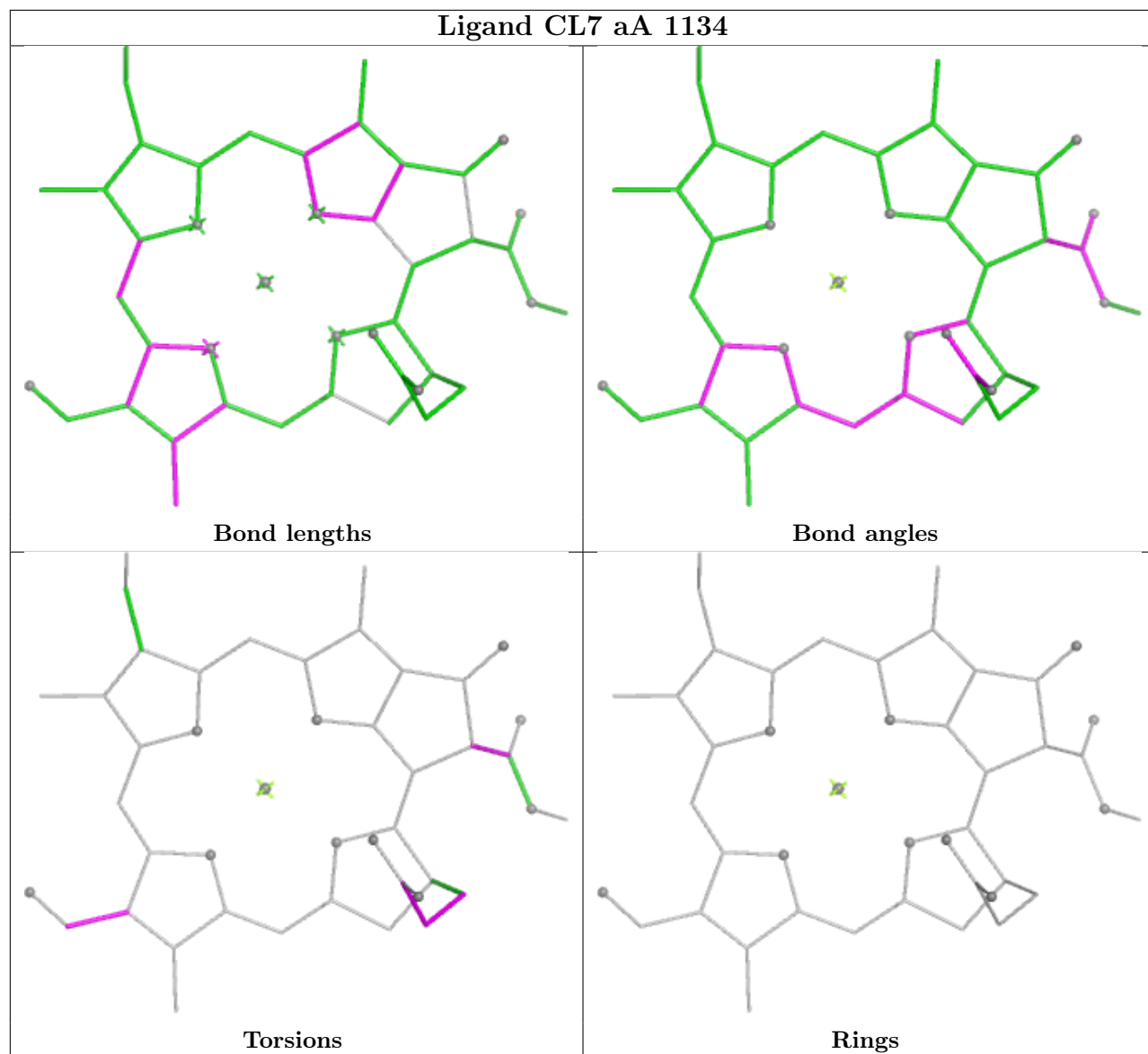




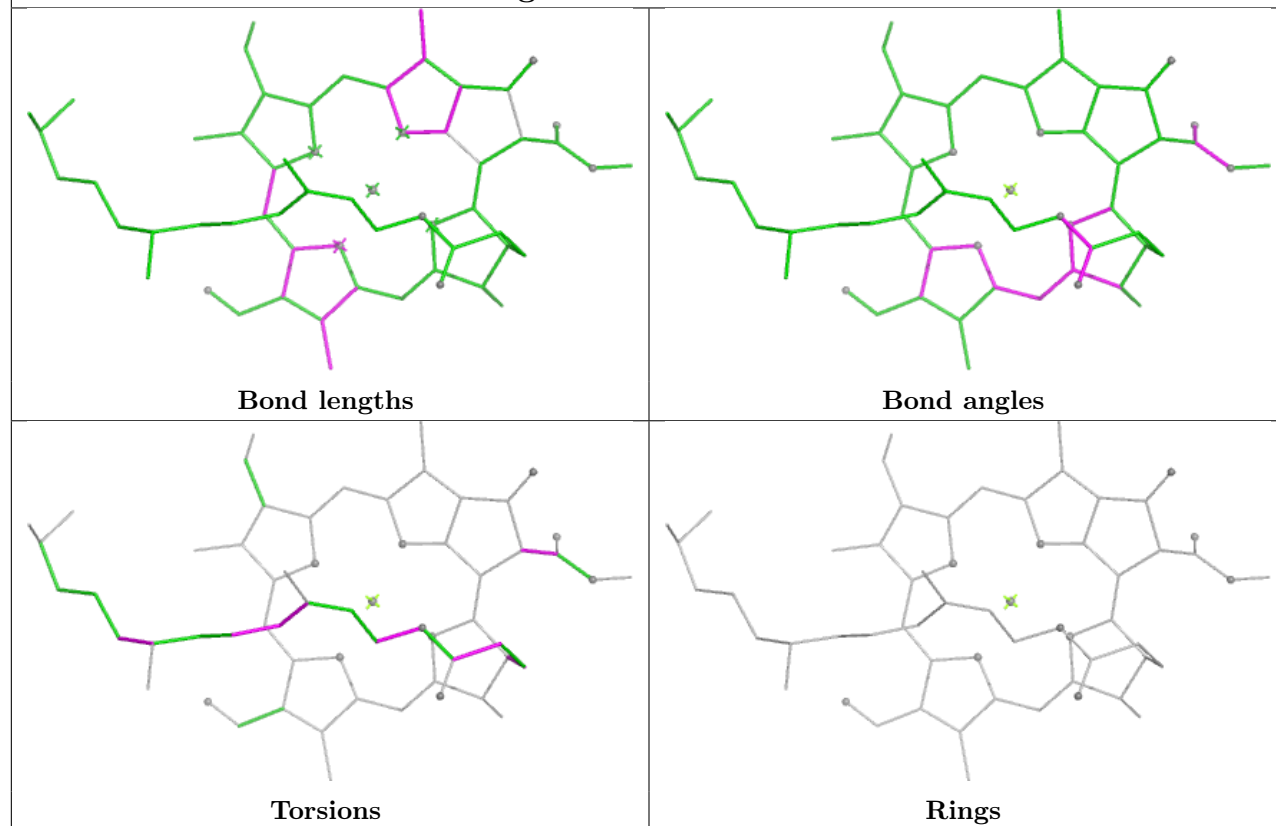
Ligand CL7 bB 1212



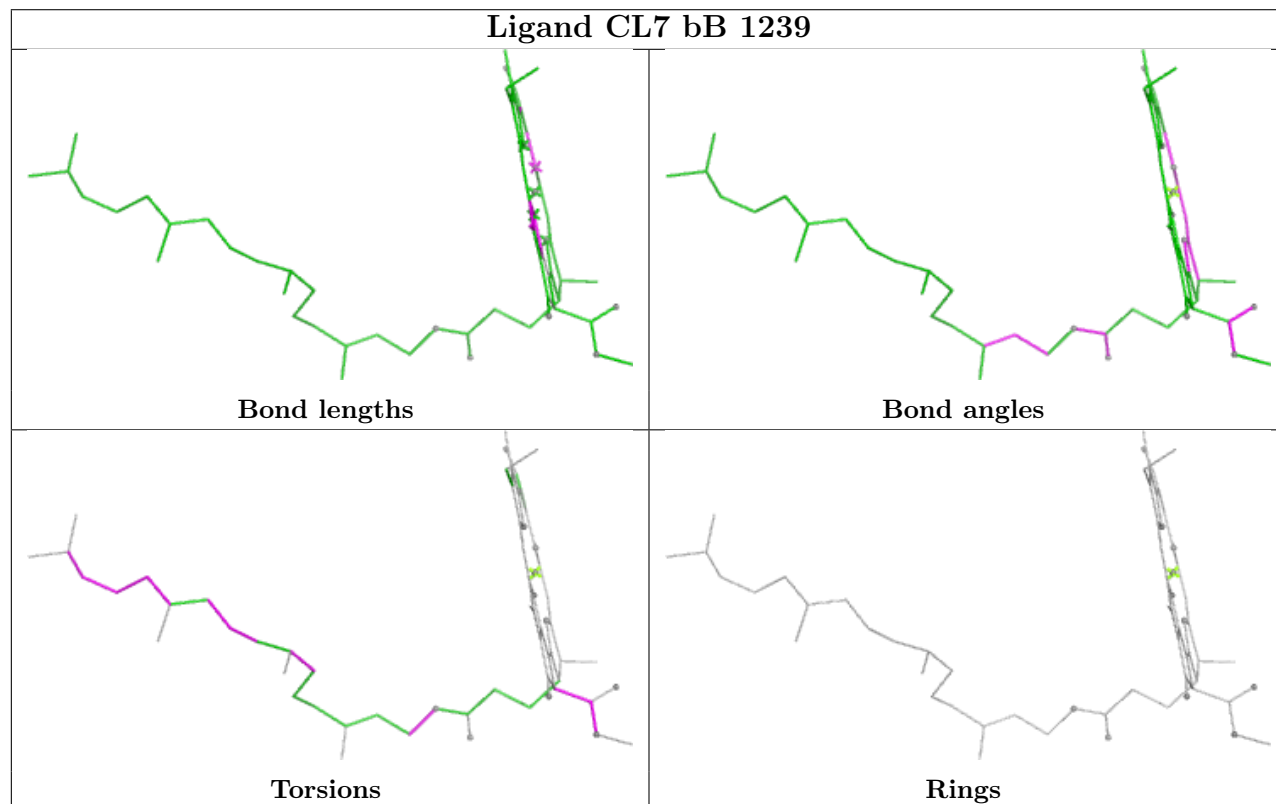


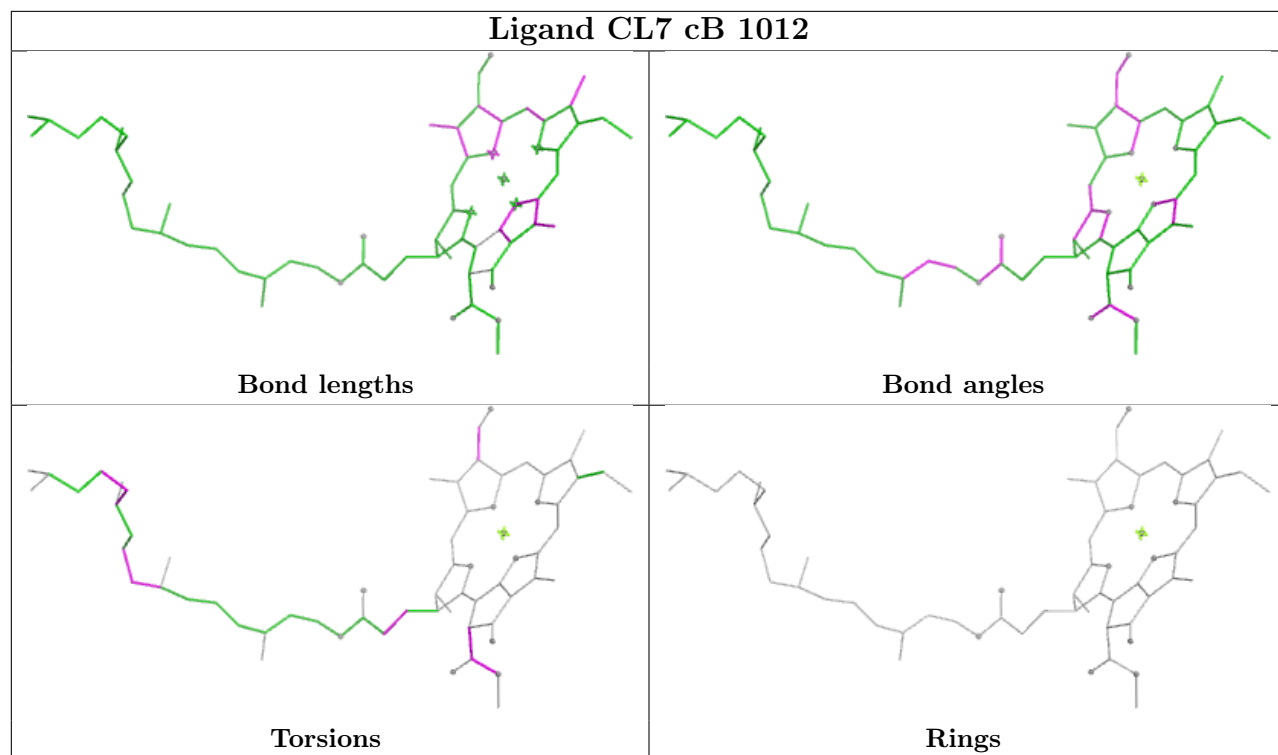


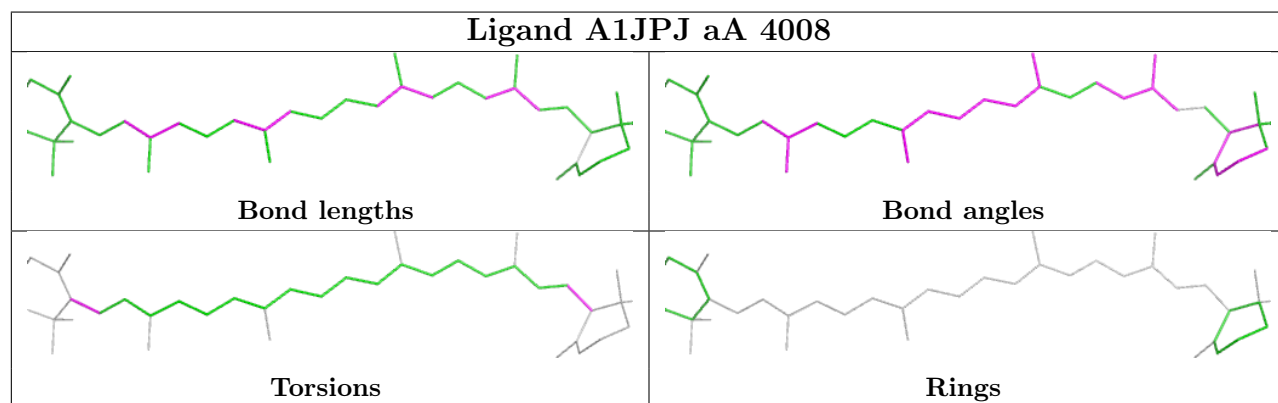
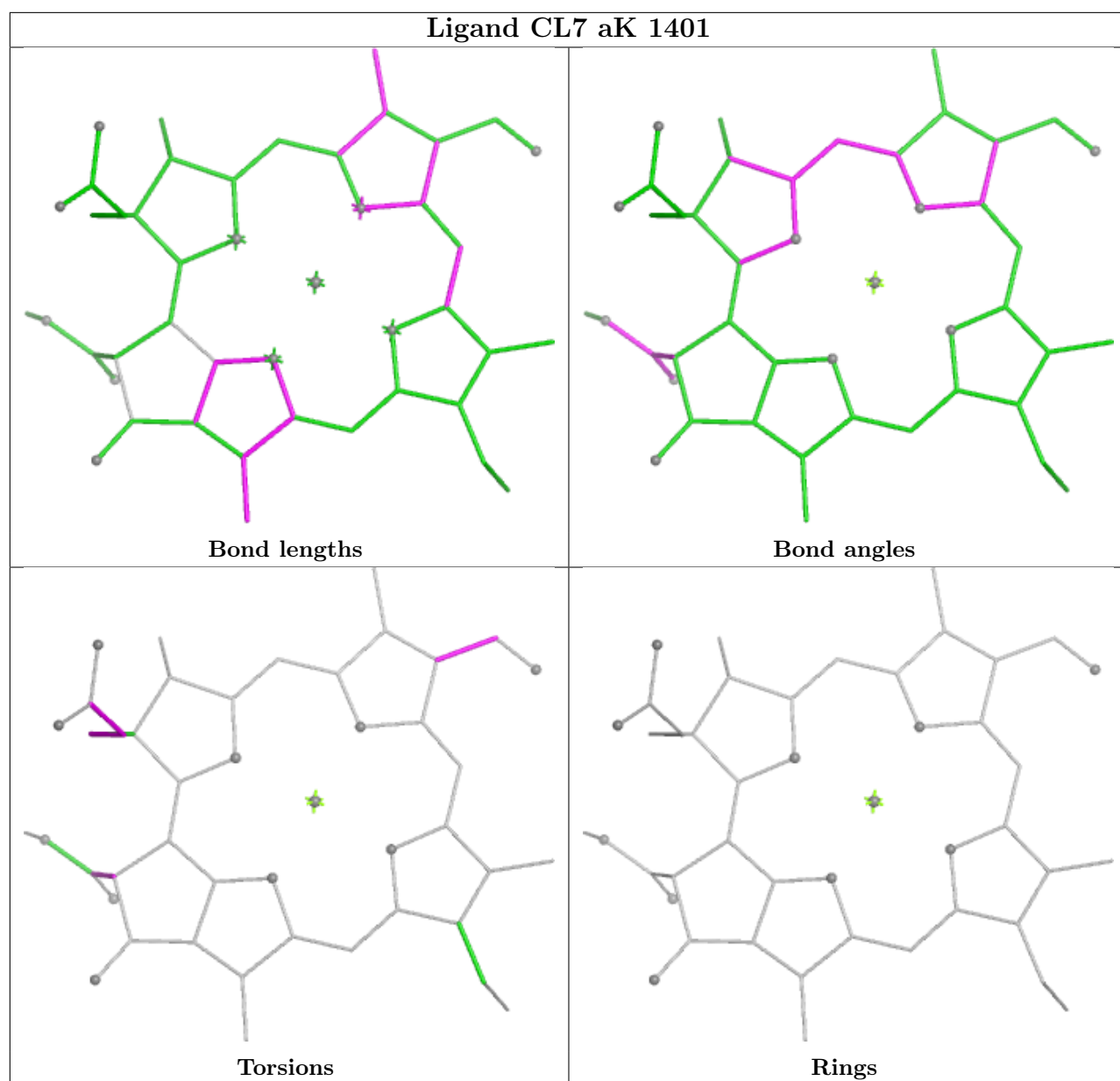
Ligand CL7 bB 1235

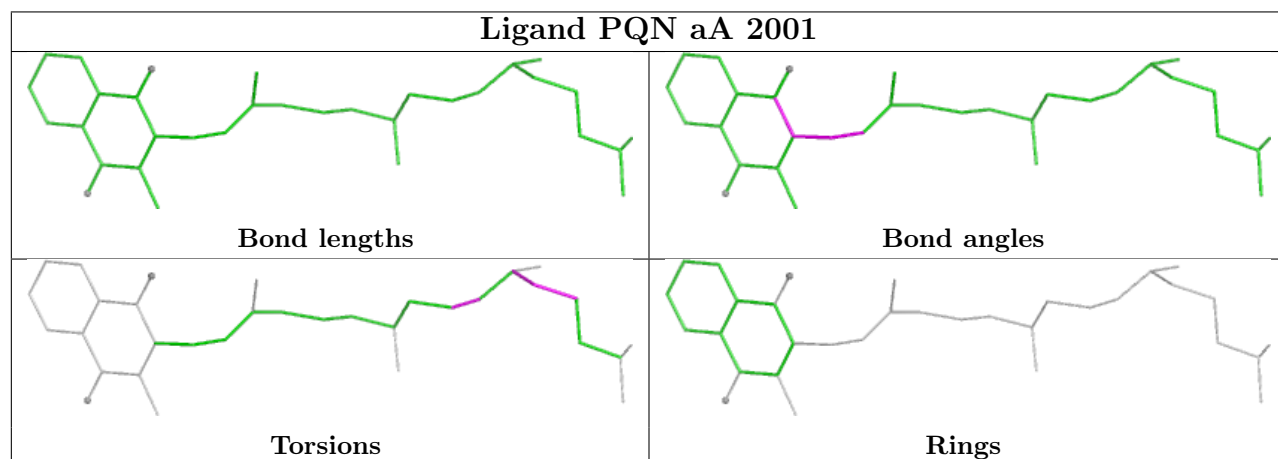
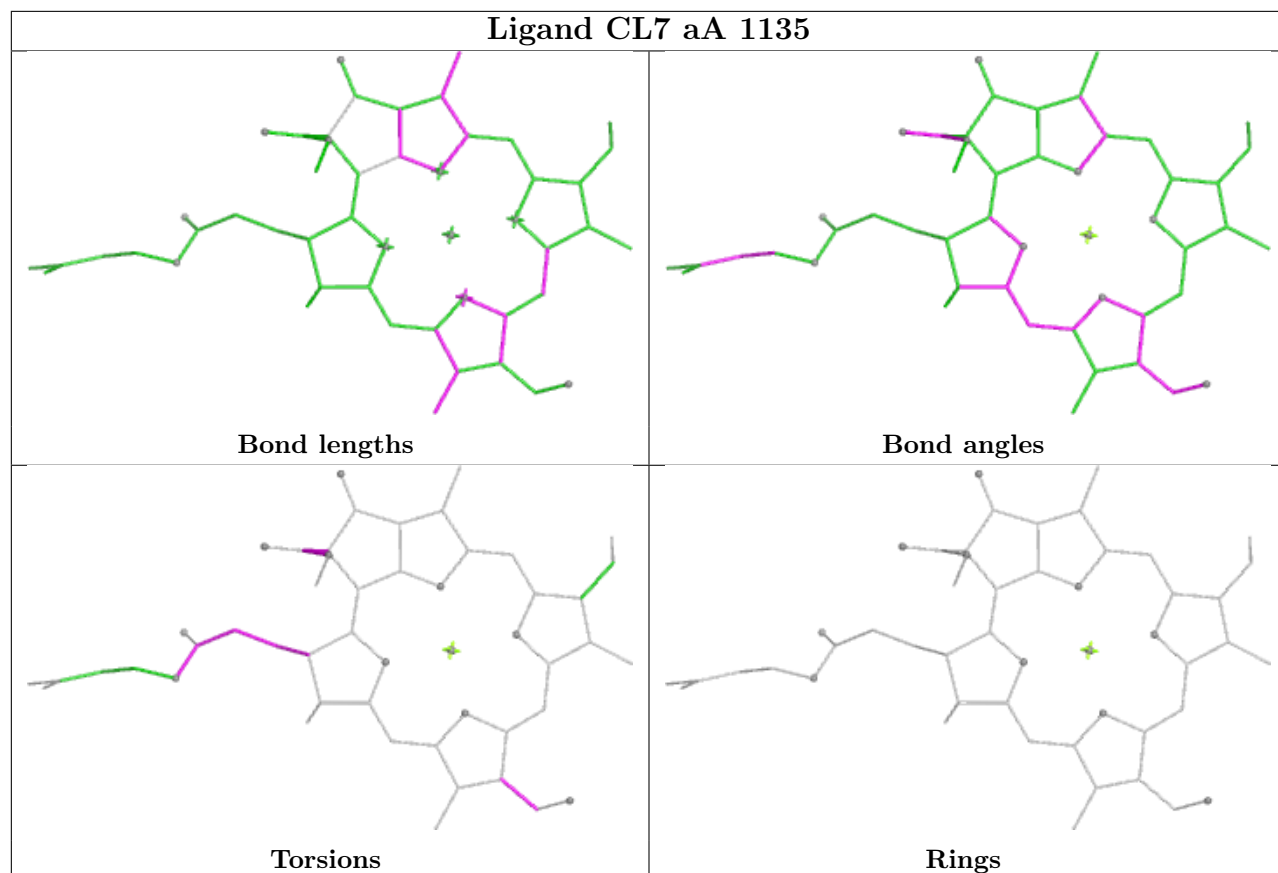


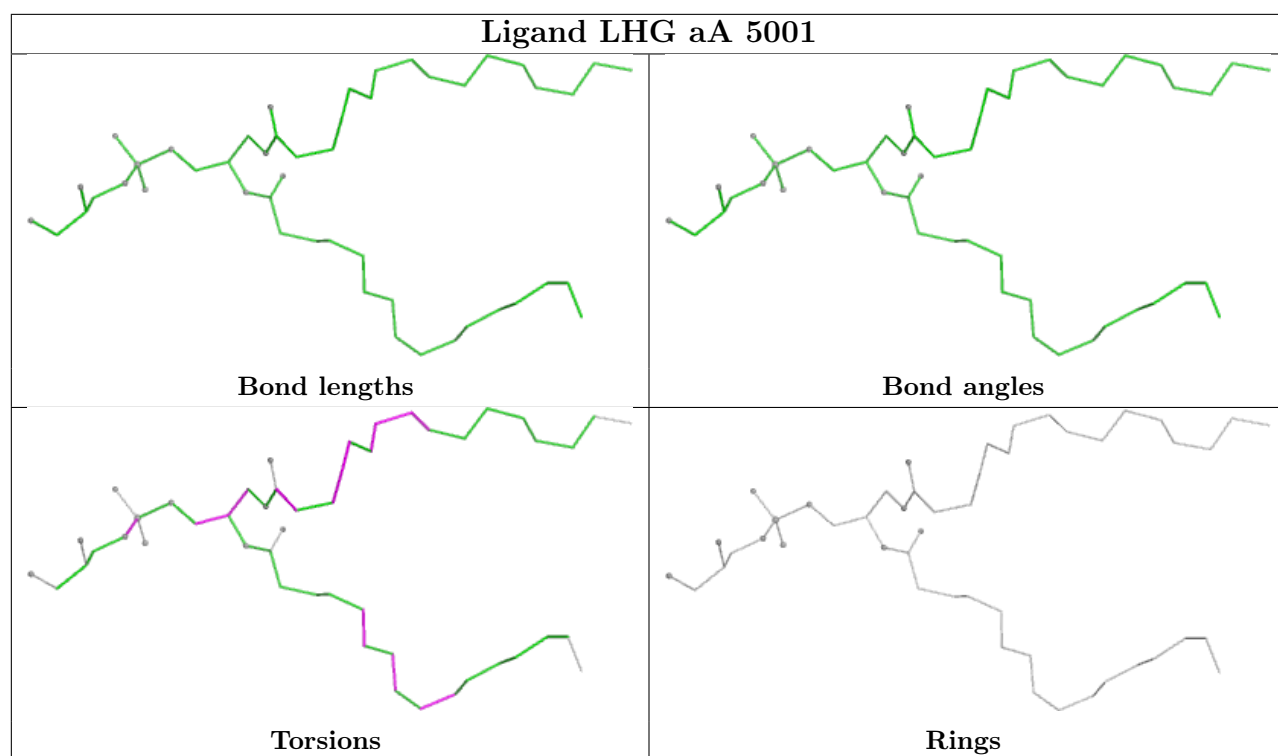
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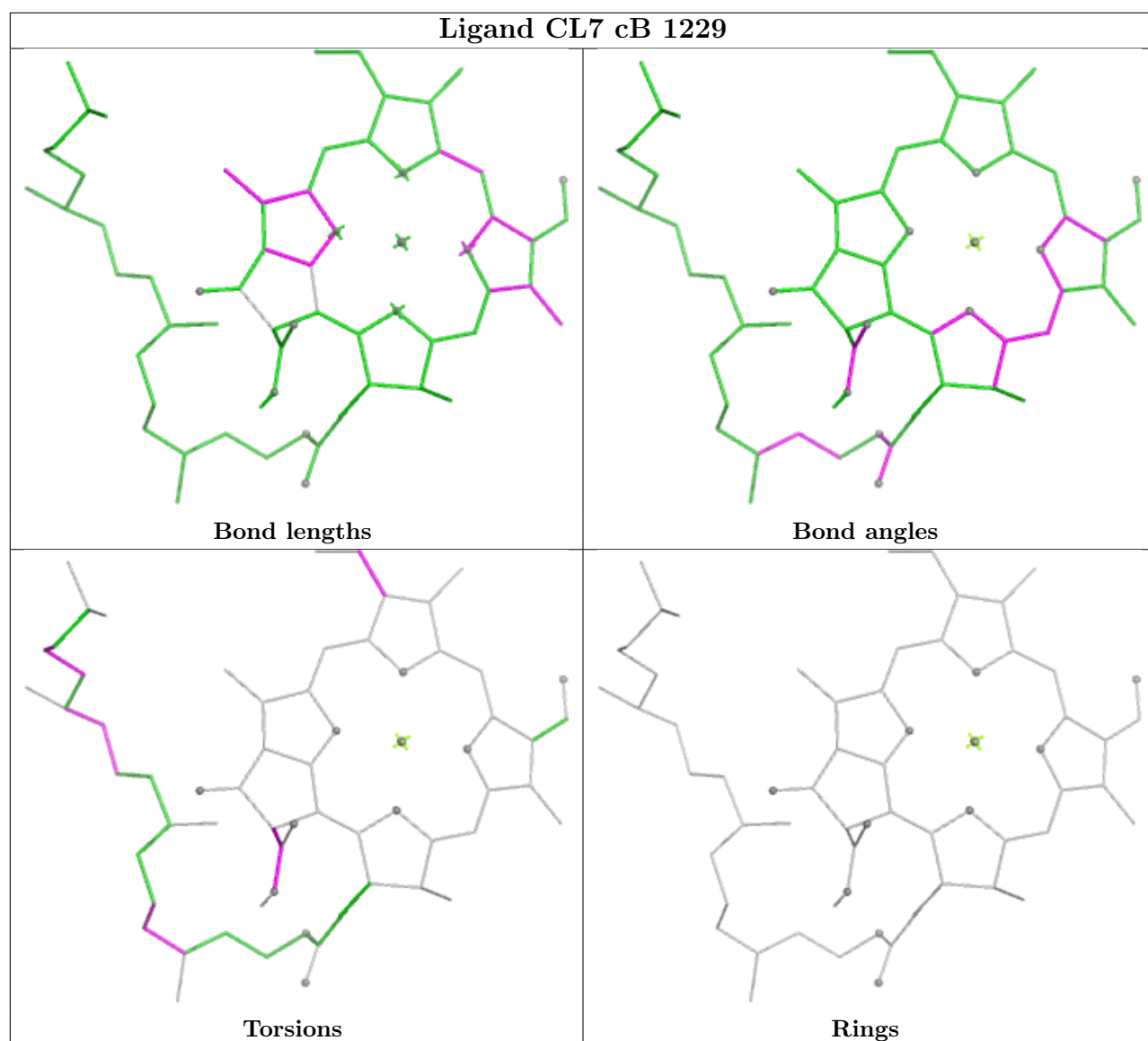




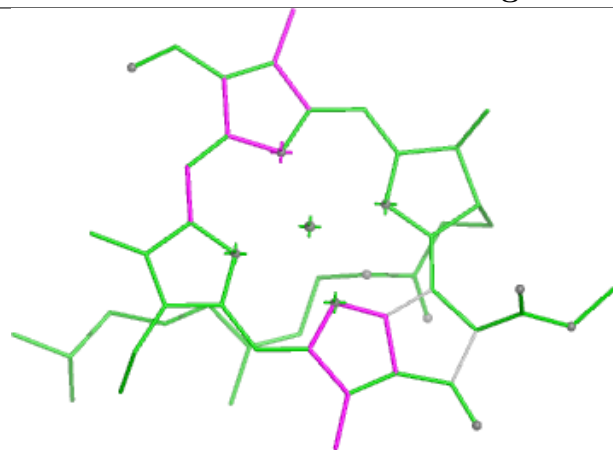




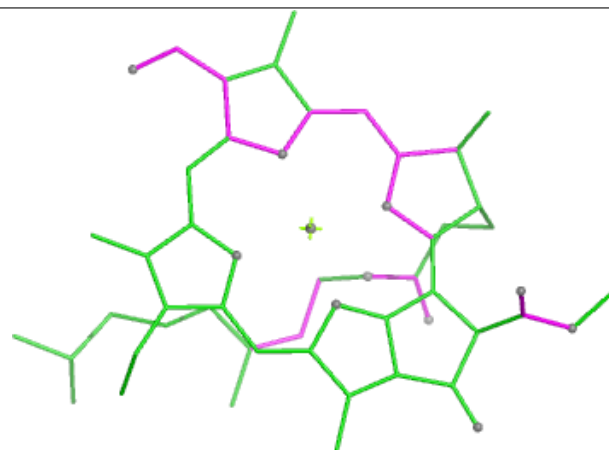




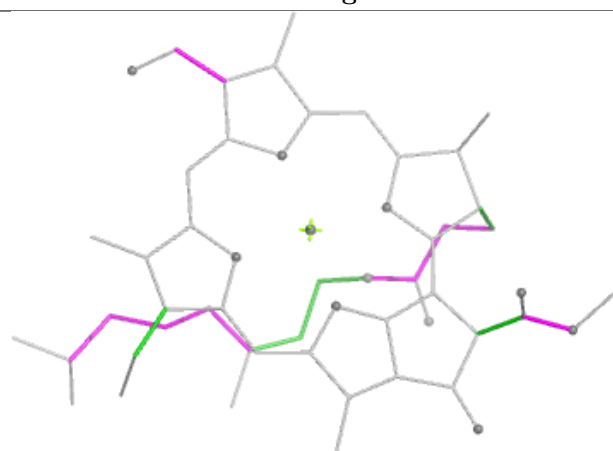
Ligand CL7 bA 1119



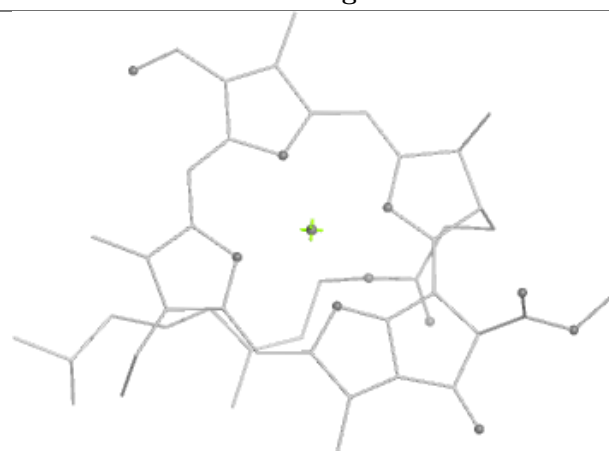
Bond lengths



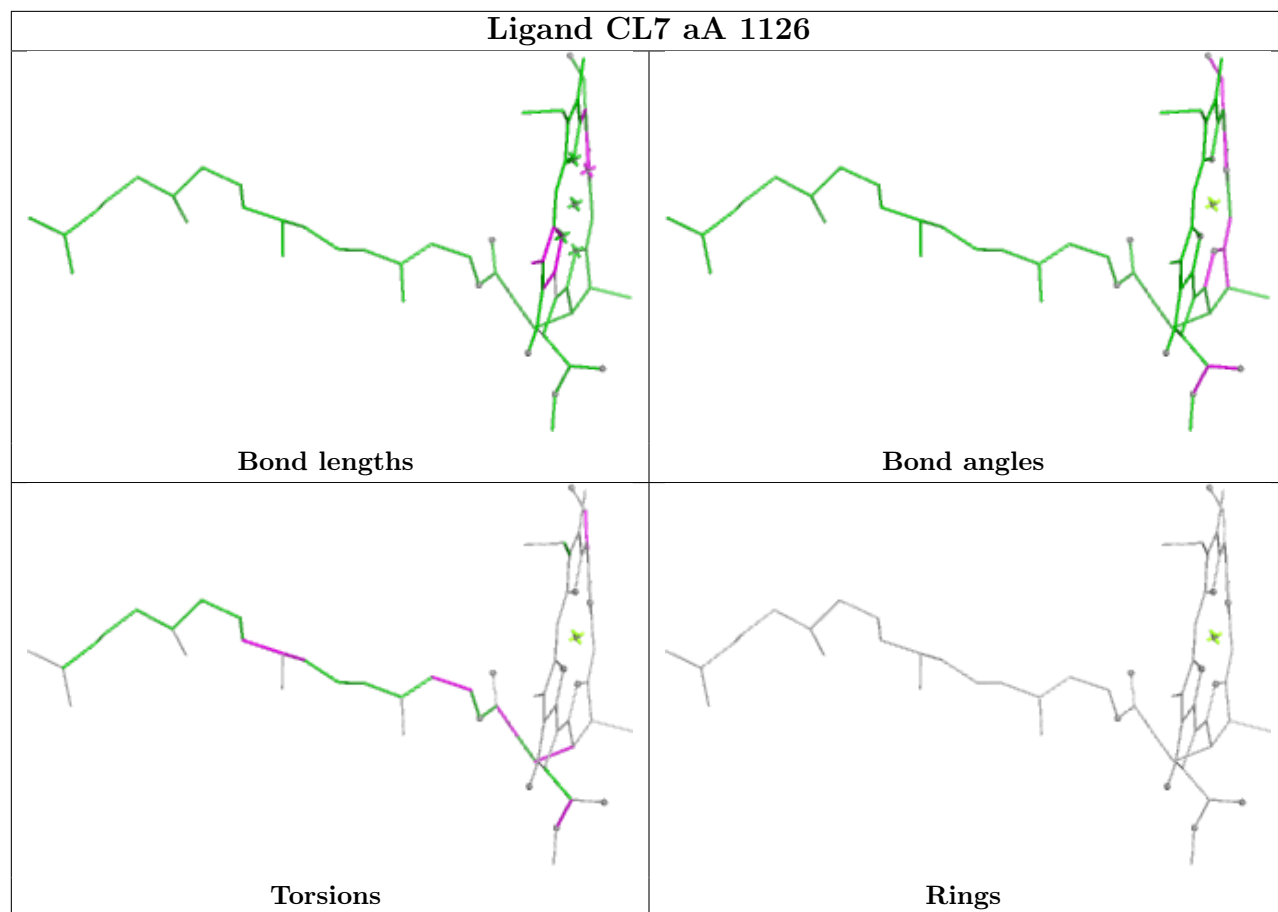
Bond angles



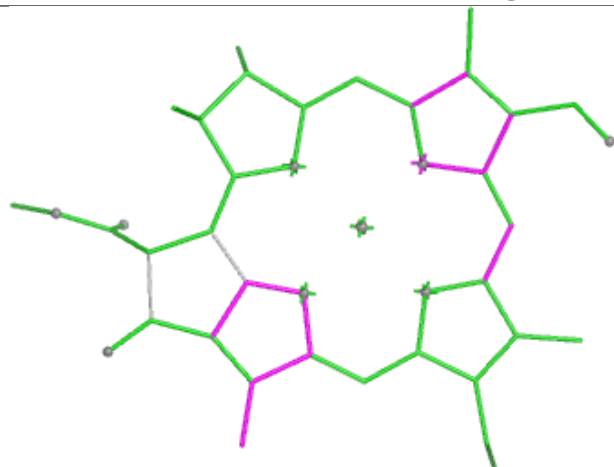
Torsions



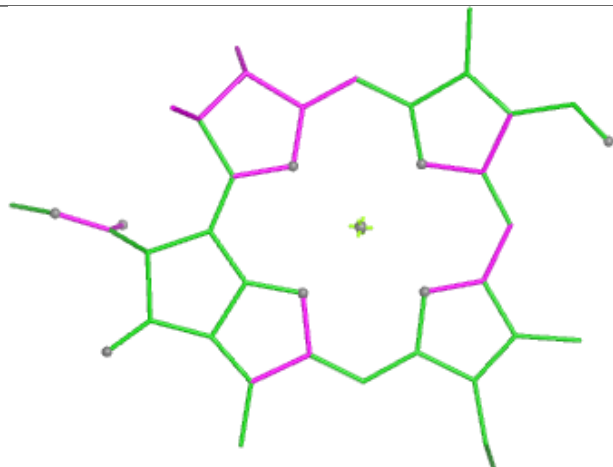
Rings



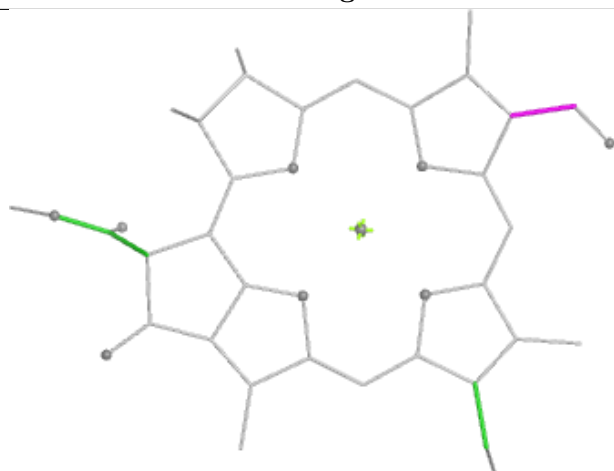
Ligand CL7 aF 1701



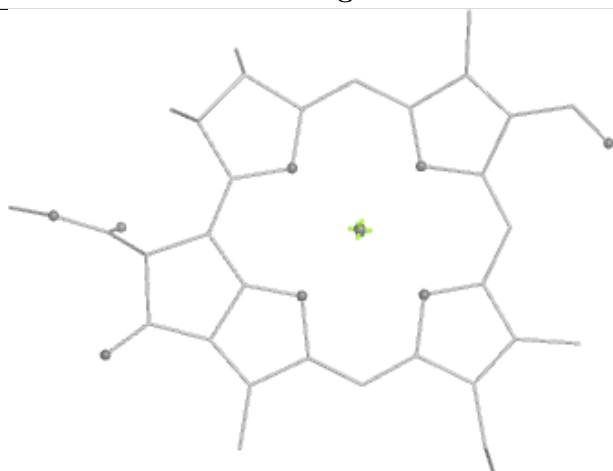
Bond lengths



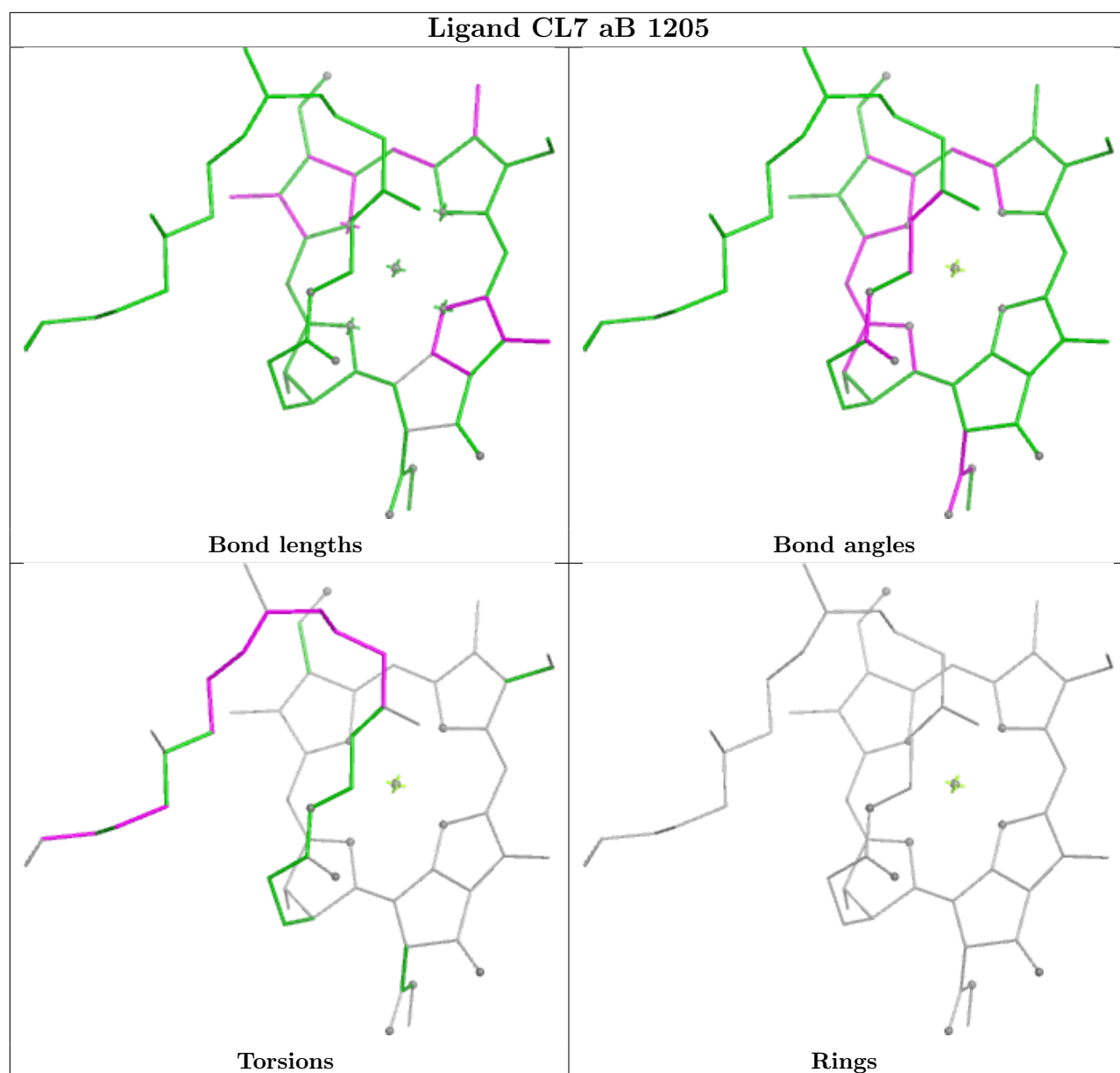
Bond angles



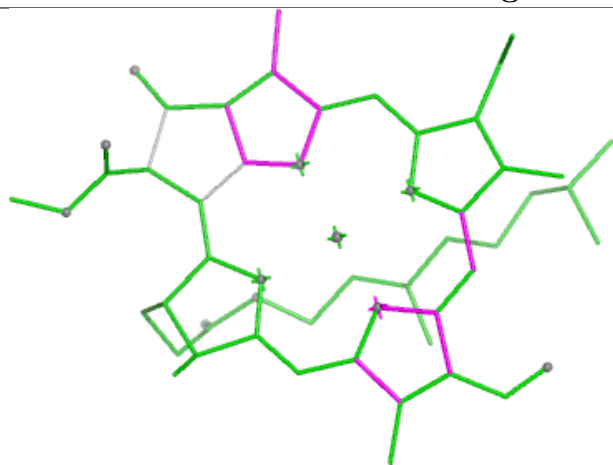
Torsions



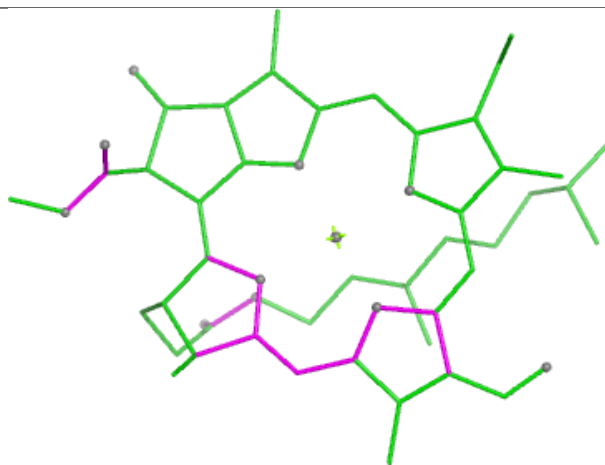
Rings



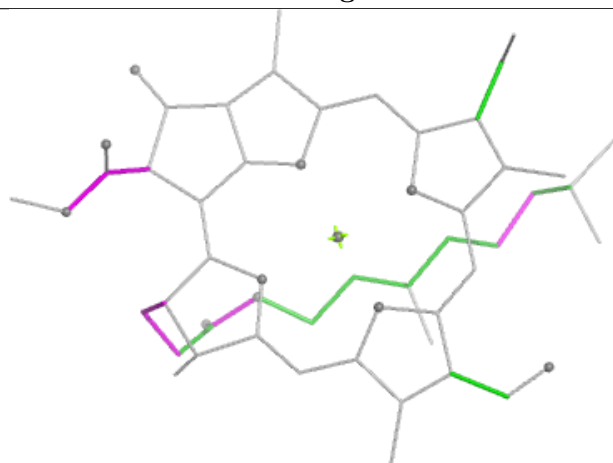
Ligand CL7 cA 1121



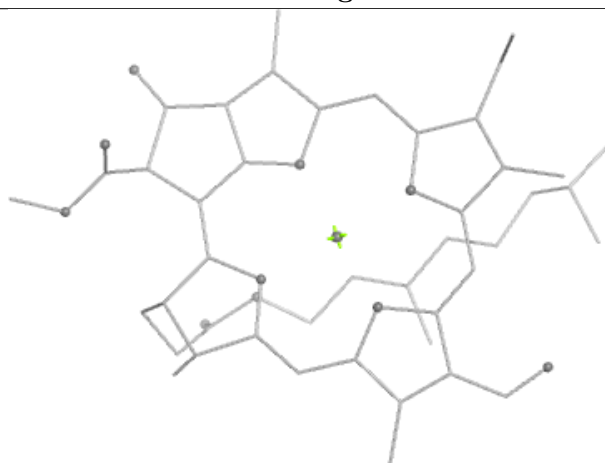
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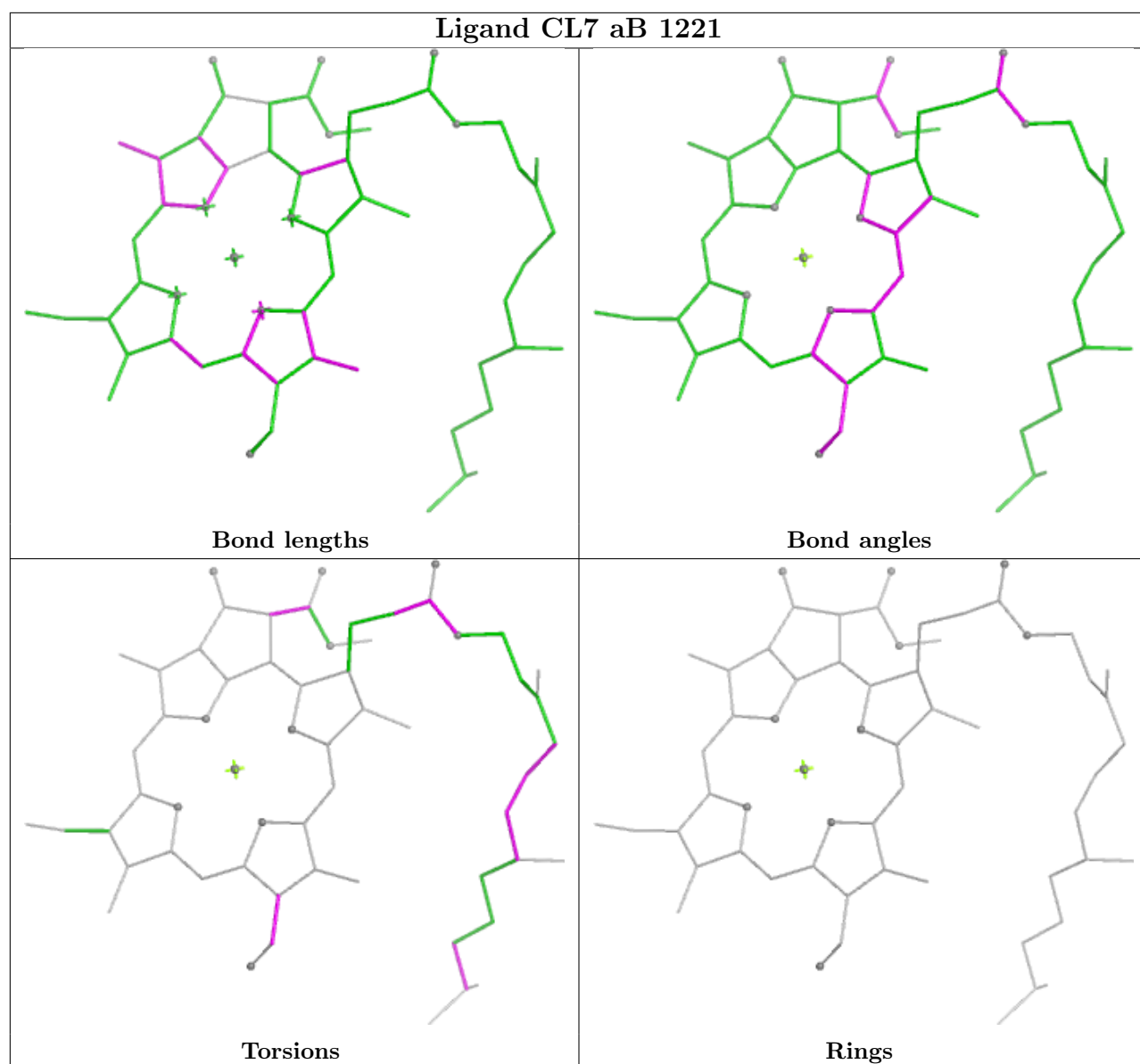
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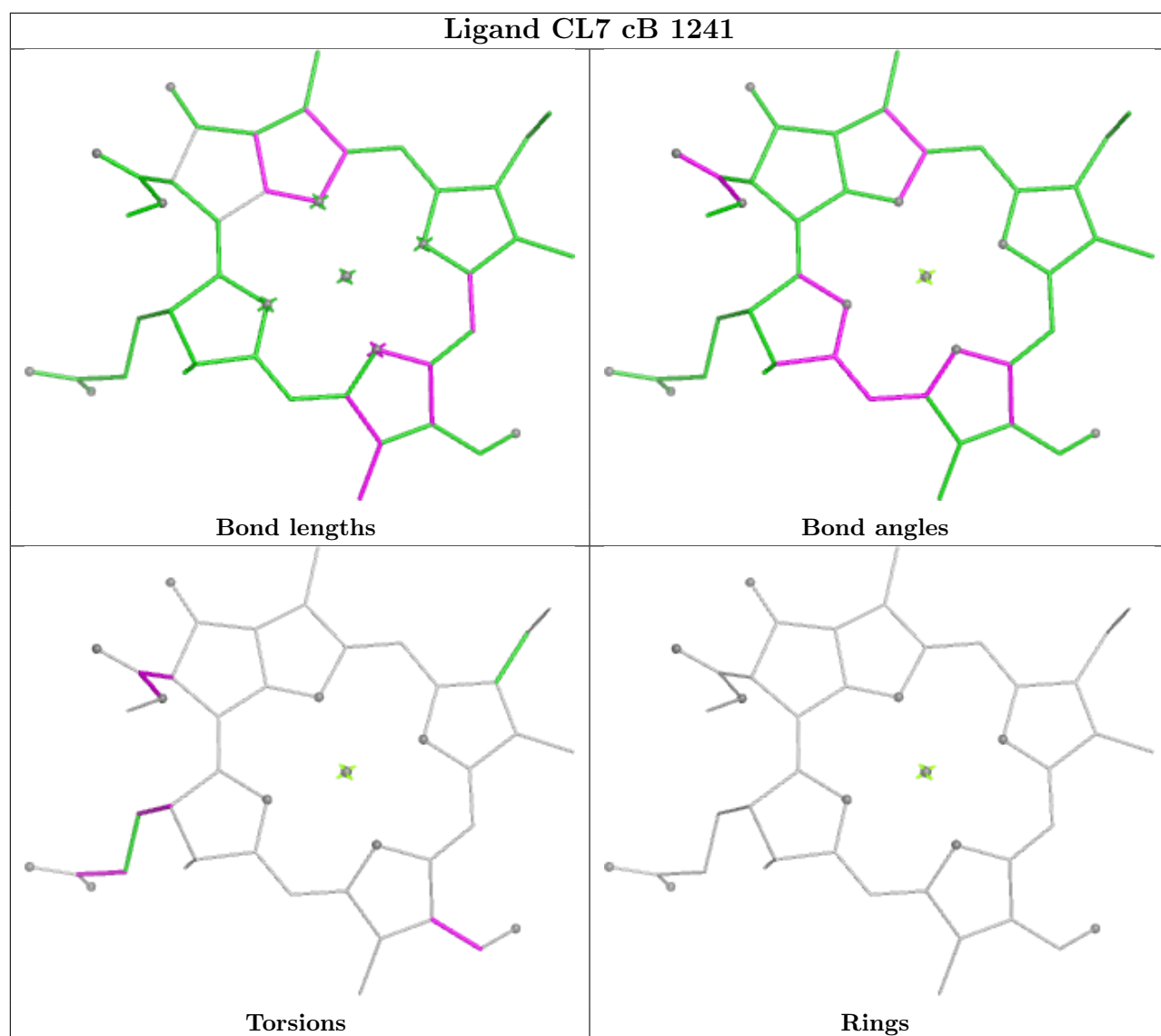


Torsions

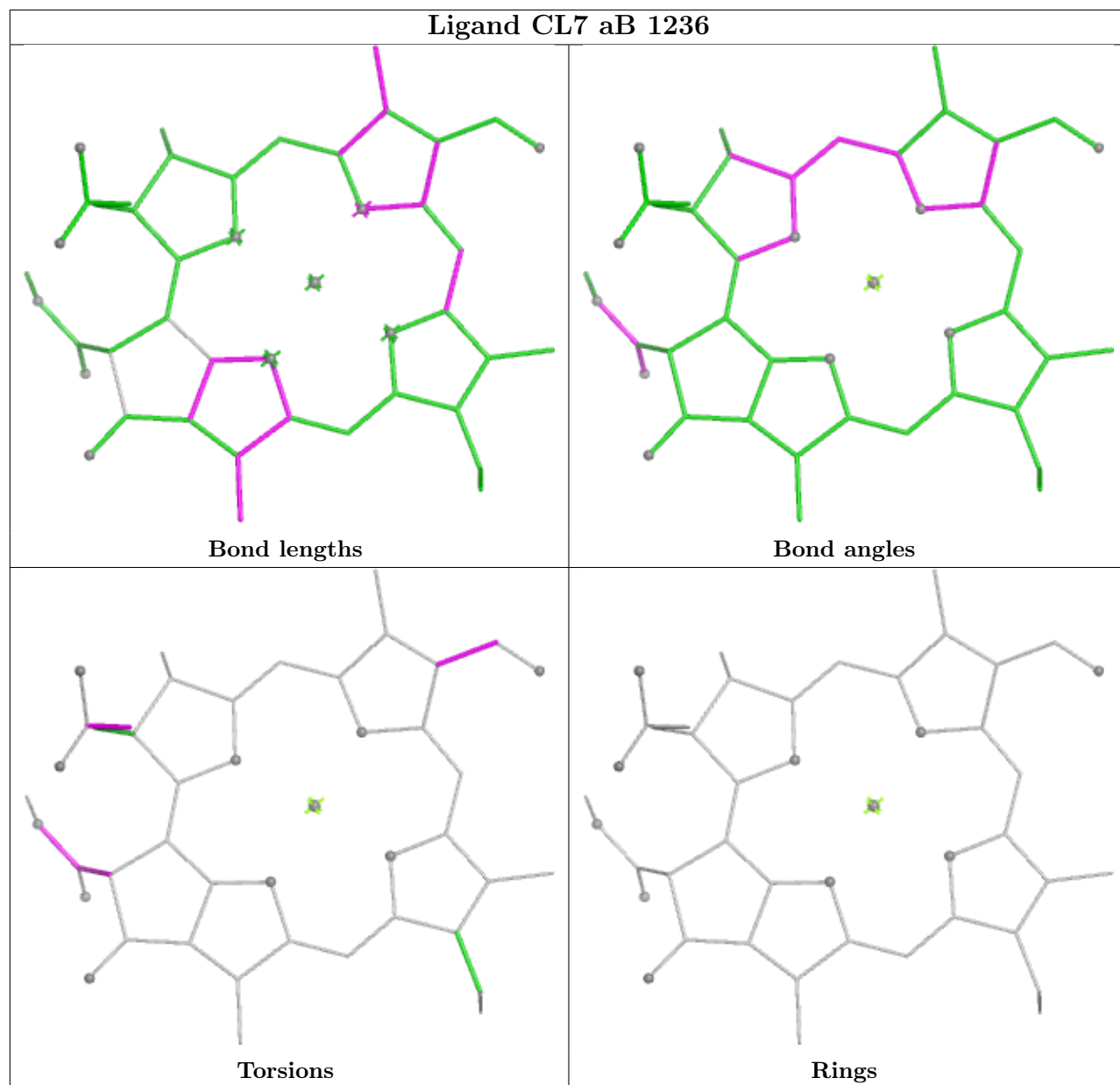


Rings

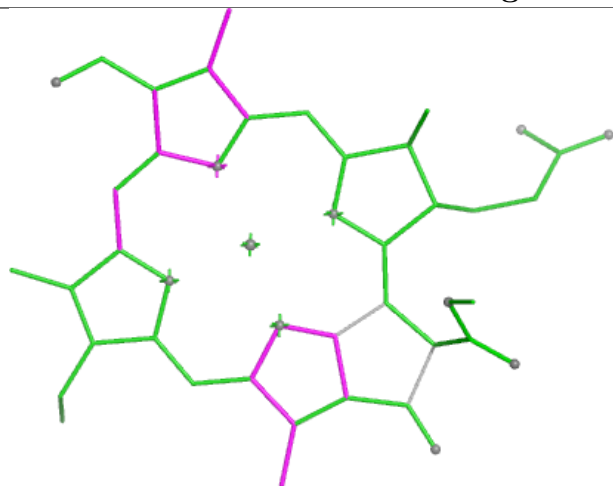




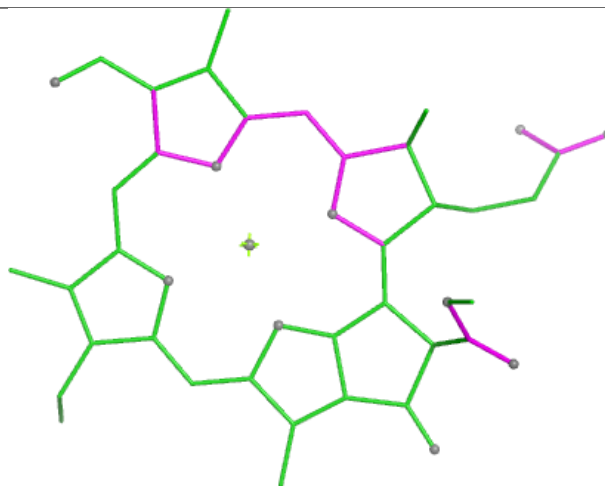
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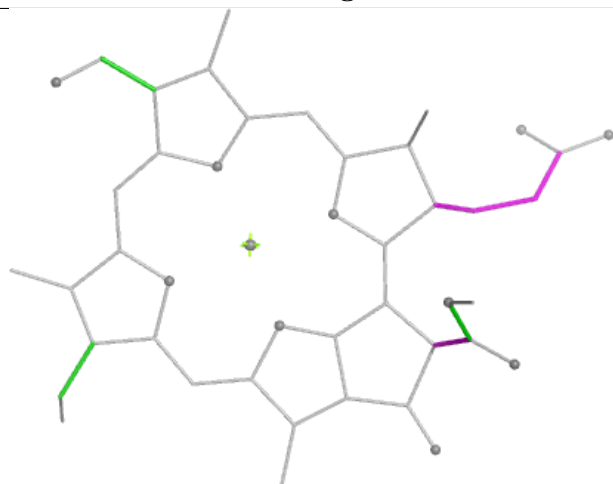
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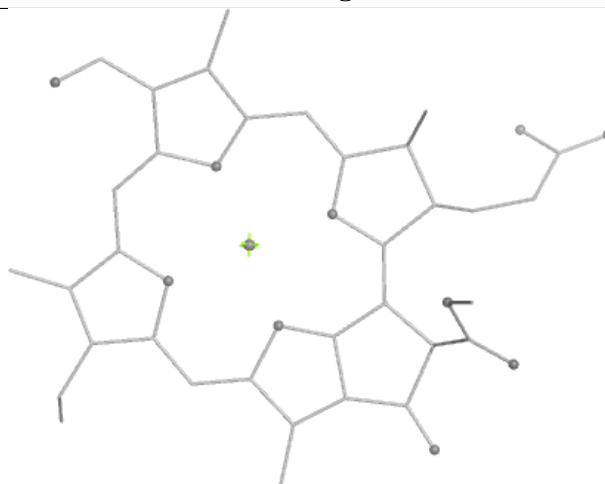
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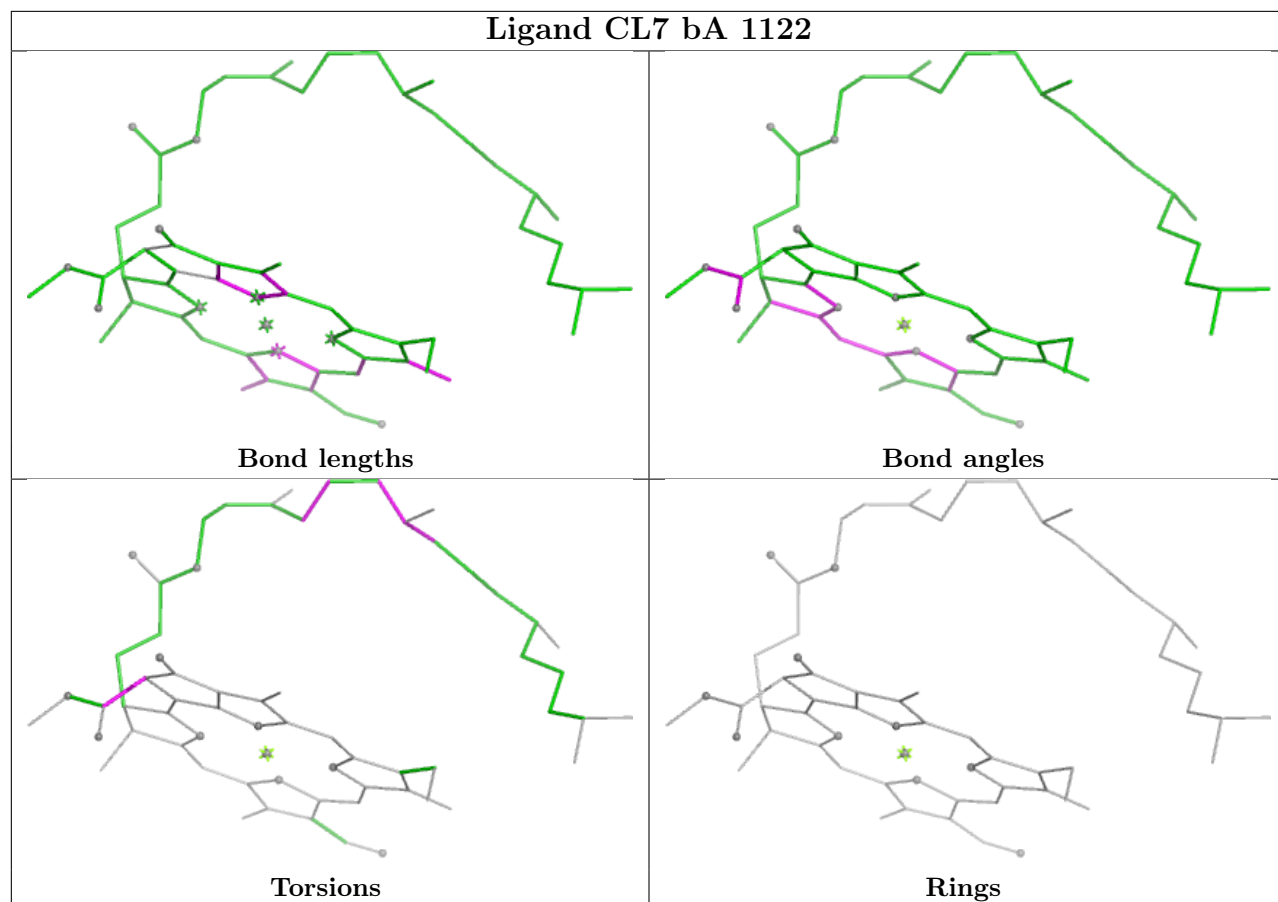
Bond angles

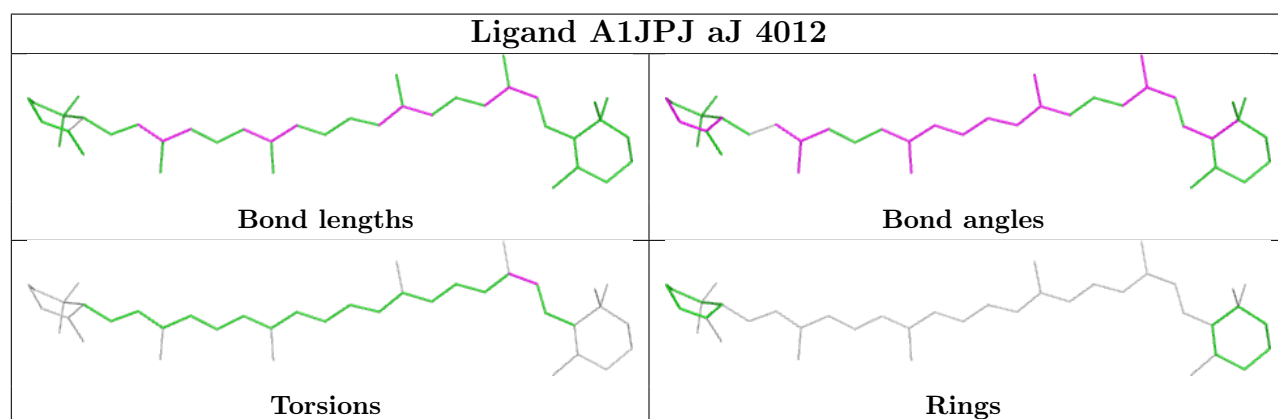
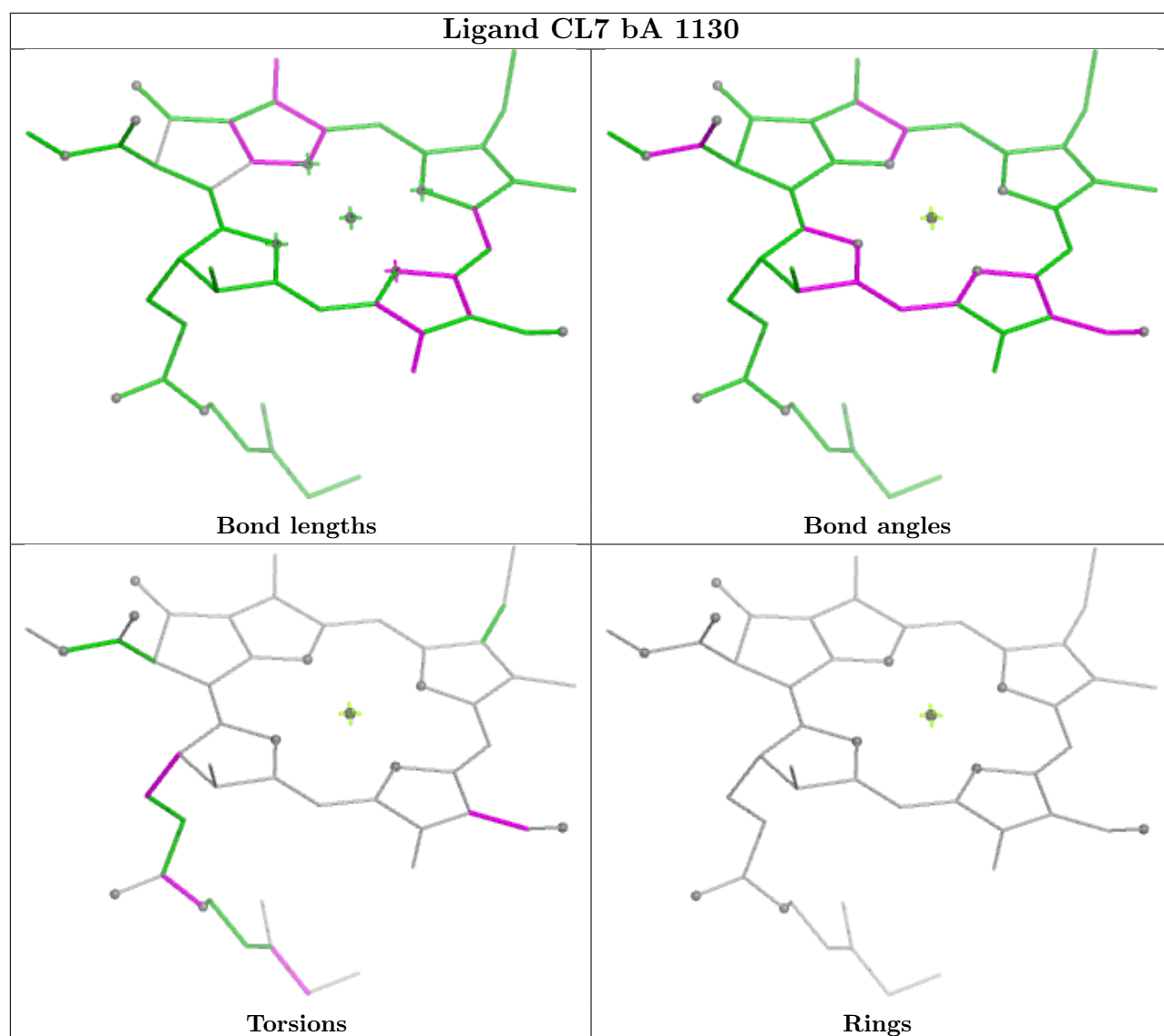


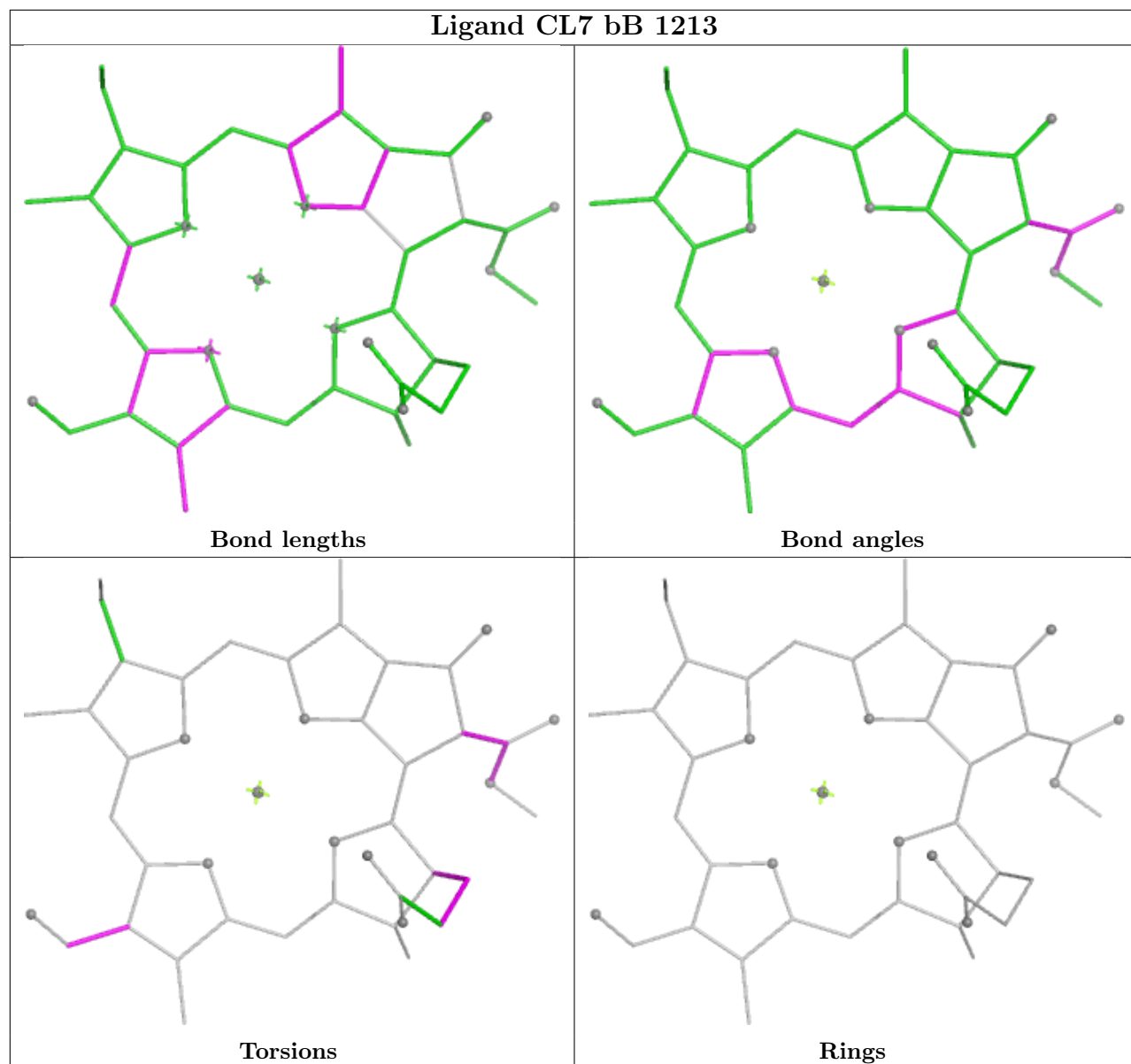
Torsions



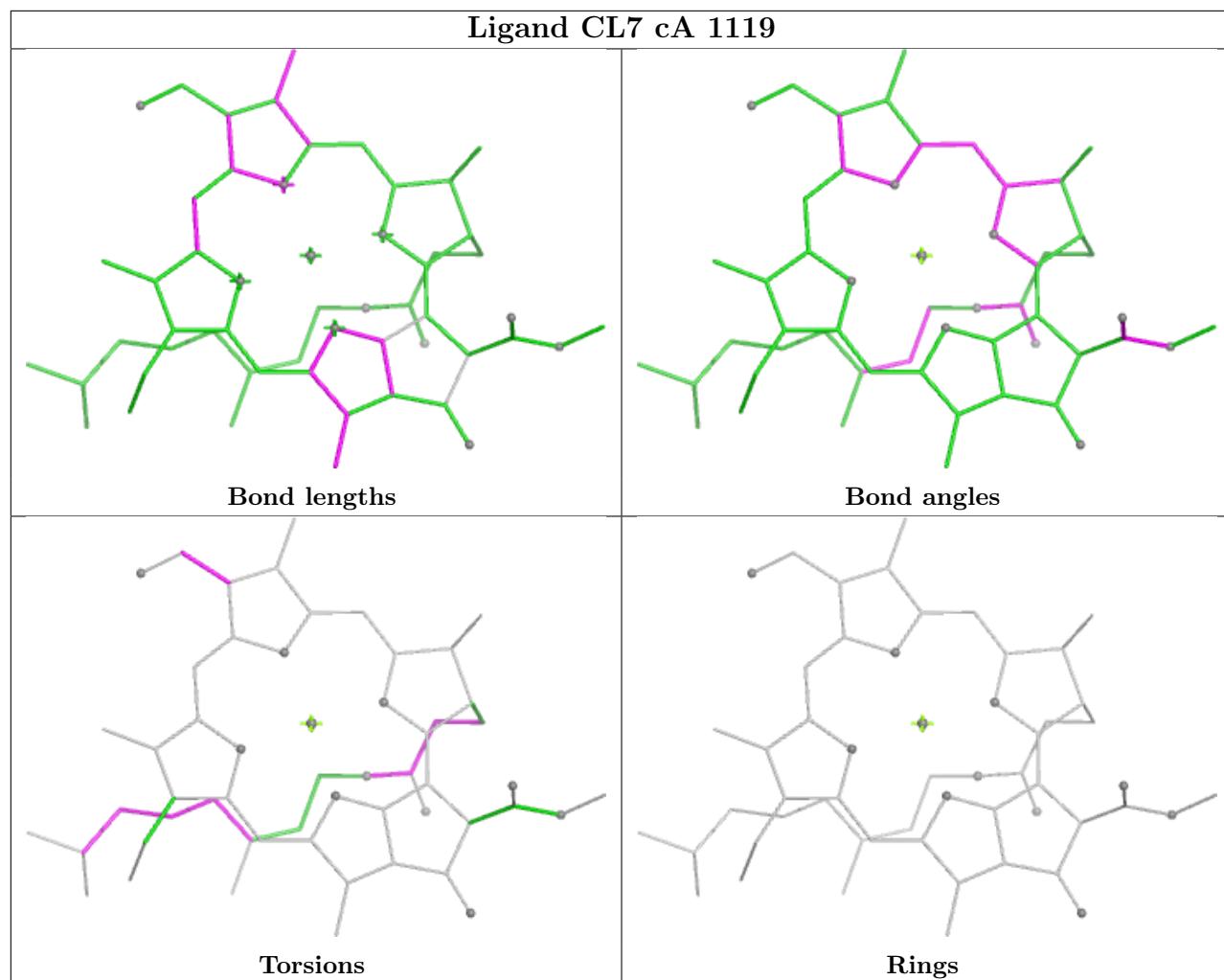
Rings

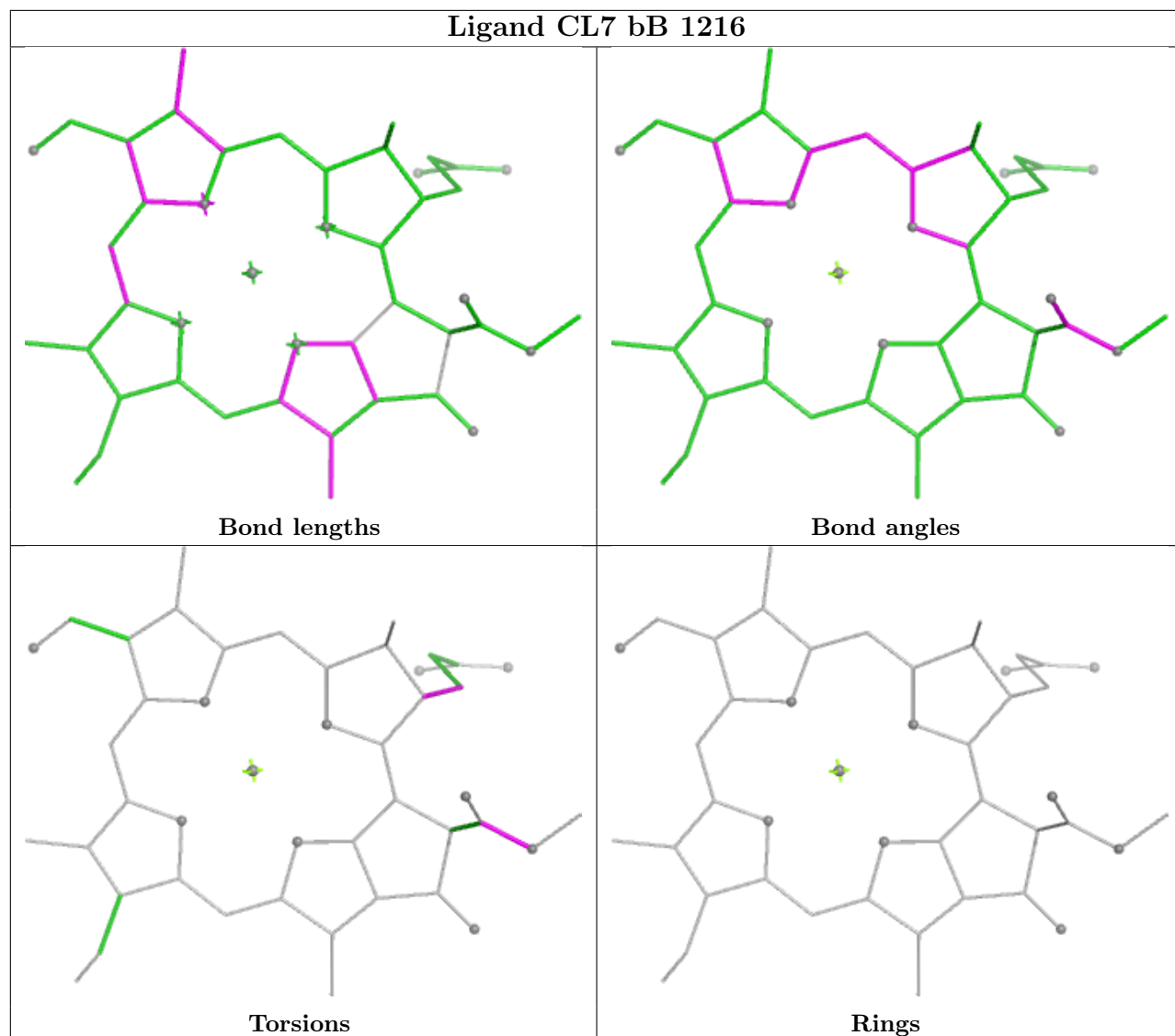


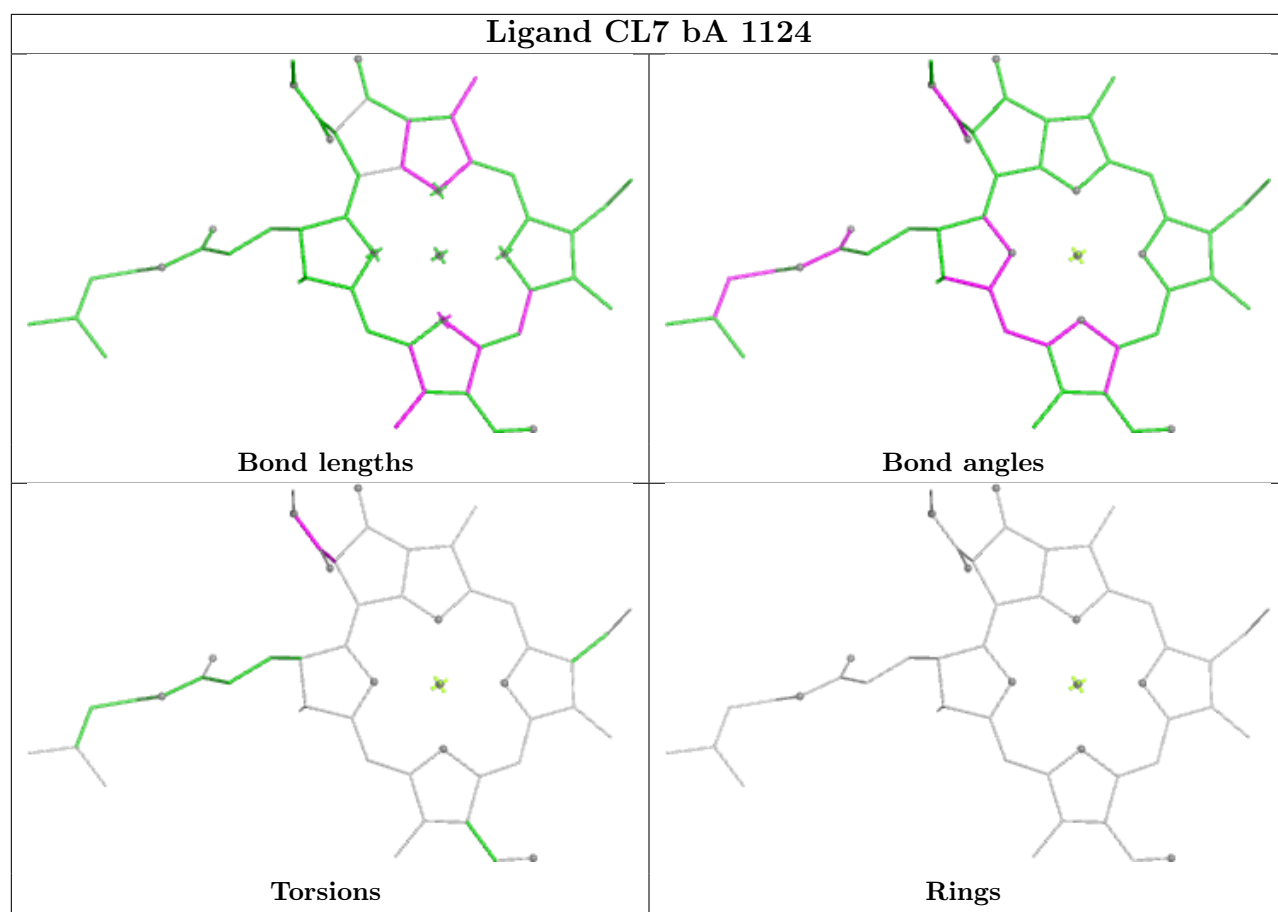




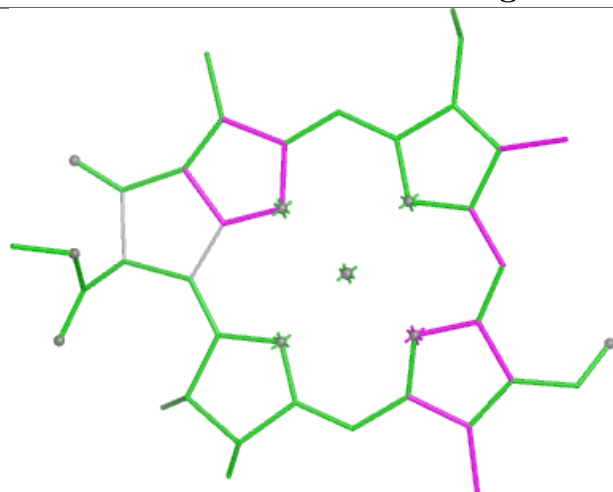
Ligand CL7 cA 1119



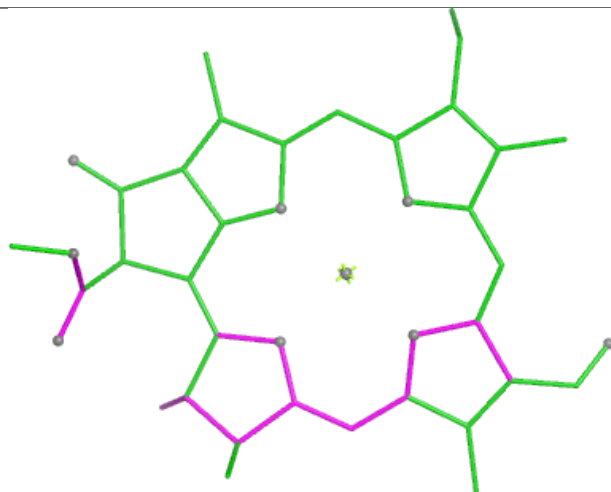




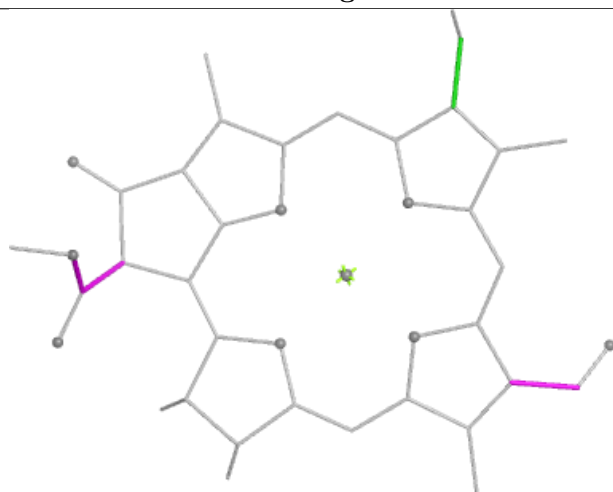
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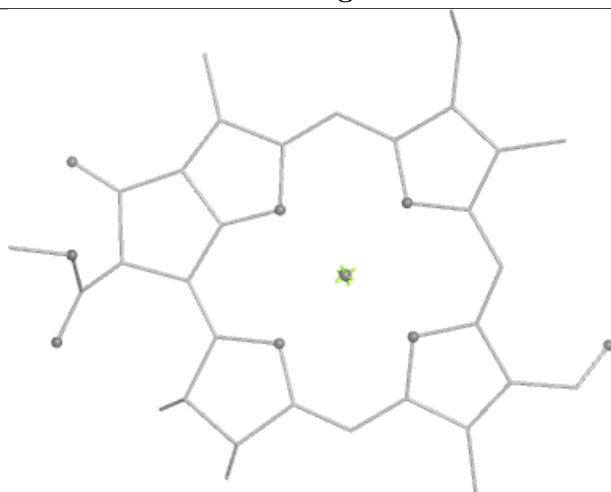
Bond lengths



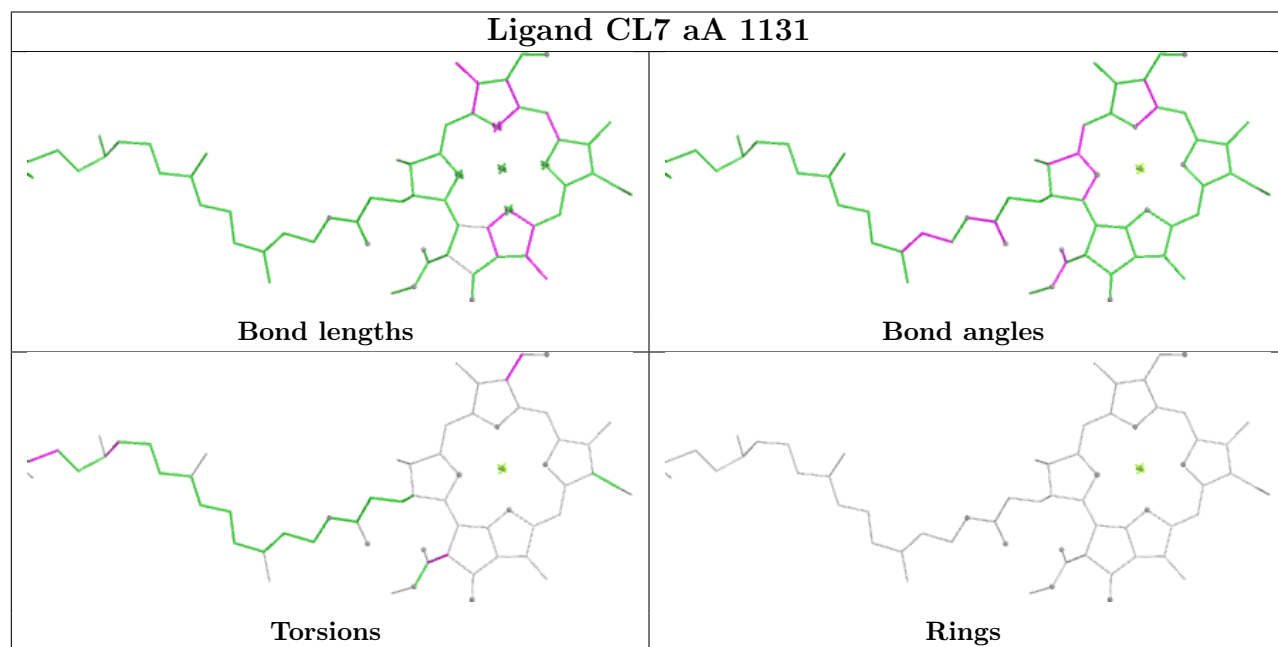
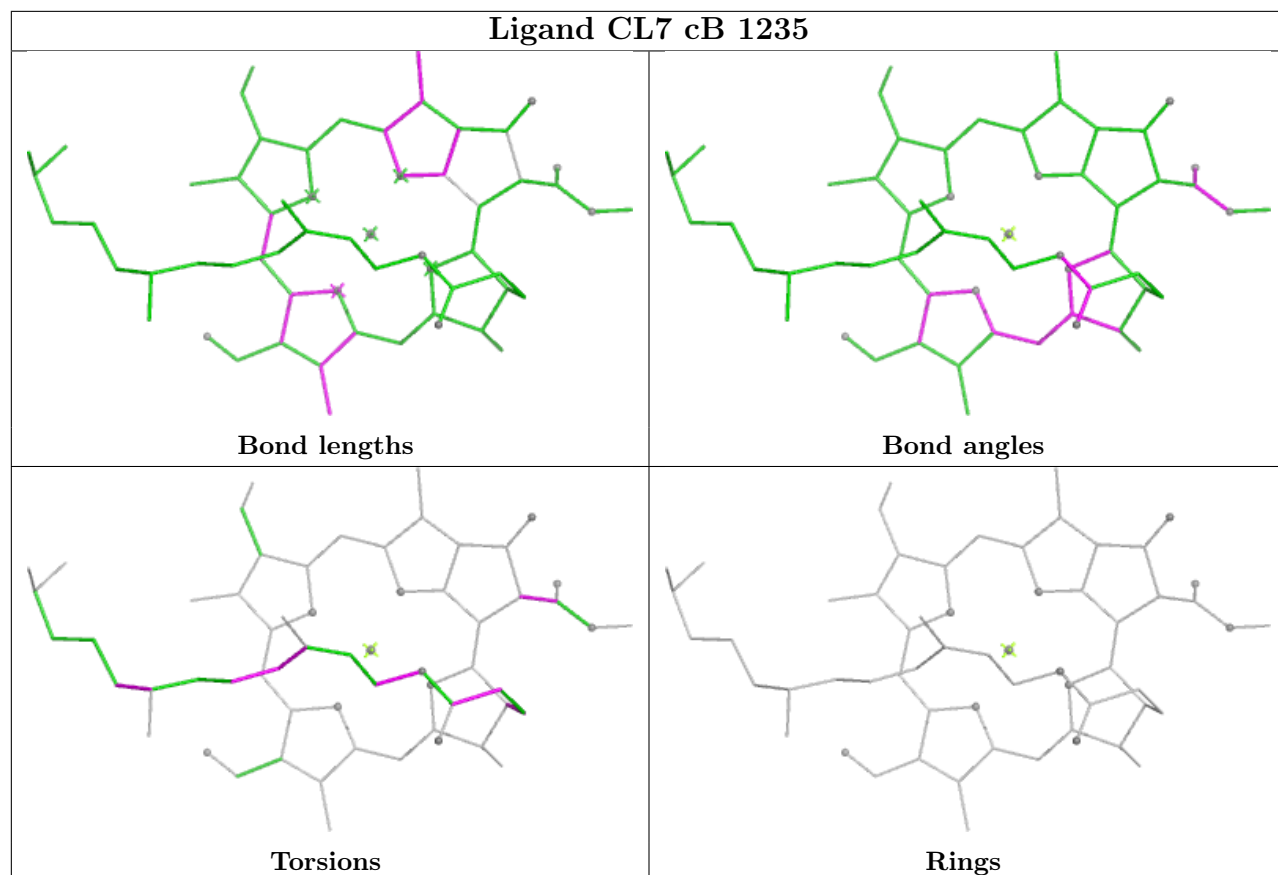
Bond angles

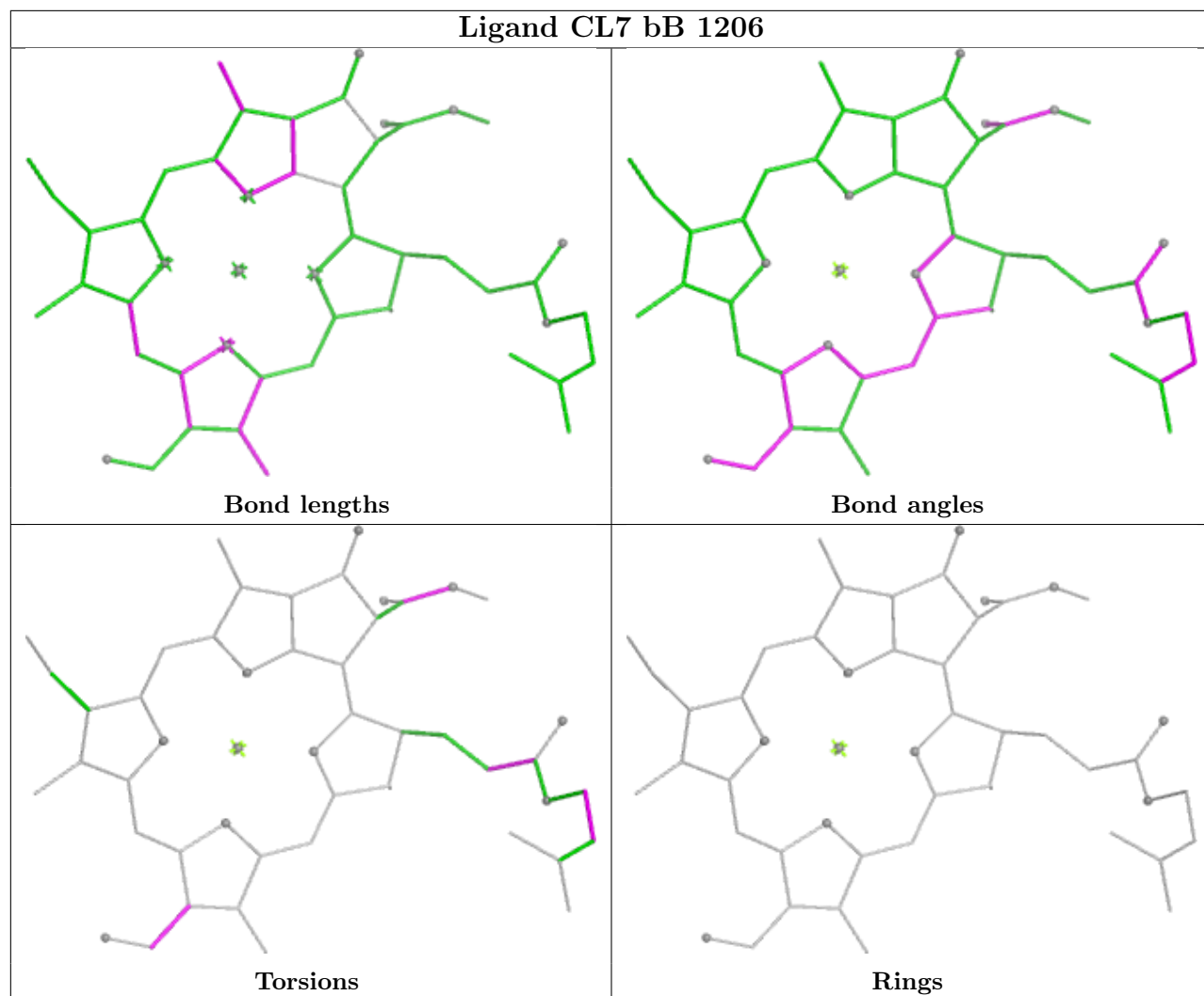


Torsions

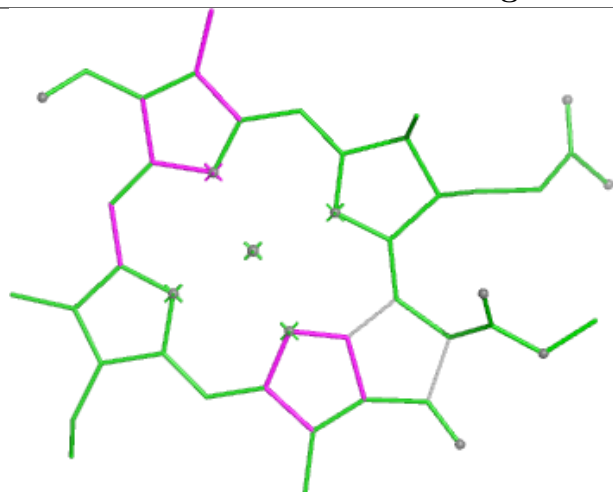


Rings

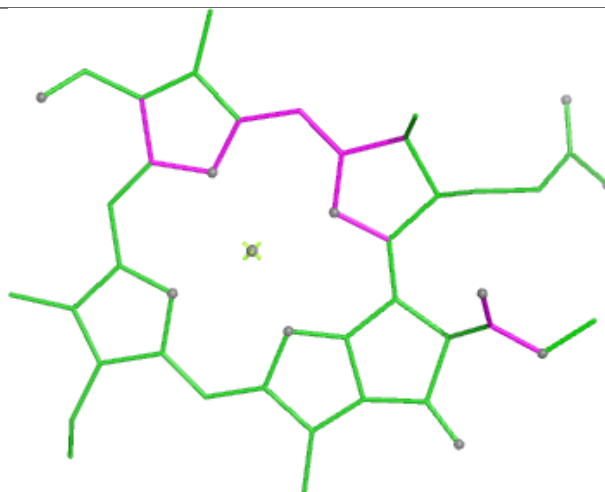




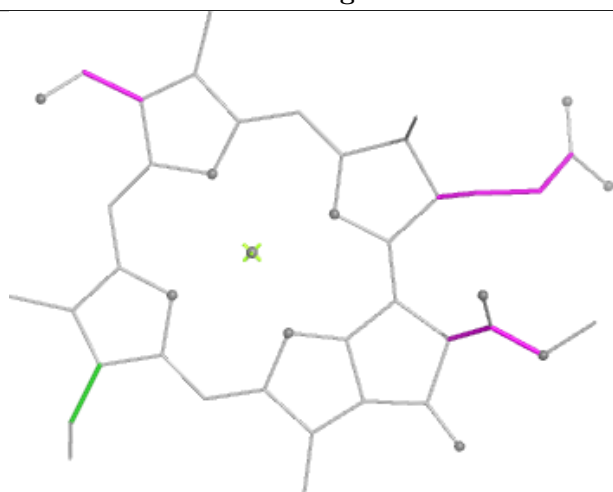
Ligand CL7 aA 1139



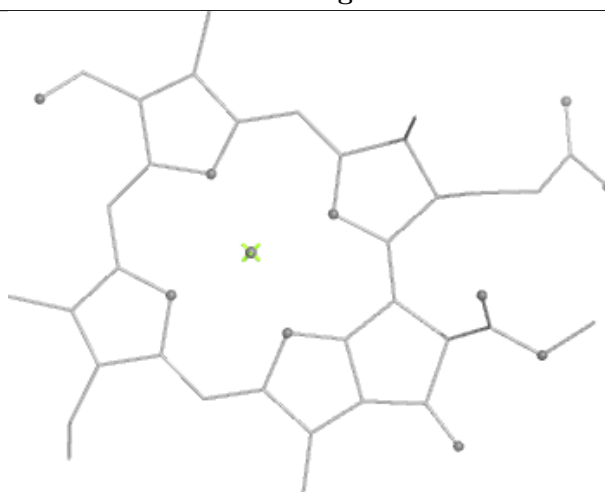
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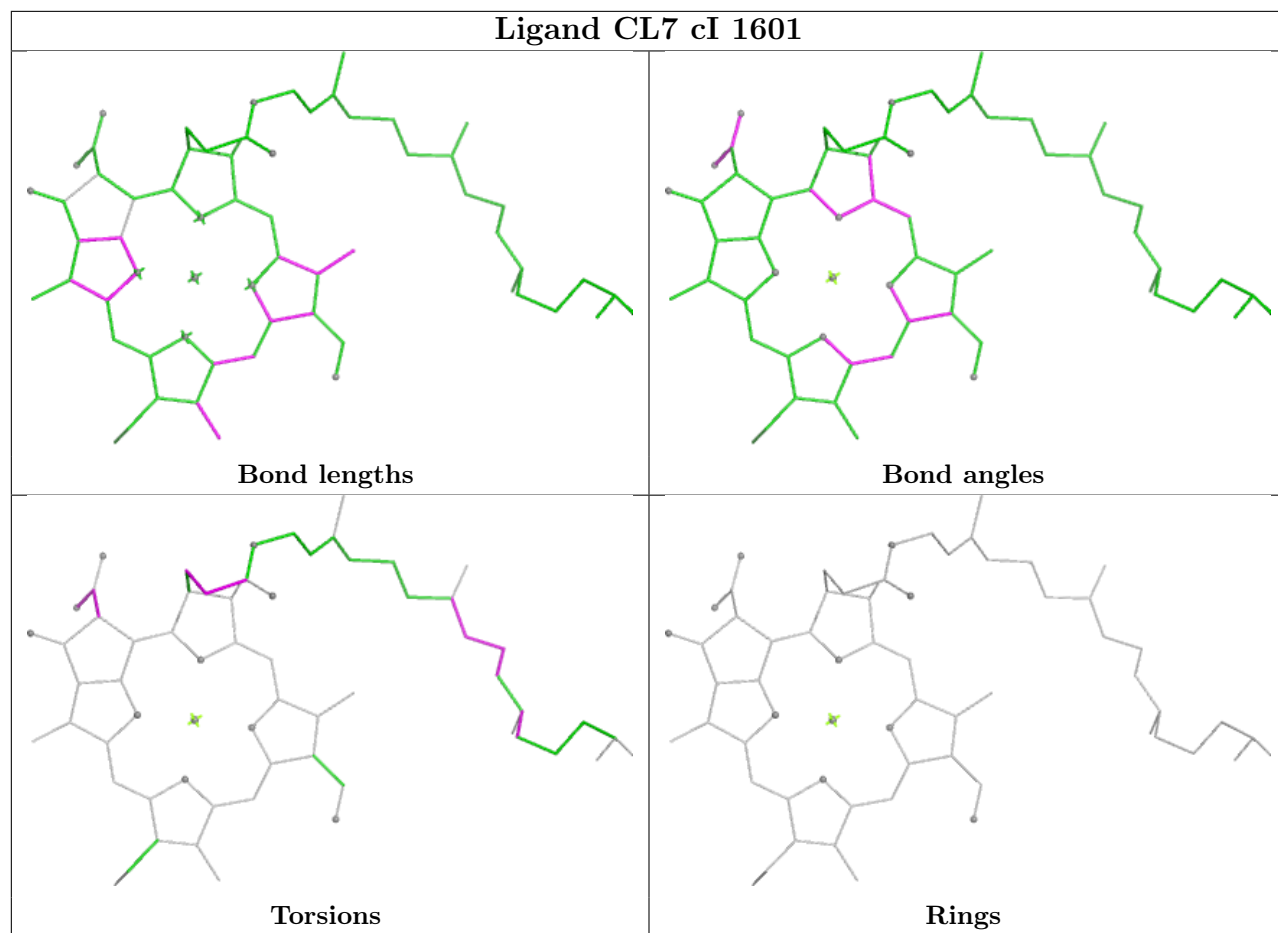
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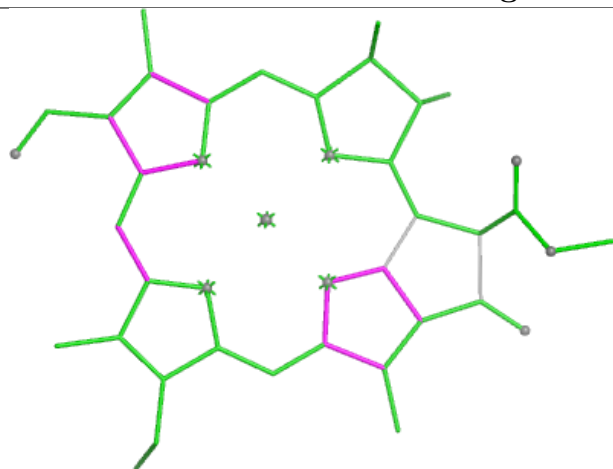
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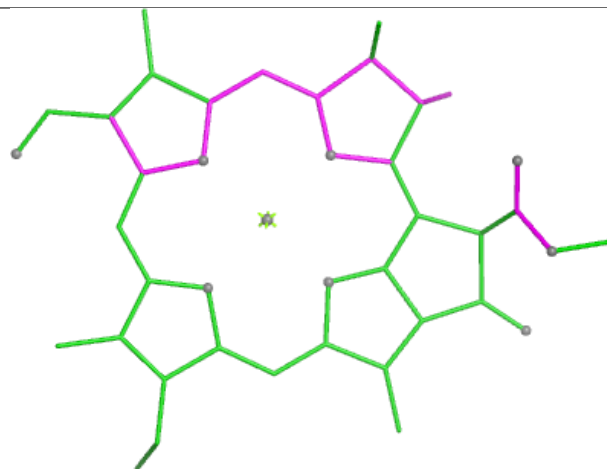
Rings



