



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:22 am BST

PDB ID : 6HQB / pdb\_00006hqb  
Title : Monomeric cyanobacterial photosystem I  
Authors : Netzer-El, S.Y.; Nelson, N.; Caspy, I.  
Deposited on : 2018-09-24  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

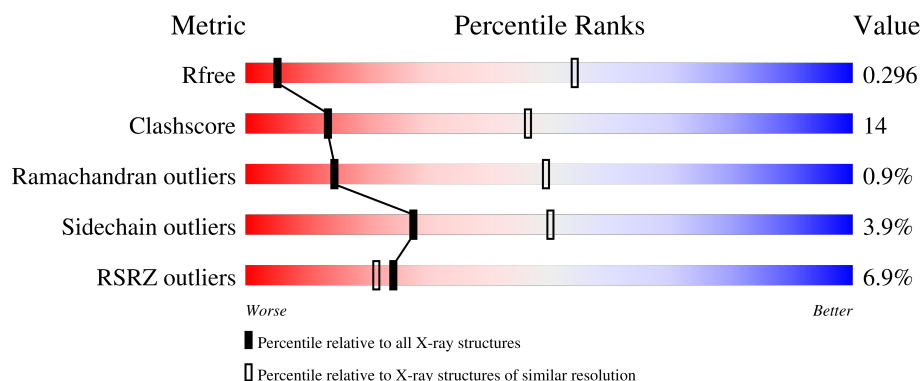
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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





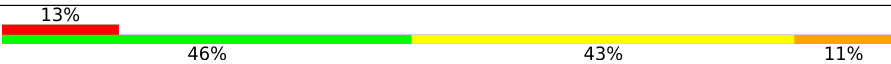
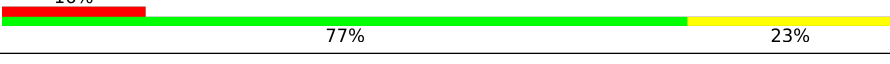
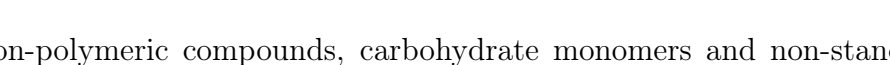
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	751	 6% 75% 24% .
2	B	731	 6% 76% 23% .
3	C	80	 4% 65% 34% .
4	D	141	 9% 76% 23% .
5	E	69	 3% 81% 16% .

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Mol	Chain	Length	Quality of chain
6	F	143	
7	I	40	
8	J	40	
9	K	70	
10	L	137	
11	M	31	

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
12	CLA	A	1011	X	-	-	-
12	CLA	A	1012	X	-	-	-
12	CLA	A	1013	X	-	-	-
12	CLA	A	1101	X	-	-	-
12	CLA	A	1102	X	-	-	-
12	CLA	A	1103	X	-	-	-
12	CLA	A	1104	X	-	-	-
12	CLA	A	1105	X	-	-	-
12	CLA	A	1106	X	-	-	-
12	CLA	A	1107	X	-	-	-
12	CLA	A	1108	X	-	-	-
12	CLA	A	1109	X	-	-	-
12	CLA	A	1110	X	-	-	-
12	CLA	A	1111	X	-	-	-
12	CLA	A	1112	X	-	-	-
12	CLA	A	1113	X	-	-	-
12	CLA	A	1114	X	-	-	-
12	CLA	A	1115	X	-	-	-
12	CLA	A	1116	X	-	-	-
12	CLA	A	1117	X	-	-	-
12	CLA	A	1118	X	-	-	-
12	CLA	A	1119	X	-	-	-
12	CLA	A	1120	X	-	-	-
12	CLA	A	1121	X	-	-	-
12	CLA	A	1122	X	-	-	-
12	CLA	A	1123	X	-	-	-
12	CLA	A	1124	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	1125	X	-	-	-
12	CLA	A	1126	X	-	-	-
12	CLA	A	1127	X	-	-	-
12	CLA	A	1128	X	-	-	-
12	CLA	A	1129	X	-	-	-
12	CLA	A	1130	X	-	-	-
12	CLA	A	1131	X	-	-	-
12	CLA	A	1132	X	-	-	-
12	CLA	A	1133	X	-	-	-
12	CLA	A	1134	X	-	-	-
12	CLA	A	1135	X	-	-	-
12	CLA	A	1136	X	-	-	-
12	CLA	A	1137	X	-	-	-
12	CLA	A	1138	X	-	-	-
12	CLA	A	1139	X	-	-	-
12	CLA	A	1140	X	-	-	-
12	CLA	A	1141	X	-	-	-
12	CLA	B	1021	X	-	-	-
12	CLA	B	1022	X	-	-	-
12	CLA	B	1023	X	-	-	-
12	CLA	B	1201	X	-	-	-
12	CLA	B	1202	X	-	-	-
12	CLA	B	1203	X	-	-	-
12	CLA	B	1204	X	-	-	-
12	CLA	B	1205	X	-	-	-
12	CLA	B	1206	X	-	-	-
12	CLA	B	1207	X	-	-	-
12	CLA	B	1208	X	-	-	-
12	CLA	B	1209	X	-	-	-
12	CLA	B	1210	X	-	-	-
12	CLA	B	1211	X	-	-	-
12	CLA	B	1212	X	-	-	-
12	CLA	B	1213	X	-	-	-
12	CLA	B	1214	X	-	-	-
12	CLA	B	1215	X	-	-	-
12	CLA	B	1216	X	-	-	-
12	CLA	B	1217	X	-	-	-
12	CLA	B	1218	X	-	-	-
12	CLA	B	1219	X	-	-	-
12	CLA	B	1220	X	-	-	-
12	CLA	B	1221	X	-	-	-
12	CLA	B	1222	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	1223	X	-	-	-
12	CLA	B	1224	X	-	-	-
12	CLA	B	1225	X	-	-	-
12	CLA	B	1226	X	-	-	-
12	CLA	B	1227	X	-	-	-
12	CLA	B	1228	X	-	-	-
12	CLA	B	1229	X	-	-	-
12	CLA	B	1230	X	-	-	-
12	CLA	B	1231	X	-	-	-
12	CLA	B	1232	X	-	-	-
12	CLA	B	1234	X	-	-	-
12	CLA	B	1235	X	-	-	-
12	CLA	B	1236	X	-	-	-
12	CLA	B	1237	X	-	-	-
12	CLA	B	1238	X	-	-	-
12	CLA	B	1239	X	-	-	-
12	CLA	B	1240	X	-	-	-
12	CLA	F	1301	X	-	-	-
12	CLA	F	1302	X	-	-	-
12	CLA	J	1302	X	-	-	-
12	CLA	J	1303	X	-	-	-
12	CLA	K	1401	X	-	-	-
12	CLA	K	1402	X	-	-	-
12	CLA	L	1502	X	-	-	-

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 23566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5876	3846	999	1003	28			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	70	Total	C	N	O	S	0	0	0
			510	337	81	87	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	137	Total	C	N	O	S	0	0	0
			1030	674	167	187	2			

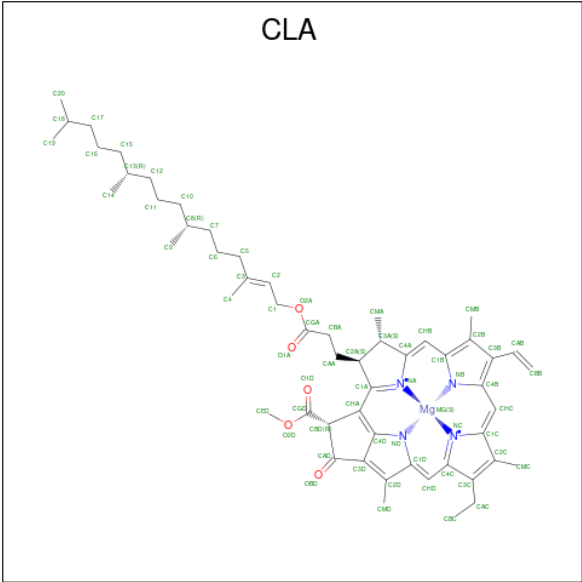
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	158	HIS	-	insertion	UNP P37277

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

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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

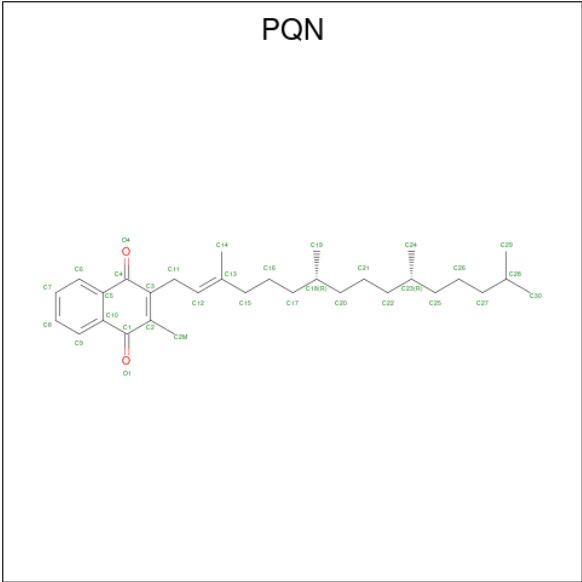
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	L	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

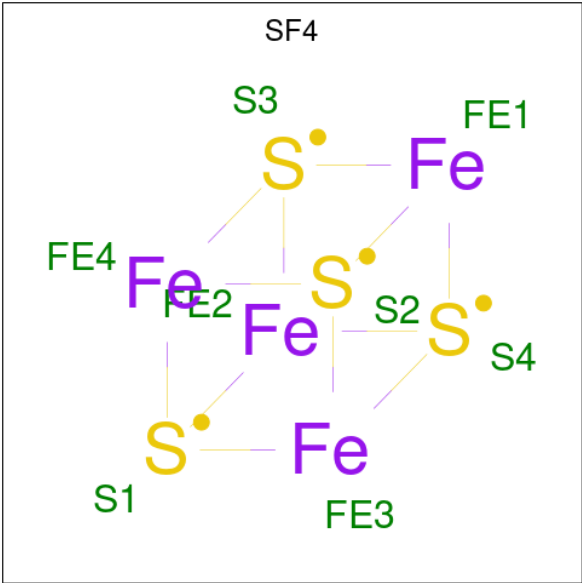
- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).





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

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



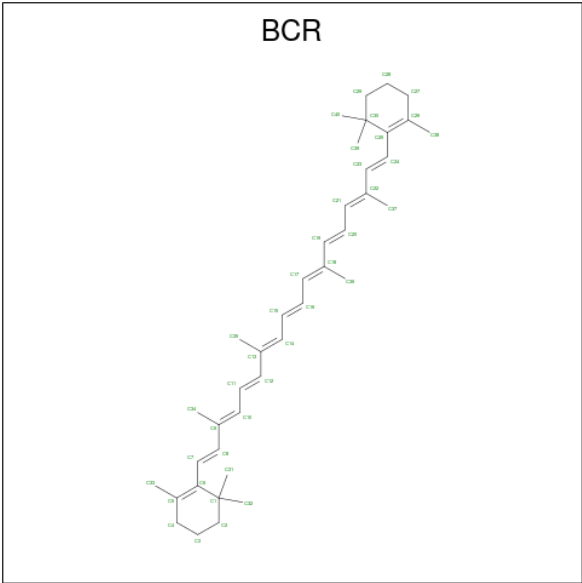
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	Fe	S	0	0
			8	4	4		
14	C	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



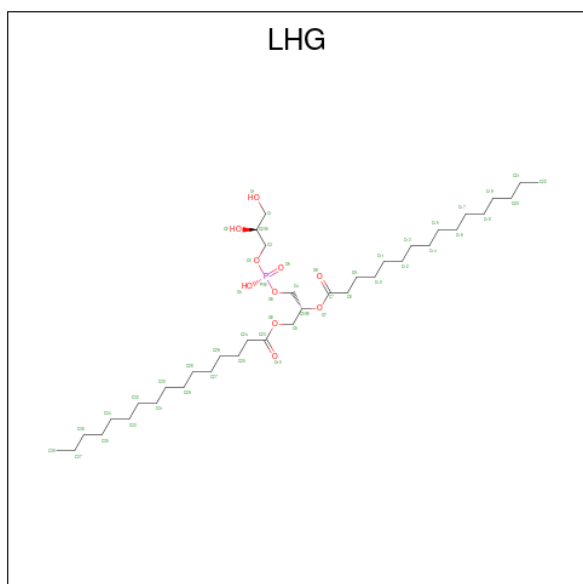
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0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

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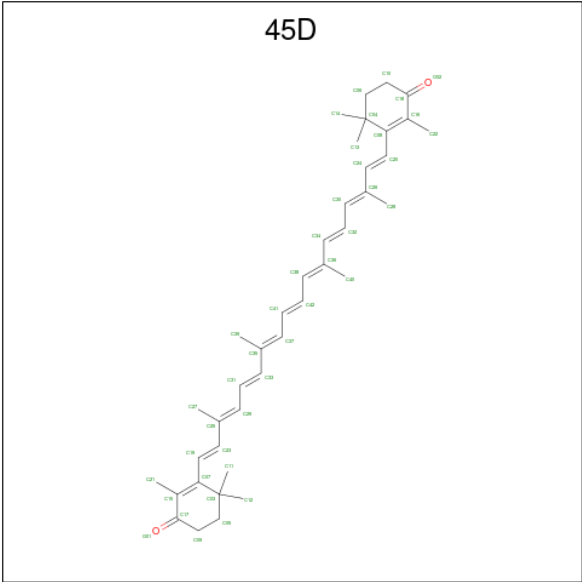
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	K	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 21 10 10 1	0	0

- Molecule 17 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula:  $C_{40}H_{52}O_2$ ).

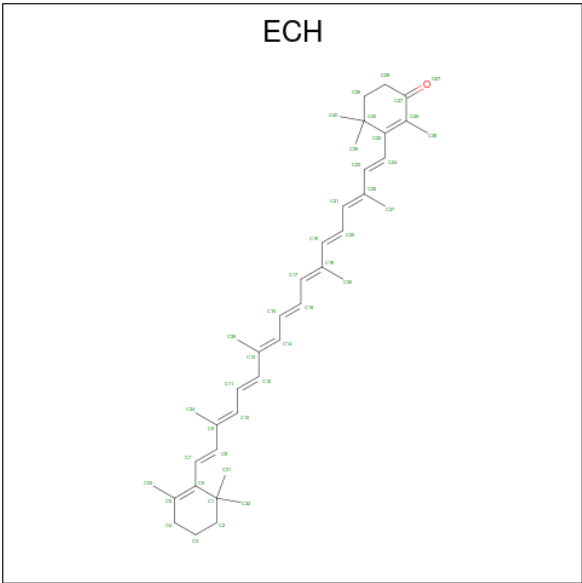


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	B	1	Total	C	O	0	0
			42	40	2		

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

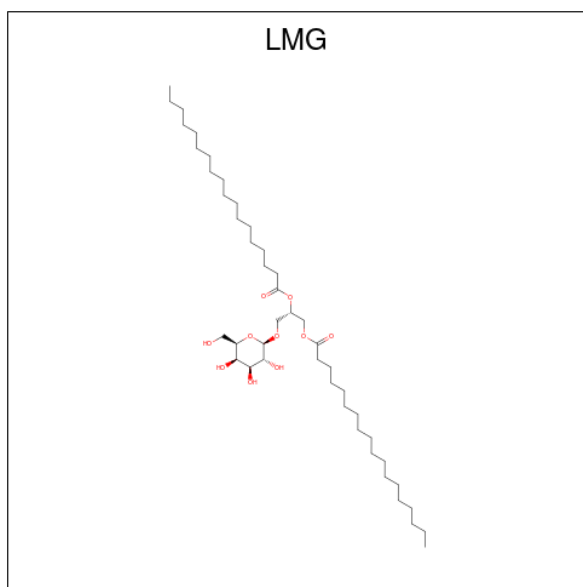
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	Cl	0	0
			1	1		

- Molecule 19 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C<sub>40</sub>H<sub>54</sub>O).



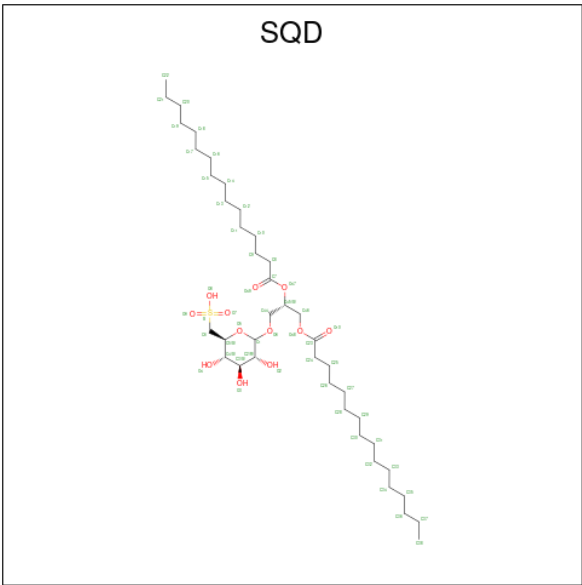
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			41	40	1		
19	M	1	Total	C	O	0	0
			41	40	1		

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			55	45	10		
20	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).

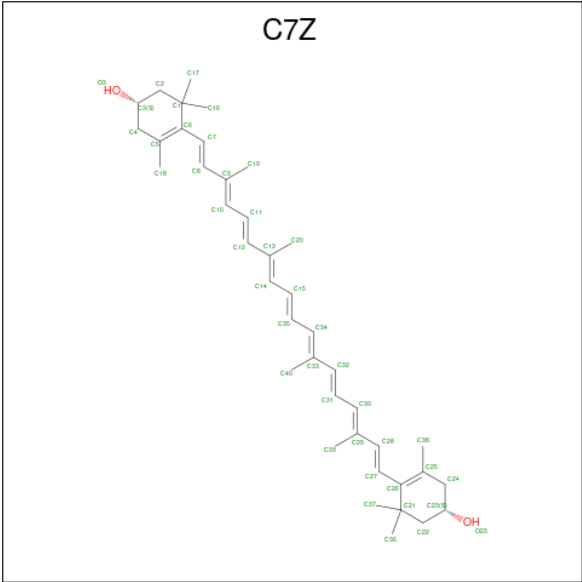


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	B	1	Total	C	O	S	0	0
			54	41	12	1		
21	F	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

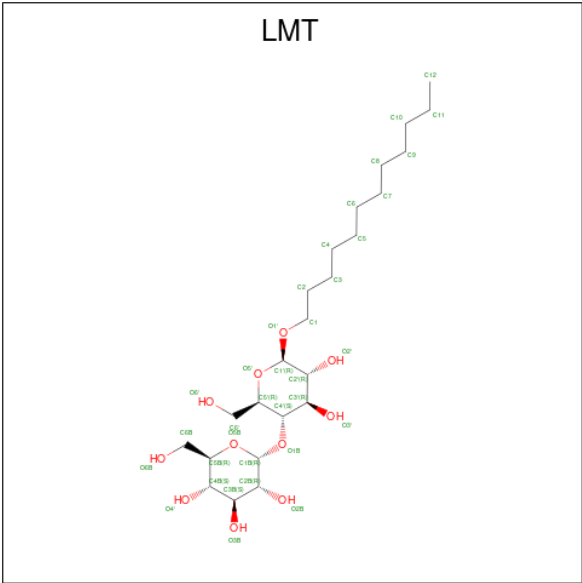
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Ca	0	0
			1	1		
22	L	1	Total	Ca	0	0
			1	1		

- Molecule 23 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



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

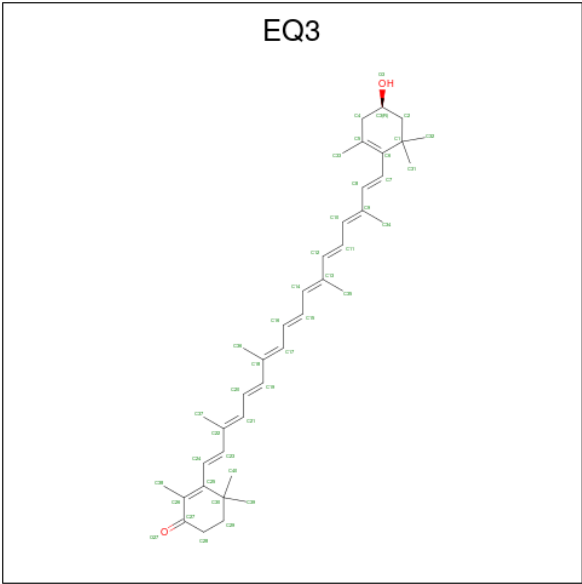
- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula:

C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>).



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



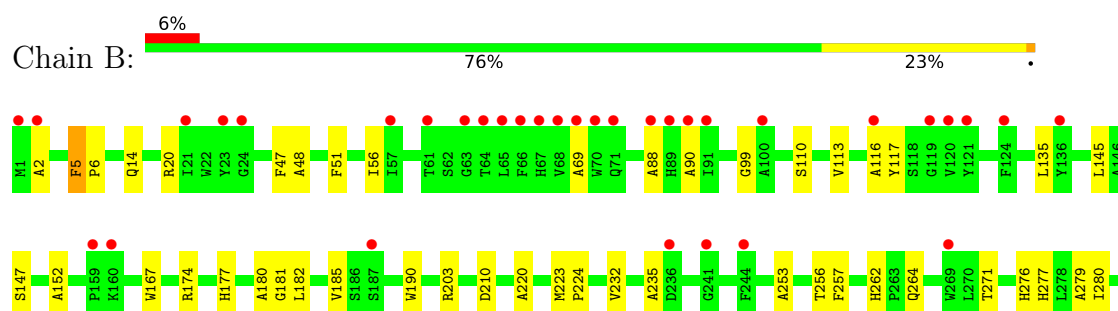
### 3 Residue-property plots

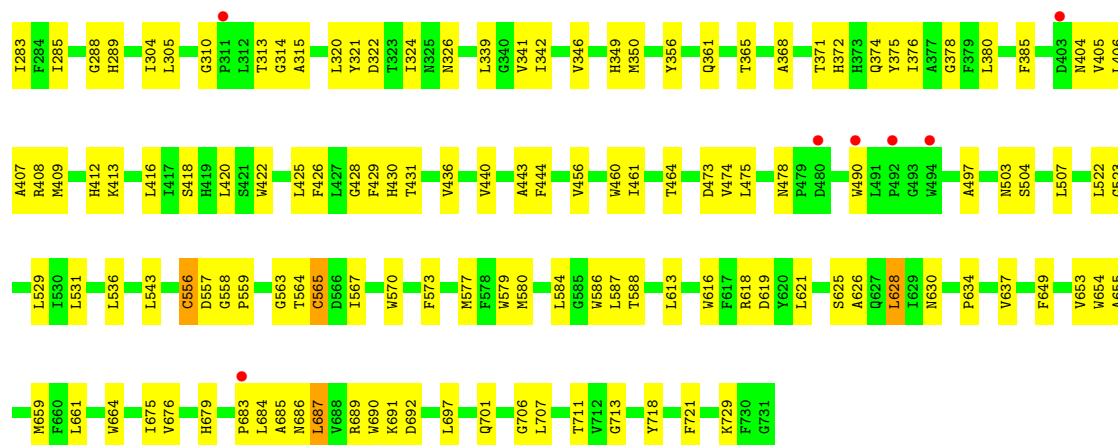
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

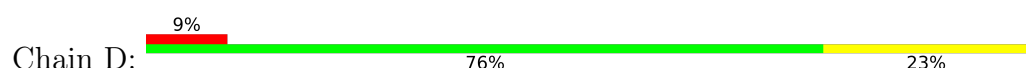




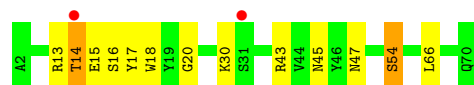
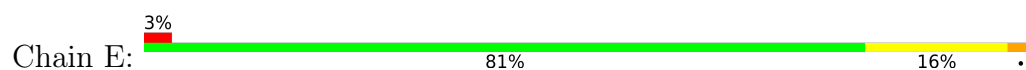
• Molecule 3: Photosystem I iron-sulfur center



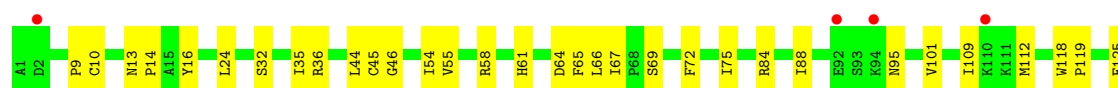
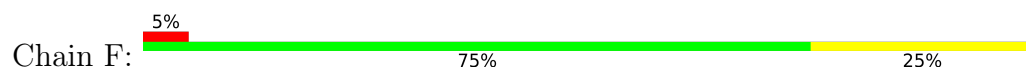
• Molecule 4: Photosystem I reaction center subunit II



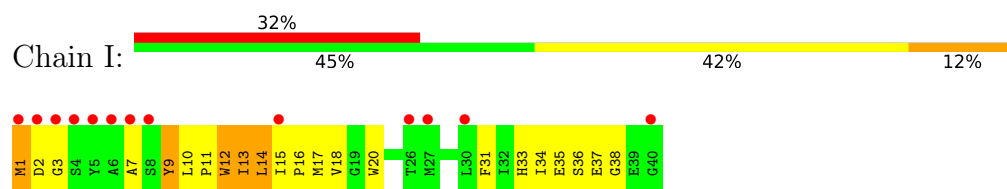
• Molecule 5: Photosystem I reaction center subunit IV



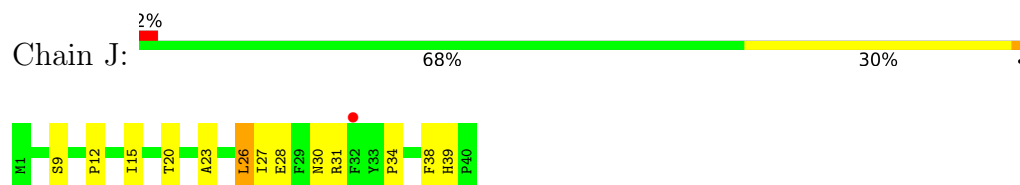
• Molecule 6: Photosystem I reaction center subunit III



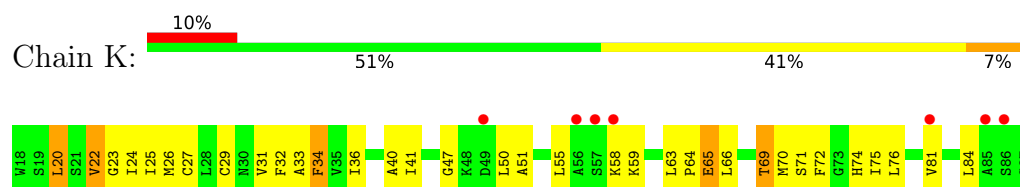
- Molecule 7: Photosystem I reaction center subunit VIII



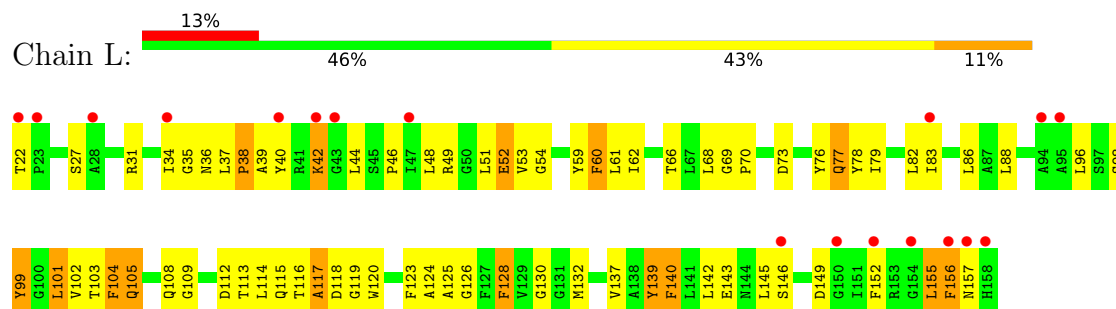
- Molecule 8: Photosystem I reaction center subunit IX



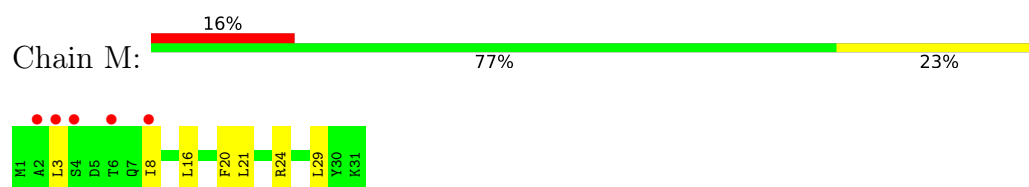
- Molecule 9: Photosystem I reaction center subunit PsaK 2



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.32Å 178.66Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 4.00 49.29 – 4.00	Depositor EDS
% Data completeness (in resolution range)	88.7 (49.29-4.00) 88.6 (49.29-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3228: ???)	Depositor
R, $R_{free}$	0.255 , 0.295 0.256 , 0.296	Depositor DCC
$R_{free}$ test set	4485 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, EQ3, BCR, PQN, CA, C7Z, 45D, CL, SQD, SF4, LMG, LHG, ECH, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/6075	0.39	0/8278
2	B	0.25	0/5994	0.40	0/8195
3	C	0.24	0/610	0.43	0/826
4	D	0.25	0/1126	0.44	0/1517
5	E	0.25	0/552	0.41	0/745
6	F	0.25	0/1143	0.40	0/1553
7	I	0.28	0/322	0.50	0/438
8	J	0.26	0/328	0.40	0/443
9	K	0.26	0/520	0.46	0/700
10	L	0.27	0/1057	0.47	0/1434
11	M	0.24	0/241	0.39	0/326
All	All	0.25	0/17968	0.41	0/24455

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5876	0	5739	157	0
2	B	5783	0	5565	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	589	18	0
4	D	1102	0	1101	17	0
5	E	543	0	525	11	0
6	F	1113	0	1110	23	0
7	I	311	0	304	19	0
8	J	319	0	328	14	0
9	K	510	0	534	27	0
10	L	1030	0	1011	60	0
11	M	238	0	260	7	0
12	A	2326	0	2027	171	0
12	B	2152	0	1801	145	0
12	F	98	0	76	3	0
12	J	98	0	76	2	0
12	K	94	0	71	0	0
12	L	49	0	38	4	0
13	A	33	0	46	2	0
13	B	33	0	46	3	0
14	A	8	0	0	1	0
14	C	16	0	0	1	0
15	A	200	0	265	21	0
15	B	200	0	264	9	0
15	F	40	0	53	9	0
15	I	40	0	52	5	0
15	J	40	0	53	9	0
15	K	40	0	53	6	0
16	A	98	0	148	5	0
16	B	70	0	83	9	0
17	B	42	0	52	5	0
18	B	1	0	0	0	0
19	B	41	0	54	4	0
19	M	41	0	54	5	0
20	B	110	0	172	7	0
21	B	54	0	77	1	0
21	F	54	0	77	3	0
22	B	1	0	0	0	0
22	L	1	0	0	0	0
23	F	42	0	0	1	0
23	J	42	0	0	0	0
24	F	35	0	45	1	0
25	I	42	0	0	1	0
All	All	23566	0	22749	666	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 14.

All (666) 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:A:210:LEU:HD11	15:A:4001:BCR:H10C	1.42	1.01
12:B:1207:CLA:HBC3	15:I:4018:BCR:H21C	1.44	0.96
10:L:35:GLY:HA2	10:L:40:TYR:HB3	1.52	0.92
12:B:1220:CLA:HAB	12:B:1227:CLA:HMD2	1.55	0.87
12:A:1125:CLA:HED1	12:A:1133:CLA:HAB	1.58	0.86
1:A:395:TRP:CD1	12:A:1126:CLA:HAB	2.11	0.85
12:A:1118:CLA:HBB1	15:K:4001:BCR:H10C	1.61	0.83
15:B:4010:BCR:H24C	15:B:4018:BCR:H392	1.60	0.82
12:A:1132:CLA:HMA2	10:L:68:LEU:HB3	1.62	0.82
1:A:250:ALA:HA	1:A:256:PHE:HB3	1.62	0.79
1:A:1:MET:CB	1:A:1:MET:C	2.51	0.78
9:K:47:GLY:HA3	9:K:64:PRO:HG2	1.66	0.78
2:B:220:ALA:HB1	2:B:224:PRO:HG2	1.65	0.78
12:A:1138:CLA:HED2	2:B:422:TRP:HB2	1.65	0.77
2:B:556:CYS:SG	2:B:557:ASP:N	2.59	0.75
9:K:55:LEU:HD23	9:K:58:LYS:HE2	1.67	0.74
1:A:433:ARG:NH2	1:A:558:SER:O	2.21	0.74
12:B:1234:CLA:HMB2	12:B:1236:CLA:HED1	1.68	0.74
1:A:500:ASN:HB3	12:A:1115:CLA:HED2	1.70	0.73
1:A:388:SER:HB3	12:A:1126:CLA:HMA1	1.70	0.73
2:B:413:LYS:HA	2:B:416:LEU:HD12	1.72	0.72
2:B:691:LYS:HD3	7:I:37:GLU:HG3	1.72	0.71
15:A:4012:BCR:HC7	8:J:26:LEU:HD23	1.73	0.71
12:B:1211:CLA:HHB	19:B:4006:ECH:H24	1.72	0.71
2:B:687:LEU:HD22	10:L:39:ALA:HB3	1.73	0.70
1:A:357:ALA:HB1	15:A:4008:BCR:H10C	1.72	0.70
12:A:1011:CLA:HBB1	12:A:1011:CLA:HMB1	1.73	0.70
12:A:1107:CLA:CAB	12:B:1230:CLA:HMD2	2.21	0.70
12:A:1129:CLA:HMA2	10:L:22:THR:HG21	1.74	0.70
13:A:2001:PQN:H142	15:F:4014:BCR:H271	1.74	0.70
12:A:1011:CLA:H2A	12:A:1011:CLA:HED2	1.74	0.69
12:A:1013:CLA:HMA1	12:A:1013:CLA:H51	1.73	0.69
2:B:718:TYR:HB2	12:B:1021:CLA:HED3	1.75	0.69
12:B:1236:CLA:HBA2	16:B:5004:LHG:H381	1.74	0.69
12:A:1012:CLA:HED2	12:B:1021:CLA:H71	1.74	0.69
12:A:1101:CLA:HBB1	15:J:4013:BCR:H292	1.74	0.69
2:B:420:LEU:HD13	2:B:529:LEU:HA	1.75	0.69
10:L:52:GLU:HB3	12:L:1502:CLA:HED3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1125:CLA:HMB1	12:A:1125:CLA:HBB1	1.75	0.68
1:A:40:ARG:NH2	5:E:54:SER:OG	2.26	0.68
4:D:39:VAL:HG22	4:D:49:ILE:HG12	1.77	0.67
12:A:1123:CLA:HMB1	12:A:1123:CLA:HBB1	1.77	0.67
12:B:1234:CLA:HMB1	12:B:1234:CLA:HBB1	1.76	0.67
9:K:51:ALA:HA	9:K:59:LYS:HD2	1.76	0.67
9:K:55:LEU:HD11	15:K:4001:BCR:H271	1.75	0.67
12:B:1220:CLA:HBB1	16:B:5004:LHG:H111	1.76	0.67
10:L:49:ARG:NH2	10:L:112:ASP:OD2	2.28	0.67
12:A:1105:CLA:H8	15:J:4013:BCR:H19C	1.77	0.66
1:A:579:ARG:HH21	1:A:582:THR:HG21	1.60	0.66
12:A:1130:CLA:H12	10:L:34:ILE:HD11	1.77	0.66
8:J:27:ILE:HG21	15:J:4013:BCR:H10C	1.77	0.66
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.76	0.66
1:A:736:ILE:HG21	12:A:1126:CLA:HMC2	1.77	0.66
12:L:1502:CLA:HED2	12:L:1502:CLA:HBA2	1.77	0.66
12:B:1204:CLA:HMA1	12:B:1205:CLA:HMB3	1.78	0.66
12:B:1218:CLA:HBB1	12:B:1218:CLA:HMB1	1.77	0.65
1:A:574:CYS:SG	1:A:575:ASP:N	2.69	0.65
2:B:174:ARG:HE	12:B:1221:CLA:HMD1	1.61	0.65
1:A:219:VAL:HG22	1:A:239:PRO:HB3	1.78	0.65
11:M:16:LEU:HD22	19:M:4021:ECH:H8	1.79	0.65
1:A:666:SER:HB2	2:B:443:ALA:HB1	1.78	0.65
12:A:1131:CLA:HHC	12:A:1131:CLA:HBB1	1.76	0.65
2:B:460:TRP:HE1	2:B:474:VAL:HG21	1.62	0.65
2:B:654:TRP:HB2	2:B:713:GLY:HA3	1.79	0.65
2:B:587:LEU:HD12	12:B:1234:CLA:HAB	1.80	0.64
1:A:82:VAL:HG22	12:A:1109:CLA:H202	1.79	0.64
6:F:75:ILE:HG23	12:F:1301:CLA:HAA1	1.80	0.64
2:B:626:ALA:O	2:B:630:ASN:ND2	2.22	0.64
2:B:580:MET:HG3	12:B:1222:CLA:HBC1	1.80	0.64
2:B:276:HIS:HB2	12:B:1214:CLA:C1B	2.28	0.63
12:B:1212:CLA:HBB1	15:B:4004:BCR:H323	1.80	0.63
2:B:684:LEU:HA	2:B:687:LEU:HD21	1.81	0.63
3:C:15:THR:HG22	3:C:28:MET:HG3	1.80	0.63
1:A:571:ARG:HD2	1:A:721:ILE:HG21	1.81	0.63
1:A:70:ARG:HH21	1:A:186:LYS:HA	1.63	0.63
2:B:378:GLY:HA3	2:B:584:LEU:HD11	1.81	0.62
9:K:55:LEU:HD13	9:K:59:LYS:HB2	1.81	0.62
9:K:71:SER:HB2	15:K:4001:BCR:H341	1.81	0.62
2:B:5:PHE:HB2	7:I:33:HIS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:GLN:HG3	20:B:5002:LMG:H142	1.82	0.62
1:A:500:ASN:HB2	12:A:1134:CLA:HED3	1.81	0.61
2:B:341:VAL:HG11	12:B:1223:CLA:H2	1.81	0.61
12:A:1138:CLA:H11	12:B:1229:CLA:HAA2	1.82	0.61
1:A:680:ALA:HB3	12:A:1013:CLA:HBB2	1.82	0.61
2:B:110:SER:O	7:I:1:MET:N	2.33	0.61
2:B:117:TYR:HA	2:B:365:THR:HG22	1.82	0.61
12:A:1122:CLA:H43	15:A:4007:BCR:H19C	1.83	0.61
9:K:22:VAL:HA	9:K:26:MET:HB2	1.83	0.61
12:B:1232:CLA:H41	20:B:5005:LMG:H182	1.82	0.61
2:B:385:PHE:HZ	12:B:1222:CLA:HAB	1.65	0.61
2:B:408:ARG:O	2:B:412:HIS:ND1	2.34	0.61
6:F:125:GLU:O	6:F:130:LYS:N	2.31	0.60
12:A:1101:CLA:HBA2	12:A:1101:CLA:HBD	1.83	0.60
12:A:1105:CLA:HMA1	12:A:1106:CLA:HMB3	1.83	0.60
12:B:1021:CLA:HMB3	12:B:1022:CLA:CAD	2.32	0.60
2:B:20:ARG:NH2	2:B:692:ASP:OD1	2.34	0.60
2:B:653:VAL:HG22	12:B:1239:CLA:HMB3	1.84	0.60
2:B:339:LEU:HD12	2:B:342:ILE:HD11	1.84	0.60
12:B:1216:CLA:HMB2	12:B:1221:CLA:HMA3	1.83	0.60
12:B:1223:CLA:HBB1	12:B:1231:CLA:HAA2	1.84	0.60
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.82	0.59
2:B:174:ARG:HH11	12:B:1210:CLA:HMD2	1.67	0.59
1:A:355:ASN:ND2	12:A:1103:CLA:OBD	2.35	0.59
1:A:478:LEU:HB2	1:A:529:THR:HG23	1.84	0.59
12:A:1107:CLA:HAB	12:B:1230:CLA:HMD2	1.83	0.59
12:A:1132:CLA:HAA1	10:L:69:GLY:HA2	1.84	0.59
2:B:375:TYR:HA	2:B:584:LEU:HD13	1.84	0.59
2:B:407:ALA:HB1	21:F:5001:SQD:H372	1.83	0.59
1:A:595:LEU:HD21	12:A:1128:CLA:HBC1	1.85	0.59
2:B:185:VAL:HG11	15:B:4005:BCR:H341	1.84	0.59
12:A:1134:CLA:HMB1	15:A:4008:BCR:H281	1.85	0.59
12:A:1011:CLA:HBB1	12:B:1021:CLA:HAA1	1.83	0.58
1:A:589:ASP:OD1	1:A:724:ARG:NH1	2.36	0.58
12:B:1234:CLA:H111	16:B:5004:LHG:H341	1.86	0.58
12:B:1203:CLA:H43	20:B:5002:LMG:H321	1.85	0.58
2:B:473:ASP:HB3	2:B:478:ASN:HD22	1.68	0.58
1:A:709:VAL:HG11	12:A:1138:CLA:HMB3	1.86	0.58
10:L:128:PHE:O	10:L:130:GLY:N	2.37	0.58
12:A:1128:CLA:HBB1	12:A:1128:CLA:HMB1	1.86	0.58
2:B:683:PRO:HB3	10:L:34:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:PRO:HG3	10:L:113:THR:HB	1.86	0.57
1:A:103:TRP:HA	1:A:110:ILE:HG21	1.85	0.57
12:A:1138:CLA:HHD	15:F:4014:BCR:H383	1.85	0.57
3:C:7:ILE:HG12	3:C:40:ALA:HB3	1.86	0.57
12:A:1138:CLA:HBB1	12:A:1138:CLA:HMB1	1.87	0.57
4:D:10:LYS:HB2	4:D:49:ILE:HB	1.84	0.57
1:A:226:LEU:HD12	1:A:236:ILE:HG23	1.86	0.57
1:A:690:ARG:HD3	2:B:563:GLY:HA3	1.87	0.57
10:L:66:THR:O	10:L:77:GLN:NE2	2.37	0.57
1:A:202:ALA:HA	1:A:305:ILE:HA	1.86	0.57
1:A:484:GLN:NE2	1:A:527:LEU:O	2.32	0.56
6:F:109:ILE:HA	6:F:112:MET:HE2	1.86	0.56
2:B:368:ALA:HB1	12:B:1224:CLA:HMA1	1.86	0.56
4:D:118:LYS:NZ	4:D:139:TYR:O	2.38	0.56
1:A:183:LYS:HD3	12:A:1108:CLA:HED3	1.87	0.56
6:F:13:ASN:ND2	6:F:46:GLY:O	2.37	0.56
1:A:738:THR:HB	12:A:1011:CLA:HED1	1.88	0.56
3:C:73:THR:H	3:C:76:SER:HG	1.52	0.56
10:L:76:TYR:HB3	10:L:79:ILE:HB	1.88	0.56
12:A:1102:CLA:H52	12:A:1109:CLA:H13	1.87	0.56
1:A:223:ILE:HG23	1:A:236:ILE:HG21	1.87	0.55
1:A:440:LEU:HB3	1:A:547:LEU:HD13	1.89	0.55
12:B:1214:CLA:HED3	12:B:1215:CLA:H12	1.87	0.55
2:B:689:ARG:HG3	10:L:103:THR:HG21	1.88	0.55
1:A:452:PHE:HE1	12:B:1022:CLA:HMA1	1.71	0.55
1:A:433:ARG:HH21	1:A:555:TYR:HA	1.72	0.55
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.88	0.55
2:B:304:ILE:HG12	12:B:1219:CLA:HED2	1.89	0.55
10:L:39:ALA:HA	10:L:49:ARG:NH2	2.22	0.55
12:A:1106:CLA:H8	15:A:4012:BCR:H372	1.88	0.55
1:A:428:ARG:HA	1:A:431:ARG:HG3	1.89	0.55
2:B:436:VAL:HG21	17:B:4011:45D:H311	1.88	0.55
4:D:121:ARG:NH1	5:E:15:GLU:OE1	2.40	0.55
12:A:1102:CLA:HBA2	12:A:1109:CLA:H51	1.88	0.55
2:B:349:HIS:HB3	12:B:1214:CLA:HED2	1.89	0.55
2:B:577:MET:HG3	2:B:707:LEU:HD21	1.88	0.55
1:A:464:LEU:HG	12:B:1206:CLA:HMC3	1.87	0.54
1:A:560:ARG:HB3	3:C:80:ALA:HB3	1.89	0.54
12:A:1116:CLA:HMB1	12:A:1116:CLA:HBB1	1.89	0.54
12:B:1218:CLA:HMD2	15:B:4004:BCR:H24C	1.89	0.54
12:B:1238:CLA:HAA2	7:I:31:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TRP:CE2	12:A:1108:CLA:HMA1	2.42	0.54
12:A:1107:CLA:HBB2	12:B:1230:CLA:CHD	2.37	0.54
1:A:254:PRO:HD2	1:A:273:ASP:HB3	1.90	0.54
12:B:1207:CLA:H43	10:L:83:ILE:HD12	1.89	0.54
1:A:56:HIS:HB2	12:A:1128:CLA:HBA1	1.89	0.54
1:A:304:PHE:CE1	12:A:1119:CLA:HAB	2.43	0.54
12:A:1011:CLA:HAB	2:B:621:LEU:HD13	1.89	0.54
12:B:1224:CLA:CGA	12:B:1224:CLA:H3A	2.37	0.54
6:F:24:LEU:O	6:F:36:ARG:NH2	2.41	0.54
1:A:42:PRO:HB3	1:A:47:TRP:CE3	2.43	0.54
12:A:1122:CLA:HMA1	12:A:1141:CLA:HAB	1.89	0.54
4:D:19:LEU:H	4:D:22:ALA:HB3	1.73	0.54
1:A:437:ILE:HG13	1:A:555:TYR:HE2	1.71	0.54
12:A:1132:CLA:H8	10:L:60:PHE:HE2	1.73	0.54
1:A:255:SER:HG	1:A:274:PHE:HD2	1.55	0.53
3:C:25:VAL:HG11	3:C:48:CYS:HB2	1.90	0.53
7:I:7:ALA:HB1	7:I:10:LEU:HD13	1.89	0.53
9:K:23:GLY:HA2	9:K:27:CYS:HB3	1.89	0.53
11:M:20:PHE:CZ	11:M:24:ARG:HD2	2.43	0.53
1:A:342:GLU:HA	1:A:345:THR:HG22	1.89	0.53
2:B:20:ARG:HH22	7:I:34:ILE:HG12	1.73	0.53
12:A:1105:CLA:H72	8:J:20:THR:HG21	1.90	0.53
1:A:263:PHE:HE1	12:A:1115:CLA:HBB1	1.74	0.53
1:A:434:ASP:OD1	1:A:555:TYR:OH	2.24	0.53
1:A:482:PHE:HB3	12:A:1135:CLA:H11	1.90	0.53
12:A:1011:CLA:CAB	12:A:1012:CLA:HED1	2.38	0.53
1:A:304:PHE:HE1	12:A:1119:CLA:HAB	1.74	0.53
12:A:1107:CLA:HBD	12:A:1107:CLA:HBA1	1.91	0.52
2:B:655:ALA:HB3	12:B:1023:CLA:HBB2	1.90	0.52
12:A:1012:CLA:HAB	2:B:579:TRP:CH2	2.44	0.52
12:A:1130:CLA:HMB1	12:B:1237:CLA:HAA2	1.90	0.52
2:B:48:ALA:HB3	11:M:29:LEU:HD21	1.89	0.52
2:B:313:THR:HG21	16:B:5004:LHG:HC11	1.91	0.52
1:A:263:PHE:CE1	12:A:1115:CLA:HBB1	2.44	0.52
12:A:1107:CLA:HMA1	8:J:27:ILE:HD13	1.92	0.52
12:A:1129:CLA:H12	16:A:5003:LHG:HC91	1.91	0.52
1:A:107:PRO:HG3	1:A:148:ARG:HH12	1.73	0.52
12:B:1235:CLA:H203	6:F:69:SER:HB2	1.91	0.52
1:A:634:ASN:O	1:A:638:SER:N	2.42	0.52
1:A:705:ASN:HD21	5:E:43:ARG:HH12	1.57	0.52
3:C:54:CYS:SG	3:C:55:GLU:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:CYS:SG	6:F:45:CYS:HB2	2.50	0.52
9:K:33:ALA:HA	9:K:36:ILE:HG12	1.91	0.52
1:A:560:ARG:NH2	4:D:15:THR:O	2.43	0.52
1:A:706:LYS:NZ	6:F:135:ASP:OD1	2.34	0.52
9:K:65:GLU:O	9:K:69:THR:HG23	2.10	0.52
1:A:583:CYS:HB2	2:B:664:TRP:HB3	1.92	0.52
3:C:72:GLU:HG2	3:C:77:MET:SD	2.50	0.52
9:K:36:ILE:O	9:K:40:ALA:HB3	2.10	0.52
1:A:369:HIS:ND1	12:A:1116:CLA:OBD	2.43	0.52
12:A:1116:CLA:HBC3	12:A:1117:CLA:HBB2	1.92	0.52
10:L:104:PHE:HD2	10:L:117:ALA:HA	1.74	0.52
1:A:190:PHE:O	1:A:192:ASN:N	2.41	0.51
1:A:740:TRP:NE1	12:A:1126:CLA:O1A	2.43	0.51
12:A:1107:CLA:C2	15:A:4012:BCR:H19C	2.40	0.51
12:B:1213:CLA:HBD	12:B:1213:CLA:HBA1	1.92	0.51
4:D:6:GLY:HA2	4:D:54:GLU:HG3	1.92	0.51
1:A:125:ILE:HG21	2:B:444:PHE:HA	1.92	0.51
2:B:375:TYR:CD2	12:B:1224:CLA:HAB	2.46	0.51
1:A:215:HIS:O	1:A:219:VAL:N	2.44	0.51
1:A:486:VAL:HG21	12:A:1135:CLA:H12	1.93	0.51
12:A:1132:CLA:H2A	12:A:1132:CLA:HED2	1.91	0.51
2:B:461:ILE:HD11	12:B:1234:CLA:H2	1.91	0.51
9:K:34:PHE:HE1	9:K:66:LEU:HA	1.75	0.51
7:I:12:TRP:O	7:I:16:PRO:HD2	2.10	0.51
1:A:319:HIS:NE2	12:A:1121:CLA:OBD	2.44	0.51
15:A:4001:BCR:H24C	9:K:72:PHE:HB2	1.92	0.51
1:A:704:HIS:NE2	12:A:1139:CLA:HAC1	2.26	0.51
2:B:490:TRP:HE1	12:B:1231:CLA:HED1	1.76	0.51
4:D:31:THR:HG22	4:D:56:LEU:HD13	1.92	0.51
2:B:5:PHE:HD1	2:B:6:PRO:HA	1.75	0.51
4:D:131:ILE:O	4:D:134:SER:OG	2.23	0.51
9:K:20:LEU:HD13	9:K:24:ILE:HD12	1.92	0.50
6:F:10:CYS:HB3	6:F:16:TYR:CE2	2.46	0.50
2:B:570:TRP:CD1	12:B:1226:CLA:HMD1	2.46	0.50
9:K:34:PHE:CZ	9:K:58:LYS:HA	2.47	0.50
2:B:371:THR:HG23	2:B:588:THR:HG21	1.92	0.50
12:A:1107:CLA:H12	15:A:4012:BCR:H17C	1.92	0.50
2:B:356:TYR:CE2	12:B:1225:CLA:HED2	2.46	0.50
12:A:1012:CLA:HMB3	12:B:1021:CLA:H18	1.93	0.50
6:F:67:ILE:HD12	8:J:39:HIS:CG	2.47	0.50
10:L:137:VAL:HA	10:L:140:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:TRP:CH2	12:B:1022:CLA:HAB	2.47	0.50
1:A:733:LEU:HD22	12:A:1140:CLA:HMA1	1.93	0.50
12:A:1102:CLA:HBD	12:A:1109:CLA:H2	1.93	0.50
12:A:1140:CLA:H161	8:J:23:ALA:HB2	1.93	0.50
6:F:55:VAL:HG12	6:F:65:PHE:HB2	1.94	0.50
24:F:6001:LMT:H42	8:J:9:SER:HB3	1.94	0.49
1:A:168:MET:O	1:A:172:MET:HG2	2.12	0.49
1:A:211:GLY:C	12:A:1112:CLA:HAB	2.32	0.49
5:E:13:ARG:O	5:E:15:GLU:N	2.44	0.49
5:E:20:GLY:HA3	6:F:139:PRO:HA	1.95	0.49
12:A:1012:CLA:HMA2	2:B:613:LEU:HD13	1.93	0.49
12:B:1216:CLA:HBA1	12:B:1221:CLA:C3B	2.41	0.49
16:B:5004:LHG:H271	16:B:5004:LHG:H121	1.93	0.49
10:L:109:GLY:H	10:L:116:THR:HG22	1.77	0.49
1:A:154:ASP:OD1	1:A:155:SER:N	2.45	0.49
1:A:607:PHE:HB3	1:A:645:TRP:HZ3	1.77	0.49
10:L:113:THR:O	10:L:116:THR:OG1	2.30	0.49
1:A:54:ASN:OD1	1:A:571:ARG:NH2	2.45	0.49
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.94	0.49
10:L:98:SER:O	10:L:102:VAL:HG13	2.12	0.49
1:A:33:HIS:HE2	12:A:1109:CLA:CGA	2.26	0.49
12:A:1138:CLA:HAB	12:A:1138:CLA:H111	1.93	0.49
2:B:324:ILE:HD12	12:B:1221:CLA:HMC2	1.94	0.49
1:A:296:HIS:HB2	12:A:1116:CLA:C1B	2.43	0.49
15:I:4018:BCR:H24C	25:I:4020:EQ3:C19	2.43	0.49
2:B:385:PHE:CZ	12:B:1222:CLA:HAB	2.47	0.49
10:L:104:PHE:CD2	10:L:117:ALA:HA	2.48	0.49
1:A:177:TRP:HB2	12:A:1109:CLA:HMC3	1.94	0.49
10:L:116:THR:OG1	10:L:119:GLY:HA3	2.13	0.49
1:A:513:THR:HG23	1:A:523:MET:HB3	1.95	0.49
12:A:1140:CLA:H61	12:A:1140:CLA:H41	1.57	0.49
2:B:659:MET:HB2	12:B:1023:CLA:C1C	2.42	0.49
6:F:118:TRP:CG	6:F:119:PRO:HD3	2.47	0.49
1:A:245:GLU:HG3	1:A:248:LYS:HE2	1.95	0.48
2:B:426:PHE:O	2:B:430:HIS:ND1	2.41	0.48
2:B:504:SER:HA	2:B:507:LEU:HD21	1.95	0.48
1:A:189:TRP:CD1	12:A:1110:CLA:HED2	2.48	0.48
17:B:4011:45D:H092	15:F:4014:BCR:H14C	1.96	0.48
1:A:538:HIS:HE1	1:A:604:ILE:HG22	1.78	0.48
12:A:1124:CLA:HAB	15:A:4008:BCR:H311	1.94	0.48
9:K:34:PHE:HE2	9:K:58:LYS:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ALA:HB1	17:B:4011:45D:C42	2.44	0.48
12:A:1140:CLA:H101	15:J:4013:BCR:H362	1.95	0.48
2:B:177:HIS:CG	12:B:1210:CLA:HMC2	2.48	0.48
2:B:413:LYS:HB2	2:B:536:LEU:HD13	1.95	0.48
12:A:1112:CLA:HBA2	12:A:1112:CLA:H3A	1.54	0.48
1:A:348:TRP:HB3	12:A:1103:CLA:HAC1	1.95	0.48
10:L:124:ALA:O	10:L:126:GLY:N	2.46	0.48
12:A:1132:CLA:H61	12:A:1132:CLA:H41	1.47	0.48
2:B:99:GLY:HA3	2:B:637:VAL:HB	1.95	0.48
2:B:456:VAL:H	12:B:1235:CLA:HMD1	1.78	0.48
1:A:531:ASP:O	1:A:535:HIS:ND1	2.38	0.48
1:A:538:HIS:CD2	12:A:1135:CLA:HAB	2.49	0.48
12:A:1132:CLA:HBD	10:L:70:PRO:HD3	1.95	0.48
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.95	0.48
2:B:210:ASP:OD1	2:B:210:ASP:N	2.46	0.48
2:B:711:THR:HB	20:B:5002:LMG:H411	1.95	0.48
10:L:38:PRO:HB3	10:L:44:LEU:HD22	1.95	0.48
2:B:167:TRP:CZ2	12:B:1208:CLA:HMA1	2.48	0.48
12:A:1109:CLA:H72	12:A:1109:CLA:H112	1.74	0.48
2:B:679:HIS:CD2	2:B:690:TRP:HZ3	2.32	0.48
9:K:31:VAL:HA	9:K:34:PHE:HB2	1.96	0.48
1:A:299:ALA:HA	12:A:1115:CLA:HMC3	1.95	0.47
12:A:1119:CLA:HMB2	12:A:1123:CLA:HMA3	1.95	0.47
1:A:573:PRO:HG3	1:A:721:ILE:HG12	1.96	0.47
1:A:576:GLY:HA2	2:B:559:PRO:HD3	1.96	0.47
12:A:1132:CLA:H8	10:L:60:PHE:CE2	2.49	0.47
2:B:147:SER:HB3	11:M:21:LEU:HD12	1.97	0.47
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.31	0.47
1:A:255:SER:HB2	1:A:271:TYR:HA	1.96	0.47
13:B:2002:PQN:H142	15:B:4017:BCR:H271	1.96	0.47
15:J:4013:BCR:H351	15:J:4013:BCR:H15C	1.68	0.47
15:A:4001:BCR:H391	9:K:41:ILE:HG12	1.96	0.47
3:C:61:ASP:OD2	5:E:16:SER:OG	2.20	0.47
2:B:182:LEU:HD13	12:B:1210:CLA:HHB	1.95	0.47
12:B:1235:CLA:H41	12:B:1235:CLA:H62	1.47	0.47
6:F:58:ARG:HD2	6:F:61:HIS:HD1	1.80	0.47
15:K:4001:BCR:H351	15:K:4001:BCR:H15C	1.64	0.47
1:A:574:CYS:SG	1:A:576:GLY:N	2.80	0.47
12:A:1122:CLA:HMA1	12:A:1141:CLA:CAB	2.44	0.47
2:B:90:ALA:HA	2:B:113:VAL:HG23	1.97	0.47
2:B:322:ASP:O	2:B:326:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:THR:HG22	12:B:1224:CLA:CAB	2.45	0.47
2:B:586:TRP:CE2	12:B:1021:CLA:H152	2.50	0.47
12:B:1205:CLA:CAD	12:B:1224:CLA:HBA1	2.45	0.47
12:B:1234:CLA:H12	12:B:1235:CLA:CGA	2.45	0.47
12:B:1202:CLA:H2	12:B:1202:CLA:H61	1.73	0.47
9:K:59:LYS:HZ3	9:K:63:LEU:HB2	1.80	0.47
1:A:577:PRO:HD3	2:B:558:GLY:HA2	1.96	0.47
12:B:1207:CLA:O1D	12:B:1207:CLA:H2	2.15	0.47
10:L:73:ASP:OD1	10:L:73:ASP:N	2.47	0.47
15:A:4001:BCR:H15C	15:A:4001:BCR:H351	1.56	0.46
12:B:1201:CLA:HMA2	11:M:29:LEU:HB3	1.97	0.46
12:B:1204:CLA:H12	7:I:14:LEU:HG	1.96	0.46
12:A:1112:CLA:NC	12:A:1114:CLA:HAB	2.29	0.46
12:B:1211:CLA:CHB	19:B:4006:ECH:H24	2.43	0.46
1:A:668:TYR:O	1:A:741:ALA:HB1	2.16	0.46
2:B:167:TRP:CZ2	12:B:1210:CLA:HAC2	2.50	0.46
2:B:289:HIS:CE1	15:B:4004:BCR:H363	2.51	0.46
12:B:1239:CLA:HBA2	12:B:1239:CLA:H3A	1.82	0.46
1:A:683:LEU:HB2	12:A:1013:CLA:HMC3	1.98	0.46
2:B:203:ARG:NH2	2:B:253:ALA:O	2.47	0.46
2:B:232:VAL:O	2:B:235:ALA:HB2	2.16	0.46
2:B:676:VAL:HG13	2:B:690:TRP:CZ2	2.51	0.46
12:B:1203:CLA:HAB	12:B:1225:CLA:HBB1	1.97	0.46
12:B:1235:CLA:H141	12:B:1235:CLA:H162	1.80	0.46
7:I:1:MET:O	7:I:3:GLY:N	2.48	0.46
1:A:320:SER:HB3	1:A:323:GLU:HG3	1.98	0.46
1:A:344:LEU:HB2	12:A:1123:CLA:HBC3	1.98	0.46
12:A:1103:CLA:H41	15:A:4003:BCR:H292	1.98	0.46
12:A:1109:CLA:H202	12:A:1109:CLA:H161	1.73	0.46
2:B:305:LEU:HD11	12:B:1221:CLA:HMC1	1.97	0.46
12:A:1011:CLA:HMB3	12:A:1012:CLA:OBD	2.15	0.46
12:A:1111:CLA:H3A	12:A:1111:CLA:HBA1	1.47	0.46
12:B:1211:CLA:HMB1	12:B:1211:CLA:HBB1	1.97	0.46
6:F:13:ASN:HB3	6:F:16:TYR:HB3	1.98	0.46
12:F:1301:CLA:C3B	15:F:4014:BCR:H10C	2.46	0.46
7:I:9:TYR:H	7:I:9:TYR:HD2	1.64	0.46
1:A:59:ASP:OD2	1:A:414:ARG:NH1	2.46	0.46
12:A:1013:CLA:HMB1	12:A:1013:CLA:HBB1	1.98	0.46
4:D:87:ARG:HH21	4:D:97:LEU:HD11	1.80	0.46
1:A:538:HIS:CE1	1:A:604:ILE:HG22	2.51	0.46
12:A:1109:CLA:H62	12:A:1109:CLA:H41	1.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:O	1:A:98:SER:OG	2.34	0.45
2:B:372:HIS:HB2	12:B:1224:CLA:C1B	2.46	0.45
2:B:440:VAL:HG21	12:B:1230:CLA:HAC2	1.98	0.45
12:B:1214:CLA:H101	12:B:1232:CLA:HMA2	1.96	0.45
19:M:4021:ECH:H24	19:M:4021:ECH:H37	1.51	0.45
1:A:597:TRP:HE1	12:B:1023:CLA:C1D	2.29	0.45
12:A:1106:CLA:H143	16:A:5001:LHG:H223	1.98	0.45
10:L:96:LEU:HG	10:L:120:TRP:HE1	1.82	0.45
10:L:139:TYR:HE1	10:L:142:LEU:HD12	1.80	0.45
1:A:435:ALA:O	1:A:439:HIS:ND1	2.32	0.45
1:A:689:GLY:HA3	2:B:565:CYS:HB2	1.98	0.45
12:A:1102:CLA:H2A	12:A:1102:CLA:HED2	1.99	0.45
12:A:1138:CLA:H43	12:B:1229:CLA:HAA2	1.99	0.45
12:B:1214:CLA:H102	12:B:1214:CLA:H61	1.37	0.45
7:I:10:LEU:N	7:I:11:PRO:HD2	2.31	0.45
8:J:31:ARG:HD3	15:J:4013:BCR:H312	1.98	0.45
10:L:99:TYR:O	10:L:102:VAL:HG22	2.16	0.45
3:C:13:GLY:HA3	3:C:38:GLN:HG3	1.99	0.45
6:F:64:ASP:HA	8:J:38:PHE:HB2	1.98	0.45
12:A:1102:CLA:HMA2	12:A:1109:CLA:HMD2	1.99	0.45
15:A:4008:BCR:H351	15:A:4008:BCR:H15C	1.68	0.45
2:B:51:PHE:HE1	12:B:1208:CLA:HBB1	1.80	0.45
2:B:279:ALA:HA	12:B:1213:CLA:HMC3	1.98	0.45
12:B:1202:CLA:H101	12:B:1210:CLA:HBA1	1.99	0.45
1:A:48:ILE:O	1:A:51:LEU:HB3	2.17	0.45
1:A:406:ALA:O	1:A:410:ILE:HG13	2.16	0.45
10:L:44:LEU:HD21	10:L:48:LEU:O	2.17	0.45
10:L:155:LEU:HD12	10:L:156:PHE:H	1.80	0.45
2:B:497:ALA:O	2:B:503:ASN:ND2	2.41	0.45
12:B:1228:CLA:HBA2	12:B:1228:CLA:H3A	1.50	0.45
6:F:9:PRO:HA	6:F:44:LEU:HA	1.99	0.45
19:M:4021:ECH:H20	19:M:4021:ECH:H36	1.57	0.45
1:A:358:LEU:HD21	12:A:1123:CLA:HMB2	1.99	0.45
2:B:56:ILE:HD11	19:M:4021:ECH:H39B	1.99	0.45
19:B:4006:ECH:H20	19:B:4006:ECH:H36	1.53	0.45
7:I:15:ILE:HB	7:I:16:PRO:HD2	1.99	0.45
1:A:202:ALA:HB2	1:A:308:GLY:HA3	1.99	0.45
1:A:332:PHE:HB2	16:A:5003:LHG:HC41	1.97	0.45
2:B:422:TRP:CZ2	12:B:1228:CLA:HAB	2.51	0.45
12:B:1237:CLA:HMC3	12:B:1238:CLA:ND	2.32	0.45
12:B:1209:CLA:HMD2	21:B:5008:SQD:H212	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:1222:CLA:HMB2	12:B:1236:CLA:HBA1	1.99	0.45
20:B:5002:LMG:H302	20:B:5002:LMG:H331	1.65	0.45
1:A:315:TRP:HB3	9:K:64:PRO:HB3	1.99	0.45
1:A:609:PHE:O	1:A:613:MET:HG2	2.17	0.45
1:A:680:ALA:C	12:A:1013:CLA:HAB	2.37	0.45
2:B:180:ALA:HA	2:B:285:ILE:HA	1.99	0.45
10:L:49:ARG:HB3	10:L:123:PHE:HA	1.98	0.45
15:A:4012:BCR:H351	15:A:4012:BCR:H15C	1.83	0.44
2:B:256:THR:OG1	2:B:271:THR:OG1	2.20	0.44
2:B:372:HIS:O	2:B:376:ILE:HG12	2.16	0.44
12:A:1012:CLA:HED2	12:B:1021:CLA:H52	2.00	0.44
12:A:1102:CLA:HMC3	12:A:1104:CLA:HED2	1.98	0.44
2:B:385:PHE:CG	2:B:531:LEU:HB3	2.53	0.44
7:I:18:VAL:HG21	15:I:4018:BCR:HC41	2.00	0.44
12:J:1302:CLA:HED2	12:J:1302:CLA:H2A	1.99	0.44
10:L:101:LEU:HD22	10:L:101:LEU:HA	1.85	0.44
12:A:1126:CLA:H3A	12:A:1126:CLA:HBA2	1.54	0.44
2:B:279:ALA:O	2:B:283:ILE:HG13	2.17	0.44
2:B:474:VAL:HG12	2:B:475:LEU:HG	1.99	0.44
2:B:523:GLY:HA2	2:B:579:TRP:HZ3	1.82	0.44
2:B:649:PHE:O	2:B:653:VAL:HG23	2.17	0.44
12:B:1204:CLA:H3A	12:B:1204:CLA:HBA2	1.61	0.44
4:D:8:PRO:O	4:D:51:ASN:ND2	2.46	0.44
1:A:199:HIS:CG	12:A:1111:CLA:HMC2	2.53	0.44
1:A:680:ALA:O	12:A:1013:CLA:HAB	2.17	0.44
12:A:1105:CLA:H141	12:A:1105:CLA:H161	1.71	0.44
12:A:1106:CLA:H93	12:A:1128:CLA:H203	1.98	0.44
12:A:1107:CLA:H2	15:A:4012:BCR:H19C	1.99	0.44
12:A:1117:CLA:HMB1	12:A:1117:CLA:HBB1	2.00	0.44
12:A:1129:CLA:HAB	12:A:1137:CLA:CBB	2.47	0.44
12:B:1238:CLA:CGD	10:L:99:TYR:CD1	3.00	0.44
1:A:588:TRP:NE1	12:A:1128:CLA:HMD1	2.33	0.44
12:A:1126:CLA:C4C	17:B:4011:45D:H061	2.48	0.44
12:B:1021:CLA:HMB3	12:B:1022:CLA:OBD	2.17	0.44
12:B:1206:CLA:H43	15:I:4018:BCR:C11	2.46	0.44
12:B:1222:CLA:C2B	15:B:4010:BCR:H363	2.48	0.44
9:K:22:VAL:O	9:K:27:CYS:N	2.25	0.44
1:A:13:LYS:HE2	1:A:314:ASN:OD1	2.17	0.44
1:A:303:LEU:HD22	12:A:1119:CLA:HMC1	1.98	0.44
2:B:310:GLY:HA3	16:B:5004:LHG:HC32	2.00	0.44
3:C:54:CYS:N	14:C:3002:SF4:S4	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:1301:CLA:C2B	15:F:4014:BCR:H10C	2.47	0.44
10:L:78:TYR:HB2	10:L:143:GLU:HG2	2.00	0.44
12:A:1102:CLA:H192	15:A:4012:BCR:H383	2.00	0.44
2:B:618:ARG:NE	2:B:619:ASP:OD1	2.50	0.44
2:B:675:ILE:HD13	12:B:1237:CLA:HMD3	1.99	0.44
1:A:651:TRP:HD1	12:B:1021:CLA:HAC2	1.83	0.44
2:B:655:ALA:O	12:B:1023:CLA:HAB	2.18	0.44
12:B:1204:CLA:HMB3	12:B:1205:CLA:HMA1	2.00	0.44
12:B:1227:CLA:HAA2	21:F:5001:SQD:O7	2.17	0.44
1:A:352:LEU:HD13	12:A:1103:CLA:C2D	2.48	0.43
12:A:1111:CLA:H2	12:A:1111:CLA:HMA2	2.00	0.43
12:A:1126:CLA:H92	12:A:1126:CLA:H62	1.79	0.43
2:B:676:VAL:HG13	2:B:690:TRP:HZ2	1.82	0.43
12:B:1222:CLA:H43	12:B:1235:CLA:HBA1	2.00	0.43
3:C:58:CYS:O	5:E:47:ASN:ND2	2.51	0.43
8:J:31:ARG:HD3	15:J:4013:BCR:C31	2.48	0.43
9:K:75:ILE:HD13	15:K:4001:BCR:H321	2.00	0.43
10:L:61:LEU:HD13	10:L:88:LEU:HD23	1.99	0.43
1:A:85:VAL:HG21	12:A:1109:CLA:H191	2.01	0.43
1:A:395:TRP:NE1	12:A:1126:CLA:HAB	2.32	0.43
12:A:1106:CLA:HBA2	12:A:1106:CLA:H3A	1.31	0.43
2:B:167:TRP:CE2	12:B:1208:CLA:HMA1	2.53	0.43
2:B:621:LEU:O	2:B:625:SER:OG	2.27	0.43
12:B:1207:CLA:HMC1	12:B:1207:CLA:HBC2	2.00	0.43
13:B:2002:PQN:H141	12:B:1238:CLA:HBB2	1.99	0.43
7:I:13:ILE:O	7:I:17:MET:HB2	2.17	0.43
9:K:70:MET:O	9:K:74:HIS:ND1	2.51	0.43
11:M:3:LEU:HD23	11:M:8:ILE:HD11	2.01	0.43
1:A:42:PRO:HG3	6:F:101:VAL:HG21	1.99	0.43
12:A:1116:CLA:H3A	12:A:1116:CLA:HBA2	1.47	0.43
12:A:1118:CLA:H3A	12:A:1118:CLA:HBA2	1.62	0.43
13:A:2001:PQN:H201	12:A:1101:CLA:H12	2.00	0.43
2:B:314:GLY:HA3	2:B:408:ARG:HH11	1.83	0.43
2:B:616:TRP:HB3	12:B:1021:CLA:H101	1.99	0.43
7:I:36:SER:O	10:L:105:GLN:NE2	2.52	0.43
1:A:263:PHE:HZ	15:A:4001:BCR:H343	1.83	0.43
2:B:167:TRP:CE2	12:B:1210:CLA:HAC2	2.53	0.43
2:B:690:TRP:HA	12:B:1238:CLA:O1D	2.18	0.43
12:B:1222:CLA:O1A	12:B:1234:CLA:HHB	2.18	0.43
3:C:66:ARG:HB3	3:C:68:TYR:CE2	2.54	0.43
6:F:32:SER:HA	6:F:35:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:10:LEU:H	7:I:11:PRO:HD2	1.83	0.43
10:L:39:ALA:HB2	10:L:114:LEU:HD23	2.00	0.43
12:A:1138:CLA:HMC3	12:A:1139:CLA:C4D	2.49	0.43
1:A:118:TRP:CE3	15:J:4013:BCR:H323	2.53	0.43
1:A:375:PRO:HB3	12:A:1117:CLA:HMA2	2.00	0.43
1:A:500:ASN:ND2	12:A:1115:CLA:OBD	2.43	0.43
12:A:1134:CLA:CHA	12:A:1134:CLA:HBA1	2.48	0.43
12:A:1102:CLA:H193	12:A:1106:CLA:H152	1.99	0.43
12:B:1205:CLA:H3A	12:B:1205:CLA:HBA2	1.74	0.43
12:B:1207:CLA:HBA2	12:B:1207:CLA:HBD	2.00	0.43
12:B:1222:CLA:HMA2	12:B:1223:CLA:HED2	2.00	0.43
5:E:14:THR:OG1	5:E:15:GLU:N	2.52	0.43
1:A:268:TRP:HZ2	15:K:4001:BCR:HC31	1.84	0.43
12:A:1106:CLA:HBB2	12:A:1126:CLA:H142	2.01	0.43
2:B:375:TYR:HB3	12:B:1224:CLA:HMC3	2.01	0.43
12:B:1021:CLA:H41	12:B:1021:CLA:H61	1.42	0.43
4:D:106:GLU:OE1	4:D:106:GLU:N	2.47	0.43
10:L:27:SER:O	10:L:31:ARG:HB2	2.19	0.43
10:L:120:TRP:HZ2	12:L:1502:CLA:HBC1	1.83	0.43
1:A:307:ALA:HB2	12:A:1119:CLA:HBC2	2.01	0.43
1:A:640:ILE:H	1:A:640:ILE:HG12	1.71	0.43
12:A:1128:CLA:H41	12:A:1128:CLA:H61	1.61	0.43
12:B:1225:CLA:H3A	12:B:1225:CLA:HBA2	1.42	0.43
15:F:4014:BCR:H15C	15:F:4014:BCR:H351	1.80	0.43
10:L:82:LEU:O	10:L:86:LEU:HG	2.19	0.43
1:A:261:THR:N	1:A:262:PRO:HD2	2.34	0.43
1:A:462:ARG:NH2	2:B:634:PRO:HG3	2.33	0.43
1:A:571:ARG:NH1	12:A:1128:CLA:OBD	2.49	0.43
12:A:1112:CLA:C1A	12:A:1114:CLA:HMB3	2.49	0.43
12:A:1121:CLA:HMB3	12:A:1141:CLA:C2C	2.49	0.43
12:A:1124:CLA:HAA2	12:A:1125:CLA:OBD	2.19	0.43
13:B:2002:PQN:H302	13:B:2002:PQN:H262	1.75	0.43
1:A:549:LEU:HD21	1:A:594:GLY:HA3	2.00	0.42
1:A:597:TRP:HE1	12:B:1023:CLA:CHD	2.32	0.42
12:A:1103:CLA:H3A	12:A:1103:CLA:HBA1	1.52	0.42
12:A:1115:CLA:H11	12:A:1115:CLA:H51	1.76	0.42
12:A:1138:CLA:H203	12:A:1139:CLA:H51	2.01	0.42
2:B:461:ILE:O	2:B:464:THR:OG1	2.24	0.42
2:B:523:GLY:HA2	2:B:579:TRP:CZ3	2.54	0.42
12:B:1202:CLA:HBD	12:B:1202:CLA:H122	2.00	0.42
19:B:4006:ECH:H8	19:B:4006:ECH:H11	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:4018:BCR:HC31	20:B:5005:LMG:H222	2.02	0.42
1:A:240:HIS:NE2	12:A:1114:CLA:O1D	2.48	0.42
12:A:1013:CLA:HBA1	2:B:425:LEU:HD12	2.01	0.42
2:B:428:GLY:HA2	2:B:522:LEU:HD22	2.01	0.42
12:B:1222:CLA:HBA2	12:B:1222:CLA:H3A	1.59	0.42
3:C:29:VAL:HG12	4:D:112:ARG:HB2	2.01	0.42
9:K:25:ILE:HG21	9:K:81:VAL:HG23	2.02	0.42
10:L:86:LEU:HD22	10:L:132:MET:SD	2.60	0.42
10:L:139:TYR:CE1	10:L:142:LEU:HD12	2.53	0.42
12:A:1011:CLA:HAA1	12:B:1021:CLA:HMB1	2.00	0.42
15:B:4010:BCR:H341	16:B:5004:LHG:H223	2.00	0.42
3:C:25:VAL:HG13	3:C:44:ARG:O	2.19	0.42
4:D:88:VAL:HG22	4:D:94:VAL:HG22	2.00	0.42
8:J:12:PRO:HA	8:J:15:ILE:HG22	2.01	0.42
10:L:82:LEU:HB2	10:L:139:TYR:HD2	1.84	0.42
10:L:99:TYR:CD1	10:L:99:TYR:C	2.92	0.42
2:B:361:GLN:OE1	2:B:361:GLN:N	2.52	0.42
2:B:661:LEU:HG	2:B:706:GLY:HA3	2.01	0.42
12:B:1229:CLA:CBB	15:F:4014:BCR:HC21	2.49	0.42
12:B:1236:CLA:C3D	16:B:5004:LHG:H372	2.50	0.42
6:F:125:GLU:HB3	6:F:130:LYS:HB3	2.02	0.42
10:L:109:GLY:N	10:L:116:THR:HG22	2.34	0.42
1:A:482:PHE:O	1:A:486:VAL:HG23	2.20	0.42
12:A:1111:CLA:HMA2	12:A:1111:CLA:C2	2.50	0.42
12:A:1119:CLA:HMA2	12:A:1123:CLA:C1C	2.50	0.42
12:A:1139:CLA:H41	12:A:1139:CLA:H61	1.37	0.42
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.54	0.42
12:B:1235:CLA:H152	23:F:4016:C7Z:C28	2.50	0.42
1:A:86:TRP:HE1	12:A:1106:CLA:HBA1	1.84	0.42
2:B:422:TRP:CD1	12:B:1229:CLA:HED2	2.55	0.42
20:B:5005:LMG:H331	20:B:5005:LMG:H302	1.85	0.42
2:B:628:LEU:HD12	2:B:721:PHE:HD1	1.85	0.42
1:A:344:LEU:HB3	1:A:351:GLN:NE2	2.35	0.42
1:A:583:CYS:HB3	14:A:3001:SF4:S4	2.60	0.42
12:A:1013:CLA:CGA	12:A:1013:CLA:H3A	2.49	0.42
2:B:152:ALA:HB2	12:B:1208:CLA:HBC2	2.02	0.42
12:A:1125:CLA:HMB3	12:A:1133:CLA:H2	2.02	0.42
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.55	0.42
2:B:461:ILE:HG12	12:B:1231:CLA:HMC3	2.02	0.42
12:B:1224:CLA:O1D	12:B:1225:CLA:HMA1	2.19	0.42
1:A:15:SER:HB2	1:A:186:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1012:CLA:HMA1	12:B:1021:CLA:H202	2.02	0.41
2:B:460:TRP:O	2:B:464:THR:HG23	2.20	0.41
2:B:679:HIS:NE2	2:B:685:ALA:O	2.53	0.41
12:B:1220:CLA:HAB	12:B:1227:CLA:CMD	2.38	0.41
12:B:1234:CLA:H111	12:B:1234:CLA:H91	1.85	0.41
7:I:35:GLU:HB2	10:L:102:VAL:HG12	2.02	0.41
10:L:112:ASP:HB3	10:L:115:GLN:HG2	2.02	0.41
2:B:2:ALA:HA	2:B:14:GLN:HA	2.03	0.41
2:B:431:THR:HG22	12:B:1021:CLA:H192	2.01	0.41
12:B:1203:CLA:H3A	12:B:1203:CLA:HBA1	1.80	0.41
9:K:34:PHE:HD1	9:K:34:PHE:HA	1.78	0.41
10:L:139:TYR:HD1	10:L:139:TYR:HA	1.68	0.41
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.87	0.41
12:B:1229:CLA:H3A	12:B:1229:CLA:HBA2	1.47	0.41
21:F:5001:SQD:H152	21:F:5001:SQD:H182	1.88	0.41
15:I:4018:BCR:H351	15:I:4018:BCR:H15C	1.67	0.41
9:K:29:CYS:HB3	9:K:76:LEU:HB2	2.01	0.41
10:L:155:LEU:C	10:L:157:ASN:H	2.23	0.41
1:A:215:HIS:HB2	12:A:1112:CLA:CHC	2.51	0.41
1:A:576:GLY:O	1:A:582:THR:OG1	2.31	0.41
12:A:1126:CLA:H62	12:A:1126:CLA:H41	1.79	0.41
2:B:654:TRP:CD2	12:B:1021:CLA:HMA2	2.55	0.41
12:B:1202:CLA:H42	12:B:1203:CLA:HBB2	2.02	0.41
3:C:5:VAL:HG11	3:C:26:LEU:HD21	2.01	0.41
5:E:17:TYR:CE2	5:E:45:ASN:HA	2.55	0.41
1:A:354:ILE:HD11	15:A:4007:BCR:HC7	2.01	0.41
12:A:1107:CLA:HBB1	15:A:4012:BCR:HC8	2.02	0.41
10:L:114:LEU:HD11	10:L:123:PHE:CD2	2.56	0.41
1:A:33:HIS:NE2	12:A:1109:CLA:O1A	2.39	0.41
1:A:194:GLU:HB3	1:A:311:TYR:HB3	2.03	0.41
12:A:1116:CLA:O1D	12:A:1117:CLA:HBB	2.20	0.41
2:B:376:ILE:O	2:B:380:LEU:HG	2.20	0.41
8:J:20:THR:HG23	15:J:4013:BCR:H351	2.02	0.41
10:L:52:GLU:O	10:L:54:GLY:N	2.54	0.41
1:A:356:LEU:HD21	12:A:1128:CLA:HAB	2.02	0.41
2:B:405:VAL:O	2:B:409:MET:HG2	2.21	0.41
8:J:30:ASN:O	8:J:34:PRO:HB3	2.20	0.41
2:B:220:ALA:CB	2:B:224:PRO:HG2	2.44	0.41
2:B:429:PHE:HZ	15:F:4014:BCR:H372	1.86	0.41
1:A:288:LEU:HD12	1:A:375:PRO:HB3	2.03	0.41
1:A:615:SER:CB	1:A:635:PHE:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ILE:HD13	12:A:1126:CLA:HMC2	2.03	0.41
12:A:1133:CLA:HMD2	12:A:1134:CLA:CAB	2.51	0.41
16:A:5001:LHG:H151	16:A:5001:LHG:H182	1.86	0.41
2:B:315:ALA:HB3	2:B:404:ASN:HA	2.02	0.41
2:B:346:VAL:O	2:B:350:MET:HG3	2.21	0.41
2:B:556:CYS:HB2	2:B:564:THR:O	2.21	0.41
2:B:697:LEU:HD22	2:B:701:GLN:NE2	2.36	0.41
12:B:1202:CLA:H61	12:B:1202:CLA:H102	1.76	0.41
12:B:1205:CLA:O1A	12:B:1224:CLA:HBD	2.21	0.41
10:L:49:ARG:HH21	10:L:114:LEU:H	1.69	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.92	0.41
1:A:483:ALA:HA	12:A:1135:CLA:HBA1	2.03	0.41
1:A:487:GLN:HA	1:A:509:PHE:HB3	2.03	0.41
1:A:674:ALA:HA	17:B:4011:45D:H371	2.03	0.41
2:B:88:ALA:HB2	2:B:116:ALA:HA	2.02	0.41
12:B:1204:CLA:HED2	7:I:11:PRO:HB3	2.03	0.41
10:L:62:ILE:O	10:L:66:THR:OG1	2.30	0.41
1:A:337:HIS:CE1	16:A:5003:LHG:HC12	2.56	0.40
1:A:395:TRP:HB3	12:A:1126:CLA:HMC3	2.02	0.40
1:A:439:HIS:O	1:A:443:VAL:HG23	2.19	0.40
2:B:305:LEU:HD12	2:B:321:TYR:HB2	2.02	0.40
12:B:1226:CLA:HBB1	12:B:1226:CLA:HMB1	2.03	0.40
1:A:340:LEU:HD21	12:A:1122:CLA:HBC3	2.02	0.40
12:A:1126:CLA:O1D	12:A:1127:CLA:HMA1	2.21	0.40
2:B:374:GLN:NE2	2:B:587:LEU:HD11	2.36	0.40
2:B:691:LYS:HZ1	7:I:37:GLU:HA	1.87	0.40
8:J:28:GLU:HG3	12:J:1302:CLA:C1C	2.51	0.40
10:L:37:LEU:HD13	12:L:1502:CLA:O1D	2.22	0.40
2:B:181:GLY:HA3	12:B:1210:CLA:HBB1	2.03	0.40
12:B:1215:CLA:H3A	12:B:1215:CLA:HBA2	1.61	0.40
12:B:1222:CLA:H42	16:B:5004:LHG:H362	2.03	0.40
12:B:1226:CLA:H2A	12:B:1226:CLA:HED2	2.03	0.40
5:E:13:ARG:HB3	5:E:16:SER:HB2	2.03	0.40
10:L:49:ARG:HA	10:L:49:ARG:HD2	1.70	0.40
1:A:704:HIS:CD2	12:A:1139:CLA:HAC1	2.56	0.40
12:A:1130:CLA:H2	2:B:683:PRO:HG2	2.04	0.40
2:B:460:TRP:CZ2	2:B:474:VAL:HG11	2.56	0.40
3:C:23:LEU:HA	4:D:66:LEU:HD13	2.03	0.40
6:F:84:ARG:O	6:F:88:ILE:HG12	2.22	0.40
10:L:36:ASN:OD1	10:L:42:LYS:NZ	2.31	0.40
1:A:360:GLY:HA2	1:A:397:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ILE:HG23	15:A:4008:BCR:H343	2.03	0.40
1:A:657:VAL:HG12	1:A:669:GLY:HA2	2.03	0.40
2:B:223:MET:HB2	2:B:224:PRO:HD3	2.04	0.40
12:B:1211:CLA:HED2	12:B:1211:CLA:H2A	2.04	0.40
12:B:1220:CLA:HMB2	12:B:1240:CLA:HBC3	2.02	0.40
12:B:1231:CLA:O1A	12:B:1232:CLA:HHB	2.21	0.40
4:D:30:ILE:HG23	4:D:32:TRP:HZ3	1.85	0.40
4:D:53:GLY:O	4:D:55:ASN:ND2	2.54	0.40
5:E:18:TRP:CH2	5:E:45:ASN:HB3	2.57	0.40
6:F:54:ILE:HB	6:F:61:HIS:ND1	2.36	0.40
6:F:72:PHE:CD1	15:F:4014:BCR:H343	2.57	0.40
9:K:59:LYS:NZ	9:K:63:LEU:HB2	2.35	0.40
11:M:20:PHE:HB2	19:M:4021:ECH:H2A	2.02	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/751 (100%)	694 (93%)	52 (7%)	3 (0%)	30	66
2	B	729/731 (100%)	685 (94%)	43 (6%)	1 (0%)	48	81
3	C	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	10	42
4	D	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
5	E	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	3	27
6	F	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9	40
7	I	38/40 (95%)	29 (76%)	6 (16%)	3 (8%)	1	12
8	J	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
9	K	68/70 (97%)	61 (90%)	6 (9%)	1 (2%)	8	40
10	L	135/137 (98%)	104 (77%)	25 (18%)	6 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
All	All	2211/2233 (99%)	2022 (92%)	168 (8%)	21 (1%)	14	49

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
10	L	105	GLN
1	A	191	GLN
5	E	14	THR
2	B	556	CYS
5	E	54	SER
7	I	2	ASP
10	L	38	PRO
10	L	117	ALA
4	D	106	GLU
9	K	84	LEU
10	L	125	ALA
10	L	146	SER
4	D	100	ALA
7	I	12	TRP
10	L	53	VAL
6	F	14	PRO
6	F	95	ASN
7	I	38	GLY
3	C	59	PRO
1	A	476	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/603 (100%)	590 (98%)	12 (2%)	50	68
2	B	583/583 (100%)	569 (98%)	14 (2%)	44	63
3	C	68/68 (100%)	66 (97%)	2 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	116/116 (100%)	110 (95%)	6 (5%)	19	43
5	E	58/58 (100%)	56 (97%)	2 (3%)	32	54
6	F	119/119 (100%)	117 (98%)	2 (2%)	56	72
7	I	32/32 (100%)	27 (84%)	5 (16%)	2	14
8	J	35/35 (100%)	34 (97%)	1 (3%)	37	58
9	K	53/54 (98%)	46 (87%)	7 (13%)	3	17
10	L	102/102 (100%)	83 (81%)	19 (19%)	1	9
11	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1793/1795 (100%)	1723 (96%)	70 (4%)	27	50

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	110	ILE
1	A	210	LEU
1	A	256	PHE
1	A	303	LEU
1	A	371	TYR
1	A	381	ILE
1	A	561	LEU
1	A	583	CYS
1	A	631	THR
1	A	704	HIS
1	A	743	PHE
2	B	5	PHE
2	B	47	PHE
2	B	145	LEU
2	B	257	PHE
2	B	406	LEU
2	B	418	SER
2	B	543	LEU
2	B	565	CYS
2	B	567	ILE
2	B	573	PHE
2	B	628	LEU
2	B	686	ASN
2	B	687	LEU
2	B	729	LYS

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Mol	Chain	Res	Type
3	C	11	CYS
3	C	72	GLU
4	D	18	LEU
4	D	66	LEU
4	D	77	LYS
4	D	96	TYR
4	D	107	LYS
4	D	108	VAL
5	E	30	LYS
5	E	66	LEU
6	F	66	LEU
6	F	132	VAL
7	I	1	MET
7	I	9	TYR
7	I	13	ILE
7	I	14	LEU
7	I	20	TRP
8	J	26	LEU
9	K	20	LEU
9	K	22	VAL
9	K	32	PHE
9	K	34	PHE
9	K	50	LEU
9	K	65	GLU
9	K	69	THR
10	L	42	LYS
10	L	51	LEU
10	L	52	GLU
10	L	59	TYR
10	L	60	PHE
10	L	77	GLN
10	L	99	TYR
10	L	101	LEU
10	L	104	PHE
10	L	108	GLN
10	L	118	ASP
10	L	128	PHE
10	L	139	TYR
10	L	140	PHE
10	L	145	LEU
10	L	149	ASP
10	L	152	PHE

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Mol	Chain	Res	Type
10	L	155	LEU
10	L	156	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	HIS
2	B	299	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 130 ligands modelled in this entry, 3 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	CLA	A	1102	12	65,73,73	1.02	7 (10%)	76,113,113	1.80	16 (21%)
12	CLA	A	1106	-	65,73,73	1.03	7 (10%)	76,113,113	1.79	15 (19%)
12	CLA	B	1201	-	49,57,73	1.18	7 (14%)	55,93,113	1.99	14 (25%)
12	CLA	B	1202	-	65,73,73	1.01	6 (9%)	76,113,113	1.79	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	LMT	F	6001	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	2 (4%)
15	BCR	A	4008	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	17 (30%)
12	CLA	B	1204	-	49,57,73	1.21	7 (14%)	55,93,113	1.94	13 (23%)
19	ECH	B	4006	-	42,42,42	0.85	1 (2%)	55,58,58	2.46	12 (21%)
14	SF4	C	3003	-	0,12,12	-	-	-	-	-
12	CLA	B	1238	-	49,57,73	1.21	8 (16%)	55,93,113	2.01	13 (23%)
12	CLA	K	1402	-	49,57,73	1.18	7 (14%)	55,93,113	2.05	16 (29%)
12	CLA	F	1302	10	49,57,73	1.18	6 (12%)	55,93,113	2.02	13 (23%)
15	BCR	B	4017	-	41,41,41	1.85	4 (9%)	56,56,56	4.45	15 (26%)
12	CLA	A	1117	-	49,57,73	1.17	7 (14%)	55,93,113	1.99	15 (27%)
12	CLA	A	1132	10	55,63,73	1.15	7 (12%)	64,101,113	1.84	13 (20%)
20	LMG	B	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.06	3 (4%)
21	SQD	B	5008	-	53,54,54	0.78	0	62,65,65	0.91	2 (3%)
12	CLA	A	1012	-	49,57,73	1.20	7 (14%)	55,93,113	1.91	13 (23%)
12	CLA	A	1101	-	49,57,73	1.19	7 (14%)	55,93,113	2.10	16 (29%)
12	CLA	B	1228	-	49,57,73	1.18	7 (14%)	55,93,113	1.98	13 (23%)
12	CLA	K	1401	-	45,53,73	1.24	7 (15%)	52,89,113	1.89	10 (19%)
12	CLA	A	1140	-	65,73,73	1.05	7 (10%)	76,113,113	1.73	13 (17%)
12	CLA	B	1203	-	49,57,73	1.17	7 (14%)	55,93,113	1.89	13 (23%)
12	CLA	A	1112	-	49,57,73	1.17	7 (14%)	55,93,113	2.00	14 (25%)
12	CLA	A	1103	-	49,57,73	1.16	7 (14%)	55,93,113	2.02	13 (23%)
12	CLA	A	1108	-	49,57,73	1.17	7 (14%)	55,93,113	1.97	13 (23%)
12	CLA	B	1023	-	49,57,73	1.17	7 (14%)	55,93,113	1.99	12 (21%)
12	CLA	A	1107	1	50,58,73	1.48	8 (16%)	58,95,113	2.19	13 (22%)
12	CLA	A	1115	-	56,64,73	1.10	7 (12%)	65,102,113	1.90	15 (23%)
13	PQN	A	2001	-	34,34,34	0.43	0	42,45,45	1.09	3 (7%)
12	CLA	B	1236	-	49,57,73	1.19	7 (14%)	55,93,113	1.98	11 (20%)
19	ECH	M	4021	-	42,42,42	0.85	1 (2%)	55,58,58	2.62	14 (25%)
12	CLA	B	1211	-	49,57,73	1.18	6 (12%)	55,93,113	2.01	14 (25%)
12	CLA	B	1231	-	49,57,73	1.19	7 (14%)	55,93,113	2.01	13 (23%)
12	CLA	A	1104	-	49,57,73	1.18	7 (14%)	55,93,113	1.94	12 (21%)
12	CLA	A	1134	1	49,57,73	1.19	7 (14%)	55,93,113	2.00	13 (23%)
12	CLA	B	1232	-	49,57,73	1.21	7 (14%)	55,93,113	1.98	14 (25%)
12	CLA	A	1113	-	49,57,73	1.19	7 (14%)	55,93,113	1.94	12 (21%)
12	CLA	A	1011	-	55,63,73	1.12	6 (10%)	64,101,113	1.96	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	B	4010	-	41,41,41	1.91	4 (9%)	56,56,56	4.49	18 (32%)
12	CLA	A	1124	-	49,57,73	1.18	7 (14%)	55,93,113	2.00	13 (23%)
12	CLA	B	1240	-	49,57,73	1.21	8 (16%)	55,93,113	2.02	13 (23%)
12	CLA	A	1116	-	49,57,73	1.17	6 (12%)	55,93,113	2.04	14 (25%)
12	CLA	B	1214	-	60,68,73	1.09	7 (11%)	70,107,113	1.75	13 (18%)
15	BCR	J	4013	-	41,41,41	1.87	4 (9%)	56,56,56	4.35	15 (26%)
12	CLA	A	1133	-	49,57,73	1.20	7 (14%)	55,93,113	1.95	12 (21%)
12	CLA	B	1218	-	49,57,73	1.17	7 (14%)	55,93,113	2.01	14 (25%)
14	SF4	A	3001	-	0,12,12	-	-	-	-	-
12	CLA	A	1121	-	49,57,73	1.17	7 (14%)	55,93,113	2.05	14 (25%)
15	BCR	I	4018	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	20 (35%)
12	CLA	A	1013	-	65,73,73	1.03	6 (9%)	76,113,113	1.74	15 (19%)
12	CLA	A	1123	-	60,68,73	1.06	8 (13%)	70,107,113	1.85	15 (21%)
12	CLA	A	1137	-	49,57,73	1.19	7 (14%)	55,93,113	1.98	12 (21%)
12	CLA	B	1223	-	49,57,73	1.24	8 (16%)	55,93,113	2.01	13 (23%)
23	C7Z	F	4016	-	43,43,43	5.36	18 (41%)	58,60,60	5.24	32 (55%)
12	CLA	A	1111	-	49,57,73	1.19	7 (14%)	55,93,113	1.89	13 (23%)
12	CLA	A	1131	-	49,57,73	1.18	7 (14%)	55,93,113	1.94	12 (21%)
15	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	18 (32%)
12	CLA	B	1209	-	49,57,73	1.20	8 (16%)	55,93,113	2.01	13 (23%)
12	CLA	B	1215	-	49,57,73	1.18	8 (16%)	55,93,113	1.98	11 (20%)
12	CLA	B	1217	-	49,57,73	1.20	7 (14%)	55,93,113	2.01	13 (23%)
15	BCR	F	4014	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
12	CLA	B	1212	-	49,57,73	1.18	7 (14%)	55,93,113	2.00	12 (21%)
25	EQ3	I	4020	-	43,43,43	4.21	25 (58%)	56,60,60	2.37	20 (35%)
12	CLA	A	1135	-	49,57,73	1.19	7 (14%)	55,93,113	2.05	13 (23%)
12	CLA	B	1226	-	49,57,73	1.20	6 (12%)	55,93,113	2.01	14 (25%)
15	BCR	A	4012	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)
15	BCR	B	4005	-	41,41,41	1.85	4 (9%)	56,56,56	4.43	14 (25%)
12	CLA	B	1205	-	49,57,73	1.20	7 (14%)	55,93,113	2.03	14 (25%)
12	CLA	B	1022	-	60,68,73	1.10	7 (11%)	70,107,113	1.82	14 (20%)
12	CLA	B	1213	-	49,57,73	1.18	8 (16%)	55,93,113	2.07	15 (27%)
13	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	3 (7%)
23	C7Z	J	4015	-	43,43,43	5.34	18 (41%)	58,60,60	5.20	31 (53%)
12	CLA	A	1114	-	49,57,73	1.20	7 (14%)	55,93,113	1.97	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	A	1109	12	65,73,73	1.03	7 (10%)	76,113,113	1.76	15 (19%)
12	CLA	B	1234	-	60,68,73	1.07	6 (10%)	70,107,113	1.87	14 (20%)
12	CLA	L	1502	-	49,57,73	1.18	8 (16%)	55,93,113	2.05	12 (21%)
15	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	15 (26%)
15	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	15 (26%)
12	CLA	A	1129	-	49,57,73	1.18	7 (14%)	55,93,113	1.97	13 (23%)
12	CLA	A	1128	-	65,73,73	1.02	6 (9%)	76,113,113	1.79	17 (22%)
12	CLA	A	1122	-	49,57,73	1.18	8 (16%)	55,93,113	2.00	12 (21%)
12	CLA	B	1219	-	49,57,73	1.19	7 (14%)	55,93,113	1.96	12 (21%)
12	CLA	J	1303	10	49,57,73	1.16	7 (14%)	55,93,113	2.00	13 (23%)
12	CLA	B	1224	-	55,63,73	1.14	6 (10%)	64,101,113	1.90	14 (21%)
16	LHG	A	5003	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
12	CLA	A	1130	-	49,57,73	1.17	7 (14%)	55,93,113	1.98	13 (23%)
12	CLA	B	1216	-	49,57,73	1.20	7 (14%)	55,93,113	1.96	12 (21%)
12	CLA	B	1206	-	49,57,73	1.17	7 (14%)	55,93,113	2.00	13 (23%)
16	LHG	B	5006	2	20,20,48	0.59	0	23,26,54	1.48	2 (8%)
15	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	16 (28%)
12	CLA	B	1225	-	49,57,73	1.19	6 (12%)	55,93,113	1.90	11 (20%)
17	45D	B	4011	-	43,43,43	3.57	16 (37%)	54,60,60	2.15	17 (31%)
15	BCR	A	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.29	16 (28%)
12	CLA	B	1237	-	49,57,73	1.17	7 (14%)	55,93,113	1.99	13 (23%)
12	CLA	B	1221	-	49,57,73	1.18	7 (14%)	55,93,113	2.00	14 (25%)
12	CLA	A	1120	-	49,57,73	1.17	8 (16%)	55,93,113	2.00	14 (25%)
16	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.04	4 (7%)
12	CLA	F	1301	-	49,57,73	1.17	6 (12%)	55,93,113	1.97	13 (23%)
12	CLA	B	1229	-	55,63,73	1.12	7 (12%)	64,101,113	1.96	15 (23%)
12	CLA	A	1138	-	65,73,73	1.02	6 (9%)	76,113,113	1.80	14 (18%)
12	CLA	B	1239	-	49,57,73	1.19	7 (14%)	55,93,113	1.94	12 (21%)
12	CLA	B	1021	-	65,73,73	1.02	6 (9%)	76,113,113	1.74	12 (15%)
12	CLA	A	1139	-	55,63,73	1.13	6 (10%)	64,101,113	1.89	12 (18%)
15	BCR	B	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	17 (30%)
12	CLA	A	1127	-	49,57,73	1.18	7 (14%)	55,93,113	1.99	14 (25%)
12	CLA	J	1302	8	49,57,73	1.18	7 (14%)	55,93,113	1.99	12 (21%)
21	SQD	F	5001	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
12	CLA	B	1220	-	49,57,73	1.20	7 (14%)	55,93,113	2.01	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	B	1210	-	49,57,73	1.17	7 (14%)	55,93,113	2.02	14 (25%)
12	CLA	B	1208	-	49,57,73	1.21	7 (14%)	55,93,113	1.92	12 (21%)
12	CLA	A	1110	-	49,57,73	1.19	7 (14%)	55,93,113	1.95	12 (21%)
12	CLA	A	1125	-	49,57,73	1.18	6 (12%)	55,93,113	2.06	14 (25%)
12	CLA	A	1126	-	60,68,73	1.08	8 (13%)	70,107,113	1.79	14 (20%)
12	CLA	B	1222	-	50,58,73	1.17	6 (12%)	58,95,113	2.02	13 (22%)
16	LHG	B	5004	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
12	CLA	B	1230	-	49,57,73	1.19	7 (14%)	55,93,113	2.04	13 (23%)
12	CLA	B	1207	-	49,57,73	1.22	7 (14%)	55,93,113	2.01	13 (23%)
12	CLA	A	1119	-	46,54,73	1.25	7 (15%)	53,90,113	1.81	11 (20%)
12	CLA	A	1118	-	50,58,73	1.16	6 (12%)	58,95,113	1.94	13 (22%)
20	LMG	B	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
14	SF4	C	3002	-	0,12,12	-	-	-	-	-
12	CLA	B	1235	-	65,73,73	1.04	7 (10%)	76,113,113	1.79	13 (17%)
12	CLA	A	1141	-	45,53,73	1.22	7 (15%)	52,89,113	1.87	11 (21%)
12	CLA	A	1136	-	49,57,73	1.20	7 (14%)	55,93,113	1.98	12 (21%)
12	CLA	B	1227	-	49,57,73	1.19	7 (14%)	55,93,113	2.06	13 (23%)
12	CLA	A	1105	-	65,73,73	1.05	7 (10%)	76,113,113	1.81	14 (18%)

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
12	CLA	A	1102	12	1/1/15/20	14/37/115/115	-
12	CLA	A	1106	-	1/1/15/20	19/37/115/115	-
12	CLA	B	1201	-	1/1/11/20	9/18/96/115	-
12	CLA	B	1202	-	1/1/15/20	16/37/115/115	-
24	LMT	F	6001	-	-	8/21/61/61	0/2/2/2
15	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
12	CLA	B	1204	-	1/1/11/20	7/18/96/115	-
19	ECH	B	4006	-	-	8/29/66/66	0/2/2/2
14	SF4	C	3003	-	-	-	0/6/5/5
12	CLA	B	1238	-	1/1/11/20	9/18/96/115	-
12	CLA	K	1402	-	1/1/11/20	12/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	F	1302	10	1/1/11/20	11/18/96/115	-
15	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
12	CLA	A	1117	-	1/1/11/20	8/18/96/115	-
12	CLA	A	1132	10	1/1/13/20	14/25/103/115	-
20	LMG	B	5005	-	-	17/50/70/70	0/1/1/1
21	SQD	B	5008	-	-	10/49/69/69	0/1/1/1
12	CLA	A	1012	-	1/1/11/20	11/18/96/115	-
12	CLA	A	1101	-	1/1/11/20	8/18/96/115	-
12	CLA	B	1228	-	1/1/11/20	10/18/96/115	-
12	CLA	K	1401	-	1/1/11/20	8/13/91/115	-
12	CLA	A	1140	-	1/1/15/20	18/37/115/115	-
12	CLA	B	1203	-	1/1/11/20	8/18/96/115	-
12	CLA	A	1112	-	1/1/11/20	12/18/96/115	-
12	CLA	A	1103	-	1/1/11/20	13/18/96/115	-
12	CLA	A	1108	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1023	-	1/1/11/20	9/18/96/115	-
12	CLA	A	1107	1	1/1/12/20	7/19/97/115	-
12	CLA	A	1115	-	1/1/13/20	7/27/105/115	-
13	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
12	CLA	B	1236	-	1/1/11/20	7/18/96/115	-
19	ECH	M	4021	-	-	12/29/66/66	0/2/2/2
12	CLA	B	1211	-	1/1/11/20	9/18/96/115	-
12	CLA	B	1231	-	1/1/11/20	6/18/96/115	-
12	CLA	A	1104	-	1/1/11/20	9/18/96/115	-
12	CLA	A	1134	1	1/1/11/20	12/18/96/115	-
12	CLA	B	1232	-	1/1/11/20	8/18/96/115	-
12	CLA	A	1113	-	1/1/11/20	14/18/96/115	-
12	CLA	A	1011	-	1/1/13/20	11/25/103/115	-
15	BCR	B	4010	-	-	11/29/63/63	0/2/2/2
12	CLA	A	1124	-	1/1/11/20	8/18/96/115	-
12	CLA	B	1240	-	1/1/11/20	12/18/96/115	-
12	CLA	A	1116	-	1/1/11/20	10/18/96/115	-
12	CLA	B	1214	-	1/1/14/20	22/31/109/115	-
15	BCR	J	4013	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1133	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1218	-	1/1/11/20	11/18/96/115	-
14	SF4	A	3001	-	-	-	0/6/5/5
12	CLA	A	1121	-	1/1/11/20	11/18/96/115	-
15	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
12	CLA	A	1013	-	1/1/15/20	15/37/115/115	-
12	CLA	A	1123	-	1/1/14/20	14/31/109/115	-
12	CLA	A	1137	-	1/1/11/20	8/18/96/115	-
12	CLA	B	1223	-	1/1/11/20	11/18/96/115	-
23	C7Z	F	4016	-	-	17/29/67/67	0/2/2/2
12	CLA	A	1111	-	1/1/11/20	13/18/96/115	-
12	CLA	A	1131	-	1/1/11/20	7/18/96/115	-
15	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
12	CLA	B	1209	-	1/1/11/20	10/18/96/115	-
12	CLA	B	1215	-	1/1/11/20	8/18/96/115	-
12	CLA	B	1217	-	1/1/11/20	7/18/96/115	-
15	BCR	F	4014	-	-	12/29/63/63	0/2/2/2
12	CLA	B	1212	-	1/1/11/20	9/18/96/115	-
25	EQ3	I	4020	-	-	15/29/68/68	0/2/2/2
12	CLA	A	1135	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1226	-	1/1/11/20	9/18/96/115	-
15	BCR	A	4012	-	-	14/29/63/63	0/2/2/2
15	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
12	CLA	B	1205	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1022	-	1/1/14/20	11/31/109/115	-
12	CLA	B	1213	-	1/1/11/20	8/18/96/115	-
13	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
23	C7Z	J	4015	-	-	14/29/67/67	0/2/2/2
12	CLA	A	1114	-	1/1/11/20	7/18/96/115	-
12	CLA	A	1109	12	1/1/15/20	18/37/115/115	-
12	CLA	B	1234	-	1/1/14/20	16/31/109/115	-
12	CLA	L	1502	-	1/1/11/20	11/18/96/115	-
15	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
15	BCR	B	4004	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1129	-	1/1/11/20	7/18/96/115	-
12	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
12	CLA	A	1122	-	1/1/11/20	8/18/96/115	-
12	CLA	B	1219	-	1/1/11/20	9/18/96/115	-
12	CLA	J	1303	10	1/1/11/20	11/18/96/115	-
12	CLA	B	1224	-	1/1/13/20	13/25/103/115	-
16	LHG	A	5003	-	-	30/53/53/53	-
12	CLA	A	1130	-	1/1/11/20	9/18/96/115	-
12	CLA	B	1216	-	1/1/11/20	12/18/96/115	-
12	CLA	B	1206	-	1/1/11/20	9/18/96/115	-
16	LHG	B	5006	2	-	11/23/23/53	-
15	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
12	CLA	B	1225	-	1/1/11/20	9/18/96/115	-
17	45D	B	4011	-	-	11/29/69/69	0/2/2/2
15	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
12	CLA	B	1237	-	1/1/11/20	9/18/96/115	-
12	CLA	B	1221	-	1/1/11/20	8/18/96/115	-
12	CLA	A	1120	-	1/1/11/20	11/18/96/115	-
16	LHG	A	5001	-	-	35/53/53/53	-
12	CLA	F	1301	-	1/1/11/20	6/18/96/115	-
12	CLA	B	1229	-	1/1/13/20	14/25/103/115	-
12	CLA	A	1138	-	1/1/15/20	13/37/115/115	-
12	CLA	B	1239	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1021	-	1/1/15/20	27/37/115/115	-
12	CLA	A	1139	-	1/1/13/20	9/25/103/115	-
15	BCR	B	4018	-	-	9/29/63/63	0/2/2/2
12	CLA	A	1127	-	1/1/11/20	9/18/96/115	-
12	CLA	J	1302	8	1/1/11/20	9/18/96/115	-
21	SQD	F	5001	-	-	17/49/69/69	0/1/1/1
12	CLA	B	1220	-	1/1/11/20	10/18/96/115	-
12	CLA	B	1210	-	1/1/11/20	13/18/96/115	-
12	CLA	B	1208	-	1/1/11/20	8/18/96/115	-
12	CLA	A	1110	-	1/1/11/20	9/18/96/115	-
12	CLA	A	1125	-	1/1/11/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1126	-	1/1/14/20	11/31/109/115	-
12	CLA	B	1222	-	1/1/12/20	7/19/97/115	-
16	LHG	B	5004	-	-	23/53/53/53	-
12	CLA	B	1230	-	1/1/11/20	10/18/96/115	-
12	CLA	B	1207	-	1/1/11/20	13/18/96/115	-
12	CLA	A	1119	-	1/1/11/20	7/15/93/115	-
12	CLA	A	1118	-	1/1/12/20	9/19/97/115	-
20	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
14	SF4	C	3002	-	-	-	0/6/5/5
12	CLA	B	1235	-	1/1/15/20	20/37/115/115	-
12	CLA	A	1141	-	1/1/11/20	11/13/91/115	-
12	CLA	A	1136	-	1/1/11/20	11/18/96/115	-
12	CLA	B	1227	-	1/1/11/20	11/18/96/115	-
12	CLA	A	1105	-	1/1/15/20	11/37/115/115	-