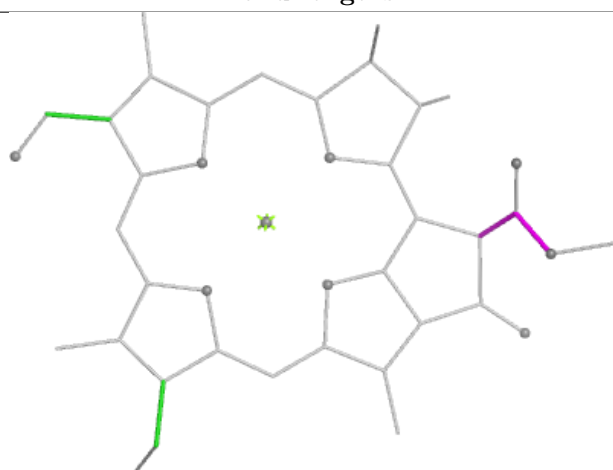
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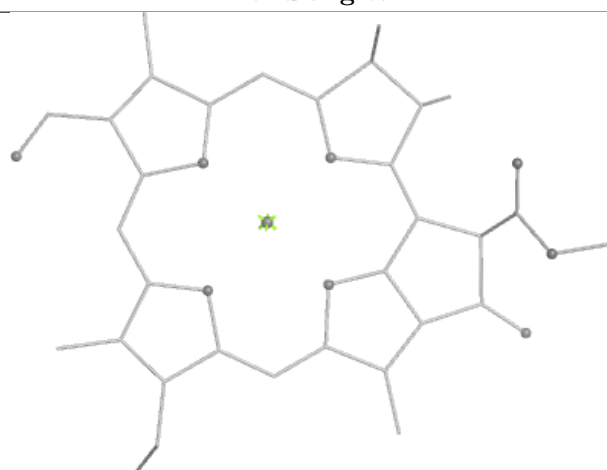
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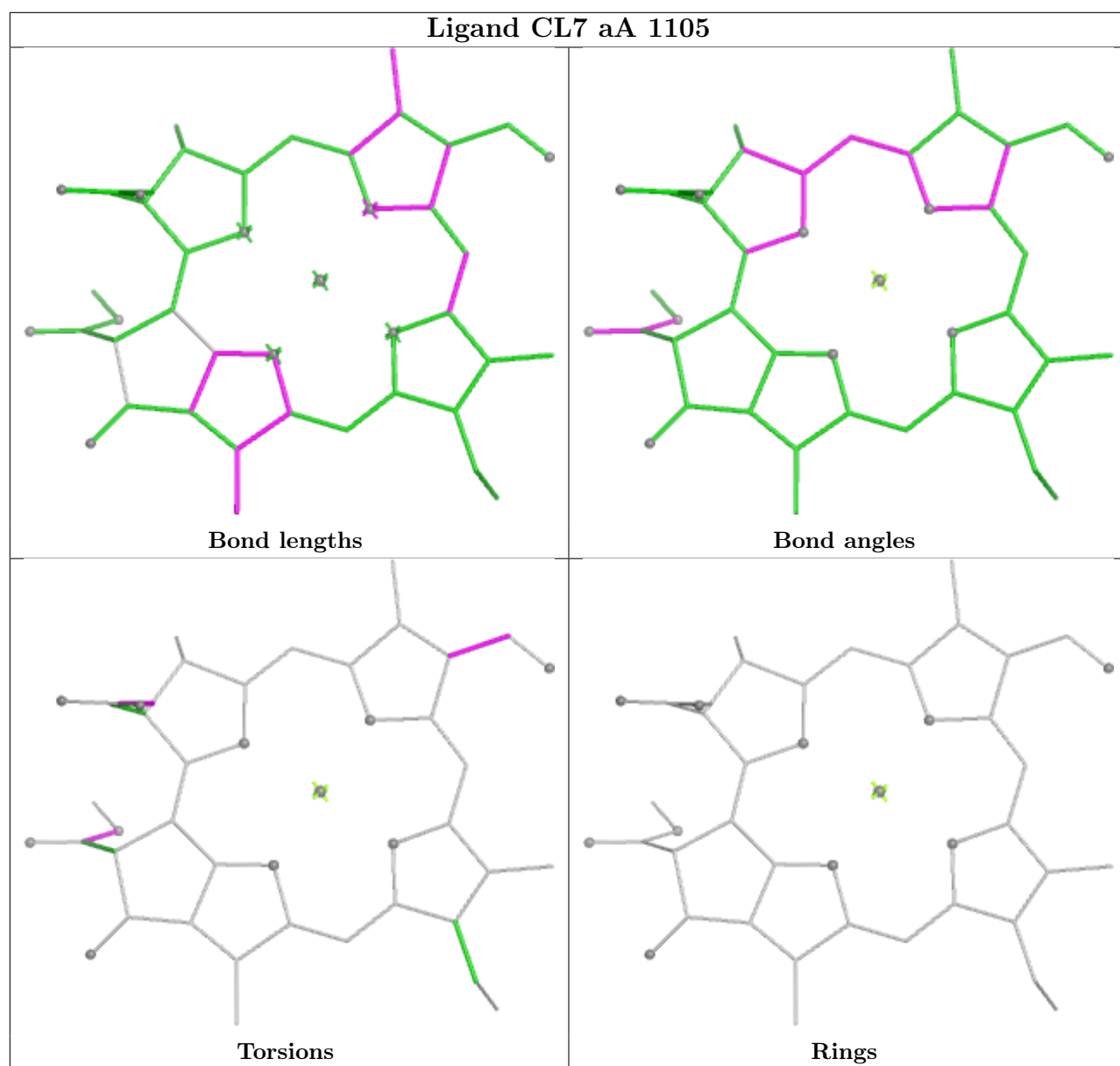
Bond angles



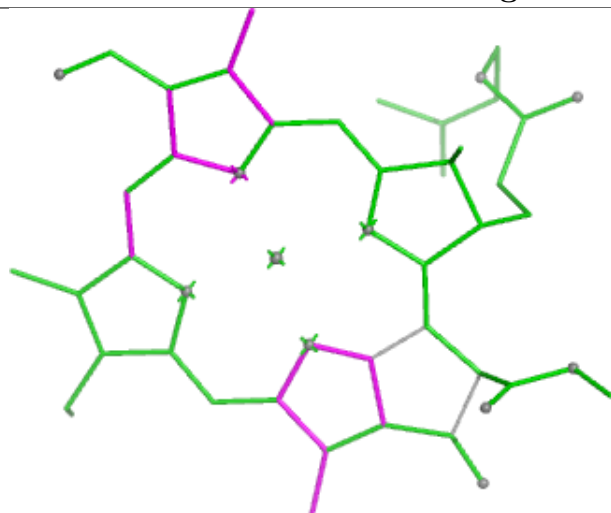
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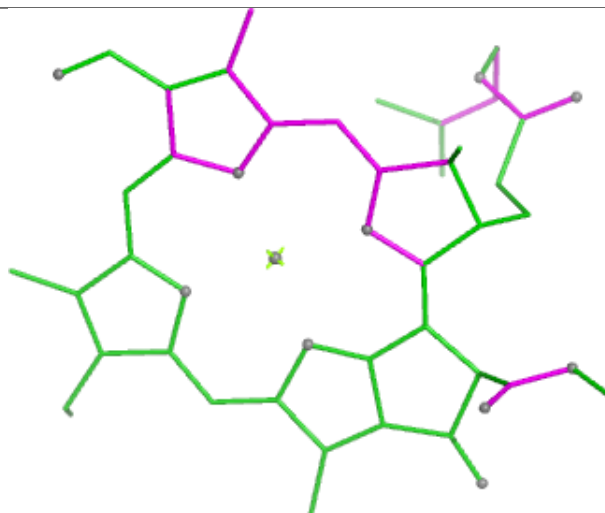
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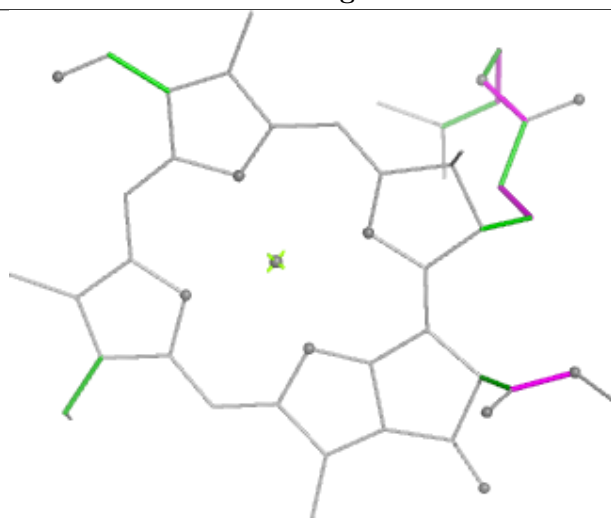
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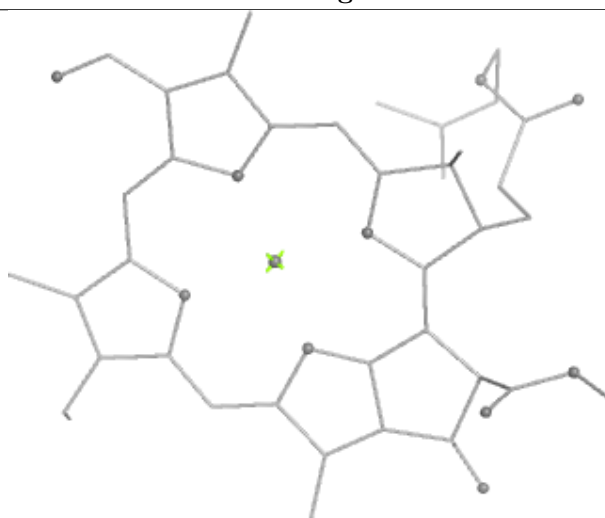
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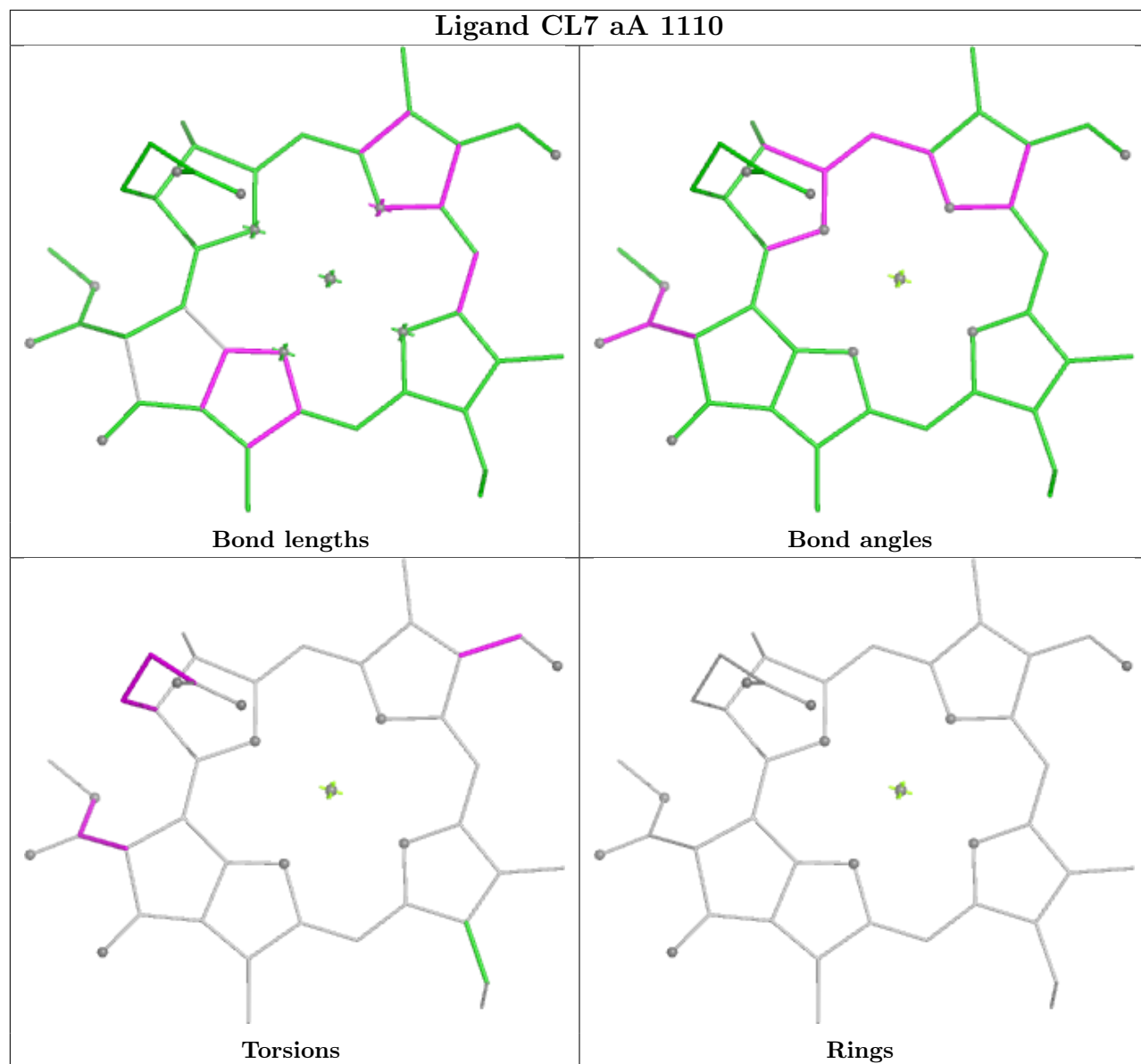
Bond angles

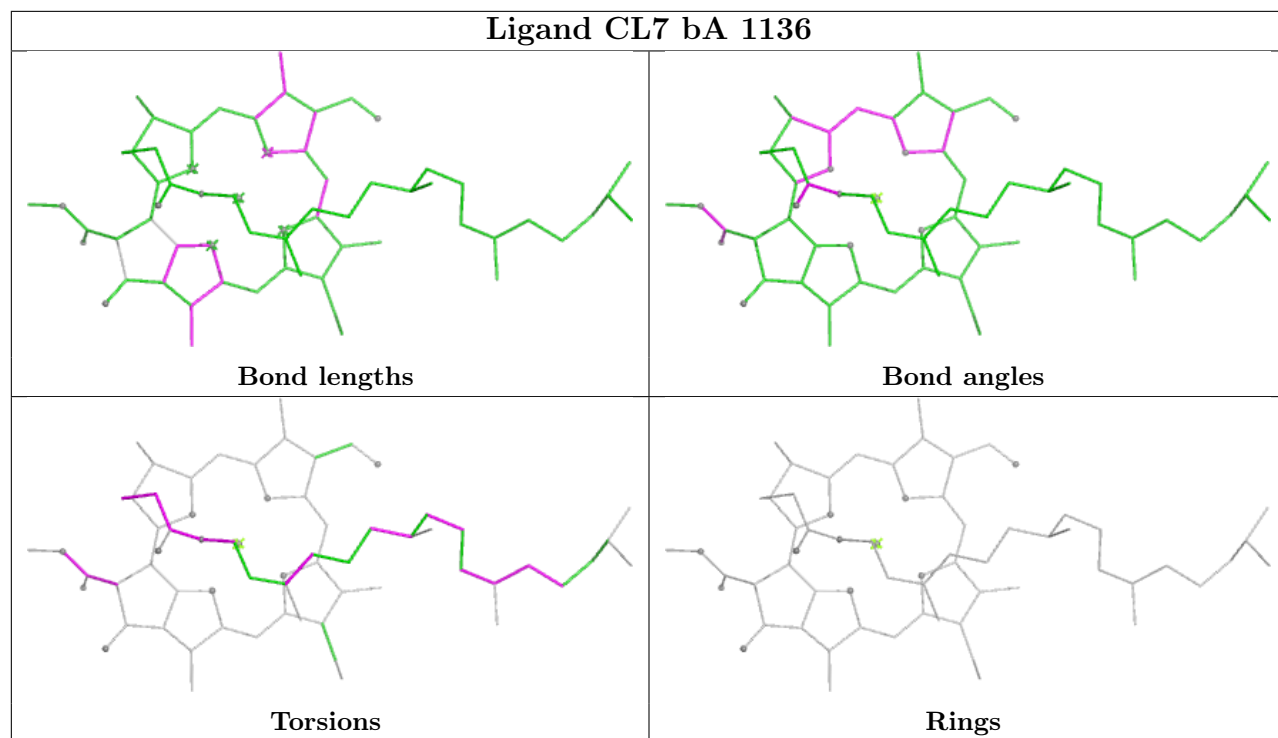


Torsions

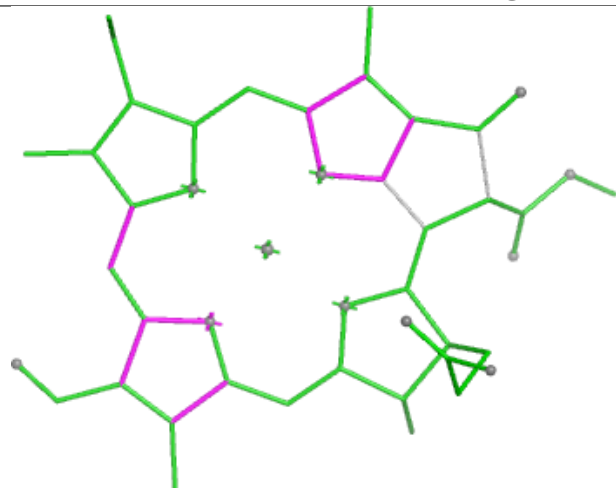


Rings

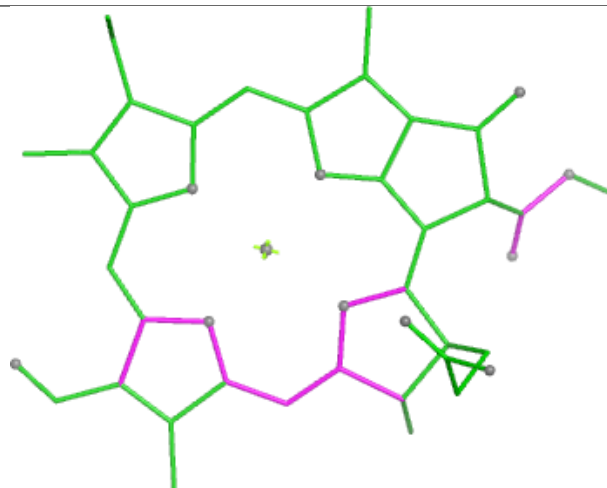




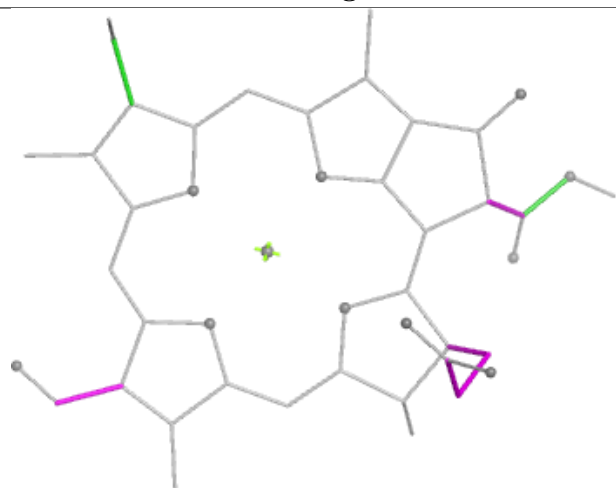
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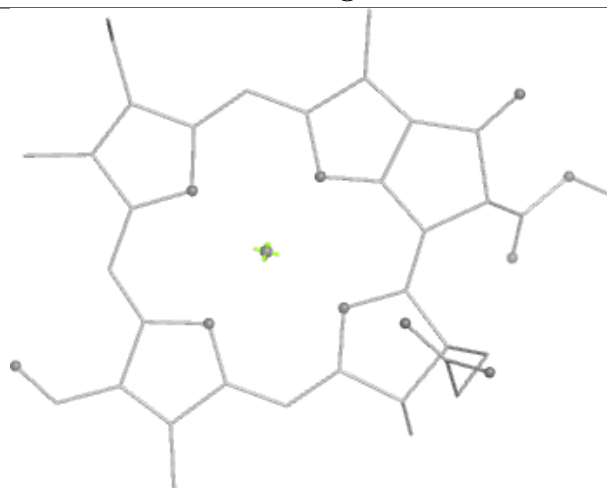
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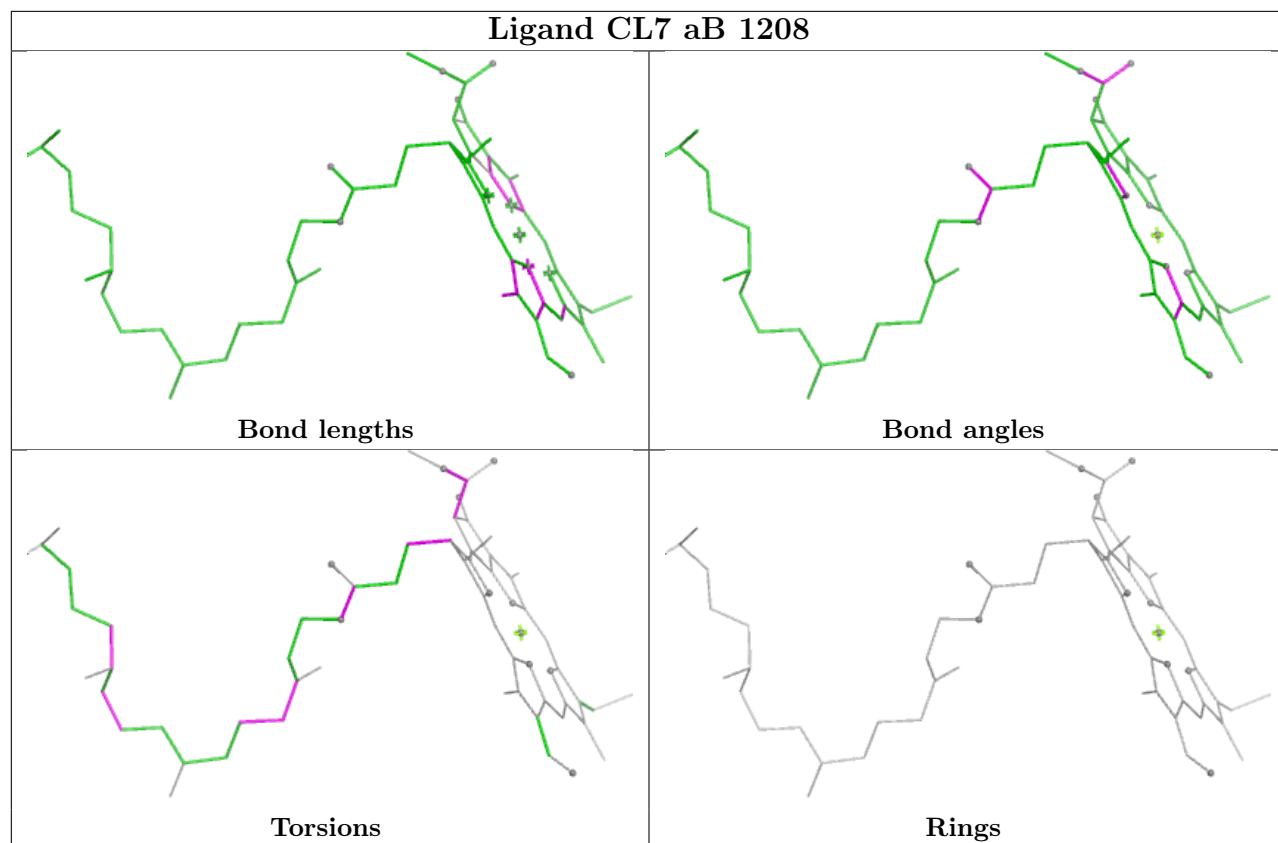
Bond angles

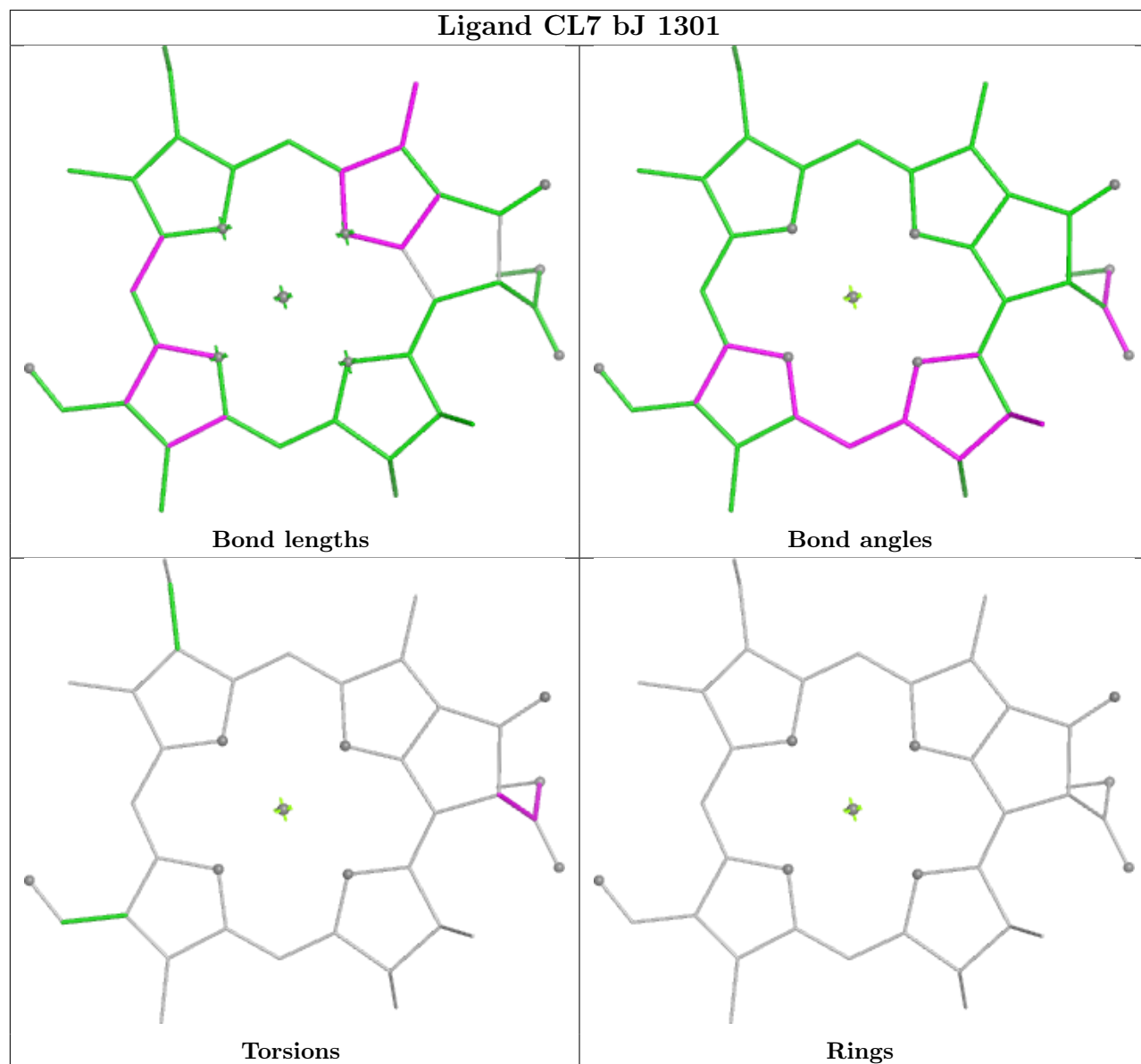


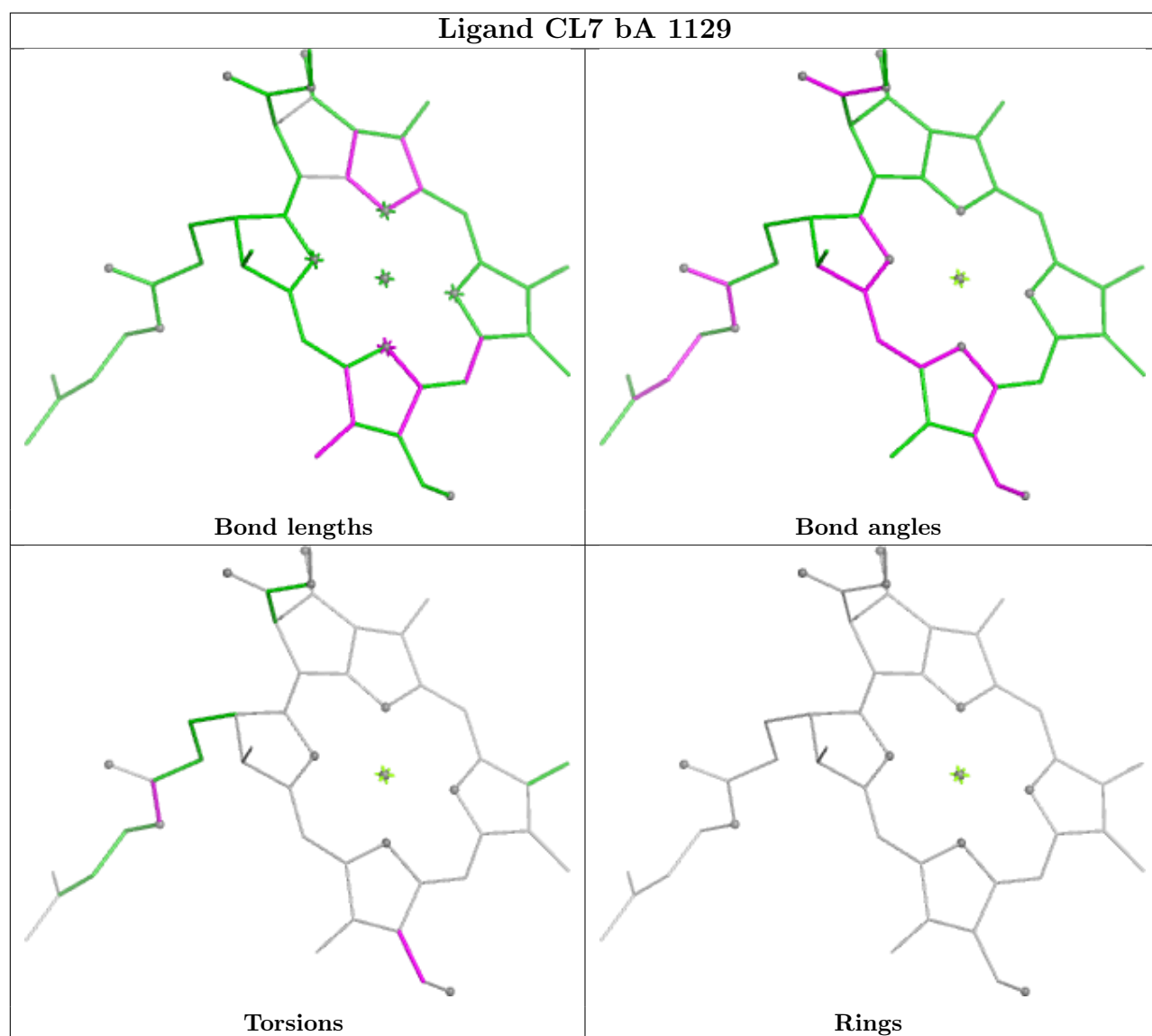
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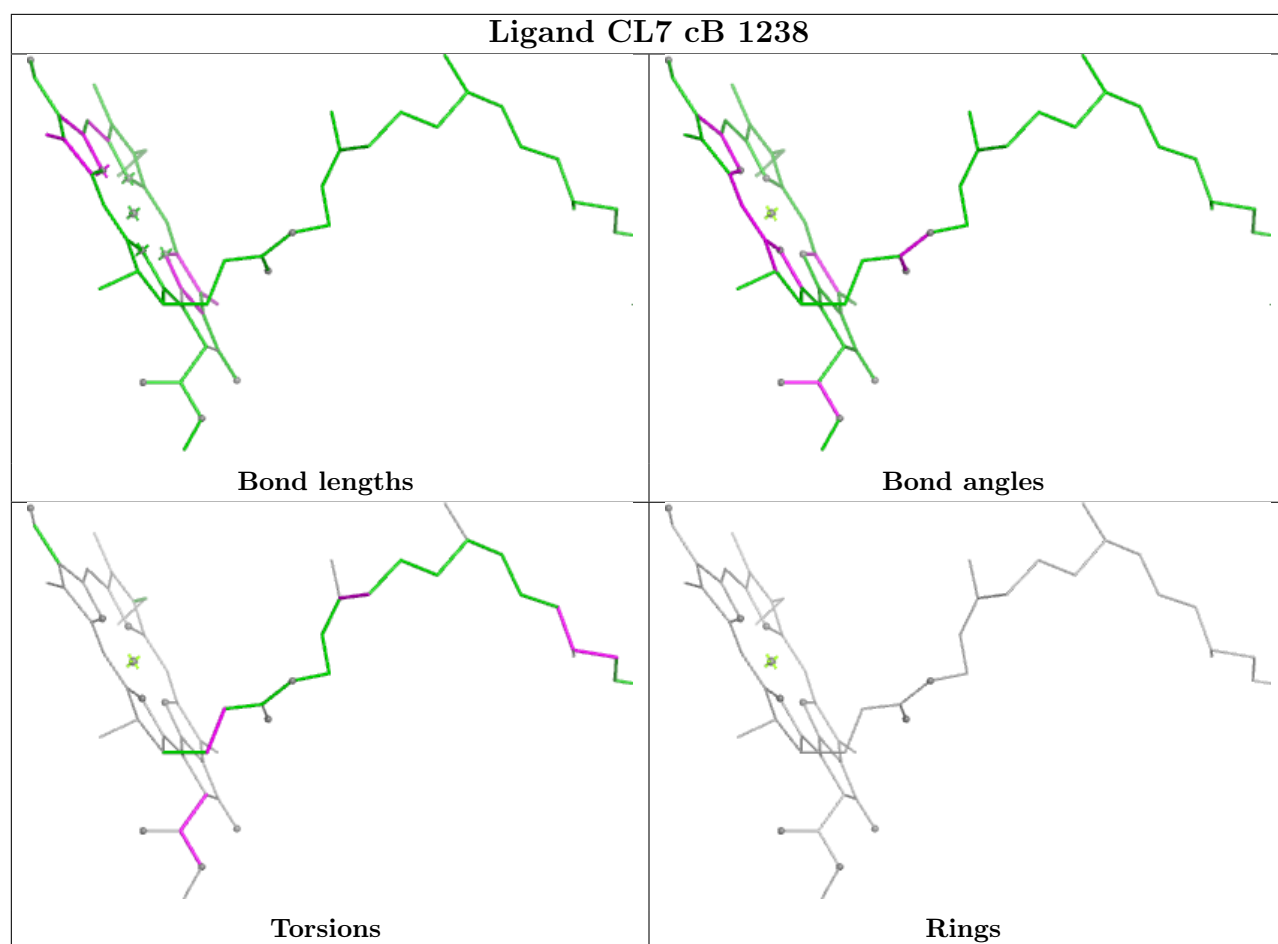


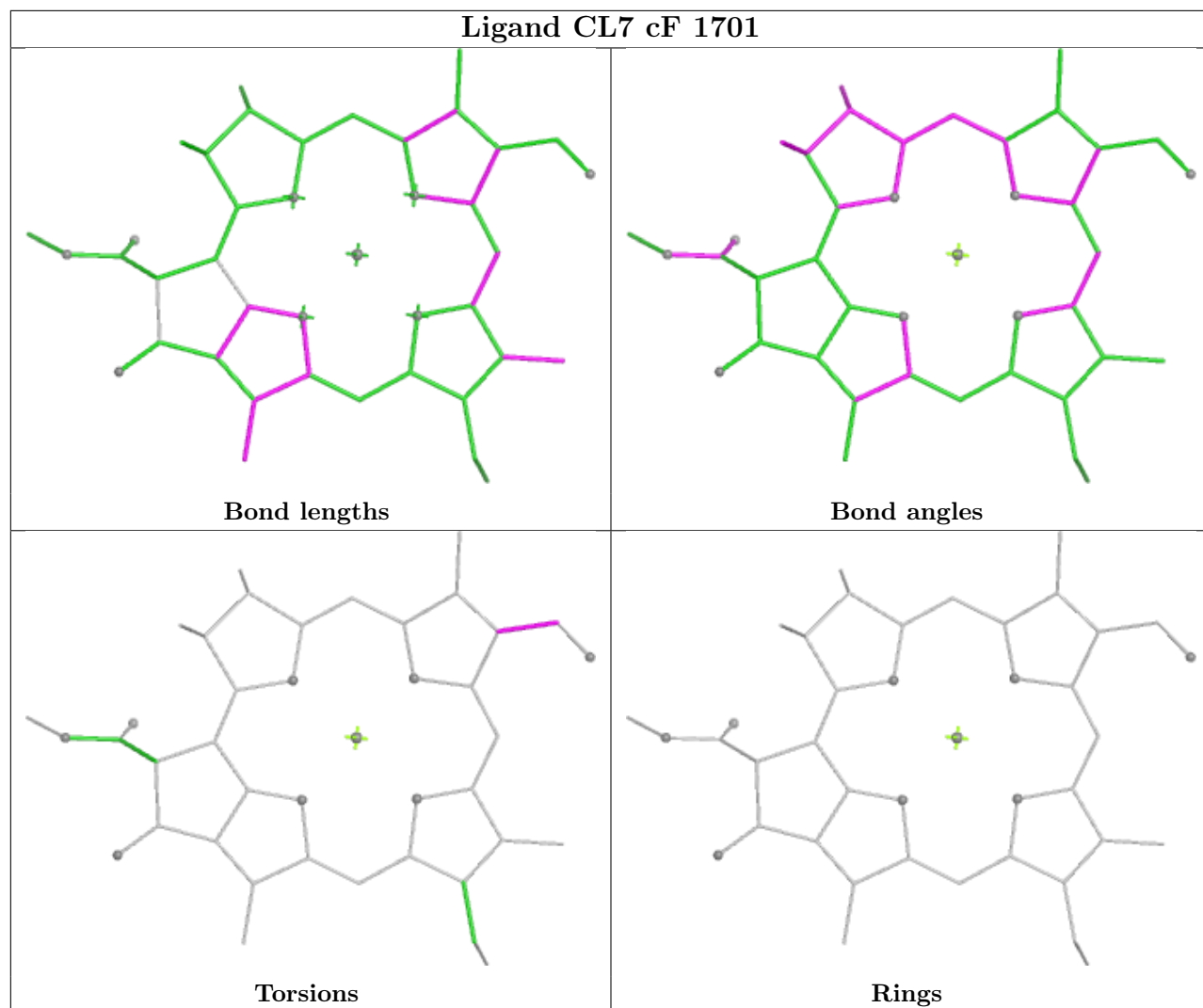
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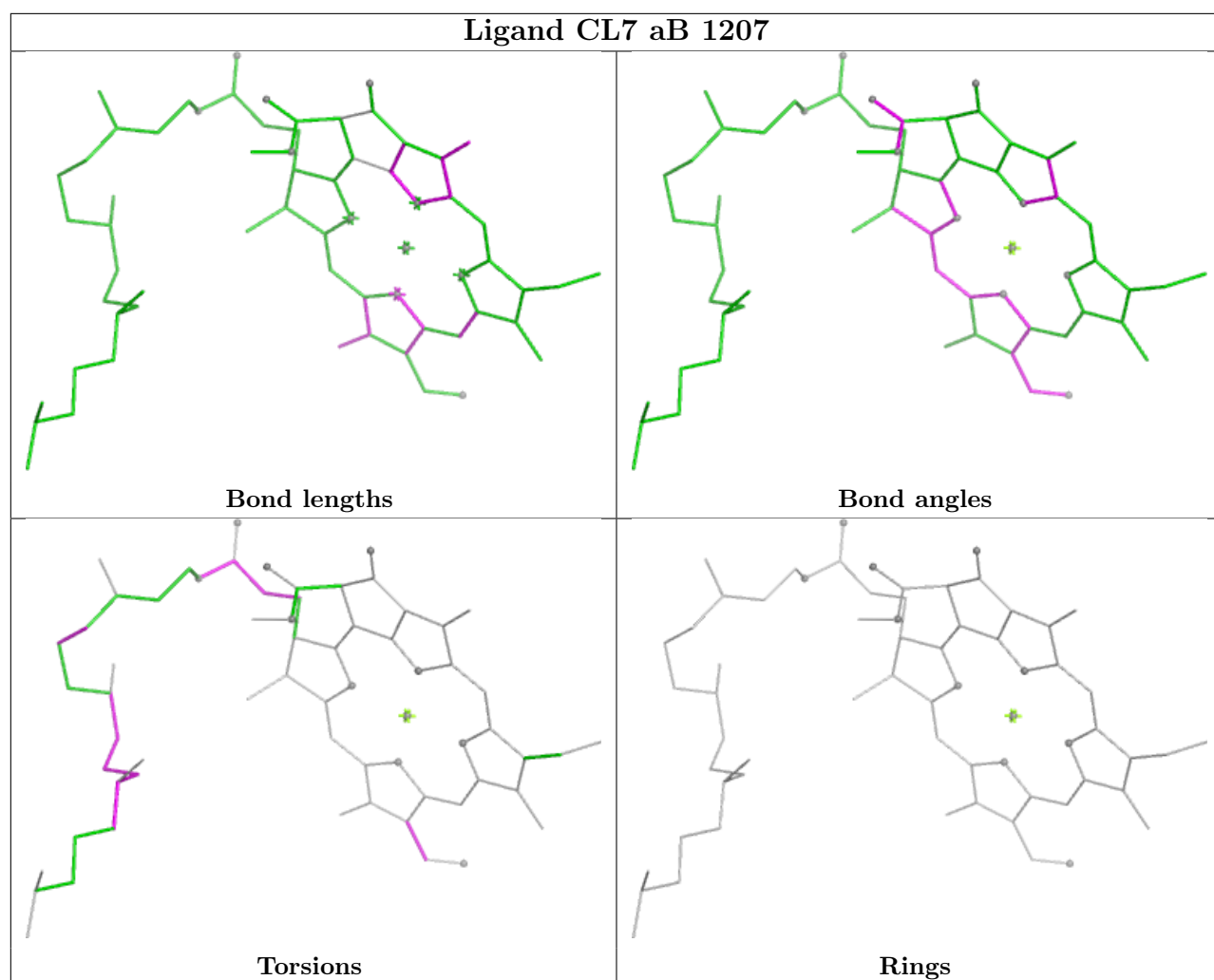


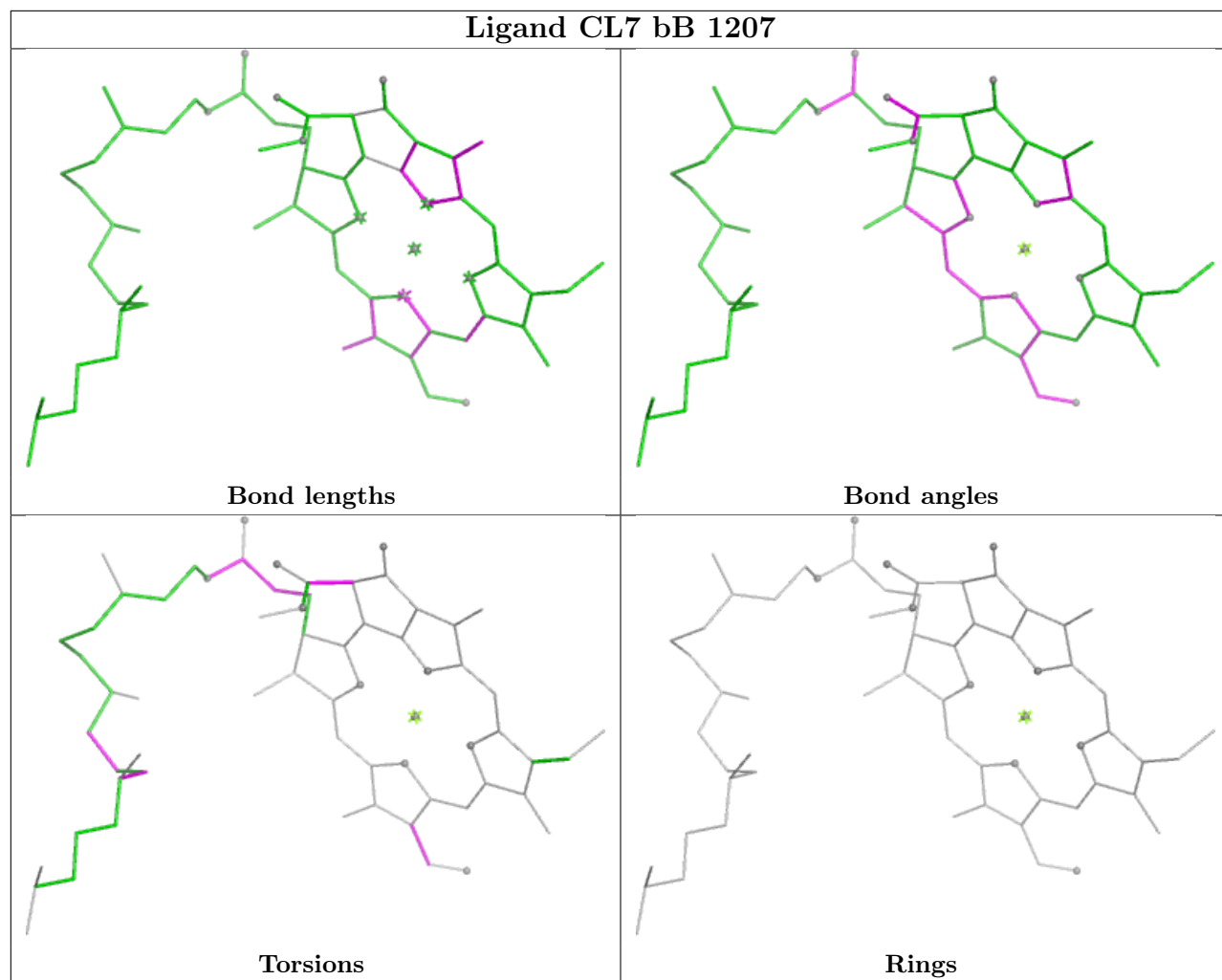




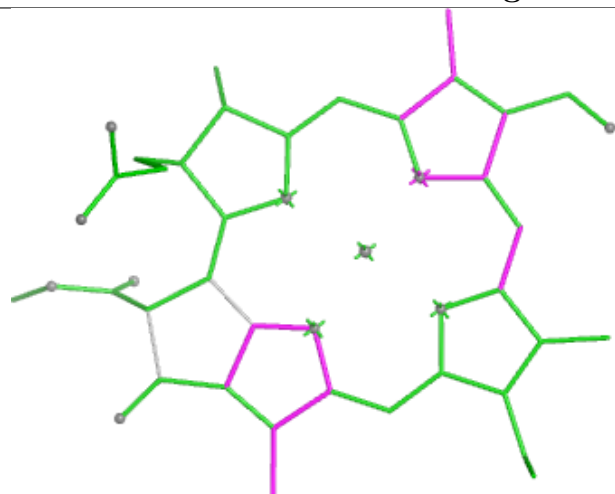




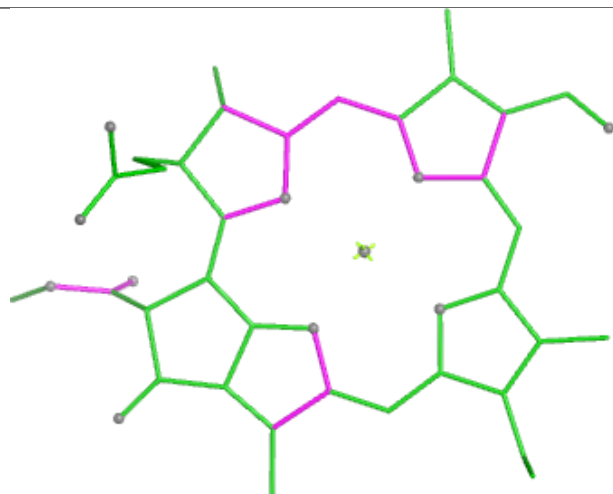




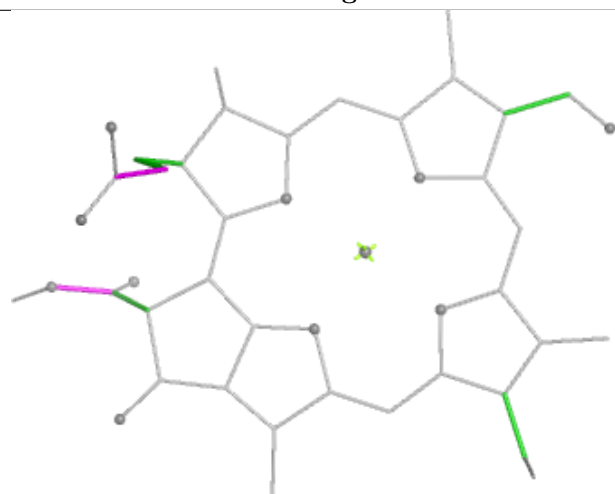
Ligand CL7 cA 1107



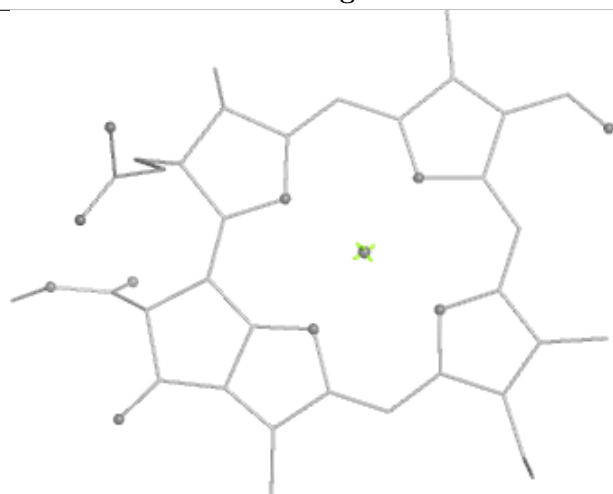
Bond lengths



Bond angles

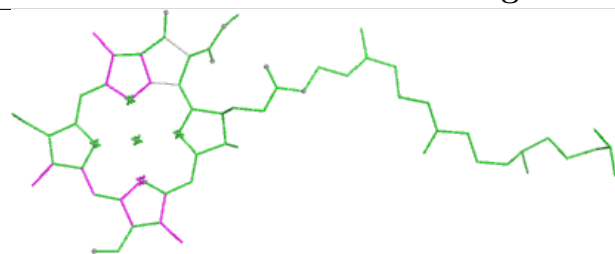


Torsions

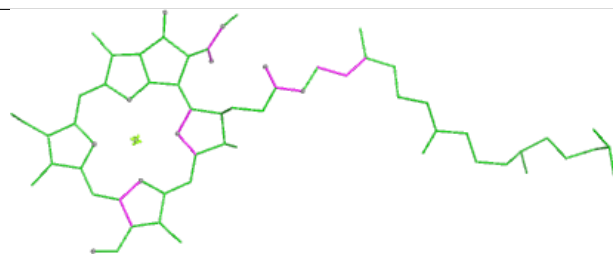


Rings

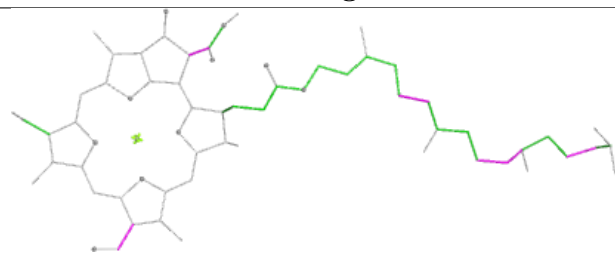
Ligand CL7 bA 1131



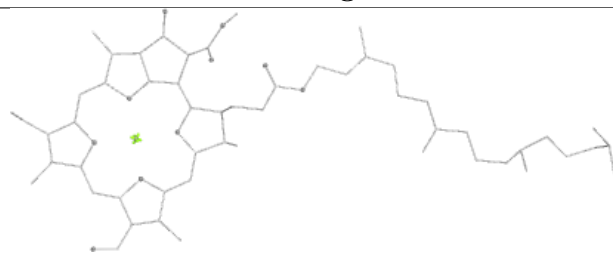
Bond lengths



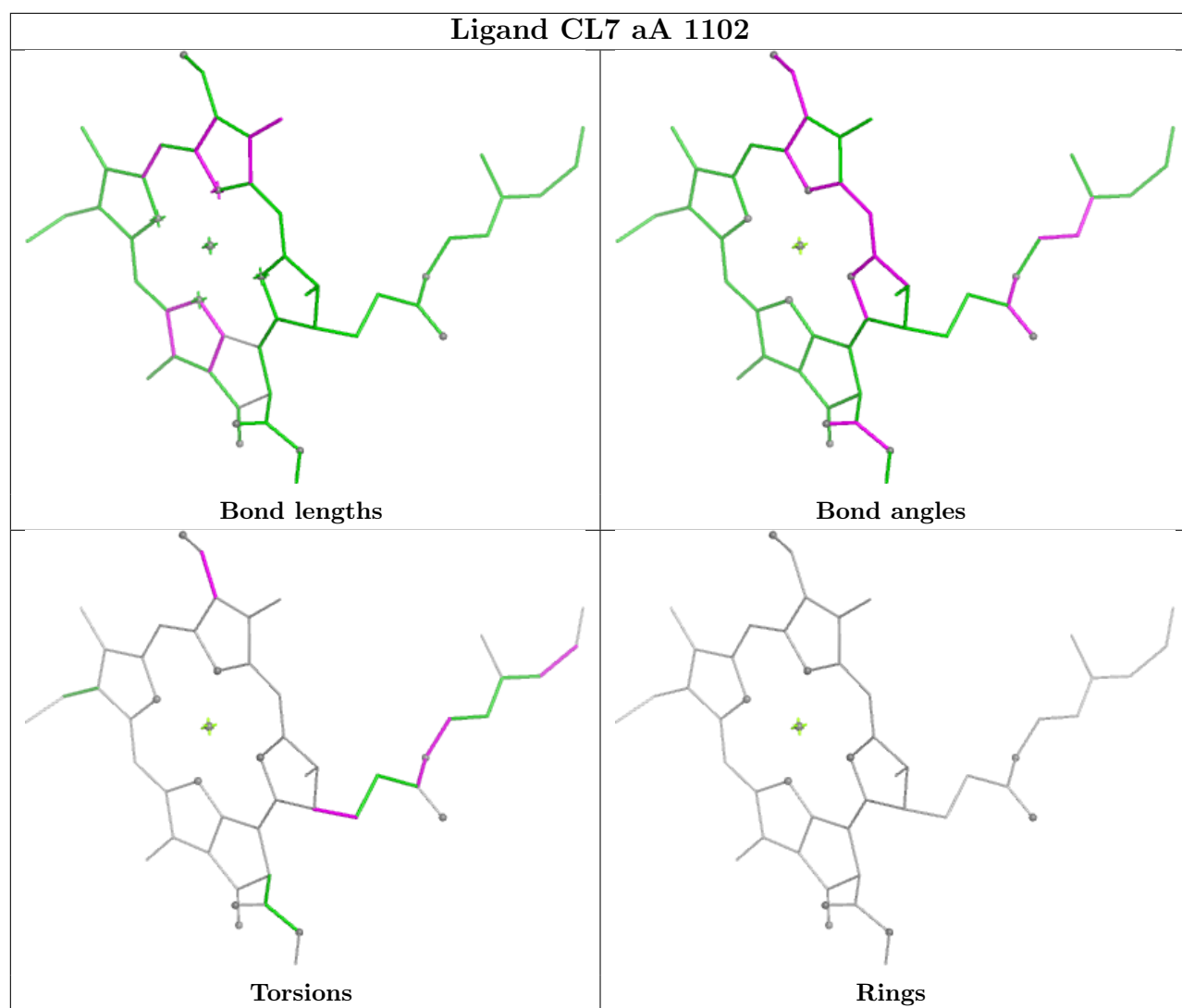
Bond angles



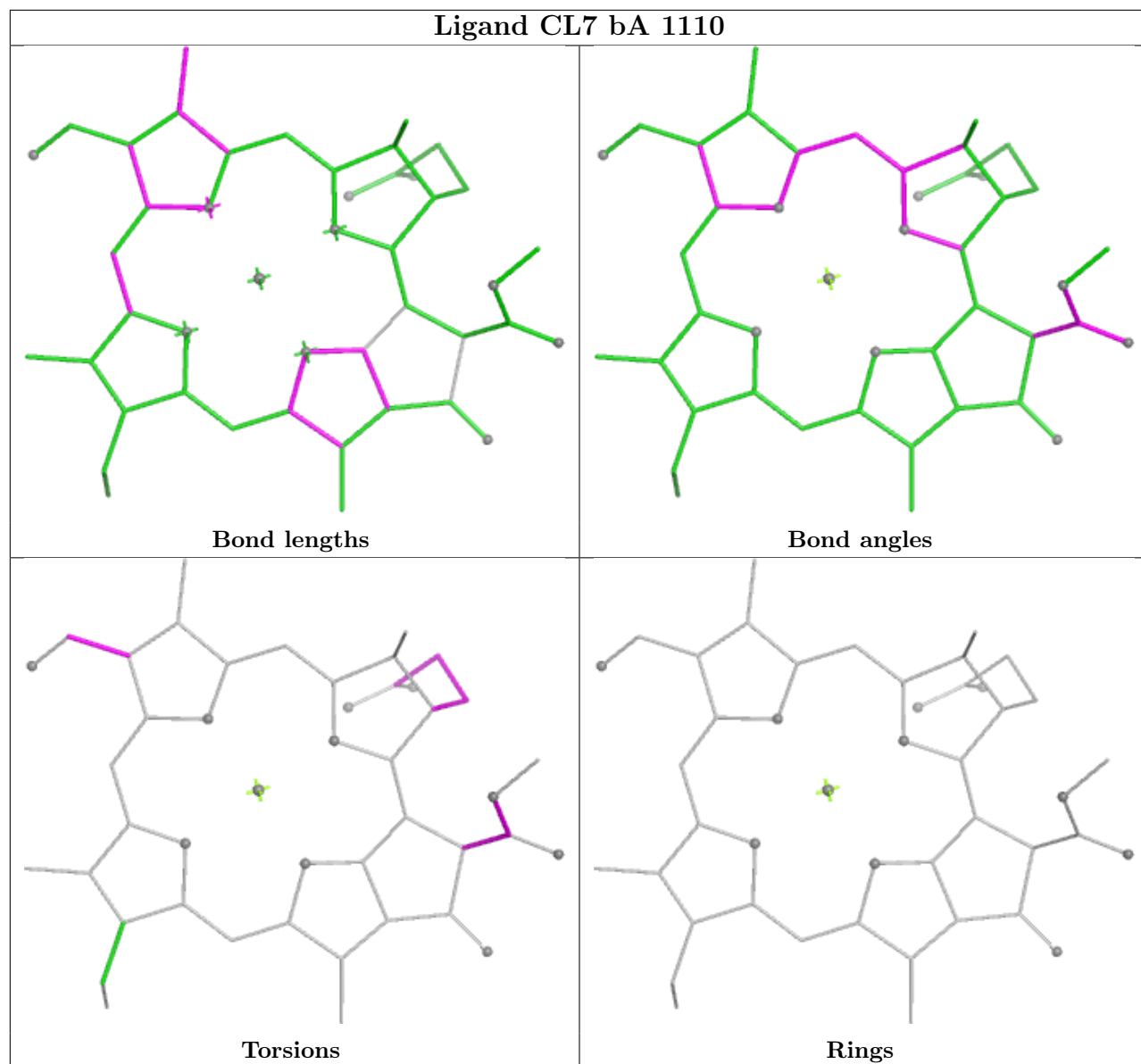
Torsions

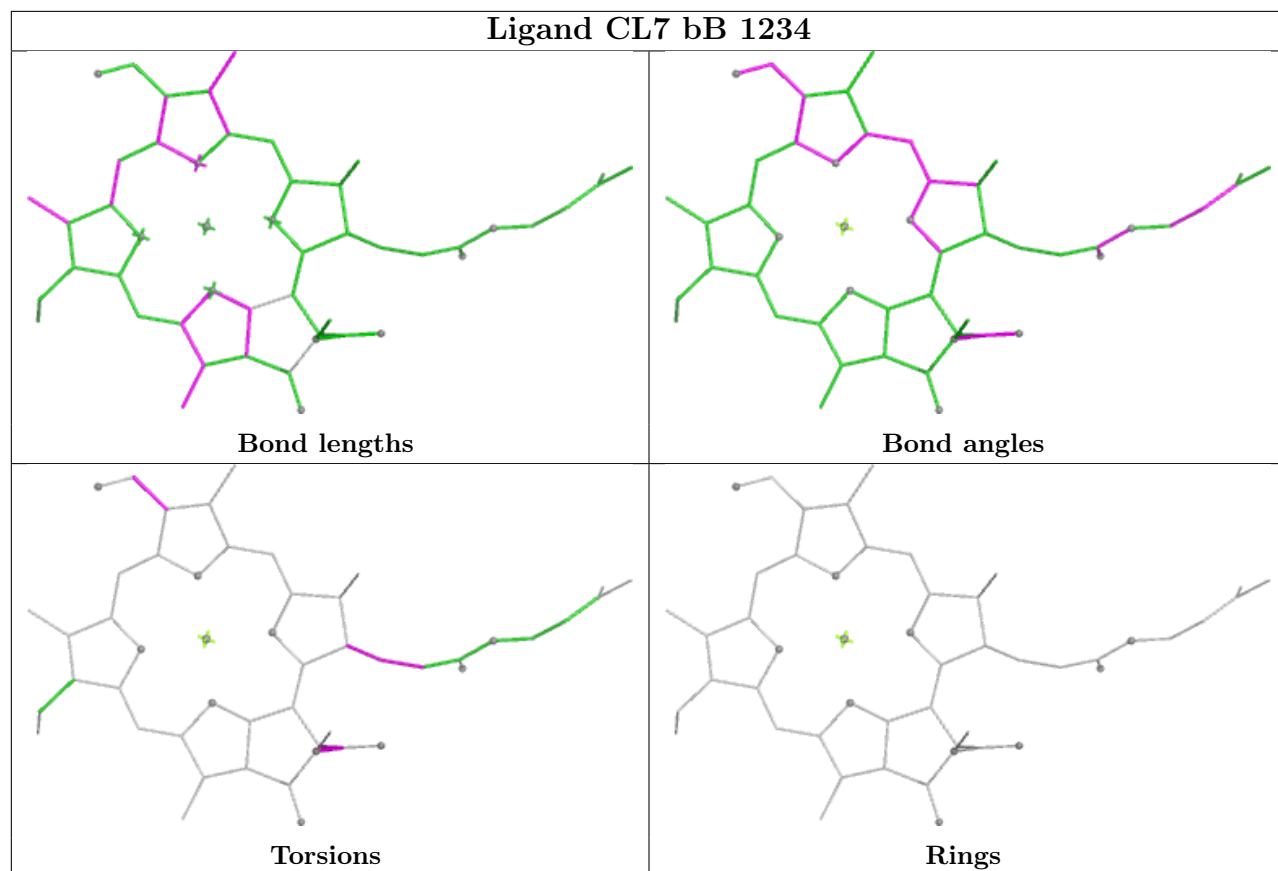


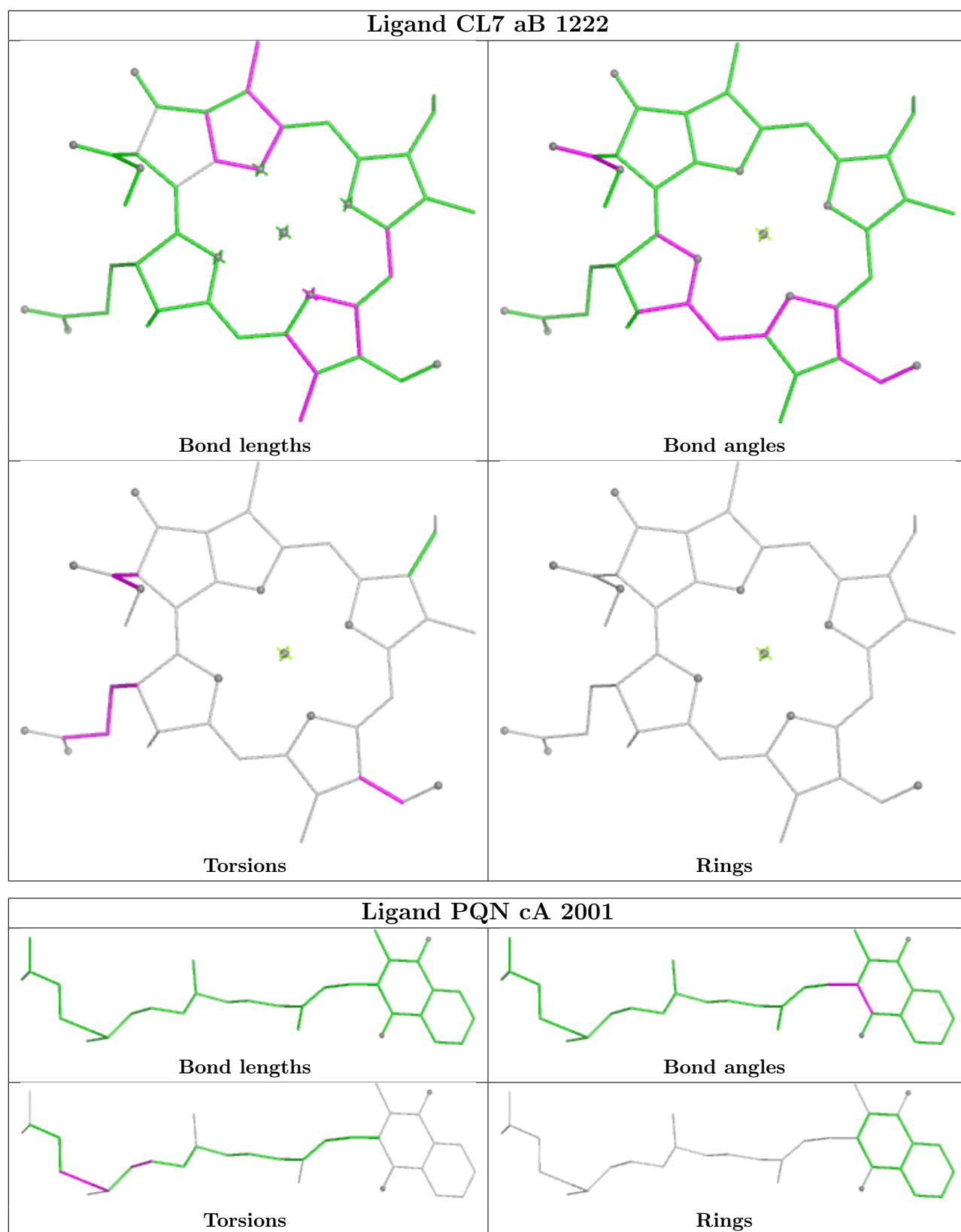
Rings



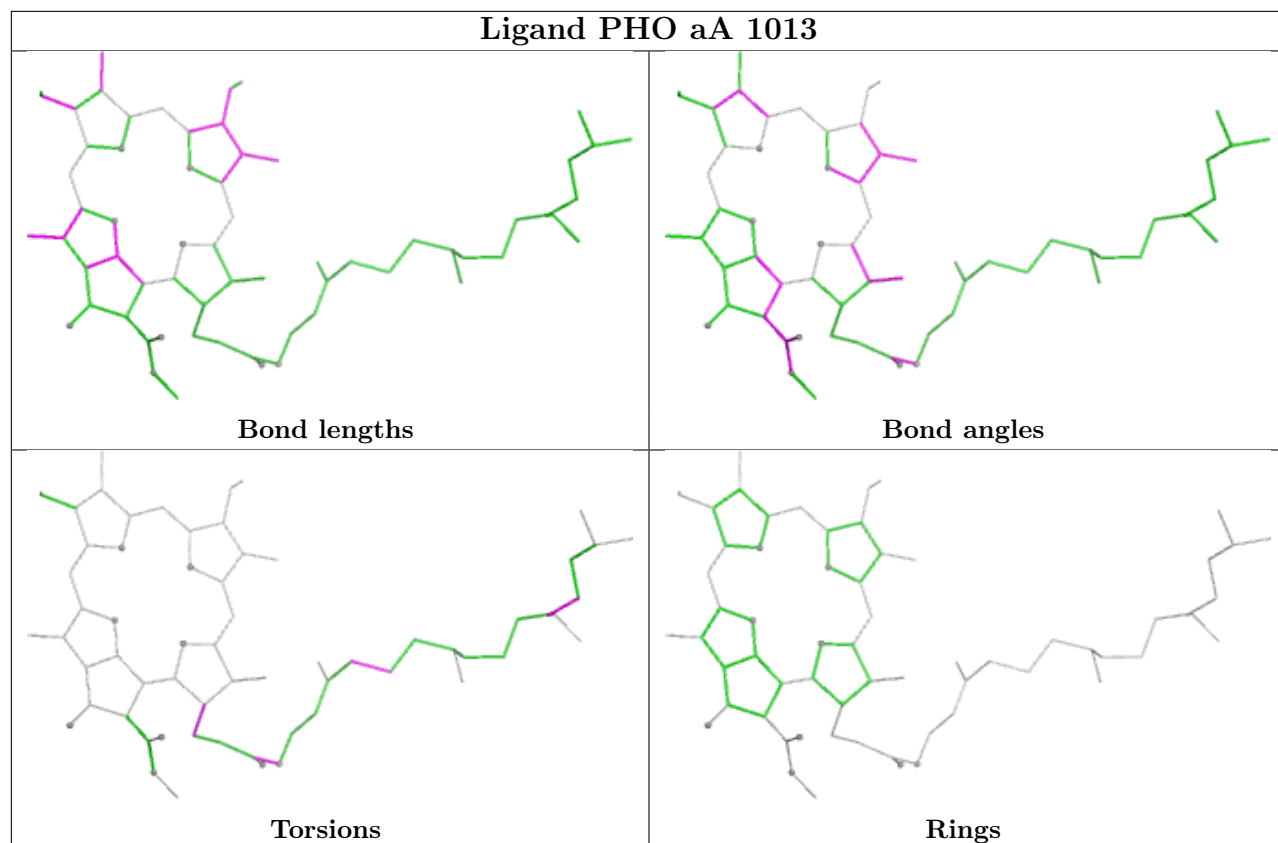
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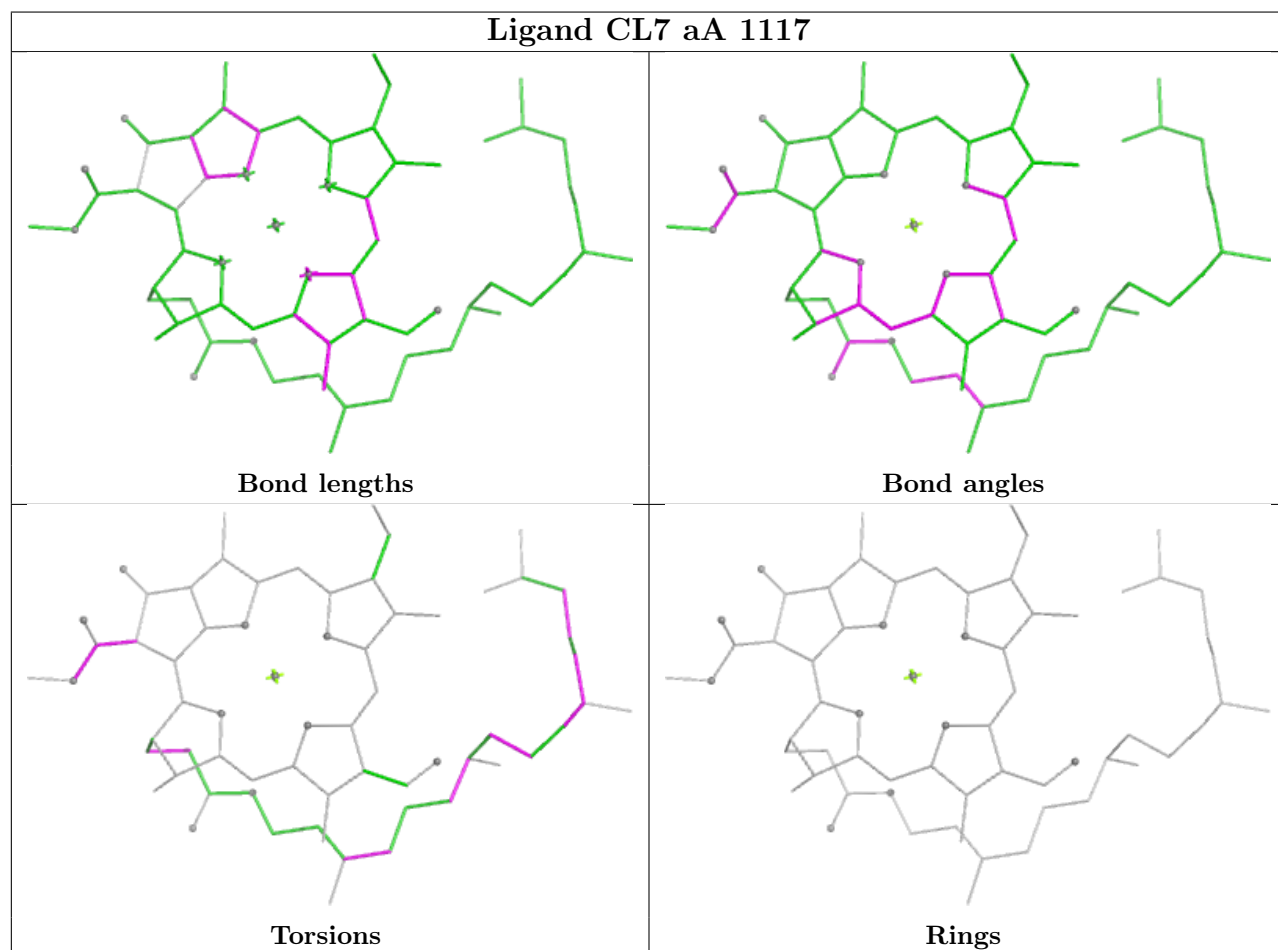


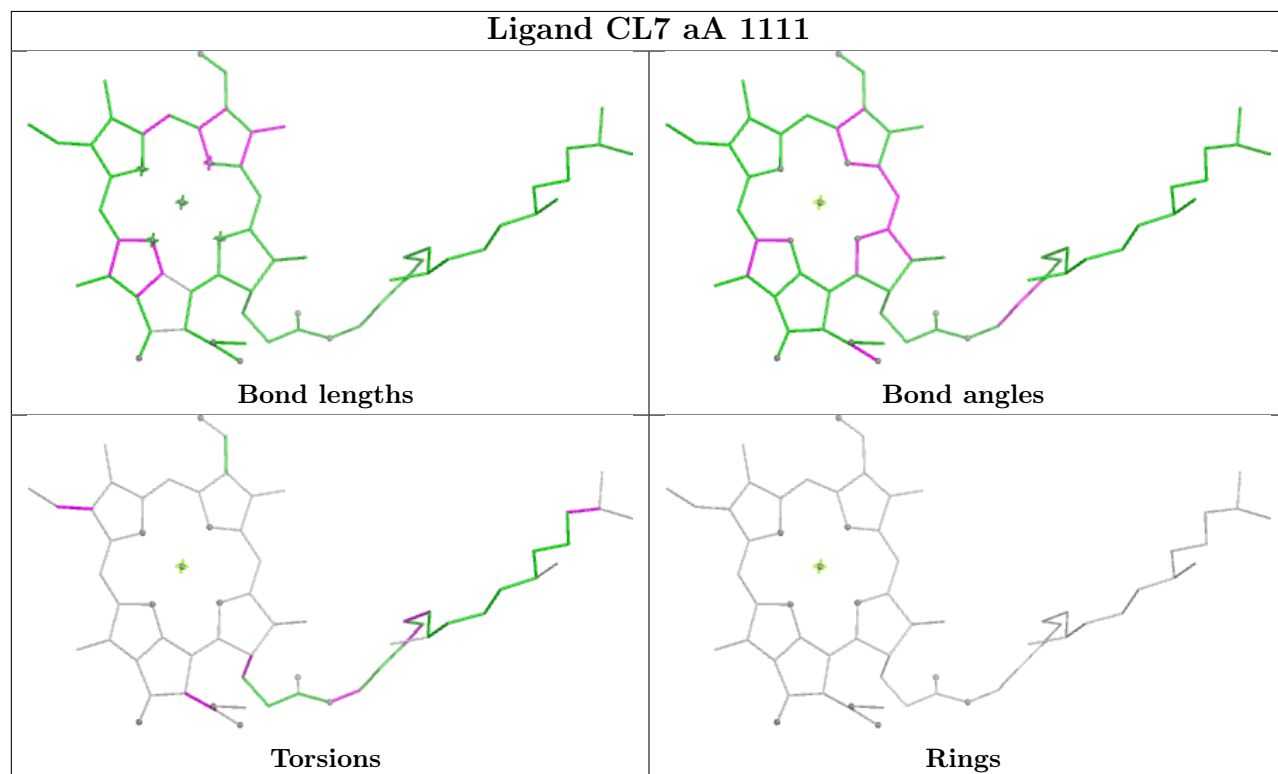
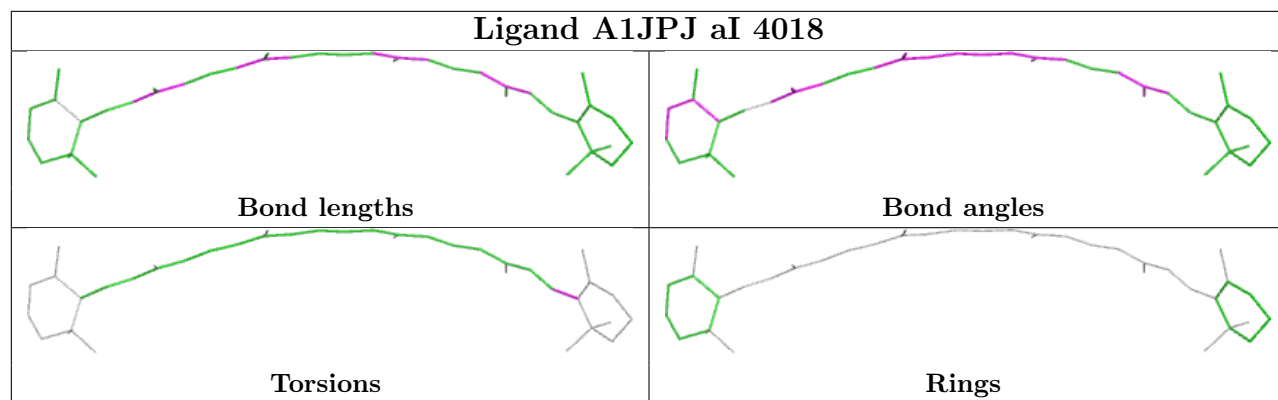


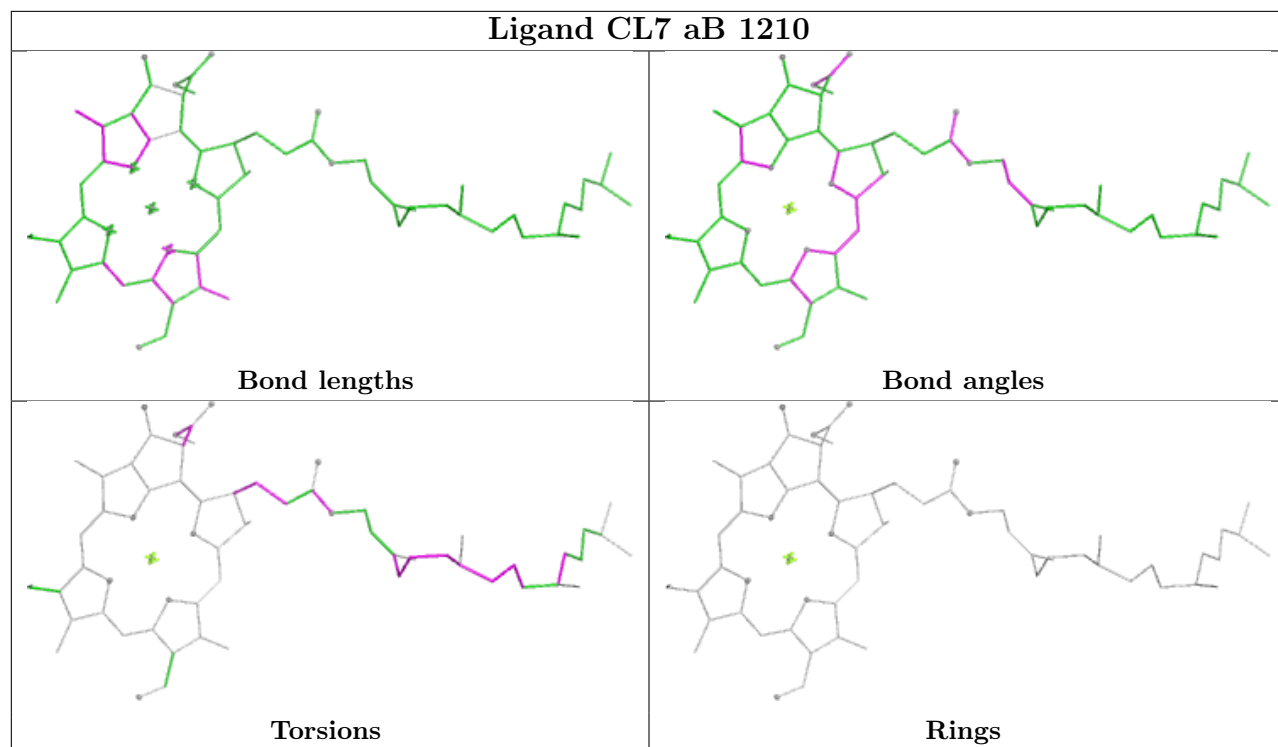
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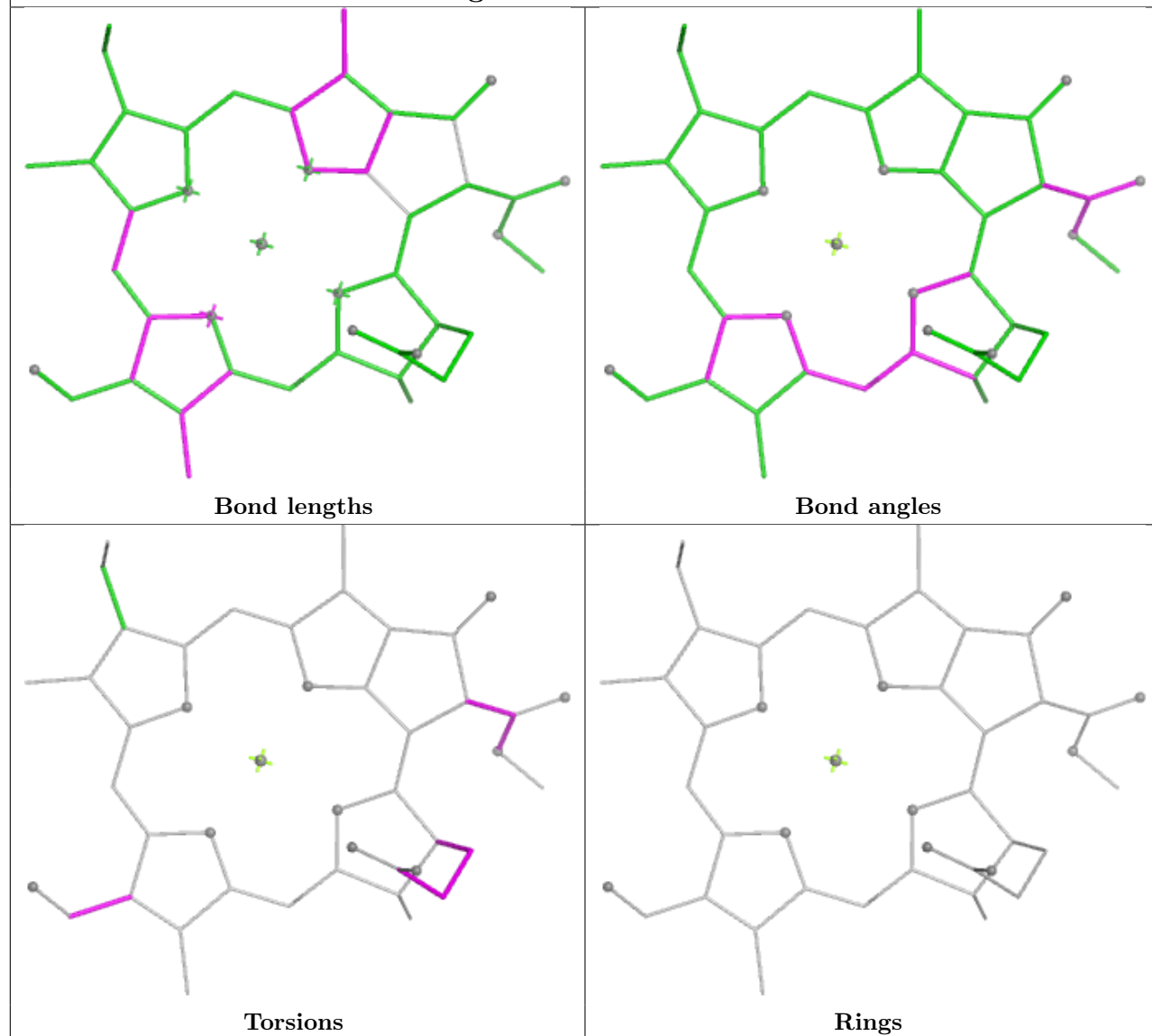
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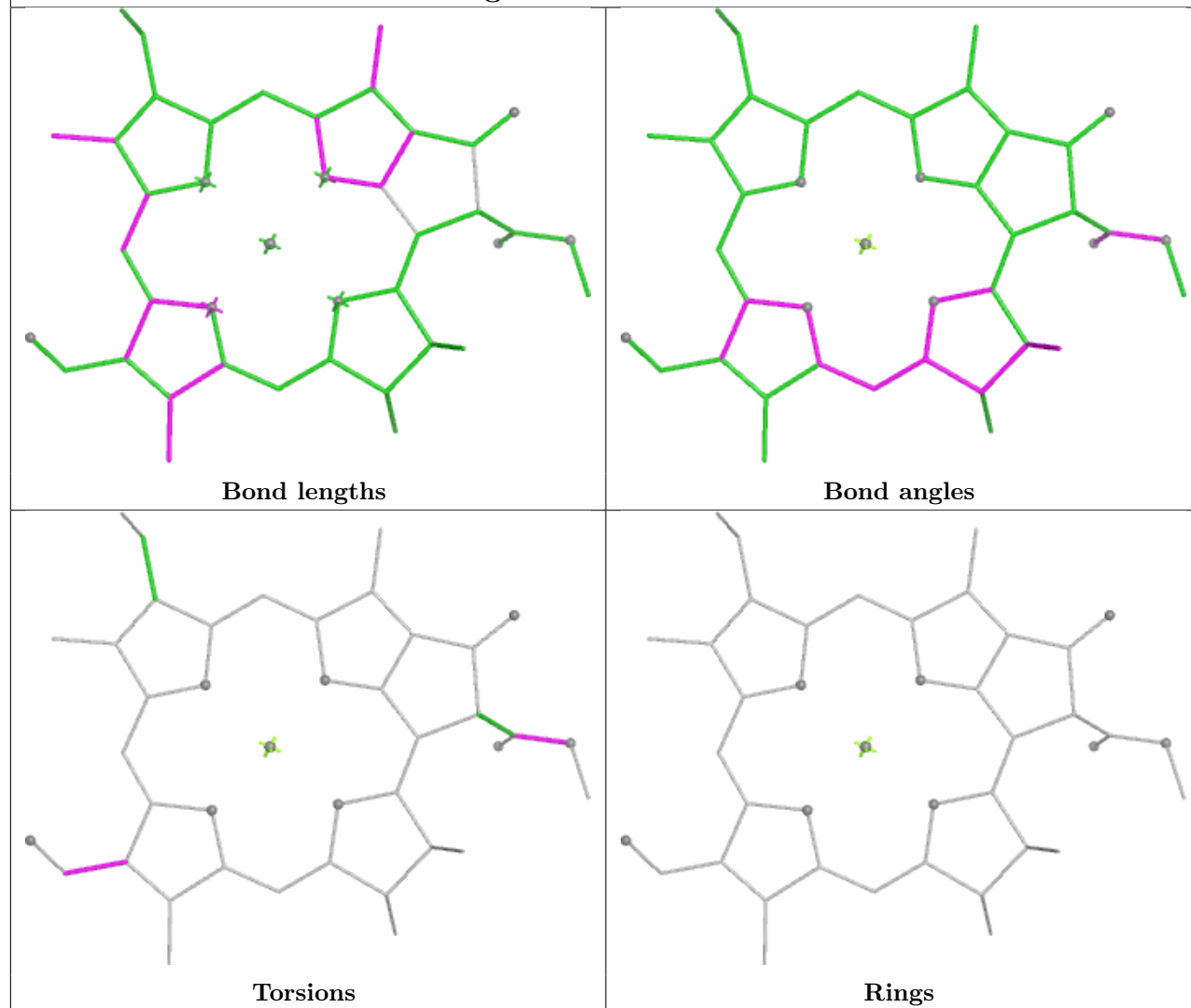




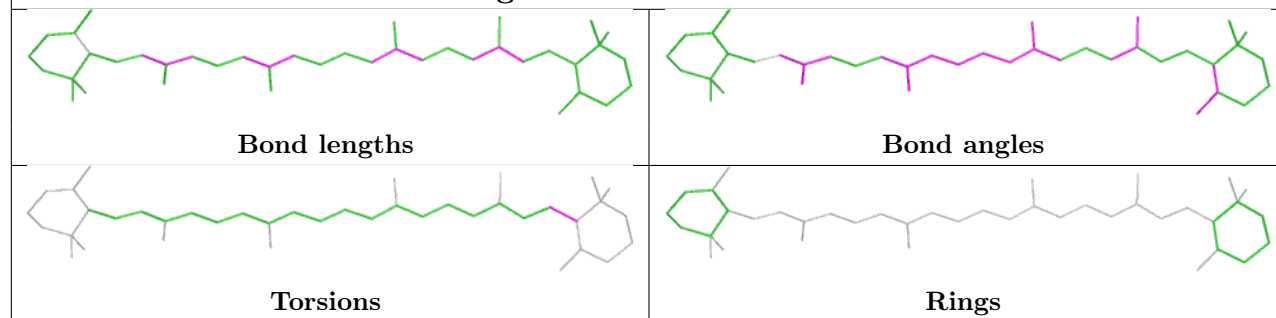
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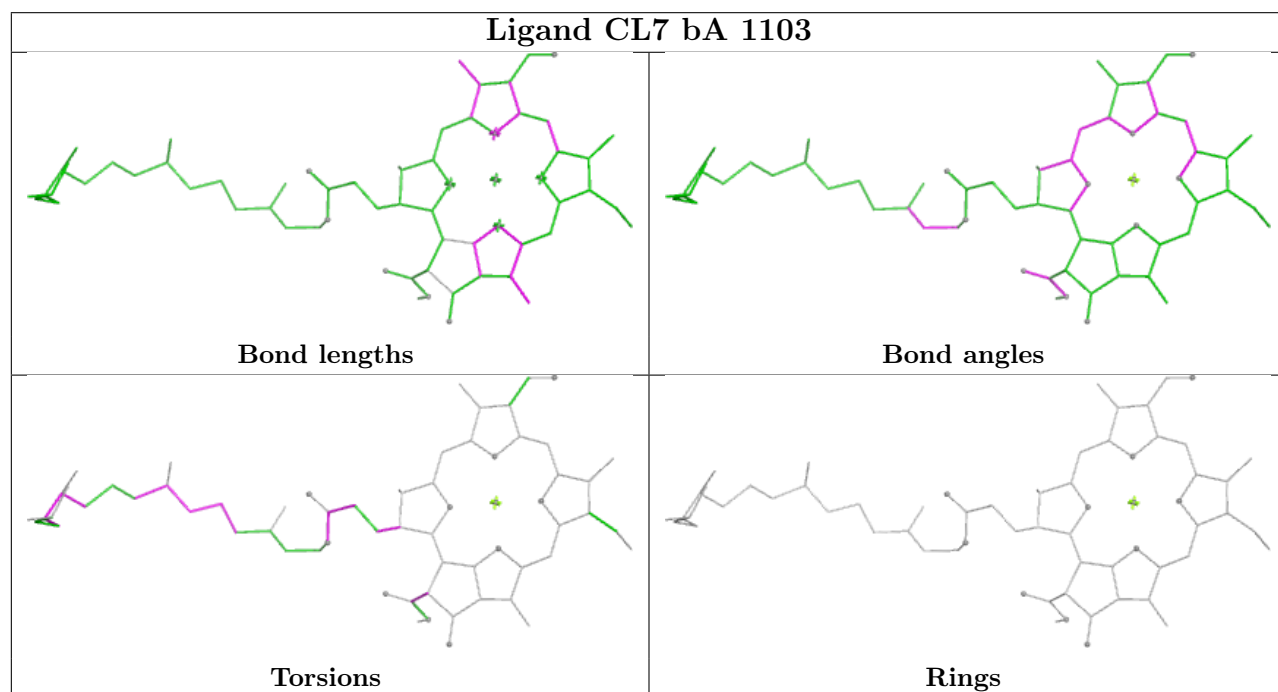
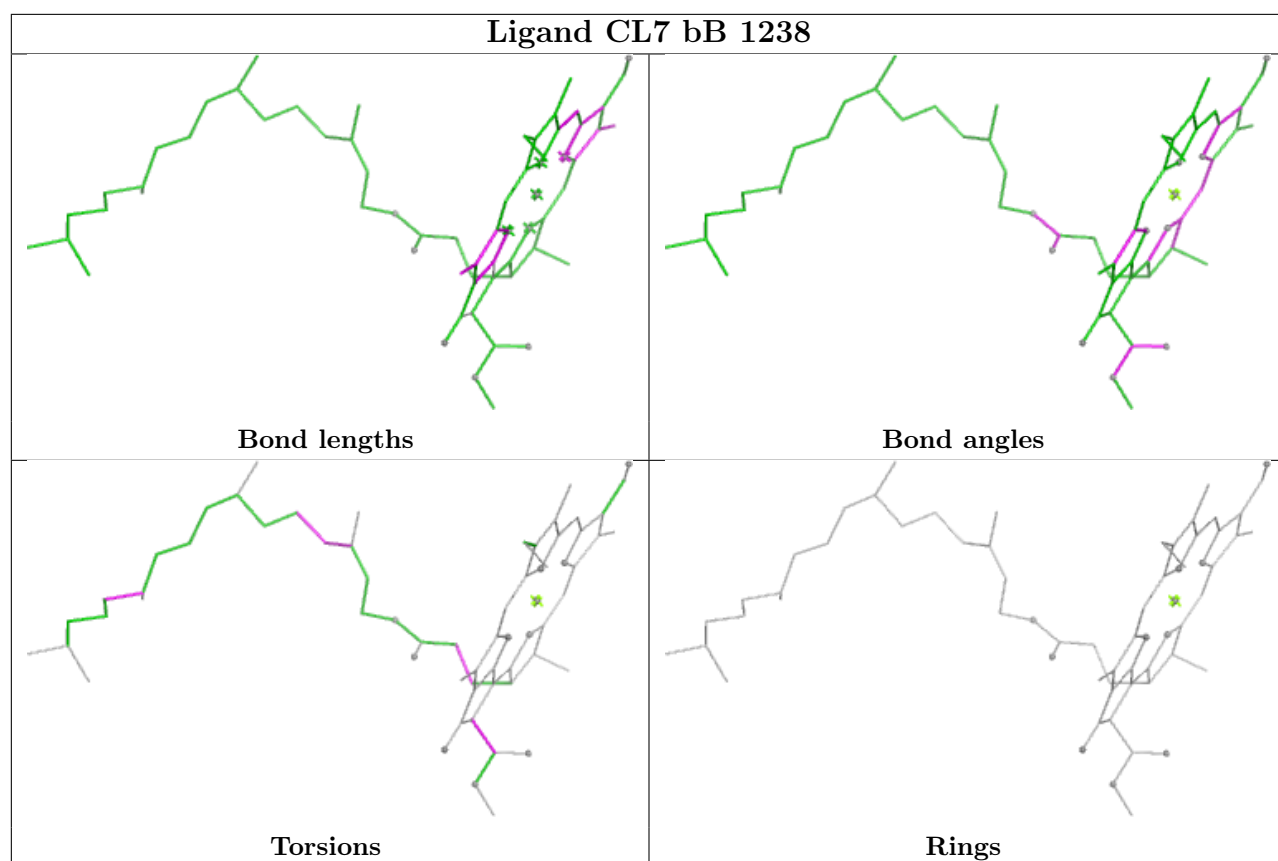


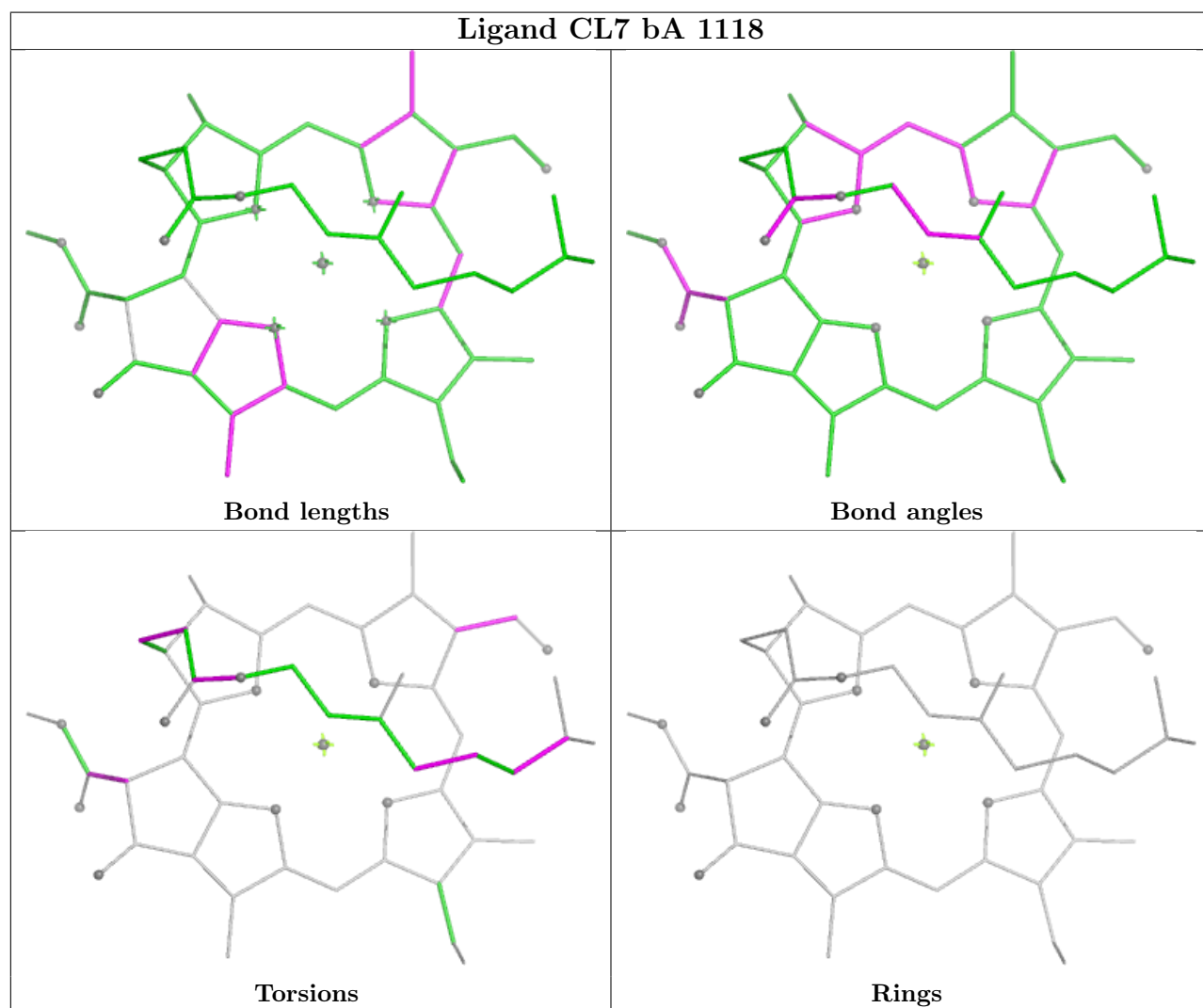
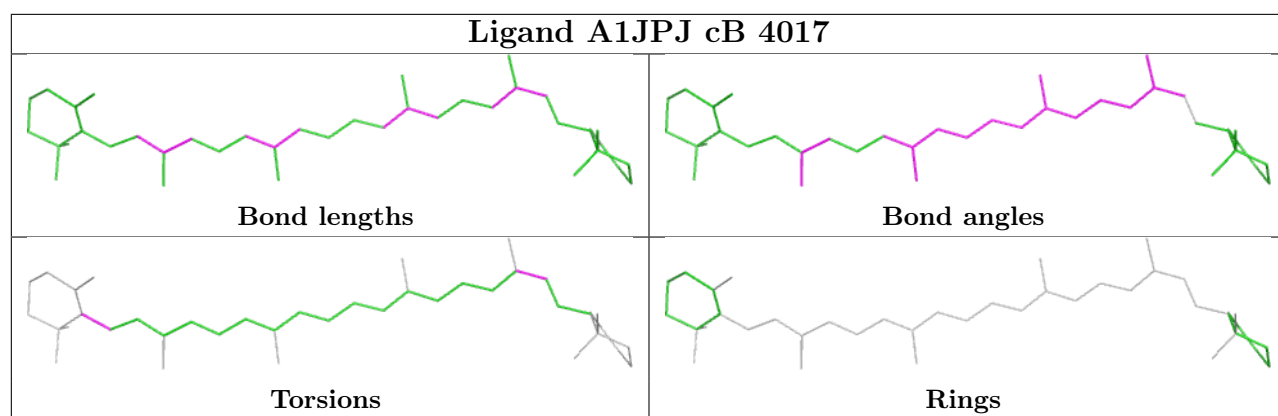
Ligand CL7 cA 1115