All (797) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	4016	C7Z	C30-C29	14.43	1.54	1.35
23	F	4016	C7Z	C14-C13	14.40	1.54	1.35
23	F	4016	C7Z	C34-C33	14.37	1.54	1.35
23	J	4015	C7Z	C30-C29	14.32	1.54	1.35
23	J	4015	C7Z	C34-C33	14.29	1.54	1.35
23	J	4015	C7Z	C14-C13	14.20	1.54	1.35
23	F	4016	C7Z	C10-C9	14.18	1.54	1.35
23	J	4015	C7Z	C10-C9	13.82	1.54	1.35
25	I	4020	EQ3	C25-C26	13.59	1.54	1.35
17	B	4011	45D	C07-C15	13.01	1.53	1.35
17	B	4011	45D	C08-C16	12.74	1.53	1.35
23	J	4015	C7Z	C25-C26	12.08	1.55	1.34
23	F	4016	C7Z	C25-C26	11.85	1.55	1.34
23	F	4016	C7Z	C5-C6	11.72	1.54	1.34
23	J	4015	C7Z	C5-C6	11.52	1.54	1.34
25	I	4020	EQ3	C4-C3	11.34	1.72	1.52
25	I	4020	EQ3	C5-C6	10.72	1.53	1.34
15	B	4010	BCR	C10-C9	7.83	1.46	1.35
15	A	4001	BCR	C10-C9	7.63	1.45	1.35
15	J	4013	BCR	C10-C9	7.55	1.45	1.35
15	B	4005	BCR	C10-C9	7.49	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	4001	BCR	C10-C9	7.41	1.45	1.35
15	B	4017	BCR	C10-C9	7.39	1.45	1.35
15	F	4014	BCR	C10-C9	7.35	1.45	1.35
15	B	4004	BCR	C10-C9	7.35	1.45	1.35
15	B	4018	BCR	C10-C9	7.30	1.45	1.35
15	I	4018	BCR	C10-C9	7.26	1.45	1.35
15	A	4003	BCR	C10-C9	7.22	1.45	1.35
15	A	4012	BCR	C10-C9	7.20	1.45	1.35
15	A	4008	BCR	C10-C9	7.07	1.45	1.35
15	A	4007	BCR	C10-C9	7.00	1.45	1.35
25	I	4020	EQ3	C2-C3	-6.20	1.43	1.52
12	A	1107	CLA	MG-NA	6.17	2.20	2.06
15	K	4001	BCR	C24-C23	5.85	1.50	1.33
15	B	4018	BCR	C24-C23	5.83	1.50	1.33
15	F	4014	BCR	C24-C23	5.82	1.50	1.33
15	A	4003	BCR	C24-C23	5.79	1.50	1.33
15	J	4013	BCR	C24-C23	5.76	1.50	1.33
15	A	4007	BCR	C24-C23	5.75	1.50	1.33
15	A	4012	BCR	C24-C23	5.75	1.50	1.33
15	A	4008	BCR	C24-C23	5.74	1.50	1.33
15	B	4017	BCR	C24-C23	5.73	1.50	1.33
15	B	4010	BCR	C24-C23	5.72	1.50	1.33
15	A	4001	BCR	C24-C23	5.72	1.50	1.33
15	B	4005	BCR	C24-C23	5.69	1.50	1.33
15	B	4004	BCR	C24-C23	5.69	1.50	1.33
15	I	4018	BCR	C24-C23	5.62	1.50	1.33
15	B	4010	BCR	C11-C12	-5.18	1.21	1.34
15	A	4007	BCR	C11-C12	-5.18	1.21	1.34
15	A	4008	BCR	C11-C12	-5.16	1.21	1.34
17	B	4011	45D	C23-C25	5.13	1.57	1.45
15	F	4014	BCR	C11-C12	-5.13	1.21	1.34
15	B	4004	BCR	C11-C12	-5.11	1.21	1.34
15	A	4012	BCR	C11-C12	-5.10	1.21	1.34
15	A	4003	BCR	C11-C12	-5.08	1.21	1.34
15	J	4013	BCR	C11-C12	-5.08	1.21	1.34
15	I	4018	BCR	C11-C12	-5.02	1.21	1.34
15	B	4017	BCR	C11-C12	-5.01	1.21	1.34
15	B	4018	BCR	C11-C12	-5.01	1.21	1.34
15	B	4005	BCR	C11-C12	-4.97	1.21	1.34
15	K	4001	BCR	C11-C12	-4.96	1.21	1.34
25	I	4020	EQ3	C15-C14	4.93	1.58	1.43
25	I	4020	EQ3	C23-C22	4.89	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	4001	BCR	C11-C12	-4.88	1.22	1.34
25	I	4020	EQ3	C1-C6	-4.77	1.47	1.53
17	B	4011	45D	C24-C26	4.76	1.56	1.45
17	B	4011	45D	C33-C35	4.72	1.56	1.45
25	I	4020	EQ3	C11-C10	4.68	1.57	1.43
25	I	4020	EQ3	C4-C5	-4.48	1.44	1.51
17	B	4011	45D	C34-C36	4.36	1.55	1.45
15	I	4018	BCR	C16-C17	-4.35	1.30	1.43
25	I	4020	EQ3	C12-C13	4.26	1.55	1.45
15	A	4007	BCR	C16-C17	-4.23	1.30	1.43
15	A	4008	BCR	C16-C17	-4.22	1.30	1.43
15	A	4012	BCR	C16-C17	-4.22	1.30	1.43
15	A	4001	BCR	C16-C17	-4.21	1.30	1.43
15	B	4017	BCR	C16-C17	-4.20	1.30	1.43
15	B	4004	BCR	C16-C17	-4.18	1.30	1.43
15	A	4003	BCR	C16-C17	-4.18	1.30	1.43
25	I	4020	EQ3	C19-C18	4.17	1.54	1.45
15	B	4010	BCR	C16-C17	-4.16	1.30	1.43
25	I	4020	EQ3	C7-C6	4.16	1.59	1.45
15	J	4013	BCR	C16-C17	-4.15	1.30	1.43
15	B	4005	BCR	C16-C17	-4.14	1.30	1.43
15	F	4014	BCR	C16-C17	-4.12	1.30	1.43
15	B	4018	BCR	C16-C17	-4.10	1.30	1.43
15	K	4001	BCR	C16-C17	-4.09	1.30	1.43
17	B	4011	45D	C42-C38	3.84	1.55	1.43
17	B	4011	45D	C41-C37	3.78	1.55	1.43
23	F	4016	C7Z	C35-C34	3.74	1.55	1.43
23	J	4015	C7Z	C35-C34	3.73	1.55	1.43
23	F	4016	C7Z	C15-C14	3.69	1.54	1.43
23	F	4016	C7Z	C12-C13	3.67	1.53	1.45
23	J	4015	C7Z	C15-C14	3.65	1.54	1.43
23	J	4015	C7Z	C12-C13	3.65	1.53	1.45
17	B	4011	45D	C31-C29	3.63	1.54	1.43
17	B	4011	45D	C32-C30	3.61	1.54	1.43
23	F	4016	C7Z	C11-C10	3.55	1.54	1.43
23	J	4015	C7Z	C31-C30	3.55	1.54	1.43
25	I	4020	EQ3	C2-C1	3.54	1.65	1.54
23	J	4015	C7Z	C11-C10	3.47	1.54	1.43
12	A	1107	CLA	MG-ND	-3.47	1.98	2.05
23	F	4016	C7Z	C31-C30	3.47	1.54	1.43
23	J	4015	C7Z	C27-C26	3.42	1.57	1.45
12	A	1013	CLA	CBB-CAB	3.39	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1201	CLA	CBB-CAB	3.39	1.51	1.29
12	B	1236	CLA	CBB-CAB	3.39	1.51	1.29
12	A	1117	CLA	CBB-CAB	3.38	1.51	1.29
12	A	1141	CLA	CBB-CAB	3.38	1.51	1.29
12	A	1131	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1215	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1109	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1011	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1202	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1112	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1103	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1123	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1012	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1116	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1206	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1102	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1128	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1021	CLA	CBB-CAB	3.37	1.51	1.29
12	K	1401	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1211	CLA	CBB-CAB	3.37	1.51	1.29
12	B	1240	CLA	CBB-CAB	3.37	1.51	1.29
12	A	1132	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1209	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1222	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1105	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1120	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1135	CLA	CBB-CAB	3.36	1.51	1.29
12	L	1502	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1126	CLA	CBB-CAB	3.36	1.51	1.29
12	J	1302	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1223	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1121	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1230	CLA	CBB-CAB	3.36	1.51	1.29
12	K	1402	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1212	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1218	CLA	CBB-CAB	3.36	1.51	1.29
12	B	1213	CLA	CBB-CAB	3.36	1.51	1.29
12	J	1303	CLA	CBB-CAB	3.36	1.51	1.29
12	A	1133	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1023	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1205	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1234	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	1301	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1104	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1221	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1239	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1134	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1224	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1110	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1231	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1226	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1204	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1214	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1227	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1124	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1217	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1228	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1122	CLA	CBB-CAB	3.35	1.51	1.29
12	F	1302	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1136	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1232	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1137	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1139	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1106	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1210	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1127	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1207	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1119	CLA	CBB-CAB	3.35	1.51	1.29
12	B	1208	CLA	CBB-CAB	3.35	1.51	1.29
12	A	1111	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1114	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1118	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1113	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1130	CLA	CBB-CAB	3.34	1.51	1.29
12	B	1235	CLA	CBB-CAB	3.34	1.51	1.29
12	B	1216	CLA	CBB-CAB	3.34	1.51	1.29
12	B	1220	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1108	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1138	CLA	CBB-CAB	3.33	1.51	1.29
12	A	1125	CLA	CBB-CAB	3.33	1.51	1.29
12	B	1219	CLA	CBB-CAB	3.33	1.51	1.29
12	A	1129	CLA	CBB-CAB	3.33	1.51	1.29
12	A	1101	CLA	CBB-CAB	3.33	1.51	1.29
12	A	1140	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1022	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1237	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1107	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1225	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1203	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1238	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1229	CLA	CBB-CAB	3.28	1.51	1.29
12	A	1115	CLA	CBB-CAB	3.27	1.51	1.29
23	J	4015	C7Z	C28-C29	3.25	1.52	1.45
25	I	4020	EQ3	C16-C17	3.24	1.53	1.43
20	B	5005	LMG	C19-C18	-3.24	1.33	1.51
20	B	5002	LMG	C19-C18	-3.23	1.33	1.51
12	B	1226	CLA	MG-ND	-3.23	1.99	2.05
20	B	5005	LMG	C22-C21	-3.23	1.33	1.51
20	B	5005	LMG	C25-C24	-3.23	1.33	1.51
20	B	5002	LMG	C22-C21	-3.22	1.33	1.51
20	B	5005	LMG	C43-C42	-3.21	1.33	1.51
20	B	5005	LMG	C37-C36	-3.20	1.33	1.51
20	B	5002	LMG	C40-C39	-3.20	1.33	1.51
20	B	5002	LMG	C25-C24	-3.20	1.33	1.51
20	B	5002	LMG	C43-C42	-3.20	1.33	1.51
20	B	5002	LMG	C37-C36	-3.19	1.33	1.51
20	B	5005	LMG	C40-C39	-3.19	1.33	1.51
17	B	4011	45D	C20-C08	3.15	1.56	1.45
17	B	4011	45D	C19-C07	3.13	1.56	1.45
25	I	4020	EQ3	C20-C21	3.10	1.53	1.43
12	B	1023	CLA	MG-ND	-3.08	1.99	2.05
12	B	1220	CLA	MG-ND	-3.08	1.99	2.05
12	B	1205	CLA	MG-ND	-3.08	1.99	2.05
23	F	4016	C7Z	C28-C29	3.07	1.52	1.45
25	I	4020	EQ3	O3-C3	-3.06	1.34	1.43
12	A	1123	CLA	MG-ND	-3.06	1.99	2.05
12	B	1206	CLA	MG-ND	-3.05	1.99	2.05
23	J	4015	C7Z	C7-C6	3.04	1.55	1.45
12	A	1128	CLA	MG-ND	-3.04	1.99	2.05
12	B	1224	CLA	MG-ND	-3.04	1.99	2.05
25	I	4020	EQ3	C35-C13	3.04	1.57	1.50
25	I	4020	EQ3	C24-C25	3.03	1.55	1.45
12	A	1012	CLA	MG-ND	-3.03	1.99	2.05
23	F	4016	C7Z	C7-C6	3.03	1.55	1.45
12	B	1217	CLA	MG-ND	-3.02	1.99	2.05
12	B	1221	CLA	MG-ND	-3.02	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1213	CLA	MG-ND	-3.02	1.99	2.05
12	A	1125	CLA	MG-ND	-3.01	1.99	2.05
12	B	1022	CLA	MG-ND	-3.01	1.99	2.05
12	B	1239	CLA	MG-ND	-3.01	1.99	2.05
12	F	1301	CLA	MG-ND	-3.01	1.99	2.05
25	I	4020	EQ3	C38-C26	3.01	1.57	1.50
12	A	1133	CLA	MG-ND	-3.00	1.99	2.05
23	F	4016	C7Z	C27-C26	3.00	1.55	1.45
12	A	1115	CLA	MG-ND	-3.00	1.99	2.05
12	B	1214	CLA	MG-ND	-2.99	1.99	2.05
12	B	1022	CLA	C3B-C2B	-2.99	1.36	1.40
12	B	1240	CLA	MG-ND	-2.98	1.99	2.05
12	A	1116	CLA	MG-ND	-2.98	1.99	2.05
12	B	1229	CLA	C3B-C2B	-2.98	1.36	1.40
12	A	1129	CLA	MG-ND	-2.98	1.99	2.05
12	B	1207	CLA	MG-ND	-2.98	1.99	2.05
12	A	1127	CLA	MG-ND	-2.98	1.99	2.05
12	L	1502	CLA	MG-ND	-2.98	1.99	2.05
12	A	1112	CLA	MG-ND	-2.98	1.99	2.05
23	J	4015	C7Z	C32-C33	2.97	1.52	1.45
12	B	1204	CLA	MG-ND	-2.97	1.99	2.05
12	A	1101	CLA	MG-ND	-2.97	1.99	2.05
12	A	1111	CLA	MG-ND	-2.96	1.99	2.05
12	B	1211	CLA	MG-ND	-2.96	1.99	2.05
12	B	1216	CLA	MG-ND	-2.96	1.99	2.05
12	B	1231	CLA	MG-ND	-2.96	1.99	2.05
12	A	1119	CLA	MG-ND	-2.96	1.99	2.05
23	F	4016	C7Z	C32-C33	2.96	1.52	1.45
12	A	1011	CLA	MG-ND	-2.95	1.99	2.05
12	B	1223	CLA	MG-ND	-2.95	1.99	2.05
12	A	1132	CLA	MG-ND	-2.94	2.00	2.05
12	A	1134	CLA	MG-ND	-2.94	2.00	2.05
12	A	1013	CLA	MG-ND	-2.94	2.00	2.05
12	B	1237	CLA	MG-ND	-2.94	2.00	2.05
12	A	1122	CLA	MG-ND	-2.94	2.00	2.05
12	B	1235	CLA	MG-ND	-2.93	2.00	2.05
12	J	1303	CLA	MG-ND	-2.93	2.00	2.05
12	A	1106	CLA	MG-ND	-2.93	2.00	2.05
12	A	1109	CLA	MG-ND	-2.93	2.00	2.05
12	B	1219	CLA	C3B-C2B	-2.92	1.36	1.40
12	B	1203	CLA	MG-ND	-2.92	2.00	2.05
12	A	1135	CLA	MG-ND	-2.92	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1113	CLA	MG-ND	-2.92	2.00	2.05
12	A	1141	CLA	MG-ND	-2.91	2.00	2.05
12	A	1118	CLA	MG-ND	-2.91	2.00	2.05
12	A	1138	CLA	MG-ND	-2.91	2.00	2.05
12	B	1234	CLA	MG-ND	-2.91	2.00	2.05
12	A	1117	CLA	MG-ND	-2.91	2.00	2.05
12	B	1202	CLA	MG-ND	-2.91	2.00	2.05
12	B	1210	CLA	MG-ND	-2.91	2.00	2.05
12	B	1201	CLA	MG-ND	-2.91	2.00	2.05
12	B	1218	CLA	MG-ND	-2.91	2.00	2.05
12	B	1225	CLA	MG-ND	-2.91	2.00	2.05
12	A	1120	CLA	MG-ND	-2.90	2.00	2.05
12	B	1232	CLA	C3B-C2B	-2.90	1.36	1.40
12	A	1108	CLA	MG-ND	-2.90	2.00	2.05
12	A	1136	CLA	MG-ND	-2.90	2.00	2.05
12	B	1021	CLA	MG-ND	-2.90	2.00	2.05
12	B	1216	CLA	C3B-C2B	-2.90	1.36	1.40
12	B	1209	CLA	MG-ND	-2.89	2.00	2.05
12	B	1232	CLA	MG-ND	-2.89	2.00	2.05
12	A	1110	CLA	MG-ND	-2.89	2.00	2.05
12	A	1114	CLA	MG-ND	-2.89	2.00	2.05
12	B	1238	CLA	C3B-C2B	-2.89	1.36	1.40
12	J	1302	CLA	MG-ND	-2.89	2.00	2.05
12	A	1131	CLA	MG-ND	-2.89	2.00	2.05
12	B	1215	CLA	MG-ND	-2.89	2.00	2.05
12	A	1103	CLA	MG-ND	-2.88	2.00	2.05
12	A	1126	CLA	MG-ND	-2.88	2.00	2.05
12	K	1402	CLA	MG-ND	-2.88	2.00	2.05
25	I	4020	EQ3	C17-C18	2.87	1.39	1.35
12	B	1208	CLA	C3B-C2B	-2.87	1.36	1.40
12	B	1222	CLA	MG-ND	-2.87	2.00	2.05
12	A	1140	CLA	MG-ND	-2.87	2.00	2.05
12	B	1238	CLA	MG-ND	-2.87	2.00	2.05
12	K	1401	CLA	MG-ND	-2.86	2.00	2.05
12	B	1225	CLA	C3B-C2B	-2.86	1.36	1.40
12	A	1105	CLA	MG-ND	-2.86	2.00	2.05
12	A	1102	CLA	MG-ND	-2.86	2.00	2.05
12	A	1130	CLA	MG-ND	-2.86	2.00	2.05
12	F	1302	CLA	MG-ND	-2.86	2.00	2.05
12	B	1228	CLA	MG-ND	-2.85	2.00	2.05
12	B	1236	CLA	MG-ND	-2.85	2.00	2.05
12	B	1219	CLA	MG-ND	-2.85	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	4015	C7Z	C8-C9	2.85	1.52	1.45
12	A	1124	CLA	MG-ND	-2.85	2.00	2.05
12	B	1224	CLA	C3B-C2B	-2.85	1.36	1.40
12	A	1137	CLA	C3B-C2B	-2.84	1.36	1.40
12	B	1227	CLA	MG-ND	-2.84	2.00	2.05
12	A	1104	CLA	MG-ND	-2.84	2.00	2.05
12	A	1137	CLA	MG-ND	-2.83	2.00	2.05
12	B	1209	CLA	C3B-C2B	-2.83	1.36	1.40
12	A	1121	CLA	MG-ND	-2.83	2.00	2.05
12	B	1208	CLA	MG-ND	-2.83	2.00	2.05
12	B	1212	CLA	MG-ND	-2.83	2.00	2.05
12	B	1207	CLA	C3B-C2B	-2.83	1.36	1.40
12	A	1114	CLA	C3B-C2B	-2.82	1.36	1.40
12	B	1227	CLA	C3B-C2B	-2.82	1.36	1.40
12	A	1012	CLA	C3B-C2B	-2.82	1.36	1.40
12	A	1139	CLA	MG-ND	-2.82	2.00	2.05
12	A	1140	CLA	C3B-C2B	-2.82	1.36	1.40
23	F	4016	C7Z	C8-C9	2.81	1.52	1.45
12	B	1230	CLA	MG-ND	-2.81	2.00	2.05
12	B	1239	CLA	C3B-C2B	-2.79	1.36	1.40
12	A	1139	CLA	C3B-C2B	-2.79	1.36	1.40
12	A	1110	CLA	C3B-C2B	-2.79	1.36	1.40
12	B	1220	CLA	C3B-C2B	-2.79	1.36	1.40
12	B	1217	CLA	C3B-C2B	-2.77	1.36	1.40
12	B	1230	CLA	C3B-C2B	-2.77	1.36	1.40
12	K	1401	CLA	C3B-C2B	-2.77	1.36	1.40
12	A	1133	CLA	C3B-C2B	-2.76	1.36	1.40
12	A	1105	CLA	C3B-C2B	-2.75	1.36	1.40
12	A	1131	CLA	C3B-C2B	-2.75	1.36	1.40
12	B	1236	CLA	C3B-C2B	-2.75	1.36	1.40
12	A	1132	CLA	C3B-C2B	-2.74	1.36	1.40
12	F	1302	CLA	C3B-C2B	-2.74	1.36	1.40
12	A	1113	CLA	C3B-C2B	-2.73	1.36	1.40
12	A	1136	CLA	C3B-C2B	-2.72	1.36	1.40
12	B	1204	CLA	C3B-C2B	-2.71	1.36	1.40
25	I	4020	EQ3	C27-C26	2.71	1.53	1.47
12	B	1240	CLA	C1C-NC	-2.70	1.33	1.37
25	I	4020	EQ3	C33-C5	2.70	1.55	1.50
12	A	1101	CLA	C3B-C2B	-2.69	1.36	1.40
12	B	1212	CLA	C3B-C2B	-2.69	1.36	1.40
12	J	1302	CLA	C3B-C2B	-2.69	1.36	1.40
12	A	1125	CLA	C1C-NC	-2.69	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1240	CLA	C3B-C2B	-2.69	1.36	1.40
25	I	4020	EQ3	C28-C27	2.68	1.54	1.50
12	B	1229	CLA	C1C-NC	-2.67	1.33	1.37
12	B	1225	CLA	C1C-NC	-2.67	1.33	1.37
12	B	1236	CLA	C1C-NC	-2.67	1.33	1.37
12	B	1214	CLA	C3B-C2B	-2.67	1.36	1.40
12	A	1134	CLA	C3B-C2B	-2.66	1.36	1.40
12	A	1131	CLA	C1C-NC	-2.66	1.33	1.37
12	B	1237	CLA	C1C-NC	-2.65	1.33	1.37
12	A	1011	CLA	C1C-NC	-2.65	1.33	1.37
12	L	1502	CLA	C3B-C2B	-2.64	1.36	1.40
12	B	1229	CLA	MG-ND	-2.64	2.00	2.05
12	A	1137	CLA	C1C-NC	-2.64	1.33	1.37
12	B	1222	CLA	C3B-C2B	-2.64	1.36	1.40
12	B	1203	CLA	C1C-NC	-2.64	1.33	1.37
12	B	1216	CLA	C1C-NC	-2.64	1.33	1.37
12	B	1205	CLA	C3B-C2B	-2.64	1.36	1.40
12	B	1023	CLA	C1C-NC	-2.63	1.33	1.37
12	A	1126	CLA	C3B-C2B	-2.63	1.36	1.40
12	B	1231	CLA	C1C-NC	-2.63	1.33	1.37
12	K	1401	CLA	C1C-NC	-2.63	1.33	1.37
12	A	1105	CLA	C1C-NC	-2.62	1.33	1.37
12	B	1207	CLA	C1C-NC	-2.62	1.33	1.37
12	B	1223	CLA	OBD-CAD	-2.62	1.18	1.22
12	A	1138	CLA	C1C-NC	-2.62	1.33	1.37
24	F	6001	LMT	O3'-C3'	-2.62	1.36	1.43
12	B	1223	CLA	C3B-C2B	-2.61	1.36	1.40
12	A	1107	CLA	C1C-C2C	2.61	1.49	1.44
12	A	1122	CLA	C1C-NC	-2.61	1.33	1.37
12	A	1109	CLA	C1C-NC	-2.61	1.33	1.37
12	J	1302	CLA	C1C-NC	-2.61	1.33	1.37
12	B	1214	CLA	C1C-NC	-2.60	1.33	1.37
12	B	1238	CLA	C1C-NC	-2.60	1.33	1.37
12	B	1204	CLA	C1C-NC	-2.60	1.33	1.37
12	A	1129	CLA	C1C-NC	-2.60	1.33	1.37
12	A	1119	CLA	C3B-C2B	-2.60	1.36	1.40
17	B	4011	45D	C17-C15	2.60	1.53	1.47
12	A	1122	CLA	C3B-C2B	-2.60	1.36	1.40
12	B	1228	CLA	C1C-C2C	2.60	1.49	1.44
12	B	1021	CLA	C3B-C2B	-2.60	1.36	1.40
12	A	1128	CLA	C1C-NC	-2.59	1.33	1.37
12	A	1111	CLA	C3B-C2B	-2.59	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1238	CLA	C1C-C2C	2.59	1.49	1.44
12	A	1105	CLA	C1C-C2C	2.59	1.49	1.44
12	F	1301	CLA	C1C-NC	-2.59	1.33	1.37
23	J	4015	C7Z	C18-C5	2.59	1.55	1.50
12	B	1220	CLA	C1C-NC	-2.58	1.34	1.37
12	B	1231	CLA	C3B-C2B	-2.58	1.36	1.40
12	B	1205	CLA	C1C-NC	-2.58	1.34	1.37
12	A	1139	CLA	C1C-NC	-2.58	1.34	1.37
12	B	1021	CLA	C1C-NC	-2.58	1.34	1.37
12	A	1134	CLA	C1C-NC	-2.57	1.34	1.37
12	A	1132	CLA	C1C-NC	-2.57	1.34	1.37
12	A	1111	CLA	C1C-NC	-2.57	1.34	1.37
12	A	1133	CLA	C1C-NC	-2.57	1.34	1.37
12	A	1106	CLA	C1C-NC	-2.57	1.34	1.37
25	I	4020	EQ3	C8-C9	2.56	1.51	1.45
12	A	1101	CLA	C1C-C2C	2.56	1.49	1.44
12	A	1136	CLA	C1C-NC	-2.56	1.34	1.37
12	A	1126	CLA	C1C-NC	-2.56	1.34	1.37
12	A	1114	CLA	C1C-NC	-2.56	1.34	1.37
12	A	1115	CLA	C1C-NC	-2.55	1.34	1.37
12	A	1102	CLA	C1C-NC	-2.55	1.34	1.37
12	A	1124	CLA	C3B-C2B	-2.54	1.36	1.40
12	B	1207	CLA	C1C-C2C	2.54	1.49	1.44
12	B	1226	CLA	C1C-NC	-2.54	1.34	1.37
12	A	1104	CLA	C3B-C2B	-2.54	1.36	1.40
12	B	1234	CLA	C1C-NC	-2.54	1.34	1.37
12	A	1117	CLA	C1C-NC	-2.53	1.34	1.37
12	B	1230	CLA	C1C-NC	-2.53	1.34	1.37
12	B	1218	CLA	C1C-NC	-2.53	1.34	1.37
12	B	1232	CLA	C1C-NC	-2.53	1.34	1.37
12	B	1206	CLA	C1C-NC	-2.53	1.34	1.37
12	K	1402	CLA	C3B-C2B	-2.52	1.36	1.40
12	A	1110	CLA	C1C-NC	-2.52	1.34	1.37
12	L	1502	CLA	C1C-NC	-2.52	1.34	1.37
12	A	1130	CLA	C1C-C2C	2.52	1.49	1.44
12	B	1222	CLA	C1C-NC	-2.52	1.34	1.37
12	A	1113	CLA	C1C-C2C	2.52	1.49	1.44
12	B	1212	CLA	C1C-NC	-2.51	1.34	1.37
12	A	1112	CLA	C1C-NC	-2.51	1.34	1.37
12	J	1303	CLA	C1C-C2C	2.51	1.49	1.44
12	B	1208	CLA	C1C-C2C	2.50	1.49	1.44
12	A	1013	CLA	C1C-C2C	2.50	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1215	CLA	C1C-NC	-2.50	1.34	1.37
12	A	1141	CLA	C1C-C2C	2.50	1.49	1.44
12	B	1221	CLA	C1C-NC	-2.50	1.34	1.37
12	A	1107	CLA	CHC-C1C	2.50	1.41	1.35
12	A	1135	CLA	C1C-C2C	2.50	1.49	1.44
12	A	1104	CLA	C1C-NC	-2.50	1.34	1.37
12	A	1139	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1201	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1223	CLA	C1C-NC	-2.49	1.34	1.37
12	A	1116	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1239	CLA	C1C-NC	-2.49	1.34	1.37
12	K	1402	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1209	CLA	C1C-NC	-2.49	1.34	1.37
12	B	1217	CLA	C1C-NC	-2.49	1.34	1.37
12	A	1114	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1022	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1217	CLA	C1C-C2C	2.49	1.49	1.44
12	A	1140	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1211	CLA	C1C-NC	-2.48	1.34	1.37
12	B	1230	CLA	C1C-C2C	2.48	1.49	1.44
12	A	1121	CLA	C1C-NC	-2.48	1.34	1.37
12	A	1110	CLA	C1C-C2C	2.48	1.49	1.44
12	B	1208	CLA	C1C-NC	-2.48	1.34	1.37
12	A	1127	CLA	C1C-C2C	2.48	1.49	1.44
12	A	1128	CLA	C3B-C2B	-2.48	1.36	1.40
12	A	1124	CLA	C1C-NC	-2.48	1.34	1.37
12	B	1204	CLA	C1C-C2C	2.48	1.49	1.44
12	A	1124	CLA	C1C-C2C	2.48	1.49	1.44
12	B	1022	CLA	C1C-NC	-2.47	1.34	1.37
12	A	1109	CLA	C3B-C2B	-2.47	1.36	1.40
12	B	1210	CLA	C1C-NC	-2.47	1.34	1.37
12	A	1119	CLA	C1C-C2C	2.47	1.49	1.44
12	A	1134	CLA	C1C-C2C	2.47	1.49	1.44
12	A	1119	CLA	C1C-NC	-2.47	1.34	1.37
12	B	1203	CLA	C3B-C2B	-2.47	1.36	1.40
12	B	1202	CLA	C1C-NC	-2.47	1.34	1.37
12	B	1219	CLA	C1C-NC	-2.47	1.34	1.37
12	B	1213	CLA	C1C-NC	-2.46	1.34	1.37
12	B	1228	CLA	C1C-NC	-2.46	1.34	1.37
12	B	1202	CLA	C1C-C2C	2.46	1.49	1.44
12	B	1229	CLA	C1C-C2C	2.46	1.49	1.44
12	B	1223	CLA	C1C-C2C	2.46	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1118	CLA	C1C-NC	-2.46	1.34	1.37
12	B	1235	CLA	C1C-NC	-2.46	1.34	1.37
12	B	1227	CLA	C1C-C2C	2.46	1.49	1.44
12	B	1224	CLA	C1C-NC	-2.46	1.34	1.37
12	A	1108	CLA	C1C-NC	-2.46	1.34	1.37
12	B	1215	CLA	C1C-C2C	2.46	1.49	1.44
12	B	1219	CLA	C1C-C2C	2.46	1.49	1.44
12	A	1135	CLA	C3B-C2B	-2.45	1.37	1.40
12	A	1101	CLA	C1C-NC	-2.45	1.34	1.37
12	K	1402	CLA	C1C-NC	-2.45	1.34	1.37
12	A	1102	CLA	C1C-C2C	2.45	1.49	1.44
12	B	1214	CLA	C1B-NB	2.45	1.37	1.35
12	B	1227	CLA	C1C-NC	-2.45	1.34	1.37
12	B	1226	CLA	C3B-C2B	-2.45	1.37	1.40
12	A	1118	CLA	C3B-C2B	-2.45	1.37	1.40
12	A	1121	CLA	C3B-C2B	-2.45	1.37	1.40
12	B	1201	CLA	C1C-NC	-2.45	1.34	1.37
12	B	1209	CLA	C1C-C2C	2.45	1.49	1.44
12	B	1215	CLA	C3B-C2B	-2.45	1.37	1.40
12	B	1232	CLA	C1C-C2C	2.44	1.49	1.44
12	A	1130	CLA	C1C-NC	-2.44	1.34	1.37
12	B	1206	CLA	C3B-C2B	-2.44	1.37	1.40
12	B	1221	CLA	C3B-C2B	-2.44	1.37	1.40
12	A	1113	CLA	C1C-NC	-2.44	1.34	1.37
12	F	1302	CLA	C1C-NC	-2.44	1.34	1.37
12	A	1135	CLA	C1C-NC	-2.44	1.34	1.37
12	A	1125	CLA	C1C-C2C	2.44	1.49	1.44
12	F	1302	CLA	C1C-C2C	2.44	1.49	1.44
12	A	1108	CLA	C1C-C2C	2.43	1.49	1.44
12	B	1235	CLA	C1C-C2C	2.43	1.49	1.44
12	A	1127	CLA	C1C-NC	-2.43	1.34	1.37
12	A	1141	CLA	C1C-NC	-2.43	1.34	1.37
12	A	1104	CLA	C1C-C2C	2.43	1.49	1.44
25	I	4020	EQ3	C40-C30	2.43	1.58	1.53
12	A	1012	CLA	C1C-NC	-2.42	1.34	1.37
12	A	1140	CLA	C1B-NB	2.42	1.37	1.35
12	B	1218	CLA	C1C-C2C	2.42	1.49	1.44
12	A	1120	CLA	C1C-NC	-2.42	1.34	1.37
12	A	1106	CLA	C1C-C2C	2.42	1.49	1.44
12	B	1212	CLA	C1C-C2C	2.42	1.49	1.44
12	A	1136	CLA	C1C-C2C	2.42	1.49	1.44
12	B	1210	CLA	C1C-C2C	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1224	CLA	C1C-C2C	2.42	1.49	1.44
12	A	1116	CLA	C1C-NC	-2.42	1.34	1.37
12	F	1301	CLA	C3B-C2B	-2.42	1.37	1.40
12	A	1120	CLA	C1C-C2C	2.41	1.49	1.44
12	B	1234	CLA	C1C-C2C	2.41	1.49	1.44
12	B	1204	CLA	C1B-NB	2.41	1.37	1.35
12	A	1132	CLA	C1C-C2C	2.41	1.49	1.44
12	A	1013	CLA	C1C-NC	-2.41	1.34	1.37
12	J	1303	CLA	C1C-NC	-2.41	1.34	1.37
12	A	1107	CLA	MG-NC	2.41	2.12	2.06
12	A	1129	CLA	C3B-C2B	-2.41	1.37	1.40
12	A	1013	CLA	CHC-C1C	2.40	1.41	1.35
12	A	1103	CLA	C1C-C2C	2.40	1.49	1.44
12	A	1103	CLA	C3B-C2B	-2.40	1.37	1.40
12	B	1239	CLA	C1C-C2C	2.40	1.49	1.44
12	B	1202	CLA	C3B-C2B	-2.40	1.37	1.40
12	A	1133	CLA	C1B-NB	2.40	1.37	1.35
12	J	1302	CLA	C1C-C2C	2.40	1.49	1.44
12	A	1012	CLA	C1C-C2C	2.40	1.49	1.44
12	B	1213	CLA	C1C-C2C	2.40	1.49	1.44
12	B	1231	CLA	C1C-C2C	2.40	1.49	1.44
12	A	1123	CLA	C1C-NC	-2.39	1.34	1.37
12	A	1103	CLA	C1C-NC	-2.39	1.34	1.37
12	B	1240	CLA	C1C-C2C	2.39	1.49	1.44
12	A	1137	CLA	C1C-C2C	2.39	1.49	1.44
12	B	1225	CLA	C1C-C2C	2.39	1.49	1.44
12	A	1123	CLA	C1C-C2C	2.39	1.49	1.44
12	A	1126	CLA	C1C-C2C	2.38	1.49	1.44
12	B	1023	CLA	C3B-C2B	-2.38	1.37	1.40
17	B	4011	45D	O02-C18	-2.38	1.18	1.23
12	B	1235	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1141	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1112	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1115	CLA	C1C-C2C	2.37	1.49	1.44
12	B	1221	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1105	CLA	C1B-NB	2.37	1.37	1.35
12	B	1214	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1106	CLA	C3B-C2B	-2.37	1.37	1.40
12	A	1138	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1107	CLA	C1C-NC	-2.37	1.34	1.37
12	A	1013	CLA	C3B-C2B	-2.37	1.37	1.40
12	B	1229	CLA	CHC-C1C	2.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1129	CLA	C1C-C2C	2.36	1.49	1.44
12	A	1121	CLA	C1C-C2C	2.35	1.49	1.44
12	A	1117	CLA	C1C-C2C	2.35	1.49	1.44
12	A	1118	CLA	C1C-C2C	2.35	1.49	1.44
12	B	1211	CLA	C1C-C2C	2.35	1.49	1.44
12	B	1237	CLA	C3B-C2B	-2.35	1.37	1.40
12	A	1140	CLA	C1C-NC	-2.35	1.34	1.37
23	F	4016	C7Z	C18-C5	2.35	1.54	1.50
12	A	1127	CLA	C3B-C2B	-2.35	1.37	1.40
12	B	1209	CLA	C1B-NB	2.34	1.37	1.35
12	F	1301	CLA	C1C-C2C	2.34	1.49	1.44
12	B	1213	CLA	C3B-C2B	-2.34	1.37	1.40
12	B	1205	CLA	C1C-C2C	2.34	1.49	1.44
12	B	1228	CLA	C3B-C2B	-2.33	1.37	1.40
24	F	6001	LMT	O2'-C2'	-2.33	1.37	1.43
12	B	1240	CLA	C1B-NB	2.33	1.37	1.35
12	A	1131	CLA	C1C-C2C	2.33	1.49	1.44
12	A	1141	CLA	CHC-C1C	2.32	1.40	1.35
12	B	1228	CLA	CHC-C1C	2.32	1.40	1.35
12	B	1232	CLA	C1B-NB	2.32	1.37	1.35
12	B	1238	CLA	CHC-C1C	2.32	1.40	1.35
12	B	1236	CLA	C1C-C2C	2.32	1.49	1.44
12	B	1230	CLA	C1B-NB	2.32	1.37	1.35
12	B	1021	CLA	C1C-C2C	2.32	1.49	1.44
12	B	1220	CLA	C1C-C2C	2.32	1.49	1.44
12	L	1502	CLA	C1C-C2C	2.32	1.49	1.44
12	A	1133	CLA	C1C-C2C	2.32	1.49	1.44
12	B	1208	CLA	CHC-C1C	2.32	1.40	1.35
12	B	1206	CLA	C1C-C2C	2.32	1.49	1.44
12	B	1235	CLA	C1B-NB	2.31	1.37	1.35
12	B	1210	CLA	C3B-C2B	-2.31	1.37	1.40
12	B	1203	CLA	C1C-C2C	2.31	1.49	1.44
12	A	1130	CLA	C3B-C2B	-2.31	1.37	1.40
12	A	1119	CLA	CHC-C1C	2.31	1.40	1.35
12	A	1102	CLA	C3B-C2B	-2.31	1.37	1.40
12	B	1208	CLA	C1B-NB	2.30	1.37	1.35
12	A	1115	CLA	C3B-C2B	-2.30	1.37	1.40
12	A	1120	CLA	C3B-C2B	-2.30	1.37	1.40
12	B	1201	CLA	CHC-C1C	2.30	1.40	1.35
12	A	1112	CLA	C1B-NB	2.30	1.37	1.35
12	A	1136	CLA	C1B-NB	2.29	1.37	1.35
12	K	1401	CLA	C1B-NB	2.29	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1122	CLA	C1C-C2C	2.29	1.49	1.44
12	A	1105	CLA	CHC-C1C	2.28	1.40	1.35
19	B	4006	ECH	C1-C6	-2.28	1.50	1.53
12	B	1226	CLA	C1C-C2C	2.28	1.49	1.44
12	A	1101	CLA	CHC-C1C	2.28	1.40	1.35
12	A	1140	CLA	CHC-C1C	2.28	1.40	1.35
12	A	1126	CLA	CHC-C1C	2.28	1.40	1.35
12	B	1237	CLA	C1C-C2C	2.28	1.49	1.44
12	A	1117	CLA	CHC-C1C	2.28	1.40	1.35
19	M	4021	ECH	C25-C26	-2.27	1.32	1.35
12	B	1207	CLA	CHC-C1C	2.27	1.40	1.35
12	A	1102	CLA	CHC-C1C	2.27	1.40	1.35
12	B	1219	CLA	CHC-C1C	2.27	1.40	1.35
12	B	1205	CLA	C1B-NB	2.27	1.37	1.35
12	B	1231	CLA	C1B-NB	2.26	1.37	1.35
12	A	1109	CLA	C1C-C2C	2.26	1.48	1.44
12	B	1222	CLA	C1C-C2C	2.26	1.48	1.44
12	B	1232	CLA	CHC-C1C	2.26	1.40	1.35
12	B	1215	CLA	CHC-C1C	2.26	1.40	1.35
12	A	1011	CLA	C3B-C2B	-2.25	1.37	1.40
12	K	1402	CLA	CHC-C1C	2.25	1.40	1.35
12	A	1126	CLA	C1B-NB	2.25	1.37	1.35
12	A	1130	CLA	CHC-C1C	2.25	1.40	1.35
12	A	1116	CLA	CHC-C1C	2.25	1.40	1.35
12	A	1134	CLA	CHC-C1C	2.25	1.40	1.35
12	A	1117	CLA	C3B-C2B	-2.25	1.37	1.40
24	F	6001	LMT	O3B-C3B	-2.25	1.37	1.43
12	B	1218	CLA	CHC-C1C	2.25	1.40	1.35
12	B	1216	CLA	C1C-C2C	2.25	1.48	1.44
12	B	1209	CLA	CHC-C1C	2.25	1.40	1.35
12	K	1401	CLA	C1C-C2C	2.25	1.48	1.44
12	A	1011	CLA	C1C-C2C	2.25	1.48	1.44
24	F	6001	LMT	O2B-C2B	-2.25	1.37	1.43
12	A	1108	CLA	C1B-NB	2.24	1.37	1.35
12	A	1103	CLA	CHC-C1C	2.24	1.40	1.35
12	A	1139	CLA	CHC-C1C	2.24	1.40	1.35
12	J	1303	CLA	CHC-C1C	2.24	1.40	1.35
12	B	1223	CLA	CHC-C1C	2.24	1.40	1.35
12	A	1113	CLA	CHC-C1C	2.24	1.40	1.35
12	A	1120	CLA	CHC-C1C	2.24	1.40	1.35
12	B	1201	CLA	C3B-C2B	-2.24	1.37	1.40
17	B	4011	45D	C18-C16	2.23	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1215	CLA	C1B-NB	2.23	1.37	1.35
12	A	1112	CLA	C1C-C2C	2.23	1.48	1.44
12	B	1239	CLA	C1B-NB	2.23	1.37	1.35
12	A	1110	CLA	CHC-C1C	2.23	1.40	1.35
12	A	1114	CLA	C1B-NB	2.23	1.37	1.35
12	A	1101	CLA	C1B-NB	2.23	1.37	1.35
12	A	1108	CLA	CHC-C1C	2.23	1.40	1.35
12	A	1121	CLA	C1B-NB	2.23	1.37	1.35
12	A	1114	CLA	CHC-C1C	2.23	1.40	1.35
12	A	1121	CLA	CHC-C1C	2.23	1.40	1.35
12	A	1108	CLA	C3B-C2B	-2.23	1.37	1.40
12	B	1227	CLA	CHC-C1C	2.23	1.40	1.35
12	A	1124	CLA	CHC-C1C	2.22	1.40	1.35
12	A	1125	CLA	CHC-C1C	2.22	1.40	1.35
12	A	1138	CLA	C3B-C2B	-2.22	1.37	1.40
12	B	1224	CLA	CHC-C1C	2.22	1.40	1.35
12	B	1202	CLA	CHC-C1C	2.22	1.40	1.35
12	A	1127	CLA	CHC-C1C	2.22	1.40	1.35
12	B	1225	CLA	CHC-C1C	2.22	1.40	1.35
12	B	1217	CLA	C1B-NB	2.22	1.37	1.35
12	A	1122	CLA	CHC-C1C	2.21	1.40	1.35
12	F	1302	CLA	CHC-C1C	2.21	1.40	1.35
12	B	1230	CLA	CHC-C1C	2.21	1.40	1.35
12	A	1104	CLA	CHC-C1C	2.21	1.40	1.35
12	B	1023	CLA	C1C-C2C	2.21	1.48	1.44
12	B	1211	CLA	CHC-C1C	2.21	1.40	1.35
12	B	1235	CLA	CHC-C1C	2.21	1.40	1.35
12	B	1023	CLA	CHC-C1C	2.21	1.40	1.35
12	B	1227	CLA	C1B-NB	2.21	1.37	1.35
12	B	1221	CLA	CHC-C1C	2.20	1.40	1.35
12	A	1132	CLA	CHC-C1C	2.20	1.40	1.35
12	A	1129	CLA	CHC-C1C	2.20	1.40	1.35
12	B	1240	CLA	CHC-C1C	2.20	1.40	1.35
12	B	1239	CLA	CHC-C1C	2.20	1.40	1.35
12	A	1118	CLA	CHC-C1C	2.20	1.40	1.35
12	B	1237	CLA	C1B-NB	2.20	1.37	1.35
12	B	1229	CLA	C1B-NB	2.20	1.37	1.35
12	B	1234	CLA	C3B-C2B	-2.20	1.37	1.40
12	B	1222	CLA	CHC-C1C	2.20	1.40	1.35
12	A	1115	CLA	C1B-NB	2.19	1.37	1.35
12	A	1137	CLA	CHC-C1C	2.19	1.40	1.35
12	B	1231	CLA	CHC-C1C	2.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1113	CLA	C1B-NB	2.19	1.37	1.35
12	A	1136	CLA	CHC-C1C	2.19	1.40	1.35
12	B	1022	CLA	C1B-NB	2.19	1.37	1.35
12	B	1213	CLA	CHC-C1C	2.18	1.40	1.35
12	A	1116	CLA	C3B-C2B	-2.18	1.37	1.40
17	B	4011	45D	C23-C19	2.18	1.39	1.33
12	A	1119	CLA	C1B-NB	2.18	1.37	1.35
12	B	1212	CLA	CHC-C1C	2.18	1.40	1.35
12	K	1401	CLA	CHC-C1C	2.18	1.40	1.35
12	B	1228	CLA	C1B-NB	2.18	1.37	1.35
12	A	1110	CLA	C1B-NB	2.17	1.37	1.35
12	B	1204	CLA	CHC-C1C	2.17	1.40	1.35
12	B	1219	CLA	C1B-NB	2.17	1.37	1.35
12	A	1138	CLA	CHC-C1C	2.17	1.40	1.35
12	A	1135	CLA	CHC-C1C	2.17	1.40	1.35
12	A	1112	CLA	CHC-C1C	2.17	1.40	1.35
12	B	1203	CLA	CHC-C1C	2.16	1.40	1.35
12	B	1217	CLA	CHC-C1C	2.16	1.40	1.35
12	A	1109	CLA	CHC-C1C	2.16	1.40	1.35
12	A	1129	CLA	C1B-NB	2.16	1.37	1.35
12	B	1210	CLA	CHC-C1C	2.16	1.40	1.35
12	A	1137	CLA	C1B-NB	2.16	1.37	1.35
12	A	1111	CLA	C1C-C2C	2.16	1.48	1.44
12	B	1226	CLA	CHC-C1C	2.15	1.40	1.35
12	A	1125	CLA	C3B-C2B	-2.15	1.37	1.40
12	A	1123	CLA	C1B-NB	2.15	1.37	1.35
12	A	1135	CLA	C1B-NB	2.15	1.37	1.35
12	B	1022	CLA	CHC-C1C	2.14	1.40	1.35
12	J	1302	CLA	CHC-C1C	2.14	1.40	1.35
12	A	1133	CLA	CHC-C1C	2.14	1.40	1.35
12	B	1207	CLA	C1B-NB	2.14	1.37	1.35
12	A	1134	CLA	C1B-NB	2.14	1.37	1.35
12	L	1502	CLA	C1B-NB	2.14	1.37	1.35
12	J	1303	CLA	C3B-C2B	-2.13	1.37	1.40
12	B	1218	CLA	C3B-C2B	-2.13	1.37	1.40
12	B	1216	CLA	CHC-C1C	2.13	1.40	1.35
12	A	1115	CLA	CHC-C1C	2.13	1.40	1.35
12	B	1210	CLA	C1B-NB	2.13	1.37	1.35
12	A	1127	CLA	C1B-NB	2.13	1.37	1.35
12	J	1302	CLA	C1B-NB	2.13	1.37	1.35
12	B	1211	CLA	C3B-C2B	-2.12	1.37	1.40
12	B	1234	CLA	CHC-C1C	2.12	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1012	CLA	CHC-C1C	2.12	1.40	1.35
12	B	1212	CLA	C1B-NB	2.12	1.37	1.35
12	F	1301	CLA	CHC-C1C	2.12	1.40	1.35
12	A	1123	CLA	CHC-C1C	2.12	1.40	1.35
12	A	1124	CLA	C1B-NB	2.12	1.37	1.35
12	B	1201	CLA	C1B-NB	2.12	1.37	1.35
12	B	1236	CLA	CHC-C1C	2.11	1.40	1.35
12	B	1218	CLA	C1B-NB	2.11	1.37	1.35
12	B	1238	CLA	C1B-NB	2.11	1.37	1.35
12	A	1111	CLA	CHC-C1C	2.11	1.40	1.35
12	B	1205	CLA	CHC-C1C	2.11	1.40	1.35
12	L	1502	CLA	CHC-C1C	2.11	1.40	1.35
12	A	1106	CLA	CHC-C1C	2.10	1.40	1.35
12	B	1214	CLA	CHC-C1C	2.10	1.40	1.35
12	B	1237	CLA	CHC-C1C	2.10	1.40	1.35
12	A	1132	CLA	C1B-NB	2.10	1.37	1.35
12	A	1109	CLA	C1B-NB	2.10	1.37	1.35
12	B	1236	CLA	C1B-NB	2.10	1.37	1.35
12	A	1120	CLA	C1B-NB	2.10	1.37	1.35
12	A	1011	CLA	CHC-C1C	2.10	1.40	1.35
12	B	1021	CLA	CHC-C1C	2.09	1.40	1.35
12	B	1216	CLA	C1B-NB	2.09	1.37	1.35
12	K	1402	CLA	C1B-NB	2.09	1.37	1.35
12	A	1130	CLA	C1B-NB	2.09	1.37	1.35
12	B	1238	CLA	C3D-C4D	-2.09	1.39	1.44
12	A	1128	CLA	C1C-C2C	2.09	1.48	1.44
12	A	1123	CLA	C3B-C2B	-2.09	1.37	1.40
12	B	1213	CLA	C1B-NB	2.08	1.37	1.35
12	A	1128	CLA	CHC-C1C	2.08	1.40	1.35
12	A	1106	CLA	C1B-NB	2.08	1.37	1.35
12	B	1220	CLA	CHC-C1C	2.08	1.40	1.35
12	A	1117	CLA	C1B-NB	2.07	1.37	1.35
12	A	1131	CLA	CHC-C1C	2.07	1.40	1.35
12	A	1122	CLA	C1B-NB	2.07	1.37	1.35
23	J	4015	C7Z	C38-C25	2.07	1.54	1.50
23	F	4016	C7Z	C38-C25	2.07	1.54	1.50
12	L	1502	CLA	C1A-CHA	2.06	1.51	1.43
12	A	1012	CLA	C1A-CHA	2.06	1.51	1.43
12	A	1111	CLA	C1B-NB	2.05	1.37	1.35
12	B	1221	CLA	C1A-CHA	2.05	1.51	1.43
12	A	1104	CLA	C1B-NB	2.05	1.37	1.35
24	F	6001	LMT	O4'-C4B	-2.05	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1203	CLA	C1B-NB	2.04	1.37	1.35
12	A	1107	CLA	C3B-C2B	-2.04	1.37	1.40
12	A	1103	CLA	C1B-NB	2.03	1.37	1.35
12	B	1209	CLA	C1A-CHA	2.03	1.51	1.43
12	A	1131	CLA	C1B-NB	2.03	1.37	1.35
12	A	1122	CLA	C1A-CHA	2.03	1.51	1.43
12	J	1303	CLA	C1B-NB	2.02	1.37	1.35
12	A	1123	CLA	C1A-CHA	2.02	1.51	1.43
12	A	1102	CLA	C1A-CHA	2.02	1.51	1.43
12	B	1223	CLA	C1B-NB	2.02	1.37	1.35
12	B	1215	CLA	C1A-CHA	2.02	1.51	1.43
12	B	1206	CLA	C1A-CHA	2.01	1.51	1.43
12	B	1213	CLA	C1A-CHA	2.01	1.51	1.43
12	B	1023	CLA	C1A-CHA	2.01	1.51	1.43
12	A	1141	CLA	C1A-CHA	2.01	1.51	1.43
12	A	1126	CLA	C3D-C4D	-2.01	1.39	1.44
12	B	1240	CLA	C1A-CHA	2.01	1.51	1.43
12	A	1120	CLA	C1A-CHA	2.00	1.51	1.43
12	B	1220	CLA	C1A-CHA	2.00	1.51	1.43
12	B	1206	CLA	CHC-C1C	2.00	1.40	1.35

All (1610) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4010	BCR	C10-C11-C12	18.17	179.93	123.22
15	B	4017	BCR	C10-C11-C12	17.87	178.98	123.22
15	K	4001	BCR	C10-C11-C12	17.67	178.35	123.22
15	B	4004	BCR	C10-C11-C12	17.57	178.06	123.22
15	B	4018	BCR	C10-C11-C12	17.57	178.04	123.22
15	F	4014	BCR	C10-C11-C12	17.49	177.81	123.22
15	A	4008	BCR	C10-C11-C12	17.49	177.79	123.22
15	A	4007	BCR	C10-C11-C12	17.43	177.61	123.22
15	B	4005	BCR	C10-C11-C12	17.36	177.41	123.22
15	A	4003	BCR	C10-C11-C12	17.23	177.00	123.22
15	J	4013	BCR	C10-C11-C12	17.21	176.91	123.22
15	A	4001	BCR	C10-C11-C12	17.19	176.86	123.22
15	A	4012	BCR	C10-C11-C12	16.74	175.47	123.22
15	I	4018	BCR	C10-C11-C12	16.25	173.94	123.22
23	F	4016	C7Z	C18-C5-C6	-14.85	107.85	124.53
15	B	4017	BCR	C16-C15-C14	14.77	153.73	123.47
15	B	4005	BCR	C16-C15-C14	14.77	153.73	123.47
15	B	4004	BCR	C16-C15-C14	14.49	153.16	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4001	BCR	C16-C15-C14	14.39	152.95	123.47
15	A	4007	BCR	C16-C15-C14	14.19	152.55	123.47
15	I	4018	BCR	C11-C10-C9	14.04	147.35	127.31
15	I	4018	BCR	C16-C15-C14	14.03	152.22	123.47
15	B	4010	BCR	C16-C15-C14	14.00	152.16	123.47
15	J	4013	BCR	C16-C15-C14	13.76	151.65	123.47
15	A	4012	BCR	C11-C10-C9	13.53	146.62	127.31
15	K	4001	BCR	C21-C20-C19	13.50	165.35	123.22
15	B	4005	BCR	C11-C10-C9	13.42	146.46	127.31
15	A	4003	BCR	C11-C10-C9	13.31	146.30	127.31
15	K	4001	BCR	C11-C10-C9	13.23	146.19	127.31
23	J	4015	C7Z	C18-C5-C6	-13.13	109.79	124.53
15	A	4008	BCR	C11-C10-C9	13.02	145.90	127.31
15	F	4014	BCR	C11-C10-C9	13.02	145.89	127.31
15	A	4008	BCR	C16-C15-C14	12.97	150.04	123.47
15	B	4004	BCR	C11-C10-C9	12.95	145.80	127.31
15	A	4001	BCR	C21-C20-C19	12.94	163.59	123.22
15	K	4001	BCR	C16-C15-C14	12.89	149.89	123.47
15	A	4007	BCR	C11-C10-C9	12.79	145.57	127.31
15	J	4013	BCR	C11-C10-C9	12.77	145.53	127.31
15	A	4003	BCR	C16-C15-C14	12.72	149.54	123.47
15	B	4004	BCR	C21-C20-C19	12.71	162.87	123.22
15	F	4014	BCR	C21-C20-C19	12.60	162.53	123.22
15	A	4008	BCR	C21-C20-C19	12.55	162.40	123.22
15	A	4012	BCR	C21-C20-C19	12.45	162.06	123.22
15	B	4017	BCR	C11-C10-C9	12.39	144.99	127.31
15	B	4010	BCR	C11-C10-C9	12.25	144.79	127.31
15	B	4018	BCR	C16-C15-C14	12.21	148.48	123.47
15	B	4017	BCR	C21-C20-C19	11.97	160.58	123.22
15	B	4010	BCR	C21-C20-C19	11.93	160.44	123.22
15	A	4007	BCR	C21-C20-C19	11.91	160.38	123.22
15	J	4013	BCR	C21-C20-C19	11.90	160.36	123.22
15	B	4018	BCR	C11-C10-C9	11.82	144.18	127.31
23	F	4016	C7Z	C38-C25-C26	-11.64	111.45	124.53
15	F	4014	BCR	C16-C15-C14	11.64	147.32	123.47
15	A	4012	BCR	C16-C15-C14	11.33	146.69	123.47
15	A	4001	BCR	C11-C10-C9	11.29	143.43	127.31
23	F	4016	C7Z	C15-C14-C13	-10.95	111.69	127.31
15	A	4012	BCR	C11-C12-C13	10.83	156.85	126.42
15	B	4005	BCR	C21-C20-C19	10.81	156.96	123.22
23	J	4015	C7Z	C38-C25-C26	-10.74	112.47	124.53
15	B	4018	BCR	C11-C12-C13	10.70	156.47	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4003	BCR	C21-C20-C19	10.69	156.58	123.22
15	F	4014	BCR	C11-C12-C13	10.67	156.40	126.42
23	J	4015	C7Z	C11-C10-C9	-10.64	112.12	127.31
23	F	4016	C7Z	C35-C34-C33	-10.61	112.17	127.31
15	B	4010	BCR	C11-C12-C13	10.55	156.05	126.42
23	J	4015	C7Z	C15-C14-C13	-10.53	112.28	127.31
15	A	4008	BCR	C11-C12-C13	10.41	155.67	126.42
15	A	4003	BCR	C11-C12-C13	10.37	155.55	126.42
15	I	4018	BCR	C21-C20-C19	10.37	155.58	123.22
12	A	1107	CLA	C4A-NA-C1A	10.21	111.30	106.71
15	B	4017	BCR	C11-C12-C13	10.15	154.93	126.42
15	B	4004	BCR	C11-C12-C13	9.93	154.31	126.42
23	F	4016	C7Z	C31-C30-C29	-9.91	113.17	127.31
23	J	4015	C7Z	C35-C34-C33	-9.87	113.22	127.31
15	A	4007	BCR	C11-C12-C13	9.86	154.11	126.42
23	J	4015	C7Z	C31-C30-C29	-9.86	113.24	127.31
23	J	4015	C7Z	C19-C9-C10	-9.83	109.16	122.92
15	B	4018	BCR	C21-C20-C19	9.82	153.87	123.22
15	K	4001	BCR	C11-C12-C13	9.78	153.88	126.42
15	B	4005	BCR	C11-C12-C13	9.69	153.65	126.42
15	J	4013	BCR	C11-C12-C13	9.68	153.61	126.42
23	J	4015	C7Z	C39-C29-C30	-9.65	109.40	122.92
23	F	4016	C7Z	C40-C33-C34	-9.64	109.42	122.92
23	F	4016	C7Z	C11-C10-C9	-9.62	113.58	127.31
23	J	4015	C7Z	C20-C13-C14	-9.61	109.46	122.92
15	A	4001	BCR	C11-C12-C13	9.51	153.14	126.42
15	I	4018	BCR	C20-C19-C18	9.48	153.06	126.42
23	F	4016	C7Z	C39-C29-C30	-9.47	109.66	122.92
15	B	4005	BCR	C20-C19-C18	9.29	152.52	126.42
23	F	4016	C7Z	C19-C9-C10	-9.26	109.95	122.92
23	J	4015	C7Z	C40-C33-C34	-9.23	109.99	122.92
19	M	4021	ECH	C16-C17-C18	-9.20	114.18	127.31
25	I	4020	EQ3	C16-C17-C18	-9.18	114.21	127.31
19	M	4021	ECH	C20-C21-C22	-9.15	114.25	127.31
23	F	4016	C7Z	C20-C13-C14	-9.07	110.22	122.92
15	I	4018	BCR	C11-C12-C13	8.74	150.97	126.42
19	B	4006	ECH	C16-C17-C18	-8.28	115.49	127.31
15	A	4007	BCR	C20-C19-C18	8.11	149.21	126.42
15	B	4010	BCR	C20-C19-C18	8.07	149.10	126.42
15	J	4013	BCR	C20-C19-C18	7.97	148.81	126.42
23	J	4015	C7Z	C21-C26-C25	-7.80	111.63	122.61
15	B	4017	BCR	C20-C19-C18	7.70	148.05	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	4014	BCR	C20-C19-C18	7.22	146.70	126.42
15	A	4003	BCR	C20-C19-C18	7.21	146.66	126.42
15	B	4004	BCR	C20-C19-C18	7.15	146.52	126.42
15	A	4008	BCR	C20-C19-C18	7.15	146.51	126.42
15	A	4012	BCR	C20-C19-C18	7.12	146.42	126.42
17	B	4011	45D	C20-C24-C26	-7.06	115.56	126.23
15	A	4001	BCR	C20-C19-C18	7.06	146.26	126.42
23	F	4016	C7Z	C28-C29-C30	-6.88	108.38	118.94
19	B	4006	ECH	C11-C10-C9	-6.85	117.53	127.31
23	J	4015	C7Z	C32-C33-C34	-6.57	108.86	118.94
23	F	4016	C7Z	C8-C9-C10	-6.31	109.25	118.94
23	J	4015	C7Z	C8-C9-C10	-6.23	109.38	118.94
15	K	4001	BCR	C20-C19-C18	6.22	143.90	126.42
12	B	1220	CLA	O2A-C1-C2	6.13	123.30	108.97
19	M	4021	ECH	C24-C23-C22	-6.11	117.00	126.23
23	J	4015	C7Z	C12-C13-C14	-6.09	109.60	118.94
12	A	1107	CLA	O2A-C1-C2	6.02	124.44	108.64
12	B	1231	CLA	CMD-C2D-C1D	5.98	135.25	124.71
23	J	4015	C7Z	C28-C29-C30	-5.97	109.77	118.94
19	B	4006	ECH	C20-C21-C22	-5.97	118.79	127.31
12	B	1227	CLA	CMD-C2D-C1D	5.97	135.23	124.71
12	B	1240	CLA	CMD-C2D-C1D	5.96	135.22	124.71
12	A	1121	CLA	O2A-C1-C2	5.95	122.88	108.97
23	F	4016	C7Z	C12-C13-C14	-5.93	109.85	118.94
12	A	1122	CLA	CMD-C2D-C1D	5.89	135.10	124.71
12	A	1121	CLA	CMD-C2D-C1D	5.89	135.09	124.71
12	B	1231	CLA	O2A-C1-C2	5.87	122.70	108.97
12	B	1227	CLA	O2D-CGD-CBD	5.87	121.69	111.27
12	A	1139	CLA	CMD-C2D-C1D	5.85	135.03	124.71
12	K	1402	CLA	O2A-C1-C2	5.85	122.65	108.97
12	B	1216	CLA	O2A-C1-C2	5.84	122.63	108.97
12	B	1230	CLA	CMD-C2D-C1D	5.84	135.00	124.71
12	A	1109	CLA	CMD-C2D-C1D	5.83	134.99	124.71
12	A	1129	CLA	O2A-C1-C2	5.83	122.59	108.97
12	A	1101	CLA	O2A-C1-C2	5.82	122.58	108.97
23	J	4015	C7Z	C1-C6-C5	-5.82	114.42	122.61
15	B	4018	BCR	C20-C19-C18	5.81	142.73	126.42
12	B	1234	CLA	O2A-C1-C2	5.80	123.89	108.64
12	B	1224	CLA	CMD-C2D-C1D	5.79	134.91	124.71
12	L	1502	CLA	CMD-C2D-C1D	5.79	134.91	124.71
12	A	1138	CLA	CMD-C2D-C1D	5.78	134.90	124.71
12	A	1135	CLA	O2A-C1-C2	5.77	122.46	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1205	CLA	O2D-CGD-CBD	5.77	121.52	111.27
17	B	4011	45D	C31-C29-C25	-5.76	119.09	127.31
12	A	1011	CLA	CMD-C2D-C1D	5.76	134.87	124.71
12	B	1223	CLA	CMD-C2D-C1D	5.76	134.86	124.71
12	B	1213	CLA	O2D-CGD-CBD	5.75	121.48	111.27
12	A	1126	CLA	CMD-C2D-C1D	5.75	134.84	124.71
12	A	1118	CLA	CMD-C2D-C1D	5.74	134.84	124.71
12	A	1119	CLA	CMD-C2D-C1D	5.74	134.83	124.71
12	B	1230	CLA	O2D-CGD-CBD	5.74	121.47	111.27
12	B	1229	CLA	CMD-C2D-C1D	5.74	134.83	124.71
12	B	1206	CLA	CMD-C2D-C1D	5.74	134.83	124.71
12	A	1105	CLA	CMD-C2D-C1D	5.72	134.80	124.71
12	B	1207	CLA	CMD-C2D-C1D	5.71	134.78	124.71
12	B	1240	CLA	O2D-CGD-CBD	5.70	121.39	111.27
12	A	1135	CLA	CMD-C2D-C1D	5.69	134.75	124.71
12	B	1238	CLA	CMD-C2D-C1D	5.69	134.74	124.71
12	A	1134	CLA	CMD-C2D-C1D	5.69	134.74	124.71
12	J	1303	CLA	CMD-C2D-C1D	5.67	134.71	124.71
12	B	1215	CLA	O2A-C1-C2	5.67	122.22	108.97
12	A	1132	CLA	CMD-C2D-C1D	5.67	134.70	124.71
12	A	1103	CLA	CMD-C2D-C1D	5.66	134.69	124.71
12	A	1013	CLA	O2A-C1-C2	5.66	123.51	108.64
12	B	1210	CLA	O2A-C1-C2	5.66	122.20	108.97
12	B	1230	CLA	O2A-C1-C2	5.66	122.20	108.97
12	A	1137	CLA	O2A-C1-C2	5.66	122.20	108.97
23	F	4016	C7Z	C40-C33-C32	-5.65	109.17	118.08
12	B	1232	CLA	CMD-C2D-C1D	5.63	134.64	124.71
12	K	1401	CLA	CMD-C2D-C1D	5.63	134.64	124.71
12	B	1234	CLA	CMD-C2D-C1D	5.63	134.63	124.71
12	B	1217	CLA	O2A-C1-C2	5.63	122.13	108.97
12	B	1209	CLA	CMD-C2D-C1D	5.62	134.63	124.71
12	B	1201	CLA	CMD-C2D-C1D	5.62	134.62	124.71
12	A	1106	CLA	O2D-CGD-CBD	5.62	121.26	111.27
12	B	1239	CLA	CMD-C2D-C1D	5.62	134.62	124.71
12	A	1131	CLA	CMD-C2D-C1D	5.61	134.61	124.71
12	B	1203	CLA	CMD-C2D-C1D	5.61	134.61	124.71
12	B	1212	CLA	CMD-C2D-C1D	5.61	134.61	124.71
12	A	1116	CLA	CMD-C2D-C1D	5.61	134.60	124.71
12	A	1141	CLA	CMD-C2D-C1D	5.61	134.60	124.71
12	A	1128	CLA	O2D-CGD-CBD	5.61	121.24	111.27
12	B	1217	CLA	CMD-C2D-C1D	5.61	134.60	124.71
12	B	1205	CLA	O2A-C1-C2	5.60	122.08	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1136	CLA	CMD-C2D-C1D	5.60	134.59	124.71
12	B	1209	CLA	O2D-CGD-CBD	5.60	121.22	111.27
12	B	1229	CLA	O2D-CGD-CBD	5.59	121.21	111.27
12	B	1205	CLA	CMD-C2D-C1D	5.59	134.57	124.71
12	A	1101	CLA	CMD-C2D-C1D	5.59	134.57	124.71
12	B	1022	CLA	CMD-C2D-C1D	5.59	134.57	124.71
12	J	1302	CLA	CMD-C2D-C1D	5.59	134.57	124.71
12	B	1213	CLA	CMD-C2D-C1D	5.59	134.56	124.71
12	A	1114	CLA	CMD-C2D-C1D	5.58	134.56	124.71
12	A	1137	CLA	CMD-C2D-C1D	5.58	134.55	124.71
12	A	1112	CLA	O2A-C1-C2	5.58	122.02	108.97
23	F	4016	C7Z	C19-C9-C8	-5.58	109.29	118.08
12	B	1226	CLA	O2A-C1-C2	5.58	122.01	108.97
12	K	1402	CLA	CMD-C2D-C1D	5.58	134.54	124.71
12	A	1104	CLA	CMD-C2D-C1D	5.57	134.54	124.71
12	B	1210	CLA	CMD-C2D-C1D	5.57	134.54	124.71
12	B	1216	CLA	CMD-C2D-C1D	5.57	134.53	124.71
12	A	1133	CLA	CMD-C2D-C1D	5.57	134.53	124.71
12	B	1237	CLA	CMD-C2D-C1D	5.57	134.53	124.71
12	B	1202	CLA	CMD-C2D-C1D	5.56	134.52	124.71
12	B	1221	CLA	O2A-C1-C2	5.56	121.97	108.97
12	A	1130	CLA	CMD-C2D-C1D	5.56	134.51	124.71
12	B	1222	CLA	CMD-C2D-C1D	5.56	134.51	124.71
12	F	1301	CLA	CMD-C2D-C1D	5.55	134.50	124.71
12	B	1214	CLA	CMD-C2D-C1D	5.55	134.50	124.71
12	A	1125	CLA	CMD-C2D-C1D	5.55	134.49	124.71
12	B	1221	CLA	O2D-CGD-CBD	5.55	121.13	111.27
12	A	1124	CLA	CMD-C2D-C1D	5.55	134.49	124.71
12	F	1302	CLA	O2D-CGD-CBD	5.53	121.10	111.27
12	B	1232	CLA	O2A-C1-C2	5.53	121.91	108.97
12	B	1218	CLA	CMD-C2D-C1D	5.53	134.46	124.71
12	B	1208	CLA	CMD-C2D-C1D	5.53	134.46	124.71
12	F	1302	CLA	CMD-C2D-C1D	5.53	134.45	124.71
12	A	1102	CLA	CMD-C2D-C1D	5.52	134.45	124.71
12	A	1110	CLA	CMD-C2D-C1D	5.52	134.45	124.71
12	B	1225	CLA	O2A-C1-C2	5.52	121.87	108.97
12	A	1113	CLA	CMD-C2D-C1D	5.51	134.43	124.71
12	L	1502	CLA	O2D-CGD-CBD	5.51	121.06	111.27
12	A	1120	CLA	CMD-C2D-C1D	5.51	134.43	124.71
12	A	1115	CLA	CMD-C2D-C1D	5.51	134.42	124.71
12	B	1211	CLA	CMD-C2D-C1D	5.50	134.41	124.71
12	A	1140	CLA	CMD-C2D-C1D	5.50	134.41	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1238	CLA	O2D-CGD-CBD	5.50	121.05	111.27
12	A	1129	CLA	CMD-C2D-C1D	5.50	134.41	124.71
12	A	1117	CLA	CMD-C2D-C1D	5.50	134.41	124.71
12	F	1301	CLA	O2A-C1-C2	5.50	121.83	108.97
12	A	1106	CLA	CMD-C2D-C1D	5.50	134.40	124.71
12	B	1237	CLA	O2A-C1-C2	5.50	121.82	108.97
12	A	1138	CLA	O2A-C1-C2	5.49	123.06	108.64
12	B	1213	CLA	O2A-C1-C2	5.48	121.79	108.97
12	A	1127	CLA	CMD-C2D-C1D	5.48	134.38	124.71
12	B	1201	CLA	O2A-C1-C2	5.48	121.79	108.97
12	A	1108	CLA	CMD-C2D-C1D	5.48	134.37	124.71
25	I	4020	EQ3	C7-C8-C9	-5.48	117.95	126.23
12	A	1103	CLA	O2A-C1-C2	5.47	121.76	108.97
12	B	1228	CLA	CMD-C2D-C1D	5.47	134.35	124.71
12	B	1228	CLA	O2A-C1-C2	5.47	121.75	108.97
12	B	1202	CLA	O2D-CGD-CBD	5.47	120.98	111.27
12	B	1212	CLA	O2A-C1-C2	5.47	121.75	108.97
12	B	1239	CLA	O2A-C1-C2	5.46	121.75	108.97
12	B	1023	CLA	O2A-C1-C2	5.46	121.74	108.97
12	A	1135	CLA	O2D-CGD-CBD	5.45	120.96	111.27
12	A	1111	CLA	CMD-C2D-C1D	5.45	134.32	124.71
12	A	1112	CLA	CMD-C2D-C1D	5.44	134.30	124.71
12	B	1235	CLA	O2A-C1-C2	5.44	122.93	108.64
12	B	1236	CLA	CMD-C2D-C1D	5.44	134.29	124.71
12	L	1502	CLA	O2A-C1-C2	5.43	121.67	108.97
12	A	1117	CLA	O2A-C1-C2	5.43	121.67	108.97
12	A	1112	CLA	O2D-CGD-CBD	5.43	120.92	111.27
12	B	1219	CLA	CMD-C2D-C1D	5.42	134.27	124.71
12	A	1122	CLA	O2A-C1-C2	5.42	121.64	108.97
12	A	1125	CLA	O2A-C1-C2	5.42	121.64	108.97
12	B	1219	CLA	O2A-C1-C2	5.41	121.63	108.97
12	A	1128	CLA	O2A-C1-C2	5.41	122.86	108.64
12	A	1011	CLA	O2D-CGD-CBD	5.41	120.88	111.27
19	B	4006	ECH	C24-C23-C22	-5.41	118.07	126.23
12	A	1012	CLA	O2A-C1-C2	5.40	121.60	108.97
12	A	1127	CLA	O2A-C1-C2	5.40	121.60	108.97
12	A	1108	CLA	O2A-C1-C2	5.40	121.59	108.97
12	J	1303	CLA	O2D-CGD-CBD	5.39	120.85	111.27
12	A	1128	CLA	CMD-C2D-C1D	5.39	134.22	124.71
12	B	1204	CLA	CMD-C2D-C1D	5.38	134.20	124.71
12	B	1236	CLA	O2D-CGD-CBD	5.38	120.83	111.27
12	A	1134	CLA	O2D-CGD-CBD	5.38	120.82	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1130	CLA	O2A-C1-C2	5.38	121.54	108.97
12	B	1227	CLA	O2A-C1-C2	5.37	121.53	108.97
12	B	1226	CLA	O2D-CGD-CBD	5.37	120.81	111.27
12	B	1236	CLA	O2A-C1-C2	5.37	121.52	108.97
12	A	1120	CLA	O2A-C1-C2	5.36	121.51	108.97
12	F	1302	CLA	O2A-C1-C2	5.36	121.51	108.97
12	A	1102	CLA	O2D-CGD-CBD	5.36	120.79	111.27
12	A	1104	CLA	O2A-C1-C2	5.36	121.50	108.97
12	B	1223	CLA	O2A-C1-C2	5.35	121.48	108.97
12	A	1105	CLA	O2D-CGD-CBD	5.34	120.77	111.27
12	B	1204	CLA	O2A-C1-C2	5.34	121.46	108.97
12	B	1226	CLA	CMD-C2D-C1D	5.34	134.13	124.71
12	A	1116	CLA	O2D-CGD-CBD	5.34	120.76	111.27
12	B	1225	CLA	CMD-C2D-C1D	5.34	134.12	124.71
12	B	1220	CLA	CMD-C2D-C1D	5.34	134.12	124.71
12	B	1238	CLA	O2A-C1-C2	5.33	121.42	108.97
12	B	1211	CLA	O2A-C1-C2	5.32	121.42	108.97
12	K	1401	CLA	O2D-CGD-CBD	5.32	120.72	111.27
12	A	1133	CLA	O2A-C1-C2	5.32	121.41	108.97
12	J	1302	CLA	O2D-CGD-CBD	5.32	120.72	111.27
12	A	1124	CLA	O2A-C1-C2	5.32	121.41	108.97
12	B	1218	CLA	O2A-C1-C2	5.32	121.40	108.97
12	A	1101	CLA	O2D-CGD-CBD	5.31	120.70	111.27
12	A	1136	CLA	O2A-C1-C2	5.30	121.36	108.97
12	A	1116	CLA	O2A-C1-C2	5.30	121.36	108.97
23	F	4016	C7Z	C20-C13-C12	-5.30	109.73	118.08
12	B	1235	CLA	CMD-C2D-C1D	5.30	134.04	124.71
12	J	1302	CLA	O2A-C1-C2	5.29	121.34	108.97
12	B	1215	CLA	CMD-C2D-C1D	5.28	134.03	124.71
12	B	1023	CLA	CMD-C2D-C1D	5.28	134.02	124.71
23	F	4016	C7Z	C32-C33-C34	-5.27	110.85	118.94
12	A	1131	CLA	O2A-C1-C2	5.27	121.30	108.97
12	A	1111	CLA	O2A-C1-C2	5.27	121.28	108.97
12	A	1114	CLA	O2A-C1-C2	5.26	121.27	108.97
12	A	1106	CLA	O2A-C1-C2	5.24	122.40	108.64
12	B	1209	CLA	O2A-C1-C2	5.23	121.21	108.97
12	A	1123	CLA	CMD-C2D-C1D	5.23	133.94	124.71
12	A	1123	CLA	O2D-CGD-CBD	5.23	120.56	111.27
12	B	1206	CLA	O2A-C1-C2	5.22	121.19	108.97
12	A	1013	CLA	CMD-C2D-C1D	5.22	133.92	124.71
12	B	1221	CLA	CMD-C2D-C1D	5.22	133.92	124.71
12	A	1136	CLA	O2D-CGD-CBD	5.21	120.53	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1120	CLA	O2D-CGD-CBD	5.21	120.52	111.27
12	B	1211	CLA	O2D-CGD-CBD	5.20	120.51	111.27
12	A	1113	CLA	O2D-CGD-CBD	5.20	120.50	111.27
12	A	1123	CLA	C4A-NA-C1A	5.20	109.04	106.71
23	J	4015	C7Z	C39-C29-C28	-5.19	109.89	118.08
12	B	1207	CLA	O2D-CGD-CBD	5.19	120.49	111.27
12	L	1502	CLA	C4A-NA-C1A	5.19	109.04	106.71
12	B	1021	CLA	O2A-C1-C2	5.18	122.26	108.64
12	B	1219	CLA	O2D-CGD-CBD	5.18	120.47	111.27
12	A	1125	CLA	O2D-CGD-CBD	5.18	120.47	111.27
12	B	1208	CLA	O2A-C1-C2	5.17	121.06	108.97
12	B	1222	CLA	O2A-C1-C2	5.16	122.20	108.64
12	A	1105	CLA	O2A-C1-C2	5.16	122.19	108.64
12	A	1124	CLA	O2D-CGD-CBD	5.16	120.43	111.27
12	B	1203	CLA	O2A-C1-C2	5.16	121.03	108.97
12	A	1134	CLA	O2A-C1-C2	5.16	121.03	108.97
12	B	1217	CLA	O2D-CGD-CBD	5.15	120.43	111.27
12	B	1207	CLA	O2A-C1-C2	5.15	121.01	108.97
12	A	1115	CLA	O2A-C1-C2	5.15	122.17	108.64
12	B	1228	CLA	O2D-CGD-CBD	5.15	120.42	111.27
23	J	4015	C7Z	C20-C13-C12	-5.13	109.99	118.08
12	B	1220	CLA	O2D-CGD-CBD	5.13	120.39	111.27
12	B	1234	CLA	O2D-CGD-CBD	5.13	120.39	111.27
12	J	1303	CLA	O2A-C1-C2	5.13	120.96	108.97
12	A	1110	CLA	O2A-C1-C2	5.13	120.96	108.97
12	A	1103	CLA	O2D-CGD-CBD	5.12	120.37	111.27
12	B	1240	CLA	O2A-C1-C2	5.12	120.94	108.97
12	B	1212	CLA	O2D-CGD-CBD	5.12	120.36	111.27
12	B	1235	CLA	O2D-CGD-CBD	5.12	120.36	111.27
12	A	1115	CLA	O2D-CGD-CBD	5.11	120.35	111.27
23	J	4015	C7Z	C19-C9-C8	-5.11	110.03	118.08
23	F	4016	C7Z	C7-C6-C5	-5.11	109.09	121.46
12	A	1113	CLA	O2A-C1-C2	5.10	120.90	108.97
12	B	1210	CLA	O2D-CGD-CBD	5.10	120.33	111.27
12	B	1205	CLA	C4A-NA-C1A	5.10	109.00	106.71
12	A	1107	CLA	CMD-C2D-C1D	5.09	133.68	124.71
12	A	1121	CLA	O2D-CGD-CBD	5.08	120.29	111.27
12	A	1012	CLA	CMD-C2D-C1D	5.08	133.66	124.71
12	A	1130	CLA	O2D-CGD-CBD	5.07	120.28	111.27
12	B	1022	CLA	O2D-CGD-CBD	5.06	120.25	111.27
12	B	1222	CLA	O2D-CGD-CBD	5.06	120.25	111.27
12	A	1011	CLA	C4A-NA-C1A	5.04	108.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4015	C7Z	C40-C33-C32	-5.04	110.13	118.08
12	B	1215	CLA	O2D-CGD-CBD	5.04	120.22	111.27
12	B	1021	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	F	4016	C7Z	C39-C29-C28	-5.03	110.16	118.08
12	A	1118	CLA	O2D-CGD-CBD	5.02	120.20	111.27
12	A	1011	CLA	O2A-C1-C2	5.02	121.84	108.64
12	A	1104	CLA	O2D-CGD-CBD	5.02	120.19	111.27
12	B	1218	CLA	O2D-CGD-CBD	5.02	120.18	111.27
12	B	1208	CLA	O2D-CGD-CBD	5.01	120.18	111.27
12	A	1131	CLA	O2D-CGD-CBD	5.00	120.16	111.27
12	A	1140	CLA	O2D-CGD-CBD	4.99	120.14	111.27
12	B	1022	CLA	O2A-C1-C2	4.99	121.75	108.64
12	B	1223	CLA	O2D-CGD-CBD	4.99	120.14	111.27
12	A	1126	CLA	O2D-CGD-CBD	4.99	120.13	111.27
12	F	1301	CLA	O2D-CGD-CBD	4.98	120.11	111.27
12	A	1133	CLA	O2D-CGD-CBD	4.97	120.11	111.27
12	B	1239	CLA	O2D-CGD-CBD	4.97	120.10	111.27
12	A	1110	CLA	O2D-CGD-CBD	4.96	120.08	111.27
12	A	1139	CLA	O2A-C1-C2	4.94	121.63	108.64
12	A	1108	CLA	O2D-CGD-CBD	4.94	120.05	111.27
12	B	1204	CLA	O2D-CGD-CBD	4.94	120.04	111.27
12	A	1109	CLA	O2A-C1-C2	4.94	121.61	108.64
12	A	1132	CLA	O2A-C1-C2	4.94	121.61	108.64
16	B	5006	LHG	O7-C7-C8	4.93	120.16	111.09
12	B	1237	CLA	O2D-CGD-CBD	4.93	120.03	111.27
12	B	1201	CLA	O2D-CGD-CBD	4.93	120.03	111.27
12	A	1114	CLA	O2D-CGD-CBD	4.92	120.02	111.27
12	B	1202	CLA	O2A-C1-C2	4.92	121.56	108.64
12	A	1140	CLA	O2A-C1-C2	4.92	121.56	108.64
12	B	1216	CLA	O2D-CGD-CBD	4.91	119.99	111.27
12	B	1021	CLA	C4A-NA-C1A	4.90	108.91	106.71
12	A	1129	CLA	O2D-CGD-CBD	4.90	119.97	111.27
12	A	1117	CLA	O2D-CGD-CBD	4.89	119.96	111.27
12	A	1103	CLA	C4A-NA-C1A	4.89	108.91	106.71
12	B	1023	CLA	C4A-NA-C1A	4.88	108.90	106.71
12	A	1106	CLA	C4A-NA-C1A	4.88	108.90	106.71
12	A	1137	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	F	4016	C7Z	C27-C26-C25	-4.86	109.70	121.46
12	A	1127	CLA	O2D-CGD-CBD	4.86	119.90	111.27
12	B	1206	CLA	C4A-NA-C1A	4.84	108.88	106.71
12	A	1111	CLA	O2D-CGD-CBD	4.84	119.86	111.27
12	B	1021	CLA	O2D-CGD-CBD	4.82	119.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1232	CLA	O2D-CGD-CBD	4.81	119.82	111.27
12	B	1224	CLA	O2D-CGD-CBD	4.81	119.82	111.27
12	A	1012	CLA	C4A-NA-C1A	4.79	108.86	106.71
12	A	1122	CLA	O2D-CGD-CBD	4.79	119.77	111.27
12	A	1126	CLA	C4A-NA-C1A	4.78	108.86	106.71
12	A	1102	CLA	C4A-NA-C1A	4.78	108.85	106.71
12	B	1214	CLA	O2D-CGD-CBD	4.77	119.74	111.27
12	A	1141	CLA	O2D-CGD-CBD	4.76	119.72	111.27
12	B	1224	CLA	O2A-C1-C2	4.75	121.13	108.64
12	B	1237	CLA	C4A-NA-C1A	4.74	108.84	106.71
12	B	1218	CLA	C4A-NA-C1A	4.72	108.83	106.71
17	B	4011	45D	C41-C37-C35	-4.71	120.58	127.31
12	A	1119	CLA	O2D-CGD-CBD	4.71	119.63	111.27
12	A	1112	CLA	C4A-NA-C1A	4.69	108.81	106.71
12	B	1202	CLA	C4A-NA-C1A	4.69	108.81	106.71
12	B	1211	CLA	C4A-NA-C1A	4.69	108.81	106.71
12	B	1214	CLA	C4A-NA-C1A	4.69	108.81	106.71
12	K	1402	CLA	O2D-CGD-CBD	4.68	119.59	111.27
12	A	1120	CLA	C4A-NA-C1A	4.68	108.81	106.71
12	B	1215	CLA	C4A-NA-C1A	4.68	108.81	106.71
12	B	1229	CLA	C2D-C1D-ND	4.68	113.55	110.10
12	B	1213	CLA	C4A-NA-C1A	4.67	108.81	106.71
25	I	4020	EQ3	C16-C15-C14	-4.66	113.92	123.47
12	A	1115	CLA	C4A-NA-C1A	4.65	108.80	106.71
12	B	1220	CLA	C4A-NA-C1A	4.64	108.79	106.71
12	A	1122	CLA	C4A-NA-C1A	4.64	108.79	106.71
12	B	1217	CLA	C4A-NA-C1A	4.64	108.79	106.71
12	A	1138	CLA	C4A-NA-C1A	4.64	108.79	106.71
25	I	4020	EQ3	C33-C5-C6	-4.64	119.32	124.53
12	A	1132	CLA	O2D-CGD-CBD	4.62	119.47	111.27
12	A	1109	CLA	O2D-CGD-CBD	4.62	119.47	111.27
12	A	1012	CLA	O2D-CGD-CBD	4.61	119.46	111.27
12	A	1141	CLA	C4A-NA-C1A	4.61	108.78	106.71
12	A	1139	CLA	O2D-CGD-CBD	4.61	119.45	111.27
12	A	1110	CLA	C4A-NA-C1A	4.59	108.77	106.71
12	A	1127	CLA	C4A-NA-C1A	4.59	108.77	106.71
12	A	1118	CLA	C4A-NA-C1A	4.59	108.77	106.71
12	B	1209	CLA	C4A-NA-C1A	4.59	108.77	106.71
23	F	4016	C7Z	C18-C5-C4	-4.58	105.86	114.36
12	A	1123	CLA	O2A-C1-C2	4.58	120.66	108.64
12	B	1210	CLA	C4A-NA-C1A	4.57	108.76	106.71
12	A	1102	CLA	O2A-C1-C2	4.57	120.64	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	4021	ECH	C20-C19-C18	-4.56	113.59	126.42
12	B	1206	CLA	O2D-CGD-CBD	4.56	119.37	111.27
12	B	1225	CLA	O2D-CGD-CBD	4.56	119.37	111.27
12	B	1240	CLA	C4A-NA-C1A	4.56	108.76	106.71
12	A	1116	CLA	C4A-NA-C1A	4.55	108.75	106.71
19	B	4006	ECH	C33-C5-C6	-4.55	119.42	124.53
12	B	1229	CLA	O2A-C1-C2	4.53	120.54	108.64
12	B	1221	CLA	C4A-NA-C1A	4.51	108.73	106.71
12	A	1118	CLA	O2A-C1-C2	4.51	120.48	108.64
12	A	1124	CLA	C4A-NA-C1A	4.51	108.73	106.71
12	B	1222	CLA	C4A-NA-C1A	4.50	108.73	106.71
12	A	1125	CLA	C4A-NA-C1A	4.50	108.73	106.71
19	B	4006	ECH	C16-C15-C14	-4.50	114.26	123.47
12	B	1212	CLA	C4A-NA-C1A	4.49	108.72	106.71
12	B	1235	CLA	C4A-NA-C1A	4.49	108.72	106.71
12	F	1301	CLA	C4A-NA-C1A	4.49	108.72	106.71
12	B	1236	CLA	C4A-NA-C1A	4.47	108.72	106.71
12	B	1204	CLA	C4A-NA-C1A	4.46	108.71	106.71
12	F	1302	CLA	C4A-NA-C1A	4.46	108.71	106.71
12	A	1108	CLA	C4A-NA-C1A	4.46	108.71	106.71
12	K	1402	CLA	C4A-NA-C1A	4.45	108.71	106.71
12	A	1013	CLA	O2D-CGD-CBD	4.45	119.17	111.27
12	B	1216	CLA	C4A-NA-C1A	4.44	108.70	106.71
12	A	1132	CLA	C4A-NA-C1A	4.44	108.70	106.71
12	A	1114	CLA	C4A-NA-C1A	4.44	108.70	106.71
12	B	1228	CLA	C4A-NA-C1A	4.43	108.70	106.71
12	B	1227	CLA	C4A-NA-C1A	4.43	108.70	106.71
12	B	1023	CLA	O2D-CGD-CBD	4.42	119.12	111.27
12	A	1133	CLA	C4A-NA-C1A	4.40	108.69	106.71
12	B	1239	CLA	C4A-NA-C1A	4.40	108.68	106.71
12	B	1232	CLA	C4A-NA-C1A	4.40	108.68	106.71
12	J	1302	CLA	C4A-NA-C1A	4.40	108.68	106.71
12	B	1229	CLA	CHD-C1D-ND	-4.39	120.42	124.45
12	B	1223	CLA	C4A-NA-C1A	4.39	108.68	106.71
12	K	1401	CLA	C4A-NA-C1A	4.39	108.68	106.71
23	J	4015	C7Z	C27-C28-C29	-4.37	119.64	126.23
12	A	1138	CLA	O2D-CGD-CBD	4.36	119.02	111.27
12	B	1207	CLA	C4A-NA-C1A	4.36	108.67	106.71
12	B	1234	CLA	C4A-NA-C1A	4.36	108.67	106.71
12	A	1117	CLA	C4A-NA-C1A	4.36	108.67	106.71
23	F	4016	C7Z	C21-C26-C25	-4.36	116.48	122.61
12	B	1231	CLA	C4A-NA-C1A	4.35	108.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1230	CLA	C4A-NA-C1A	4.35	108.66	106.71
12	B	1231	CLA	O2D-CGD-CBD	4.33	118.96	111.27
12	B	1023	CLA	C2D-C1D-ND	4.33	113.30	110.10
12	B	1201	CLA	C4A-NA-C1A	4.33	108.65	106.71
12	B	1229	CLA	C1D-ND-C4D	-4.32	103.27	106.33
12	A	1121	CLA	C4A-NA-C1A	4.31	108.64	106.71
12	B	1219	CLA	C4A-NA-C1A	4.31	108.64	106.71
12	A	1105	CLA	C4A-NA-C1A	4.31	108.64	106.71
19	M	4021	ECH	C16-C15-C14	-4.31	114.65	123.47
12	A	1140	CLA	C4A-NA-C1A	4.30	108.64	106.71
12	B	1203	CLA	O2D-CGD-CBD	4.30	118.90	111.27
12	B	1231	CLA	CHD-C1D-ND	-4.29	120.51	124.45
12	A	1109	CLA	C4A-NA-C1A	4.28	108.63	106.71
12	A	1130	CLA	C4A-NA-C1A	4.28	108.63	106.71
19	B	4006	ECH	C28-C27-C26	-4.27	114.71	118.65
12	A	1134	CLA	C4A-NA-C1A	4.27	108.62	106.71
12	B	1238	CLA	CHD-C1D-ND	-4.26	120.54	124.45
12	J	1303	CLA	C4A-NA-C1A	4.26	108.62	106.71
12	A	1104	CLA	C4A-NA-C1A	4.24	108.61	106.71
15	B	4004	BCR	C33-C5-C6	-4.24	119.77	124.53
12	A	1135	CLA	C4A-NA-C1A	4.23	108.61	106.71
15	A	4001	BCR	C15-C14-C13	-4.22	121.29	127.31
12	A	1136	CLA	C4A-NA-C1A	4.21	108.60	106.71
23	J	4015	C7Z	C18-C5-C4	-4.21	106.56	114.36
15	B	4018	BCR	C19-C18-C17	4.21	125.40	118.94
12	A	1137	CLA	C4A-NA-C1A	4.20	108.59	106.71
12	B	1229	CLA	C4A-NA-C1A	4.20	108.59	106.71
12	A	1126	CLA	O2A-C1-C2	4.19	119.66	108.64
12	A	1129	CLA	C4A-NA-C1A	4.16	108.58	106.71
12	A	1139	CLA	C4A-NA-C1A	4.16	108.58	106.71
15	J	4013	BCR	C33-C5-C6	-4.16	119.86	124.53
12	A	1113	CLA	C4A-NA-C1A	4.15	108.57	106.71
12	A	1131	CLA	C4A-NA-C1A	4.15	108.57	106.71
12	B	1222	CLA	C1-C2-C3	-4.15	120.03	126.75
12	A	1141	CLA	C2D-C1D-ND	4.13	113.14	110.10
12	B	1226	CLA	C4A-NA-C1A	4.12	108.56	106.71
12	A	1105	CLA	C2D-C1D-ND	4.12	113.14	110.10
12	A	1125	CLA	C2D-C1D-ND	4.12	113.14	110.10
12	A	1121	CLA	CHD-C1D-ND	-4.11	120.68	124.45
12	A	1128	CLA	C4A-NA-C1A	4.11	108.55	106.71
12	A	1101	CLA	C4A-NA-C1A	4.10	108.55	106.71
12	B	1227	CLA	CHD-C1D-ND	-4.10	120.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4015	C7Z	C7-C6-C5	-4.09	111.56	121.46
12	A	1013	CLA	C2D-C1D-ND	4.09	113.11	110.10
12	A	1101	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
12	B	1021	CLA	C1-C2-C3	-4.08	118.98	126.04
16	A	5003	LHG	O7-C7-C8	4.08	120.30	111.50
12	A	1119	CLA	CHD-C1D-ND	-4.07	120.71	124.45
12	B	1225	CLA	C2D-C1D-ND	4.07	113.10	110.10
12	A	1116	CLA	C2D-C1D-ND	4.06	113.09	110.10
12	B	1236	CLA	C2D-C1D-ND	4.06	113.09	110.10
12	A	1137	CLA	C2D-C1D-ND	4.05	113.09	110.10
12	A	1111	CLA	C4A-NA-C1A	4.05	108.53	106.71
19	M	4021	ECH	C33-C5-C6	-4.05	119.98	124.53
15	B	4010	BCR	C15-C14-C13	-4.04	121.54	127.31
25	I	4020	EQ3	C19-C18-C17	4.04	125.14	118.94
12	A	1109	CLA	CHD-C1D-ND	-4.04	120.74	124.45
12	B	1022	CLA	CHD-C1D-ND	-4.04	120.75	124.45
12	B	1212	CLA	C2D-C1D-ND	4.04	113.08	110.10
12	B	1022	CLA	C4A-NA-C1A	4.03	108.52	106.71
12	A	1119	CLA	C4A-NA-C1A	4.03	108.52	106.71
12	B	1231	CLA	C2D-C1D-ND	4.02	113.07	110.10
12	B	1235	CLA	C1-C2-C3	-4.02	119.09	126.04
12	B	1224	CLA	C4A-NA-C1A	4.01	108.51	106.71
12	A	1131	CLA	C2D-C1D-ND	4.01	113.06	110.10
12	K	1402	CLA	C2D-C1D-ND	4.01	113.06	110.10
12	B	1215	CLA	C2D-C1D-ND	4.01	113.06	110.10
12	B	1212	CLA	CHD-C1D-ND	-4.01	120.77	124.45
15	B	4004	BCR	C15-C14-C13	-4.00	121.60	127.31
12	B	1224	CLA	CHD-C1D-ND	-4.00	120.78	124.45
23	F	4016	C7Z	C1-C6-C5	-3.99	117.00	122.61
12	A	1124	CLA	C2D-C1D-ND	3.99	113.04	110.10
12	B	1221	CLA	C2D-C1D-ND	3.98	113.04	110.10
12	A	1013	CLA	C4A-NA-C1A	3.98	108.50	106.71
12	K	1402	CLA	CHD-C1D-ND	-3.98	120.80	124.45
12	B	1222	CLA	CHD-C1D-ND	-3.98	120.80	124.45
12	A	1103	CLA	C2D-C1D-ND	3.98	113.03	110.10
16	B	5004	LHG	O7-C7-C8	3.97	120.06	111.50
12	A	1102	CLA	C2D-C1D-ND	3.97	113.03	110.10
12	A	1118	CLA	CHD-C1D-ND	-3.96	120.82	124.45
12	A	1103	CLA	CHD-C1D-ND	-3.95	120.83	124.45
12	A	1114	CLA	C2D-C1D-ND	3.95	113.01	110.10
19	M	4021	ECH	C11-C10-C9	-3.94	121.68	127.31
12	B	1203	CLA	C4A-NA-C1A	3.94	108.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1209	CLA	C2D-C1D-ND	3.94	113.01	110.10
12	B	1230	CLA	CHD-C1D-ND	-3.94	120.83	124.45
12	A	1102	CLA	CHD-C1D-ND	-3.94	120.83	124.45
12	B	1225	CLA	C4A-NA-C1A	3.93	108.47	106.71
15	B	4005	BCR	C33-C5-C6	-3.93	120.11	124.53
12	B	1223	CLA	C2D-C1D-ND	3.93	113.00	110.10
12	B	1238	CLA	C2D-C1D-ND	3.93	113.00	110.10
12	J	1302	CLA	C2D-C1D-ND	3.93	113.00	110.10
12	A	1123	CLA	C2D-C1D-ND	3.93	113.00	110.10
12	B	1203	CLA	C2D-C1D-ND	3.93	113.00	110.10
12	A	1110	CLA	C2D-C1D-ND	3.92	113.00	110.10
12	A	1140	CLA	CHD-C1D-ND	-3.92	120.85	124.45
12	A	1122	CLA	C2D-C1D-ND	3.92	112.99	110.10
12	B	1228	CLA	CHD-C1D-ND	-3.91	120.86	124.45
12	B	1021	CLA	C2D-C1D-ND	3.91	112.99	110.10
12	A	1105	CLA	CHD-C1D-ND	-3.91	120.86	124.45
20	B	5005	LMG	O7-C10-C11	3.91	119.93	111.50
12	B	1204	CLA	C2D-C1D-ND	3.91	112.98	110.10
12	B	1201	CLA	CHD-C1D-ND	-3.91	120.86	124.45
12	B	1224	CLA	C2D-C1D-ND	3.91	112.98	110.10
12	B	1234	CLA	CHD-C1D-ND	-3.91	120.86	124.45
12	B	1235	CLA	CHD-C1D-ND	-3.91	120.86	124.45
12	F	1302	CLA	C2D-C1D-ND	3.91	112.98	110.10
12	B	1210	CLA	CHD-C1D-ND	-3.90	120.87	124.45
12	A	1138	CLA	CHD-C1D-ND	-3.90	120.87	124.45
12	A	1134	CLA	CHD-C1D-ND	-3.90	120.87	124.45
15	A	4003	BCR	C33-C5-C6	-3.90	120.15	124.53
12	B	1217	CLA	C2D-C1D-ND	3.90	112.98	110.10
12	B	1228	CLA	C2D-C1D-ND	3.90	112.98	110.10
12	A	1126	CLA	CHD-C1D-ND	-3.90	120.87	124.45
12	A	1115	CLA	CHD-C1D-ND	-3.90	120.87	124.45
12	A	1124	CLA	CHD-C1D-ND	-3.89	120.88	124.45
12	A	1118	CLA	C2D-C1D-ND	3.89	112.97	110.10
12	B	1230	CLA	C2D-C1D-ND	3.89	112.97	110.10
12	A	1011	CLA	CHD-C1D-ND	-3.89	120.88	124.45
12	B	1214	CLA	O2A-C1-C2	3.88	118.84	108.64
12	A	1101	CLA	C2D-C1D-ND	3.88	112.97	110.10
12	A	1104	CLA	CHD-C1D-ND	-3.88	120.89	124.45
12	A	1130	CLA	C2D-C1D-ND	3.88	112.96	110.10
12	F	1302	CLA	CHD-C1D-ND	-3.88	120.89	124.45
12	B	1214	CLA	C2D-C1D-ND	3.88	112.96	110.10
12	A	1133	CLA	CHD-C1D-ND	-3.87	120.90	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4018	BCR	C36-C18-C17	-3.87	117.50	122.92
12	A	1135	CLA	CHD-C1D-ND	-3.87	120.90	124.45
12	A	1134	CLA	C2D-C1D-ND	3.87	112.95	110.10
12	K	1401	CLA	CHD-C1D-ND	-3.86	120.90	124.45
23	J	4015	C7Z	C7-C8-C9	-3.86	120.40	126.23
12	A	1131	CLA	CHD-C1D-ND	-3.86	120.91	124.45
12	A	1136	CLA	CHD-C1D-ND	-3.85	120.91	124.45
12	A	1133	CLA	C2D-C1D-ND	3.85	112.94	110.10
12	B	1219	CLA	C2D-C1D-ND	3.85	112.94	110.10
12	B	1226	CLA	CHD-C1D-ND	-3.85	120.92	124.45
12	A	1141	CLA	CHD-C1D-ND	-3.85	120.92	124.45
12	J	1302	CLA	CHD-C1D-ND	-3.85	120.92	124.45
12	A	1128	CLA	CHD-C1D-ND	-3.85	120.92	124.45
12	B	1210	CLA	C2D-C1D-ND	3.85	112.94	110.10
12	A	1013	CLA	CHD-C1D-ND	-3.85	120.92	124.45
12	F	1301	CLA	C2D-C1D-ND	3.85	112.94	110.10
12	B	1219	CLA	CHD-C1D-ND	-3.84	120.92	124.45
12	B	1207	CLA	CHD-C1D-ND	-3.84	120.92	124.45
12	B	1208	CLA	CHD-C1D-ND	-3.84	120.93	124.45
16	A	5001	LHG	O7-C7-C8	3.83	119.76	111.50
12	B	1222	CLA	C2D-C1D-ND	3.83	112.93	110.10
12	A	1139	CLA	CHD-C1D-ND	-3.83	120.93	124.45
12	A	1127	CLA	C2D-C1D-ND	3.83	112.93	110.10
12	B	1227	CLA	C2D-C1D-ND	3.83	112.93	110.10
12	A	1132	CLA	CHD-C1D-ND	-3.83	120.94	124.45
12	A	1113	CLA	C2D-C1D-ND	3.83	112.92	110.10
12	B	1232	CLA	C2D-C1D-ND	3.83	112.92	110.10
12	B	1239	CLA	C2D-C1D-ND	3.83	112.92	110.10
12	B	1022	CLA	C2D-C1D-ND	3.83	112.92	110.10
12	F	1301	CLA	CHD-C1D-ND	-3.82	120.94	124.45
12	A	1114	CLA	CHD-C1D-ND	-3.82	120.94	124.45
12	B	1232	CLA	CHD-C1D-ND	-3.82	120.94	124.45
12	B	1237	CLA	CHD-C1D-ND	-3.82	120.95	124.45
12	A	1129	CLA	CHD-C1D-ND	-3.82	120.95	124.45
12	A	1108	CLA	CHD-C1D-ND	-3.81	120.95	124.45
12	B	1203	CLA	CHD-C1D-ND	-3.81	120.95	124.45
12	B	1211	CLA	CHD-C1D-ND	-3.81	120.95	124.45
12	J	1303	CLA	CHD-C1D-ND	-3.81	120.95	124.45
20	B	5002	LMG	O7-C10-C11	3.81	119.71	111.50
12	A	1011	CLA	C2D-C1D-ND	3.81	112.91	110.10
15	A	4012	BCR	C33-C5-C6	-3.81	120.25	124.53
12	A	1140	CLA	C2D-C1D-ND	3.81	112.91	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1218	CLA	C2D-C1D-ND	3.80	112.91	110.10
12	A	1127	CLA	CHD-C1D-ND	-3.80	120.96	124.45
12	B	1234	CLA	C2D-C1D-ND	3.80	112.91	110.10
12	A	1136	CLA	C2D-C1D-ND	3.80	112.90	110.10
12	B	1206	CLA	CHD-C1D-ND	-3.80	120.96	124.45
12	K	1401	CLA	C2D-C1D-ND	3.80	112.90	110.10
12	A	1122	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	M	4021	ECH	C7-C8-C9	-3.78	120.52	126.23
12	B	1218	CLA	CHD-C1D-ND	-3.78	120.98	124.45
12	B	1238	CLA	C1D-ND-C4D	-3.78	103.65	106.33
12	A	1108	CLA	C2D-C1D-ND	3.78	112.89	110.10
21	F	5001	SQD	O7-S-C6	-3.77	102.45	106.94
12	A	1115	CLA	C2D-C1D-ND	3.77	112.89	110.10
12	B	1206	CLA	C2D-C1D-ND	3.77	112.89	110.10
12	A	1137	CLA	CHD-C1D-ND	-3.77	120.99	124.45
12	B	1202	CLA	C2D-C1D-ND	3.77	112.88	110.10
12	B	1236	CLA	CHD-C1D-ND	-3.77	120.99	124.45
12	A	1101	CLA	CHD-C1D-ND	-3.77	120.99	124.45
12	A	1105	CLA	C1D-ND-C4D	-3.77	103.66	106.33
12	B	1238	CLA	C4A-NA-C1A	3.76	108.40	106.71
12	A	1112	CLA	C2D-C1D-ND	3.76	112.88	110.10
12	A	1116	CLA	CHD-C1D-ND	-3.76	121.00	124.45
12	B	1214	CLA	CHD-C1D-ND	-3.75	121.01	124.45
12	B	1023	CLA	CHD-C1D-ND	-3.74	121.01	124.45
12	A	1105	CLA	C1-C2-C3	-3.74	119.57	126.04
19	M	4021	ECH	C28-C27-C26	-3.74	115.20	118.65
12	A	1120	CLA	C2D-C1D-ND	3.74	112.86	110.10
12	A	1117	CLA	CHD-C1D-ND	-3.73	121.02	124.45
12	B	1202	CLA	CHD-C1D-ND	-3.73	121.03	124.45
12	J	1303	CLA	C2D-C1D-ND	3.73	112.85	110.10
12	A	1117	CLA	C2D-C1D-ND	3.73	112.85	110.10
12	B	1237	CLA	C2D-C1D-ND	3.72	112.85	110.10
12	A	1135	CLA	C2D-C1D-ND	3.72	112.84	110.10
23	F	4016	C7Z	C7-C8-C9	-3.72	120.62	126.23
12	B	1235	CLA	C2D-C1D-ND	3.72	112.84	110.10
12	A	1130	CLA	CHD-C1D-ND	-3.71	121.04	124.45
12	B	1208	CLA	C4A-NA-C1A	3.71	108.38	106.71
12	A	1129	CLA	C2D-C1D-ND	3.71	112.84	110.10
12	A	1119	CLA	C2D-C1D-ND	3.71	112.84	110.10
12	A	1113	CLA	CHD-C1D-ND	-3.71	121.05	124.45
12	B	1239	CLA	CHD-C1D-ND	-3.71	121.05	124.45
12	B	1216	CLA	CHD-C1D-ND	-3.71	121.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1106	CLA	CHD-C1D-ND	-3.70	121.05	124.45
12	A	1139	CLA	C1-C2-C3	-3.70	119.65	126.04
15	B	4018	BCR	C27-C26-C25	-3.69	117.37	122.73
12	A	1126	CLA	C2D-C1D-ND	3.69	112.83	110.10
12	B	1208	CLA	C2D-C1D-ND	3.69	112.82	110.10
12	B	1213	CLA	CHD-C1D-ND	-3.69	121.06	124.45
12	B	1223	CLA	CHD-C1D-ND	-3.69	121.06	124.45
12	B	1213	CLA	C2D-C1D-ND	3.68	112.82	110.10
12	B	1207	CLA	C2D-C1D-ND	3.68	112.81	110.10
12	B	1209	CLA	CHD-C1D-ND	-3.67	121.08	124.45
12	A	1110	CLA	CHD-C1D-ND	-3.67	121.08	124.45
12	B	1204	CLA	CHD-C1D-ND	-3.67	121.08	124.45
12	A	1112	CLA	CHD-C1D-ND	-3.65	121.10	124.45
12	A	1104	CLA	C2D-C1D-ND	3.65	112.79	110.10
12	A	1111	CLA	CHD-C1D-ND	-3.65	121.10	124.45
12	A	1106	CLA	C2D-C1D-ND	3.64	112.79	110.10
15	I	4018	BCR	C4-C5-C6	-3.64	117.45	122.73
12	B	1201	CLA	C2D-C1D-ND	3.64	112.78	110.10
12	A	1109	CLA	C2D-C1D-ND	3.64	112.78	110.10
12	B	1205	CLA	C2D-C1D-ND	3.63	112.78	110.10
12	B	1225	CLA	CHD-C1D-ND	-3.63	121.12	124.45
12	B	1231	CLA	C1D-ND-C4D	-3.63	103.76	106.33
12	B	1211	CLA	C2D-C1D-ND	3.62	112.78	110.10
12	B	1217	CLA	CHD-C1D-ND	-3.62	121.12	124.45
12	B	1224	CLA	C1-C2-C3	-3.62	119.78	126.04
12	A	1118	CLA	C1-C2-C3	-3.62	120.90	126.75
12	A	1120	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	B	4011	45D	C42-C38-C36	-3.59	122.18	127.31
12	B	1220	CLA	C2D-C1D-ND	3.59	112.75	110.10
12	A	1012	CLA	C2D-C1D-ND	3.59	112.75	110.10
12	B	1240	CLA	CHD-C1D-ND	-3.58	121.16	124.45
12	L	1502	CLA	CHD-C1D-ND	-3.58	121.16	124.45
12	B	1204	CLA	C1D-ND-C4D	-3.58	103.79	106.33
12	K	1402	CLA	C1D-ND-C4D	-3.58	103.79	106.33
12	A	1138	CLA	C2D-C1D-ND	3.58	112.74	110.10
12	B	1240	CLA	CMA-C3A-C4A	3.58	121.39	111.77
12	L	1502	CLA	C2D-C1D-ND	3.57	112.74	110.10
12	A	1131	CLA	C1D-ND-C4D	-3.56	103.81	106.33
12	B	1215	CLA	CHD-C1D-ND	-3.55	121.19	124.45
12	B	1225	CLA	C1D-ND-C4D	-3.55	103.81	106.33
25	I	4020	EQ3	C36-C18-C17	-3.55	117.96	122.92
12	B	1021	CLA	CHD-C1D-ND	-3.54	121.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1125	CLA	CHD-C1D-ND	-3.54	121.20	124.45
15	B	4017	BCR	C33-C5-C6	-3.54	120.56	124.53
12	A	1103	CLA	C1D-ND-C4D	-3.53	103.83	106.33
12	A	1123	CLA	CHD-C1D-ND	-3.53	121.21	124.45
12	A	1121	CLA	C2D-C1D-ND	3.53	112.71	110.10
12	B	1230	CLA	C1D-ND-C4D	-3.53	103.83	106.33
12	A	1127	CLA	C1D-ND-C4D	-3.53	103.83	106.33
12	B	1216	CLA	C2D-C1D-ND	3.53	112.70	110.10
12	B	1227	CLA	C1D-ND-C4D	-3.53	103.83	106.33
12	B	1205	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	B	4011	45D	C22-C16-C08	-3.52	118.45	124.11
12	A	1116	CLA	C1D-ND-C4D	-3.52	103.83	106.33
12	A	1134	CLA	C1D-ND-C4D	-3.51	103.84	106.33
12	A	1136	CLA	C1D-ND-C4D	-3.51	103.84	106.33
12	A	1141	CLA	C1D-ND-C4D	-3.51	103.84	106.33
12	A	1139	CLA	C2D-C1D-ND	3.51	112.69	110.10
15	A	4007	BCR	C33-C5-C6	-3.51	120.59	124.53
12	B	1208	CLA	C1D-ND-C4D	-3.50	103.85	106.33
15	K	4001	BCR	C19-C18-C17	3.50	124.31	118.94
21	B	5008	SQD	O7-S-C6	-3.50	102.78	106.94
15	I	4018	BCR	C33-C5-C4	3.49	120.33	113.62
12	B	1202	CLA	C1-C2-C3	-3.48	120.02	126.04
25	I	4020	EQ3	C21-C20-C19	-3.48	112.35	123.22
12	B	1023	CLA	C1D-ND-C4D	-3.48	103.86	106.33
12	A	1107	CLA	O2D-CGD-CBD	3.48	117.46	111.27
12	A	1122	CLA	C1D-ND-C4D	-3.48	103.87	106.33
12	A	1114	CLA	C1D-ND-C4D	-3.46	103.87	106.33
15	B	4018	BCR	C30-C25-C26	-3.46	117.74	122.61
12	A	1137	CLA	C1D-ND-C4D	-3.46	103.88	106.33
12	J	1302	CLA	C1D-ND-C4D	-3.46	103.88	106.33
12	B	1236	CLA	C1D-ND-C4D	-3.46	103.88	106.33
12	B	1221	CLA	CHD-C1D-ND	-3.46	121.28	124.45
12	A	1133	CLA	C1D-ND-C4D	-3.45	103.88	106.33
15	A	4012	BCR	C36-C18-C17	-3.45	118.09	122.92
12	A	1128	CLA	C2D-C1D-ND	3.45	112.64	110.10
12	A	1132	CLA	C2D-C1D-ND	3.44	112.64	110.10
12	A	1124	CLA	C1D-ND-C4D	-3.44	103.89	106.33
12	B	1212	CLA	C1D-ND-C4D	-3.43	103.90	106.33
12	A	1119	CLA	C1D-ND-C4D	-3.43	103.90	106.33
12	A	1111	CLA	C2D-C1D-ND	3.43	112.63	110.10
12	B	1203	CLA	C1D-ND-C4D	-3.42	103.90	106.33
23	J	4015	C7Z	C24-C25-C26	-3.42	113.22	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1108	CLA	C1D-ND-C4D	-3.42	103.90	106.33
12	B	1222	CLA	C1D-ND-C4D	-3.42	103.91	106.33
12	F	1302	CLA	C1D-ND-C4D	-3.42	103.91	106.33
15	B	4010	BCR	C28-C27-C26	-3.42	107.98	114.08
12	K	1401	CLA	C1D-ND-C4D	-3.41	103.91	106.33
12	B	1209	CLA	C1D-ND-C4D	-3.41	103.92	106.33
12	A	1101	CLA	C1D-ND-C4D	-3.40	103.92	106.33
12	A	1011	CLA	C1D-ND-C4D	-3.40	103.92	106.33
12	B	1232	CLA	C1D-ND-C4D	-3.40	103.92	106.33
12	B	1219	CLA	C1D-ND-C4D	-3.40	103.92	106.33
12	A	1118	CLA	C1D-ND-C4D	-3.40	103.92	106.33
12	B	1220	CLA	CHD-C1D-ND	-3.39	121.34	124.45
19	B	4006	ECH	C11-C12-C13	-3.39	116.90	126.42
12	A	1110	CLA	C1D-ND-C4D	-3.39	103.93	106.33
12	B	1240	CLA	C2D-C1D-ND	3.39	112.60	110.10
12	B	1214	CLA	C1D-ND-C4D	-3.39	103.93	106.33
12	B	1210	CLA	C1D-ND-C4D	-3.38	103.93	106.33
12	A	1012	CLA	CHD-C1D-ND	-3.38	121.34	124.45
17	B	4011	45D	C28-C26-C30	-3.38	118.19	122.92
15	F	4014	BCR	C19-C18-C17	3.38	124.12	118.94
12	A	1102	CLA	C1D-ND-C4D	-3.38	103.94	106.33
15	J	4013	BCR	C15-C14-C13	-3.36	122.52	127.31
12	B	1223	CLA	C1D-ND-C4D	-3.36	103.95	106.33
15	F	4014	BCR	C36-C18-C17	-3.36	118.22	122.92
15	K	4001	BCR	C36-C18-C17	-3.35	118.22	122.92
12	A	1107	CLA	CHD-C1D-ND	-3.35	121.38	124.45
12	A	1126	CLA	C1D-ND-C4D	-3.35	103.95	106.33
12	A	1138	CLA	C1-C2-C3	-3.35	120.25	126.04
12	A	1135	CLA	C1D-ND-C4D	-3.34	103.96	106.33
12	B	1211	CLA	C1D-ND-C4D	-3.34	103.96	106.33
12	B	1217	CLA	C1D-ND-C4D	-3.33	103.97	106.33
12	B	1235	CLA	C1D-ND-C4D	-3.33	103.97	106.33
12	B	1228	CLA	C1D-ND-C4D	-3.33	103.97	106.33
15	A	4012	BCR	C19-C18-C17	3.33	124.05	118.94
15	A	4003	BCR	C33-C5-C4	3.32	120.00	113.62
12	A	1115	CLA	C1D-ND-C4D	-3.32	103.98	106.33
12	A	1112	CLA	C1D-ND-C4D	-3.32	103.98	106.33
12	A	1121	CLA	C1D-ND-C4D	-3.32	103.98	106.33
12	A	1140	CLA	C1D-ND-C4D	-3.32	103.98	106.33
12	B	1022	CLA	C1D-ND-C4D	-3.32	103.98	106.33
23	F	4016	C7Z	C28-C27-C26	-3.31	117.90	127.20
12	A	1125	CLA	C1D-ND-C4D	-3.31	103.98	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1237	CLA	C1D-ND-C4D	-3.31	103.99	106.33
12	B	1229	CLA	C1-C2-C3	-3.30	120.33	126.04
12	B	1207	CLA	C1D-ND-C4D	-3.30	103.99	106.33
12	B	1224	CLA	C1D-ND-C4D	-3.30	103.99	106.33
23	J	4015	C7Z	C4-C5-C6	-3.30	113.50	120.85
12	B	1215	CLA	C1D-ND-C4D	-3.29	104.00	106.33
12	A	1130	CLA	C1D-ND-C4D	-3.29	104.00	106.33
12	B	1234	CLA	C1D-ND-C4D	-3.29	104.00	106.33
25	I	4020	EQ3	C2-C3-C4	-3.28	105.81	110.30
12	F	1301	CLA	C1D-ND-C4D	-3.28	104.01	106.33
15	B	4010	BCR	C33-C5-C4	3.27	119.90	113.62
12	A	1104	CLA	C1D-ND-C4D	-3.27	104.01	106.33
12	A	1013	CLA	C1D-ND-C4D	-3.26	104.02	106.33
12	B	1021	CLA	C1D-ND-C4D	-3.26	104.02	106.33
12	A	1139	CLA	C1D-ND-C4D	-3.26	104.02	106.33
12	A	1123	CLA	CMA-C3A-C4A	3.26	120.52	111.77
12	A	1109	CLA	C1D-ND-C4D	-3.25	104.02	106.33
12	B	1201	CLA	C1D-ND-C4D	-3.25	104.02	106.33
12	A	1117	CLA	C1D-ND-C4D	-3.25	104.03	106.33
12	J	1303	CLA	C1D-ND-C4D	-3.25	104.03	106.33
12	B	1234	CLA	C1-C2-C3	-3.25	120.42	126.04
12	B	1205	CLA	C1D-ND-C4D	-3.24	104.03	106.33
12	A	1132	CLA	C1-C2-C3	-3.23	120.46	126.04
12	A	1106	CLA	C1D-ND-C4D	-3.21	104.05	106.33
12	A	1139	CLA	CMA-C3A-C4A	3.21	120.40	111.77
12	A	1113	CLA	C1D-ND-C4D	-3.21	104.06	106.33
12	L	1502	CLA	CMA-C3A-C4A	3.21	120.40	111.77
12	B	1216	CLA	C1D-ND-C4D	-3.21	104.06	106.33
12	B	1239	CLA	C1D-ND-C4D	-3.20	104.06	106.33
15	I	4018	BCR	C1-C6-C5	-3.20	118.11	122.61
19	B	4006	ECH	C20-C19-C18	-3.20	117.44	126.42
12	B	1213	CLA	C1D-ND-C4D	-3.19	104.07	106.33
12	A	1109	CLA	C1-C2-C3	-3.19	120.52	126.04
15	B	4017	BCR	C15-C14-C13	-3.19	122.76	127.31
12	A	1106	CLA	C1-C2-C3	-3.18	120.54	126.04
12	B	1226	CLA	C2D-C1D-ND	3.18	112.45	110.10
12	B	1218	CLA	C1D-ND-C4D	-3.17	104.08	106.33
15	A	4001	BCR	C33-C5-C4	3.17	119.70	113.62
15	B	4005	BCR	C23-C24-C25	-3.16	118.32	127.20
12	A	1129	CLA	C1D-ND-C4D	-3.16	104.09	106.33
12	A	1138	CLA	C1D-ND-C4D	-3.16	104.09	106.33
12	A	1120	CLA	C1D-ND-C4D	-3.15	104.09	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1202	CLA	C1D-ND-C4D	-3.15	104.10	106.33
12	A	1123	CLA	C1D-ND-C4D	-3.15	104.10	106.33
15	K	4001	BCR	C33-C5-C6	-3.15	121.00	124.53
12	A	1117	CLA	CMA-C3A-C4A	3.14	120.22	111.77
12	A	1123	CLA	C1-C2-C3	-3.14	120.61	126.04
12	L	1502	CLA	C1D-ND-C4D	-3.13	104.11	106.33
12	B	1220	CLA	CMA-C3A-C4A	3.13	120.19	111.77
12	B	1206	CLA	C1D-ND-C4D	-3.13	104.11	106.33
12	B	1022	CLA	C1-C2-C3	-3.13	120.64	126.04
12	B	1221	CLA	C1D-ND-C4D	-3.13	104.11	106.33
12	A	1130	CLA	CMA-C3A-C4A	3.12	120.15	111.77
12	A	1135	CLA	CMA-C3A-C4A	3.11	120.14	111.77
13	B	2002	PQN	C11-C12-C13	-3.11	121.61	126.79
15	B	4010	BCR	C37-C22-C21	-3.11	118.57	122.92
12	B	1240	CLA	C1D-ND-C4D	-3.10	104.13	106.33
12	A	1115	CLA	C1-C2-C3	-3.10	120.68	126.04
15	B	4010	BCR	C33-C5-C6	-3.09	121.05	124.53
13	B	2002	PQN	C14-C13-C15	3.09	120.47	115.27
12	A	1011	CLA	C1-C2-C3	-3.09	120.70	126.04
12	J	1303	CLA	CMA-C3A-C4A	3.08	120.06	111.77
12	A	1122	CLA	CMA-C3A-C4A	3.08	120.05	111.77
12	A	1113	CLA	CMA-C3A-C4A	3.08	120.05	111.77
12	A	1102	CLA	C1-C2-C3	-3.08	120.72	126.04
12	A	1115	CLA	CMA-C3A-C4A	3.07	120.03	111.77
17	B	4011	45D	C19-C23-C25	-3.07	121.60	126.23
25	I	4020	EQ3	C37-C22-C23	3.07	122.91	118.08
15	K	4001	BCR	C37-C22-C21	-3.07	118.62	122.92
12	B	1209	CLA	CMA-C3A-C4A	3.07	120.02	111.77
12	A	1121	CLA	CMA-C3A-C4A	3.07	120.02	111.77
12	A	1120	CLA	CMA-C3A-C4A	3.07	120.01	111.77
12	F	1302	CLA	CMA-C3A-C4A	3.06	120.01	111.77
12	A	1125	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	K	4001	BCR	C15-C14-C13	-3.06	122.95	127.31
12	B	1022	CLA	CMA-C3A-C4A	3.06	119.98	111.77
12	B	1208	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	A	1109	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	A	1107	CLA	C2D-C1D-ND	3.05	112.35	110.10
12	B	1237	CLA	CMA-C3A-C4A	3.05	119.96	111.77
12	B	1213	CLA	CMA-C3A-C4A	3.03	119.92	111.77
12	B	1214	CLA	CMA-C3A-C4A	3.03	119.91	111.77
12	A	1107	CLA	C1D-ND-C4D	-3.02	104.19	106.33
12	A	1105	CLA	CMA-C3A-C4A	3.02	119.88	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4001	BCR	C33-C5-C6	-3.02	121.14	124.53
15	A	4012	BCR	C33-C5-C4	3.02	119.41	113.62
15	B	4018	BCR	C4-C5-C6	-3.01	118.36	122.73
15	A	4003	BCR	C36-C18-C17	-3.01	118.70	122.92
12	A	1136	CLA	CMA-C3A-C4A	3.01	119.87	111.77
12	A	1110	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	B	4005	BCR	C27-C26-C25	-3.01	118.36	122.73
15	B	4017	BCR	C36-C18-C17	-3.01	118.71	122.92
16	B	5006	LHG	C5-O7-C7	-3.00	112.30	117.90
17	B	4011	45D	C23-C19-C07	-3.00	118.76	127.20
12	K	1401	CLA	CMA-C3A-C4A	3.00	119.85	111.77
12	B	1218	CLA	CMA-C3A-C4A	3.00	119.83	111.77
12	B	1232	CLA	CMA-C3A-C4A	3.00	119.83	111.77
12	B	1235	CLA	CMA-C3A-C4A	2.99	119.82	111.77
12	B	1202	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
15	B	4017	BCR	C33-C5-C4	2.99	119.36	113.62
12	A	1140	CLA	C1-C2-C3	-2.99	120.87	126.04
23	F	4016	C7Z	C24-C25-C26	-2.99	114.19	120.85
12	B	1223	CLA	CMA-C3A-C4A	2.98	119.79	111.77
12	K	1402	CLA	CMA-C3A-C4A	2.98	119.78	111.77
25	I	4020	EQ3	C34-C9-C10	-2.98	118.75	122.92
12	B	1217	CLA	CMA-C3A-C4A	2.97	119.76	111.77
12	A	1134	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	A	1126	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	B	1226	CLA	C1D-ND-C4D	-2.96	104.23	106.33
12	A	1013	CLA	CMB-C2B-C3B	2.96	130.22	124.68
15	B	4004	BCR	C33-C5-C4	2.96	119.30	113.62
12	B	1219	CLA	CMA-C3A-C4A	2.96	119.72	111.77
12	A	1114	CLA	CMA-C3A-C4A	2.96	119.72	111.77
15	B	4010	BCR	C27-C26-C25	-2.95	118.45	122.73
12	J	1302	CLA	CMA-C3A-C4A	2.95	119.70	111.77
17	B	4011	45D	C24-C26-C30	2.94	123.45	118.94
12	A	1137	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	B	4018	BCR	C33-C5-C4	2.93	119.25	113.62
12	B	1207	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	F	4014	BCR	C33-C5-C6	-2.93	121.24	124.53
12	B	1212	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	A	1108	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	A	1012	CLA	C1D-ND-C4D	-2.92	104.26	106.33
12	A	1124	CLA	CMA-C3A-C4A	2.92	119.62	111.77
12	B	1211	CLA	CMA-C3A-C4A	2.92	119.62	111.77
12	A	1132	CLA	C1D-ND-C4D	-2.92	104.26	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4008	BCR	C15-C14-C13	-2.92	123.15	127.31
12	A	1127	CLA	CMA-C3A-C4A	2.91	119.59	111.77
12	A	1128	CLA	C1D-ND-C4D	-2.90	104.27	106.33
19	B	4006	ECH	C8-C7-C6	-2.90	119.05	127.20
12	B	1230	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	B	1226	CLA	CMB-C2B-C3B	2.90	130.10	124.68
15	I	4018	BCR	C23-C24-C25	-2.89	119.08	127.20
12	A	1138	CLA	CMA-C3A-C4A	2.89	119.53	111.77
13	A	2001	PQN	C14-C13-C15	2.88	120.12	115.27
12	B	1227	CLA	CMA-C3A-C4A	2.88	119.50	111.77
12	L	1502	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	B	4017	BCR	C23-C24-C25	-2.87	119.14	127.20
15	A	4008	BCR	C36-C18-C17	-2.86	118.91	122.92
19	B	4006	ECH	C7-C8-C9	-2.86	121.92	126.23
12	B	1228	CLA	CMA-C3A-C4A	2.85	119.44	111.77
12	A	1111	CLA	C1D-ND-C4D	-2.85	104.31	106.33
17	B	4011	45D	C41-C42-C38	-2.85	117.64	123.47
12	B	1222	CLA	CMA-C3A-C4A	2.85	119.43	111.77
12	B	1220	CLA	C1D-ND-C4D	-2.85	104.31	106.33
12	B	1205	CLA	CMA-C3A-C4A	2.85	119.42	111.77
12	B	1234	CLA	CMA-C3A-C4A	2.84	119.41	111.77
12	B	1206	CLA	CMA-C3A-C4A	2.83	119.39	111.77
12	B	1225	CLA	CMA-C3A-C4A	2.83	119.37	111.77
12	B	1207	CLA	O2A-CGA-CBA	2.82	120.77	111.91
12	B	1226	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
15	A	4008	BCR	C34-C9-C10	-2.81	118.98	122.92
12	A	1138	CLA	CMB-C2B-C3B	2.81	129.93	124.68
12	A	1129	CLA	CMA-C3A-C4A	2.81	119.32	111.77
12	A	1140	CLA	CMA-C3A-C4A	2.81	119.32	111.77
12	B	1216	CLA	CMA-C3A-C4A	2.81	119.31	111.77
20	B	5002	LMG	O8-C28-C29	2.80	120.70	111.91
12	A	1102	CLA	O2A-CGA-CBA	2.80	120.69	111.91
12	B	1202	CLA	O2A-CGA-CBA	2.80	120.69	111.91
15	I	4018	BCR	C38-C26-C25	-2.79	121.39	124.53
15	F	4014	BCR	C33-C5-C4	2.79	118.98	113.62
12	A	1126	CLA	C1-C2-C3	-2.79	121.22	126.04
12	A	1116	CLA	CMA-C3A-C4A	2.78	119.23	111.77
12	B	1227	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	A	4008	BCR	C33-C5-C6	-2.77	121.42	124.53
12	A	1128	CLA	CMA-C3A-C4A	2.77	119.21	111.77
12	B	1215	CLA	CMA-C3A-C4A	2.77	119.21	111.77
15	A	4001	BCR	C37-C22-C21	-2.76	119.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1218	CLA	CMB-C2B-C3B	2.75	129.83	124.68
12	A	1128	CLA	C1-C2-C3	-2.75	121.28	126.04
12	B	1214	CLA	C1-C2-C3	-2.75	121.28	126.04
19	M	4021	ECH	C11-C12-C13	-2.75	118.69	126.42
12	B	1201	CLA	CMB-C2B-C3B	2.75	129.82	124.68
12	B	1240	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
12	A	1128	CLA	CMB-C2B-C3B	2.74	129.80	124.68
12	A	1116	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	A	4007	BCR	C36-C18-C17	-2.73	119.09	122.92
12	A	1101	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
12	A	1107	CLA	CMA-C3A-C4A	2.73	119.11	111.77
20	B	5005	LMG	O8-C28-C29	2.73	120.46	111.91
15	A	4008	BCR	C37-C22-C21	-2.72	119.11	122.92
12	B	1226	CLA	CMA-C3A-C4A	2.72	119.08	111.77
15	I	4018	BCR	C34-C9-C10	-2.72	119.12	122.92
24	F	6001	LMT	C3'-C4'-C5'	-2.72	104.70	110.93
12	B	1234	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	J	4013	BCR	C33-C5-C4	2.71	118.83	113.62
12	F	1302	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
12	B	1210	CLA	CMA-C3A-C4A	2.71	119.06	111.77
15	B	4010	BCR	C38-C26-C27	2.71	118.82	113.62
12	A	1128	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	A	4008	BCR	C33-C5-C4	2.69	118.78	113.62
12	A	1125	CLA	CMB-C2B-C3B	2.69	129.71	124.68
12	A	1120	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
12	B	1224	CLA	O2A-CGA-CBA	2.68	120.33	111.91
12	B	1224	CLA	CMA-C3A-C4A	2.68	118.98	111.77
15	A	4007	BCR	C27-C26-C25	-2.68	118.84	122.73
25	I	4020	EQ3	C38-C26-C27	2.68	119.47	115.48
13	A	2001	PQN	C11-C12-C13	-2.68	122.33	126.79
12	B	1209	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	F	4016	C7Z	C38-C25-C24	-2.68	109.40	114.36
12	B	1204	CLA	CMA-C3A-C4A	2.67	118.95	111.77
15	J	4013	BCR	C36-C18-C17	-2.67	119.18	122.92
12	A	1141	CLA	CMA-C3A-C4A	2.66	118.93	111.77
12	K	1401	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
12	A	1104	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
12	B	1236	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
15	F	4014	BCR	C37-C22-C21	-2.66	119.20	122.92
12	A	1103	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
12	A	1102	CLA	CMA-C3A-C4A	2.66	118.92	111.77
15	F	4014	BCR	C34-C9-C10	-2.66	119.20	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1201	CLA	CMA-C3A-C4A	2.65	118.91	111.77
12	A	1012	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
15	I	4018	BCR	C37-C22-C23	2.65	122.25	118.08
12	B	1239	CLA	CMA-C3A-C4A	2.64	118.88	111.77
25	I	4020	EQ3	C33-C5-C4	2.64	119.25	114.36
12	B	1213	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
12	A	1135	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
17	B	4011	45D	C30-C32-C34	-2.63	115.00	123.22
12	J	1303	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
12	A	1117	CLA	CMB-C2B-C3B	2.63	129.60	124.68
25	I	4020	EQ3	C38-C26-C25	-2.62	119.89	124.11
19	M	4021	ECH	C15-C14-C13	-2.62	123.56	127.31
12	B	1238	CLA	CMA-C3A-C4A	2.62	118.82	111.77
12	B	1205	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
12	A	1132	CLA	CMA-C3A-C4A	2.62	118.80	111.77
17	B	4011	45D	C21-C15-C07	-2.61	119.92	124.11
15	B	4018	BCR	C28-C27-C26	-2.61	109.42	114.08
12	F	1301	CLA	CMA-C3A-C4A	2.60	118.77	111.77
12	A	1113	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
12	A	1112	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	A	4001	BCR	C27-C26-C25	-2.59	118.96	122.73
15	A	4007	BCR	C38-C26-C27	2.59	118.60	113.62
12	A	1011	CLA	CMA-C3A-C4A	2.59	118.73	111.77
19	B	4006	ECH	C23-C24-C25	-2.59	119.93	127.20
16	A	5003	LHG	O8-C23-C24	2.59	120.03	111.91
15	B	4017	BCR	C27-C26-C25	-2.59	118.98	122.73
12	B	1222	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
12	B	1207	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
12	A	1106	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
17	B	4011	45D	C05-C03-C07	2.58	114.45	110.48
15	B	4005	BCR	C38-C26-C27	2.58	118.57	113.62
12	J	1302	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
12	A	1141	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	I	4018	BCR	C38-C26-C27	2.57	118.56	113.62
12	A	1110	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	A	4007	BCR	C23-C24-C25	-2.57	119.98	127.20
12	J	1303	CLA	CMB-C2B-C3B	2.57	129.49	124.68
12	A	1116	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
16	B	5004	LHG	O8-C23-C24	2.57	119.97	111.91
12	A	1013	CLA	C1-O2A-CGA	2.57	123.18	116.44
17	B	4011	45D	C21-C15-C17	2.57	119.30	115.48
12	A	1101	CLA	CMA-C3A-C4A	2.56	118.67	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4001	BCR	C36-C18-C17	-2.56	119.33	122.92
15	B	4018	BCR	C34-C9-C10	-2.56	119.34	122.92
12	A	1131	CLA	CMA-C3A-C4A	2.56	118.65	111.77
24	F	6001	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
12	B	1208	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
12	B	1220	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
12	B	1229	CLA	CMA-C3A-C4A	2.55	118.62	111.77
15	K	4001	BCR	C23-C22-C21	2.54	122.85	118.94
12	B	1201	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
12	B	1219	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
12	K	1402	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
15	B	4010	BCR	C4-C5-C6	-2.54	119.04	122.73
12	B	1229	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
20	B	5005	LMG	C8-O7-C10	-2.53	111.56	117.79
15	B	4004	BCR	C37-C22-C21	-2.53	119.38	122.92
12	B	1210	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
16	A	5001	LHG	O8-C23-C24	2.53	119.84	111.91
12	B	1221	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
12	A	1101	CLA	O2A-CGA-CBA	2.53	119.83	111.91
12	B	1202	CLA	CMA-C3A-C4A	2.52	118.56	111.77
12	B	1234	CLA	CMB-C2B-C3B	2.52	129.40	124.68
12	A	1134	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	B	4017	BCR	C19-C18-C17	2.52	122.81	118.94
12	B	1229	CLA	C3D-C2D-C1D	-2.51	102.40	105.83
12	A	1140	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
12	A	1128	CLA	O2A-CGA-CBA	2.51	119.79	111.91
12	A	1125	CLA	C3D-C2D-C1D	-2.51	102.41	105.83
12	B	1240	CLA	CMD-C2D-C3D	-2.51	121.84	127.61
12	A	1136	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
12	A	1139	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
12	B	1221	CLA	O2A-CGA-CBA	2.50	119.75	111.91
12	B	1206	CLA	O2A-CGA-CBA	2.50	119.75	111.91
12	A	1121	CLA	O2A-CGA-CBA	2.49	119.74	111.91
12	B	1223	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
12	B	1211	CLA	CMB-C2B-C3B	2.49	129.34	124.68
12	A	1128	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
15	J	4013	BCR	C34-C9-C10	-2.49	119.44	122.92
12	A	1111	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
12	B	1236	CLA	CMA-C3A-C4A	2.49	118.45	111.77
15	B	4005	BCR	C15-C14-C13	-2.49	123.76	127.31
12	A	1106	CLA	CMA-C3A-C4A	2.49	118.45	111.77
12	B	1238	CLA	O1D-CGD-CBD	-2.48	119.40	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1023	CLA	O2A-CGA-CBA	2.48	119.70	111.91
12	B	1239	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
12	A	1121	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
15	B	4010	BCR	C23-C22-C21	2.47	122.73	118.94
15	A	4012	BCR	C35-C13-C12	2.47	121.97	118.08
12	A	1108	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
12	B	1212	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
12	A	1105	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	J	4015	C7Z	C1-C6-C7	-2.47	108.80	115.78
15	A	4001	BCR	C4-C5-C6	-2.46	119.16	122.73
12	A	1102	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
12	A	1012	CLA	CMA-C3A-C4A	2.46	118.38	111.77
12	B	1023	CLA	CMB-C2B-C3B	2.46	129.28	124.68
12	B	1235	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
15	I	4018	BCR	C36-C18-C19	2.45	121.94	118.08
17	B	4011	45D	C31-C33-C35	-2.45	119.53	126.42
12	A	1124	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
12	B	1228	CLA	CMB-C2B-C3B	2.45	129.26	124.68
12	A	1104	CLA	CMA-C3A-C4A	2.45	118.35	111.77
15	B	4005	BCR	C33-C5-C4	2.44	118.31	113.62
12	A	1111	CLA	CMA-C3A-C4A	2.44	118.34	111.77
15	A	4012	BCR	C37-C22-C21	-2.44	119.50	122.92
12	A	1102	CLA	CMB-C2B-C3B	2.44	129.24	124.68
12	A	1120	CLA	CMB-C2B-C3B	2.44	129.24	124.68
12	B	1238	CLA	C3D-C2D-C1D	-2.44	102.50	105.83
12	B	1022	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
12	B	1227	CLA	CMD-C2D-C3D	-2.43	122.01	127.61
15	A	4007	BCR	C15-C14-C13	-2.43	123.84	127.31
12	A	1127	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
12	A	1013	CLA	O2A-CGA-CBA	2.43	119.54	111.91
15	B	4018	BCR	C1-C6-C5	-2.42	119.20	122.61
12	A	1116	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
12	B	1218	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
16	A	5001	LHG	C5-O7-C7	-2.42	111.84	117.79
12	A	1130	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
12	A	1139	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
12	B	1232	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
12	A	1125	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
12	A	1124	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
12	B	1217	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	B	4018	BCR	C38-C26-C27	2.41	118.24	113.62
12	A	1118	CLA	O2D-CGD-O1D	-2.41	119.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1230	CLA	CMA-C3A-C4A	2.41	118.24	111.77
15	B	4004	BCR	C34-C9-C10	-2.41	119.55	122.92
12	F	1301	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
12	B	1231	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
12	B	1211	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
15	A	4001	BCR	C34-C9-C10	-2.40	119.56	122.92
25	I	4020	EQ3	C10-C11-C12	-2.40	115.72	123.22
12	A	1121	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
12	B	1239	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
12	B	1216	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
12	A	1112	CLA	CMA-C3A-C4A	2.40	118.22	111.77
15	A	4007	BCR	C33-C5-C4	2.40	118.22	113.62
12	A	1129	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
12	A	1105	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
12	B	1223	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
12	A	1115	CLA	CMB-C2B-C3B	2.39	129.16	124.68
12	B	1220	CLA	O2A-CGA-CBA	2.39	119.42	111.91
23	F	4016	C7Z	C31-C32-C33	-2.39	119.70	126.42
12	A	1103	CLA	CMA-C3A-C4A	2.39	118.20	111.77
12	A	1011	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
12	B	1212	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
15	A	4003	BCR	C38-C26-C27	2.39	118.20	113.62
15	I	4018	BCR	C15-C14-C13	-2.39	123.90	127.31
12	A	1116	CLA	O2A-CGA-CBA	2.39	119.40	111.91
15	A	4003	BCR	C34-C9-C10	-2.39	119.58	122.92
12	A	1122	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
12	B	1023	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
12	J	1302	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
12	K	1402	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
12	B	1218	CLA	C3D-C2D-C1D	-2.38	102.58	105.83
12	B	1218	CLA	O2A-CGA-CBA	2.38	119.39	111.91
15	B	4004	BCR	C38-C26-C27	2.38	118.19	113.62
12	A	1141	CLA	C3D-C2D-C1D	-2.38	102.58	105.83
12	A	1138	CLA	O2A-CGA-CBA	2.38	119.37	111.91
12	A	1137	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
12	A	1125	CLA	OBD-CAD-C3D	-2.37	122.81	128.52
12	B	1203	CLA	O2A-CGA-CBA	2.37	119.35	111.91
15	J	4013	BCR	C37-C22-C21	-2.37	119.60	122.92
12	A	1123	CLA	CMB-C2B-C3B	2.37	129.11	124.68
12	A	1130	CLA	CMB-C2B-C3B	2.37	129.11	124.68
12	B	1228	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
12	A	1131	CLA	O2D-CGD-O1D	-2.37	119.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4008	BCR	C19-C18-C17	2.37	122.57	118.94
15	B	4017	BCR	C38-C26-C27	2.37	118.16	113.62
12	B	1214	CLA	O2A-CGA-CBA	2.37	119.33	111.91
19	M	4021	ECH	C8-C7-C6	-2.36	120.56	127.20
12	B	1226	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
12	A	1103	CLA	CMB-C2B-C3B	2.36	129.10	124.68
12	B	1224	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
12	A	1125	CLA	O2A-CGA-CBA	2.36	119.31	111.91
12	B	1209	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
12	A	1141	CLA	CMB-C2B-C3B	2.36	129.09	124.68
12	B	1217	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
12	B	1236	CLA	C3D-C2D-C1D	-2.36	102.62	105.83
12	A	1136	CLA	O2A-CGA-CBA	2.35	119.30	111.91
12	B	1231	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
12	A	1108	CLA	O2A-CGA-CBA	2.35	119.28	111.91
12	A	1102	CLA	C3D-C2D-C1D	-2.35	102.63	105.83
12	A	1138	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
12	B	1023	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
12	A	1131	CLA	C3D-C2D-C1D	-2.35	102.63	105.83
12	A	1109	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
25	I	4020	EQ3	C7-C6-C5	-2.35	115.78	121.46
12	F	1302	CLA	C1-O2A-CGA	2.34	122.59	116.44
12	A	1114	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
12	B	1229	CLA	O2A-CGA-CBA	2.34	119.25	111.91
12	A	1123	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
12	A	1133	CLA	CMA-C3A-C4A	2.34	118.06	111.77
12	A	1130	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
12	A	1109	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
12	A	1012	CLA	OBD-CAD-C3D	-2.34	122.90	128.52
12	A	1137	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
12	A	1111	CLA	CAC-C3C-C4C	2.33	127.84	124.81
12	A	1123	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
12	B	1221	CLA	CMB-C2B-C3B	2.33	129.04	124.68
12	B	1221	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
12	B	1230	CLA	O2A-CGA-CBA	2.33	119.22	111.91
12	A	1119	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
12	B	1204	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
12	A	1113	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
12	L	1502	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
12	A	1115	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
12	A	1134	CLA	C3D-C2D-C1D	-2.33	102.66	105.83
12	B	1221	CLA	CMA-C3A-C4A	2.33	118.03	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1127	CLA	CMB-C2B-C3B	2.33	129.03	124.68
12	A	1129	CLA	CMB-C2B-C3B	2.32	129.03	124.68
12	A	1101	CLA	C1-O2A-CGA	2.32	122.54	116.44
12	A	1118	CLA	O2A-CGA-CBA	2.32	119.20	111.91
12	A	1129	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
12	B	1215	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
12	B	1234	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
12	A	1124	CLA	O2A-CGA-CBA	2.32	119.19	111.91
12	A	1118	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
12	B	1230	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
12	B	1215	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
12	J	1302	CLA	O2A-CGA-CBA	2.32	119.17	111.91
15	A	4003	BCR	C19-C18-C17	2.31	122.49	118.94
12	B	1022	CLA	O2A-CGA-CBA	2.31	119.16	111.91
12	B	1202	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
12	B	1203	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
12	A	1013	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
16	A	5003	LHG	C5-O7-C7	-2.31	112.10	117.79
12	A	1137	CLA	O2A-CGA-CBA	2.31	119.16	111.91
12	A	1107	CLA	O2A-CGA-CBA	2.31	119.15	111.91
12	A	1011	CLA	CMB-C2B-C3B	2.31	129.00	124.68
21	B	5008	SQD	O3-C3-C2	-2.31	105.01	110.35
12	B	1223	CLA	O2A-CGA-CBA	2.31	119.14	111.91
12	A	1126	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
12	B	1205	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
12	B	1022	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
12	A	1126	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
12	B	1231	CLA	O2A-CGA-CBA	2.30	119.13	111.91
12	A	1117	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
12	B	1023	CLA	CAC-C3C-C4C	2.30	127.79	124.81
12	A	1122	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
15	A	4008	BCR	C38-C26-C25	-2.30	121.95	124.53
12	B	1231	CLA	C1-O2A-CGA	2.30	122.47	116.44
12	B	1230	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
12	A	1011	CLA	O2A-CGA-CBA	2.30	119.11	111.91
12	A	1119	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
12	J	1303	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
12	B	1022	CLA	OBD-CAD-C3D	-2.29	123.00	128.52
12	B	1214	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
16	B	5004	LHG	C5-O7-C7	-2.29	112.15	117.79
12	B	1228	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
12	J	1303	CLA	O2A-CGA-CBA	2.29	119.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1103	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
12	A	1107	CLA	CHA-C4D-ND	2.29	137.28	132.50
12	A	1135	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
12	B	1202	CLA	CMB-C2B-C3B	2.29	128.96	124.68
12	B	1210	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
12	A	1126	CLA	O2A-CGA-CBA	2.28	119.08	111.91
12	K	1402	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
12	B	1206	CLA	C3D-C2D-C1D	-2.28	102.71	105.83
12	A	1109	CLA	CMB-C2B-C3B	2.28	128.95	124.68
12	B	1235	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
15	I	4018	BCR	C35-C13-C12	2.28	121.67	118.08
23	F	4016	C7Z	C1-C6-C7	-2.28	109.33	115.78
12	A	1110	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
12	K	1401	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
12	K	1402	CLA	O2A-CGA-CBA	2.28	119.06	111.91
12	B	1201	CLA	O2A-CGA-CBA	2.28	119.05	111.91
12	B	1219	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
12	A	1136	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
12	B	1222	CLA	O2A-CGA-CBA	2.27	119.05	111.91
12	A	1114	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
12	B	1237	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
12	A	1011	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
12	B	1220	CLA	C1-O2A-CGA	2.27	122.40	116.44
12	B	1240	CLA	O2A-CGA-CBA	2.27	119.03	111.91
12	A	1109	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
12	A	1101	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
12	B	1222	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
12	B	1225	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
12	B	1213	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
12	A	1133	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
12	F	1301	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
12	A	1114	CLA	O2A-CGA-CBA	2.26	119.01	111.91
12	B	1205	CLA	O2A-CGA-CBA	2.26	119.01	111.91
12	F	1302	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
12	A	1011	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
12	B	1209	CLA	O2A-CGA-CBA	2.26	119.00	111.91
12	A	1120	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
12	A	1133	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
12	B	1237	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
12	A	1132	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
23	J	4015	C7Z	C27-C26-C25	-2.26	116.00	121.46
12	B	1227	CLA	C3D-C2D-C1D	-2.25	102.75	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1106	CLA	CMB-C2B-C3B	2.25	128.90	124.68
12	A	1013	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
21	F	5001	SQD	O3-C3-C2	-2.25	105.14	110.35
12	B	1207	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
15	K	4001	BCR	C38-C26-C25	-2.25	122.00	124.53
12	B	1232	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
12	F	1301	CLA	CMB-C2B-C3B	2.25	128.89	124.68
12	A	1115	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
12	B	1227	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
12	A	1108	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
12	B	1206	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
12	A	1012	CLA	O2A-CGA-CBA	2.24	118.93	111.91
15	A	4008	BCR	C38-C26-C27	2.24	117.92	113.62
12	B	1213	CLA	CMB-C2B-C3B	2.24	128.87	124.68
15	A	4008	BCR	C29-C28-C27	2.24	116.38	111.38
15	B	4004	BCR	C38-C26-C25	-2.24	122.02	124.53
12	A	1126	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
15	I	4018	BCR	C23-C22-C21	-2.24	115.51	118.94
12	A	1119	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
12	A	1122	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
12	B	1225	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
12	B	1217	CLA	O2A-CGA-CBA	2.23	118.92	111.91
12	B	1207	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
12	B	1229	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
12	B	1225	CLA	O2A-CGA-CBA	2.23	118.91	111.91
12	B	1224	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
12	A	1132	CLA	O2A-CGA-CBA	2.23	118.91	111.91
12	B	1238	CLA	O2A-CGA-CBA	2.23	118.91	111.91
12	A	1121	CLA	C1-O2A-CGA	2.23	122.29	116.44
23	F	4016	C7Z	C4-C5-C6	-2.23	115.88	120.85
12	A	1105	CLA	O2A-CGA-CBA	2.23	118.89	111.91
12	A	1118	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
12	B	1237	CLA	O2A-CGA-CBA	2.22	118.88	111.91
12	A	1109	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
17	B	4011	45D	C27-C25-C29	-2.22	119.81	122.92
12	B	1201	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
12	B	1213	CLA	C1-O2A-CGA	2.22	122.27	116.44
15	B	4010	BCR	C30-C25-C24	2.22	122.06	115.78
15	A	4001	BCR	C8-C7-C6	-2.22	120.97	127.20
15	A	4012	BCR	C23-C24-C25	-2.22	120.97	127.20
12	A	1111	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
15	J	4013	BCR	C23-C24-C25	-2.22	120.97	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1208	CLA	O2A-CGA-CBA	2.22	118.86	111.91
12	A	1106	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
12	B	1215	CLA	O2A-CGA-CBA	2.22	118.86	111.91
12	A	1140	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
12	L	1502	CLA	O2A-CGA-CBA	2.21	118.84	111.91
12	B	1204	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
12	B	1213	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
12	B	1213	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
12	A	1011	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
12	B	1237	CLA	CMB-C2B-C3B	2.21	128.81	124.68
12	A	1107	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
12	B	1216	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
12	A	1135	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
12	B	1221	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
12	B	1226	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
12	A	1121	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
15	B	4005	BCR	C34-C9-C10	-2.20	119.84	122.92
12	A	1131	CLA	O2A-CGA-CBA	2.20	118.82	111.91
12	B	1205	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	M	4021	ECH	C23-C24-C25	-2.20	121.02	127.20
12	B	1239	CLA	O2A-CGA-CBA	2.20	118.81	111.91
12	B	1220	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
12	L	1502	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
15	I	4018	BCR	C30-C25-C24	2.20	122.00	115.78
12	A	1135	CLA	O2A-CGA-CBA	2.20	118.80	111.91
19	M	4021	ECH	C19-C18-C17	2.20	122.31	118.94
12	A	1106	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
15	J	4013	BCR	C38-C26-C25	-2.20	122.06	124.53
15	A	4003	BCR	C23-C24-C25	-2.19	121.04	127.20
12	B	1238	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
12	A	1104	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
12	B	1224	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
12	B	1217	CLA	CAC-C3C-C4C	2.19	127.65	124.81
12	A	1102	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
12	B	1201	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
12	A	1127	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
15	A	4003	BCR	C35-C13-C12	2.19	121.52	118.08
12	J	1303	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
12	A	1108	CLA	CMB-C2B-C3B	2.18	128.76	124.68
25	I	4020	EQ3	C8-C9-C10	2.18	122.29	118.94
12	A	1013	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
12	A	1112	CLA	C3D-C2D-C1D	-2.18	102.85	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1103	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
12	B	1208	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
12	B	1232	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
12	A	1120	CLA	O2A-CGA-CBA	2.18	118.74	111.91
12	A	1134	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
12	A	1127	CLA	O2A-CGA-CBA	2.18	118.73	111.91
12	A	1117	CLA	O2A-CGA-CBA	2.17	118.73	111.91
12	B	1210	CLA	CAC-C3C-C4C	2.17	127.63	124.81
12	B	1210	CLA	O2A-CGA-CBA	2.17	118.73	111.91
12	B	1236	CLA	O2A-CGA-CBA	2.17	118.73	111.91
15	A	4007	BCR	C31-C1-C6	-2.17	106.78	110.30
12	B	1213	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
15	A	4001	BCR	C19-C18-C17	2.17	122.27	118.94
12	A	1130	CLA	O2A-CGA-CBA	2.17	118.72	111.91
12	A	1112	CLA	CMB-C2B-C3B	2.17	128.74	124.68
12	B	1211	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
12	A	1110	CLA	O2A-CGA-CBA	2.17	118.71	111.91
12	B	1232	CLA	C1-O2A-CGA	2.17	122.13	116.44
12	B	1210	CLA	CMB-C2B-C3B	2.17	128.73	124.68
12	B	1232	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
12	A	1132	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
12	B	1205	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
12	K	1401	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
12	A	1105	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
12	A	1138	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
12	A	1101	CLA	CBA-CAA-C2A	2.16	120.23	113.86
12	A	1128	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
12	A	1104	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
12	B	1207	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
15	J	4013	BCR	C38-C26-C27	2.15	117.74	113.62
15	A	4001	BCR	C38-C26-C27	2.14	117.73	113.62
12	A	1136	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
12	A	1134	CLA	O2A-CGA-CBA	2.14	118.62	111.91
12	A	1101	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
12	A	1013	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
15	A	4007	BCR	C37-C22-C21	-2.14	119.93	122.92
12	A	1119	CLA	CMB-C2B-C3B	2.14	128.68	124.68
12	A	1139	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
12	B	1234	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
12	A	1113	CLA	O2A-CGA-CBA	2.13	118.61	111.91
12	A	1112	CLA	O2A-CGA-CBA	2.13	118.60	111.91
12	A	1121	CLA	CMB-C2B-C3B	2.13	128.67	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4004	BCR	C23-C24-C25	-2.13	121.21	127.20
12	B	1235	CLA	CMB-C2B-C3B	2.13	128.67	124.68
12	B	1223	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
12	B	1226	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
15	A	4003	BCR	C27-C26-C25	-2.13	119.64	122.73
15	A	4012	BCR	C38-C26-C25	-2.13	122.14	124.53
12	K	1402	CLA	C1-O2A-CGA	2.13	122.03	116.44
12	B	1203	CLA	CMA-C3A-C4A	2.13	117.50	111.77
12	B	1203	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
12	A	1129	CLA	O2A-CGA-CBA	2.13	118.58	111.91
12	B	1237	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
12	B	1203	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
12	K	1402	CLA	CMB-C2B-C3B	2.13	128.65	124.68
12	B	1240	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
12	A	1104	CLA	O2A-CGA-CBA	2.12	118.57	111.91
12	B	1216	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
12	B	1240	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
12	A	1106	CLA	C1-O2A-CGA	2.12	122.01	116.44
12	B	1226	CLA	O2A-CGA-CBA	2.12	118.57	111.91
12	A	1133	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
12	B	1206	CLA	CMB-C2B-C3B	2.12	128.65	124.68
12	A	1013	CLA	C1-C2-C3	-2.12	122.38	126.04
12	A	1109	CLA	O2A-CGA-CBA	2.12	118.56	111.91
12	A	1119	CLA	CMA-C3A-C4A	2.12	117.47	111.77
12	B	1021	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
12	B	1022	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
12	B	1208	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
12	A	1123	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
16	A	5001	LHG	C37-C36-C35	-2.12	95.66	115.30
13	A	2001	PQN	C2M-C2-C3	-2.12	120.95	124.40
12	B	1204	CLA	O2A-CGA-CBA	2.12	118.55	111.91
15	B	4005	BCR	C30-C25-C26	-2.11	119.64	122.61
12	B	1210	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
15	K	4001	BCR	C38-C26-C27	2.11	117.67	113.62
12	B	1222	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
12	F	1301	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
12	B	1238	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
17	B	4011	45D	C22-C16-C18	2.11	118.62	115.48
12	A	1101	CLA	CHA-C1A-NA	-2.11	121.56	126.40
12	A	1117	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
12	B	1209	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
15	A	4003	BCR	C38-C26-C25	-2.11	122.16	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1106	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
12	A	1131	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
12	B	1021	CLA	O2A-CGA-CBA	2.11	118.52	111.91
25	I	4020	EQ3	C1-C6-C5	-2.11	119.65	122.61
12	B	1229	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
12	B	1224	CLA	CMB-C2B-C3B	2.11	128.62	124.68
12	B	1209	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
12	B	1211	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
12	A	1132	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
12	A	1102	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
12	A	1140	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
12	A	1127	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
12	A	1140	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
12	B	1205	CLA	CAC-C3C-C4C	2.10	127.53	124.81
12	B	1217	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
12	B	1021	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
12	A	1126	CLA	CMB-C2B-C3B	2.10	128.60	124.68
15	A	4007	BCR	C30-C25-C26	-2.10	119.66	122.61
12	A	1103	CLA	O2A-CGA-CBA	2.09	118.48	111.91
12	B	1214	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
12	A	1115	CLA	C1-O2A-CGA	2.09	121.93	116.44
15	B	4010	BCR	C36-C18-C17	-2.09	119.99	122.92
12	B	1202	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
23	J	4015	C7Z	C38-C25-C24	-2.09	110.48	114.36
12	B	1203	CLA	CMB-C2B-C3B	2.09	128.59	124.68
12	F	1302	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
12	A	1128	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
12	B	1211	CLA	O2A-CGA-CBA	2.09	118.47	111.91
12	B	1212	CLA	O2A-CGA-CBA	2.09	118.46	111.91
12	A	1114	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
15	F	4014	BCR	C31-C1-C6	-2.09	106.91	110.30
12	B	1204	CLA	C1-O2A-CGA	2.09	121.92	116.44
12	B	1231	CLA	CMA-C3A-C4A	2.09	117.38	111.77
12	A	1133	CLA	O2A-CGA-CBA	2.09	118.46	111.91
23	F	4016	C7Z	C11-C12-C13	-2.09	120.55	126.42
12	B	1228	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
12	A	1107	CLA	C1-O2A-CGA	2.09	121.92	116.44
12	B	1227	CLA	O2A-CGA-CBA	2.09	118.45	111.91
12	A	1141	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
12	A	1105	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
12	B	1214	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
12	A	1125	CLA	CAA-C2A-C3A	-2.08	107.07	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1219	CLA	O2A-CGA-CBA	2.08	118.45	111.91
12	A	1115	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
12	B	1212	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
23	J	4015	C7Z	C11-C12-C13	-2.08	120.57	126.42
12	B	1021	CLA	CMB-C2B-C3B	2.08	128.57	124.68
12	A	1120	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
12	A	1118	CLA	CMB-C2B-C3B	2.08	128.57	124.68
23	F	4016	C7Z	C27-C28-C29	-2.08	123.09	126.23
12	B	1239	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
12	A	1110	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
15	B	4010	BCR	C34-C9-C10	-2.08	120.01	122.92
25	I	4020	EQ3	C15-C14-C13	-2.08	124.35	127.31
12	B	1232	CLA	O2A-CGA-CBA	2.07	118.42	111.91
12	A	1112	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
12	A	1111	CLA	O2A-CGA-CBA	2.07	118.41	111.91
12	A	1130	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
12	B	1216	CLA	O2A-CGA-CBA	2.07	118.40	111.91
12	A	1108	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
12	A	1137	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
12	J	1302	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
13	B	2002	PQN	C2M-C2-C3	-2.07	121.03	124.40
12	K	1402	CLA	CAA-CBA-CGA	-2.07	107.22	113.25
12	B	1206	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
12	A	1138	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
12	A	1128	CLA	C1-O2A-CGA	2.06	121.86	116.44
12	A	1116	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
12	A	1124	CLA	CMB-C2B-C3B	2.06	128.54	124.68
12	A	1120	CLA	CAC-C3C-C4C	2.06	127.48	124.81
12	A	1134	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
25	I	4020	EQ3	C11-C10-C9	-2.06	124.37	127.31
12	A	1111	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
12	B	1228	CLA	O2A-CGA-CBA	2.06	118.37	111.91
12	K	1402	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
12	A	1123	CLA	O2A-CGA-CBA	2.06	118.36	111.91
12	A	1122	CLA	C1-O2A-CGA	2.05	121.83	116.44
15	I	4018	BCR	C33-C5-C6	-2.05	122.22	124.53
12	A	1128	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
12	A	1117	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
25	I	4020	EQ3	C35-C13-C12	2.05	121.30	118.08
12	A	1011	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	J	4015	C7Z	C22-C23-C24	2.05	113.11	110.30
15	B	4017	BCR	C34-C9-C10	-2.05	120.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1223	CLA	CMB-C2B-C3B	2.04	128.50	124.68
12	A	1113	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
15	F	4014	BCR	C4-C5-C6	-2.04	119.77	122.73
12	B	1229	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
12	B	1201	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
12	A	1102	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
12	B	1220	CLA	CAC-C3C-C4C	2.04	127.45	124.81
12	A	1129	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
12	A	1112	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
12	A	1117	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
12	F	1301	CLA	O2A-CGA-CBA	2.03	118.29	111.91
12	B	1218	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
12	B	1231	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
12	A	1107	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
15	B	4004	BCR	C27-C26-C25	-2.02	119.79	122.73
12	B	1218	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
12	B	1211	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
15	A	4008	BCR	C4-C5-C6	-2.02	119.80	122.73
12	A	1116	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
12	A	1115	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
12	A	1124	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
12	B	1230	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
12	B	1234	CLA	C1-O2A-CGA	2.02	121.74	116.44
12	A	1127	CLA	C1-O2A-CGA	2.02	121.74	116.44
12	A	1135	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
12	F	1302	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
15	K	4001	BCR	C33-C5-C4	2.02	117.49	113.62
12	B	1220	CLA	CAA-CBA-CGA	-2.01	107.36	113.25
12	B	1204	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
12	A	1012	CLA	CHA-C1A-NA	-2.01	121.79	126.40
15	A	4001	BCR	C35-C13-C14	-2.01	120.11	122.92
12	A	1123	CLA	CAC-C3C-C4C	2.01	127.42	124.81
12	B	1221	CLA	CHA-C1A-NA	-2.01	121.80	126.40
12	A	1012	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
12	A	1117	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
15	B	4018	BCR	C37-C22-C23	2.00	121.23	118.08
12	B	1219	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
12	B	1235	CLA	O2A-CGA-CBA	2.00	118.19	111.91