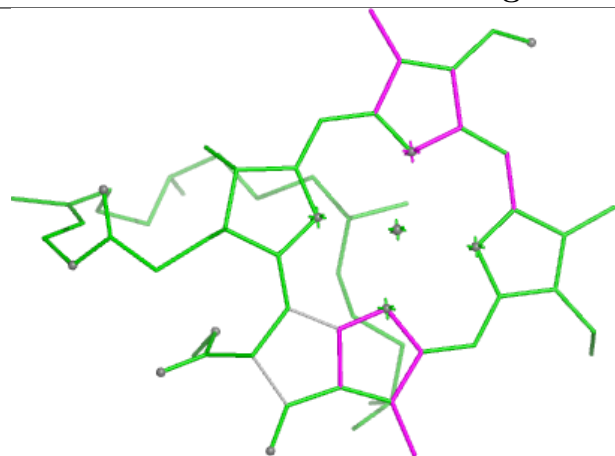
Ligand A1JPJ bA 4003



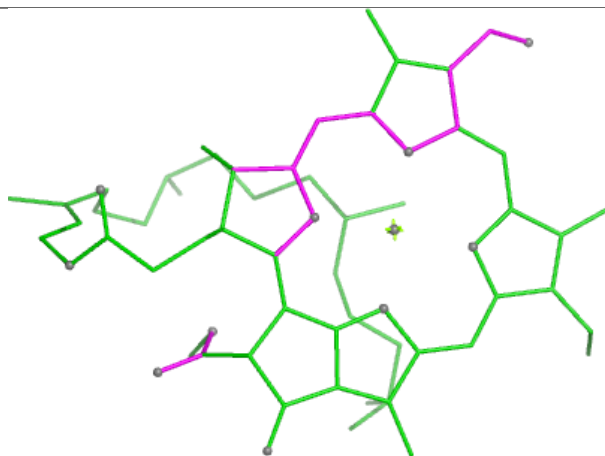




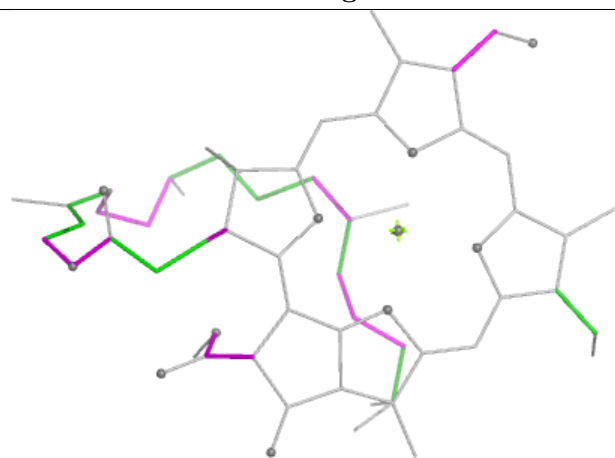
Ligand CL7 aA 1104



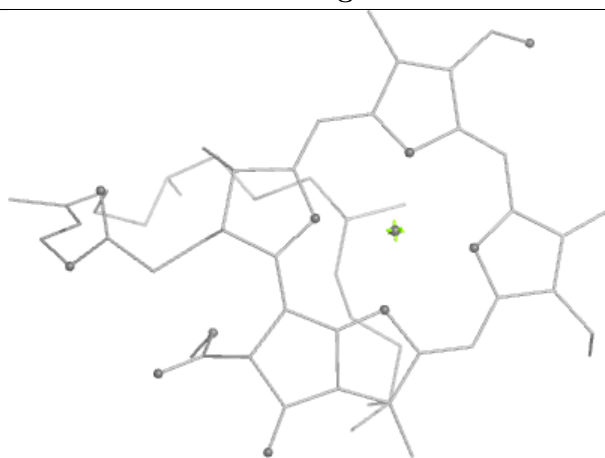
Bond lengths



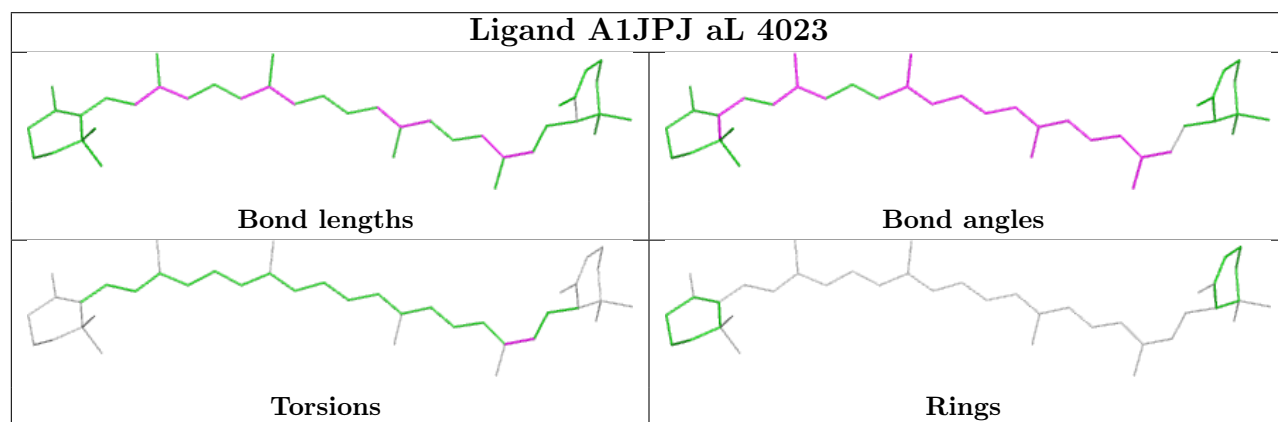
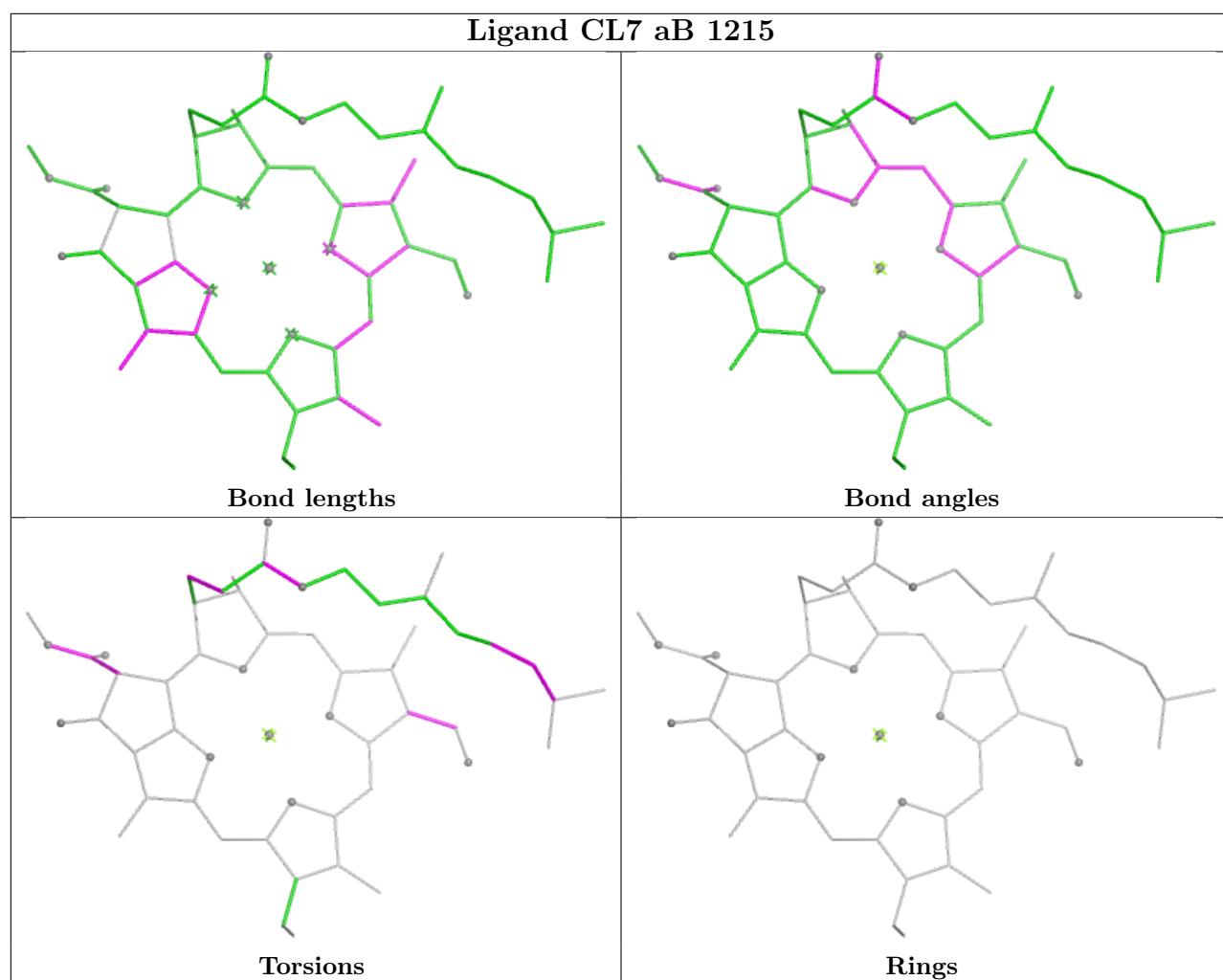
Bond angles

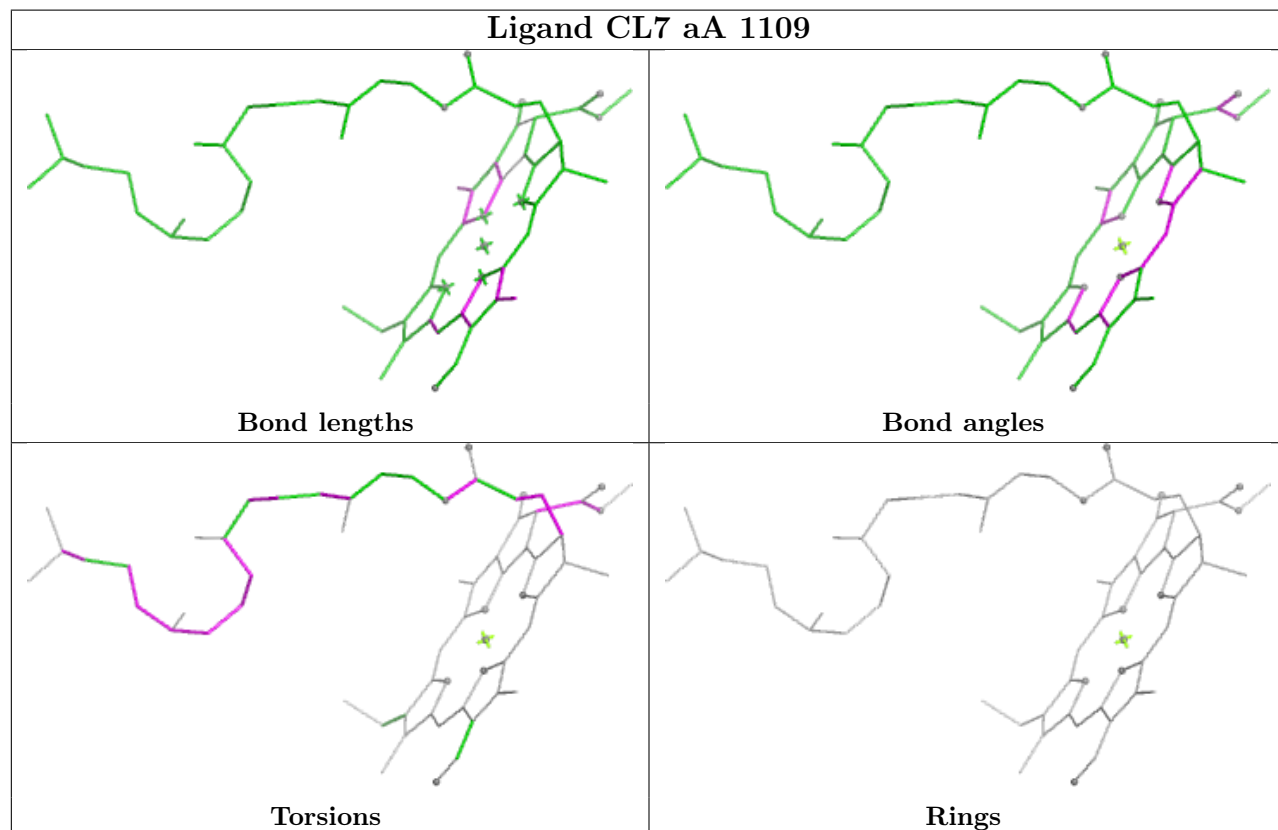
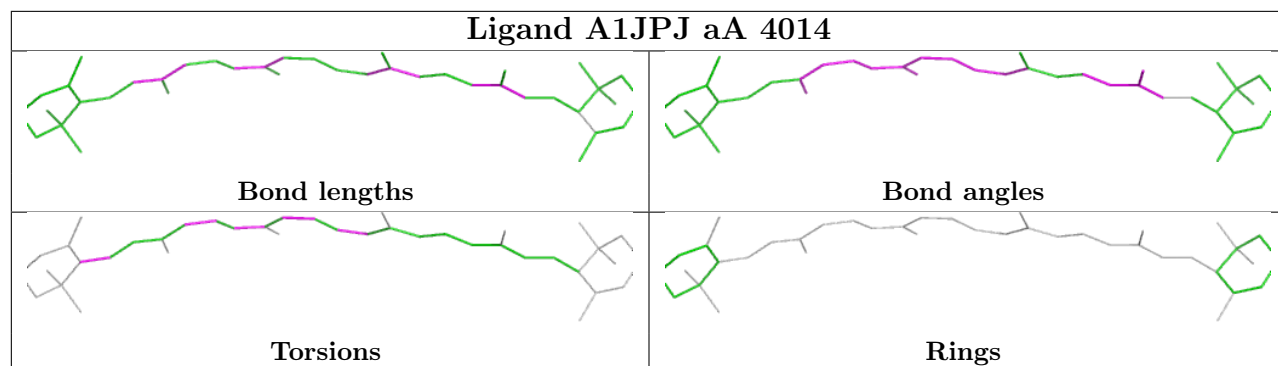


Torsions

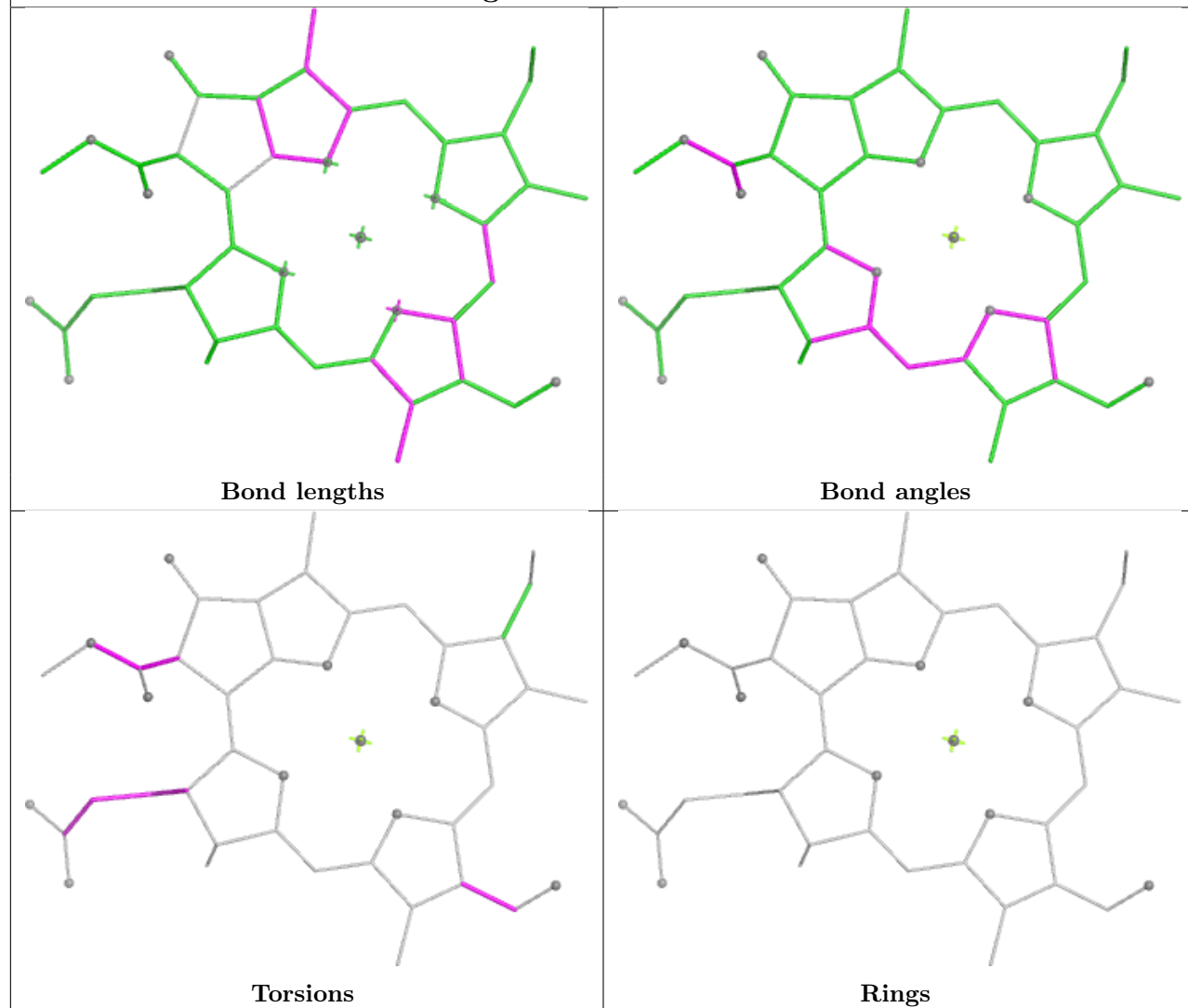


Rings

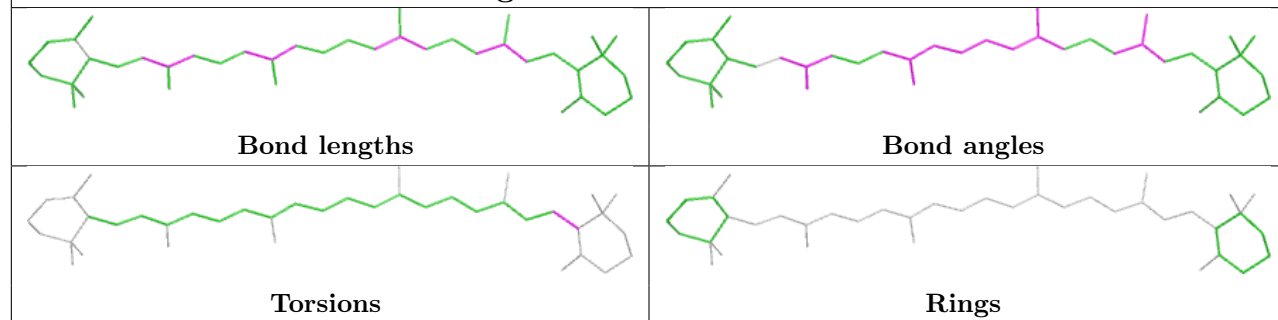


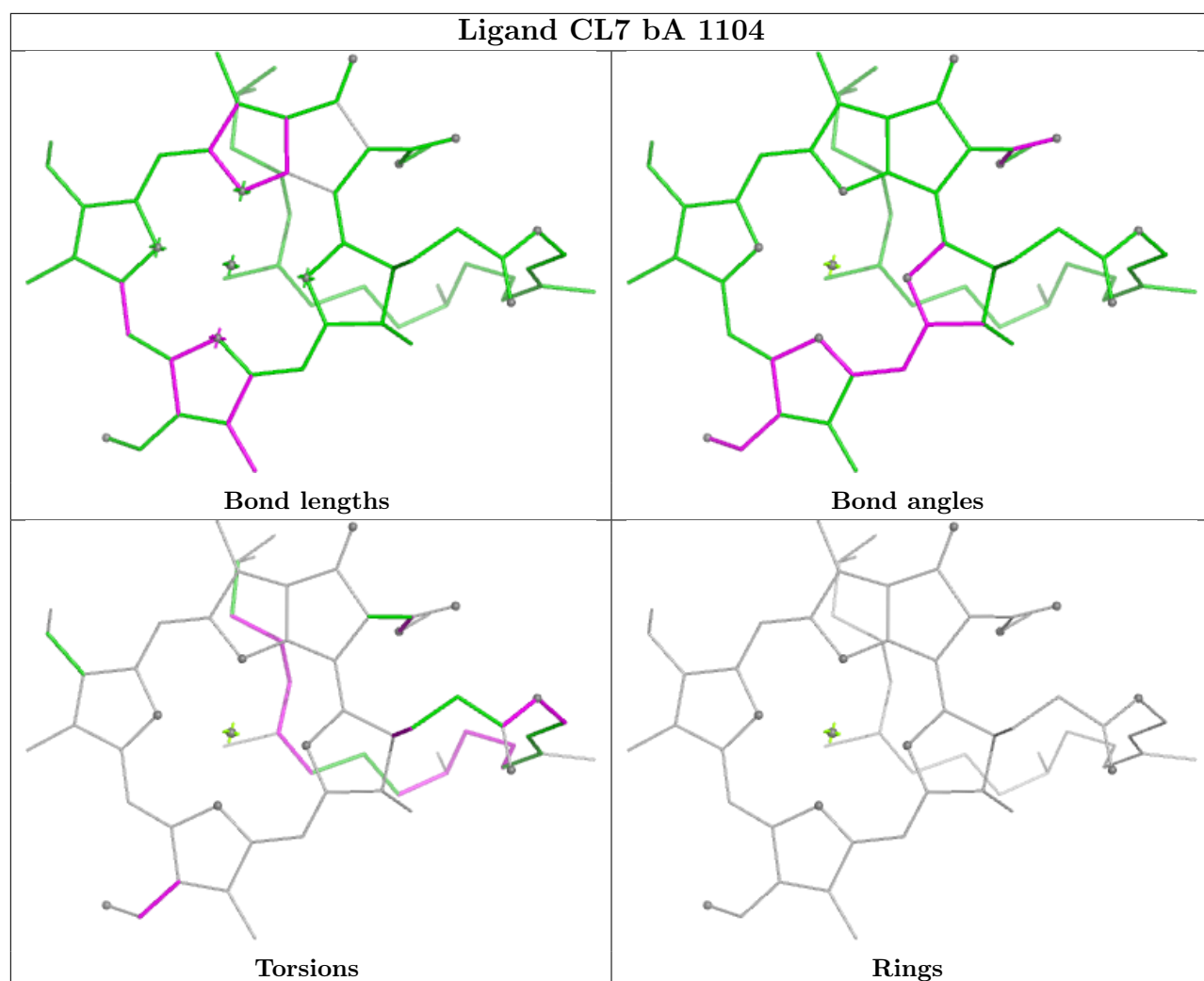


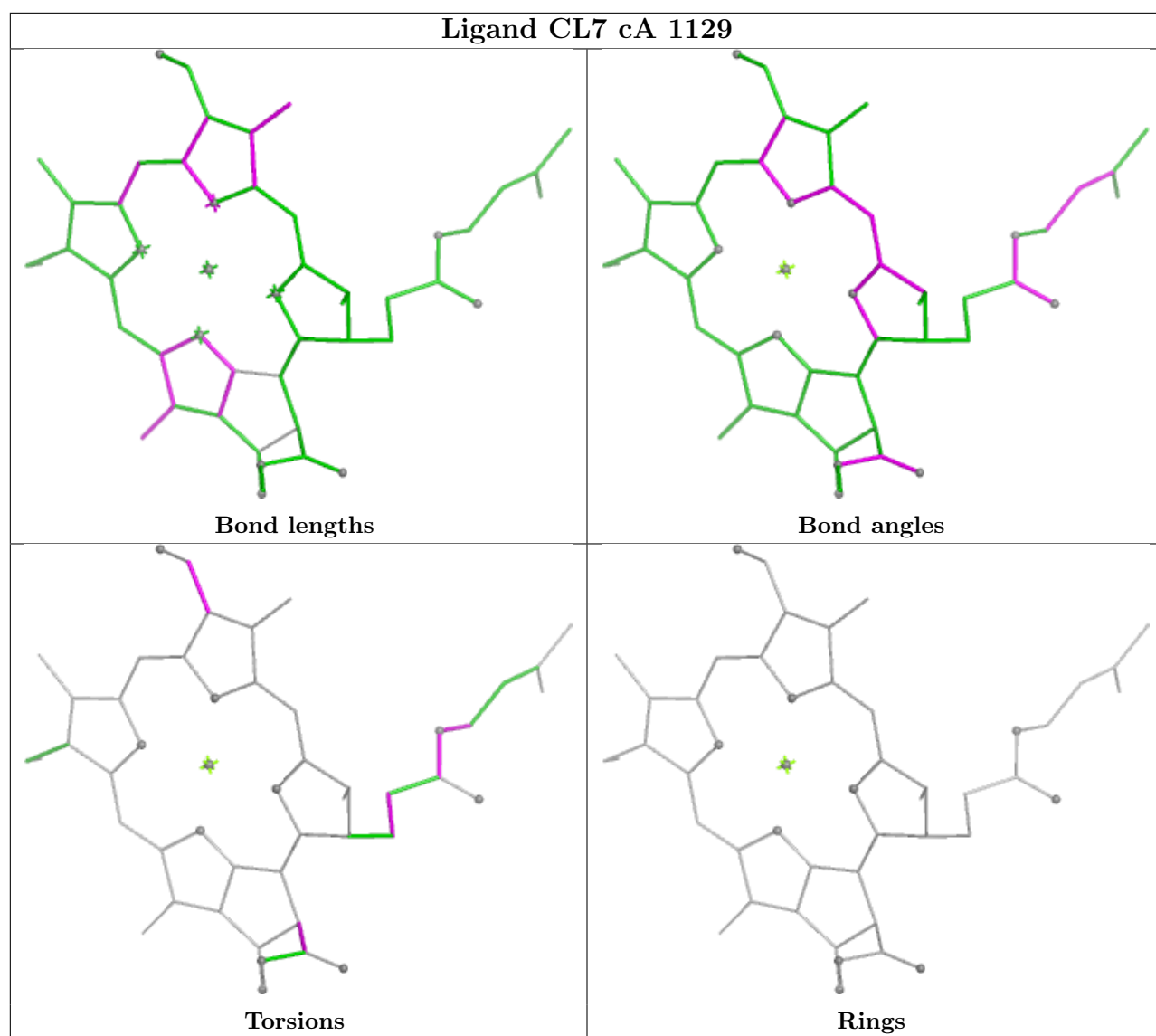
Ligand CL7 cA 1139

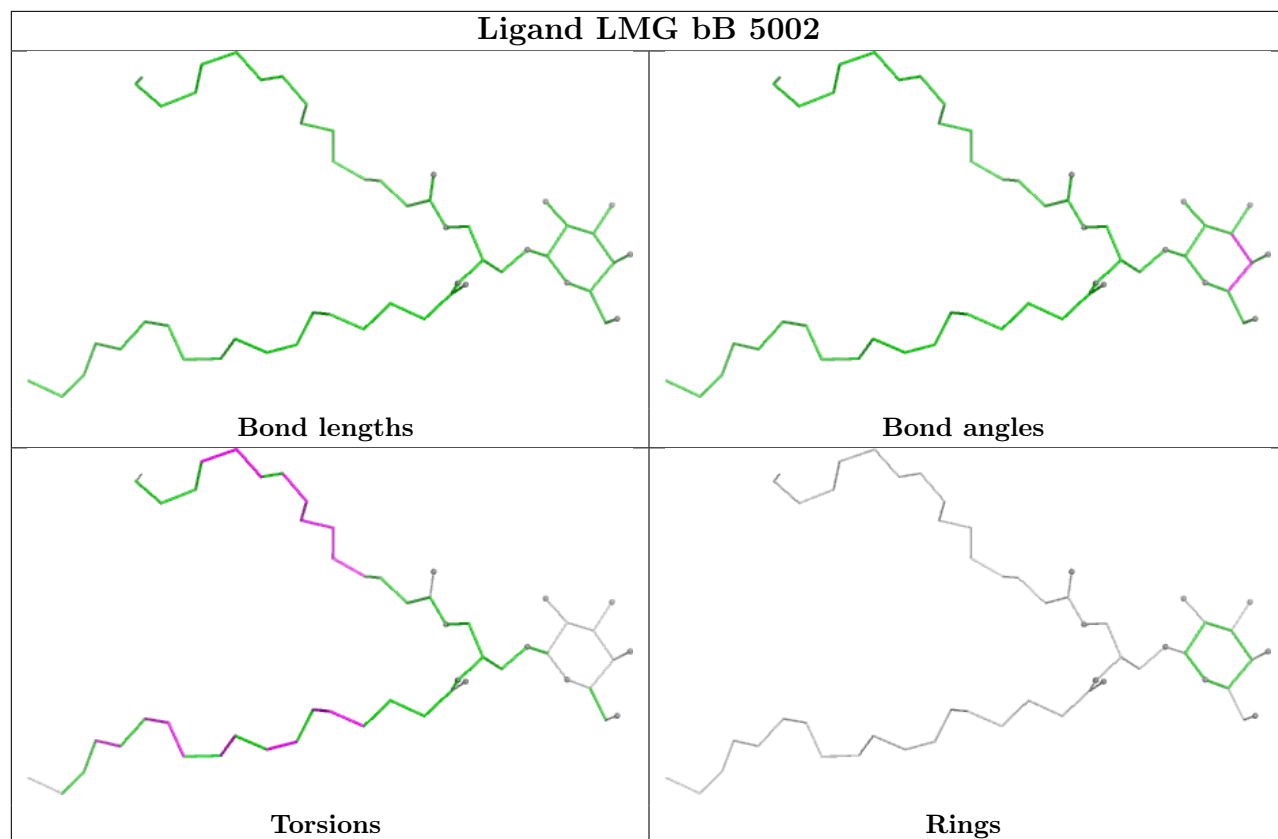


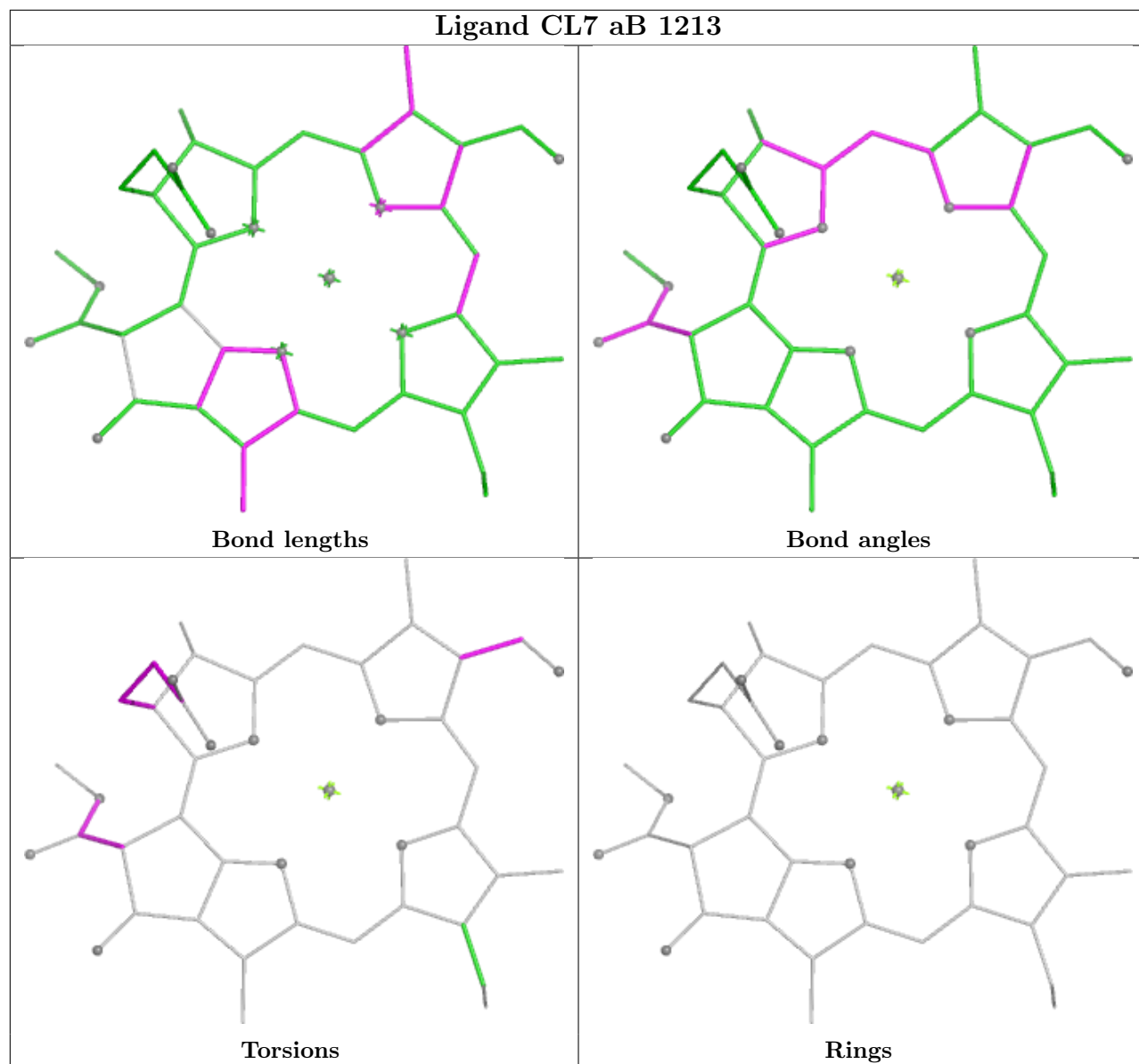
Ligand A1JPJ bA 4002



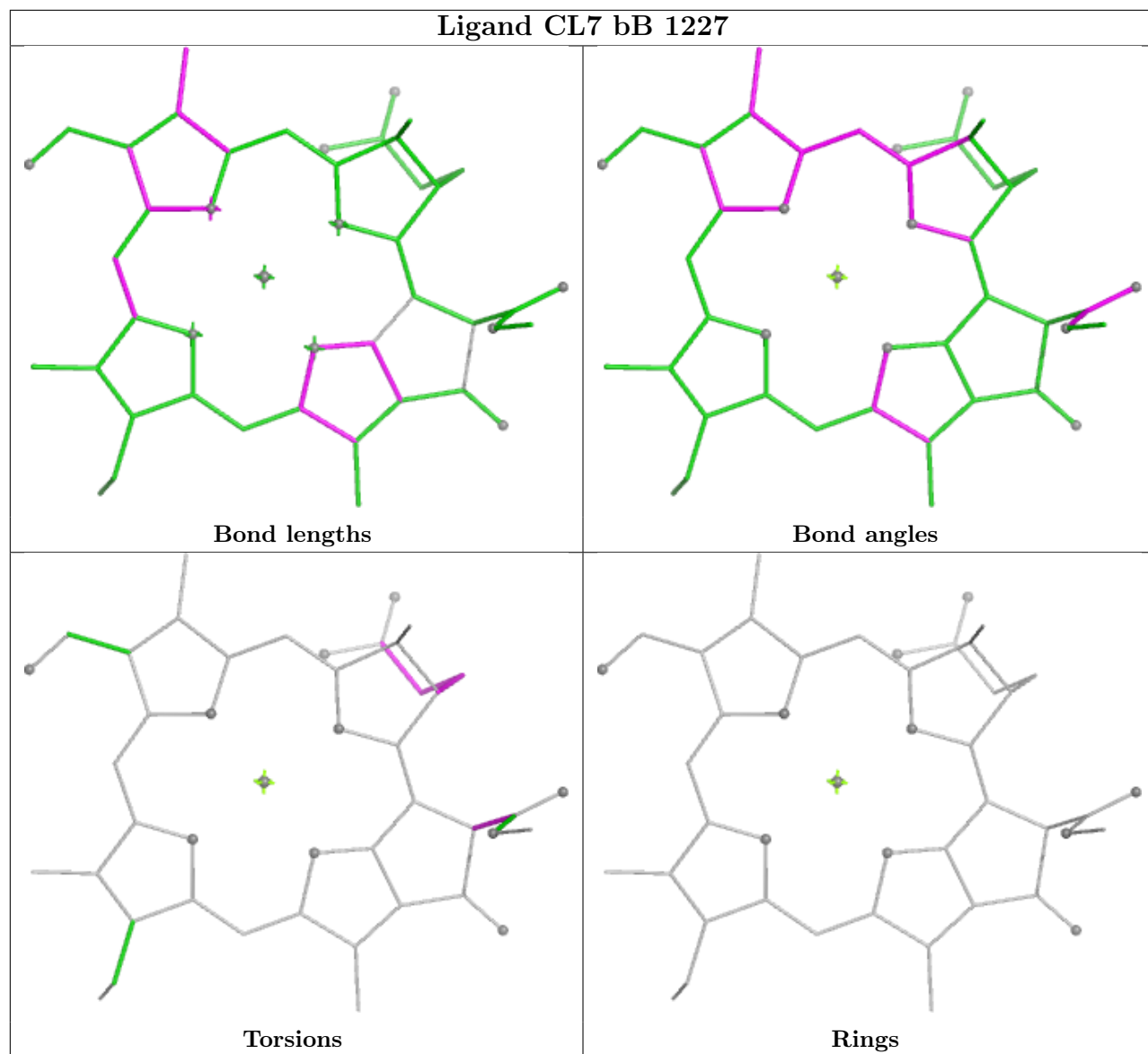


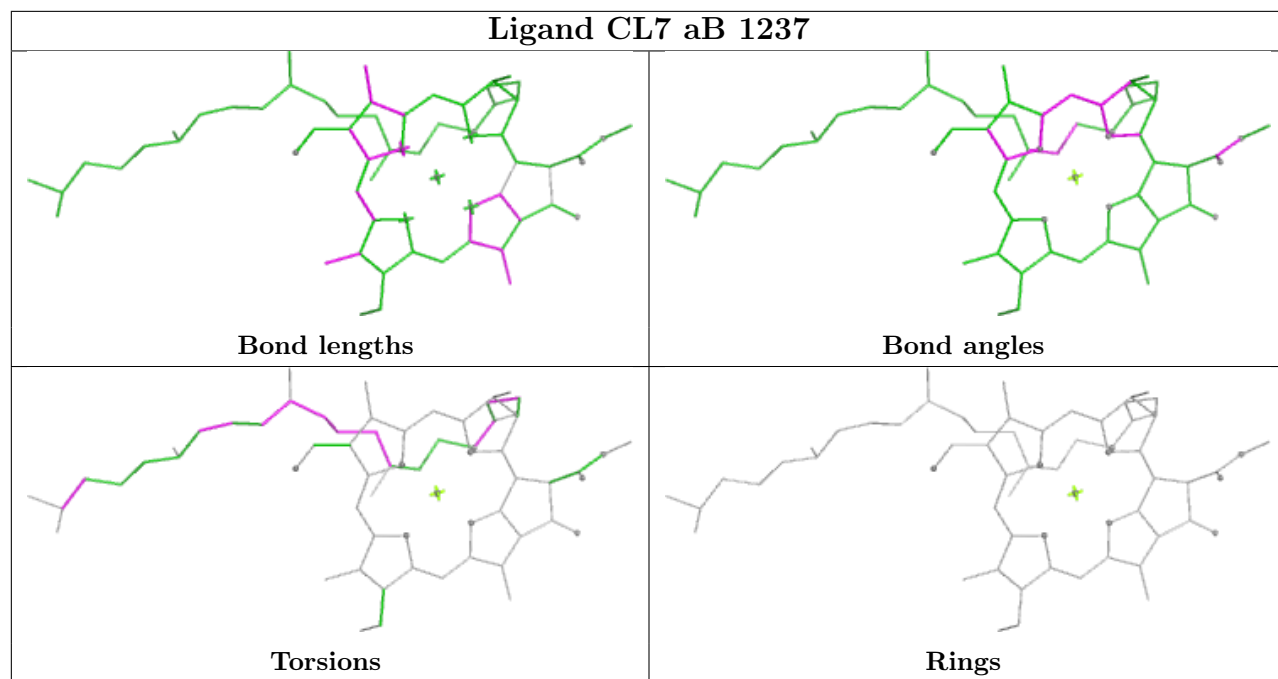




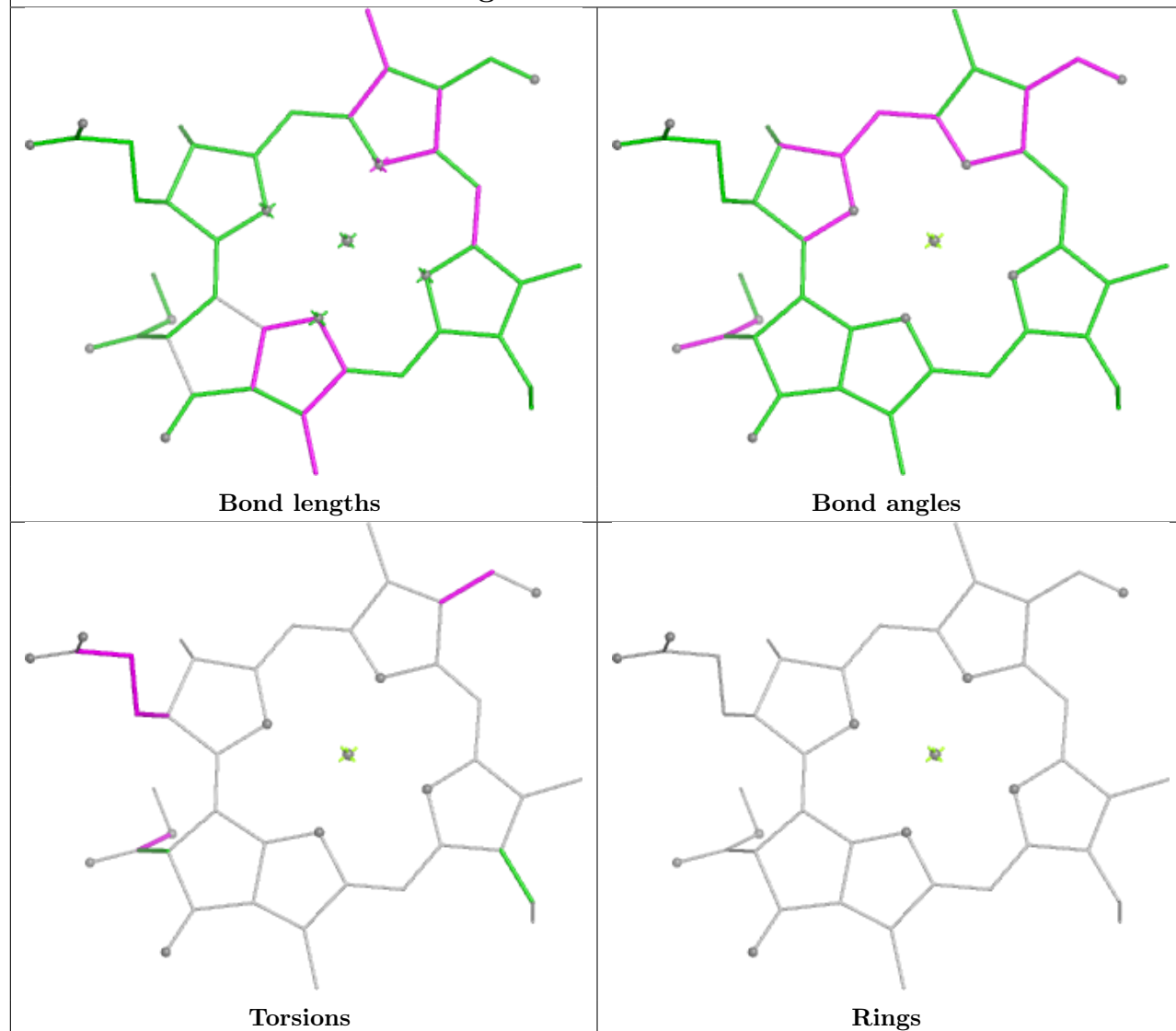


Ligand CL7 bB 1227

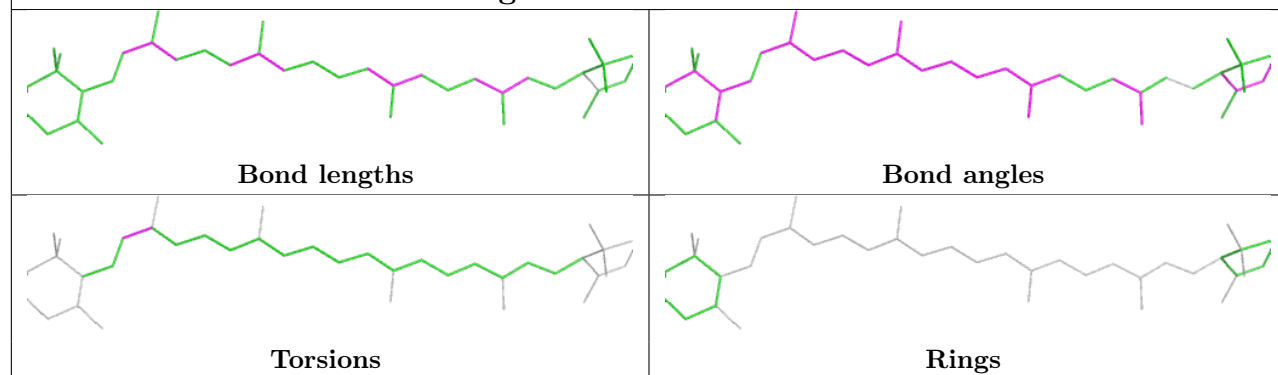




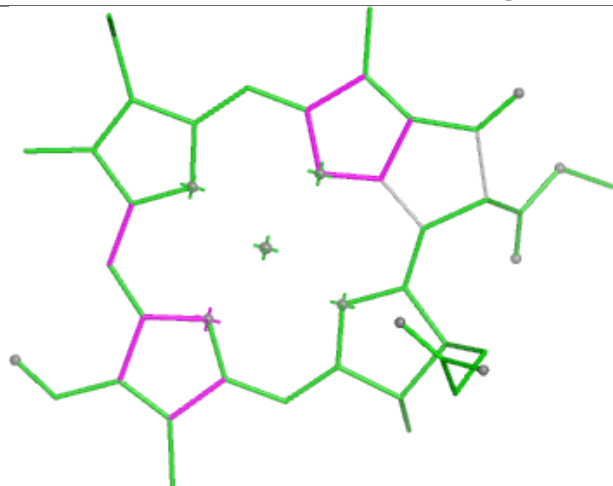
Ligand CL7 cB 1222



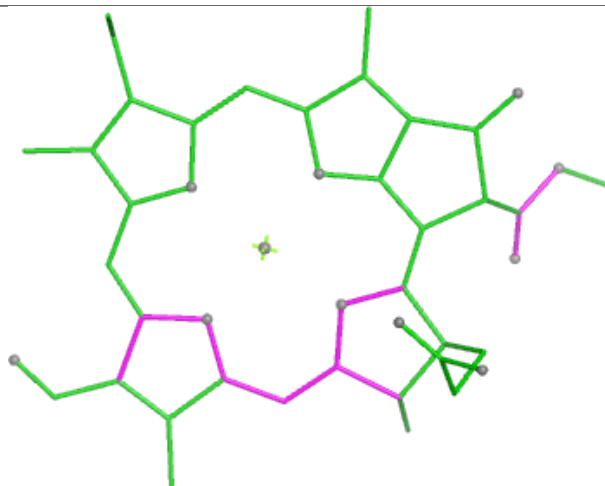
Ligand A1JPJ aB 4015



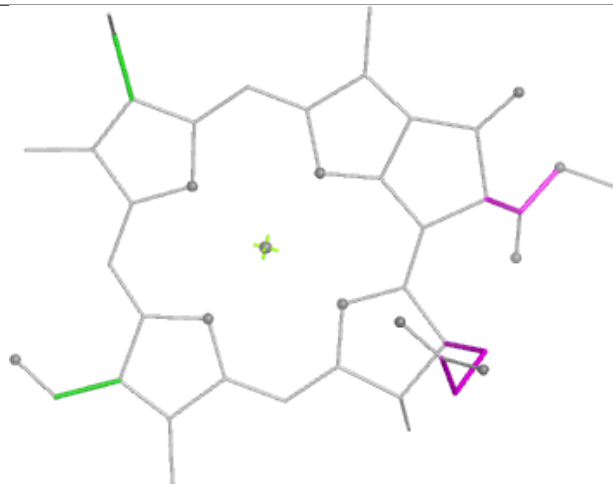
Ligand CL7 bB 1209



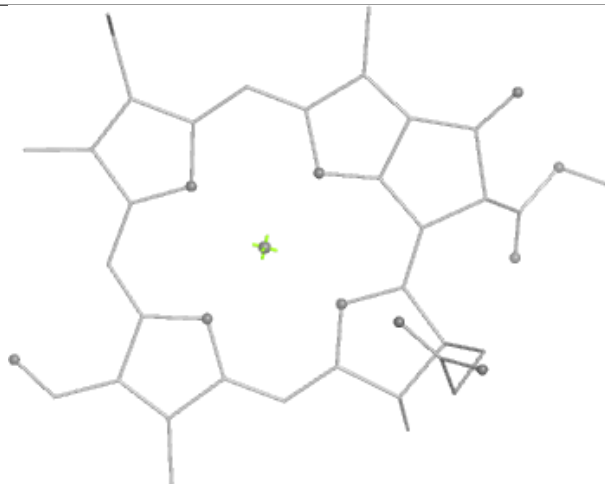
Bond lengths



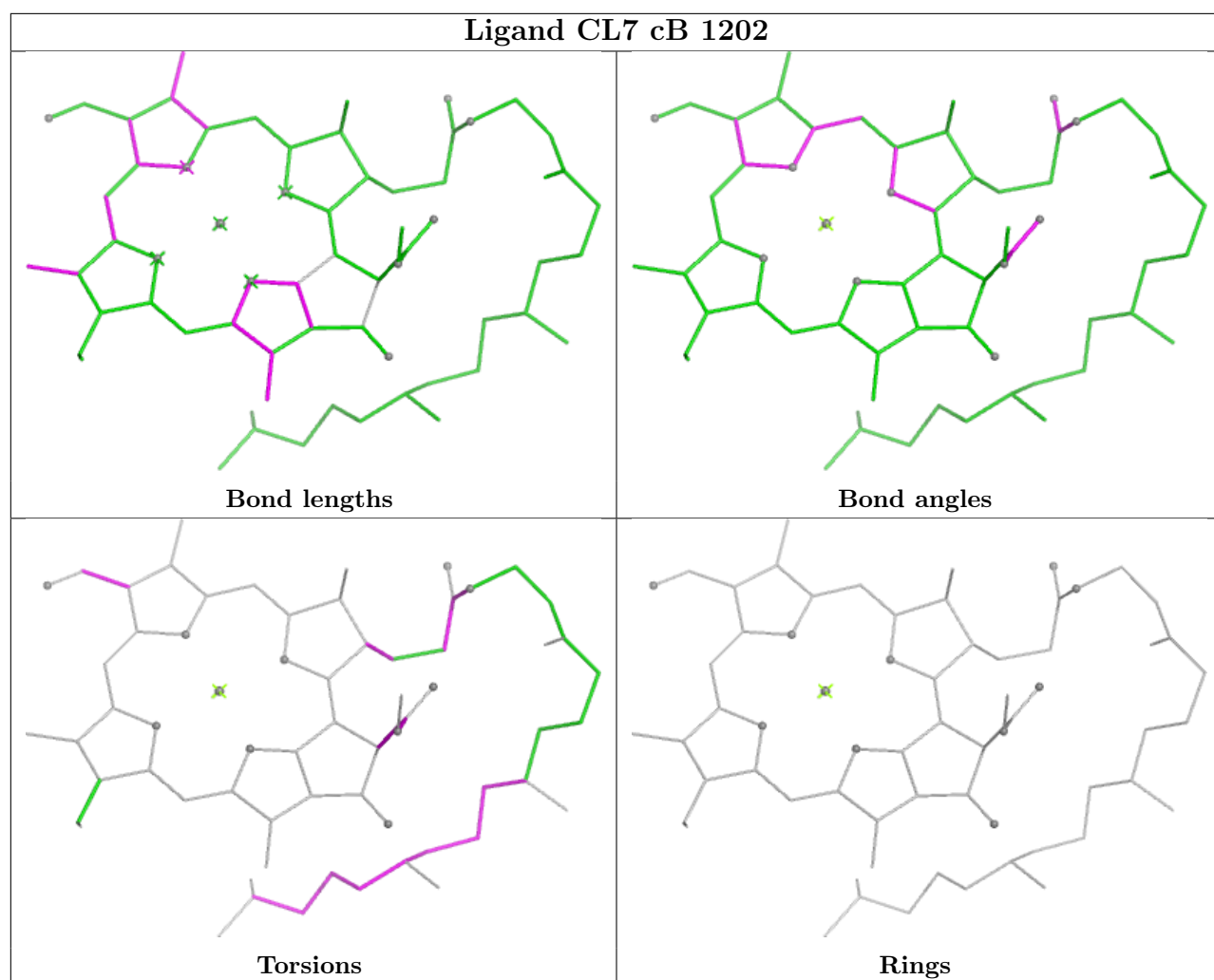
Bond angles

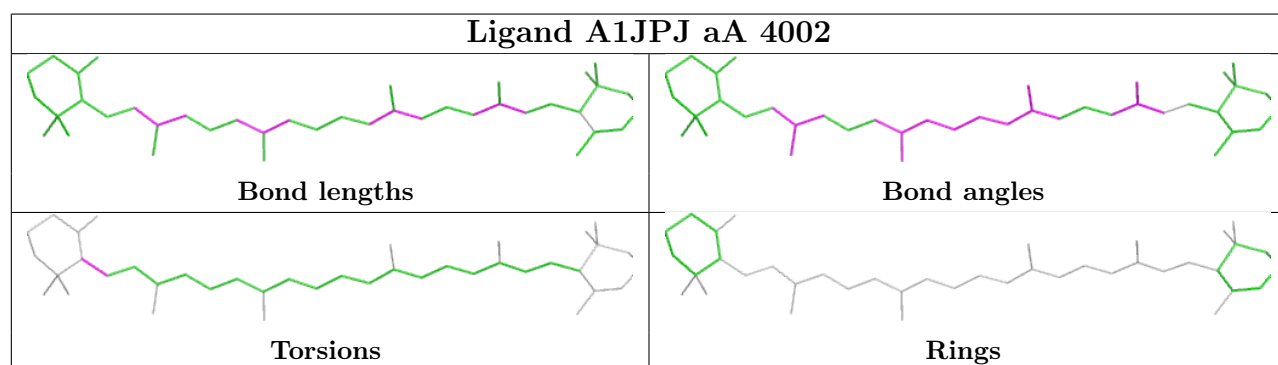
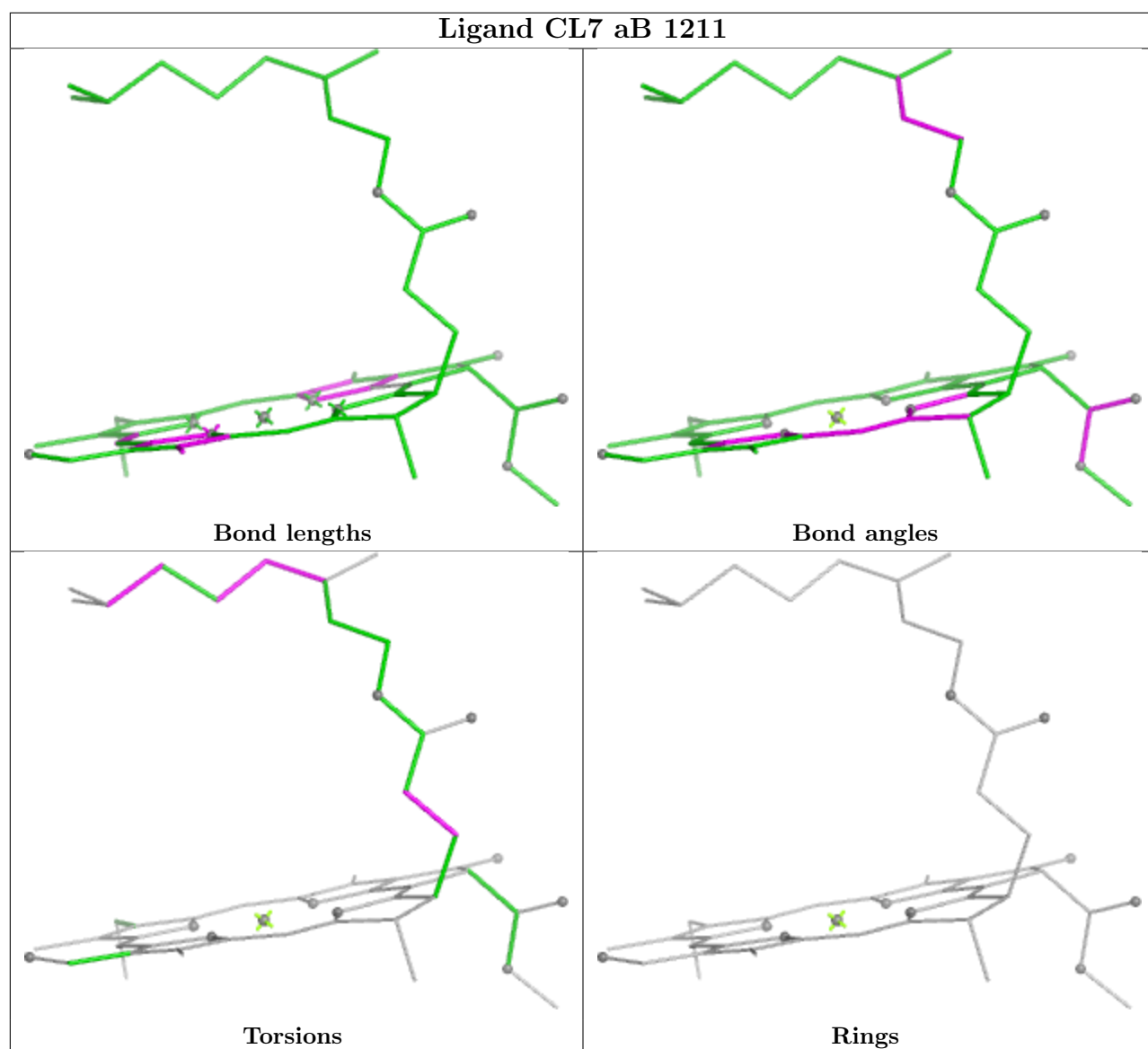


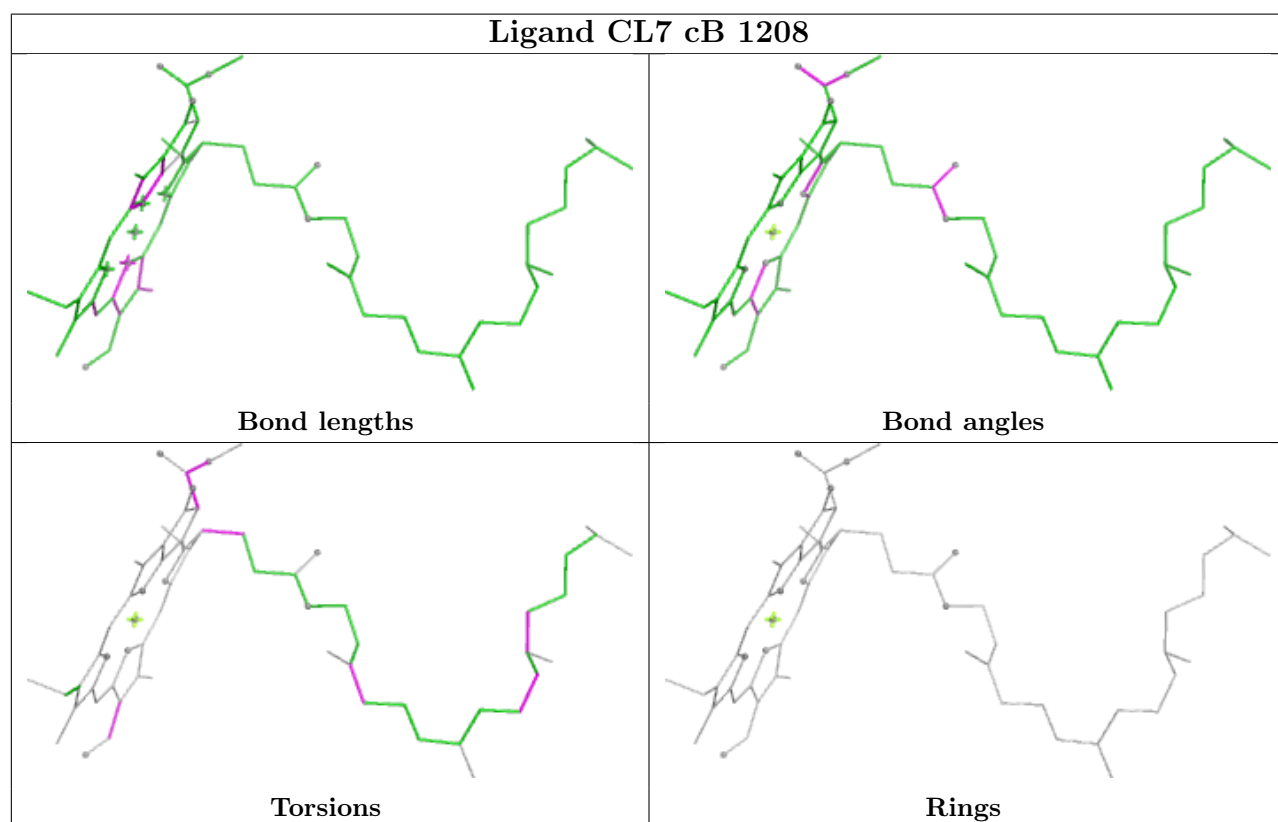
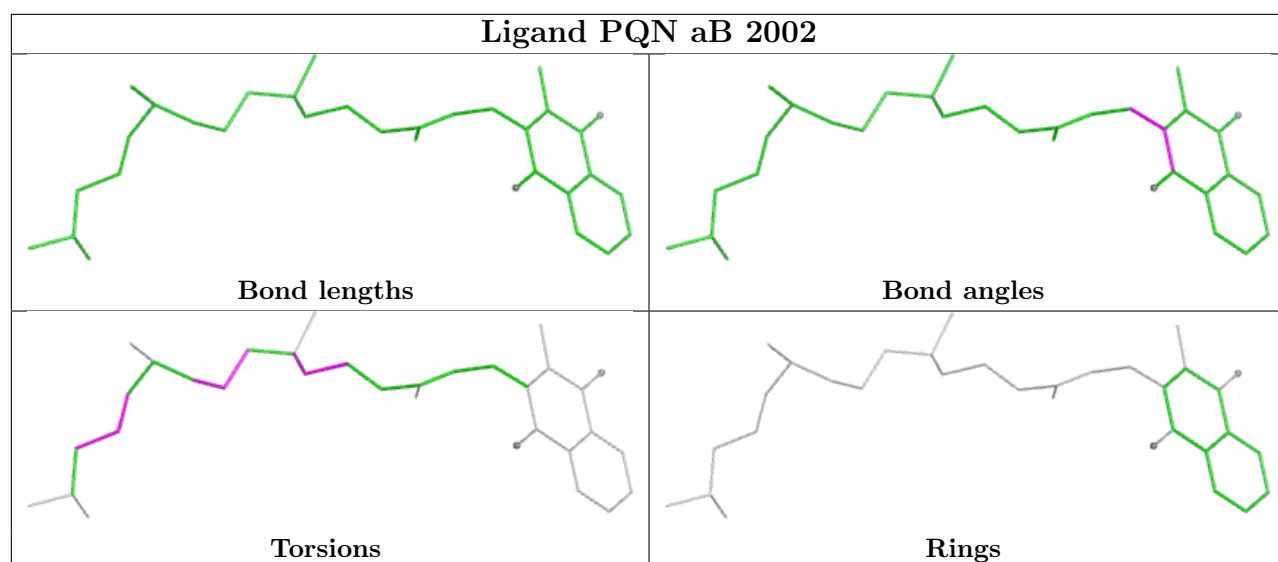
Torsions

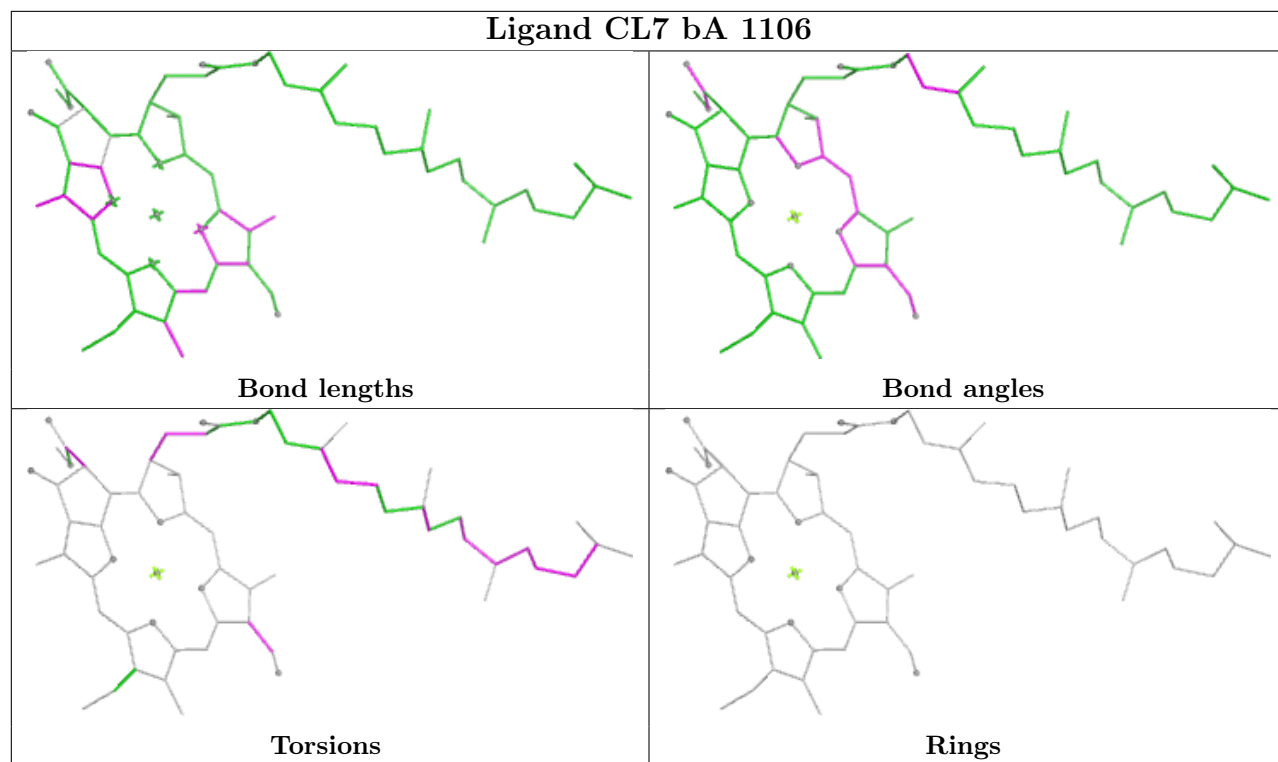


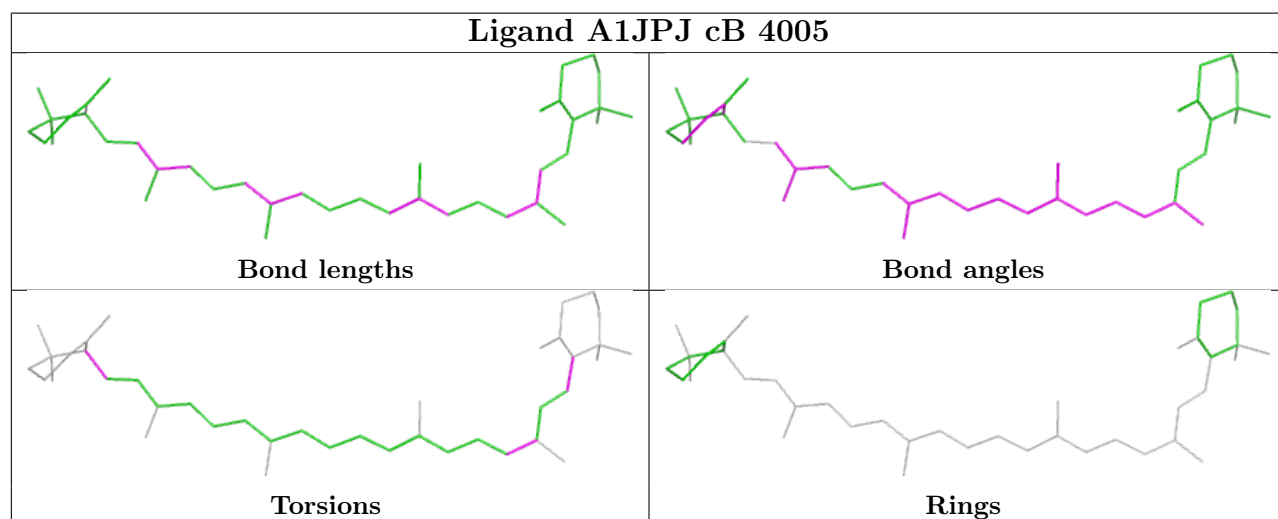
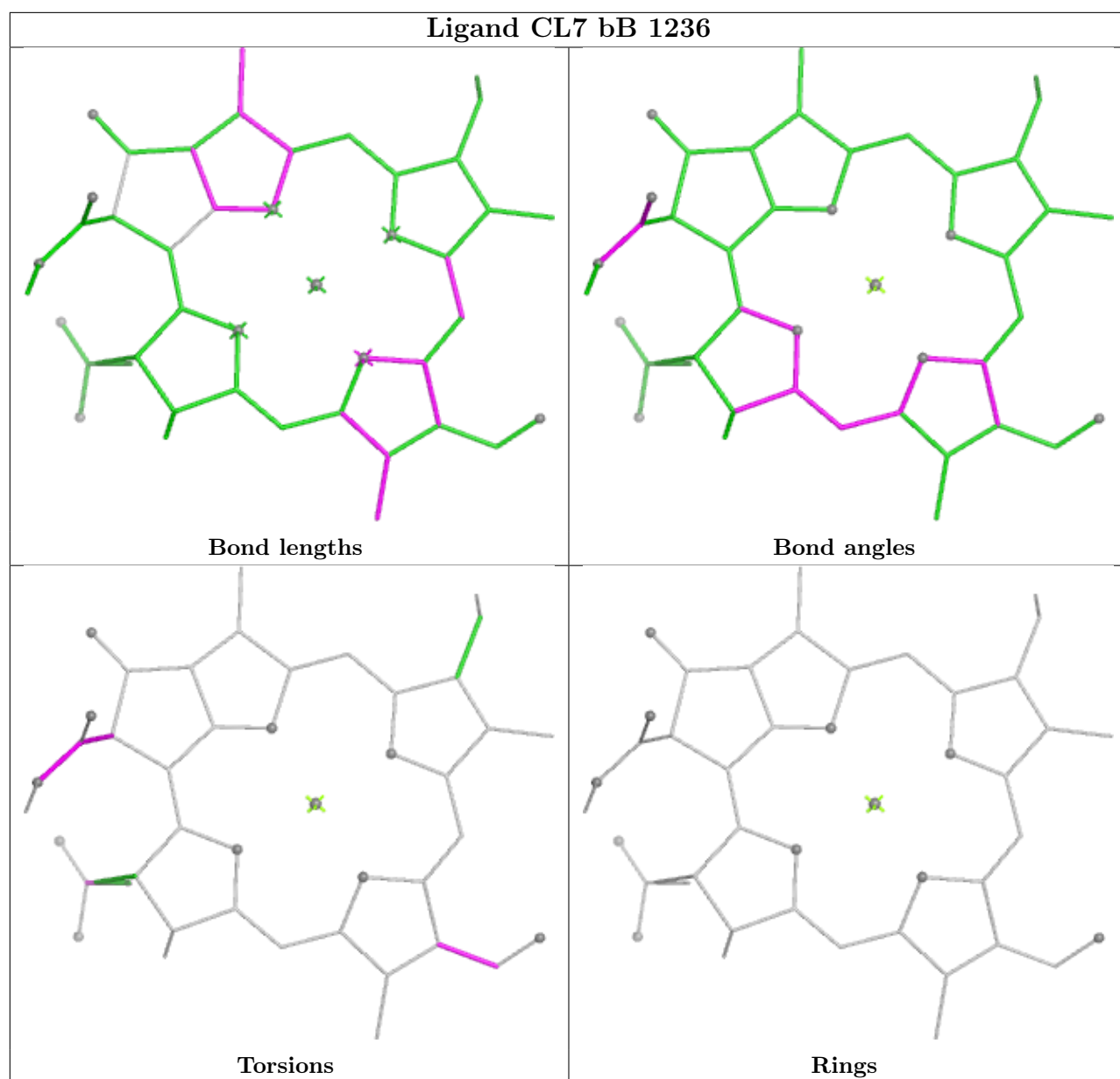
Rings

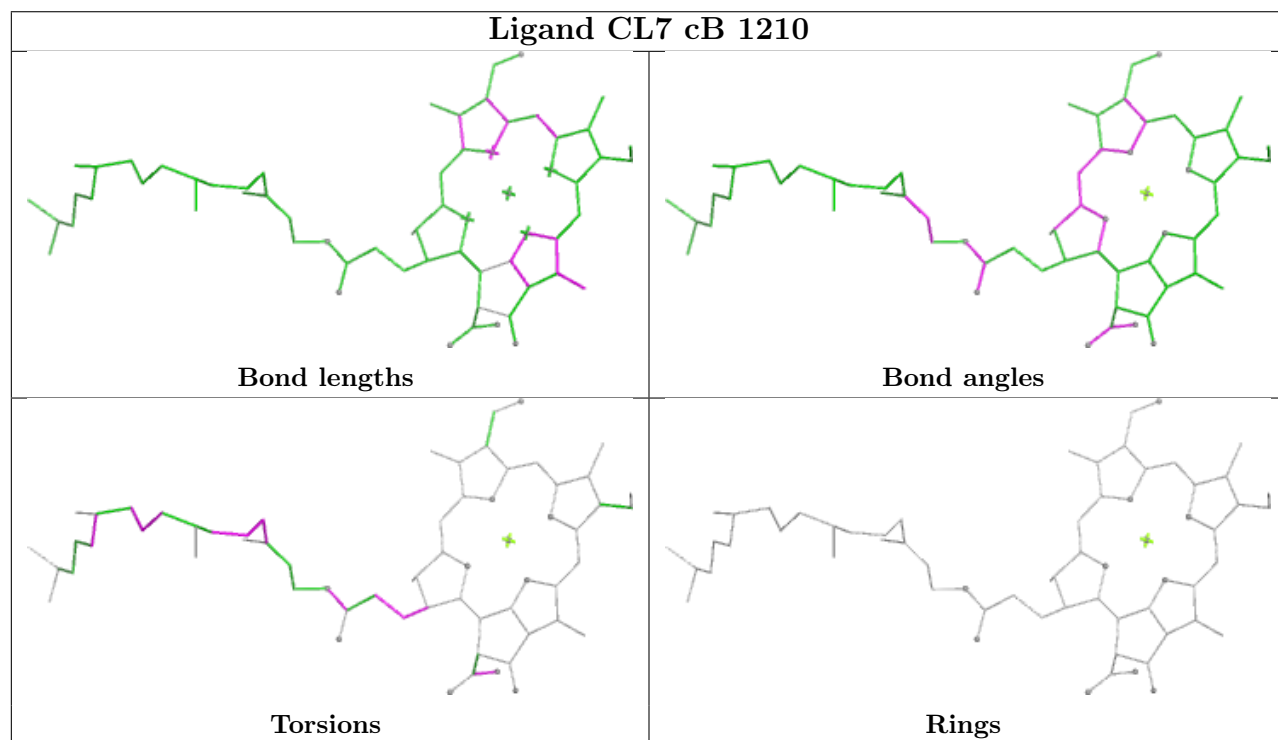
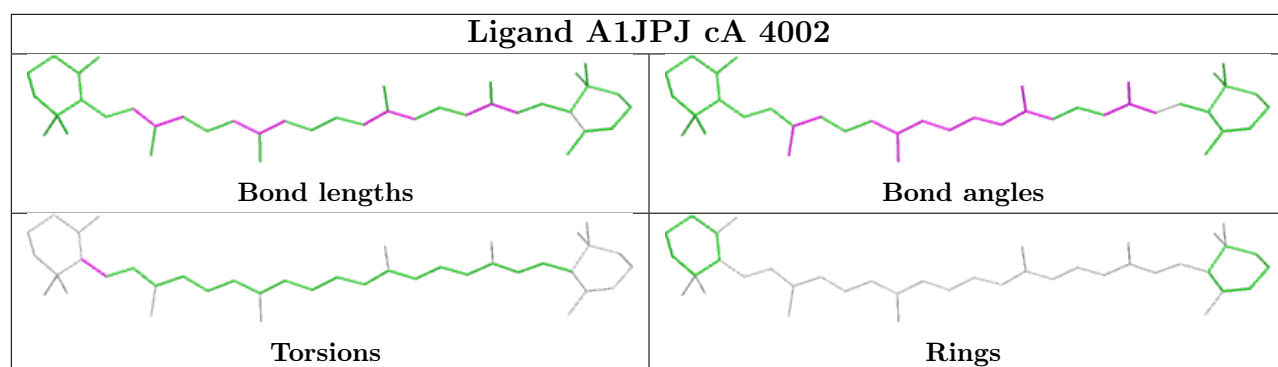


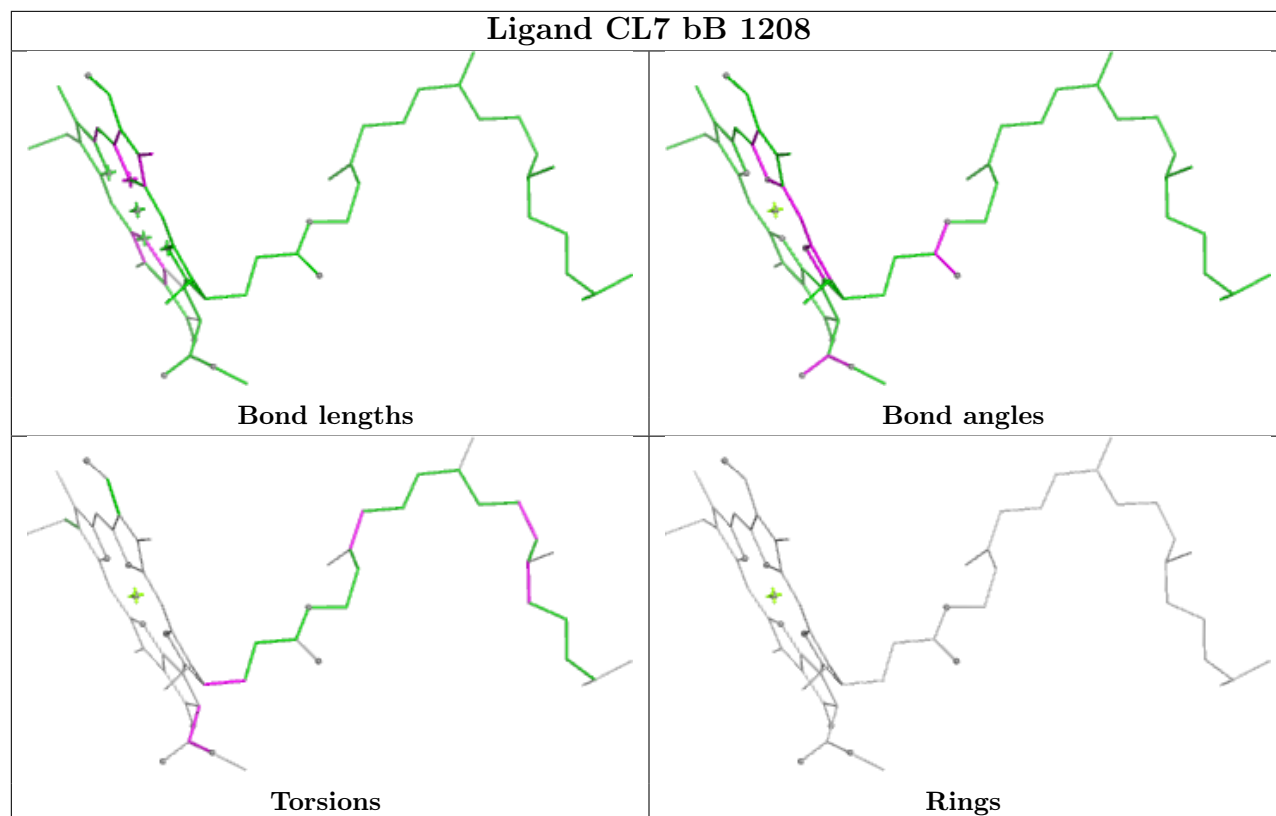


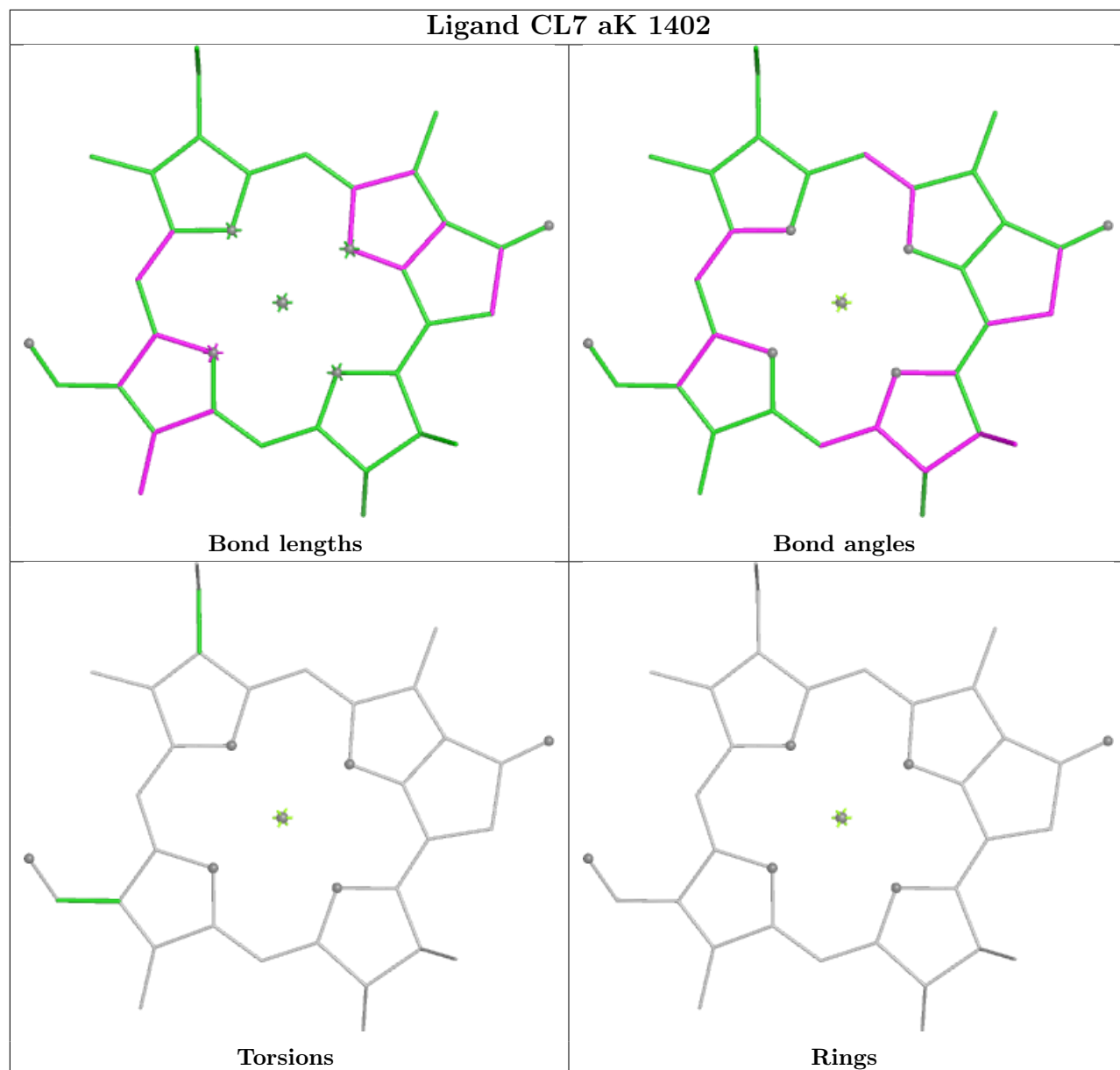


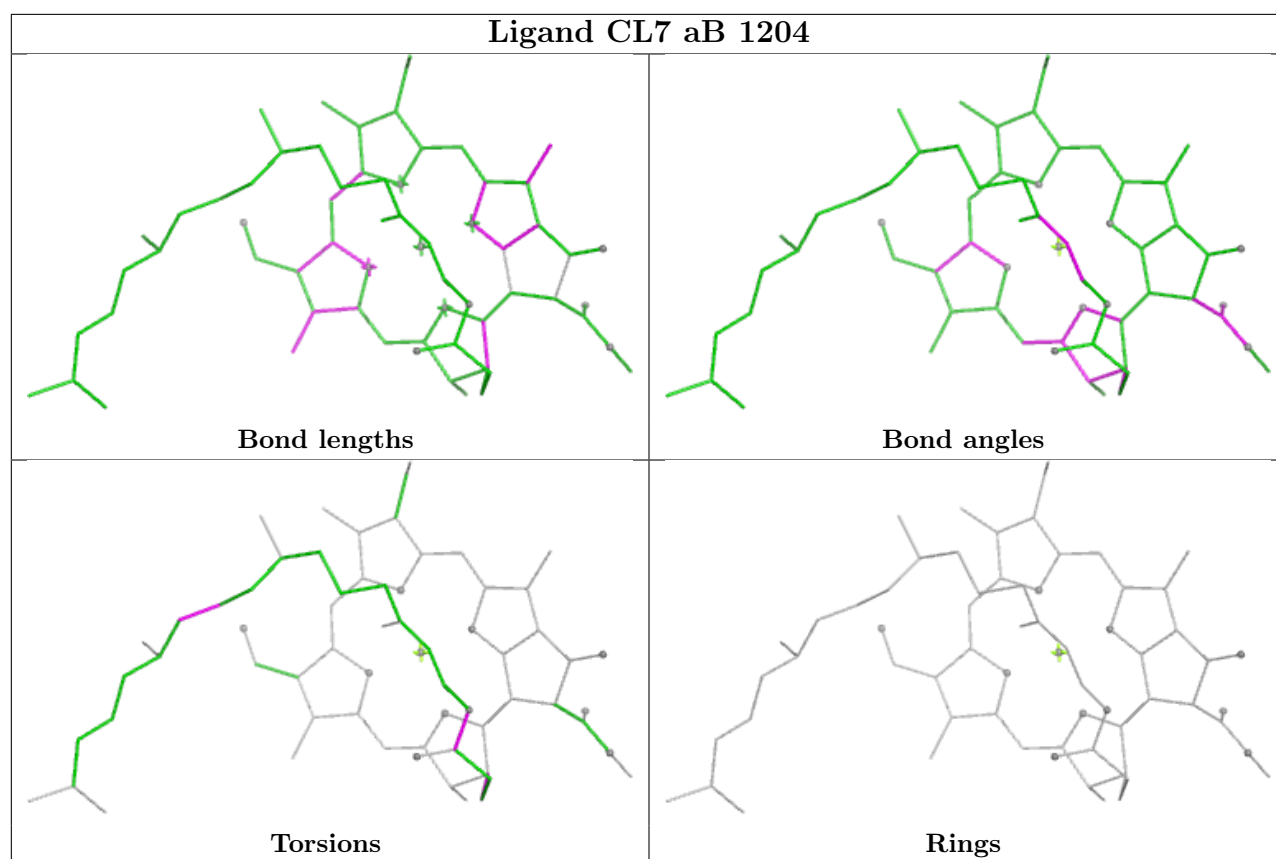




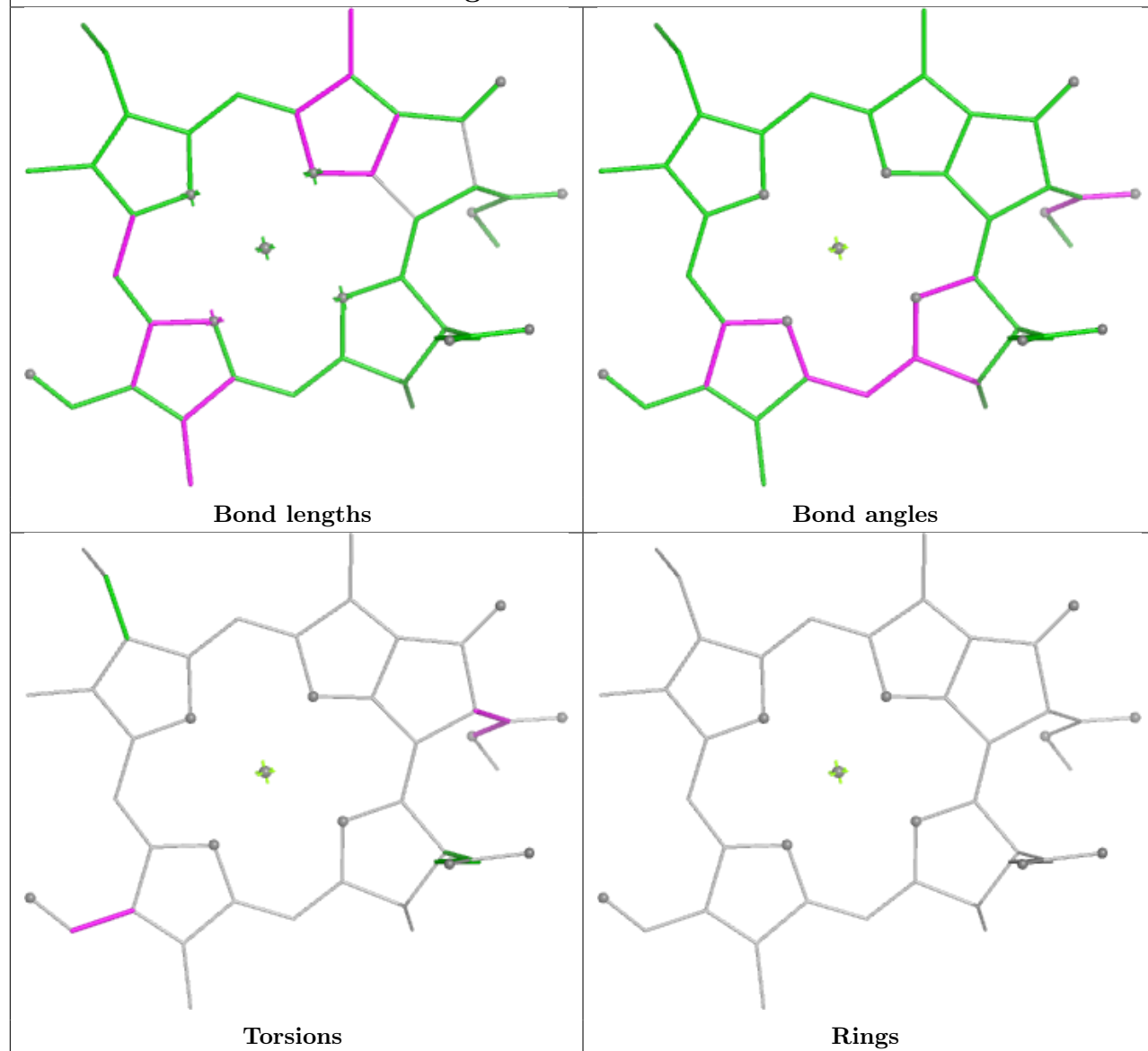


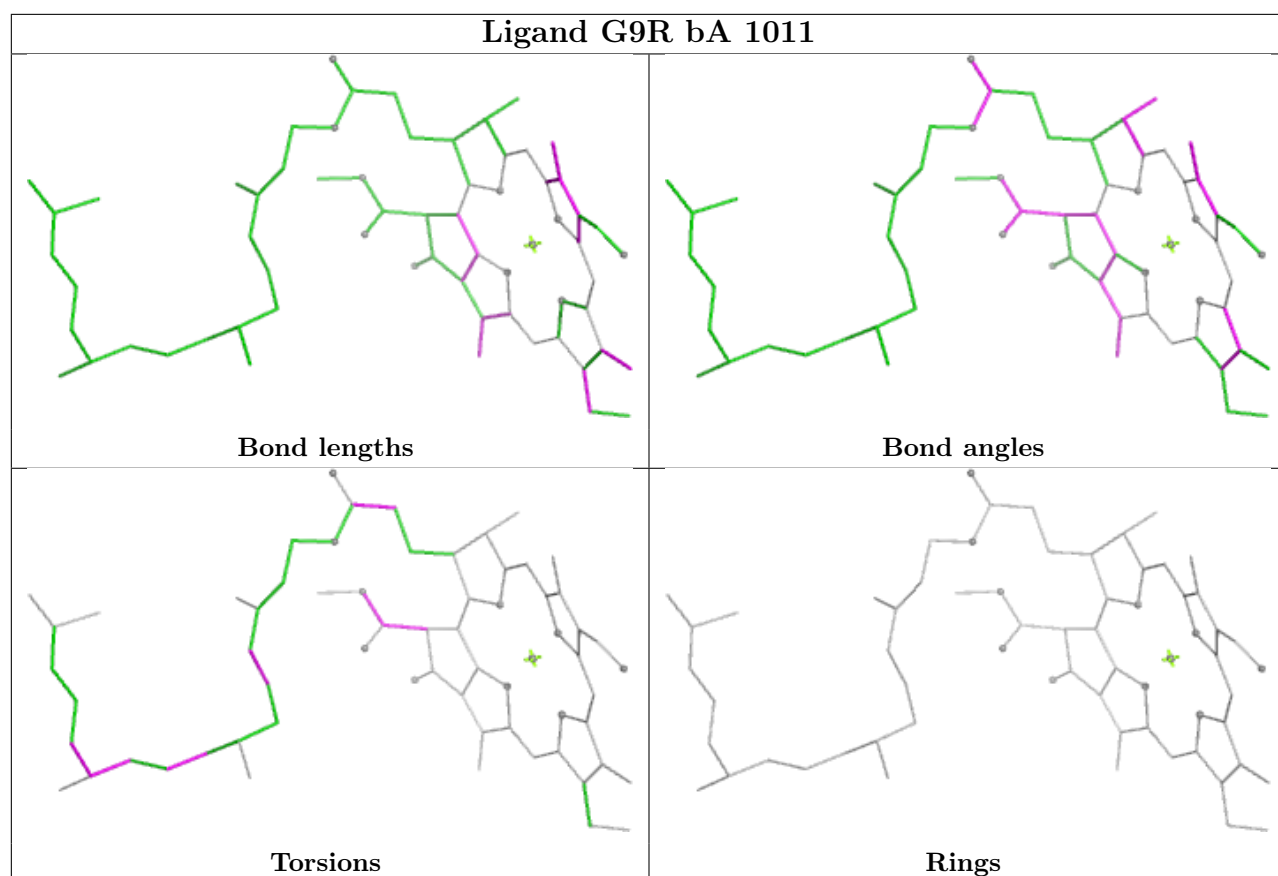


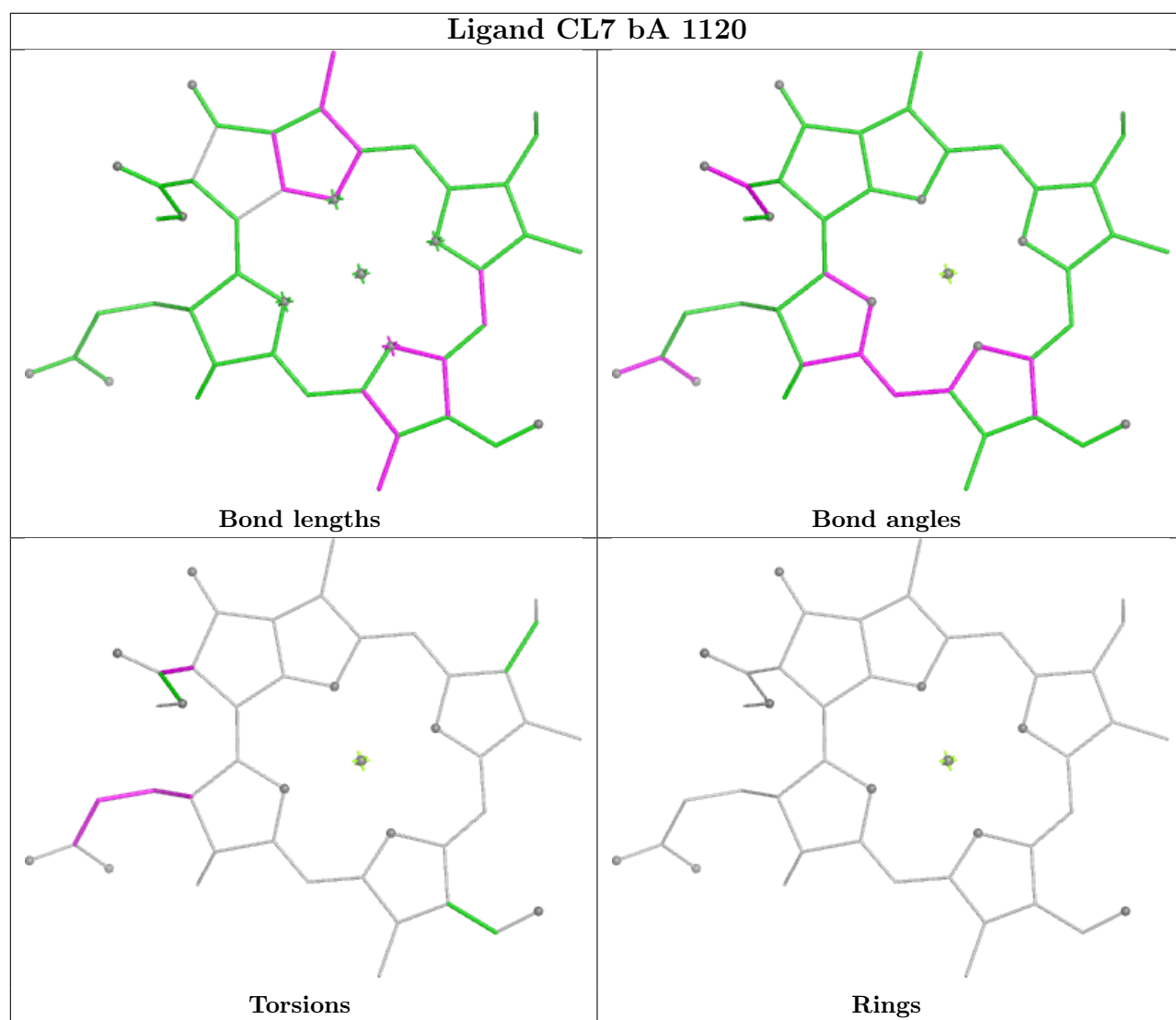


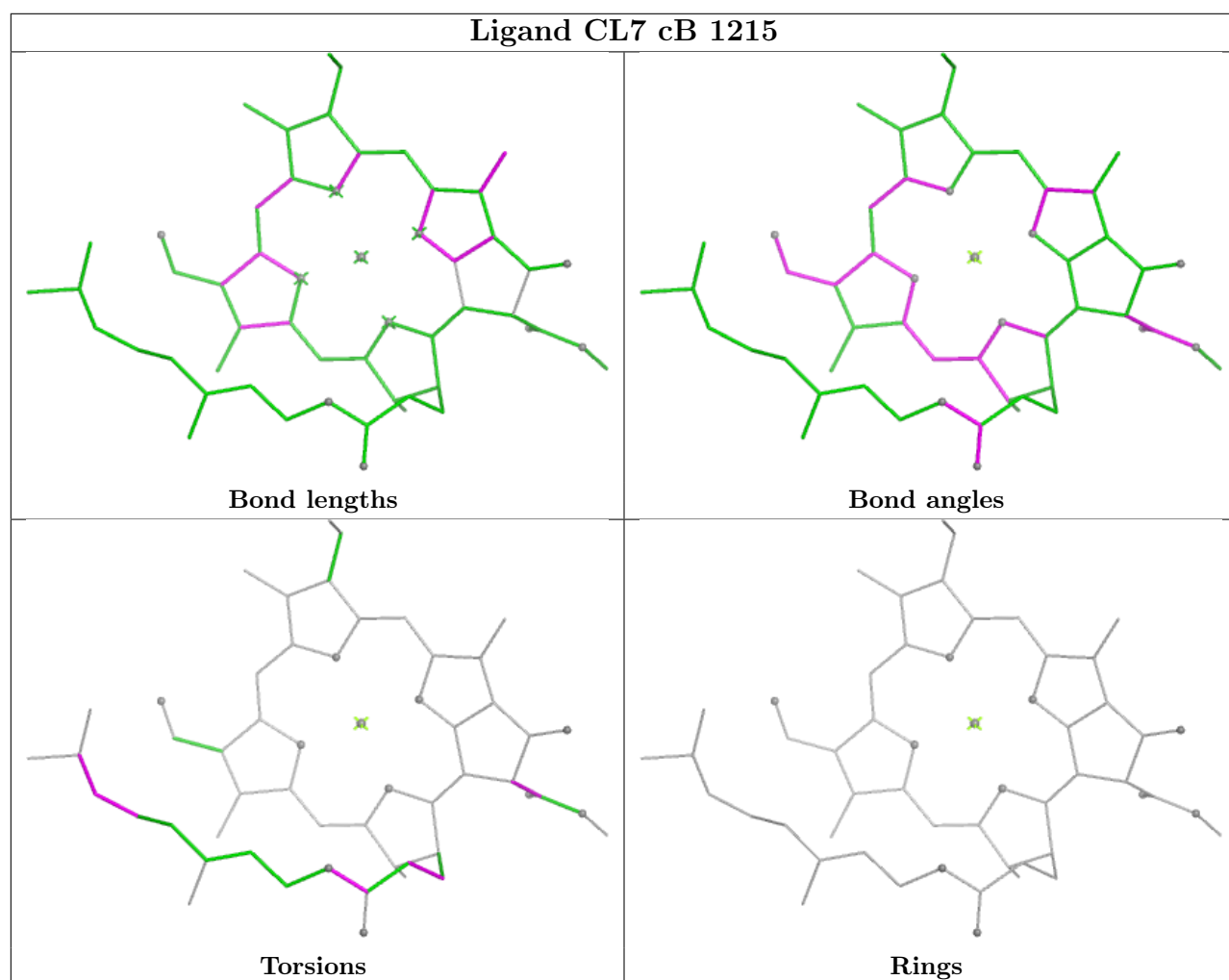
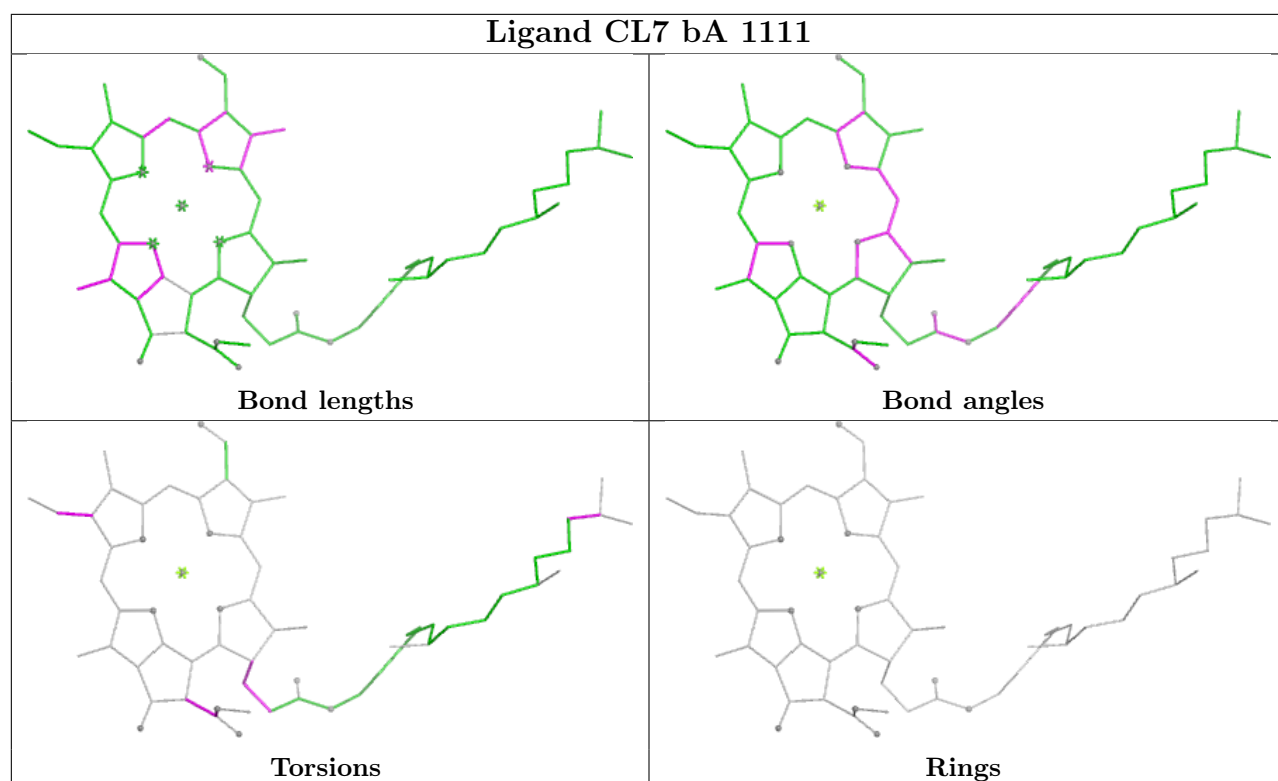


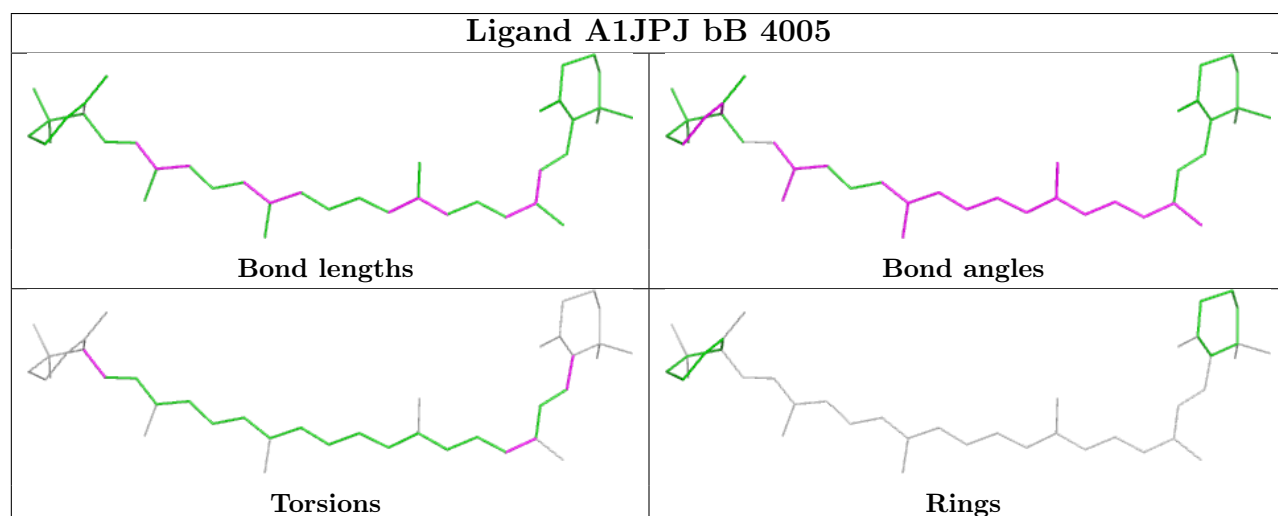
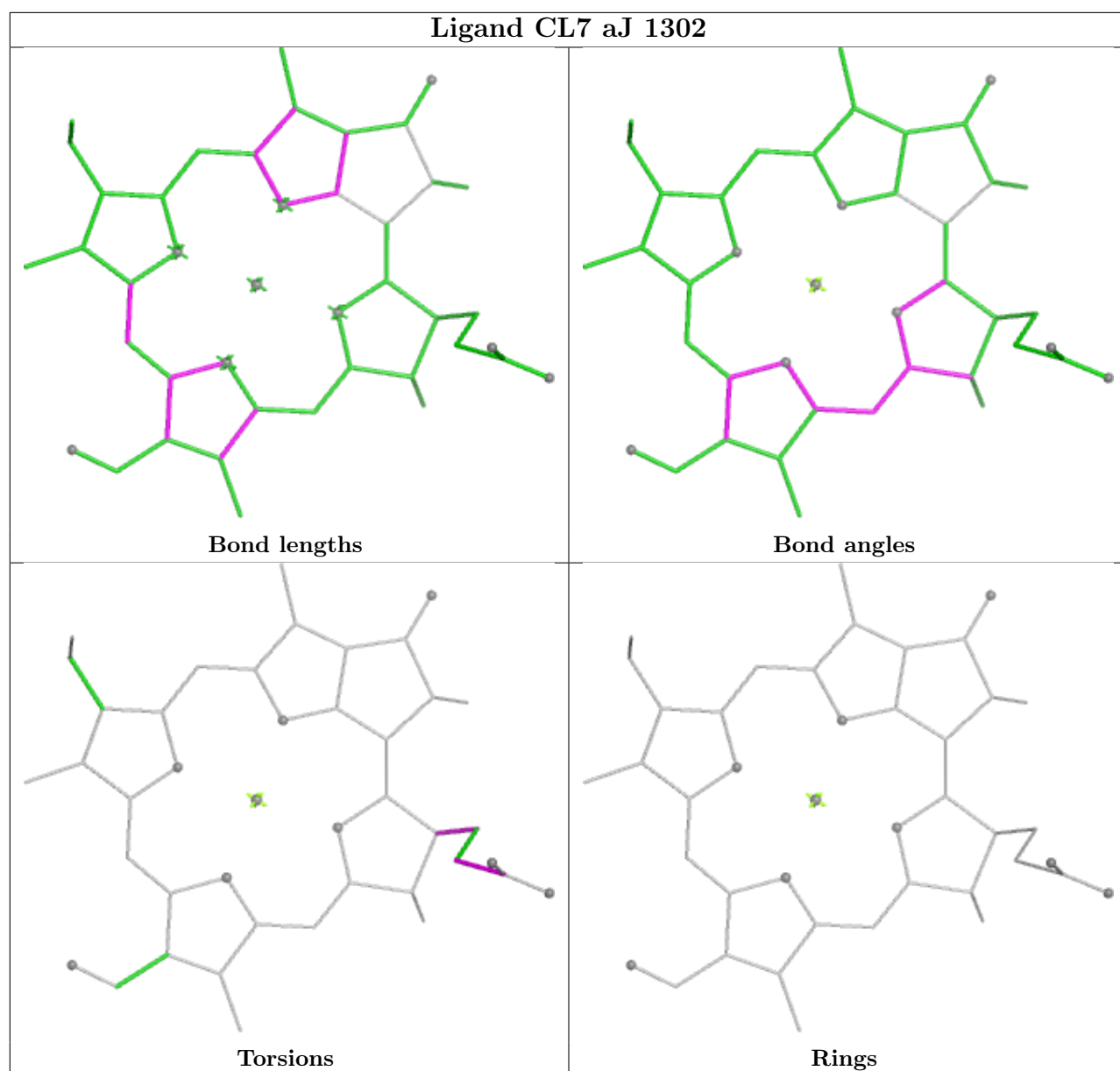
Ligand CL7 bA 1105