All (93) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
12	A	1011	CLA	ND
12	A	1012	CLA	ND
12	A	1013	CLA	ND
12	A	1102	CLA	ND
12	A	1103	CLA	ND
12	A	1104	CLA	ND
12	A	1105	CLA	ND
12	A	1106	CLA	ND
12	A	1107	CLA	ND
12	A	1108	CLA	ND
12	A	1109	CLA	ND
12	A	1110	CLA	ND
12	A	1111	CLA	ND
12	A	1112	CLA	ND
12	A	1113	CLA	ND
12	A	1114	CLA	ND
12	A	1115	CLA	ND
12	A	1116	CLA	ND
12	A	1117	CLA	ND
12	A	1118	CLA	ND
12	A	1119	CLA	ND
12	A	1120	CLA	ND
12	A	1121	CLA	ND
12	A	1122	CLA	ND
12	A	1123	CLA	ND
12	A	1124	CLA	ND
12	A	1125	CLA	ND
12	A	1126	CLA	ND
12	A	1127	CLA	ND
12	A	1128	CLA	ND
12	A	1129	CLA	ND
12	A	1131	CLA	ND
12	A	1133	CLA	ND
12	A	1134	CLA	ND
12	A	1135	CLA	ND
12	A	1136	CLA	ND
12	A	1137	CLA	ND
12	A	1138	CLA	ND
12	A	1139	CLA	ND
12	A	1140	CLA	ND
12	A	1141	CLA	ND

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Mol	Chain	Res	Type	Atom
12	A	1101	CLA	ND
12	A	1130	CLA	ND
12	A	1132	CLA	ND
12	B	1237	CLA	ND
12	B	1021	CLA	ND
12	B	1022	CLA	ND
12	B	1023	CLA	ND
12	B	1201	CLA	ND
12	B	1202	CLA	ND
12	B	1203	CLA	ND
12	B	1204	CLA	ND
12	B	1205	CLA	ND
12	B	1206	CLA	ND
12	B	1207	CLA	ND
12	B	1208	CLA	ND
12	B	1209	CLA	ND
12	B	1210	CLA	ND
12	B	1211	CLA	ND
12	B	1212	CLA	ND
12	B	1213	CLA	ND
12	B	1214	CLA	ND
12	B	1215	CLA	ND
12	B	1216	CLA	ND
12	B	1217	CLA	ND
12	B	1218	CLA	ND
12	B	1219	CLA	ND
12	B	1220	CLA	ND
12	B	1221	CLA	ND
12	B	1222	CLA	ND
12	B	1223	CLA	ND
12	B	1224	CLA	ND
12	B	1225	CLA	ND
12	B	1226	CLA	ND
12	B	1227	CLA	ND
12	B	1228	CLA	ND
12	B	1229	CLA	ND
12	B	1230	CLA	ND
12	B	1231	CLA	ND
12	B	1232	CLA	ND
12	B	1234	CLA	ND
12	B	1235	CLA	ND
12	B	1236	CLA	ND

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Mol	Chain	Res	Type	Atom
12	B	1239	CLA	ND
12	B	1240	CLA	ND
12	B	1238	CLA	ND
12	F	1301	CLA	ND
12	F	1302	CLA	ND
12	J	1303	CLA	ND
12	J	1302	CLA	ND
12	K	1401	CLA	ND
12	K	1402	CLA	ND
12	L	1502	CLA	ND

All (1428) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1012	CLA	CAD-CBD-CGD-O1D
12	A	1012	CLA	CAD-CBD-CGD-O2D
12	A	1013	CLA	C2-C1-O2A-CGA
12	A	1013	CLA	CHA-CBD-CGD-O1D
12	A	1013	CLA	CHA-CBD-CGD-O2D
12	A	1103	CLA	C1A-C2A-CAA-CBA
12	A	1103	CLA	C3A-C2A-CAA-CBA
12	A	1103	CLA	CHA-CBD-CGD-O1D
12	A	1103	CLA	CHA-CBD-CGD-O2D
12	A	1103	CLA	CAD-CBD-CGD-O1D
12	A	1103	CLA	CBD-CGD-O2D-CED
12	A	1104	CLA	CBD-CGD-O2D-CED
12	A	1105	CLA	C1A-C2A-CAA-CBA
12	A	1105	CLA	C3A-C2A-CAA-CBA
12	A	1106	CLA	C3A-C2A-CAA-CBA
12	A	1106	CLA	CHA-CBD-CGD-O1D
12	A	1106	CLA	CHA-CBD-CGD-O2D
12	A	1107	CLA	C1A-C2A-CAA-CBA
12	A	1107	CLA	C2-C1-O2A-CGA
12	A	1107	CLA	CBD-CGD-O2D-CED
12	A	1108	CLA	C1A-C2A-CAA-CBA
12	A	1108	CLA	CHA-CBD-CGD-O1D
12	A	1108	CLA	CHA-CBD-CGD-O2D
12	A	1108	CLA	CBD-CGD-O2D-CED
12	A	1110	CLA	C1A-C2A-CAA-CBA
12	A	1110	CLA	C3A-C2A-CAA-CBA
12	A	1110	CLA	CBD-CGD-O2D-CED
12	A	1111	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	1111	CLA	C3A-C2A-CAA-CBA
12	A	1111	CLA	C2-C1-O2A-CGA
12	A	1111	CLA	CHA-CBD-CGD-O1D
12	A	1111	CLA	CHA-CBD-CGD-O2D
12	A	1111	CLA	CAD-CBD-CGD-O1D
12	A	1111	CLA	CBD-CGD-O2D-CED
12	A	1112	CLA	C1A-C2A-CAA-CBA
12	A	1112	CLA	CHA-CBD-CGD-O1D
12	A	1112	CLA	CHA-CBD-CGD-O2D
12	A	1113	CLA	C1A-C2A-CAA-CBA
12	A	1113	CLA	CHA-CBD-CGD-O1D
12	A	1113	CLA	CBD-CGD-O2D-CED
12	A	1115	CLA	CBD-CGD-O2D-CED
12	A	1116	CLA	C3A-C2A-CAA-CBA
12	A	1116	CLA	CBD-CGD-O2D-CED
12	A	1117	CLA	CHA-CBD-CGD-O1D
12	A	1117	CLA	CHA-CBD-CGD-O2D
12	A	1117	CLA	CBD-CGD-O2D-CED
12	A	1118	CLA	CBD-CGD-O2D-CED
12	A	1119	CLA	CHA-CBD-CGD-O1D
12	A	1119	CLA	CHA-CBD-CGD-O2D
12	A	1119	CLA	CBD-CGD-O2D-CED
12	A	1120	CLA	CHA-CBD-CGD-O1D
12	A	1120	CLA	CHA-CBD-CGD-O2D
12	A	1120	CLA	CAD-CBD-CGD-O1D
12	A	1120	CLA	CBD-CGD-O2D-CED
12	A	1121	CLA	CBA-CGA-O2A-C1
12	A	1121	CLA	O1A-CGA-O2A-C1
12	A	1121	CLA	CBD-CGD-O2D-CED
12	A	1122	CLA	CHA-CBD-CGD-O1D
12	A	1122	CLA	CHA-CBD-CGD-O2D
12	A	1123	CLA	C1A-C2A-CAA-CBA
12	A	1123	CLA	C3A-C2A-CAA-CBA
12	A	1123	CLA	C2-C1-O2A-CGA
12	A	1124	CLA	C3A-C2A-CAA-CBA
12	A	1124	CLA	CBD-CGD-O2D-CED
12	A	1125	CLA	C1A-C2A-CAA-CBA
12	A	1125	CLA	C3A-C2A-CAA-CBA
12	A	1125	CLA	C2A-CAA-CBA-CGA
12	A	1125	CLA	CBD-CGD-O2D-CED
12	A	1126	CLA	C1A-C2A-CAA-CBA
12	A	1126	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	1126	CLA	C2-C1-O2A-CGA
12	A	1126	CLA	CHA-CBD-CGD-O1D
12	A	1126	CLA	CHA-CBD-CGD-O2D
12	A	1127	CLA	CHA-CBD-CGD-O1D
12	A	1127	CLA	CHA-CBD-CGD-O2D
12	A	1128	CLA	C2-C1-O2A-CGA
12	A	1128	CLA	CHA-CBD-CGD-O2D
12	A	1129	CLA	CHA-CBD-CGD-O1D
12	A	1129	CLA	CHA-CBD-CGD-O2D
12	A	1134	CLA	C1A-C2A-CAA-CBA
12	A	1135	CLA	CHA-CBD-CGD-O1D
12	A	1135	CLA	CHA-CBD-CGD-O2D
12	A	1136	CLA	CHA-CBD-CGD-O1D
12	A	1136	CLA	CHA-CBD-CGD-O2D
12	A	1137	CLA	CHA-CBD-CGD-O1D
12	A	1137	CLA	CHA-CBD-CGD-O2D
12	A	1138	CLA	C2-C1-O2A-CGA
12	A	1138	CLA	CBD-CGD-O2D-CED
12	A	1140	CLA	C2-C3-C5-C6
12	A	1140	CLA	C4-C3-C5-C6
12	A	1141	CLA	C1A-C2A-CAA-CBA
12	A	1141	CLA	C3A-C2A-CAA-CBA
12	A	1141	CLA	CAD-CBD-CGD-O1D
12	A	1141	CLA	CAD-CBD-CGD-O2D
12	A	1141	CLA	CBD-CGD-O2D-CED
12	A	1101	CLA	C1A-C2A-CAA-CBA
12	A	1130	CLA	CBD-CGD-O2D-CED
12	A	1132	CLA	CBD-CGD-O2D-CED
12	B	1237	CLA	CBD-CGD-O2D-CED
12	B	1021	CLA	C1A-C2A-CAA-CBA
12	B	1021	CLA	C3A-C2A-CAA-CBA
12	B	1021	CLA	CHA-CBD-CGD-O1D
12	B	1021	CLA	CHA-CBD-CGD-O2D
12	B	1021	CLA	CBD-CGD-O2D-CED
12	B	1022	CLA	CBD-CGD-O2D-CED
12	B	1023	CLA	C2-C1-O2A-CGA
12	B	1023	CLA	CHA-CBD-CGD-O1D
12	B	1023	CLA	CHA-CBD-CGD-O2D
12	B	1023	CLA	CBD-CGD-O2D-CED
12	B	1201	CLA	C2-C1-O2A-CGA
12	B	1201	CLA	CHA-CBD-CGD-O1D
12	B	1201	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	B	1202	CLA	C3A-C2A-CAA-CBA
12	B	1202	CLA	CHA-CBD-CGD-O1D
12	B	1202	CLA	CHA-CBD-CGD-O2D
12	B	1202	CLA	CAD-CBD-CGD-O1D
12	B	1202	CLA	CAD-CBD-CGD-O2D
12	B	1203	CLA	C2-C1-O2A-CGA
12	B	1204	CLA	C1A-C2A-CAA-CBA
12	B	1204	CLA	CHA-CBD-CGD-O1D
12	B	1204	CLA	CHA-CBD-CGD-O2D
12	B	1205	CLA	CHA-CBD-CGD-O1D
12	B	1205	CLA	CHA-CBD-CGD-O2D
12	B	1206	CLA	C2-C1-O2A-CGA
12	B	1206	CLA	CBD-CGD-O2D-CED
12	B	1207	CLA	C1A-C2A-CAA-CBA
12	B	1207	CLA	CBD-CGD-O2D-CED
12	B	1209	CLA	C1A-C2A-CAA-CBA
12	B	1209	CLA	C3A-C2A-CAA-CBA
12	B	1209	CLA	CHA-CBD-CGD-O1D
12	B	1209	CLA	CHA-CBD-CGD-O2D
12	B	1210	CLA	C1A-C2A-CAA-CBA
12	B	1210	CLA	CBD-CGD-O2D-CED
12	B	1211	CLA	CBD-CGD-O2D-CED
12	B	1212	CLA	CBD-CGD-O2D-CED
12	B	1213	CLA	C1A-C2A-CAA-CBA
12	B	1213	CLA	C3A-C2A-CAA-CBA
12	B	1213	CLA	CHA-CBD-CGD-O1D
12	B	1213	CLA	CHA-CBD-CGD-O2D
12	B	1214	CLA	C2-C1-O2A-CGA
12	B	1214	CLA	CBD-CGD-O2D-CED
12	B	1215	CLA	C3A-C2A-CAA-CBA
12	B	1215	CLA	CBD-CGD-O2D-CED
12	B	1216	CLA	C1A-C2A-CAA-CBA
12	B	1216	CLA	C3A-C2A-CAA-CBA
12	B	1216	CLA	CBD-CGD-O2D-CED
12	B	1217	CLA	C1A-C2A-CAA-CBA
12	B	1217	CLA	C3A-C2A-CAA-CBA
12	B	1217	CLA	CBD-CGD-O2D-CED
12	B	1218	CLA	C1A-C2A-CAA-CBA
12	B	1218	CLA	C3A-C2A-CAA-CBA
12	B	1218	CLA	CHA-CBD-CGD-O1D
12	B	1218	CLA	CHA-CBD-CGD-O2D
12	B	1218	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	1219	CLA	CBD-CGD-O2D-CED
12	B	1220	CLA	CHA-CBD-CGD-O1D
12	B	1220	CLA	CBD-CGD-O2D-CED
12	B	1223	CLA	C1A-C2A-CAA-CBA
12	B	1223	CLA	C3A-C2A-CAA-CBA
12	B	1223	CLA	CHA-CBD-CGD-O1D
12	B	1223	CLA	CHA-CBD-CGD-O2D
12	B	1223	CLA	CBD-CGD-O2D-CED
12	B	1224	CLA	CHA-CBD-CGD-O1D
12	B	1225	CLA	C1A-C2A-CAA-CBA
12	B	1225	CLA	C3A-C2A-CAA-CBA
12	B	1225	CLA	CHA-CBD-CGD-O1D
12	B	1225	CLA	CHA-CBD-CGD-O2D
12	B	1227	CLA	CHA-CBD-CGD-O2D
12	B	1228	CLA	C1A-C2A-CAA-CBA
12	B	1228	CLA	C3A-C2A-CAA-CBA
12	B	1229	CLA	C3A-C2A-CAA-CBA
12	B	1229	CLA	C2-C1-O2A-CGA
12	B	1229	CLA	CBD-CGD-O2D-CED
12	B	1230	CLA	C3A-C2A-CAA-CBA
12	B	1230	CLA	CHA-CBD-CGD-O2D
12	B	1232	CLA	C2-C1-O2A-CGA
12	B	1234	CLA	CBD-CGD-O2D-CED
12	B	1234	CLA	C11-C10-C8-C9
12	B	1235	CLA	CHA-CBD-CGD-O1D
12	B	1235	CLA	CHA-CBD-CGD-O2D
12	B	1235	CLA	C2-C3-C5-C6
12	B	1235	CLA	C4-C3-C5-C6
12	B	1239	CLA	C1A-C2A-CAA-CBA
12	B	1239	CLA	C3A-C2A-CAA-CBA
12	B	1239	CLA	CBD-CGD-O2D-CED
12	F	1302	CLA	CHA-CBD-CGD-O1D
12	F	1302	CLA	CHA-CBD-CGD-O2D
12	J	1303	CLA	CHA-CBD-CGD-O1D
12	J	1303	CLA	CHA-CBD-CGD-O2D
12	K	1401	CLA	CHA-CBD-CGD-O1D
12	K	1401	CLA	CHA-CBD-CGD-O2D
12	L	1502	CLA	C1A-C2A-CAA-CBA
12	L	1502	CLA	CBA-CGA-O2A-C1
15	A	4001	BCR	C7-C8-C9-C10
15	A	4001	BCR	C7-C8-C9-C34
15	A	4001	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	A	4001	BCR	C11-C10-C9-C34
15	A	4001	BCR	C17-C18-C19-C20
15	A	4001	BCR	C36-C18-C19-C20
15	A	4001	BCR	C21-C22-C23-C24
15	A	4003	BCR	C7-C8-C9-C10
15	A	4003	BCR	C7-C8-C9-C34
15	A	4003	BCR	C11-C10-C9-C8
15	A	4003	BCR	C11-C10-C9-C34
15	A	4003	BCR	C11-C12-C13-C35
15	A	4003	BCR	C21-C22-C23-C24
15	A	4003	BCR	C37-C22-C23-C24
15	A	4003	BCR	C23-C24-C25-C26
15	A	4003	BCR	C23-C24-C25-C30
15	A	4007	BCR	C11-C10-C9-C8
15	A	4007	BCR	C11-C10-C9-C34
15	A	4007	BCR	C10-C11-C12-C13
15	A	4007	BCR	C36-C18-C19-C20
15	A	4008	BCR	C1-C6-C7-C8
15	A	4008	BCR	C7-C8-C9-C10
15	A	4008	BCR	C7-C8-C9-C34
15	A	4008	BCR	C11-C10-C9-C8
15	A	4008	BCR	C11-C10-C9-C34
15	A	4008	BCR	C10-C11-C12-C13
15	A	4008	BCR	C37-C22-C23-C24
15	A	4008	BCR	C23-C24-C25-C26
15	A	4012	BCR	C11-C10-C9-C34
15	A	4012	BCR	C10-C11-C12-C13
15	A	4012	BCR	C11-C12-C13-C14
15	A	4012	BCR	C11-C12-C13-C35
15	A	4012	BCR	C21-C22-C23-C24
15	A	4012	BCR	C37-C22-C23-C24
15	B	4004	BCR	C1-C6-C7-C8
15	B	4004	BCR	C5-C6-C7-C8
15	B	4004	BCR	C11-C10-C9-C8
15	B	4004	BCR	C11-C10-C9-C34
15	B	4004	BCR	C10-C11-C12-C13
15	B	4004	BCR	C23-C24-C25-C26
15	B	4004	BCR	C23-C24-C25-C30
15	B	4005	BCR	C11-C10-C9-C8
15	B	4005	BCR	C11-C10-C9-C34
15	B	4005	BCR	C9-C10-C11-C12
15	B	4005	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	B	4005	BCR	C17-C18-C19-C20
15	B	4005	BCR	C36-C18-C19-C20
15	B	4005	BCR	C21-C22-C23-C24
15	B	4005	BCR	C37-C22-C23-C24
15	B	4010	BCR	C7-C8-C9-C10
15	B	4010	BCR	C7-C8-C9-C34
15	B	4010	BCR	C11-C10-C9-C8
15	B	4010	BCR	C11-C10-C9-C34
15	B	4010	BCR	C10-C11-C12-C13
15	B	4010	BCR	C19-C20-C21-C22
15	B	4010	BCR	C23-C24-C25-C26
15	B	4010	BCR	C23-C24-C25-C30
15	B	4017	BCR	C11-C10-C9-C8
15	B	4017	BCR	C11-C10-C9-C34
15	B	4017	BCR	C10-C11-C12-C13
15	B	4017	BCR	C17-C18-C19-C20
15	B	4017	BCR	C36-C18-C19-C20
15	B	4018	BCR	C11-C10-C9-C8
15	B	4018	BCR	C11-C10-C9-C34
15	F	4014	BCR	C7-C8-C9-C10
15	F	4014	BCR	C7-C8-C9-C34
15	F	4014	BCR	C11-C10-C9-C8
15	F	4014	BCR	C11-C10-C9-C34
15	F	4014	BCR	C10-C11-C12-C13
15	F	4014	BCR	C17-C18-C19-C20
15	F	4014	BCR	C36-C18-C19-C20
15	I	4018	BCR	C7-C8-C9-C34
15	I	4018	BCR	C10-C11-C12-C13
15	I	4018	BCR	C17-C18-C19-C20
15	I	4018	BCR	C36-C18-C19-C20
15	J	4013	BCR	C11-C10-C9-C8
15	J	4013	BCR	C11-C10-C9-C34
15	J	4013	BCR	C10-C11-C12-C13
15	J	4013	BCR	C17-C18-C19-C20
15	J	4013	BCR	C36-C18-C19-C20
15	K	4001	BCR	C11-C10-C9-C8
15	K	4001	BCR	C11-C10-C9-C34
15	K	4001	BCR	C9-C10-C11-C12
15	K	4001	BCR	C10-C11-C12-C13
15	K	4001	BCR	C17-C18-C19-C20
15	K	4001	BCR	C36-C18-C19-C20
16	A	5001	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	A	5001	LHG	C1-C2-C3-O3
16	A	5001	LHG	O2-C2-C3-O3
16	A	5001	LHG	C4-O6-P-O3
16	A	5001	LHG	C4-O6-P-O5
16	A	5003	LHG	C1-C2-C3-O3
16	A	5003	LHG	C3-O3-P-O4
16	A	5003	LHG	C3-O3-P-O5
16	A	5003	LHG	C3-O3-P-O6
16	B	5004	LHG	C3-O3-P-O4
16	B	5004	LHG	C3-O3-P-O5
16	B	5004	LHG	C3-O3-P-O6
16	B	5006	LHG	O1-C1-C2-C3
16	B	5006	LHG	C4-O6-P-O5
17	B	4011	45D	C31-C33-C35-C37
17	B	4011	45D	C31-C33-C35-C39
19	M	4021	ECH	C5-C6-C7-C8
19	M	4021	ECH	C7-C8-C9-C34
20	B	5005	LMG	C11-C10-O7-C8
21	B	5008	SQD	C8-C7-O47-C45
21	F	5001	SQD	O49-C7-O47-C45
21	F	5001	SQD	O5-C5-C6-S
23	F	4016	C7Z	C5-C6-C7-C8
23	F	4016	C7Z	C11-C10-C9-C19
23	F	4016	C7Z	C11-C12-C13-C20
23	F	4016	C7Z	C11-C12-C13-C14
23	F	4016	C7Z	C12-C13-C14-C15
23	F	4016	C7Z	C40-C33-C34-C35
23	F	4016	C7Z	C32-C33-C34-C35
23	F	4016	C7Z	C39-C29-C30-C31
23	F	4016	C7Z	C27-C28-C29-C30
23	F	4016	C7Z	C27-C28-C29-C39
23	J	4015	C7Z	C7-C8-C9-C10
23	J	4015	C7Z	C11-C10-C9-C19
23	J	4015	C7Z	C11-C12-C13-C14
23	J	4015	C7Z	C20-C13-C14-C15
23	J	4015	C7Z	C40-C33-C34-C35
23	J	4015	C7Z	C31-C32-C33-C34
23	J	4015	C7Z	C31-C32-C33-C40
23	J	4015	C7Z	C39-C29-C30-C31
23	J	4015	C7Z	C27-C28-C29-C39
24	F	6001	LMT	C2-C1-O1'-C1'
25	I	4020	EQ3	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
25	I	4020	EQ3	C11-C12-C13-C14
25	I	4020	EQ3	C21-C22-C23-C24
25	I	4020	EQ3	C37-C22-C23-C24
16	B	5006	LHG	C8-C7-O7-C5
12	A	1139	CLA	O1D-CGD-O2D-CED
12	B	1203	CLA	O1D-CGD-O2D-CED
12	B	1206	CLA	O1D-CGD-O2D-CED
16	B	5006	LHG	O9-C7-O7-C5
12	A	1109	CLA	O1D-CGD-O2D-CED
12	A	1127	CLA	O1D-CGD-O2D-CED
12	A	1138	CLA	O1D-CGD-O2D-CED
12	B	1021	CLA	O1D-CGD-O2D-CED
12	B	1023	CLA	O1D-CGD-O2D-CED
12	B	1201	CLA	O1D-CGD-O2D-CED
12	B	1231	CLA	O1D-CGD-O2D-CED
12	B	1232	CLA	O1D-CGD-O2D-CED
12	K	1402	CLA	O1D-CGD-O2D-CED
12	A	1011	CLA	CBD-CGD-O2D-CED
12	A	1012	CLA	CBD-CGD-O2D-CED
12	A	1013	CLA	CBD-CGD-O2D-CED
12	A	1102	CLA	CBD-CGD-O2D-CED
12	A	1105	CLA	CBD-CGD-O2D-CED
12	A	1106	CLA	CBD-CGD-O2D-CED
12	A	1109	CLA	CBD-CGD-O2D-CED
12	A	1112	CLA	CBD-CGD-O2D-CED
12	A	1114	CLA	CBD-CGD-O2D-CED
12	A	1122	CLA	CBD-CGD-O2D-CED
12	A	1126	CLA	CBD-CGD-O2D-CED
12	A	1127	CLA	CBD-CGD-O2D-CED
12	A	1129	CLA	CBD-CGD-O2D-CED
12	A	1131	CLA	CBD-CGD-O2D-CED
12	A	1133	CLA	CBD-CGD-O2D-CED
12	A	1134	CLA	CBD-CGD-O2D-CED
12	A	1136	CLA	CBD-CGD-O2D-CED
12	A	1137	CLA	CBD-CGD-O2D-CED
12	A	1139	CLA	CBD-CGD-O2D-CED
12	A	1140	CLA	CBD-CGD-O2D-CED
12	A	1101	CLA	CBD-CGD-O2D-CED
12	B	1201	CLA	CBD-CGD-O2D-CED
12	B	1202	CLA	CBD-CGD-O2D-CED
12	B	1203	CLA	CBD-CGD-O2D-CED
12	B	1205	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	1208	CLA	CBD-CGD-O2D-CED
12	B	1209	CLA	CBD-CGD-O2D-CED
12	B	1213	CLA	CBD-CGD-O2D-CED
12	B	1222	CLA	CBD-CGD-O2D-CED
12	B	1224	CLA	CBD-CGD-O2D-CED
12	B	1225	CLA	CBD-CGD-O2D-CED
12	B	1226	CLA	CBD-CGD-O2D-CED
12	B	1227	CLA	CBD-CGD-O2D-CED
12	B	1228	CLA	CBD-CGD-O2D-CED
12	B	1230	CLA	CBD-CGD-O2D-CED
12	B	1231	CLA	CBD-CGD-O2D-CED
12	B	1232	CLA	CBD-CGD-O2D-CED
12	B	1236	CLA	CBD-CGD-O2D-CED
12	B	1240	CLA	CBD-CGD-O2D-CED
12	F	1301	CLA	CBD-CGD-O2D-CED
12	F	1302	CLA	CBD-CGD-O2D-CED
12	J	1303	CLA	CBD-CGD-O2D-CED
12	J	1302	CLA	CBD-CGD-O2D-CED
12	K	1401	CLA	CBD-CGD-O2D-CED
12	K	1402	CLA	CBD-CGD-O2D-CED
12	L	1502	CLA	CBD-CGD-O2D-CED
12	L	1502	CLA	O1A-CGA-O2A-C1
12	A	1013	CLA	O1D-CGD-O2D-CED
12	A	1104	CLA	O1D-CGD-O2D-CED
12	A	1114	CLA	O1D-CGD-O2D-CED
12	A	1120	CLA	O1D-CGD-O2D-CED
12	A	1126	CLA	O1D-CGD-O2D-CED
12	A	1129	CLA	O1D-CGD-O2D-CED
12	A	1131	CLA	O1D-CGD-O2D-CED
12	A	1133	CLA	O1D-CGD-O2D-CED
12	A	1134	CLA	O1D-CGD-O2D-CED
12	A	1140	CLA	O1D-CGD-O2D-CED
12	B	1207	CLA	O1D-CGD-O2D-CED
12	B	1224	CLA	O1D-CGD-O2D-CED
12	B	1228	CLA	O1D-CGD-O2D-CED
12	B	1229	CLA	O1D-CGD-O2D-CED
12	F	1301	CLA	O1D-CGD-O2D-CED
12	L	1502	CLA	O1D-CGD-O2D-CED
12	A	1103	CLA	O1D-CGD-O2D-CED
12	A	1107	CLA	O1D-CGD-O2D-CED
12	A	1110	CLA	O1D-CGD-O2D-CED
12	A	1113	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	1115	CLA	O1D-CGD-O2D-CED
12	A	1118	CLA	O1D-CGD-O2D-CED
12	A	1119	CLA	O1D-CGD-O2D-CED
12	A	1121	CLA	O1D-CGD-O2D-CED
12	A	1124	CLA	O1D-CGD-O2D-CED
12	A	1125	CLA	O1D-CGD-O2D-CED
12	A	1130	CLA	O1D-CGD-O2D-CED
12	A	1132	CLA	O1D-CGD-O2D-CED
12	B	1210	CLA	O1D-CGD-O2D-CED
12	B	1211	CLA	O1D-CGD-O2D-CED
12	B	1214	CLA	O1D-CGD-O2D-CED
12	B	1215	CLA	O1D-CGD-O2D-CED
12	B	1219	CLA	O1D-CGD-O2D-CED
12	B	1220	CLA	O1D-CGD-O2D-CED
12	B	1223	CLA	O1D-CGD-O2D-CED
12	A	1128	CLA	CBD-CGD-O2D-CED
12	A	1135	CLA	CBD-CGD-O2D-CED
12	B	1221	CLA	CBD-CGD-O2D-CED
12	B	1235	CLA	CBD-CGD-O2D-CED
12	A	1102	CLA	O1A-CGA-O2A-C1
12	A	1109	CLA	O1A-CGA-O2A-C1
12	A	1110	CLA	O1A-CGA-O2A-C1
12	A	1114	CLA	O1A-CGA-O2A-C1
12	A	1129	CLA	O1A-CGA-O2A-C1
12	B	1206	CLA	O1A-CGA-O2A-C1
12	B	1212	CLA	O1A-CGA-O2A-C1
12	B	1235	CLA	O1A-CGA-O2A-C1
12	B	1238	CLA	O1A-CGA-O2A-C1
12	K	1402	CLA	O1A-CGA-O2A-C1
12	A	1108	CLA	O1D-CGD-O2D-CED
12	A	1116	CLA	O1D-CGD-O2D-CED
12	A	1117	CLA	O1D-CGD-O2D-CED
12	A	1141	CLA	O1D-CGD-O2D-CED
12	B	1237	CLA	O1D-CGD-O2D-CED
12	B	1022	CLA	O1D-CGD-O2D-CED
12	B	1212	CLA	O1D-CGD-O2D-CED
12	B	1217	CLA	O1D-CGD-O2D-CED
12	B	1218	CLA	O1D-CGD-O2D-CED
12	B	1239	CLA	O1D-CGD-O2D-CED
12	A	1111	CLA	O1D-CGD-O2D-CED
12	B	1208	CLA	O1D-CGD-O2D-CED
12	B	1216	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	1225	CLA	O1D-CGD-O2D-CED
12	B	1234	CLA	O1D-CGD-O2D-CED
12	A	1012	CLA	O1D-CGD-O2D-CED
12	A	1102	CLA	O1D-CGD-O2D-CED
12	A	1137	CLA	O1D-CGD-O2D-CED
12	A	1101	CLA	O1D-CGD-O2D-CED
12	J	1302	CLA	O1D-CGD-O2D-CED
20	B	5005	LMG	O9-C10-O7-C8
21	B	5008	SQD	O49-C7-O47-C45
12	A	1119	CLA	O1A-CGA-O2A-C1
12	A	1139	CLA	C3-C5-C6-C7
12	A	1140	CLA	C3-C5-C6-C7
12	A	1013	CLA	CBA-CGA-O2A-C1
12	A	1109	CLA	CBA-CGA-O2A-C1
12	A	1110	CLA	CBA-CGA-O2A-C1
12	A	1120	CLA	CBA-CGA-O2A-C1
12	A	1128	CLA	CBA-CGA-O2A-C1
12	A	1138	CLA	CBA-CGA-O2A-C1
12	B	1212	CLA	CBA-CGA-O2A-C1
12	B	1240	CLA	CBA-CGA-O2A-C1
21	F	5001	SQD	C8-C7-O47-C45
12	A	1105	CLA	O1D-CGD-O2D-CED
12	B	1202	CLA	O1D-CGD-O2D-CED
12	B	1207	CLA	C2C-C3C-CAC-CBC
12	A	1119	CLA	CBA-CGA-O2A-C1
12	A	1133	CLA	C2A-CAA-CBA-CGA
12	A	1136	CLA	C2A-CAA-CBA-CGA
12	B	1228	CLA	C2A-CAA-CBA-CGA
12	J	1302	CLA	C2A-CAA-CBA-CGA
20	B	5002	LMG	C20-C21-C22-C23
20	B	5002	LMG	C23-C24-C25-C26
20	B	5002	LMG	C35-C36-C37-C38
20	B	5005	LMG	C38-C39-C40-C41
20	B	5005	LMG	C41-C42-C43-C44
12	A	1013	CLA	C3-C5-C6-C7
12	A	1109	CLA	C3-C5-C6-C7
12	A	1102	CLA	CBA-CGA-O2A-C1
12	A	1104	CLA	CBA-CGA-O2A-C1
12	A	1114	CLA	CBA-CGA-O2A-C1
12	A	1123	CLA	CBA-CGA-O2A-C1
12	A	1127	CLA	CBA-CGA-O2A-C1
12	A	1129	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	A	1136	CLA	CBA-CGA-O2A-C1
12	A	1130	CLA	CBA-CGA-O2A-C1
12	B	1023	CLA	CBA-CGA-O2A-C1
12	B	1206	CLA	CBA-CGA-O2A-C1
12	B	1211	CLA	CBA-CGA-O2A-C1
12	B	1215	CLA	CBA-CGA-O2A-C1
12	B	1221	CLA	CBA-CGA-O2A-C1
12	B	1227	CLA	CBA-CGA-O2A-C1
12	B	1228	CLA	CBA-CGA-O2A-C1
12	B	1230	CLA	CBA-CGA-O2A-C1
12	B	1235	CLA	CBA-CGA-O2A-C1
12	B	1238	CLA	CBA-CGA-O2A-C1
12	J	1303	CLA	CBA-CGA-O2A-C1
12	K	1402	CLA	CBA-CGA-O2A-C1
12	B	1209	CLA	O1D-CGD-O2D-CED
12	B	1236	CLA	O1D-CGD-O2D-CED
12	B	1227	CLA	O1D-CGD-O2D-CED
12	B	1230	CLA	O1D-CGD-O2D-CED
12	B	1240	CLA	O1D-CGD-O2D-CED
12	A	1013	CLA	O1A-CGA-O2A-C1
12	A	1120	CLA	O1A-CGA-O2A-C1
12	A	1123	CLA	O1A-CGA-O2A-C1
12	A	1126	CLA	O1A-CGA-O2A-C1
12	A	1128	CLA	O1A-CGA-O2A-C1
12	A	1136	CLA	O1A-CGA-O2A-C1
12	A	1138	CLA	O1A-CGA-O2A-C1
12	B	1237	CLA	O1A-CGA-O2A-C1
12	B	1209	CLA	O1A-CGA-O2A-C1
12	B	1219	CLA	O1A-CGA-O2A-C1
12	B	1221	CLA	O1A-CGA-O2A-C1
12	B	1228	CLA	O1A-CGA-O2A-C1
12	B	1207	CLA	C4C-C3C-CAC-CBC
12	A	1011	CLA	O1D-CGD-O2D-CED
12	A	1112	CLA	O1D-CGD-O2D-CED
12	F	1302	CLA	O1D-CGD-O2D-CED
12	J	1303	CLA	O1D-CGD-O2D-CED
12	K	1401	CLA	O1D-CGD-O2D-CED
15	B	4017	BCR	C9-C10-C11-C12
15	I	4018	BCR	C9-C10-C11-C12
23	J	4015	C7Z	C29-C30-C31-C32
25	I	4020	EQ3	C13-C14-C15-C16
12	A	1106	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	1136	CLA	O1D-CGD-O2D-CED
12	B	1205	CLA	O1D-CGD-O2D-CED
12	A	1011	CLA	CBA-CGA-O2A-C1
12	A	1126	CLA	CBA-CGA-O2A-C1
12	A	1131	CLA	CBA-CGA-O2A-C1
12	A	1135	CLA	CBA-CGA-O2A-C1
12	B	1209	CLA	CBA-CGA-O2A-C1
12	B	1219	CLA	CBA-CGA-O2A-C1
12	A	1130	CLA	O1A-CGA-O2A-C1
12	B	1227	CLA	O1A-CGA-O2A-C1
12	B	1240	CLA	O1A-CGA-O2A-C1
12	B	1213	CLA	O1D-CGD-O2D-CED
12	B	1222	CLA	O1D-CGD-O2D-CED
16	A	5001	LHG	C8-C7-O7-C5
16	B	5004	LHG	C11-C12-C13-C14
12	B	1226	CLA	O1D-CGD-O2D-CED
16	A	5001	LHG	C11-C12-C13-C14
12	A	1122	CLA	O1D-CGD-O2D-CED
12	B	1229	CLA	C3-C5-C6-C7
12	A	1134	CLA	CBA-CGA-O2A-C1
12	B	1237	CLA	CBA-CGA-O2A-C1
12	A	1104	CLA	O1A-CGA-O2A-C1
12	A	1127	CLA	O1A-CGA-O2A-C1
12	A	1135	CLA	O1A-CGA-O2A-C1
12	B	1023	CLA	O1A-CGA-O2A-C1
12	B	1211	CLA	O1A-CGA-O2A-C1
12	B	1215	CLA	O1A-CGA-O2A-C1
12	B	1230	CLA	O1A-CGA-O2A-C1
12	J	1303	CLA	O1A-CGA-O2A-C1
12	A	1109	CLA	C4-C3-C5-C6
12	A	1139	CLA	C4-C3-C5-C6
12	A	1132	CLA	C4-C3-C5-C6
12	B	1021	CLA	C4-C3-C5-C6
12	A	1109	CLA	C2-C3-C5-C6
12	A	1139	CLA	C2-C3-C5-C6
12	A	1132	CLA	C2-C3-C5-C6
12	B	1021	CLA	C2-C3-C5-C6
12	A	1129	CLA	C2A-CAA-CBA-CGA
12	L	1502	CLA	C2A-CAA-CBA-CGA
12	A	1011	CLA	O1A-CGA-O2A-C1
12	A	1131	CLA	O1A-CGA-O2A-C1
12	A	1111	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	1239	CLA	CBA-CGA-O2A-C1
12	A	1128	CLA	O1D-CGD-O2D-CED
12	A	1134	CLA	O1A-CGA-O2A-C1
12	B	1239	CLA	O1A-CGA-O2A-C1
12	F	1302	CLA	O1A-CGA-O2A-C1
12	A	1105	CLA	C3-C5-C6-C7
12	A	1106	CLA	C3-C5-C6-C7
12	B	1235	CLA	O1D-CGD-O2D-CED
12	A	1106	CLA	CBA-CGA-O2A-C1
12	A	1113	CLA	CBA-CGA-O2A-C1
12	A	1118	CLA	CBA-CGA-O2A-C1
12	A	1122	CLA	CBA-CGA-O2A-C1
12	A	1137	CLA	CBA-CGA-O2A-C1
12	B	1202	CLA	CBA-CGA-O2A-C1
12	B	1214	CLA	CBA-CGA-O2A-C1
12	B	1218	CLA	CBA-CGA-O2A-C1
12	B	1222	CLA	CBA-CGA-O2A-C1
12	F	1302	CLA	CBA-CGA-O2A-C1
15	B	4017	BCR	C15-C16-C17-C18
12	B	1202	CLA	C13-C15-C16-C17
12	B	1214	CLA	C5-C6-C7-C8
13	A	2001	PQN	C18-C20-C21-C22
16	A	5003	LHG	O2-C2-C3-O3
20	B	5005	LMG	C28-C29-C30-C31
12	A	1118	CLA	O1A-CGA-O2A-C1
12	A	1102	CLA	C11-C10-C8-C9
12	A	1105	CLA	C14-C13-C15-C16
12	A	1106	CLA	C14-C13-C15-C16
12	A	1128	CLA	C11-C12-C13-C14
12	A	1140	CLA	C11-C12-C13-C14
12	A	1135	CLA	O1D-CGD-O2D-CED
12	B	1221	CLA	O1D-CGD-O2D-CED
12	A	1123	CLA	CBD-CGD-O2D-CED
12	A	1106	CLA	C2A-CAA-CBA-CGA
12	A	1135	CLA	C2A-CAA-CBA-CGA
15	A	4001	BCR	C11-C12-C13-C35
15	A	4001	BCR	C37-C22-C23-C24
15	A	4012	BCR	C36-C18-C19-C20
15	B	4004	BCR	C7-C8-C9-C34
15	B	4010	BCR	C37-C22-C23-C24
15	F	4014	BCR	C37-C22-C23-C24
15	J	4013	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	K	4001	BCR	C7-C8-C9-C34
17	B	4011	45D	C19-C23-C25-C27
23	F	4016	C7Z	C31-C32-C33-C40
25	I	4020	EQ3	C7-C8-C9-C34
15	A	4003	BCR	C11-C12-C13-C14
15	B	4004	BCR	C7-C8-C9-C10
15	F	4014	BCR	C21-C22-C23-C24
17	B	4011	45D	C19-C23-C25-C29
25	I	4020	EQ3	C7-C8-C9-C10
16	A	5001	LHG	O9-C7-O7-C5
12	A	1106	CLA	O1A-CGA-O2A-C1
12	B	1202	CLA	O1A-CGA-O2A-C1
12	B	1214	CLA	O1A-CGA-O2A-C1
12	B	1218	CLA	O1A-CGA-O2A-C1
24	F	6001	LMT	O5'-C5'-C6'-O6'
12	A	1109	CLA	C13-C15-C16-C17
12	A	1140	CLA	C10-C11-C12-C13
16	A	5001	LHG	C23-C24-C25-C26
12	A	1123	CLA	C10-C11-C12-C13
12	A	1132	CLA	C5-C6-C7-C8
12	B	1214	CLA	C3-C5-C6-C7
12	A	1011	CLA	C2-C1-O2A-CGA
12	A	1108	CLA	C2-C1-O2A-CGA
12	A	1110	CLA	C2-C1-O2A-CGA
12	A	1112	CLA	C2-C1-O2A-CGA
12	A	1113	CLA	C2-C1-O2A-CGA
12	A	1114	CLA	C2-C1-O2A-CGA
12	A	1118	CLA	C2-C1-O2A-CGA
12	A	1120	CLA	C2-C1-O2A-CGA
12	A	1124	CLA	C2-C1-O2A-CGA
12	A	1125	CLA	C2-C1-O2A-CGA
12	A	1127	CLA	C2-C1-O2A-CGA
12	A	1134	CLA	C2-C1-O2A-CGA
12	A	1135	CLA	C2-C1-O2A-CGA
12	A	1136	CLA	C2-C1-O2A-CGA
12	A	1140	CLA	C2-C1-O2A-CGA
12	A	1130	CLA	C2-C1-O2A-CGA
12	B	1237	CLA	C2-C1-O2A-CGA
12	B	1022	CLA	C2-C1-O2A-CGA
12	B	1207	CLA	C2-C1-O2A-CGA
12	B	1208	CLA	C2-C1-O2A-CGA
12	B	1209	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	1211	CLA	C2-C1-O2A-CGA
12	B	1220	CLA	C2-C1-O2A-CGA
12	B	1223	CLA	C2-C1-O2A-CGA
12	B	1230	CLA	C2-C1-O2A-CGA
12	B	1231	CLA	C2-C1-O2A-CGA
12	B	1240	CLA	C2-C1-O2A-CGA
12	F	1301	CLA	C2-C1-O2A-CGA
12	F	1302	CLA	C2-C1-O2A-CGA
12	J	1303	CLA	C2-C1-O2A-CGA
12	K	1402	CLA	C2-C1-O2A-CGA
12	A	1140	CLA	C13-C15-C16-C17
12	B	1021	CLA	C13-C15-C16-C17
12	B	1234	CLA	C5-C6-C7-C8
16	A	5003	LHG	C23-C24-C25-C26
12	A	1102	CLA	C12-C13-C15-C16
12	B	1021	CLA	C6-C7-C8-C10
12	B	1214	CLA	C6-C7-C8-C10
12	A	1113	CLA	O1A-CGA-O2A-C1
12	A	1122	CLA	O1A-CGA-O2A-C1
15	A	4008	BCR	C19-C20-C21-C22
15	B	4010	BCR	C13-C14-C15-C16
15	B	4018	BCR	C13-C14-C15-C16
15	K	4001	BCR	C15-C16-C17-C18
19	M	4021	ECH	C9-C10-C11-C12
12	A	1112	CLA	CBA-CGA-O2A-C1
12	A	1011	CLA	C2A-CAA-CBA-CGA
12	A	1112	CLA	C2A-CAA-CBA-CGA
12	B	1207	CLA	C2A-CAA-CBA-CGA
12	F	1302	CLA	C2A-CAA-CBA-CGA
12	A	1013	CLA	C10-C11-C12-C13
13	B	2002	PQN	C25-C26-C27-C28
12	A	1137	CLA	O1A-CGA-O2A-C1
12	B	1222	CLA	O1A-CGA-O2A-C1
21	B	5008	SQD	O5-C1-O6-C44
12	A	1106	CLA	C13-C15-C16-C17
12	A	1109	CLA	C8-C10-C11-C12
15	A	4001	BCR	C10-C11-C12-C13
15	A	4003	BCR	C10-C11-C12-C13
16	B	5006	LHG	O2-C2-C3-O3
12	B	1021	CLA	C3-C5-C6-C7
12	A	1102	CLA	C10-C11-C12-C13
12	A	1126	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	B	1022	CLA	C10-C11-C12-C13
12	B	1021	CLA	CBA-CGA-O2A-C1
12	A	1111	CLA	O1A-CGA-O2A-C1
12	A	1013	CLA	C13-C15-C16-C17
12	A	1106	CLA	C8-C10-C11-C12
16	A	5003	LHG	C4-O6-P-O3
16	B	5004	LHG	C4-O6-P-O3
12	A	1124	CLA	CBA-CGA-O2A-C1
12	A	1139	CLA	CBA-CGA-O2A-C1
12	B	1203	CLA	CBA-CGA-O2A-C1
12	B	1226	CLA	CBA-CGA-O2A-C1
12	A	1128	CLA	C4-C3-C5-C6
12	A	1140	CLA	C15-C16-C17-C18
13	B	2002	PQN	C15-C16-C17-C18
12	A	1013	CLA	C2A-CAA-CBA-CGA
12	A	1120	CLA	C2A-CAA-CBA-CGA
12	A	1138	CLA	C2A-CAA-CBA-CGA
12	B	1237	CLA	C2A-CAA-CBA-CGA
12	B	1023	CLA	C2A-CAA-CBA-CGA
12	A	1140	CLA	C16-C17-C18-C20
12	B	1234	CLA	C3-C5-C6-C7
12	B	1210	CLA	CBA-CGA-O2A-C1
17	B	4011	45D	C35-C37-C41-C42
17	B	4011	45D	C36-C38-C42-C41
16	A	5001	LHG	C28-C29-C30-C31
21	B	5008	SQD	C30-C31-C32-C33
12	A	1128	CLA	C16-C17-C18-C20
12	B	1205	CLA	CBA-CGA-O2A-C1
12	B	1208	CLA	CBA-CGA-O2A-C1
12	F	1301	CLA	CBA-CGA-O2A-C1
24	F	6001	LMT	C2-C3-C4-C5
21	F	5001	SQD	C11-C10-C9-C8
12	A	1112	CLA	O1A-CGA-O2A-C1
16	A	5003	LHG	C11-C12-C13-C14
15	A	4012	BCR	C11-C10-C9-C8
20	B	5005	LMG	C2-C1-O1-C7
21	B	5008	SQD	C2-C1-O6-C44
23	F	4016	C7Z	C28-C29-C30-C31
23	J	4015	C7Z	C12-C13-C14-C15
23	J	4015	C7Z	C32-C33-C34-C35
12	B	1229	CLA	CBA-CGA-O2A-C1
16	A	5003	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
12	A	1106	CLA	C15-C16-C17-C18
12	A	1109	CLA	C15-C16-C17-C18
12	A	1013	CLA	C16-C17-C18-C20
12	B	1202	CLA	C2-C3-C5-C6
12	B	1214	CLA	C2-C3-C5-C6
13	A	2001	PQN	C19-C18-C20-C21
12	B	1214	CLA	C2A-CAA-CBA-CGA
15	I	4018	BCR	C11-C12-C13-C35
23	F	4016	C7Z	C7-C8-C9-C19
25	I	4020	EQ3	C36-C18-C19-C20
16	A	5003	LHG	O1-C1-C2-C3
16	B	5004	LHG	O1-C1-C2-C3
15	A	4008	BCR	C21-C22-C23-C24
15	B	4010	BCR	C21-C22-C23-C24
15	B	4018	BCR	C21-C22-C23-C24
15	I	4018	BCR	C11-C12-C13-C14
15	J	4013	BCR	C7-C8-C9-C10
19	M	4021	ECH	C7-C8-C9-C10
21	F	5001	SQD	C29-C30-C31-C32
16	A	5003	LHG	C9-C10-C11-C12
16	B	5004	LHG	C28-C29-C30-C31
12	A	1128	CLA	C16-C17-C18-C19
20	B	5005	LMG	C16-C17-C18-C19
12	B	1240	CLA	C2C-C3C-CAC-CBC
12	A	1124	CLA	O1A-CGA-O2A-C1
20	B	5005	LMG	C32-C33-C34-C35
12	A	1011	CLA	C3A-C2A-CAA-CBA
12	A	1104	CLA	C3A-C2A-CAA-CBA
12	A	1107	CLA	C3A-C2A-CAA-CBA
12	A	1112	CLA	C3A-C2A-CAA-CBA
12	A	1135	CLA	C3A-C2A-CAA-CBA
12	B	1204	CLA	C3A-C2A-CAA-CBA
12	B	1206	CLA	C3A-C2A-CAA-CBA
12	B	1207	CLA	C3A-C2A-CAA-CBA
12	B	1210	CLA	C3A-C2A-CAA-CBA
12	B	1219	CLA	C3A-C2A-CAA-CBA
12	B	1234	CLA	C3A-C2A-CAA-CBA
12	B	1240	CLA	C3A-C2A-CAA-CBA
12	F	1302	CLA	C3A-C2A-CAA-CBA
12	K	1401	CLA	C3A-C2A-CAA-CBA
12	K	1402	CLA	C3A-C2A-CAA-CBA
12	L	1502	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	1139	CLA	O1A-CGA-O2A-C1
12	B	1021	CLA	O1A-CGA-O2A-C1
12	B	1203	CLA	O1A-CGA-O2A-C1
20	B	5005	LMG	C12-C13-C14-C15
21	F	5001	SQD	C14-C15-C16-C17
12	B	1226	CLA	O1A-CGA-O2A-C1
12	B	1202	CLA	C4-C3-C5-C6
12	B	1214	CLA	C4-C3-C5-C6
16	A	5003	LHG	C8-C7-O7-C5
20	B	5002	LMG	C11-C10-O7-C8
16	A	5001	LHG	O1-C1-C2-O2
16	B	5006	LHG	O1-C1-C2-O2
16	A	5003	LHG	C13-C14-C15-C16
12	B	1205	CLA	O1A-CGA-O2A-C1
12	B	1210	CLA	O1A-CGA-O2A-C1
12	F	1301	CLA	O1A-CGA-O2A-C1
12	B	1229	CLA	C6-C7-C8-C9
12	A	1105	CLA	C13-C15-C16-C17
16	B	5004	LHG	C11-C10-C9-C8
16	A	5003	LHG	O9-C7-O7-C5
12	A	1012	CLA	C2-C1-O2A-CGA
12	A	1103	CLA	C2-C1-O2A-CGA
12	A	1109	CLA	C2-C1-O2A-CGA
12	A	1116	CLA	C2-C1-O2A-CGA
12	A	1117	CLA	C2-C1-O2A-CGA
12	A	1131	CLA	C2-C1-O2A-CGA
12	A	1137	CLA	C2-C1-O2A-CGA
12	A	1139	CLA	C2-C1-O2A-CGA
12	A	1101	CLA	C2-C1-O2A-CGA
12	A	1132	CLA	C2-C1-O2A-CGA
12	B	1021	CLA	C2-C1-O2A-CGA
12	B	1210	CLA	C2-C1-O2A-CGA
12	B	1213	CLA	C2-C1-O2A-CGA
12	B	1215	CLA	C2-C1-O2A-CGA
12	B	1216	CLA	C2-C1-O2A-CGA
12	B	1219	CLA	C2-C1-O2A-CGA
12	B	1225	CLA	C2-C1-O2A-CGA
12	B	1226	CLA	C2-C1-O2A-CGA
12	B	1227	CLA	C2-C1-O2A-CGA
12	B	1228	CLA	C2-C1-O2A-CGA
12	B	1235	CLA	C2-C1-O2A-CGA
12	B	1236	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	1238	CLA	C2-C1-O2A-CGA
12	J	1302	CLA	C2-C1-O2A-CGA
12	B	1229	CLA	O1A-CGA-O2A-C1
16	A	5001	LHG	C34-C35-C36-C37
16	B	5004	LHG	C32-C33-C34-C35
15	A	4008	BCR	C5-C6-C7-C8
15	A	4008	BCR	C23-C24-C25-C30
15	A	4012	BCR	C1-C6-C7-C8
15	A	4012	BCR	C5-C6-C7-C8
15	B	4005	BCR	C1-C6-C7-C8
15	B	4005	BCR	C5-C6-C7-C8
15	I	4018	BCR	C23-C24-C25-C26
15	I	4018	BCR	C23-C24-C25-C30
15	J	4013	BCR	C1-C6-C7-C8
15	J	4013	BCR	C5-C6-C7-C8
15	K	4001	BCR	C23-C24-C25-C26
15	K	4001	BCR	C23-C24-C25-C30
17	B	4011	45D	C16-C08-C20-C24
19	B	4006	ECH	C23-C24-C25-C26
19	M	4021	ECH	C1-C6-C7-C8
19	M	4021	ECH	C23-C24-C25-C26
23	F	4016	C7Z	C25-C26-C27-C28
23	J	4015	C7Z	C5-C6-C7-C8
25	I	4020	EQ3	C1-C6-C7-C8
25	I	4020	EQ3	C5-C6-C7-C8
25	I	4020	EQ3	C23-C24-C25-C26
16	A	5003	LHG	C29-C30-C31-C32
16	B	5004	LHG	C31-C32-C33-C34
13	A	2001	PQN	C23-C25-C26-C27
12	B	1208	CLA	O1A-CGA-O2A-C1
12	A	1102	CLA	C11-C10-C8-C7
12	A	1109	CLA	C11-C10-C8-C7
13	A	2001	PQN	C17-C18-C20-C21
13	B	2002	PQN	C21-C22-C23-C25
15	A	4007	BCR	C9-C10-C11-C12
20	B	5002	LMG	O9-C10-O7-C8
12	A	1012	CLA	CBA-CGA-O2A-C1
12	A	1108	CLA	C2A-CAA-CBA-CGA
12	A	1116	CLA	C2A-CAA-CBA-CGA
12	A	1121	CLA	C2A-CAA-CBA-CGA
12	B	1224	CLA	C2A-CAA-CBA-CGA
12	B	1214	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	A	1140	CLA	C8-C10-C11-C12
12	B	1235	CLA	C13-C15-C16-C17
20	B	5005	LMG	O6-C1-O1-C7
16	A	5001	LHG	C24-C25-C26-C27
12	A	1123	CLA	O1D-CGD-O2D-CED
16	B	5004	LHG	C13-C14-C15-C16
12	A	1013	CLA	C16-C17-C18-C19
12	A	1128	CLA	C2-C3-C5-C6
12	A	1102	CLA	C14-C13-C15-C16
12	B	1021	CLA	C6-C7-C8-C9
13	A	2001	PQN	C21-C22-C23-C24
13	B	2002	PQN	C21-C22-C23-C24
16	A	5003	LHG	C34-C35-C36-C37
12	B	1209	CLA	C2A-CAA-CBA-CGA
12	K	1402	CLA	C2A-CAA-CBA-CGA
20	B	5005	LMG	O6-C5-C6-O5
15	B	4018	BCR	C37-C22-C23-C24
15	F	4014	BCR	C11-C12-C13-C35
19	M	4021	ECH	C11-C12-C13-C35
15	I	4018	BCR	C7-C8-C9-C10
19	M	4021	ECH	C11-C12-C13-C14
25	I	4020	EQ3	C17-C18-C19-C20
12	A	1104	CLA	C1A-C2A-CAA-CBA
12	A	1106	CLA	C1A-C2A-CAA-CBA
12	A	1116	CLA	C1A-C2A-CAA-CBA
12	A	1120	CLA	C1A-C2A-CAA-CBA
12	A	1121	CLA	C1A-C2A-CAA-CBA
12	A	1122	CLA	C1A-C2A-CAA-CBA
12	A	1124	CLA	C1A-C2A-CAA-CBA
12	A	1127	CLA	C1A-C2A-CAA-CBA
12	A	1133	CLA	C1A-C2A-CAA-CBA
12	A	1135	CLA	C1A-C2A-CAA-CBA
12	A	1132	CLA	C1A-C2A-CAA-CBA
12	B	1202	CLA	C1A-C2A-CAA-CBA
12	B	1206	CLA	C1A-C2A-CAA-CBA
12	B	1214	CLA	C1A-C2A-CAA-CBA
12	B	1215	CLA	C1A-C2A-CAA-CBA
12	B	1219	CLA	C1A-C2A-CAA-CBA
12	B	1220	CLA	C1A-C2A-CAA-CBA
12	B	1224	CLA	C1A-C2A-CAA-CBA
12	B	1229	CLA	C1A-C2A-CAA-CBA
12	B	1230	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	1234	CLA	C1A-C2A-CAA-CBA
12	B	1240	CLA	C1A-C2A-CAA-CBA
12	B	1238	CLA	C1A-C2A-CAA-CBA
12	F	1302	CLA	C1A-C2A-CAA-CBA
12	K	1401	CLA	C1A-C2A-CAA-CBA
12	K	1402	CLA	C1A-C2A-CAA-CBA
12	A	1140	CLA	C16-C17-C18-C19
12	B	1229	CLA	C6-C7-C8-C10
15	B	4005	BCR	C15-C16-C17-C18
15	B	4017	BCR	C13-C14-C15-C16
15	F	4014	BCR	C9-C10-C11-C12
12	B	1021	CLA	C5-C6-C7-C8
20	B	5002	LMG	C34-C35-C36-C37
21	B	5008	SQD	C31-C32-C33-C34
16	A	5001	LHG	C30-C31-C32-C33
21	B	5008	SQD	O6-C44-C45-C46
16	A	5003	LHG	C7-C8-C9-C10
12	A	1012	CLA	O1A-CGA-O2A-C1
16	A	5001	LHG	C13-C14-C15-C16
20	B	5002	LMG	O6-C5-C6-O5
16	A	5003	LHG	O1-C1-C2-O2
16	A	5003	LHG	C35-C36-C37-C38
16	B	5004	LHG	C26-C27-C28-C29
12	B	1229	CLA	C4-C3-C5-C6
16	A	5001	LHG	C25-C26-C27-C28
16	A	5001	LHG	C7-C8-C9-C10
12	B	1201	CLA	CBA-CGA-O2A-C1
12	B	1231	CLA	CBA-CGA-O2A-C1
12	A	1128	CLA	C13-C15-C16-C17
12	B	1214	CLA	C8-C10-C11-C12
12	A	1134	CLA	C2A-CAA-CBA-CGA
12	B	1208	CLA	C2A-CAA-CBA-CGA
12	A	1115	CLA	C2-C1-O2A-CGA
12	A	1121	CLA	C2-C1-O2A-CGA
12	B	1212	CLA	C2-C1-O2A-CGA
12	B	1217	CLA	C2-C1-O2A-CGA
12	B	1218	CLA	C2-C1-O2A-CGA
12	L	1502	CLA	C2-C1-O2A-CGA
12	B	1240	CLA	C4C-C3C-CAC-CBC
12	A	1140	CLA	CBA-CGA-O2A-C1
12	B	1236	CLA	CBA-CGA-O2A-C1
12	A	1103	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	A	1101	CLA	CAA-CBA-CGA-O2A
12	A	1128	CLA	C10-C11-C12-C13
12	A	1128	CLA	C15-C16-C17-C18
12	A	1138	CLA	C8-C10-C11-C12
12	B	1021	CLA	CAA-CBA-CGA-O2A
16	A	5001	LHG	C11-C10-C9-C8
24	F	6001	LMT	O1'-C1-C2-C3
12	A	1123	CLA	C11-C10-C8-C7
12	A	1140	CLA	C11-C12-C13-C15
12	B	1214	CLA	C11-C10-C8-C7
12	B	1229	CLA	C2-C3-C5-C6
12	B	1234	CLA	C11-C10-C8-C7
12	B	1235	CLA	C11-C12-C13-C15
13	A	2001	PQN	C21-C22-C23-C25
12	A	1013	CLA	C14-C13-C15-C16
12	A	1123	CLA	C11-C10-C8-C9
12	B	1235	CLA	C11-C10-C8-C9
15	B	4004	BCR	C9-C10-C11-C12
12	A	1110	CLA	C2A-CAA-CBA-CGA
12	A	1132	CLA	C2A-CAA-CBA-CGA
12	B	1235	CLA	C2A-CAA-CBA-CGA
19	M	4021	ECH	C36-C18-C19-C20
15	A	4007	BCR	C17-C18-C19-C20
12	A	1123	CLA	C8-C10-C11-C12
12	B	1207	CLA	CBA-CGA-O2A-C1
12	B	1224	CLA	CBA-CGA-O2A-C1
12	B	1232	CLA	CBA-CGA-O2A-C1
12	A	1128	CLA	C5-C6-C7-C8
21	F	5001	SQD	C31-C32-C33-C34
16	A	5001	LHG	C26-C27-C28-C29
12	B	1224	CLA	C4-C3-C5-C6
16	B	5004	LHG	C10-C11-C12-C13
20	B	5005	LMG	C39-C40-C41-C42
12	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	4004	BCR	C19-C20-C21-C22
12	B	1231	CLA	O1A-CGA-O2A-C1
12	A	1106	CLA	C10-C11-C12-C13
12	A	1140	CLA	C5-C6-C7-C8
12	A	1123	CLA	C4-C3-C5-C6
12	B	1201	CLA	O1A-CGA-O2A-C1
12	B	1201	CLA	C2A-CAA-CBA-CGA
16	B	5004	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
16	A	5001	LHG	O6-C4-C5-O7
12	B	1236	CLA	O1A-CGA-O2A-C1
12	A	1140	CLA	O1A-CGA-O2A-C1
12	A	1132	CLA	C3-C5-C6-C7
16	A	5003	LHG	C31-C32-C33-C34
16	A	5001	LHG	O7-C5-C6-O8
16	A	5001	LHG	C35-C36-C37-C38
12	B	1202	CLA	C3-C5-C6-C7
12	B	1224	CLA	C2-C3-C5-C6
12	B	1021	CLA	C11-C10-C8-C9
12	B	1214	CLA	C6-C7-C8-C9
12	B	1235	CLA	C11-C12-C13-C14
12	A	1107	CLA	CBA-CGA-O2A-C1
12	B	1224	CLA	O1A-CGA-O2A-C1
16	A	5003	LHG	C10-C11-C12-C13
12	A	1141	CLA	C2A-CAA-CBA-CGA
15	A	4007	BCR	C23-C24-C25-C26
15	A	4007	BCR	C23-C24-C25-C30
15	A	4012	BCR	C23-C24-C25-C26
15	A	4012	BCR	C23-C24-C25-C30
15	J	4013	BCR	C23-C24-C25-C26
15	J	4013	BCR	C23-C24-C25-C30
19	B	4006	ECH	C23-C24-C25-C30
23	J	4015	C7Z	C21-C26-C27-C28
15	A	4012	BCR	C17-C18-C19-C20
15	K	4001	BCR	C7-C8-C9-C10
12	A	1109	CLA	C16-C17-C18-C20
16	B	5004	LHG	O6-C4-C5-C6
16	A	5003	LHG	C12-C13-C14-C15
12	A	1105	CLA	C12-C13-C15-C16
12	A	1109	CLA	C11-C12-C13-C15
12	A	1123	CLA	C2-C3-C5-C6
12	A	1128	CLA	C11-C12-C13-C15
12	A	1138	CLA	C11-C10-C8-C7
12	B	1021	CLA	C11-C10-C8-C7
12	B	1235	CLA	C11-C10-C8-C7
15	A	4001	BCR	C9-C10-C11-C12
15	A	4008	BCR	C9-C10-C11-C12
15	B	4005	BCR	C13-C14-C15-C16
15	J	4013	BCR	C9-C10-C11-C12
24	F	6001	LMT	C1-C2-C3-C4
20	B	5005	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
12	A	1116	CLA	CBA-CGA-O2A-C1
12	B	1207	CLA	O1A-CGA-O2A-C1
12	B	1232	CLA	O1A-CGA-O2A-C1
16	A	5001	LHG	C24-C23-O8-C6
12	A	1011	CLA	CAD-CBD-CGD-O2D
12	A	1103	CLA	CAD-CBD-CGD-O2D
12	A	1111	CLA	CAD-CBD-CGD-O2D
12	A	1125	CLA	CAD-CBD-CGD-O2D
12	A	1134	CLA	CAD-CBD-CGD-O2D
12	A	1132	CLA	CAD-CBD-CGD-O2D
12	B	1238	CLA	CAD-CBD-CGD-O2D
12	B	1021	CLA	C15-C16-C17-C18
12	J	1302	CLA	CAA-CBA-CGA-O2A
12	A	1101	CLA	CBA-CGA-O2A-C1
16	A	5001	LHG	C2-C3-O3-P
20	B	5005	LMG	C7-C8-C9-O8
12	A	1107	CLA	O1A-CGA-O2A-C1
12	A	1116	CLA	O1A-CGA-O2A-C1
16	A	5003	LHG	O6-C4-C5-O7
12	A	1113	CLA	CHA-CBD-CGD-O2D
12	A	1125	CLA	CHA-CBD-CGD-O1D
12	A	1128	CLA	CHA-CBD-CGD-O1D
12	A	1138	CLA	CHA-CBD-CGD-O1D
12	A	1138	CLA	CHA-CBD-CGD-O2D
12	B	1210	CLA	CHA-CBD-CGD-O1D
12	B	1210	CLA	CHA-CBD-CGD-O2D
12	B	1216	CLA	CHA-CBD-CGD-O1D
12	B	1220	CLA	CHA-CBD-CGD-O2D
12	B	1221	CLA	CHA-CBD-CGD-O1D
12	B	1221	CLA	CHA-CBD-CGD-O2D
12	B	1224	CLA	CHA-CBD-CGD-O2D
12	B	1227	CLA	CHA-CBD-CGD-O1D
12	B	1230	CLA	CHA-CBD-CGD-O1D
12	B	1234	CLA	CHA-CBD-CGD-O1D
12	B	1234	CLA	CHA-CBD-CGD-O2D
12	B	1240	CLA	CHA-CBD-CGD-O1D
12	B	1240	CLA	CHA-CBD-CGD-O2D
12	B	1238	CLA	CHA-CBD-CGD-O1D
12	J	1302	CLA	CHA-CBD-CGD-O1D
12	J	1302	CLA	CHA-CBD-CGD-O2D
12	K	1402	CLA	CHA-CBD-CGD-O1D
12	K	1402	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	5005	LMG	O7-C8-C9-O8
12	B	1234	CLA	C11-C12-C13-C15
12	B	1202	CLA	C15-C16-C17-C18
19	B	4006	ECH	C37-C22-C23-C24
19	B	4006	ECH	C21-C22-C23-C24
12	A	1011	CLA	C1A-C2A-CAA-CBA
12	A	1117	CLA	C1A-C2A-CAA-CBA
12	B	1211	CLA	C1A-C2A-CAA-CBA
12	A	1105	CLA	C2-C1-O2A-CGA
12	B	1205	CLA	C2-C1-O2A-CGA
12	B	1239	CLA	C2-C1-O2A-CGA
15	J	4013	BCR	C15-C16-C17-C18
12	A	1101	CLA	O1A-CGA-O2A-C1
16	A	5003	LHG	C4-O6-P-O5
16	B	5004	LHG	C4-O6-P-O4
12	B	1224	CLA	C6-C7-C8-C9
12	A	1131	CLA	O2A-C1-C2-C3
12	B	1218	CLA	O2A-C1-C2-C3
16	A	5001	LHG	O6-C4-C5-C6
16	A	5003	LHG	O6-C4-C5-C6
21	F	5001	SQD	C13-C14-C15-C16
12	B	1225	CLA	C2A-CAA-CBA-CGA
16	A	5003	LHG	C24-C25-C26-C27
12	A	1102	CLA	C16-C17-C18-C19
12	A	1113	CLA	CAD-CBD-CGD-O1D
12	B	1210	CLA	CAD-CBD-CGD-O1D
12	B	1220	CLA	CAD-CBD-CGD-O1D
12	B	1234	CLA	CAD-CBD-CGD-O1D
12	K	1402	CLA	CAD-CBD-CGD-O1D
12	B	1235	CLA	C3-C5-C6-C7
16	A	5001	LHG	O10-C23-O8-C6
12	B	1022	CLA	C4-C3-C5-C6
12	A	1128	CLA	C6-C7-C8-C10
12	A	1138	CLA	C11-C12-C13-C15
12	B	1021	CLA	C11-C12-C13-C15
16	B	5004	LHG	O6-C4-C5-O7
16	B	5006	LHG	O6-C4-C5-O7
15	A	4003	BCR	C19-C20-C21-C22
23	F	4016	C7Z	C33-C34-C35-C15
12	A	1012	CLA	C2A-CAA-CBA-CGA
16	A	5003	LHG	C28-C29-C30-C31
12	B	1214	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	A	2001	PQN	C13-C15-C16-C17
12	A	1109	CLA	C11-C12-C13-C14
12	A	1128	CLA	C6-C7-C8-C9
12	A	1138	CLA	C11-C10-C8-C9
12	B	1021	CLA	C14-C13-C15-C16
12	B	1229	CLA	C2C-C3C-CAC-CBC
15	A	4003	BCR	C18-C19-C20-C21
15	B	4018	BCR	C18-C19-C20-C21
19	M	4021	ECH	C17-C18-C19-C20
12	A	1012	CLA	C1-C2-C3-C4
12	A	1103	CLA	C1-C2-C3-C4
12	A	1104	CLA	C1-C2-C3-C4
12	A	1108	CLA	C1-C2-C3-C4
12	A	1110	CLA	C1-C2-C3-C4
12	A	1111	CLA	C1-C2-C3-C4
12	A	1112	CLA	C1-C2-C3-C4
12	A	1113	CLA	C1-C2-C3-C4
12	A	1116	CLA	C1-C2-C3-C4
12	A	1117	CLA	C1-C2-C3-C4
12	A	1121	CLA	C1-C2-C3-C4
12	A	1124	CLA	C1-C2-C3-C4
12	A	1125	CLA	C1-C2-C3-C4
12	A	1127	CLA	C1-C2-C3-C4
12	A	1131	CLA	C1-C2-C3-C4
12	A	1133	CLA	C1-C2-C3-C4
12	A	1134	CLA	C1-C2-C3-C4
12	A	1135	CLA	C1-C2-C3-C4
12	A	1136	CLA	C1-C2-C3-C4
12	A	1130	CLA	C1-C2-C3-C4
12	B	1237	CLA	C1-C2-C3-C4
12	B	1023	CLA	C1-C2-C3-C4
12	B	1201	CLA	C1-C2-C3-C4
12	B	1203	CLA	C1-C2-C3-C4
12	B	1204	CLA	C1-C2-C3-C4
12	B	1205	CLA	C1-C2-C3-C4
12	B	1206	CLA	C1-C2-C3-C4
12	B	1207	CLA	C1-C2-C3-C4
12	B	1208	CLA	C1-C2-C3-C4
12	B	1210	CLA	C1-C2-C3-C4
12	B	1211	CLA	C1-C2-C3-C4
12	B	1213	CLA	C1-C2-C3-C4
12	B	1216	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	B	1218	CLA	C1-C2-C3-C4
12	B	1219	CLA	C1-C2-C3-C4
12	B	1220	CLA	C1-C2-C3-C4
12	B	1221	CLA	C1-C2-C3-C4
12	B	1223	CLA	C1-C2-C3-C4
12	B	1225	CLA	C1-C2-C3-C4
12	B	1226	CLA	C1-C2-C3-C4
12	B	1227	CLA	C1-C2-C3-C4
12	B	1230	CLA	C1-C2-C3-C4
12	B	1231	CLA	C1-C2-C3-C4
12	B	1232	CLA	C1-C2-C3-C4
12	B	1236	CLA	C1-C2-C3-C4
12	B	1239	CLA	C1-C2-C3-C4
12	B	1240	CLA	C1-C2-C3-C4
12	B	1238	CLA	C1-C2-C3-C4
12	F	1301	CLA	C1-C2-C3-C4
12	F	1302	CLA	C1-C2-C3-C4
12	J	1303	CLA	C1-C2-C3-C4
12	J	1302	CLA	C1-C2-C3-C4
12	K	1402	CLA	C1-C2-C3-C4
12	L	1502	CLA	C1-C2-C3-C4
12	B	1204	CLA	C2A-CAA-CBA-CGA
12	B	1217	CLA	C2A-CAA-CBA-CGA
12	A	1104	CLA	C2-C1-O2A-CGA
12	A	1133	CLA	C2-C1-O2A-CGA
12	B	1234	CLA	C11-C12-C13-C14
12	B	1223	CLA	CBA-CGA-O2A-C1
15	A	4007	BCR	C13-C14-C15-C16
12	B	1223	CLA	O1A-CGA-O2A-C1
21	F	5001	SQD	C28-C29-C30-C31
12	B	1202	CLA	CAA-CBA-CGA-O2A
21	B	5008	SQD	O6-C44-C45-O47
16	B	5004	LHG	C29-C30-C31-C32
16	A	5001	LHG	C3-O3-P-O6
16	B	5006	LHG	C3-O3-P-O6
16	B	5006	LHG	C4-O6-P-O3
16	B	5004	LHG	C34-C35-C36-C37
12	A	1112	CLA	CAA-CBA-CGA-O2A
12	A	1116	CLA	CAA-CBA-CGA-O2A
12	B	1214	CLA	C11-C10-C8-C9
16	A	5003	LHG	C25-C26-C27-C28
21	F	5001	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
12	A	1102	CLA	C16-C17-C18-C20
12	B	1216	CLA	CBA-CGA-O2A-C1
16	A	5003	LHG	C2-C3-O3-P
15	A	4001	BCR	C11-C12-C13-C14
12	A	1132	CLA	CBA-CGA-O2A-C1
24	F	6001	LMT	O5B-C5B-C6B-O6B
16	A	5001	LHG	C12-C13-C14-C15
12	A	1132	CLA	O1A-CGA-O2A-C1
16	A	5001	LHG	C27-C28-C29-C30
12	A	1111	CLA	C2A-CAA-CBA-CGA
15	A	4007	BCR	C15-C16-C17-C18
15	B	4018	BCR	C19-C20-C21-C22
15	I	4018	BCR	C19-C20-C21-C22
12	B	1216	CLA	O1A-CGA-O2A-C1
16	B	5004	LHG	C23-C24-C25-C26
12	A	1106	CLA	C2-C1-O2A-CGA
12	B	1022	CLA	C2A-CAA-CBA-CGA
12	B	1215	CLA	C2A-CAA-CBA-CGA
12	B	1229	CLA	C2A-CAA-CBA-CGA
12	B	1205	CLA	C3A-C2A-CAA-CBA
12	B	1222	CLA	C3A-C2A-CAA-CBA
12	B	1235	CLA	C3A-C2A-CAA-CBA
16	A	5001	LHG	C33-C34-C35-C36
12	B	1022	CLA	C2-C3-C5-C6
16	A	5001	LHG	C31-C32-C33-C34
12	B	1022	CLA	C11-C10-C8-C9
12	B	1224	CLA	C6-C7-C8-C10
20	B	5005	LMG	C37-C38-C39-C40
12	A	1141	CLA	CAA-CBA-CGA-O2A
12	A	1108	CLA	CBA-CGA-O2A-C1
24	F	6001	LMT	C3-C4-C5-C6
15	I	4018	BCR	C11-C10-C9-C34
16	A	5001	LHG	C4-C5-C6-O8
17	B	4011	45D	C28-C26-C30-C32
17	B	4011	45D	C39-C35-C37-C41
19	B	4006	ECH	C11-C10-C9-C34
19	B	4006	ECH	C35-C13-C14-C15
19	M	4021	ECH	C11-C10-C9-C34
23	F	4016	C7Z	C20-C13-C14-C15
25	I	4020	EQ3	C11-C10-C9-C34
21	F	5001	SQD	C33-C34-C35-C36
12	A	1118	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	1140	CLA	C1A-C2A-CAA-CBA
12	B	1212	CLA	C1A-C2A-CAA-CBA
12	B	1222	CLA	C1A-C2A-CAA-CBA
12	A	1106	CLA	C12-C13-C15-C16
12	B	1235	CLA	C6-C7-C8-C10
12	A	1118	CLA	CAA-CBA-CGA-O2A
12	A	1141	CLA	CAA-CBA-CGA-O1A
12	A	1103	CLA	C2A-CAA-CBA-CGA
12	A	1118	CLA	C2A-CAA-CBA-CGA
12	A	1119	CLA	C2A-CAA-CBA-CGA
21	B	5008	SQD	C29-C30-C31-C32
12	B	1239	CLA	O2A-C1-C2-C3
12	B	1234	CLA	C8-C10-C11-C12
12	B	1021	CLA	C16-C17-C18-C19
15	I	4018	BCR	C11-C10-C9-C8
17	B	4011	45D	C24-C26-C30-C32
17	B	4011	45D	C33-C35-C37-C41
19	B	4006	ECH	C11-C10-C9-C8
19	B	4006	ECH	C12-C13-C14-C15
19	M	4021	ECH	C11-C10-C9-C8
25	I	4020	EQ3	C11-C10-C9-C8
12	B	1021	CLA	CAA-CBA-CGA-O1A
15	J	4013	BCR	C19-C20-C21-C22
12	A	1101	CLA	CAA-CBA-CGA-O1A
21	F	5001	SQD	O5-C1-O6-C44
12	A	1108	CLA	O1A-CGA-O2A-C1
16	B	5006	LHG	C1-C2-C3-O3
12	A	1103	CLA	CAA-CBA-CGA-O1A
15	B	4018	BCR	C1-C6-C7-C8
12	K	1401	CLA	CAA-CBA-CGA-O2A
25	I	4020	EQ3	C19-C20-C21-C22
12	B	1223	CLA	C2A-CAA-CBA-CGA
12	J	1303	CLA	C2A-CAA-CBA-CGA
16	B	5006	LHG	O6-C4-C5-C6
12	B	1021	CLA	C12-C13-C15-C16
12	B	1022	CLA	C11-C10-C8-C7
24	F	6001	LMT	C4'-C5'-C6'-O6'
16	A	5003	LHG	C30-C31-C32-C33
12	A	1013	CLA	C4-C3-C5-C6
13	B	2002	PQN	C23-C25-C26-C27
12	A	1138	CLA	C11-C12-C13-C14
12	B	1021	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	B	1235	CLA	C6-C7-C8-C9
12	A	1108	CLA	C3A-C2A-CAA-CBA
12	A	1118	CLA	C3A-C2A-CAA-CBA
12	A	1134	CLA	C3A-C2A-CAA-CBA
12	B	1022	CLA	C3A-C2A-CAA-CBA
16	B	5004	LHG	O2-C2-C3-O3
20	B	5002	LMG	O7-C10-C11-C12
12	A	1120	CLA	CAD-CBD-CGD-O2D
12	A	1123	CLA	CAD-CBD-CGD-O2D
12	B	1207	CLA	CAD-CBD-CGD-O2D
12	B	1219	CLA	CAD-CBD-CGD-O2D
12	A	1106	CLA	C5-C6-C7-C8
12	A	1136	CLA	CAA-CBA-CGA-O2A
12	L	1502	CLA	CAA-CBA-CGA-O2A
12	K	1401	CLA	CAA-CBA-CGA-O1A
15	F	4014	BCR	C11-C12-C13-C14
12	A	1113	CLA	CAA-CBA-CGA-O2A
12	A	1114	CLA	CAA-CBA-CGA-O2A
12	B	1227	CLA	CAA-CBA-CGA-O2A
12	B	1221	CLA	O2A-C1-C2-C3
12	A	1011	CLA	CHA-CBD-CGD-O2D
12	A	1012	CLA	CHA-CBD-CGD-O1D
12	A	1012	CLA	CHA-CBD-CGD-O2D
12	A	1102	CLA	CHA-CBD-CGD-O1D
12	A	1102	CLA	CHA-CBD-CGD-O2D
12	A	1104	CLA	CHA-CBD-CGD-O2D
12	A	1121	CLA	CHA-CBD-CGD-O1D
12	A	1121	CLA	CHA-CBD-CGD-O2D
12	A	1133	CLA	CHA-CBD-CGD-O1D
12	A	1133	CLA	CHA-CBD-CGD-O2D
12	A	1141	CLA	CHA-CBD-CGD-O1D
12	A	1141	CLA	CHA-CBD-CGD-O2D
12	A	1130	CLA	CHA-CBD-CGD-O1D
12	A	1130	CLA	CHA-CBD-CGD-O2D
12	A	1132	CLA	CHA-CBD-CGD-O1D
12	A	1132	CLA	CHA-CBD-CGD-O2D
12	B	1203	CLA	CHA-CBD-CGD-O1D
12	B	1203	CLA	CHA-CBD-CGD-O2D
12	B	1206	CLA	CHA-CBD-CGD-O2D
12	B	1211	CLA	CHA-CBD-CGD-O1D
12	B	1211	CLA	CHA-CBD-CGD-O2D
12	B	1212	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	B	1212	CLA	CHA-CBD-CGD-O2D
12	B	1214	CLA	CHA-CBD-CGD-O1D
12	B	1214	CLA	CHA-CBD-CGD-O2D
12	B	1216	CLA	CHA-CBD-CGD-O2D
12	B	1226	CLA	CHA-CBD-CGD-O1D
12	B	1226	CLA	CHA-CBD-CGD-O2D
12	B	1228	CLA	CHA-CBD-CGD-O1D
12	B	1228	CLA	CHA-CBD-CGD-O2D
12	B	1239	CLA	CHA-CBD-CGD-O1D
12	B	1239	CLA	CHA-CBD-CGD-O2D
12	B	1238	CLA	CHA-CBD-CGD-O2D
12	B	1210	CLA	CAA-CBA-CGA-O2A
12	B	1216	CLA	CAA-CBA-CGA-O2A
12	A	1125	CLA	CAA-CBA-CGA-O2A
12	B	1237	CLA	CAA-CBA-CGA-O2A
12	B	1220	CLA	CAA-CBA-CGA-O2A
16	A	5001	LHG	O8-C23-C24-C25
12	A	1133	CLA	CBA-CGA-O2A-C1
12	B	1232	CLA	CAA-CBA-CGA-O2A
12	A	1109	CLA	C16-C17-C18-C19
12	A	1105	CLA	CAA-CBA-CGA-O2A
15	A	4001	BCR	C19-C20-C21-C22
15	A	4003	BCR	C13-C14-C15-C16
15	A	4012	BCR	C9-C10-C11-C12
21	F	5001	SQD	C32-C33-C34-C35
12	B	1205	CLA	O2A-C1-C2-C3
12	A	1113	CLA	C2A-CAA-CBA-CGA
12	A	1117	CLA	C2A-CAA-CBA-CGA
12	A	1122	CLA	C2A-CAA-CBA-CGA
21	F	5001	SQD	O47-C7-C8-C9
12	A	1136	CLA	CAA-CBA-CGA-O1A
12	A	1126	CLA	C11-C12-C13-C15
12	A	1011	CLA	C5-C6-C7-C8
12	A	1137	CLA	C1A-C2A-CAA-CBA
12	B	1022	CLA	C1A-C2A-CAA-CBA
12	B	1205	CLA	C1A-C2A-CAA-CBA
12	B	1214	CLA	CAA-CBA-CGA-O2A
12	L	1502	CLA	CAA-CBA-CGA-O1A
12	B	1235	CLA	C8-C10-C11-C12
12	A	1134	CLA	CAA-CBA-CGA-O2A
12	B	1234	CLA	CAA-CBA-CGA-O2A
12	A	1114	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	B	1237	CLA	CAA-CBA-CGA-O1A
12	B	1216	CLA	CAA-CBA-CGA-O1A
20	B	5002	LMG	O9-C10-C11-C12
16	A	5001	LHG	C3-O3-P-O5
12	B	1210	CLA	CAA-CBA-CGA-O1A
16	A	5001	LHG	O10-C23-C24-C25
12	B	1208	CLA	O2A-C1-C2-C3
12	B	1236	CLA	O2A-C1-C2-C3
15	A	4003	BCR	C1-C6-C7-C8
15	B	4018	BCR	C5-C6-C7-C8
12	A	1113	CLA	CAA-CBA-CGA-O1A
12	B	1227	CLA	CAA-CBA-CGA-O1A
21	F	5001	SQD	O49-C7-C8-C9
12	A	1133	CLA	O1A-CGA-O2A-C1
12	A	1121	CLA	CAA-CBA-CGA-O2A
12	A	1130	CLA	CAA-CBA-CGA-O2A
20	B	5005	LMG	C13-C14-C15-C16
12	B	1204	CLA	CAA-CBA-CGA-O2A
12	A	1102	CLA	C3-C5-C6-C7
12	A	1106	CLA	CAD-CBD-CGD-O1D
12	A	1133	CLA	CAD-CBD-CGD-O1D
12	A	1139	CLA	CAD-CBD-CGD-O1D
12	B	1212	CLA	CAD-CBD-CGD-O1D
12	B	1227	CLA	CAD-CBD-CGD-O1D
21	B	5008	SQD	O5-C5-C6-S
12	B	1214	CLA	CAA-CBA-CGA-O1A
12	A	1109	CLA	C11-C10-C8-C9
12	A	1115	CLA	C6-C7-C8-C9
12	B	1220	CLA	CAA-CBA-CGA-O1A
12	B	1232	CLA	CAA-CBA-CGA-O1A
12	J	1302	CLA	CAA-CBA-CGA-O1A
12	A	1115	CLA	CAA-CBA-CGA-O2A
21	F	5001	SQD	O48-C23-C24-C25
20	B	5002	LMG	C30-C31-C32-C33
12	B	1217	CLA	O1A-CGA-O2A-C1
12	J	1303	CLA	CAA-CBA-CGA-O2A
16	B	5004	LHG	C1-C2-C3-O3
12	B	1021	CLA	C8-C10-C11-C12
12	A	1125	CLA	CAA-CBA-CGA-O1A
12	A	1113	CLA	C3A-C2A-CAA-CBA
12	A	1115	CLA	C6-C7-C8-C10
13	A	2001	PQN	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	A	1105	CLA	CAA-CBA-CGA-O1A
12	A	1134	CLA	CAA-CBA-CGA-O1A
21	F	5001	SQD	O10-C23-C24-C25
12	B	1226	CLA	CAA-CBA-CGA-O2A
16	B	5004	LHG	O8-C23-C24-C25
12	B	1207	CLA	O2A-C1-C2-C3
12	B	1238	CLA	O2A-C1-C2-C3
15	A	4007	BCR	C11-C12-C13-C14
23	F	4016	C7Z	C31-C32-C33-C34
12	A	1115	CLA	CAA-CBA-CGA-O1A
12	B	1234	CLA	CAA-CBA-CGA-O1A
12	J	1303	CLA	CAA-CBA-CGA-O1A
12	B	1222	CLA	C2A-CAA-CBA-CGA
12	A	1109	CLA	C5-C6-C7-C8

There are no ring outliers.