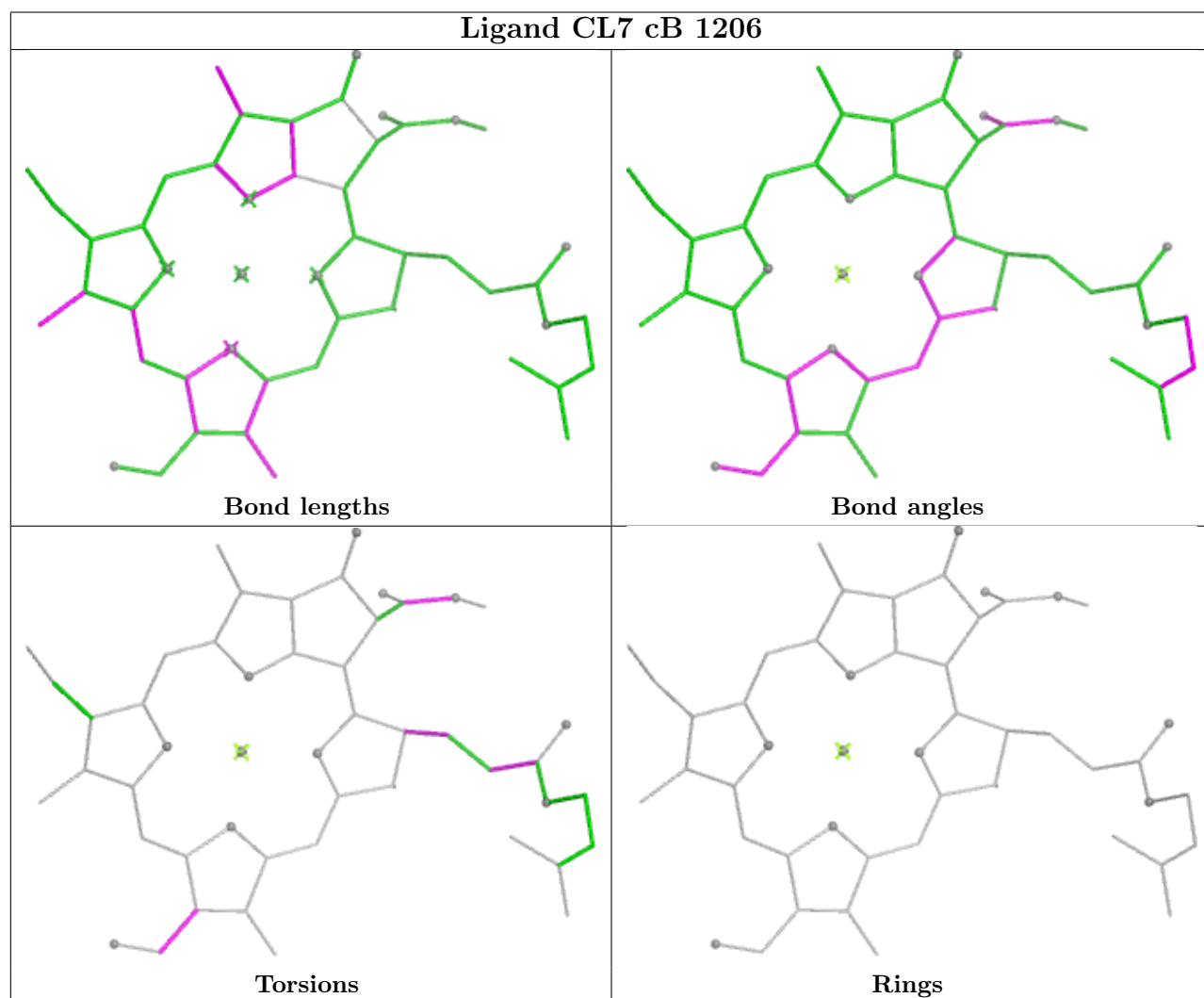
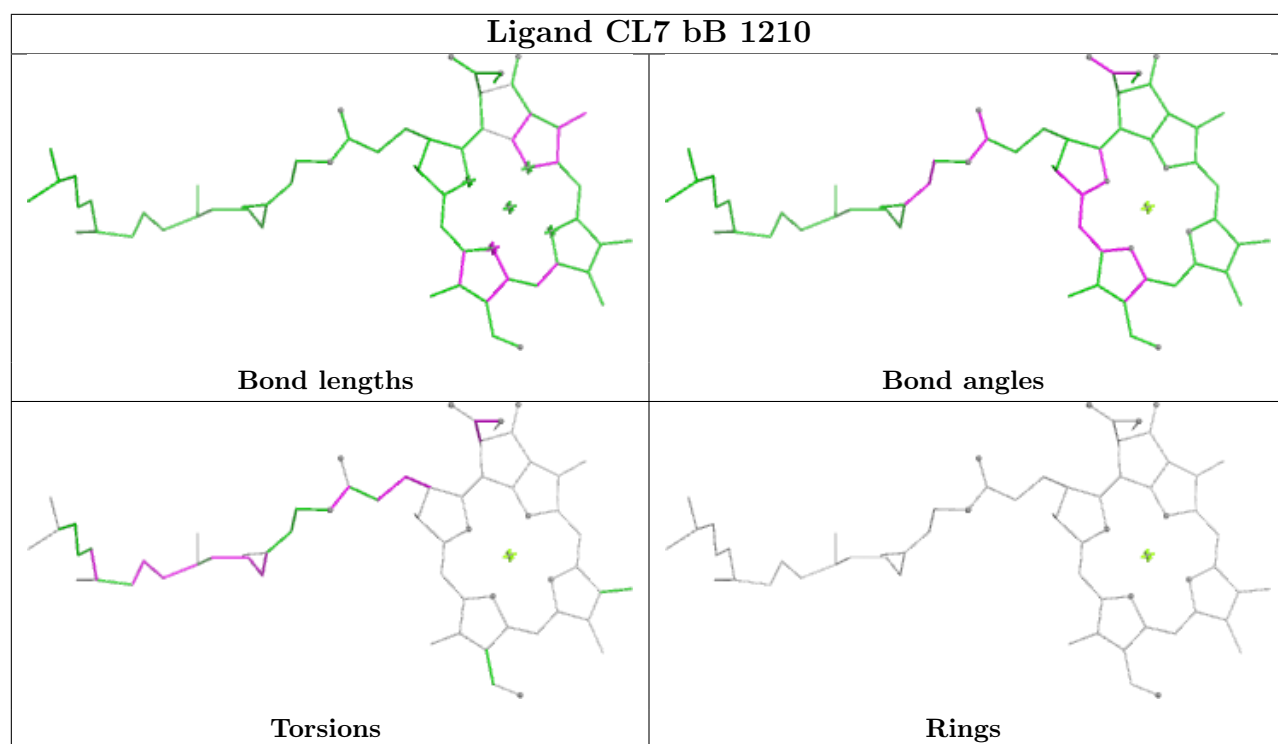


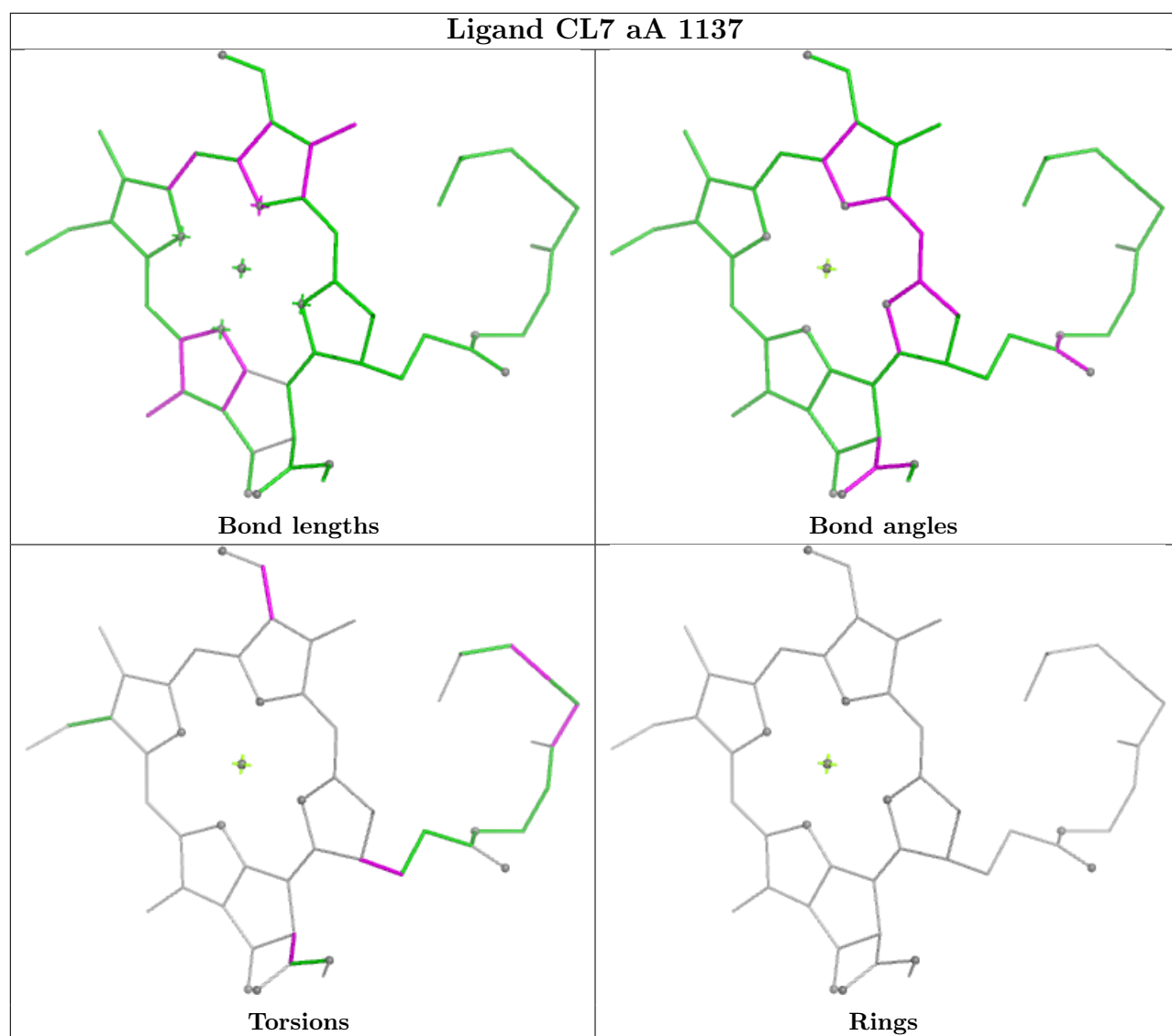


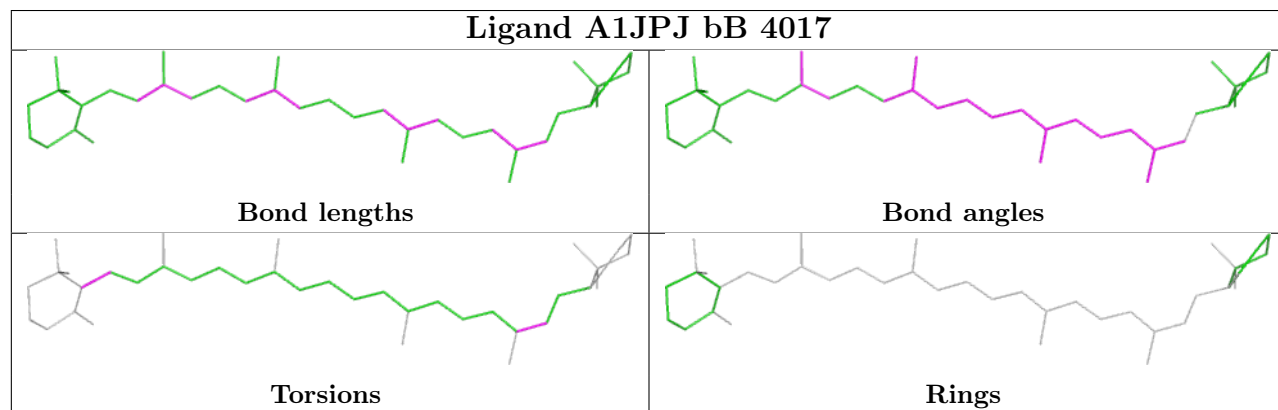
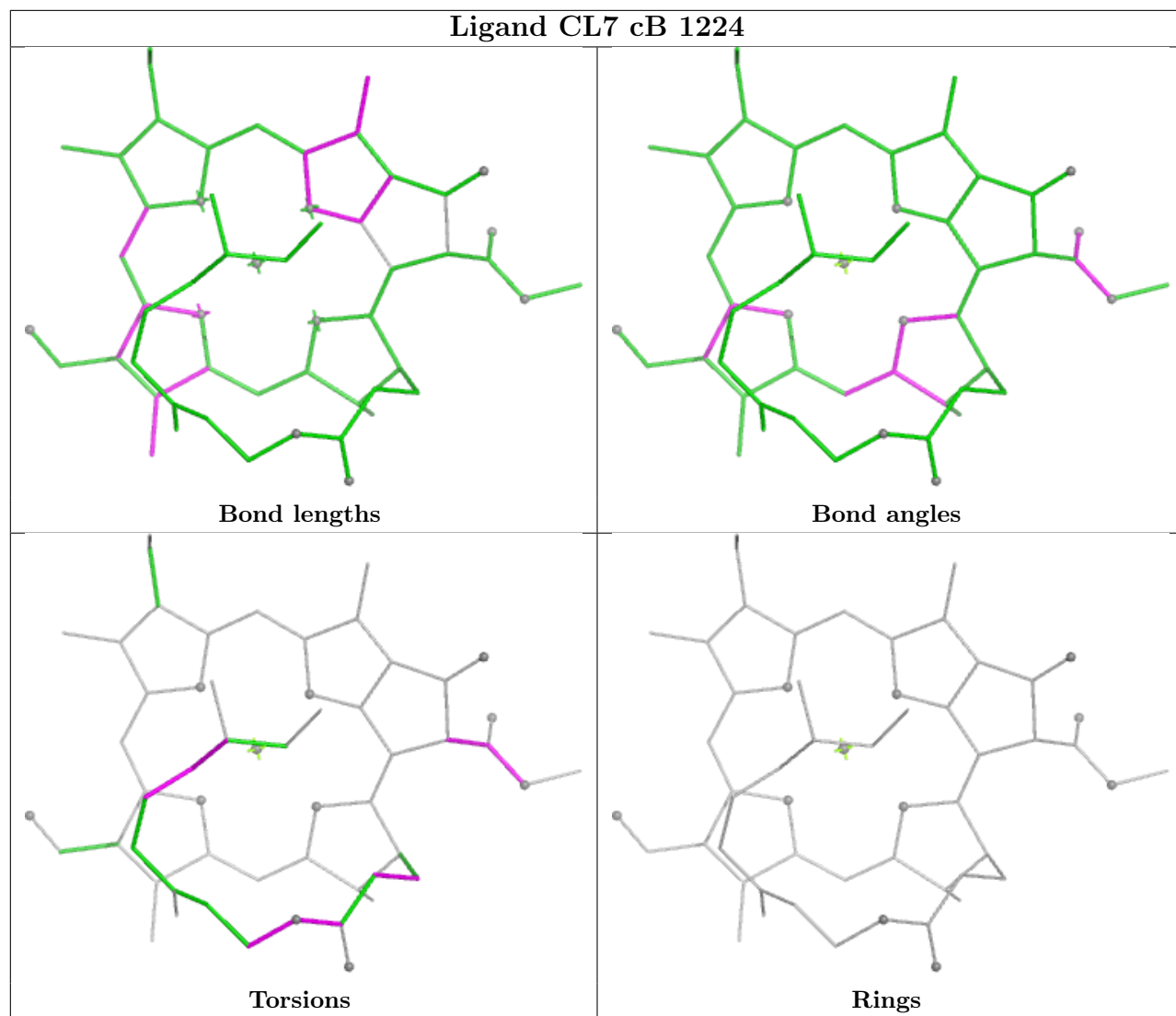


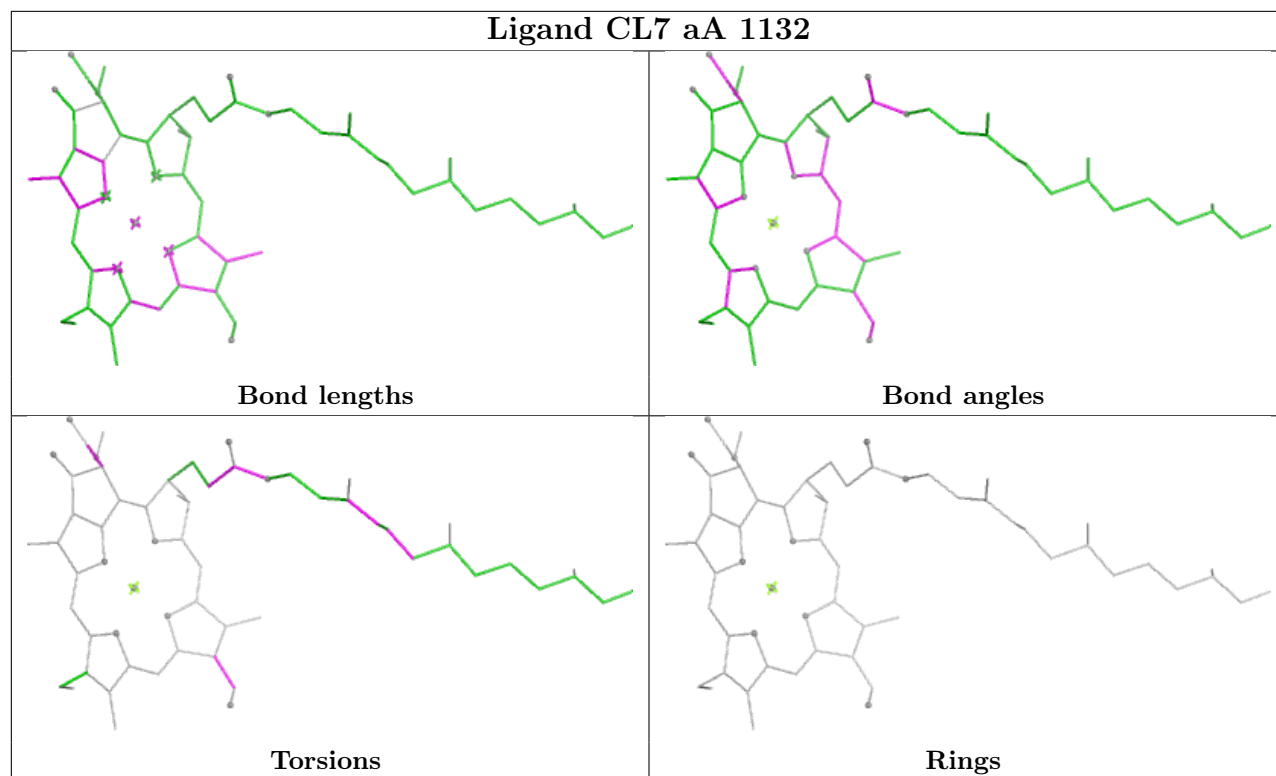


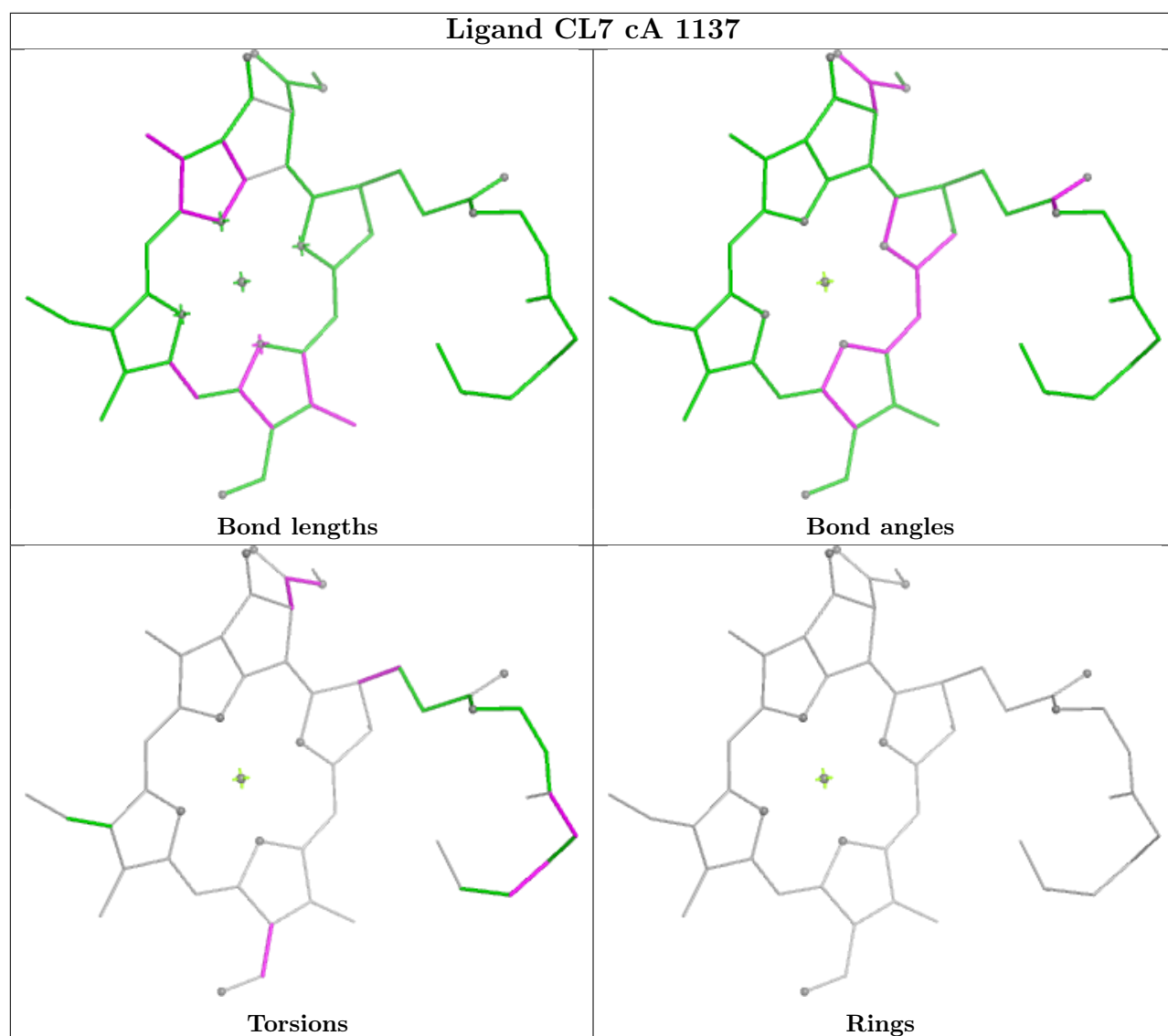


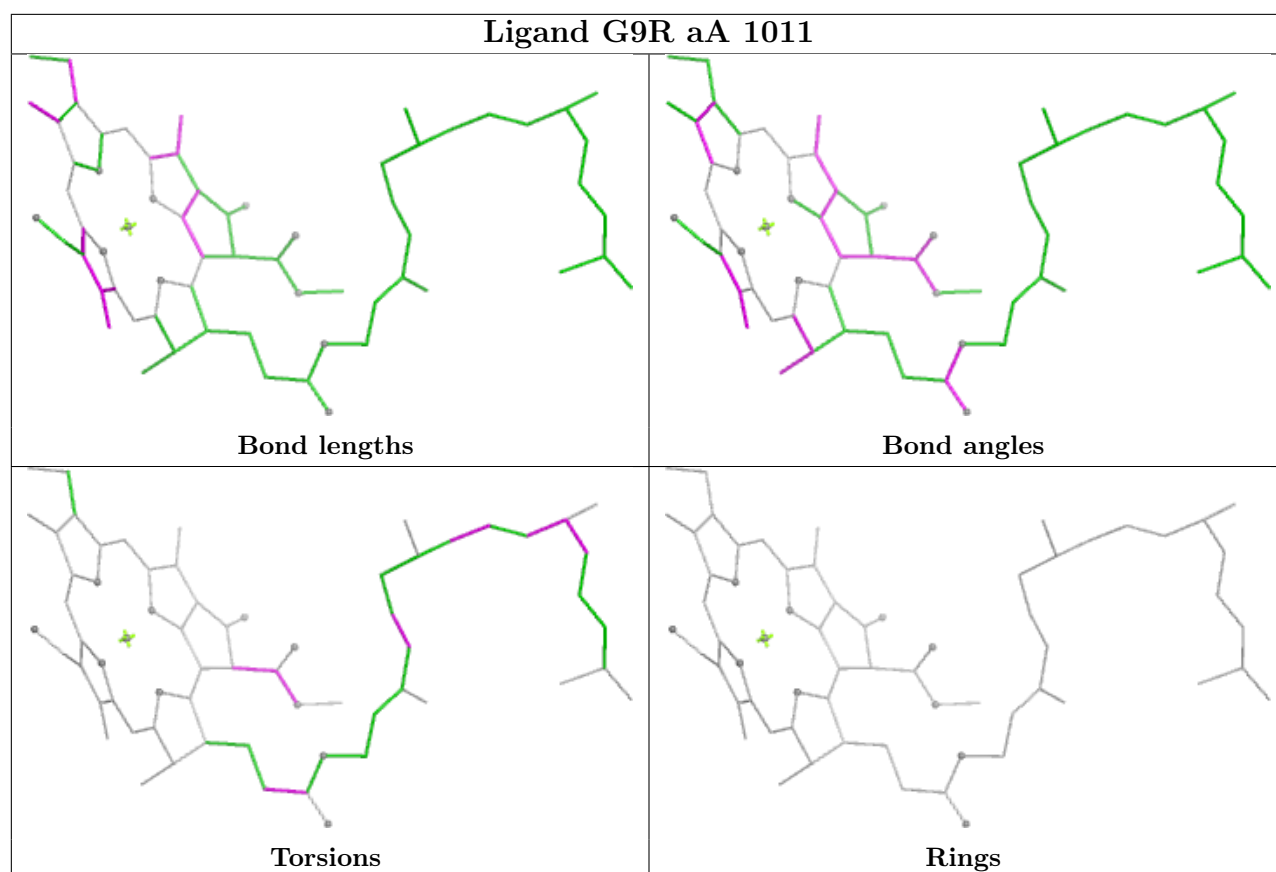


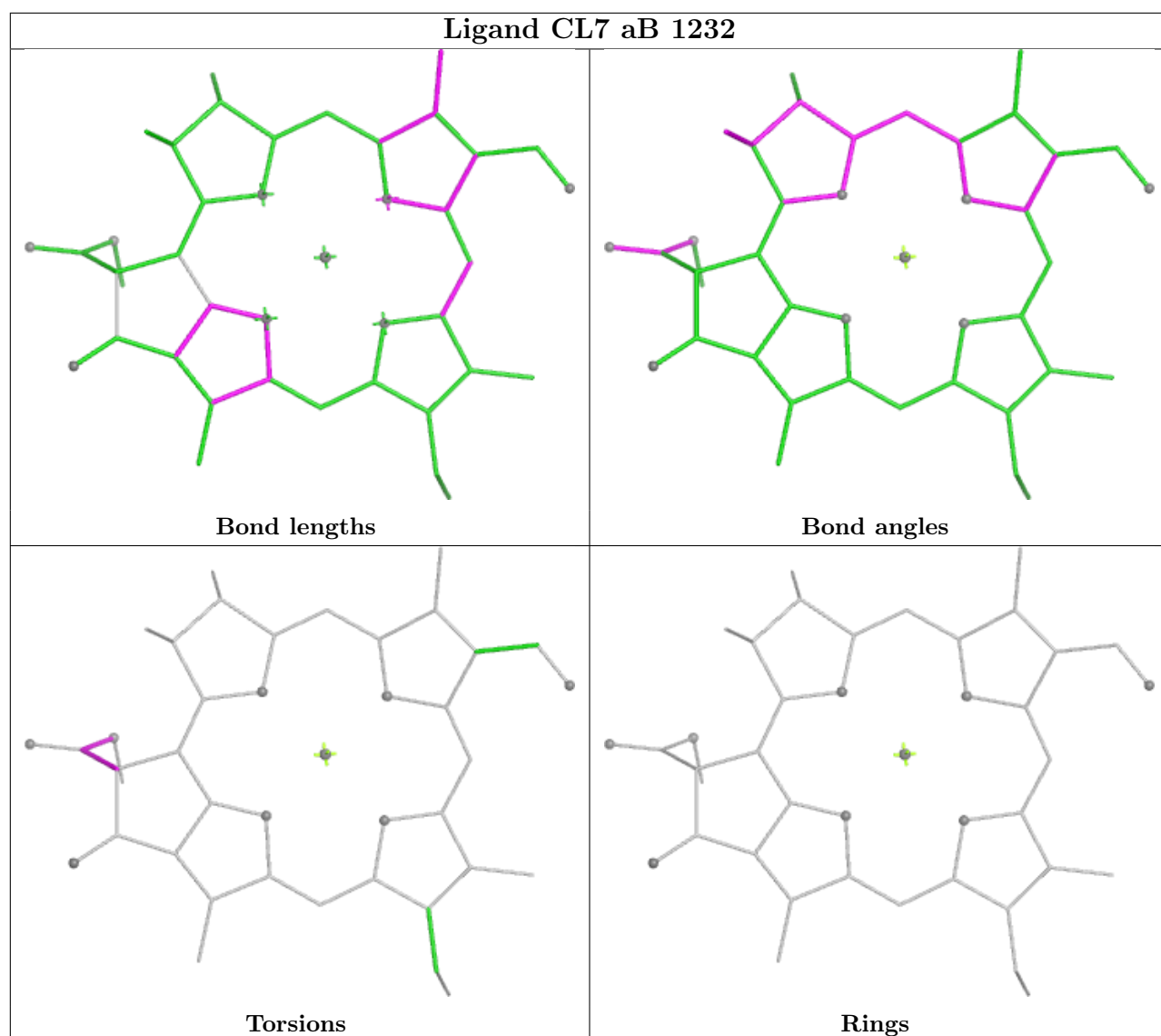




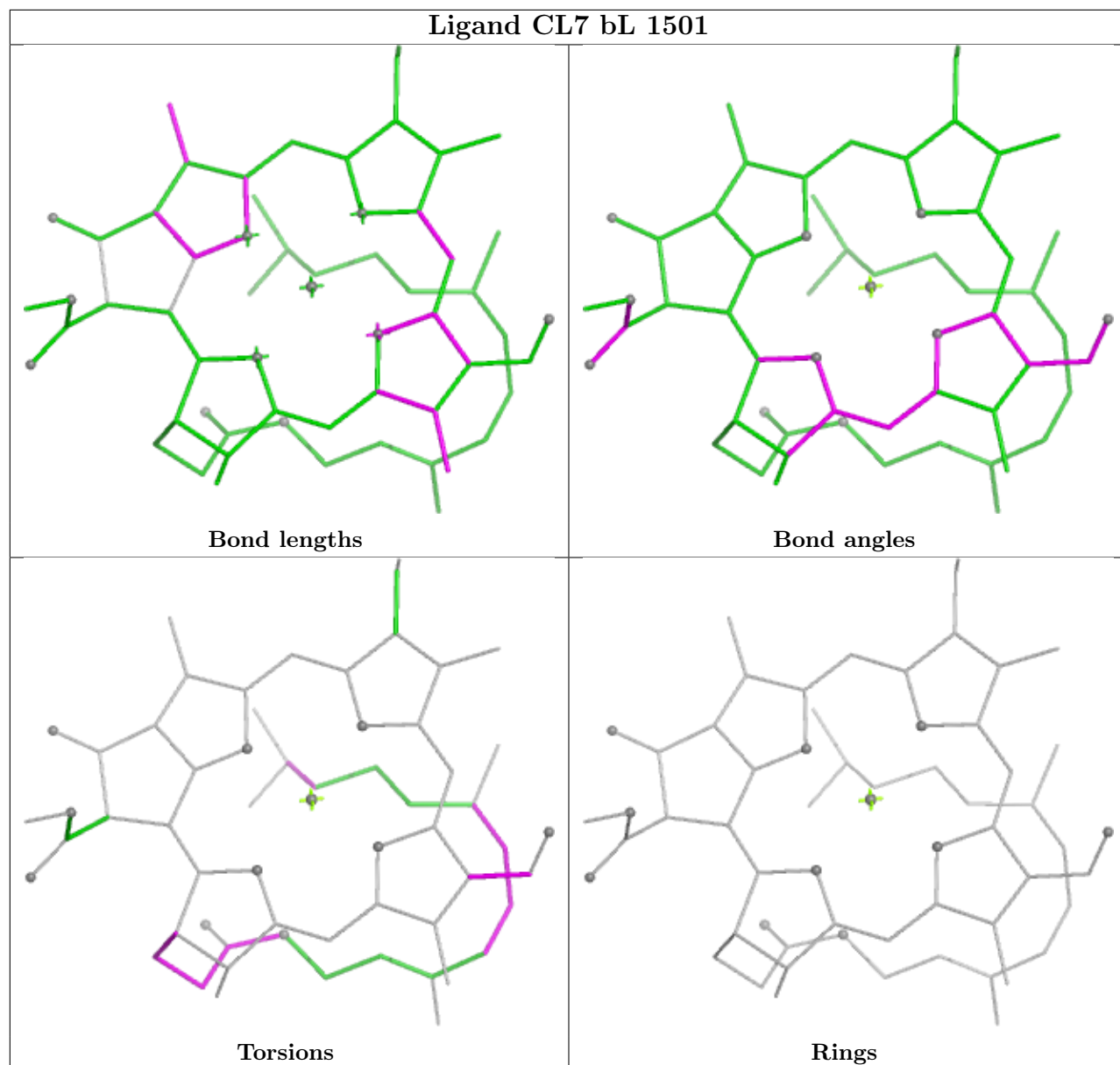


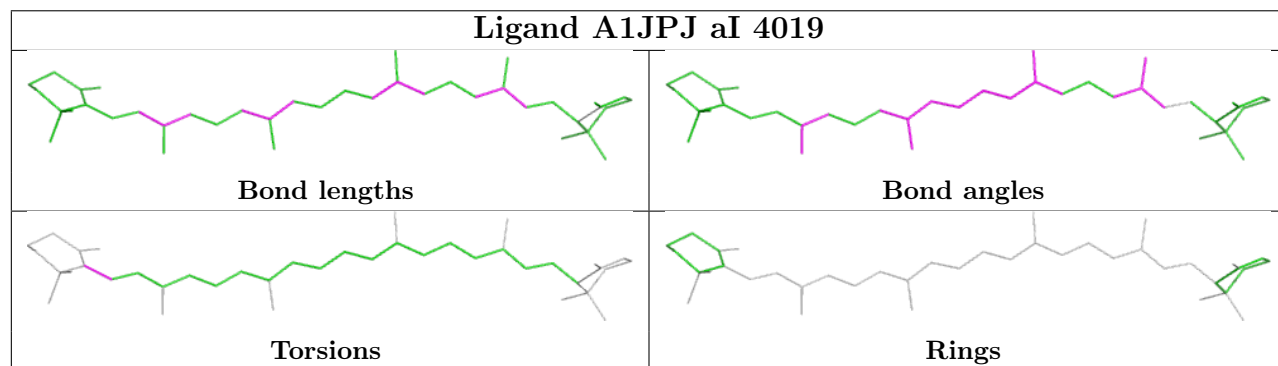
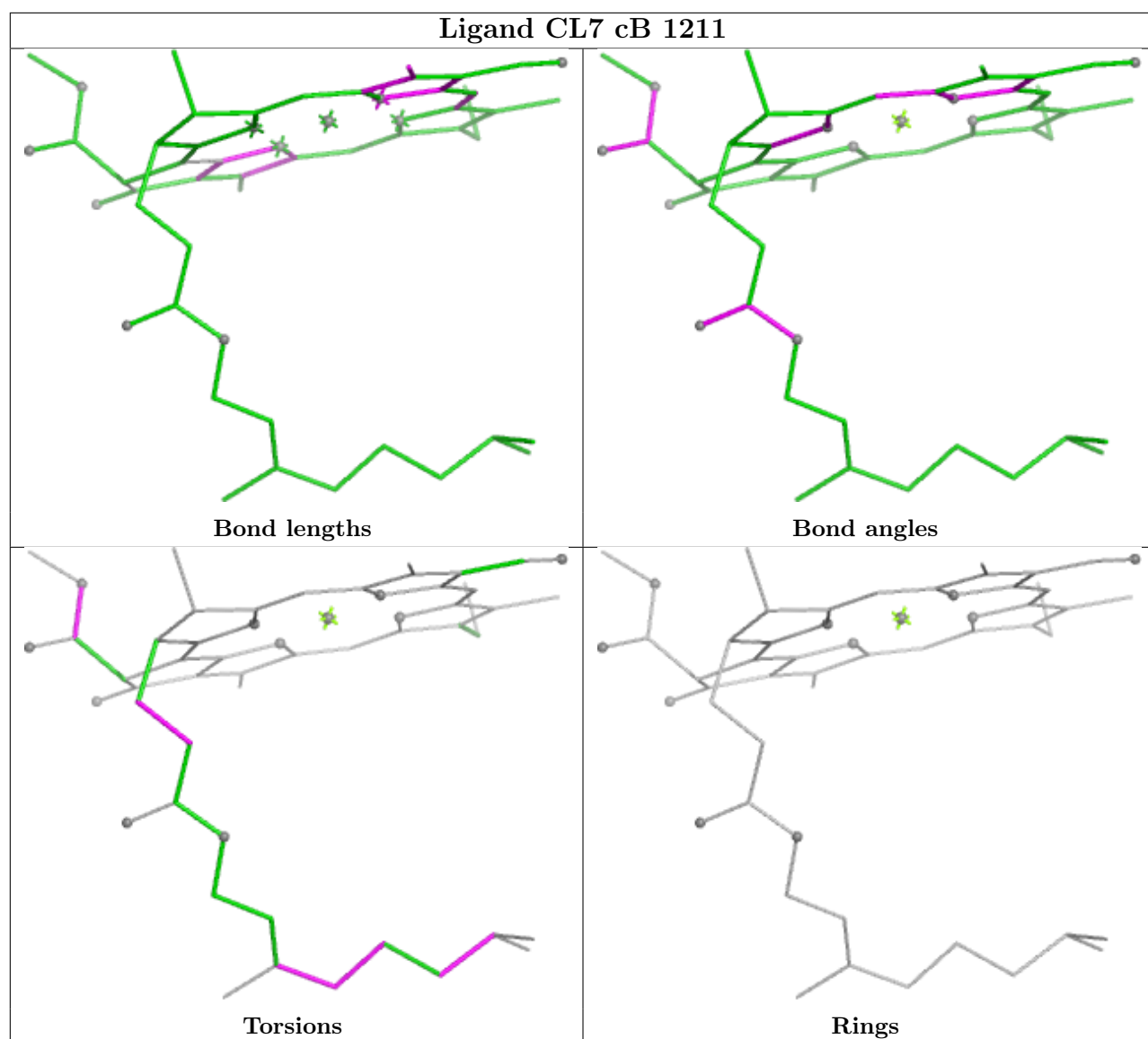


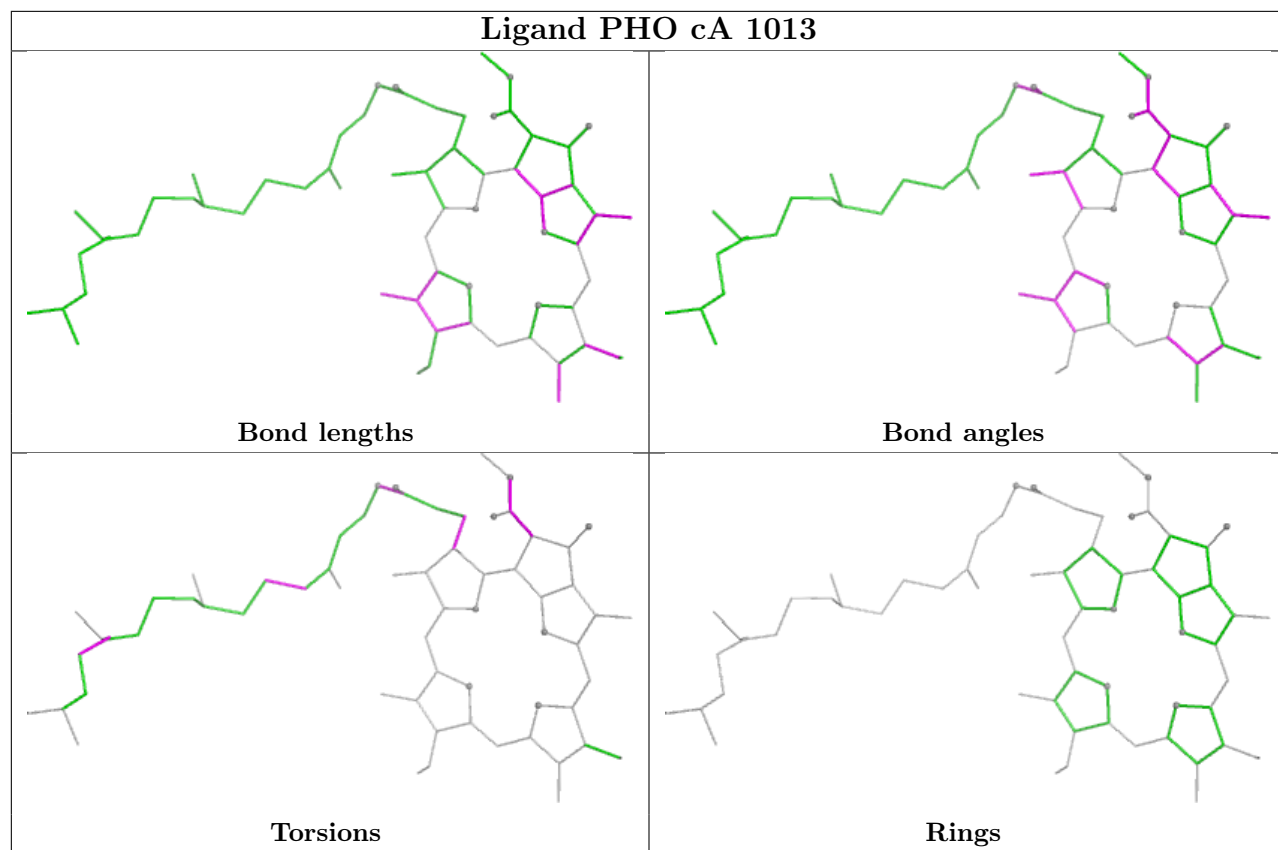


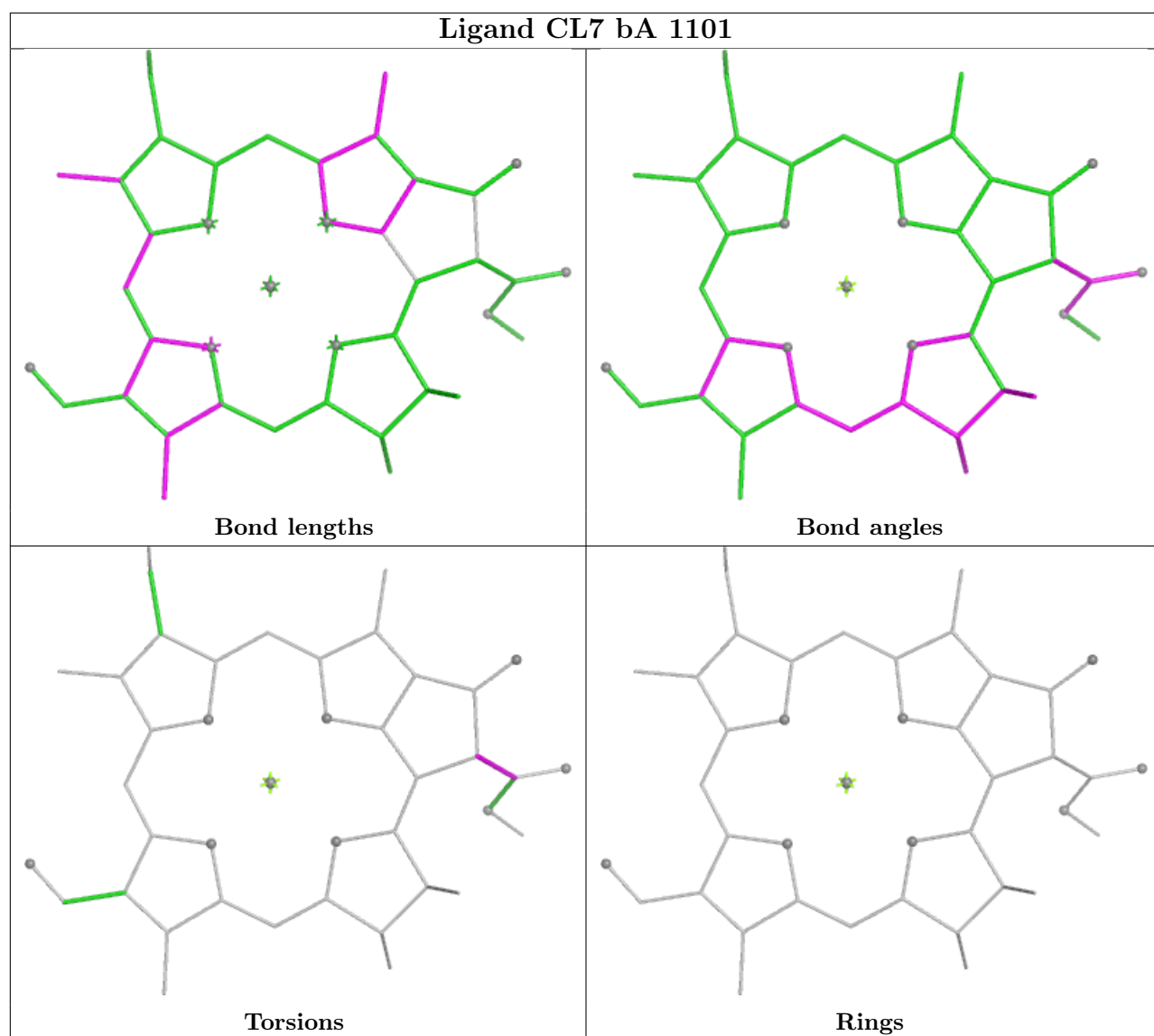


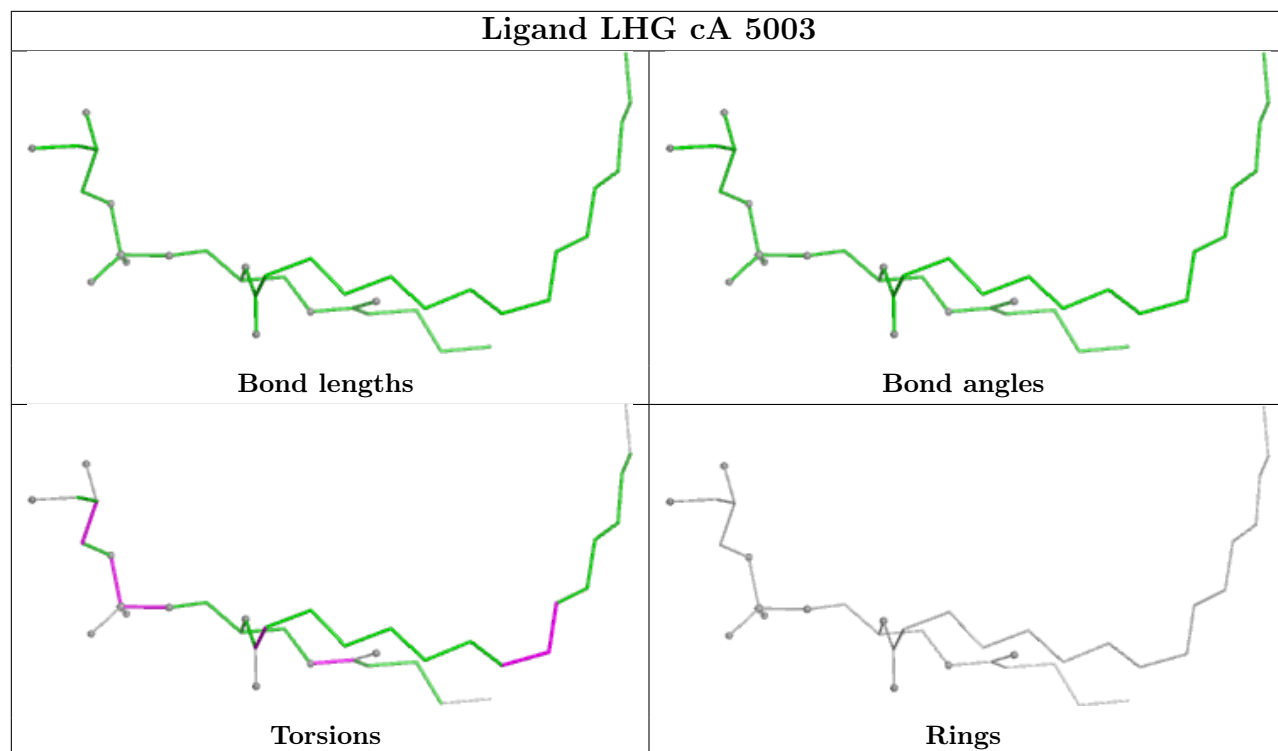
Ligand CL7 bL 1501

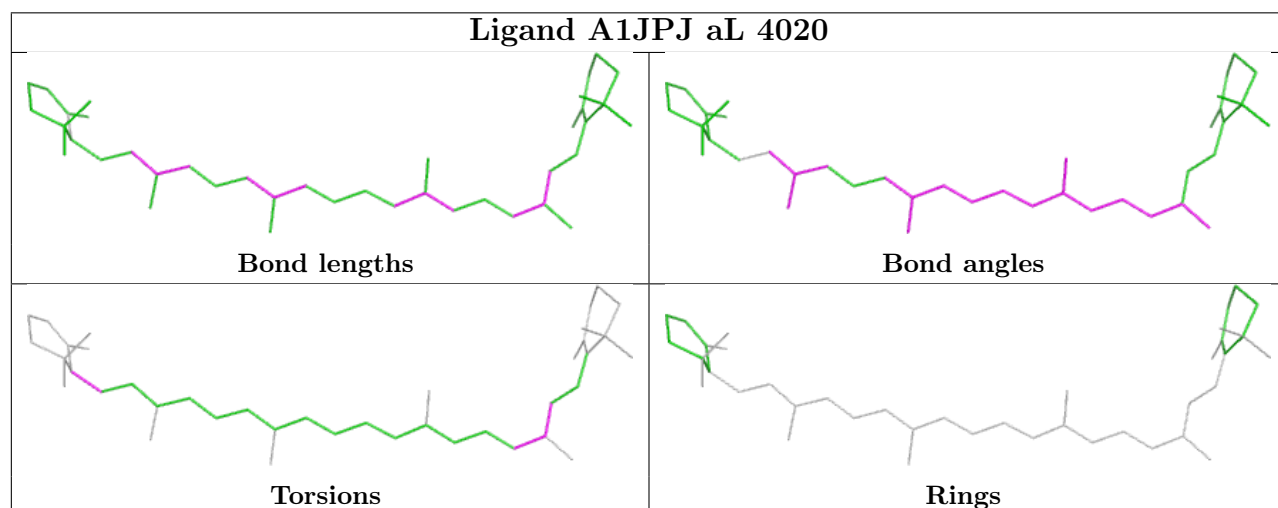
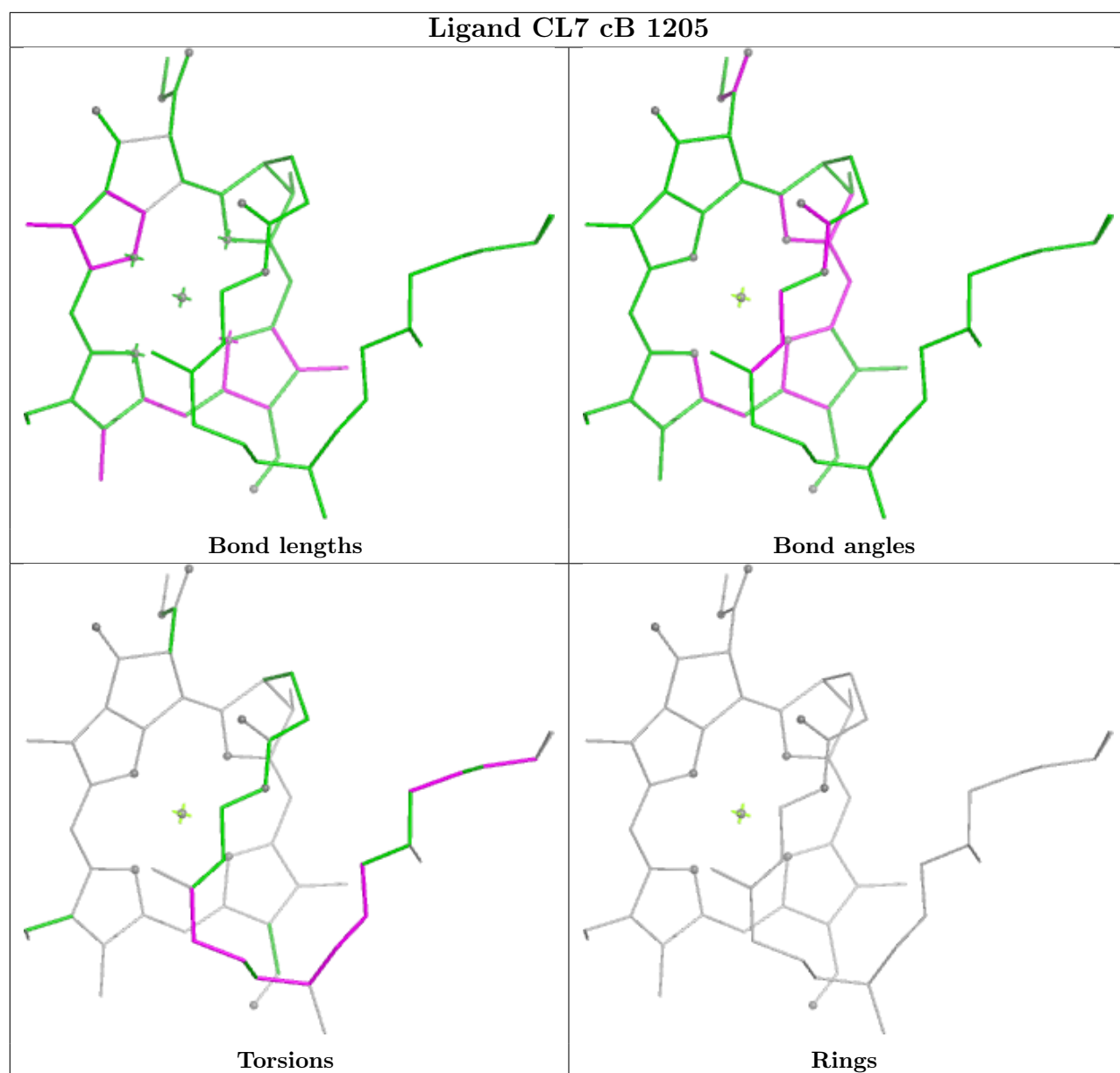


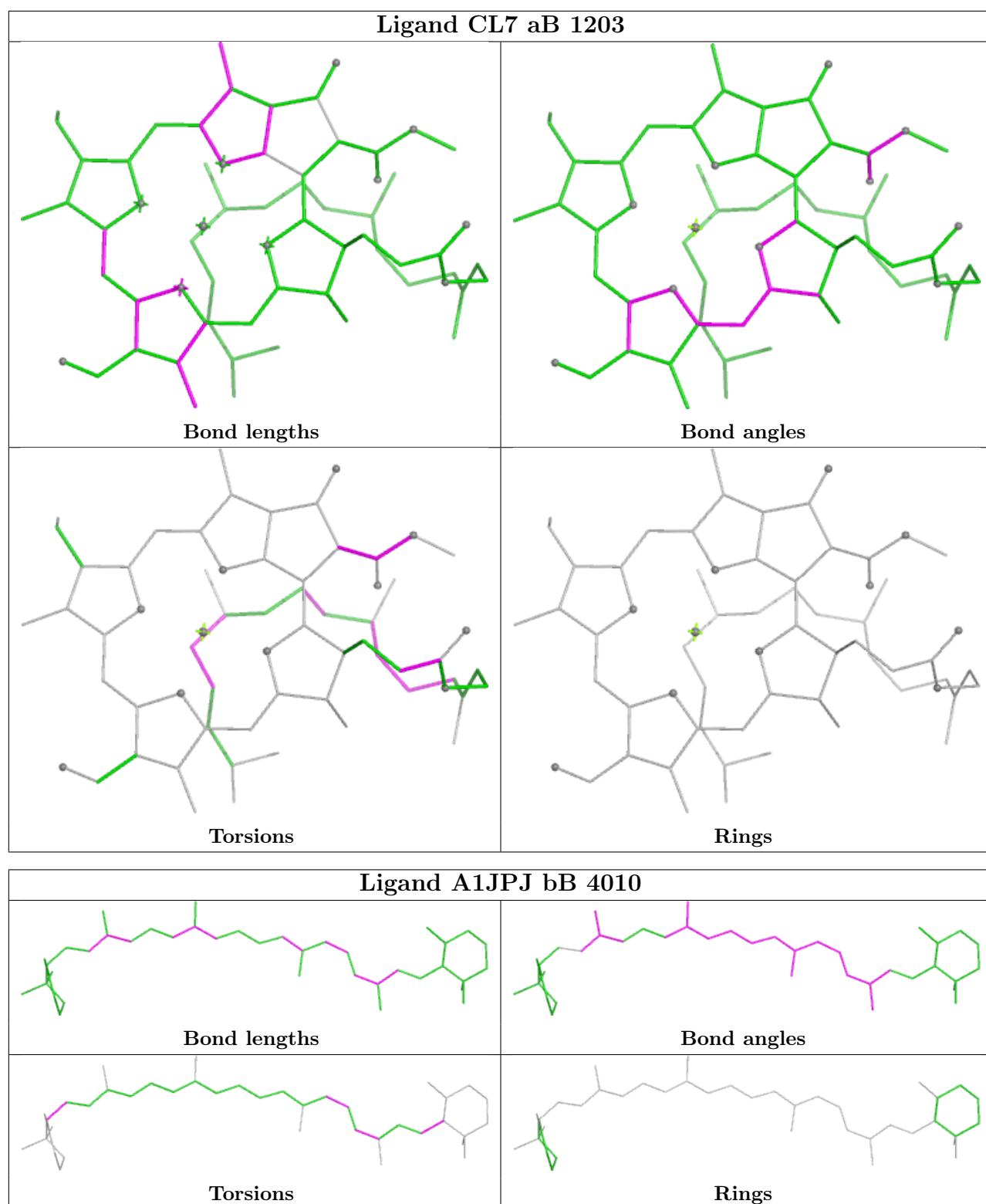


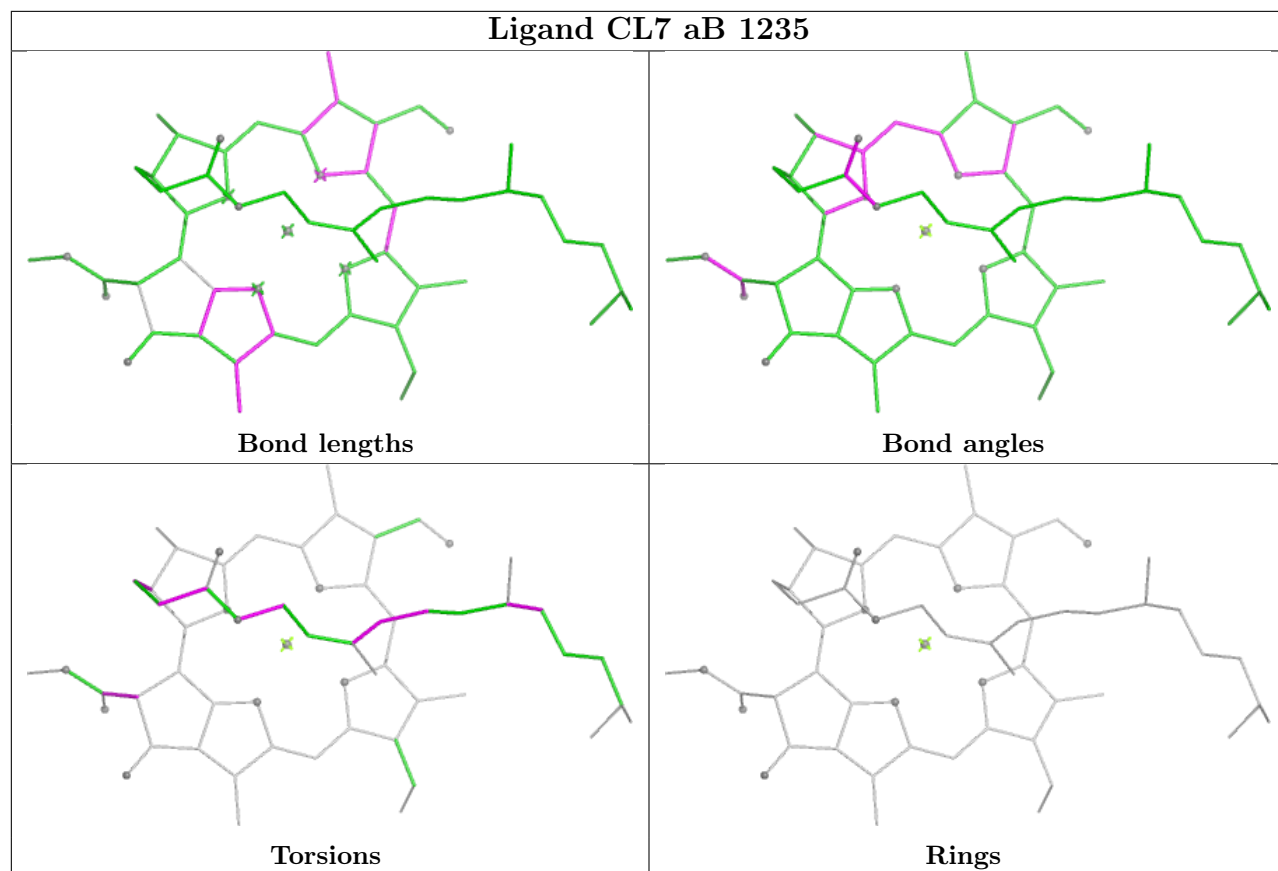


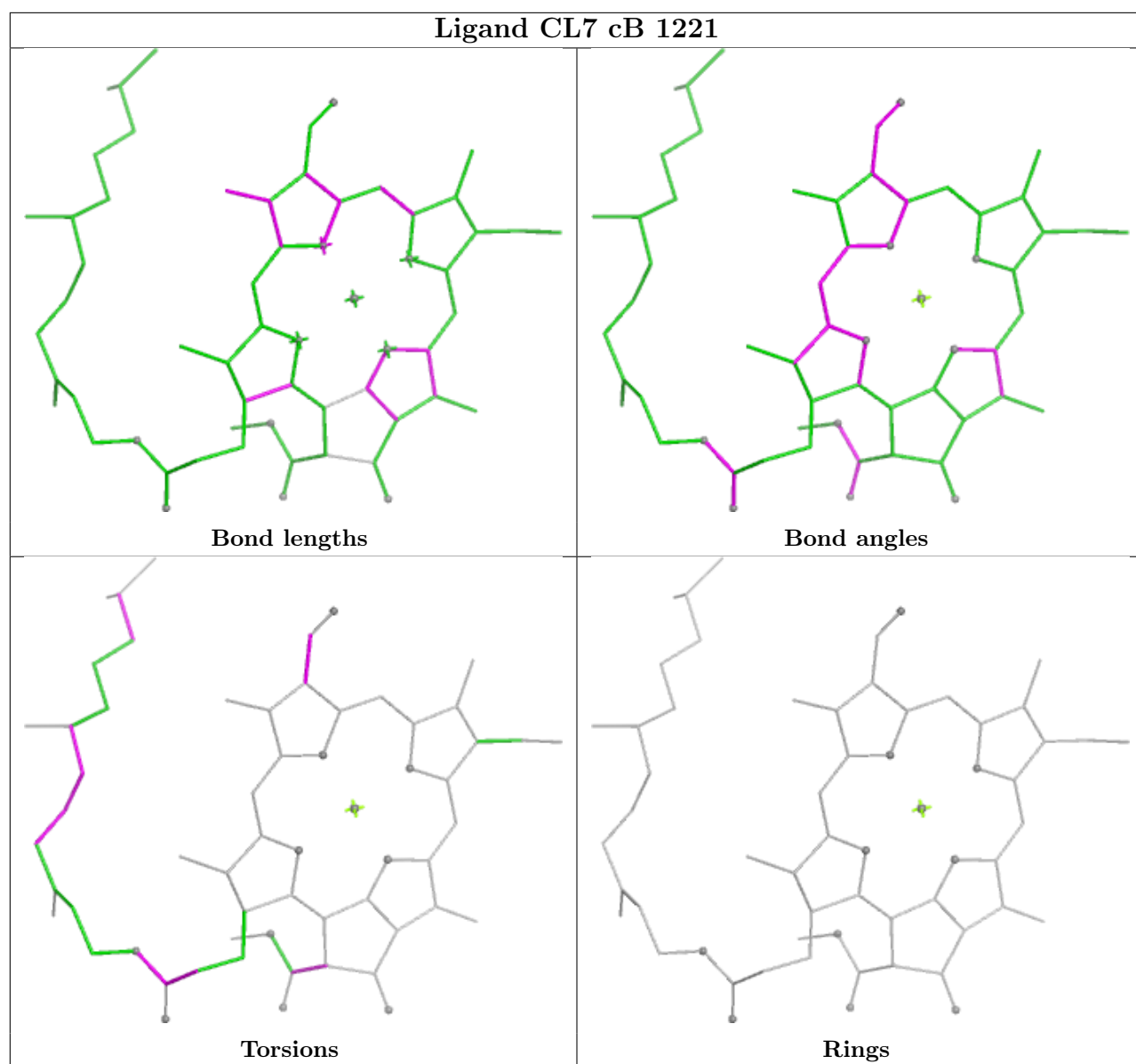


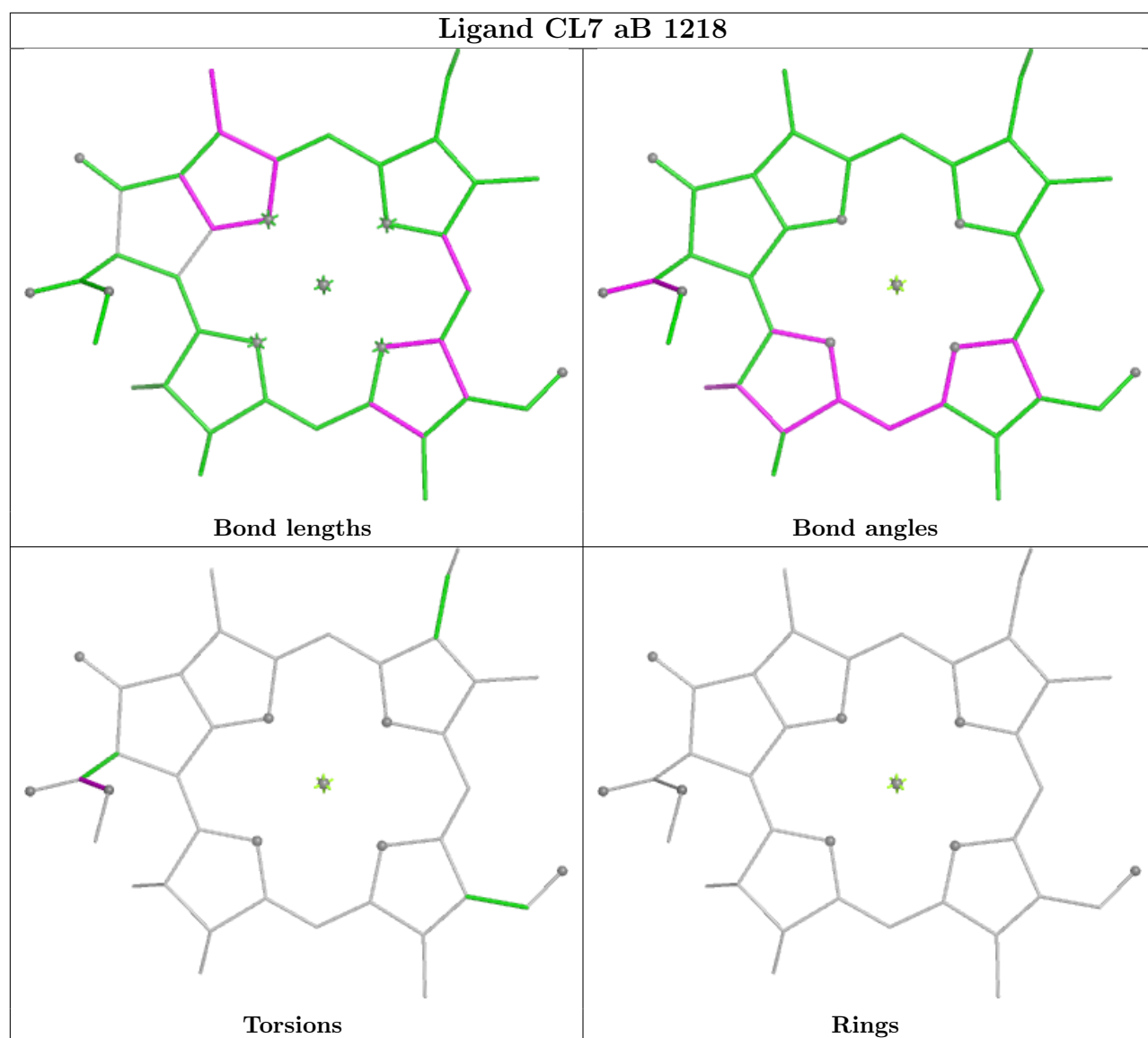


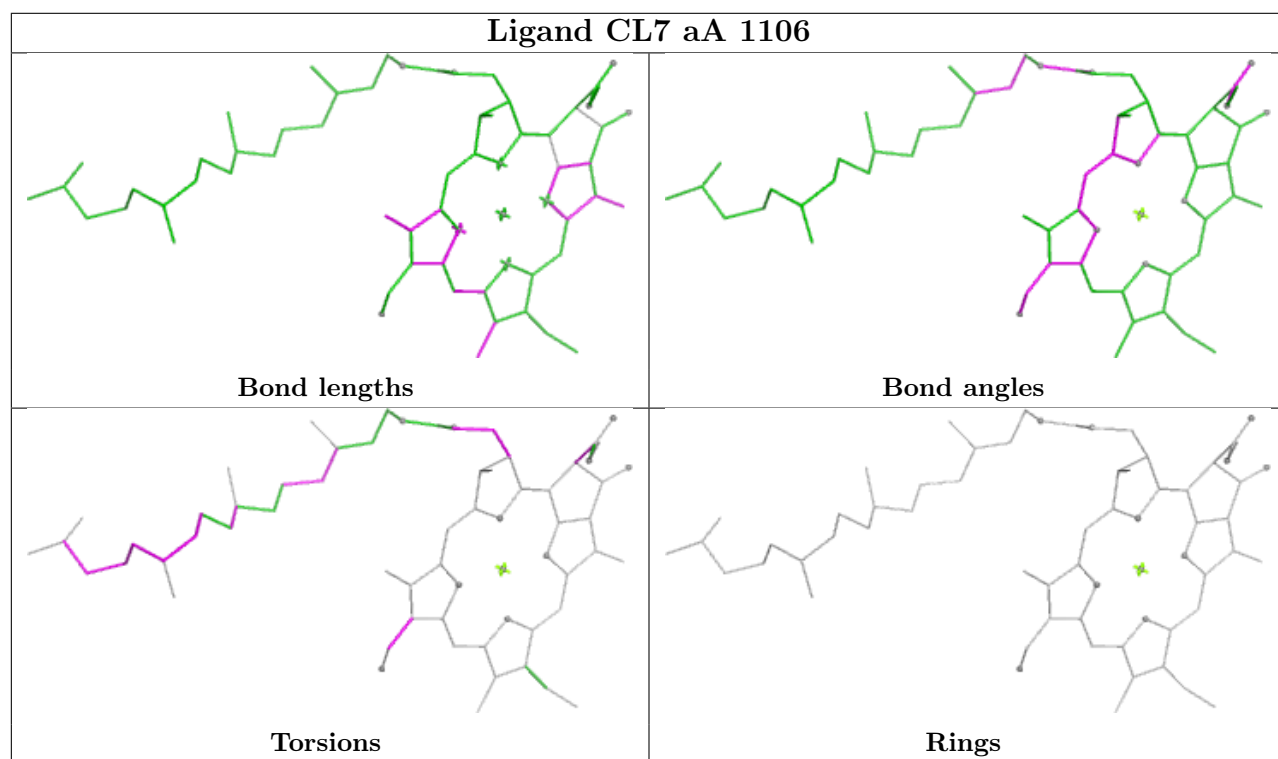
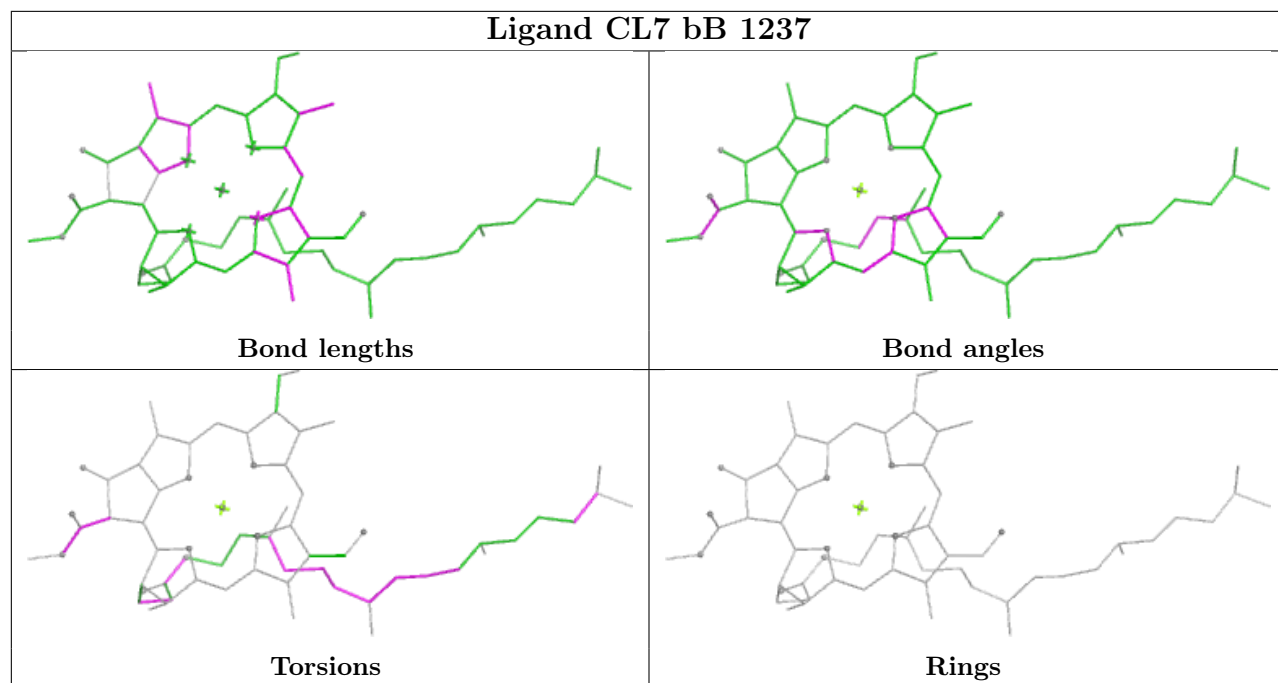




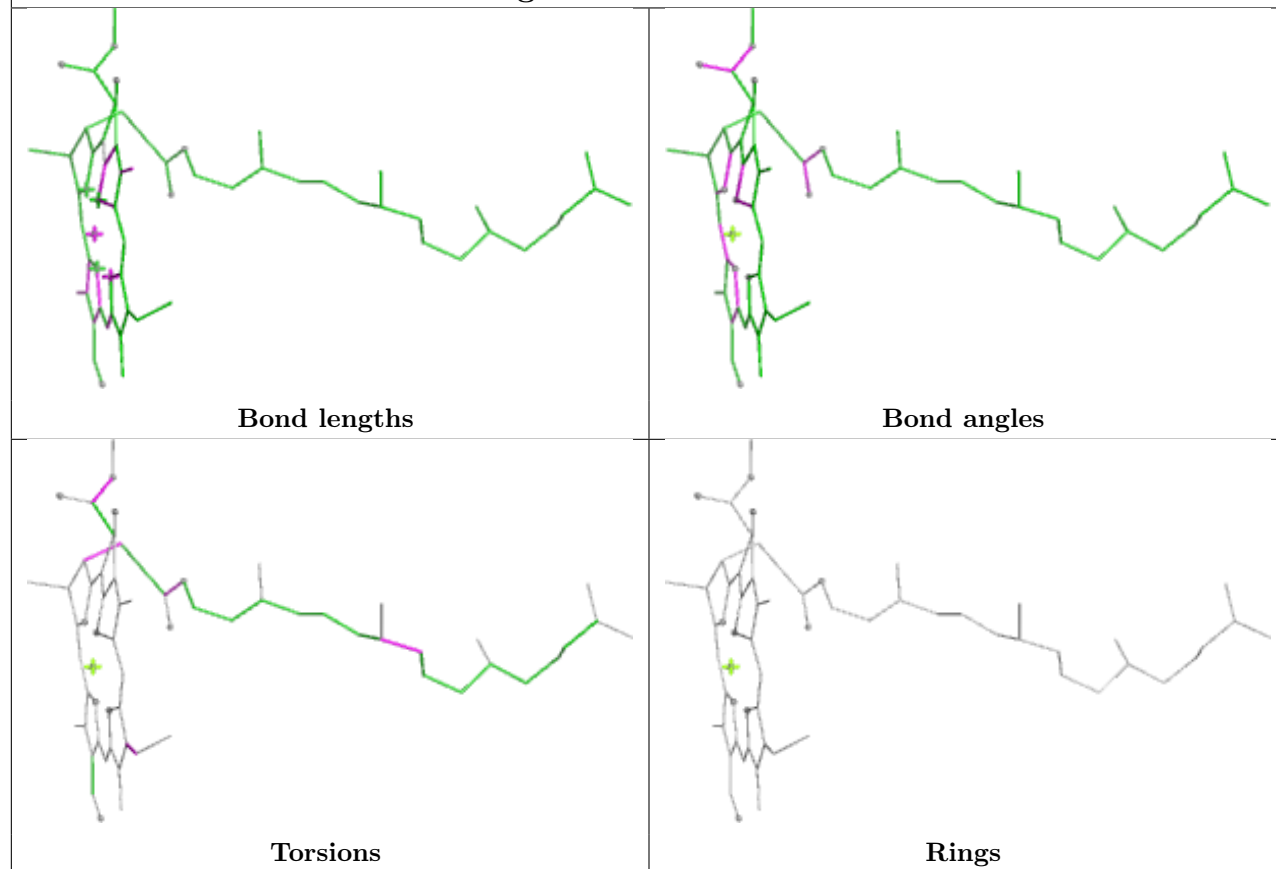




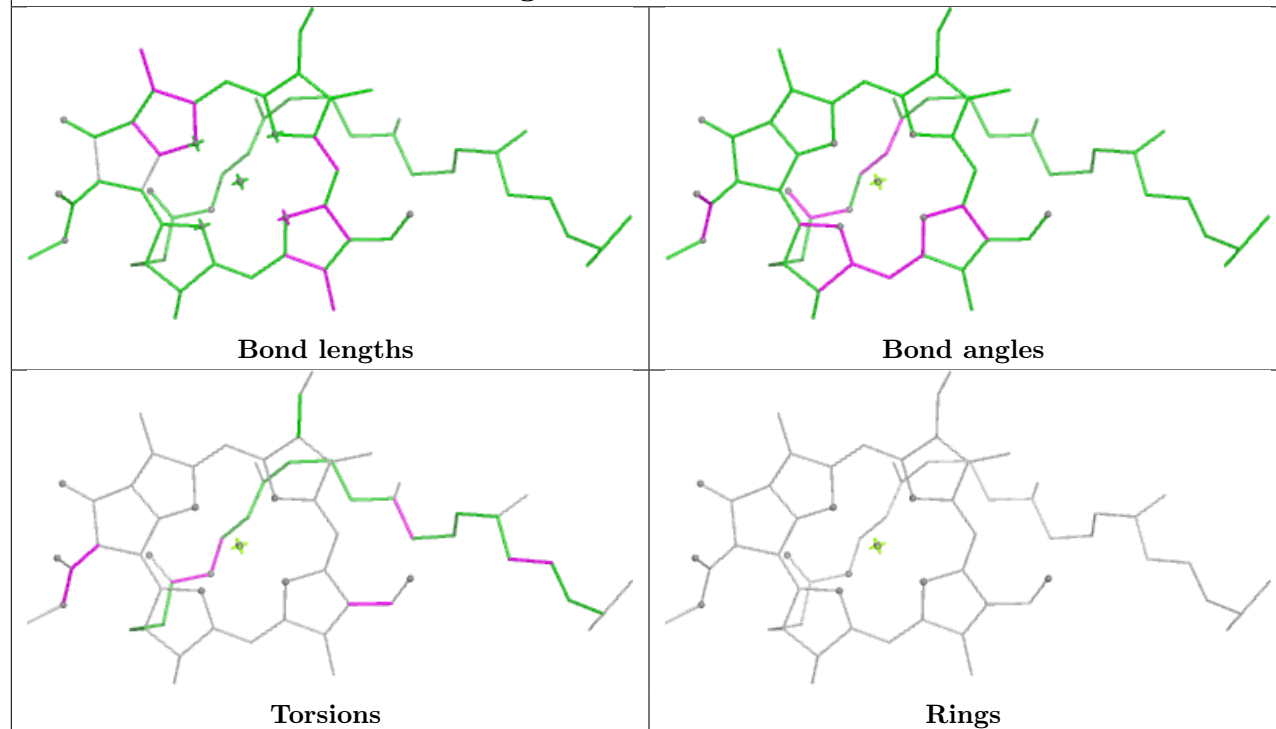


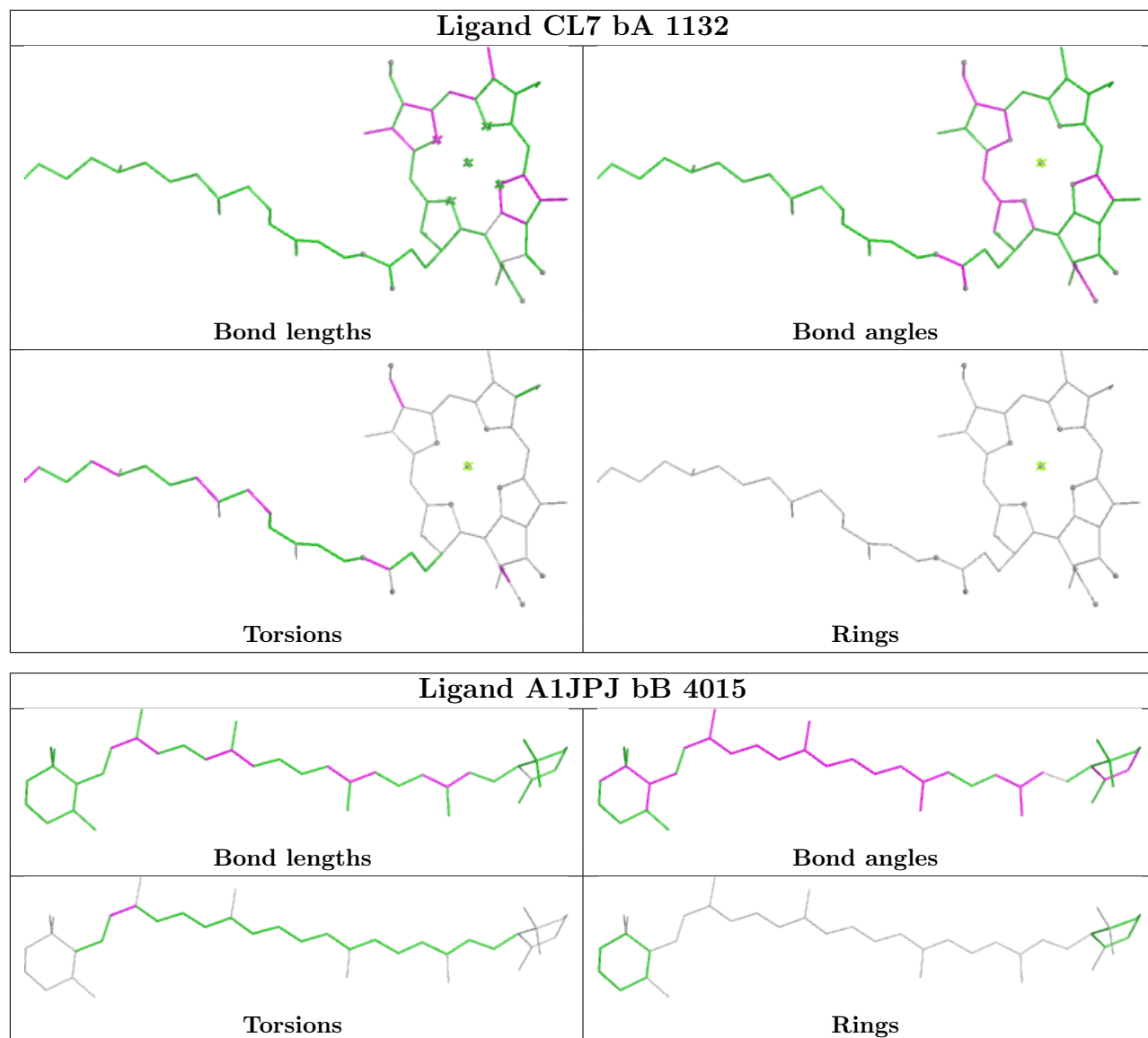


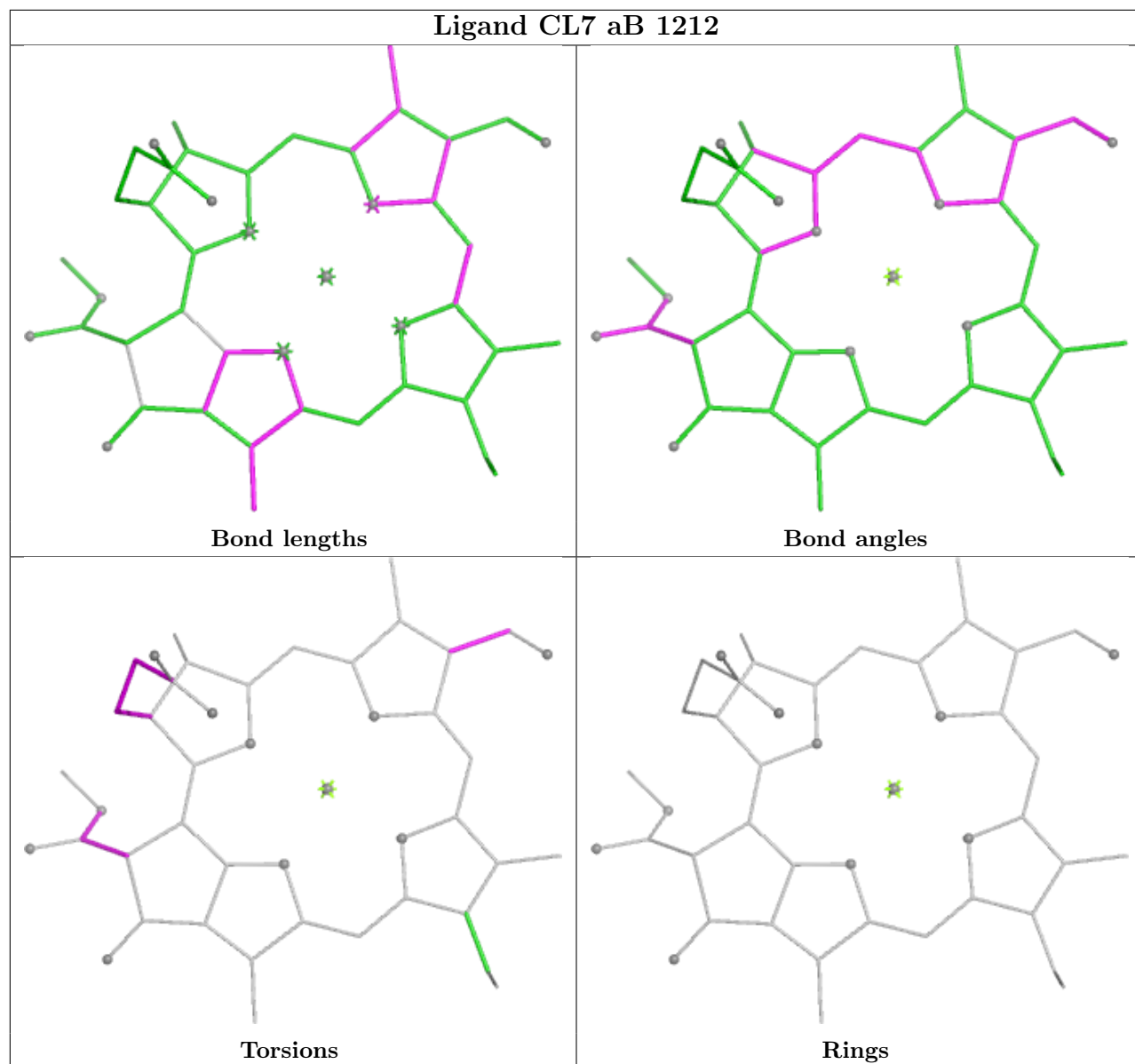
Ligand CL7 bA 1126

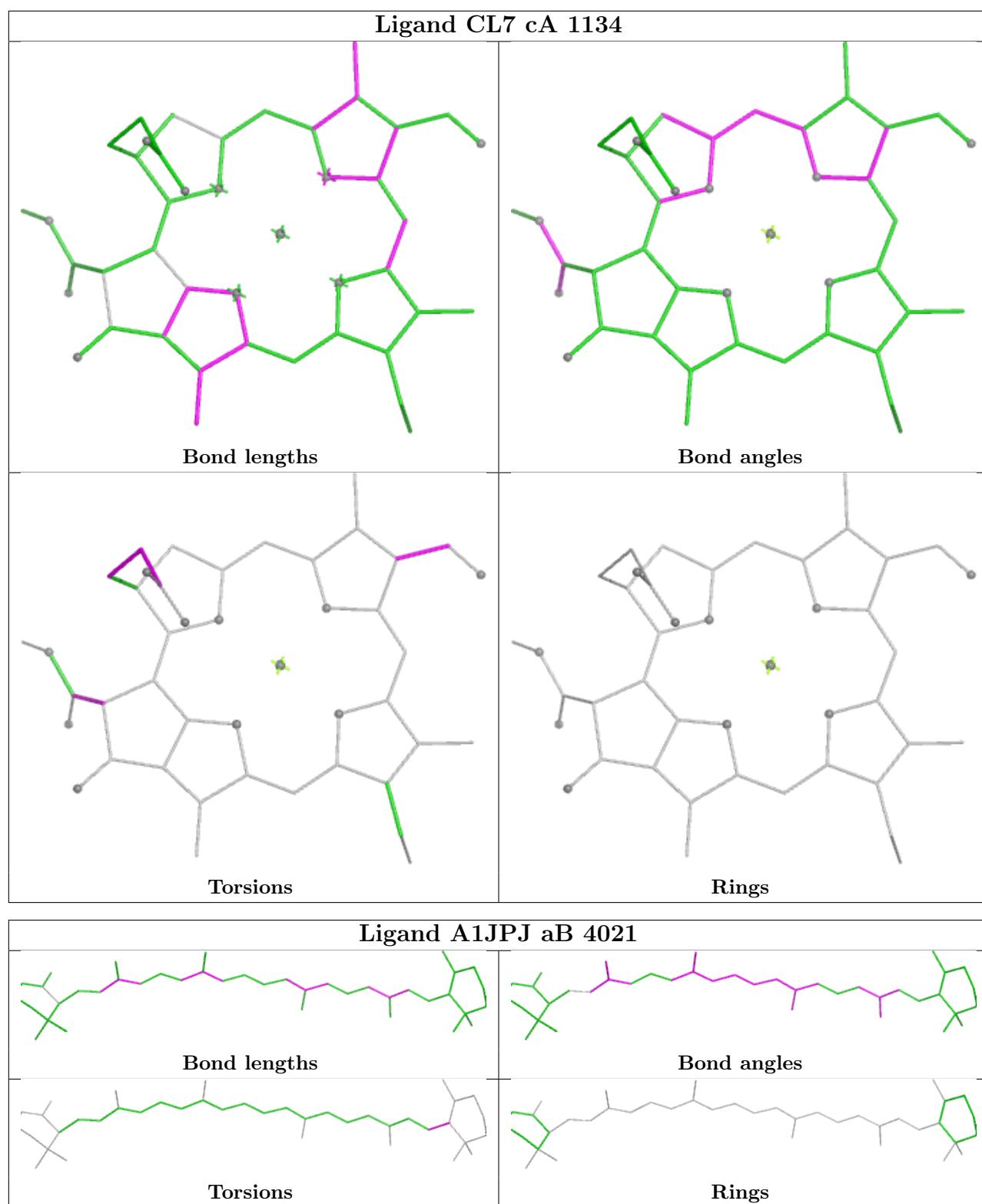


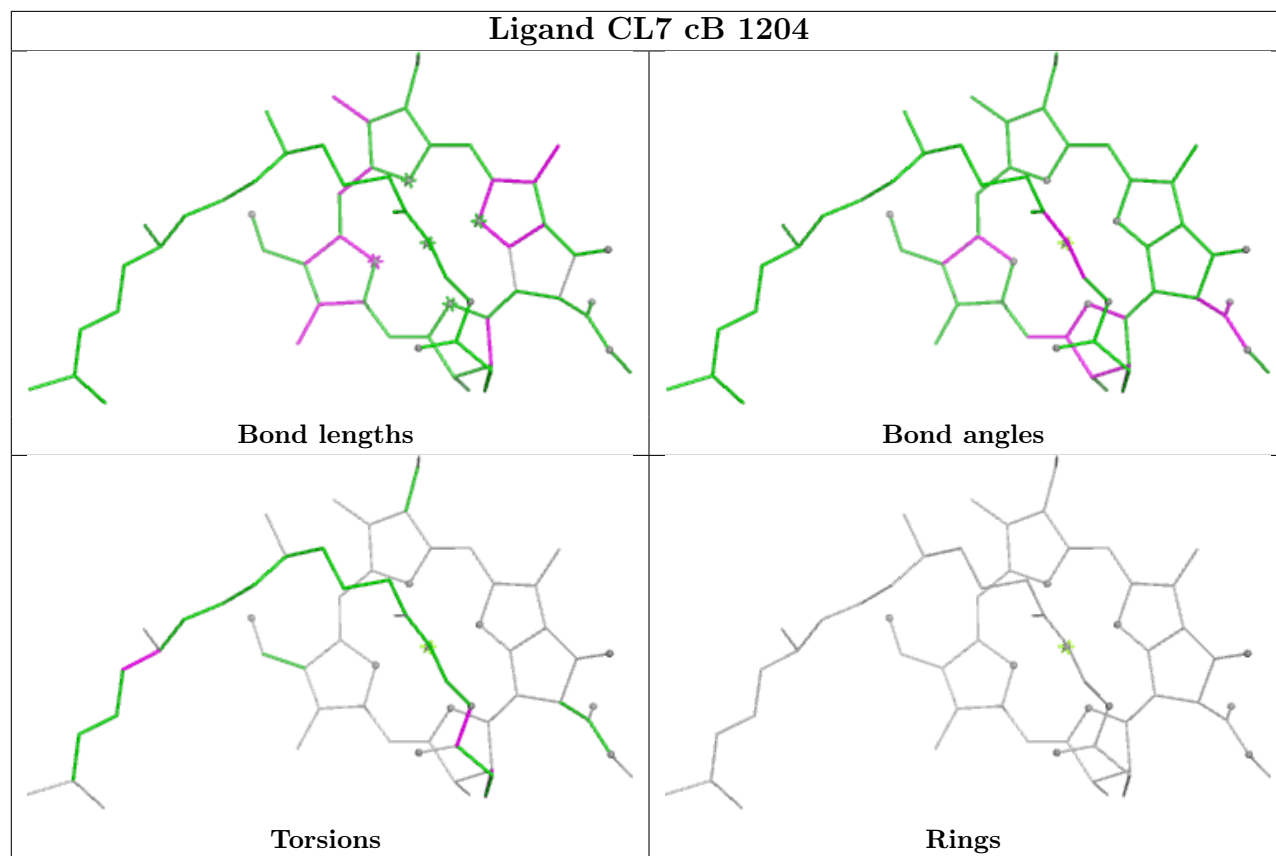
Ligand CL7 aA 1138



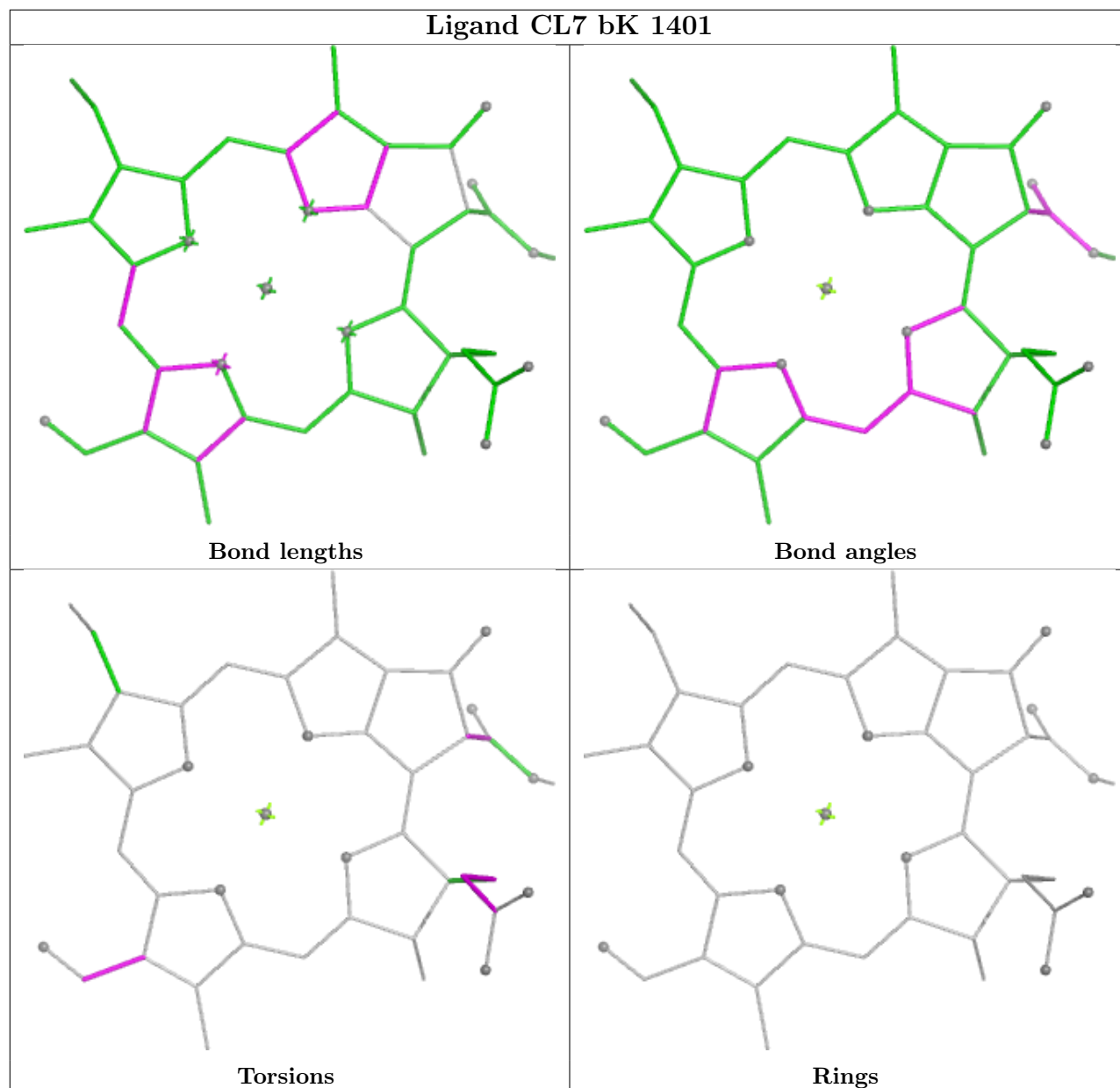




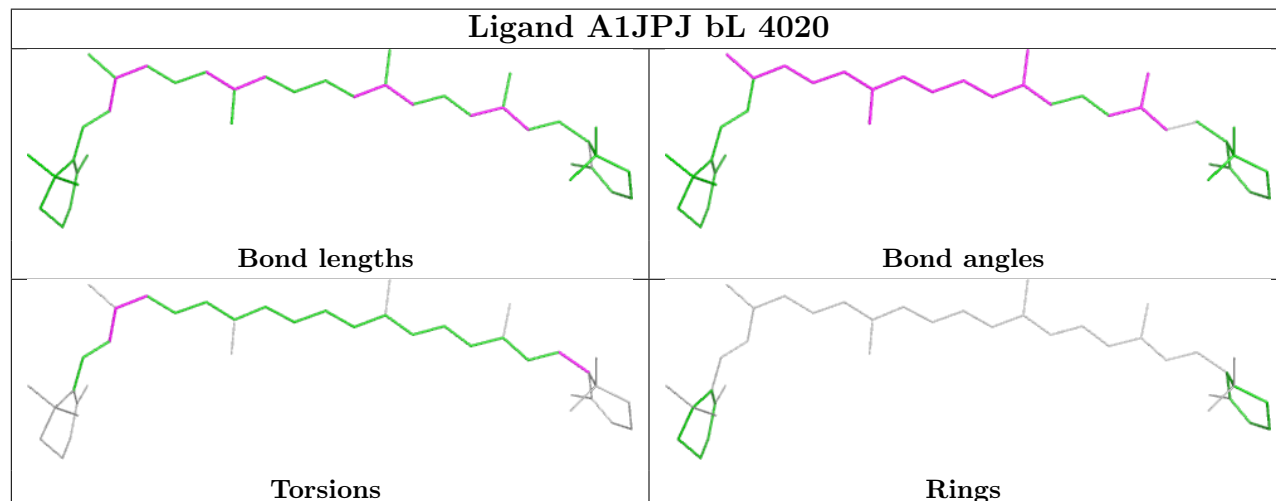




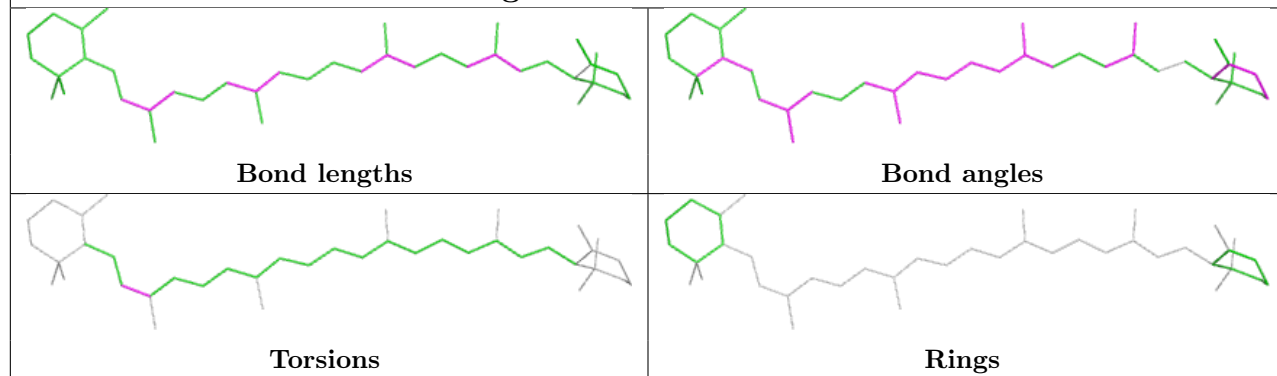
Ligand CL7 bK 1401



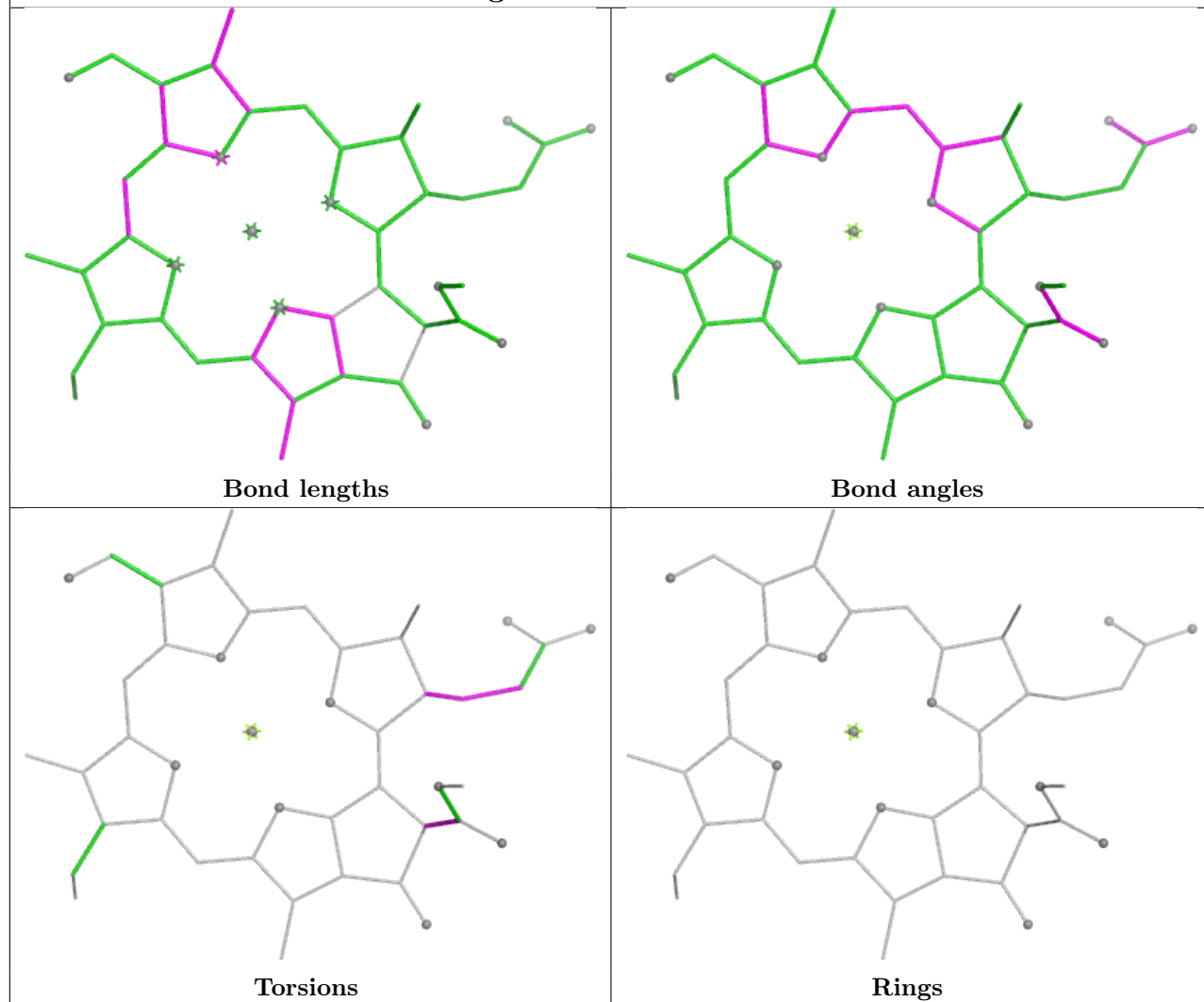
Ligand A1JPJ bL 4020

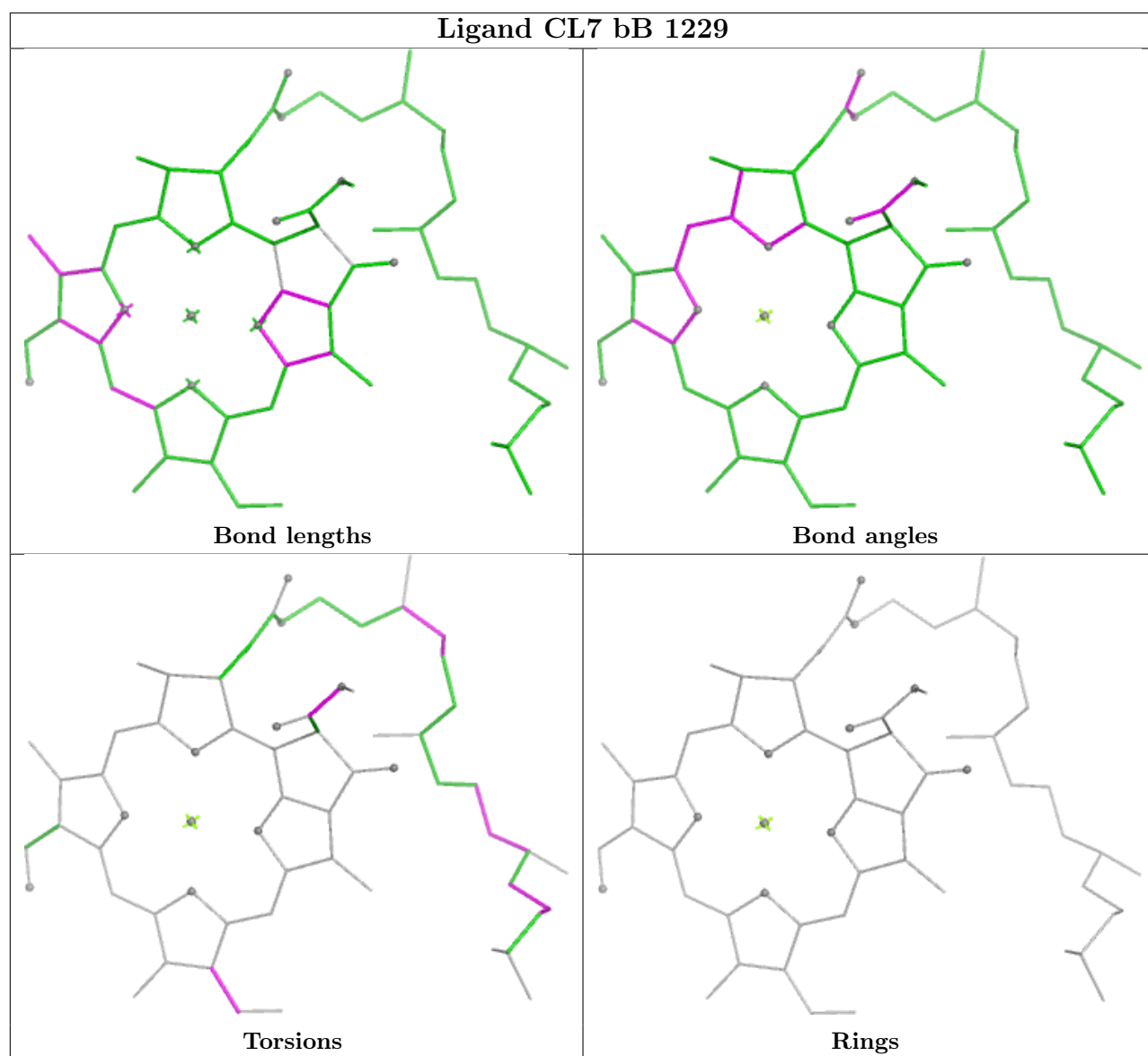


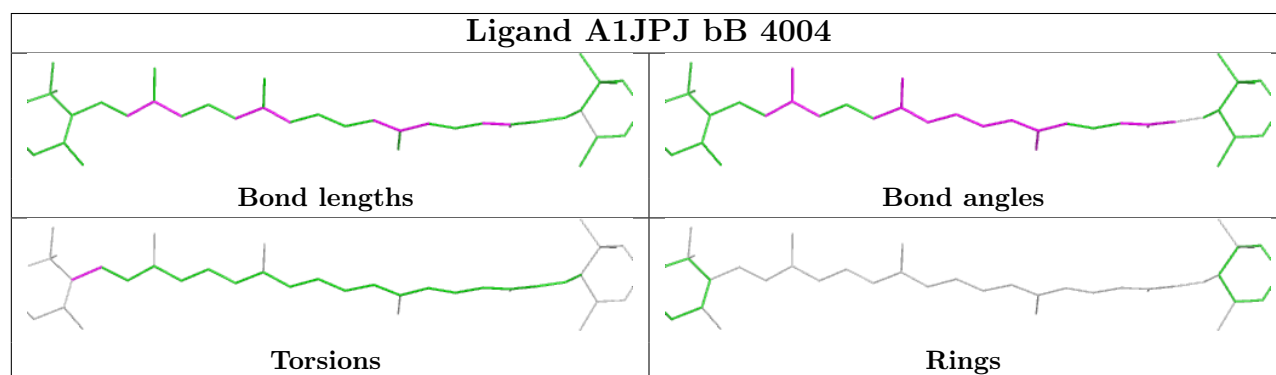
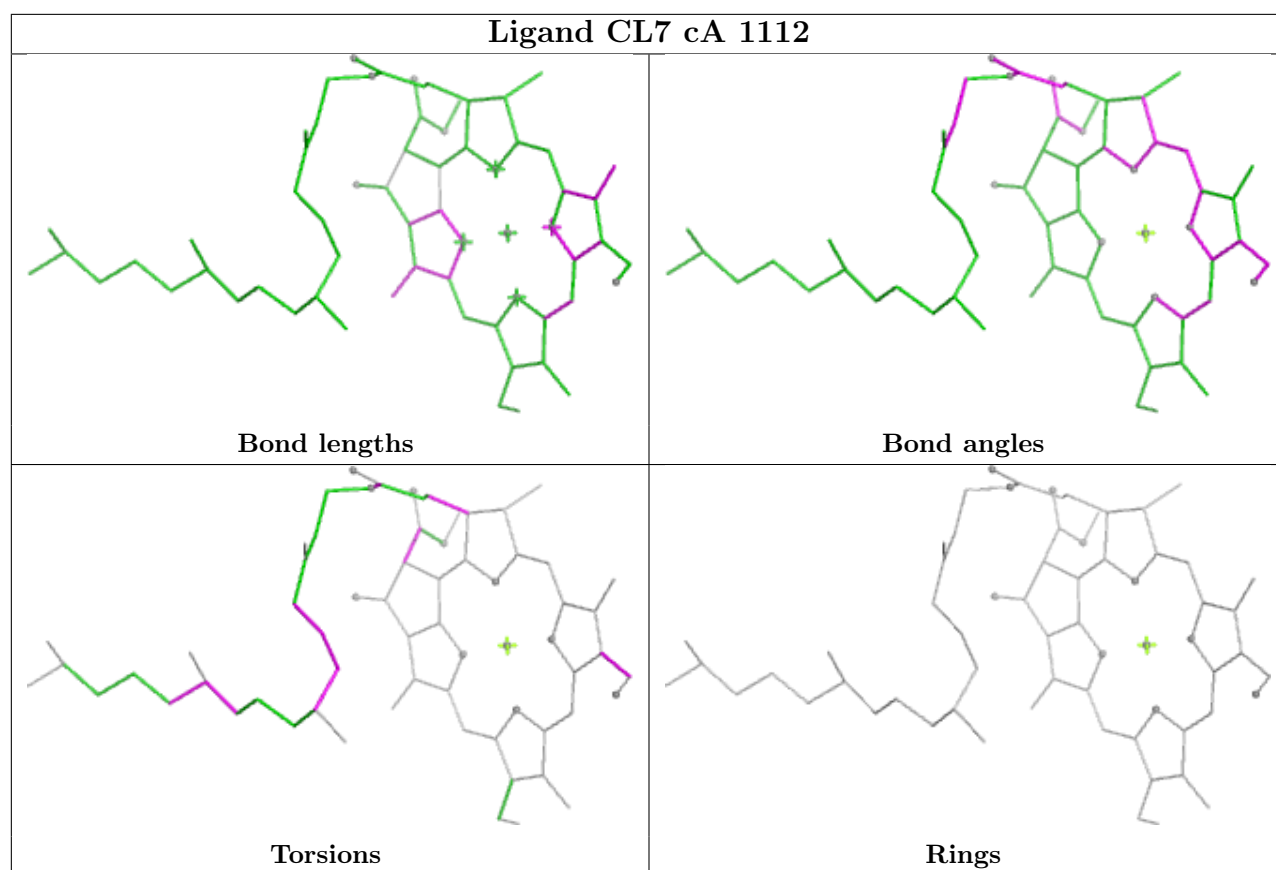
Ligand A1JPJ cJ 4012