116 monomers are involved in 375 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1102	CLA	8	0
12	A	1106	CLA	8	0
12	B	1201	CLA	1	0
12	B	1202	CLA	5	0
24	F	6001	LMT	1	0
15	A	4008	BCR	5	0
12	B	1204	CLA	5	0
19	B	4006	ECH	4	0
12	B	1238	CLA	5	0
15	B	4017	BCR	1	0
12	A	1117	CLA	4	0
12	A	1132	CLA	7	0
20	B	5005	LMG	3	0
21	B	5008	SQD	1	0
12	A	1012	CLA	8	0
12	A	1101	CLA	3	0
12	B	1228	CLA	2	0
12	A	1140	CLA	4	0
12	B	1203	CLA	4	0
12	A	1112	CLA	5	0
12	A	1103	CLA	5	0
12	A	1108	CLA	2	0
12	B	1023	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1107	CLA	9	0
12	A	1115	CLA	6	0
13	A	2001	PQN	2	0
12	B	1236	CLA	4	0
19	M	4021	ECH	5	0
12	B	1211	CLA	4	0
12	B	1231	CLA	4	0
12	A	1104	CLA	1	0
12	A	1134	CLA	4	0
12	B	1232	CLA	3	0
12	A	1011	CLA	8	0
15	B	4010	BCR	3	0
12	A	1124	CLA	2	0
12	B	1240	CLA	1	0
12	A	1116	CLA	6	0
12	B	1214	CLA	5	0
15	J	4013	BCR	9	0
12	A	1133	CLA	3	0
12	B	1218	CLA	2	0
14	A	3001	SF4	1	0
12	A	1121	CLA	2	0
15	I	4018	BCR	5	0
12	A	1013	CLA	8	0
12	A	1123	CLA	5	0
12	A	1137	CLA	1	0
12	B	1223	CLA	3	0
23	F	4016	C7Z	1	0
12	A	1111	CLA	4	0
12	A	1131	CLA	1	0
15	A	4001	BCR	5	0
12	B	1209	CLA	1	0
12	B	1215	CLA	2	0
15	F	4014	BCR	9	0
12	B	1212	CLA	1	0
25	I	4020	EQ3	1	0
12	A	1135	CLA	4	0
12	B	1226	CLA	3	0
15	A	4012	BCR	8	0
15	B	4005	BCR	1	0
12	B	1205	CLA	5	0
12	B	1022	CLA	4	0
12	B	1213	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2002	PQN	3	0
12	A	1114	CLA	3	0
12	A	1109	CLA	12	0
12	B	1234	CLA	8	0
12	L	1502	CLA	4	0
15	K	4001	BCR	6	0
15	B	4004	BCR	3	0
12	A	1129	CLA	3	0
12	A	1128	CLA	8	0
12	A	1122	CLA	4	0
12	B	1219	CLA	1	0
12	B	1224	CLA	9	0
16	A	5003	LHG	3	0
12	A	1130	CLA	3	0
12	B	1216	CLA	2	0
12	B	1206	CLA	2	0
15	A	4007	BCR	2	0
12	B	1225	CLA	4	0
17	B	4011	45D	5	0
15	A	4003	BCR	1	0
12	B	1237	CLA	3	0
12	B	1221	CLA	5	0
16	A	5001	LHG	2	0
12	F	1301	CLA	3	0
12	B	1229	CLA	5	0
12	A	1138	CLA	9	0
12	B	1239	CLA	2	0
12	B	1021	CLA	15	0
12	A	1139	CLA	5	0
15	B	4018	BCR	2	0
12	A	1127	CLA	1	0
12	J	1302	CLA	2	0
21	F	5001	SQD	3	0
12	B	1220	CLA	4	0
12	B	1210	CLA	7	0
12	B	1208	CLA	4	0
12	A	1110	CLA	1	0
12	A	1125	CLA	4	0
12	A	1126	CLA	13	0
12	B	1222	CLA	10	0
16	B	5004	LHG	9	0
12	B	1230	CLA	4	0

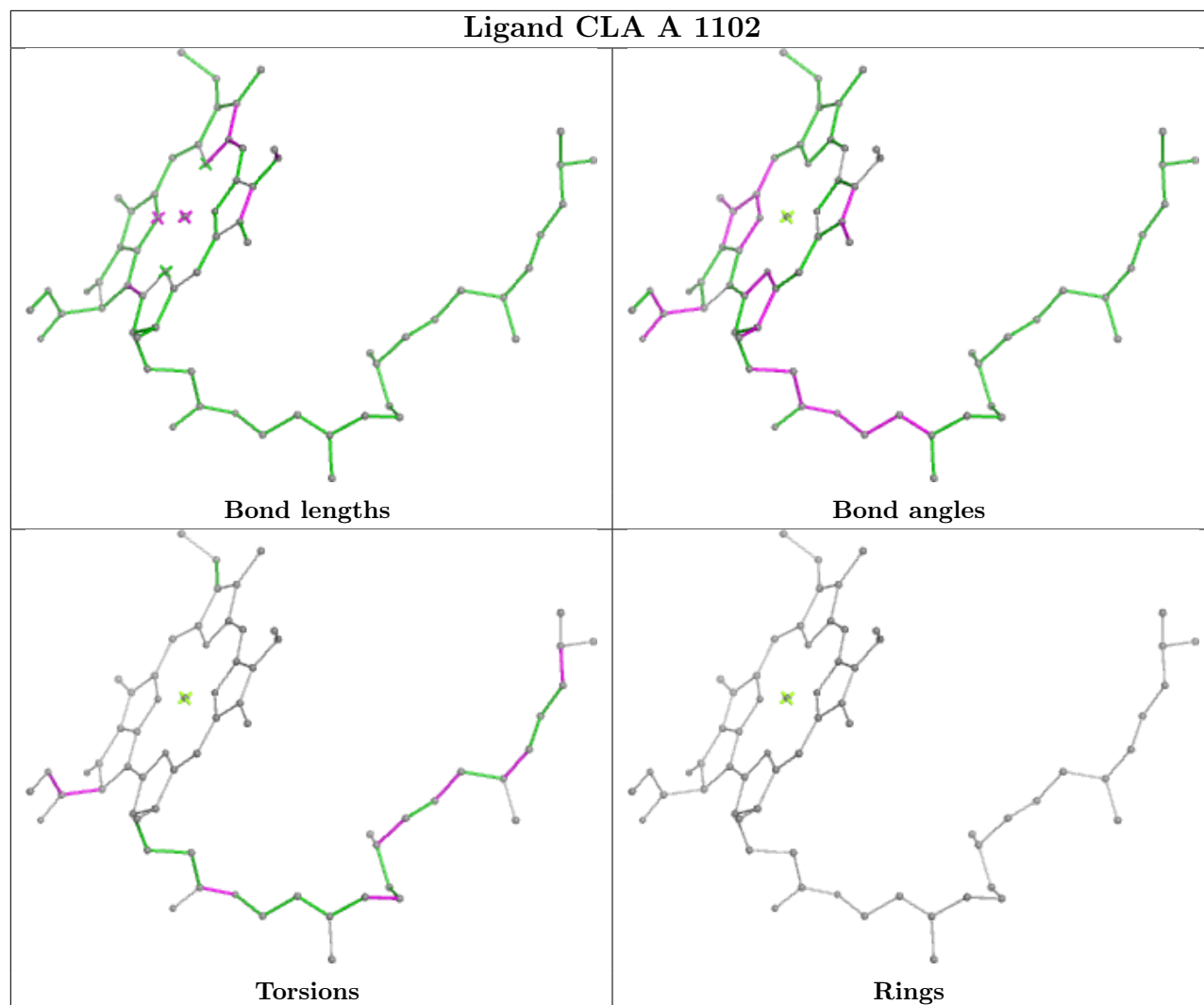
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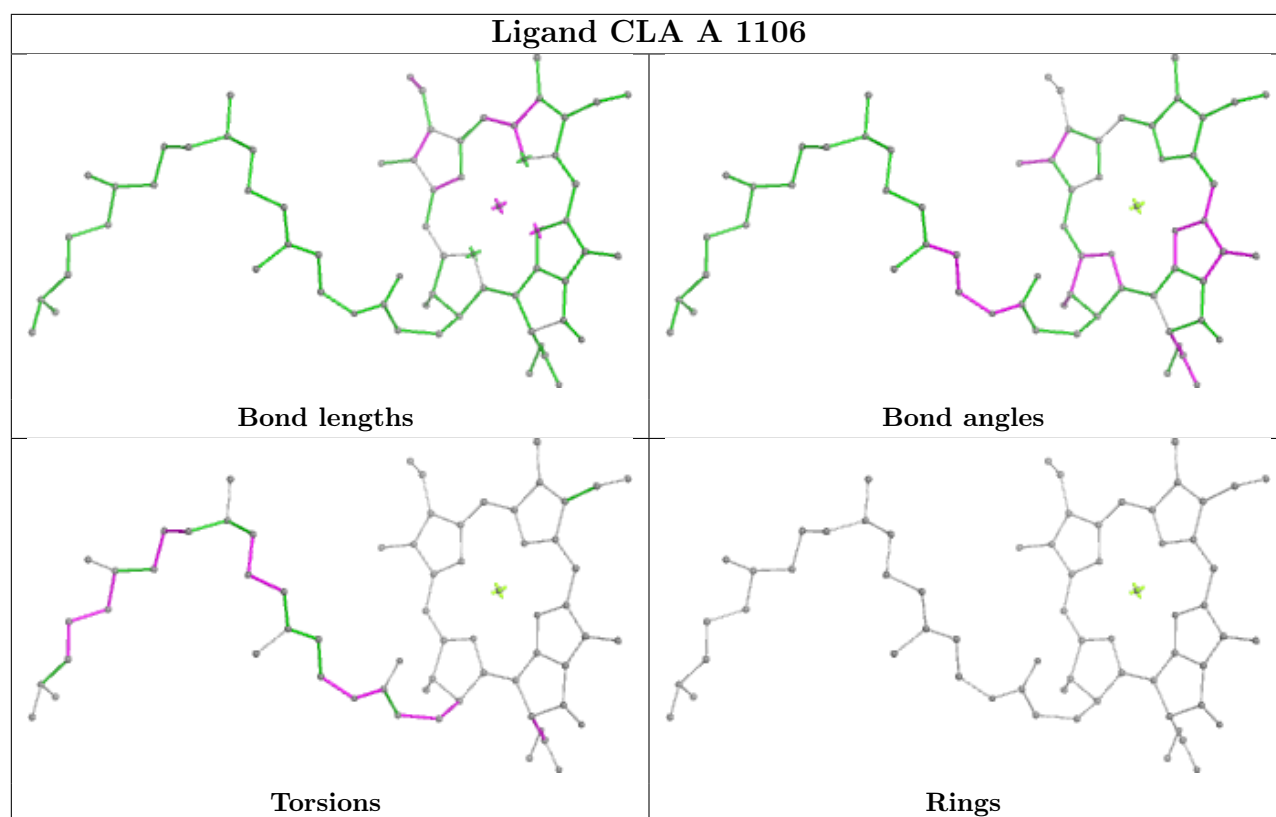
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1207	CLA	5	0
12	A	1119	CLA	6	0
12	A	1118	CLA	2	0
20	B	5002	LMG	4	0
14	C	3002	SF4	1	0
12	B	1235	CLA	7	0
12	A	1141	CLA	3	0
12	B	1227	CLA	3	0
12	A	1105	CLA	4	0

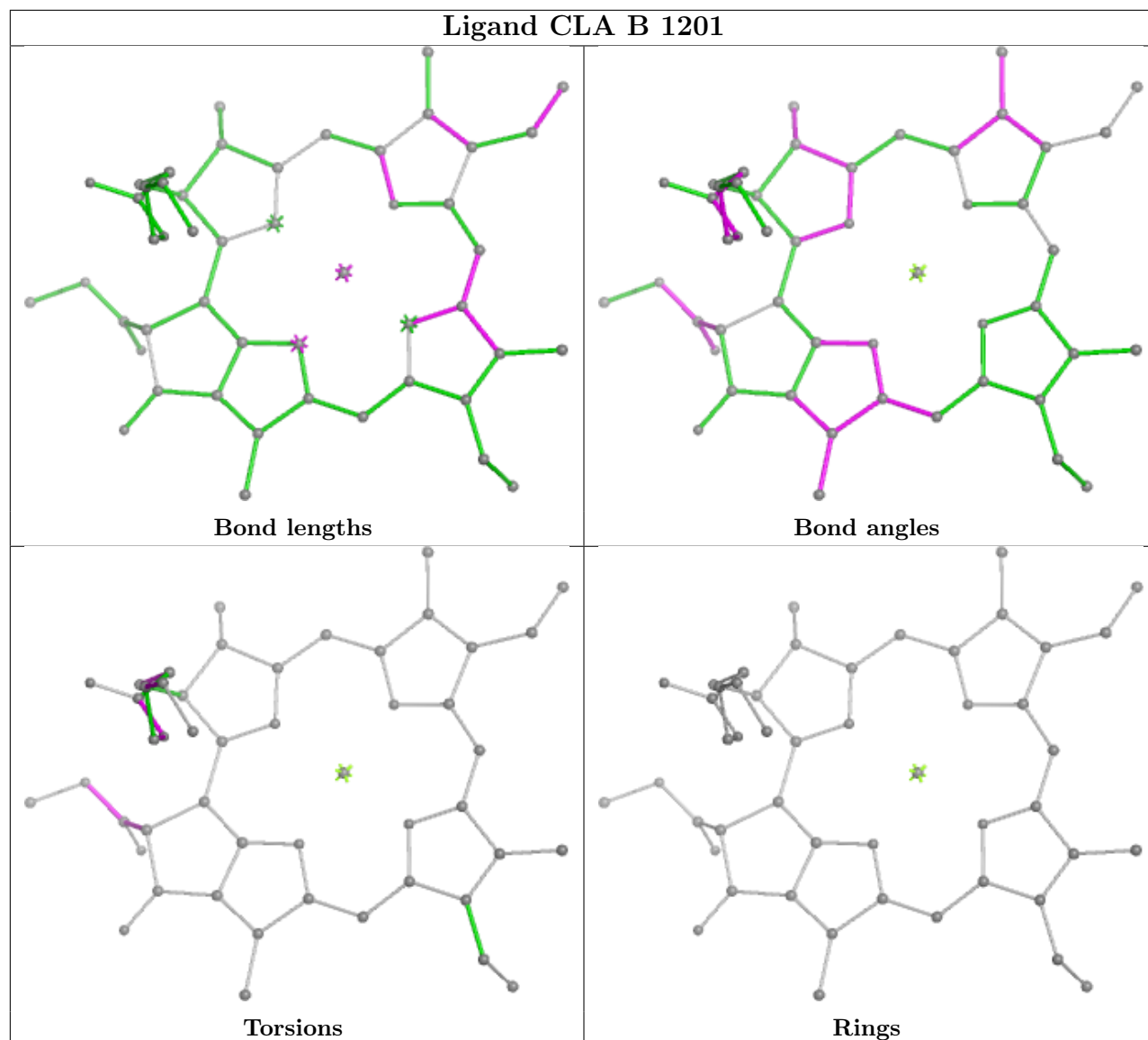
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand CLA A 1102

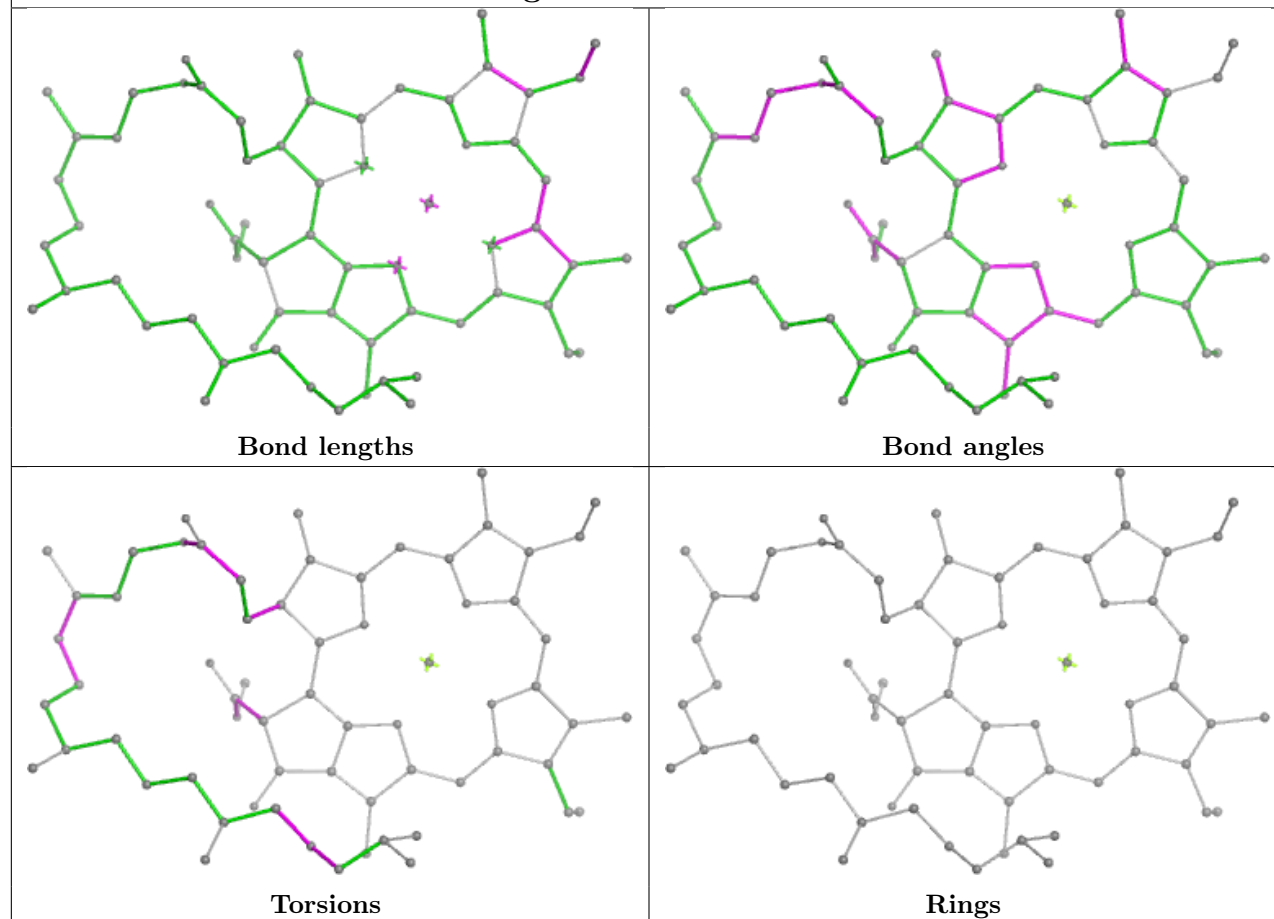




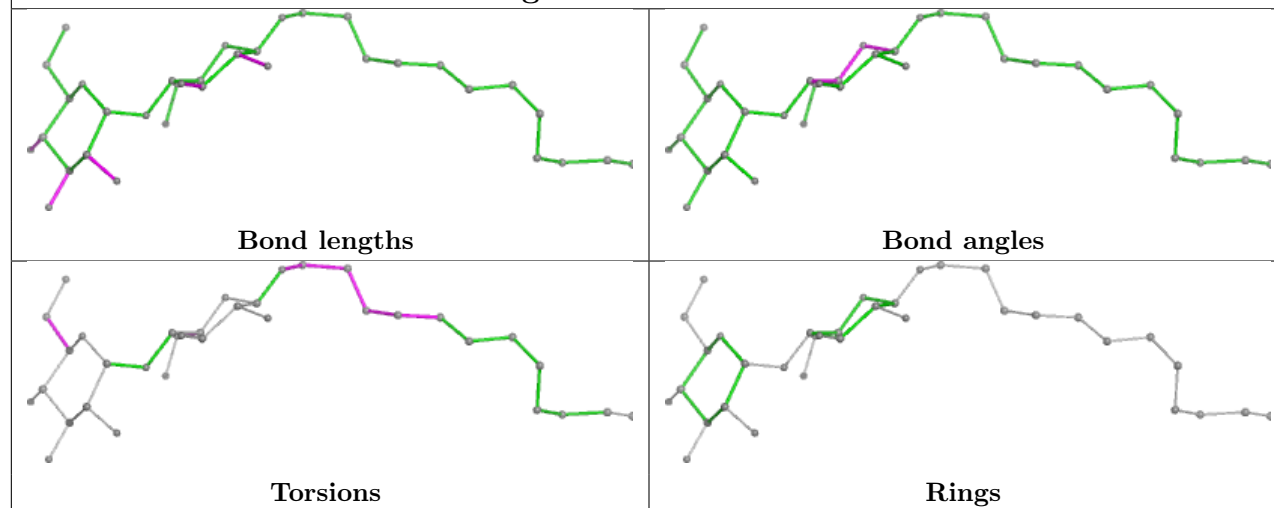
## Ligand CLA B 1201



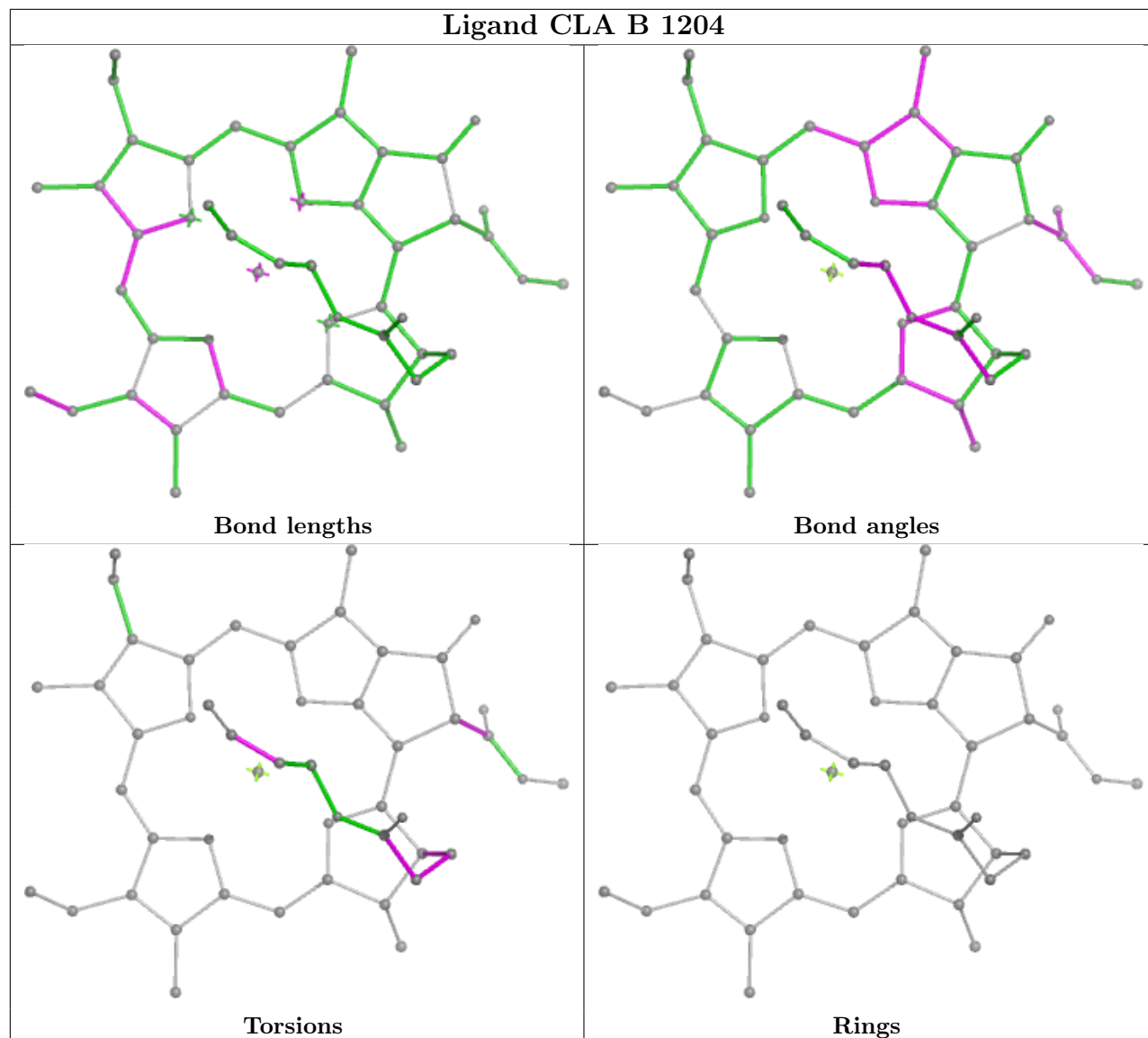
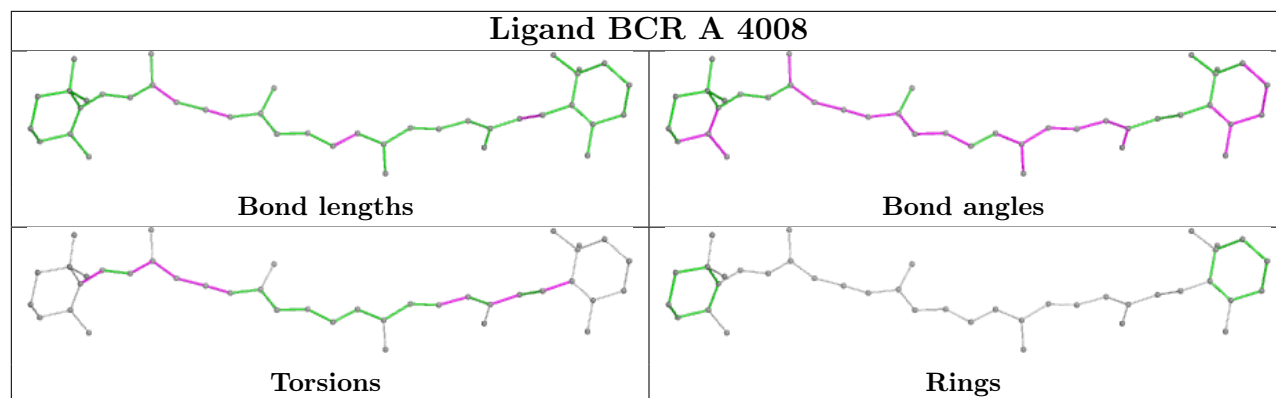
## Ligand CLA B 1202



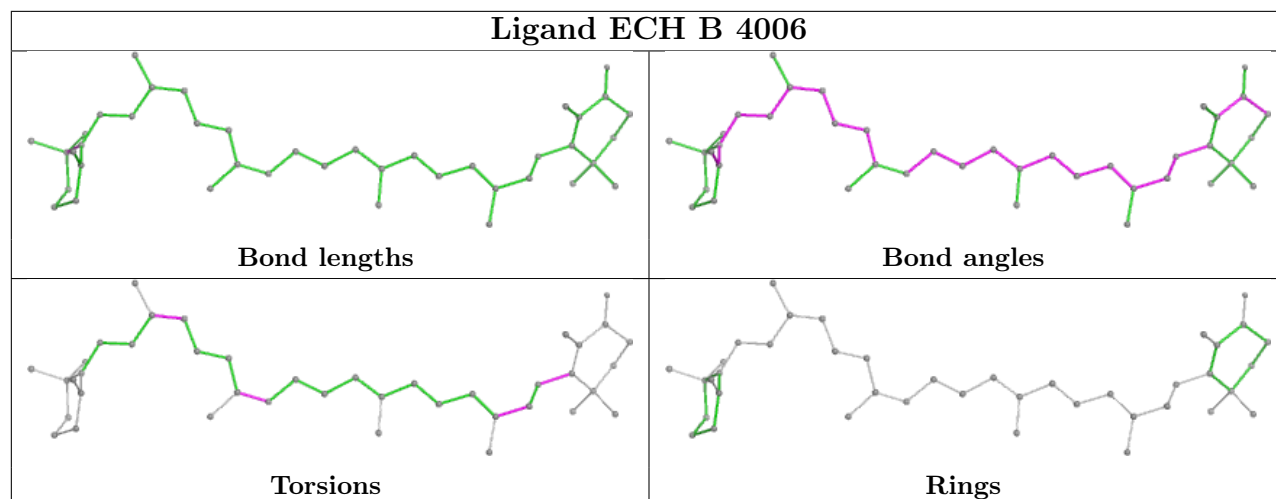
## Ligand LMT F 6001



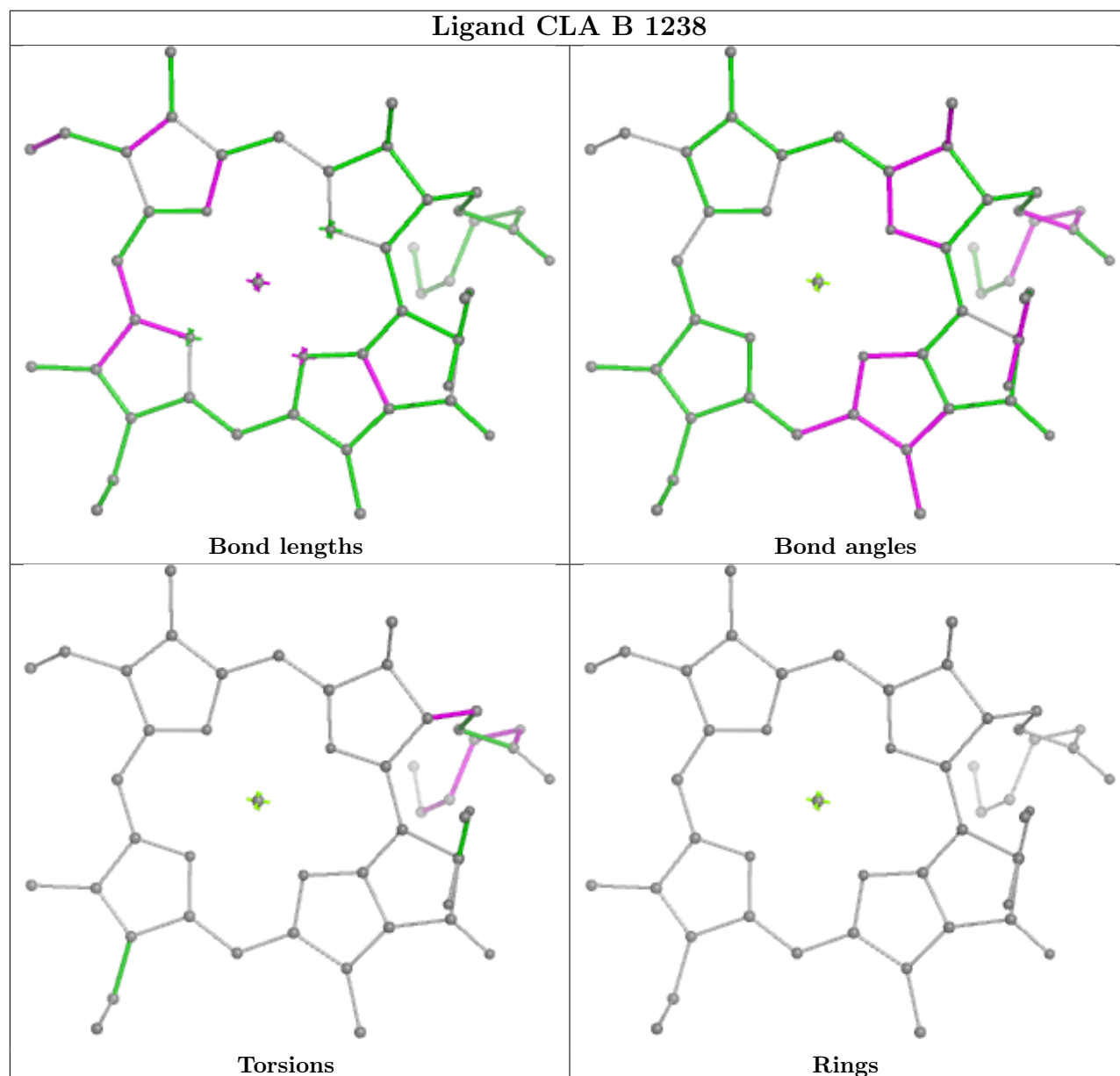




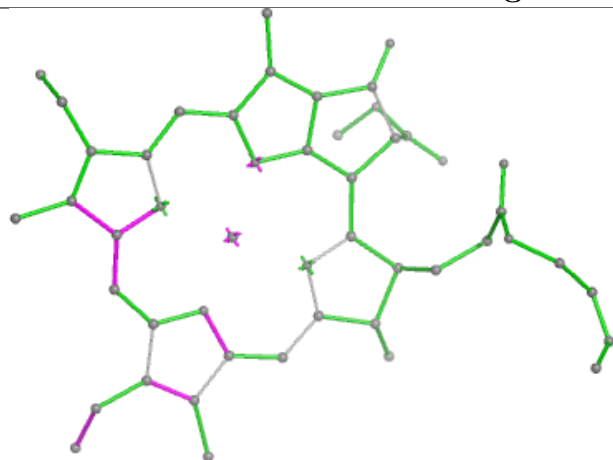
## Ligand ECH B 4006



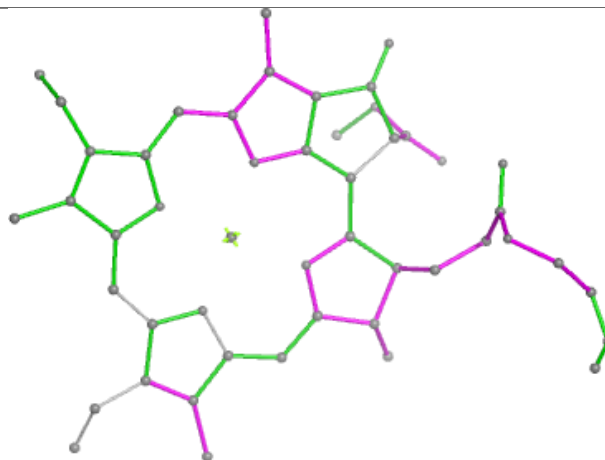
## Ligand CLA B 1238



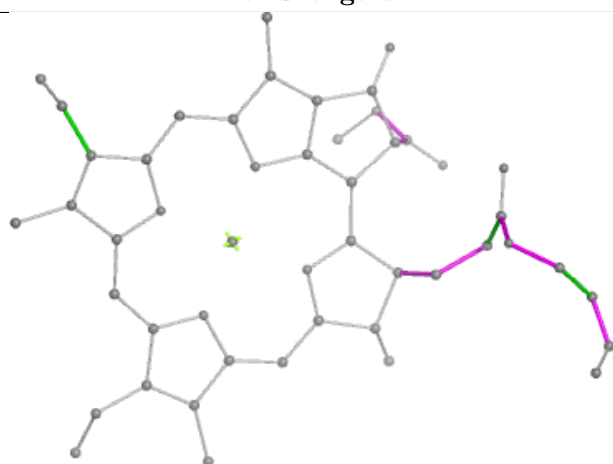
## Ligand CLA K 1402



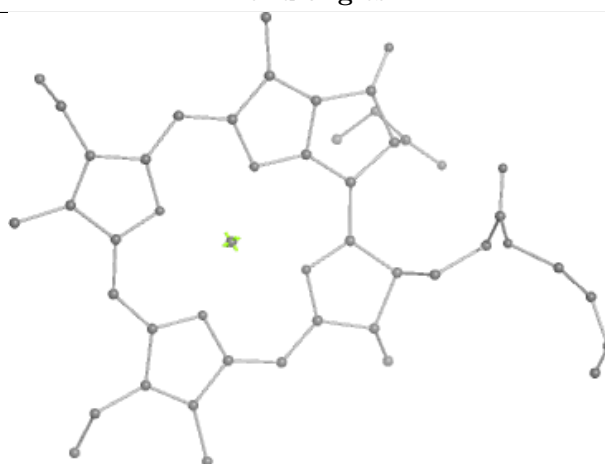
Bond lengths



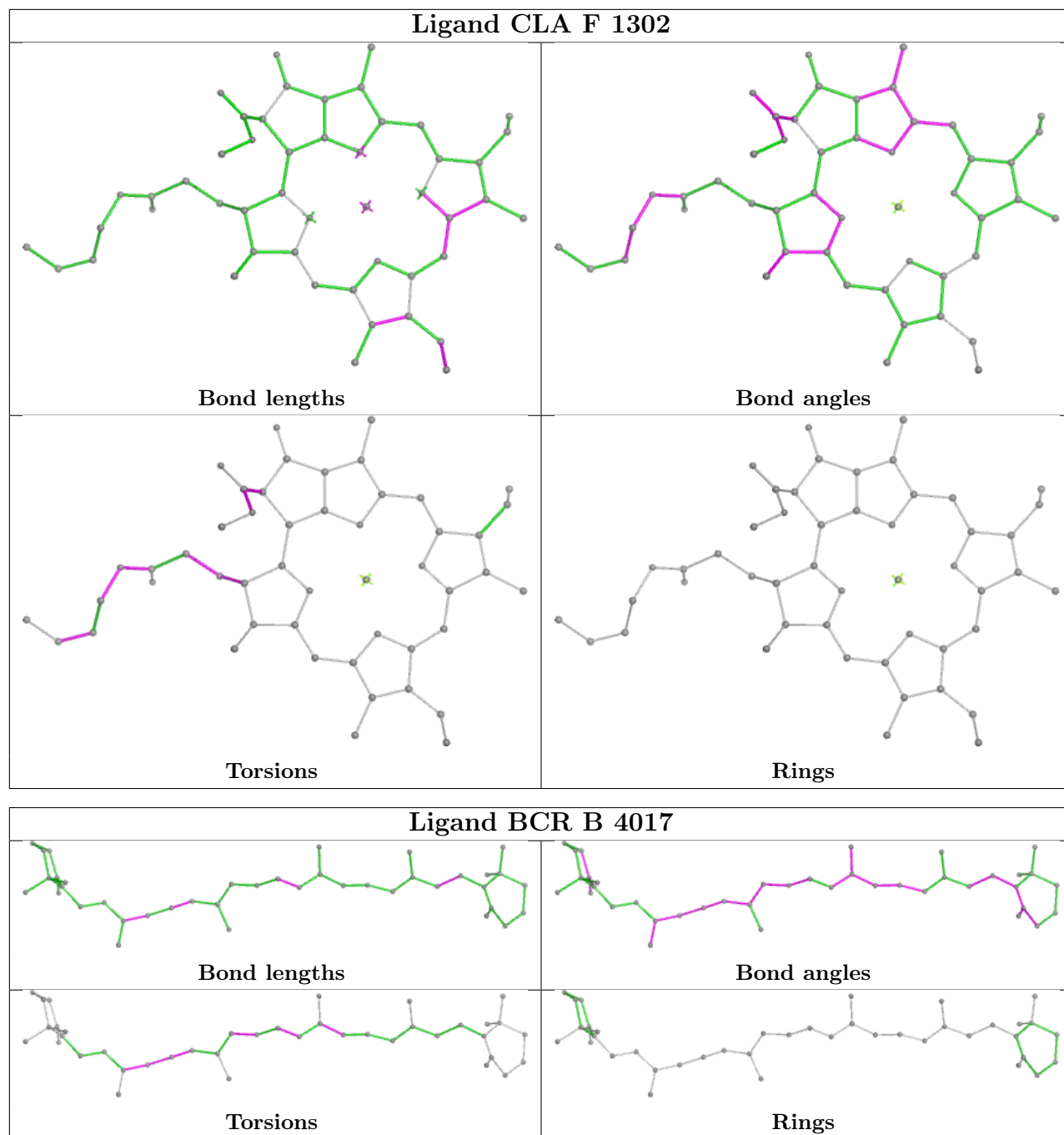
Bond angles



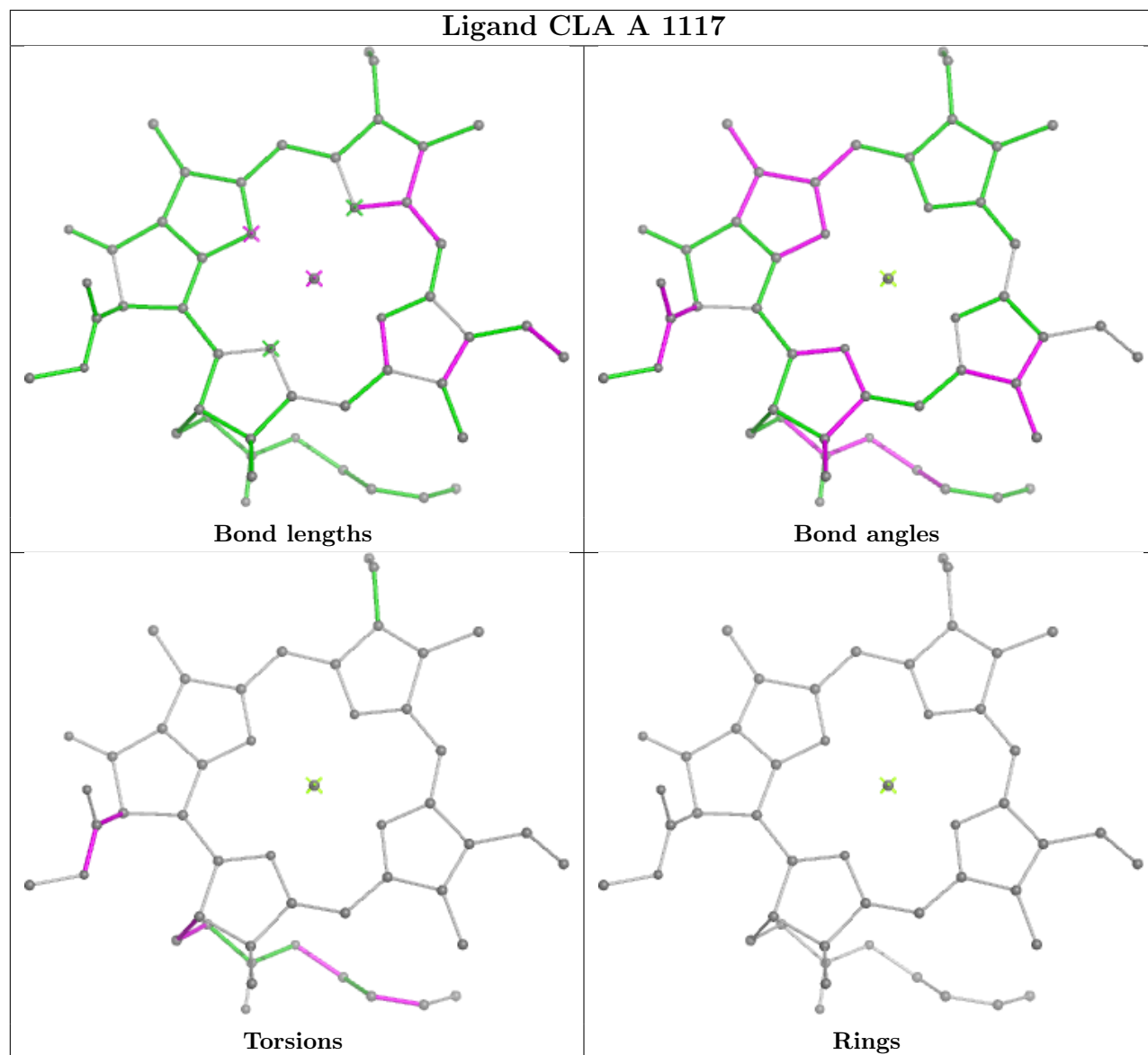
Torsions



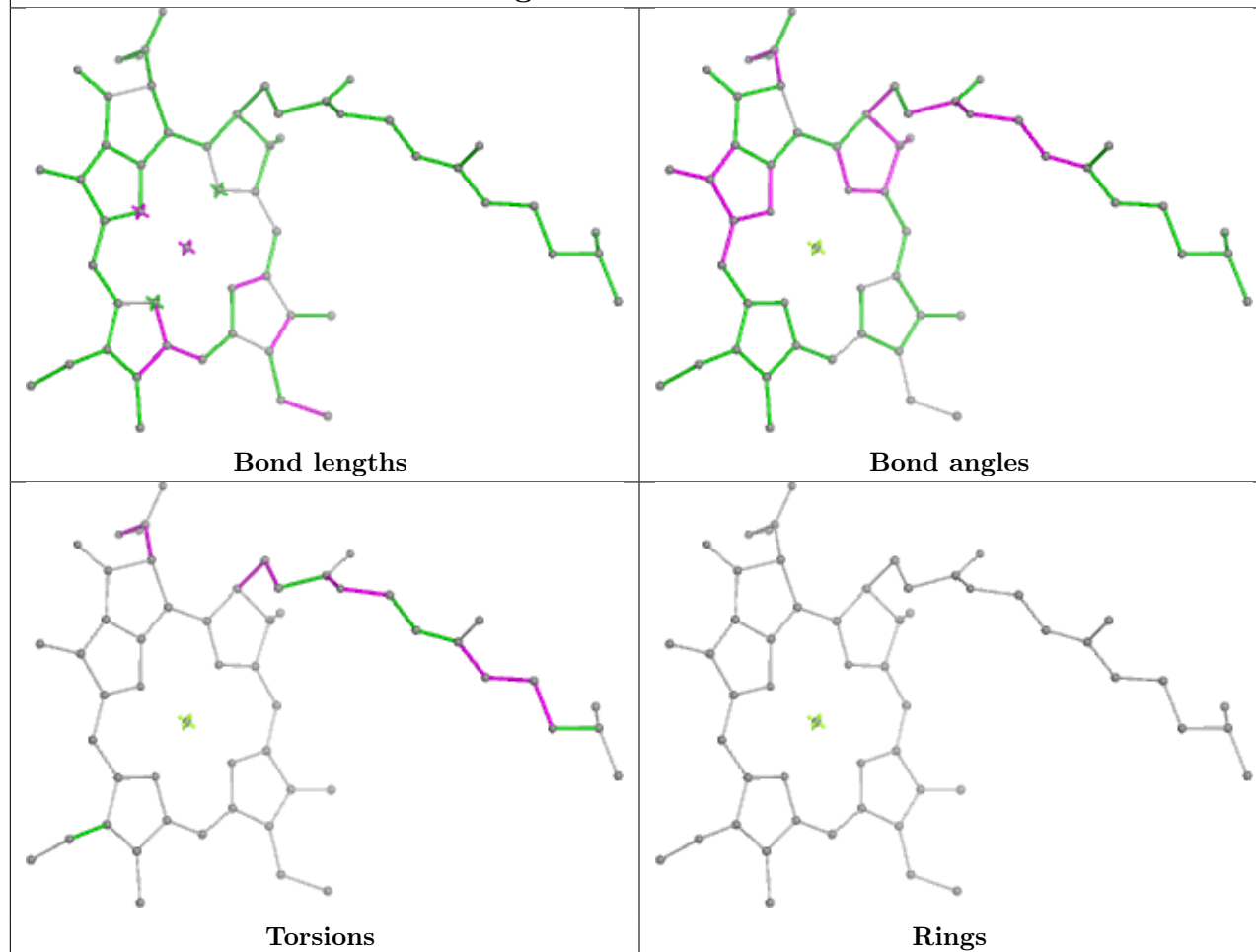
Rings



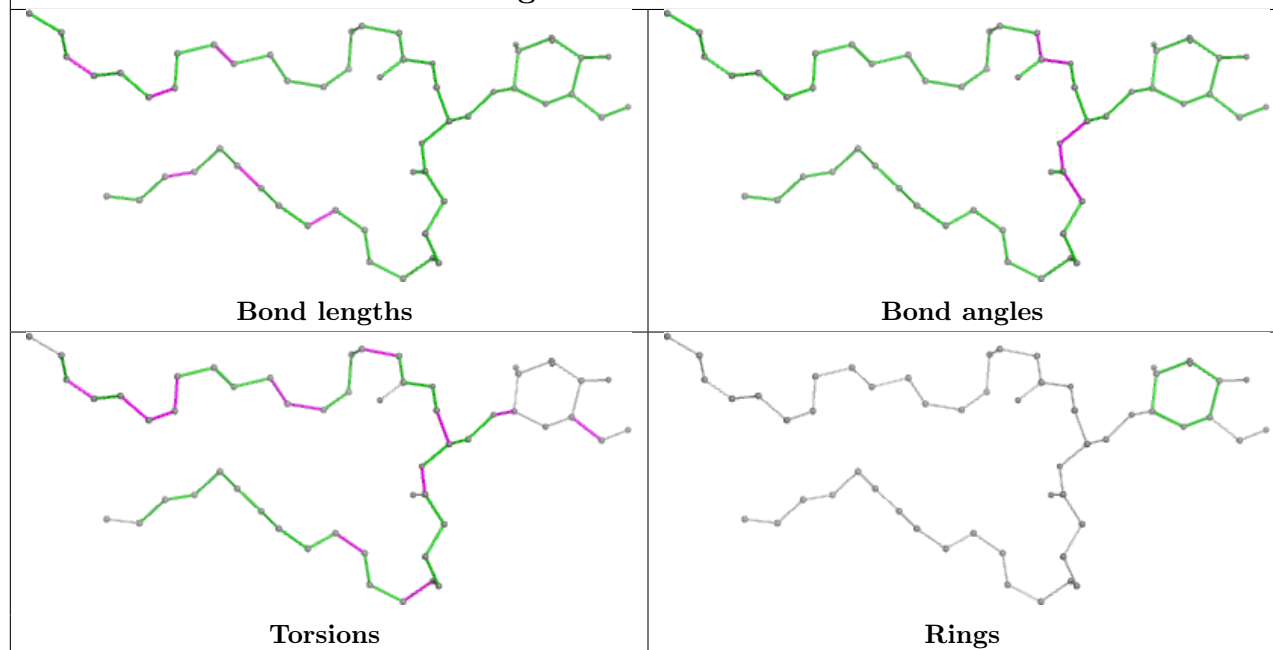
## Ligand CLA A 1117

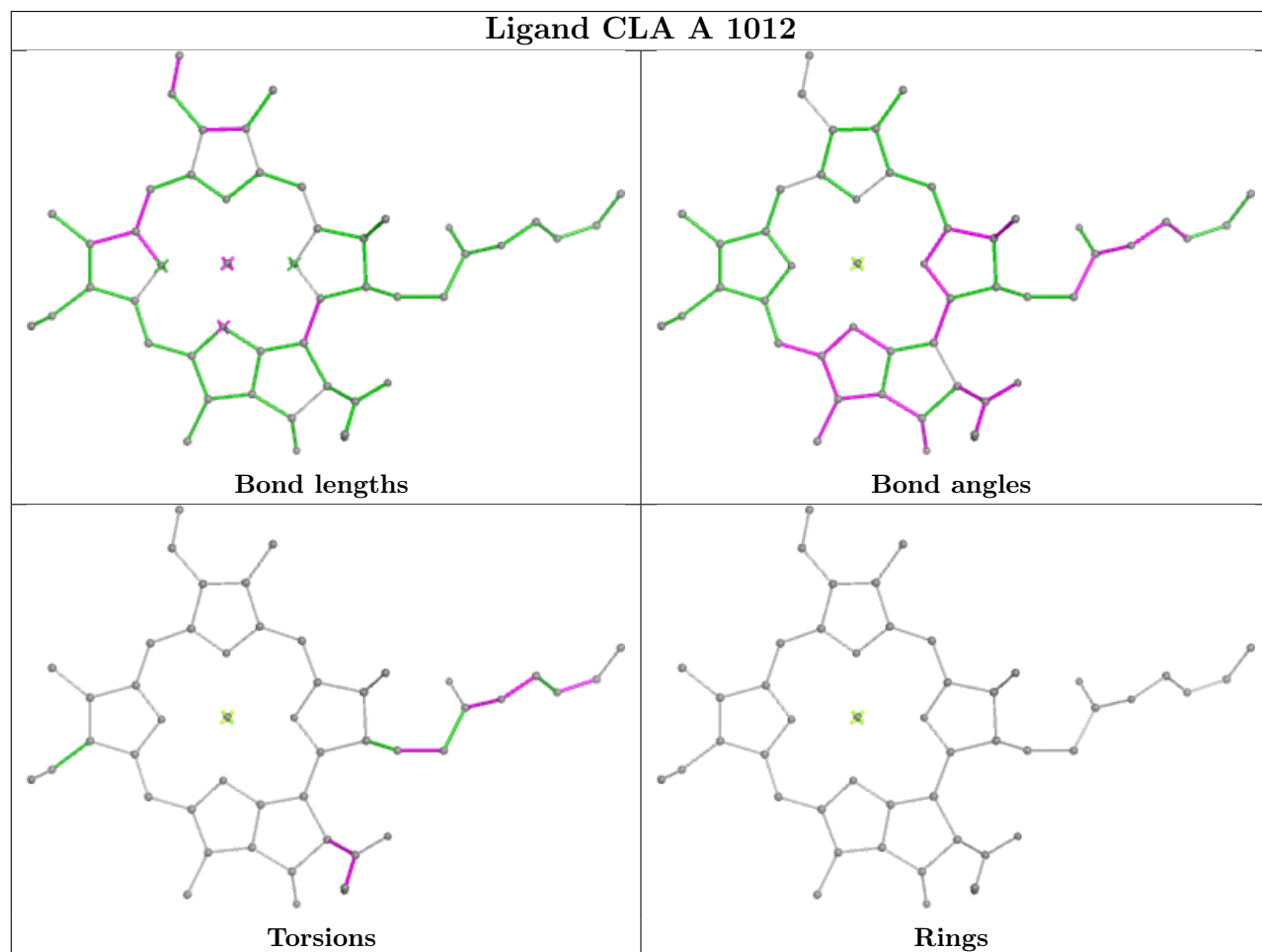
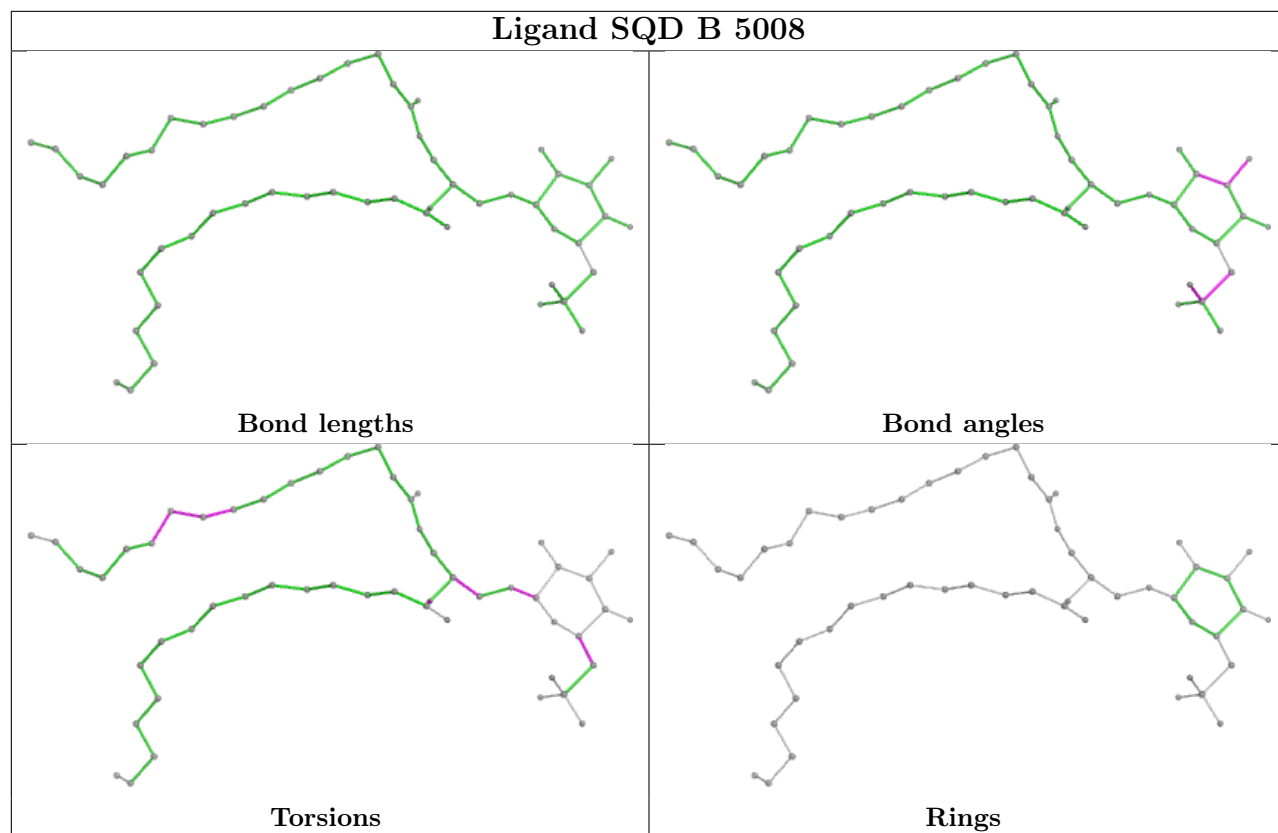