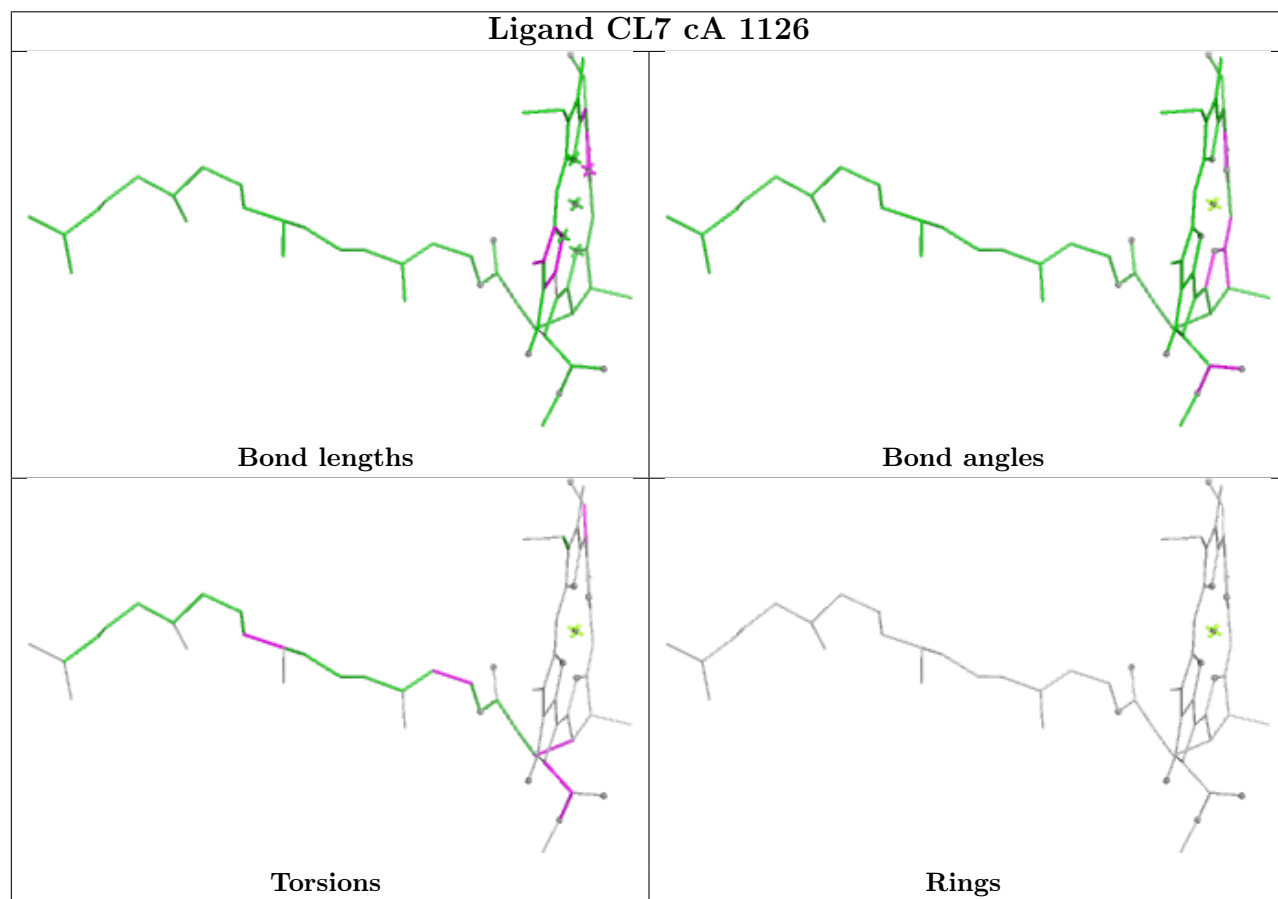
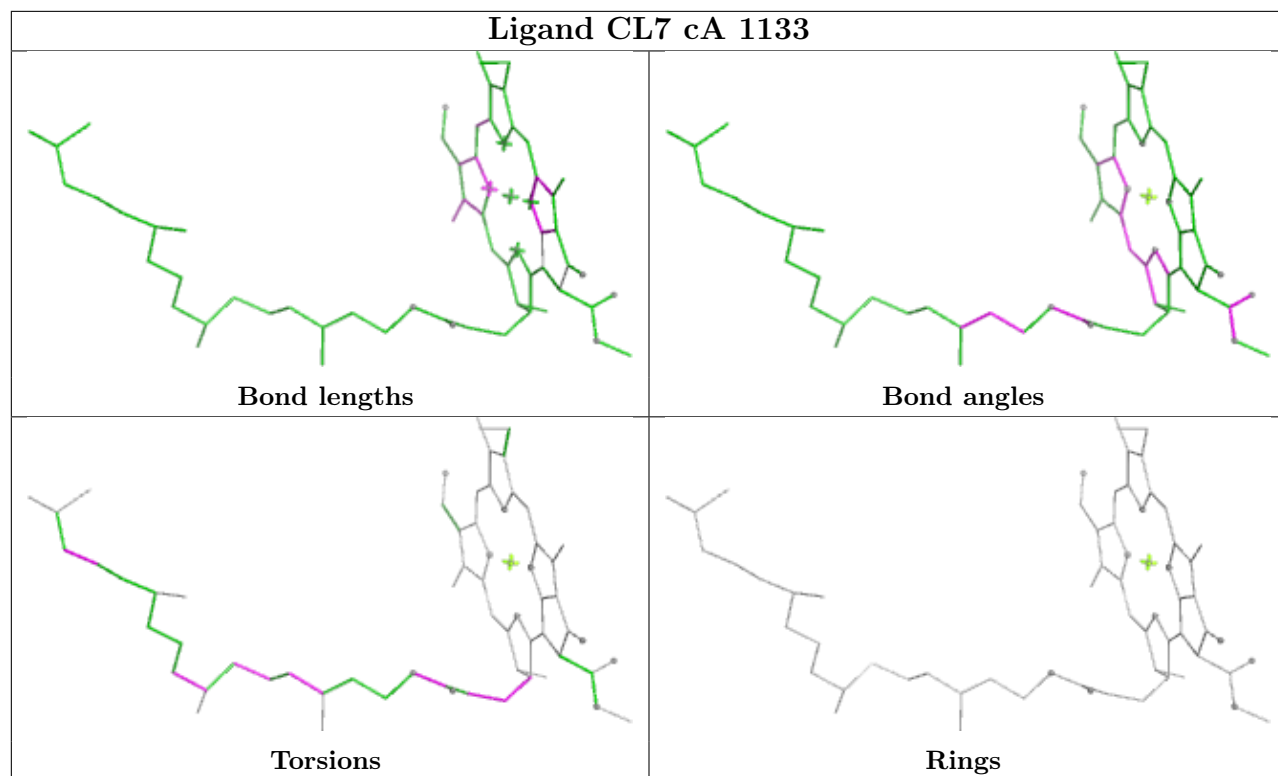


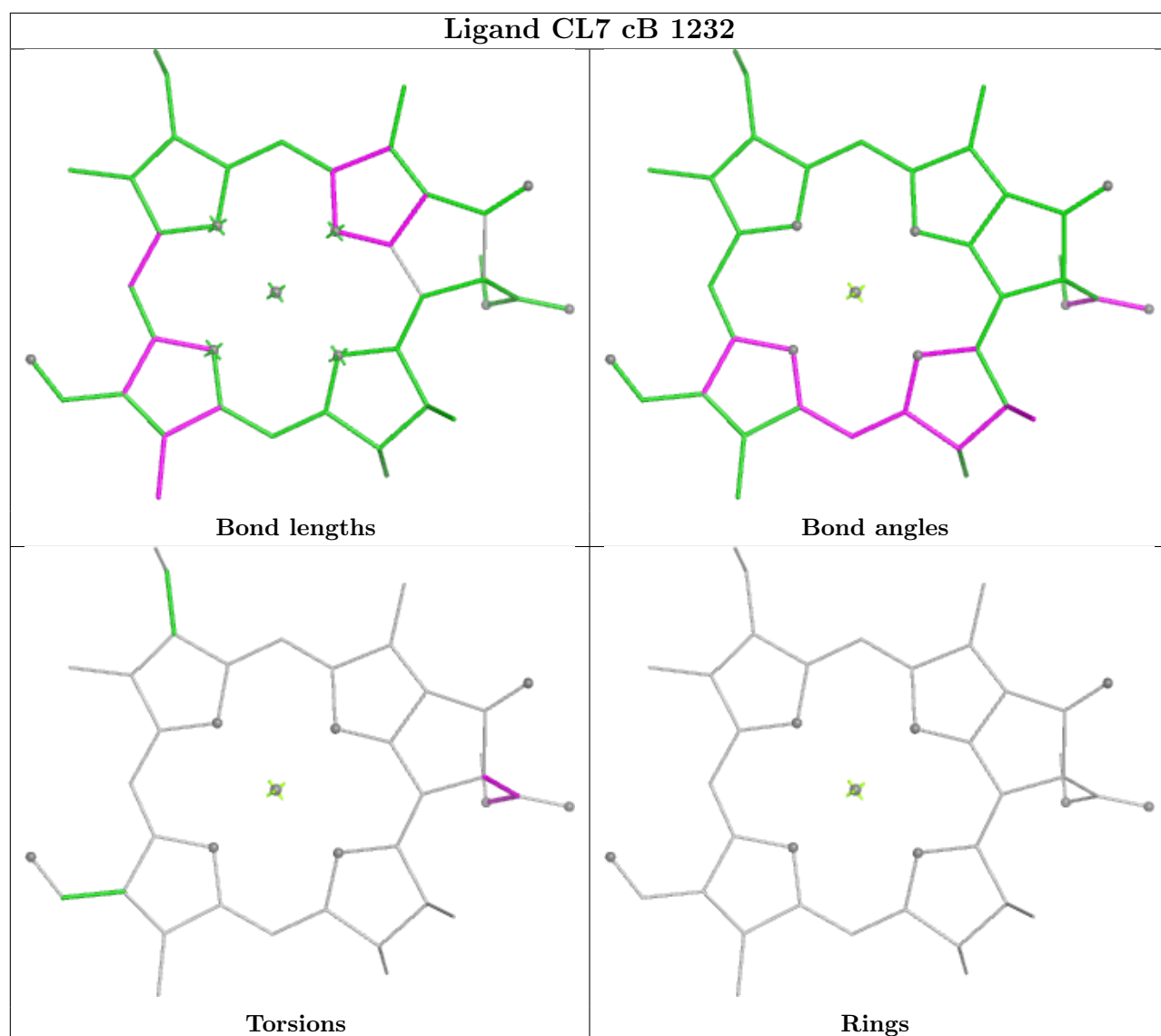
Ligand CL7 aA 1120

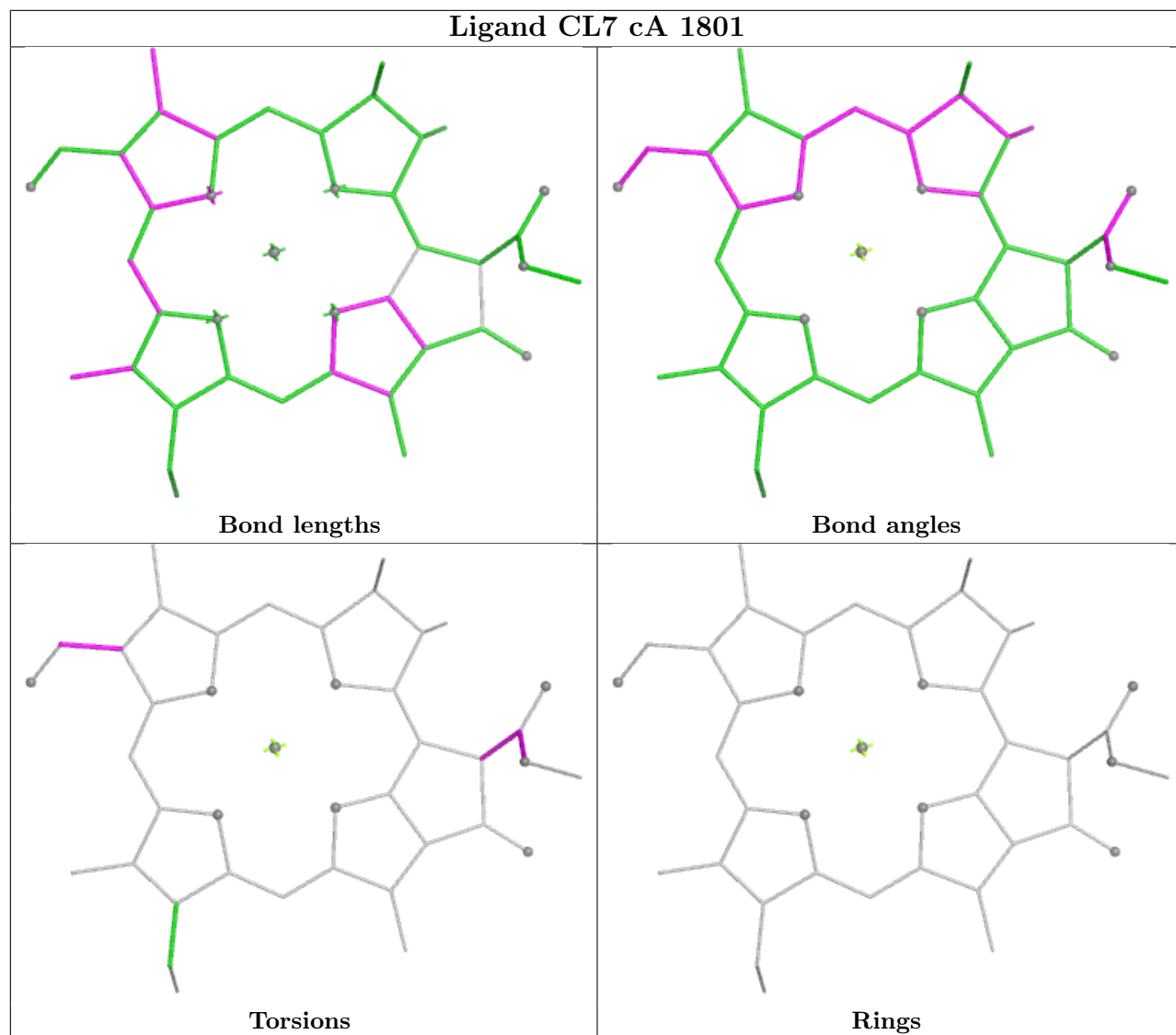


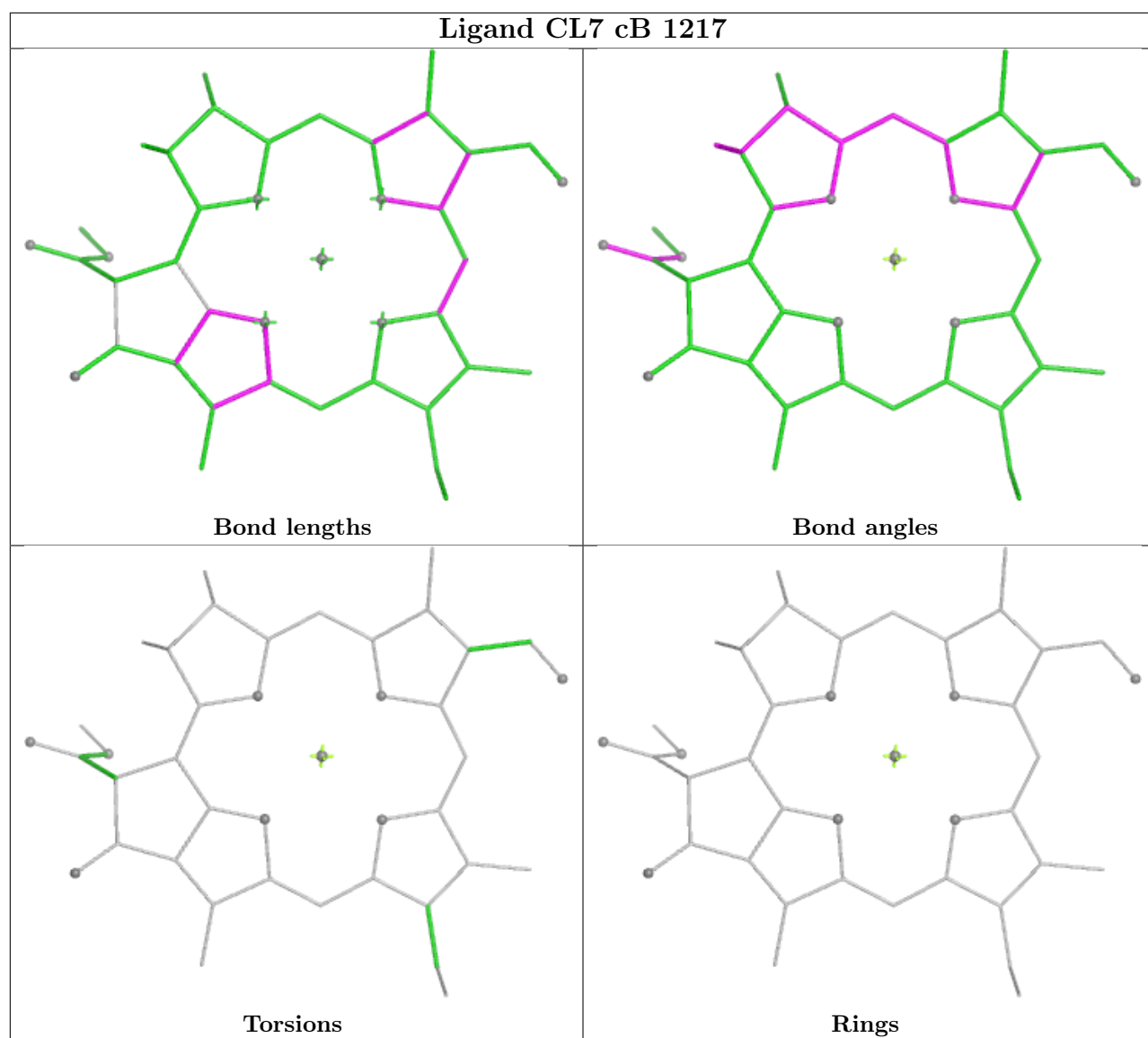


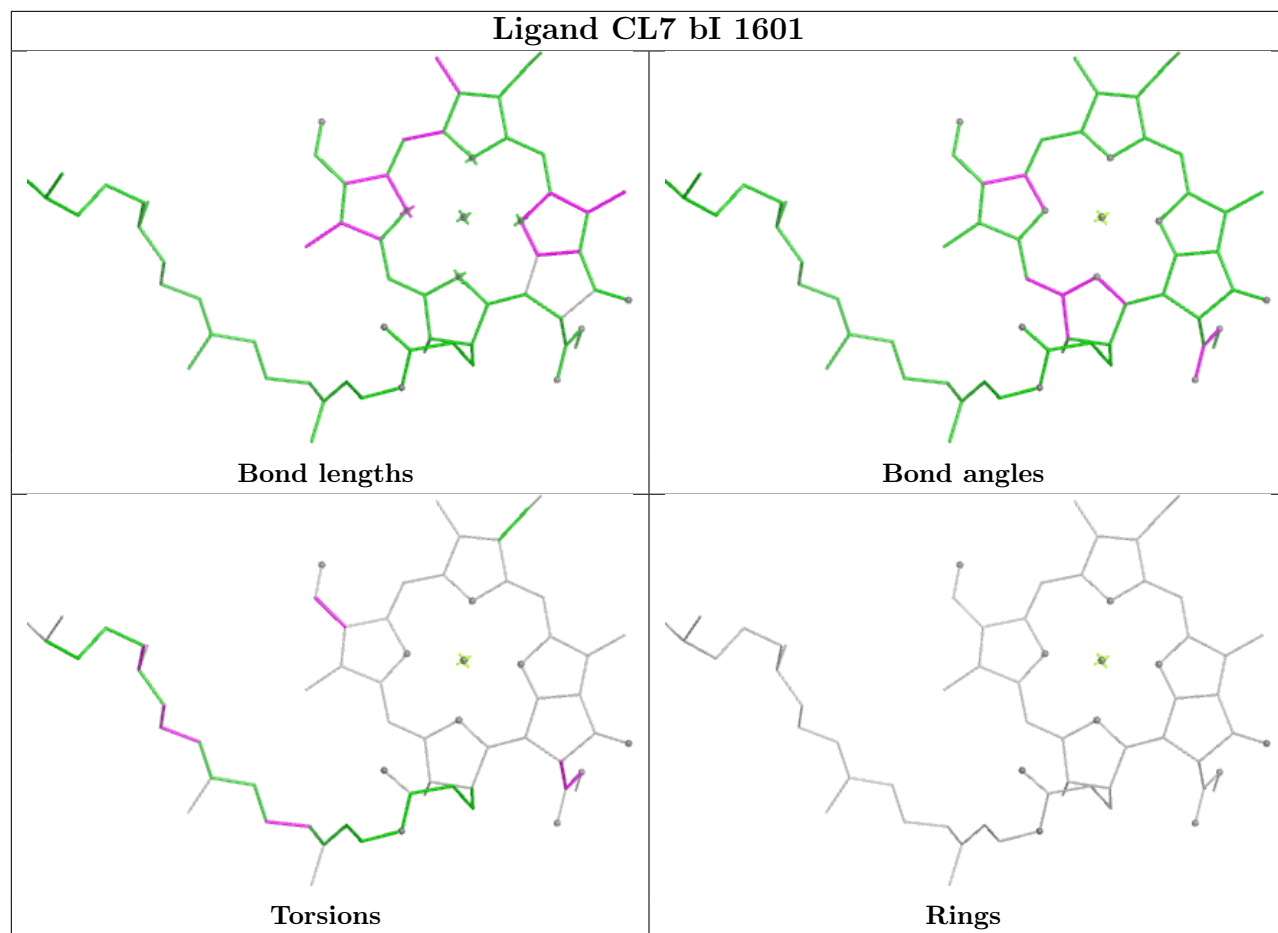




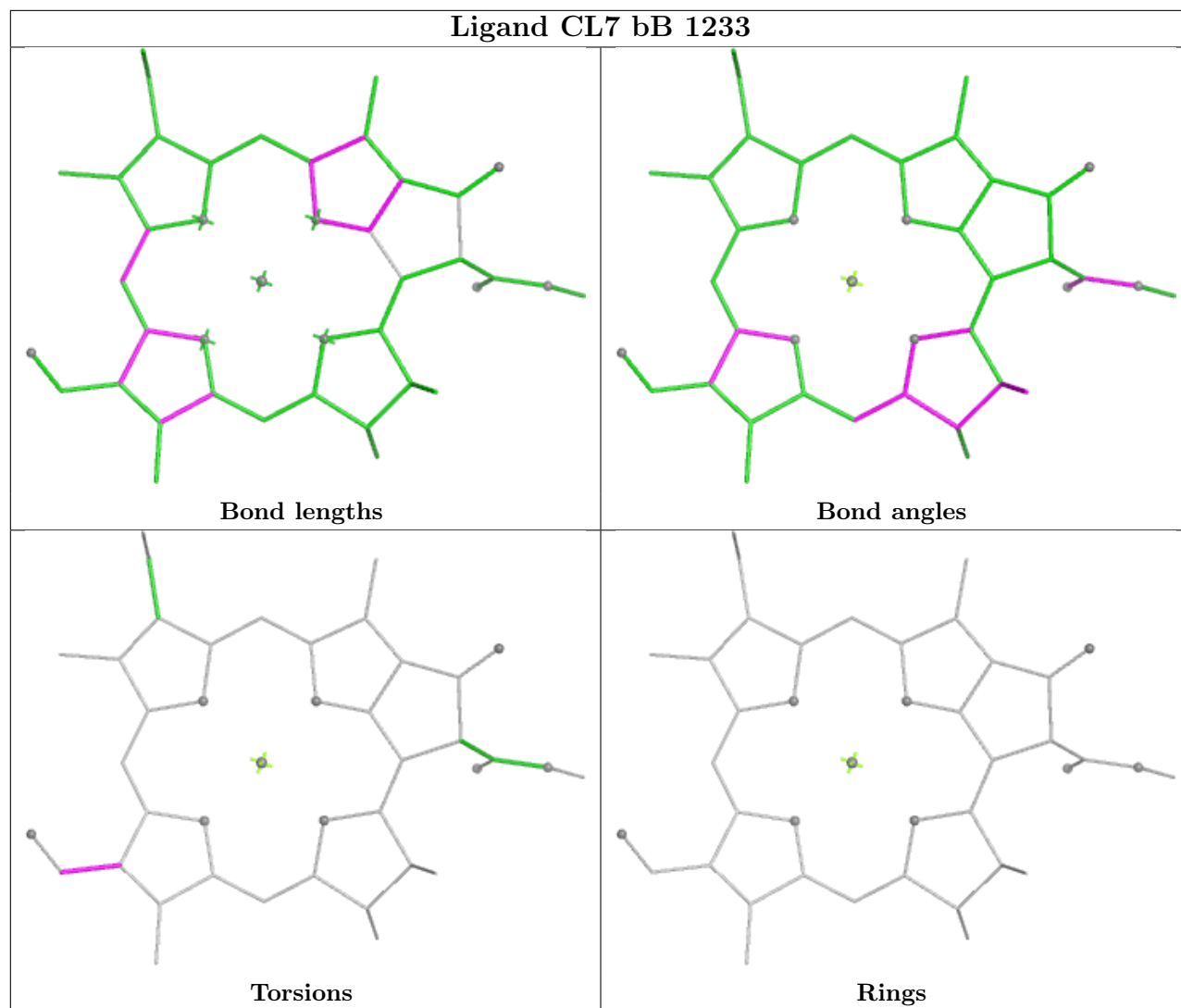


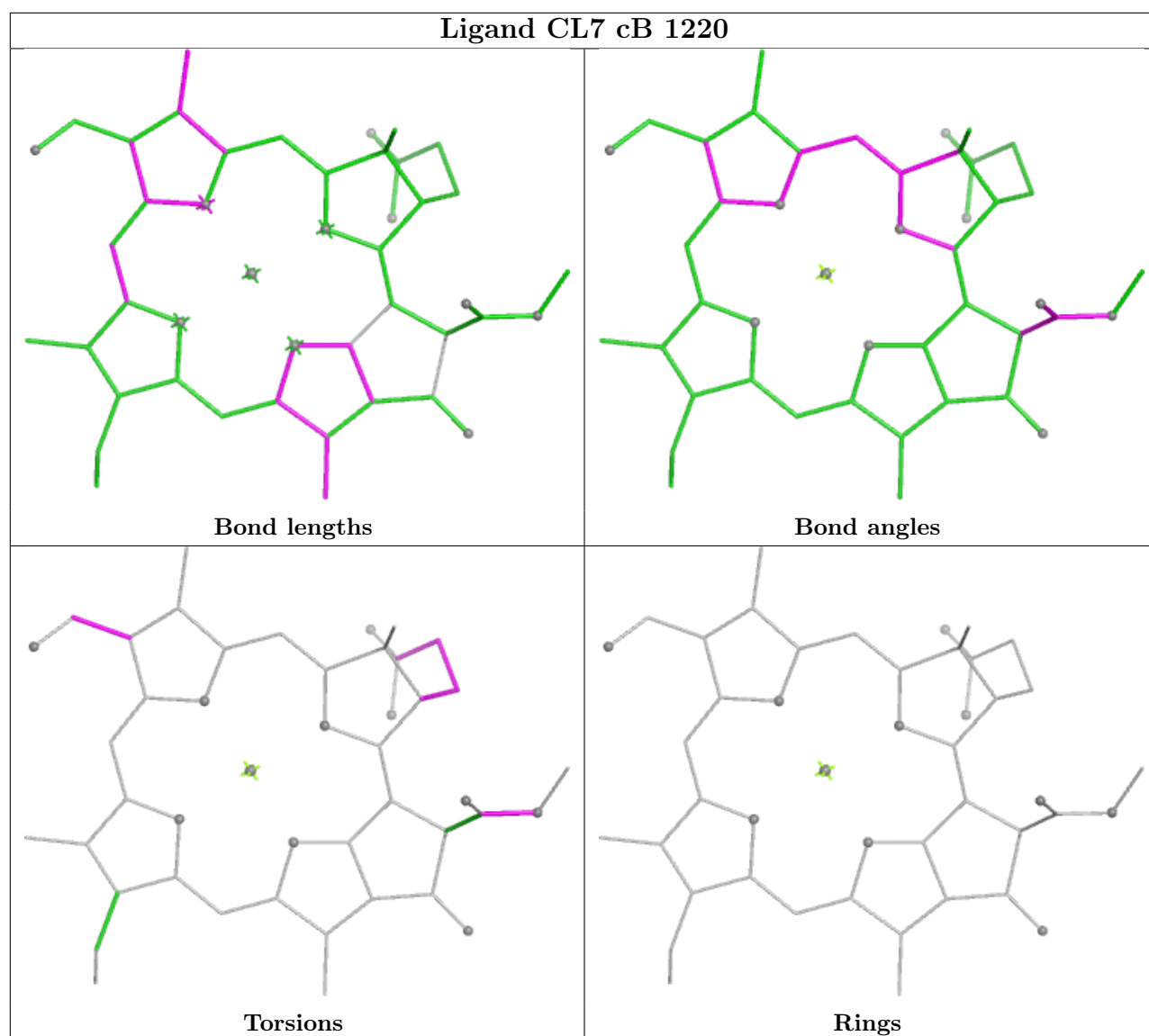




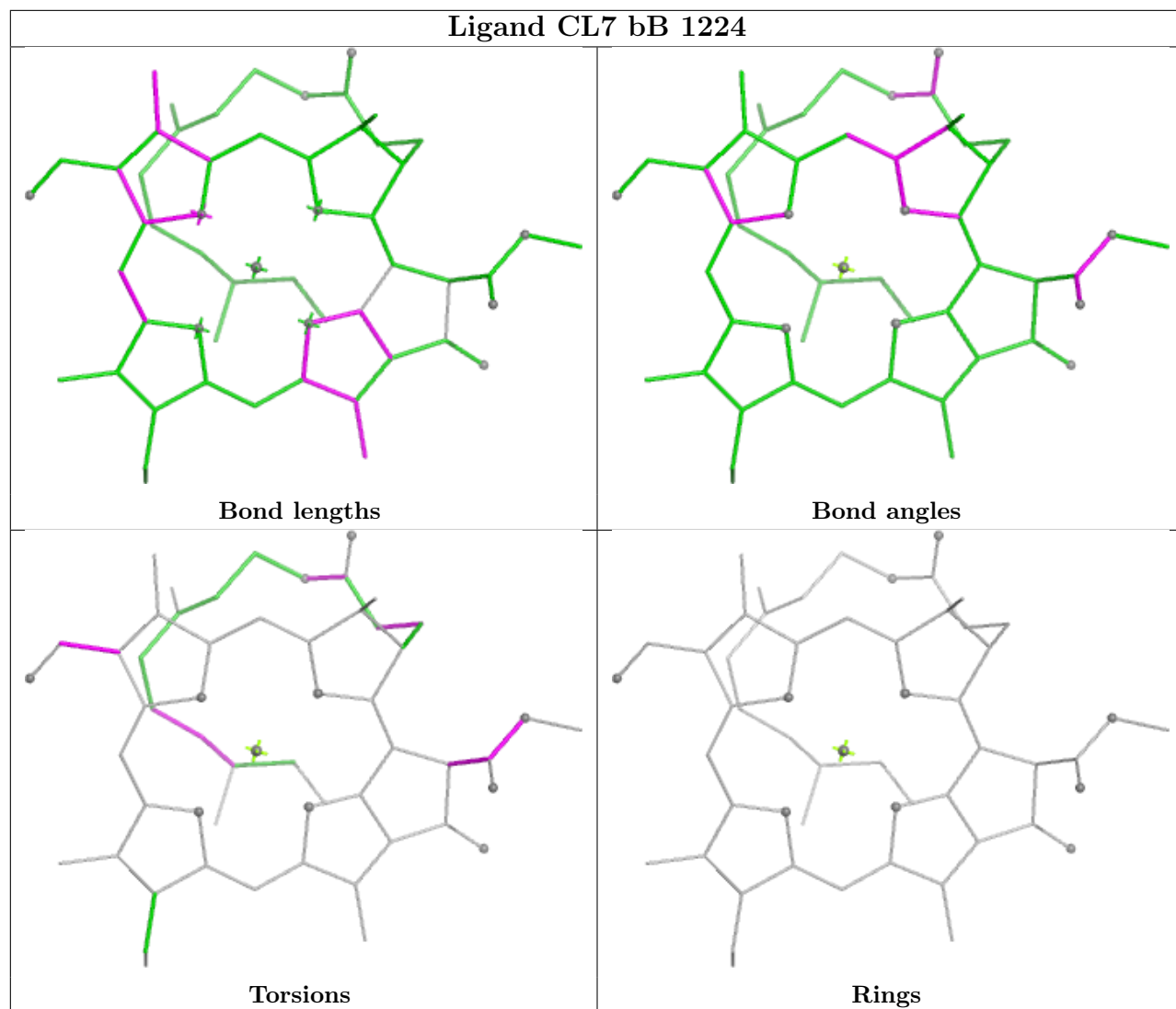


Ligand CL7 bB 1233

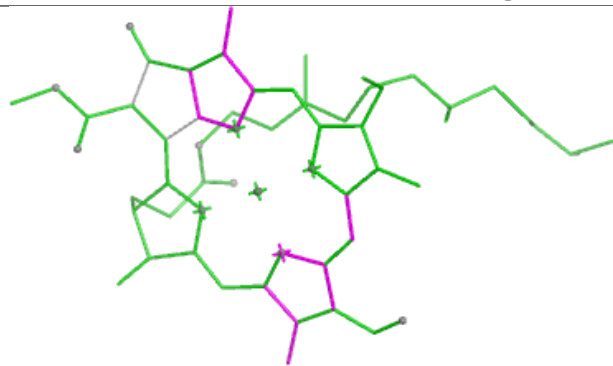




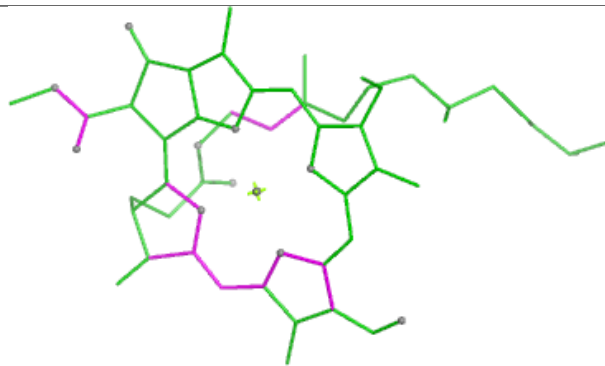
Ligand CL7 bB 1224



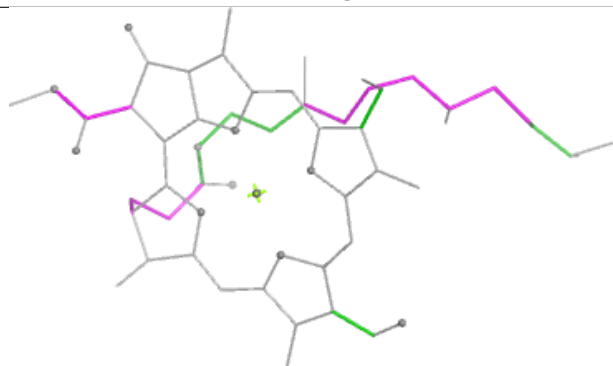
Ligand CL7 bA 1140



Bond lengths



Bond angles

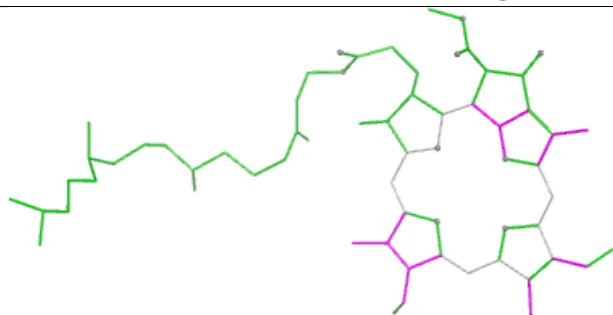


Torsions

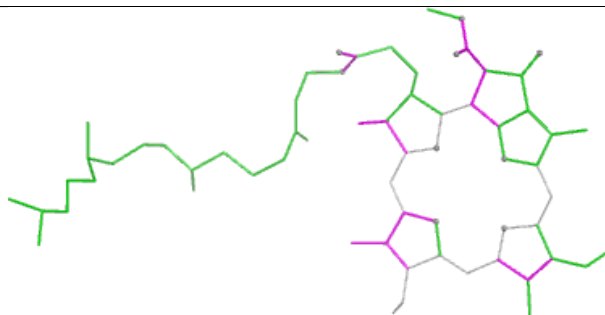


Rings

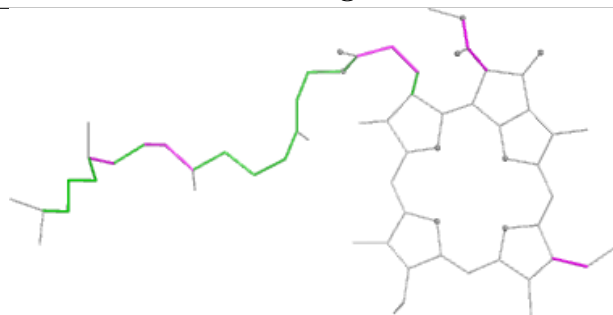
Ligand PHO aB 1023



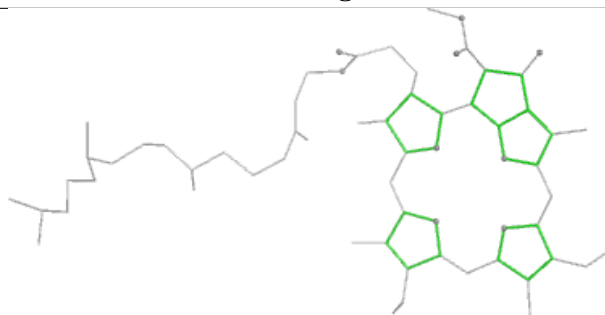
Bond lengths



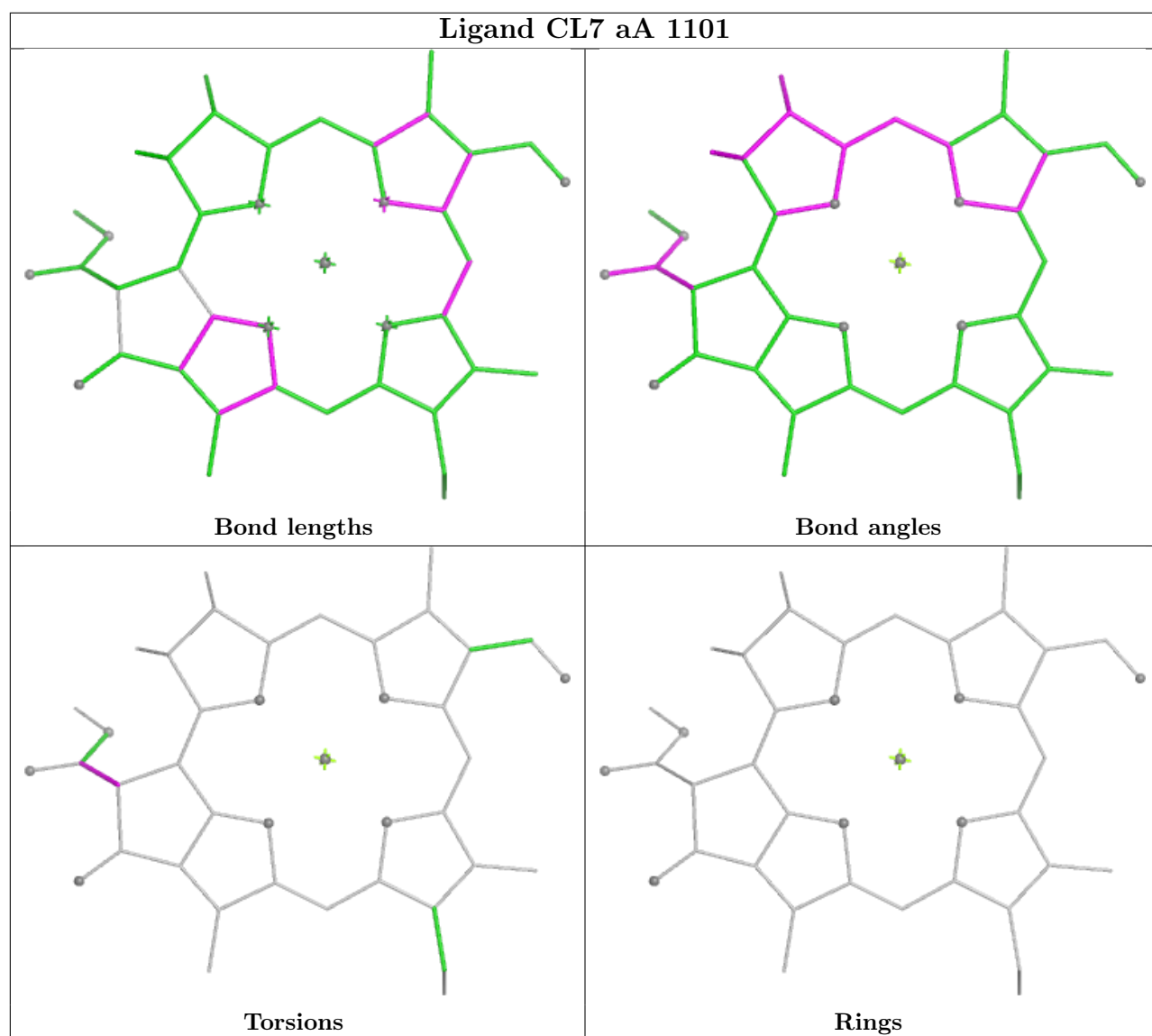
Bond angles



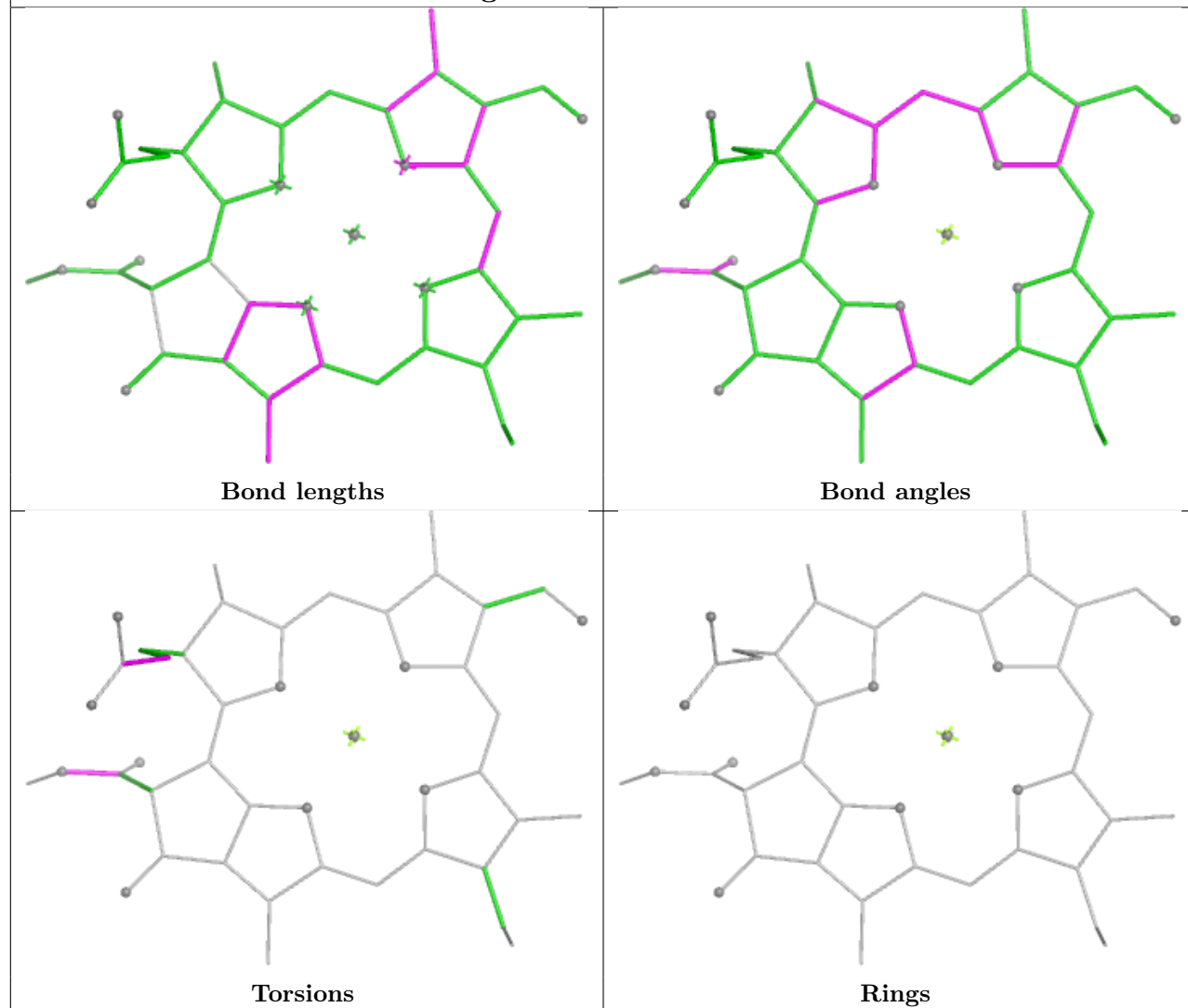
Torsions



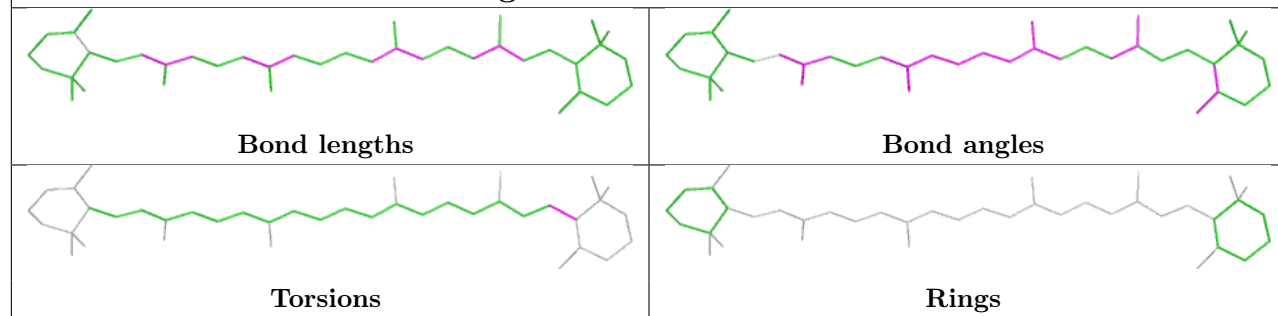
Rings

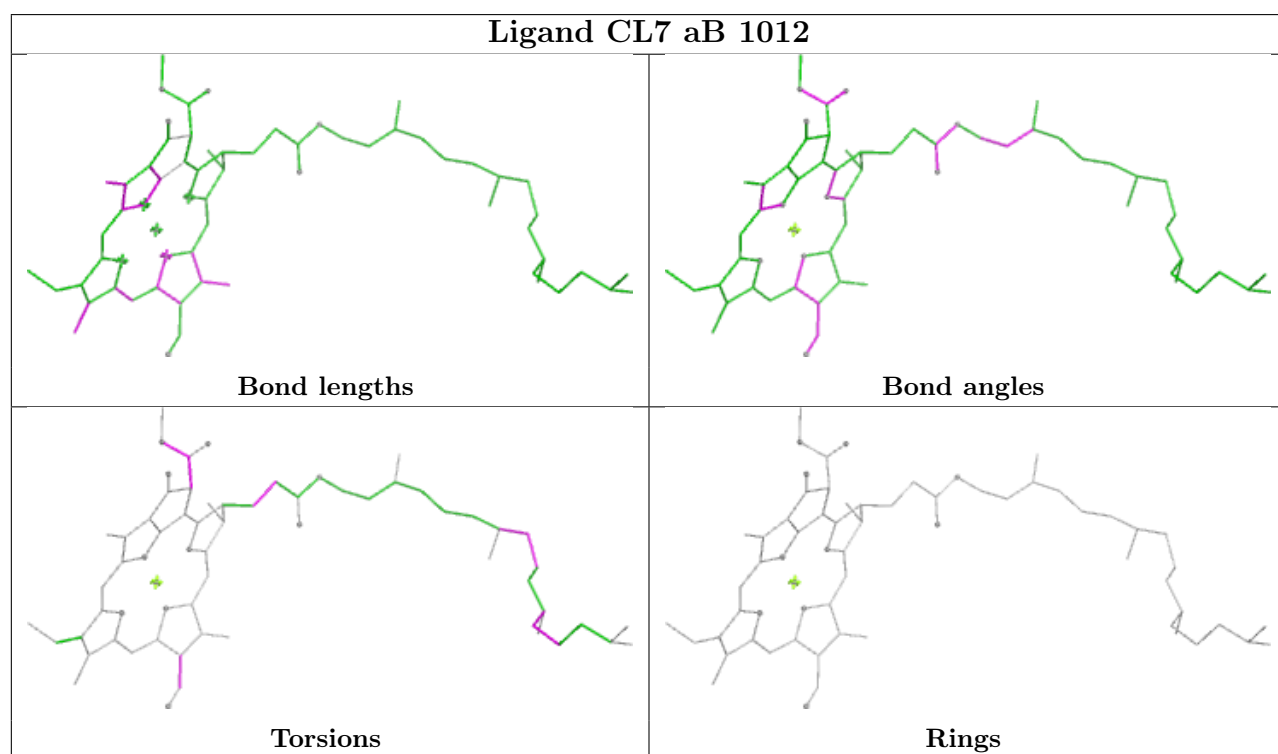
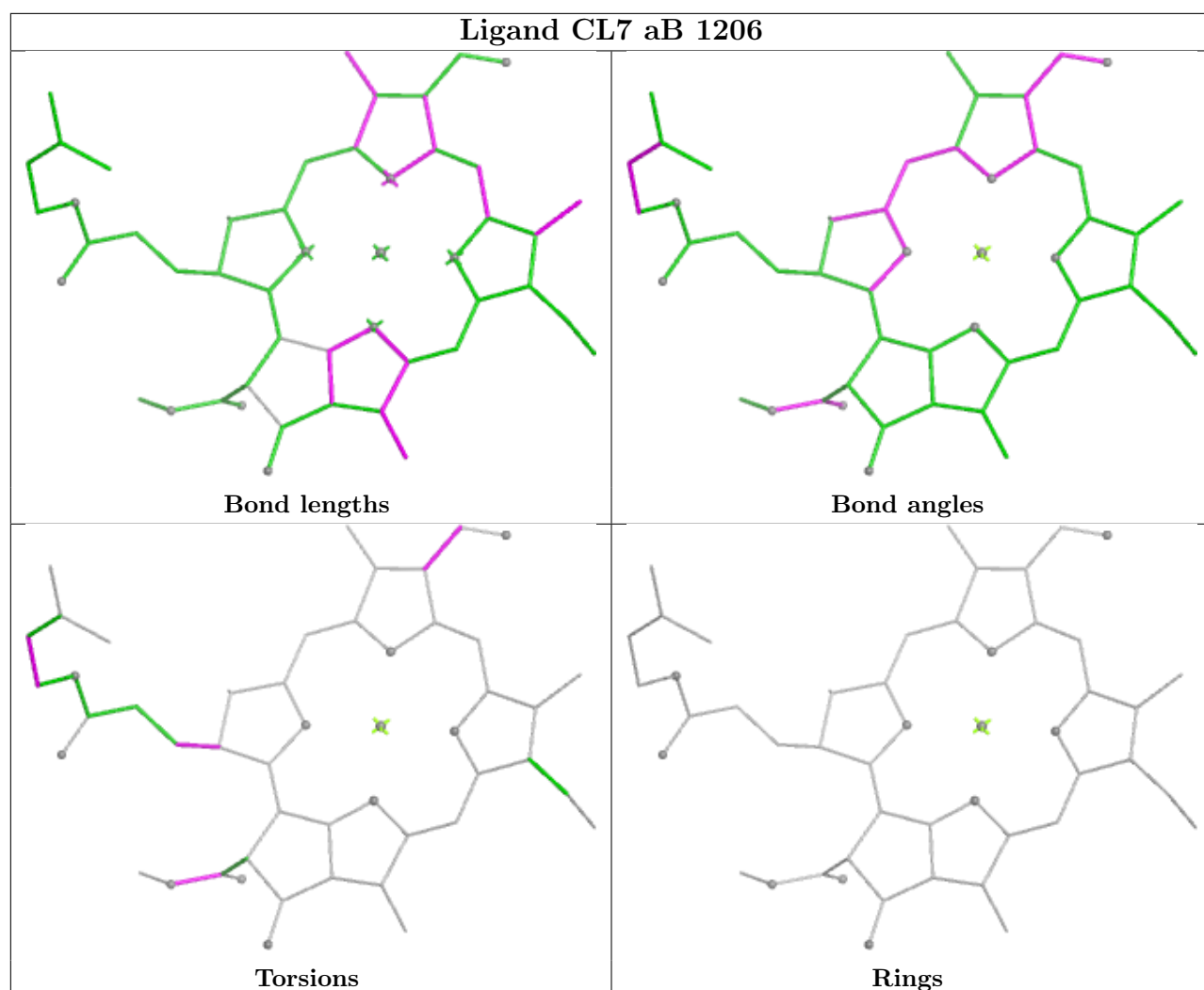


Ligand CL7 bA 1107

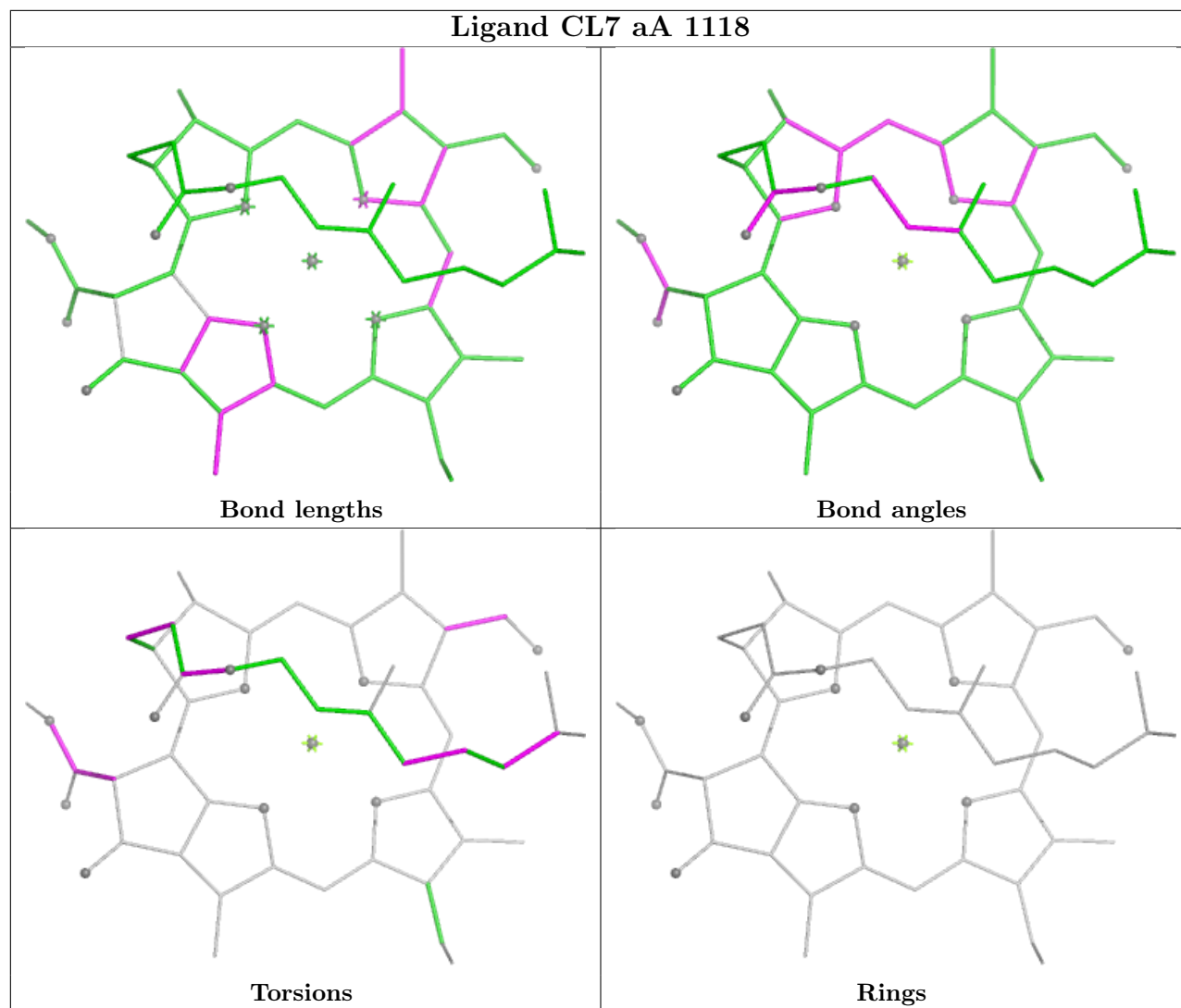


Ligand A1JPJ cA 4003

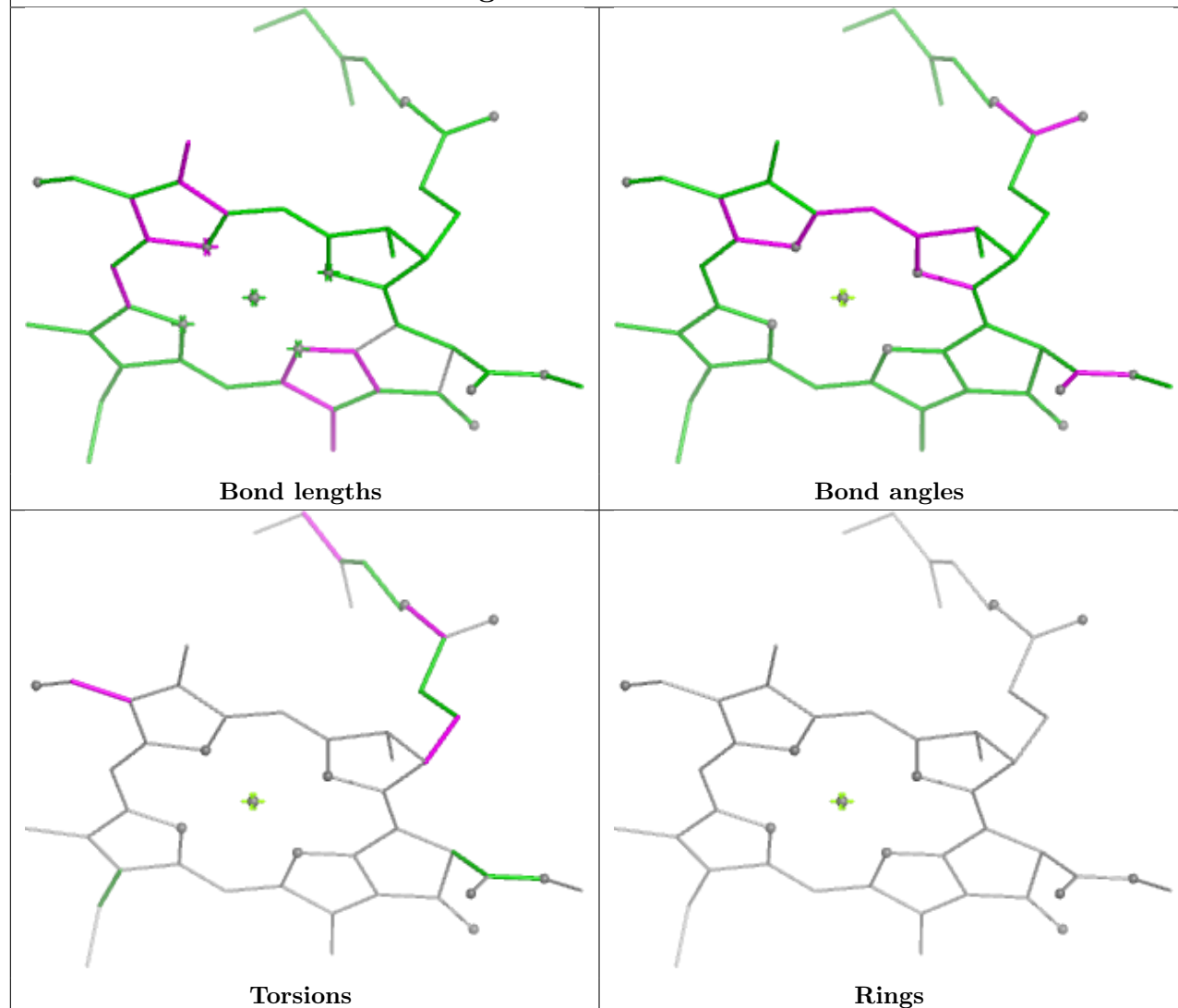




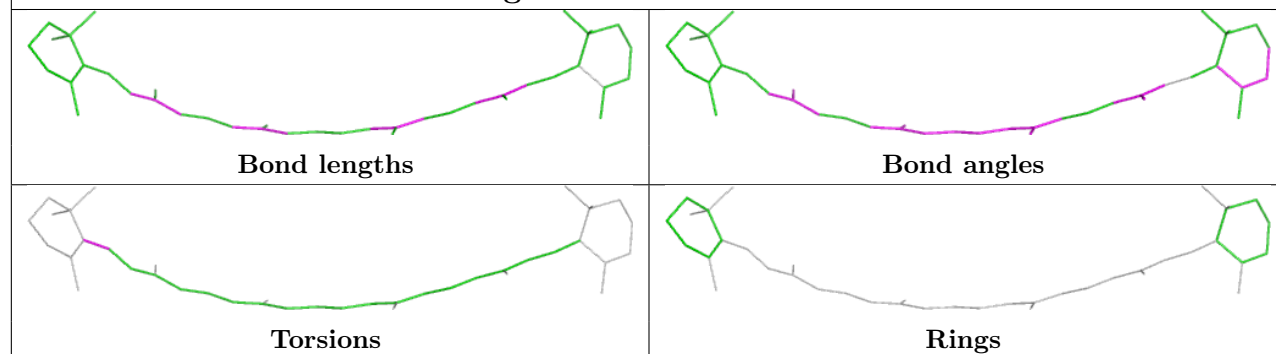
Ligand CL7 aA 1118

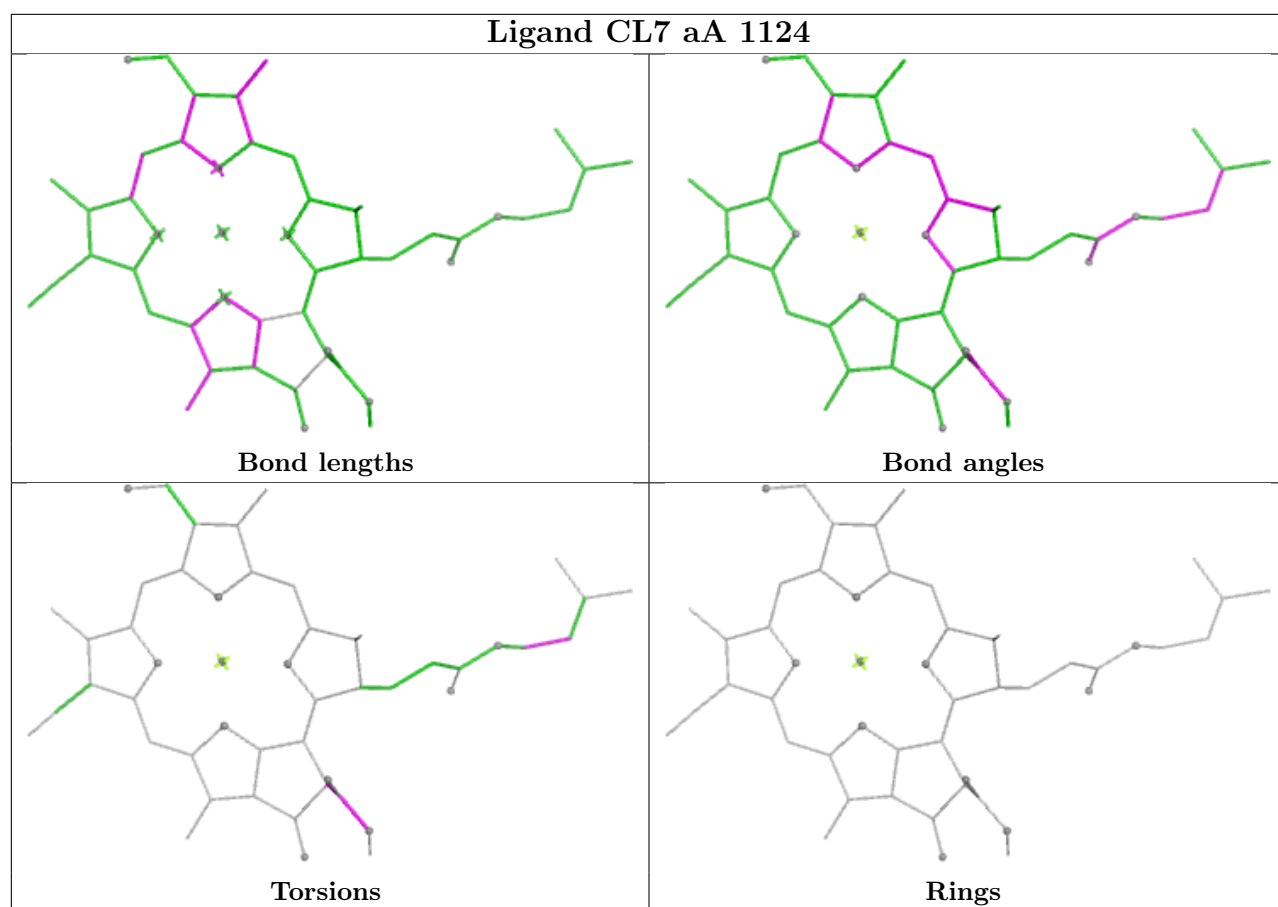


Ligand CL7 aA 1130

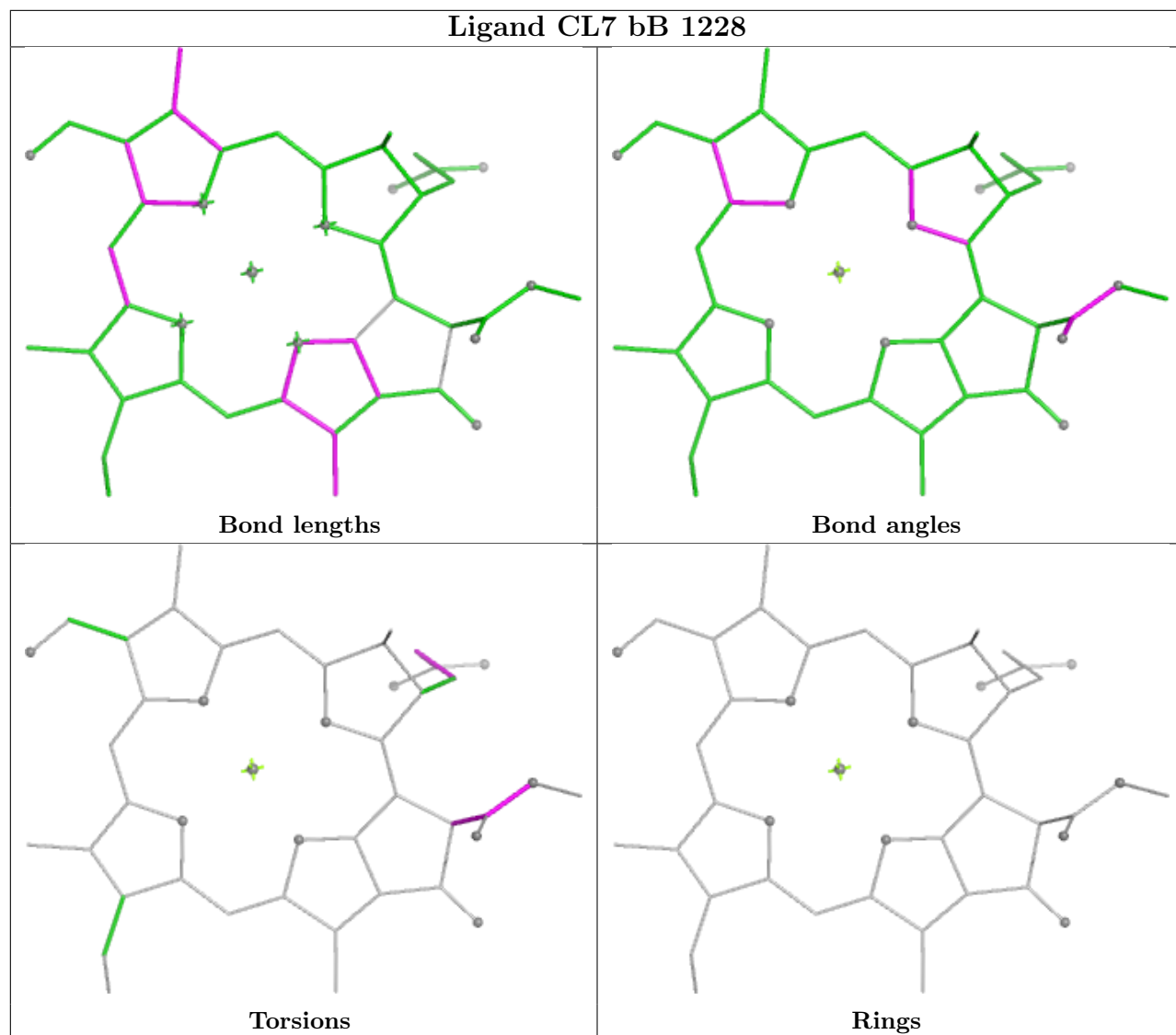


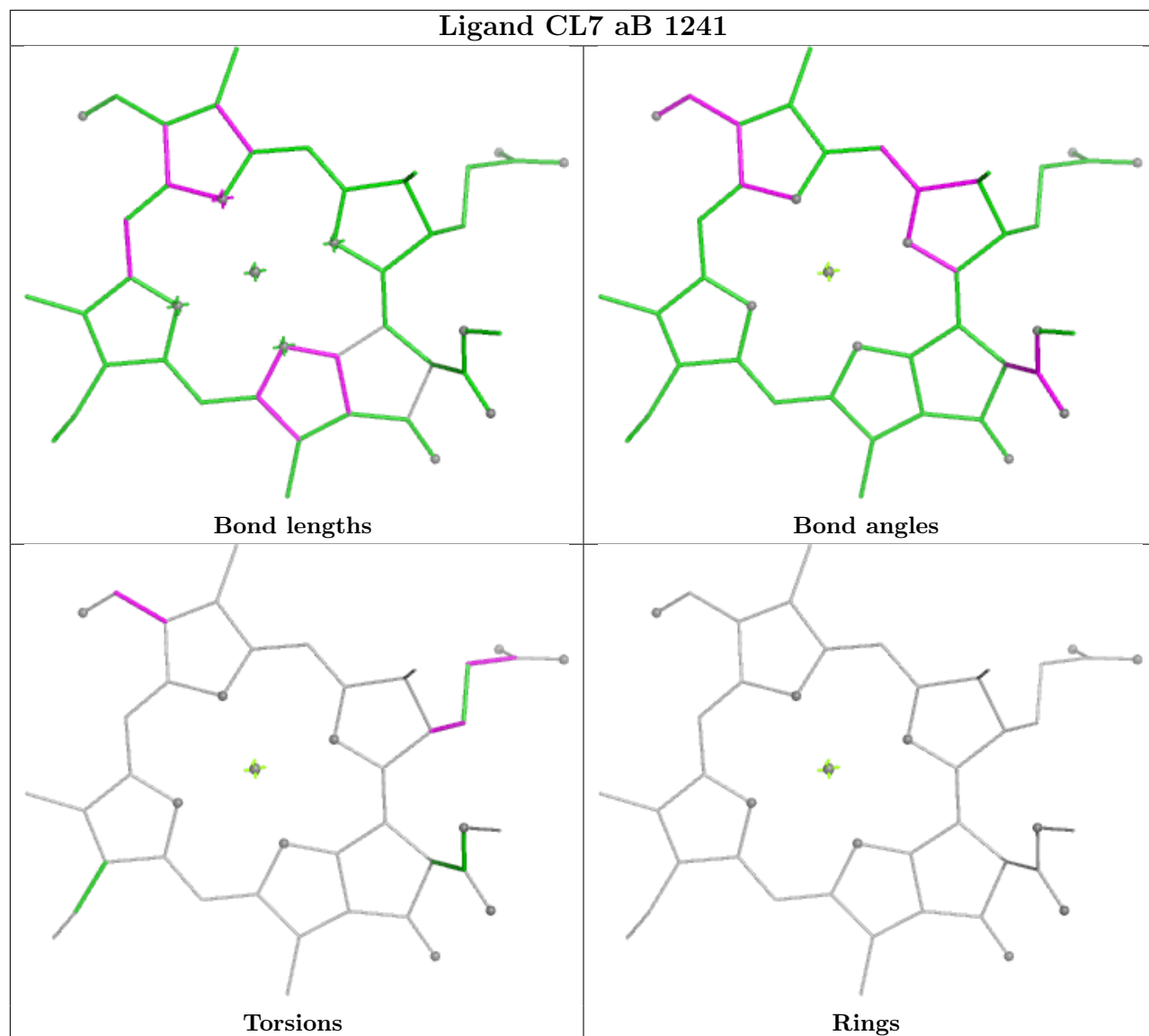
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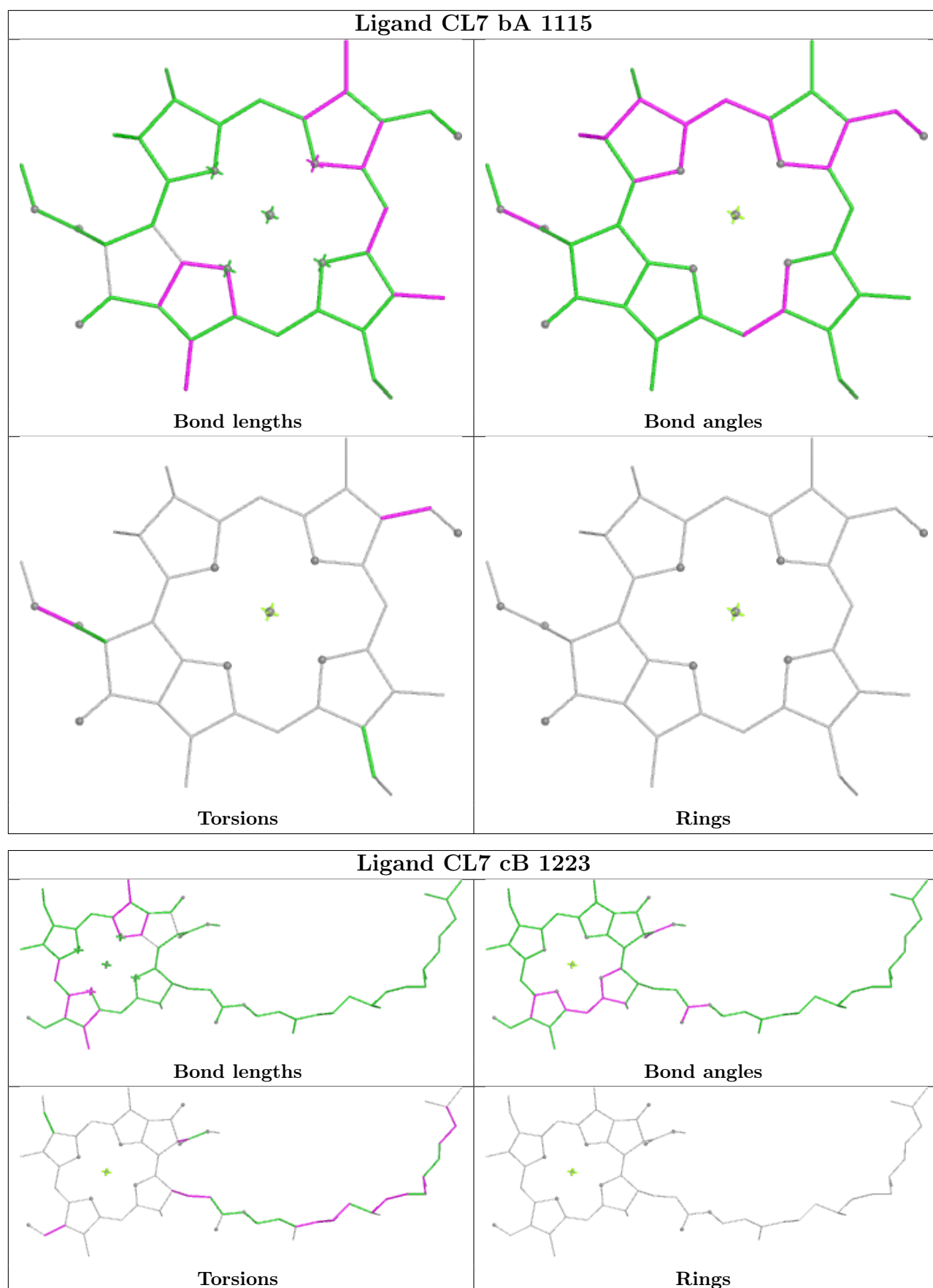




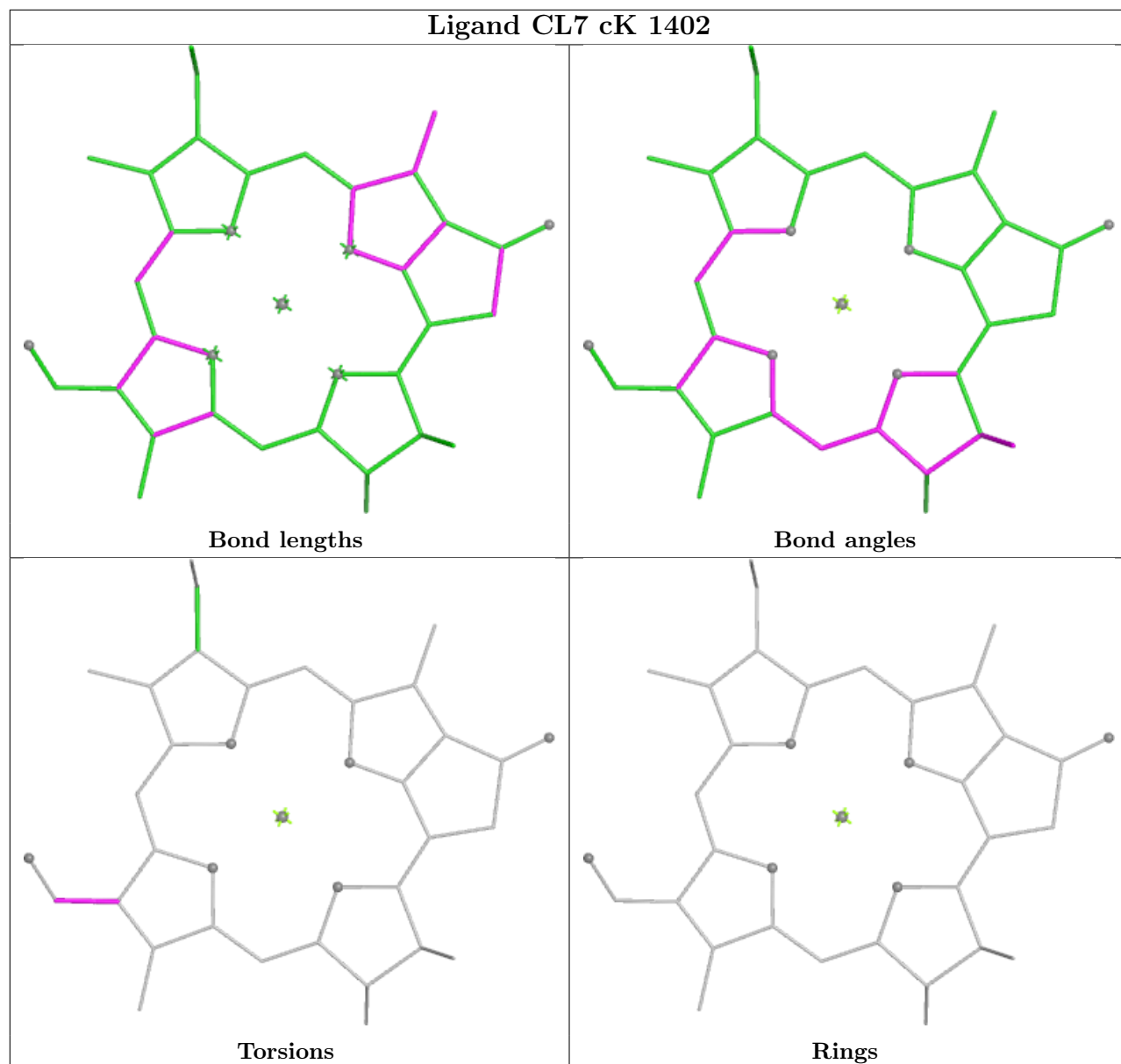
Ligand CL7 bB 1228

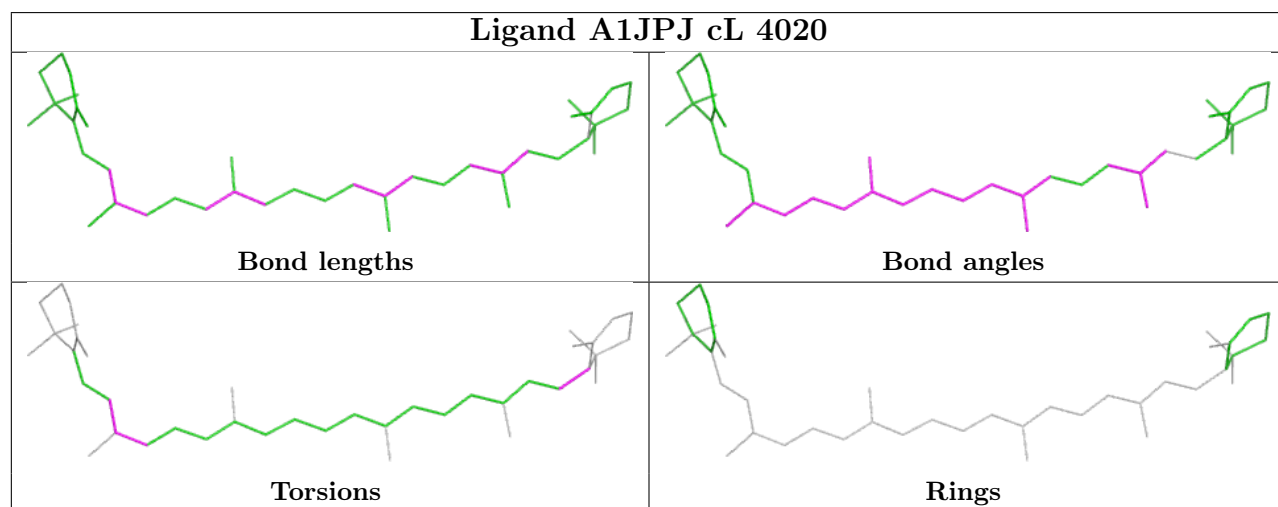
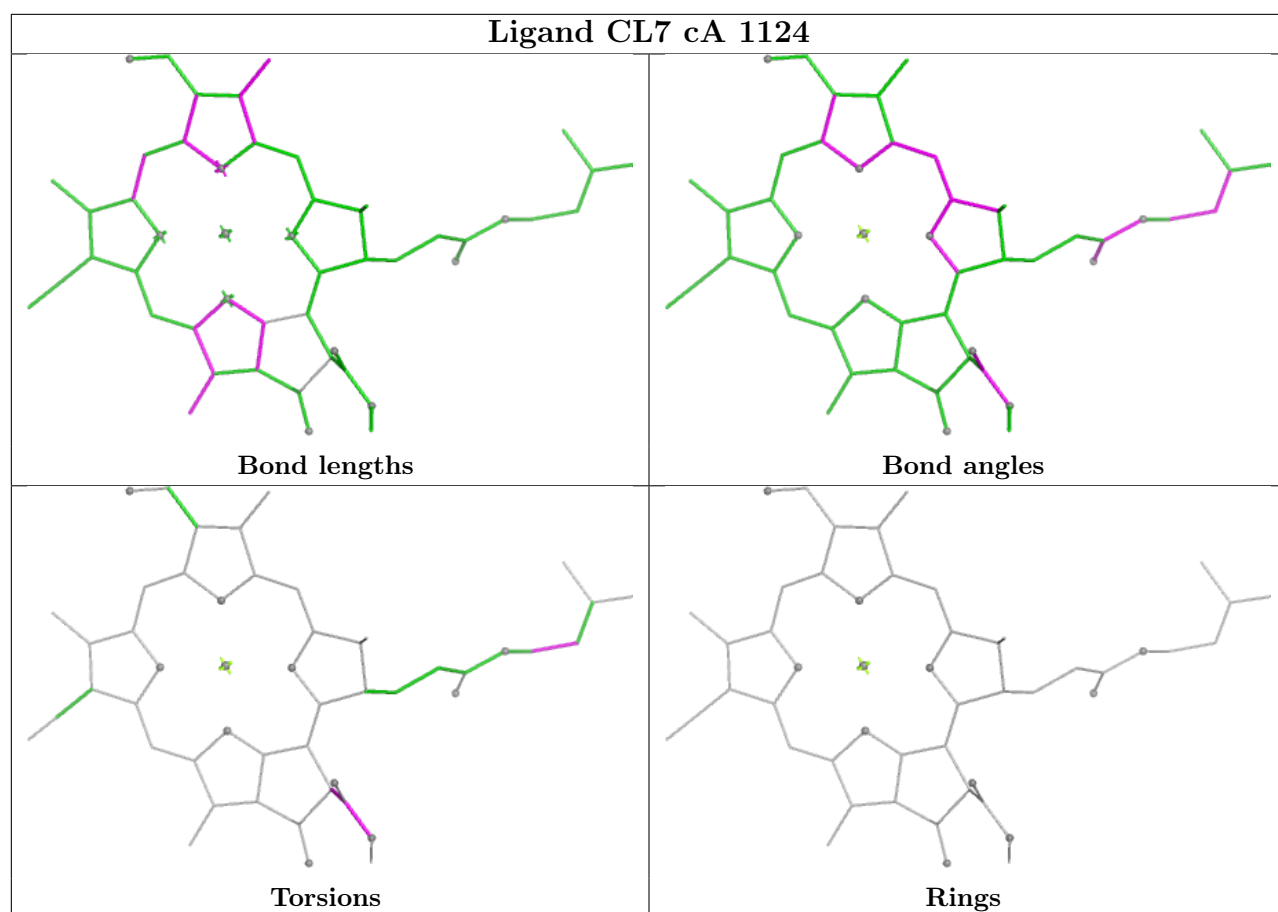


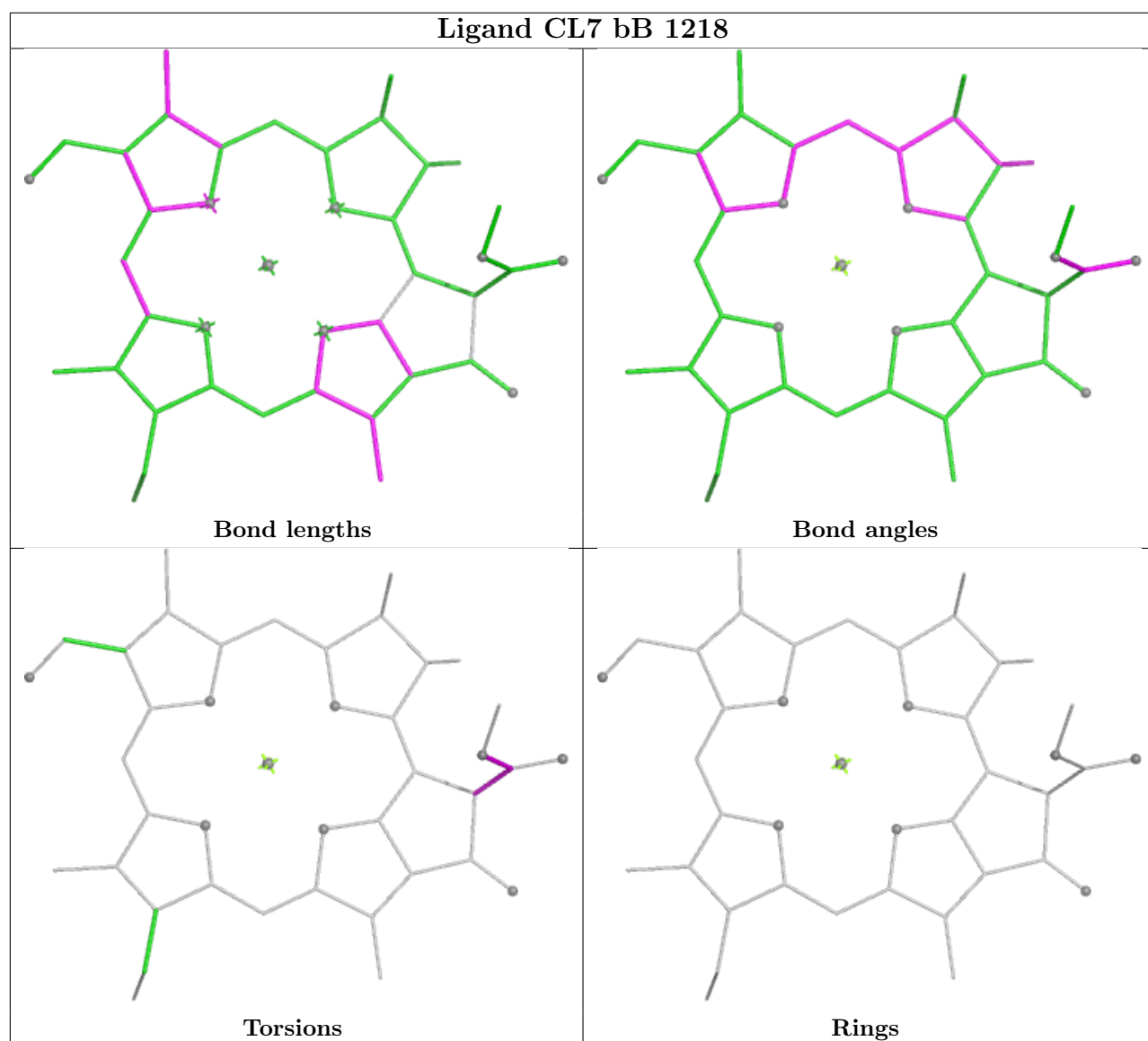




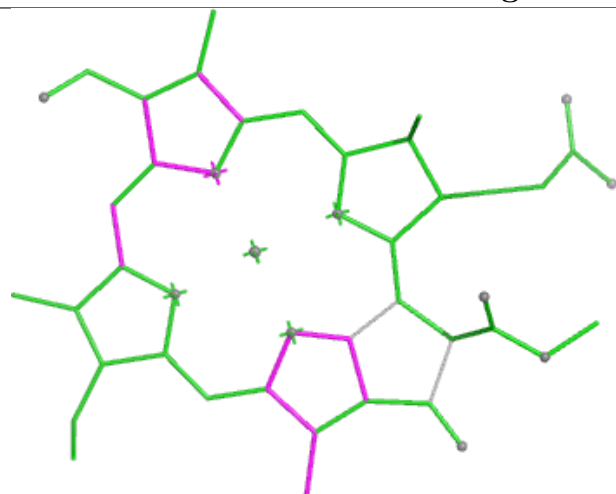
Ligand CL7 cK 1402



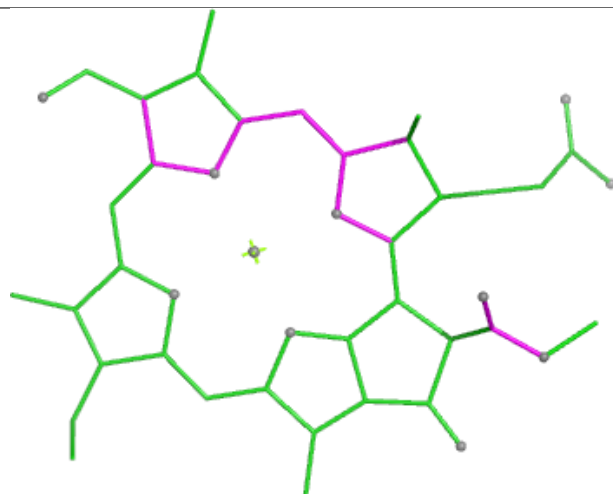




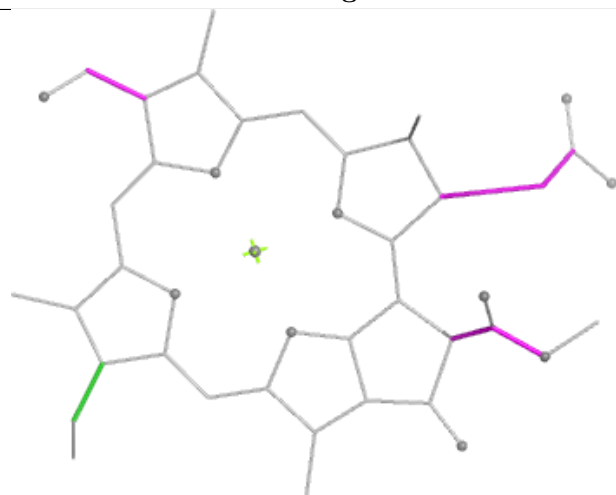
Ligand CL7 bA 1139



Bond lengths



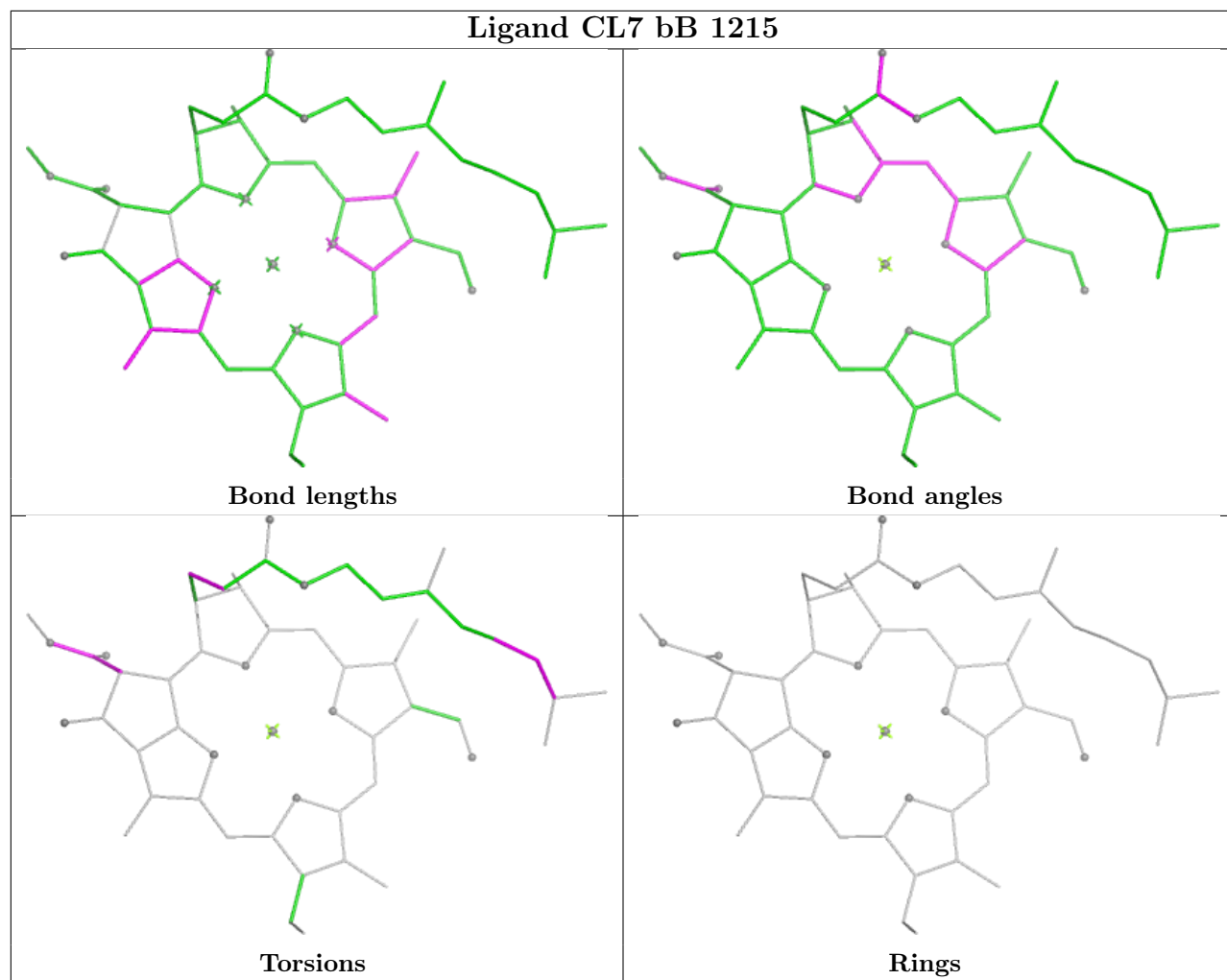
Bond angles

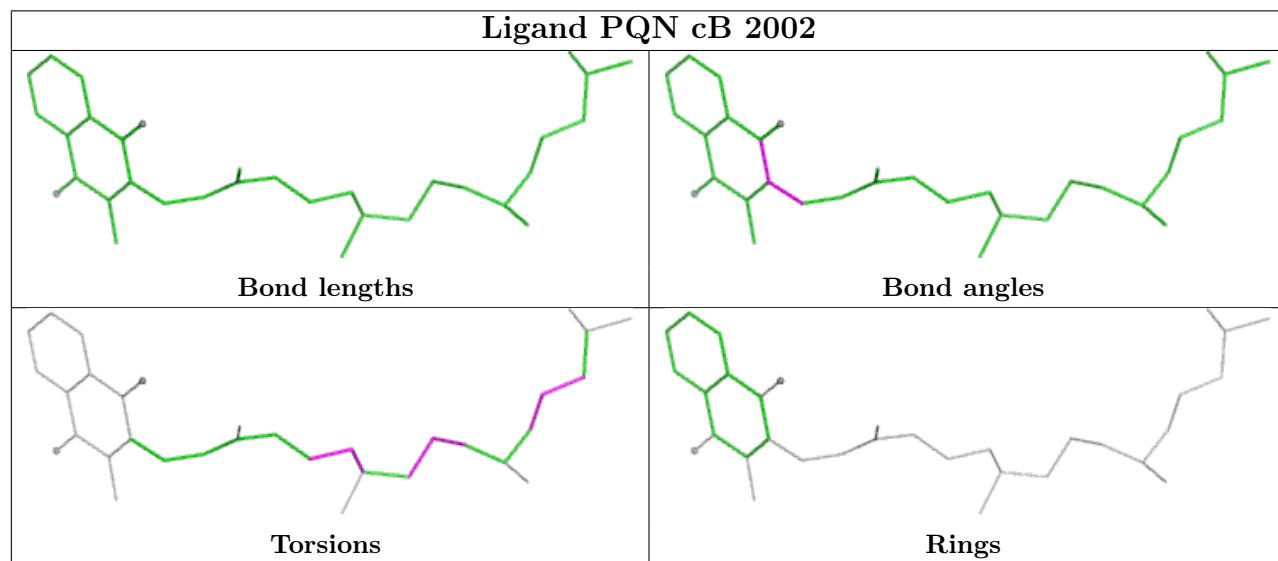
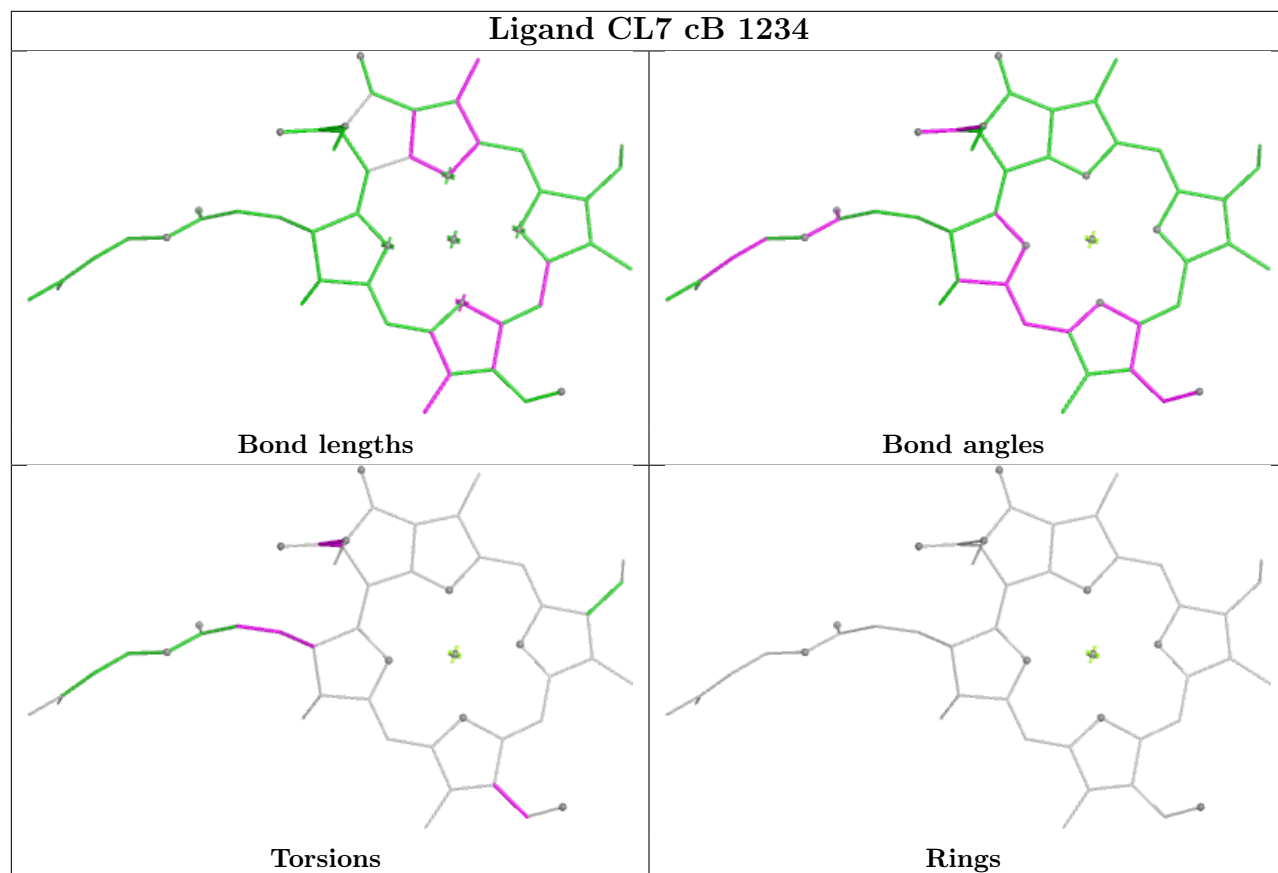