## Ligand CLA A 1132

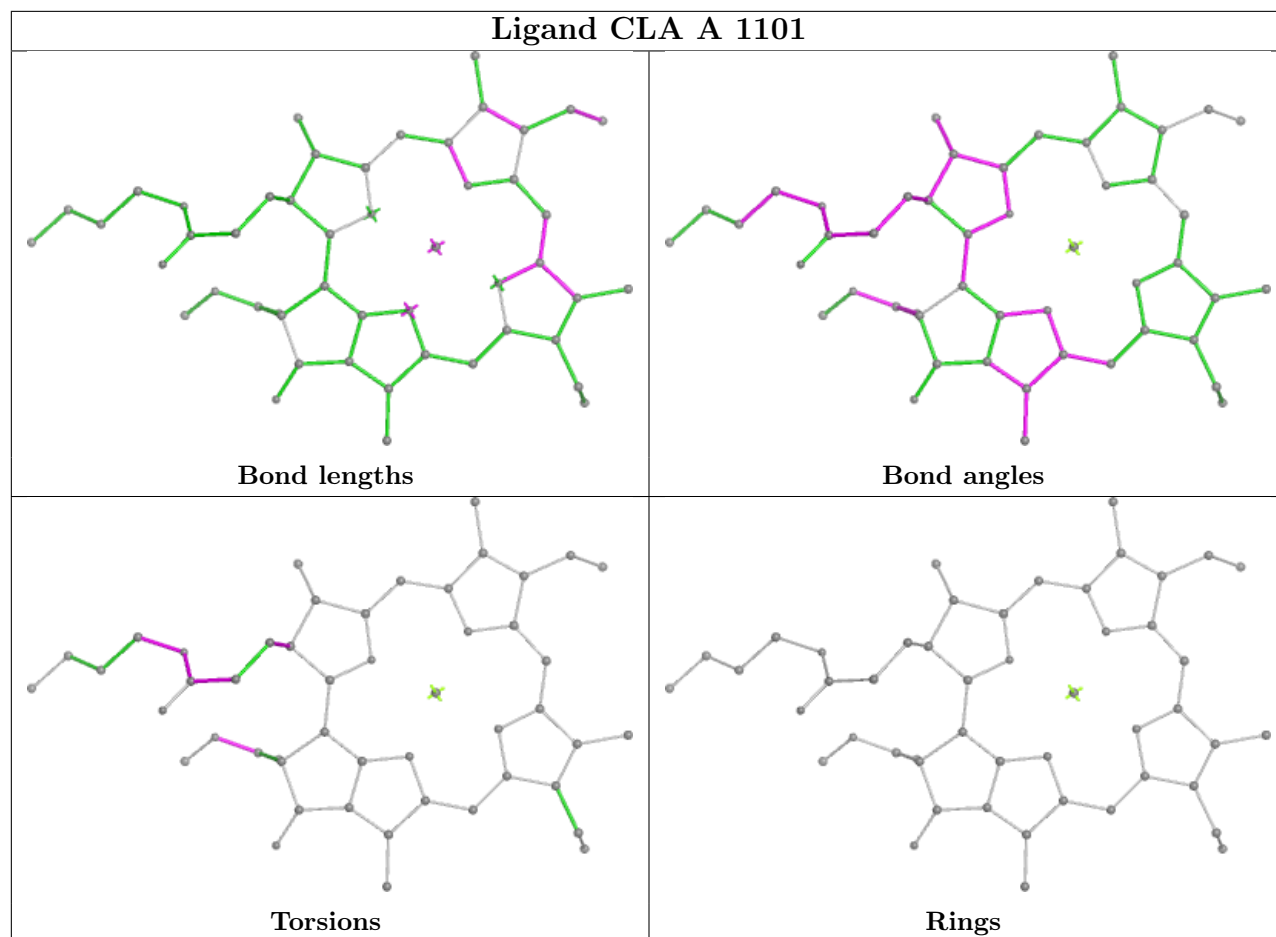


## Ligand LMG B 5005

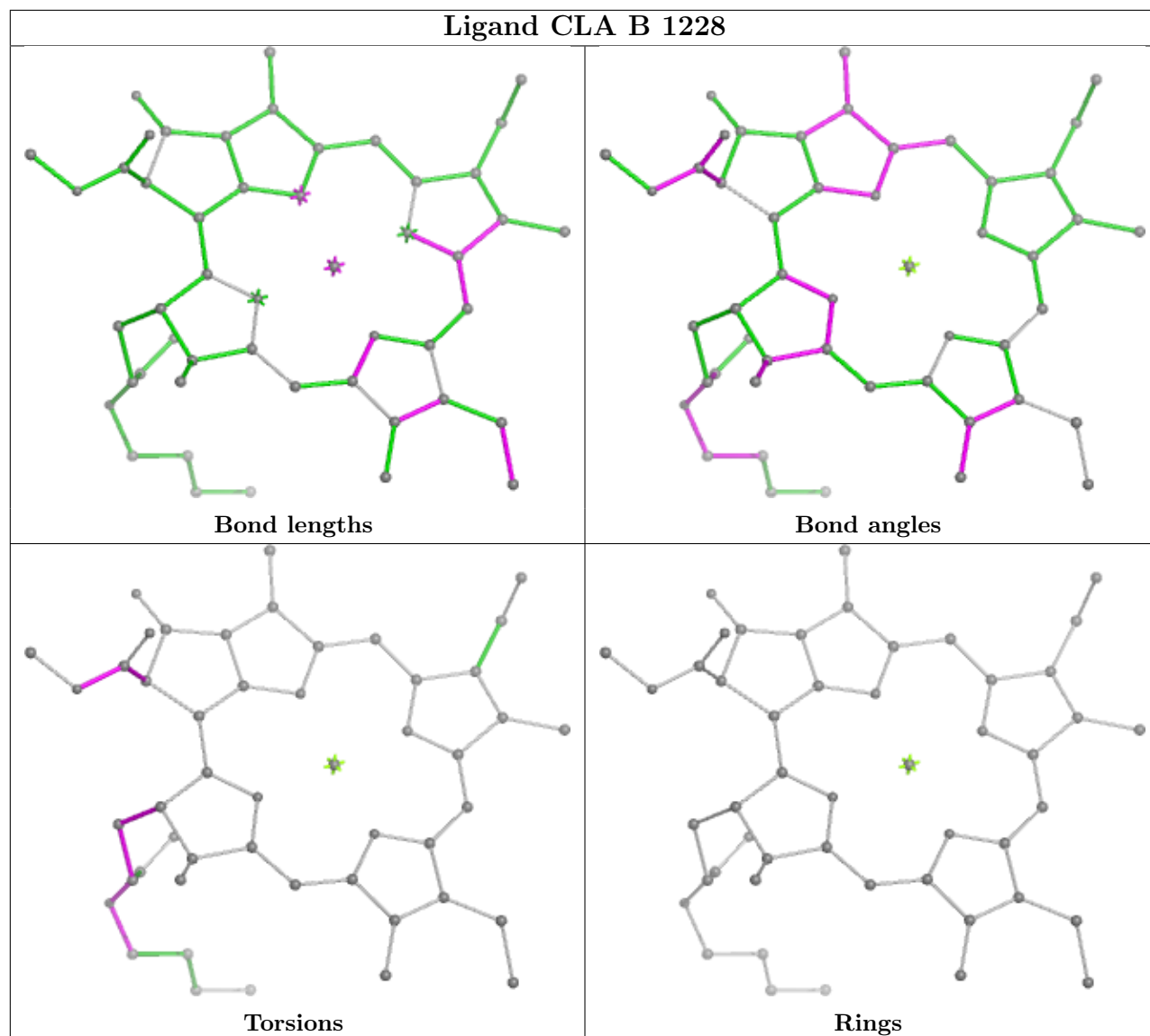




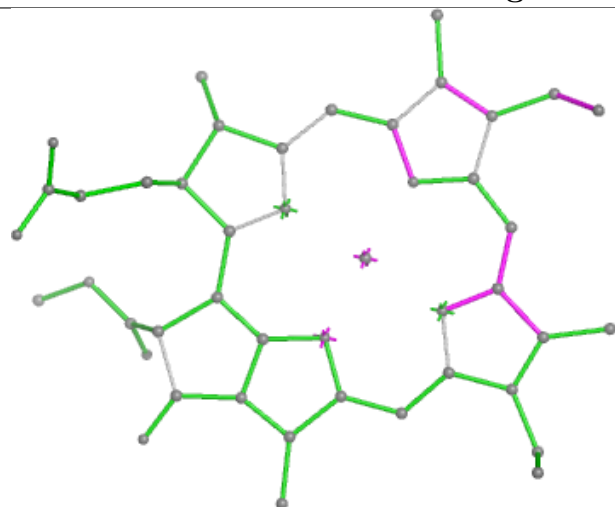
## Ligand CLA A 1101



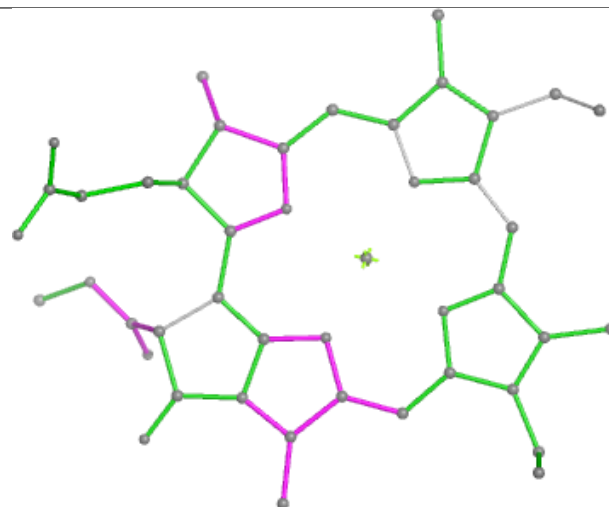




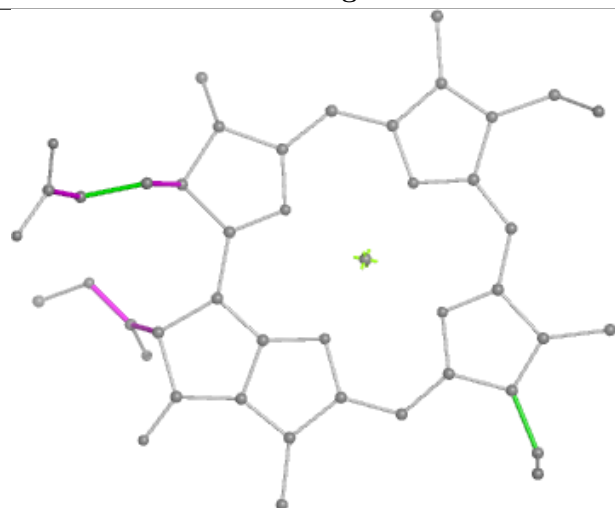
## Ligand CLA K 1401



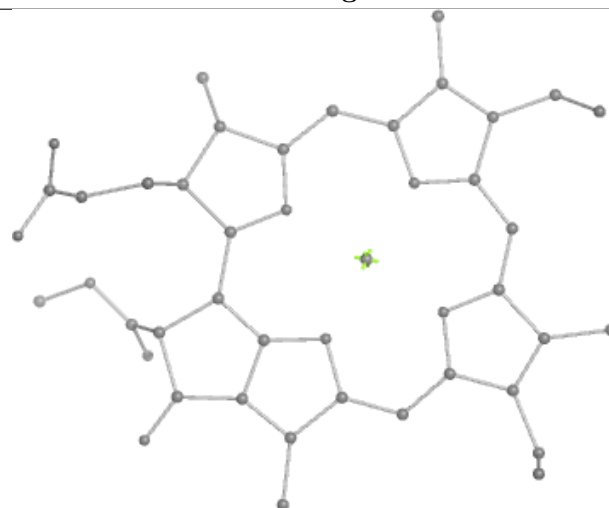
Bond lengths



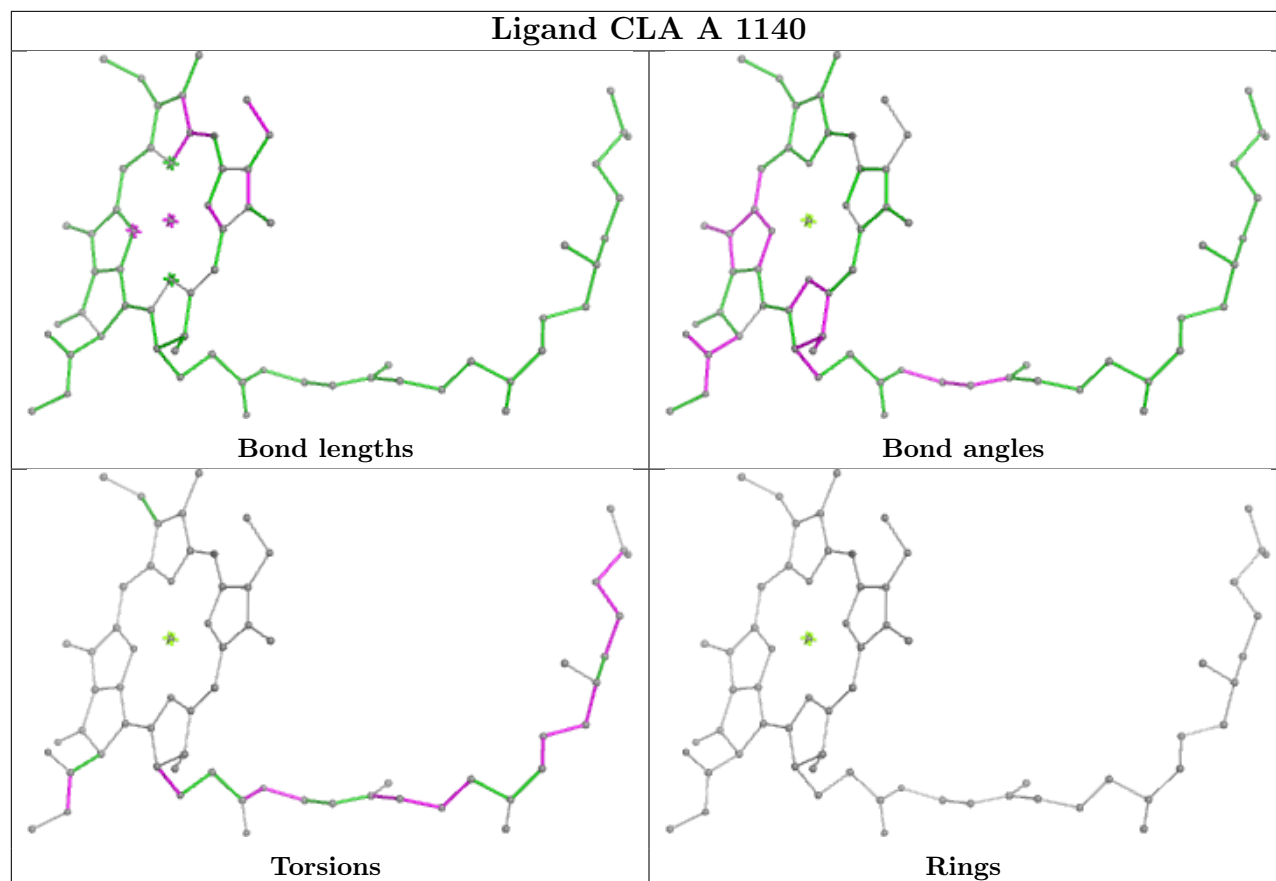
Bond angles



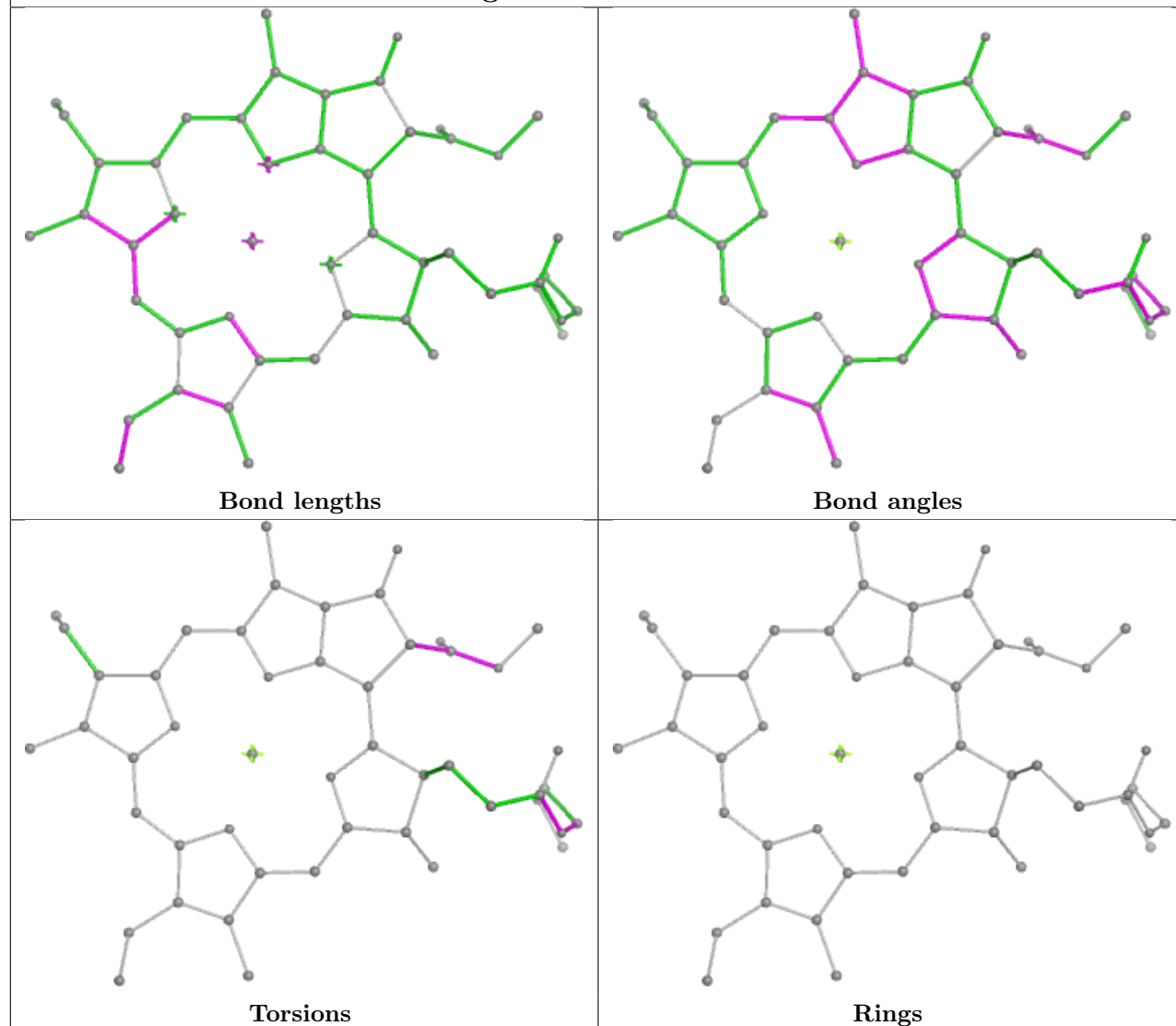
Torsions



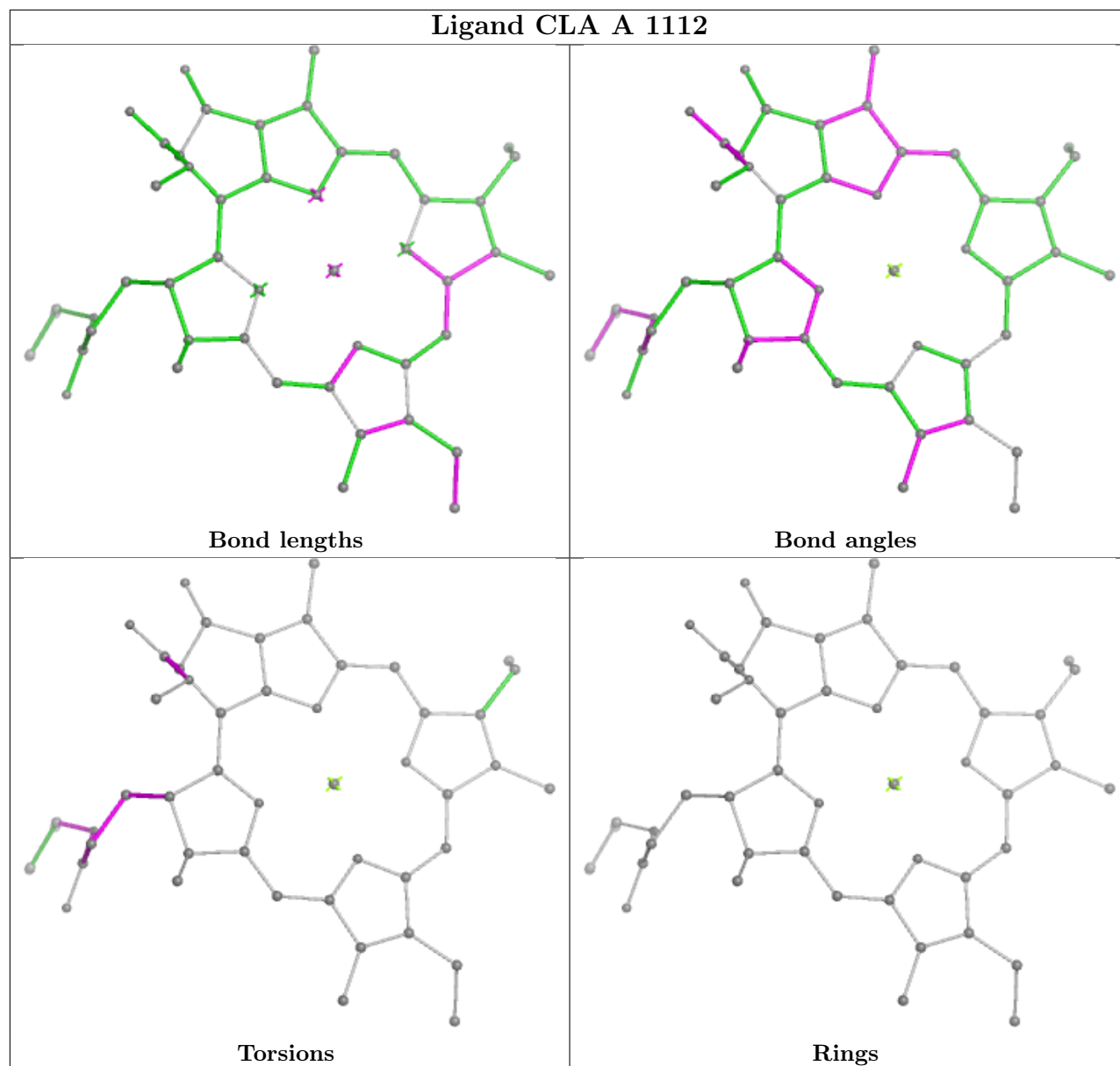
Rings



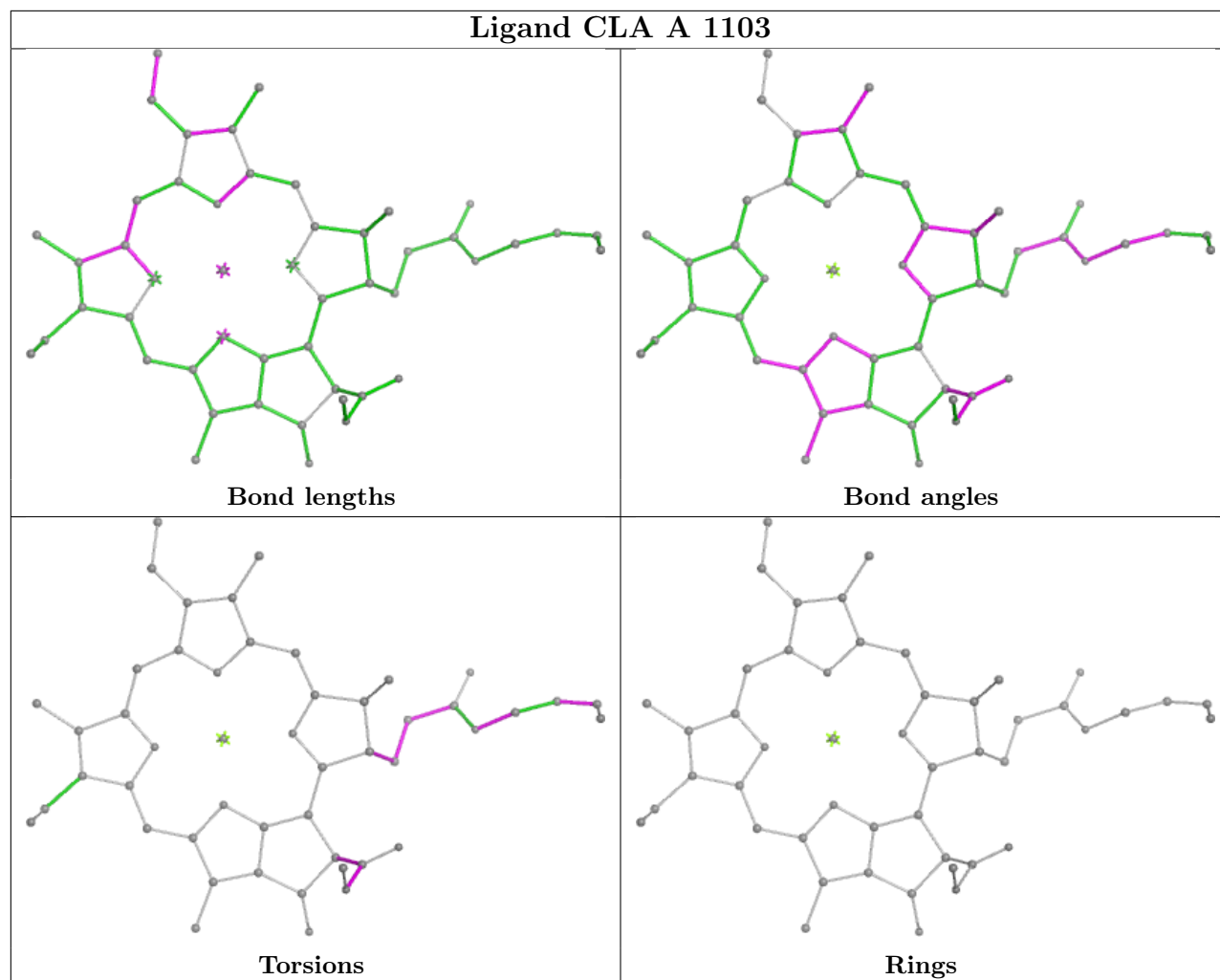
## Ligand CLA B 1203



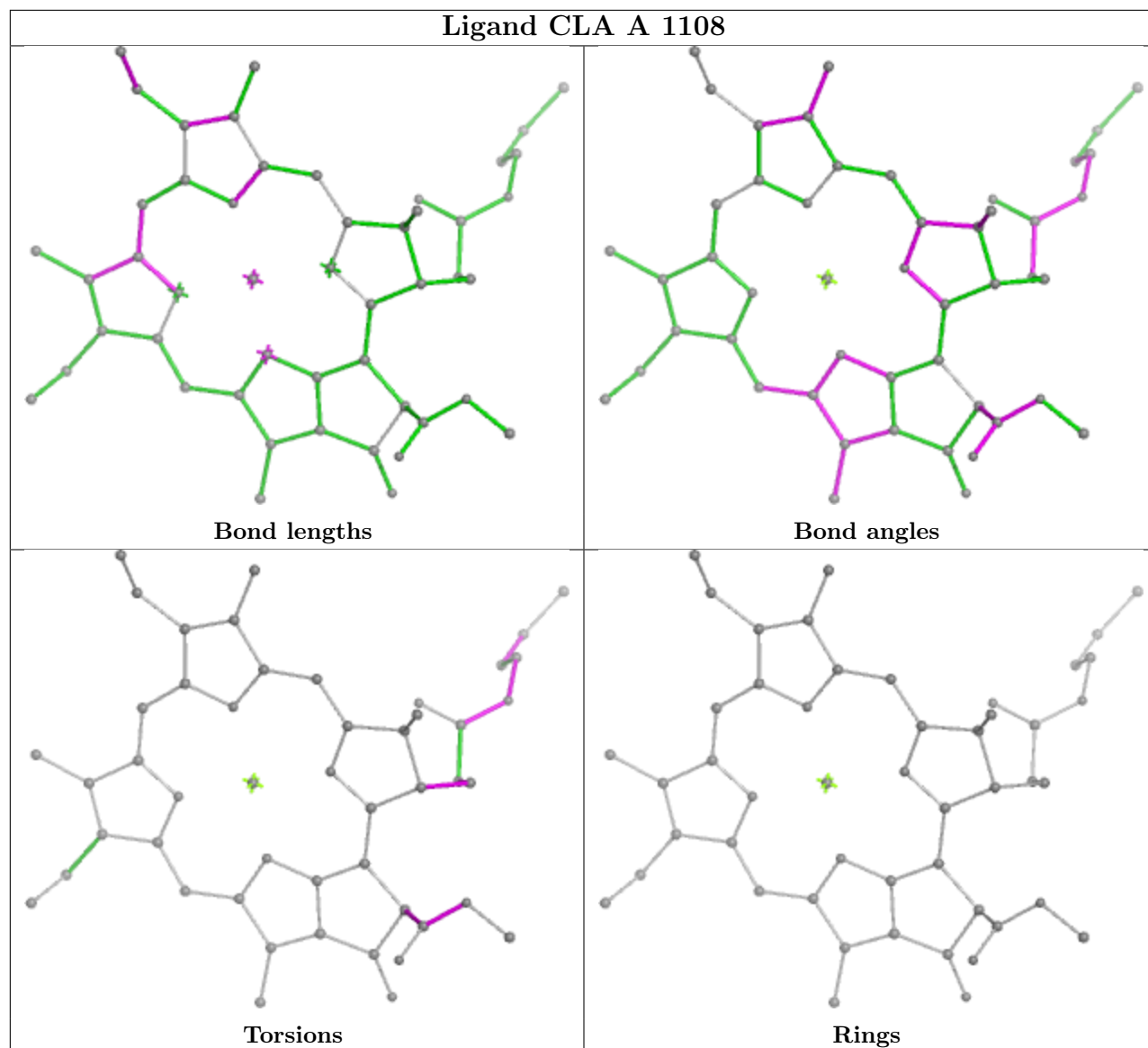
## Ligand CLA A 1112



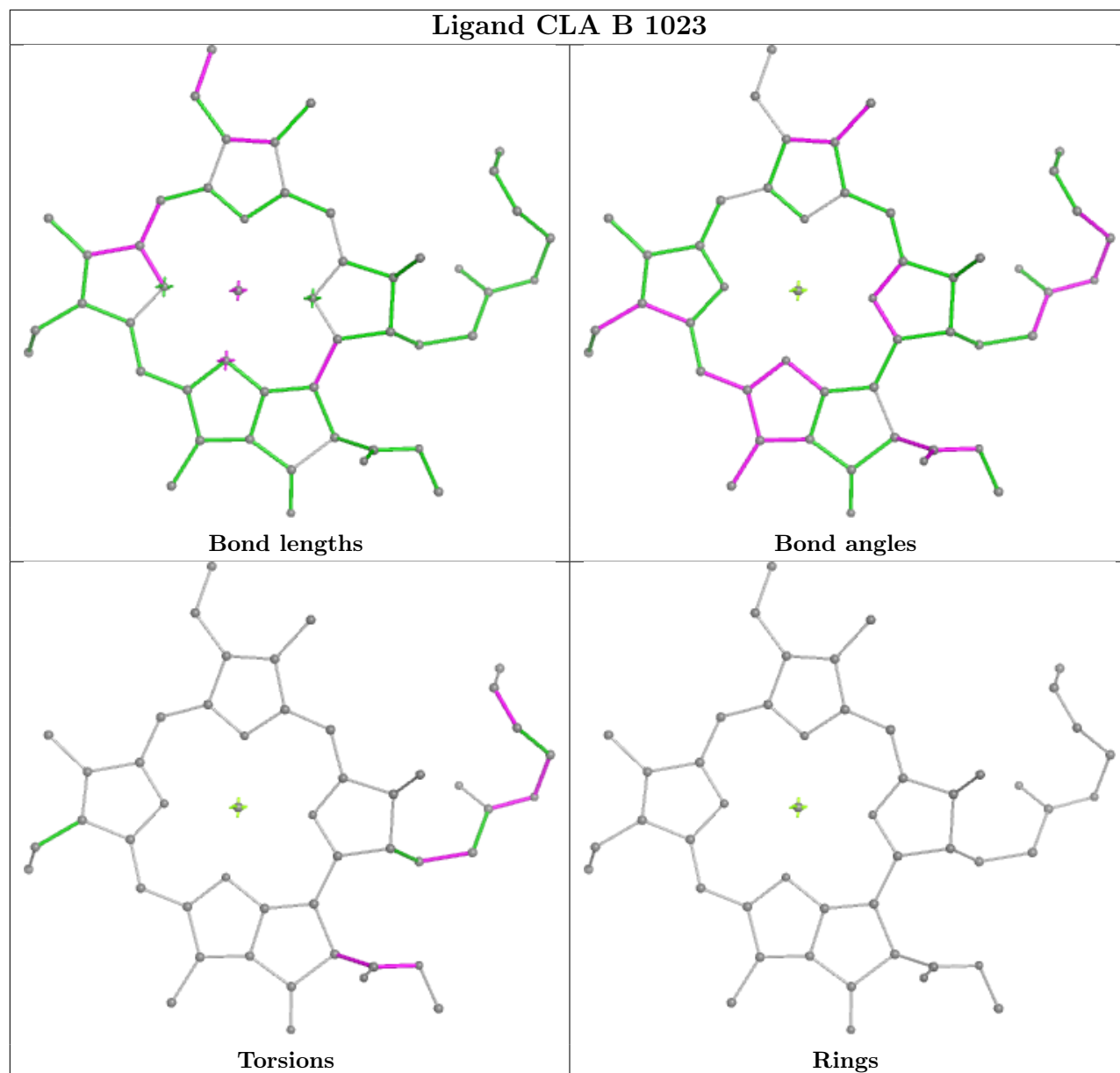
## Ligand CLA A 1103



## Ligand CLA A 1108

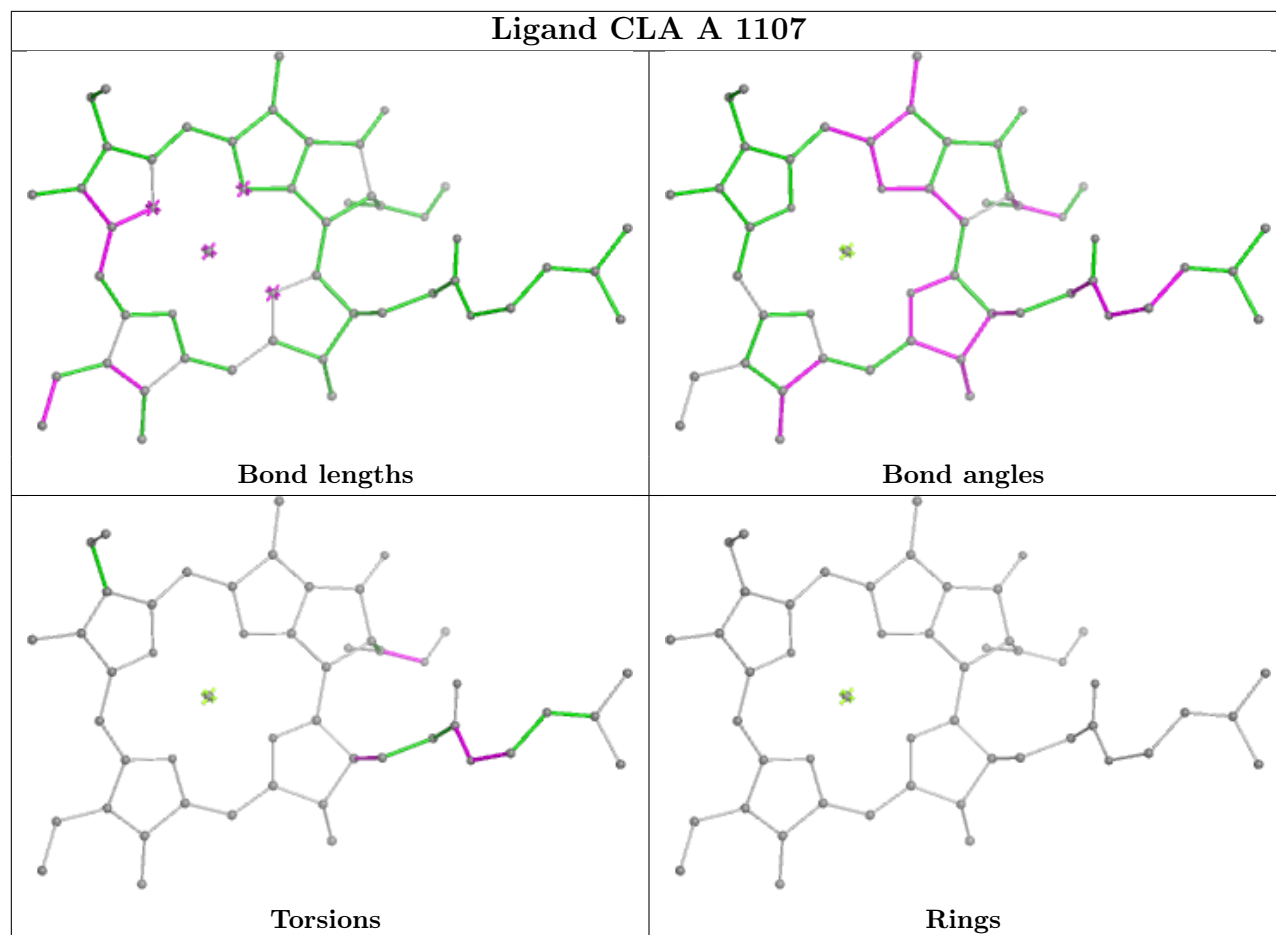


## Ligand CLA B 1023

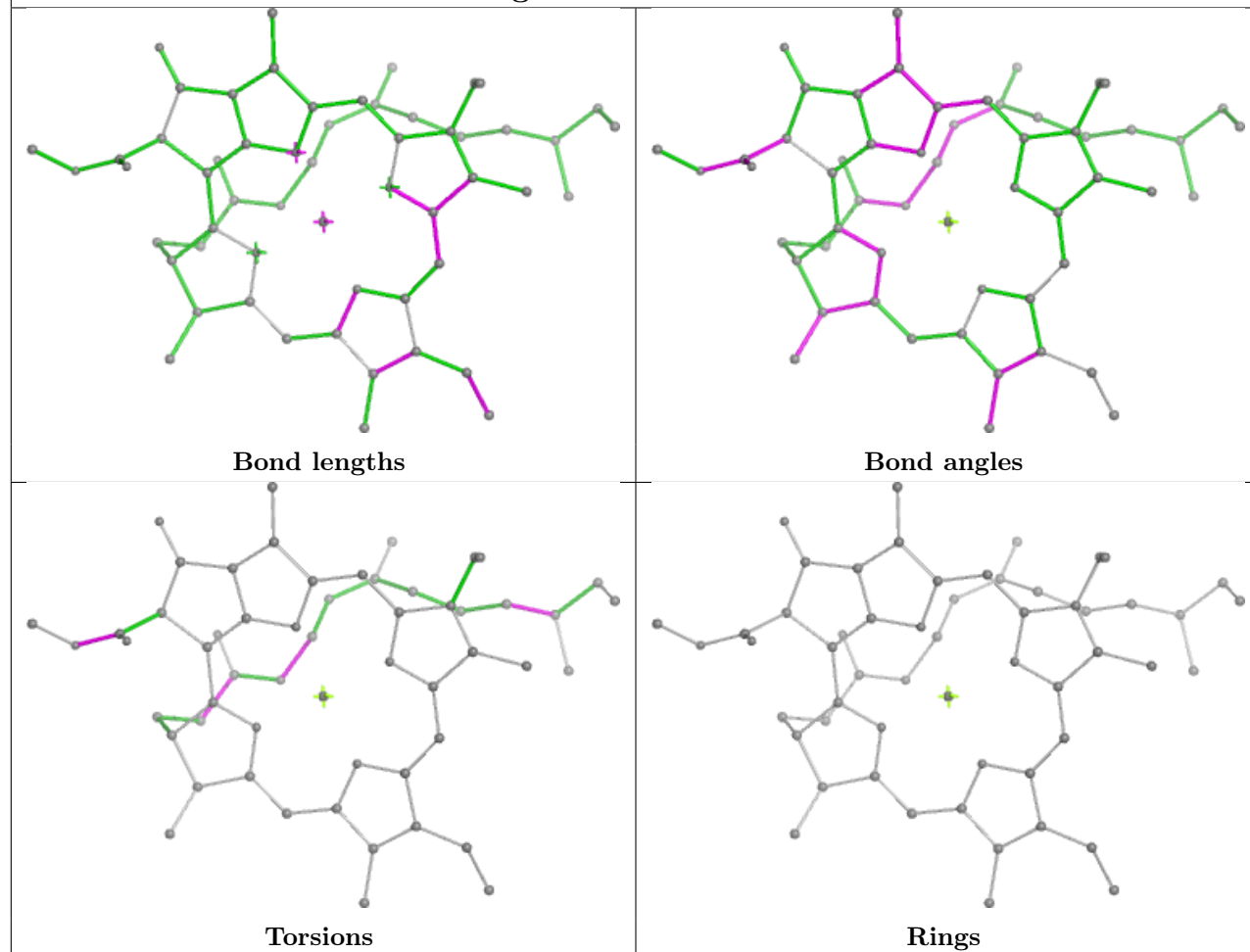




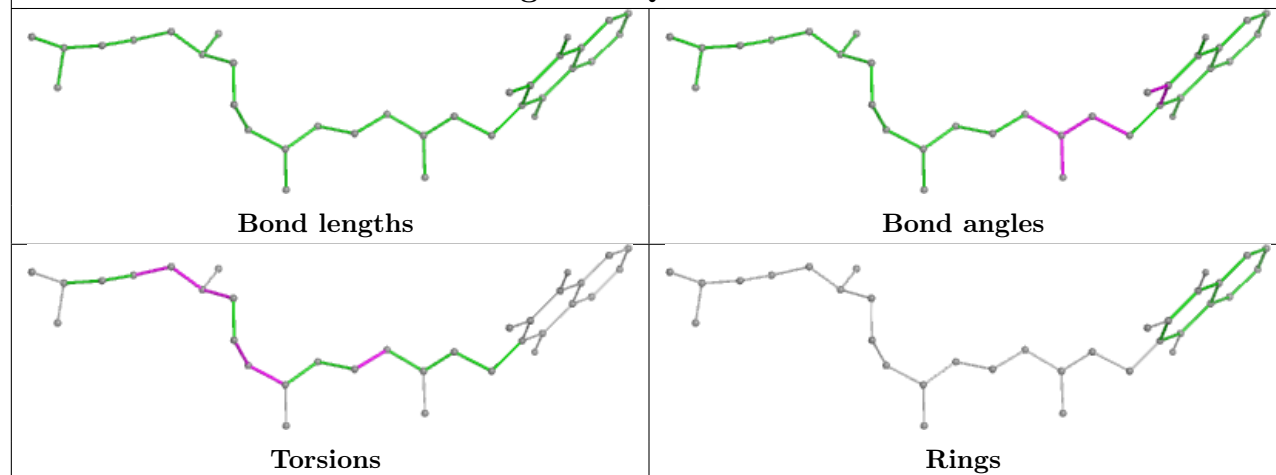
## Ligand CLA A 1107



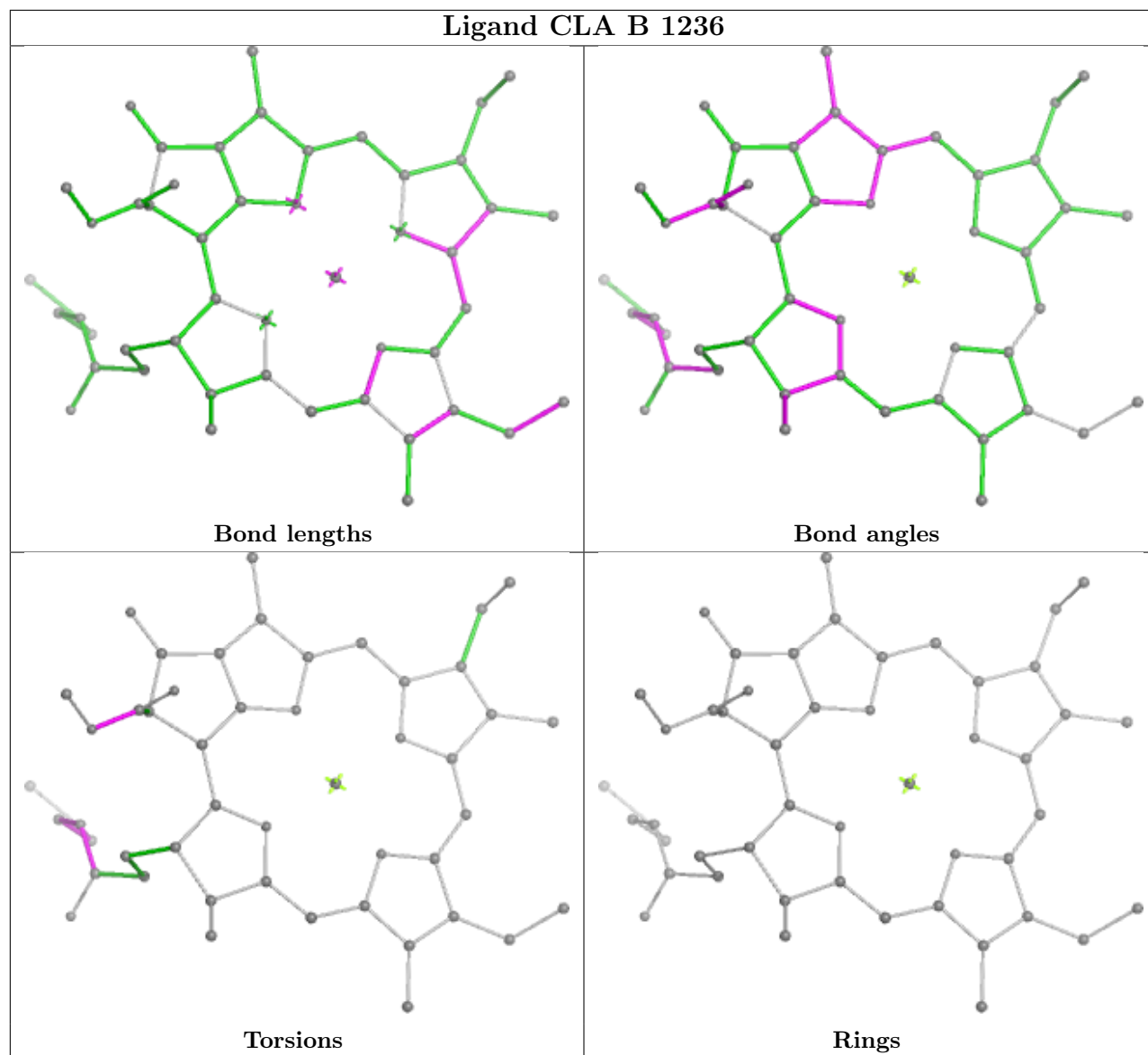
## Ligand CLA A 1115

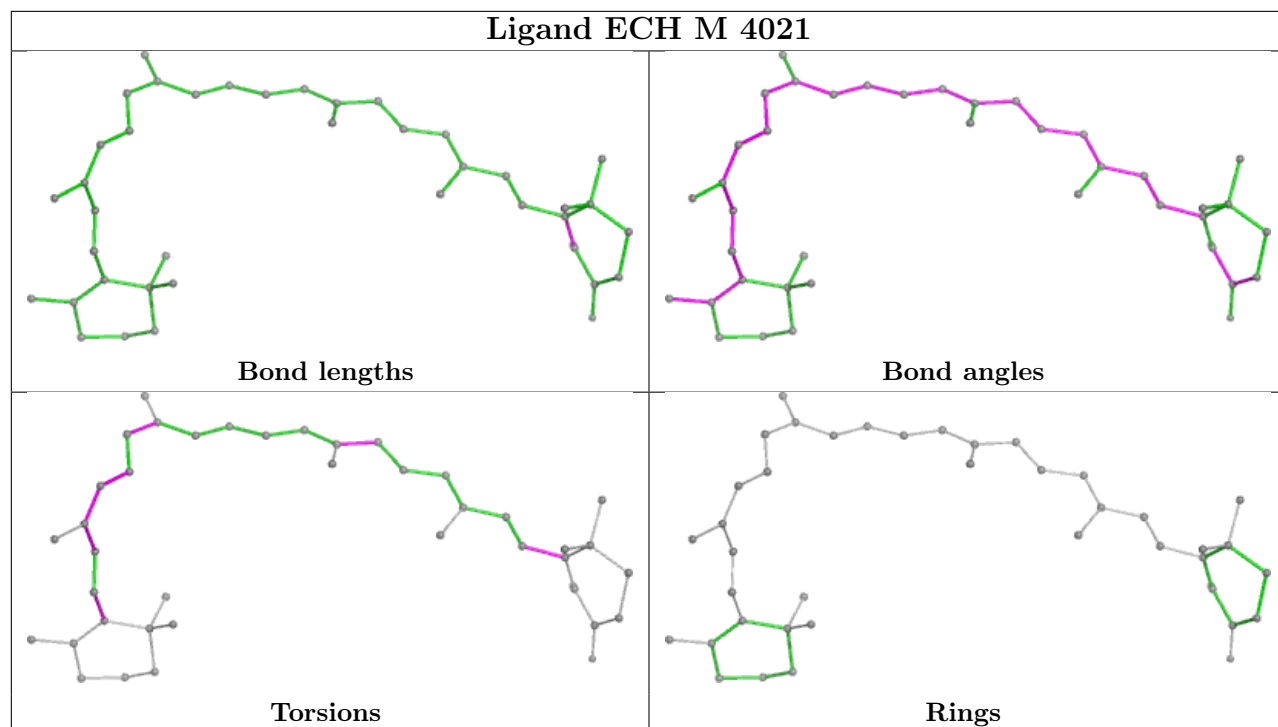


## Ligand PQN A 2001

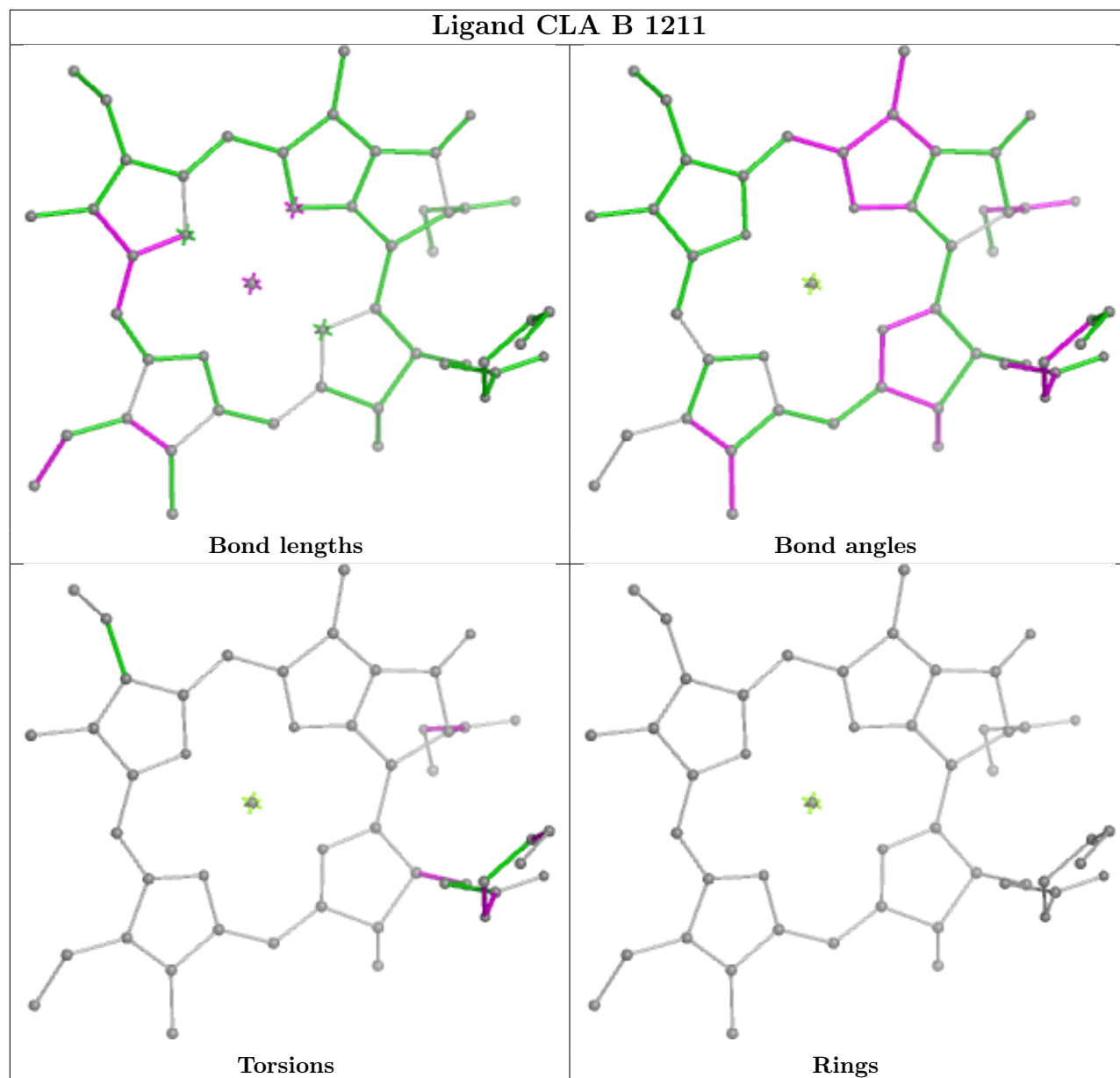


## Ligand CLA B 1236

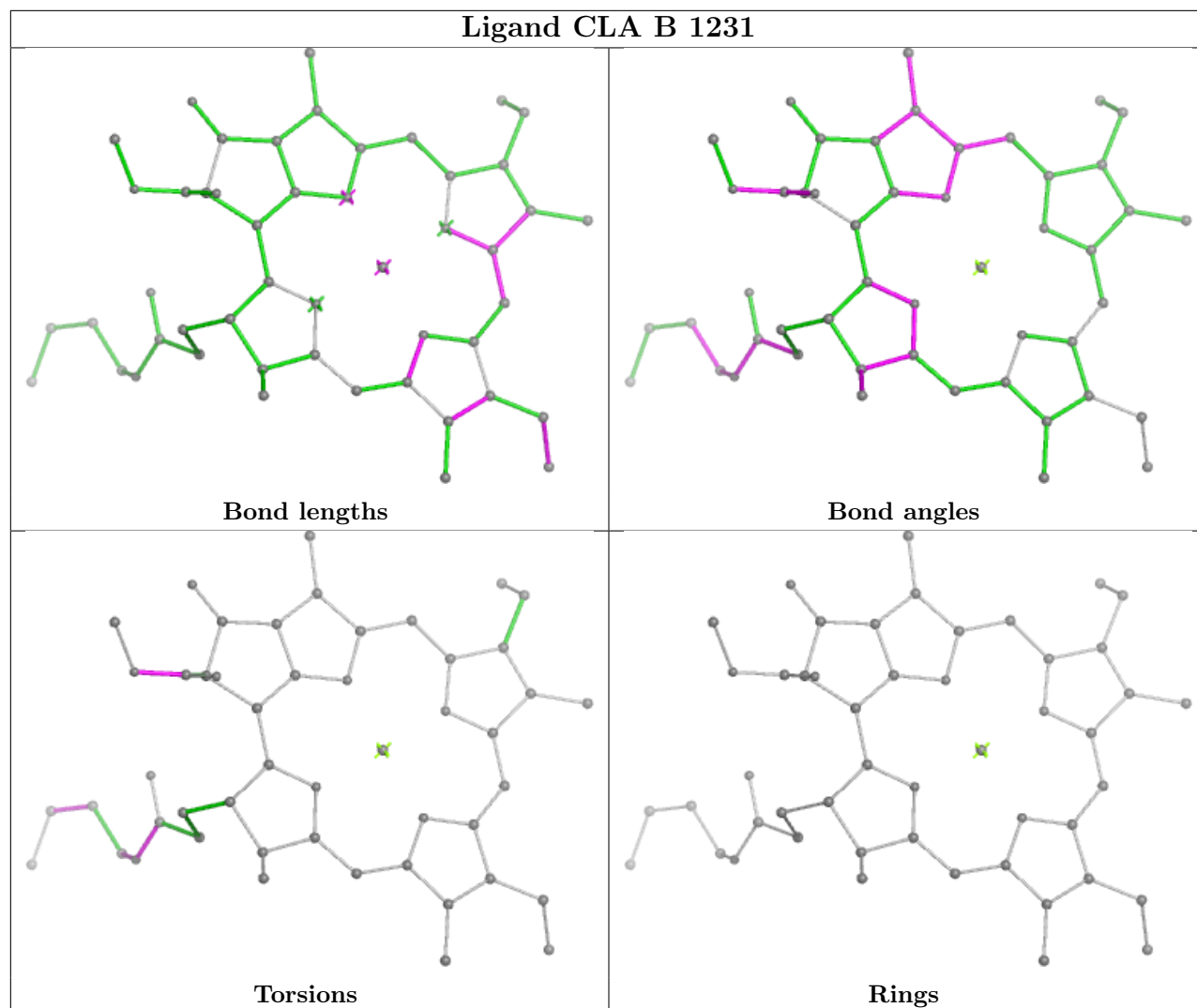




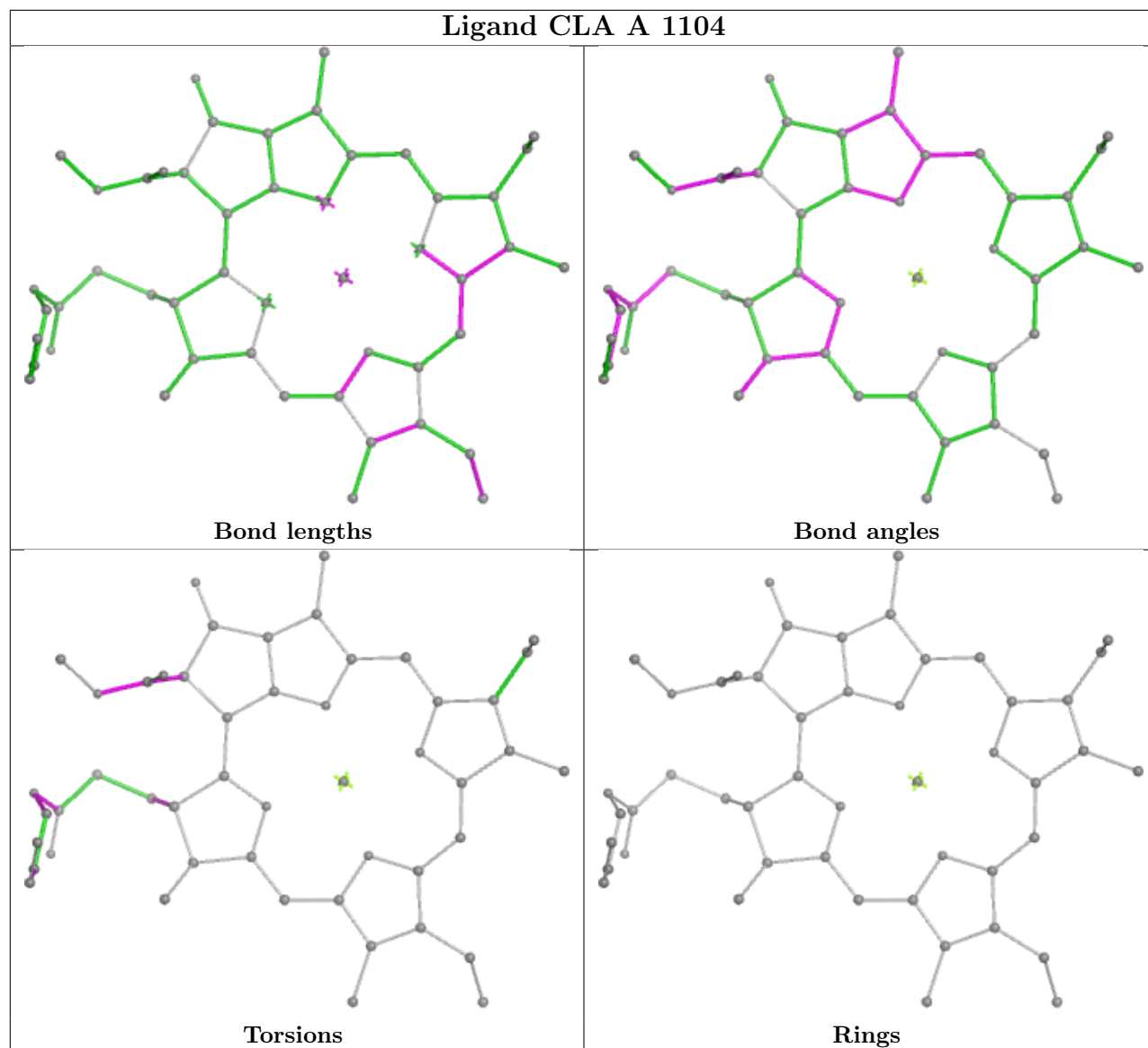
## Ligand CLA B 1211



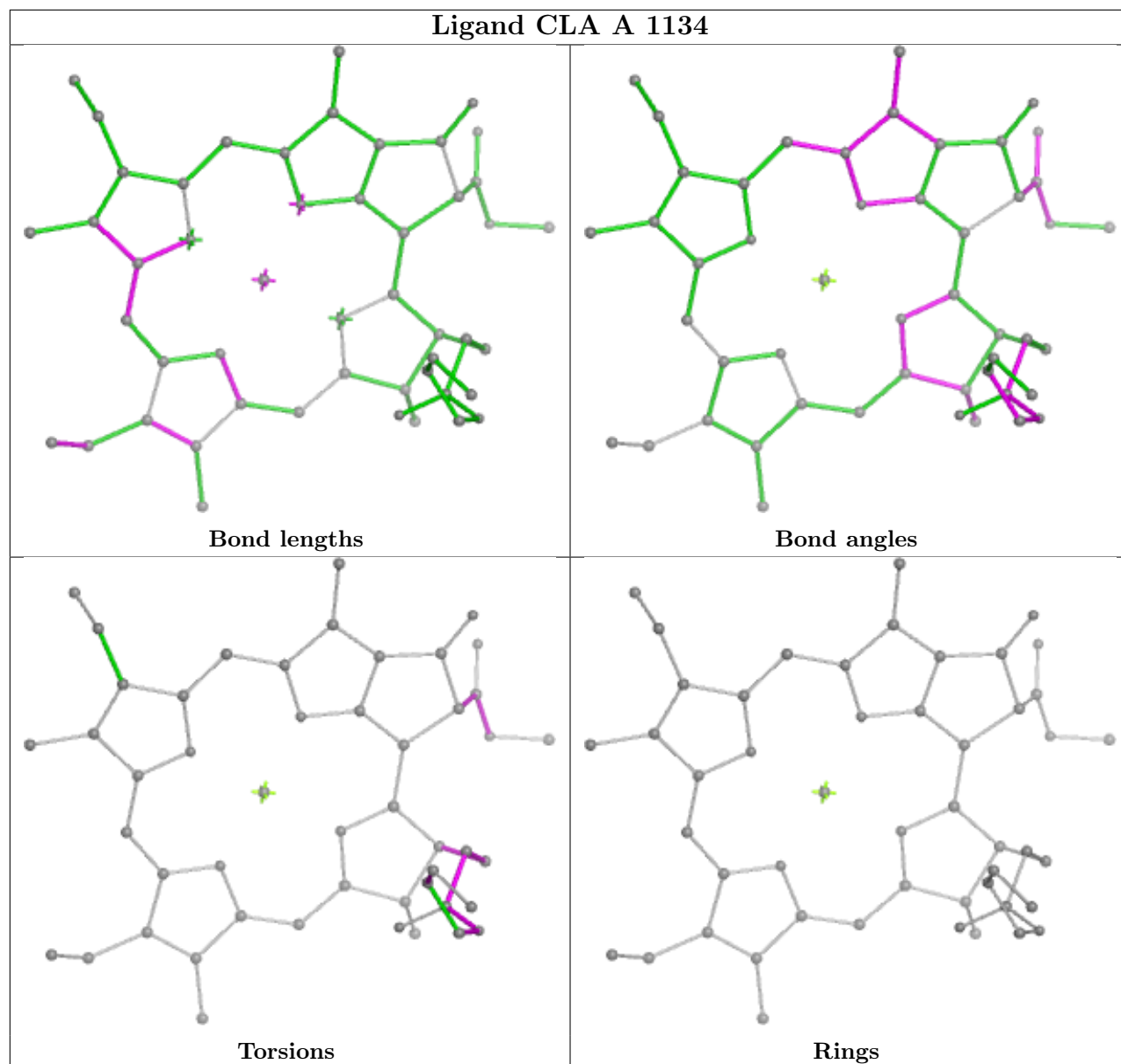
## Ligand CLA B 1231



## Ligand CLA A 1104

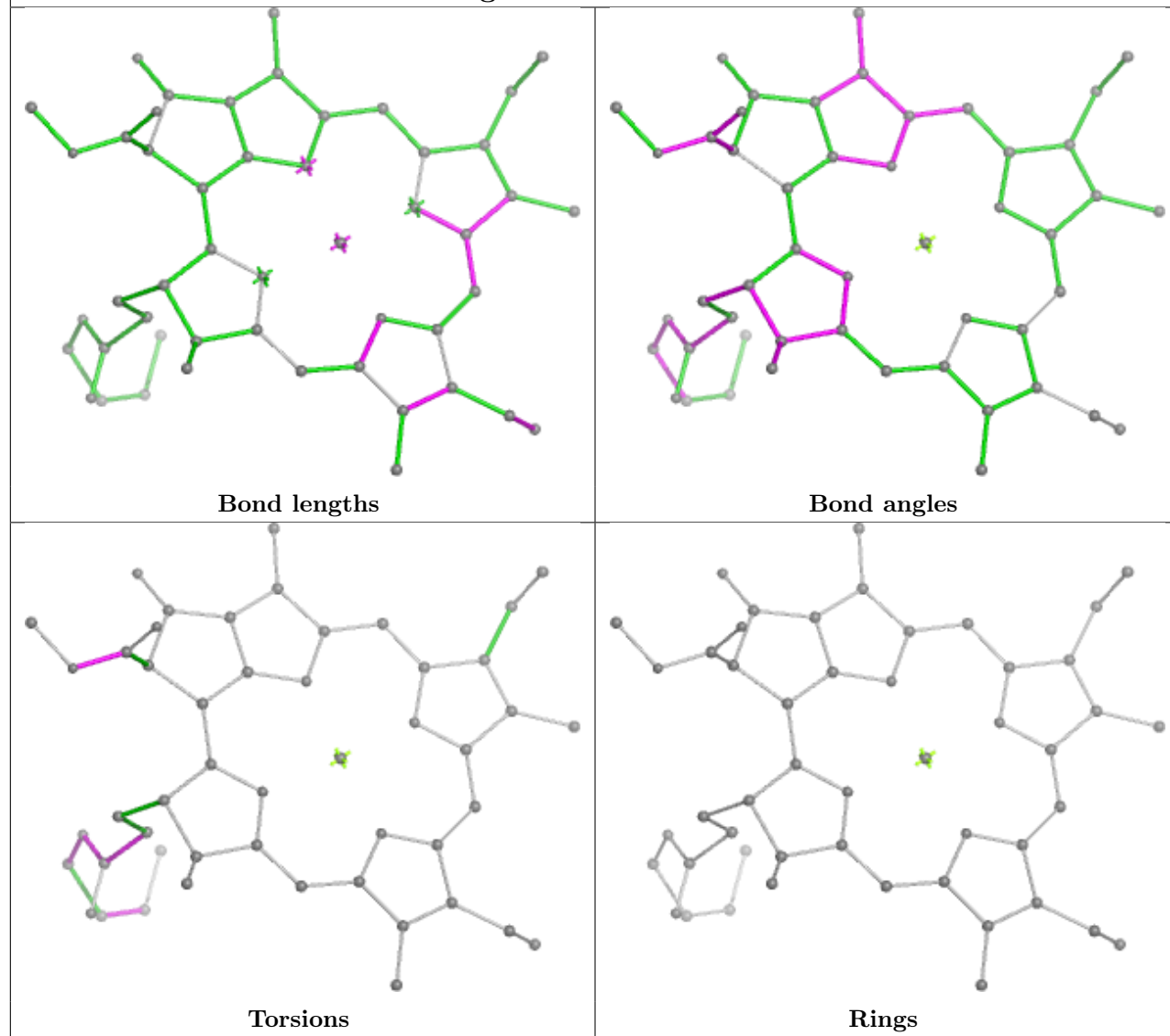


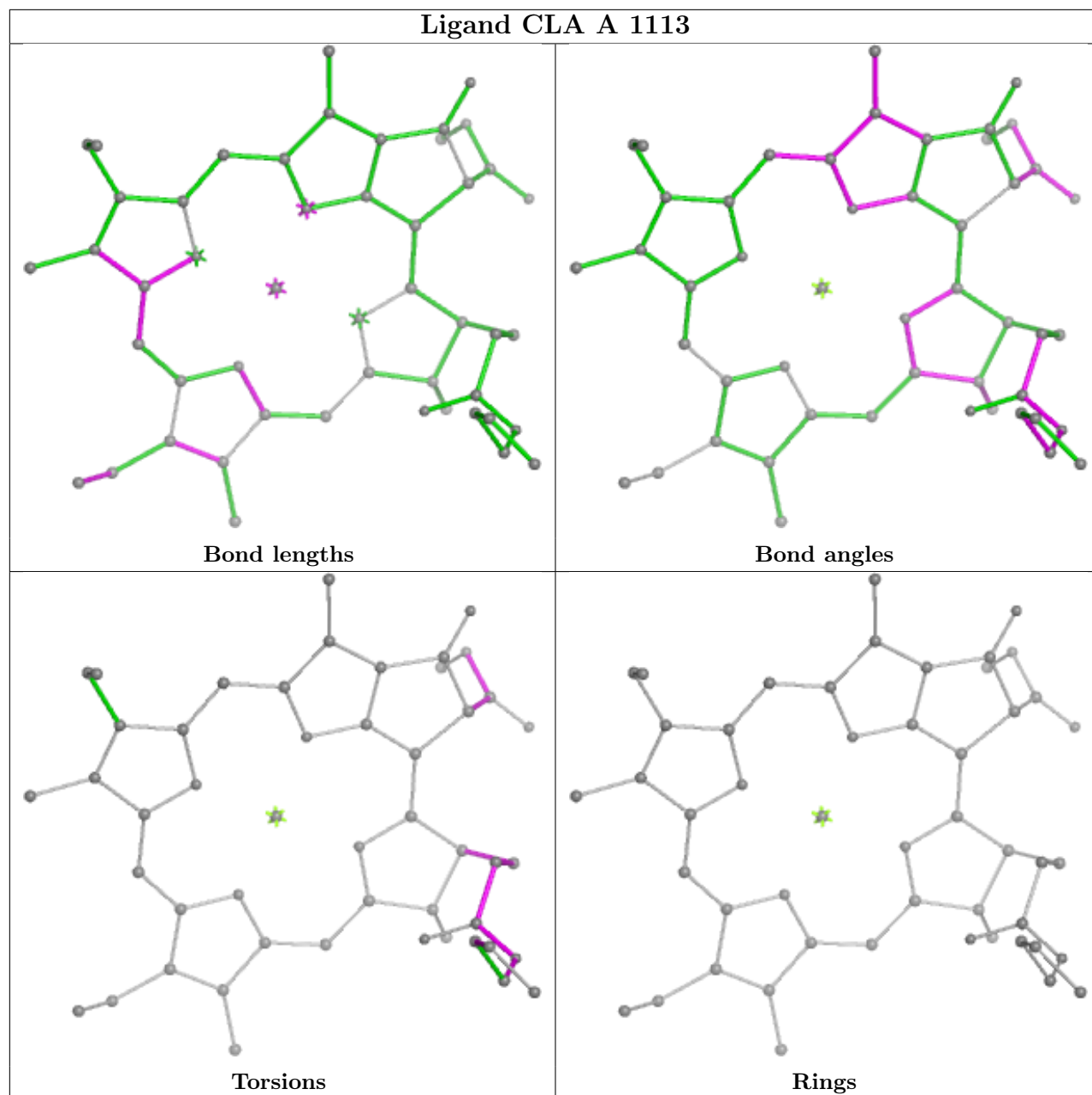
## Ligand CLA A 1134

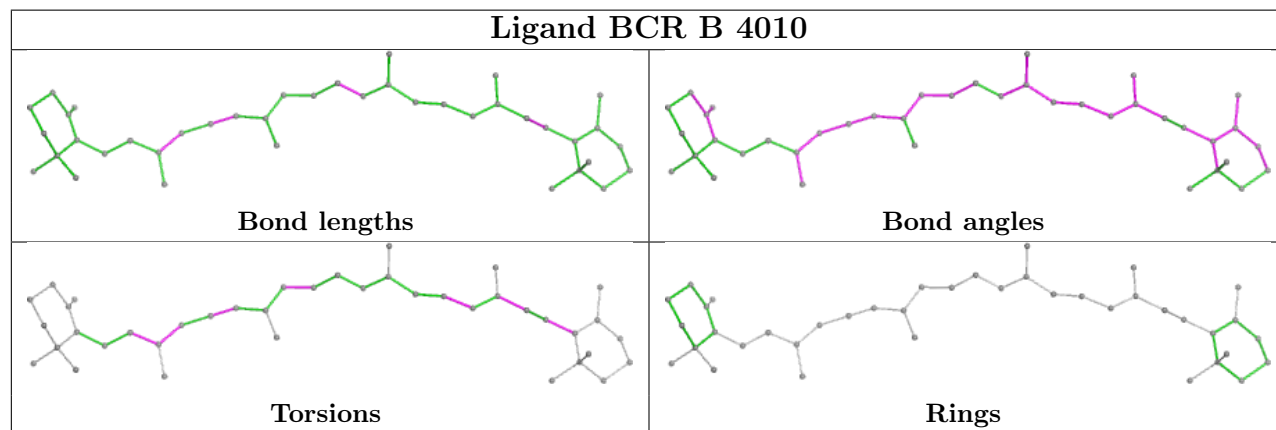
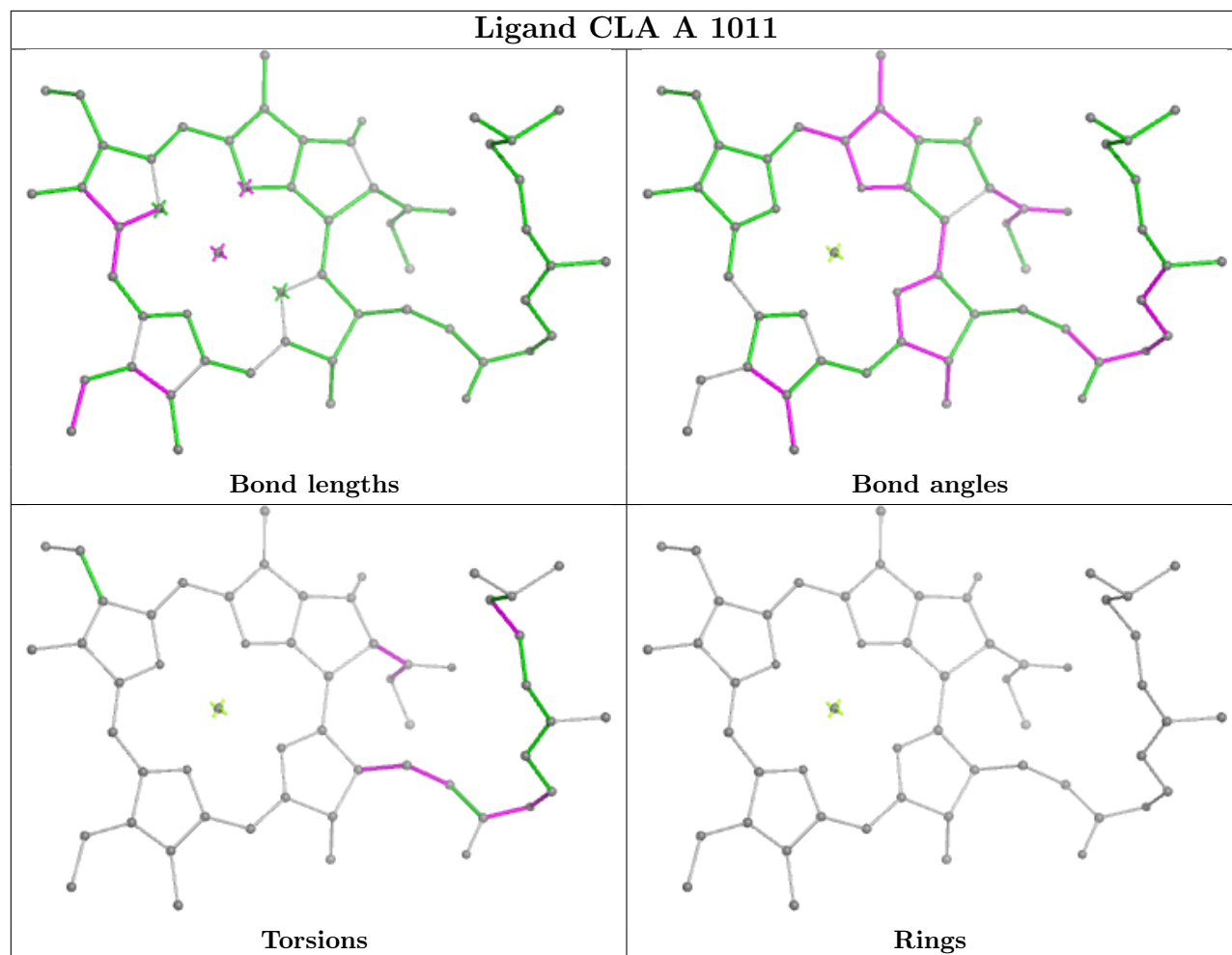




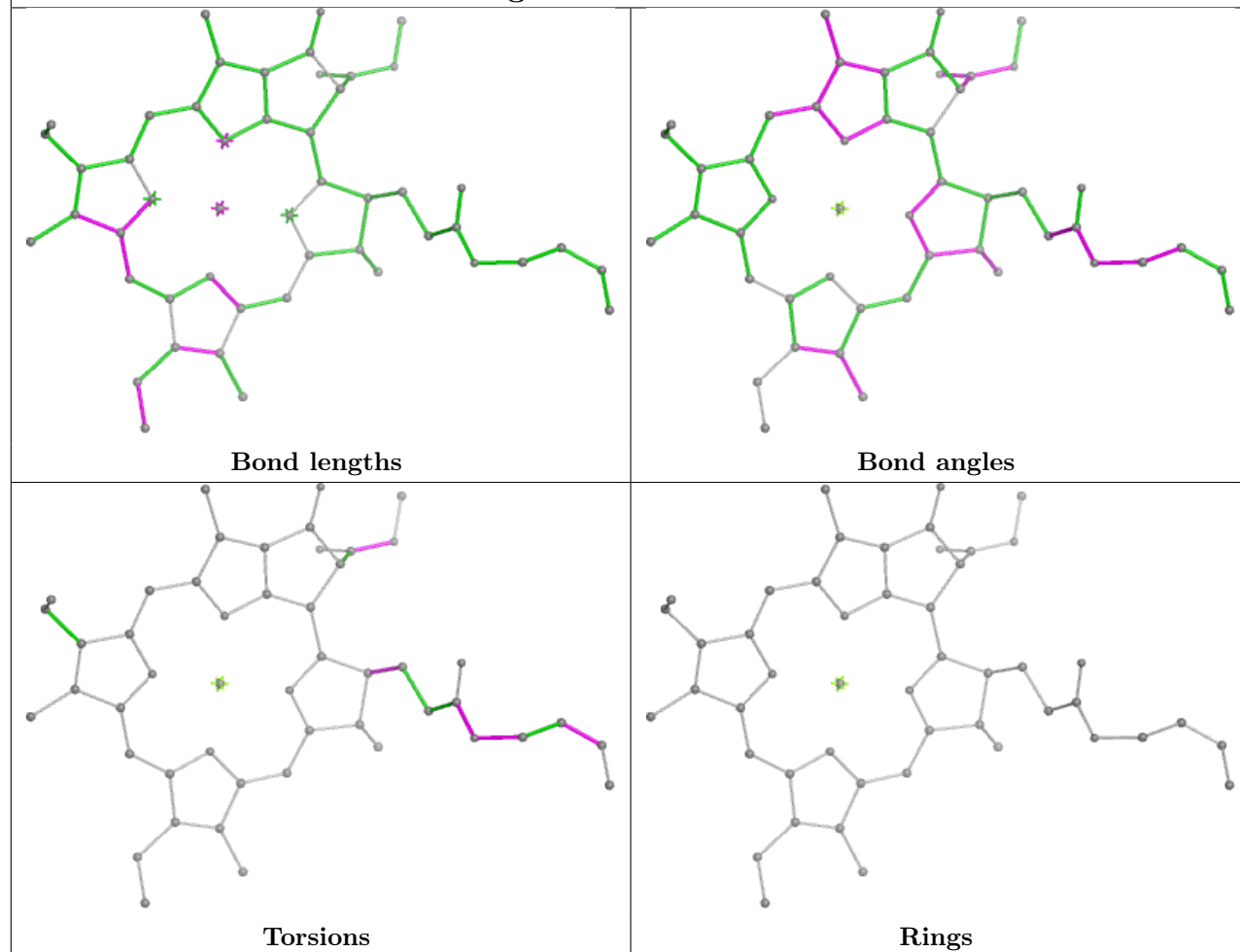
## Ligand CLA B 1232

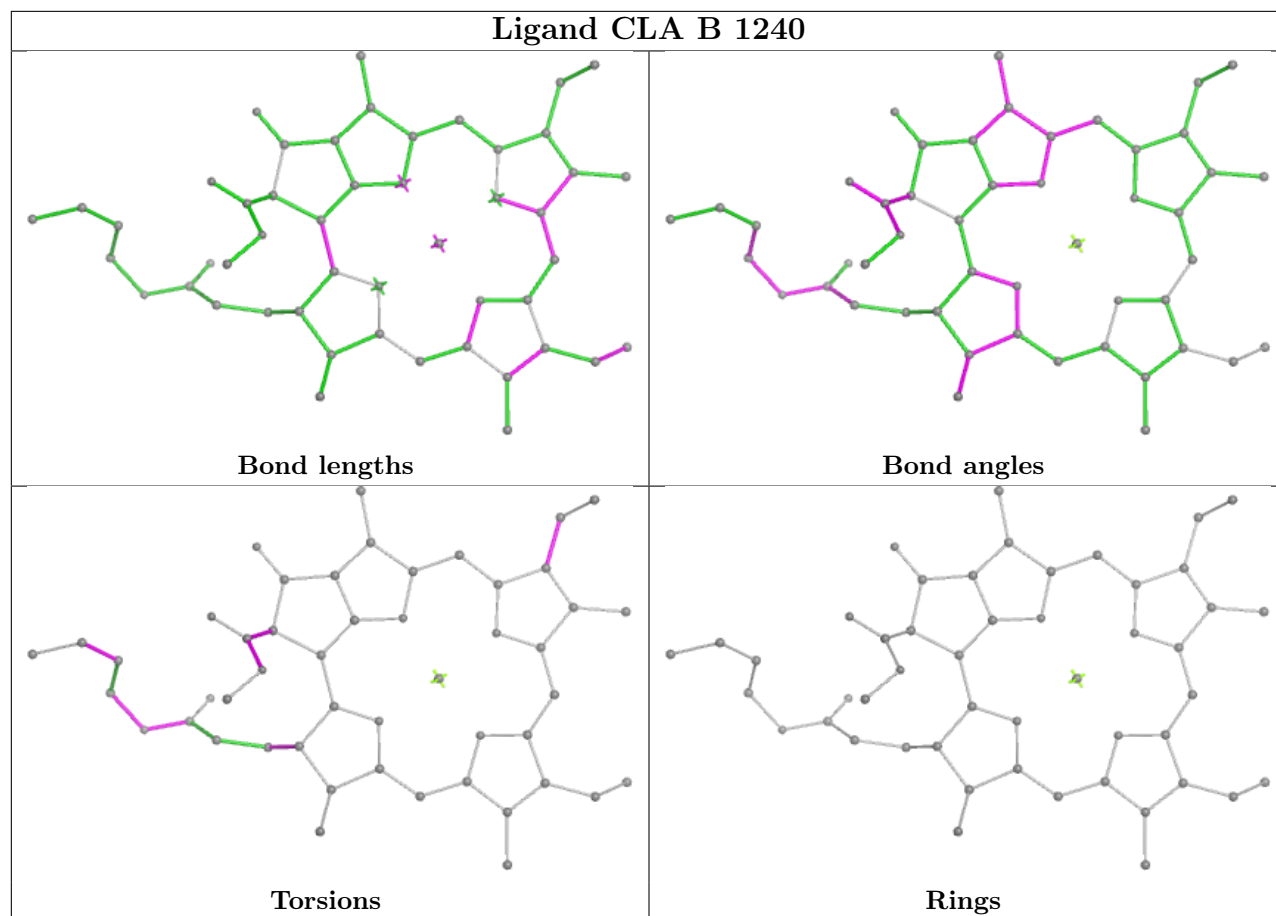


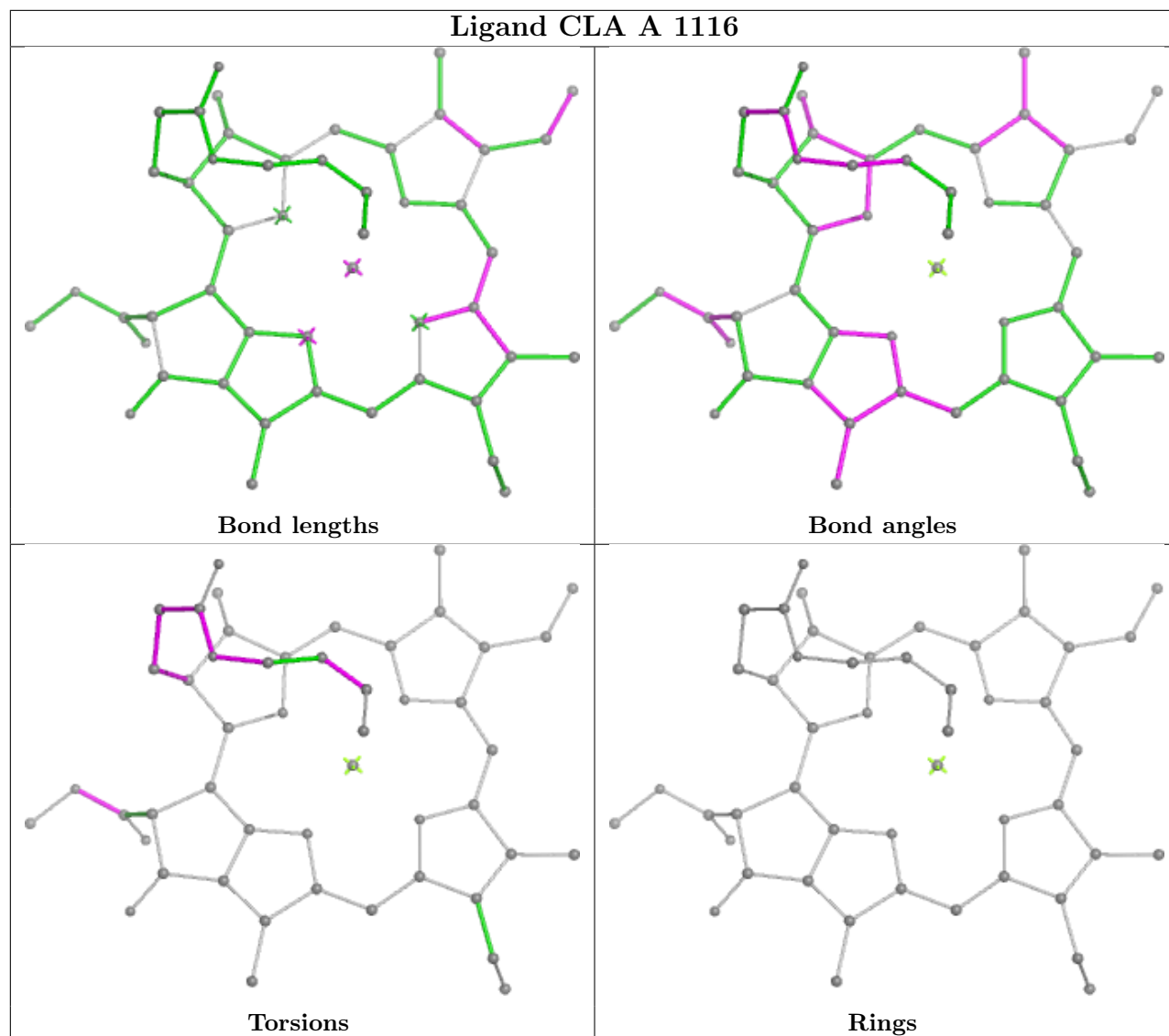




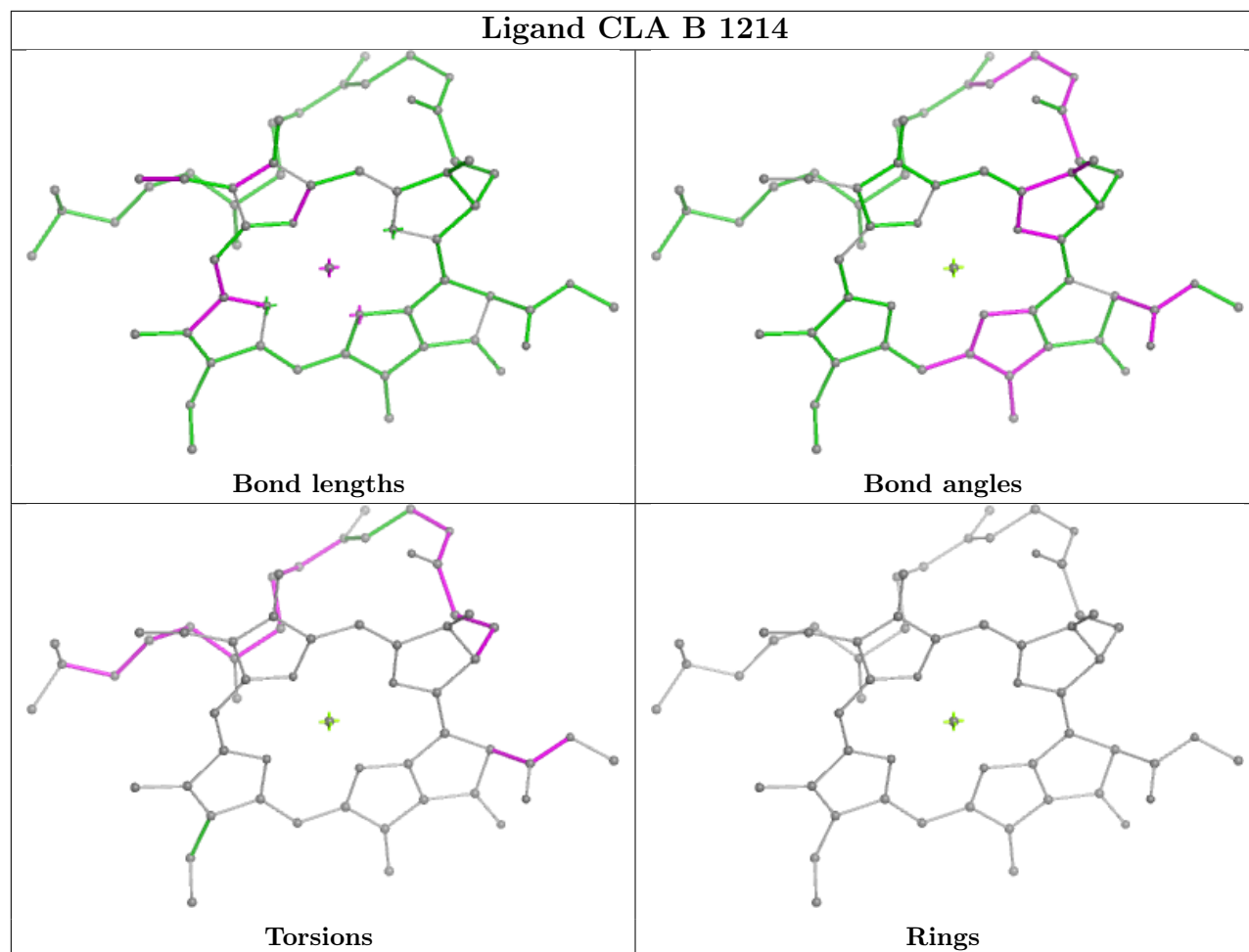
## Ligand CLA A 1124



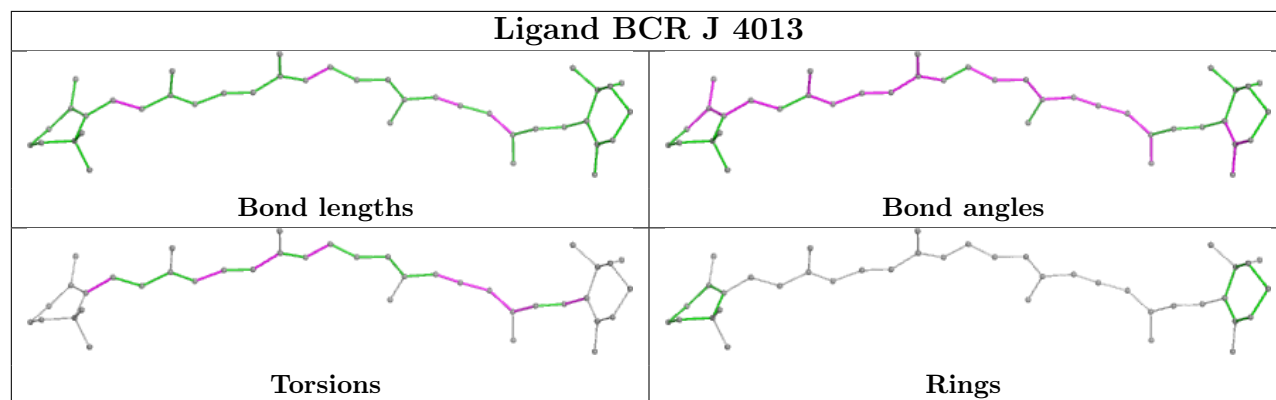




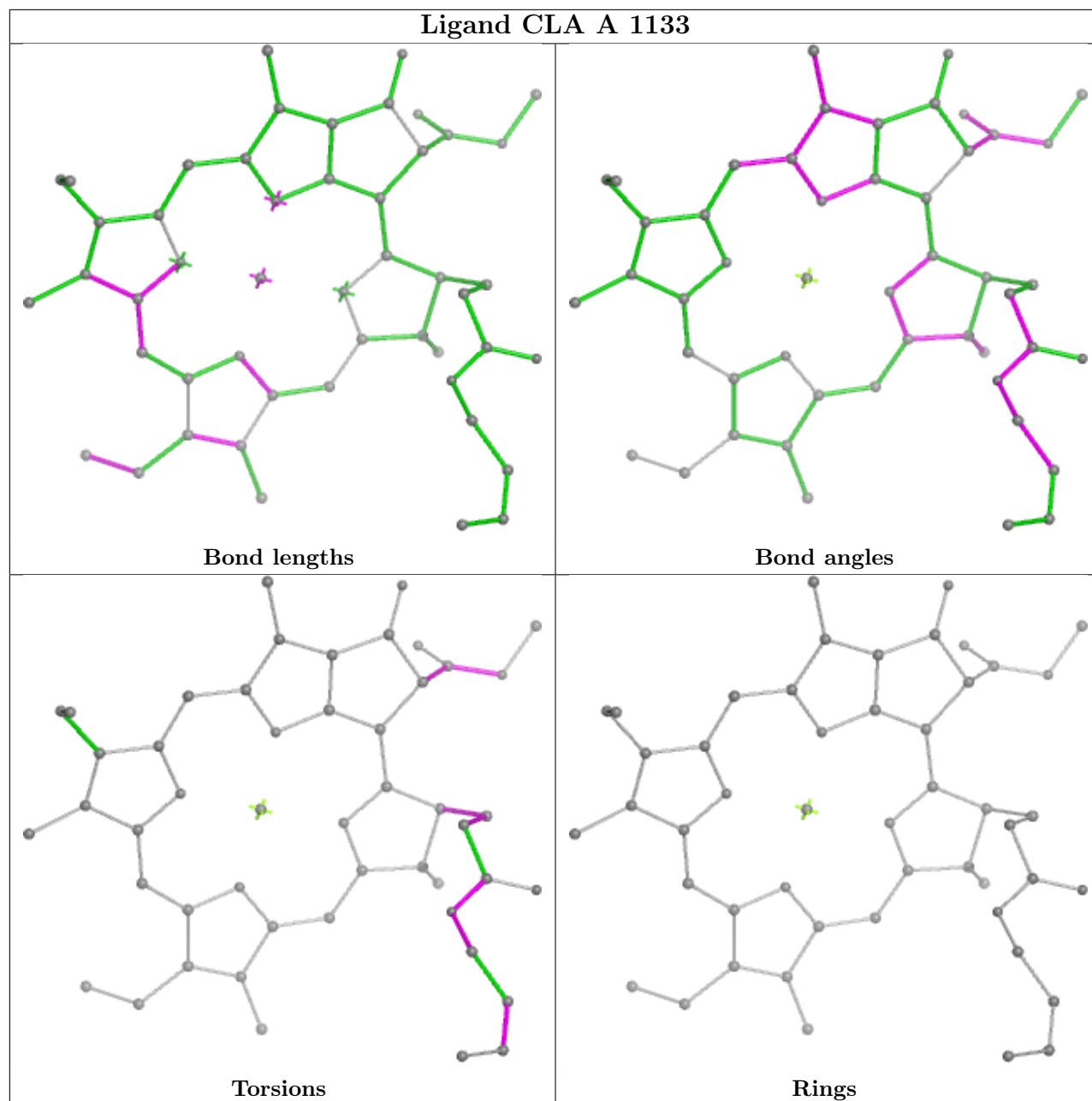
## Ligand CLA B 1214



## Ligand BCR J 4013

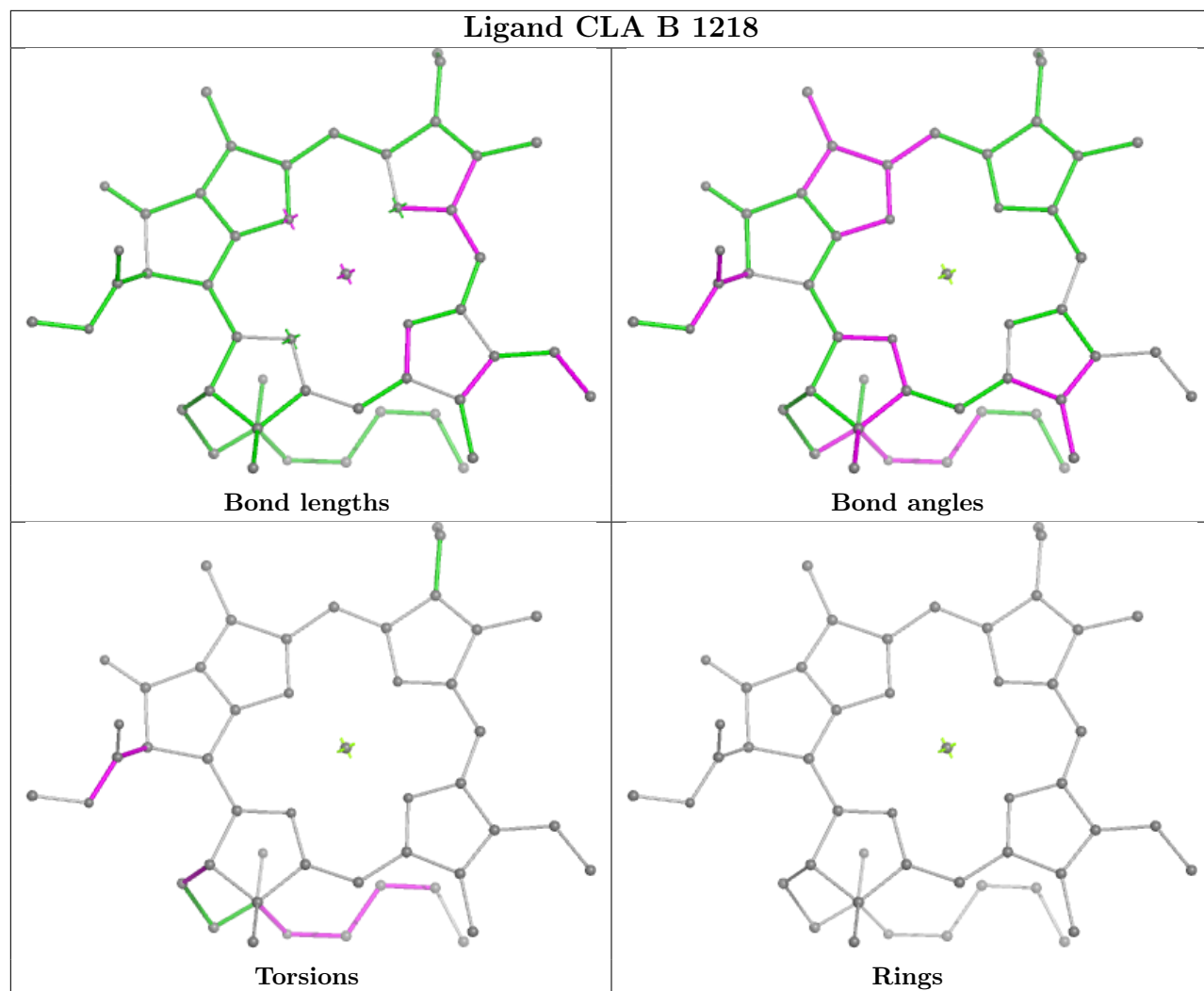


## Ligand CLA A 1133

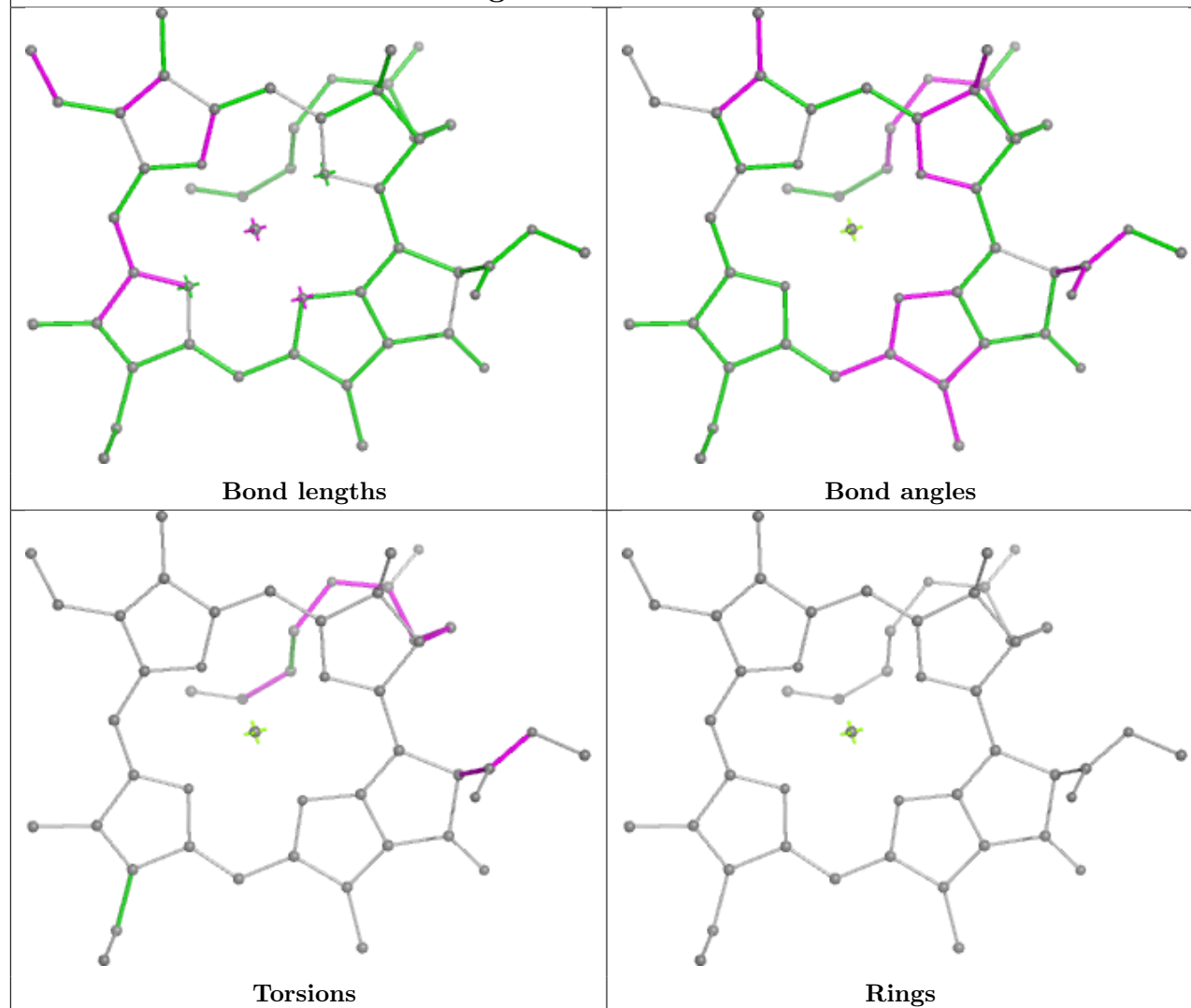




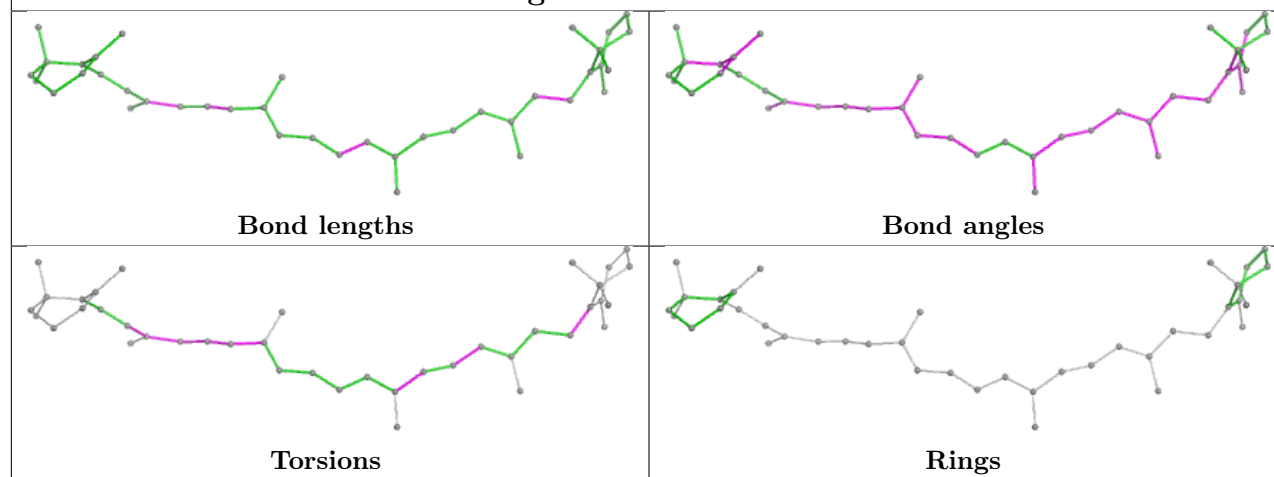
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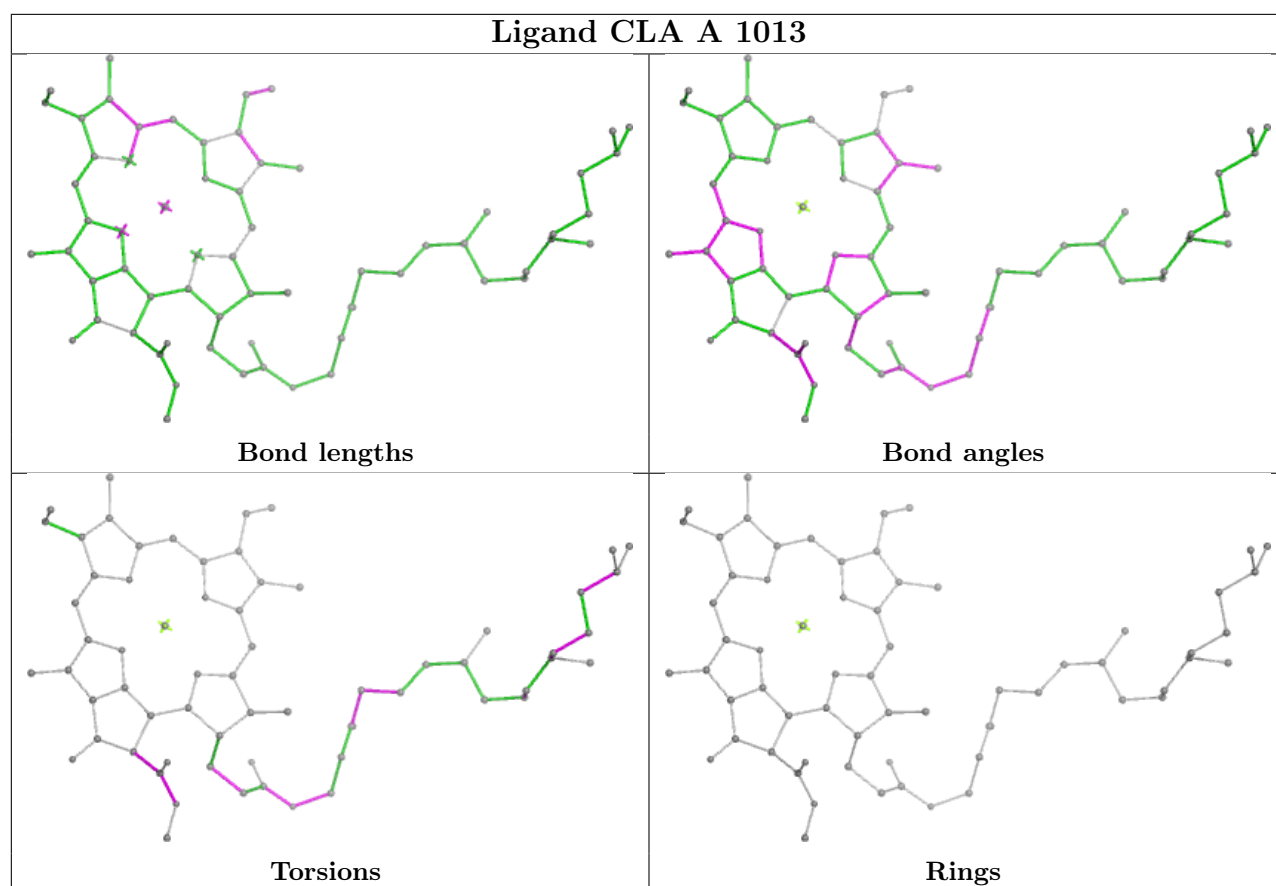


## Ligand CLA A 1121

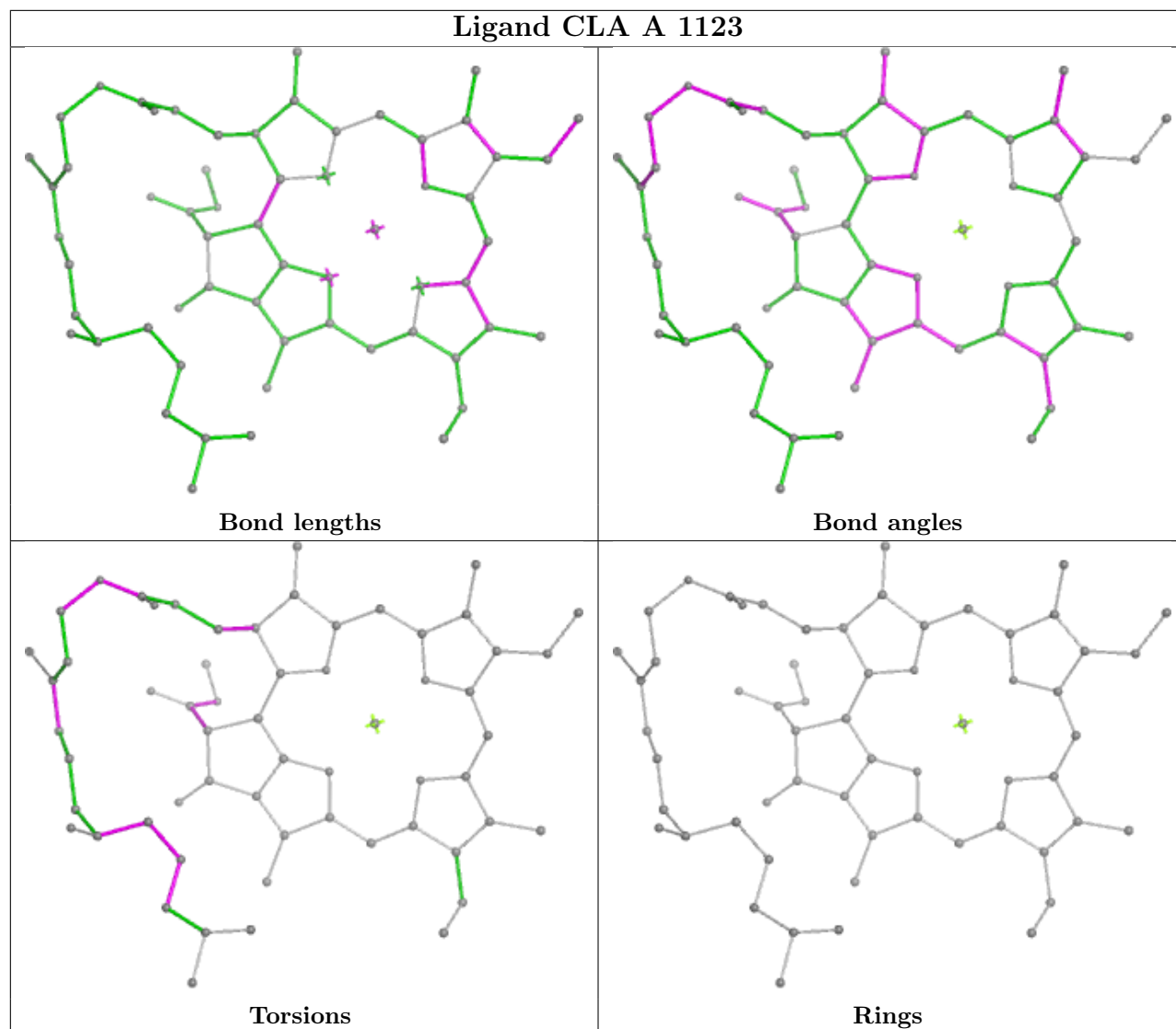


## Ligand BCR I 4018

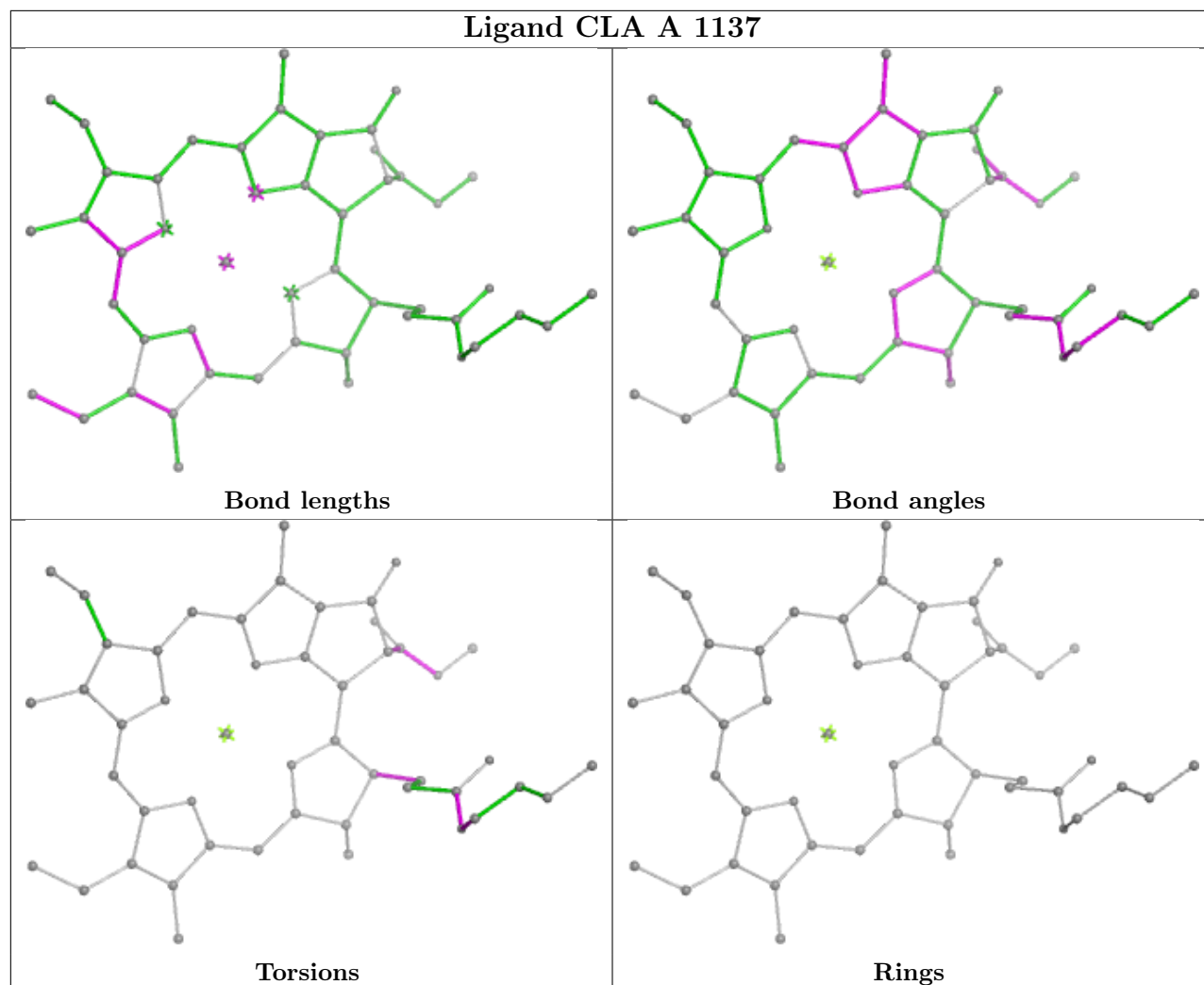


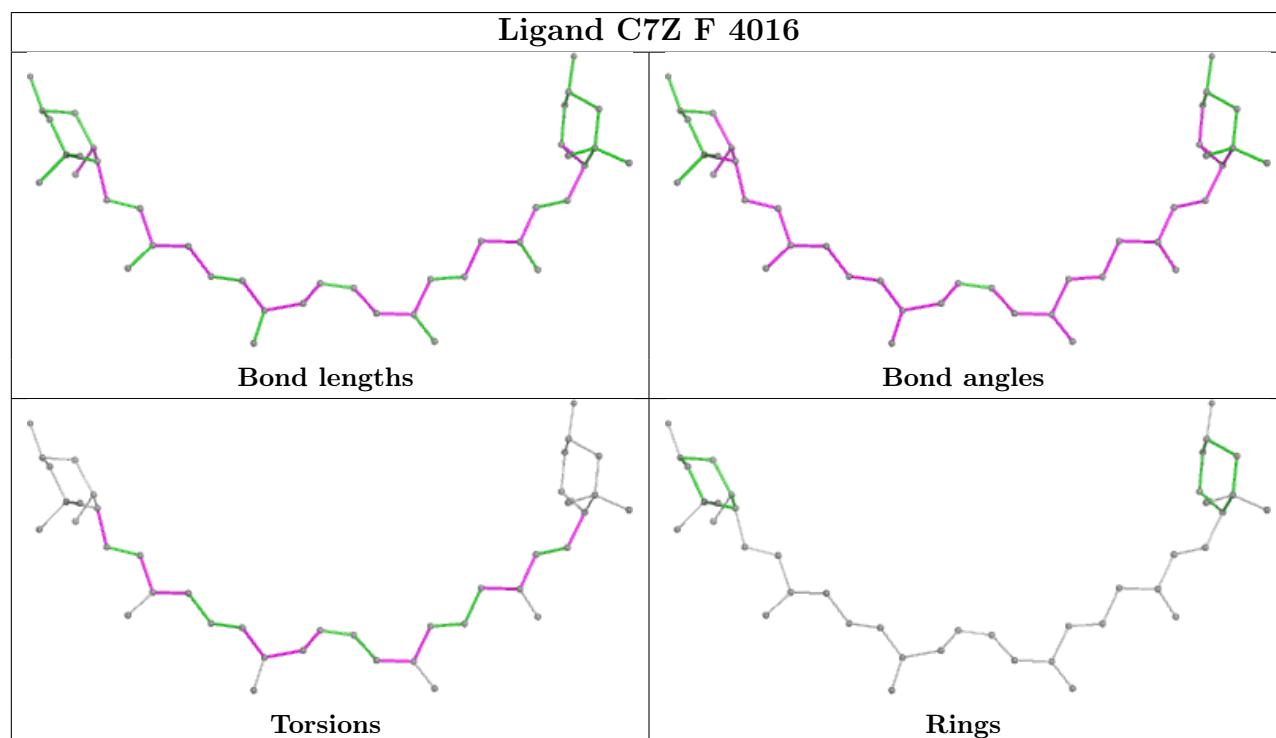
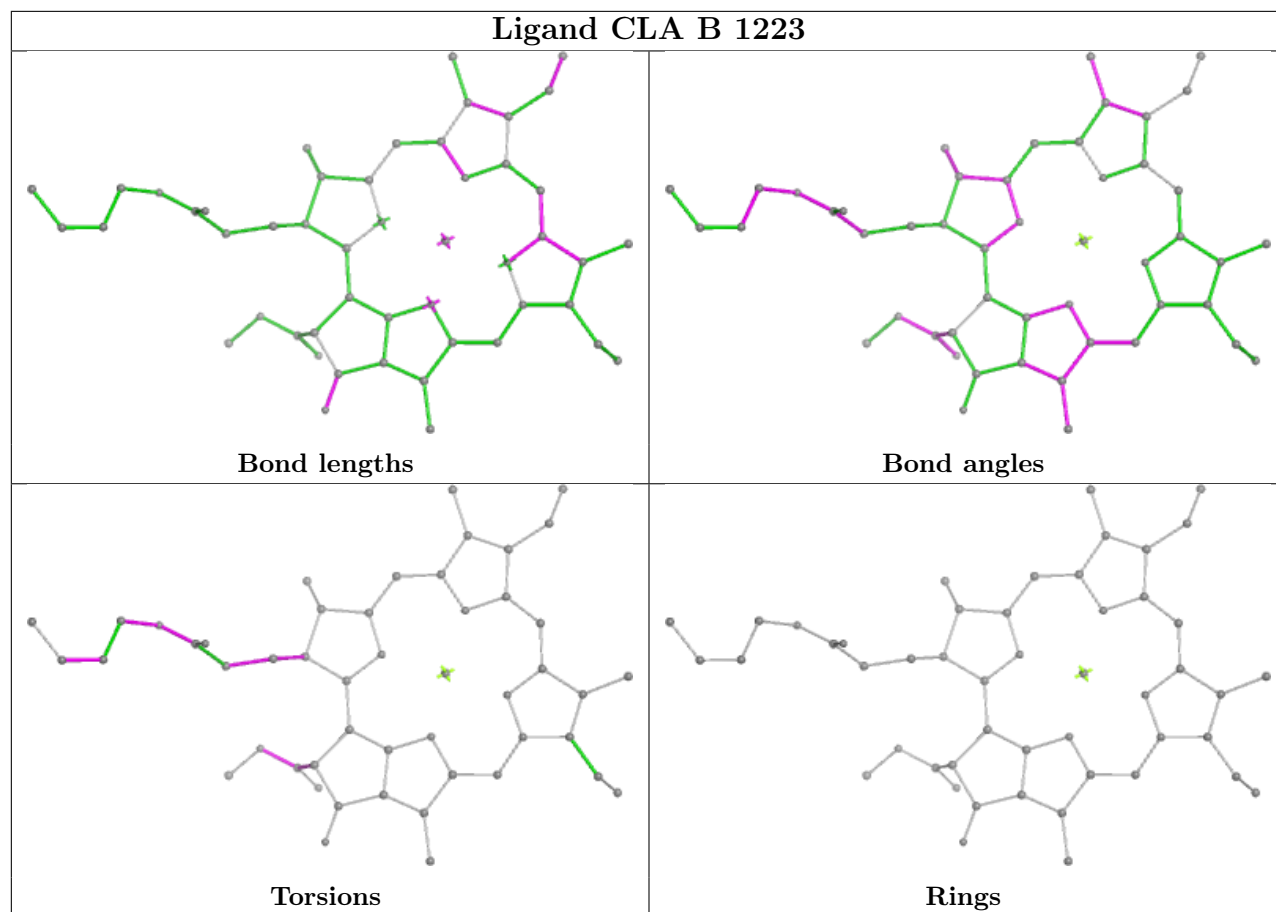


## Ligand CLA A 1123

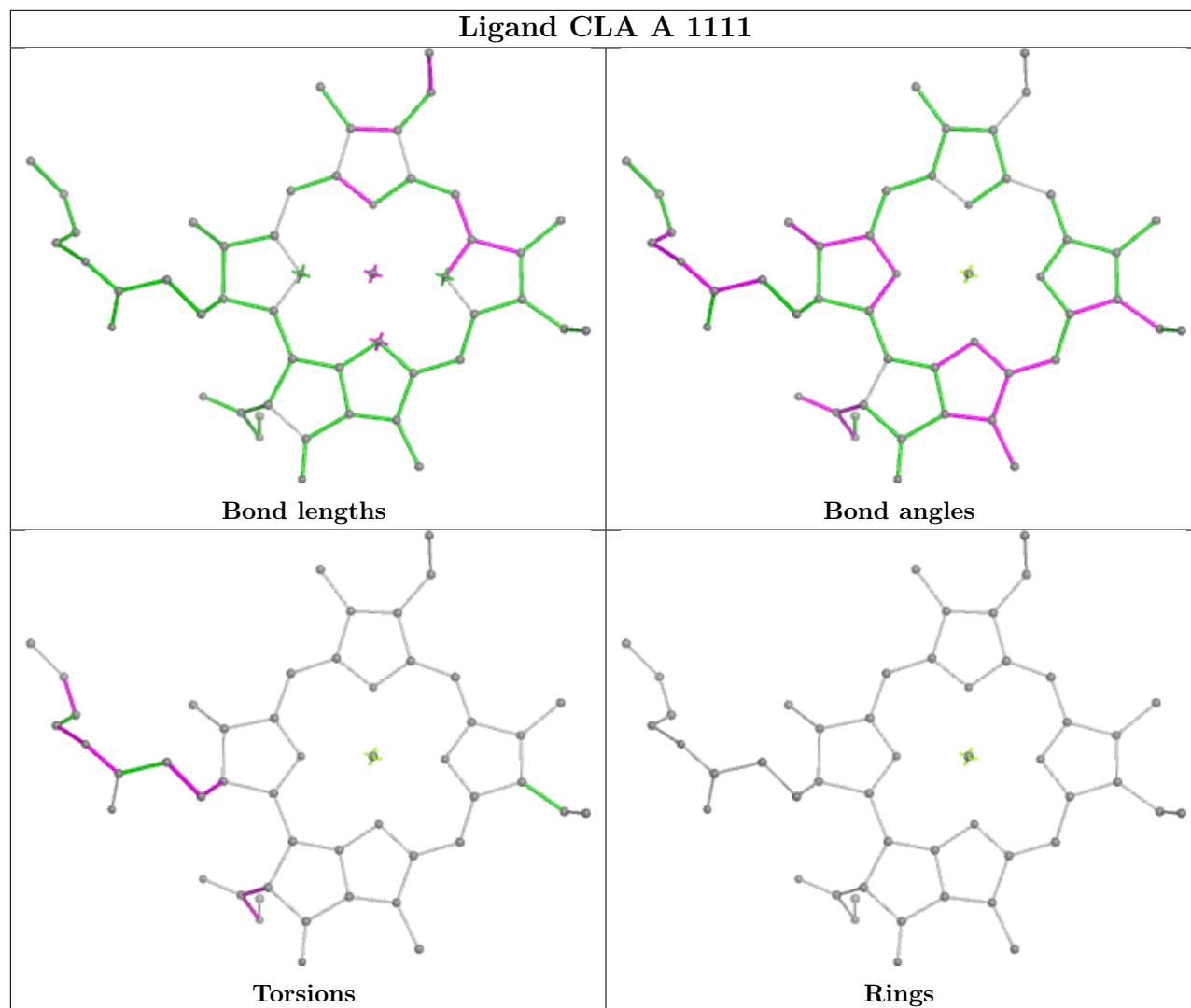


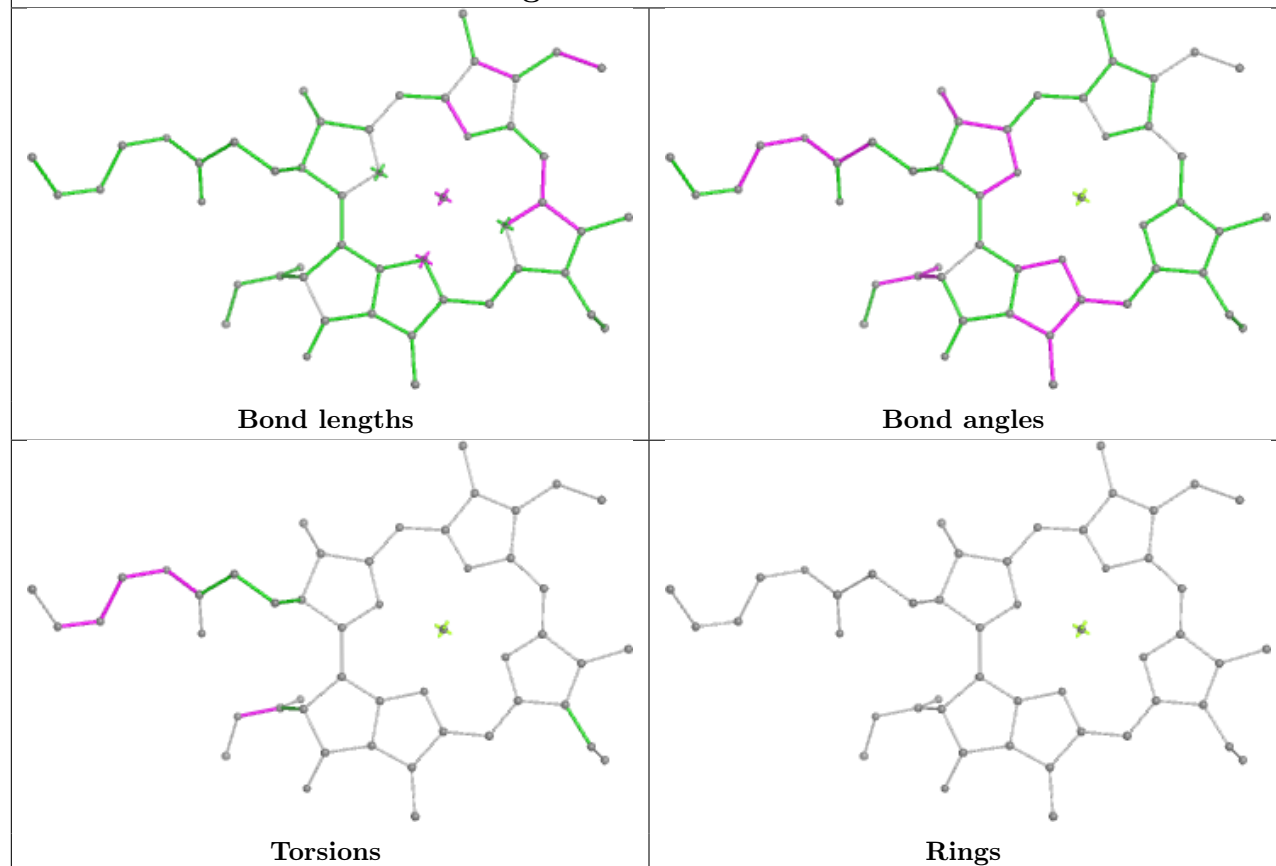
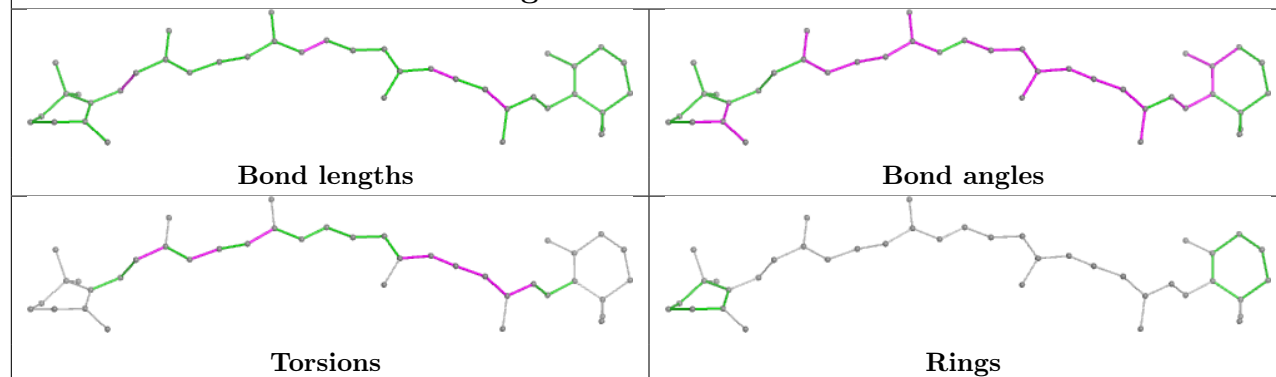
## Ligand CLA A 1137





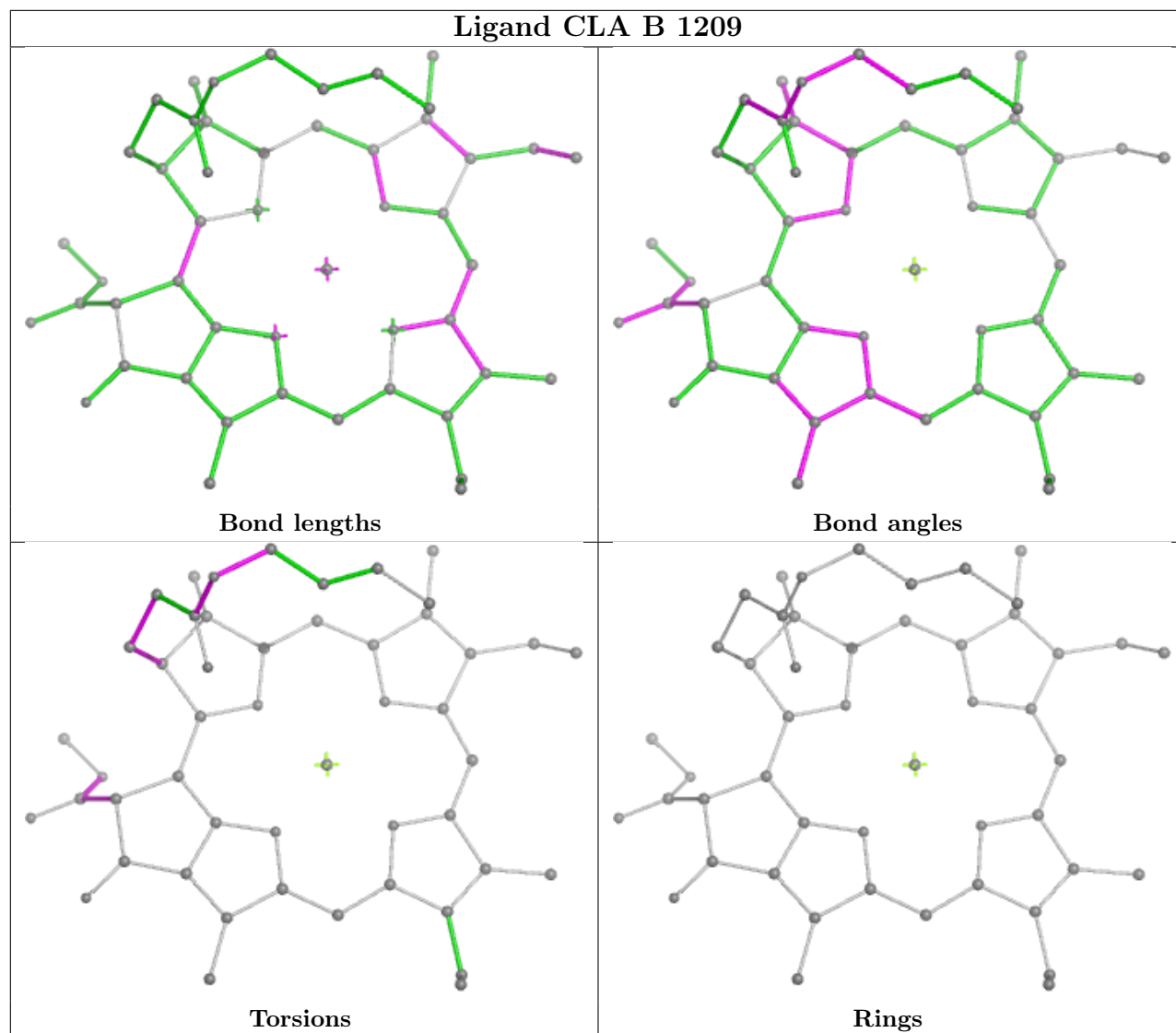
## Ligand CLA A 1111

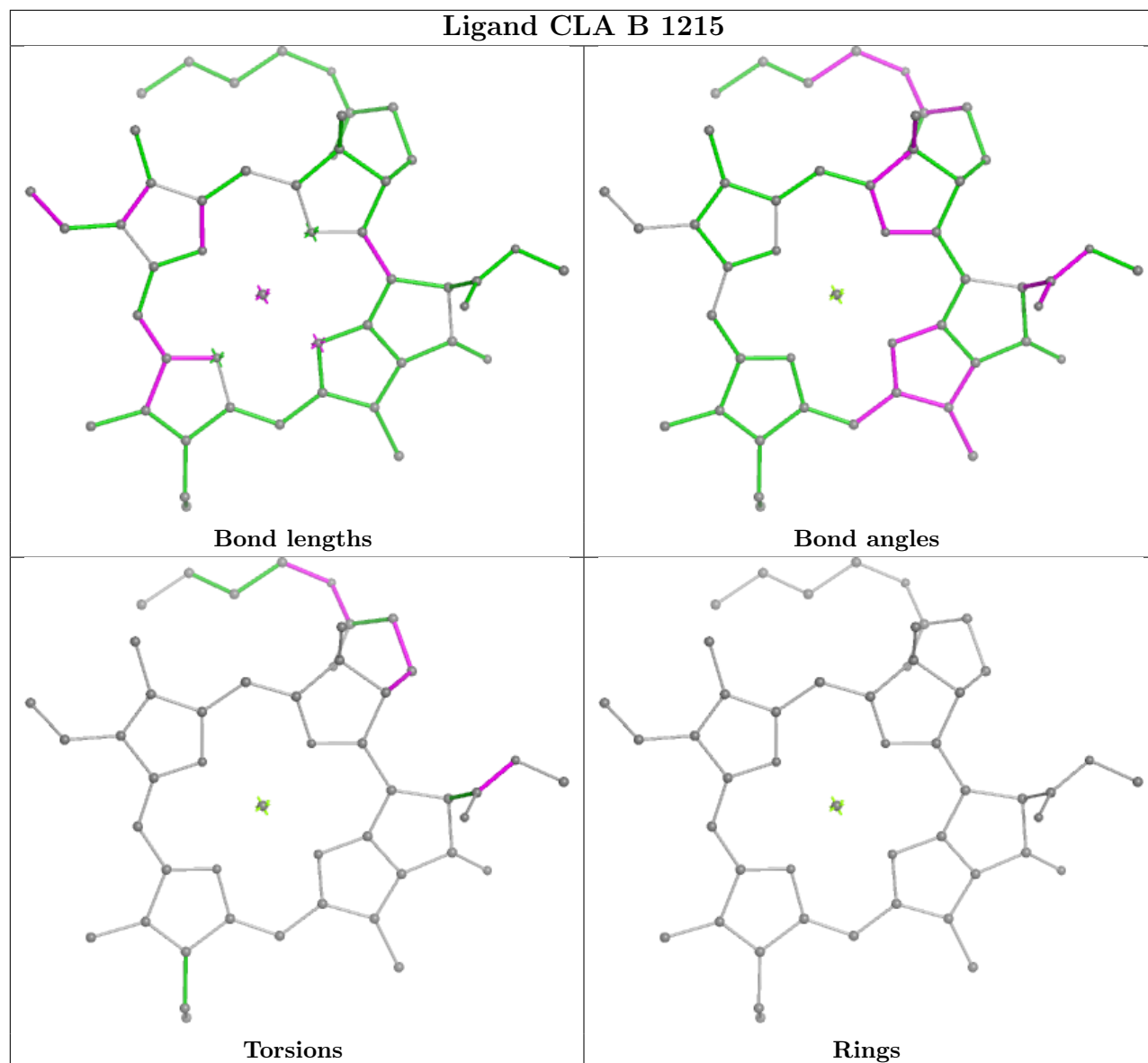


**Ligand CLA A 1131****Ligand BCR A 4001**

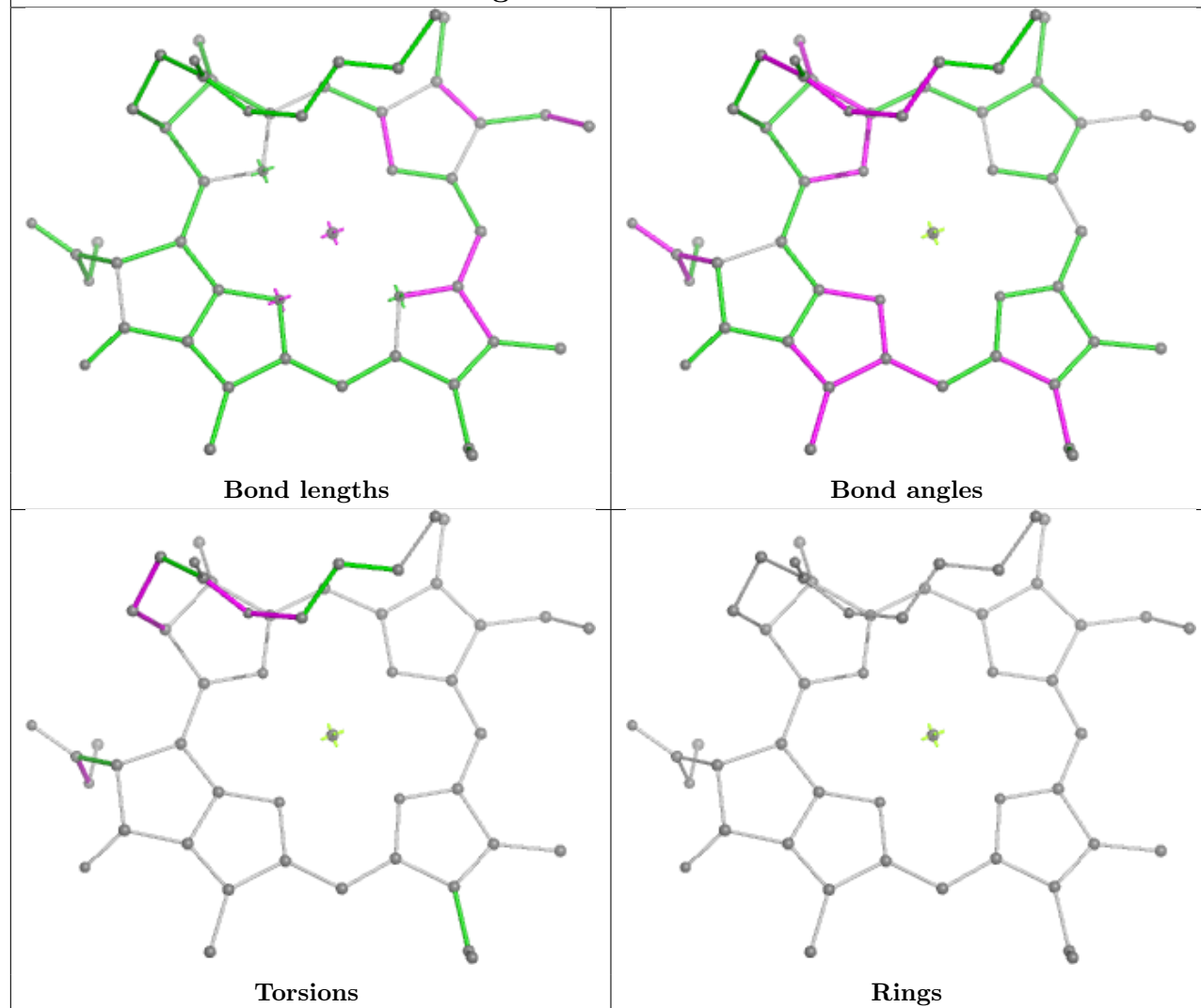


## Ligand CLA B 1209

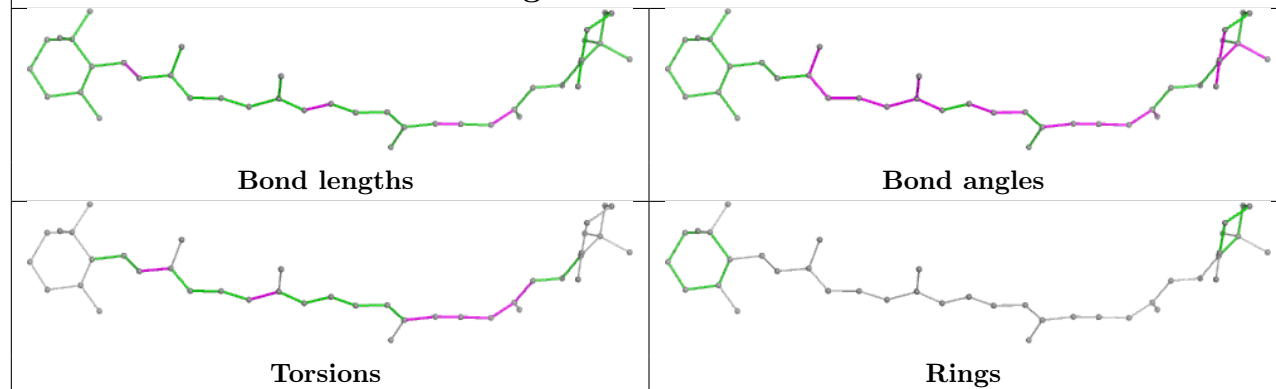




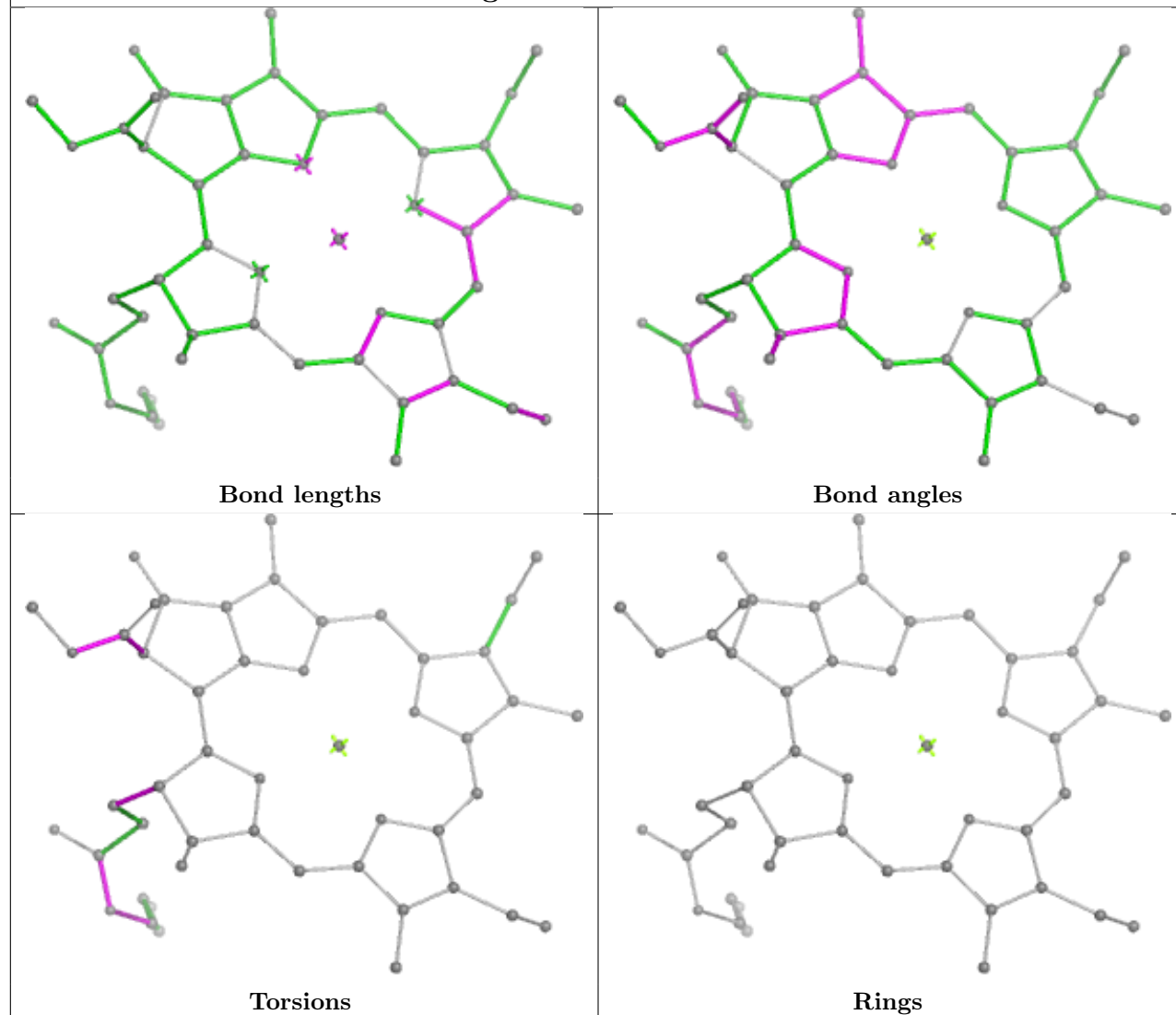
## Ligand CLA B 1217



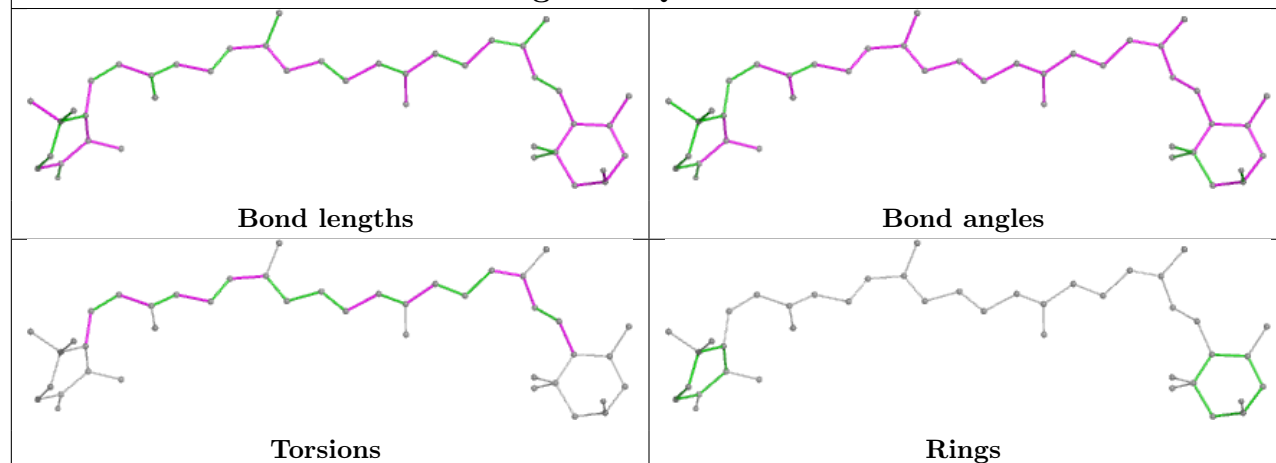
## Ligand BCR F 4014



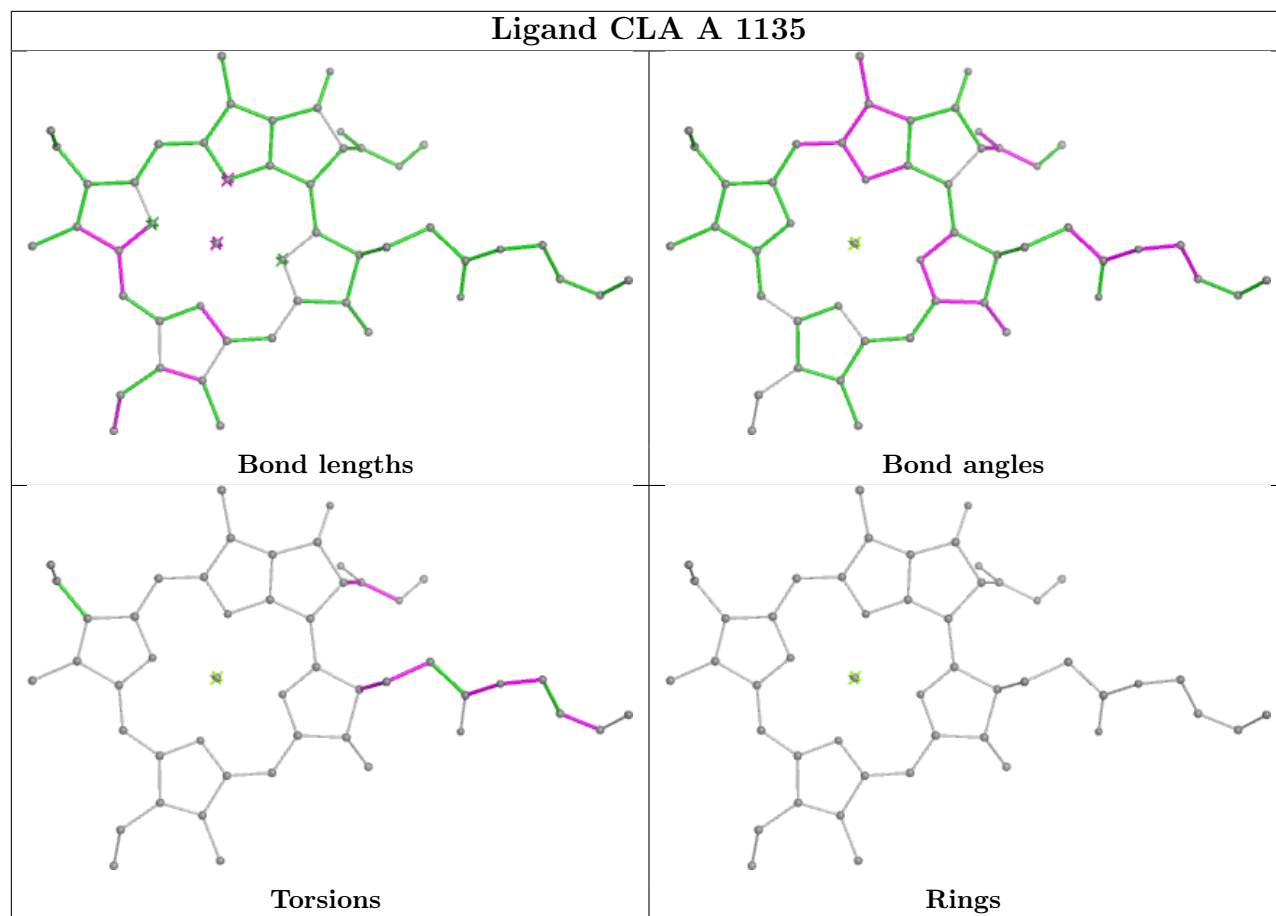
## Ligand CLA B 1212

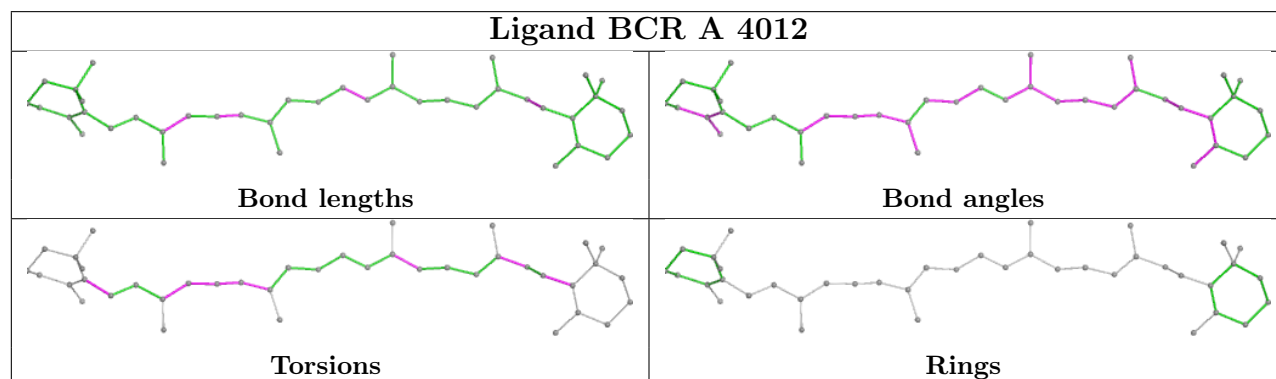
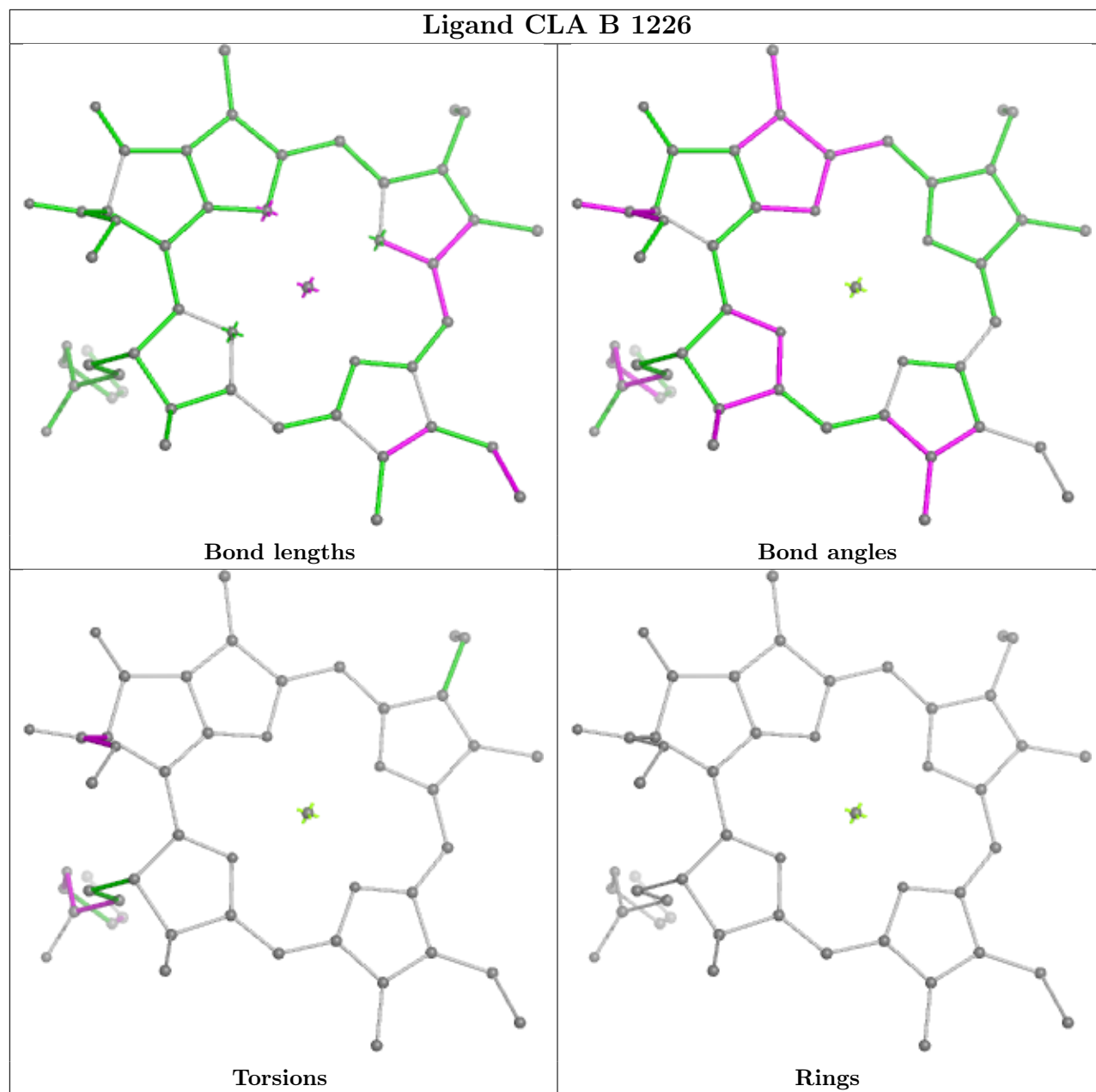


## Ligand EQ3 I 4020

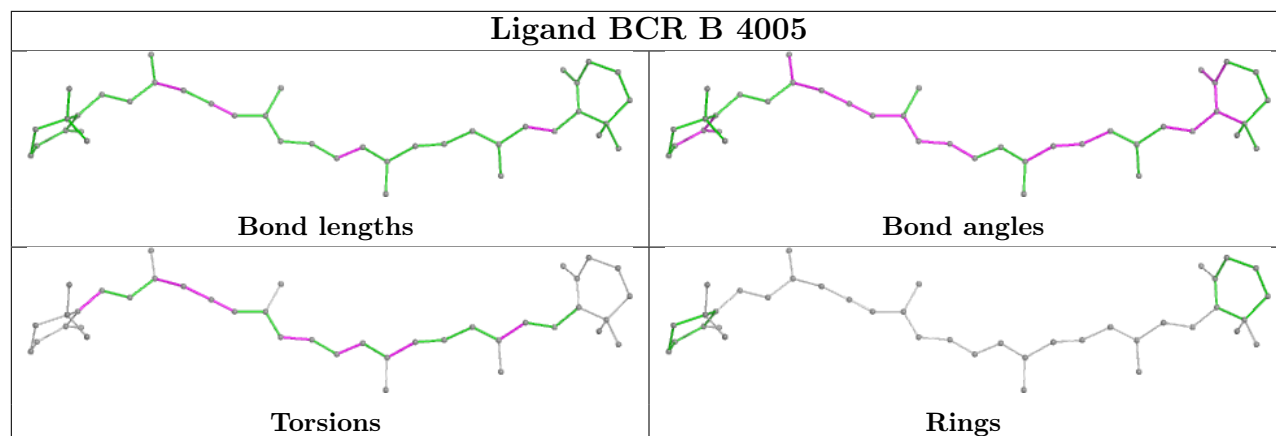


## Ligand CLA A 1135

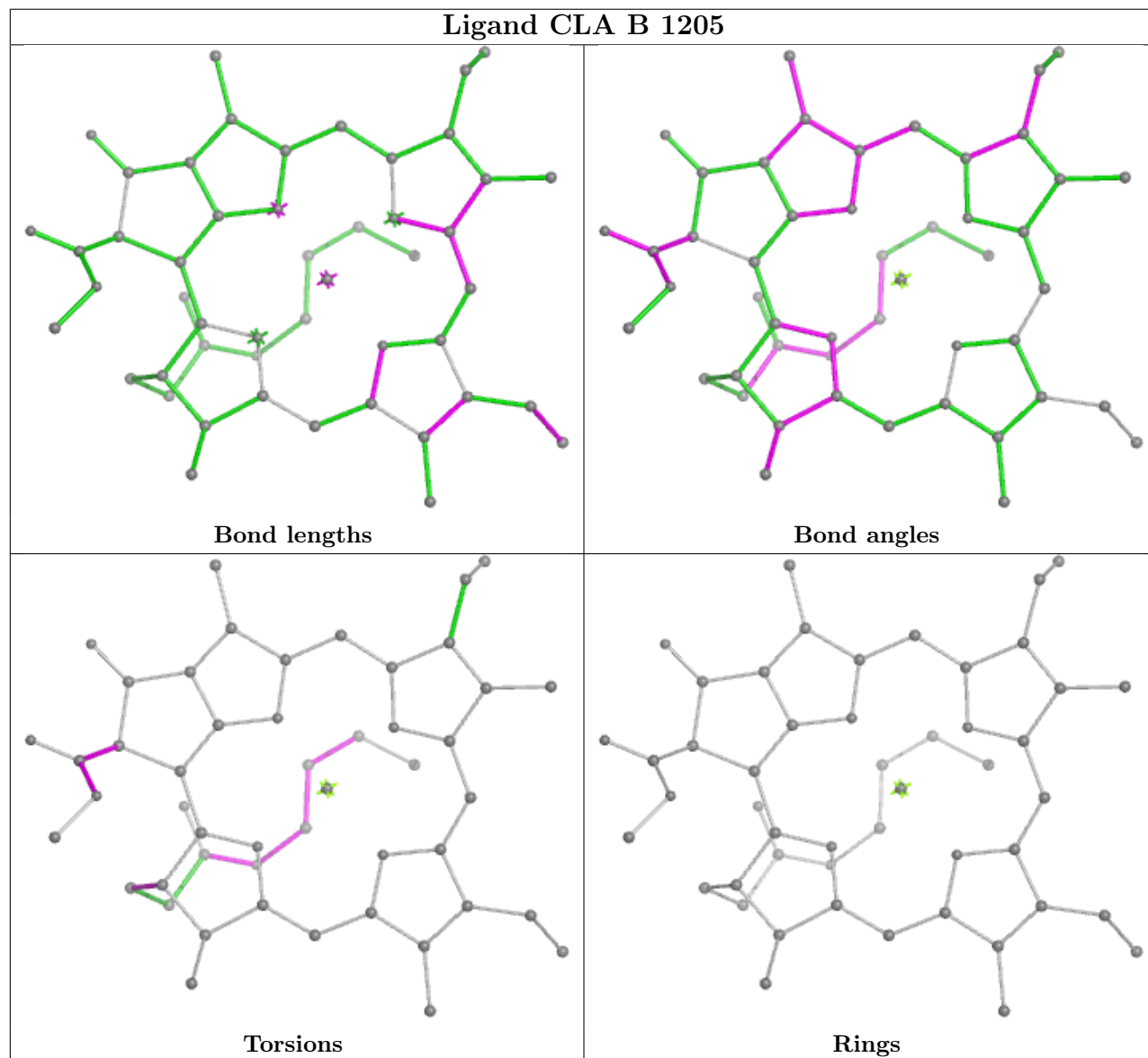


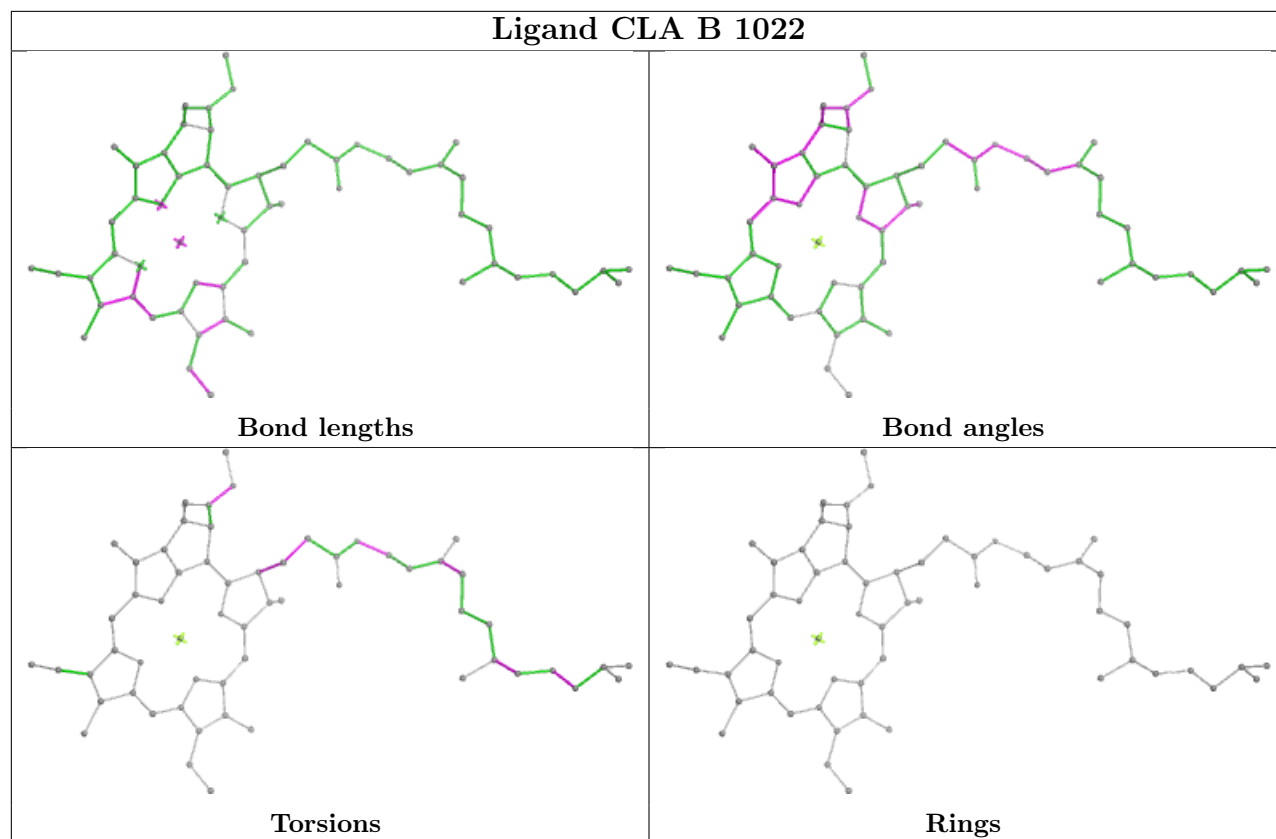


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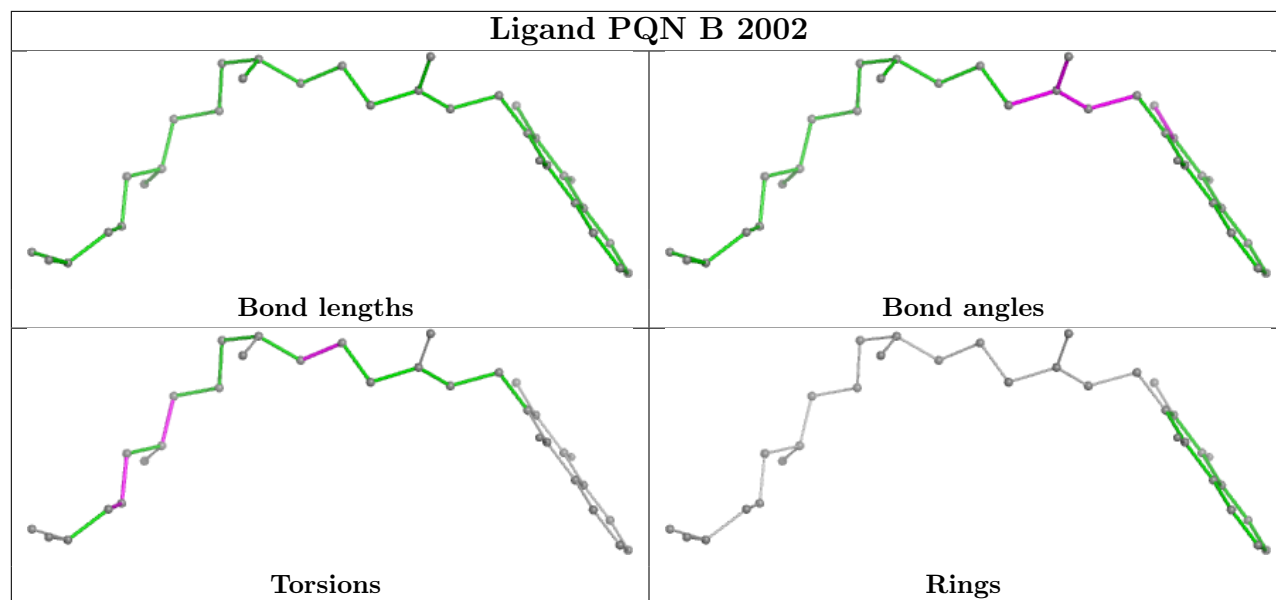
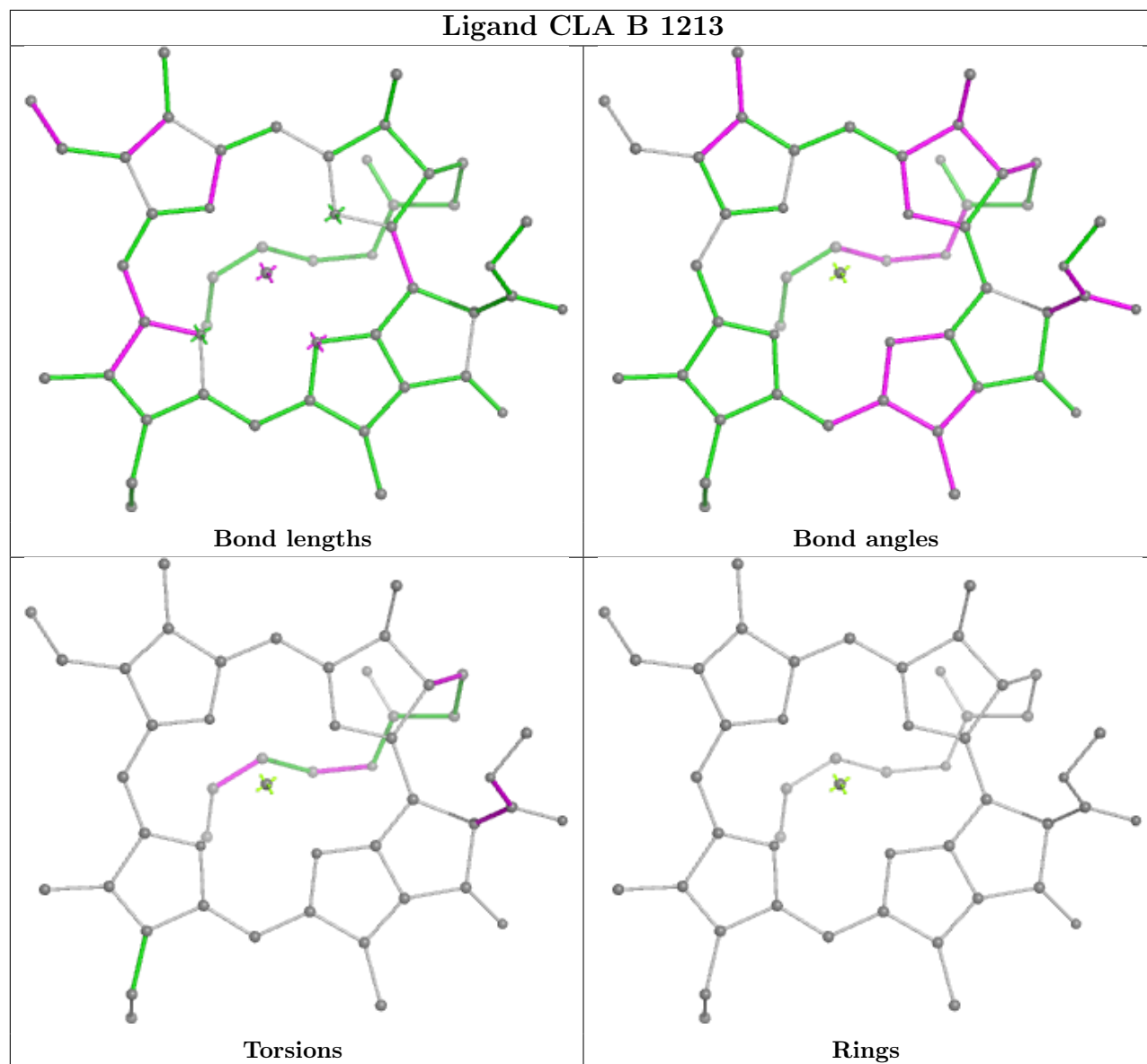