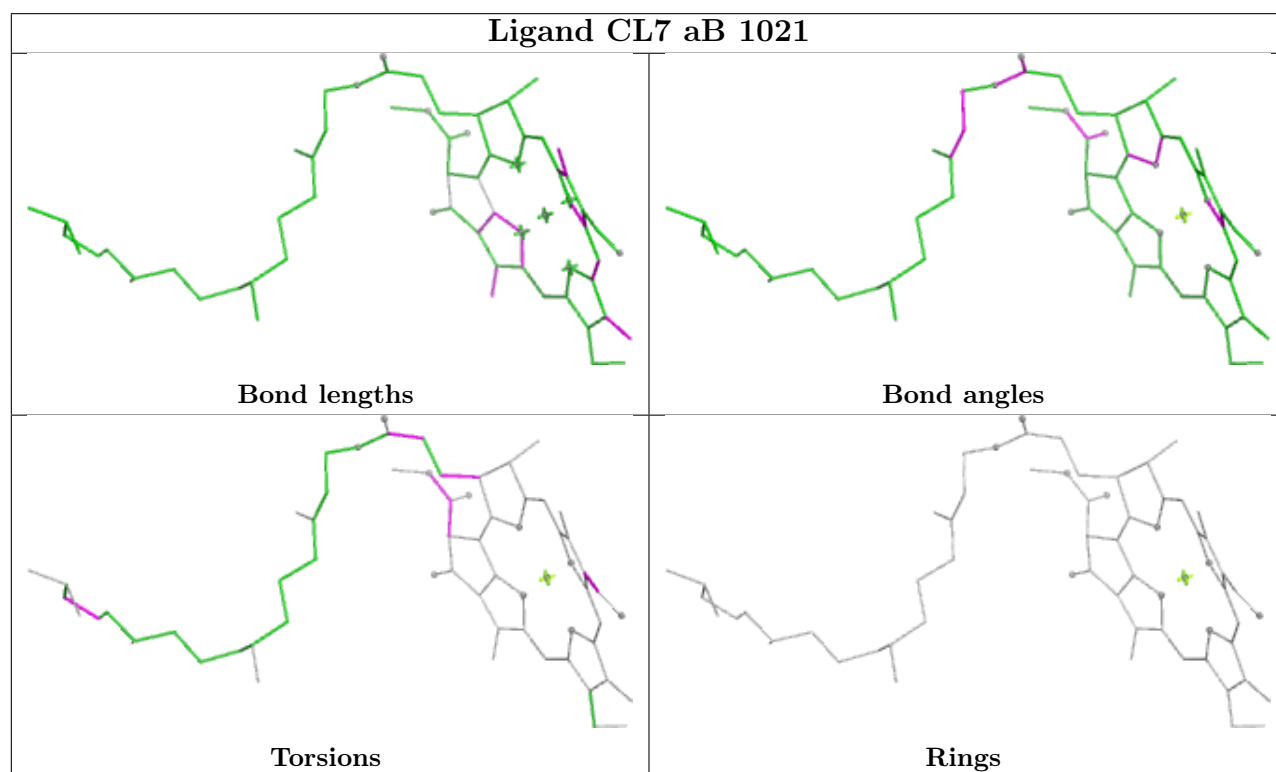
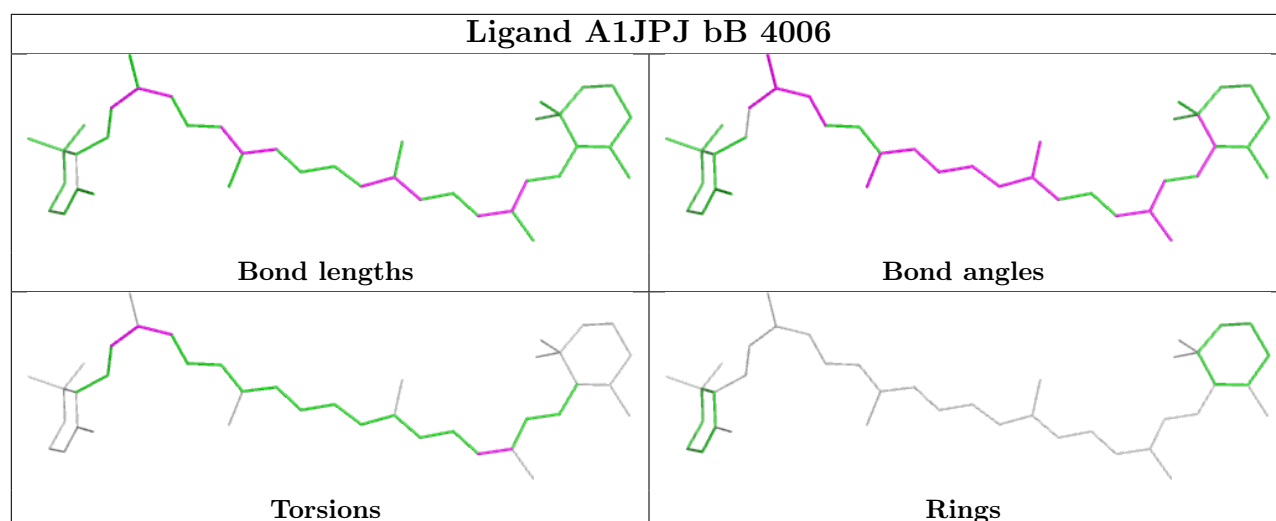
Torsions

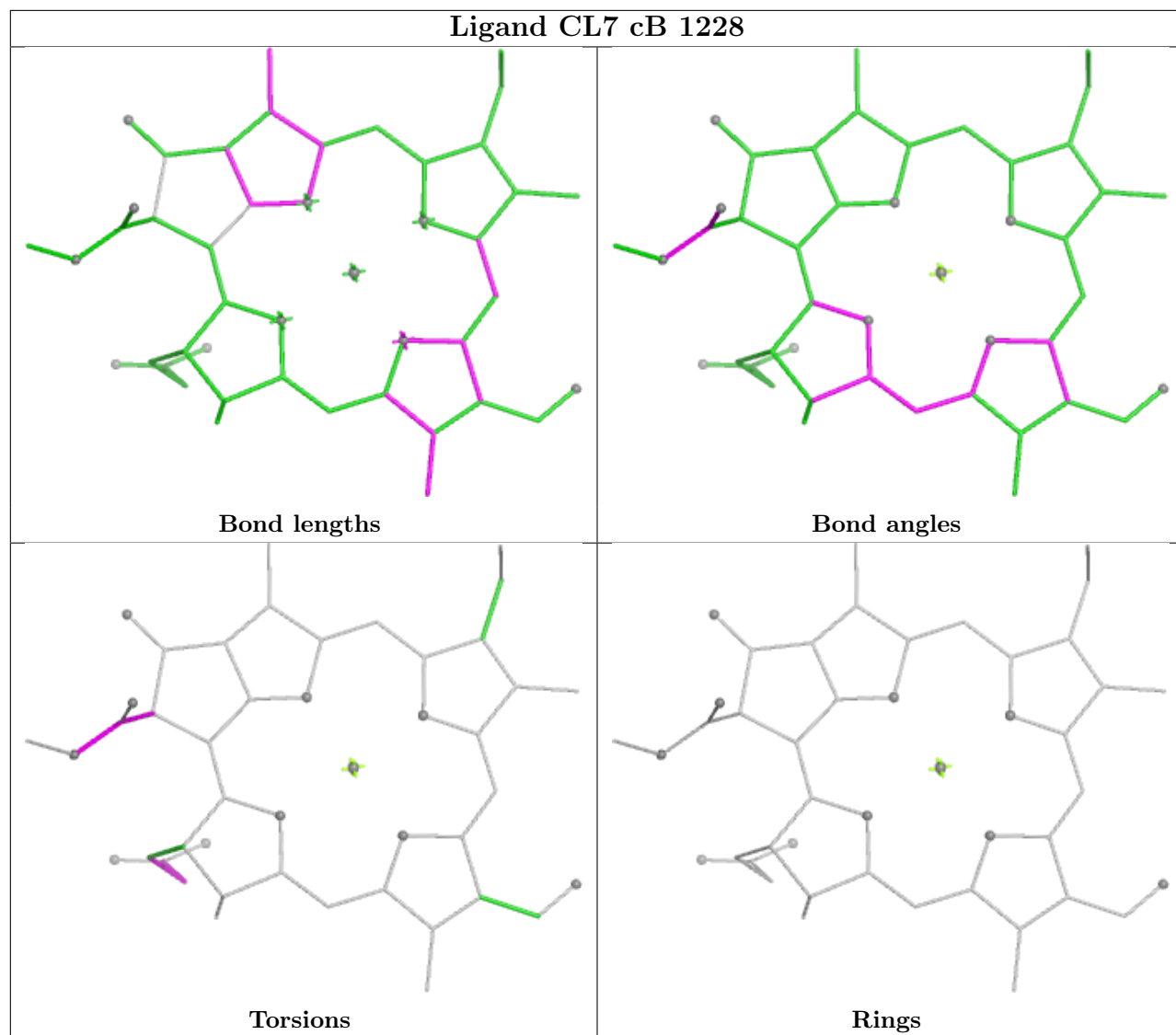


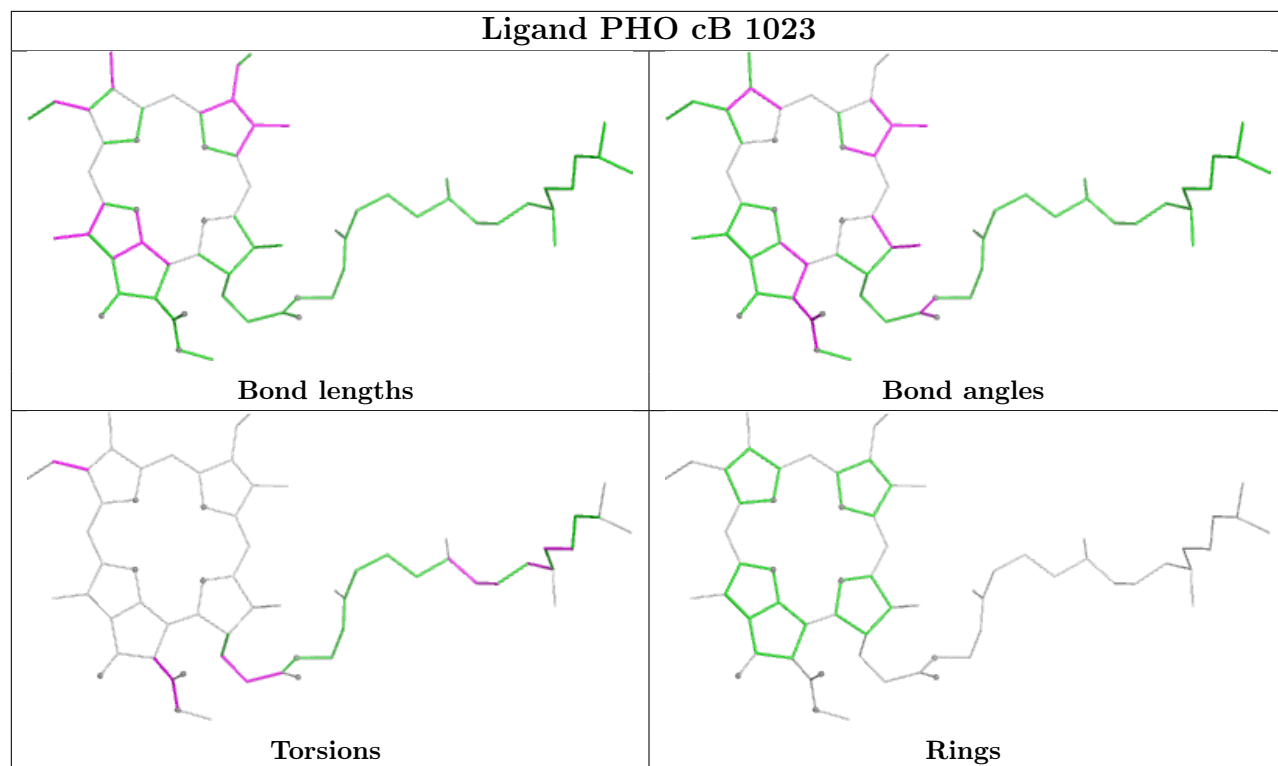
Rings



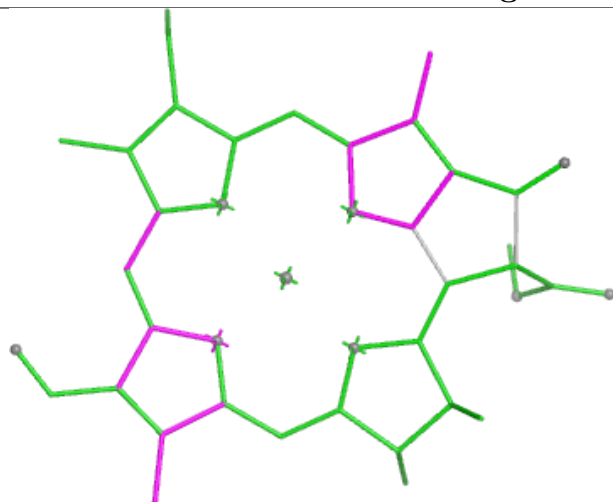




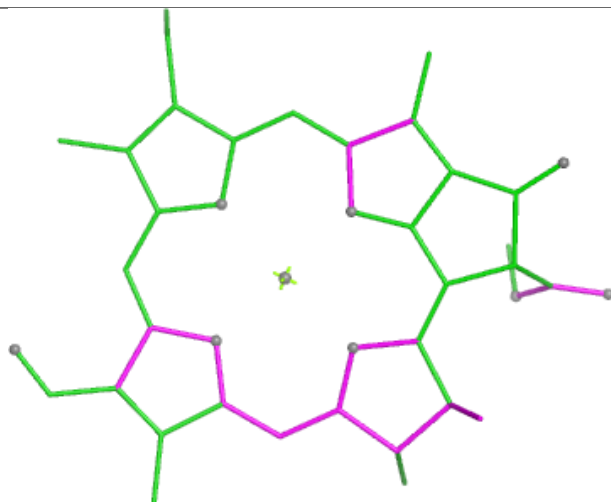




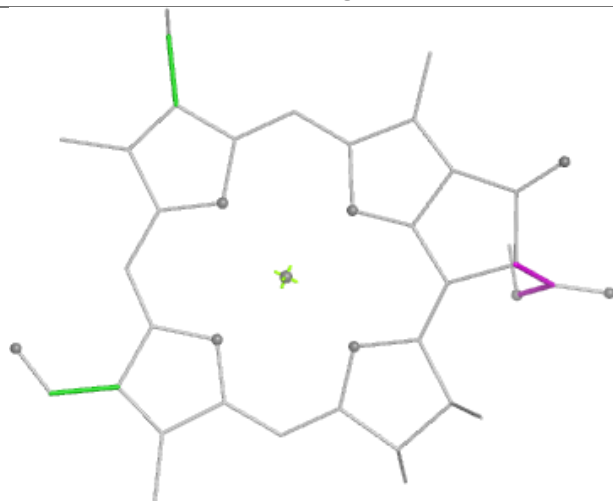
Ligand CL7 bB 1232



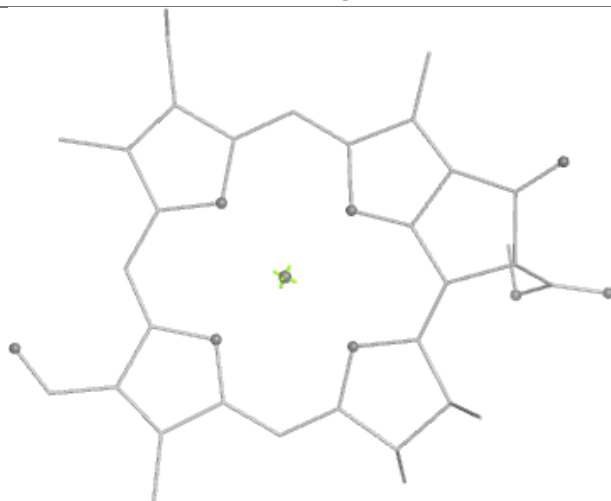
Bond lengths



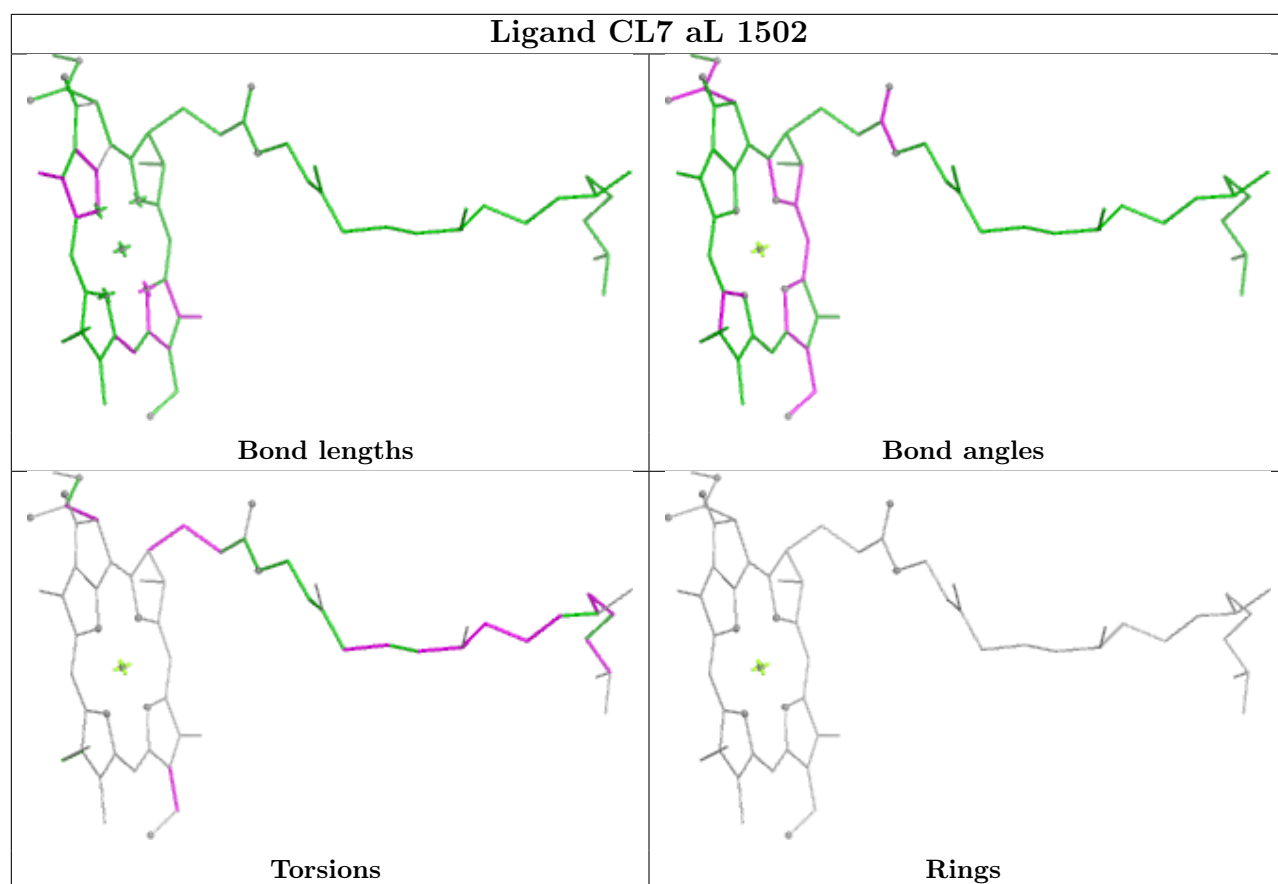
Bond angles



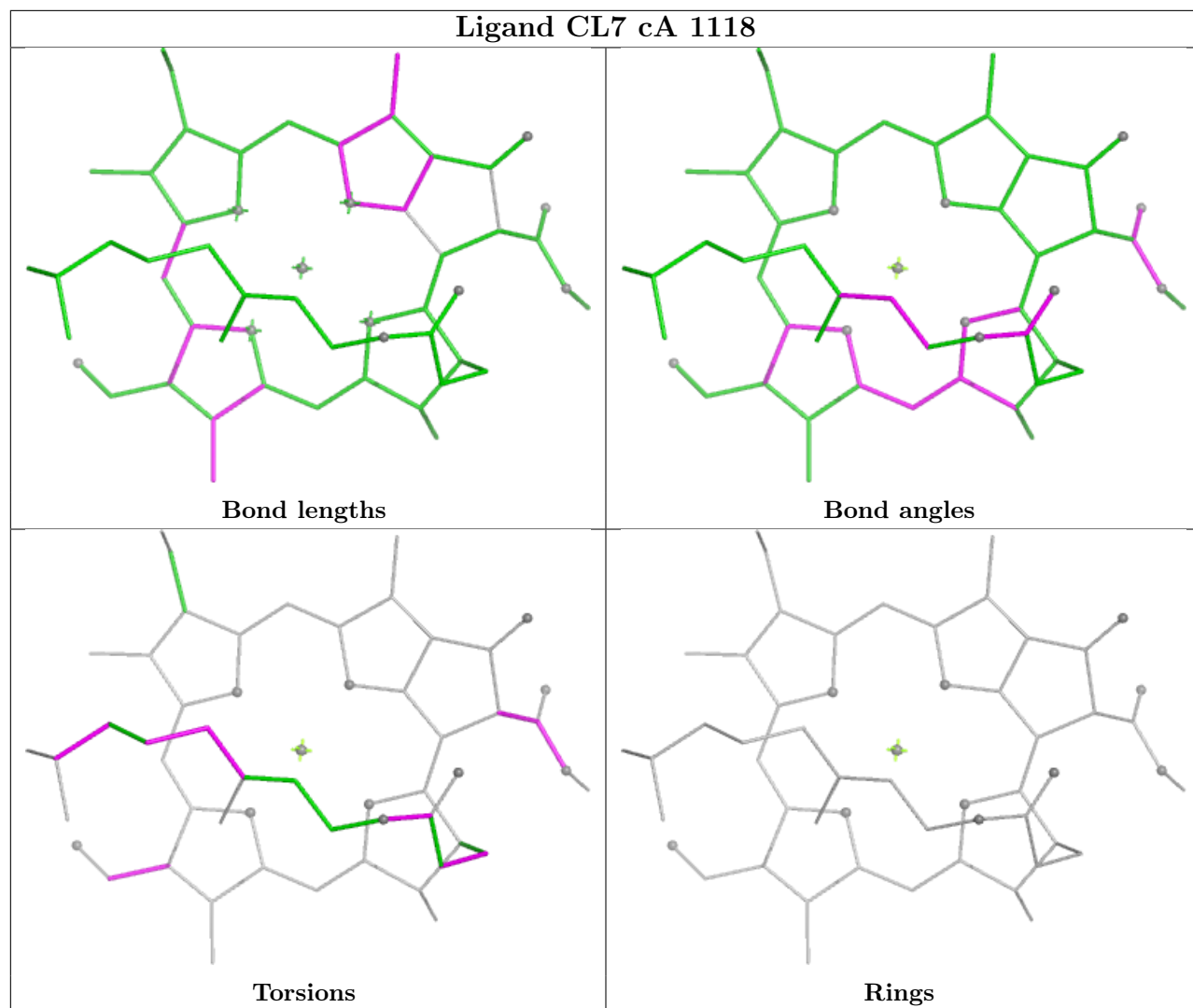
Torsions

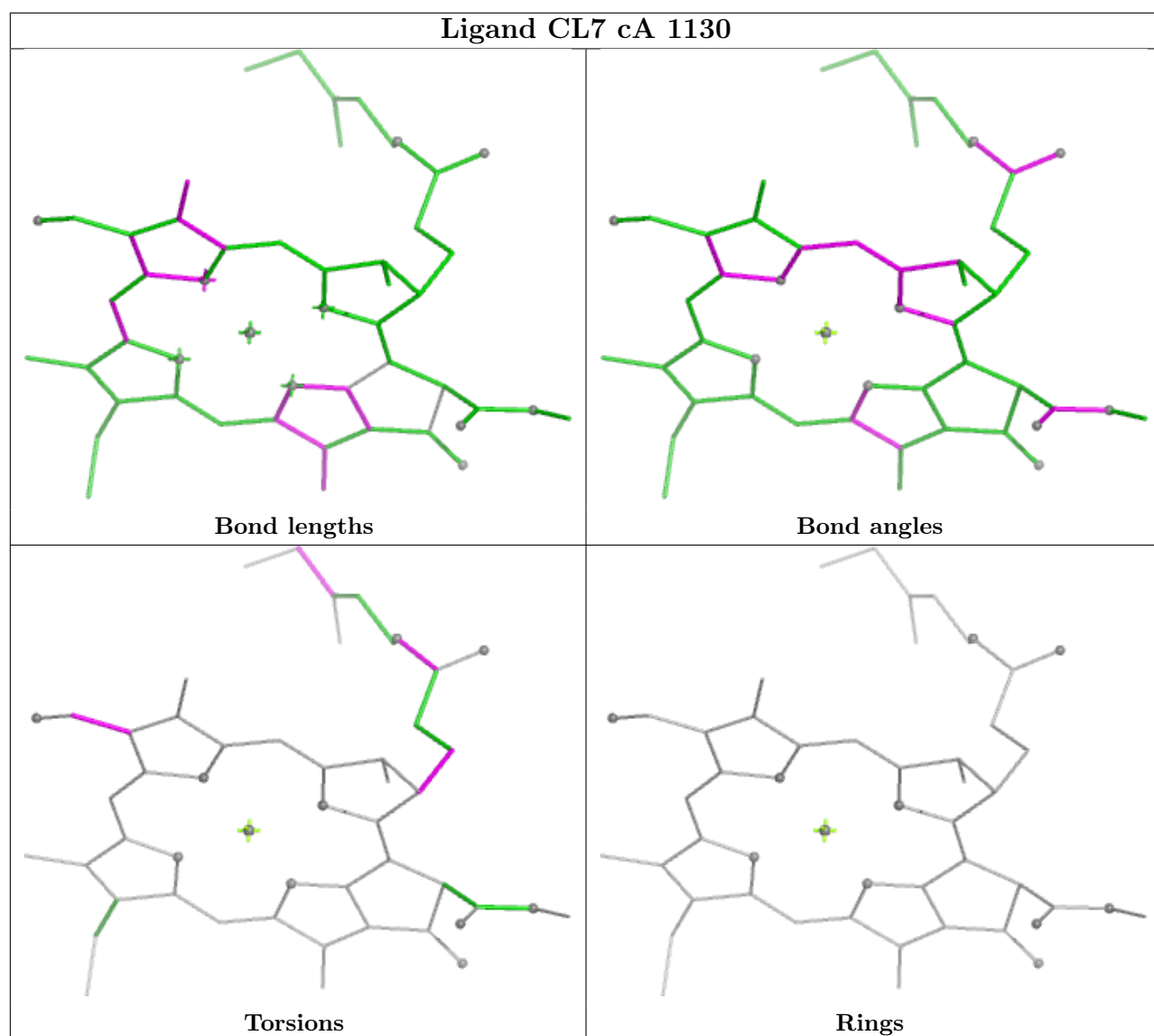


Rings

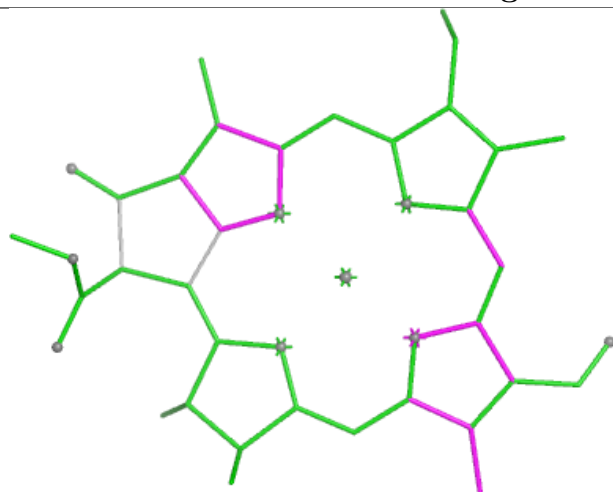


Ligand CL7 cA 1118

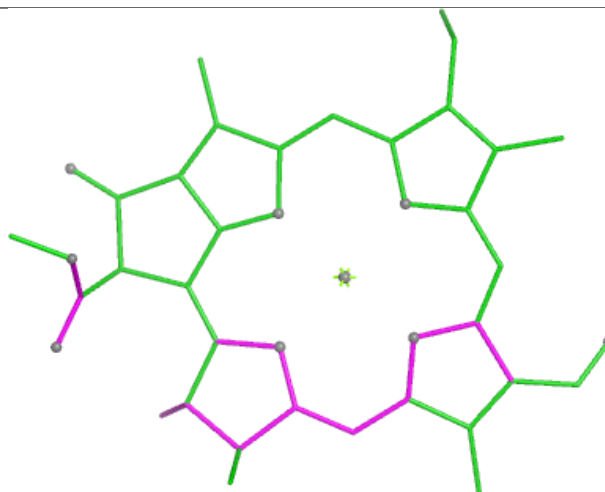




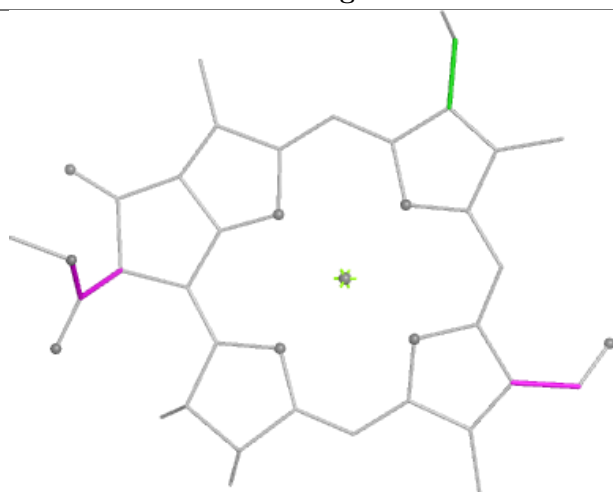
Ligand CL7 aA 1801



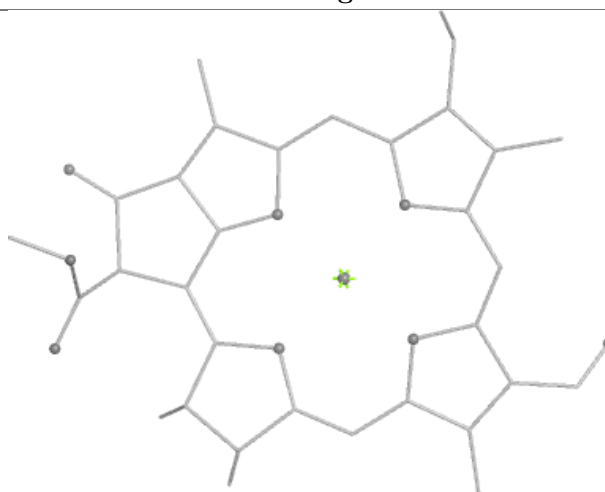
Bond lengths



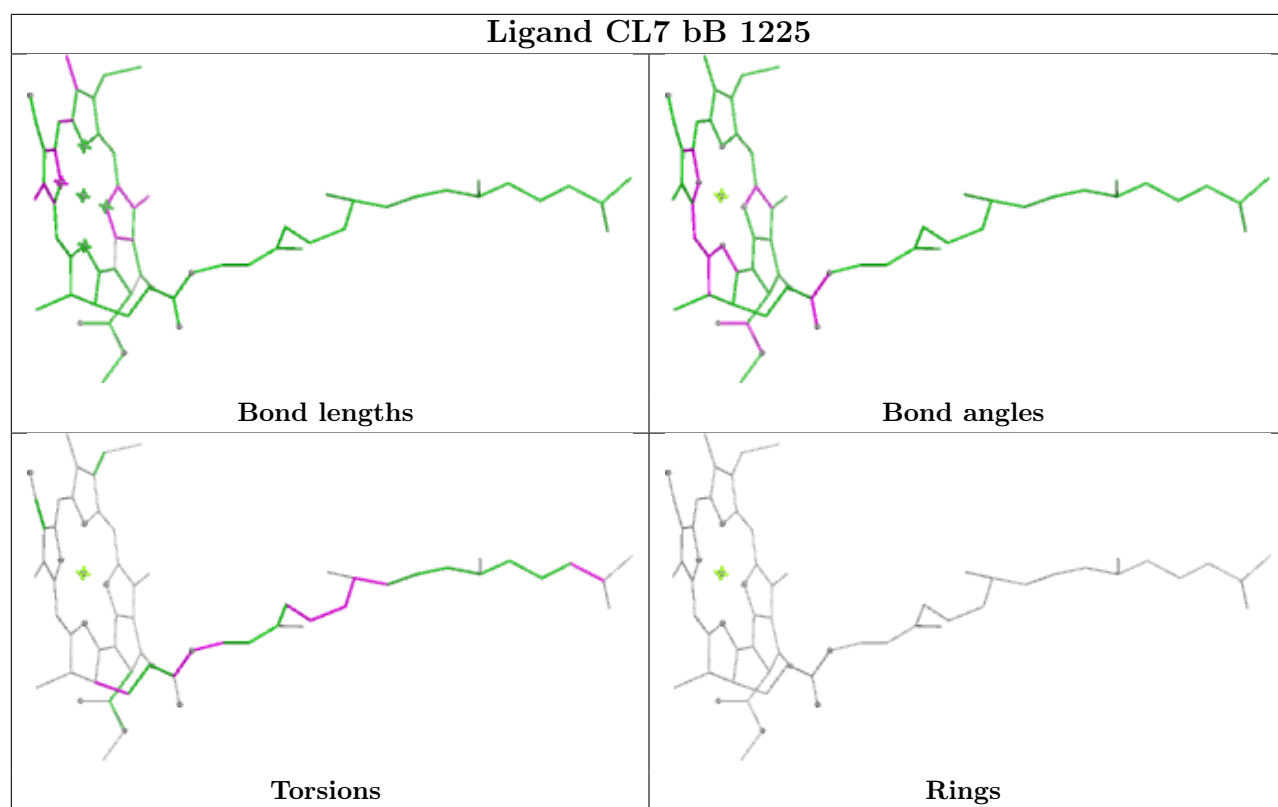
Bond angles



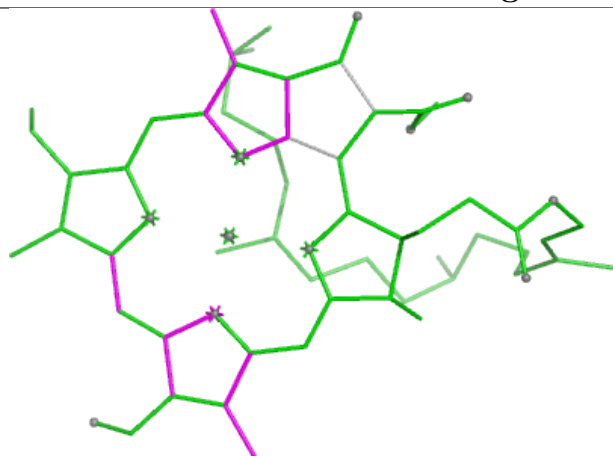
Torsions



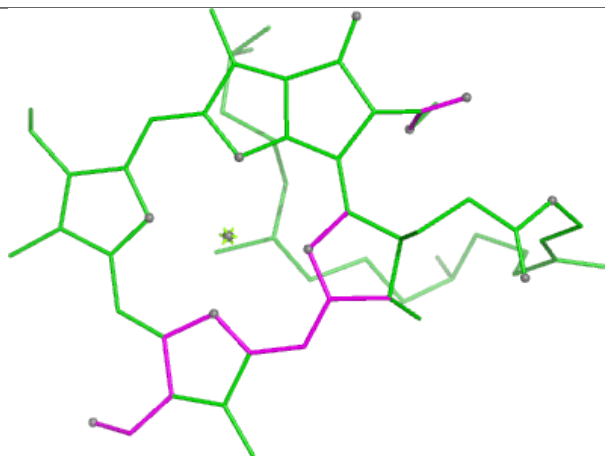
Rings



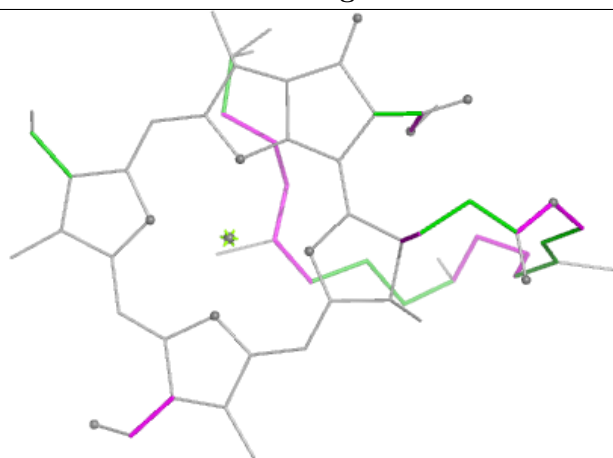
Ligand CL7 cA 1104



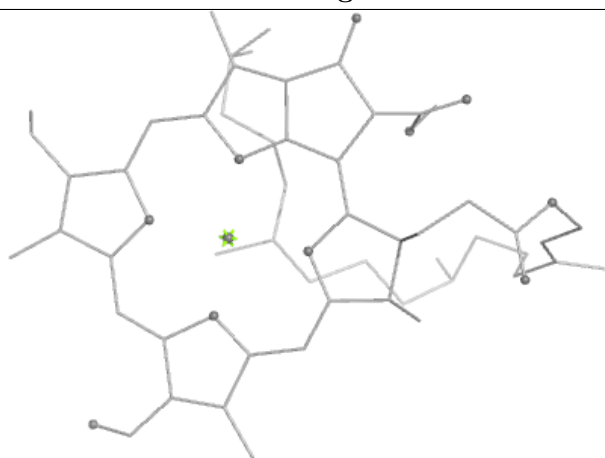
Bond lengths



Bond angles

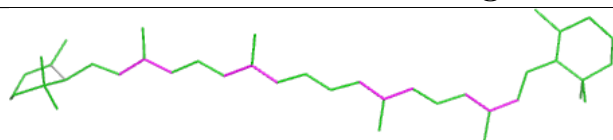


Torsions

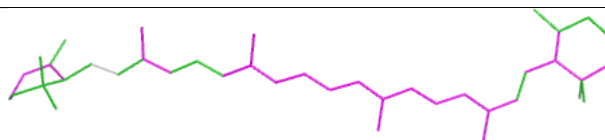


Rings

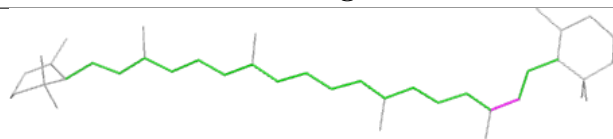
Ligand A1JPJ cB 4015



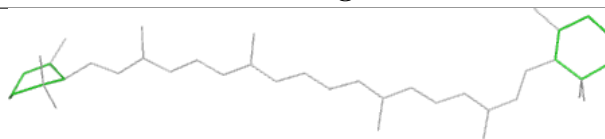
Bond lengths



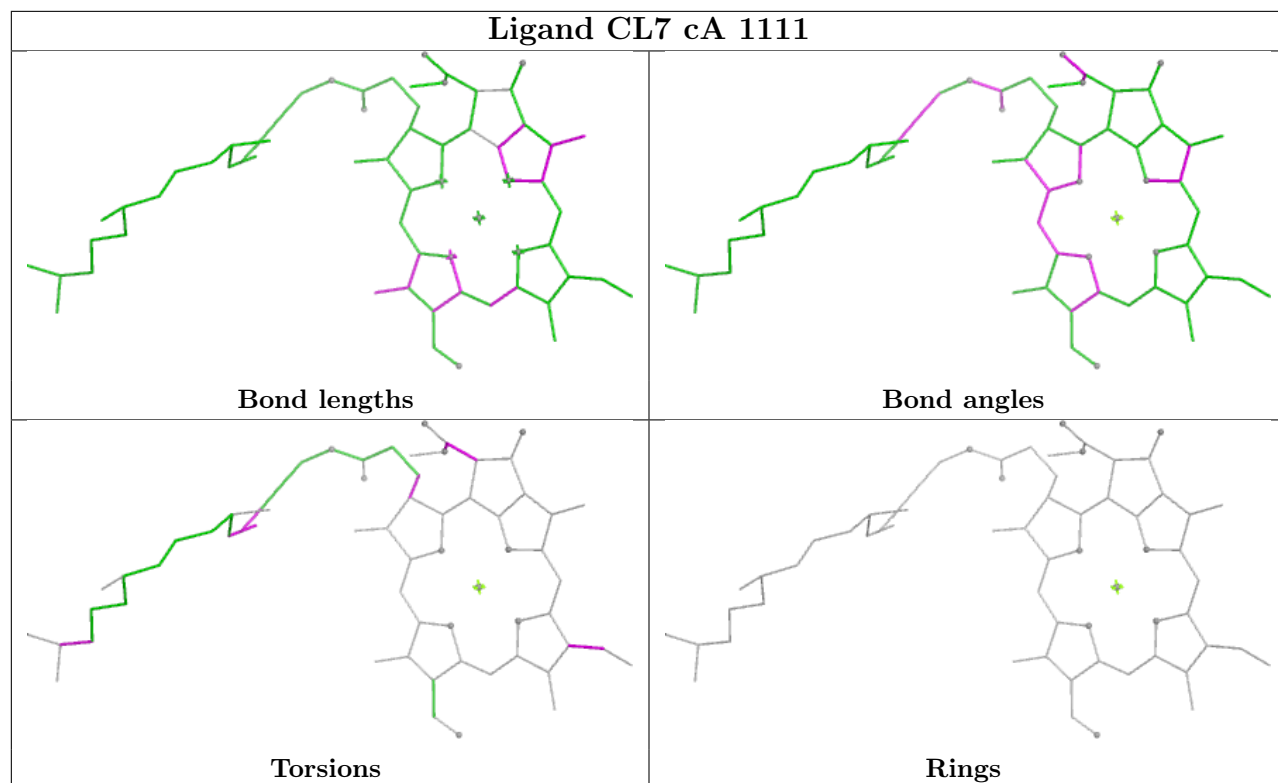
Bond angles



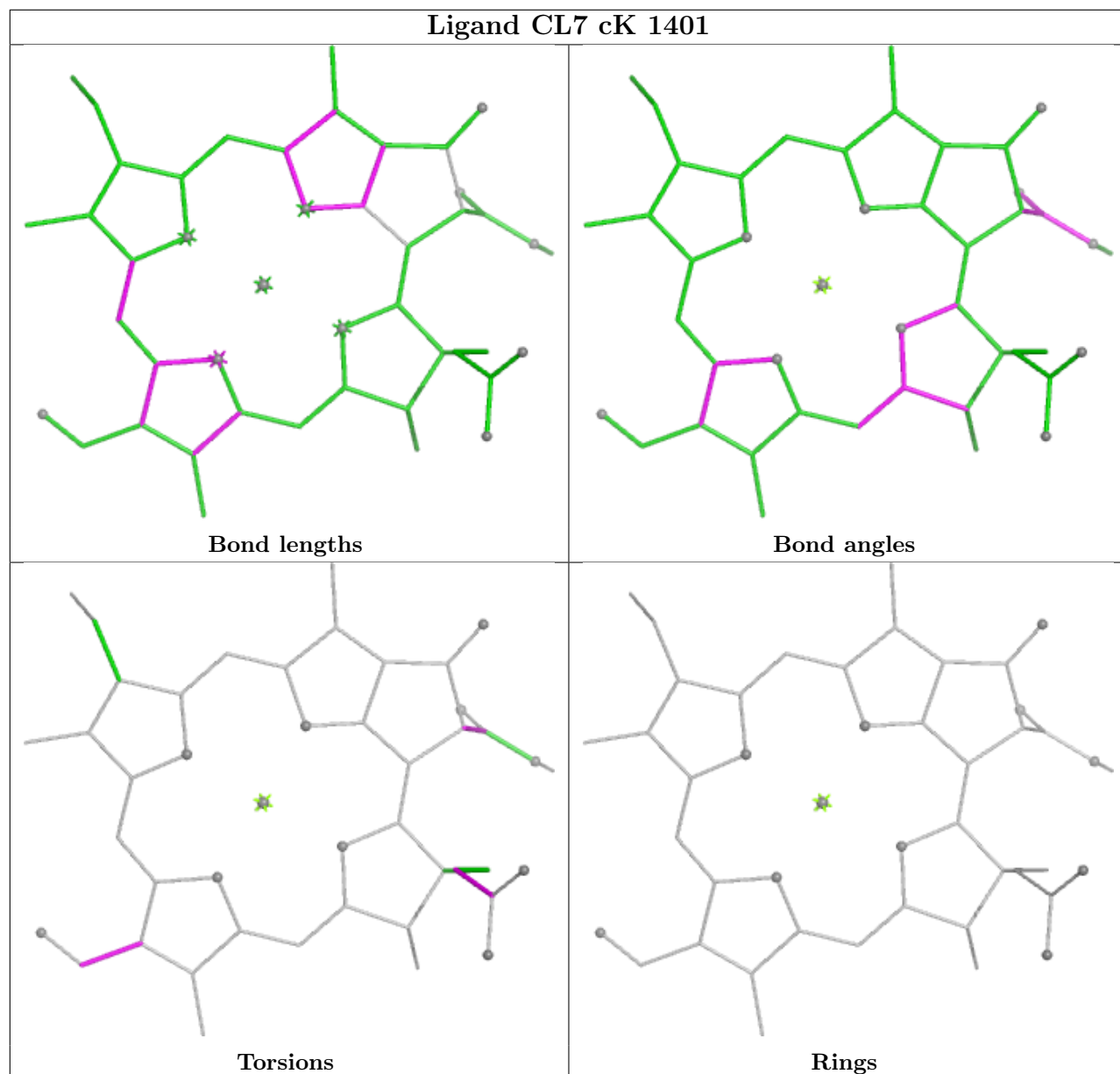
Torsions



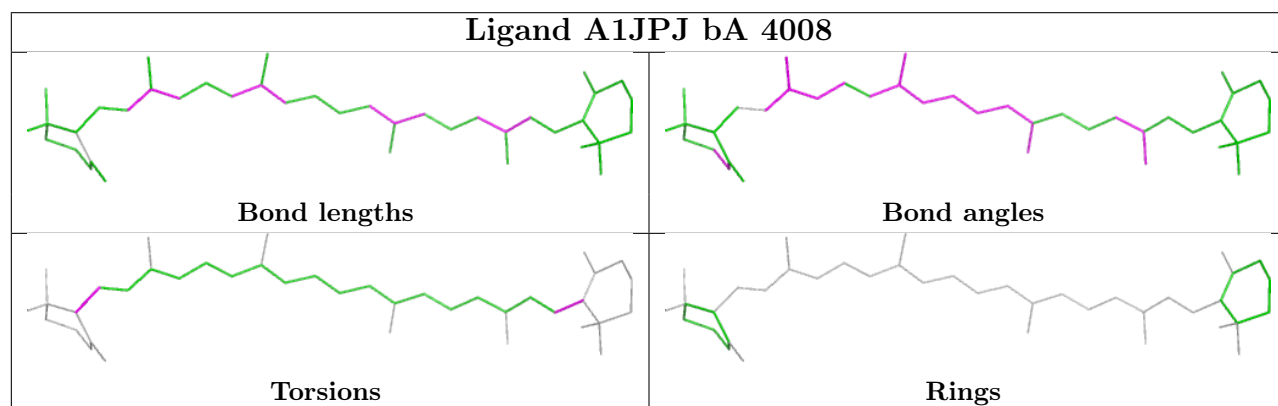
Rings

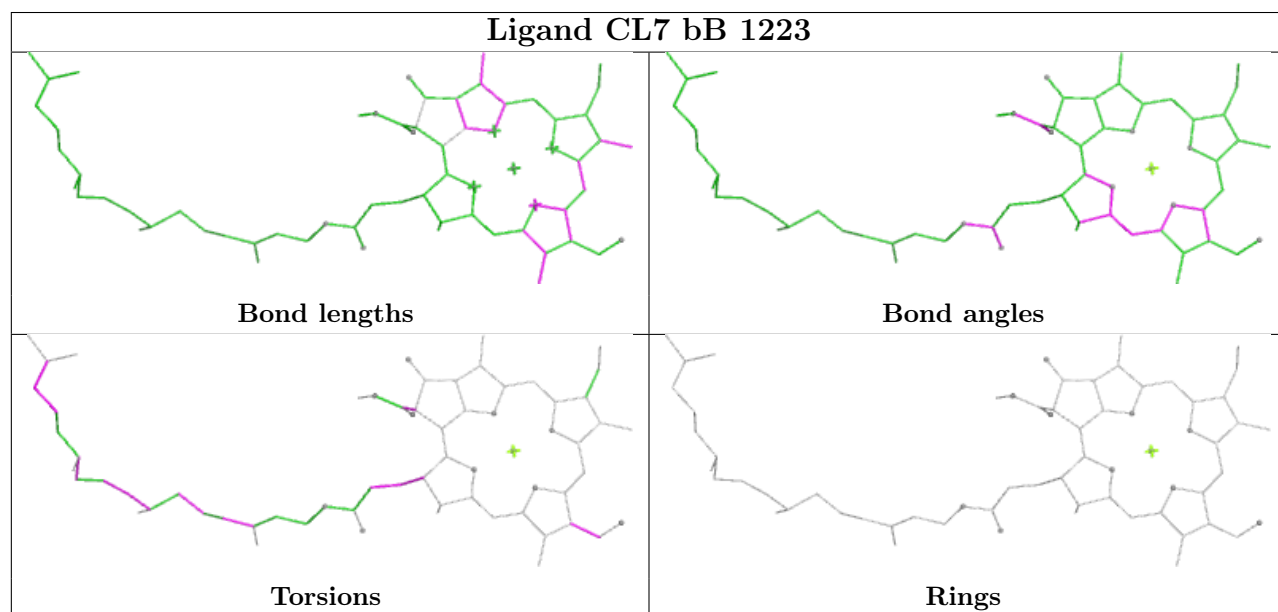
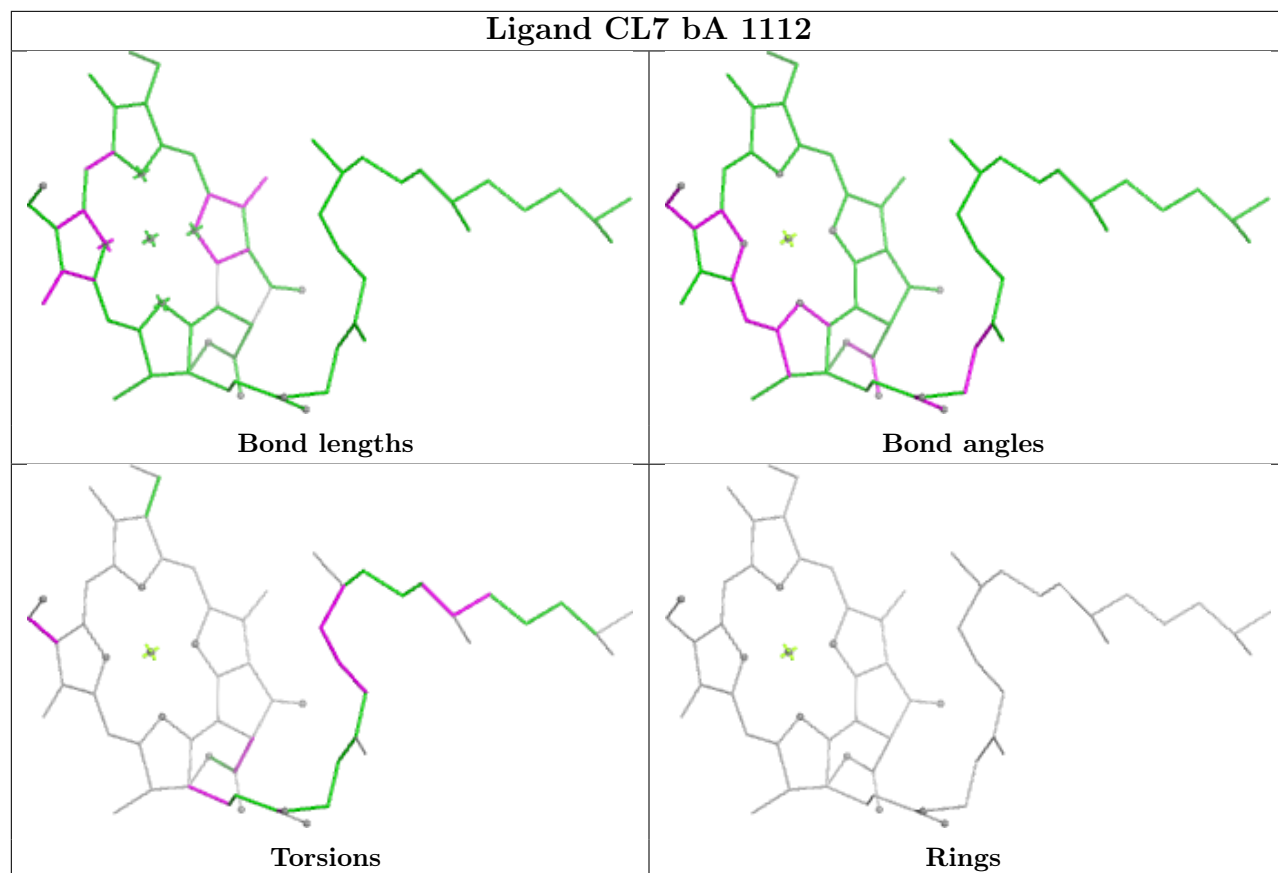


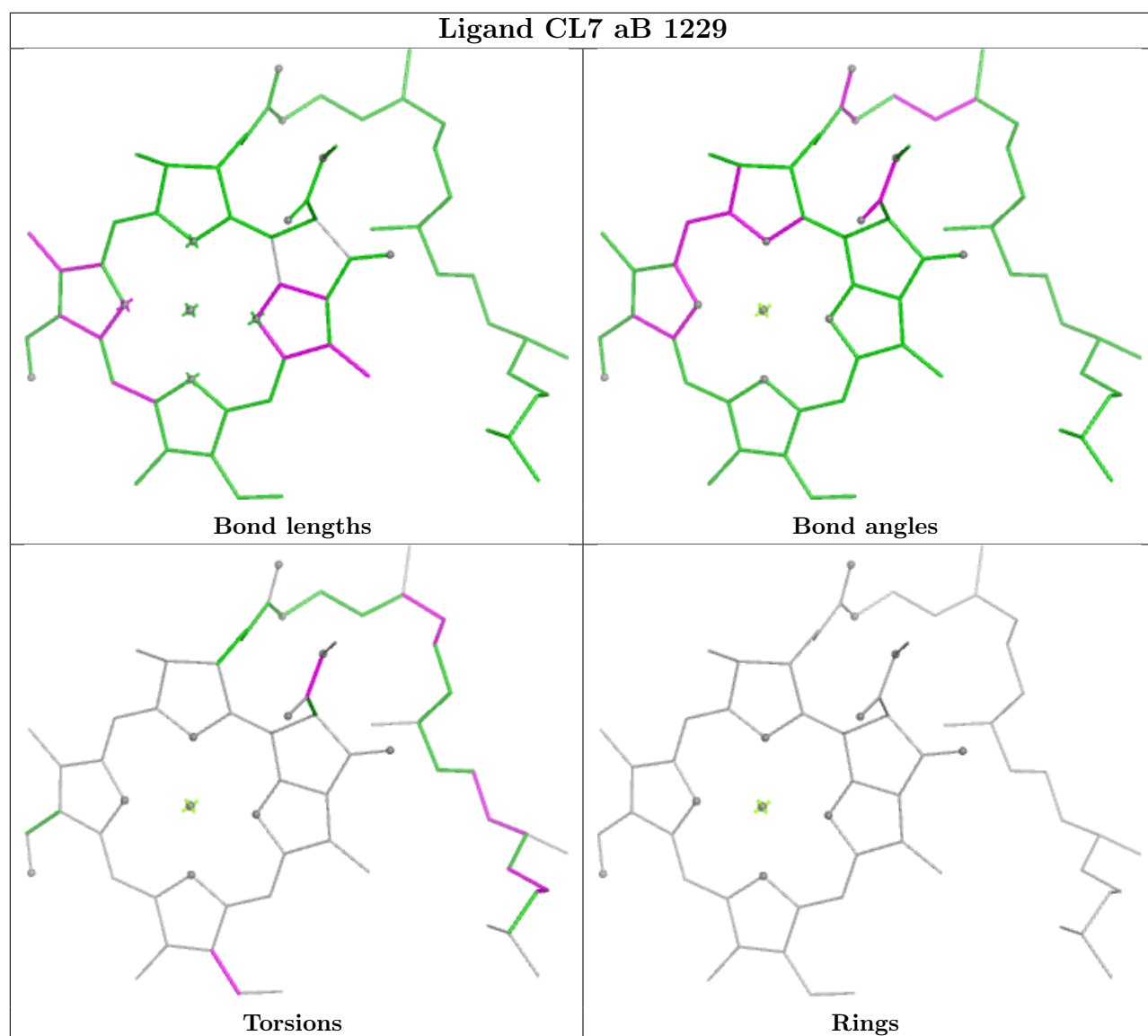
Ligand CL7 cK 1401

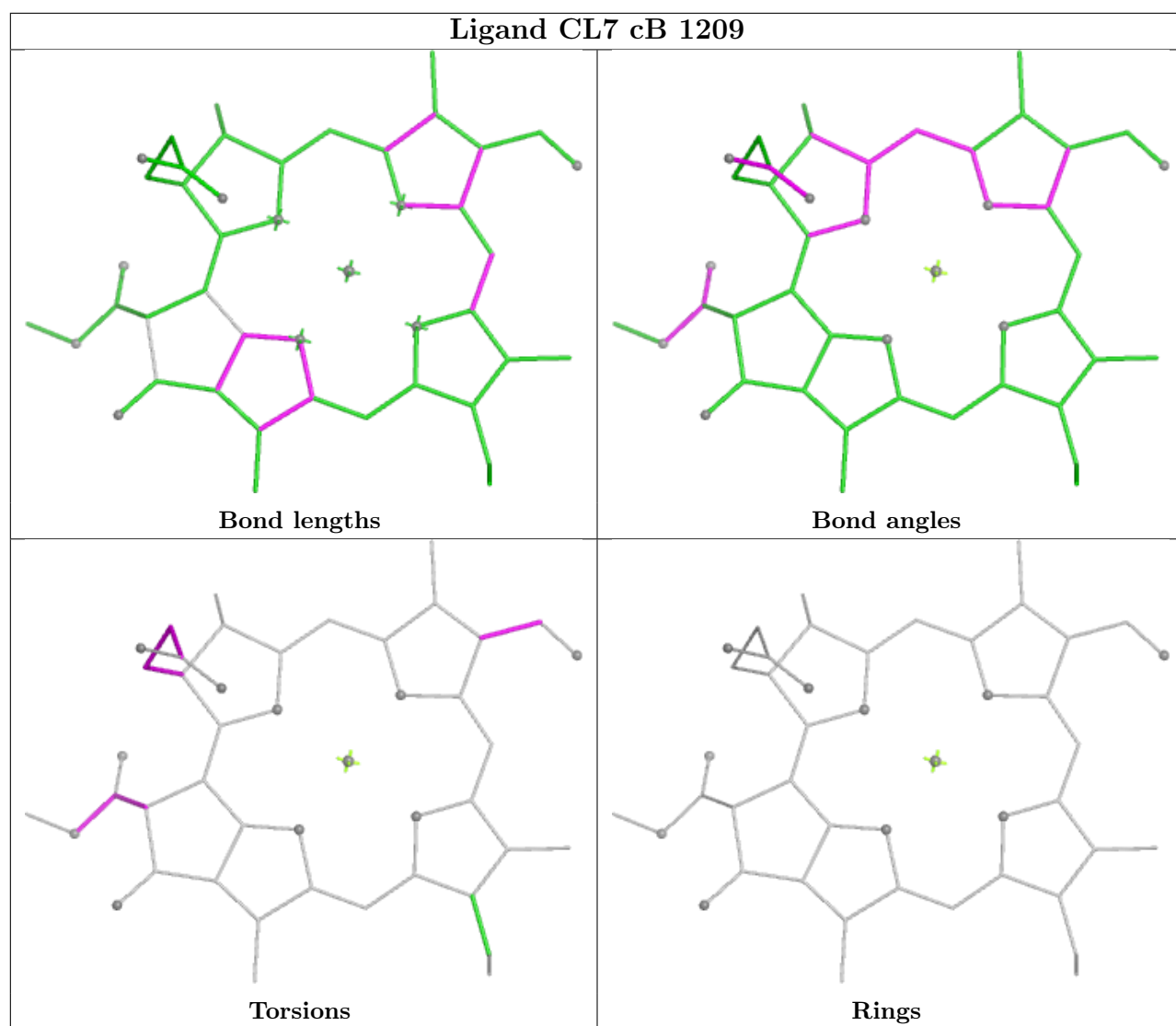


Ligand A1JPJ bA 4008

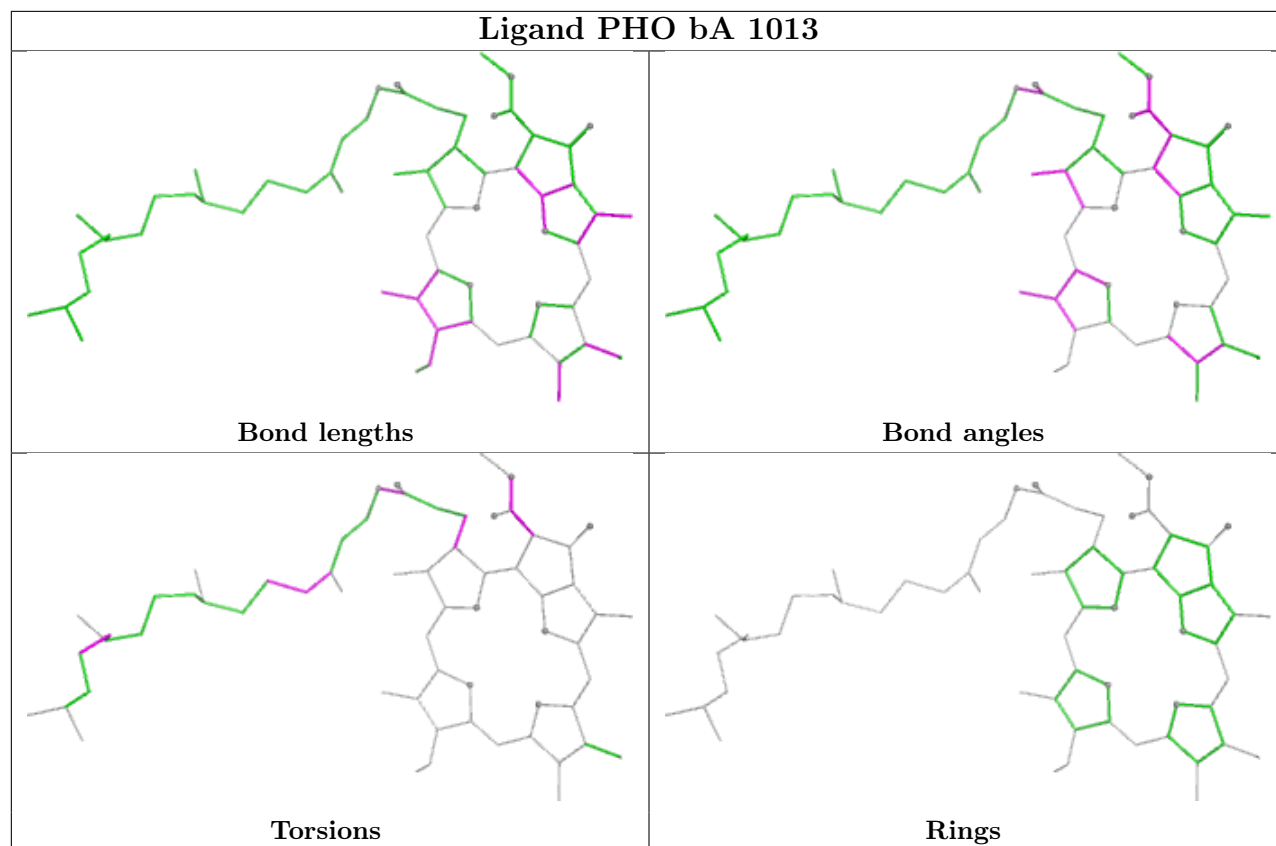




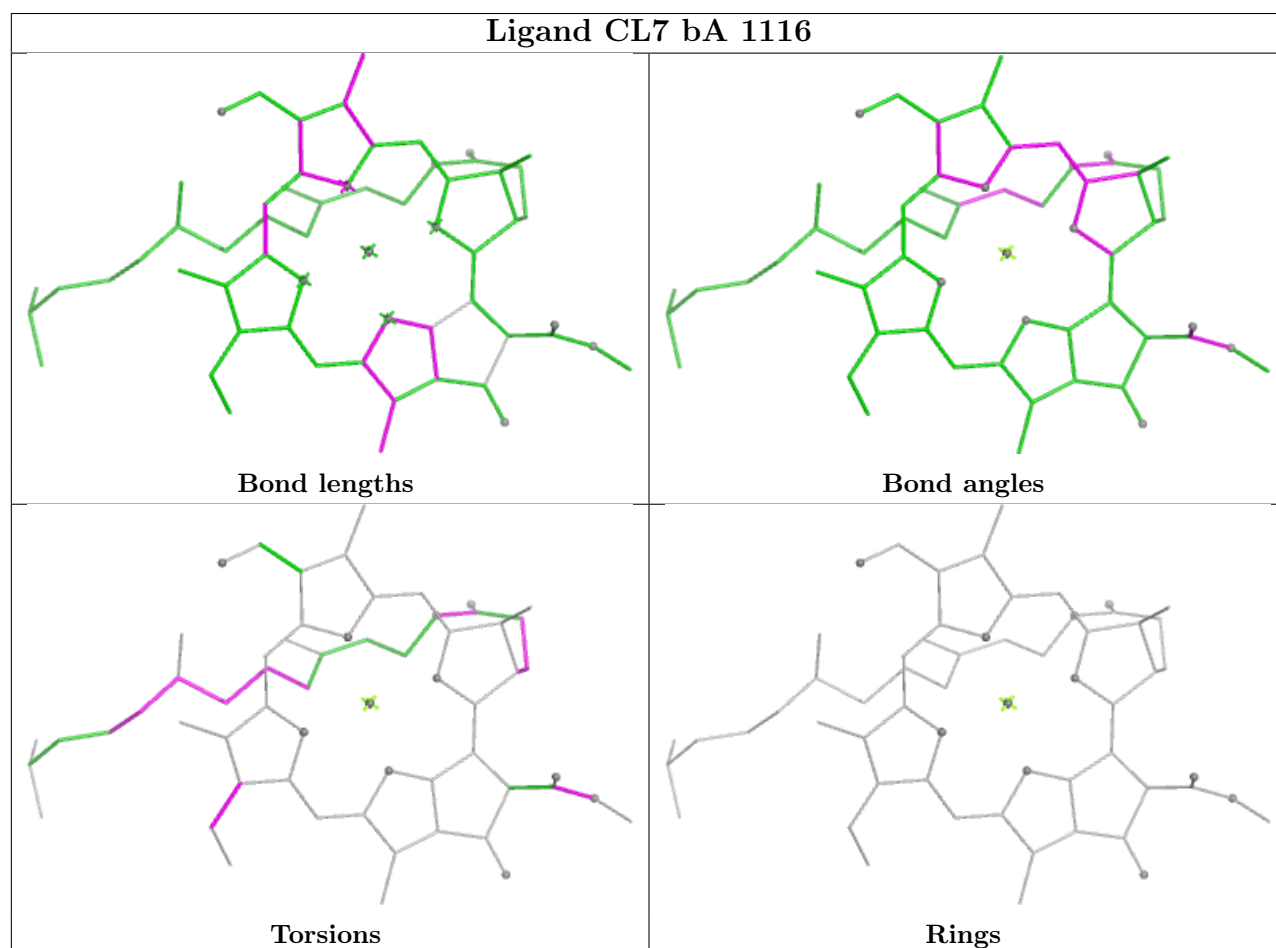




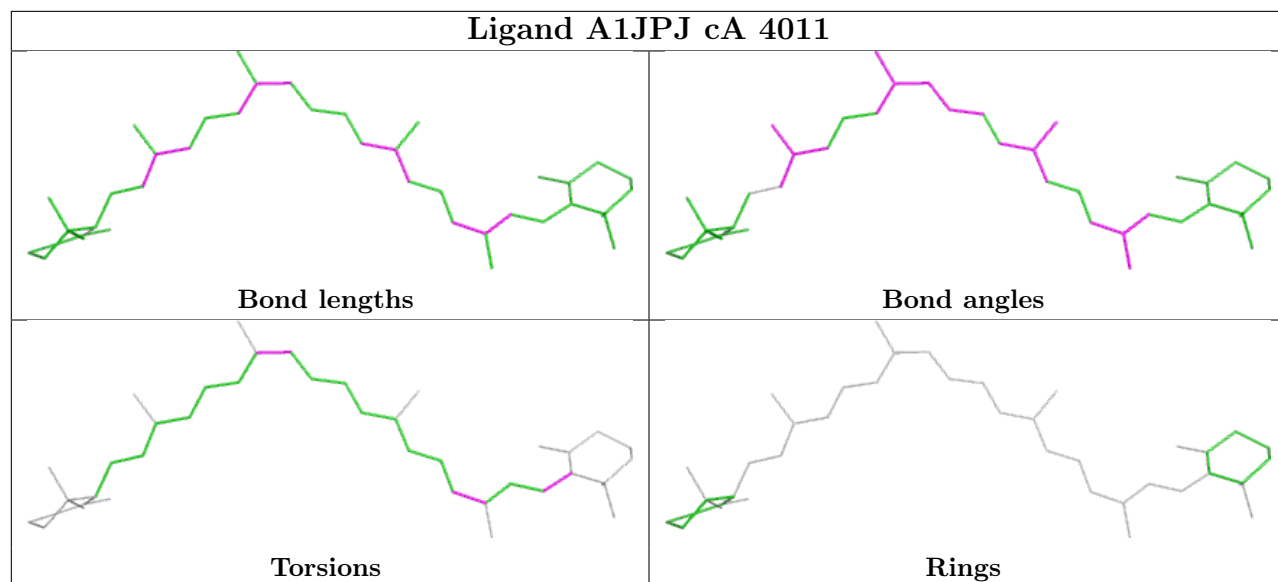
Ligand PHO bA 1013



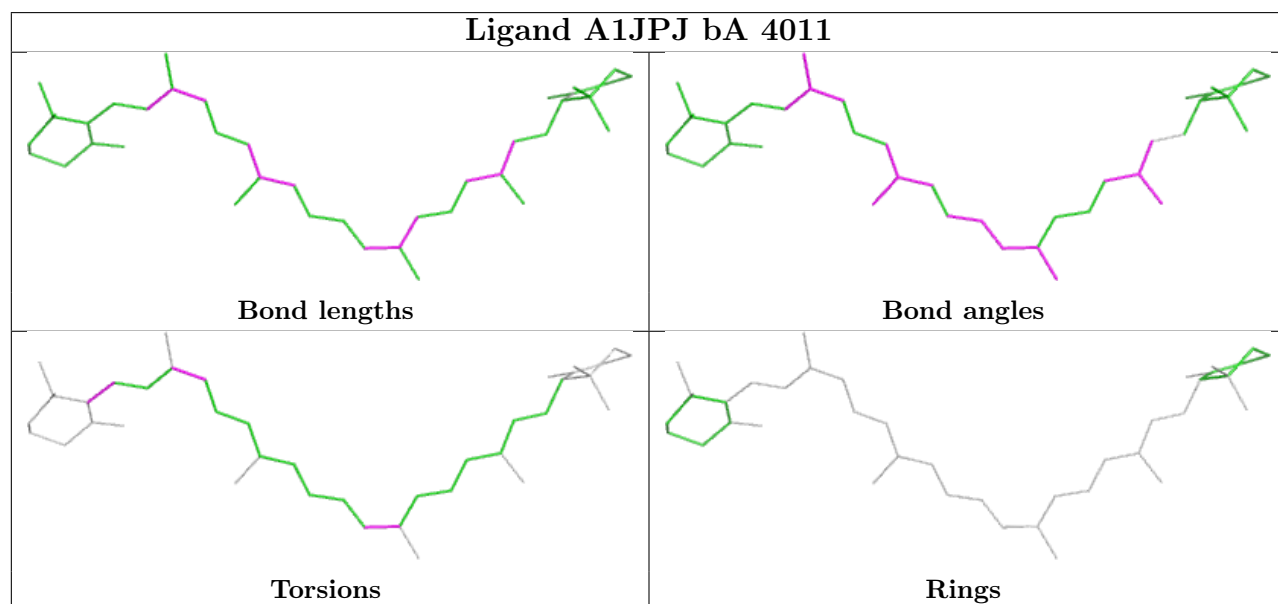
Ligand CL7 bA 1116



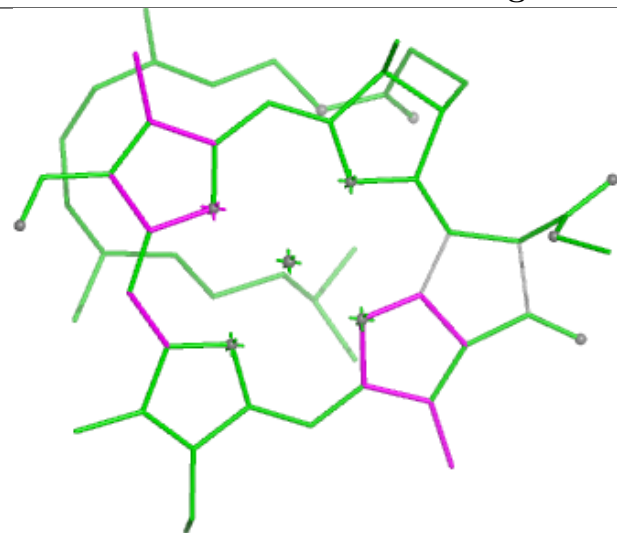
Ligand A1JPJ cA 4011



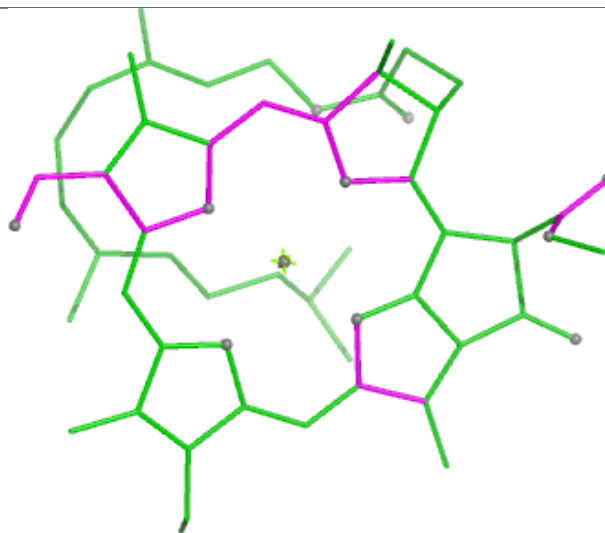
Ligand A1JPJ bA 4011



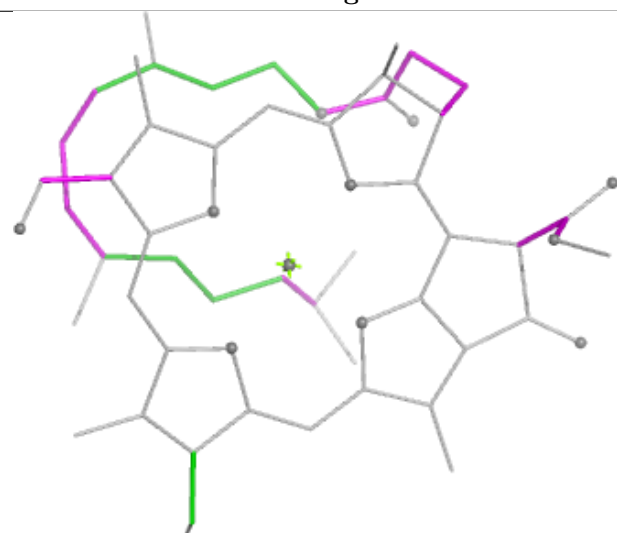
Ligand CL7 cL 1501



Bond lengths



Bond angles

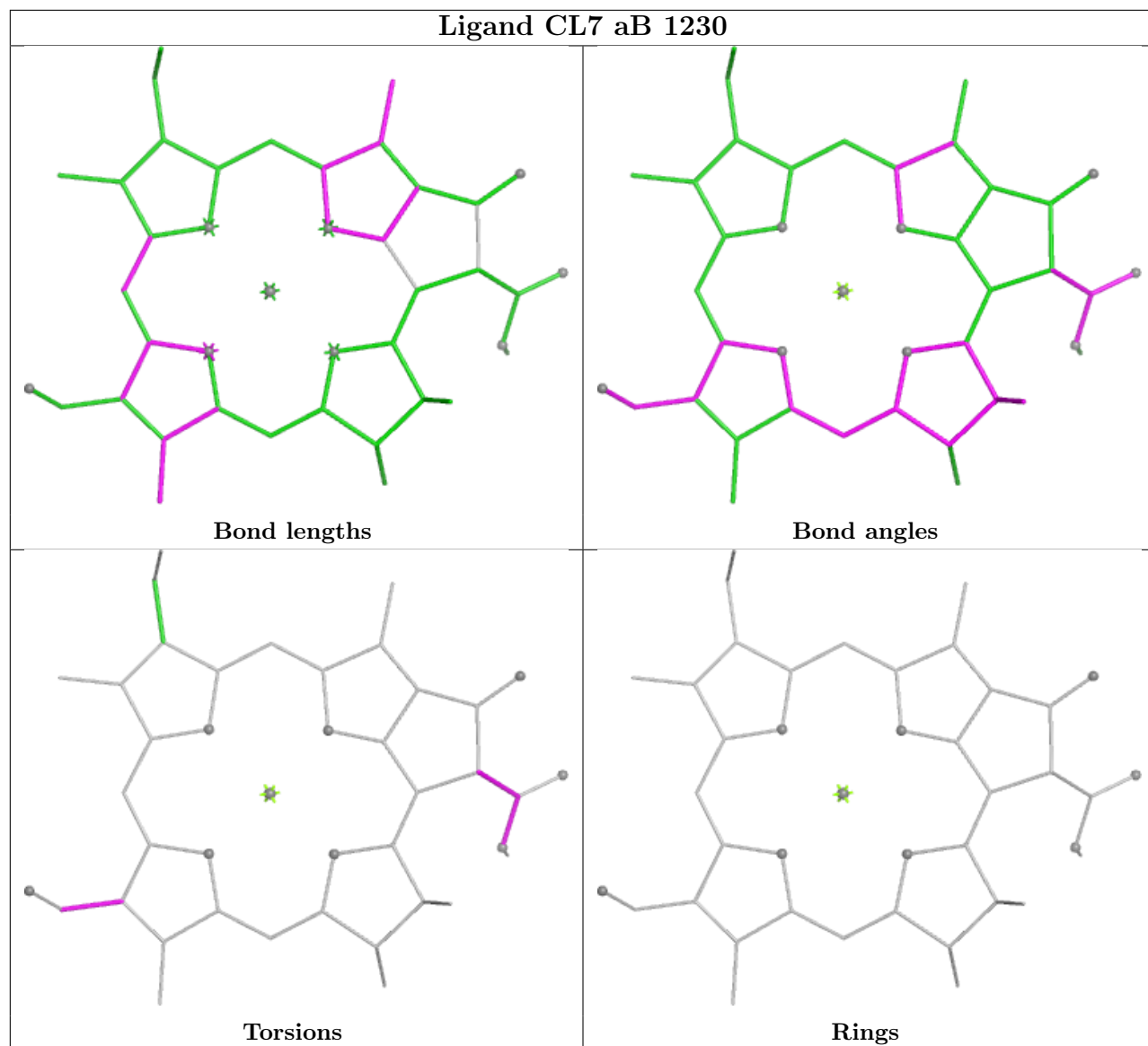


Torsions

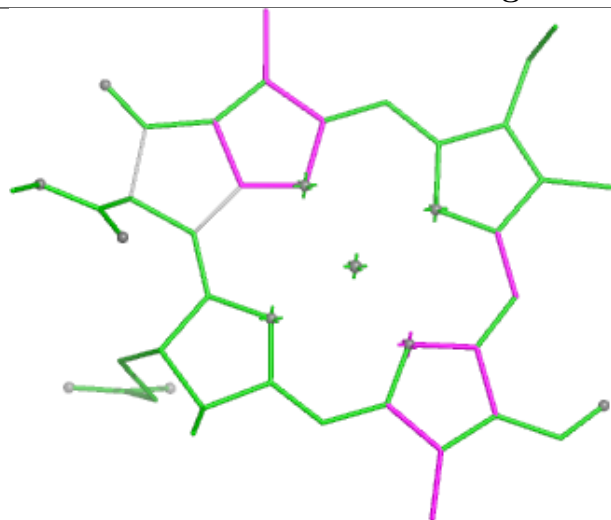


Rings

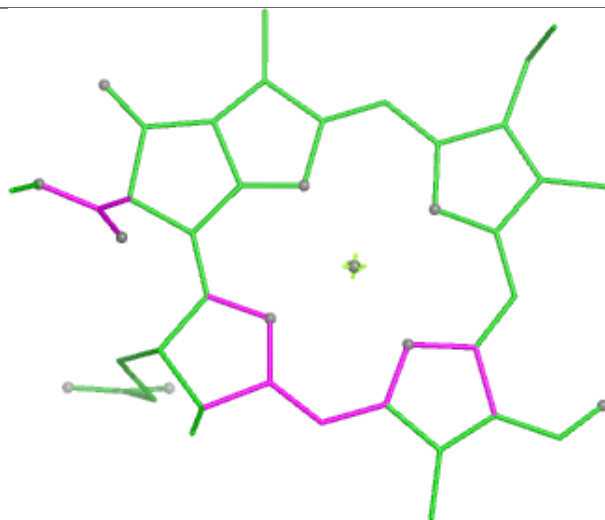
Ligand CL7 aB 1230



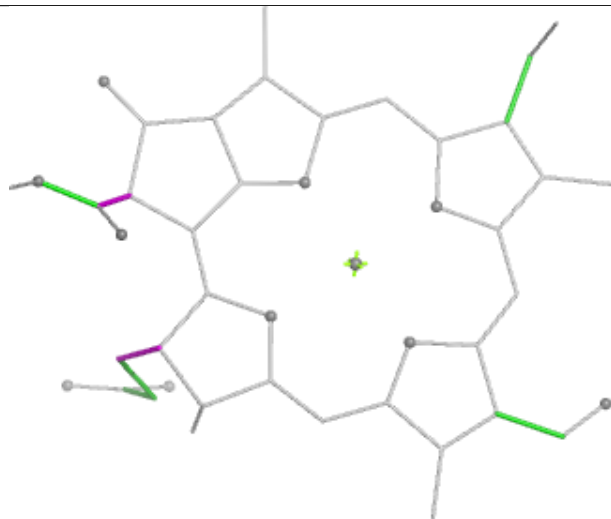
Ligand CL7 cB 1216



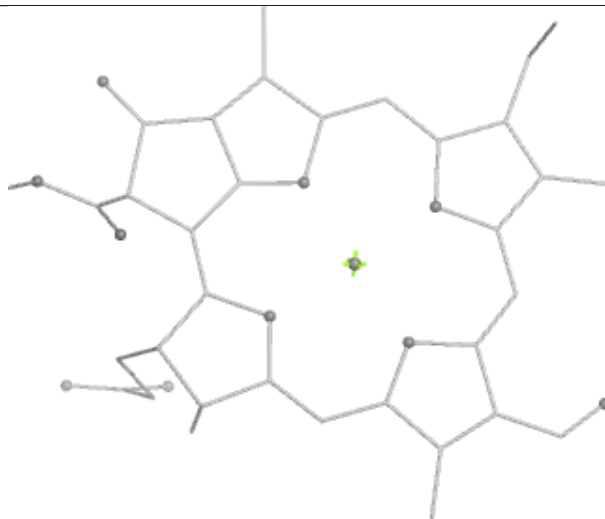
Bond lengths



Bond angles

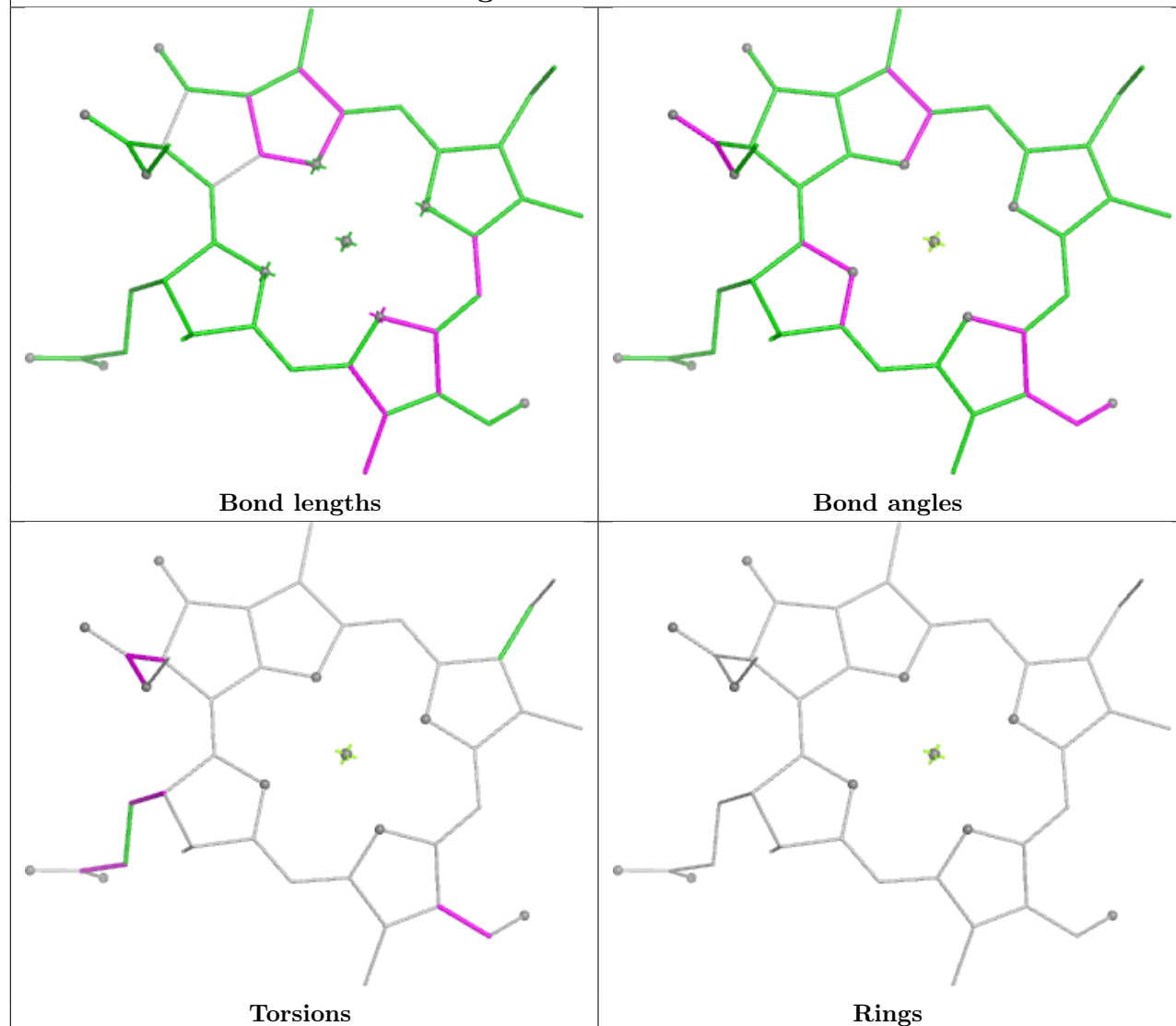


Torsions

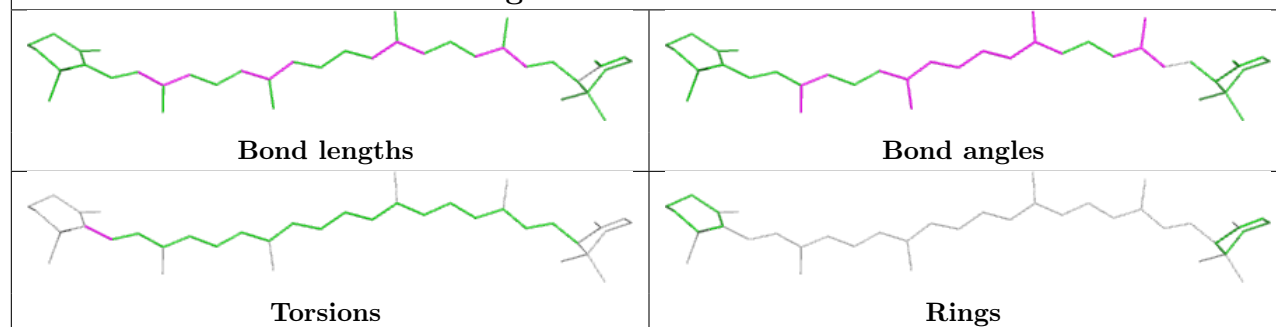


Rings

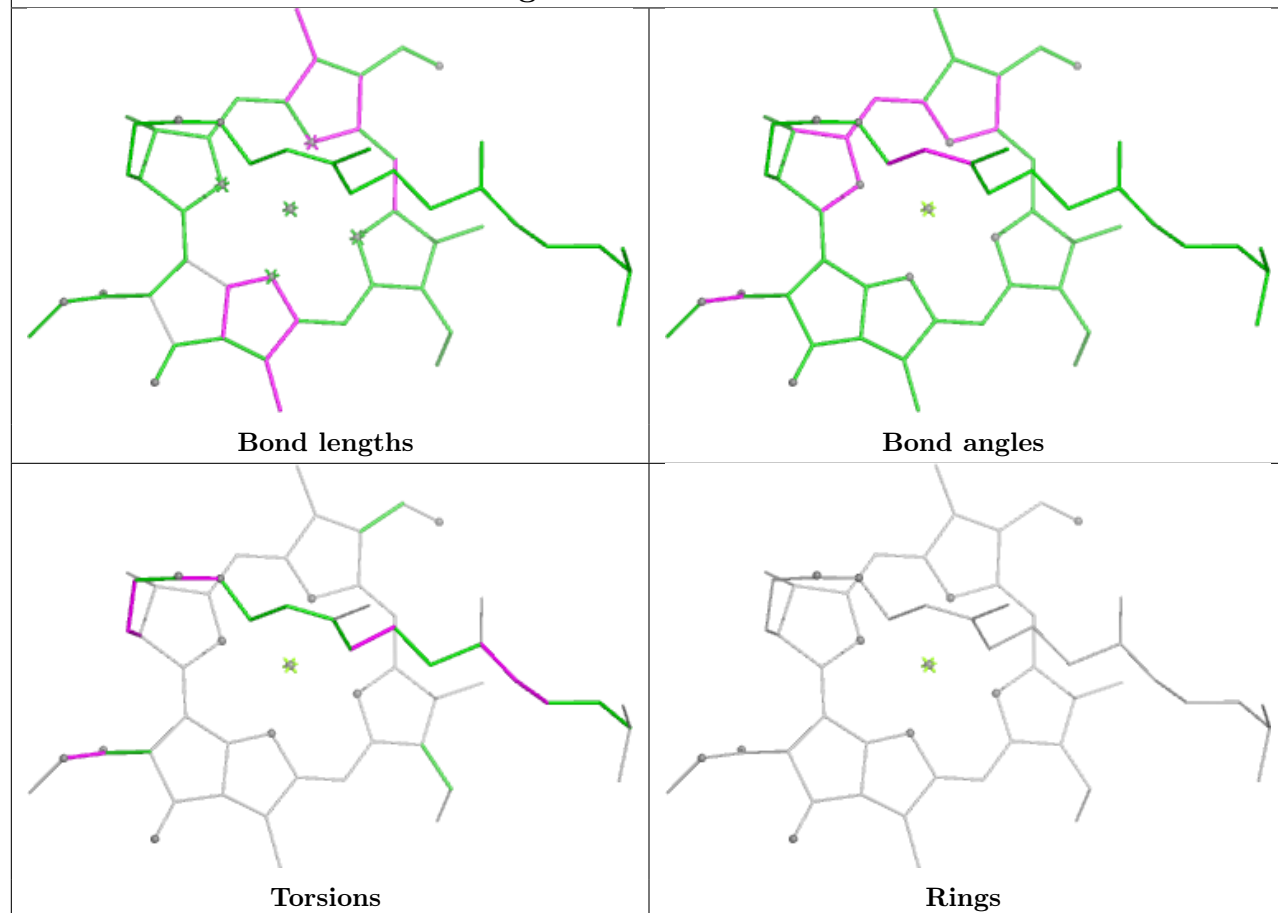
Ligand CL7 bB 1241



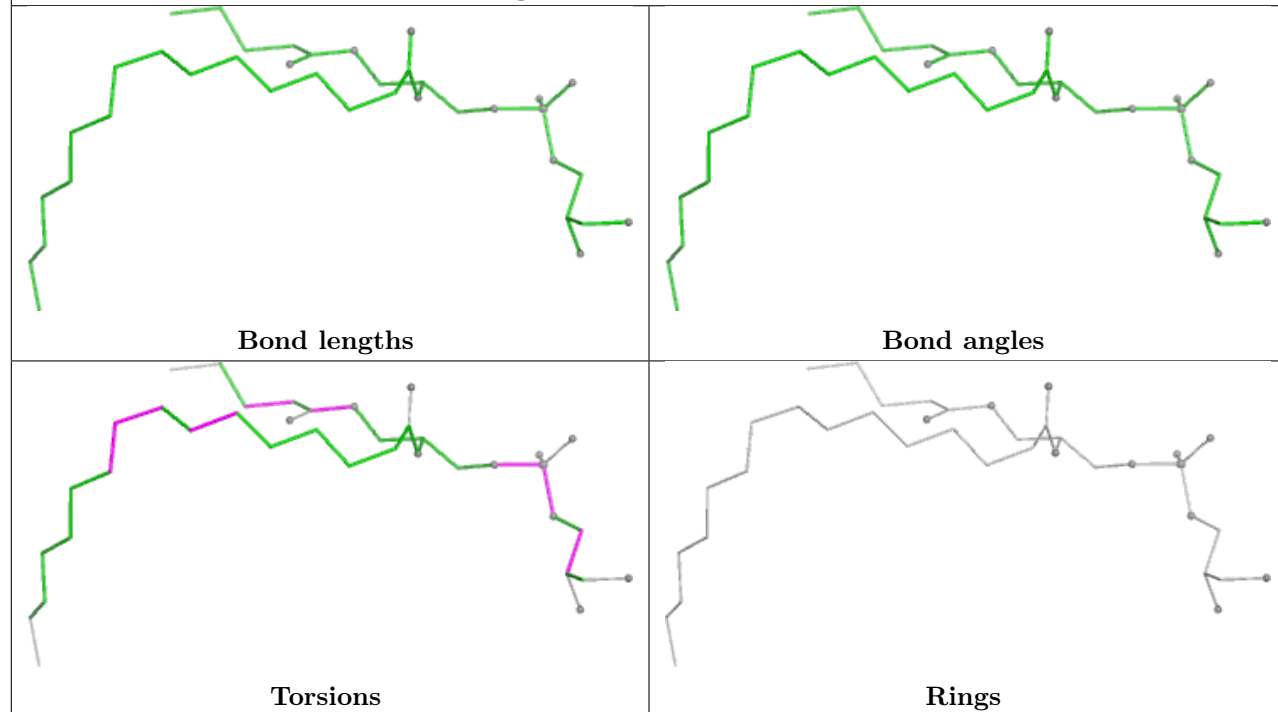
Ligand A1JPJ cI 4019

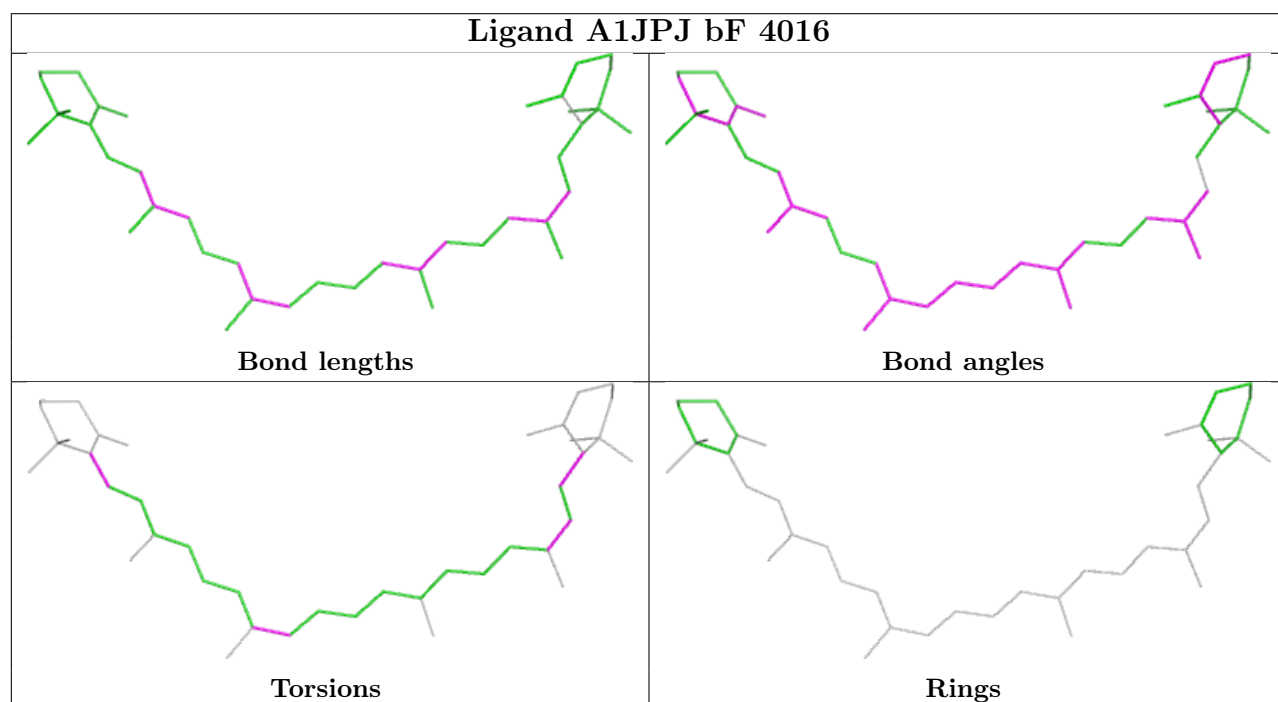
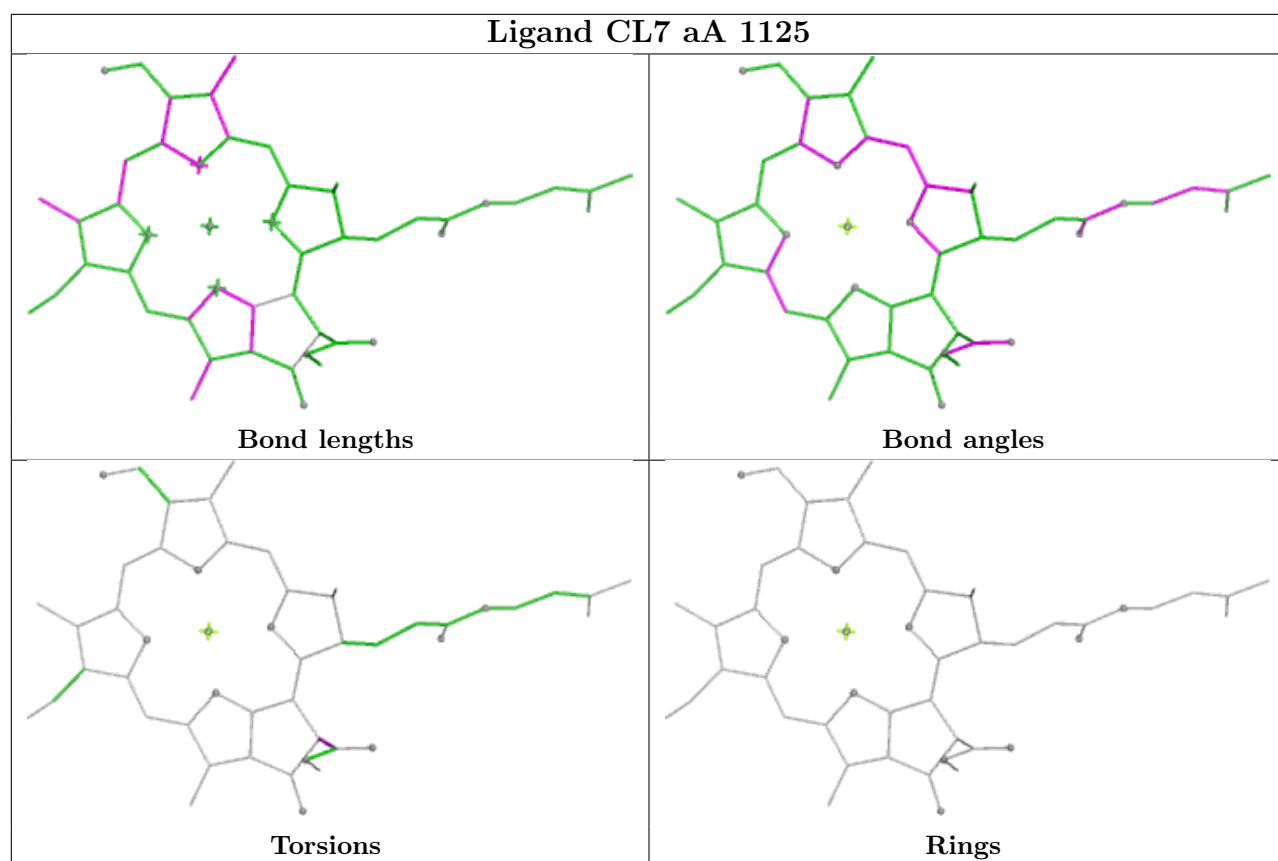