## Ligand CLA B 1205

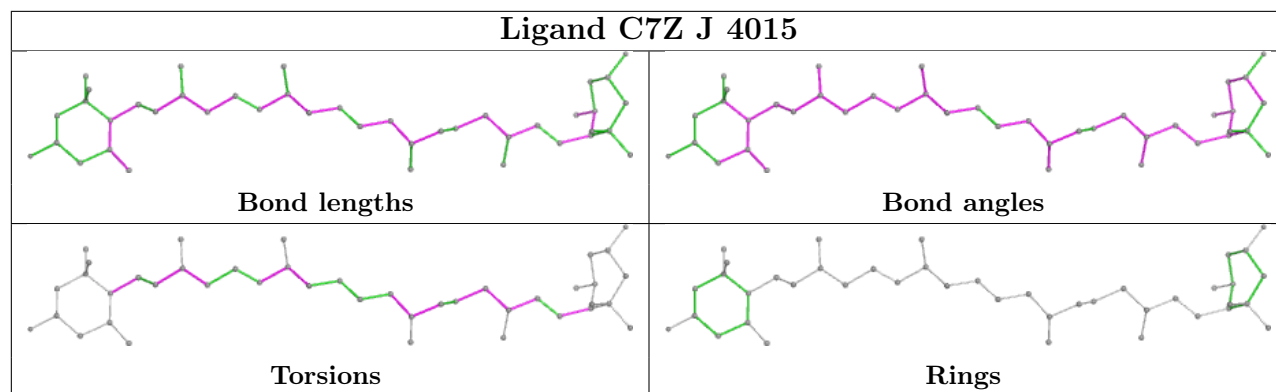




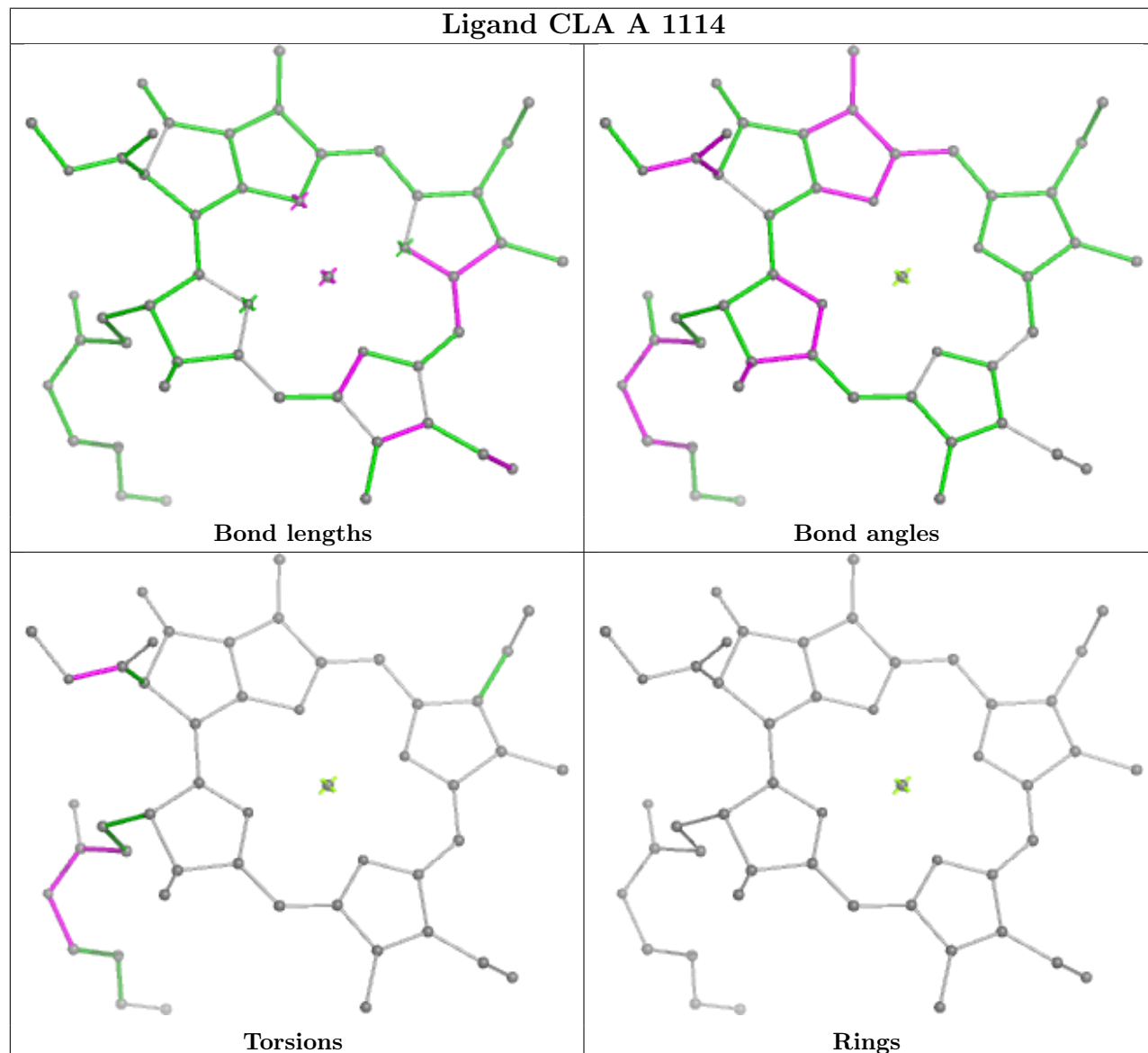


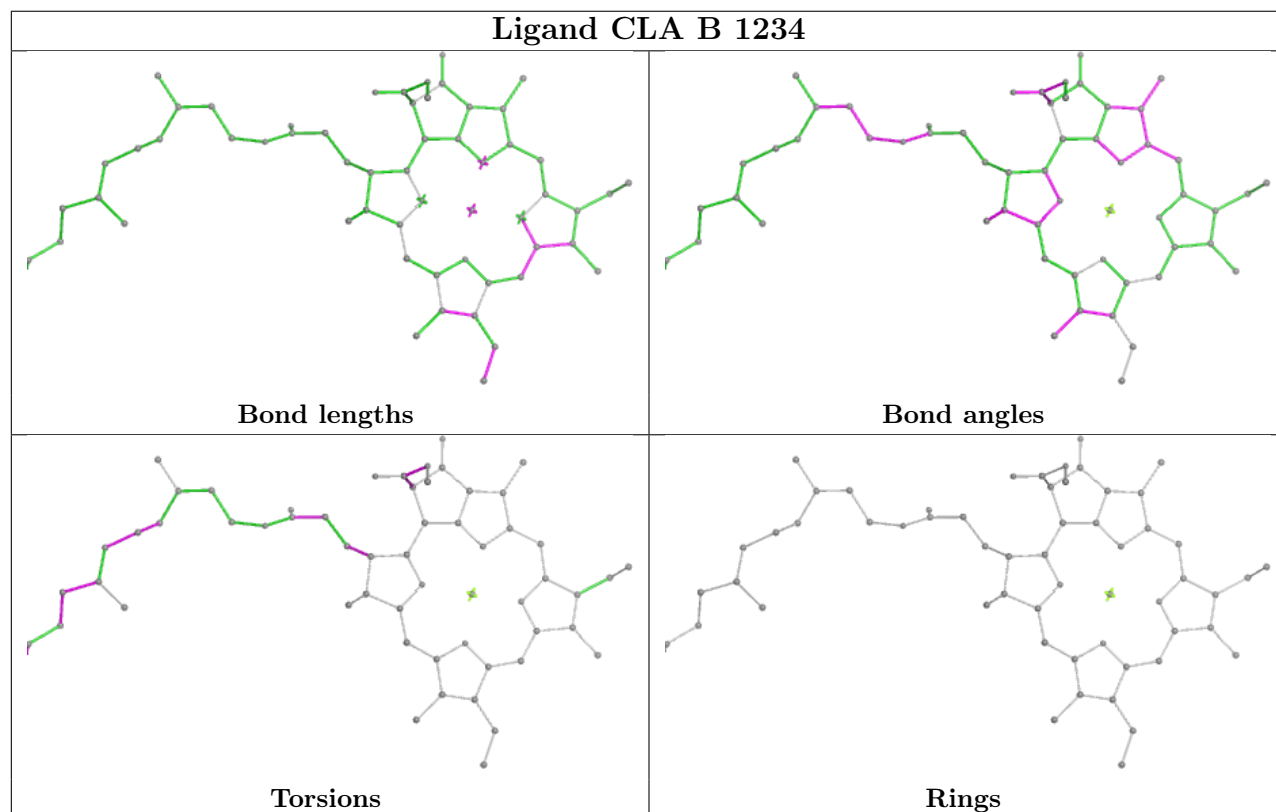
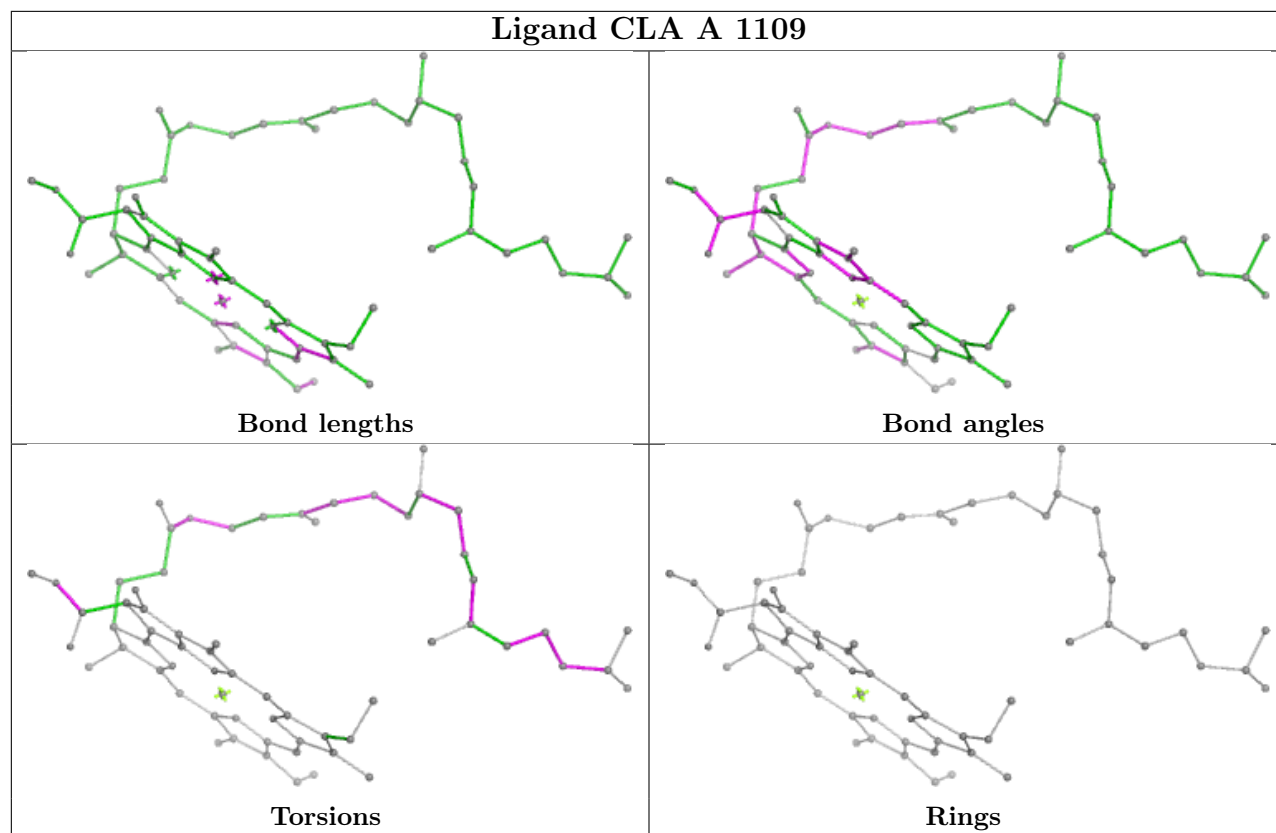


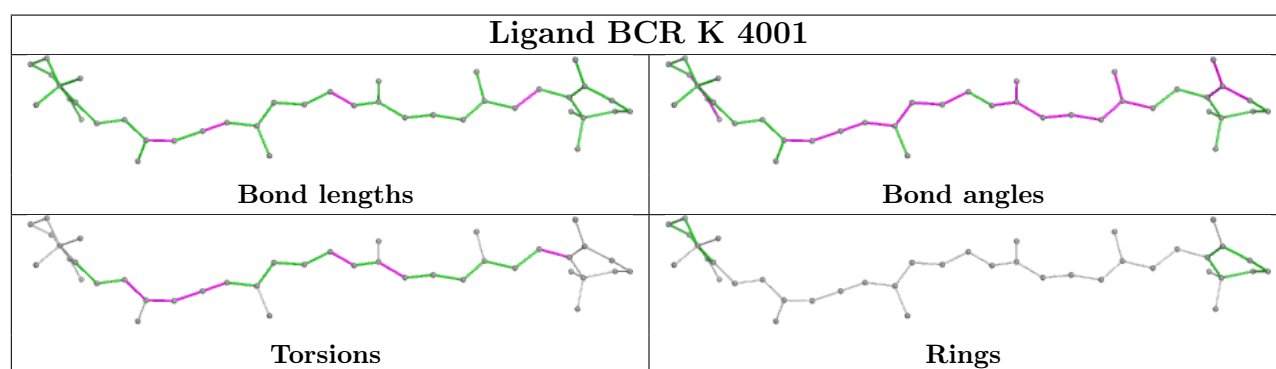
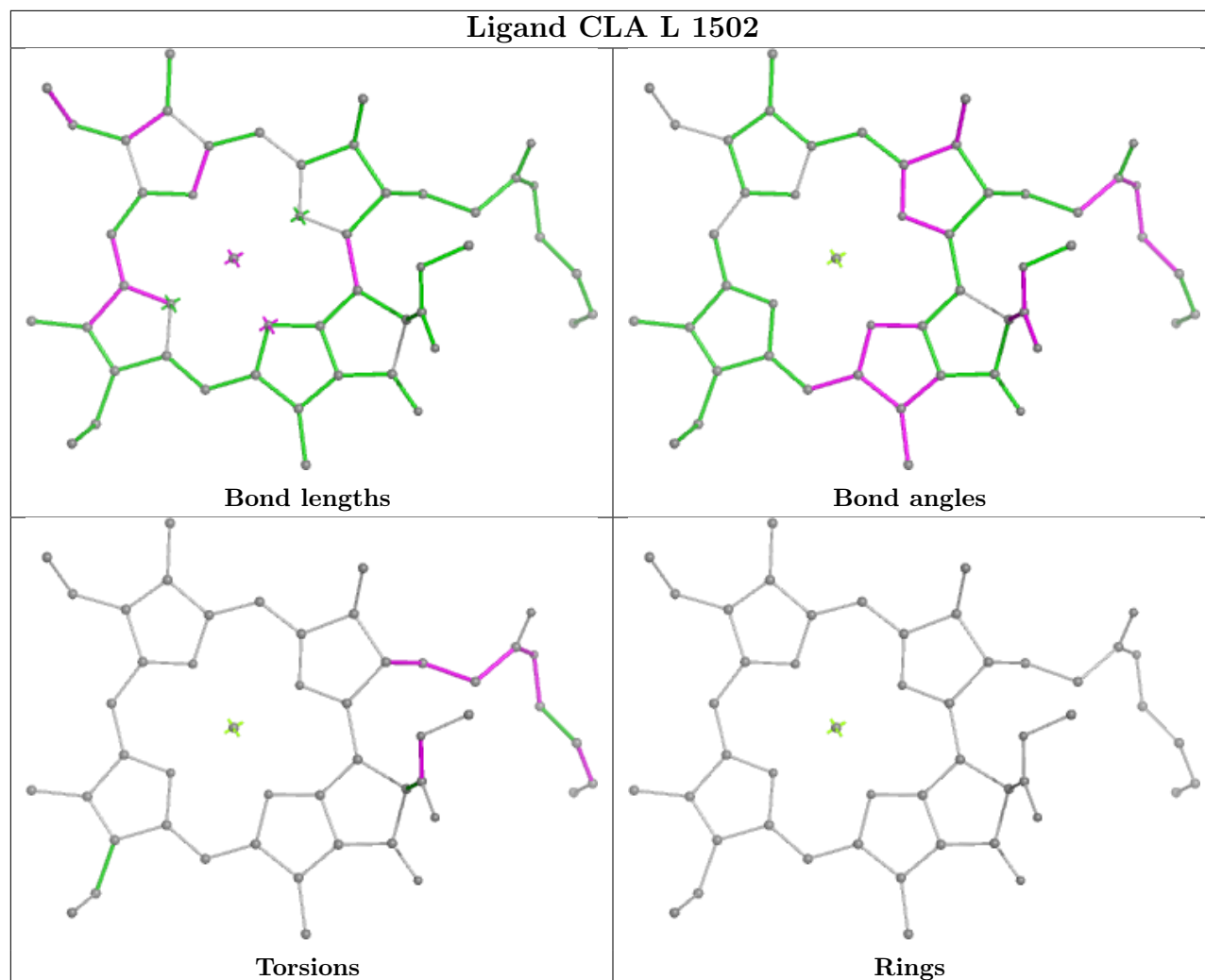
## Ligand C7Z J 4015

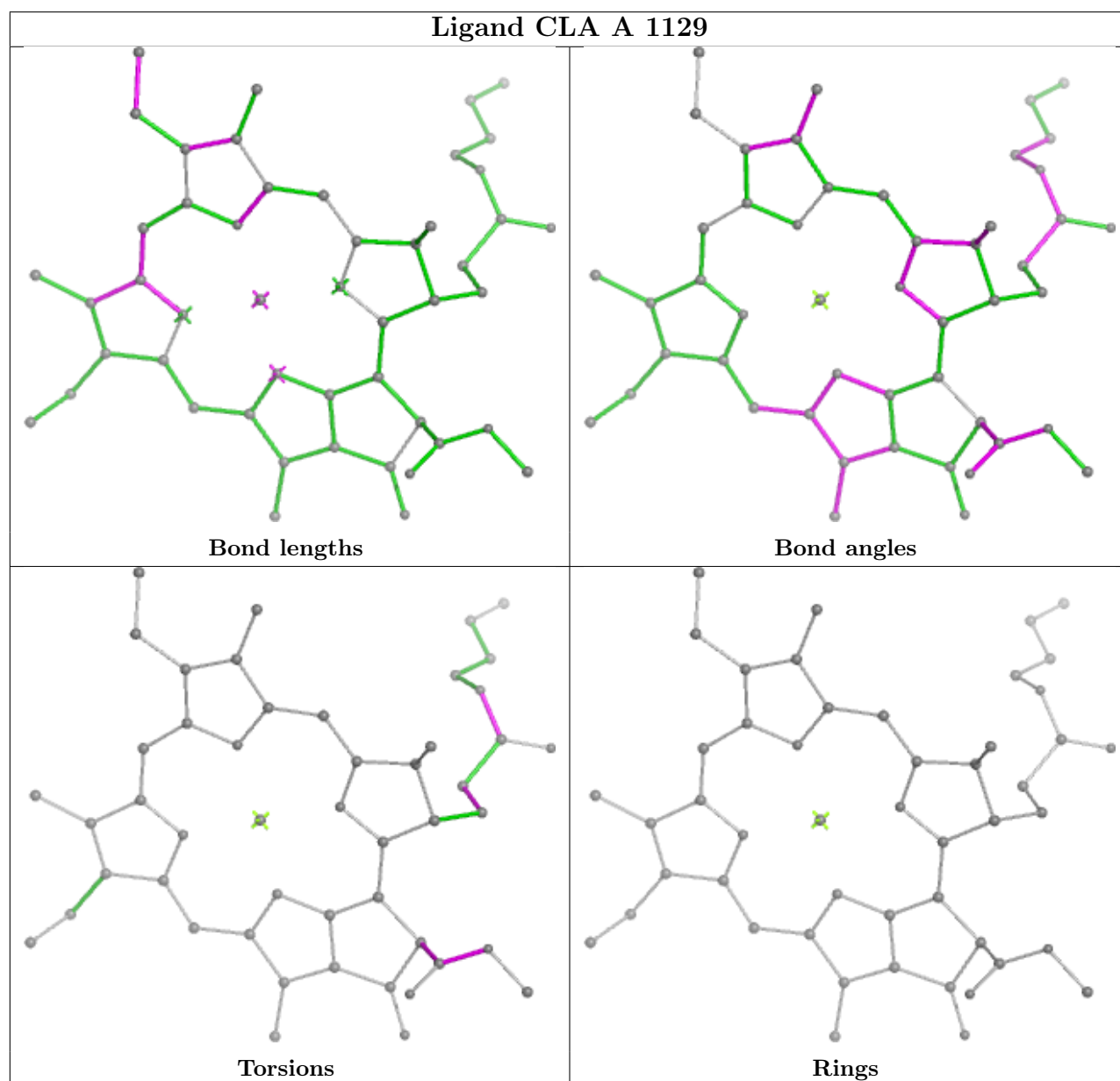
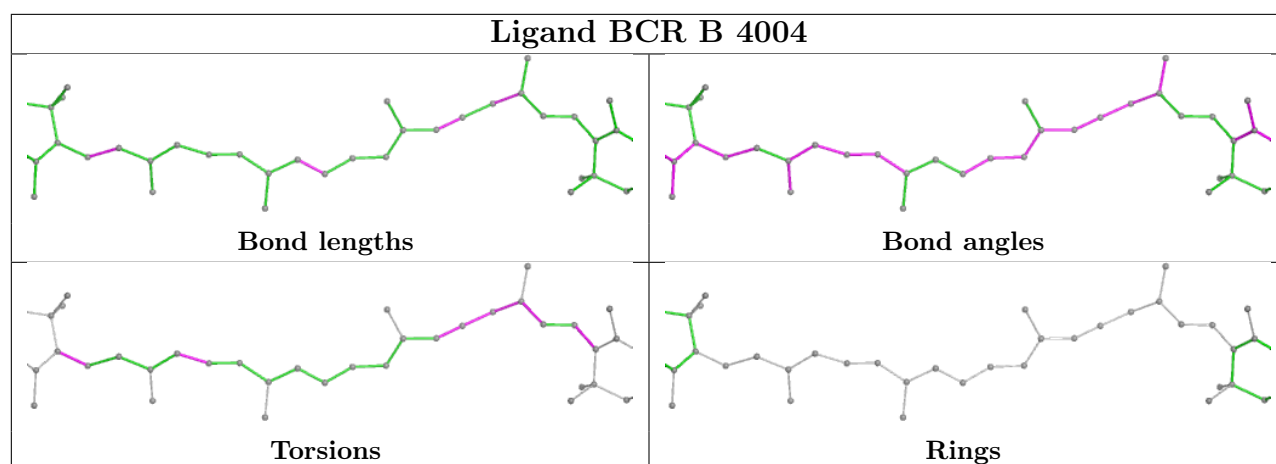


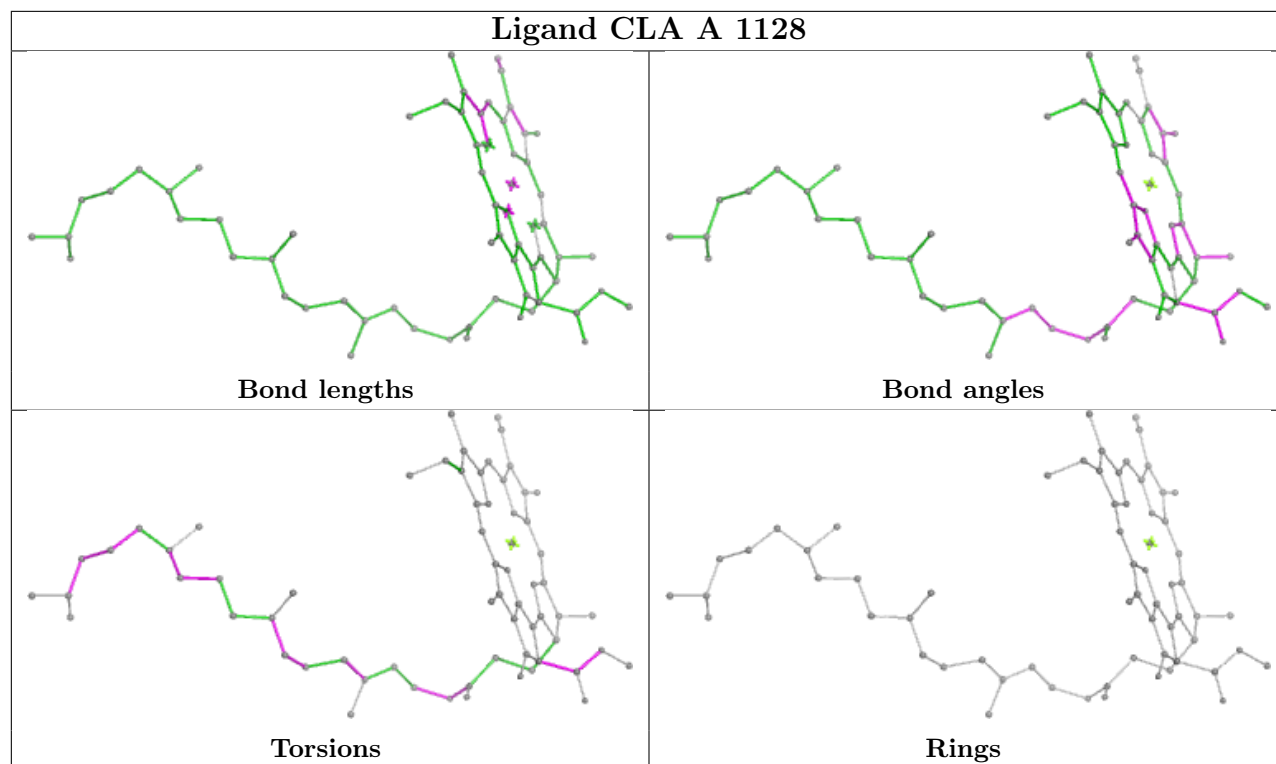
## Ligand CLA A 1114



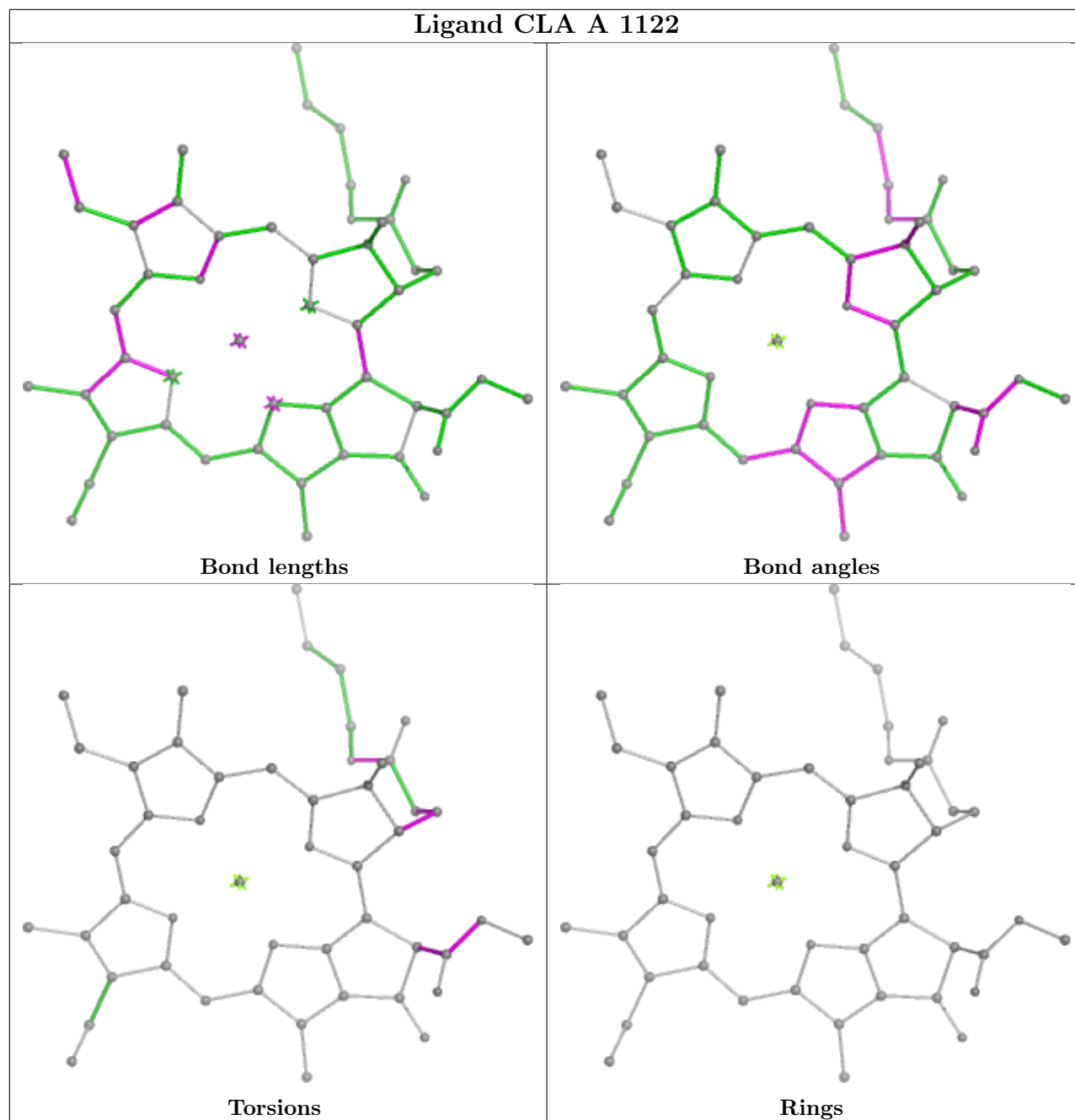


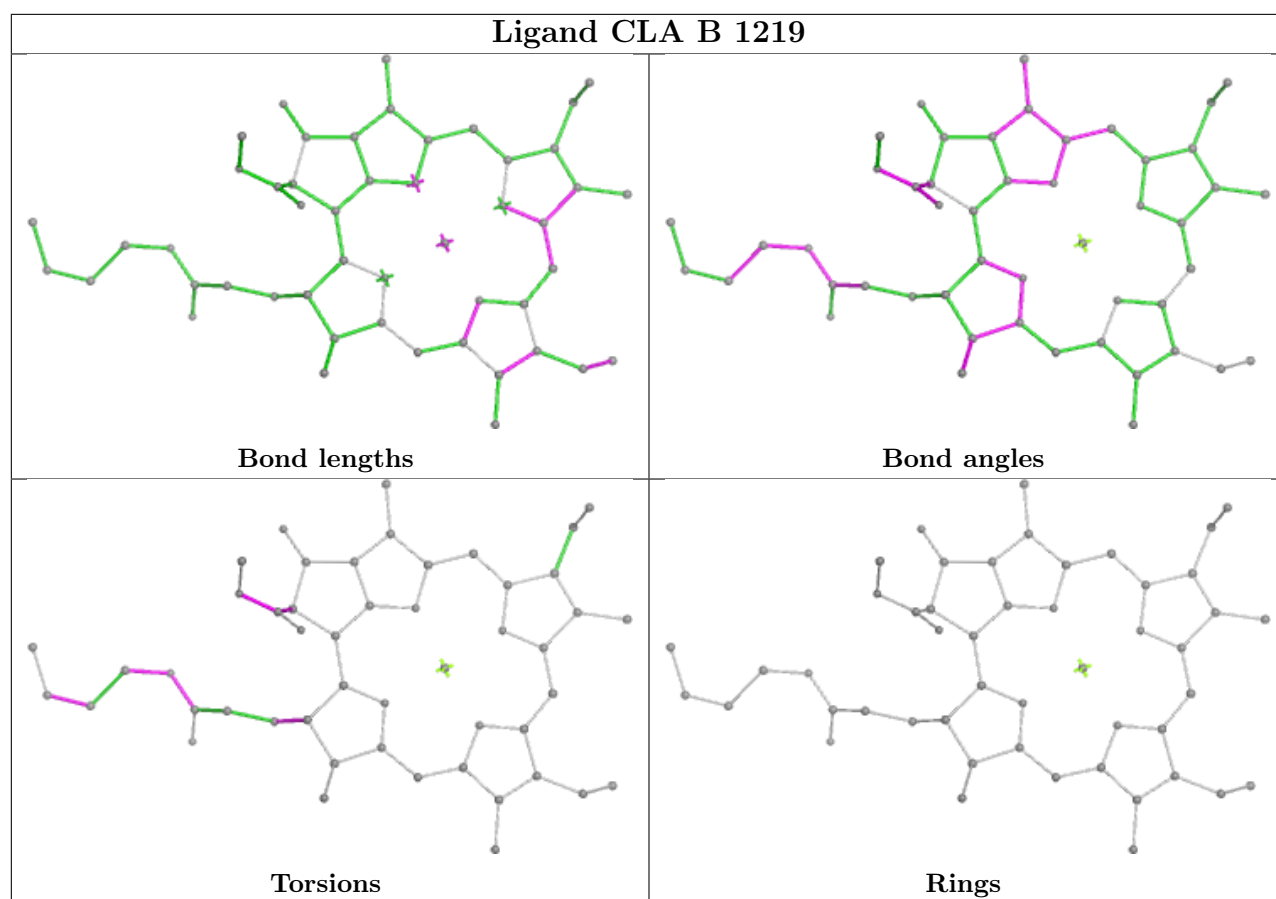




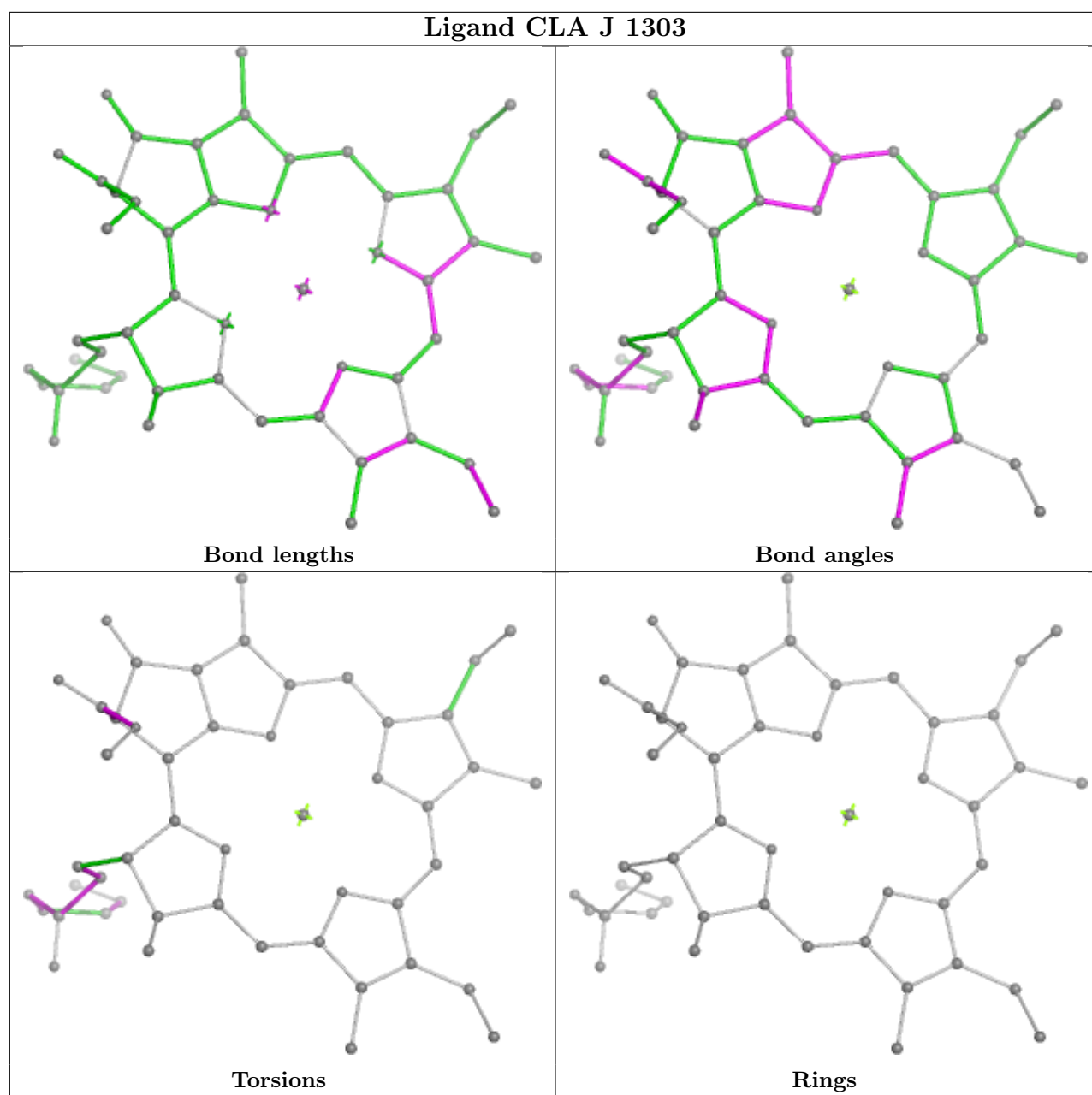


## Ligand CLA A 1122

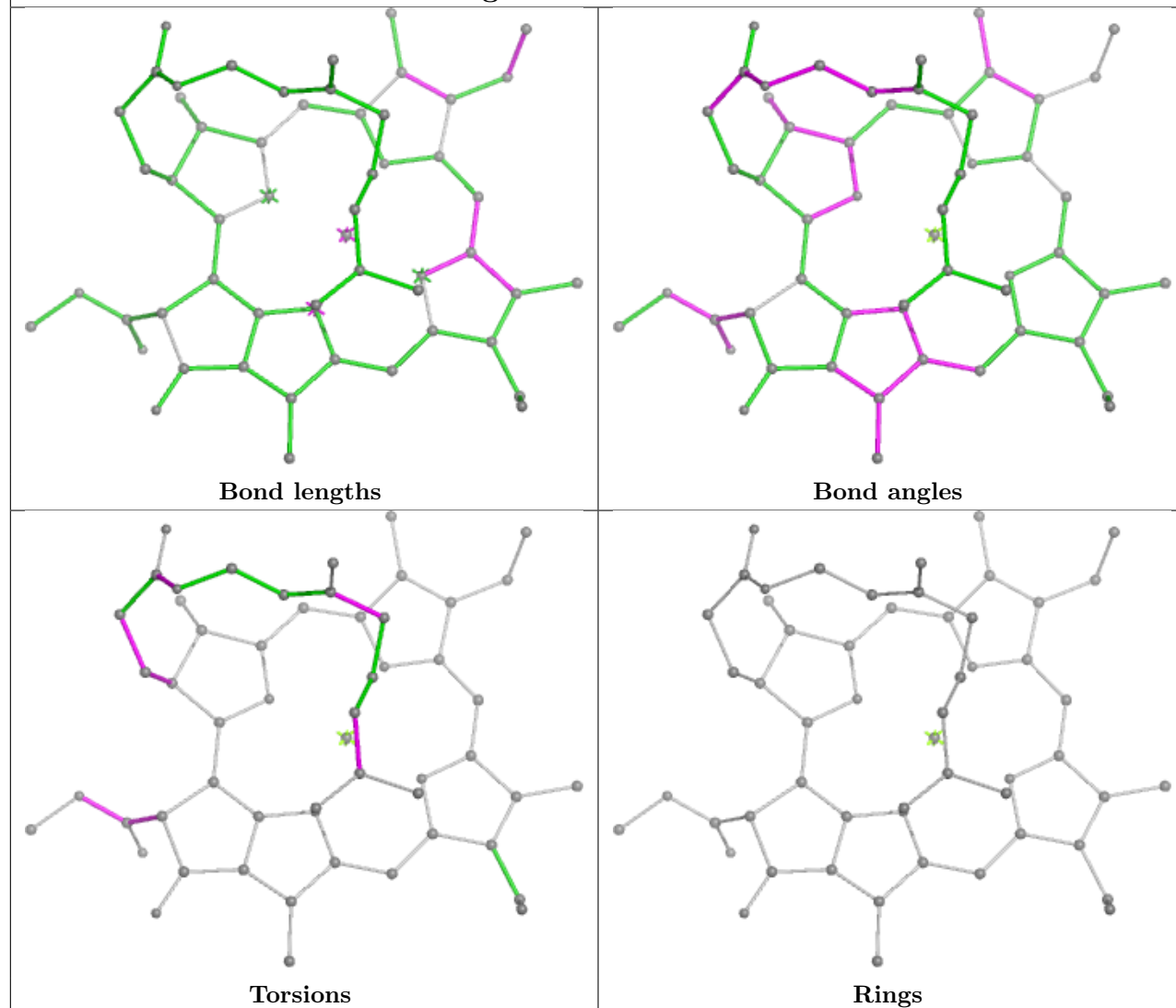




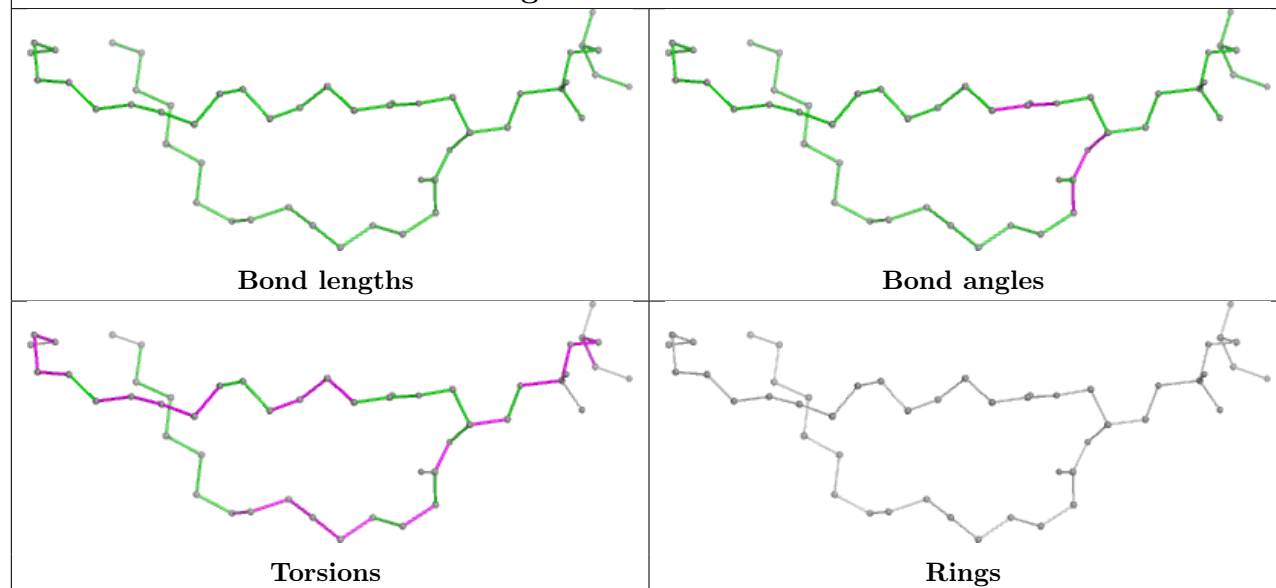


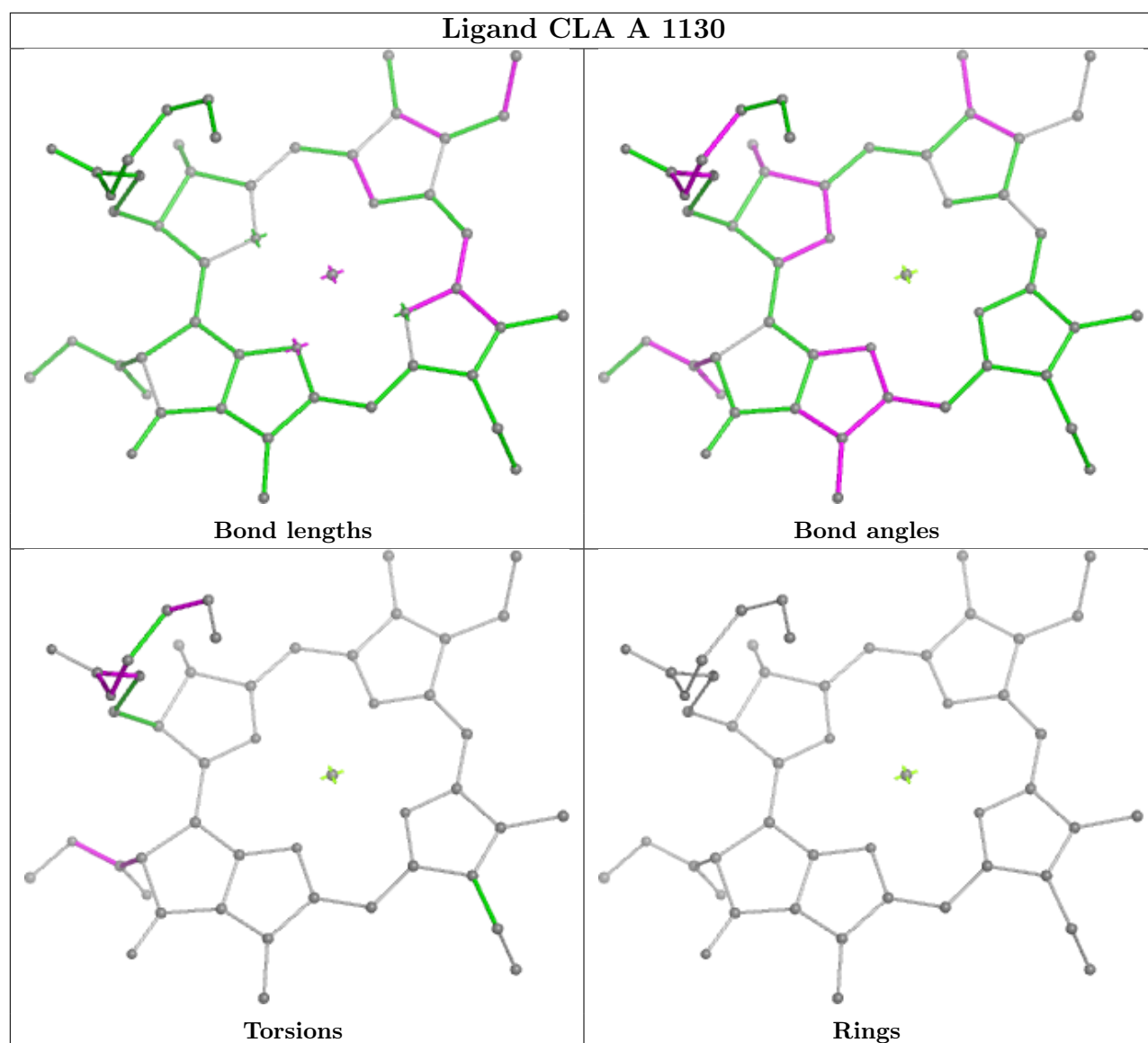


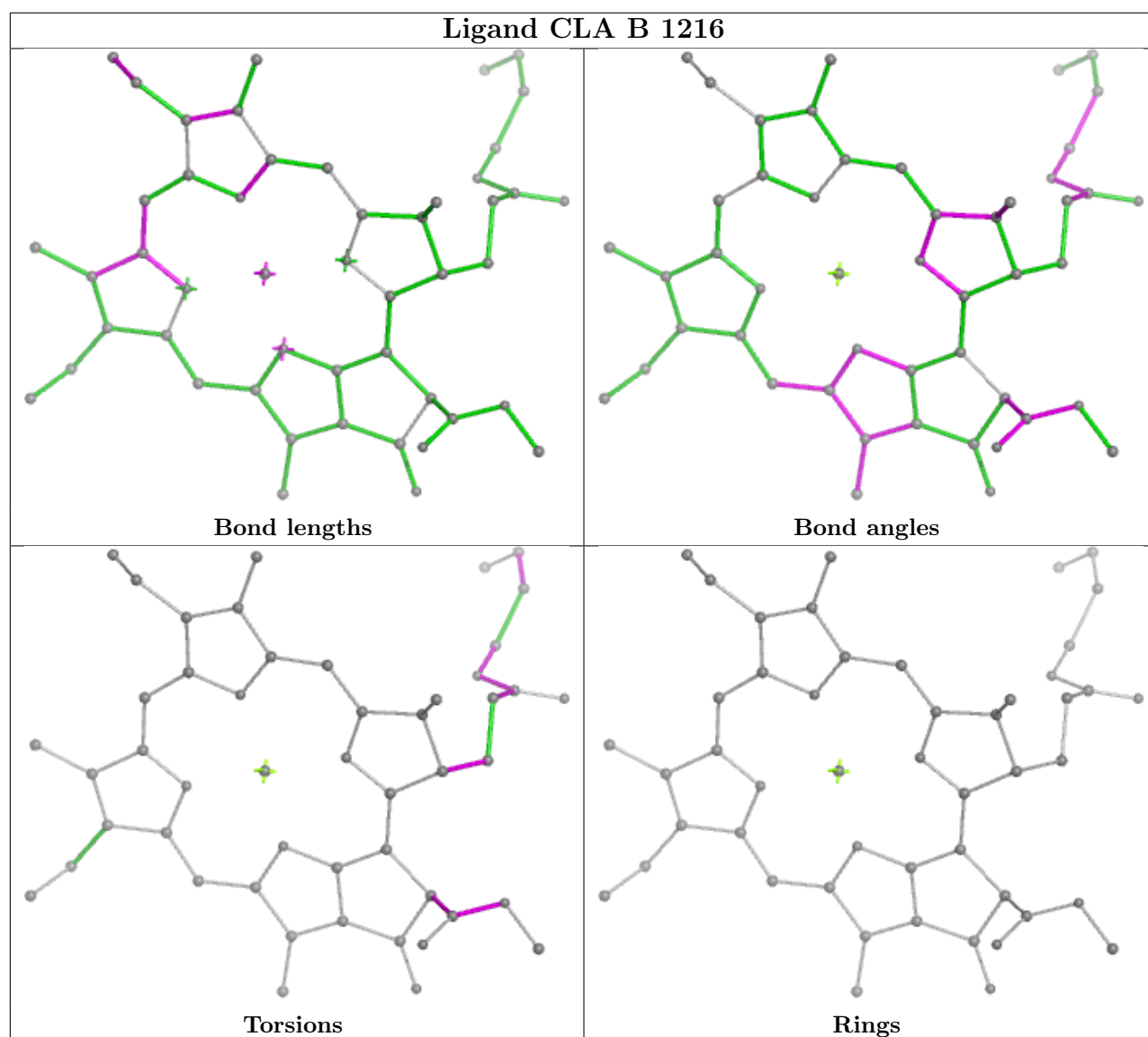
## Ligand CLA B 1224



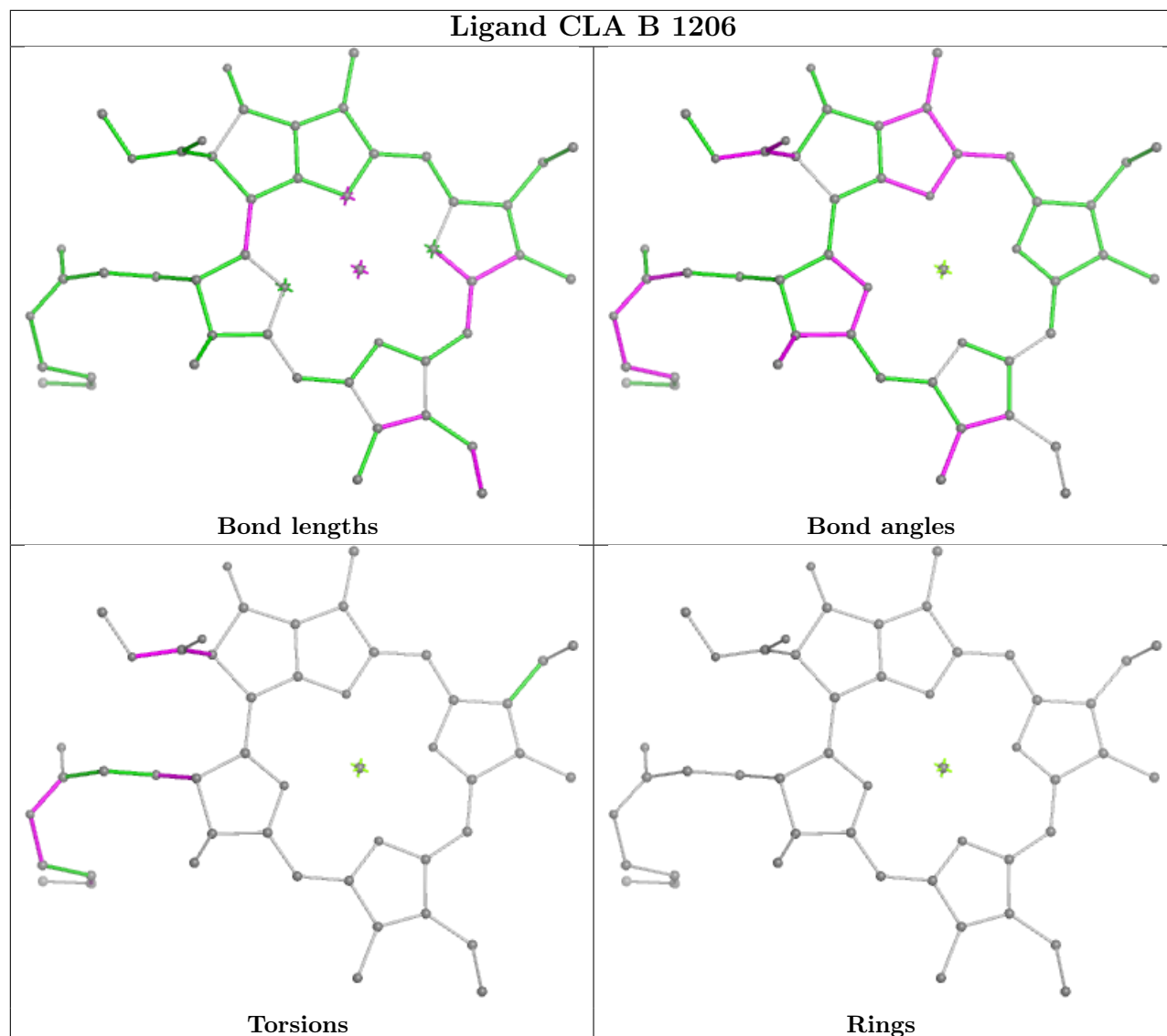
## Ligand LHG A 5003

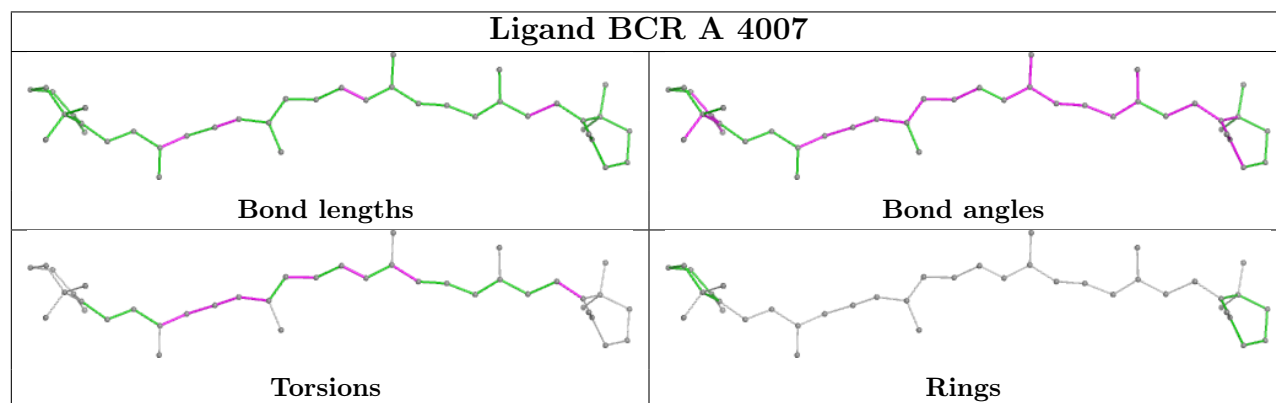
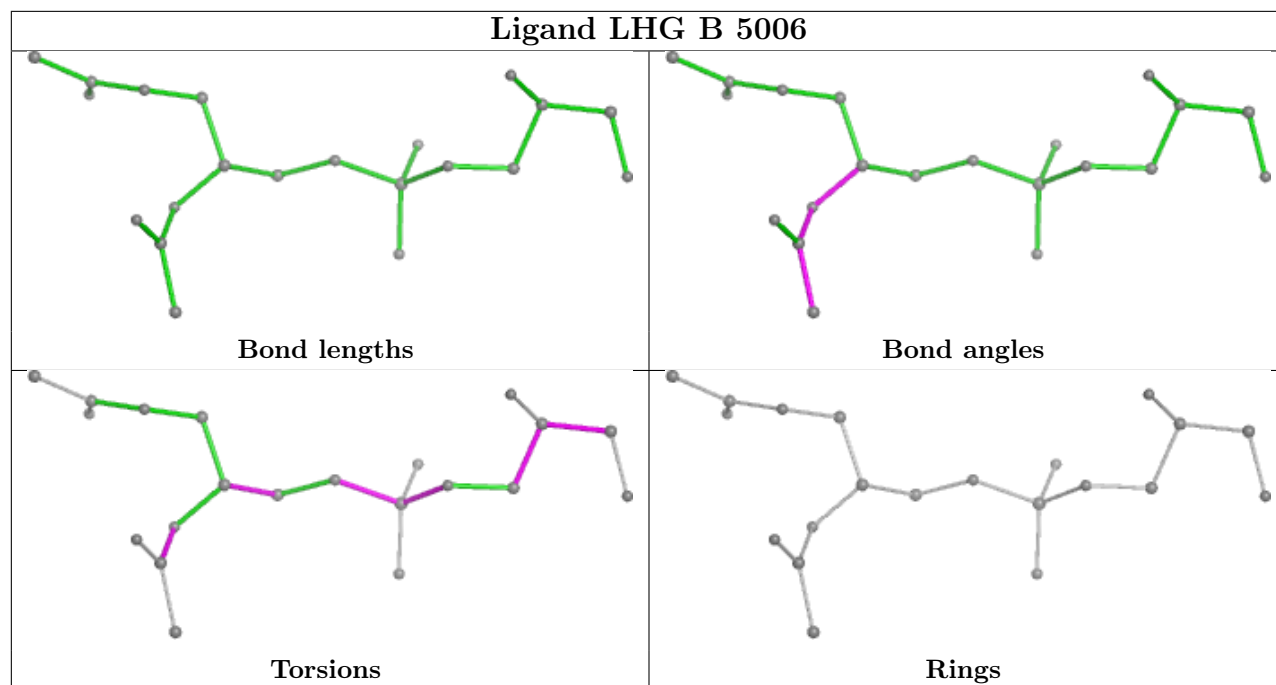




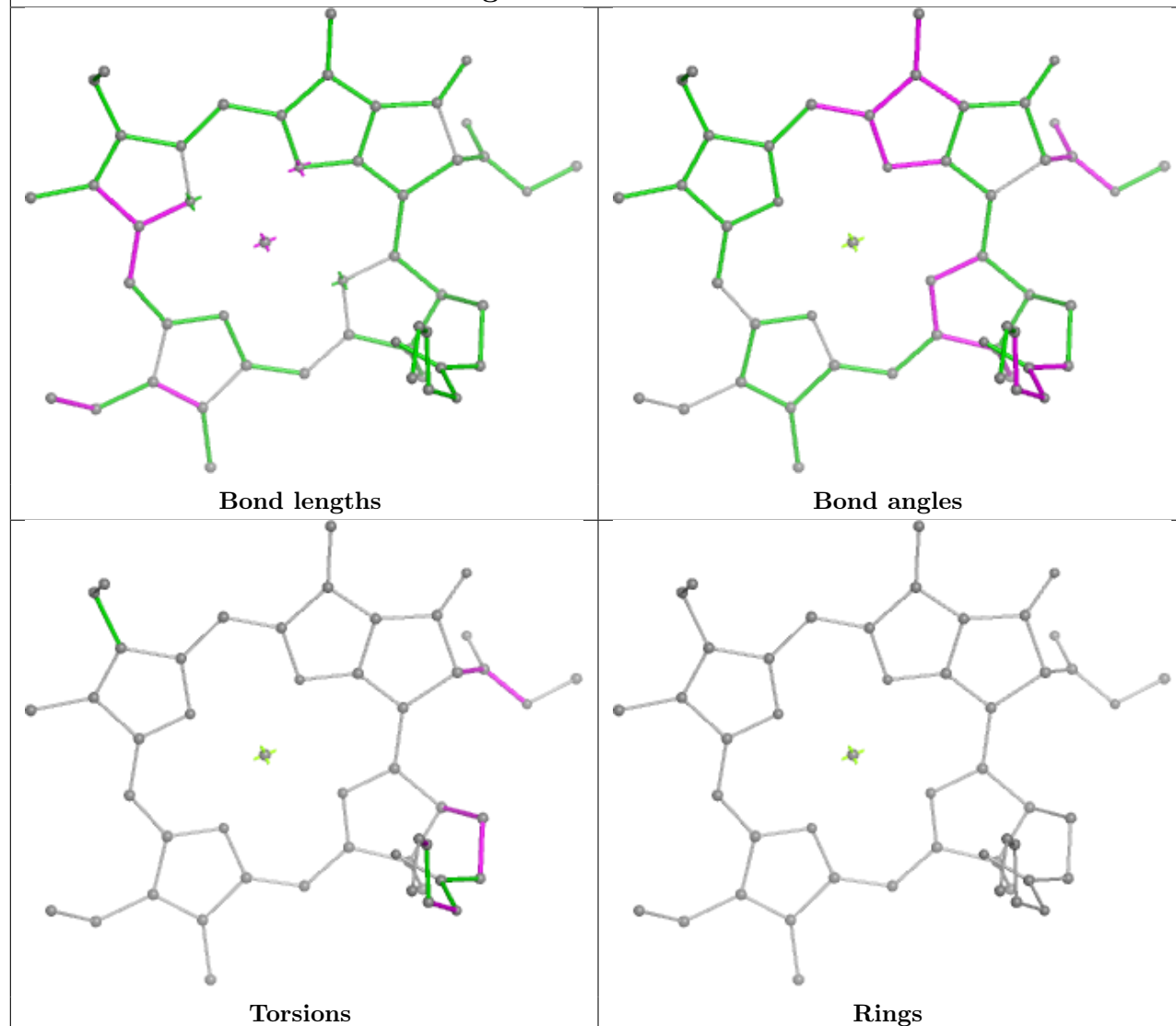


## Ligand CLA B 1206

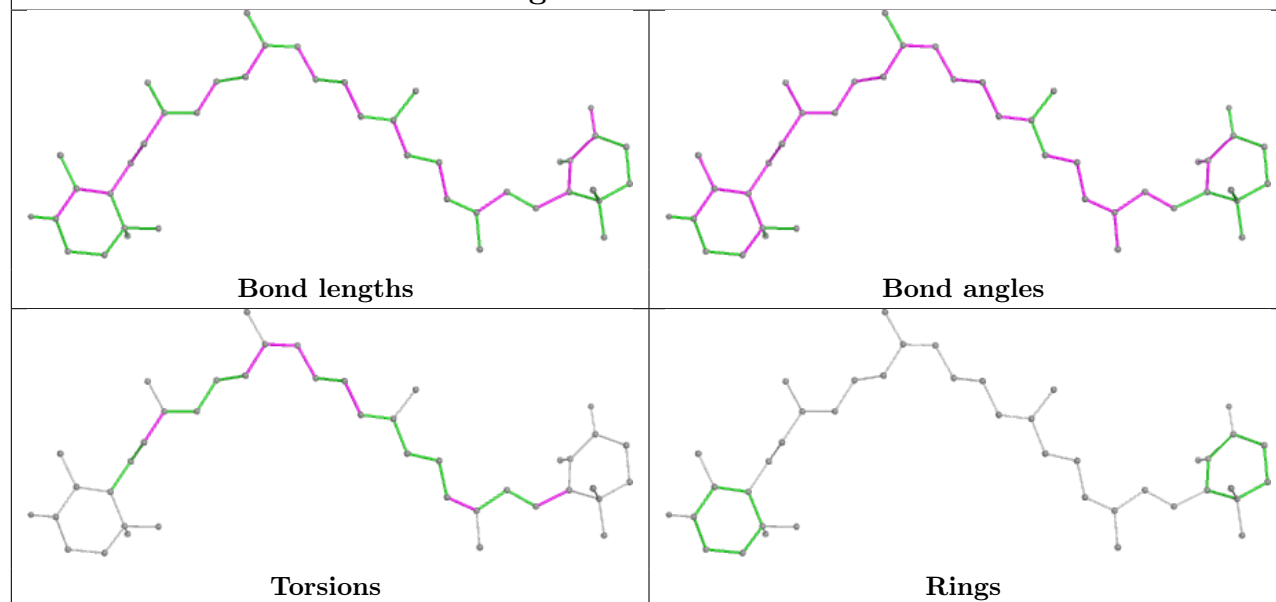




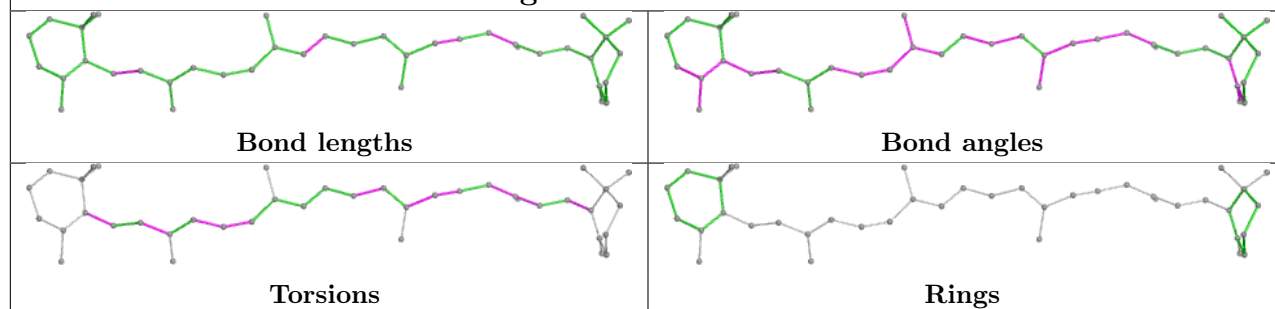
## Ligand CLA B 1225



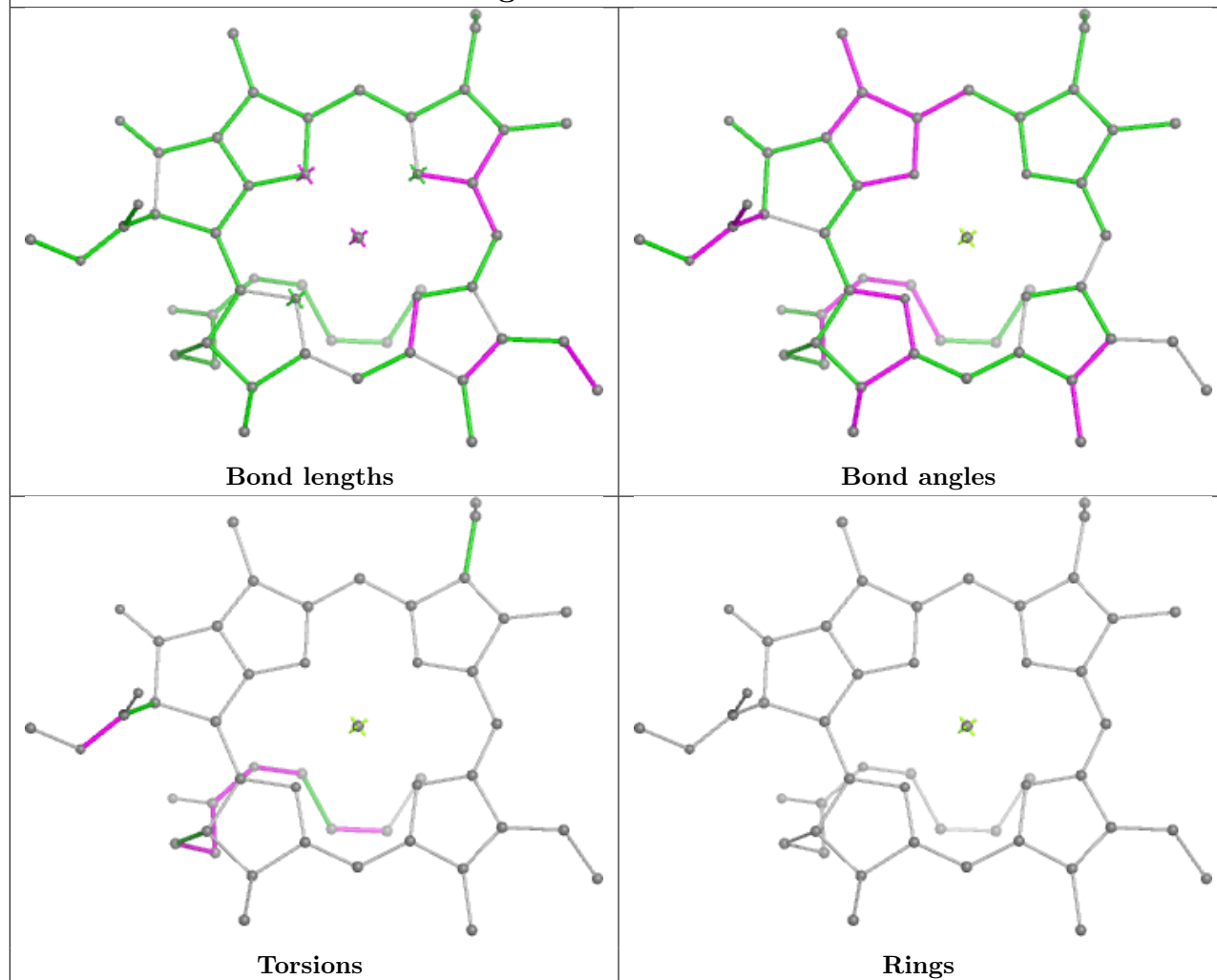
## Ligand 45D B 4011



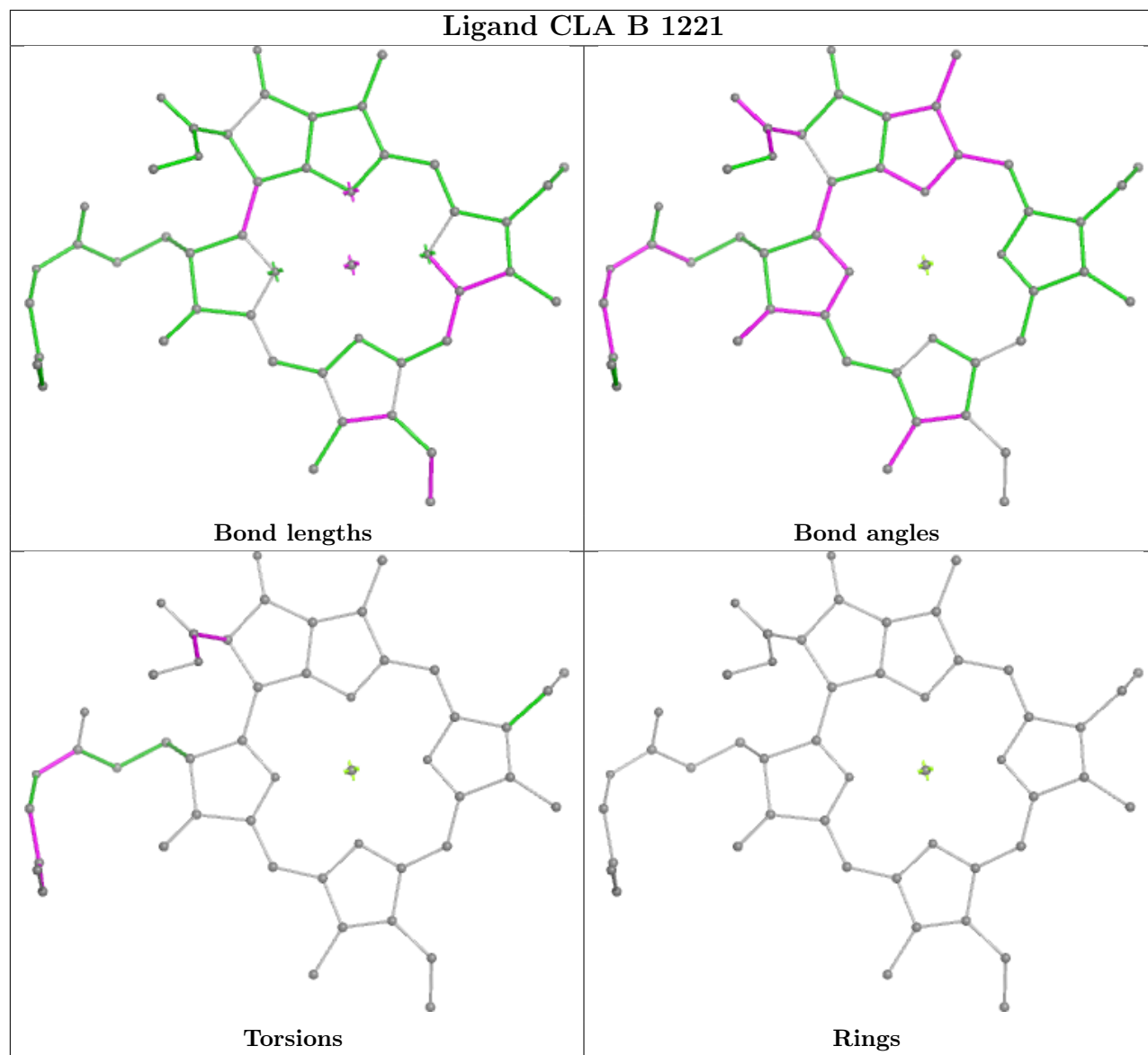
## Ligand BCR A 4003



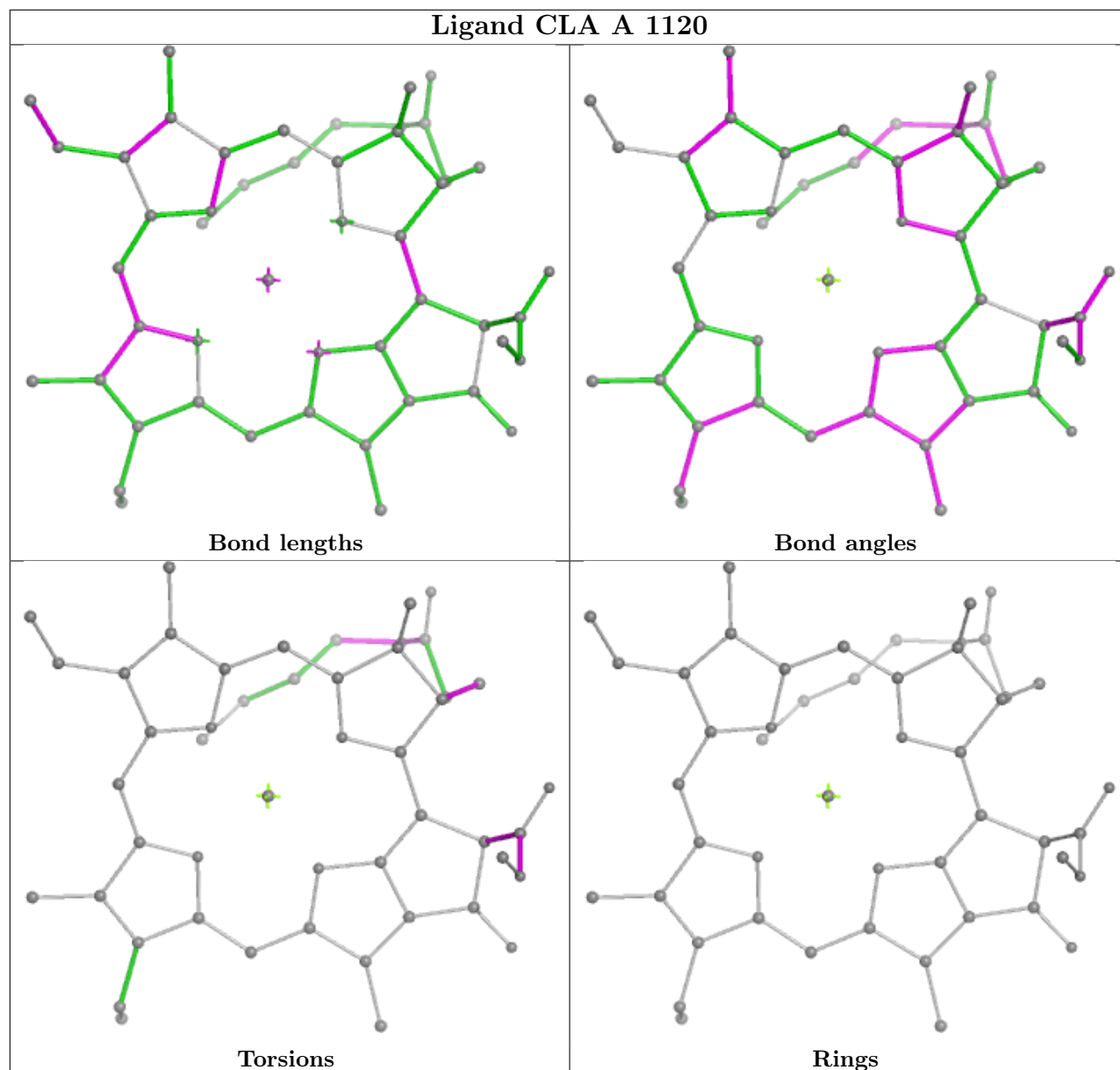
## Ligand CLA B 1237

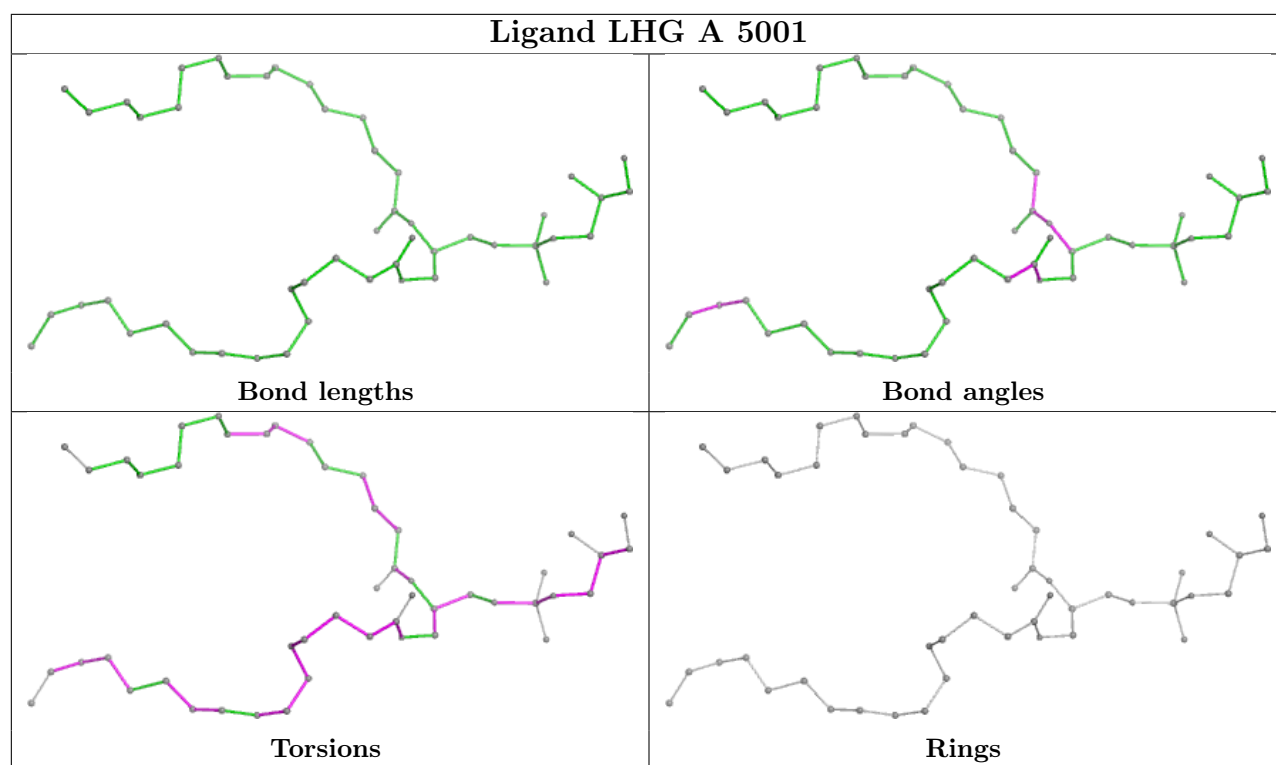




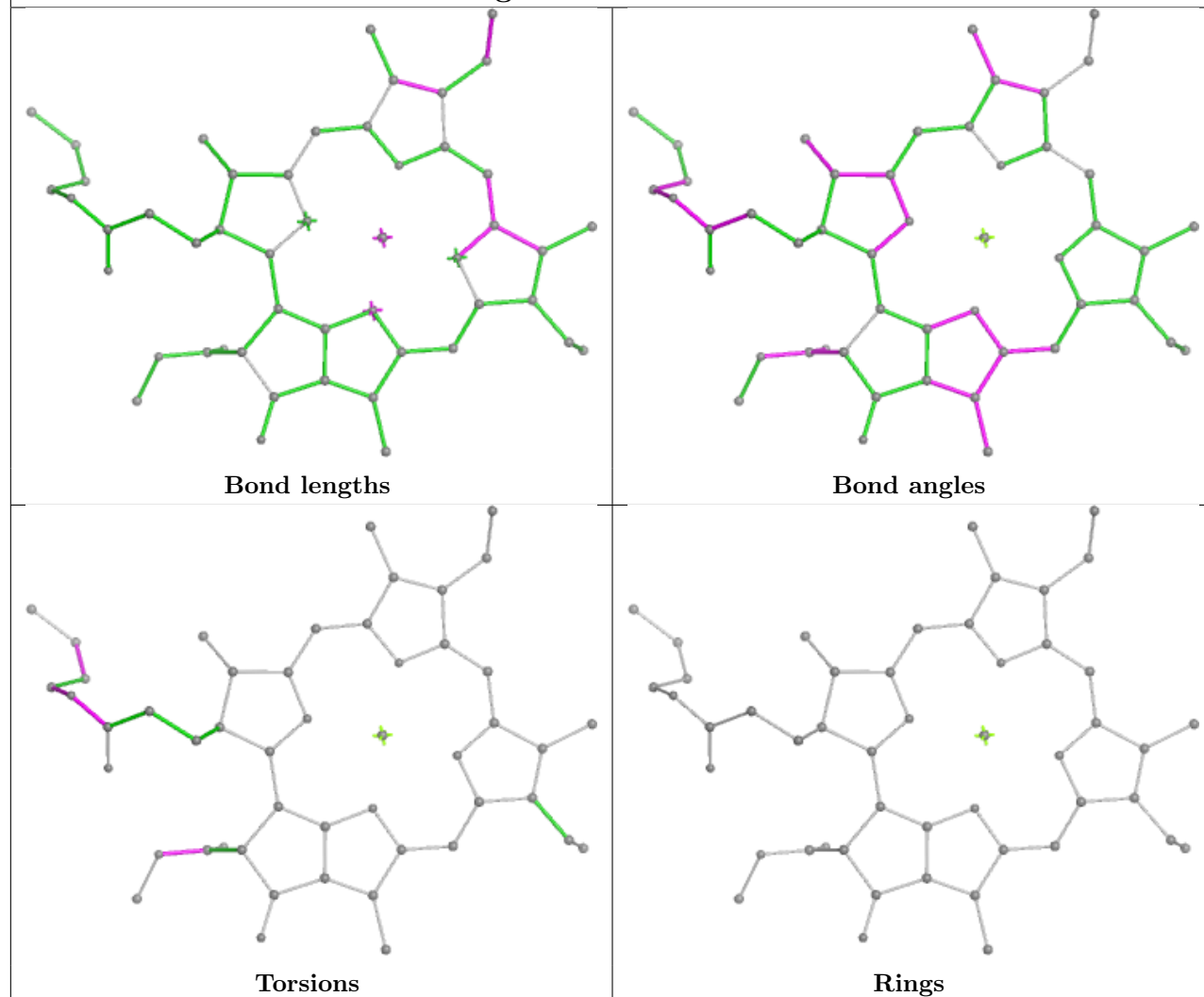


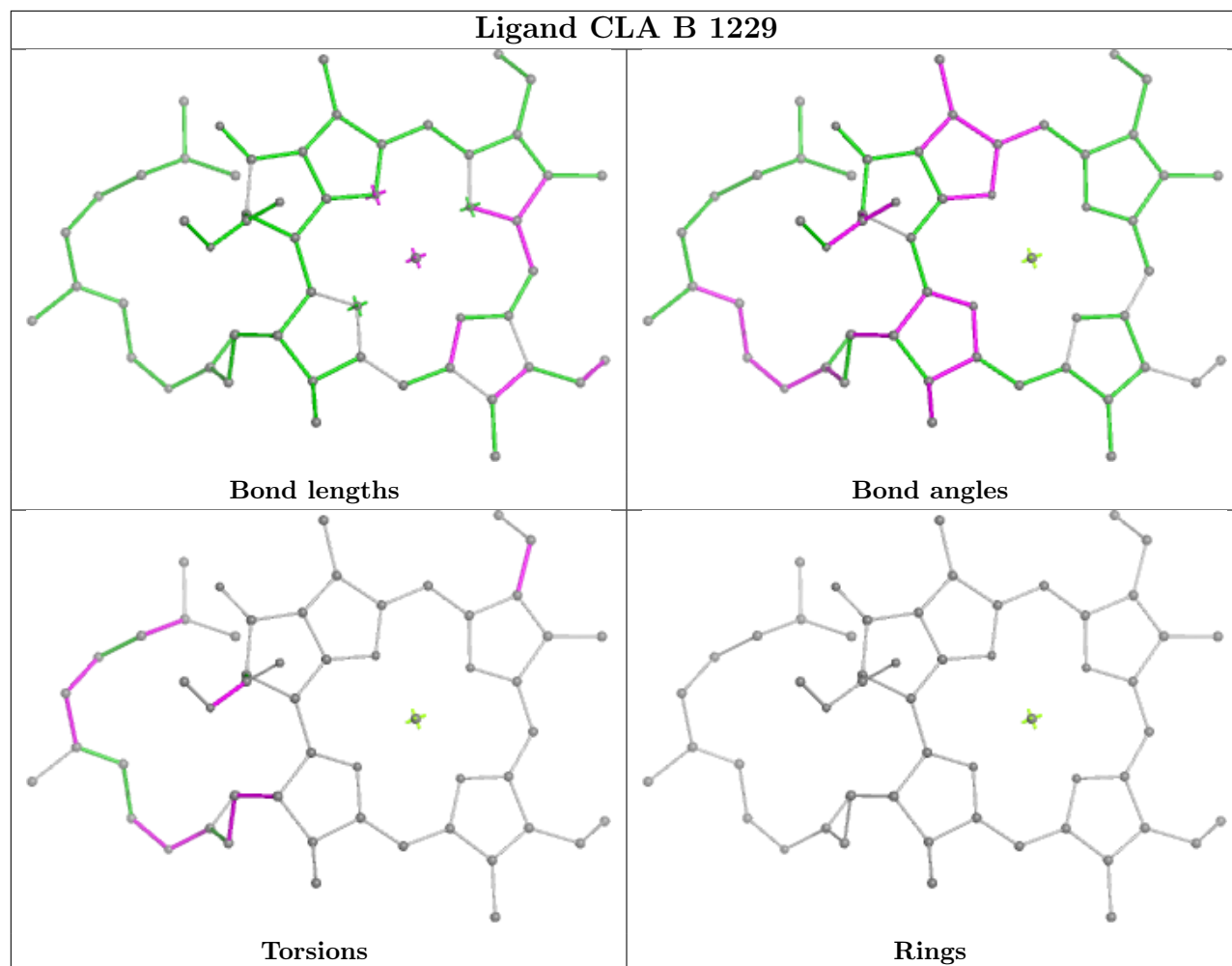
## Ligand CLA A 1120



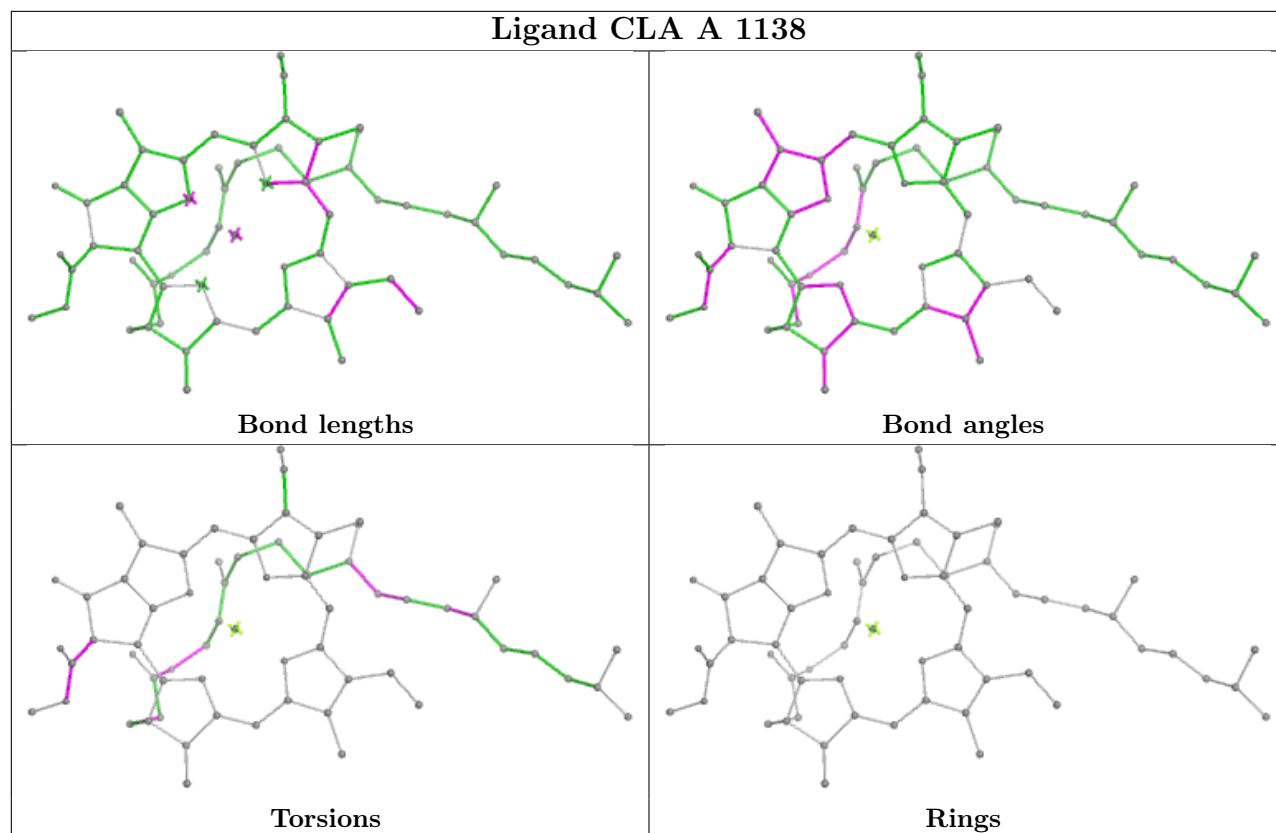


## Ligand CLA F 1301

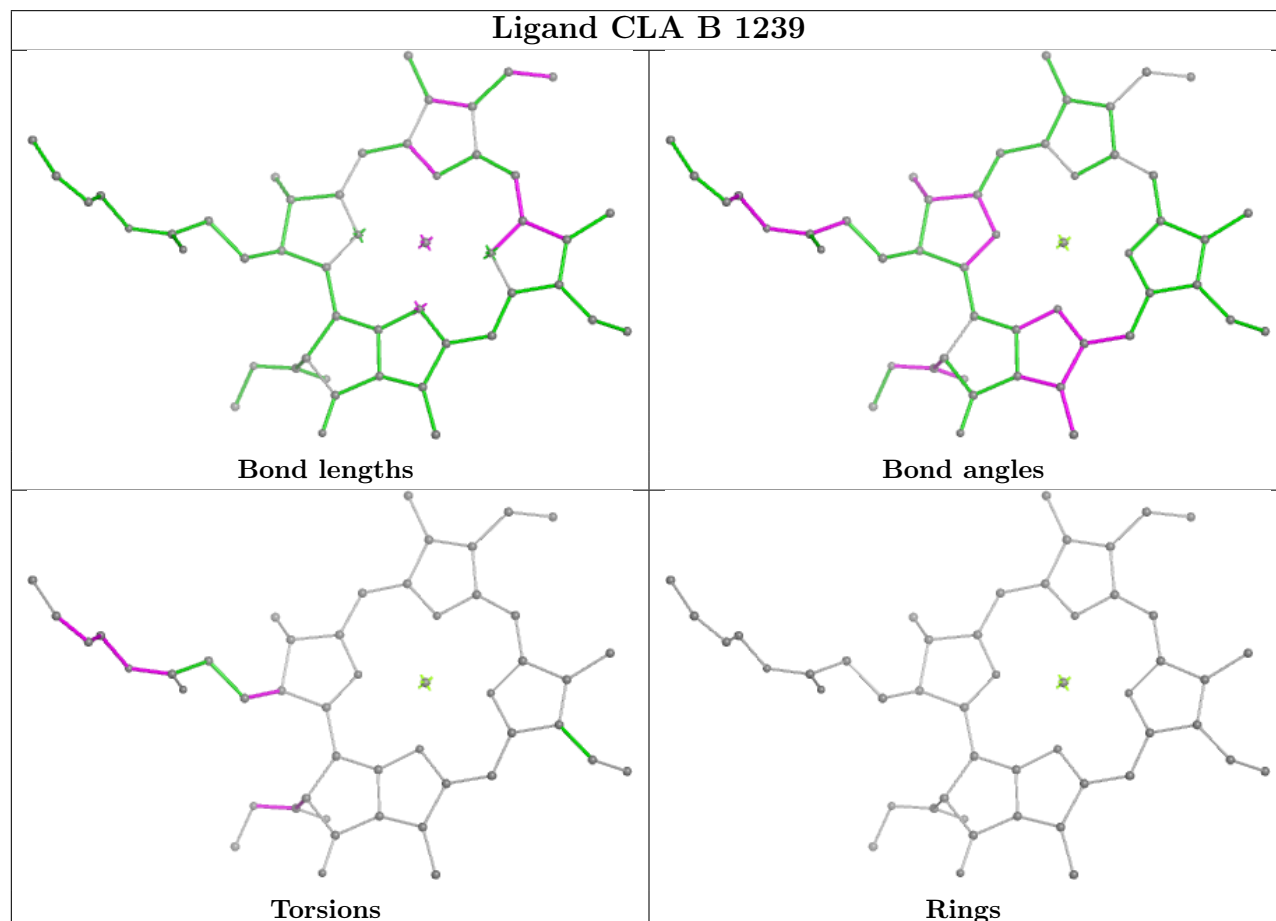


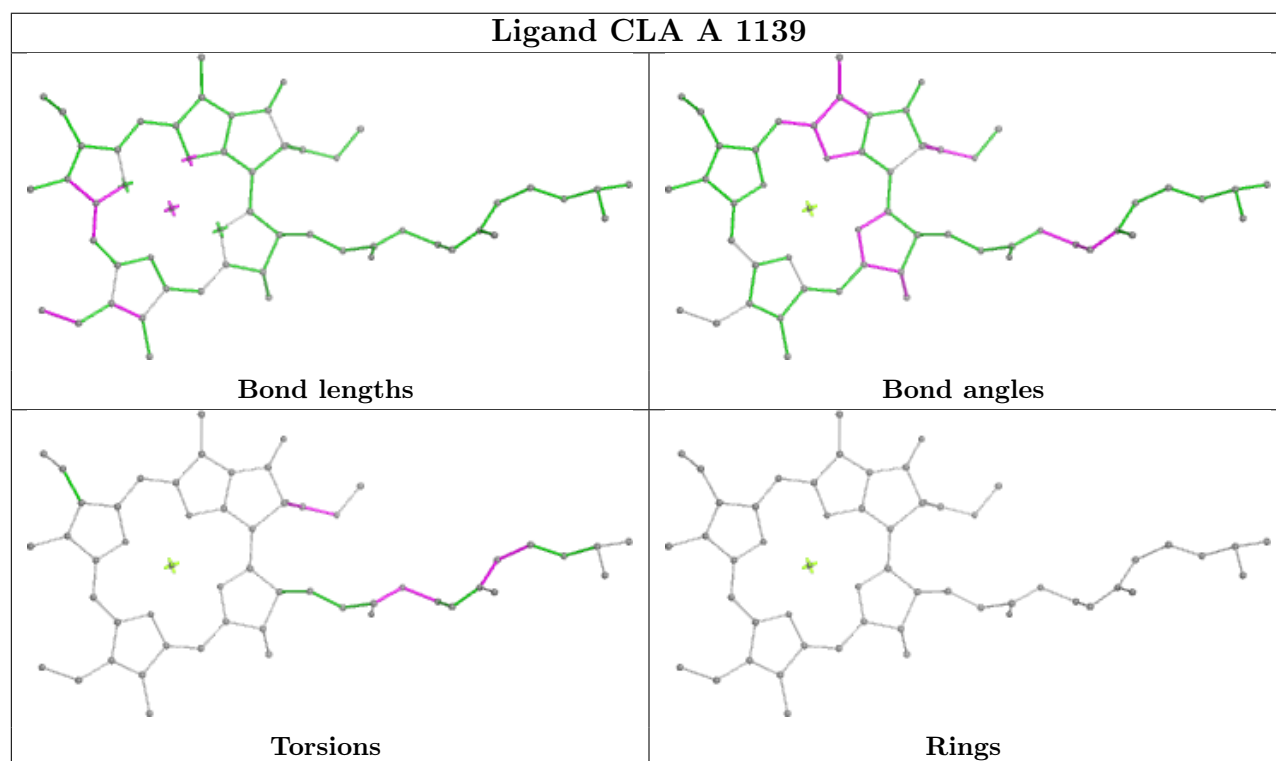
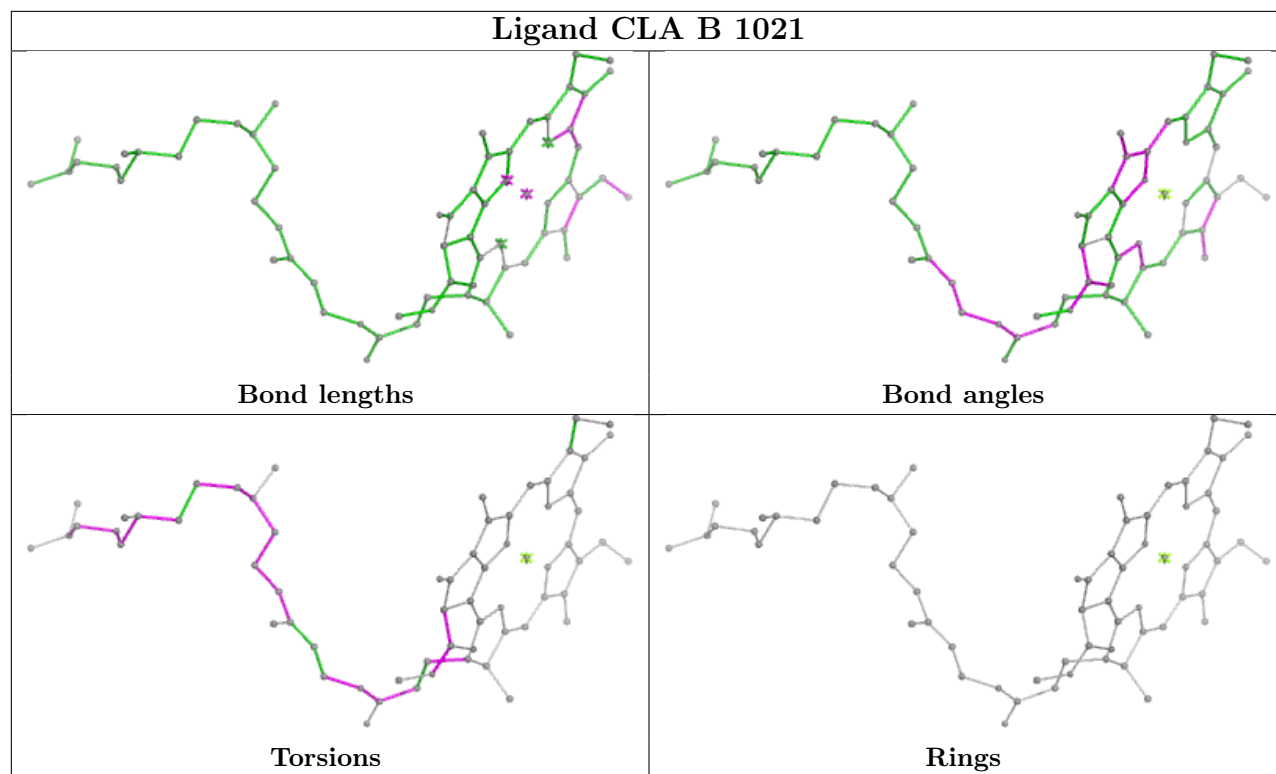


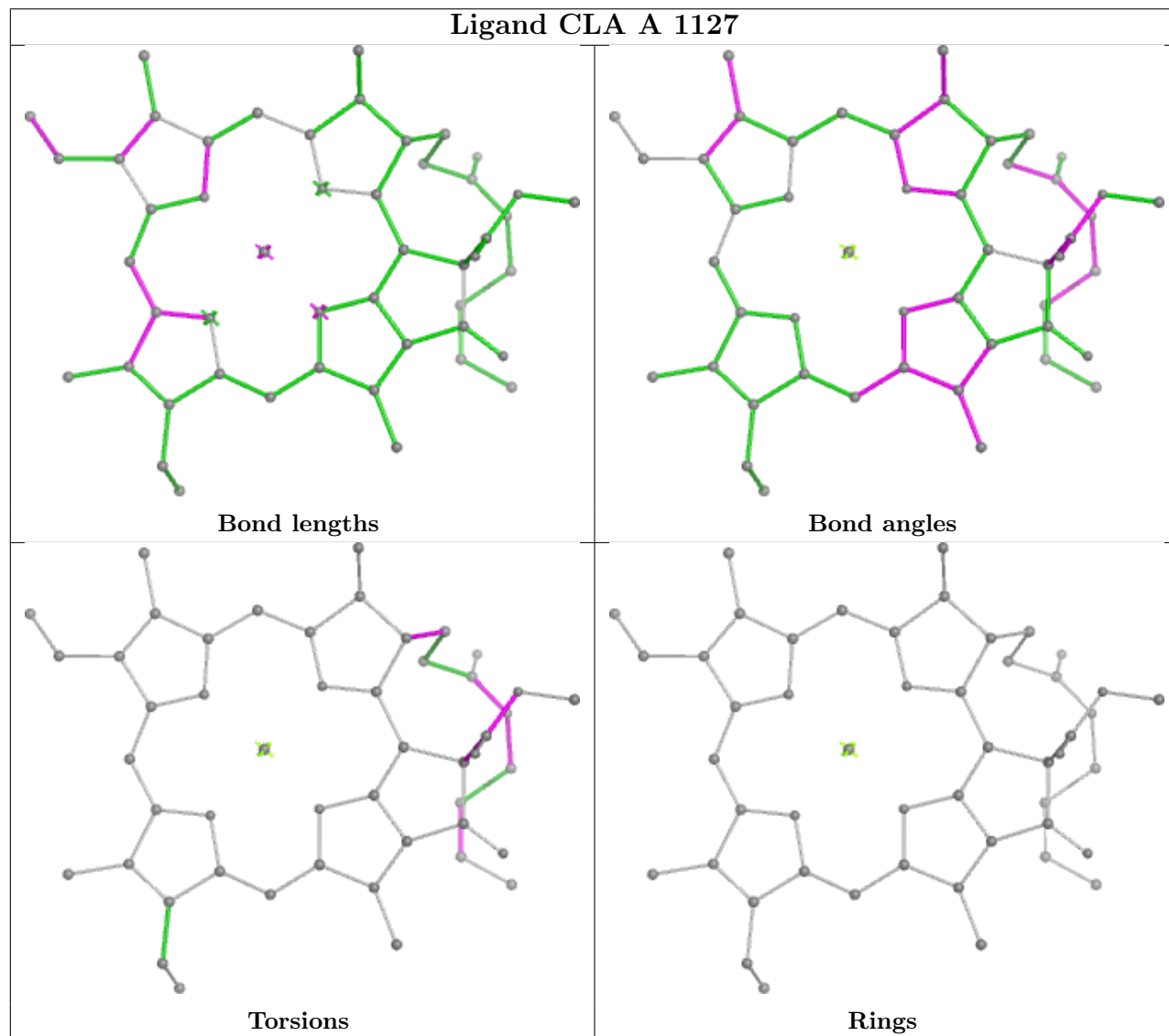
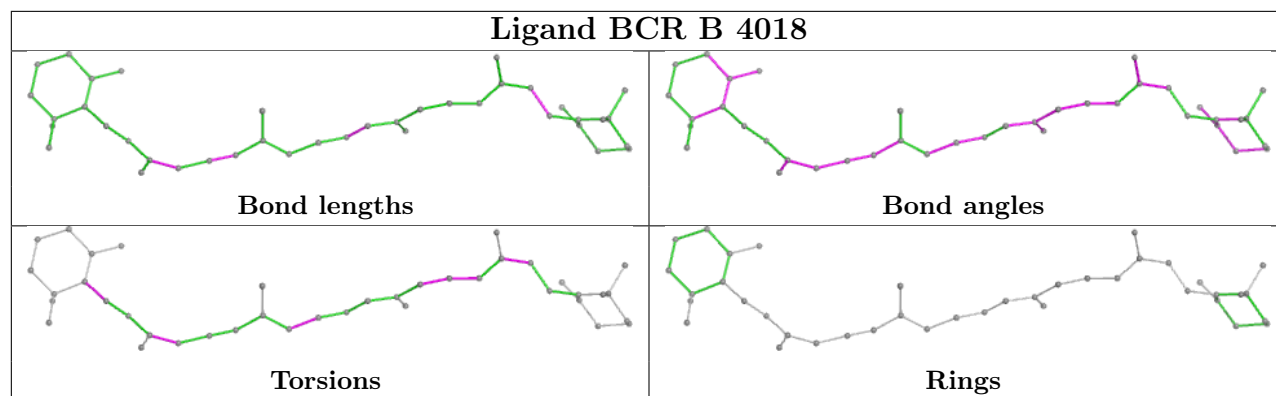
## Ligand CLA A 1138



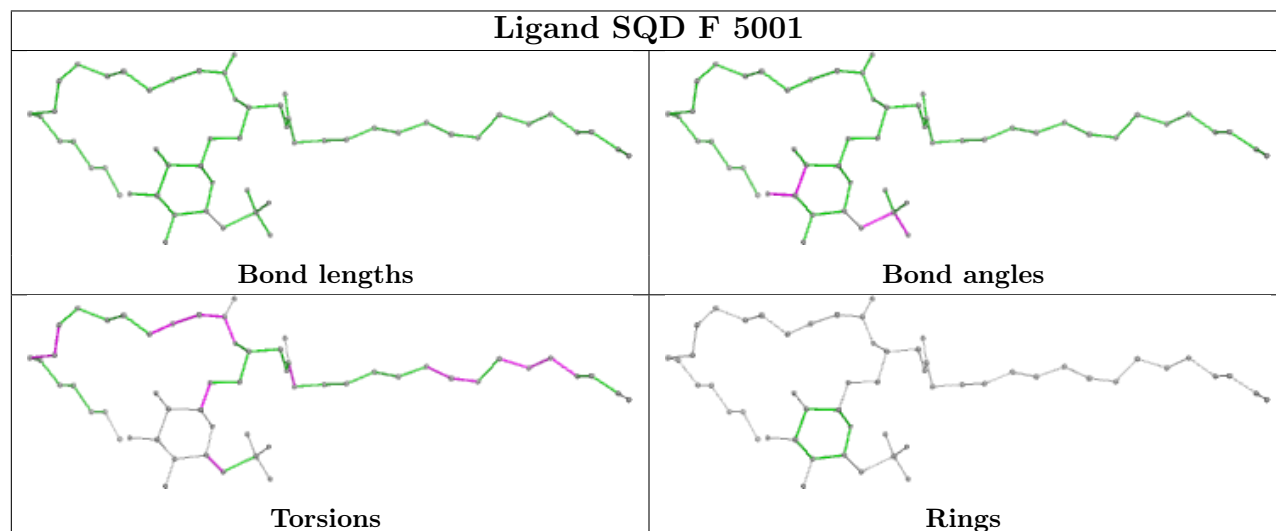
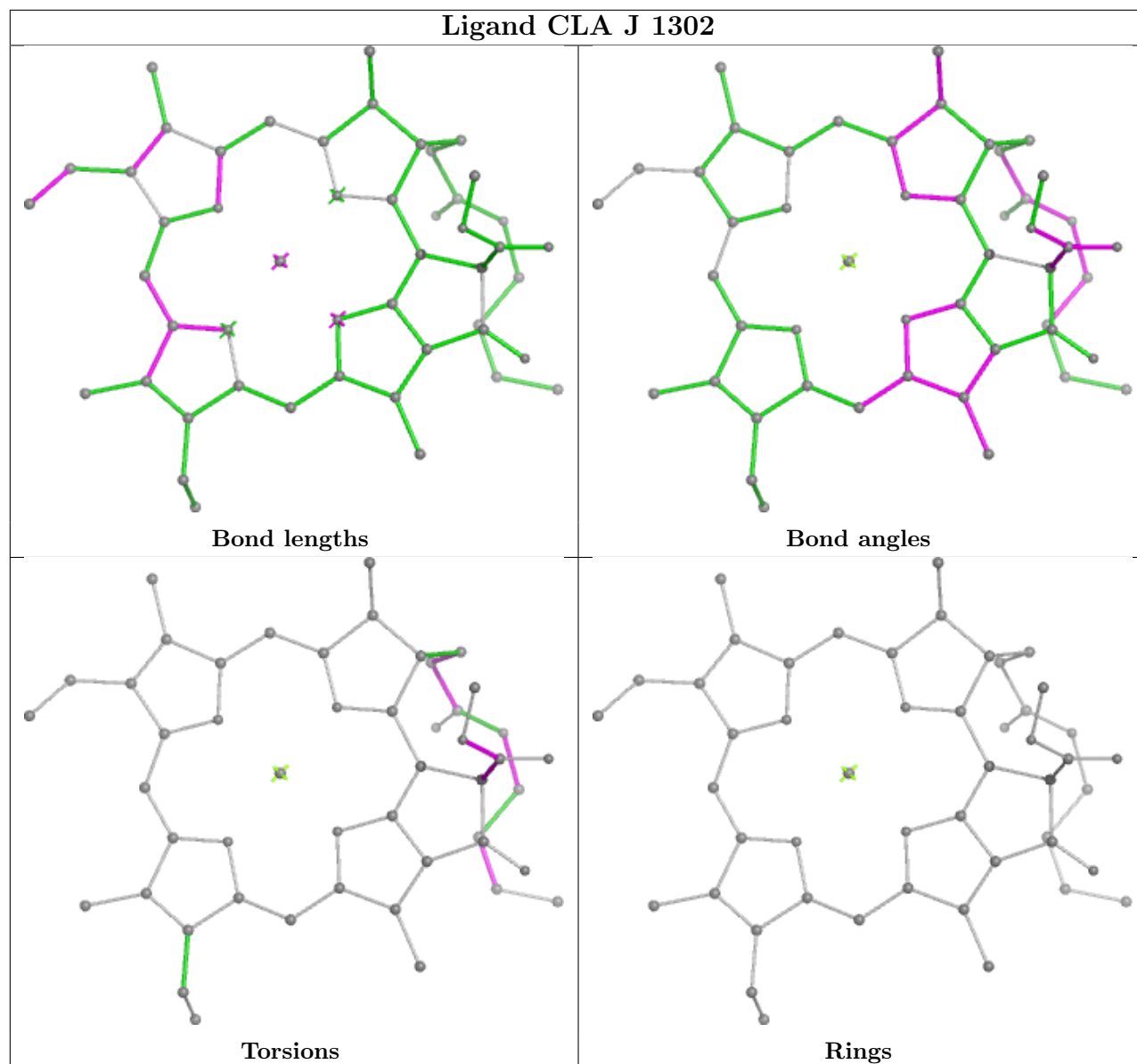
## Ligand CLA B 1239