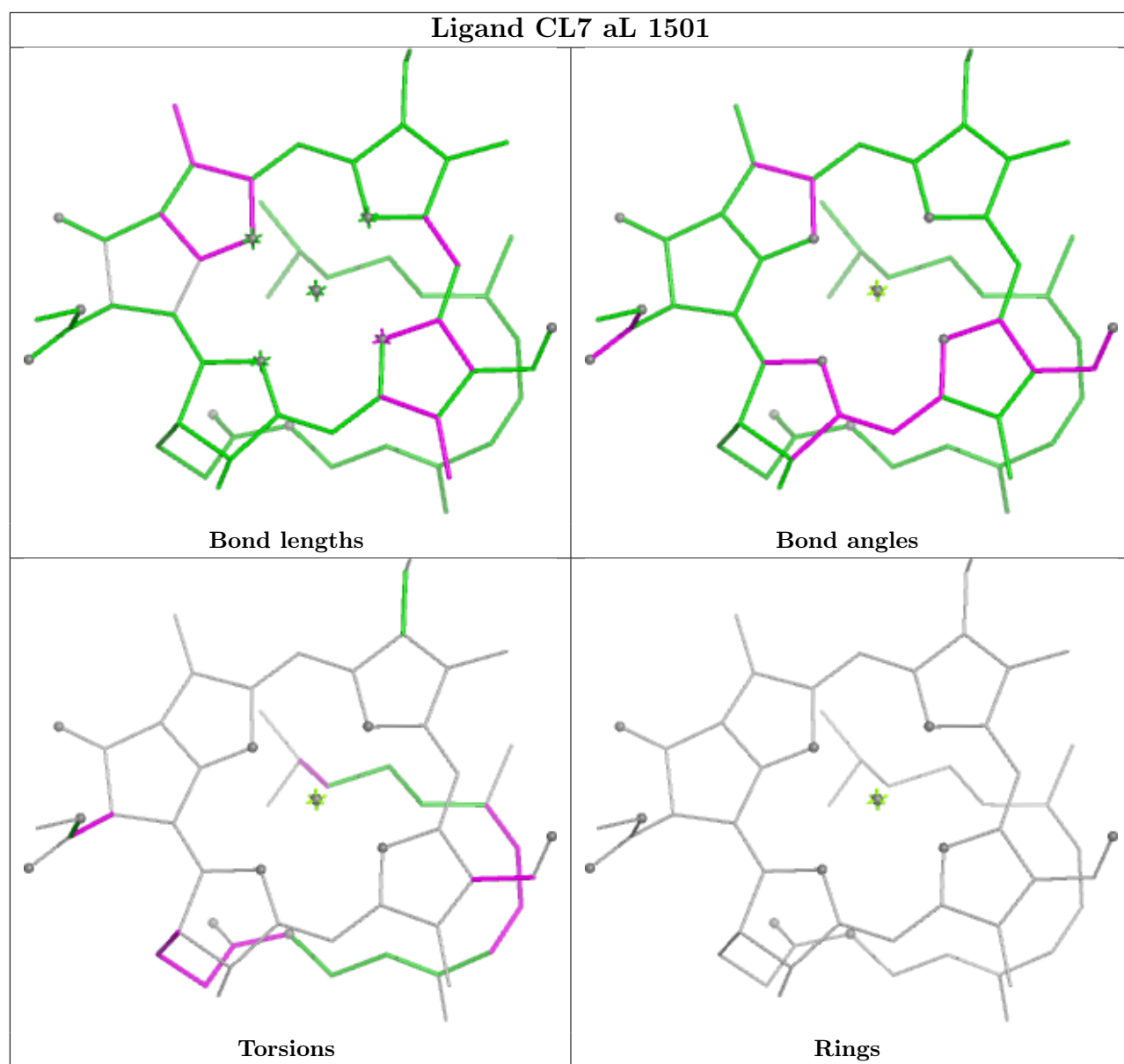
Ligand CL7 aA 1116

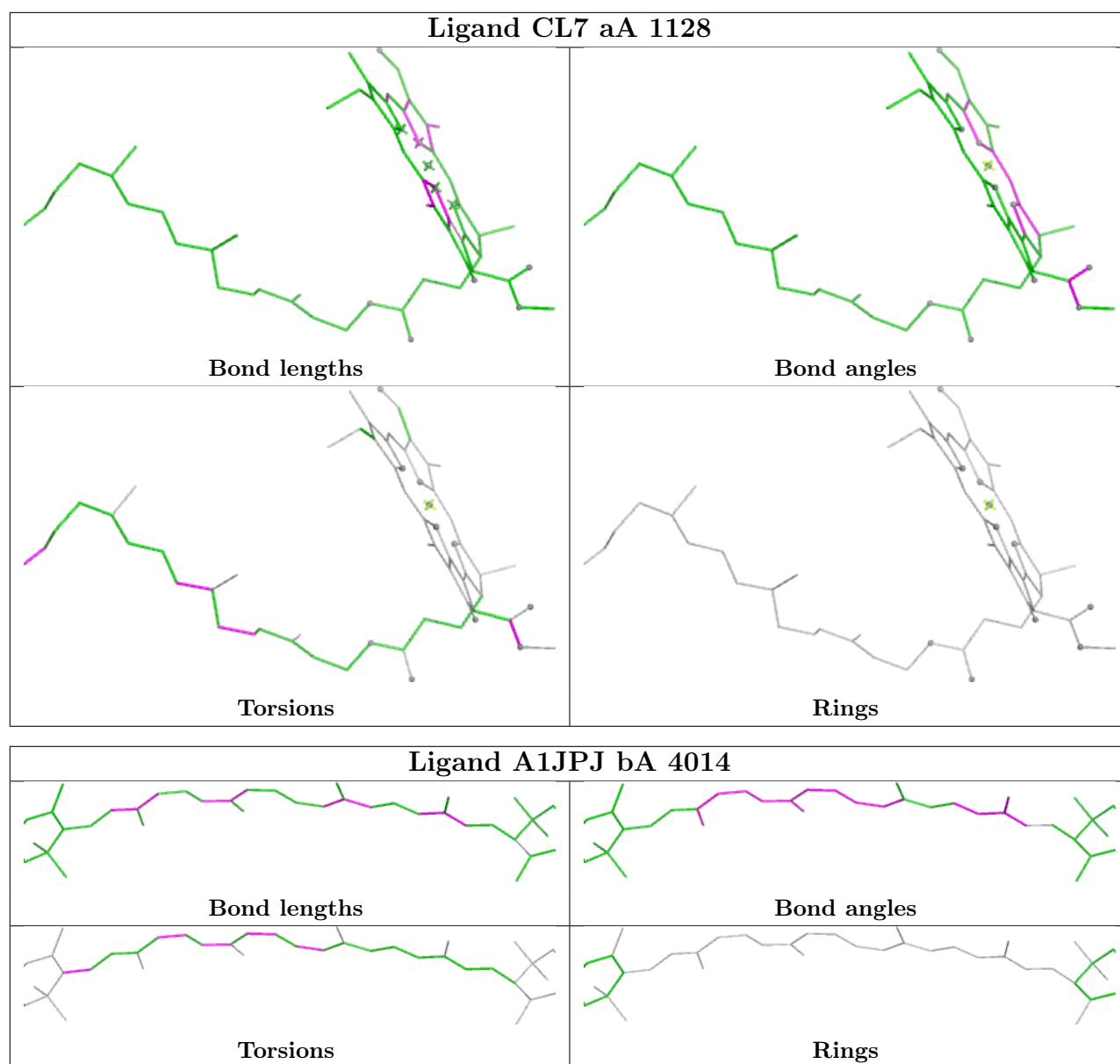


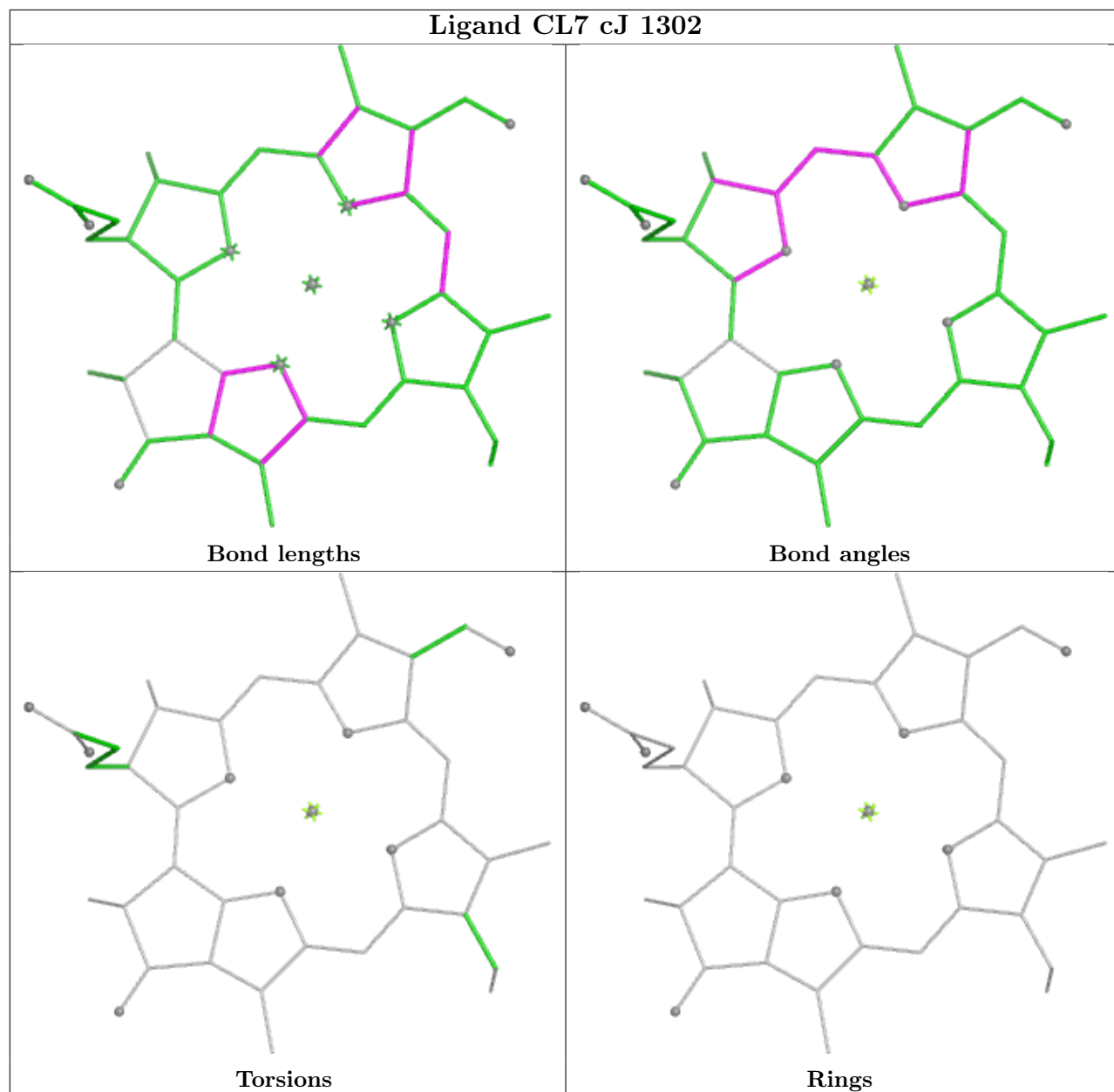
Ligand LHG aA 5003

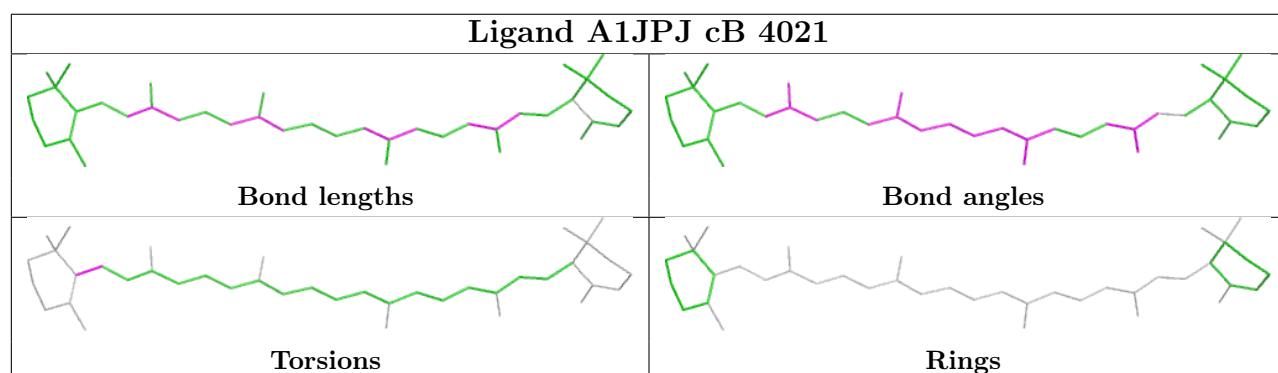
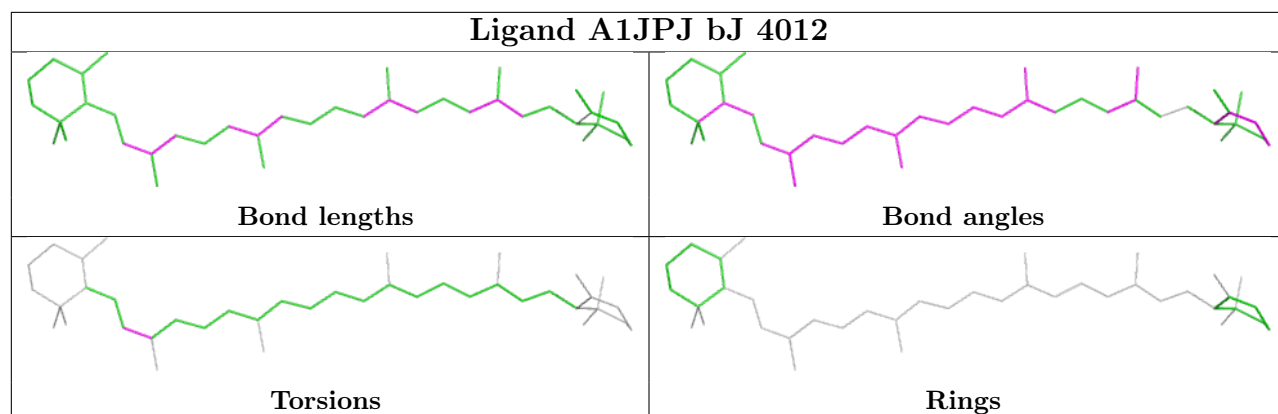
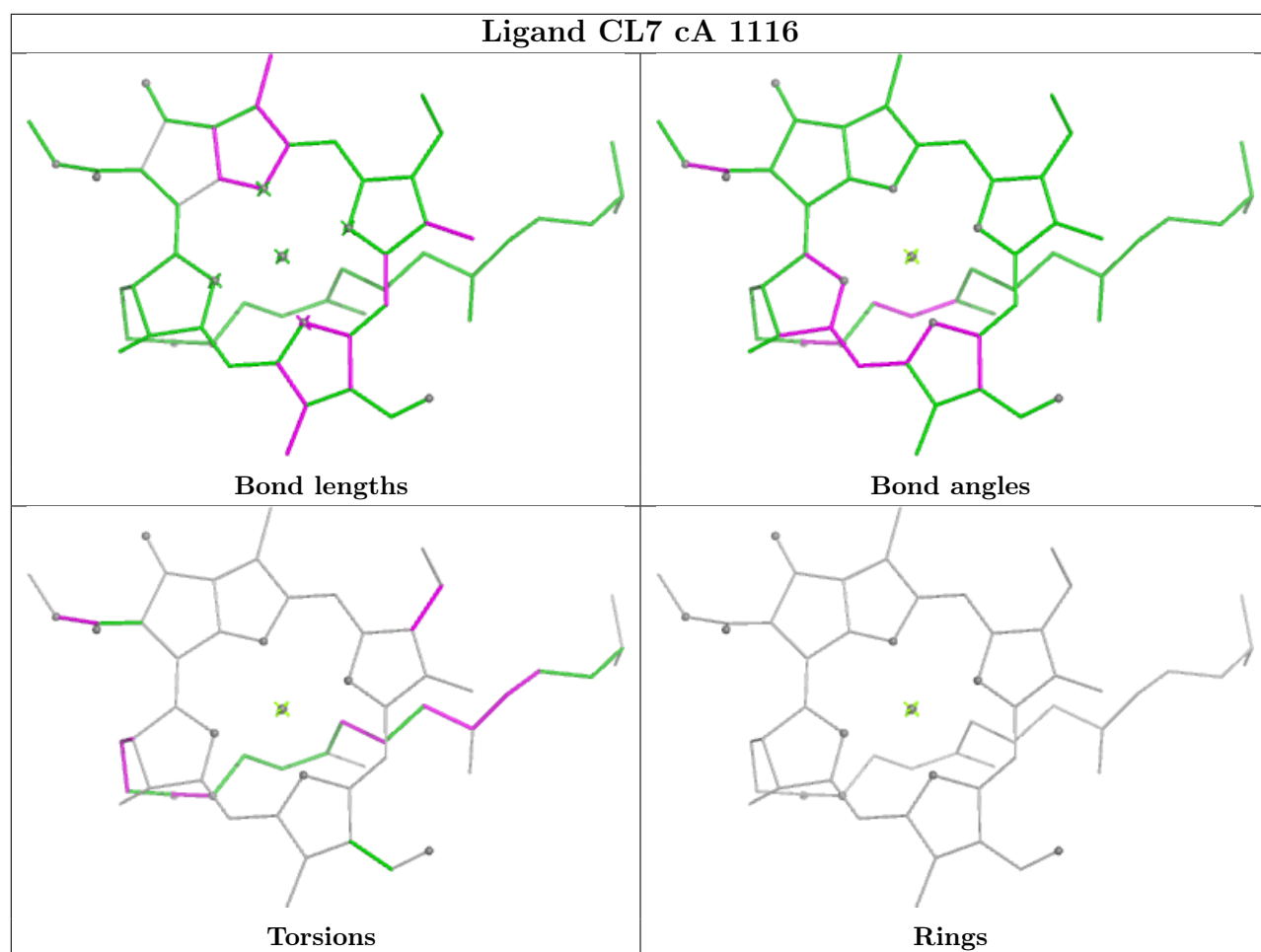




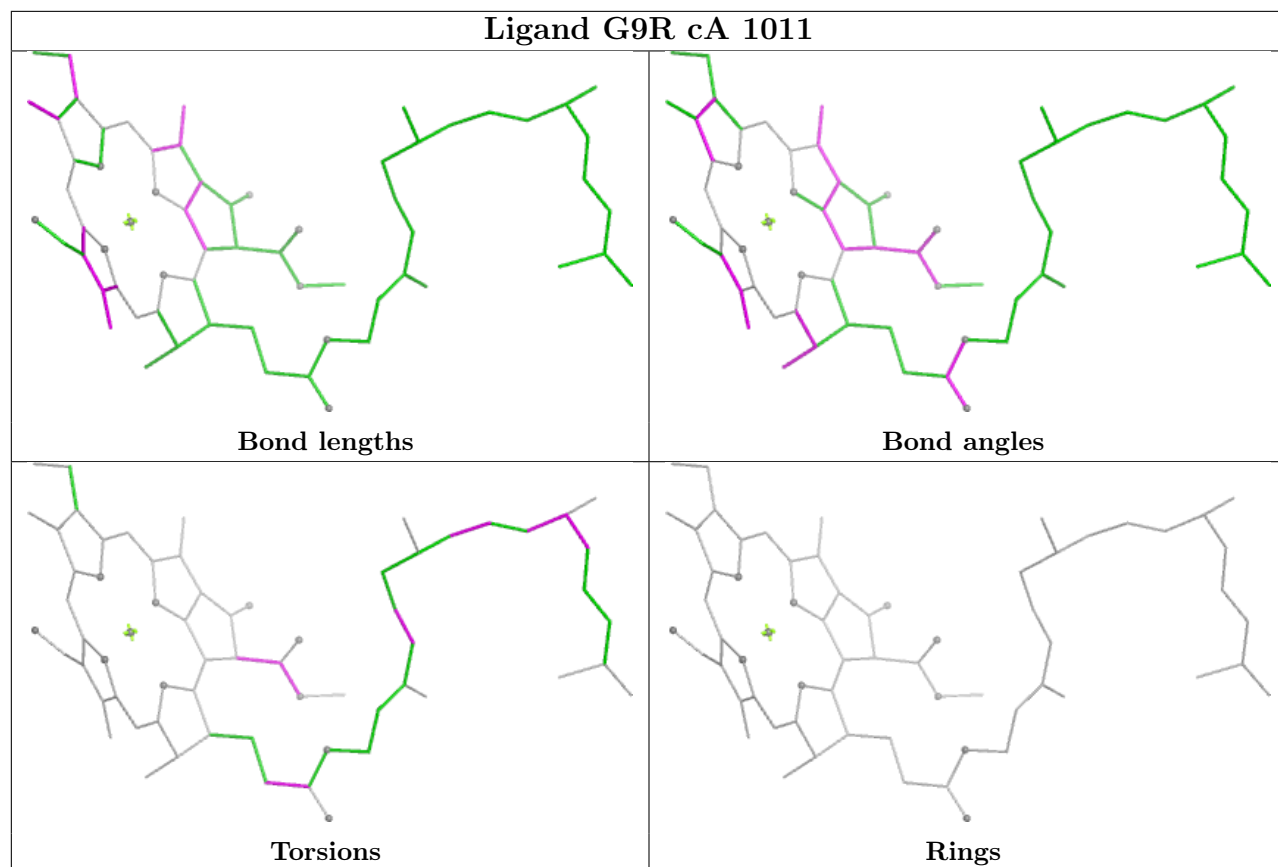




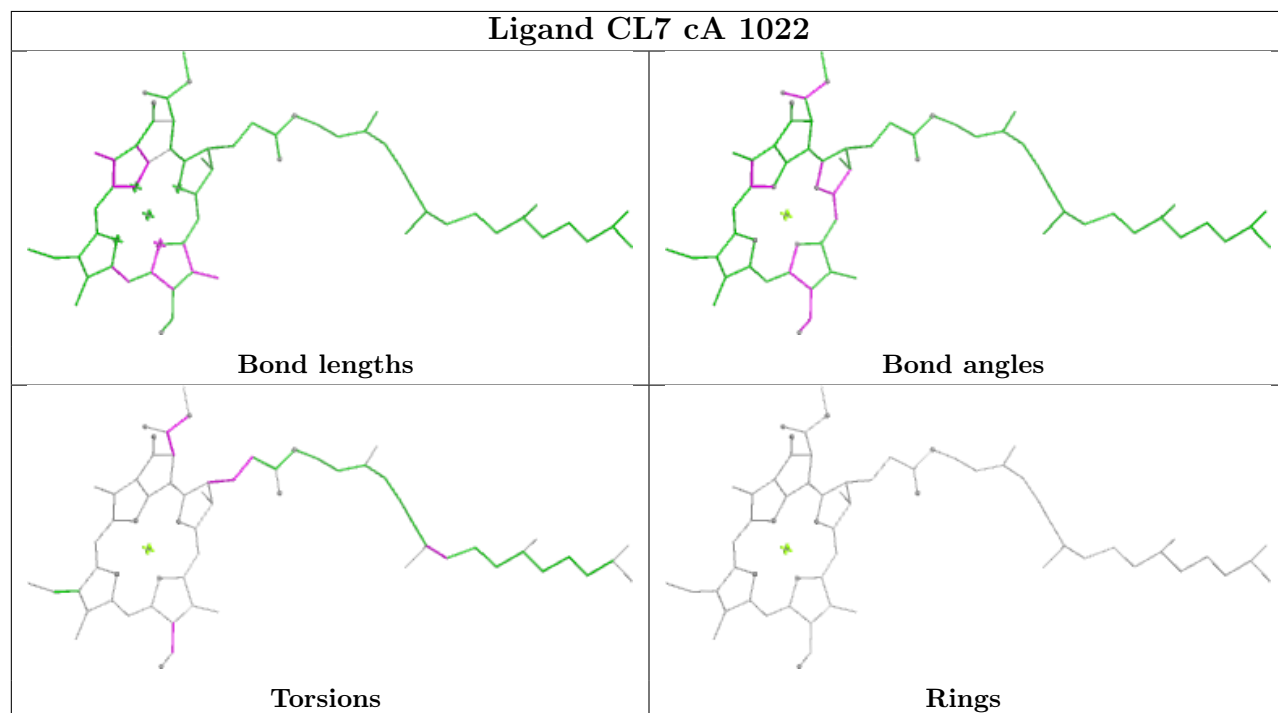


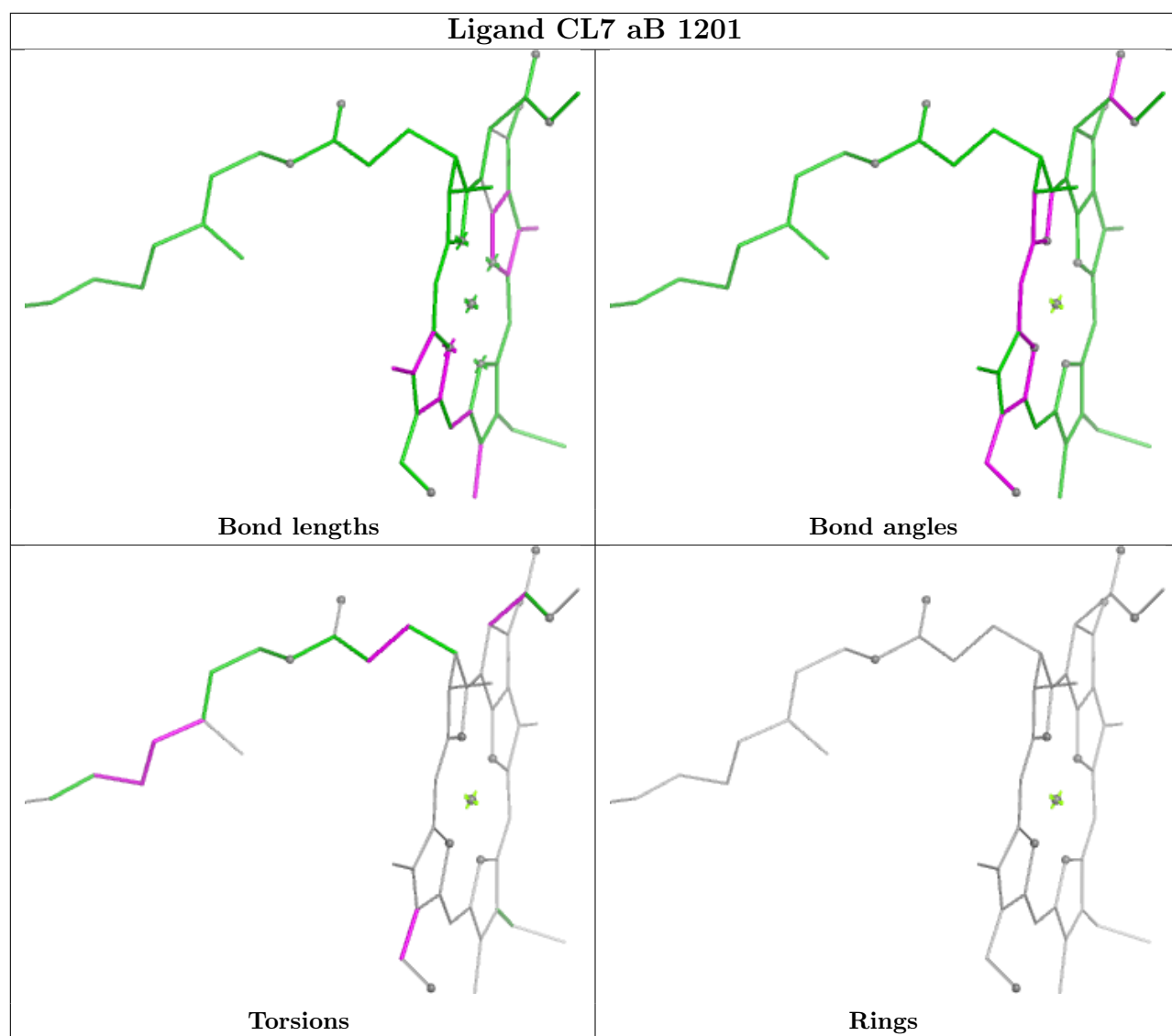


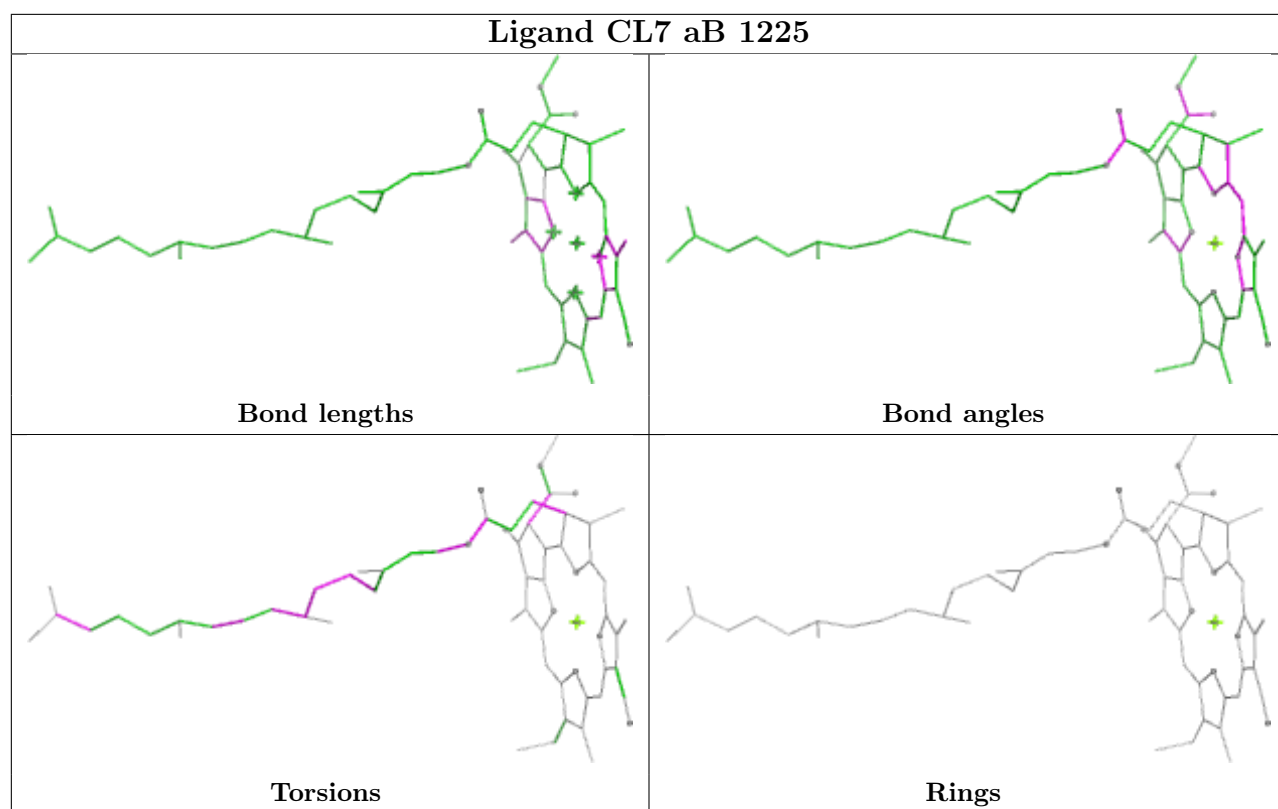
Ligand G9R cA 1011

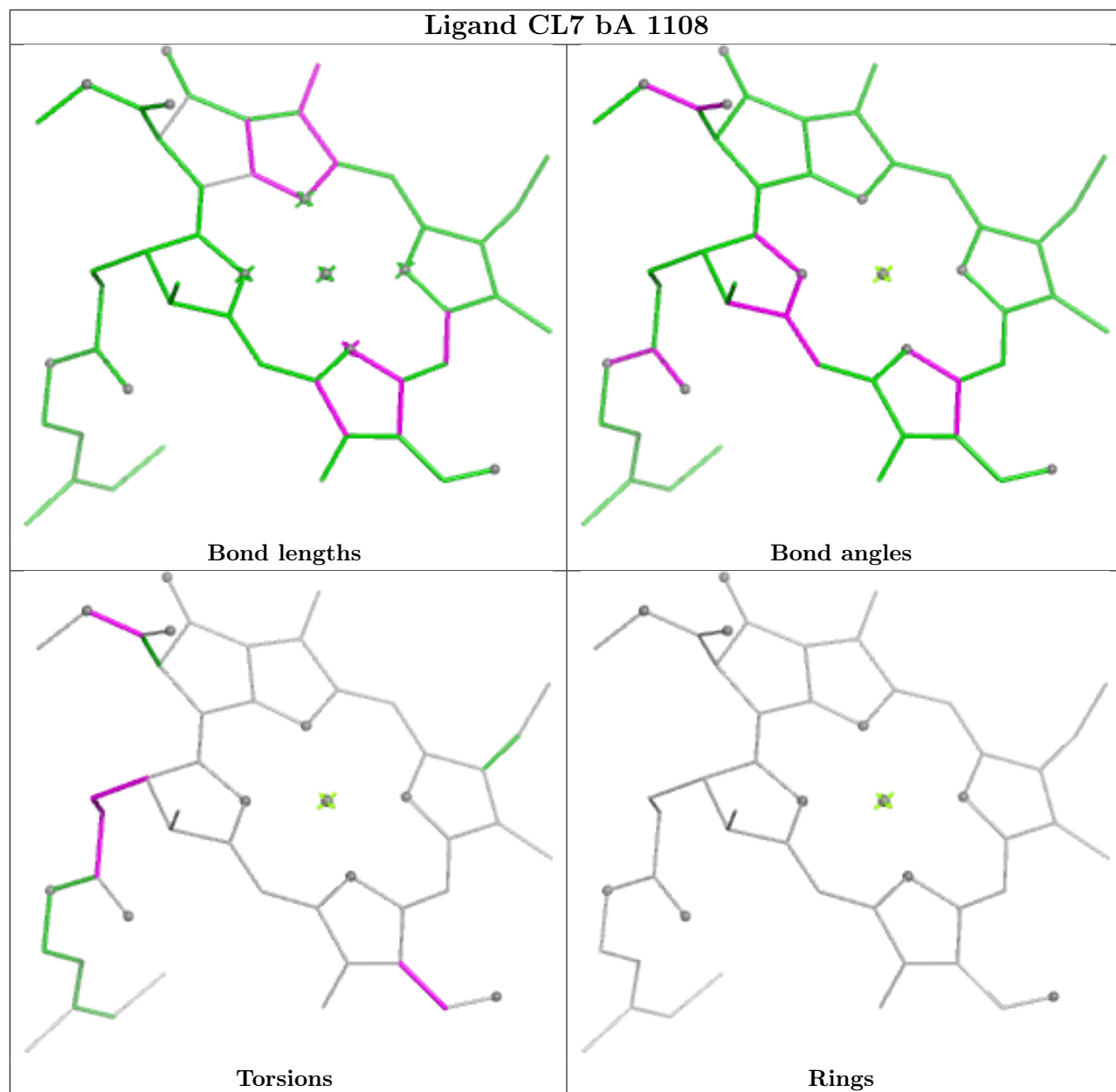


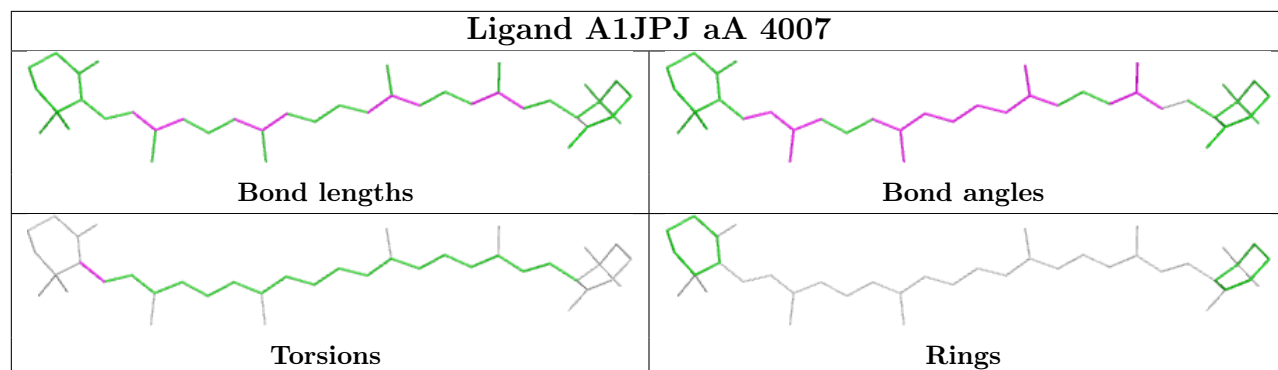
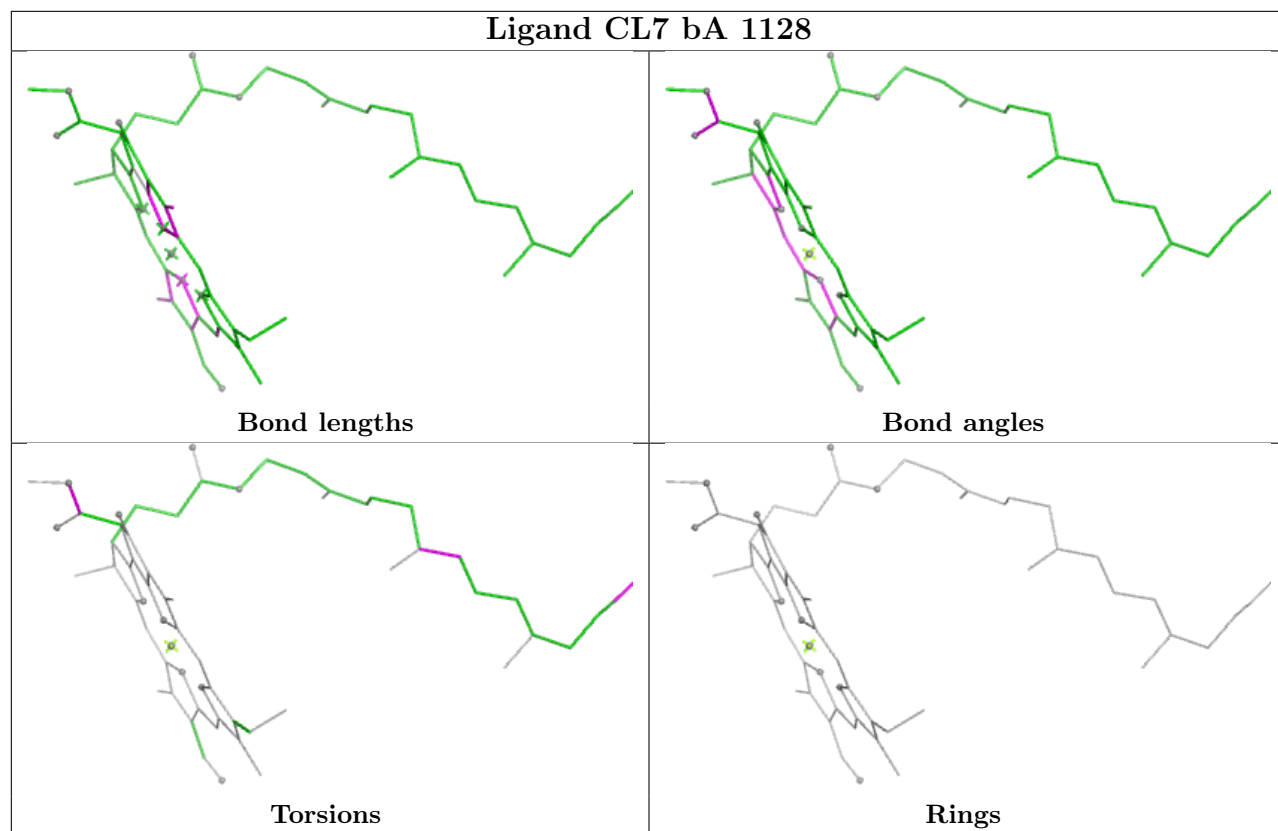
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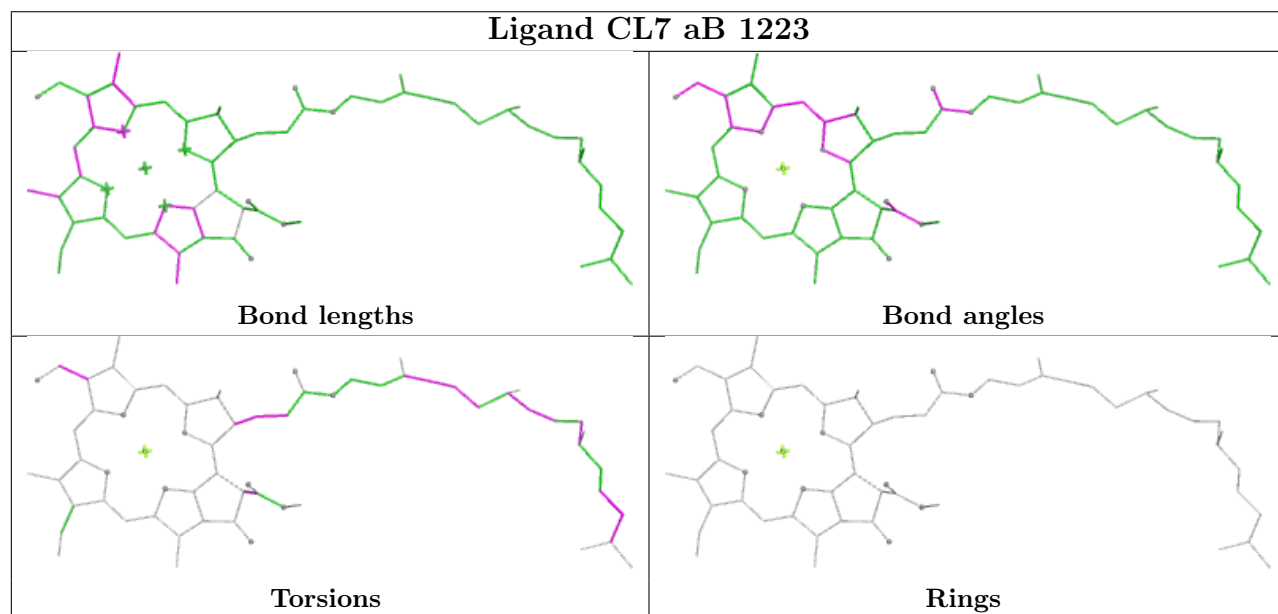
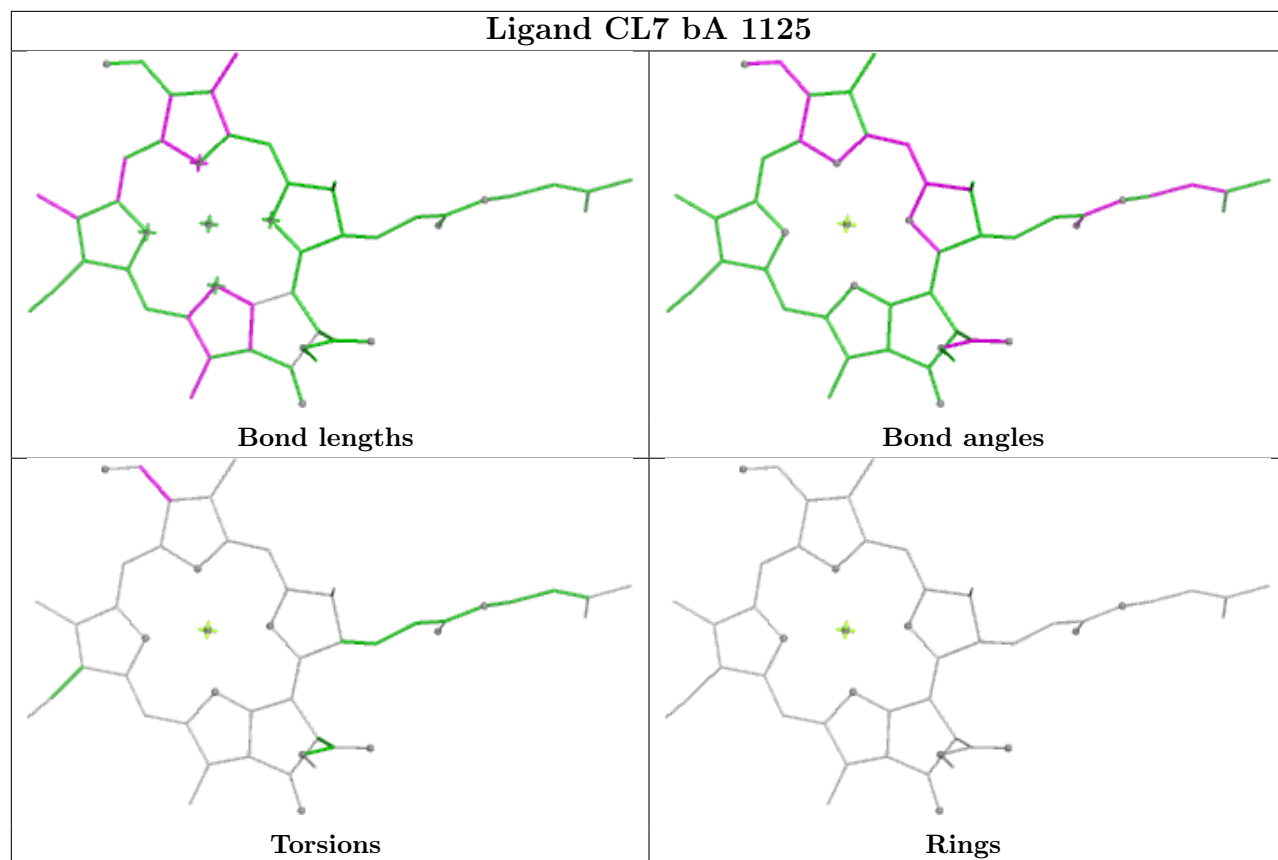


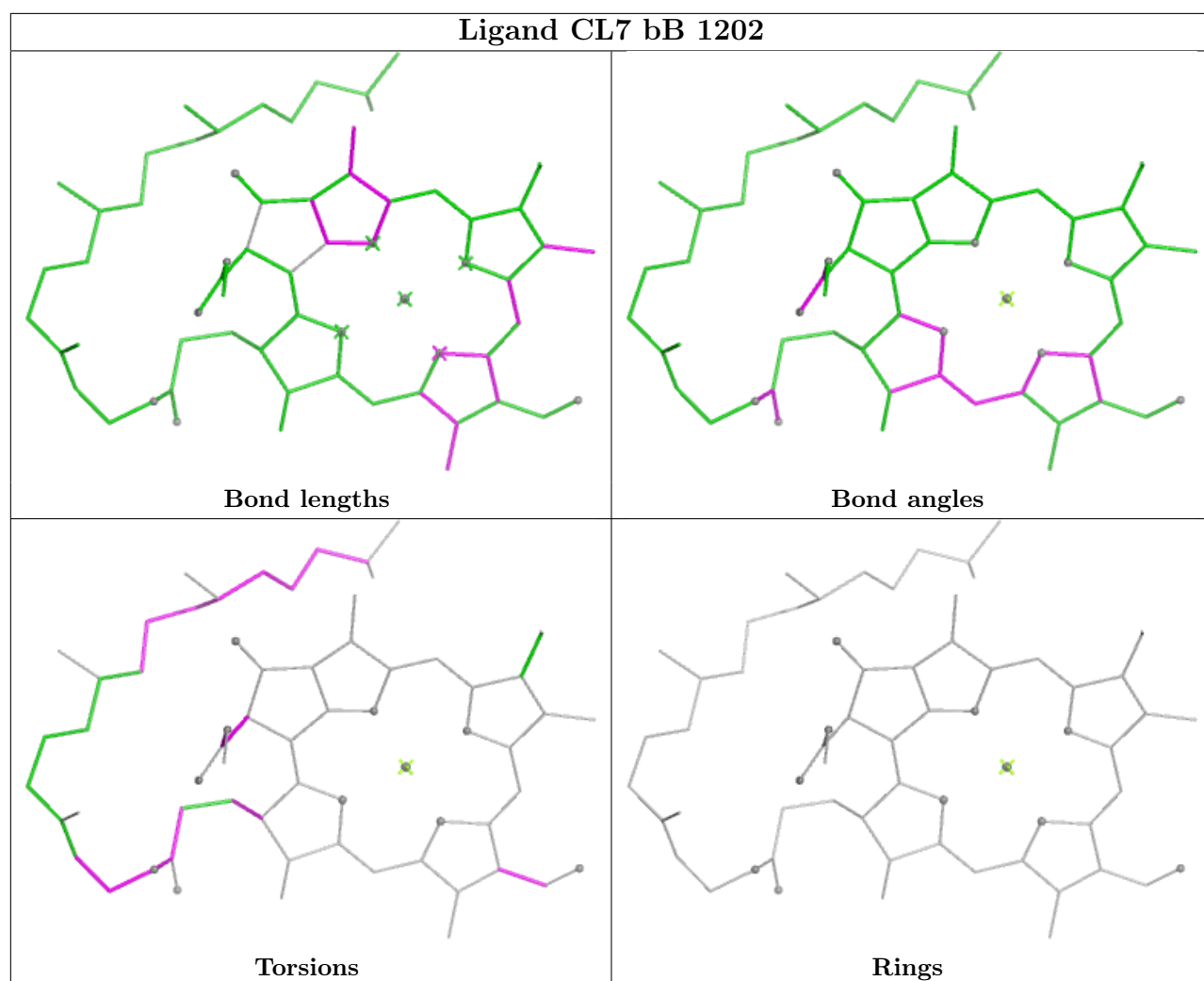


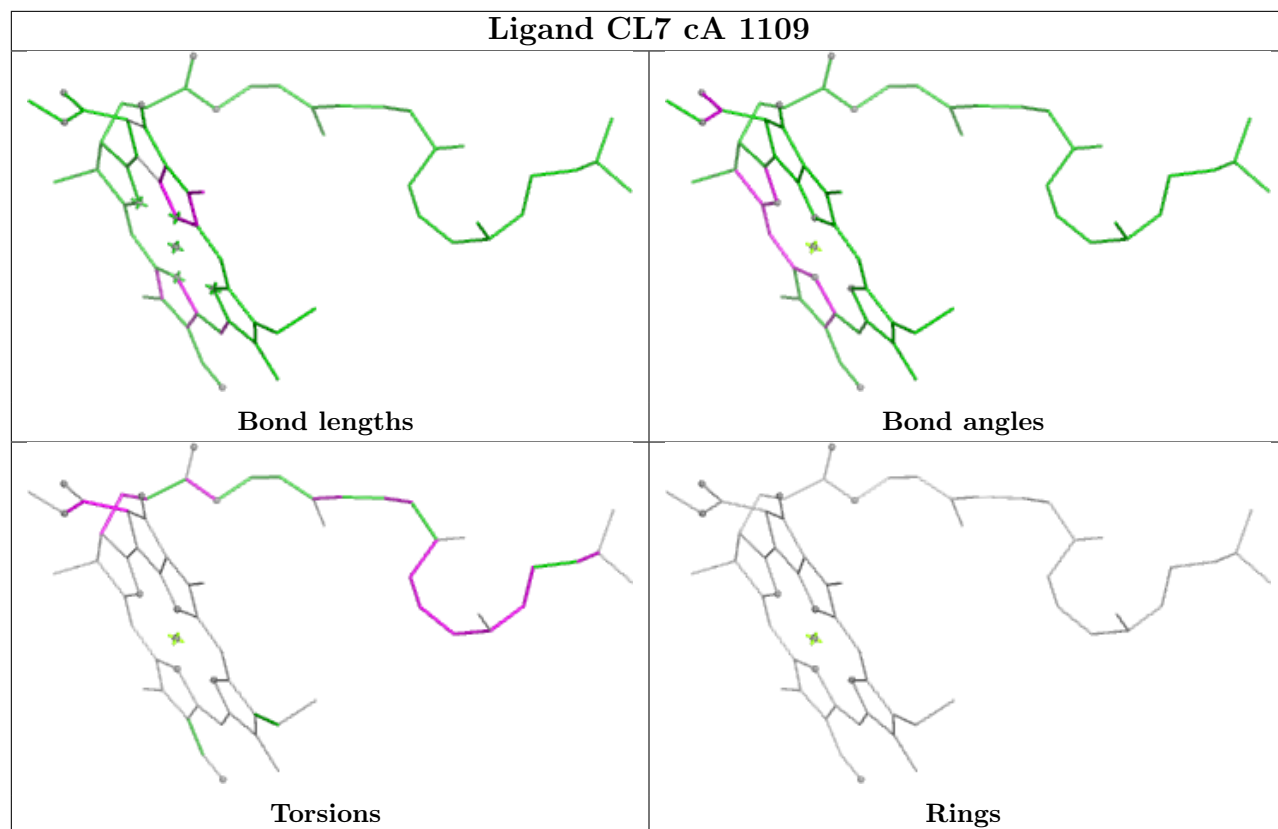


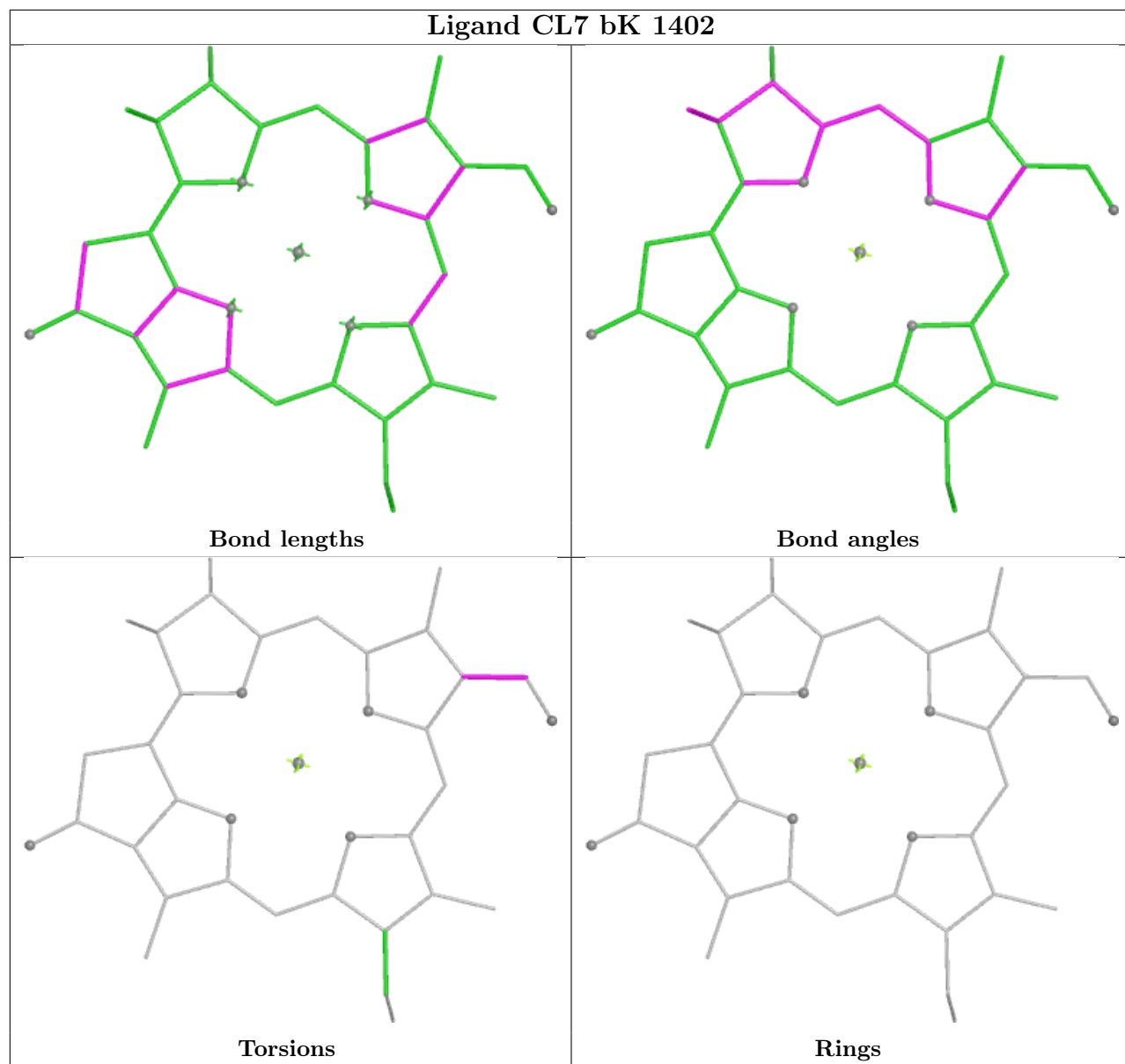


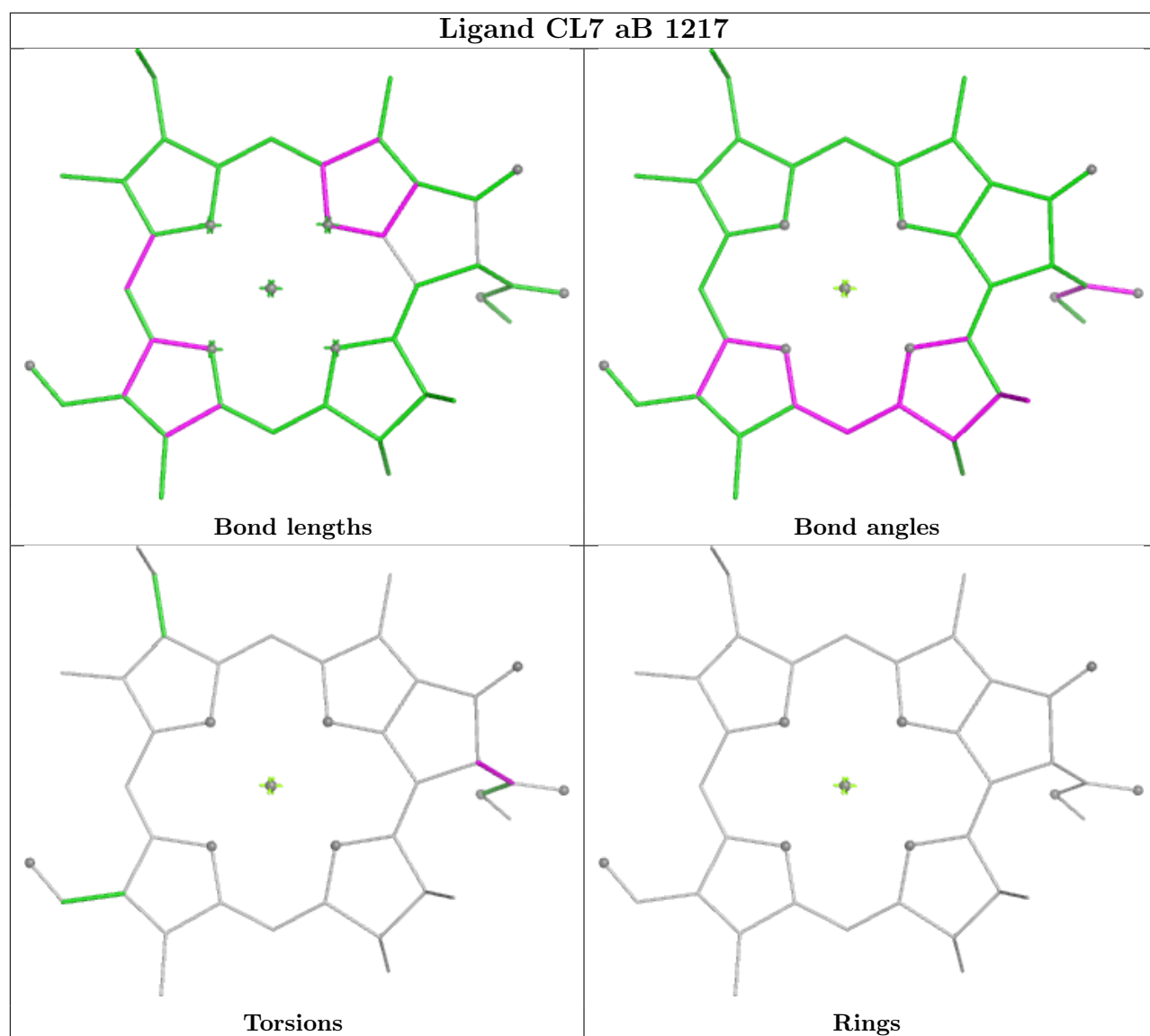




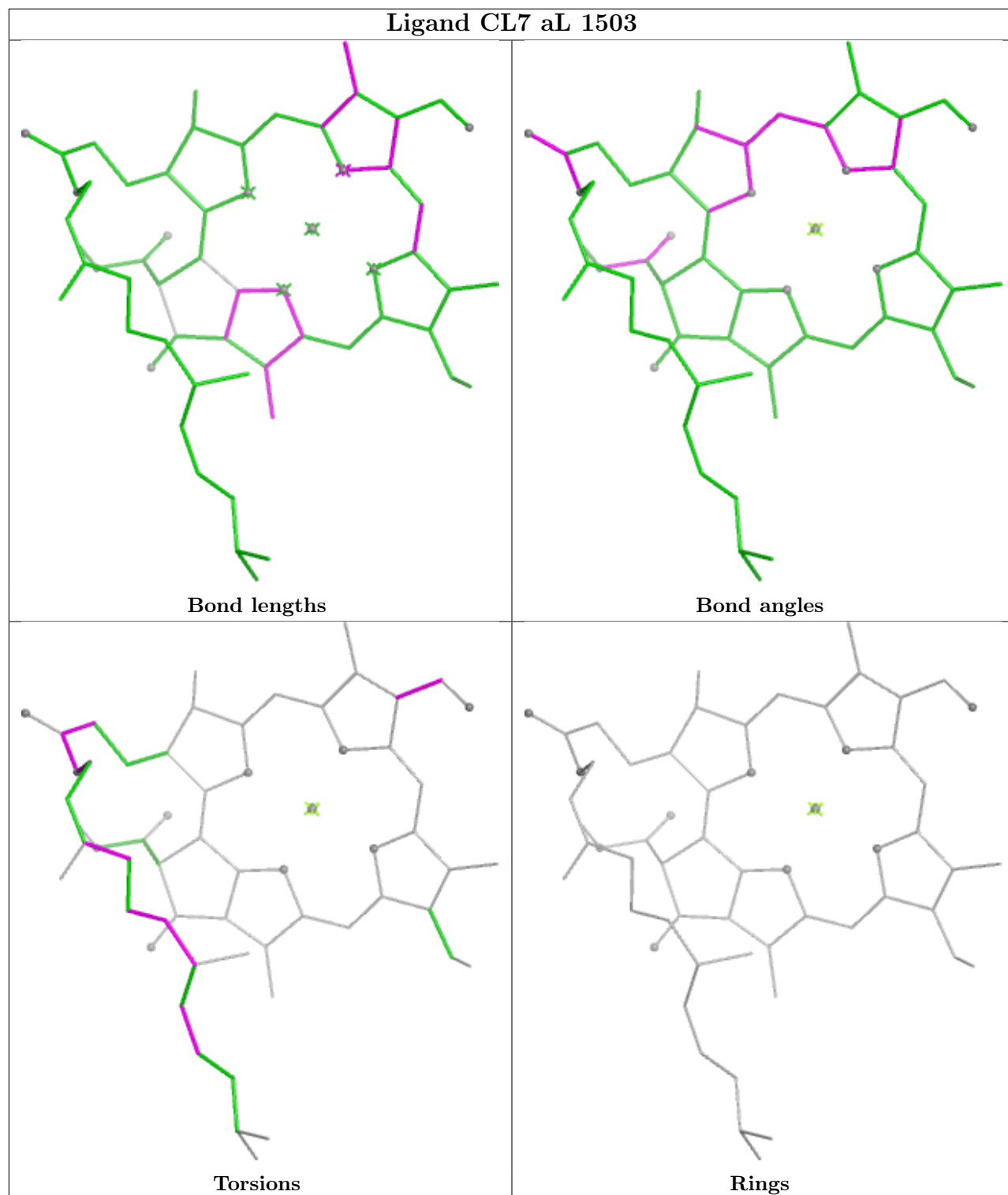




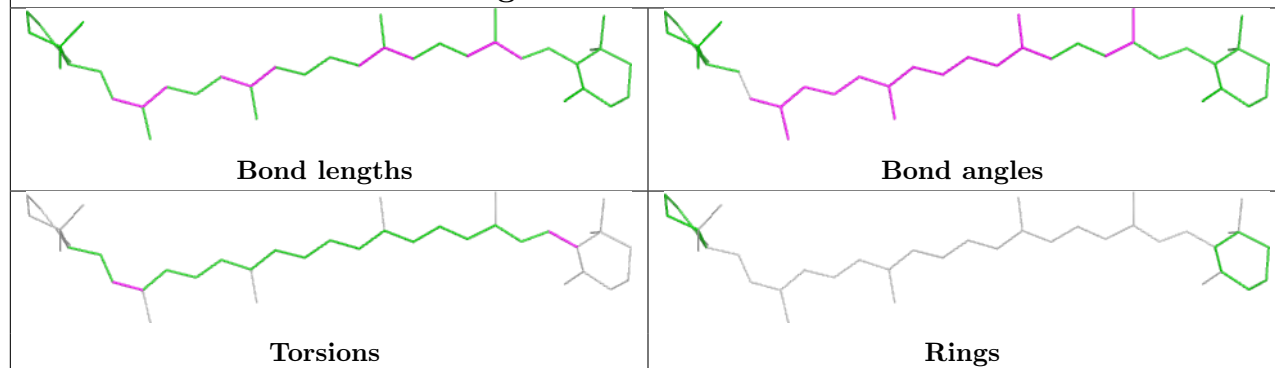




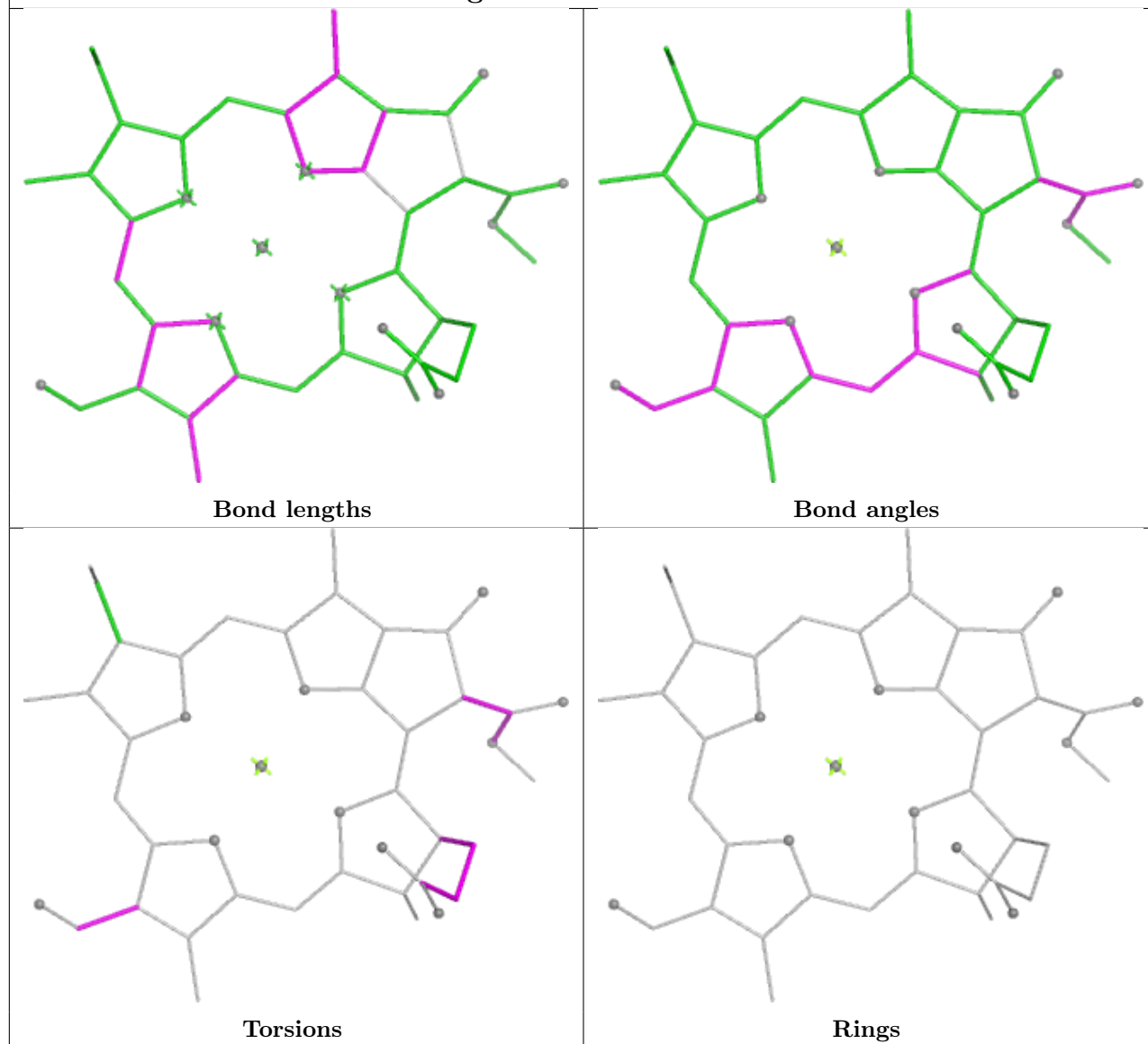
Ligand CL7 aL 1503

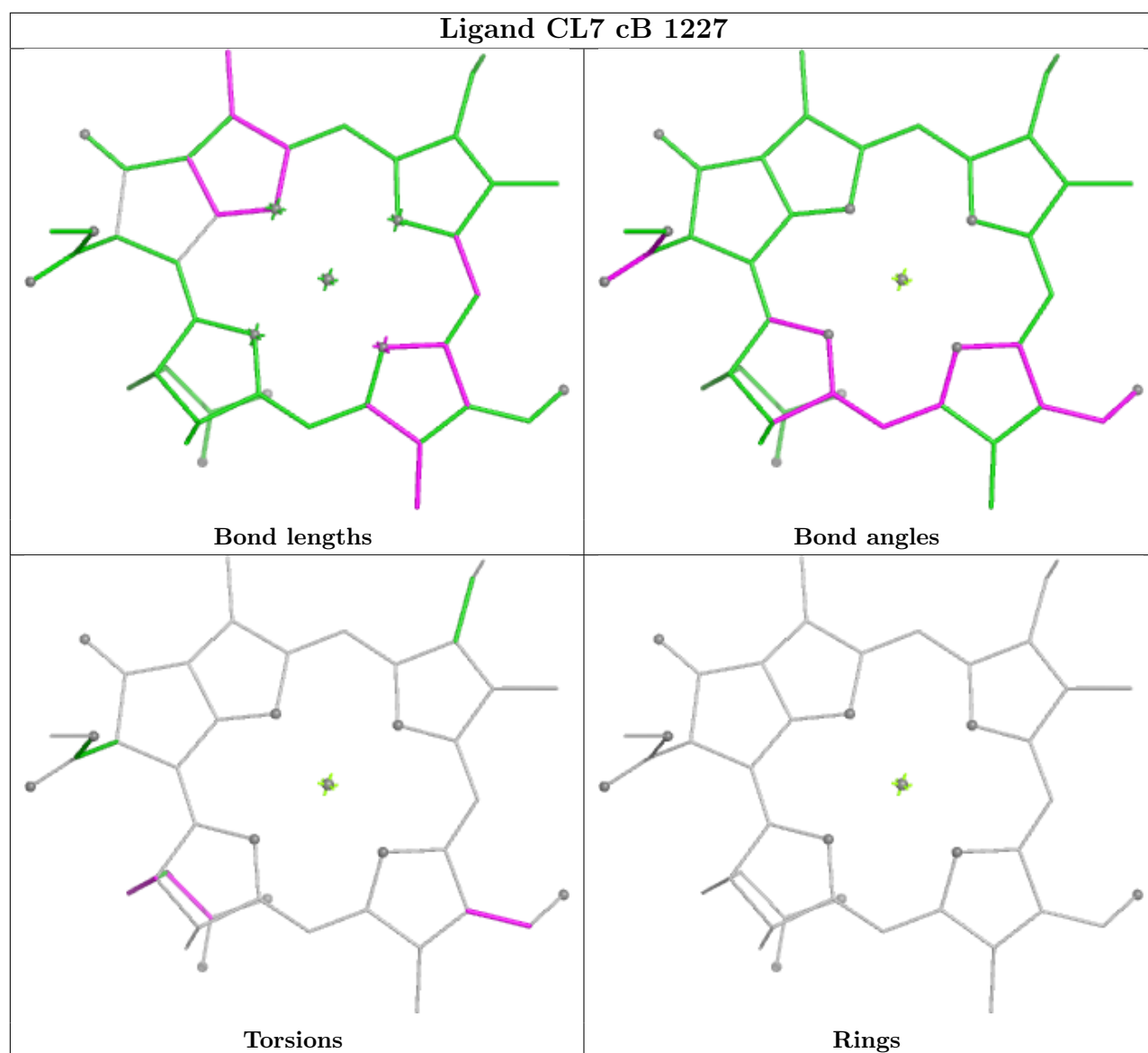


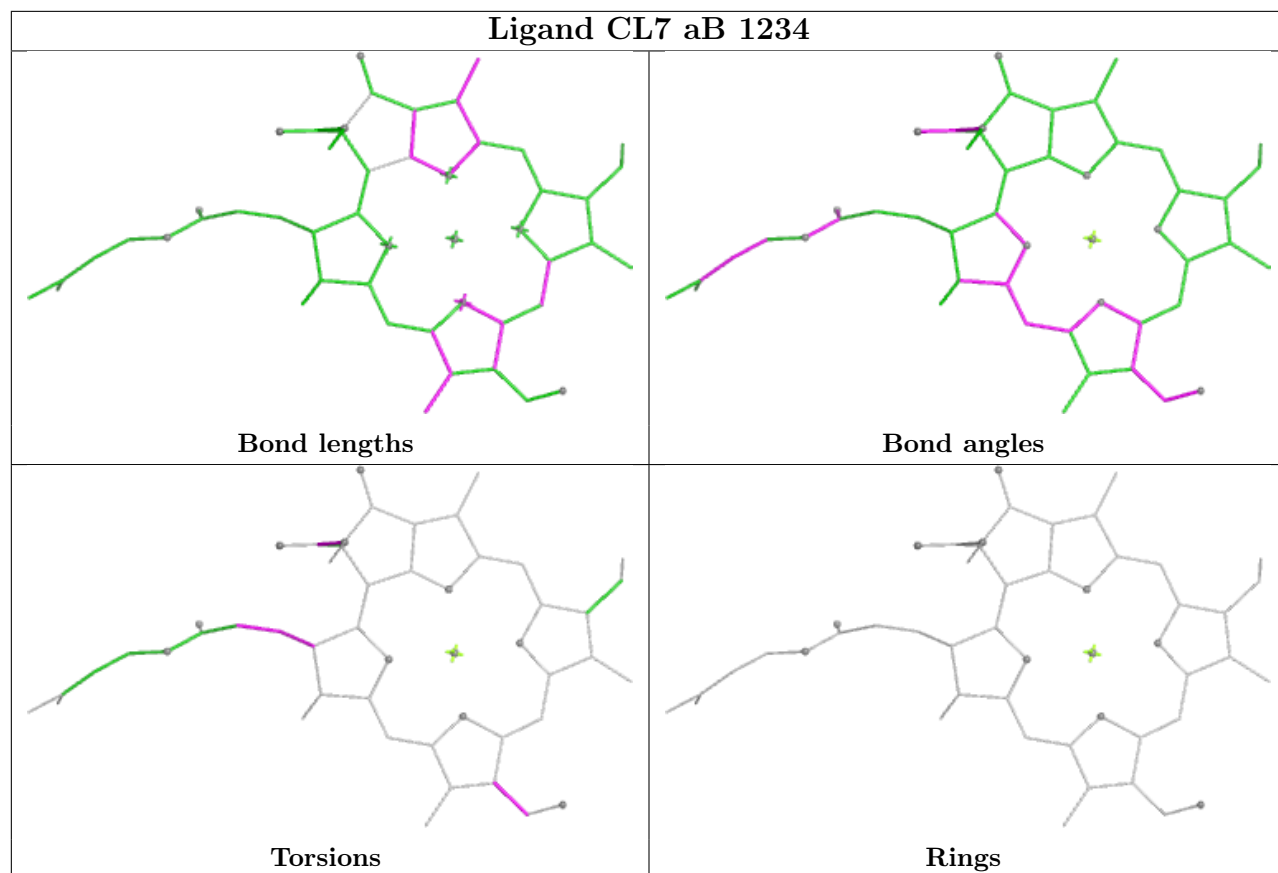
Ligand A1JPJ aB 4017



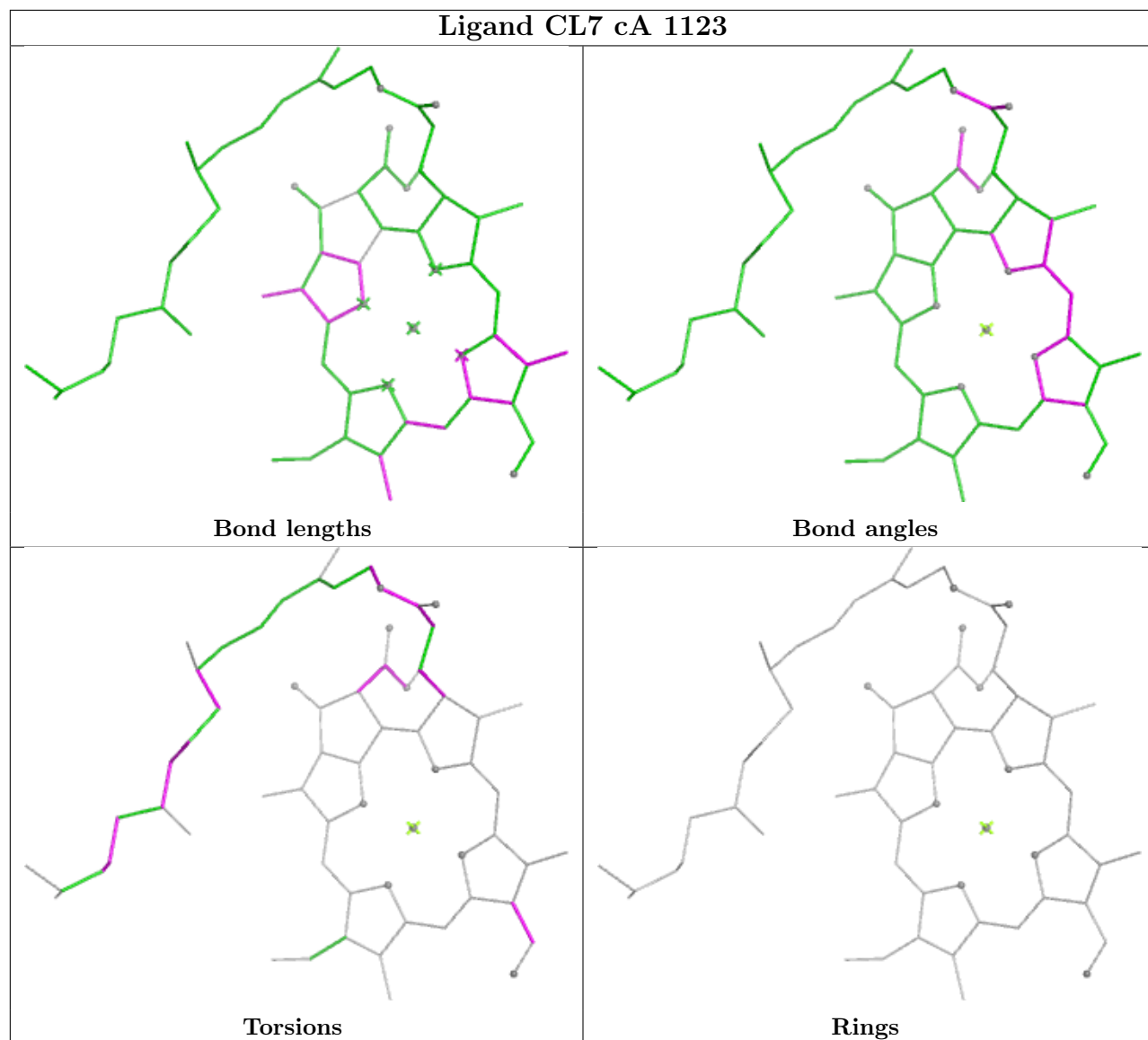
Ligand CL7 cB 1212

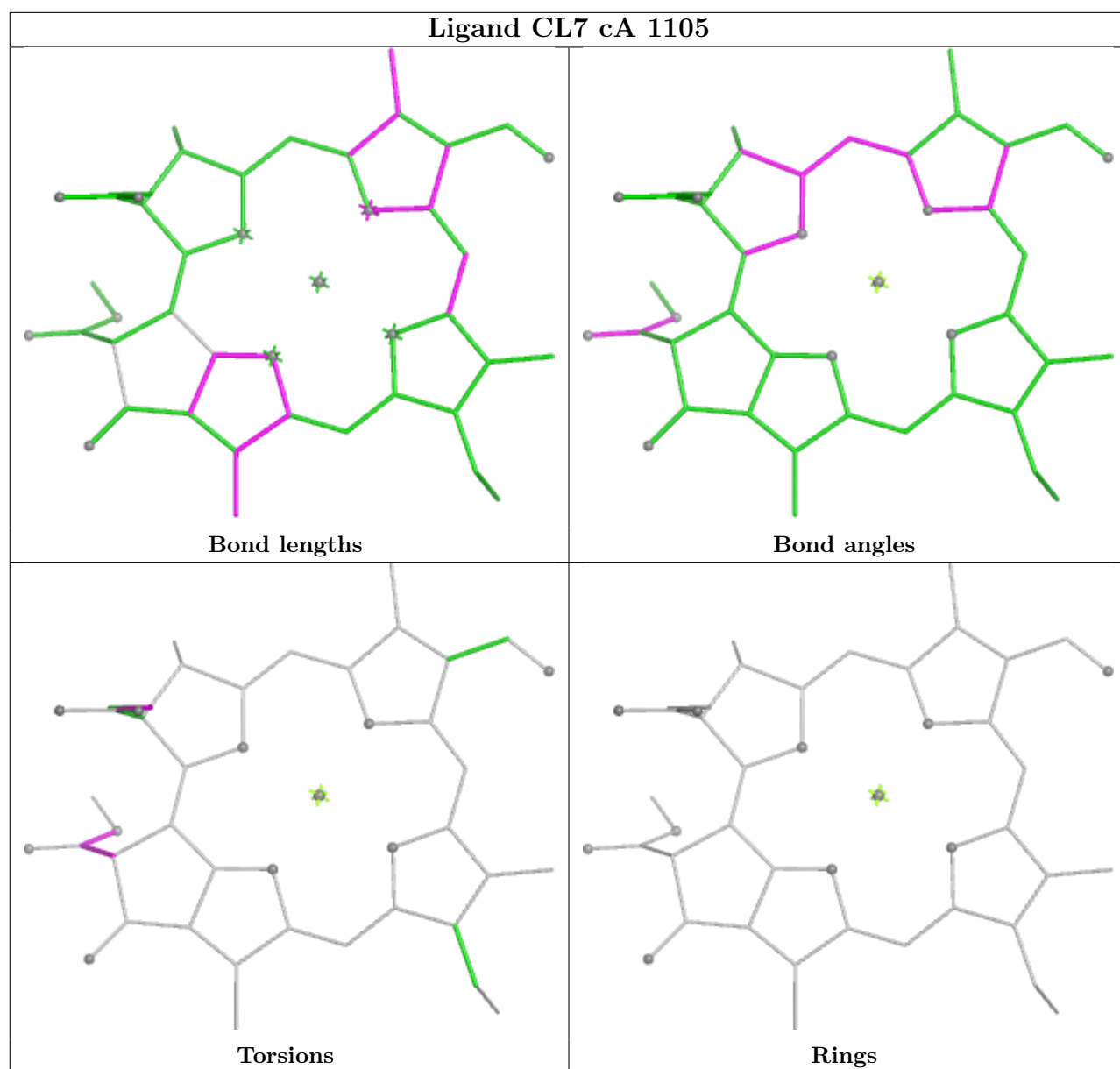


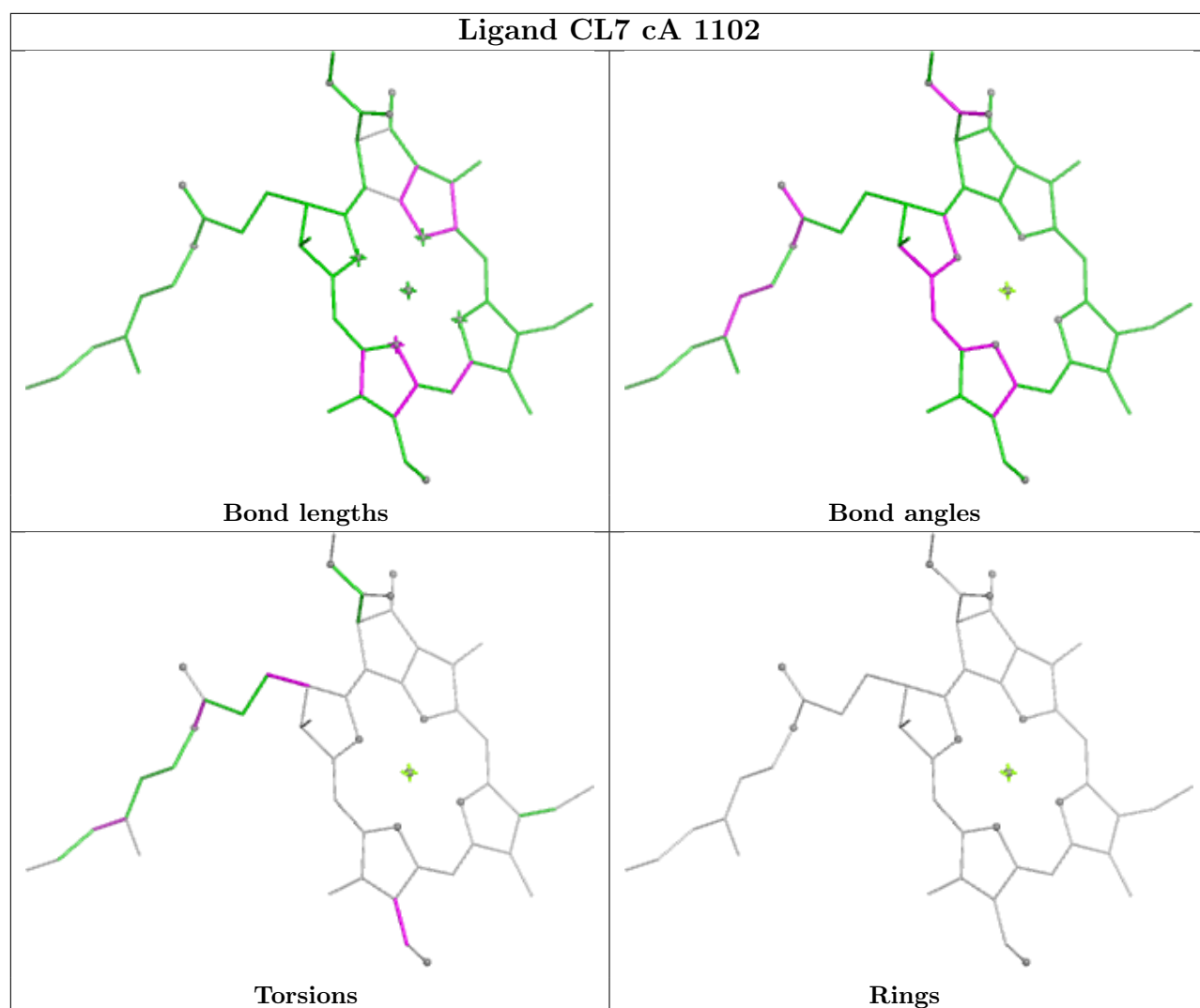




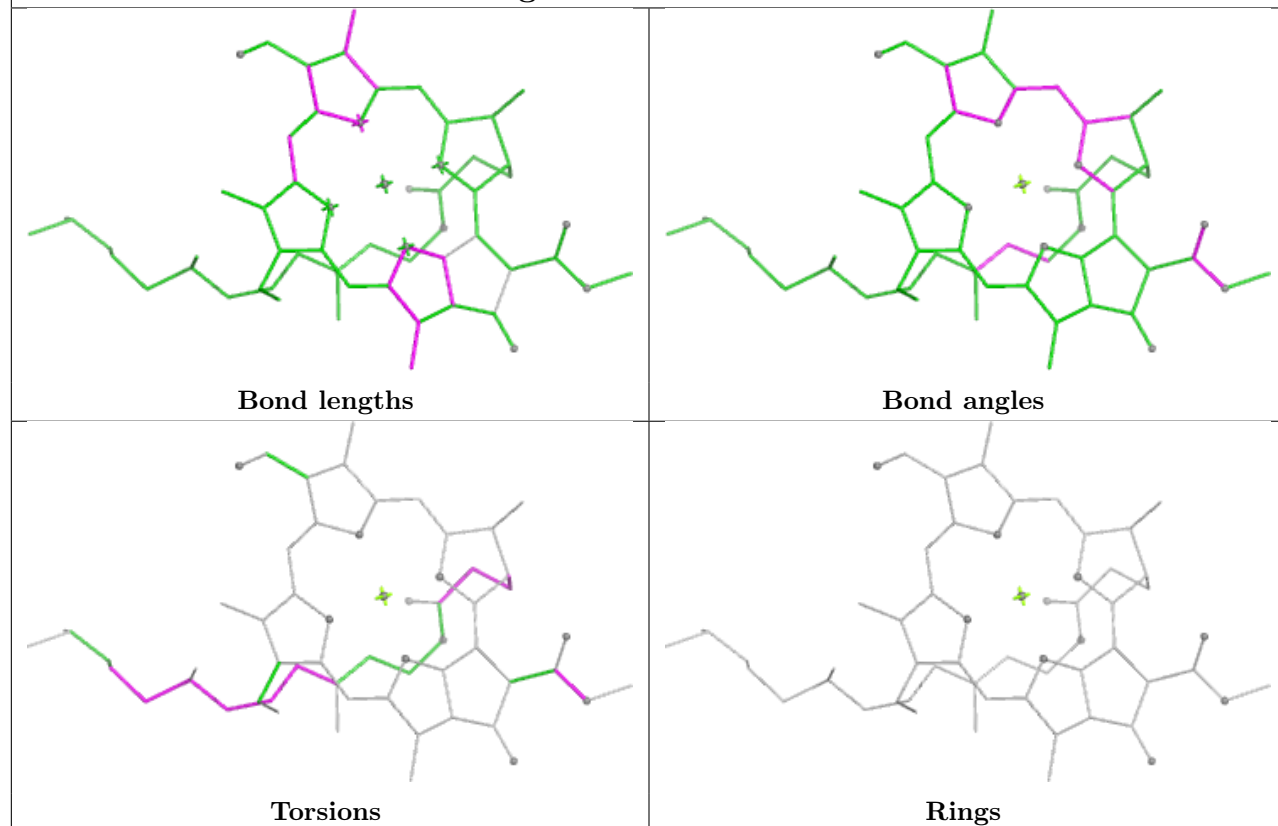
Ligand CL7 cA 1123



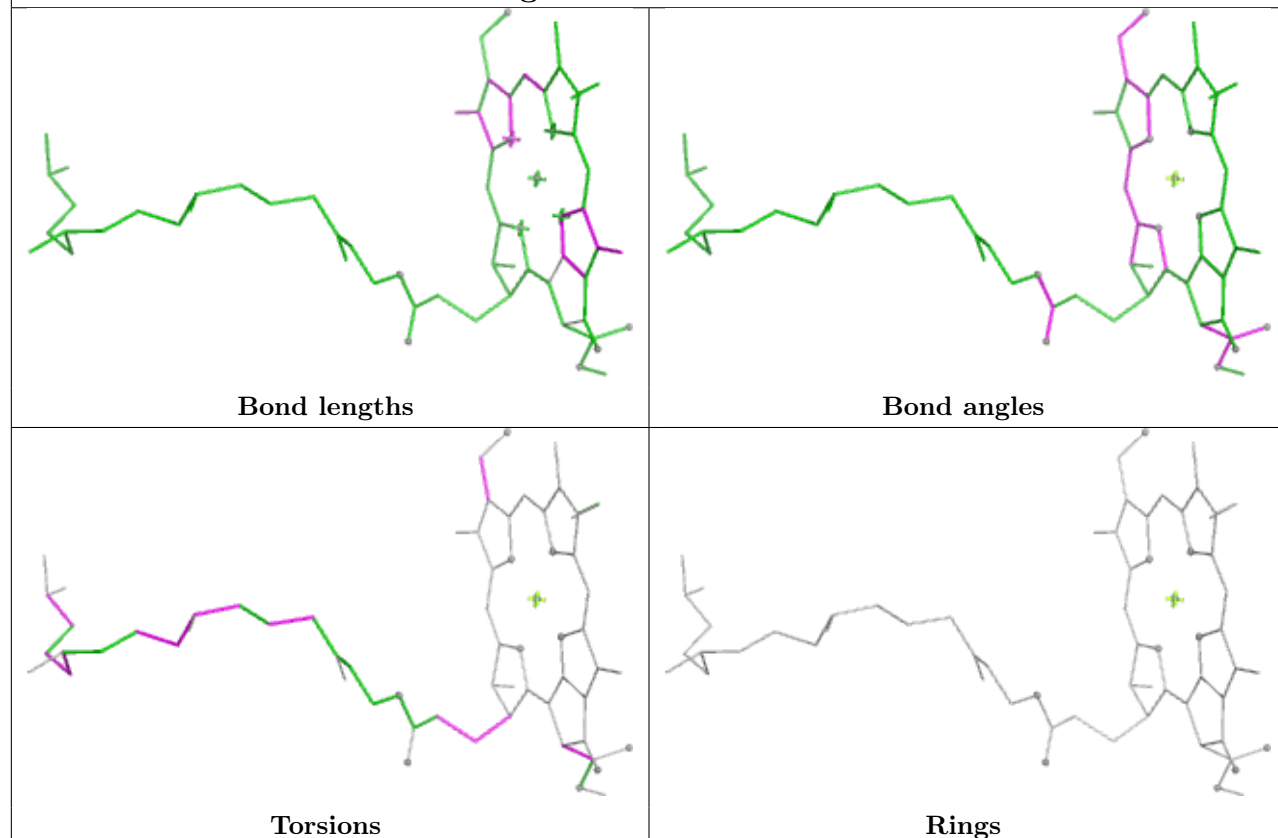


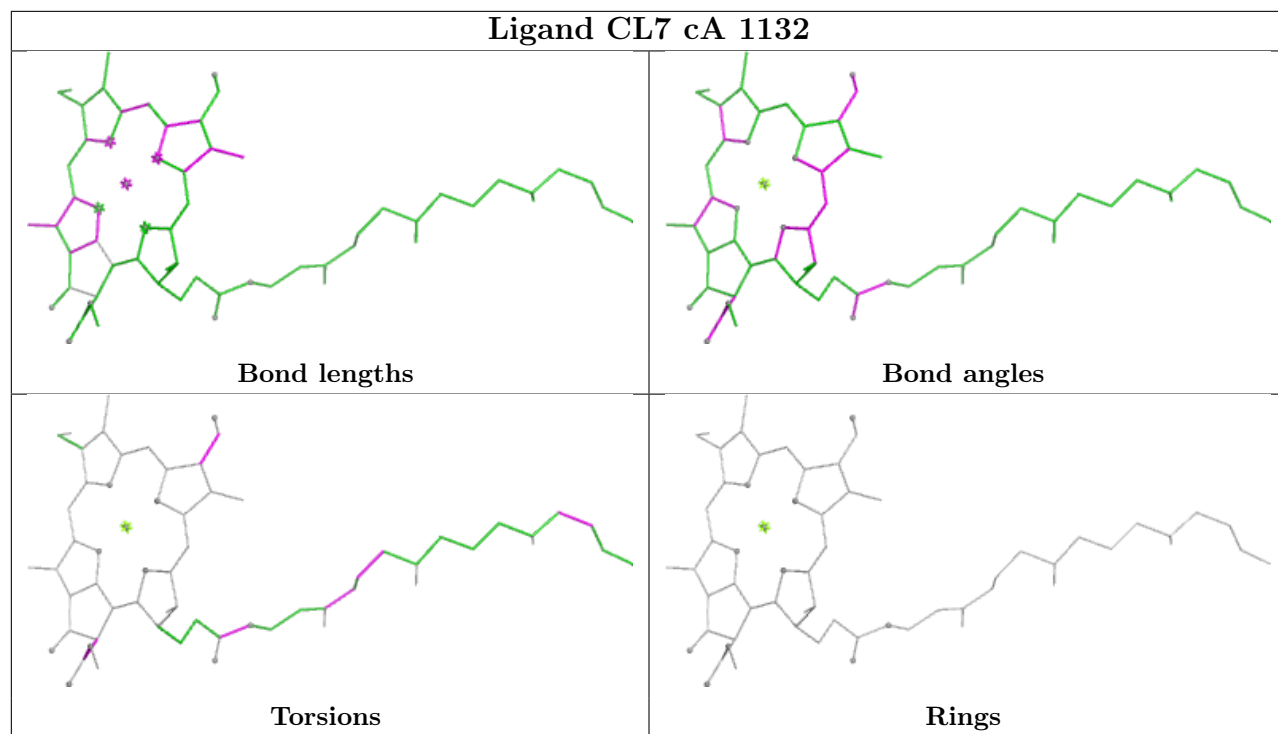
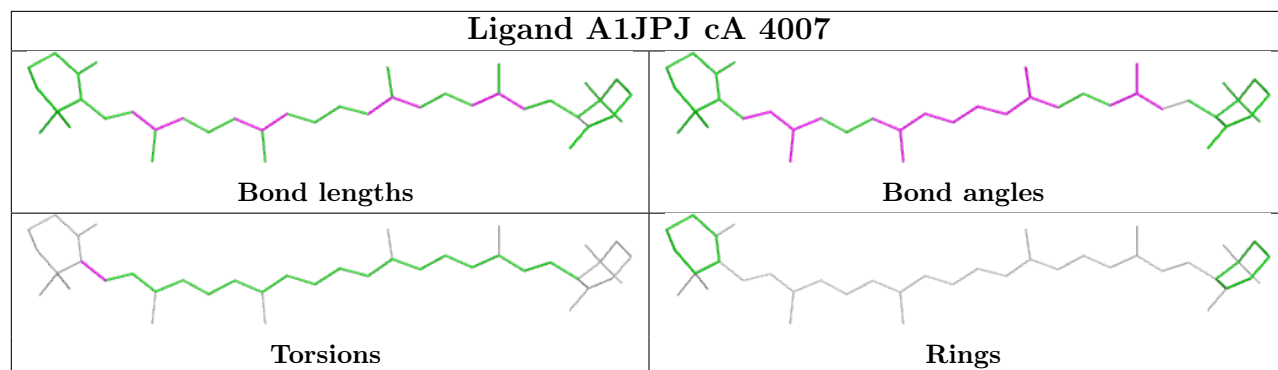