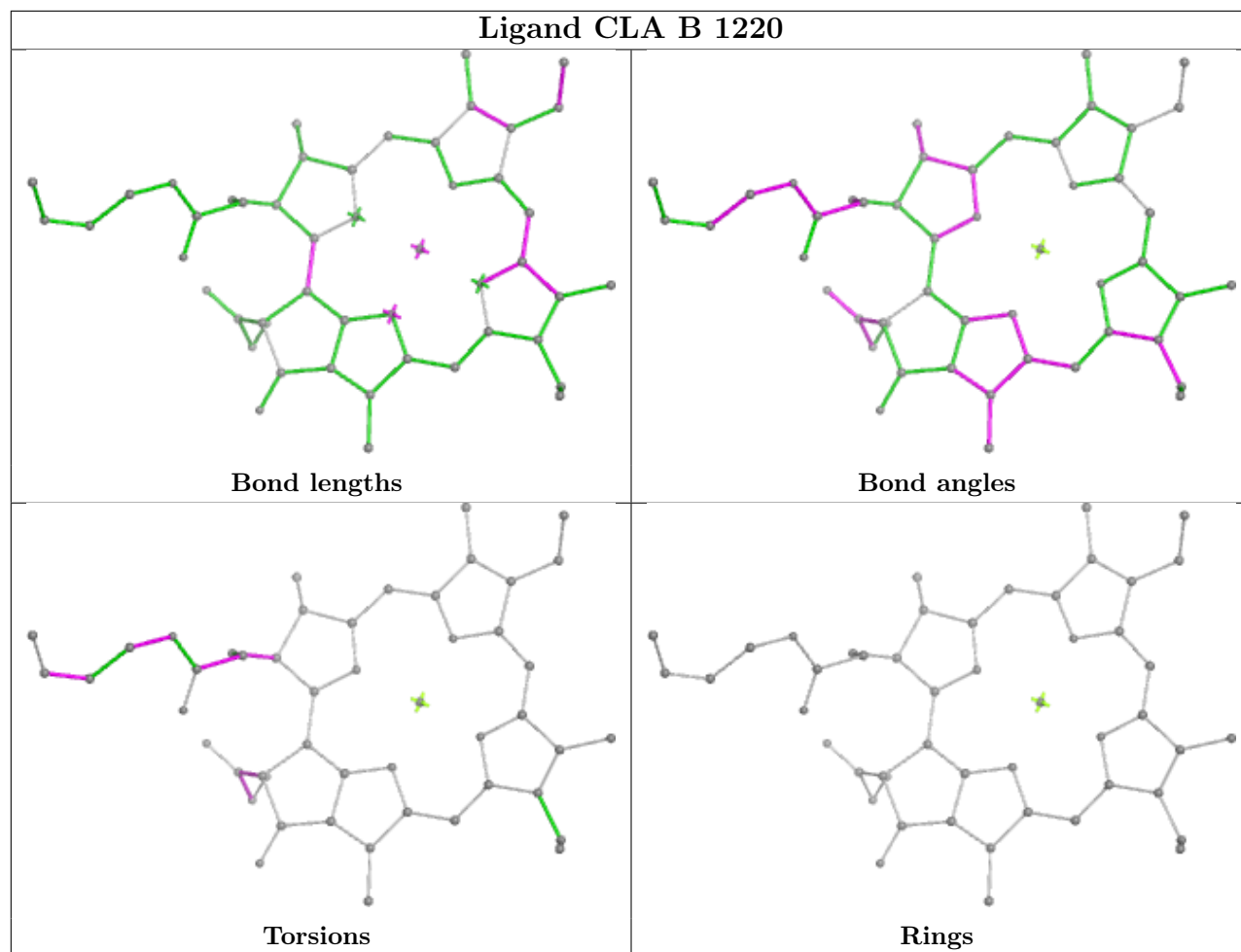


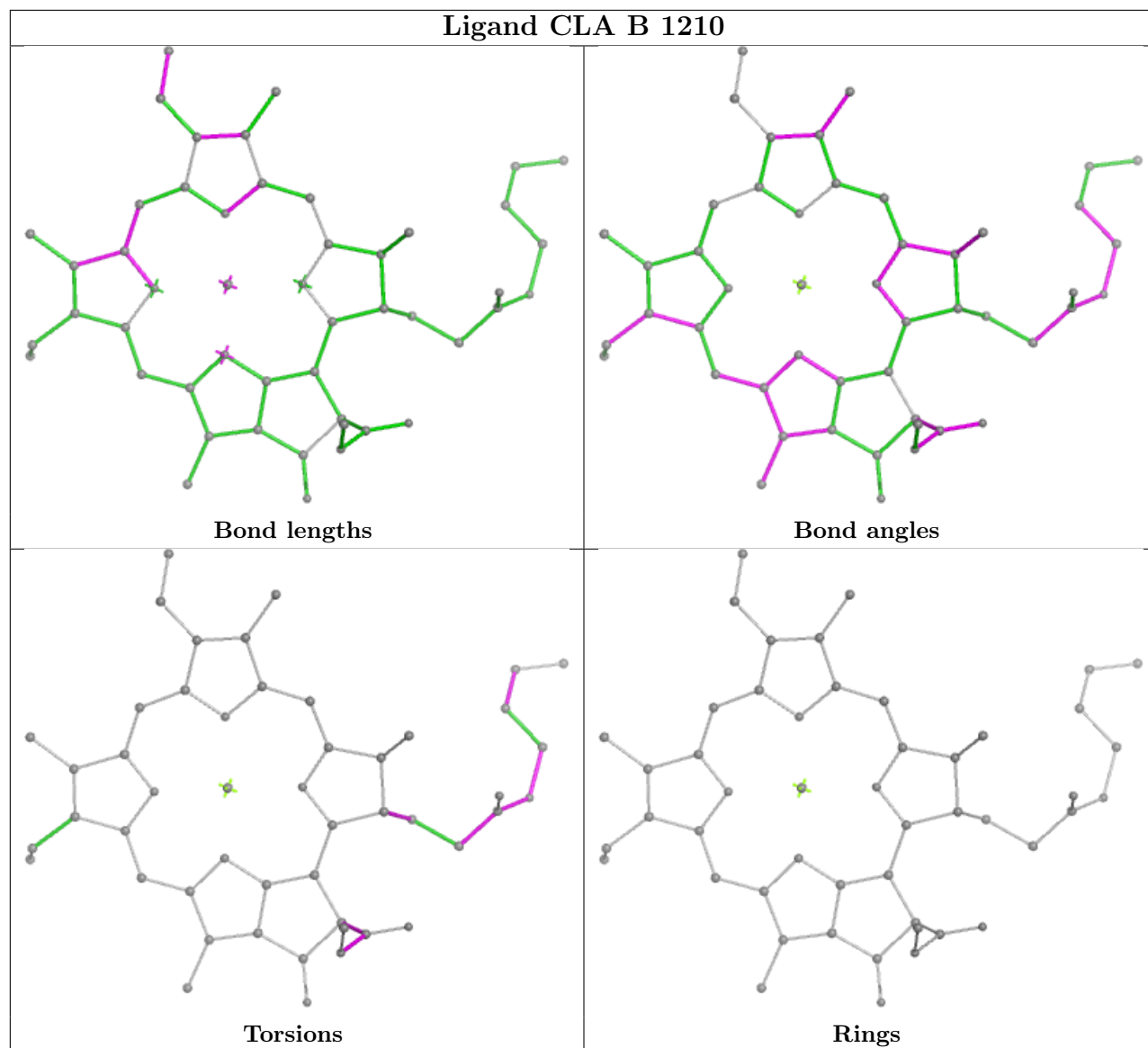


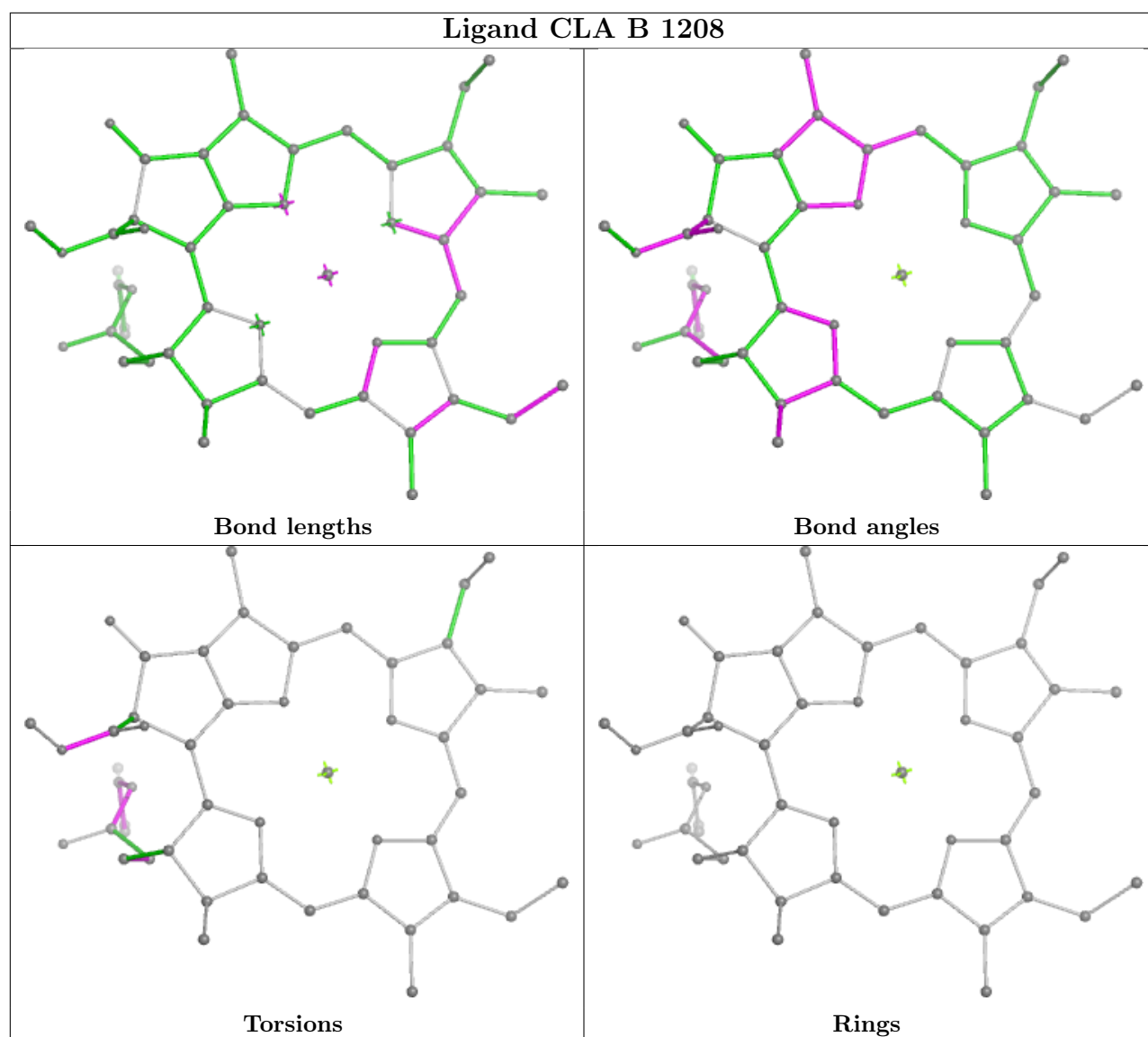




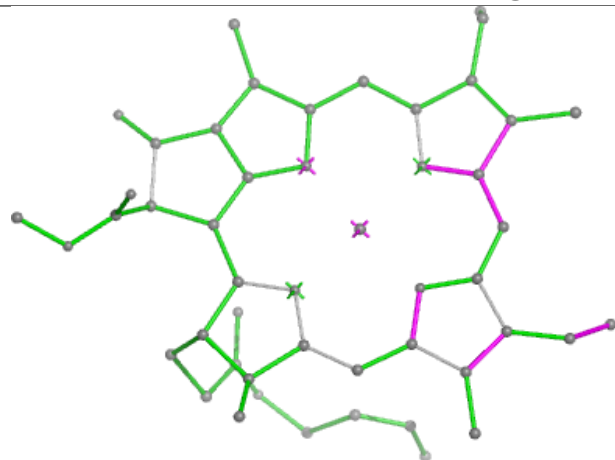




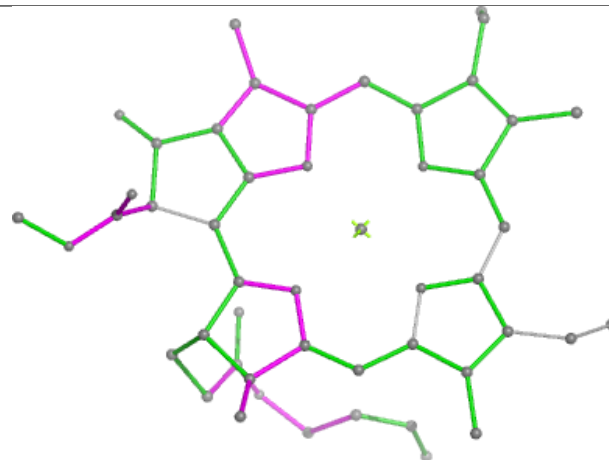




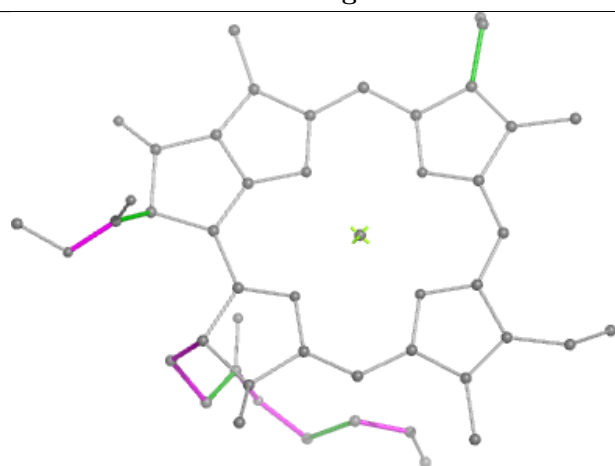
## Ligand CLA A 1110



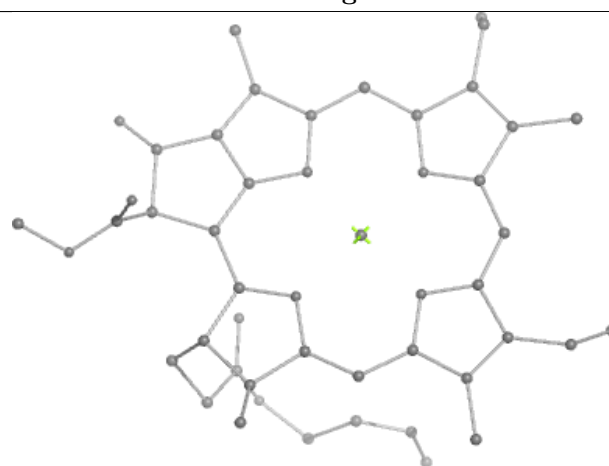
Bond lengths



Bond angles

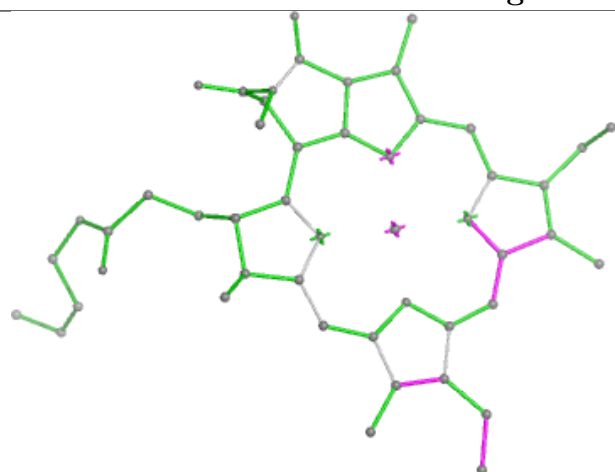


Torsions

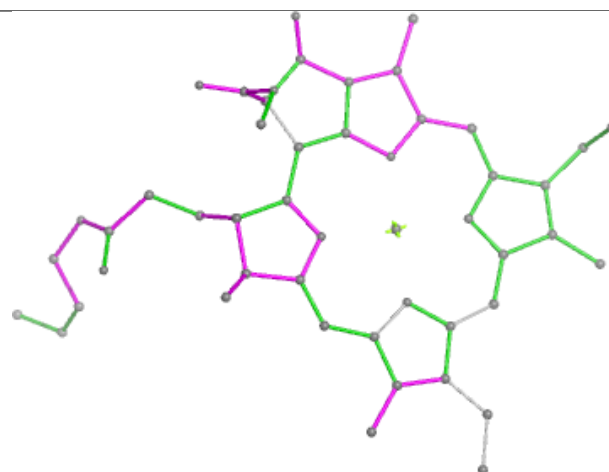


Rings

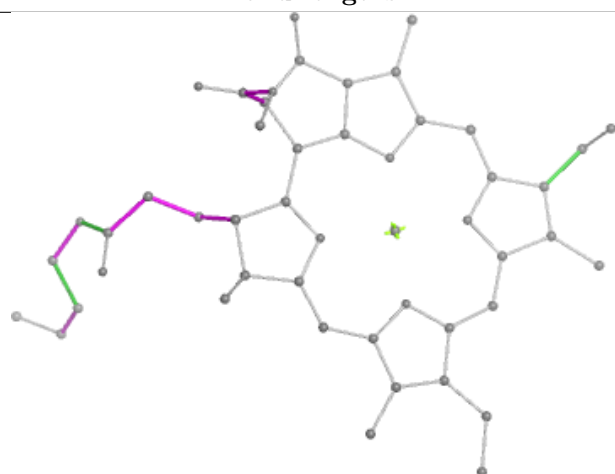
## Ligand CLA A 1125



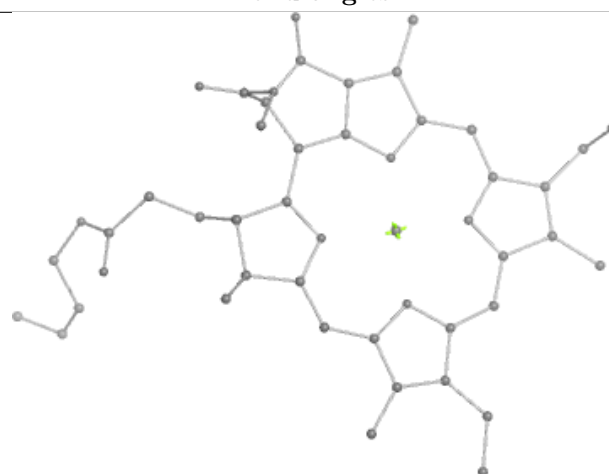
Bond lengths



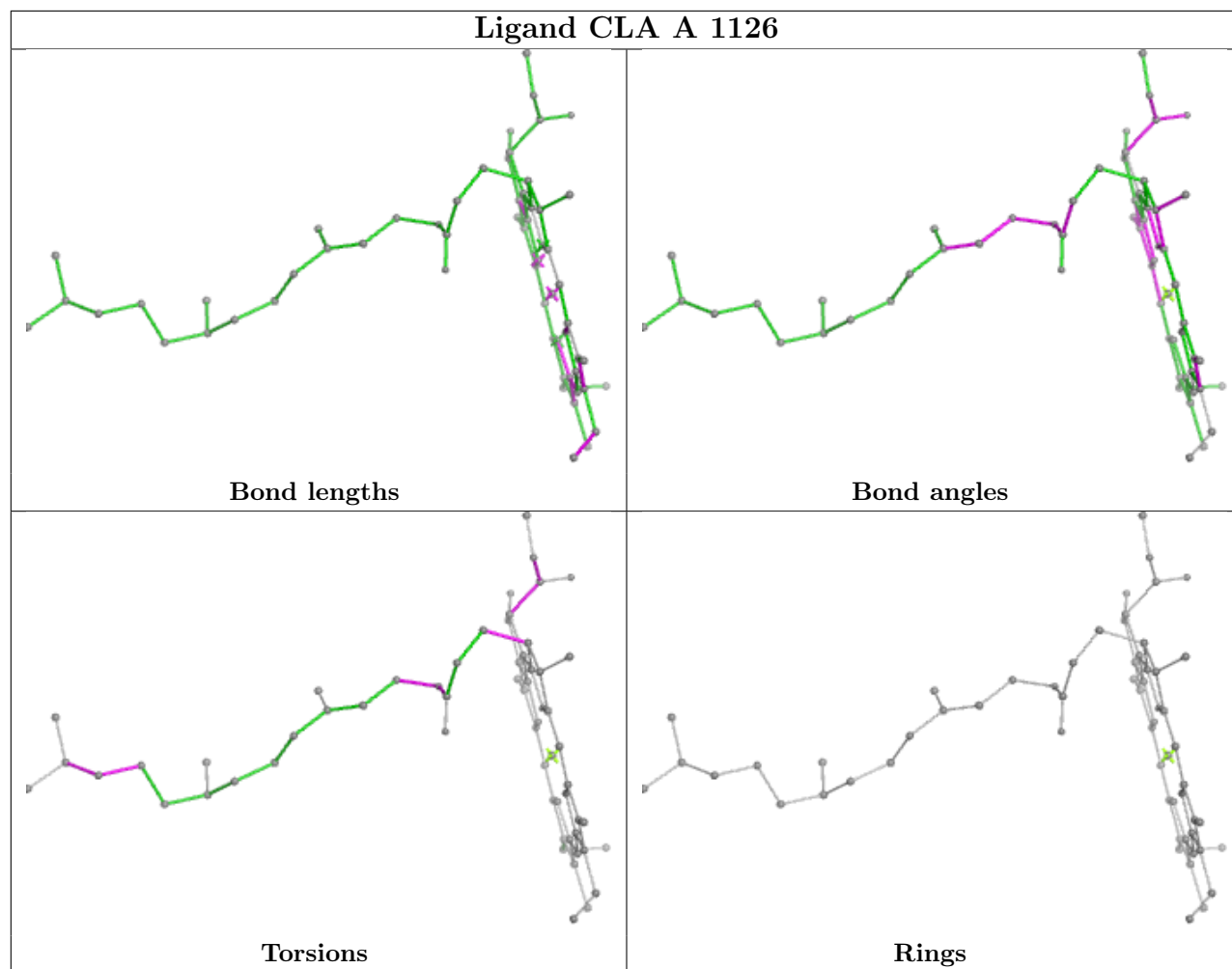
Bond angles

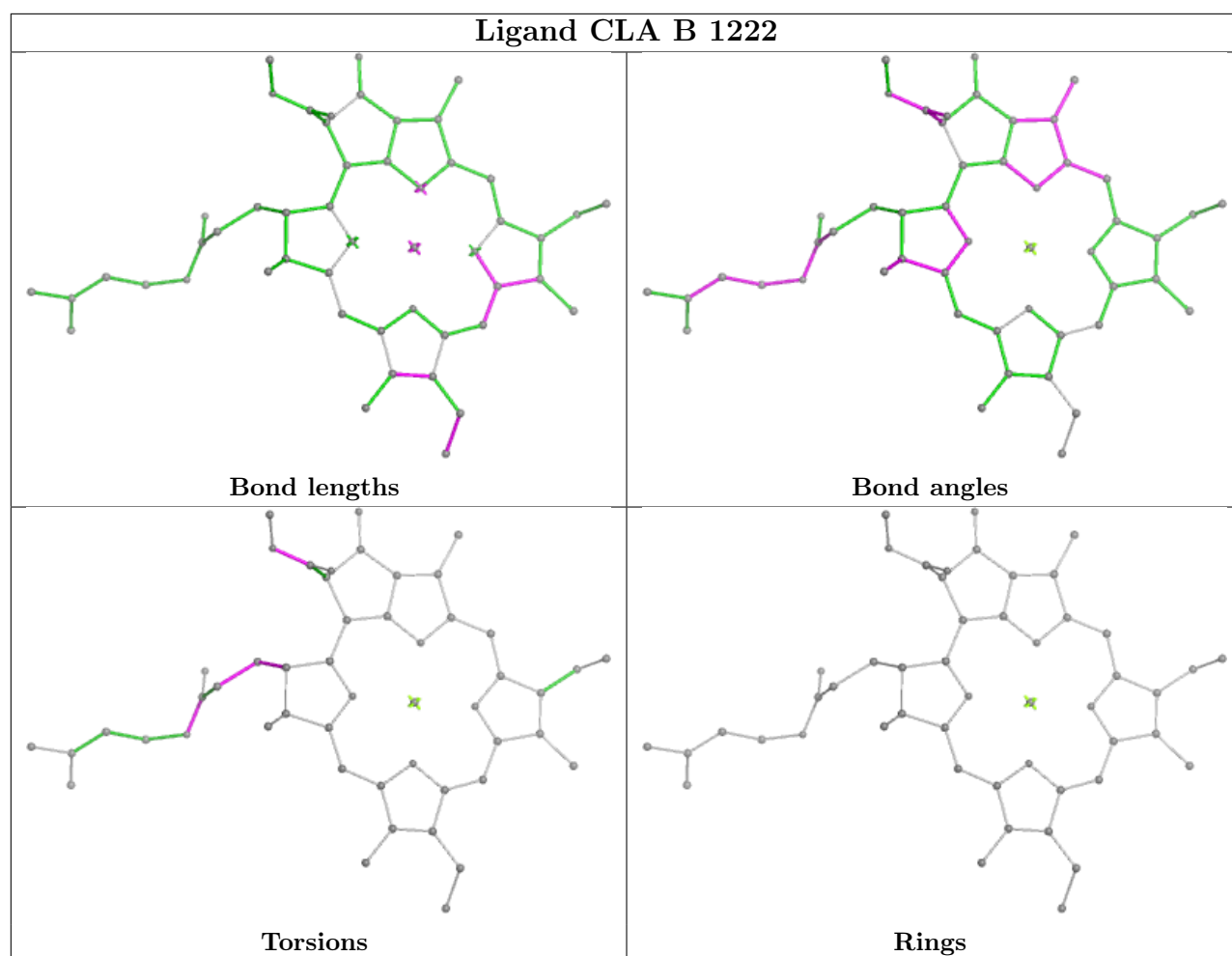


Torsions



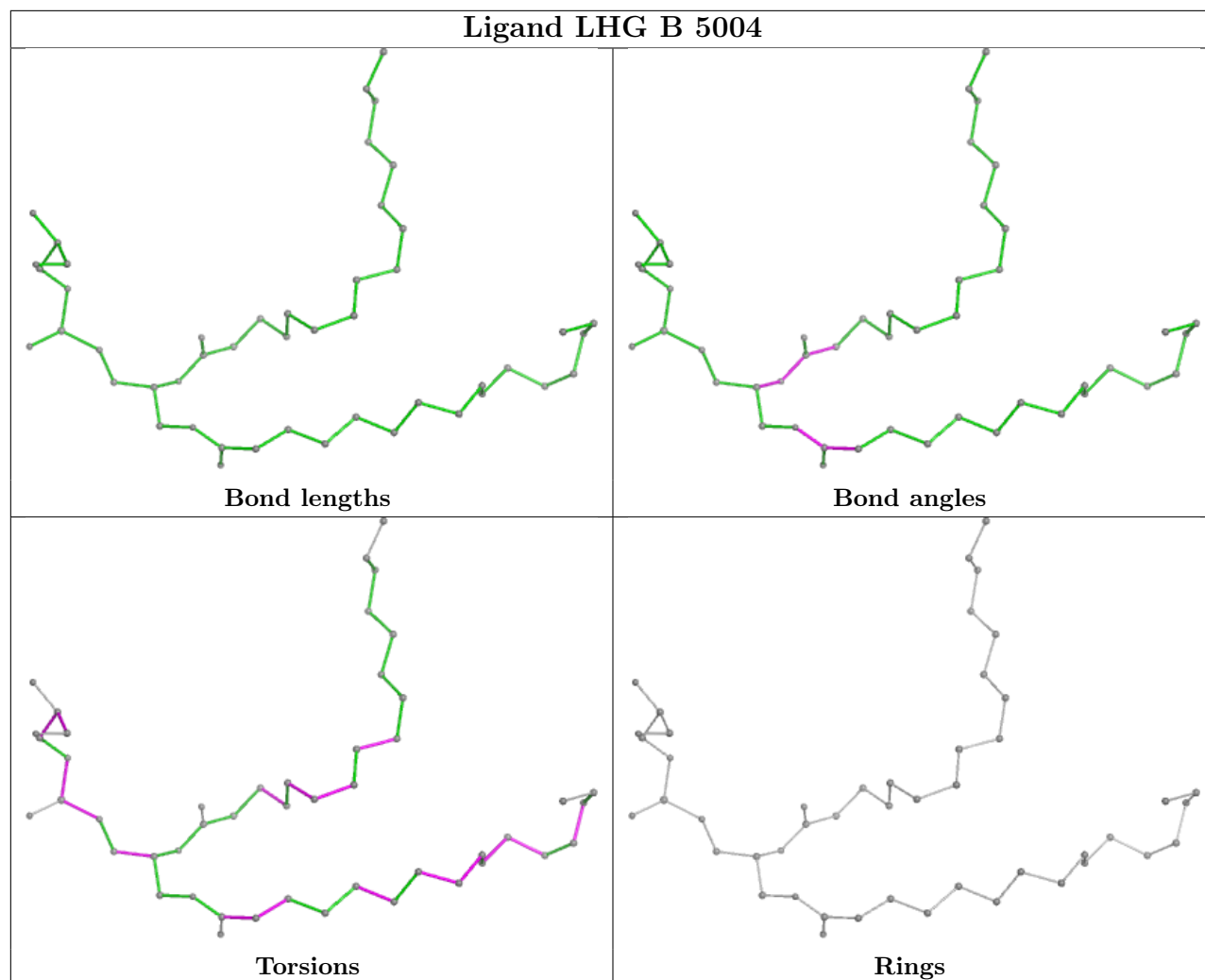
Rings



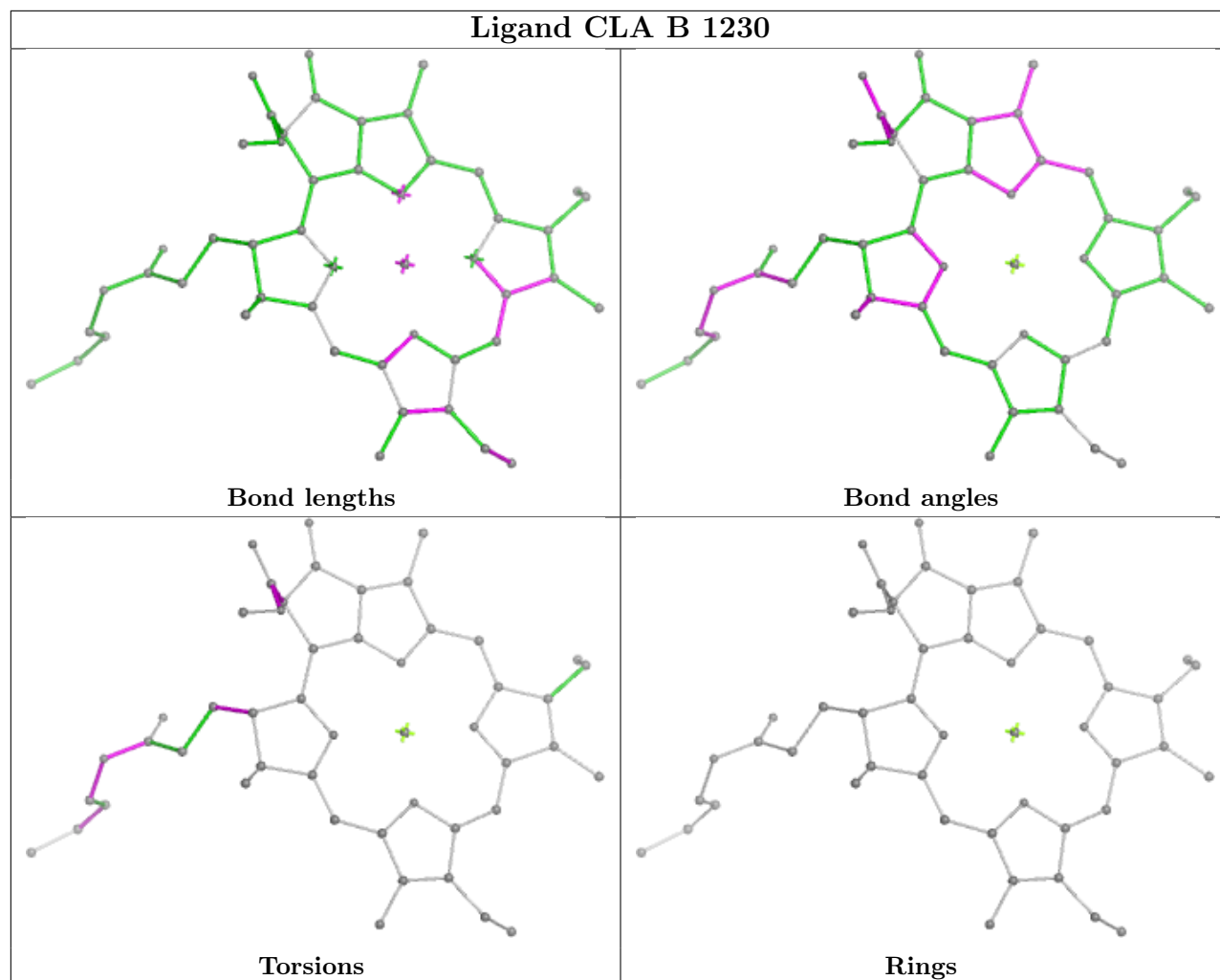




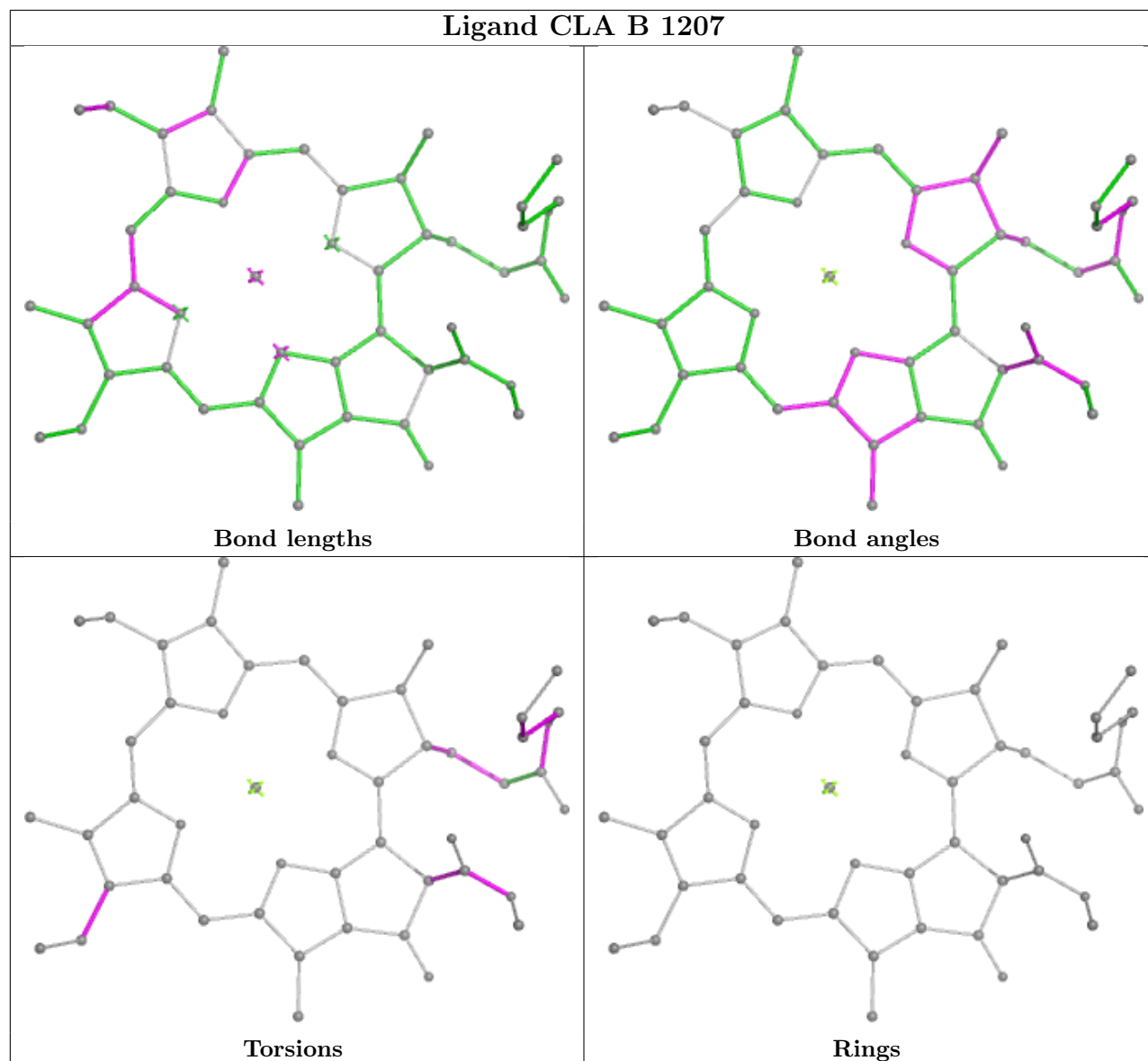
## Ligand LHG B 5004



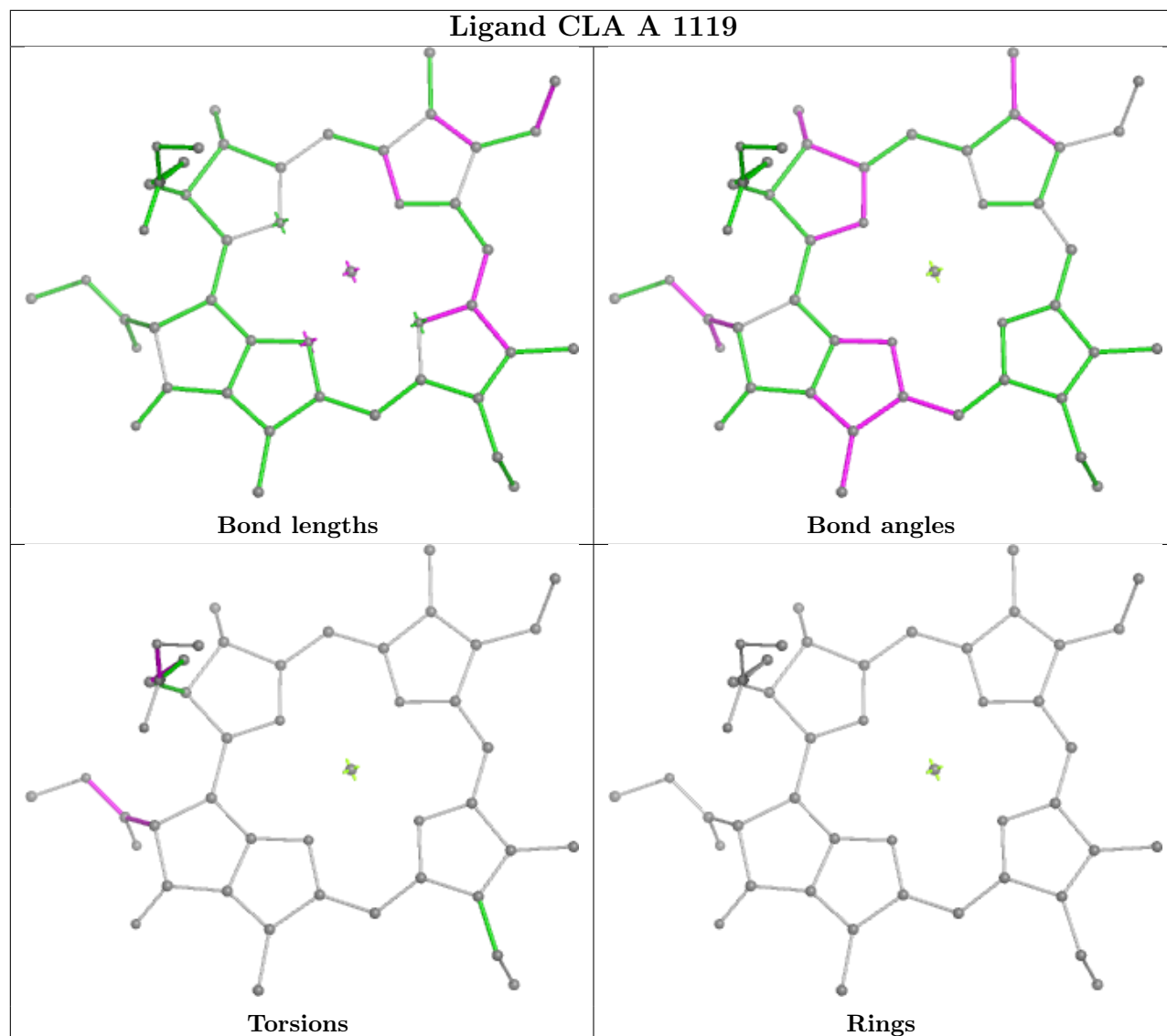
## Ligand CLA B 1230



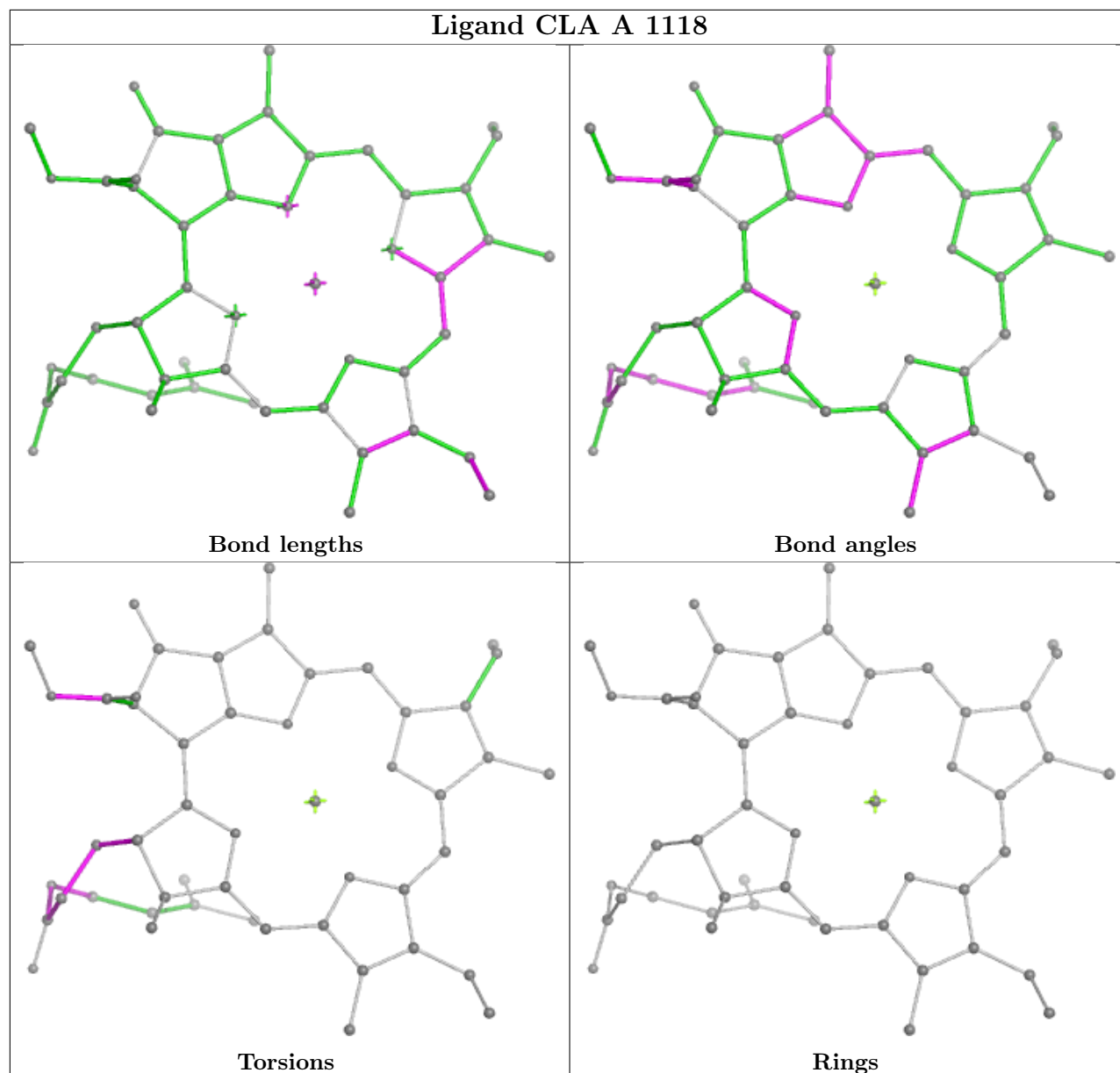
## Ligand CLA B 1207



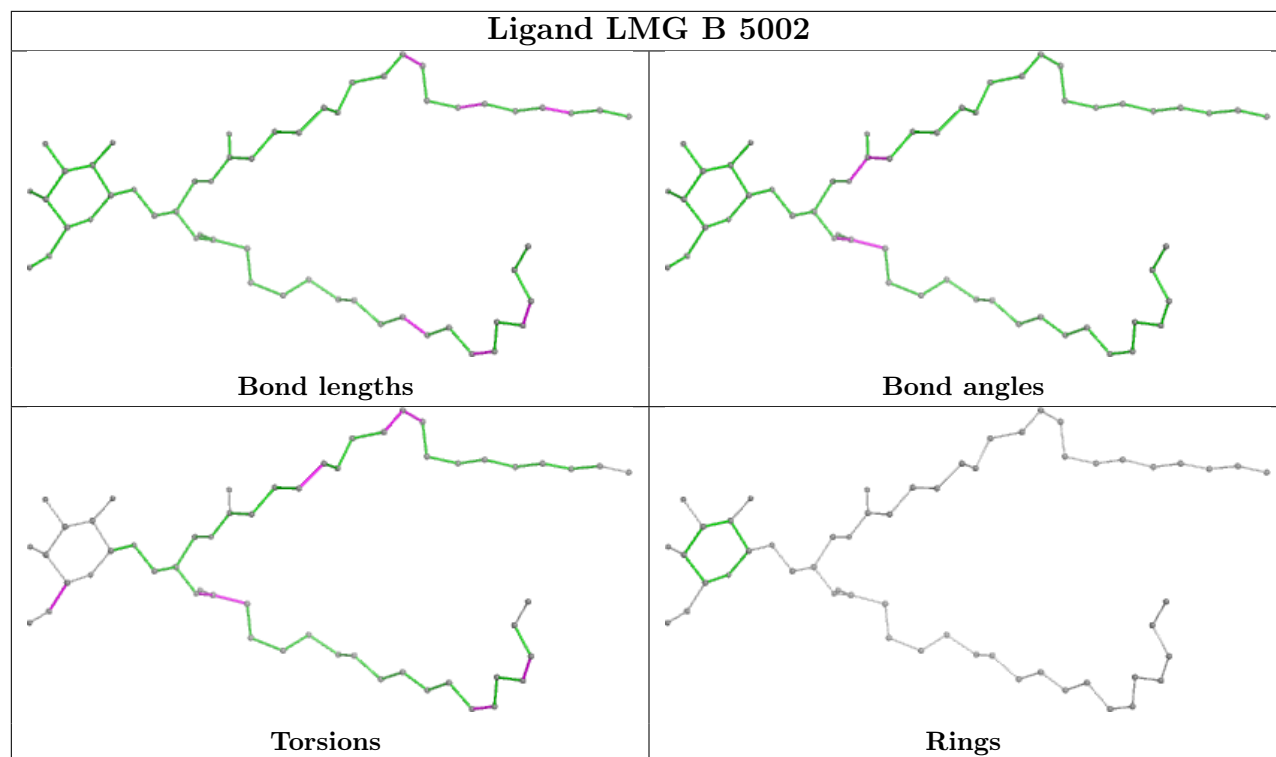
## Ligand CLA A 1119



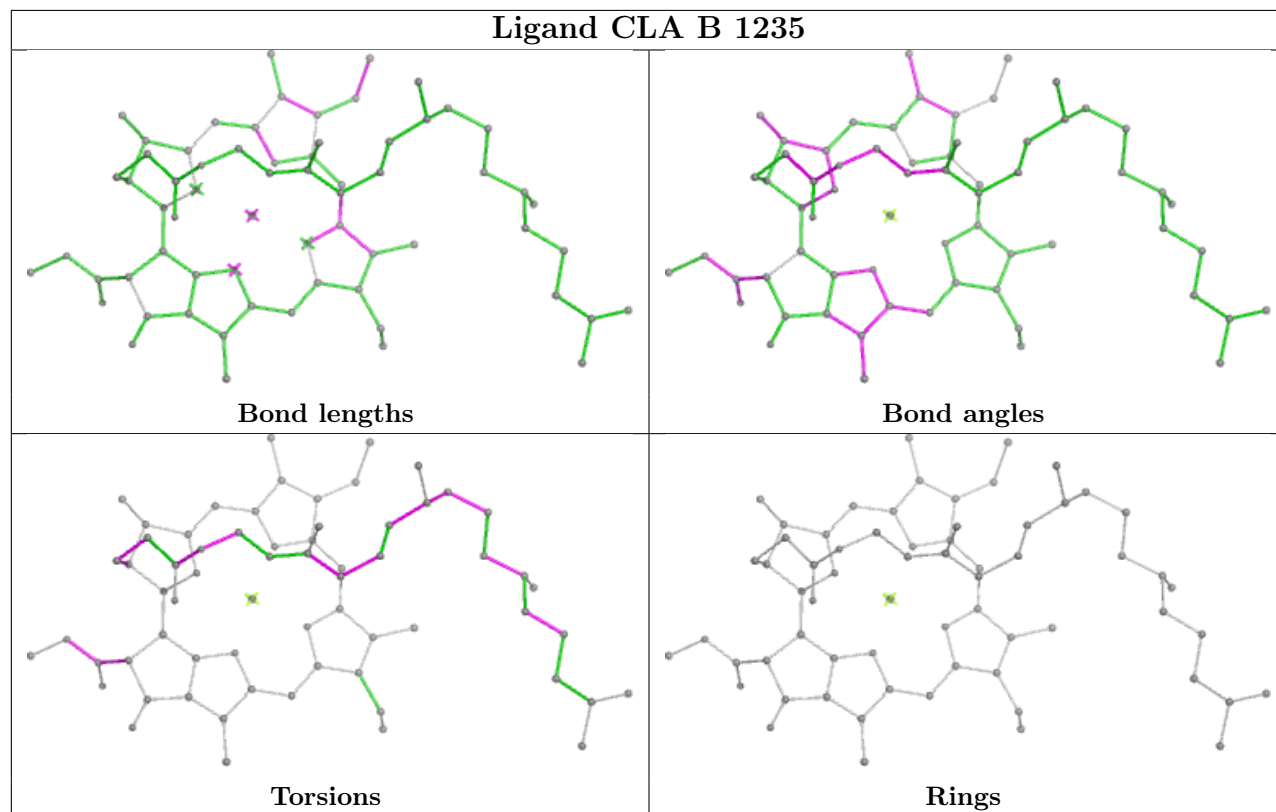
## Ligand CLA A 1118



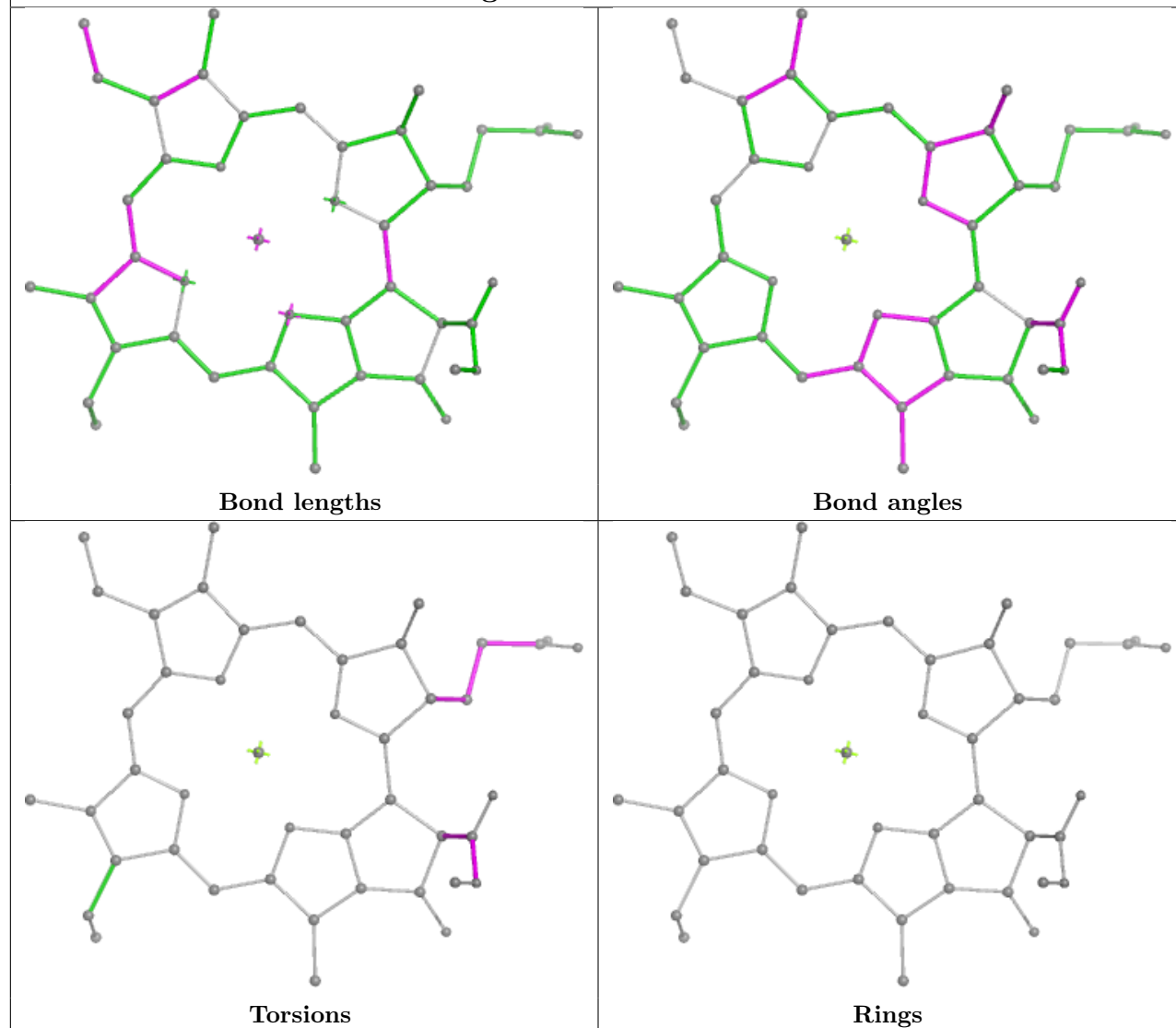
## Ligand LMG B 5002



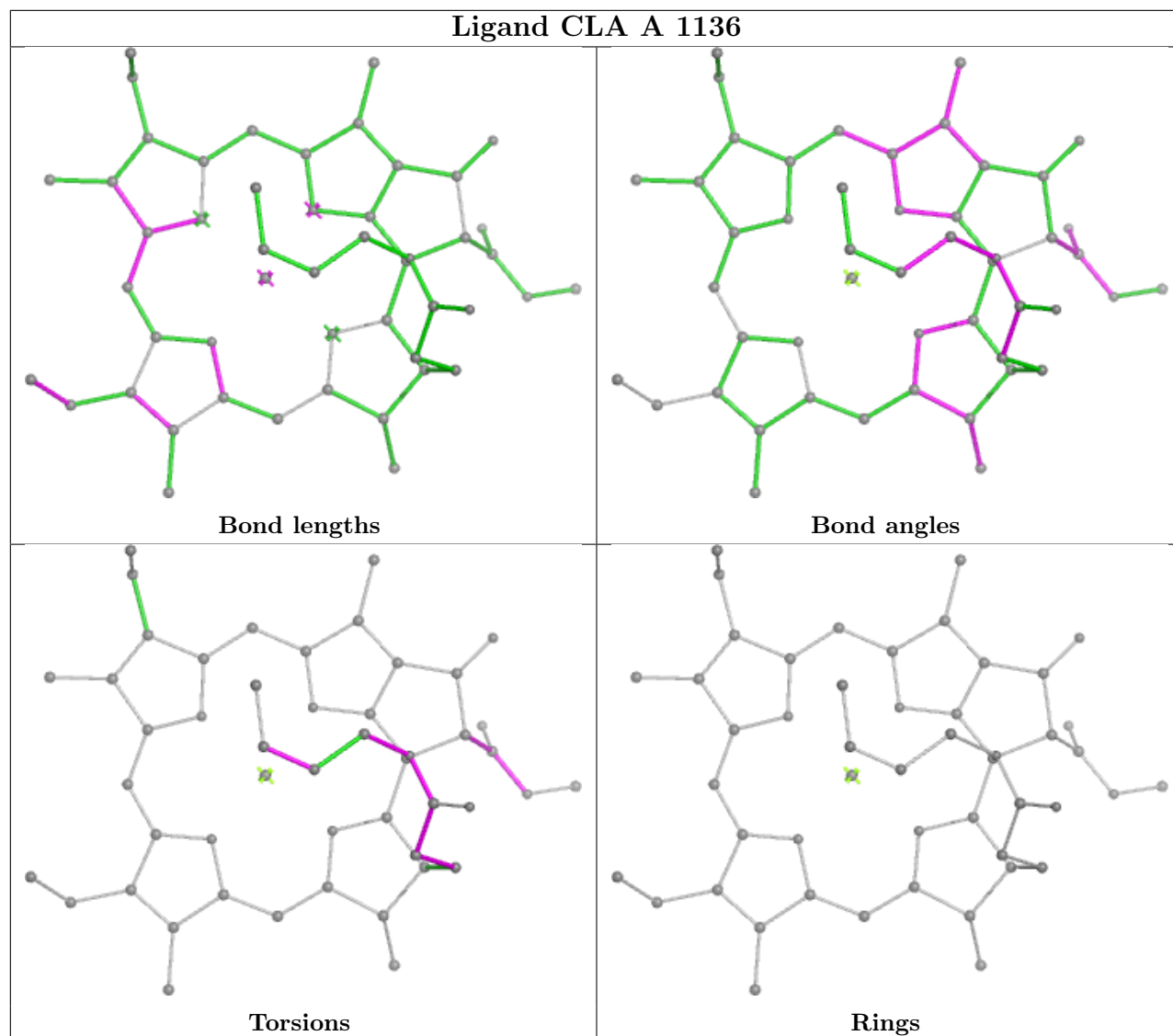
## Ligand CLA B 1235



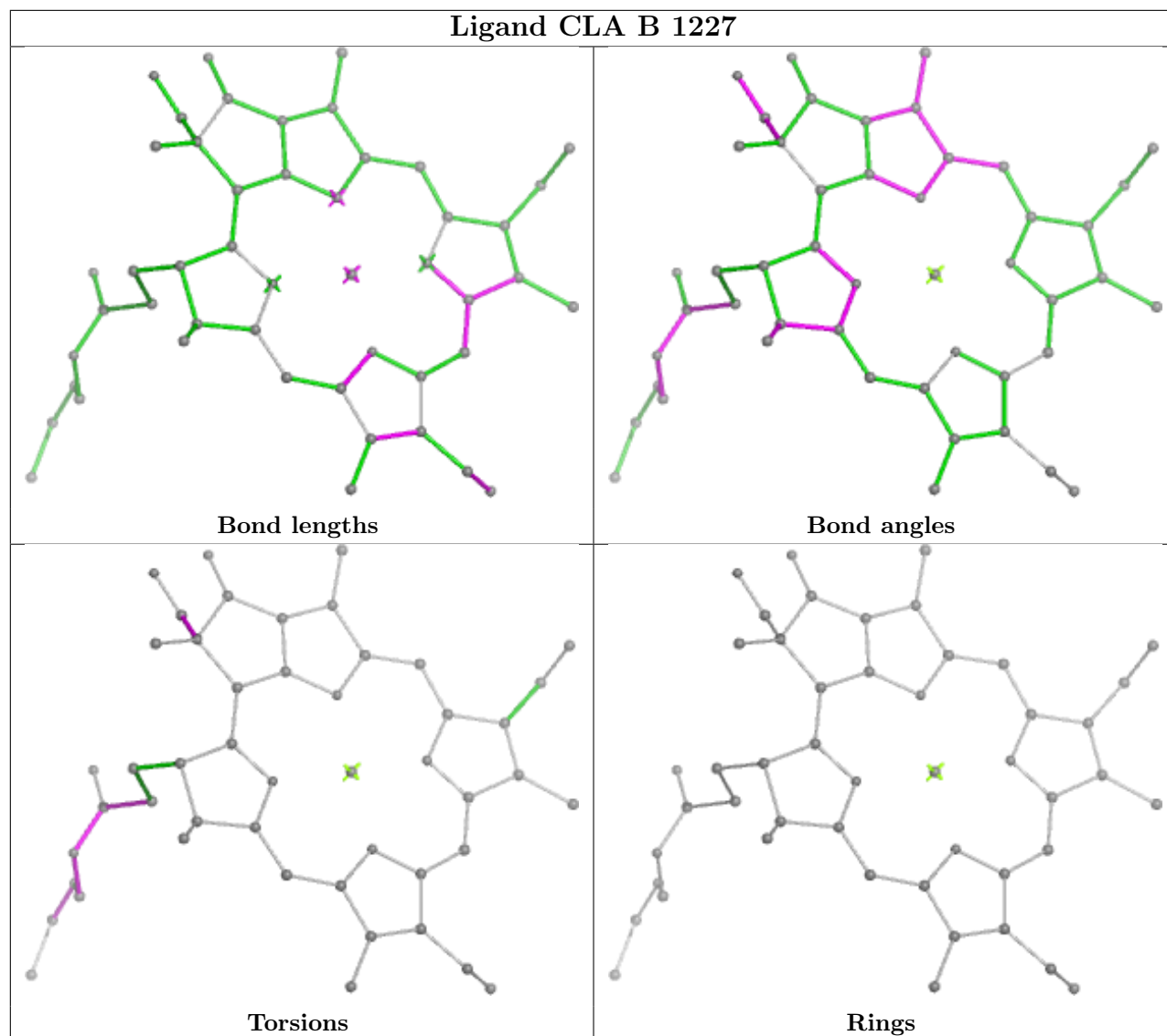
## Ligand CLA A 1141

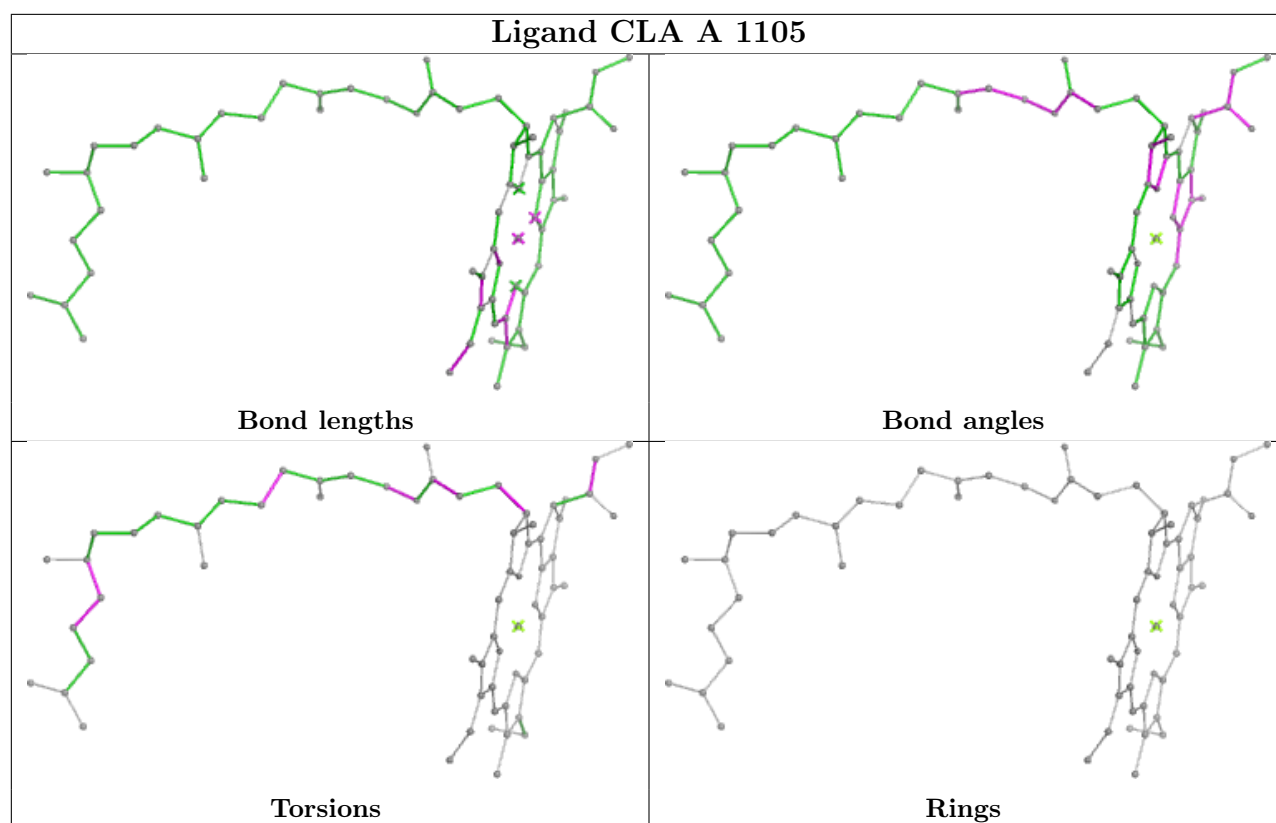


## Ligand CLA A 1136









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	751/751 (100%)	0.57	43 (5%)	30 26	27, 117, 229, 322	0
2	B	731/731 (100%)	0.48	41 (5%)	31 26	18, 95, 176, 428	0
3	C	80/80 (100%)	0.55	3 (3%)	44 34	30, 87, 122, 144	0
4	D	141/141 (100%)	0.57	13 (9%)	16 15	67, 112, 187, 399	0
5	E	69/69 (100%)	0.30	2 (2%)	54 40	45, 81, 154, 170	0
6	F	143/143 (100%)	0.46	7 (4%)	36 29	28, 98, 148, 186	0
7	I	40/40 (100%)	1.95	13 (32%)	1 2	228, 290, 404, 432	0
8	J	40/40 (100%)	0.23	1 (2%)	58 44	73, 106, 144, 149	0
9	K	70/70 (100%)	0.53	7 (10%)	14 13	150, 241, 380, 499	0
10	L	137/137 (100%)	1.03	18 (13%)	8 10	231, 373, 583, 606	0
11	M	31/31 (100%)	0.91	5 (16%)	5 8	123, 149, 199, 221	0
All	All	2233/2233 (100%)	0.57	153 (6%)	24 21	18, 108, 335, 606	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	8.3
6	F	92	GLU	8.0
7	I	8	SER	6.9
1	A	238	LEU	6.5
7	I	2	ASP	5.7
10	L	47	ILE	5.7
2	B	91	ILE	5.7
1	A	153	THR	5.4
1	A	222	PRO	5.0
2	B	23	TYR	4.9
2	B	64	THR	4.9
7	I	3	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	66	PHE	4.7
2	B	70	TRP	4.6
2	B	65	LEU	4.6
11	M	3	LEU	4.4
10	L	43	GLY	4.3
1	A	225	LYS	4.3
1	A	220	SER	4.3
1	A	481	ILE	4.2
9	K	56	ALA	4.2
3	C	2	SER	3.9
4	D	100	ALA	3.9
1	A	239	PRO	3.8
1	A	150	SER	3.8
7	I	5	TYR	3.7
1	A	241	GLU	3.7
6	F	94	LYS	3.6
2	B	61	THR	3.5
2	B	159	PRO	3.5
4	D	11	PHE	3.5
10	L	157	ASN	3.5
2	B	67	HIS	3.5
2	B	68	VAL	3.5
4	D	111	GLY	3.5
1	A	224	ASN	3.5
2	B	90	ALA	3.4
2	B	494	TRP	3.4
10	L	22	THR	3.4
11	M	2	ALA	3.4
2	B	311	PRO	3.4
5	E	31	SER	3.3
2	B	71	GLN	3.3
10	L	152	PHE	3.3
10	L	154	GLY	3.2
2	B	69	ALA	3.2
7	I	6	ALA	3.2
2	B	492	PRO	3.2
1	A	482	PHE	3.2
9	K	49	ASP	3.1
7	I	4	SER	3.1
10	L	150	GLY	3.1
9	K	86	SER	3.1
7	I	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	3.0
11	M	6	THR	2.9
4	D	101	ASP	2.9
10	L	158	HIS	2.9
1	A	214	GLY	2.9
7	I	26	THR	2.9
2	B	120	VAL	2.9
6	F	134	LYS	2.9
6	F	137	GLU	2.8
6	F	110	LYS	2.8
4	D	109	ASN	2.8
1	A	223	ILE	2.8
1	A	628	THR	2.8
9	K	58	LYS	2.8
10	L	42	LYS	2.7
2	B	116	ALA	2.7
1	A	592	PHE	2.7
1	A	485	TRP	2.7
2	B	24	GLY	2.7
9	K	85	ALA	2.7
2	B	119	GLY	2.6
7	I	15	ILE	2.6
10	L	40	TYR	2.6
1	A	7	GLU	2.6
2	B	244	PHE	2.6
1	A	299	ALA	2.6
2	B	269	TRP	2.6
10	L	83	ILE	2.6
2	B	88	ALA	2.6
2	B	403	ASP	2.5
2	B	241	GLY	2.5
2	B	57	ILE	2.5
1	A	221	MET	2.5
7	I	30	LEU	2.5
8	J	32	PHE	2.5
1	A	290	LEU	2.5
1	A	556	ALA	2.5
1	A	218	HIS	2.5
1	A	10	ALA	2.5
4	D	10	LYS	2.5
1	A	620	THR	2.5
3	C	27	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
6	F	2	ASP	2.4
7	I	27	MET	2.4
7	I	7	ALA	2.4
2	B	21	ILE	2.4
9	K	81	VAL	2.4
2	B	236	ASP	2.4
2	B	63	GLY	2.4
7	I	40	GLY	2.4
5	E	14	THR	2.4
11	M	4	SER	2.4
2	B	1	MET	2.3
2	B	124	PHE	2.3
2	B	187	SER	2.3
9	K	57	SER	2.3
1	A	279	GLY	2.3
10	L	94	ALA	2.3
2	B	100	ALA	2.3
4	D	110	GLU	2.3
11	M	8	ILE	2.2
1	A	596	PHE	2.2
2	B	160	LYS	2.2
6	F	141	SER	2.2
1	A	235	ASP	2.2
2	B	480	ASP	2.2
1	A	636	ALA	2.2
1	A	217	ILE	2.2
1	A	313	THR	2.2
1	A	170	ALA	2.2
1	A	317	ILE	2.2
1	A	479	GLN	2.1
1	A	189	TRP	2.1
1	A	291	SER	2.1
1	A	619	GLY	2.1
1	A	8	ARG	2.1
4	D	113	GLU	2.1
2	B	683	PRO	2.1
4	D	48	ALA	2.1
4	D	20	SER	2.1
2	B	490	TRP	2.1
3	C	47	ASP	2.1
10	L	23	PRO	2.1
4	D	123	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
10	L	34	ILE	2.1
1	A	335	GLU	2.1
2	B	2	ALA	2.1
10	L	95	ALA	2.1
1	A	1	MET	2.0
2	B	89	HIS	2.0
10	L	146	SER	2.0
1	A	192	ASN	2.0
1	A	503	ALA	2.0
4	D	16	GLY	2.0
2	B	121	TYR	2.0
2	B	136	TYR	2.0
10	L	156	PHE	2.0
4	D	21	LYS	2.0
10	L	28	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	CLA	L	1502	49/65	0.22	0.22	382,393,407,412	0
16	LHG	B	5006	21/49	0.39	0.20	154,179,195,201	0
20	LMG	B	5005	55/55	0.51	0.18	80,149,188,190	0
21	SQD	B	5008	54/54	0.53	0.21	92,154,193,201	0
25	EQ3	I	4020	42/42	0.53	0.27	224,232,241,245	0
24	LMT	F	6001	35/35	0.58	0.18	78,142,171,178	0
15	BCR	K	4001	40/40	0.68	0.17	129,194,221,223	0
19	ECH	M	4021	41/41	0.72	0.28	148,166,189,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	SQD	F	5001	54/54	0.72	0.26	149,164,176,178	0
15	BCR	A	4001	40/40	0.74	0.24	148,169,184,185	0
12	CLA	B	1207	49/65	0.77	0.19	131,157,223,227	0
12	CLA	K	1401	45/65	0.77	0.14	127,147,170,175	0
12	CLA	A	1113	49/65	0.77	0.16	135,160,184,192	0
12	CLA	B	1240	49/65	0.78	0.18	76,105,156,163	0
15	BCR	I	4018	40/40	0.79	0.30	161,194,217,223	0
12	CLA	B	1219	49/65	0.79	0.15	64,91,133,135	0
15	BCR	A	4003	40/40	0.79	0.35	124,164,188,189	0
12	CLA	B	1217	49/65	0.80	0.14	72,85,95,103	0
12	CLA	J	1303	49/65	0.80	0.15	145,167,176,202	0
22	CA	L	1001	1/1	0.80	0.08	156,156,156,156	0
12	CLA	A	1115	56/65	0.80	0.15	118,146,155,156	0
12	CLA	K	1402	49/65	0.80	0.16	168,189,213,218	0
12	CLA	F	1302	49/65	0.81	0.15	63,82,106,112	0
12	CLA	B	1212	49/65	0.81	0.15	124,146,166,171	0
12	CLA	B	1204	49/65	0.81	0.17	94,111,127,139	0
16	LHG	A	5003	49/49	0.81	0.17	106,135,156,160	0
12	CLA	A	1114	49/65	0.82	0.15	142,154,173,178	0
19	ECH	B	4006	41/41	0.82	0.27	111,135,146,150	0
12	CLA	J	1302	49/65	0.82	0.16	134,150,159,160	0
12	CLA	A	1133	49/65	0.83	0.17	98,115,131,133	0
15	BCR	B	4004	40/40	0.83	0.16	105,125,134,138	0
12	CLA	B	1209	49/65	0.84	0.15	107,131,139,144	0
12	CLA	A	1120	49/65	0.84	0.17	130,149,195,200	0
12	CLA	A	1108	49/65	0.85	0.14	89,101,135,142	0
12	CLA	B	1208	49/65	0.85	0.14	90,107,128,130	0
12	CLA	A	1130	49/65	0.85	0.15	77,95,130,133	0
12	CLA	A	1112	49/65	0.85	0.18	138,146,155,164	0
23	C7Z	F	4016	42/42	0.85	0.17	35,58,93,97	0
12	CLA	B	1213	49/65	0.85	0.14	105,121,132,141	0
12	CLA	B	1216	49/65	0.85	0.15	58,113,119,124	0
20	LMG	B	5002	55/55	0.86	0.20	37,69,102,118	0
12	CLA	A	1105	65/65	0.86	0.17	66,114,126,130	0
12	CLA	B	1201	49/65	0.86	0.14	77,89,106,110	0
12	CLA	A	1011	55/65	0.86	0.19	43,63,72,89	0
12	CLA	A	1111	49/65	0.86	0.20	70,113,131,146	0
12	CLA	A	1141	45/65	0.86	0.13	137,156,176,188	0
15	BCR	A	4007	40/40	0.86	0.16	66,82,134,137	0
15	BCR	A	4008	40/40	0.86	0.22	43,110,125,125	0
12	CLA	B	1211	49/65	0.87	0.18	100,120,130,134	0
12	CLA	A	1129	49/65	0.87	0.17	96,116,153,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	CLA	A	1119	46/65	0.87	0.19	106,126,144,154	0
15	BCR	A	4012	40/40	0.87	0.21	66,81,92,93	0
12	CLA	A	1134	49/65	0.87	0.13	109,140,149,156	0
15	BCR	B	4017	40/40	0.87	0.23	50,68,88,91	0
12	CLA	A	1118	50/65	0.87	0.18	120,151,195,209	0
12	CLA	B	1218	49/65	0.87	0.13	64,90,122,130	0
12	CLA	A	1121	49/65	0.87	0.13	90,117,137,142	0
12	CLA	B	1226	49/65	0.87	0.17	29,59,81,85	0
12	CLA	B	1234	60/65	0.88	0.18	55,77,106,112	0
12	CLA	A	1122	49/65	0.88	0.16	90,108,122,124	0
12	CLA	A	1110	49/65	0.88	0.19	130,154,173,179	0
22	CA	B	6001	1/1	0.88	0.12	171,171,171,171	0
12	CLA	A	1135	49/65	0.88	0.17	110,119,124,128	0
15	BCR	B	4005	40/40	0.88	0.18	31,63,141,143	0
12	CLA	B	1203	49/65	0.88	0.18	75,86,99,103	0
15	BCR	B	4018	40/40	0.88	0.20	61,121,136,140	0
15	BCR	B	4010	40/40	0.89	0.17	43,57,71,73	0
12	CLA	F	1301	49/65	0.89	0.17	80,98,136,138	0
12	CLA	A	1125	49/65	0.89	0.19	108,124,132,135	0
12	CLA	B	1205	49/65	0.89	0.19	57,73,97,106	0
15	BCR	J	4013	40/40	0.89	0.21	88,110,132,133	0
12	CLA	A	1132	55/65	0.89	0.17	107,148,273,351	0
12	CLA	B	1228	49/65	0.89	0.14	56,67,96,97	0
16	LHG	B	5004	49/49	0.89	0.18	57,80,128,133	0
12	CLA	A	1136	49/65	0.89	0.14	128,139,145,149	0
12	CLA	A	1131	49/65	0.89	0.16	111,130,156,163	0
12	CLA	A	1102	65/65	0.90	0.14	70,86,98,104	0
12	CLA	A	1109	65/65	0.90	0.14	64,113,123,126	0
12	CLA	B	1021	65/65	0.90	0.17	22,41,55,65	0
12	CLA	B	1022	60/65	0.90	0.17	31,89,94,102	0
12	CLA	B	1220	49/65	0.90	0.16	77,91,96,98	0
12	CLA	B	1221	49/65	0.90	0.17	60,105,115,122	0
12	CLA	A	1116	49/65	0.90	0.19	96,126,142,150	0
12	CLA	A	1137	49/65	0.90	0.15	92,112,121,126	0
13	PQN	B	2002	33/33	0.90	0.20	72,83,105,111	0
12	CLA	A	1107	50/65	0.90	0.13	42,53,69,94	0
12	CLA	B	1235	65/65	0.90	0.17	37,60,72,74	0
12	CLA	B	1239	49/65	0.90	0.16	36,61,108,114	0
12	CLA	B	1215	49/65	0.91	0.20	67,79,87,89	0
12	CLA	B	1238	49/65	0.91	0.18	82,108,125,127	0
17	45D	B	4011	42/42	0.91	0.18	45,59,68,68	0
12	CLA	B	1222	50/65	0.91	0.15	69,81,93,97	0

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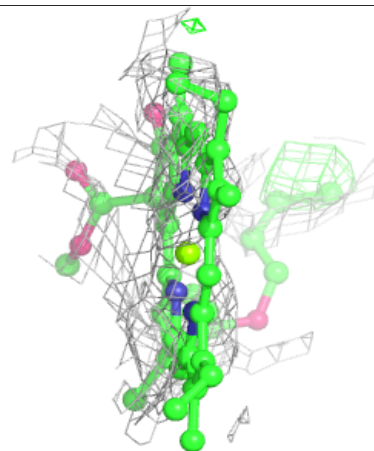
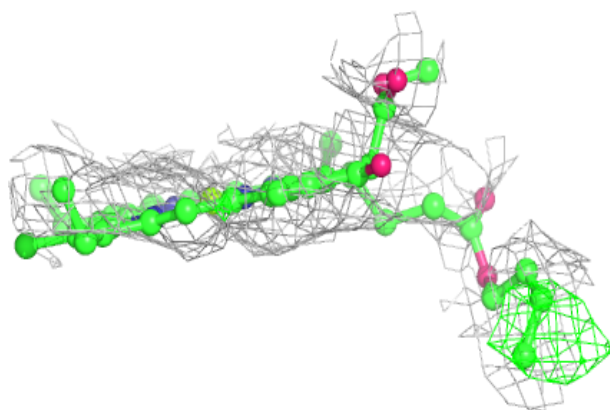
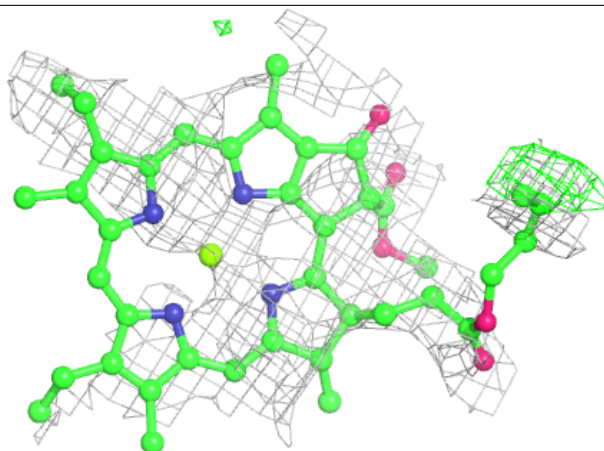
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	CLA	B	1224	55/65	0.91	0.17	13,49,70,75	0
12	CLA	B	1225	49/65	0.91	0.15	36,61,78,80	0
12	CLA	A	1101	49/65	0.91	0.15	52,74,79,86	0
12	CLA	B	1227	49/65	0.91	0.15	80,91,140,146	0
12	CLA	A	1140	65/65	0.91	0.16	16,65,78,88	0
15	BCR	F	4014	40/40	0.91	0.21	57,85,104,106	0
12	CLA	A	1013	65/65	0.91	0.17	19,57,67,79	0
12	CLA	B	1237	49/65	0.91	0.16	92,112,121,127	0
12	CLA	B	1236	49/65	0.91	0.16	49,63,76,77	0
12	CLA	B	1214	60/65	0.91	0.16	46,80,102,105	0
12	CLA	A	1117	49/65	0.92	0.18	78,99,110,116	0
12	CLA	A	1126	60/65	0.92	0.17	28,79,96,102	0
12	CLA	B	1206	49/65	0.92	0.14	75,86,127,132	0
12	CLA	A	1128	65/65	0.92	0.17	32,87,97,104	0
12	CLA	B	1202	65/65	0.92	0.13	12,70,77,79	0
12	CLA	B	1229	55/65	0.92	0.14	33,44,62,64	0
16	LHG	A	5001	49/49	0.92	0.17	38,59,91,113	0
12	CLA	B	1230	49/65	0.92	0.12	66,77,81,86	0
12	CLA	B	1232	49/65	0.92	0.10	70,82,98,101	0
23	C7Z	J	4015	42/42	0.92	0.16	60,87,96,101	0
12	CLA	A	1012	49/65	0.92	0.16	38,63,73,74	0
12	CLA	B	1223	49/65	0.92	0.20	81,96,110,113	0
12	CLA	B	1210	49/65	0.93	0.10	42,72,80,82	0
12	CLA	A	1123	60/65	0.93	0.17	67,85,100,104	0
12	CLA	A	1127	49/65	0.93	0.17	72,86,97,103	0
18	CL	B	6000	1/1	0.93	0.08	89,89,89,89	0
12	CLA	B	1231	49/65	0.93	0.15	49,85,97,109	0
12	CLA	A	1139	55/65	0.93	0.19	43,59,110,117	0
12	CLA	A	1124	49/65	0.93	0.17	100,122,134,135	0
12	CLA	A	1103	49/65	0.93	0.16	75,90,108,114	0
12	CLA	A	1106	65/65	0.94	0.16	72,95,117,130	0
12	CLA	B	1023	49/65	0.94	0.14	65,80,89,93	0
13	PQN	A	2001	33/33	0.94	0.14	13,27,42,50	0
12	CLA	A	1104	49/65	0.94	0.12	60,85,96,101	0
12	CLA	A	1138	65/65	0.95	0.13	26,55,72,76	0
14	SF4	A	3001	8/8	0.98	0.08	36,63,86,101	0
14	SF4	C	3002	8/8	0.99	0.05	32,41,89,113	0
14	SF4	C	3003	8/8	0.99	0.11	32,57,177,197	0

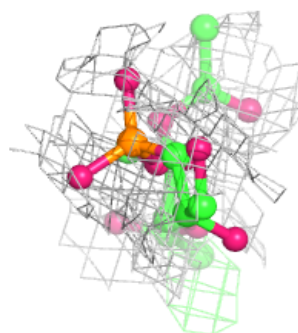
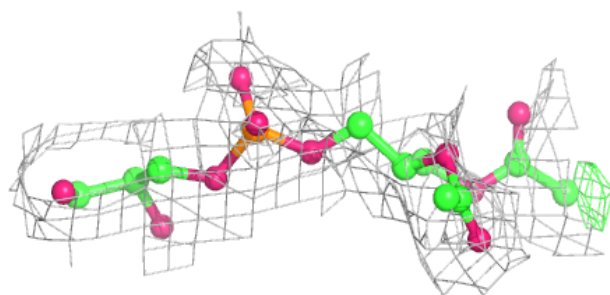
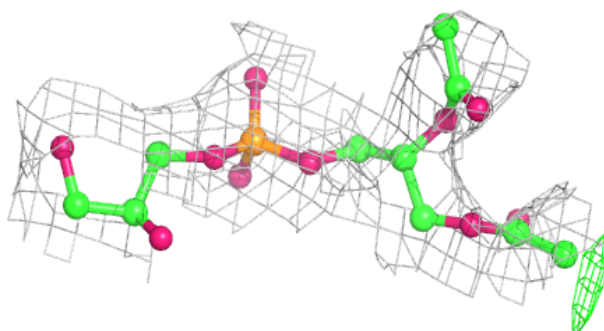
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CLA L 1502:**

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

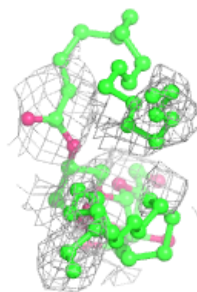
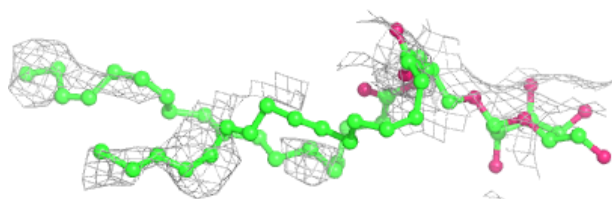
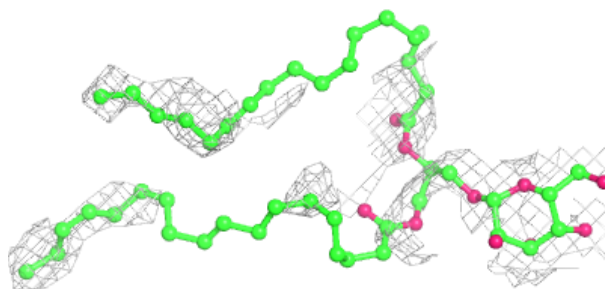
**Electron density around LHG B 5006:**

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

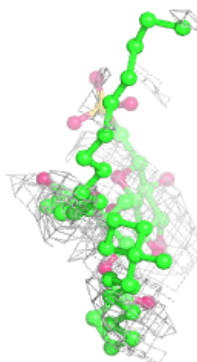
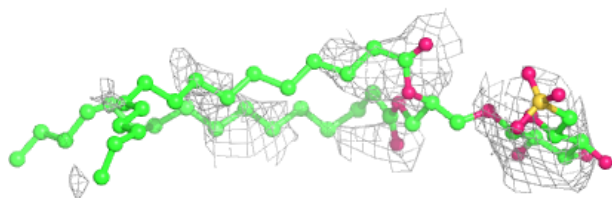
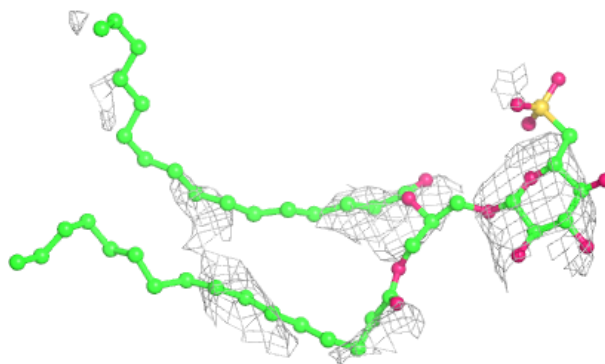


**Electron density around LMG B 5005:**

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

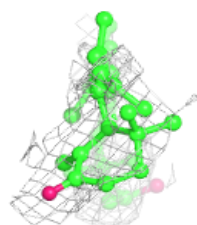
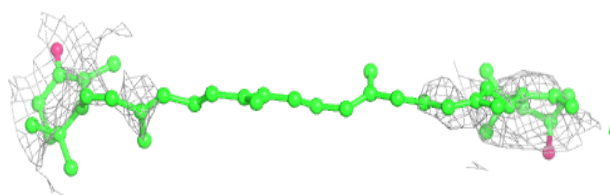
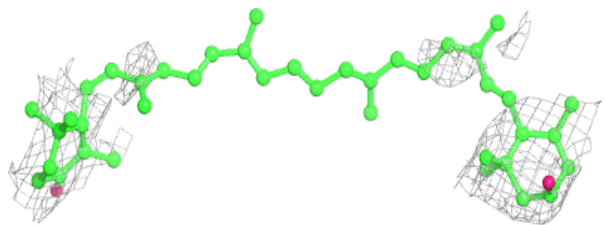
**Electron density around SQD B 5008:**

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

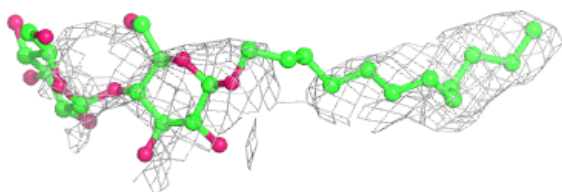
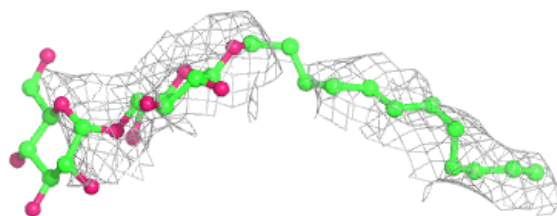


**Electron density around EQ3 I 4020:**

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and green (positive)

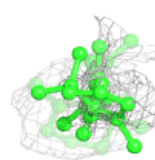
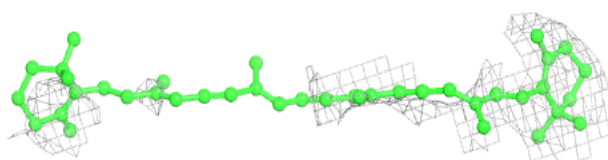
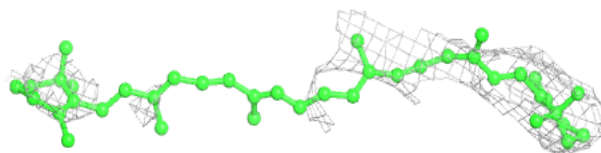
**Electron density around LMT F 6001:**

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

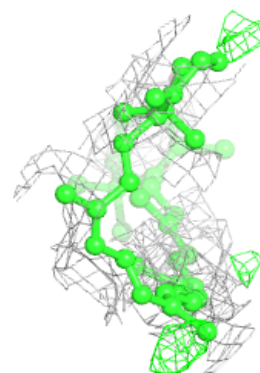
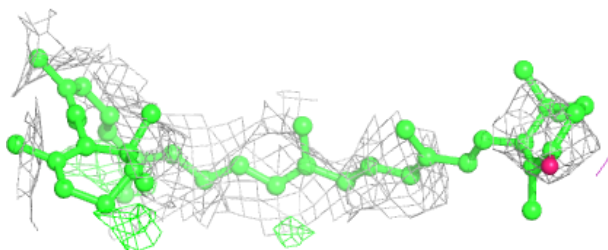
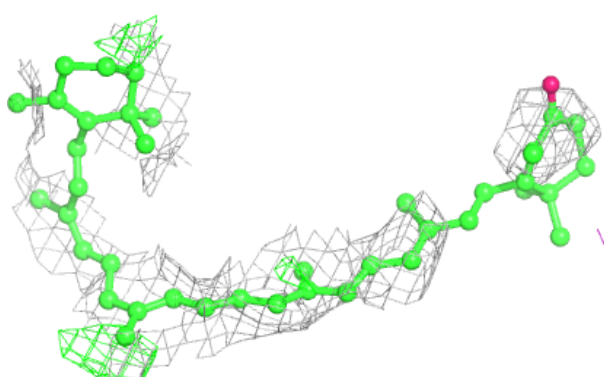


**Electron density around BCR K 4001:**

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

**Electron density around ECH M 4021:**

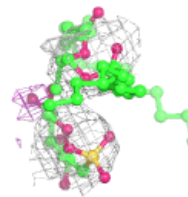
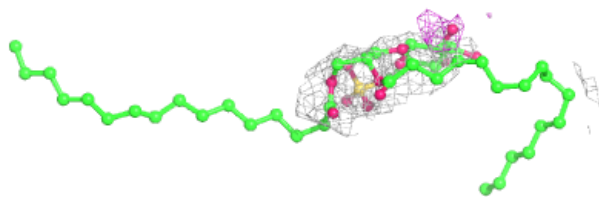
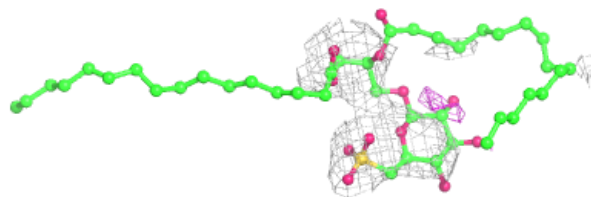
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



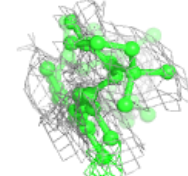
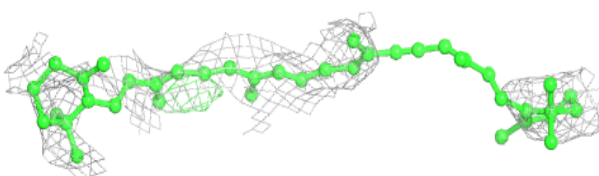
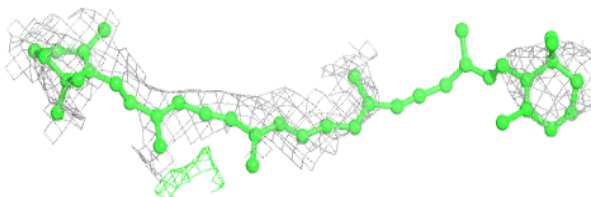


**Electron density around SQD F 5001:**

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

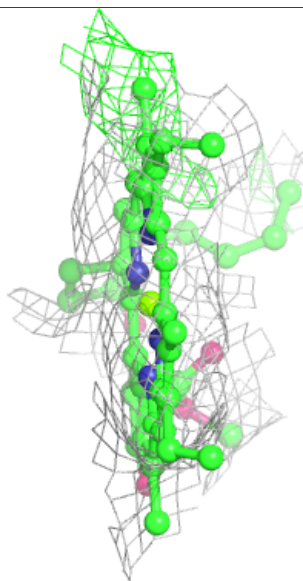
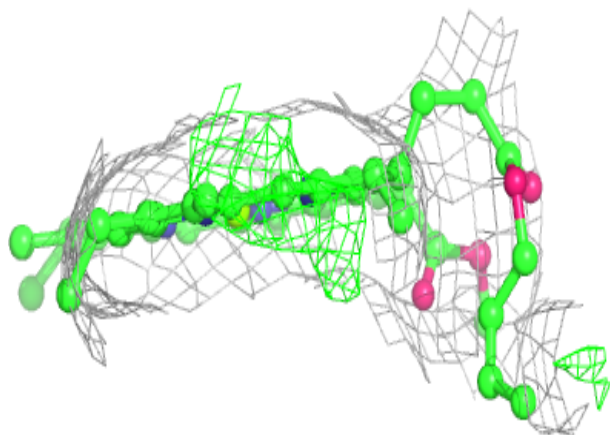
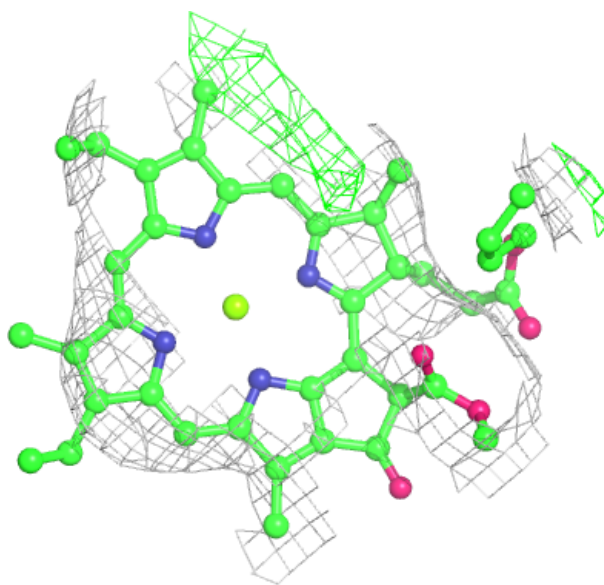
**Electron density around BCR A 4001:**

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



**Electron density around CLA B 1207:**

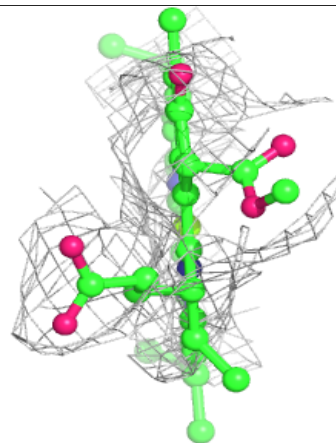
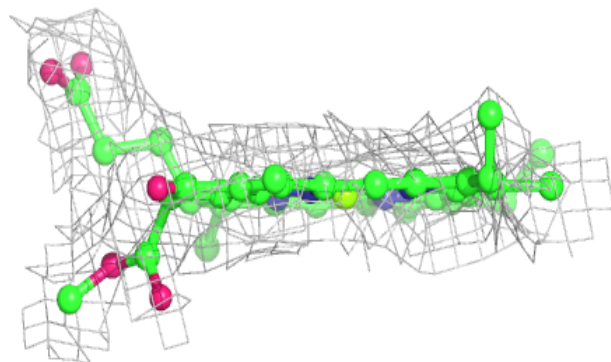
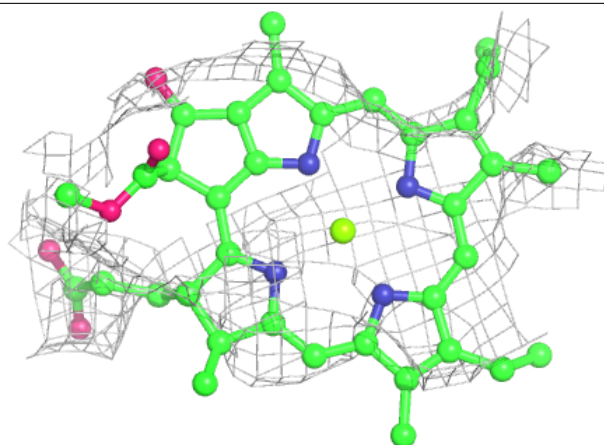
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





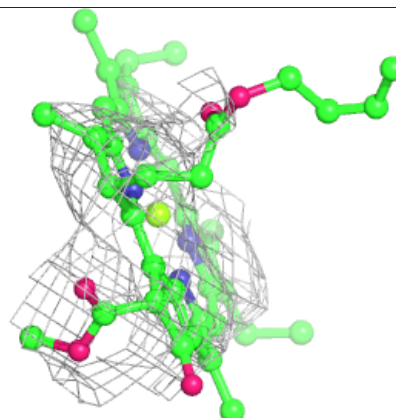
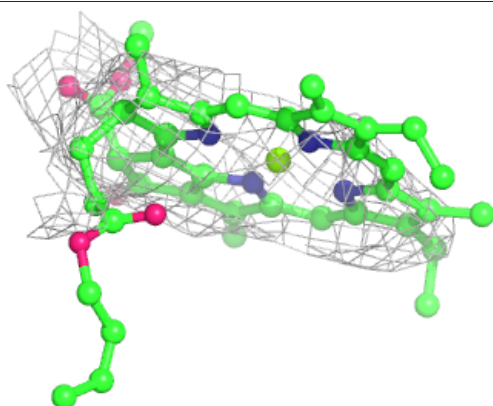
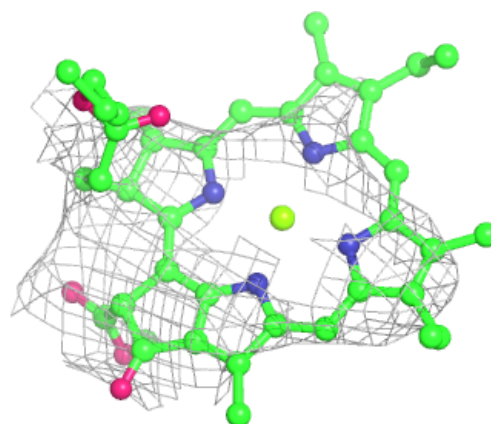
**Electron density around CLA K 1401:**

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

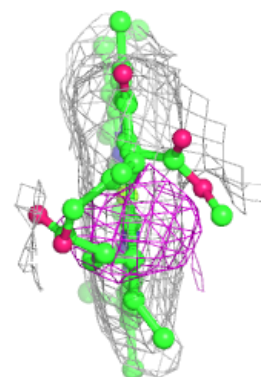
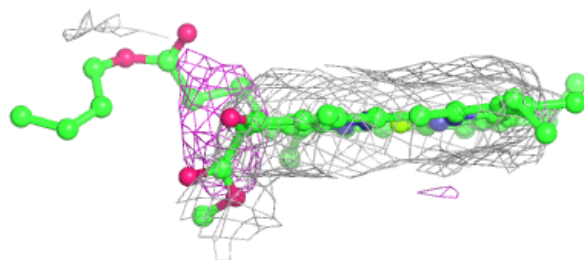
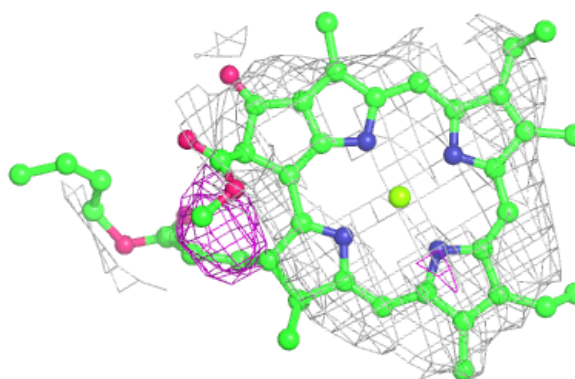


**Electron density around CLA A 1113:**

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

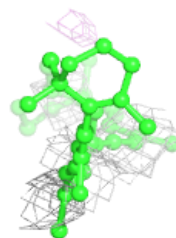
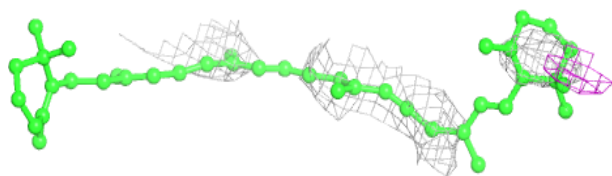
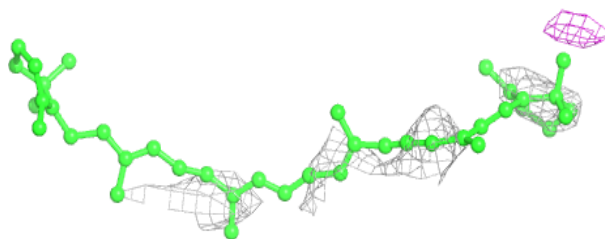
**Electron density around CLA B 1240:**

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

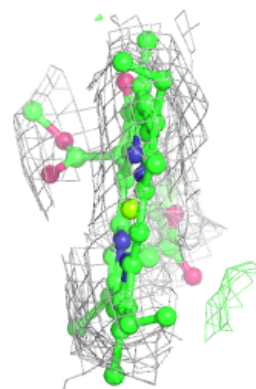
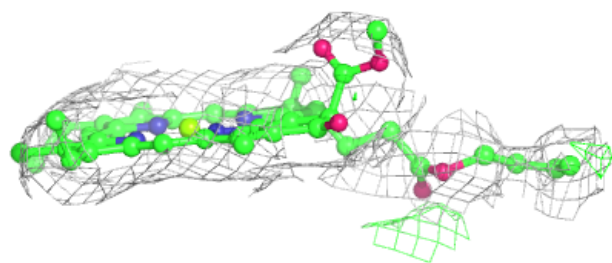
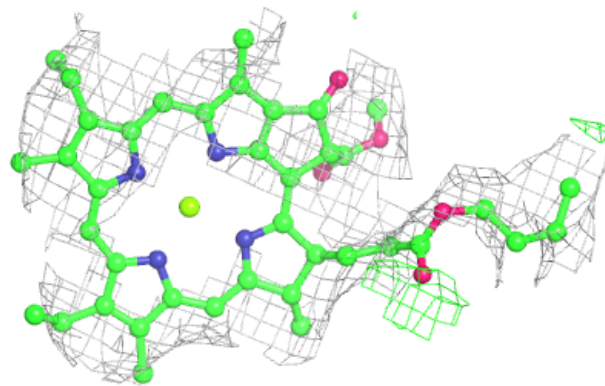


**Electron density around BCR I 4018:**

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

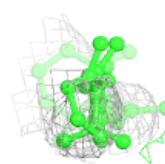
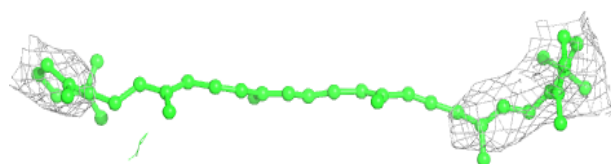
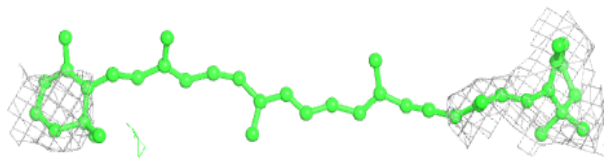
**Electron density around CLA B 1219:**

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



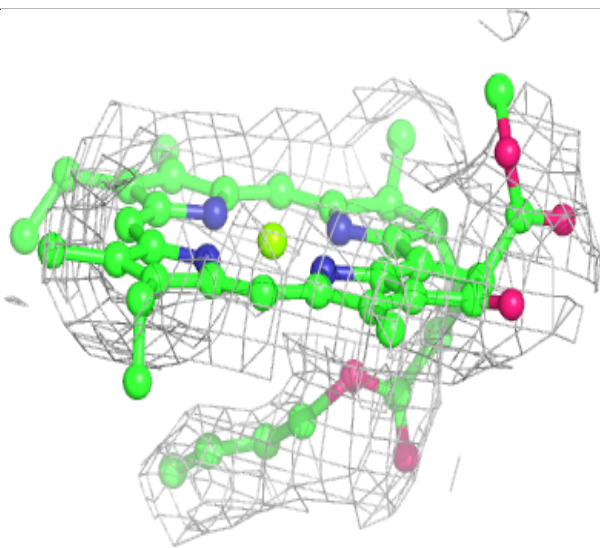
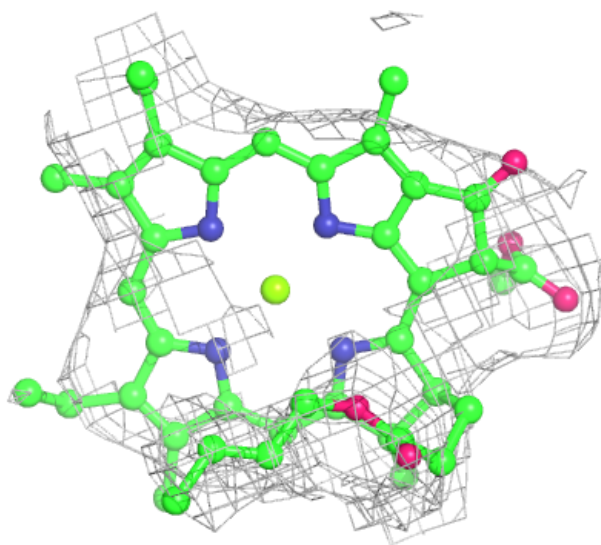
**Electron density around BCR A 4003:**

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



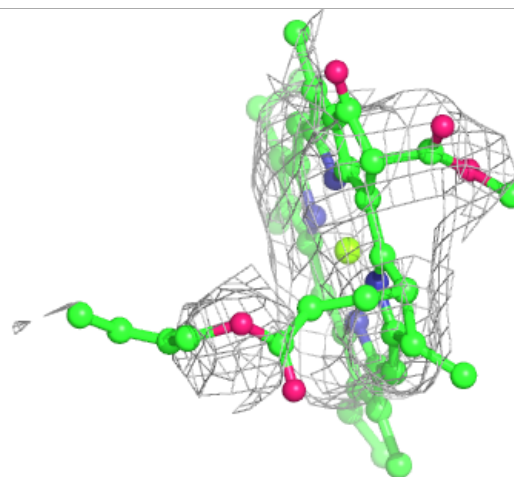
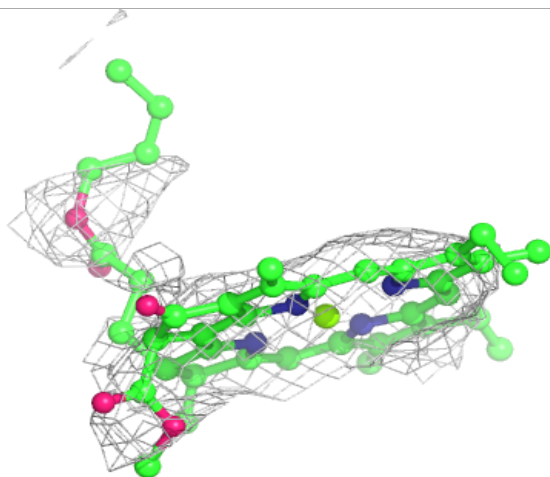
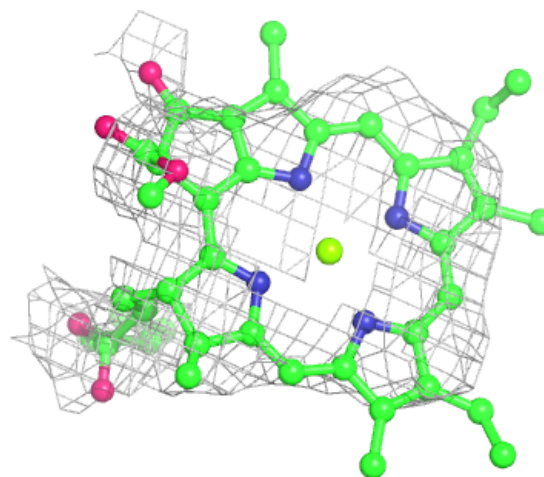
**Electron density around CLA B 1217:**

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



**Electron density around CLA J 1303:**

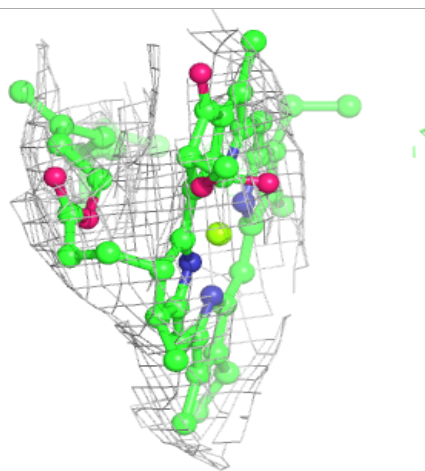
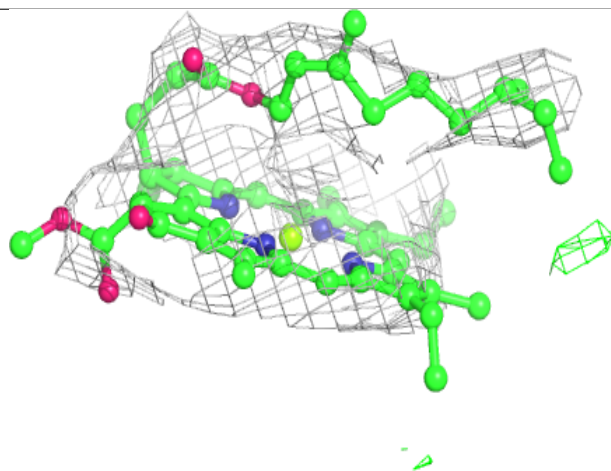
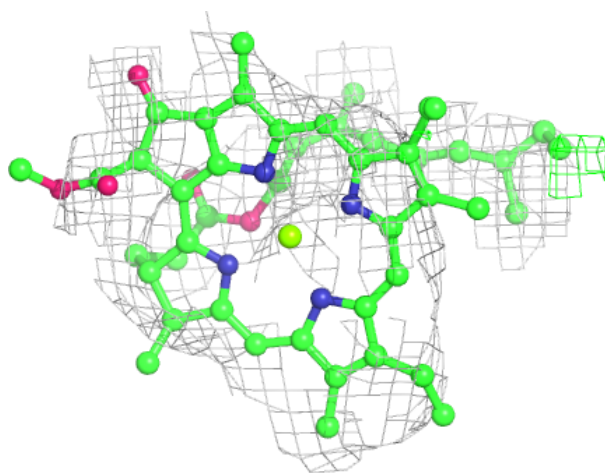
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





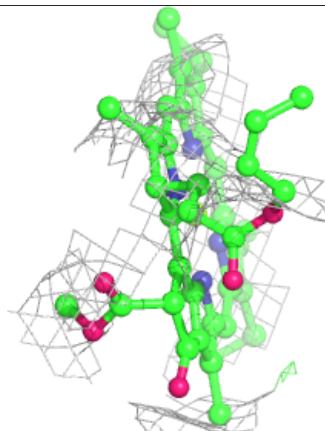
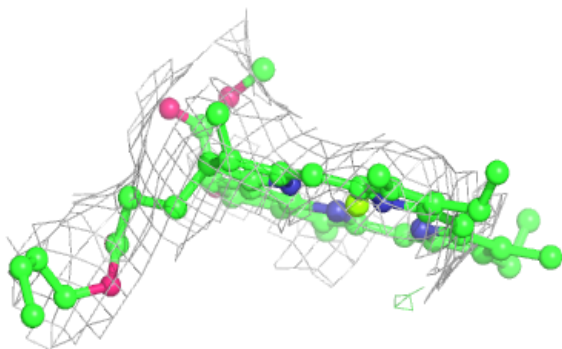
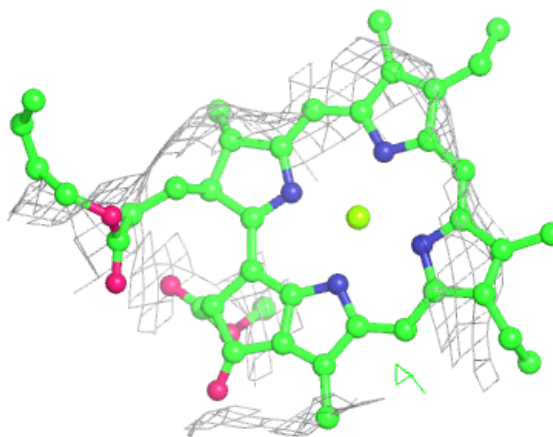
**Electron density around CLA A 1115:**

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



**Electron density around CLA K 1402:**

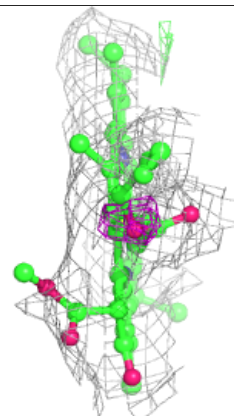
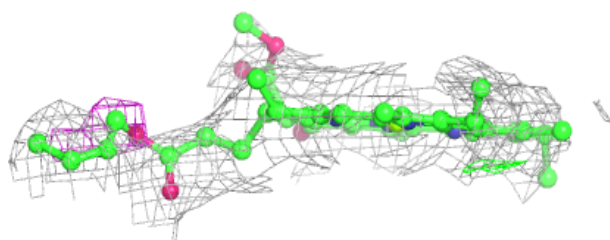
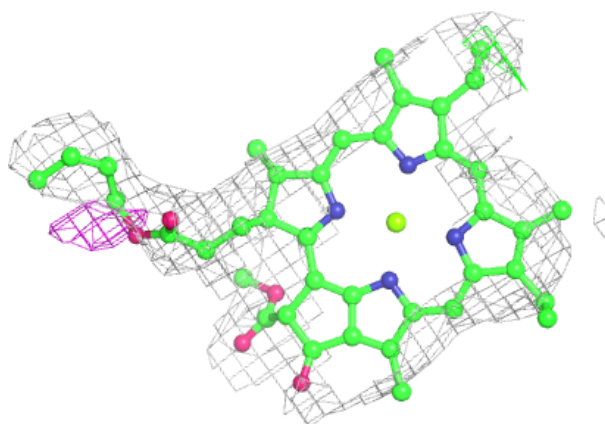
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





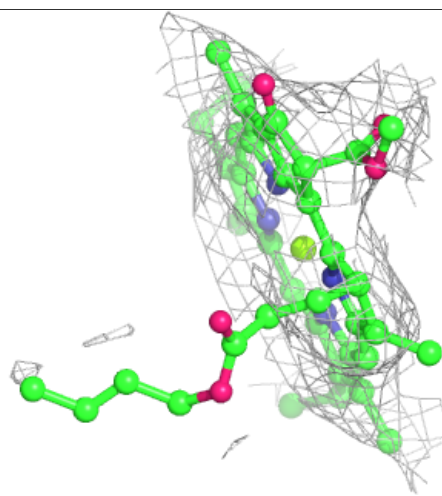
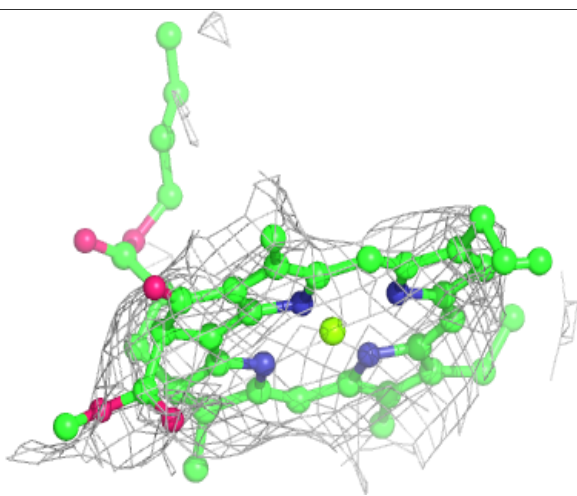
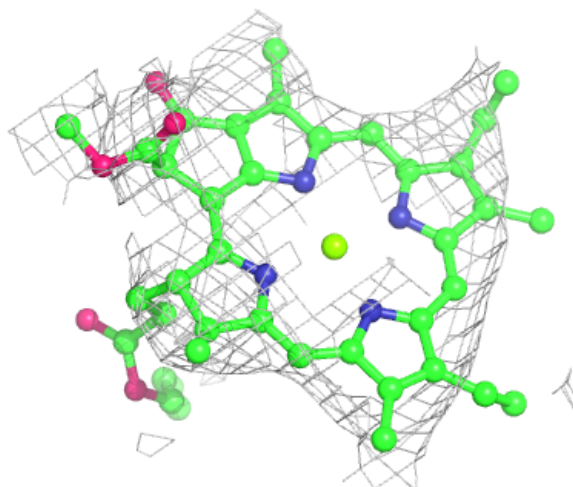
**Electron density around CLA F 1302:**

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



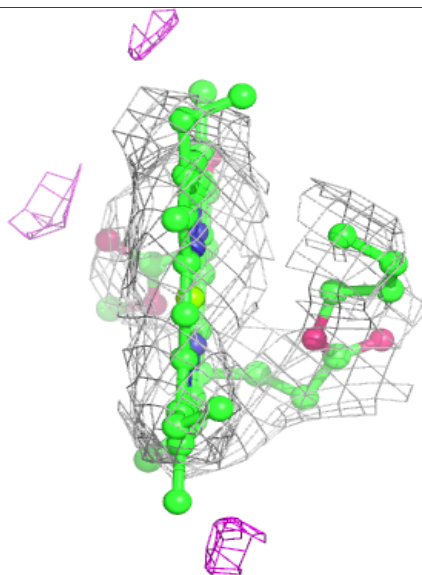
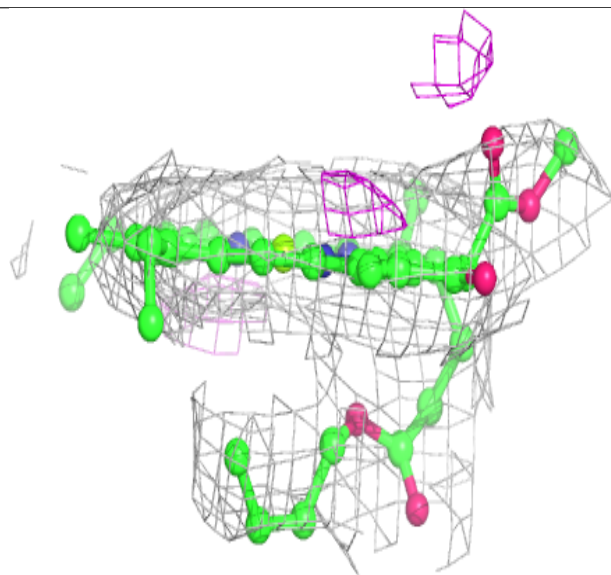
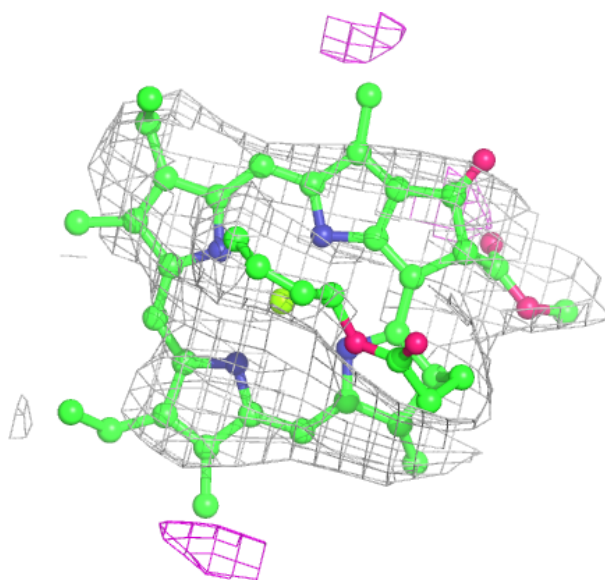
**Electron density around CLA B 1212:**