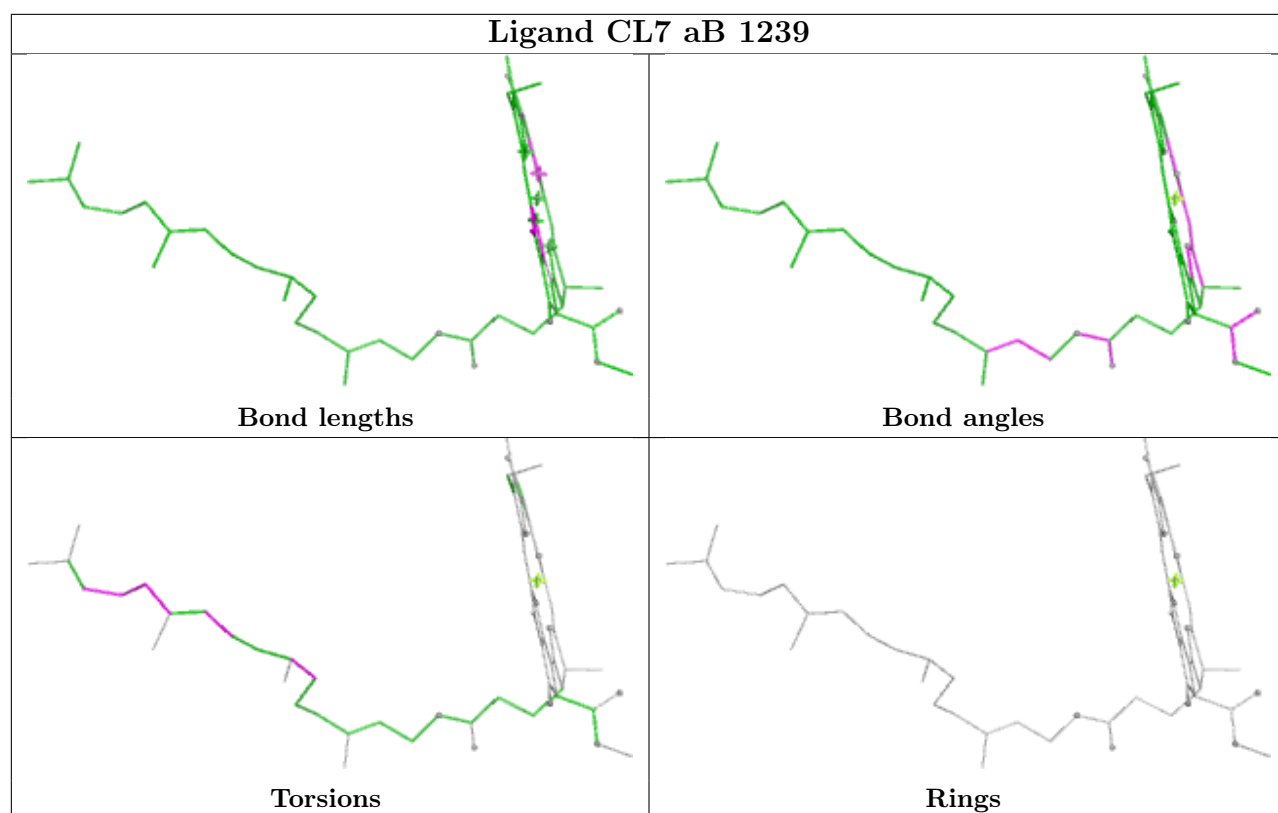
Ligand CL7 aA 1140



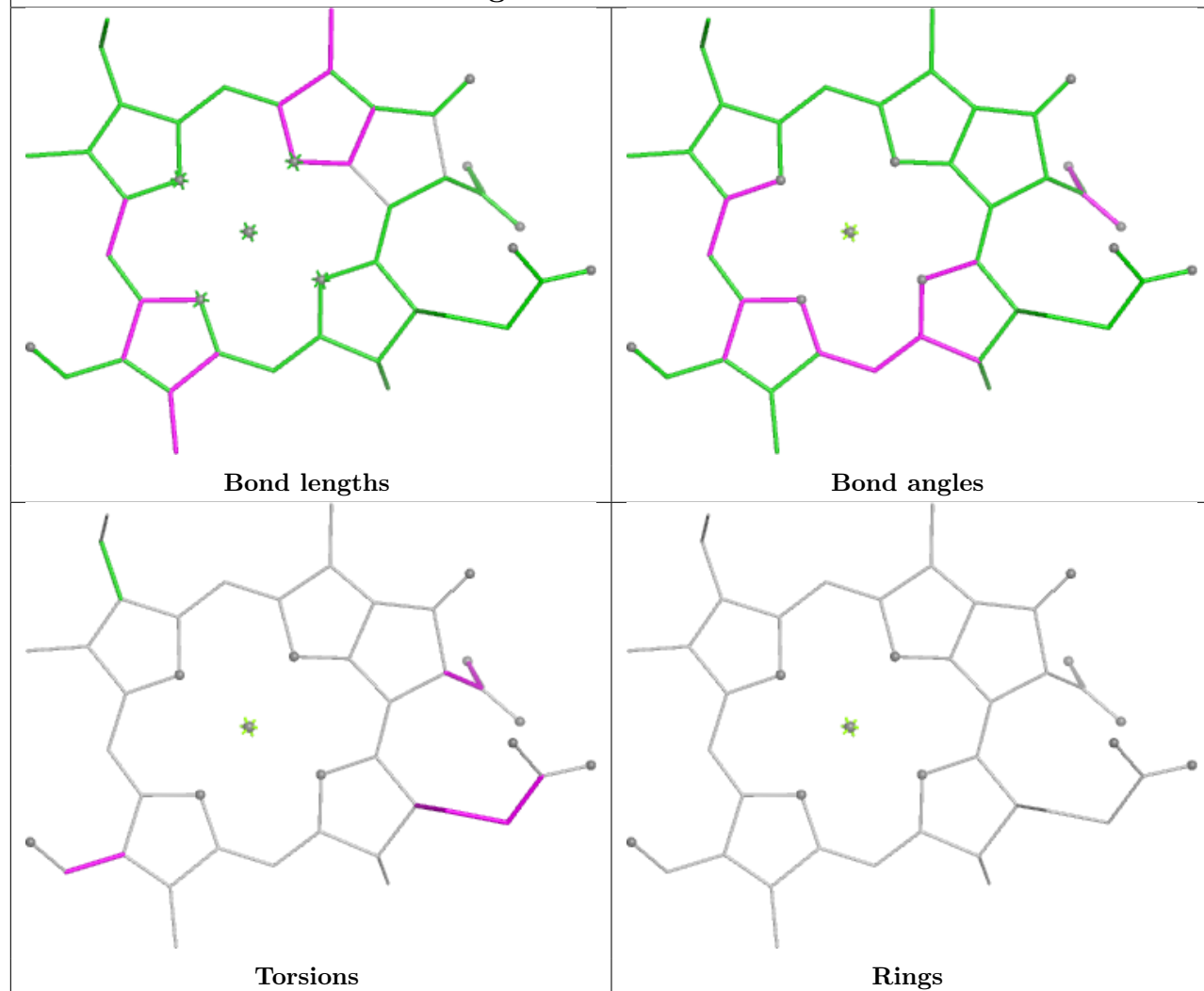
Ligand CL7 bL 1502

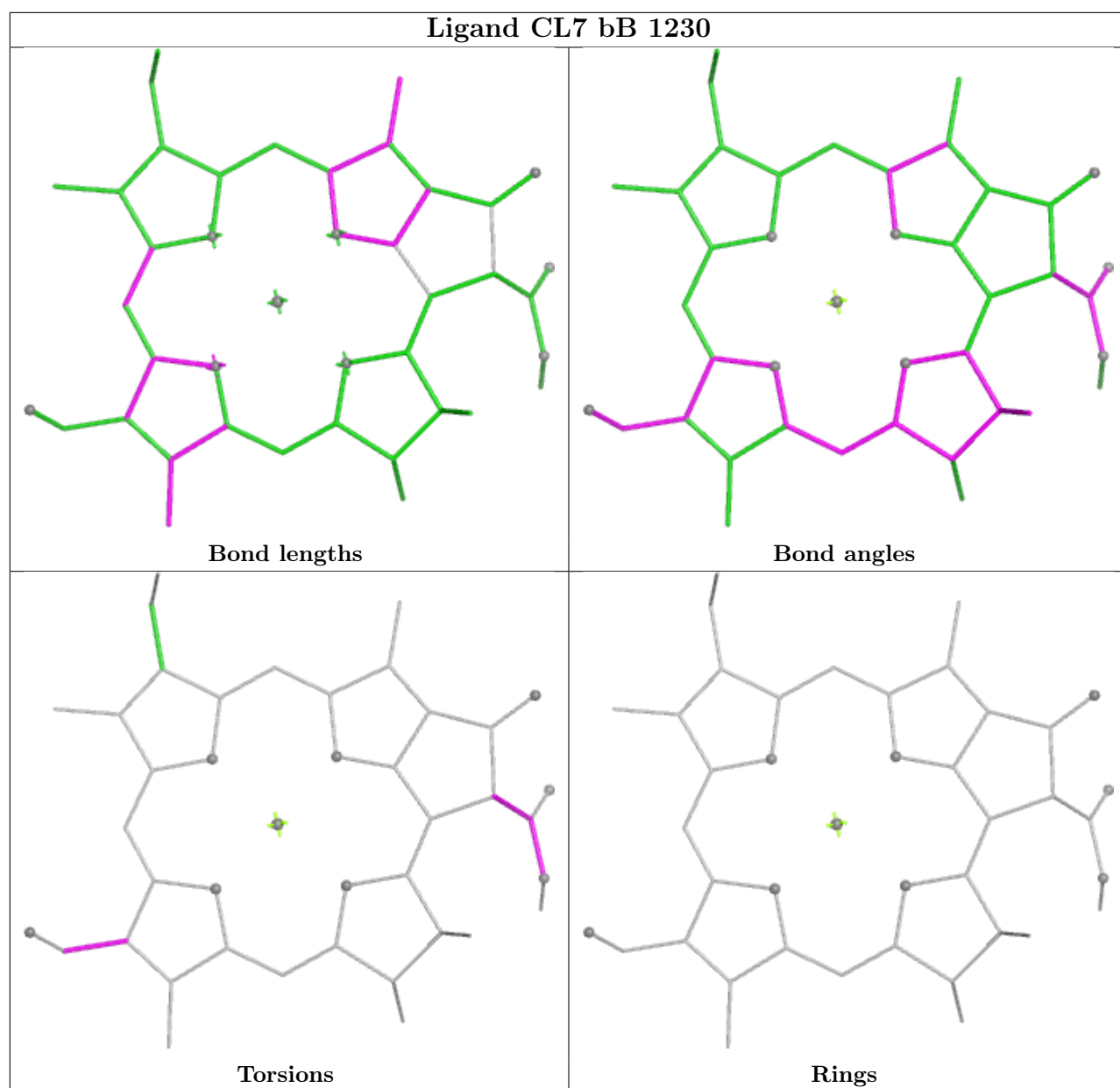


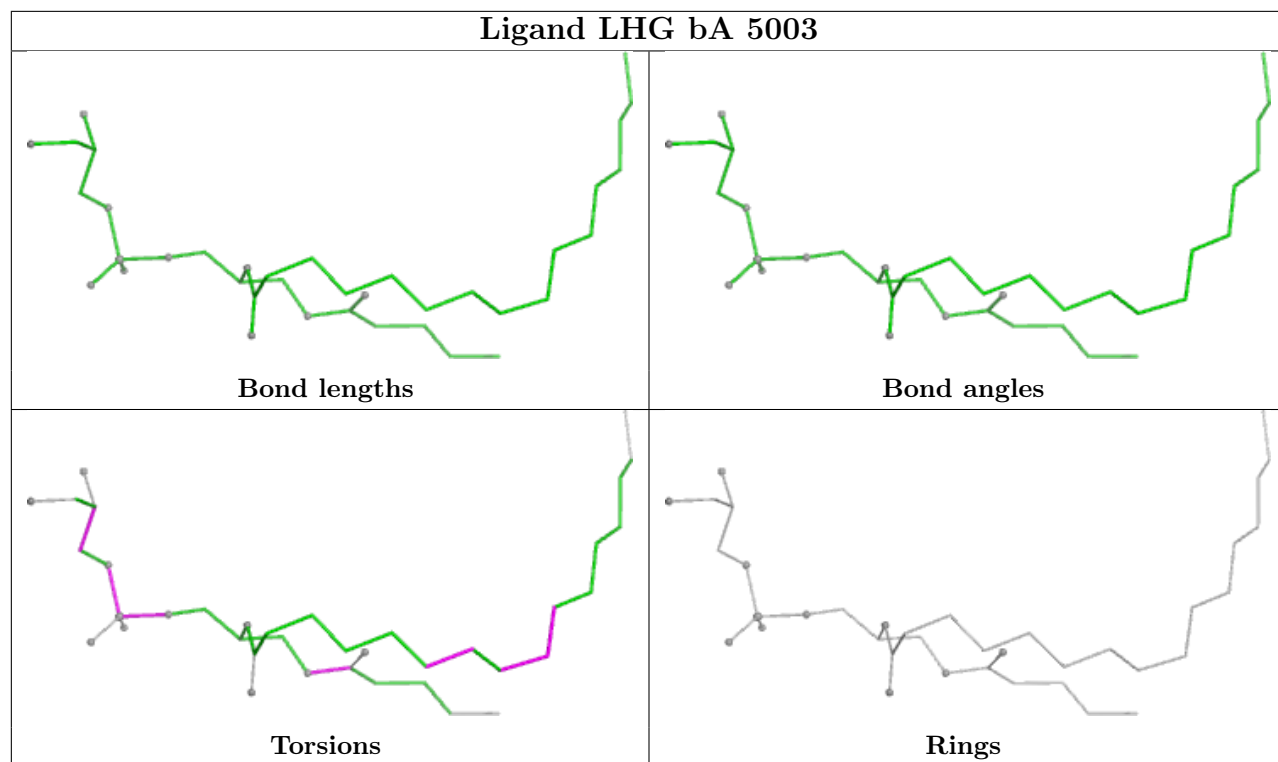


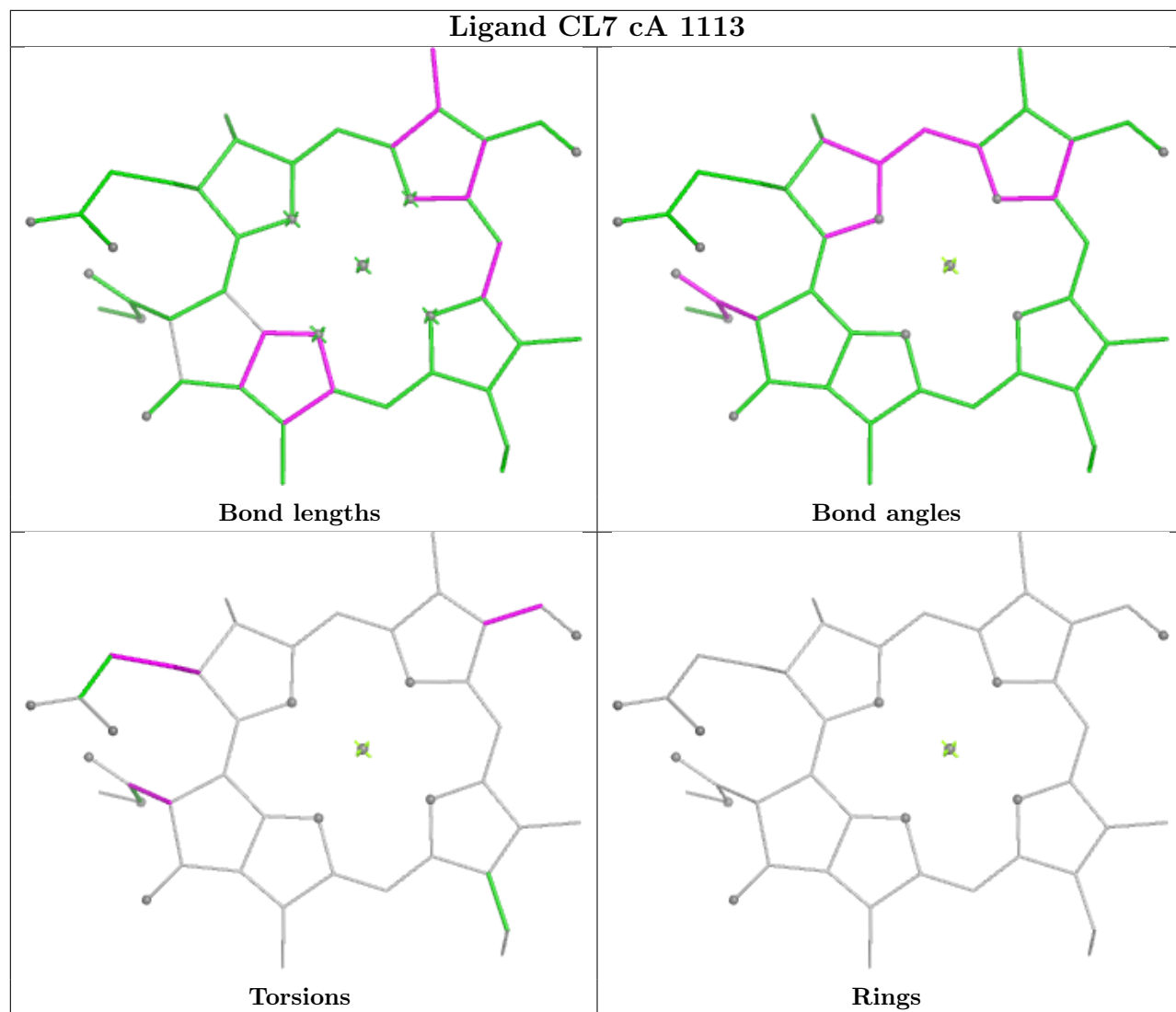


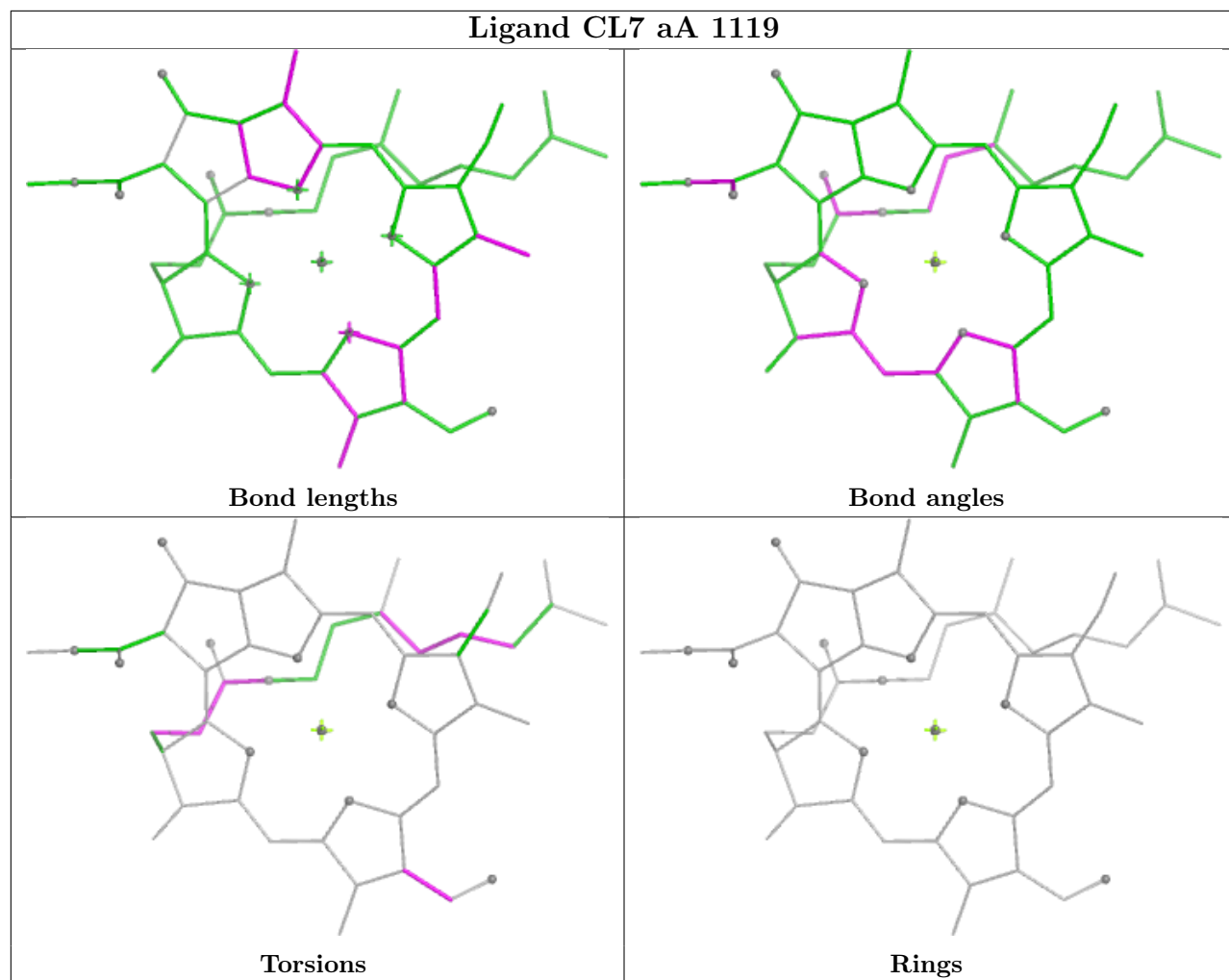
Ligand CL7 aA 1113

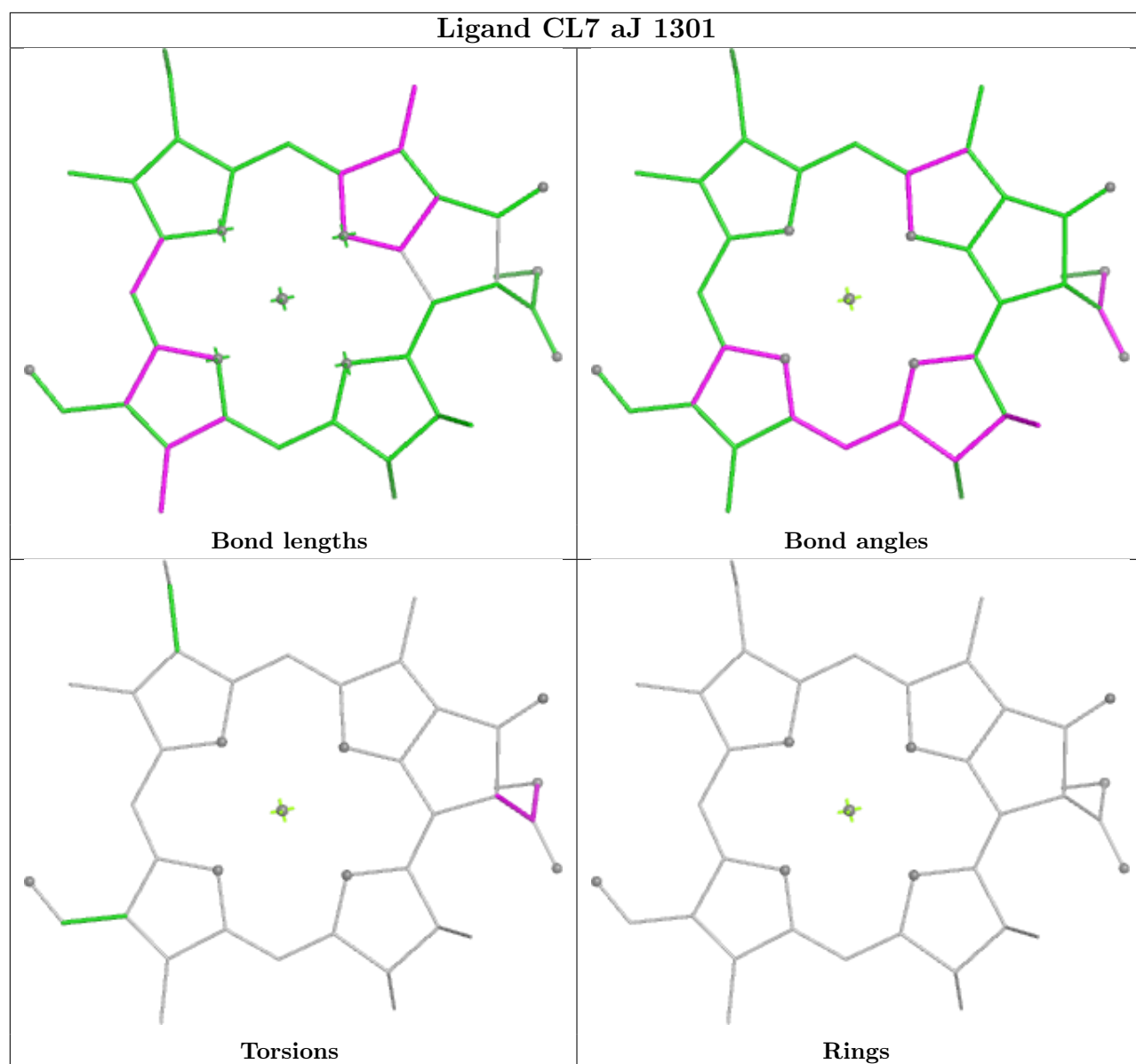


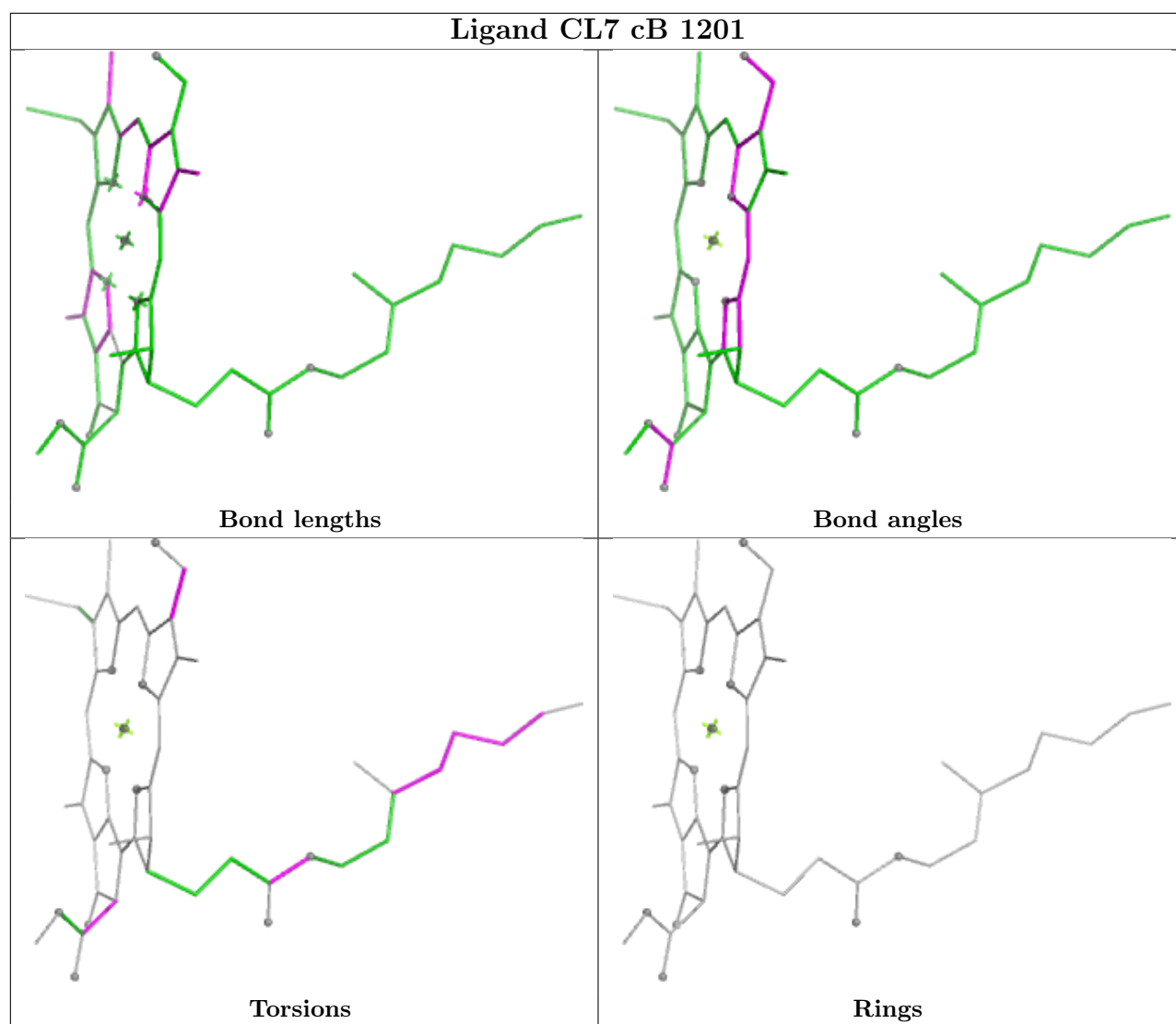


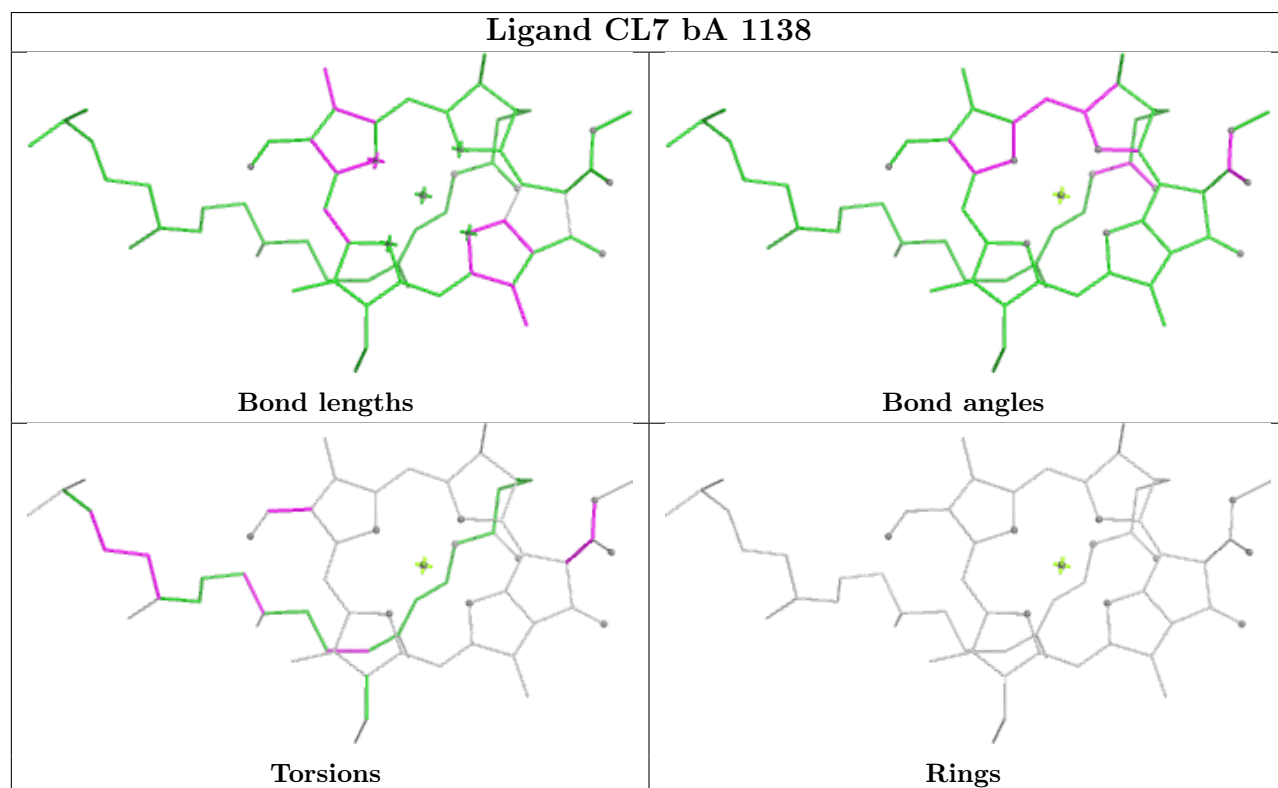
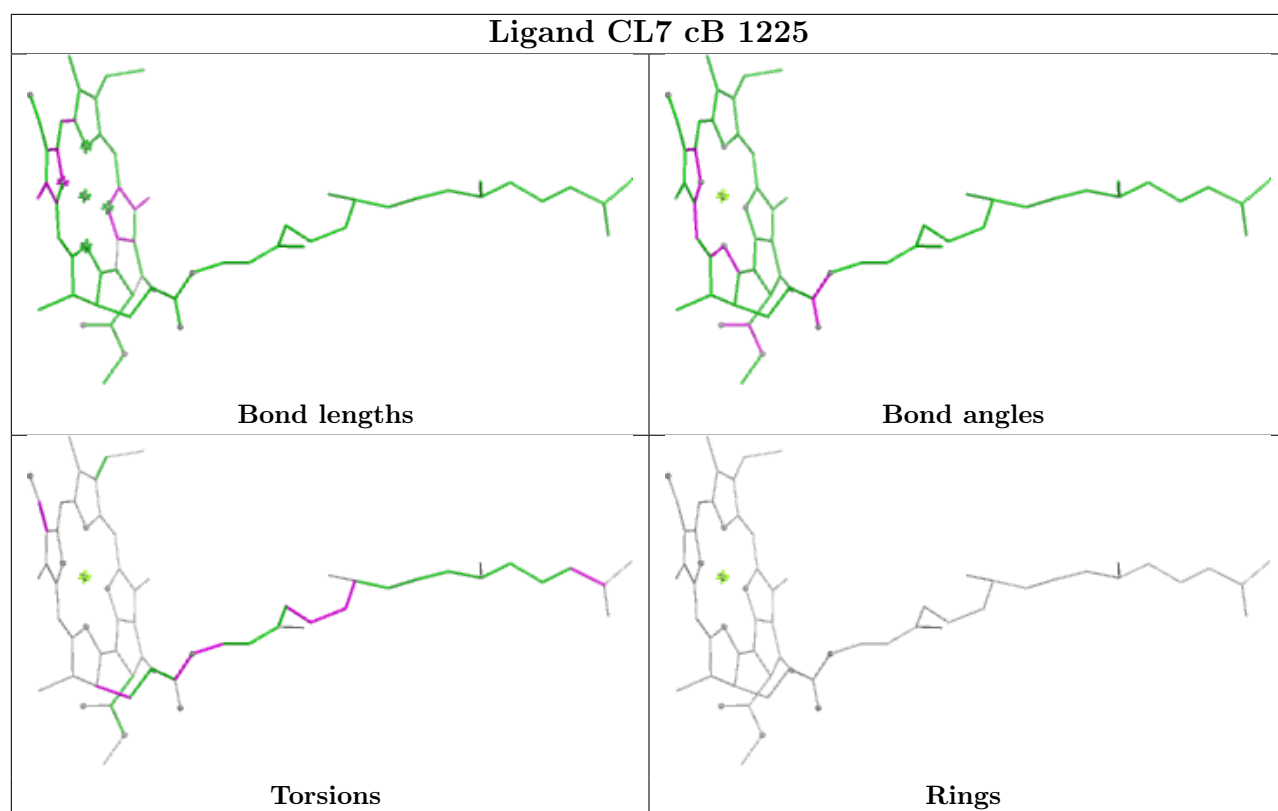


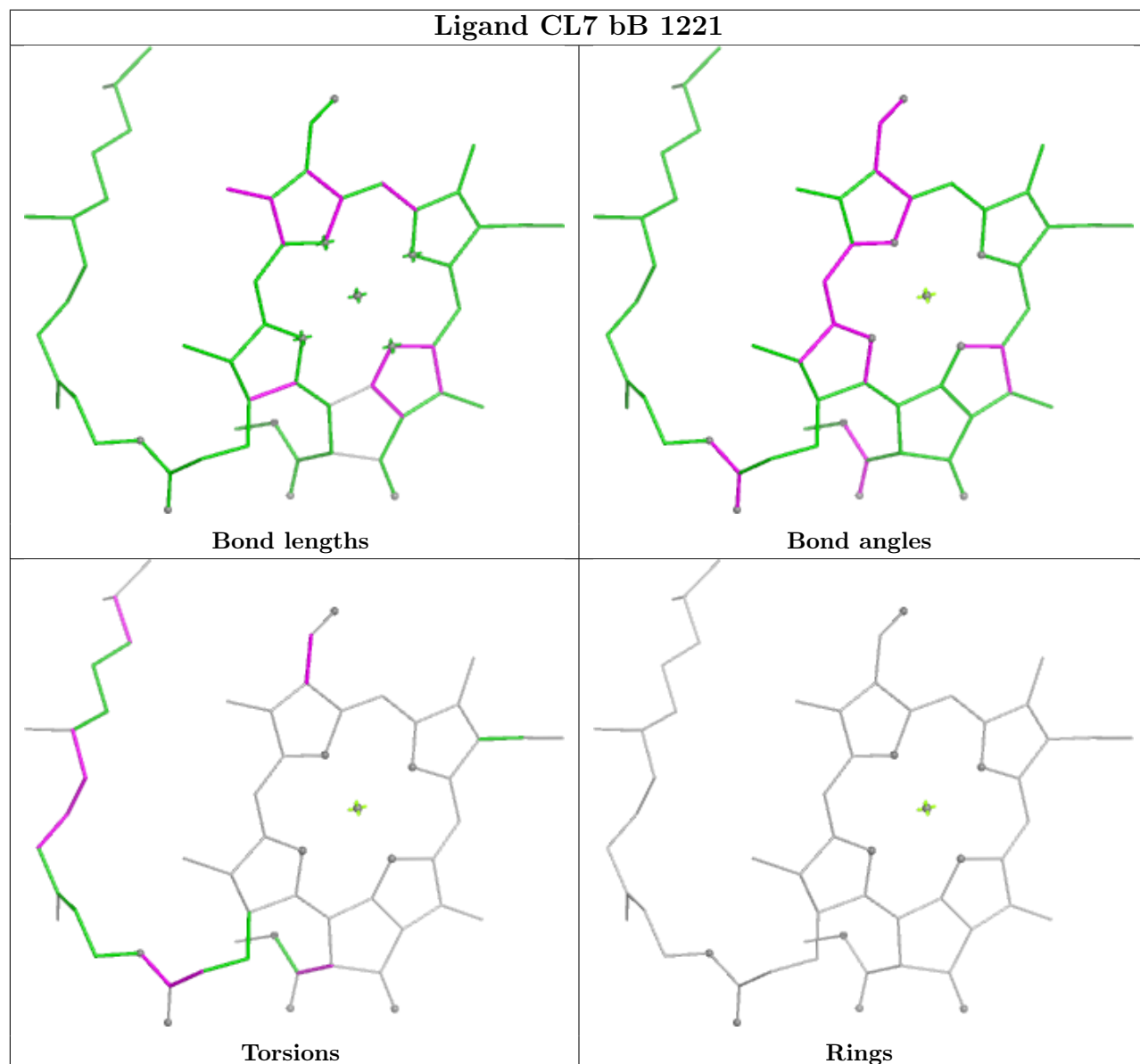
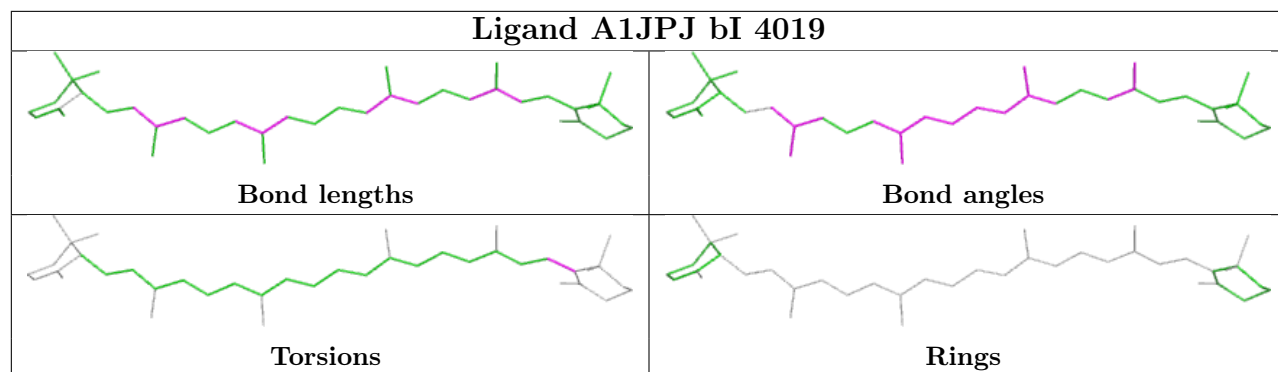


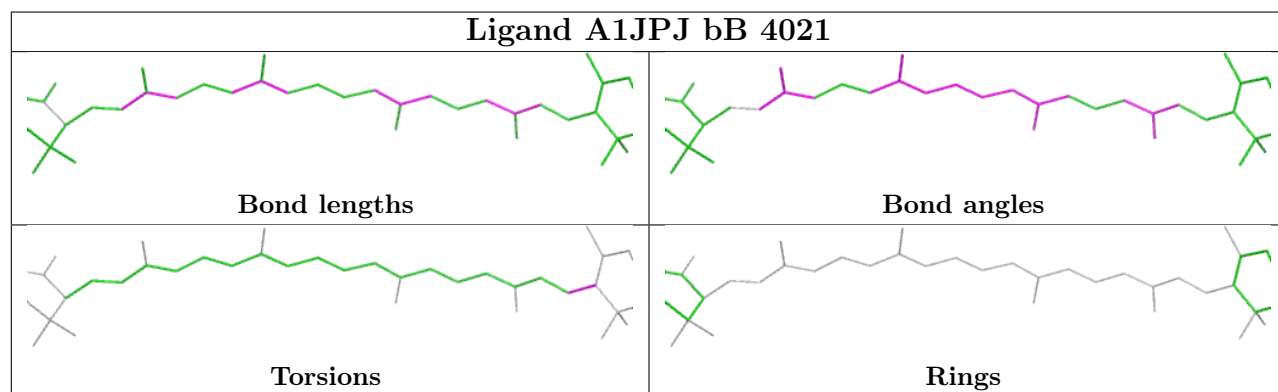
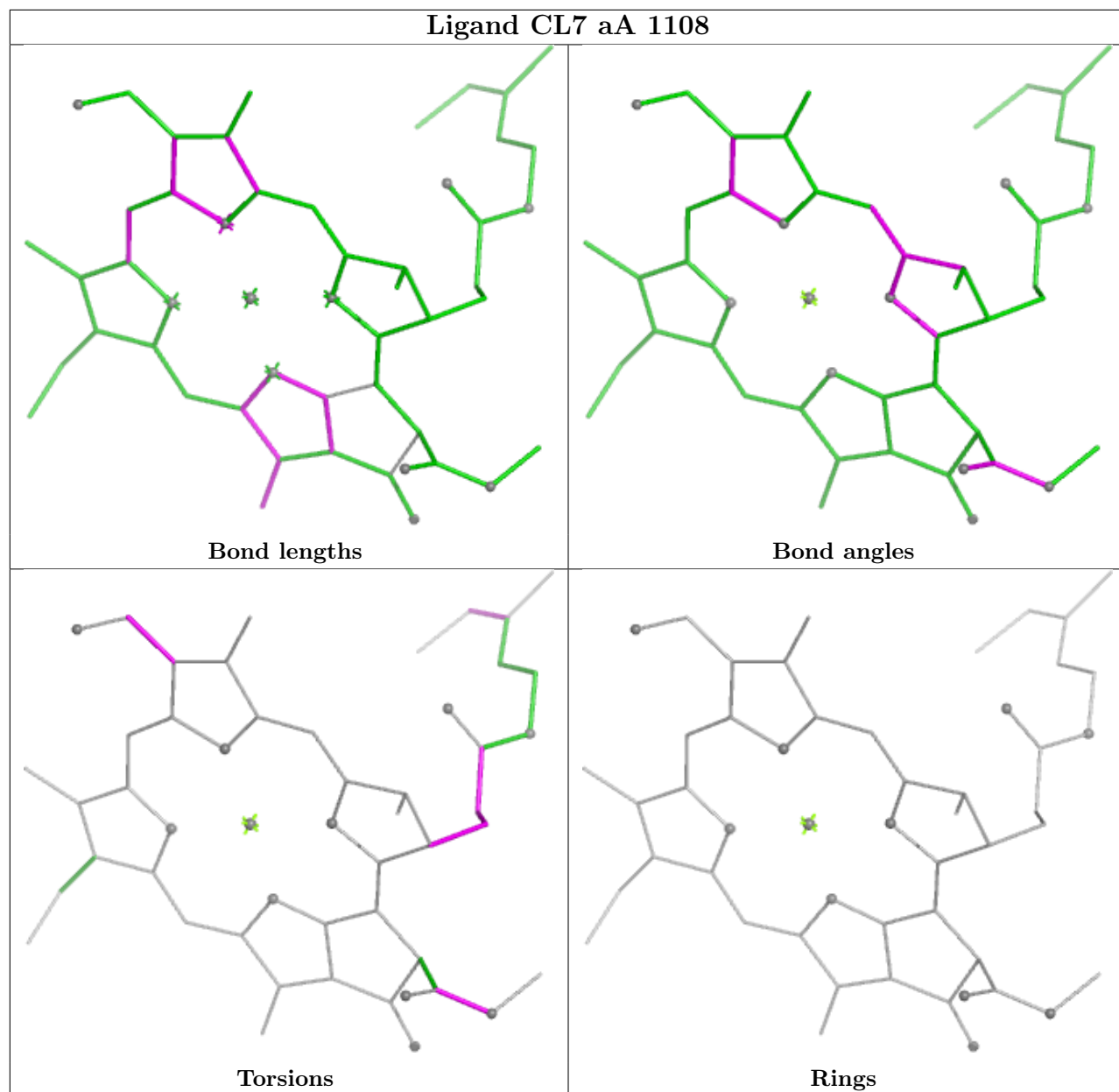




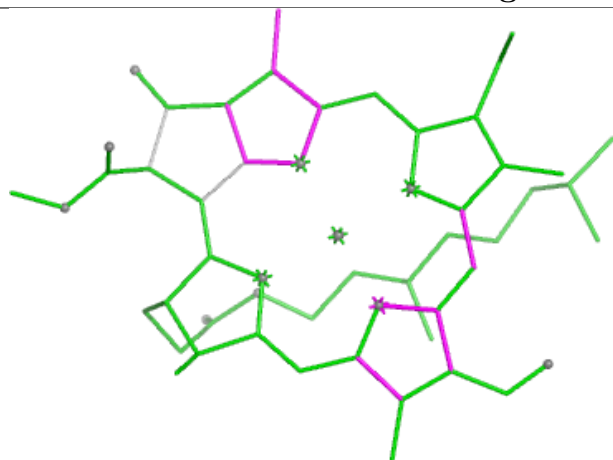




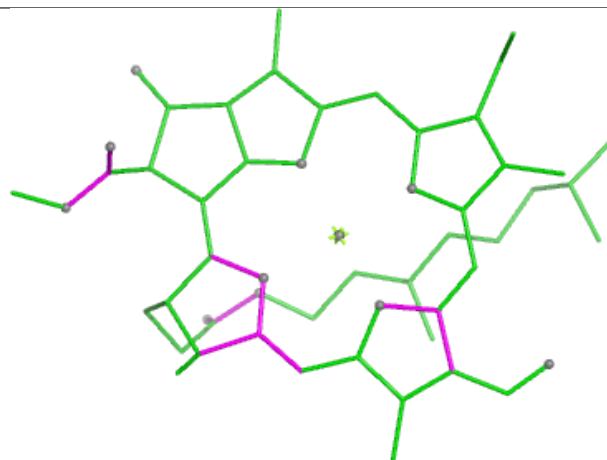




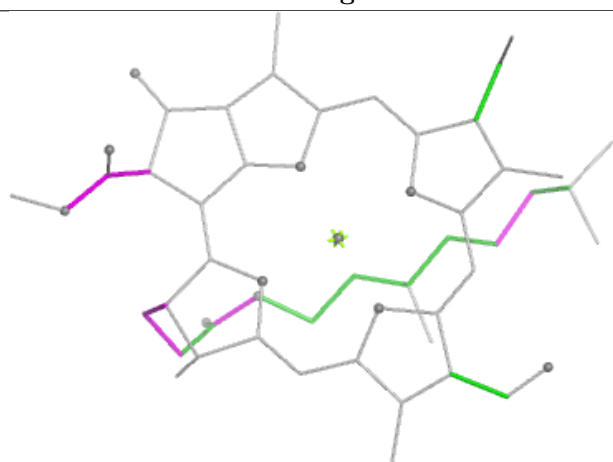
Ligand CL7 bA 1121



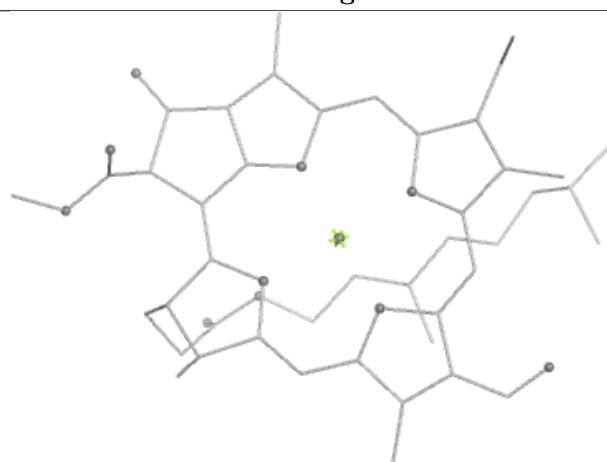
Bond lengths



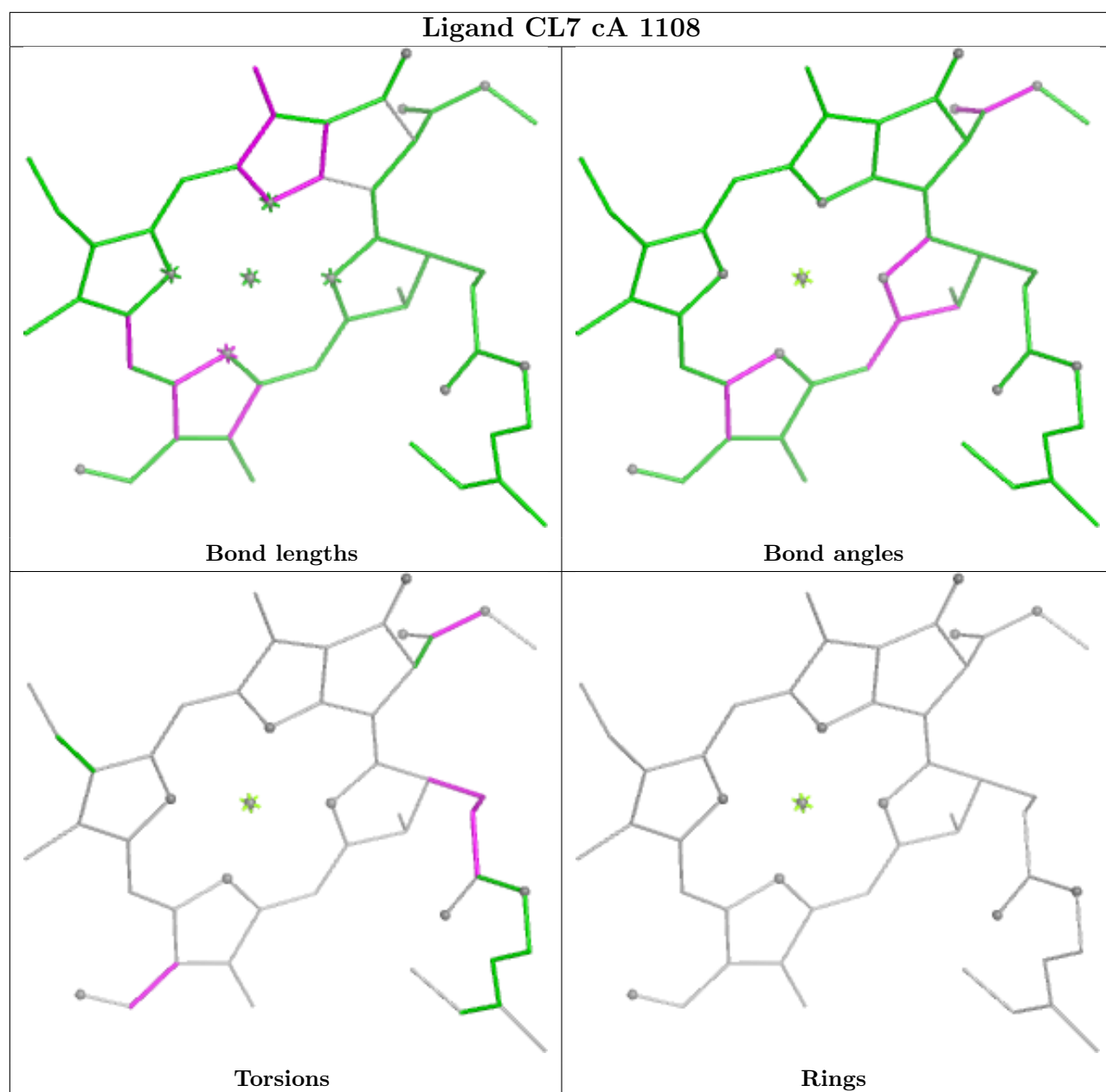
Bond angles



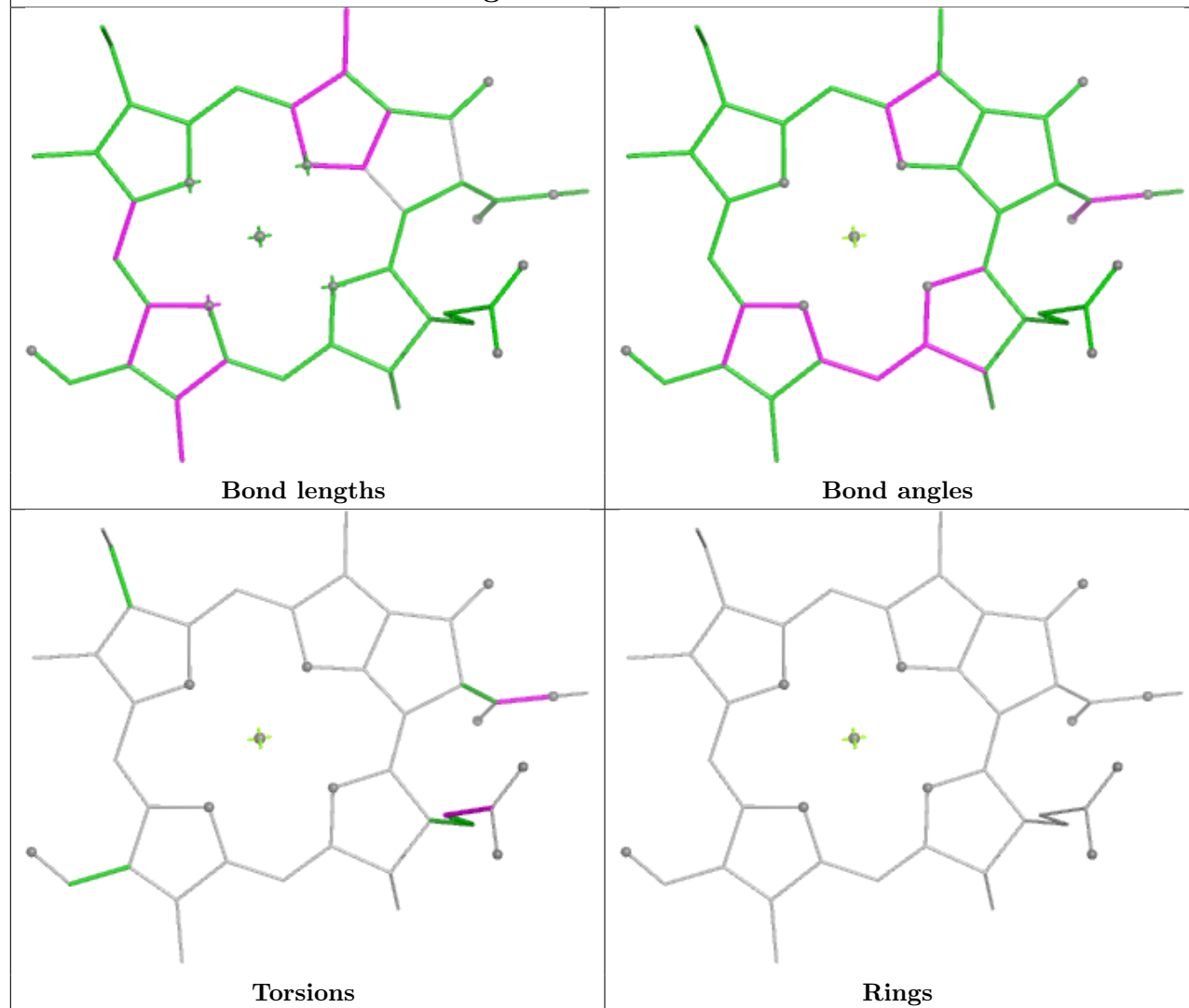
Torsions



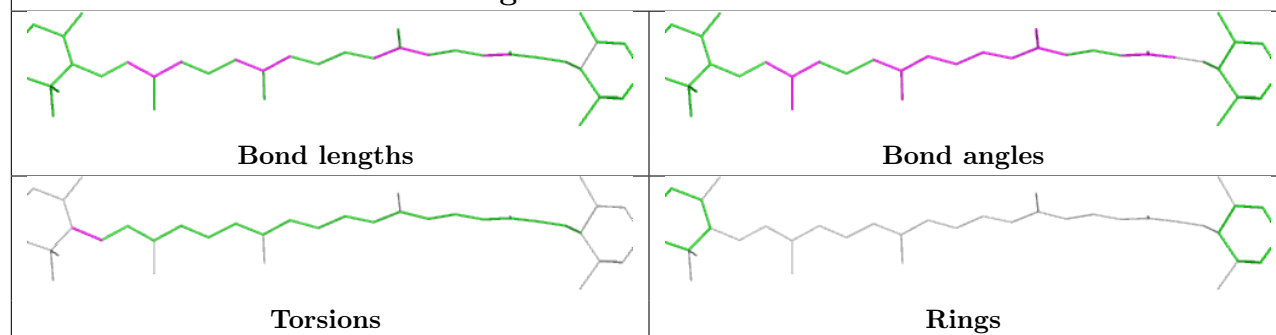
Rings

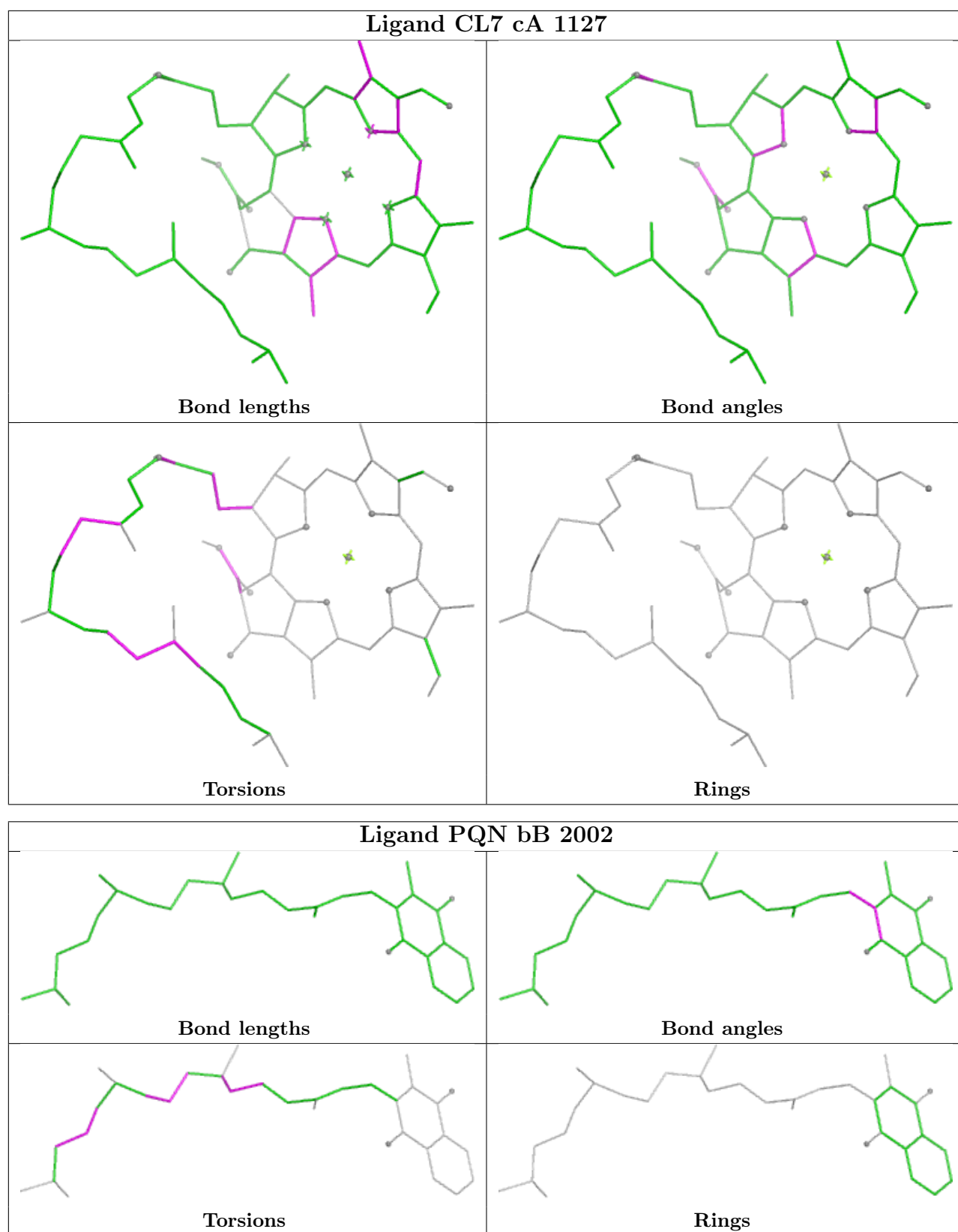


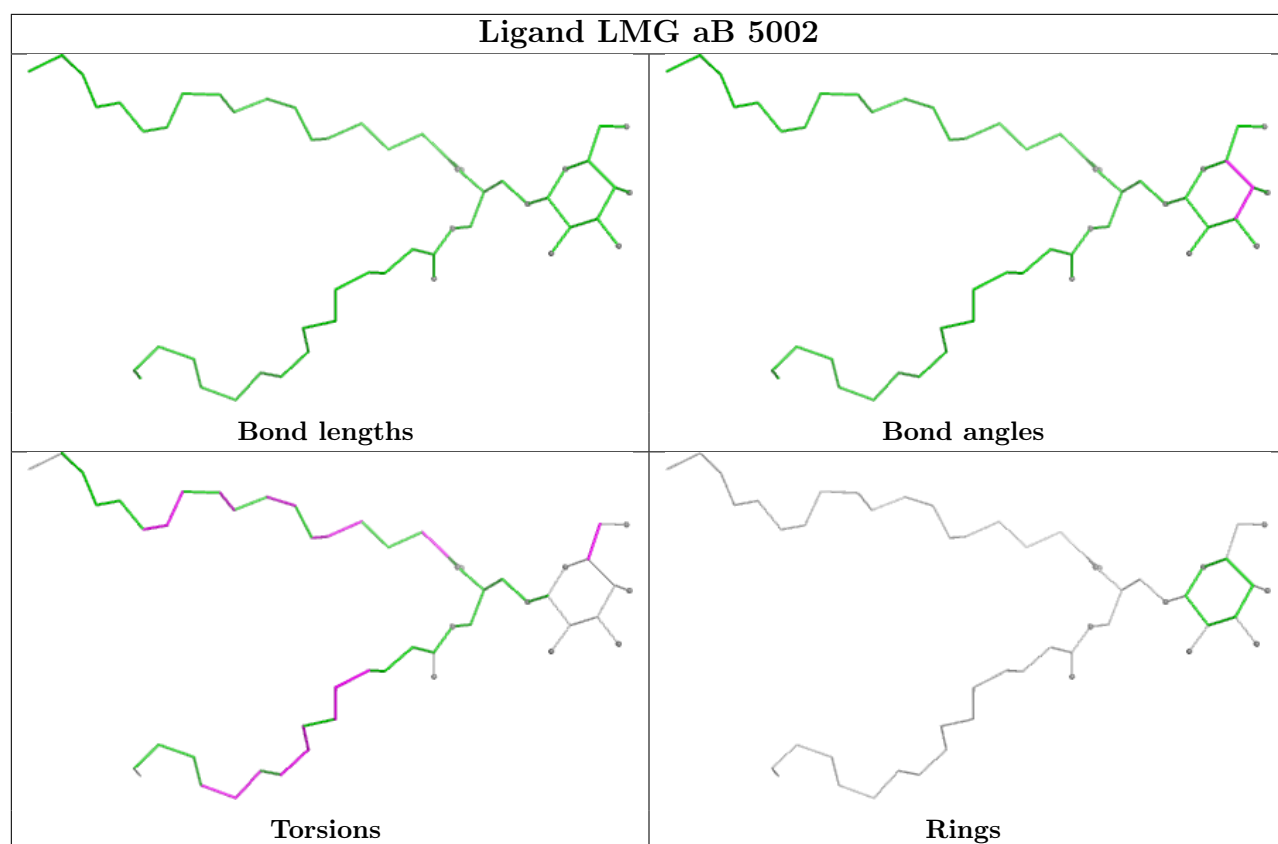
Ligand CL7 aA 1107



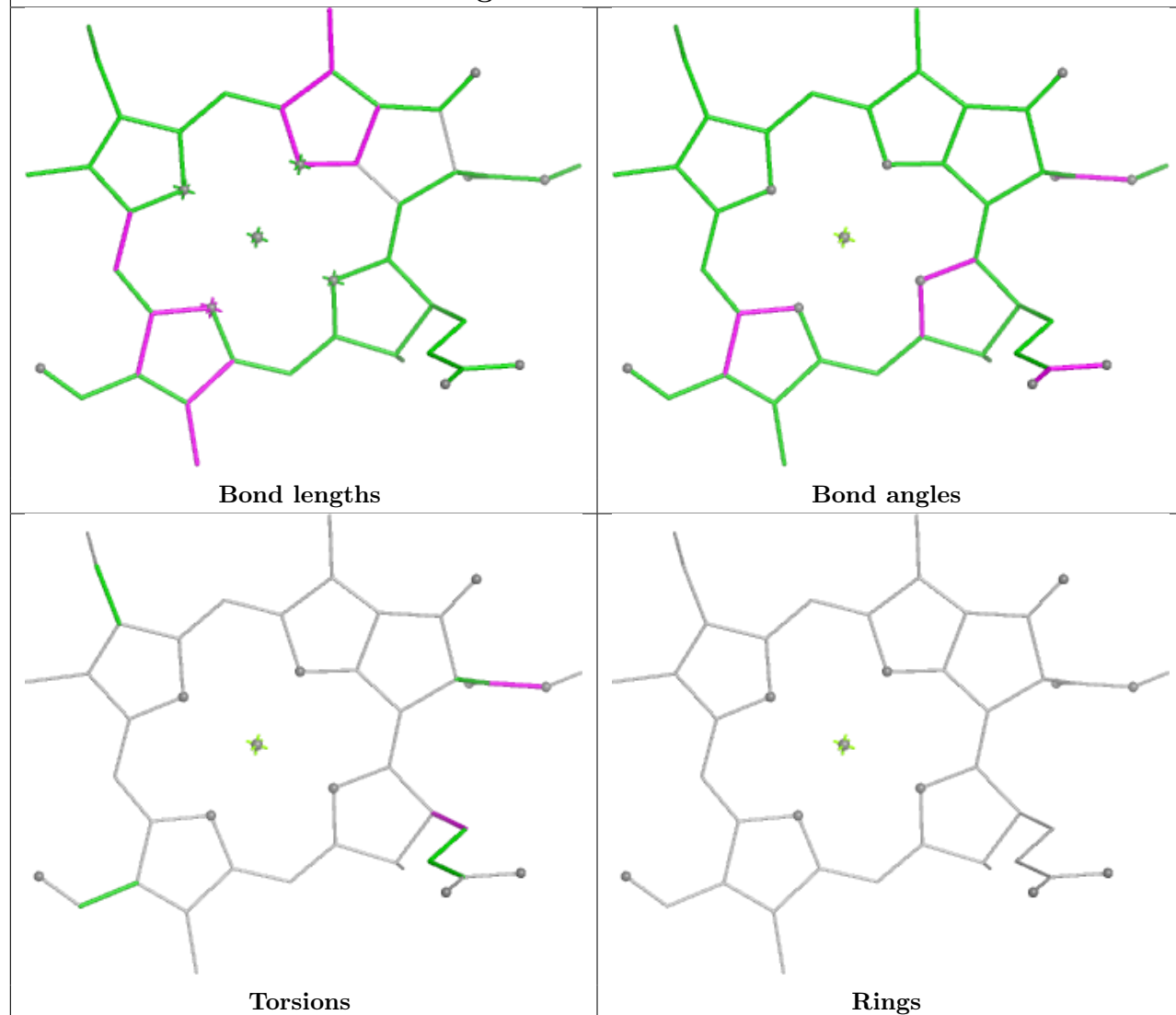
Ligand A1JPJ cB 4004

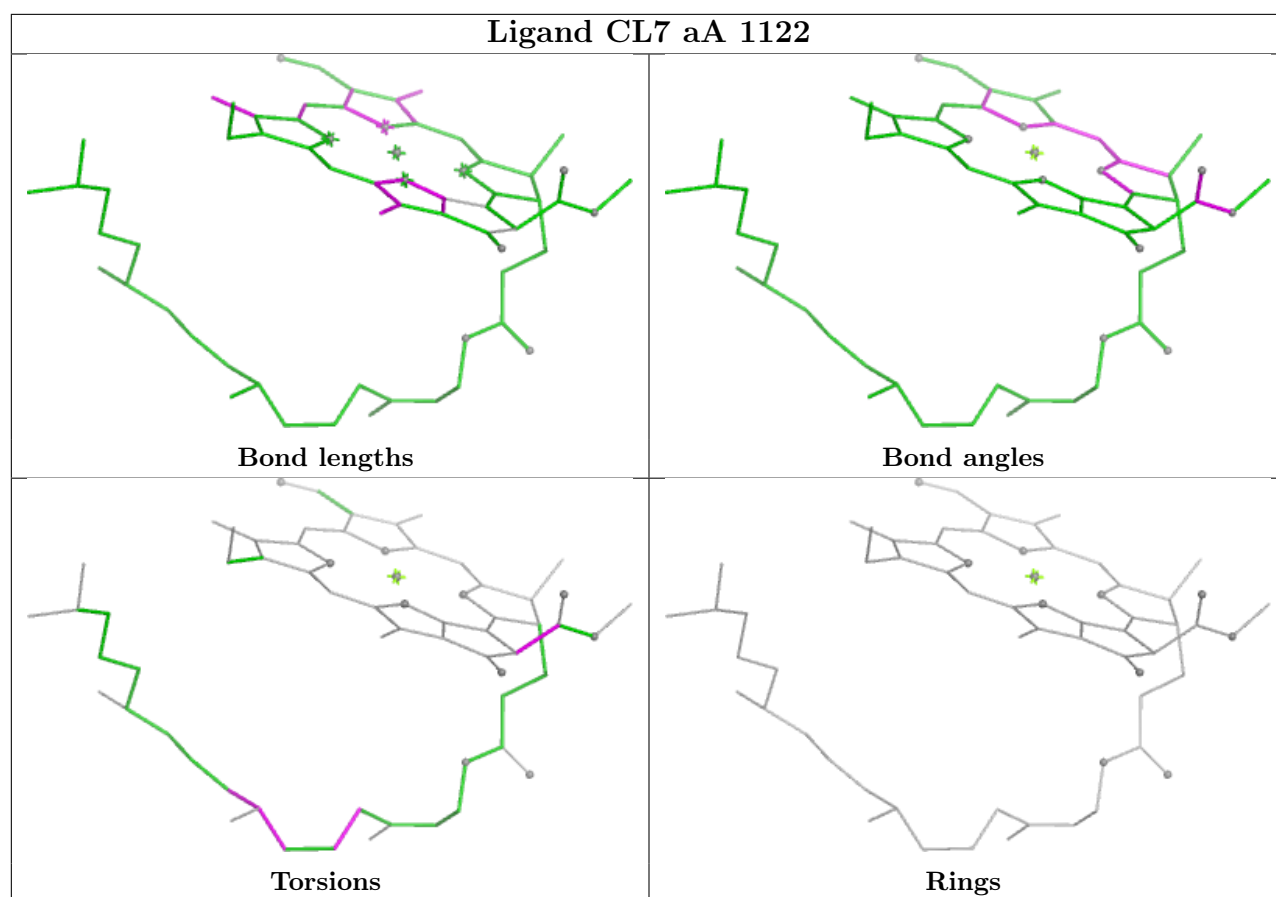






Ligand CL7 bB 1231





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.

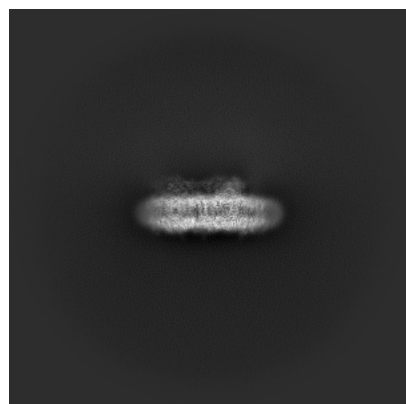
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54956. These allow visual inspection of the internal detail of the map and identification of artifacts.

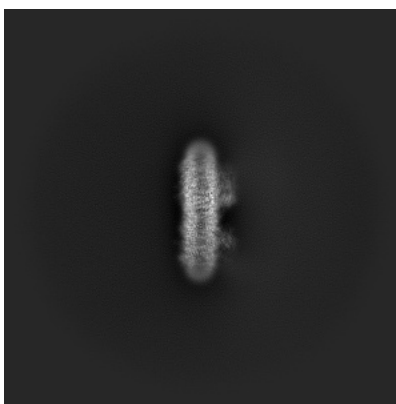
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

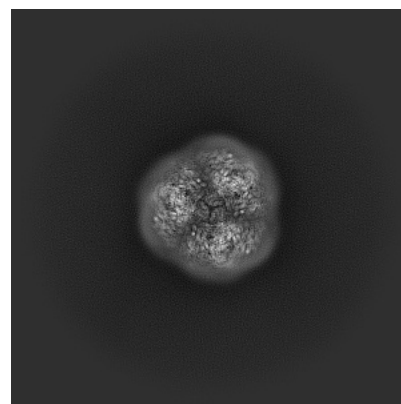
6.1.1 Primary map



X

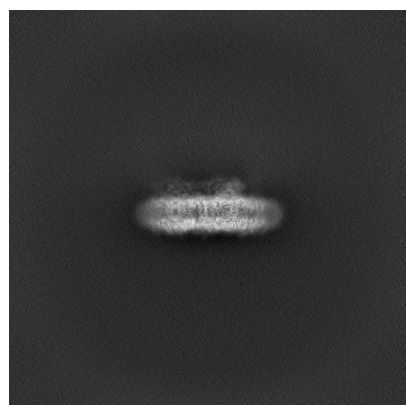


Y

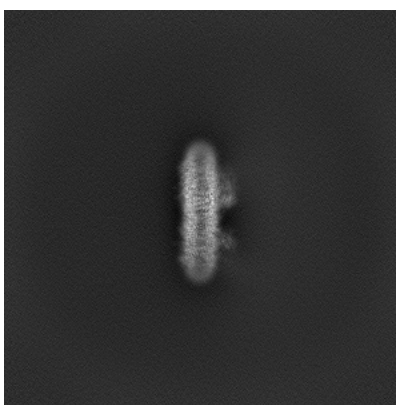


Z

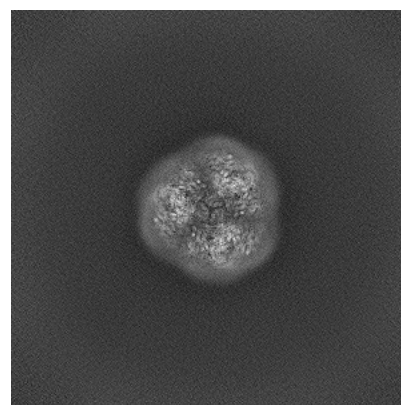
6.1.2 Raw map



X



Y

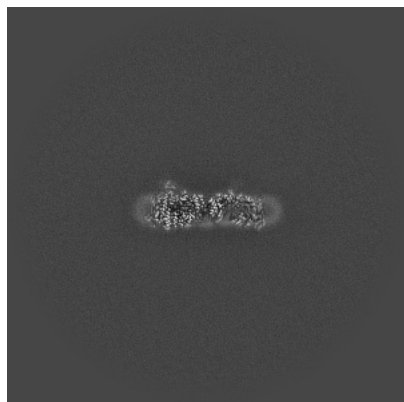


Z

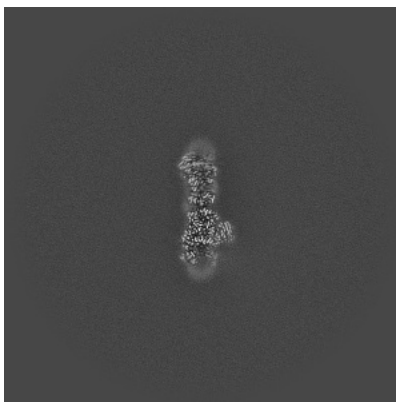
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

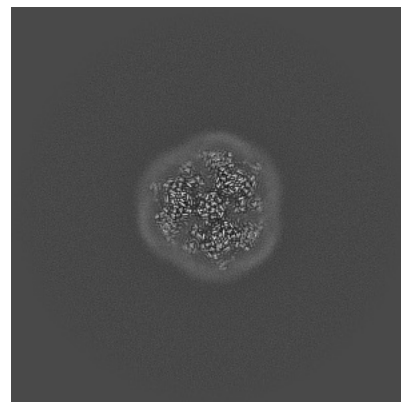
6.2.1 Primary map



X Index: 300

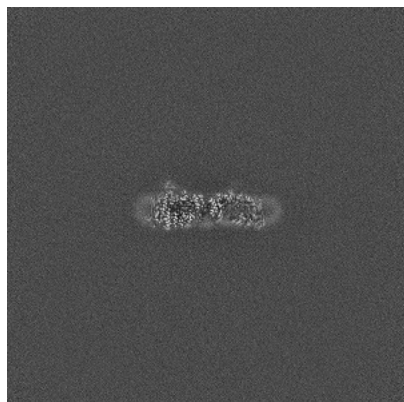


Y Index: 300

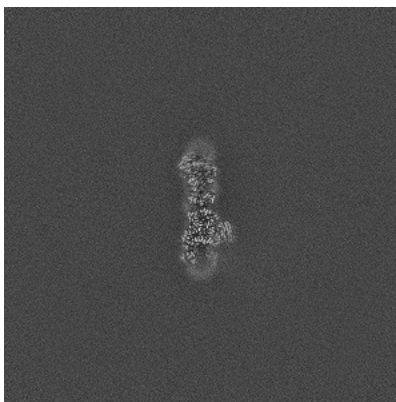


Z Index: 300

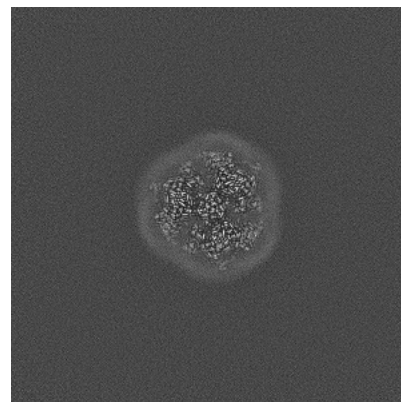
6.2.2 Raw map



X Index: 300



Y Index: 300

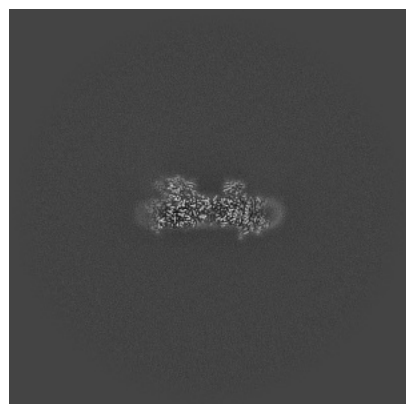


Z Index: 300

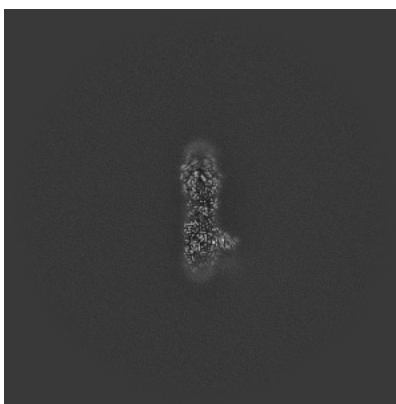
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

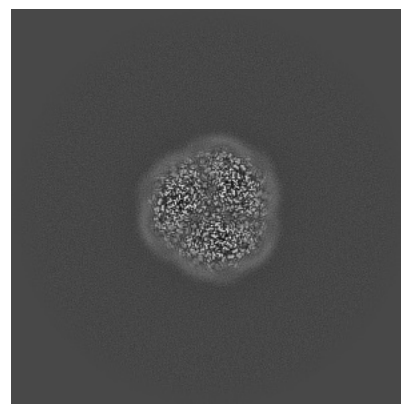
6.3.1 Primary map



X Index: 316



Y Index: 312

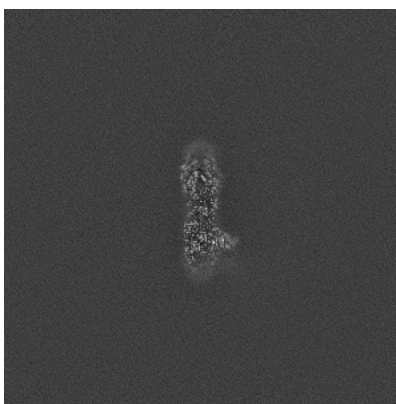


Z Index: 284

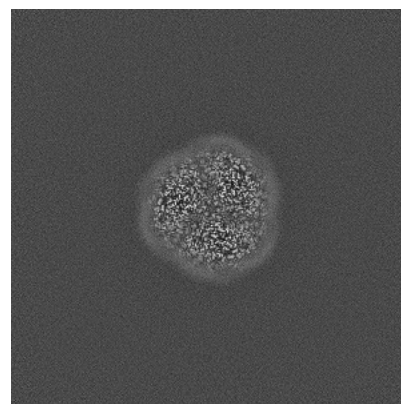
6.3.2 Raw map



X Index: 317



Y Index: 312



Z Index: 284

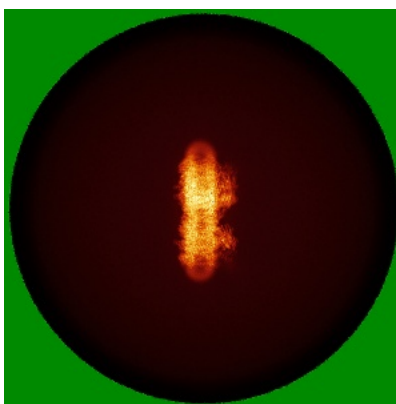
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

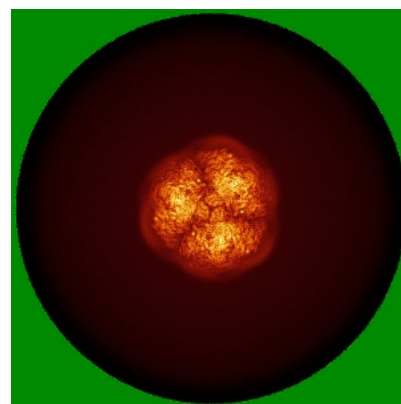
6.4.1 Primary map



X

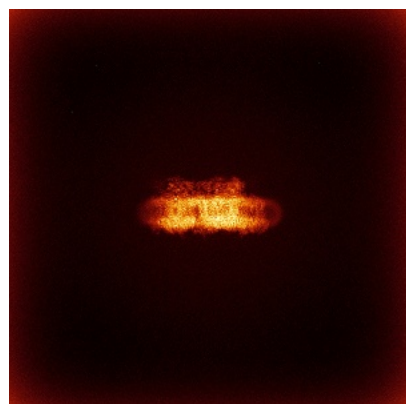


Y

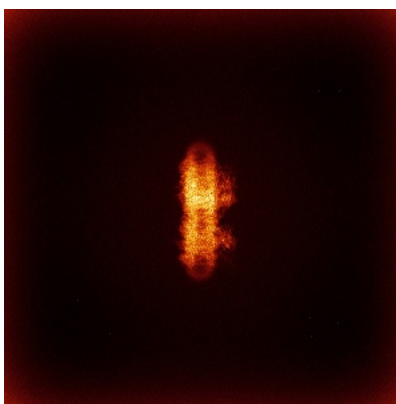


Z

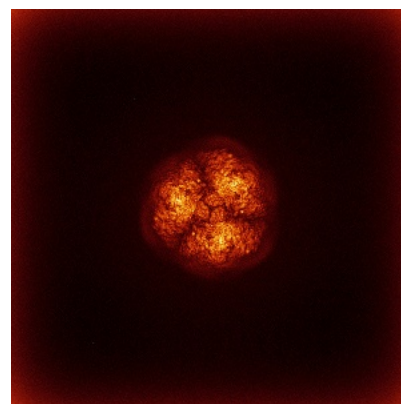
6.4.2 Raw map



X



Y

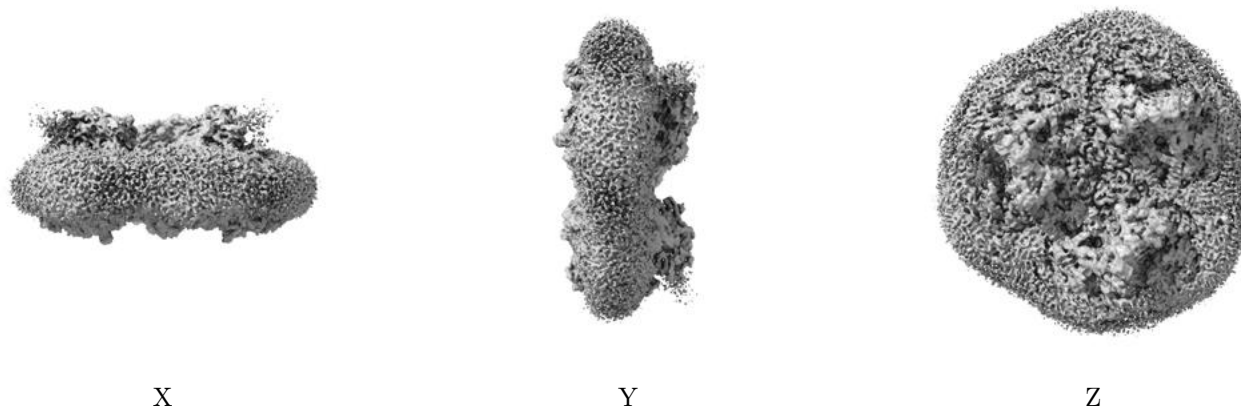


Z

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

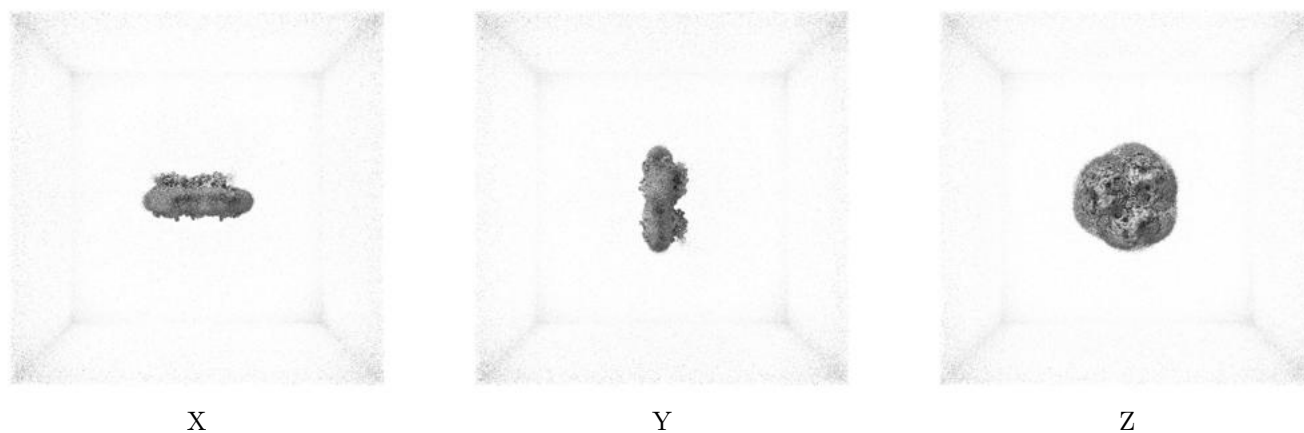
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

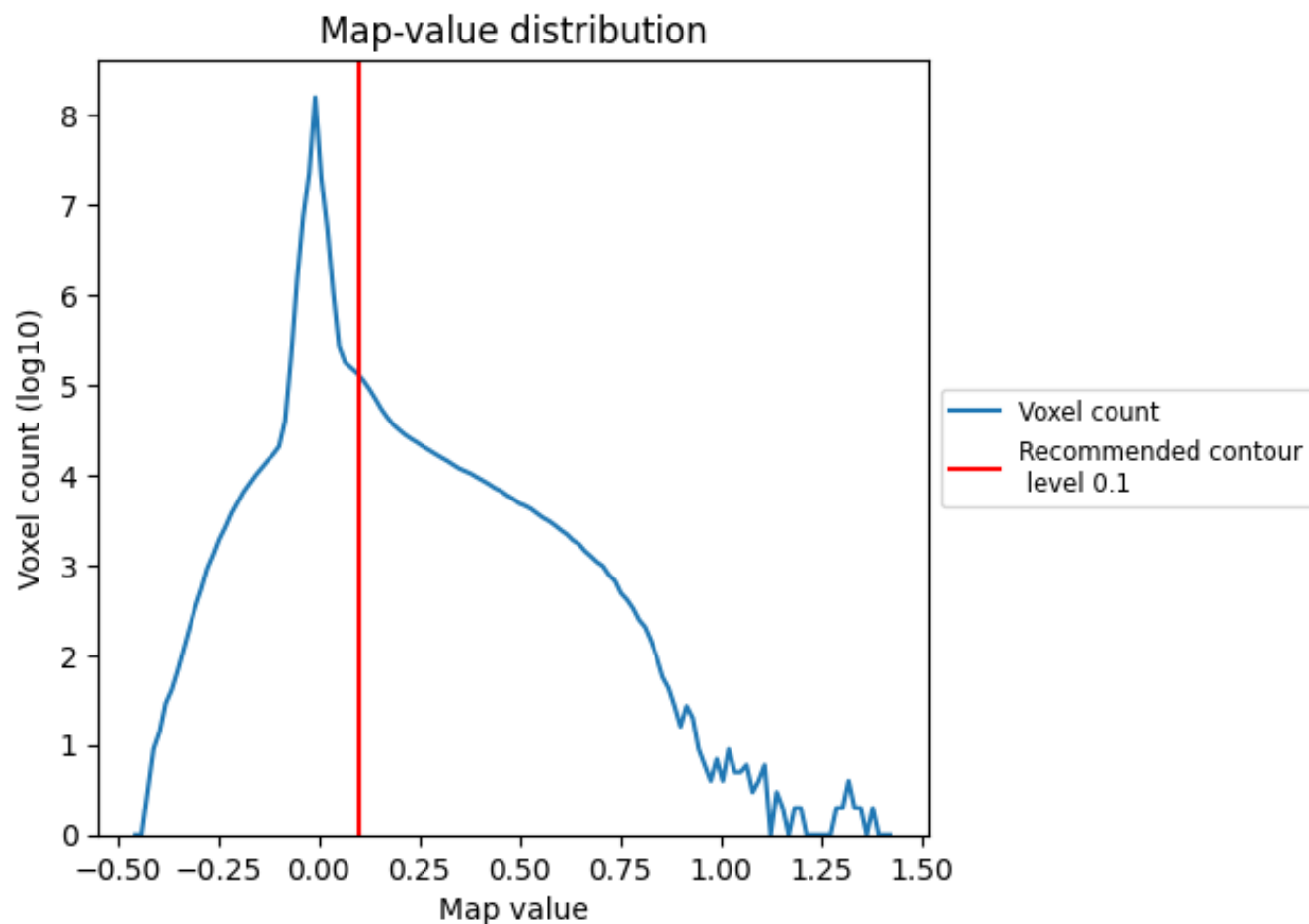
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

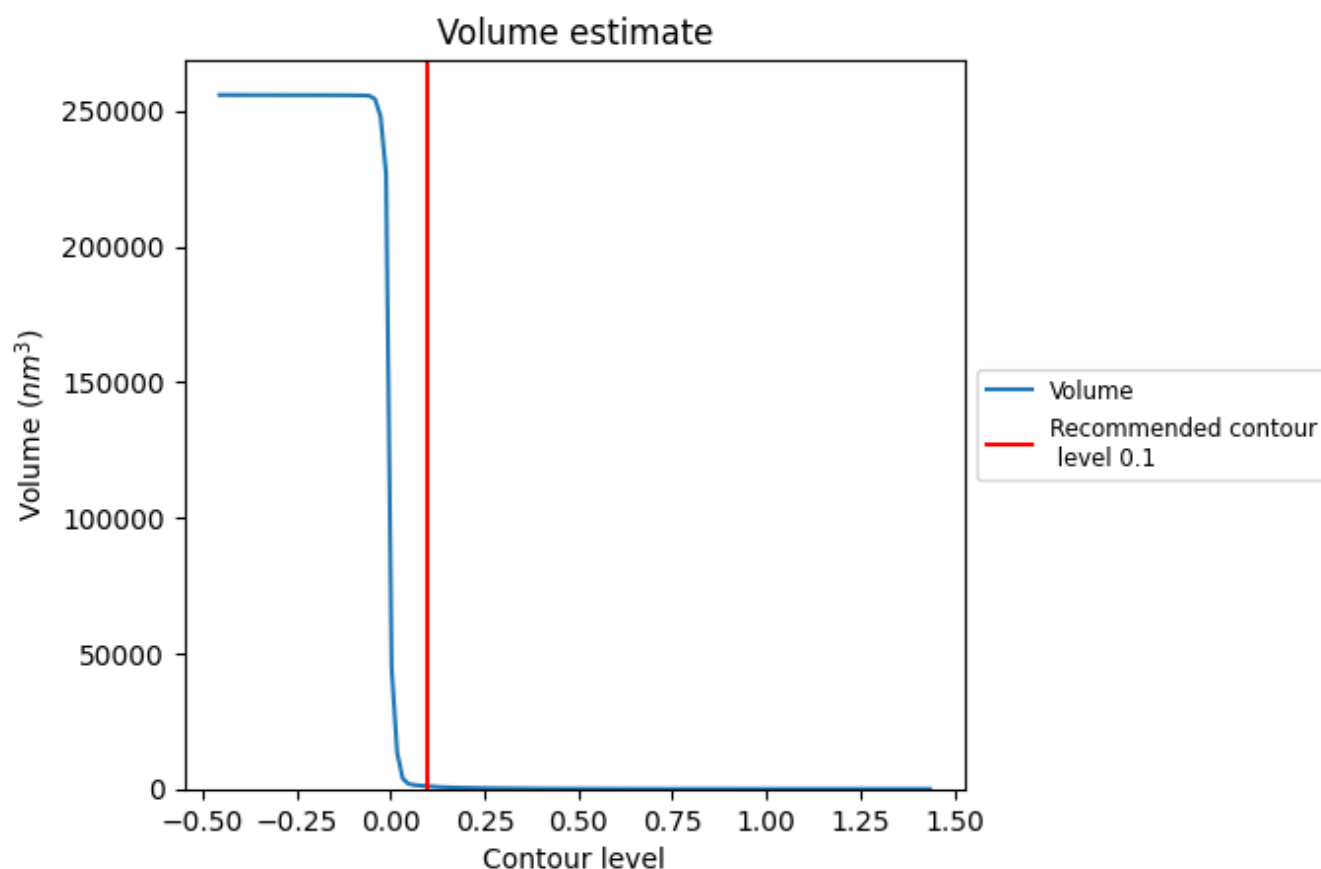
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

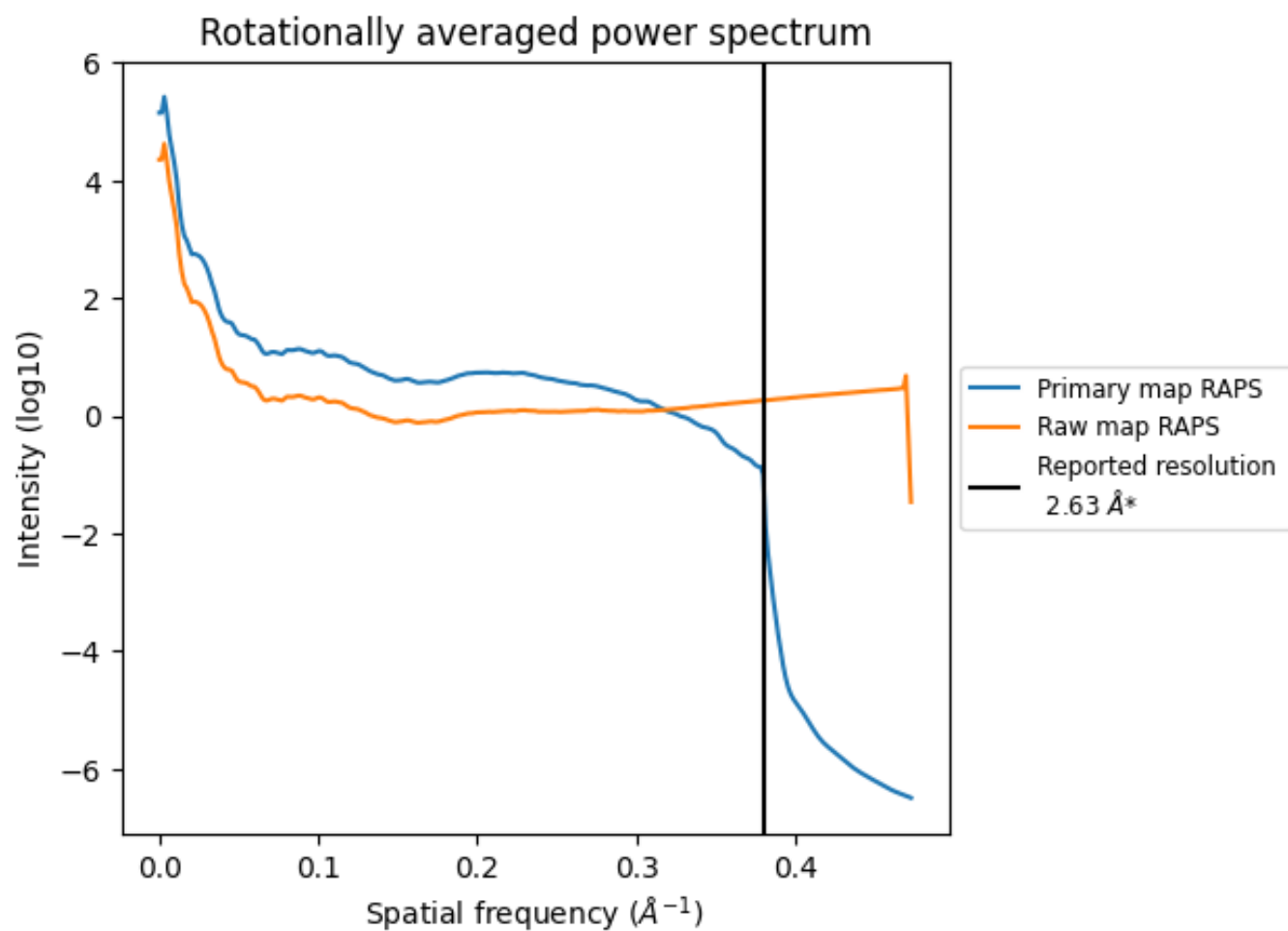
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 992 nm^3 ; this corresponds to an approximate mass of 896 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

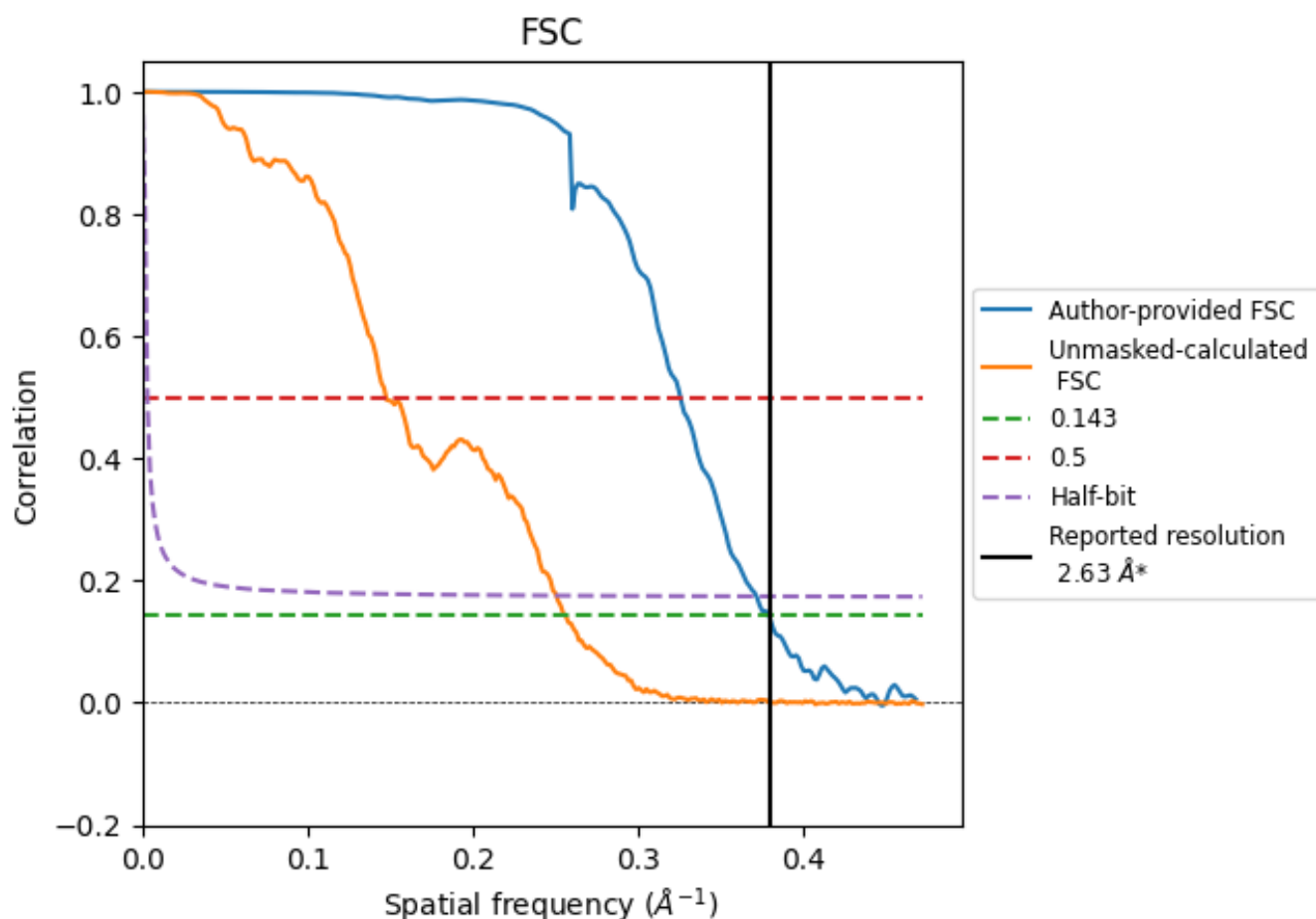


*Reported resolution corresponds to spatial frequency of 0.380 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

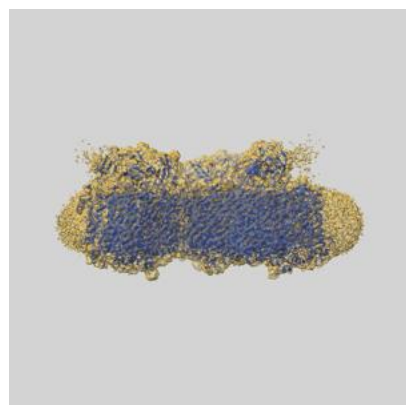
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.63	3.07	2.69
Unmasked-calculated*	3.90	6.77	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 2.63 by more than 10 %

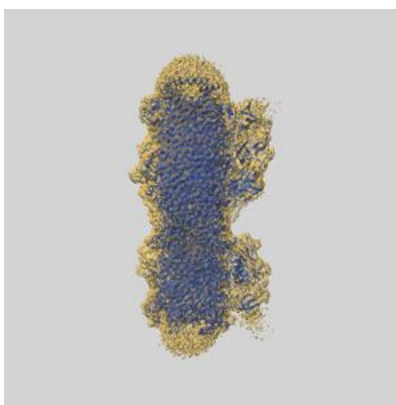
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54956 and PDB model 9SK3. Per-residue inclusion information can be found in section [3](#) on page [38](#).

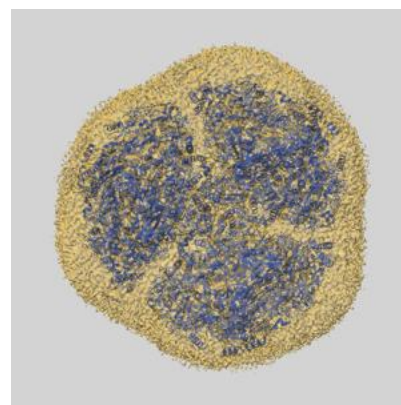
9.1 Map-model overlay [i](#)



X



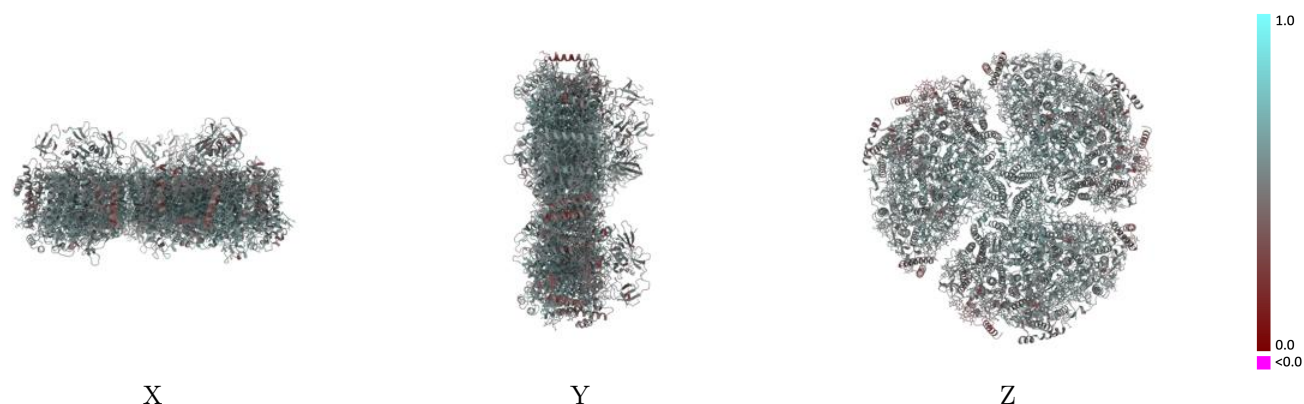
Y



Z

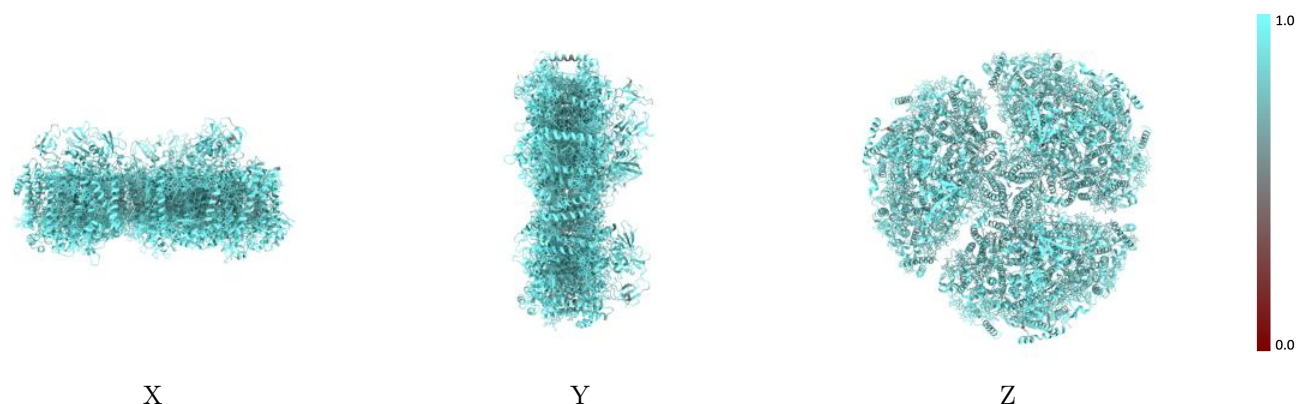
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



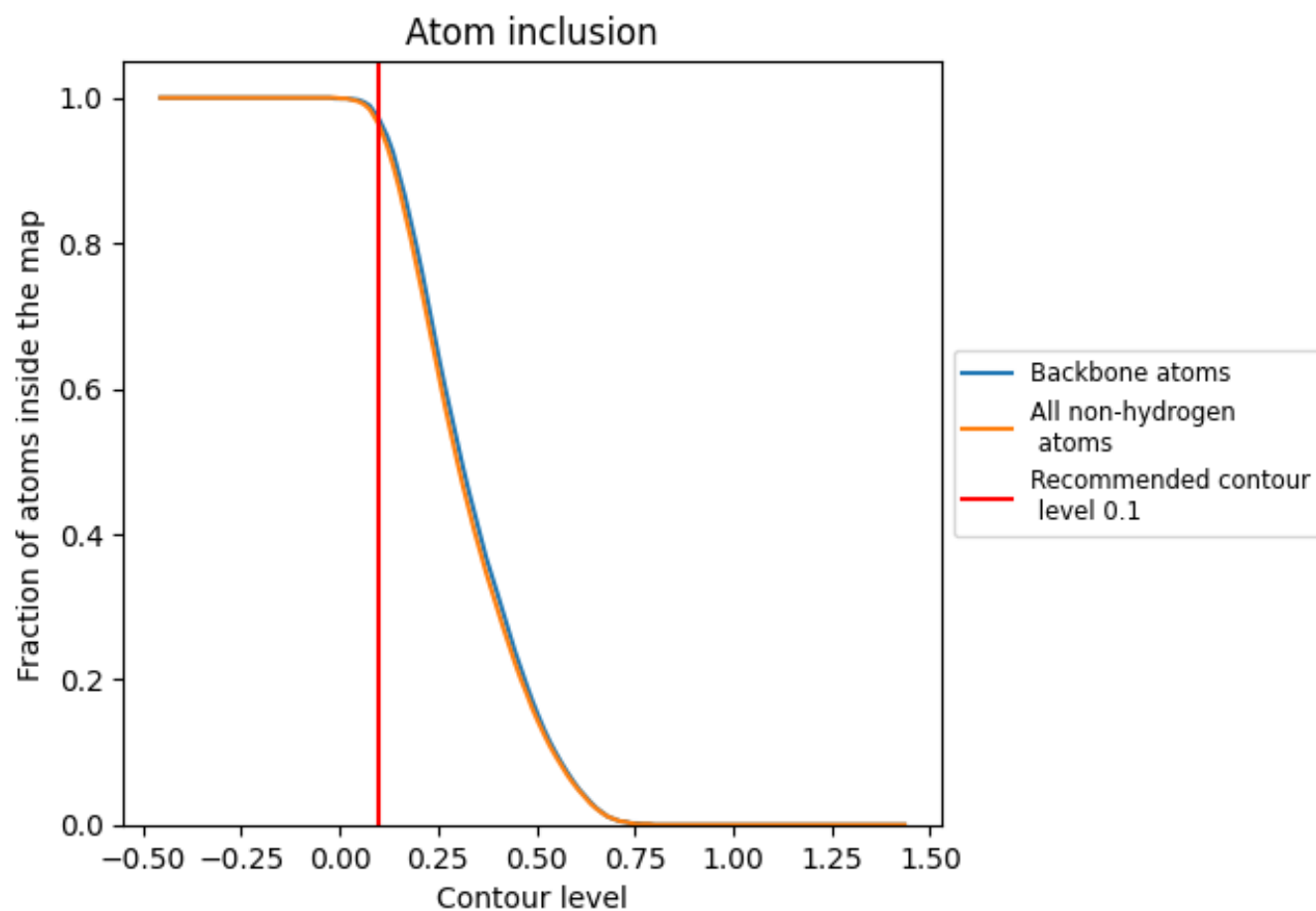
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.5330
aA	 0.9710	 0.5490
aB	 0.9700	 0.5390
aC	 0.9930	 0.5120
aD	 0.9740	 0.5010
aE	 0.8520	 0.4920
aF	 0.9290	 0.4970
aI	 0.9690	 0.5670
aJ	 0.9230	 0.4930
aK	 0.9160	 0.3890
aL	 0.9850	 0.5740
aM	 0.9240	 0.4880
aX	 0.8370	 0.3300
bA	 0.9680	 0.5480
bB	 0.9700	 0.5400
bC	 0.9870	 0.5060
bD	 0.9730	 0.5030
bE	 0.8480	 0.4790
bF	 0.9300	 0.4950
bI	 0.9720	 0.5660
bJ	 0.9010	 0.4920
bK	 0.9060	 0.3900
bL	 0.9860	 0.5740
bM	 0.9370	 0.4990
bX	 0.8210	 0.3380
cA	 0.9690	 0.5500
cB	 0.9700	 0.5390
cC	 0.9880	 0.5060
cD	 0.9700	 0.5030
cE	 0.8460	 0.4790
cF	 0.9260	 0.4910
cI	 0.9610	 0.5660
cJ	 0.9130	 0.4890
cK	 0.8990	 0.3840
cL	 0.9850	 0.5780



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
cM	 0.9330	 0.5080
cX	 0.8260	 0.3420