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



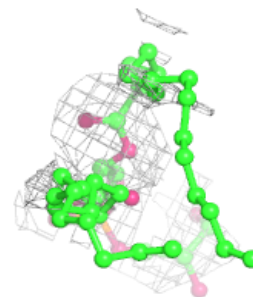
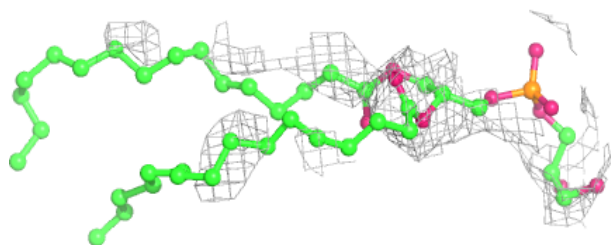
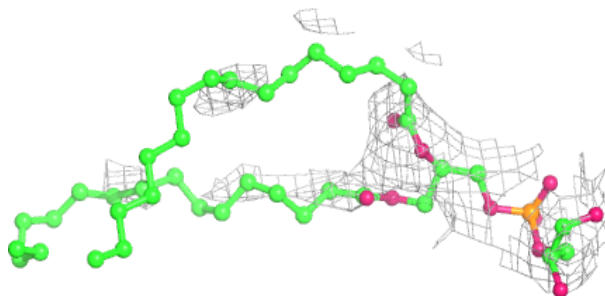
**Electron density around CLA B 1204:**

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



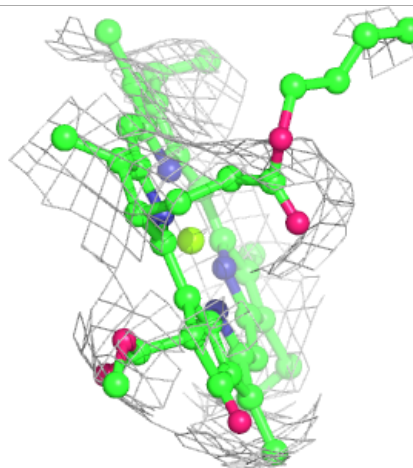
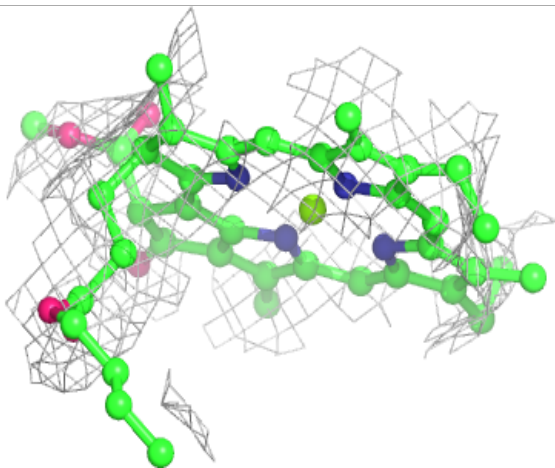
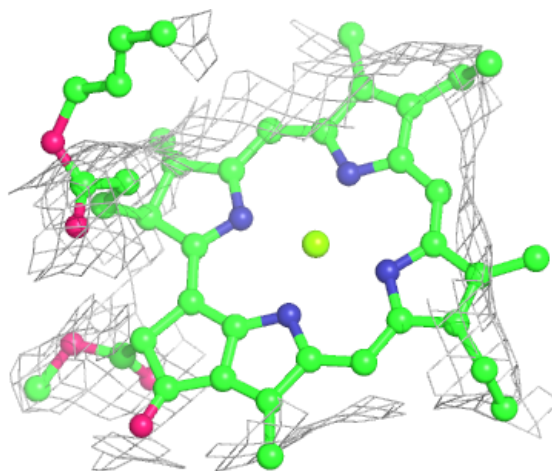
**Electron density around LHG A 5003:**

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



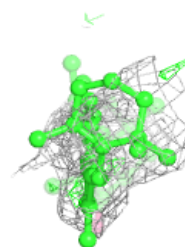
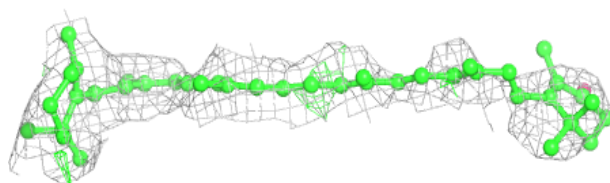
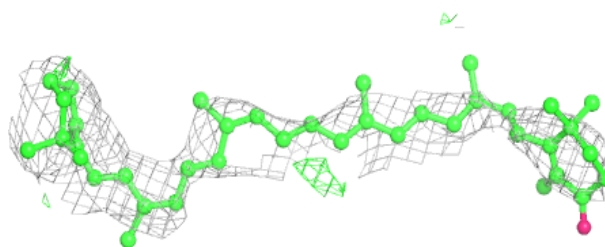
**Electron density around CLA A 1114:**

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



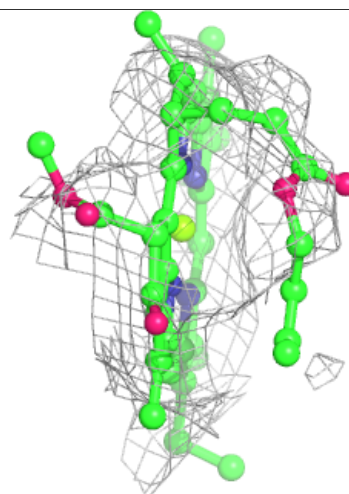
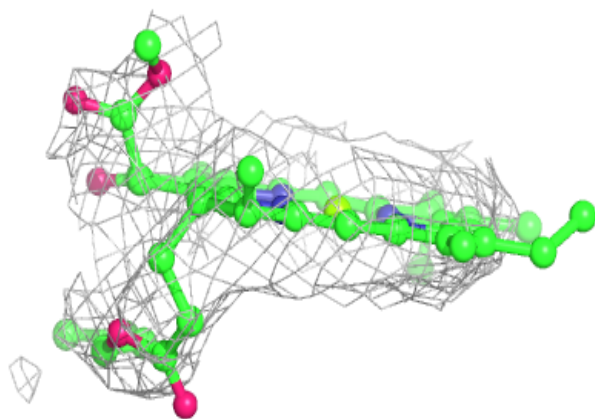
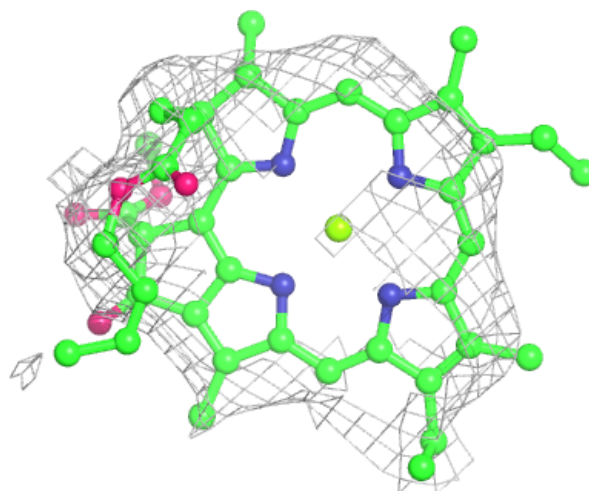
**Electron density around ECH B 4006:**

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



**Electron density around CLA J 1302:**

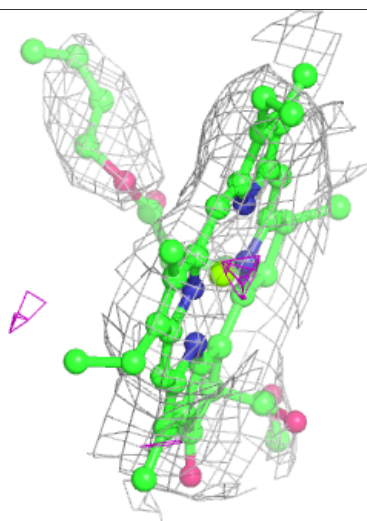
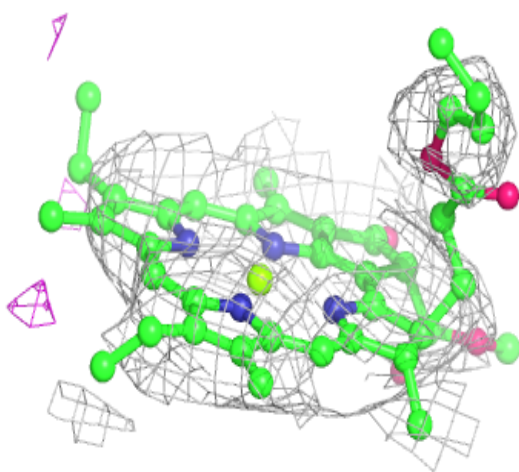
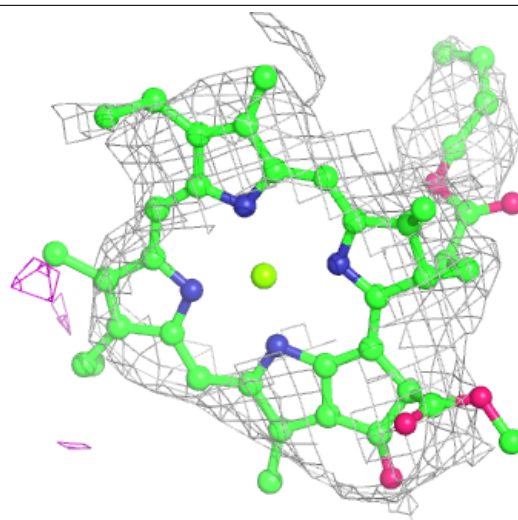
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 1133:**

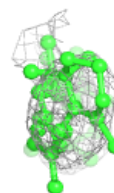
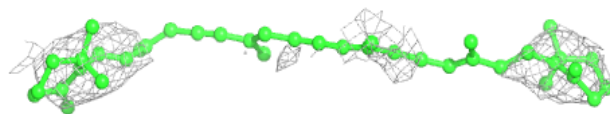
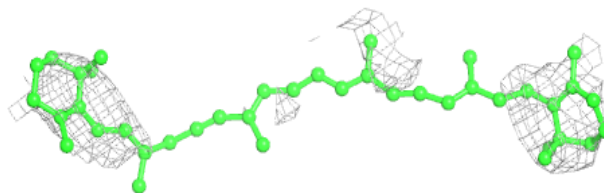
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





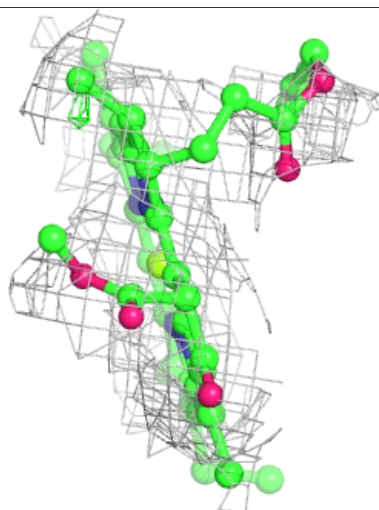
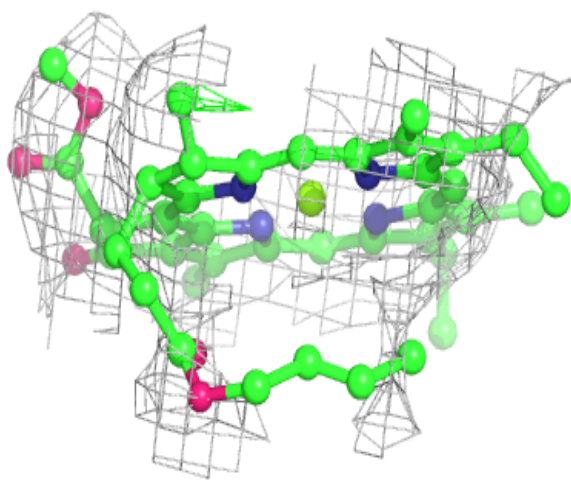
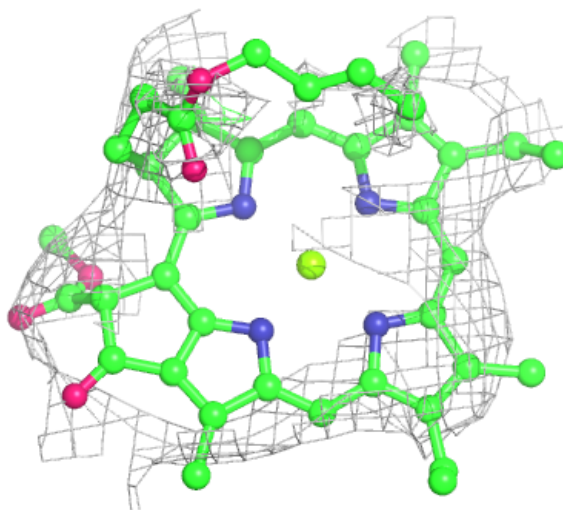
**Electron density around BCR B 4004:**

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



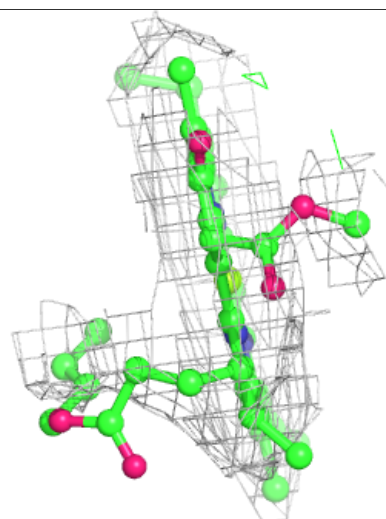
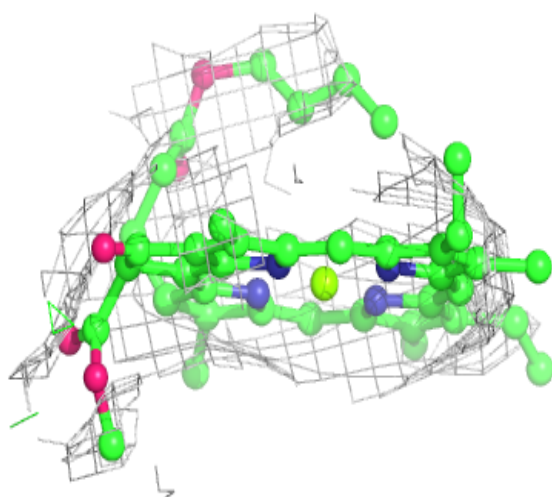
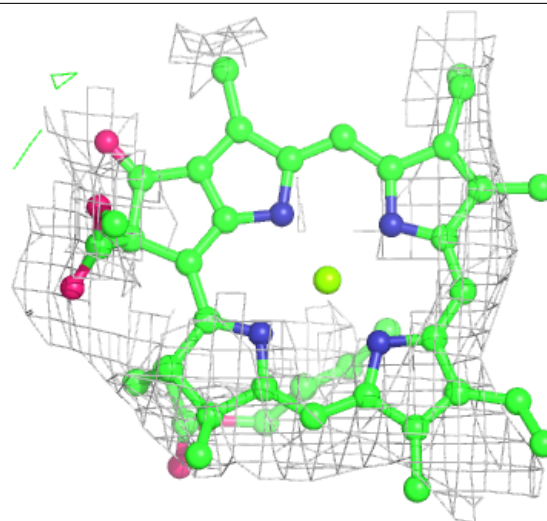
**Electron density around CLA B 1209:**

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



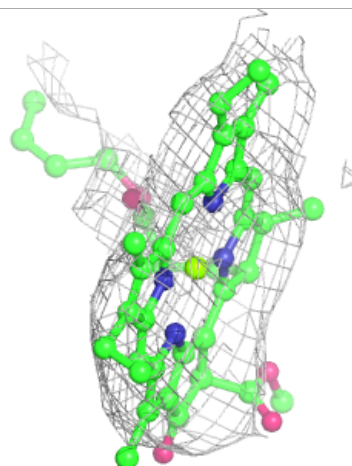
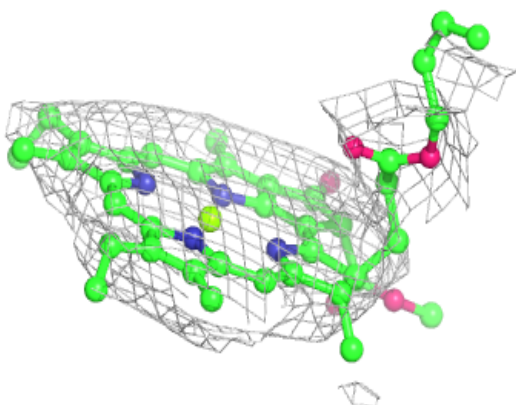
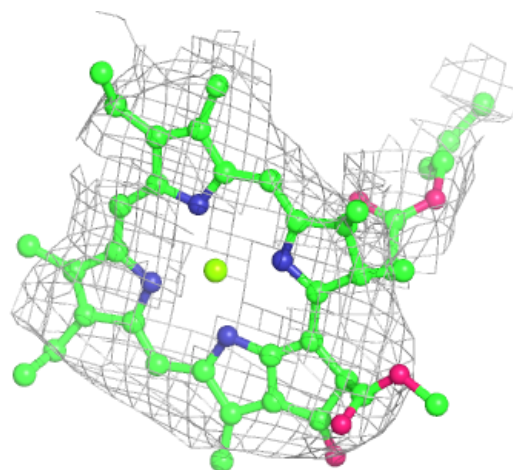
**Electron density around CLA A 1120:**

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



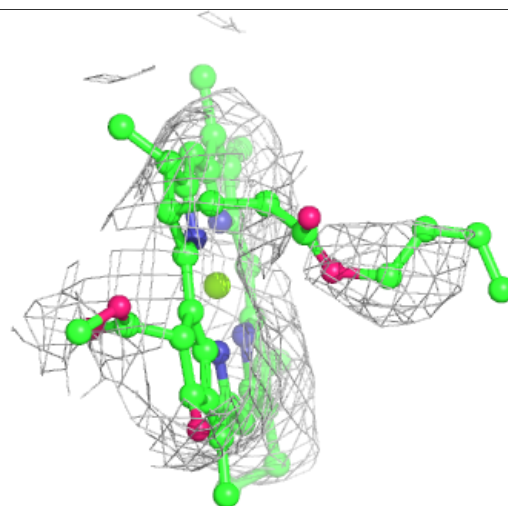
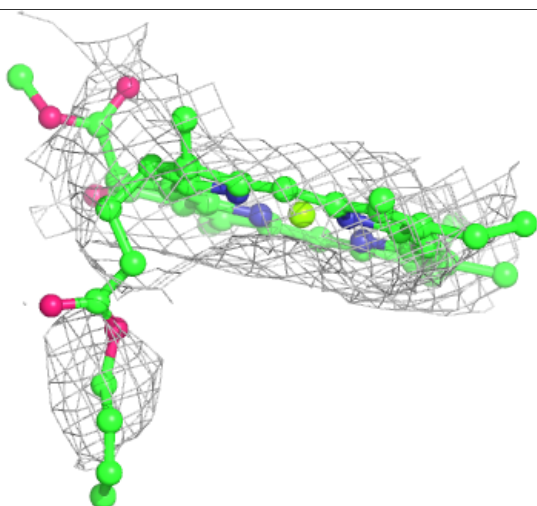
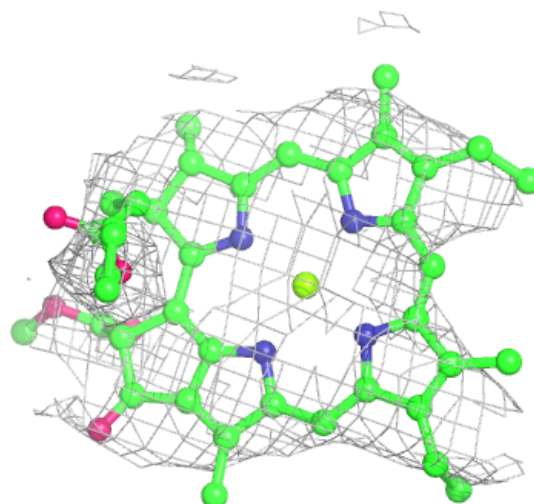
**Electron density around CLA A 1108:**

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



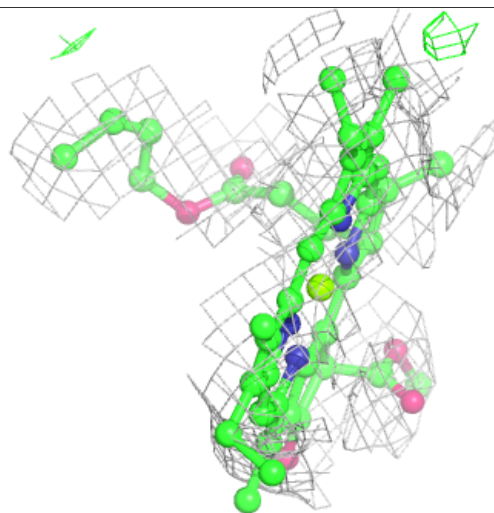
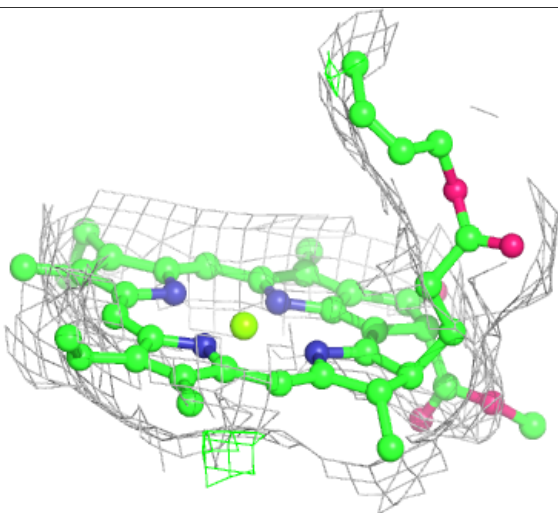
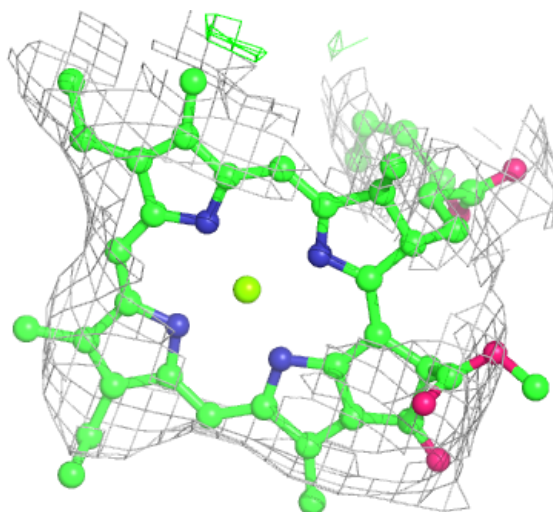
**Electron density around CLA B 1208:**

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



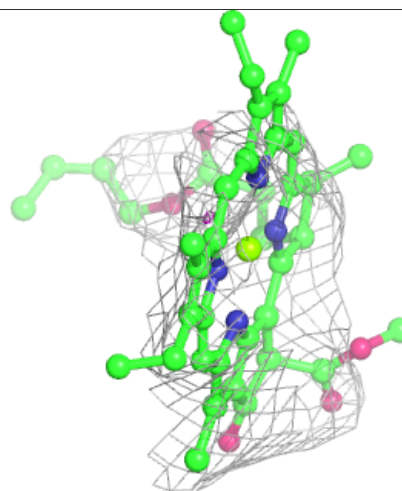
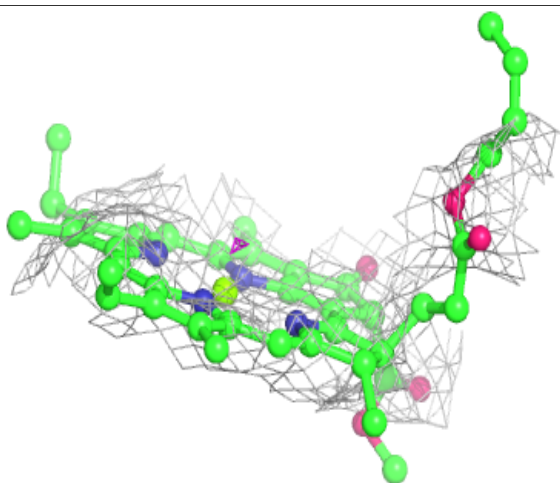
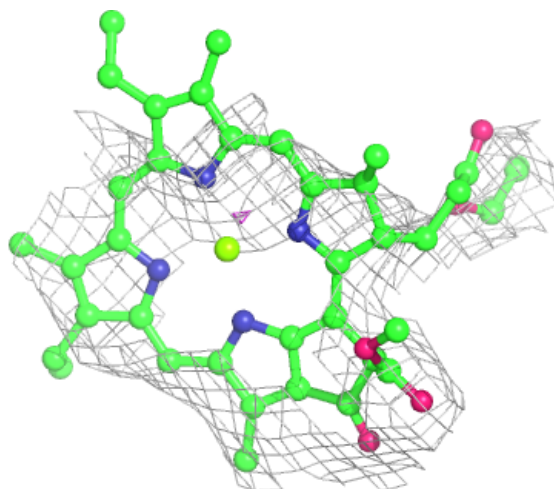
**Electron density around CLA A 1130:**

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



**Electron density around CLA A 1112:**

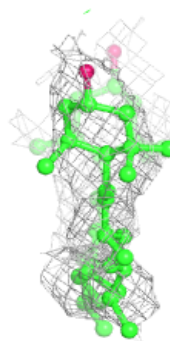
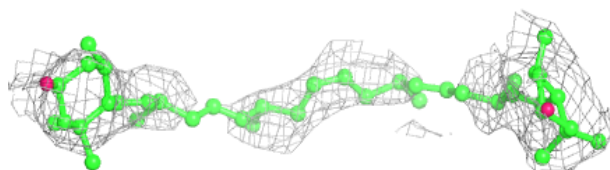
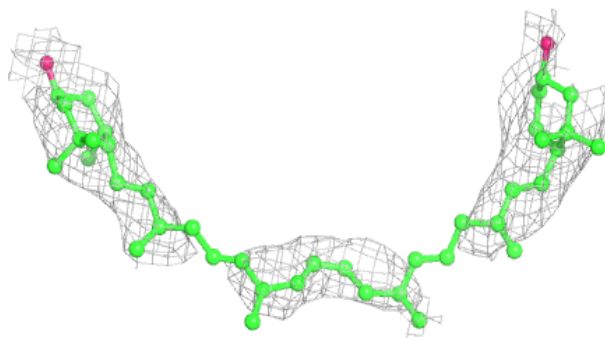
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around C7Z F 4016:**

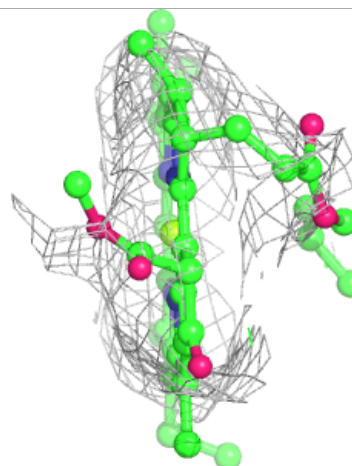
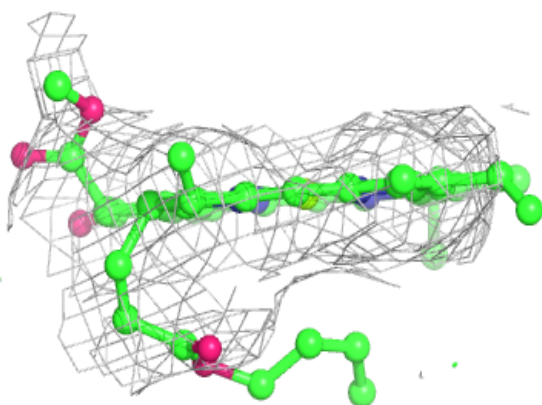
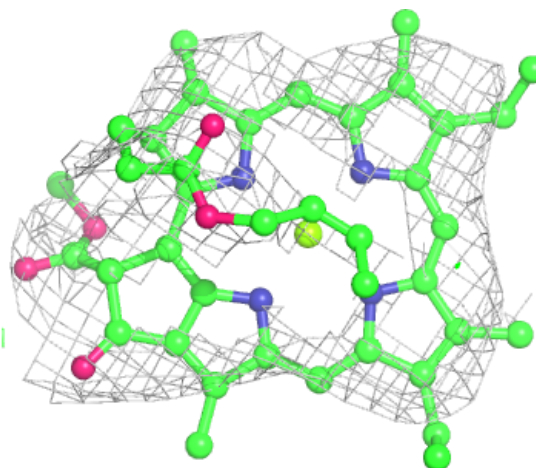
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





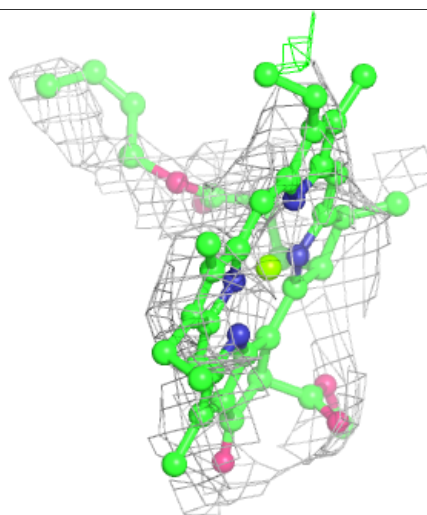
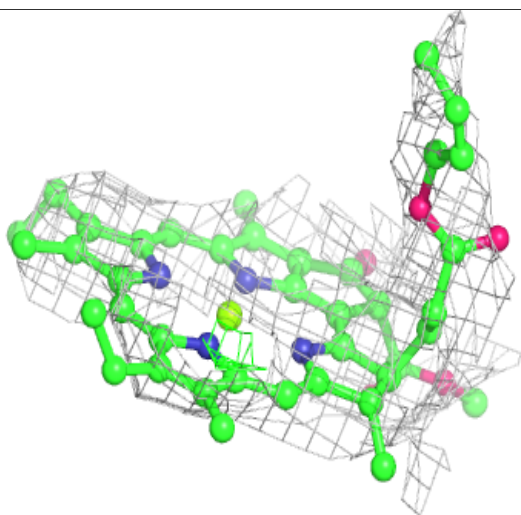
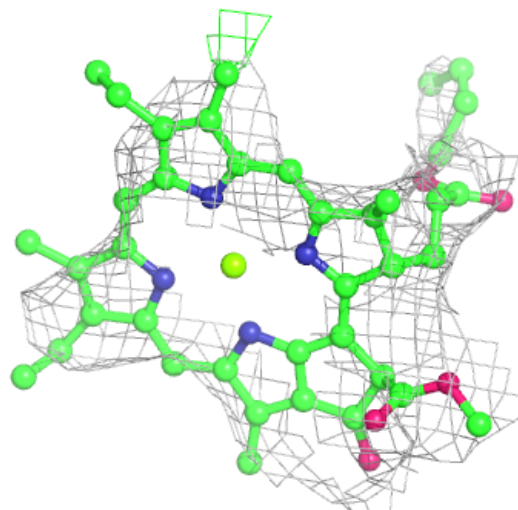
**Electron density around CLA B 1213:**

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



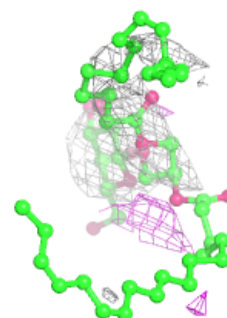
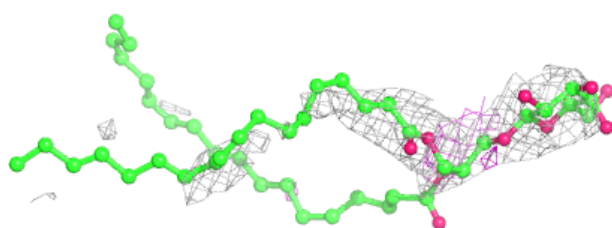
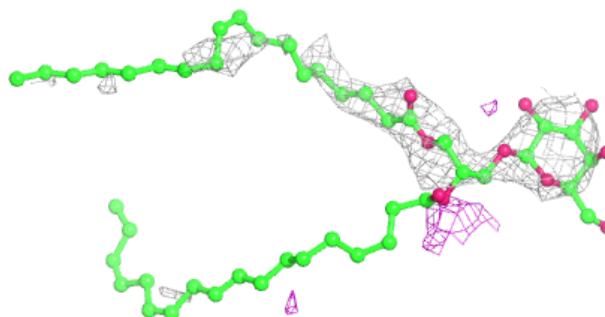
**Electron density around CLA B 1216:**

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

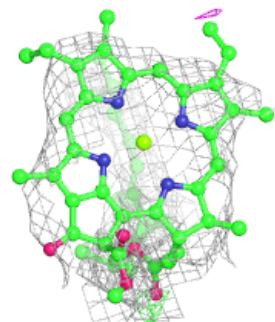
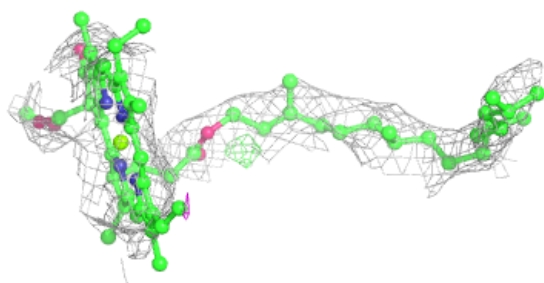
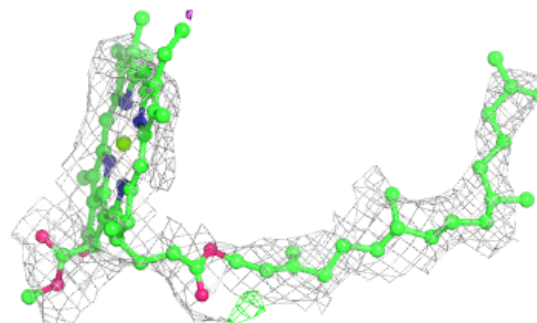


**Electron density around LMG B 5002:**

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

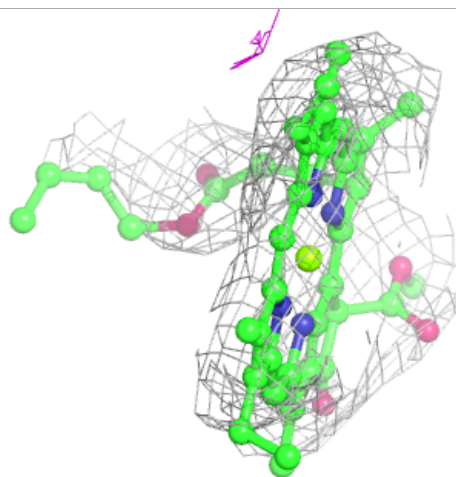
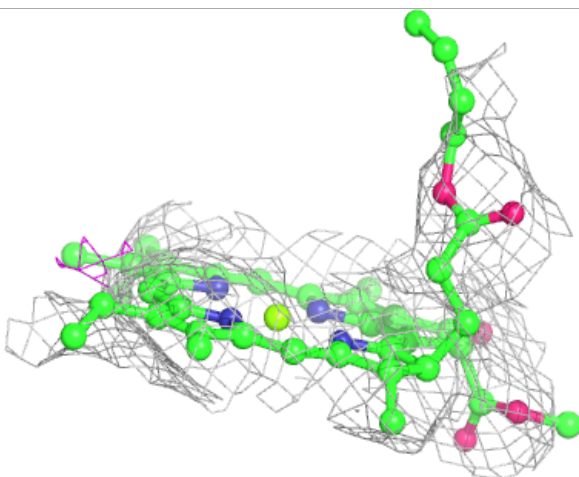
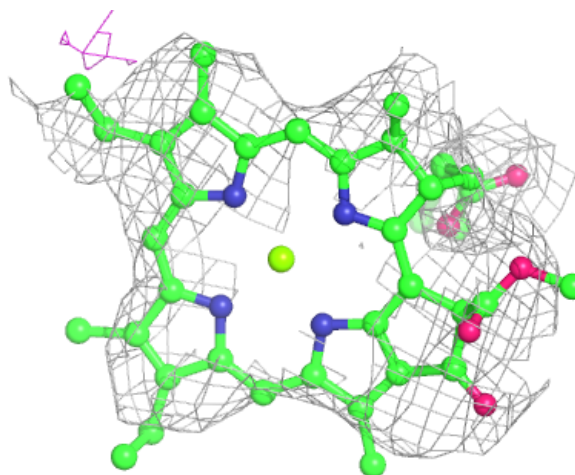
**Electron density around CLA A 1105:**

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



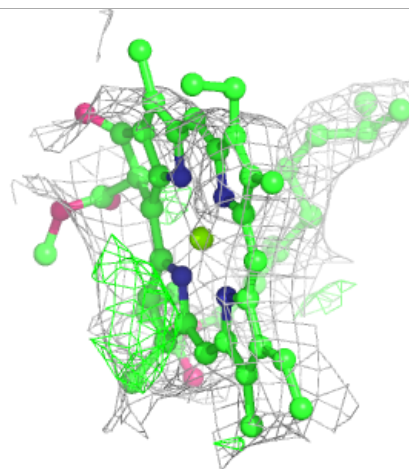
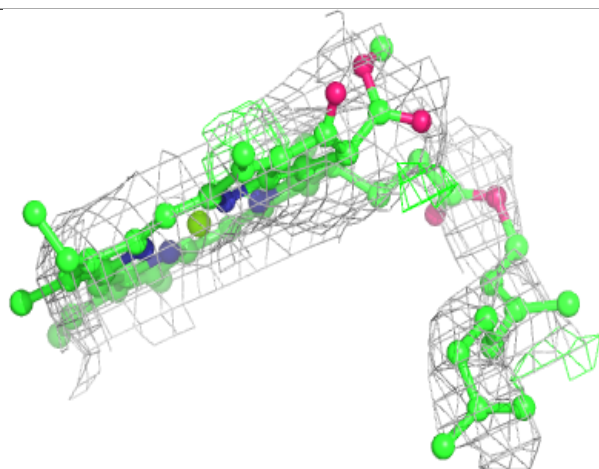
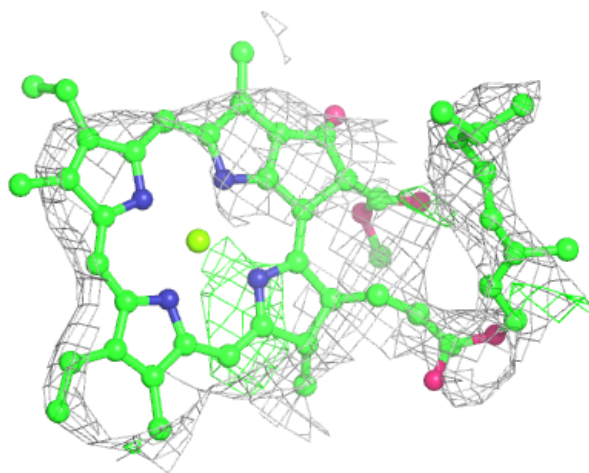
**Electron density around CLA B 1201:**

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



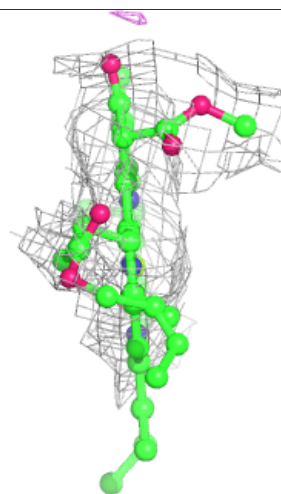
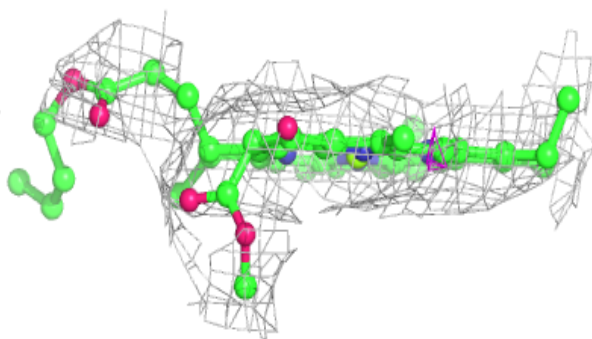
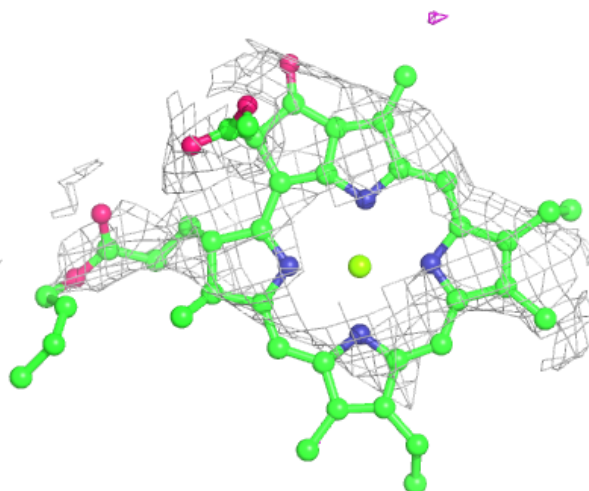
**Electron density around CLA A 1011:**

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



**Electron density around CLA A 1111:**

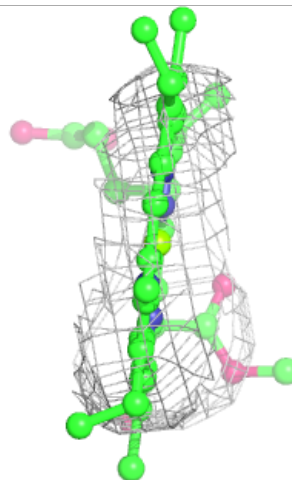
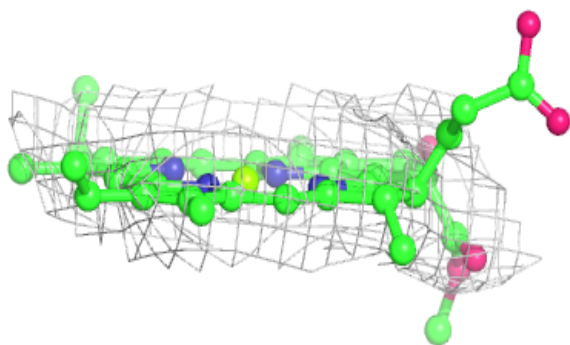
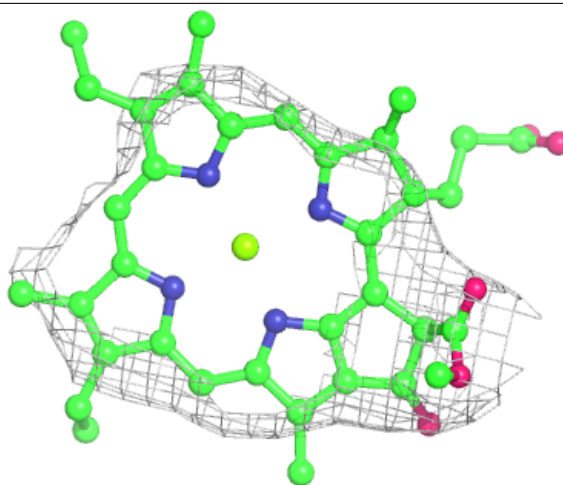
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





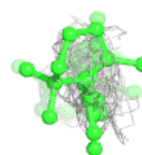
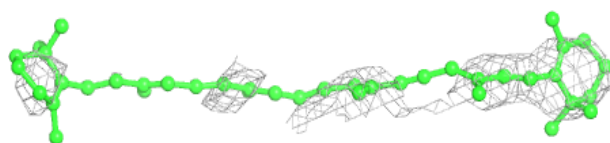
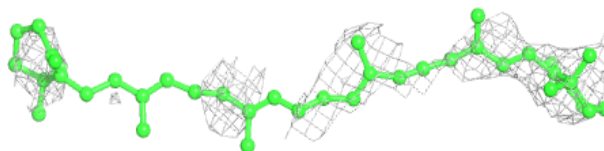
**Electron density around CLA A 1141:**

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

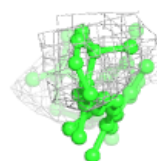
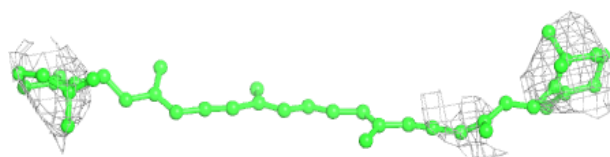
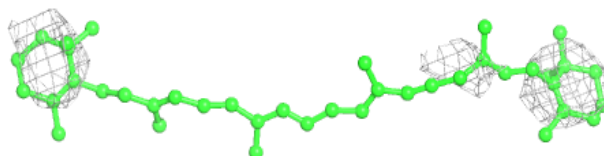


**Electron density around BCR A 4007:**

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

**Electron density around BCR A 4008:**

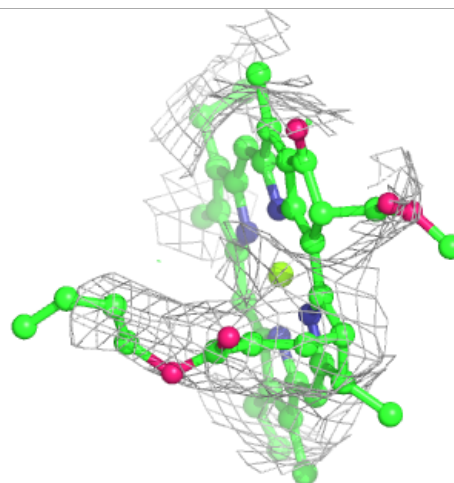
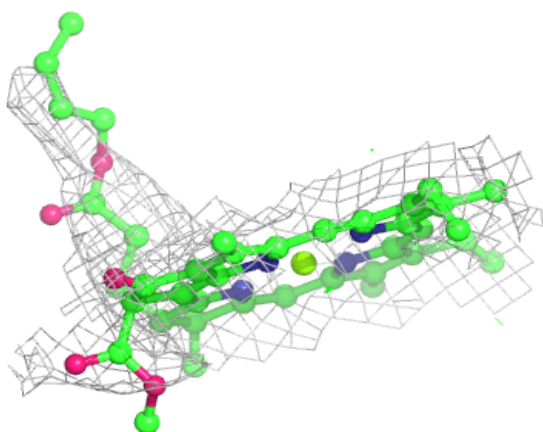
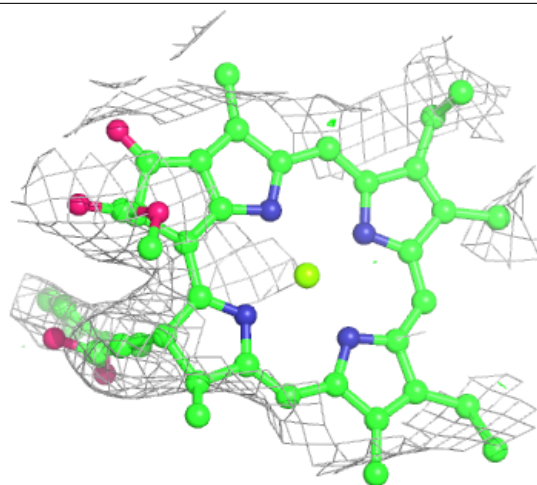
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





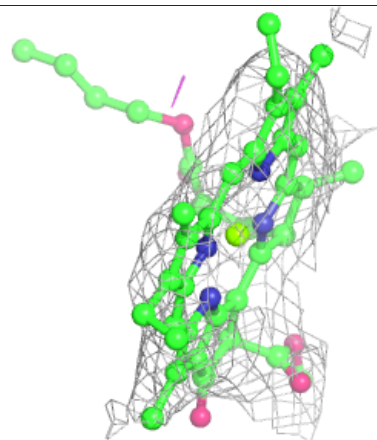
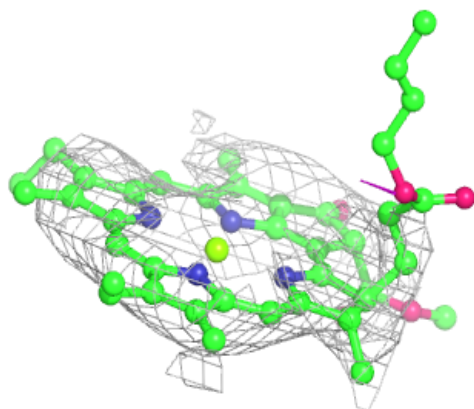
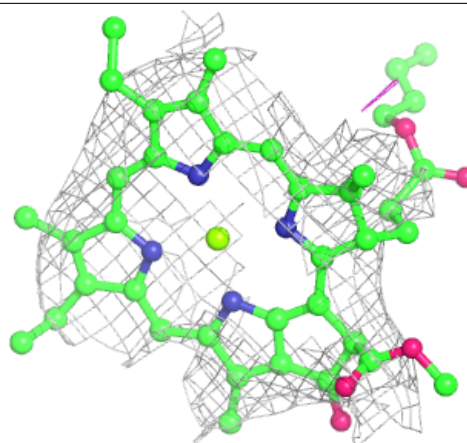
**Electron density around CLA B 1211:**

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



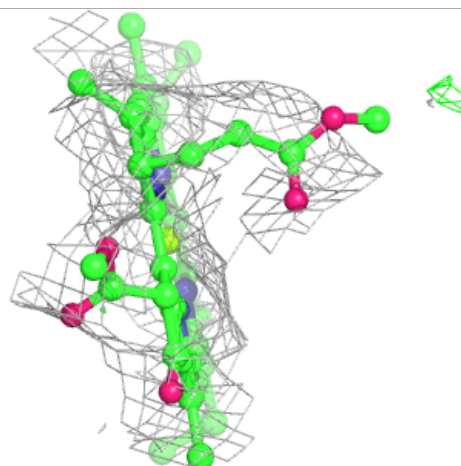
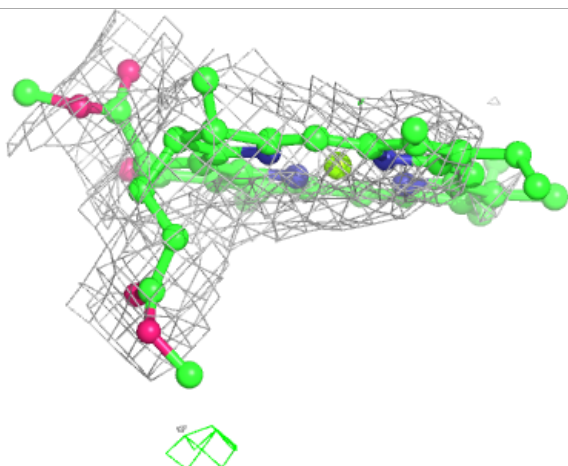
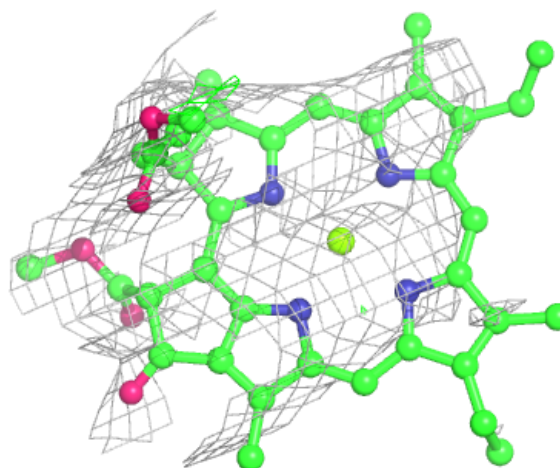
**Electron density around CLA A 1129:**

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



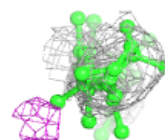
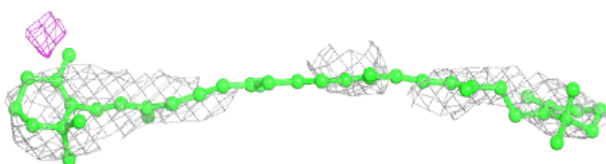
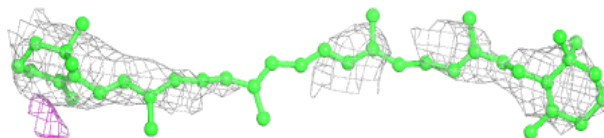
**Electron density around CLA A 1119:**

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

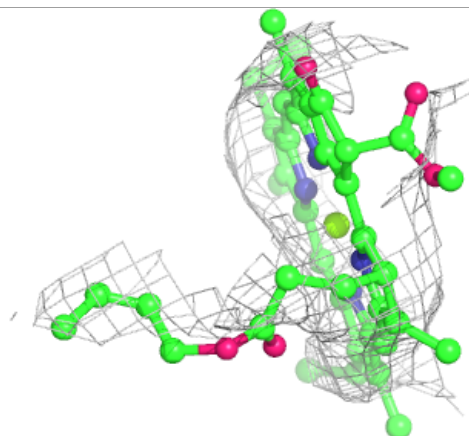
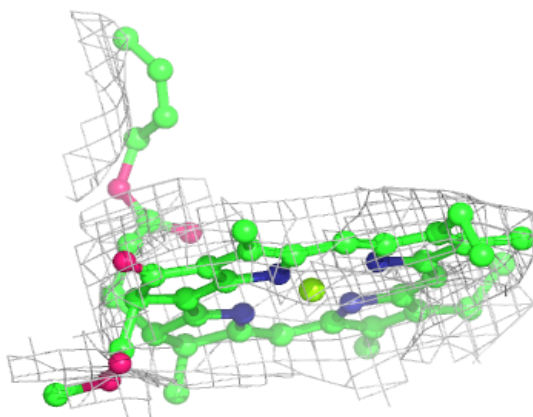
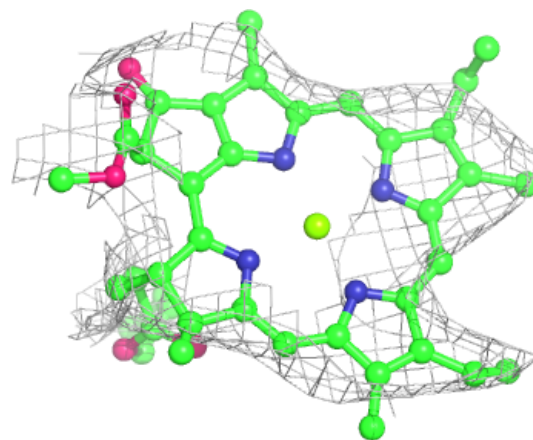


**Electron density around BCR A 4012:**

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

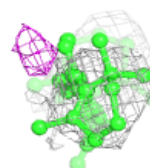
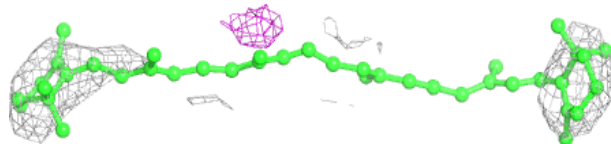
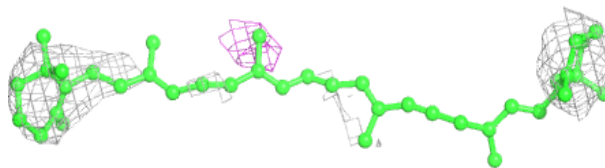
**Electron density around CLA A 1134:**

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



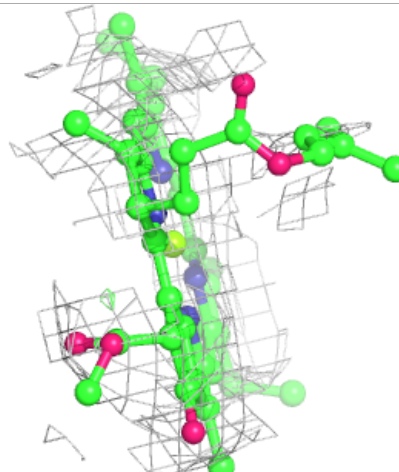
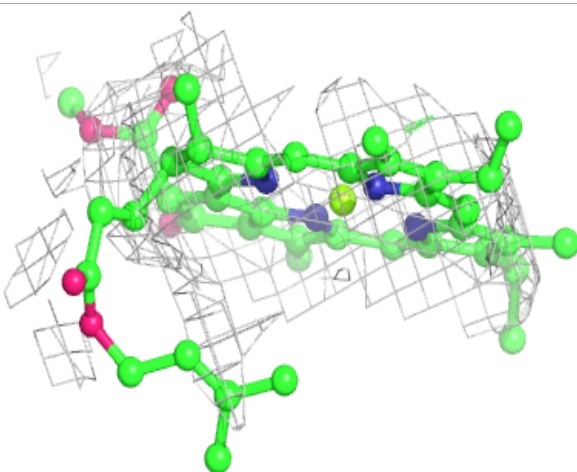
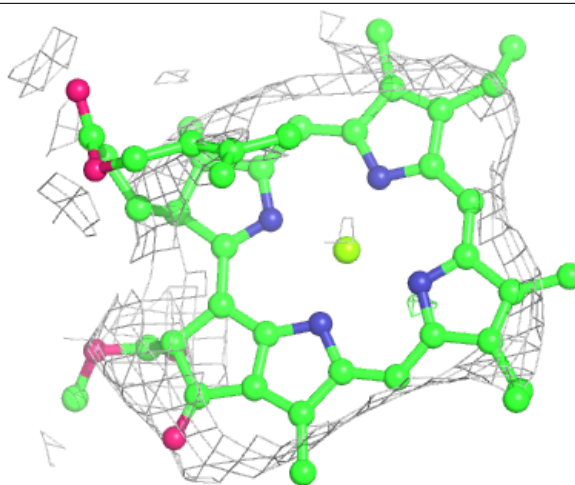
**Electron density around BCR B 4017:**

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



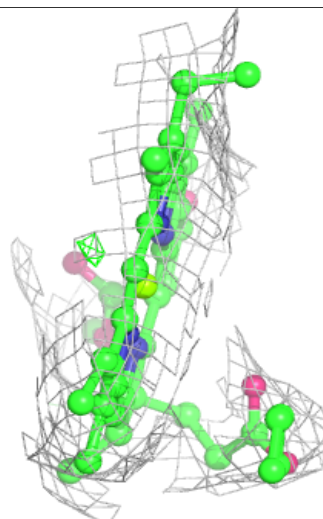
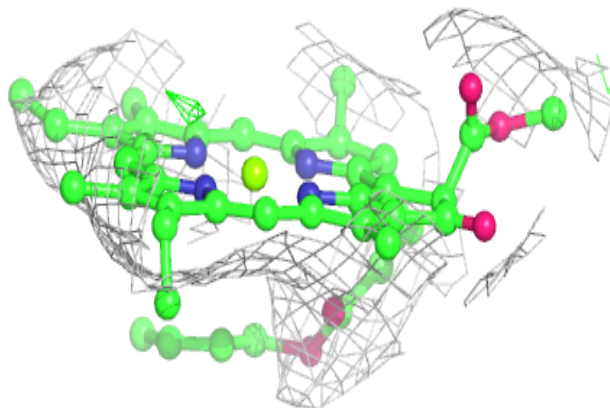
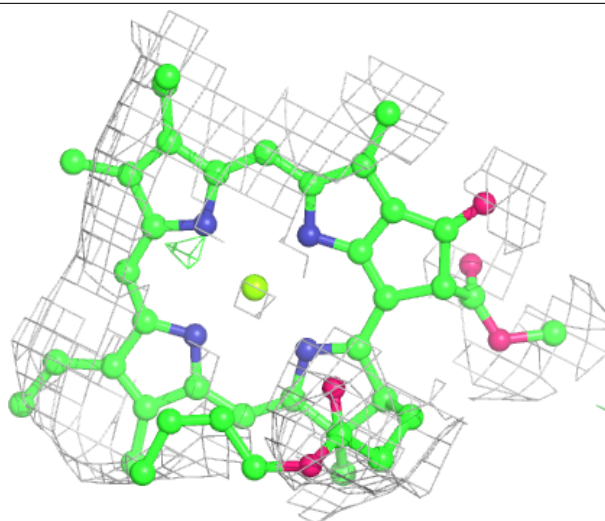
**Electron density around CLA A 1118:**

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



**Electron density around CLA B 1218:**

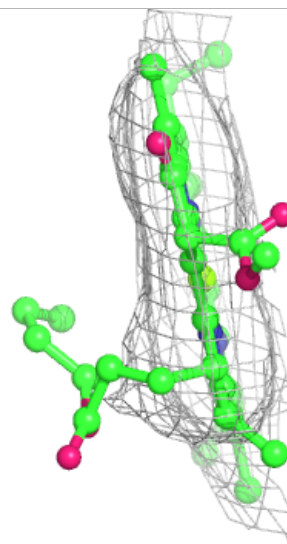
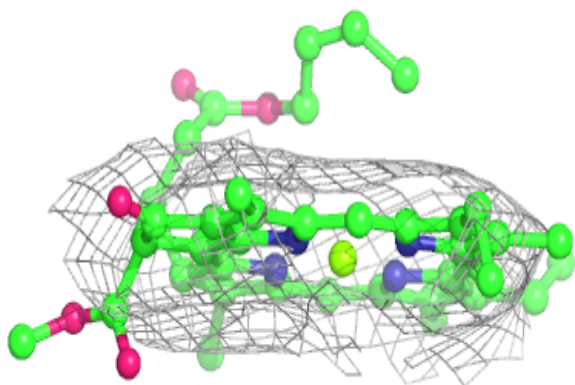
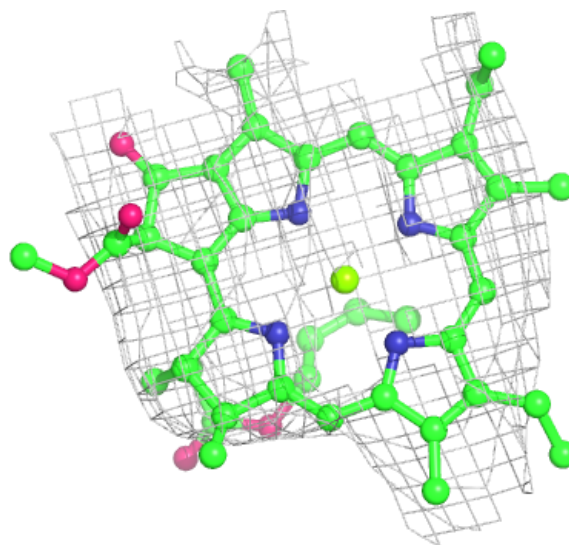
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 1121:**

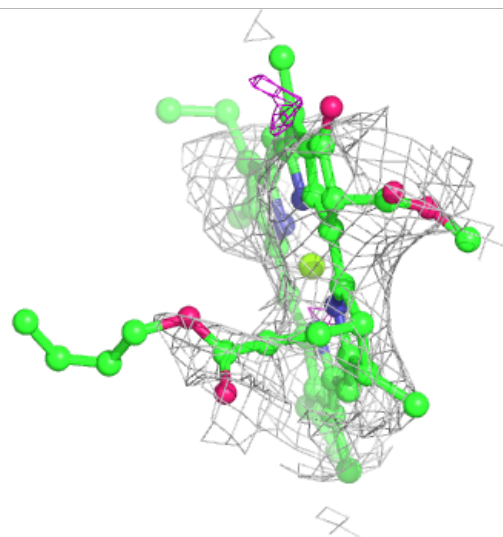
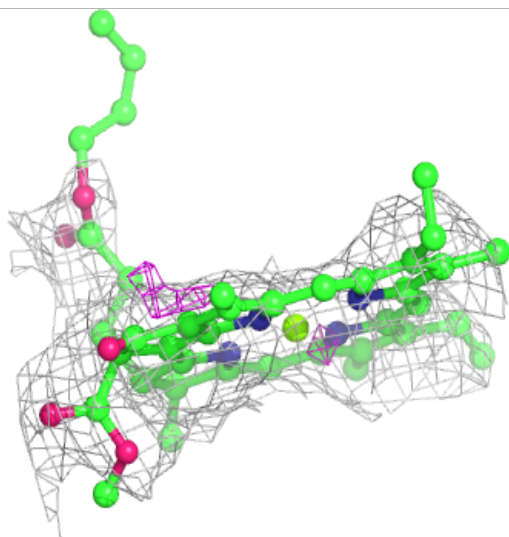
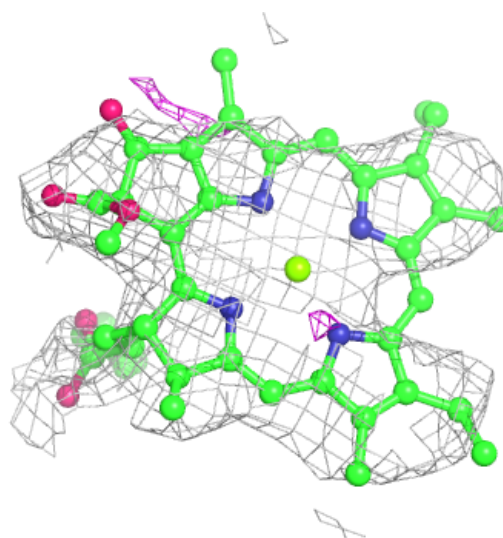
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





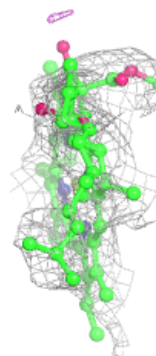
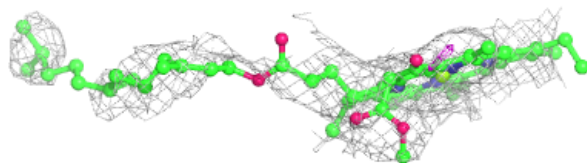
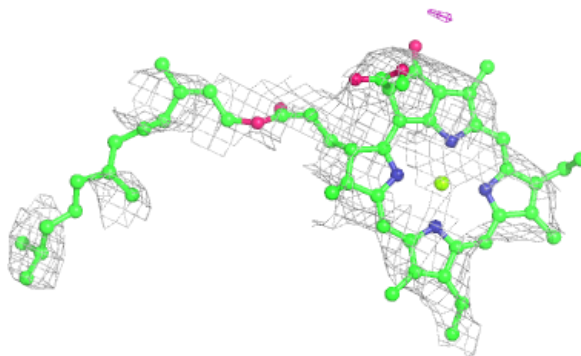
**Electron density around CLA B 1226:**

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



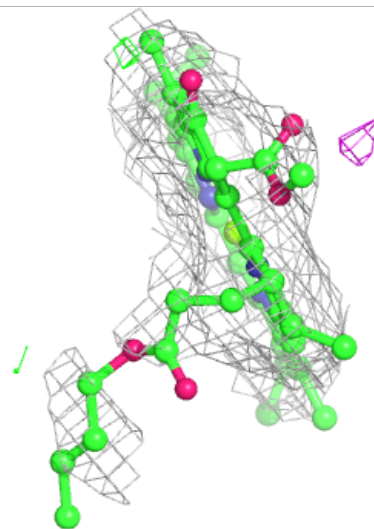
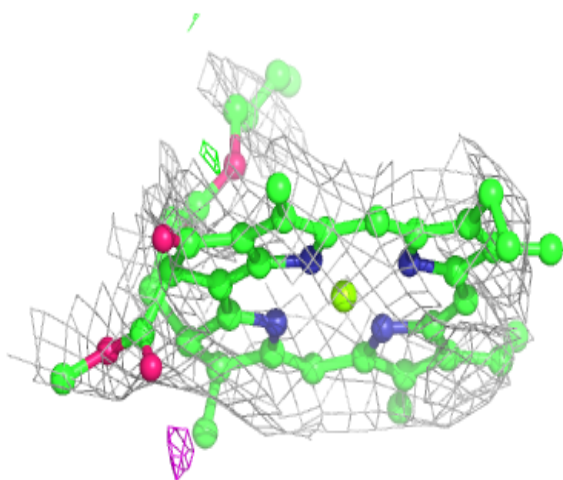
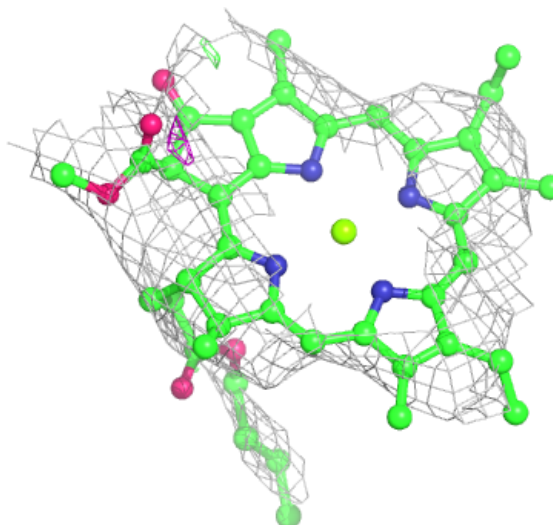
**Electron density around CLA B 1234:**

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



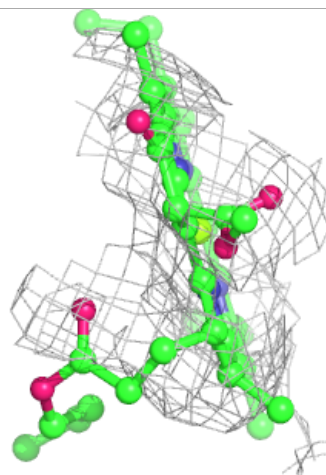
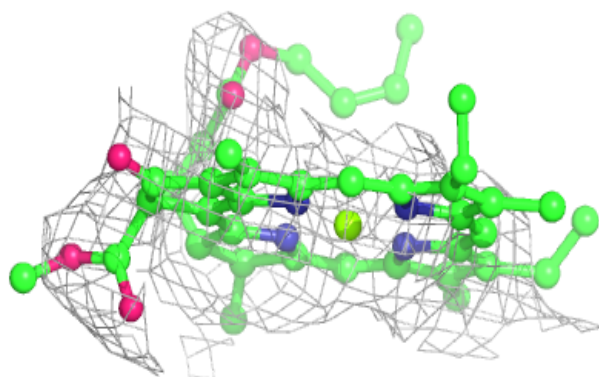
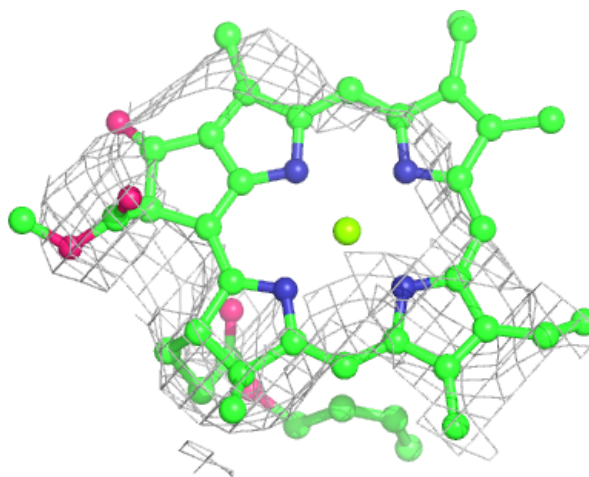
**Electron density around CLA A 1122:**

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



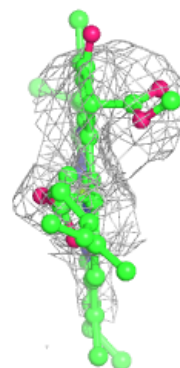
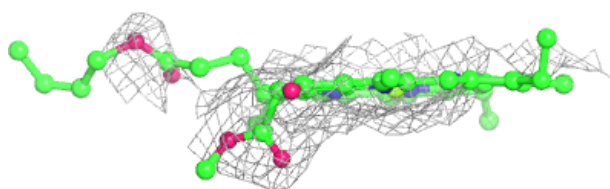
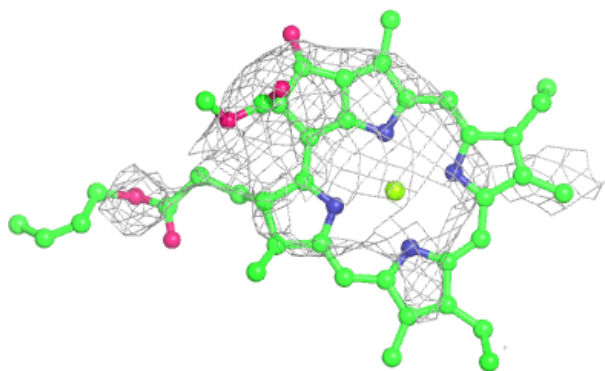
**Electron density around CLA A 1110:**

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

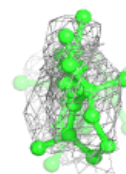
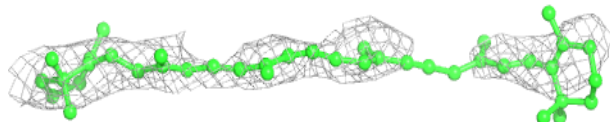
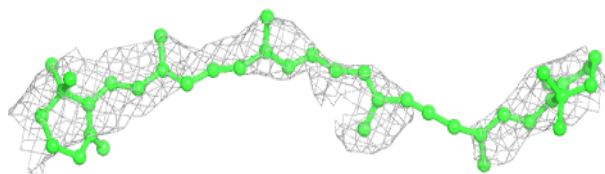


**Electron density around CLA A 1135:**

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

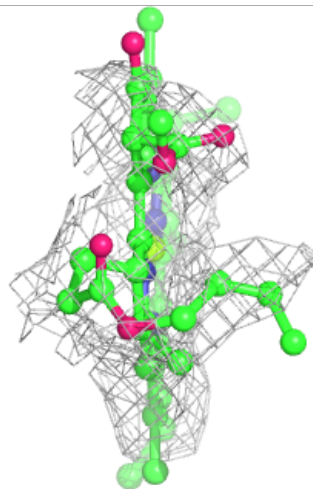
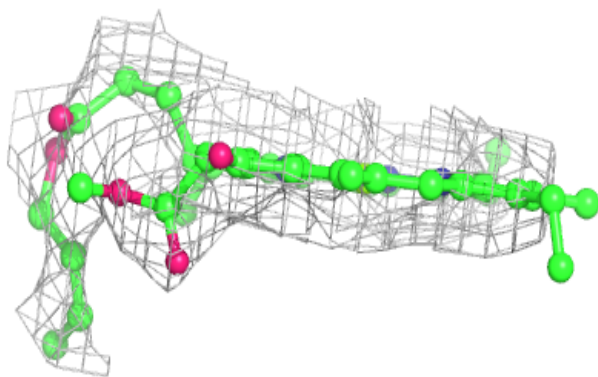
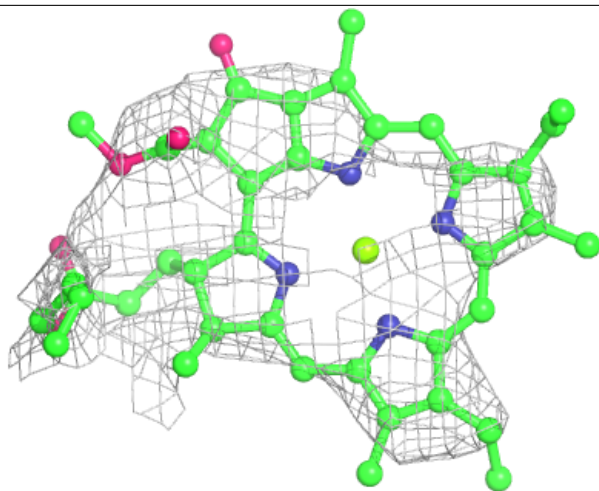
**Electron density around BCR B 4005:**

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



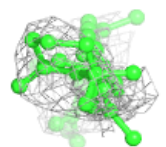
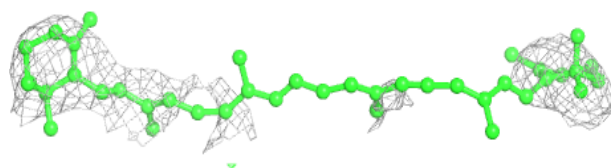
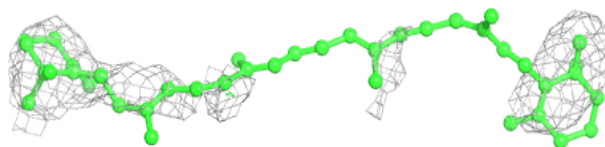
**Electron density around CLA B 1203:**

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

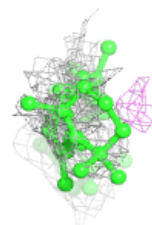
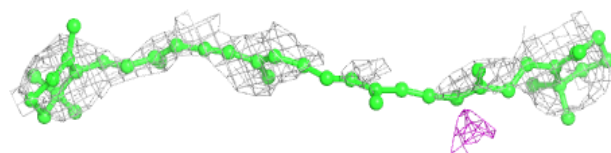
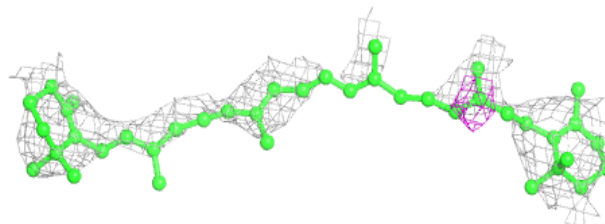


**Electron density around BCR B 4018:**

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

**Electron density around BCR B 4010:**

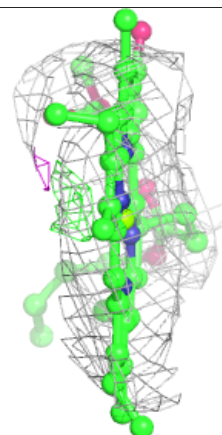
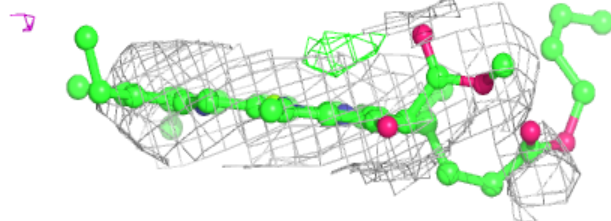
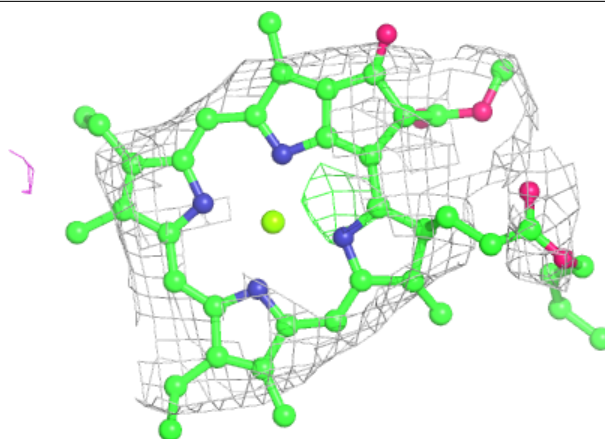
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA F 1301:**

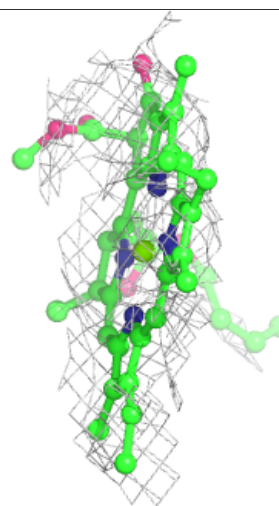
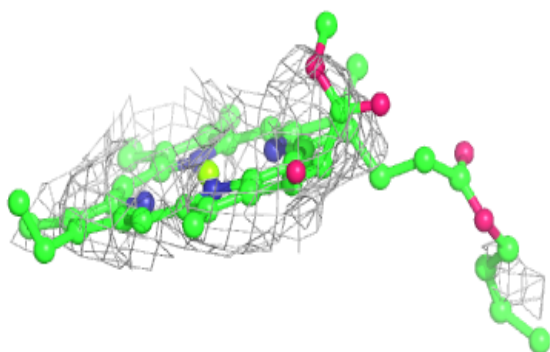
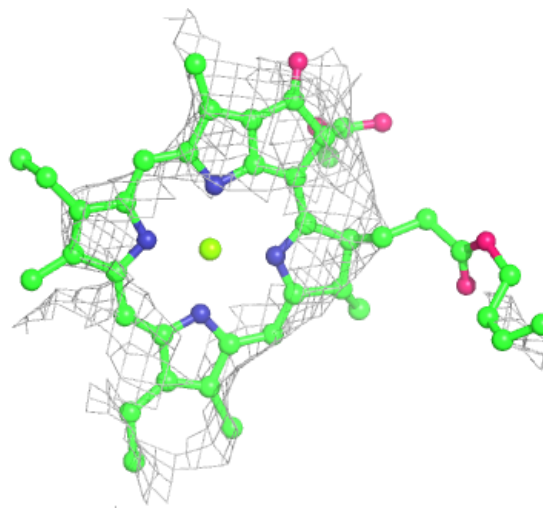
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





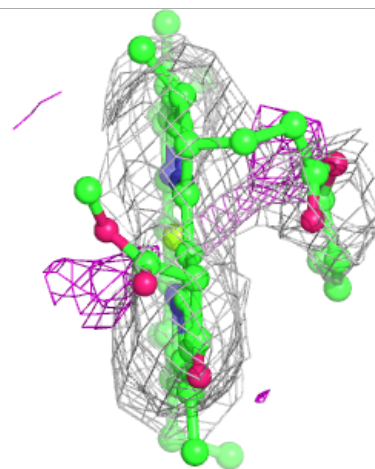
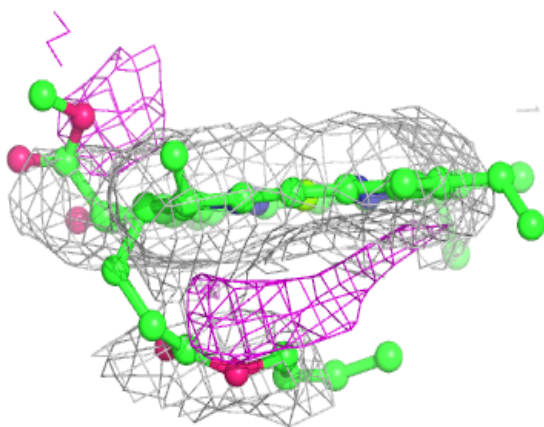
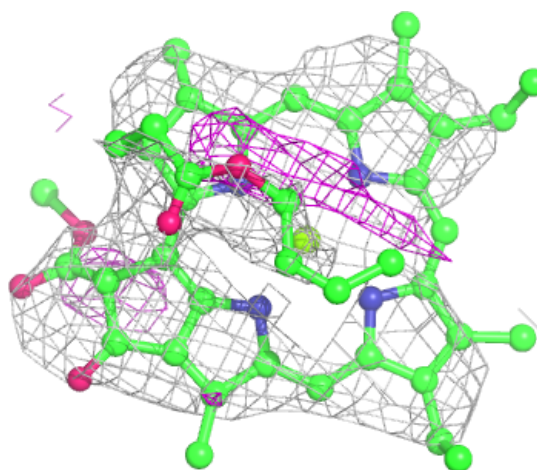
**Electron density around CLA A 1125:**

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



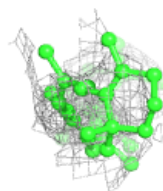
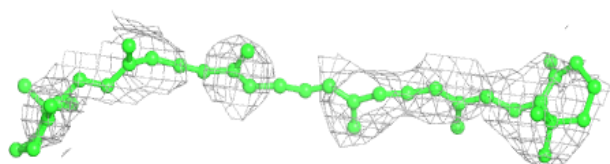
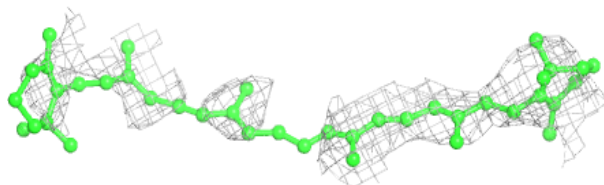
**Electron density around CLA B 1205:**

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

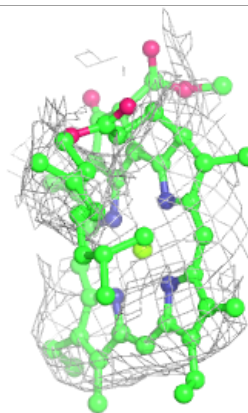
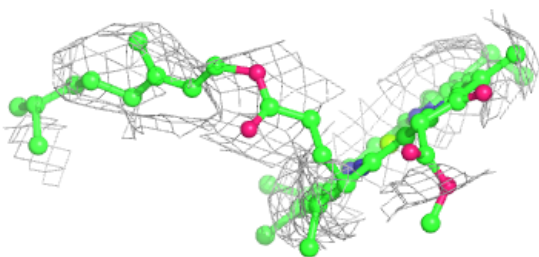
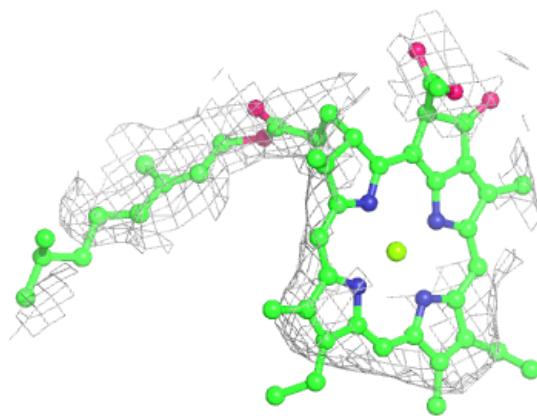


**Electron density around BCR J 4013:**

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

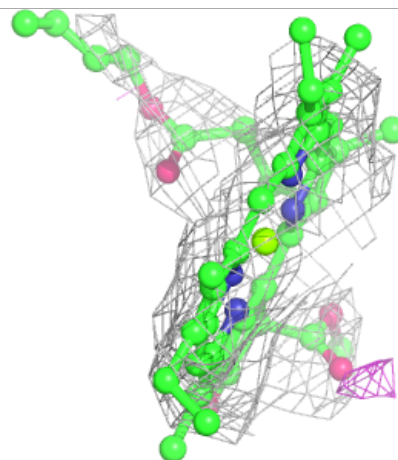
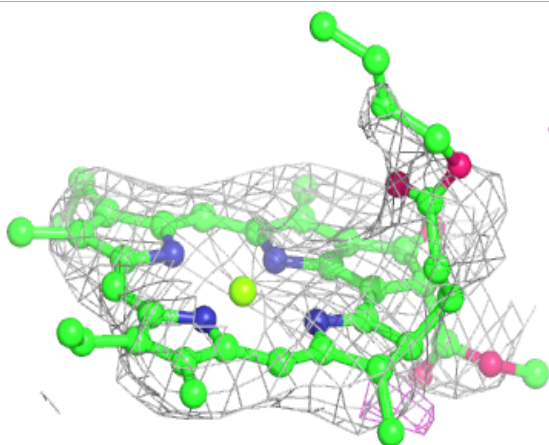
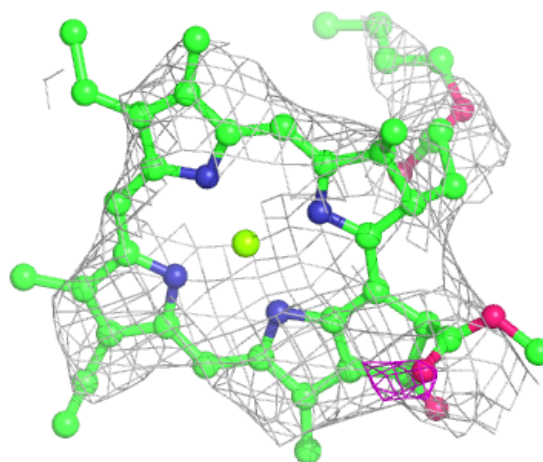
**Electron density around CLA A 1132:**

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



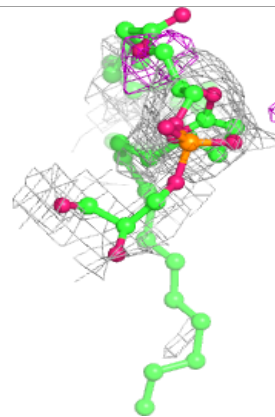
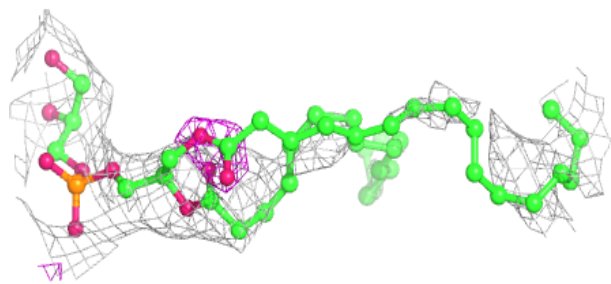
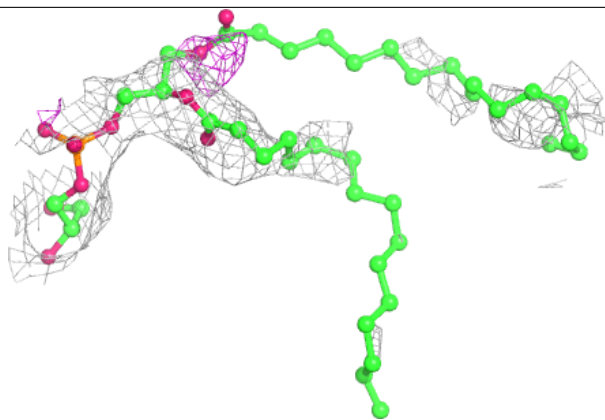
**Electron density around CLA B 1228:**

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



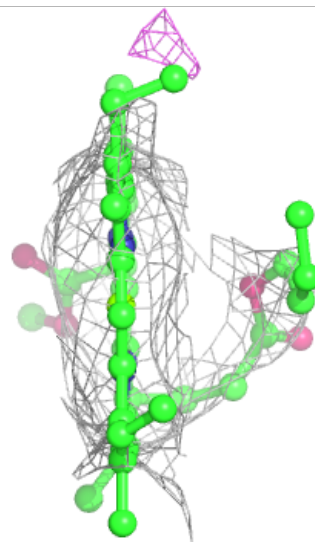
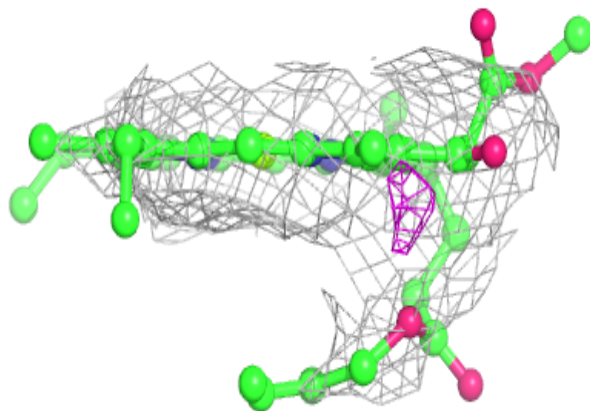
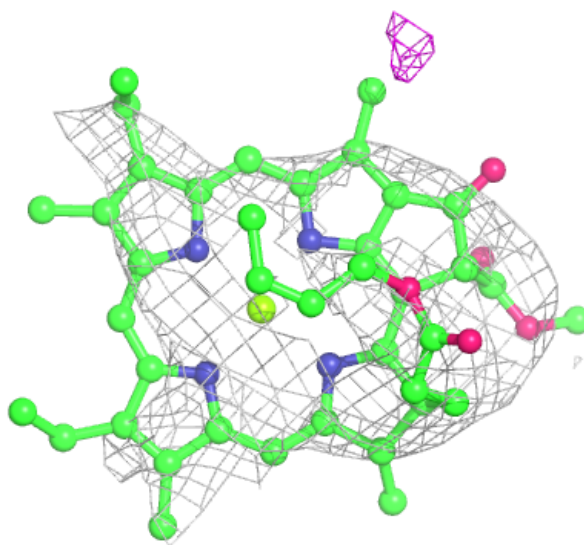
**Electron density around LHG B 5004:**

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



**Electron density around CLA A 1136:**

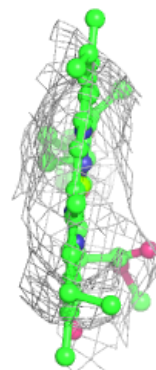
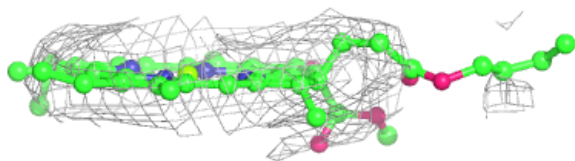
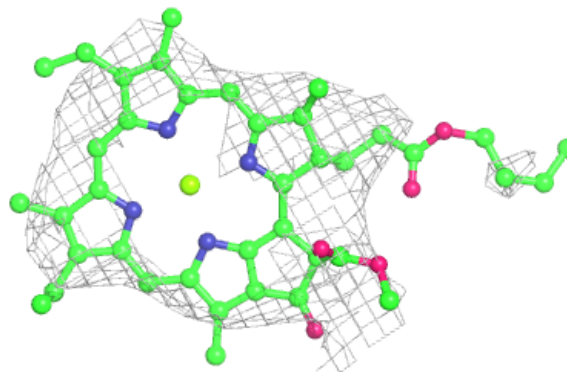
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



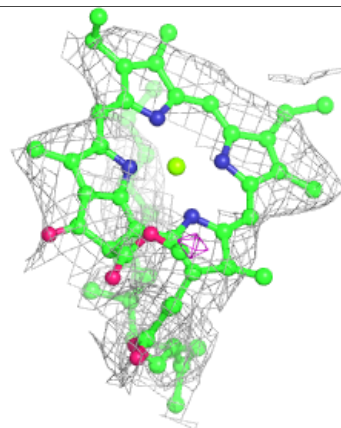
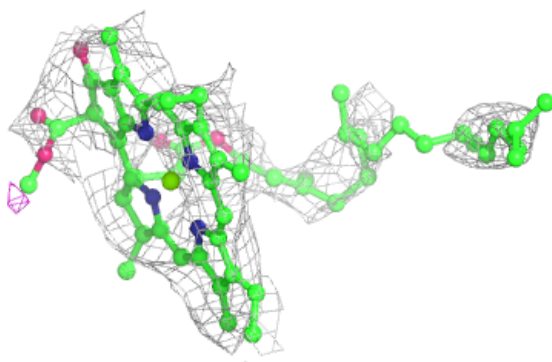
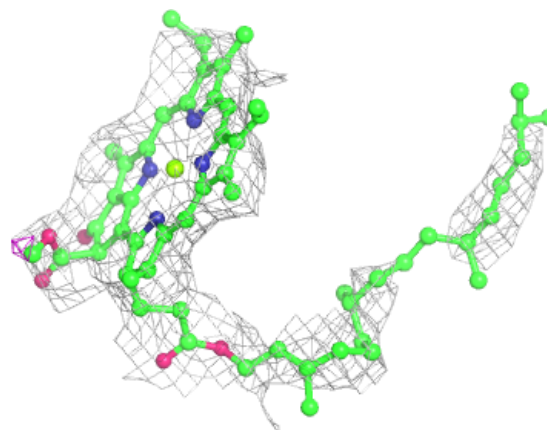


**Electron density around CLA A 1131:**

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

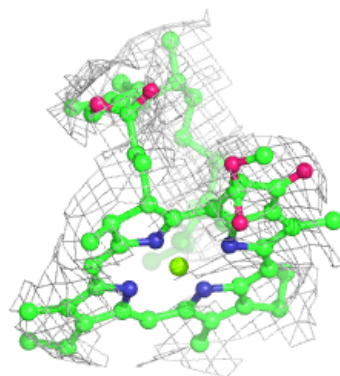
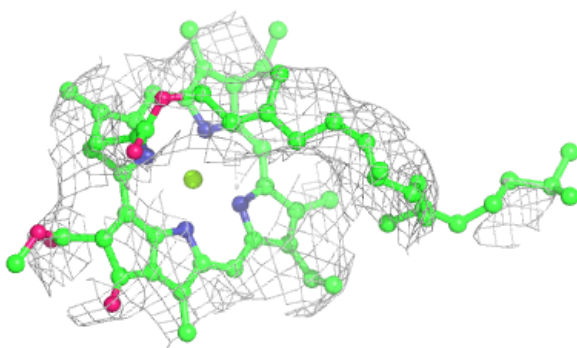
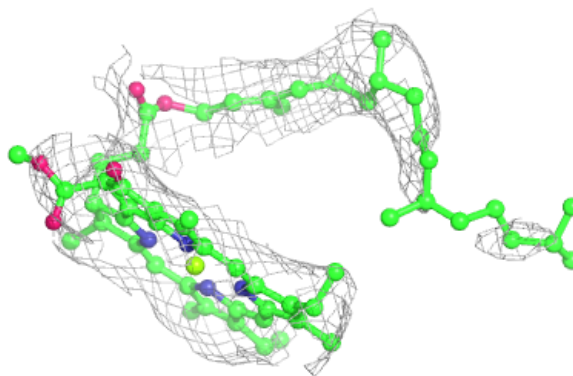
**Electron density around CLA A 1102:**

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

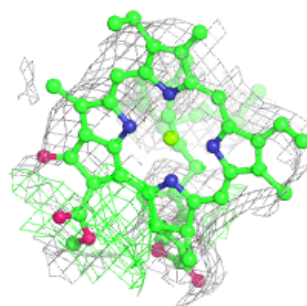
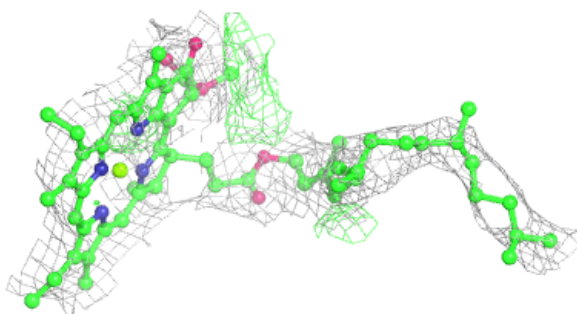
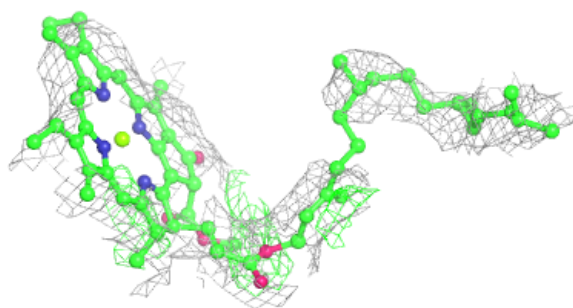


**Electron density around CLA A 1109:**

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

**Electron density around CLA B 1021:**

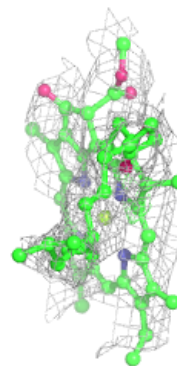
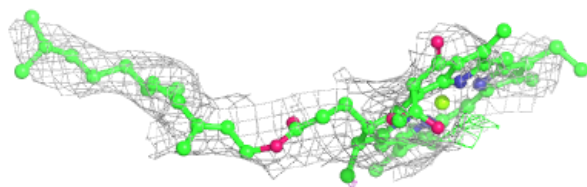
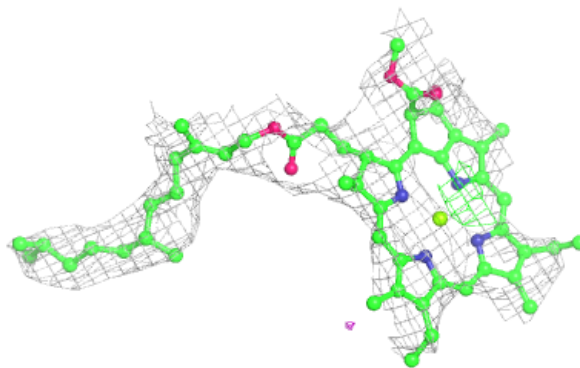
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



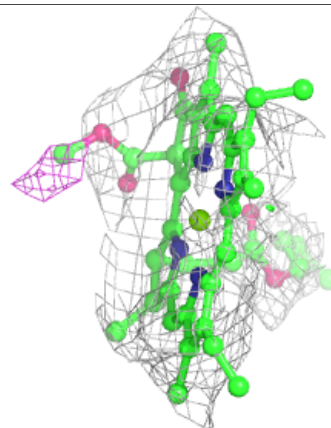
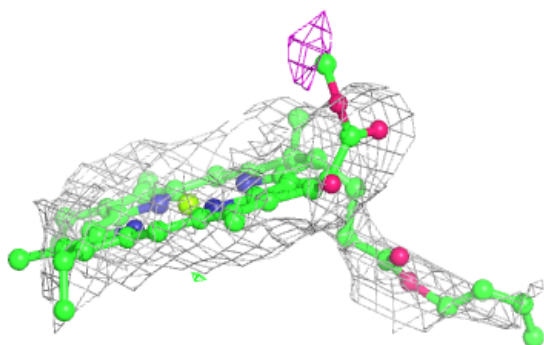
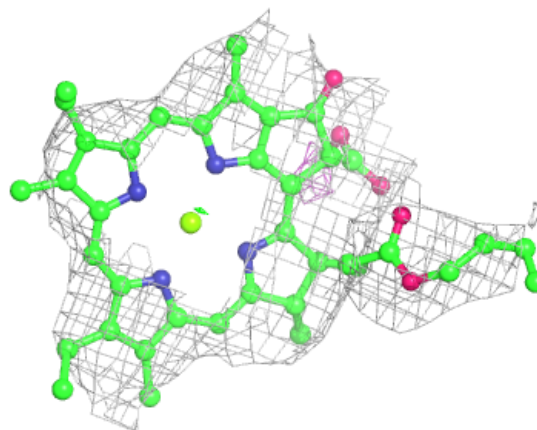


**Electron density around CLA B 1022:**

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

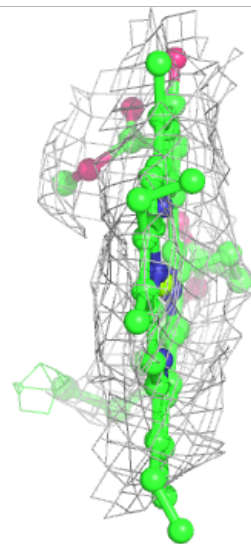
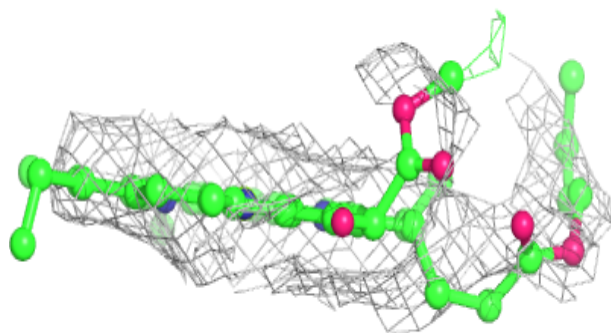
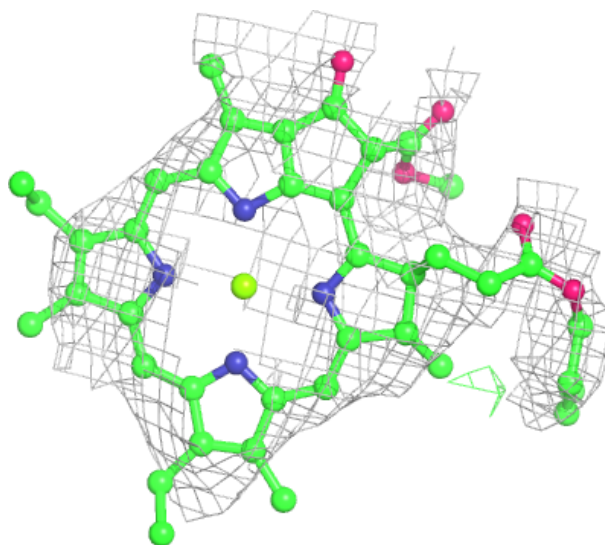
**Electron density around CLA B 1220:**

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



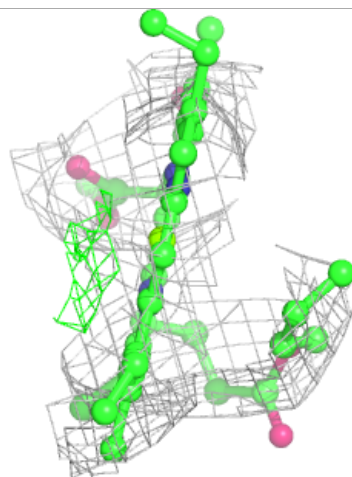
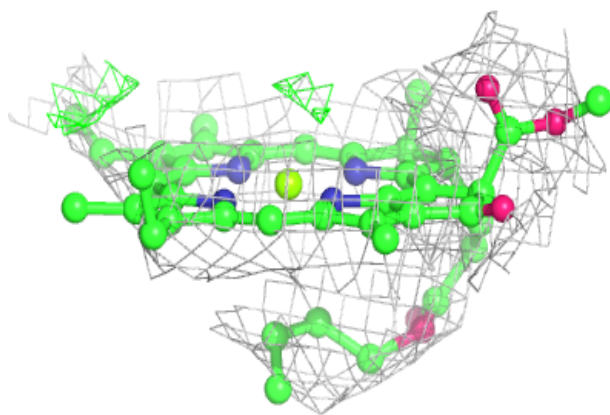
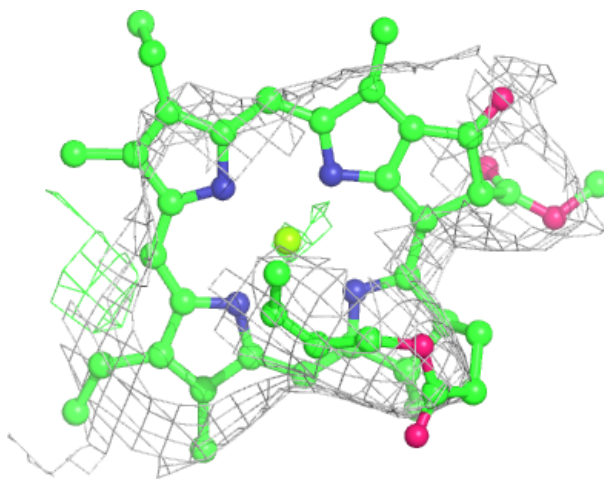
**Electron density around CLA B 1221:**

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



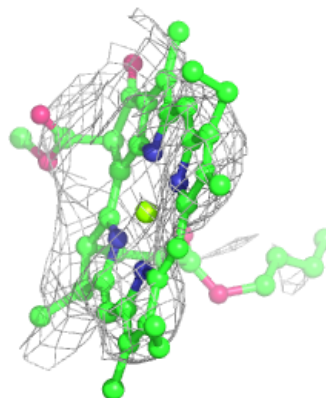
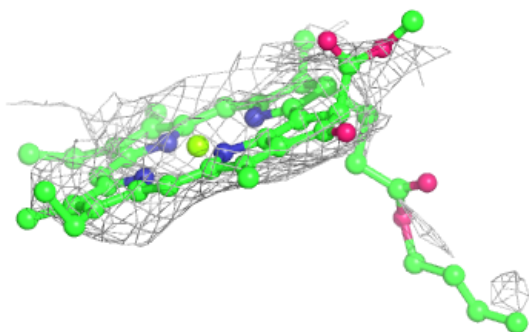
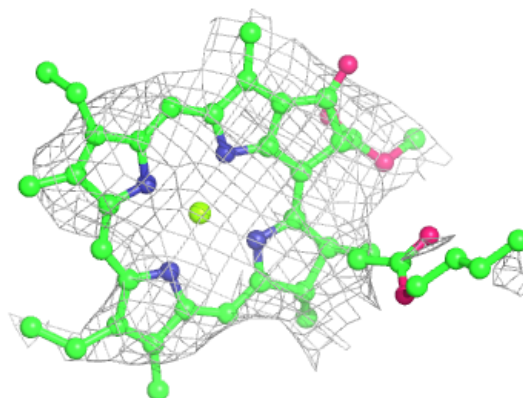
**Electron density around CLA A 1116:**

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

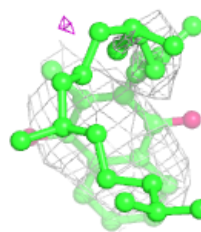
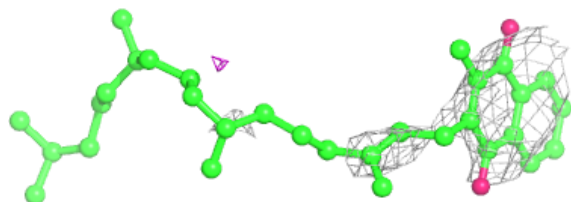
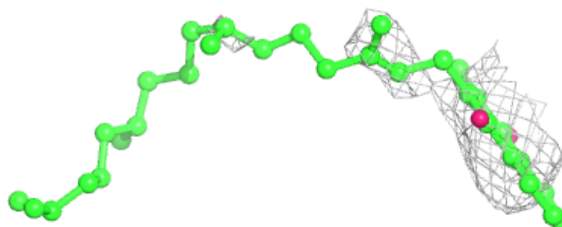


**Electron density around CLA A 1137:**

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

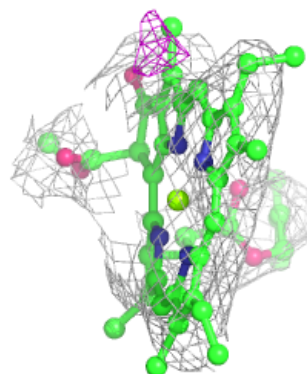
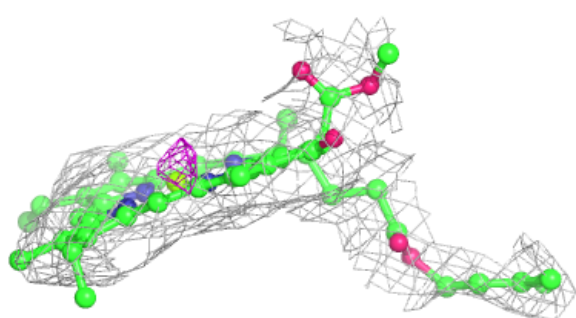
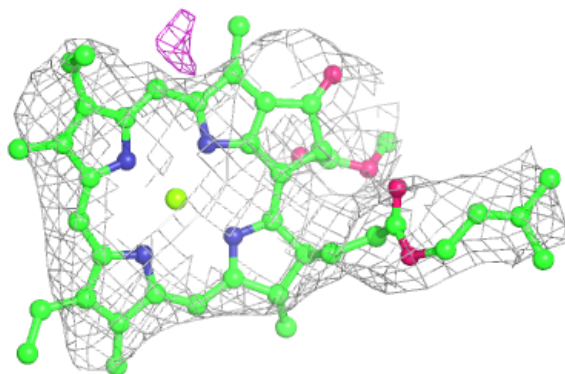
**Electron density around PQN B 2002:**

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

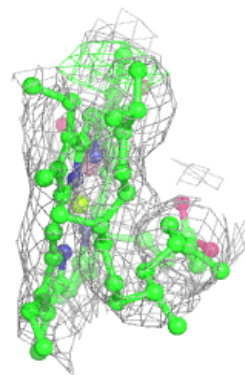
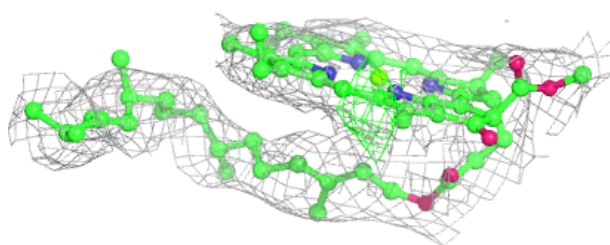
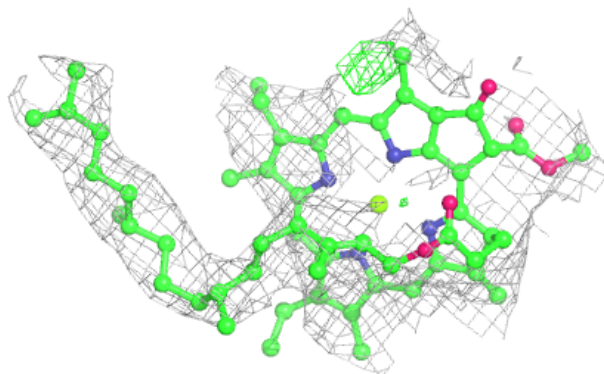


**Electron density around CLA A 1107:**

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

**Electron density around CLA B 1235:**

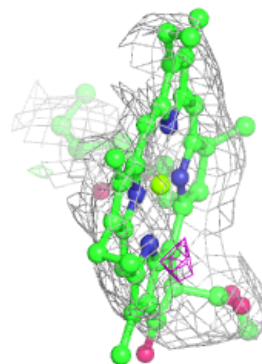
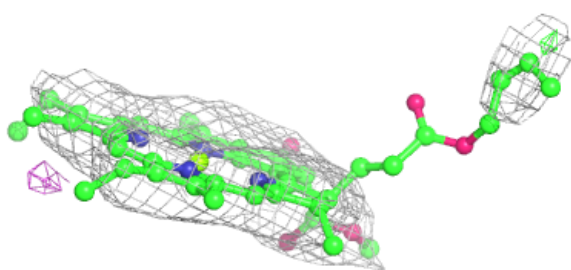
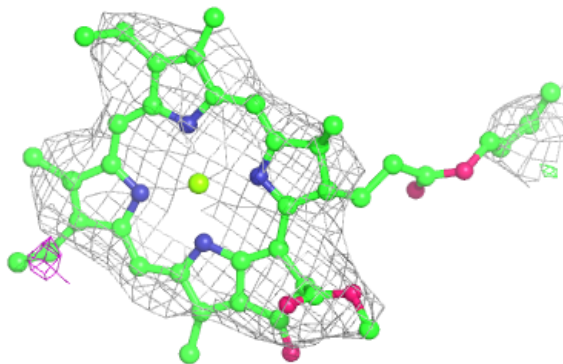
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





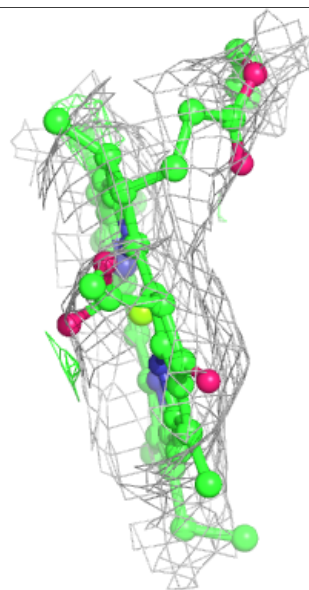
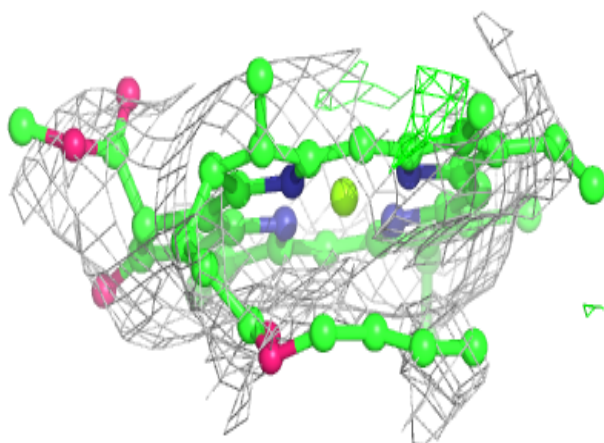
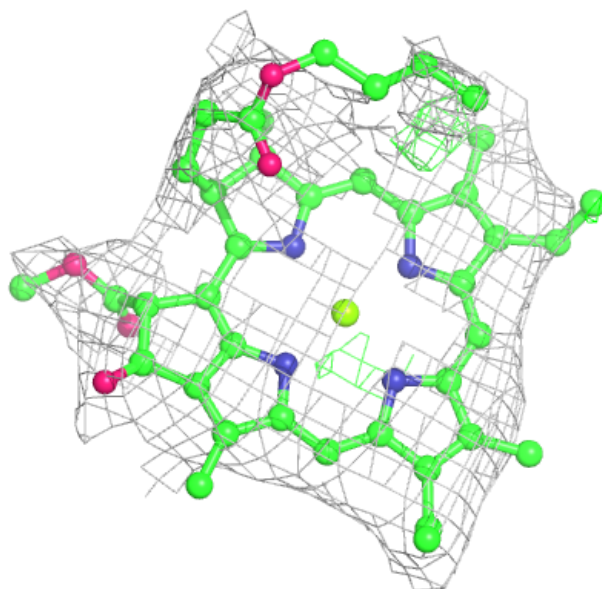
**Electron density around CLA B 1239:**

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



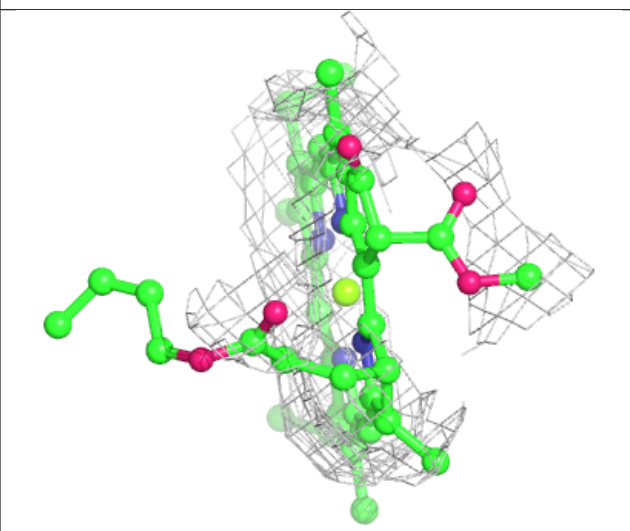
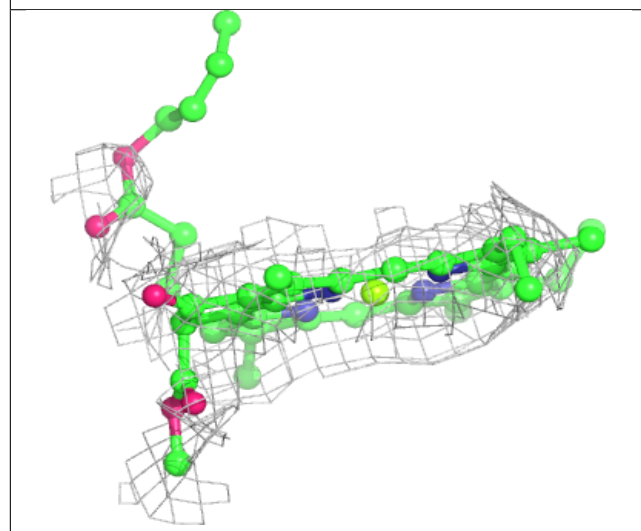
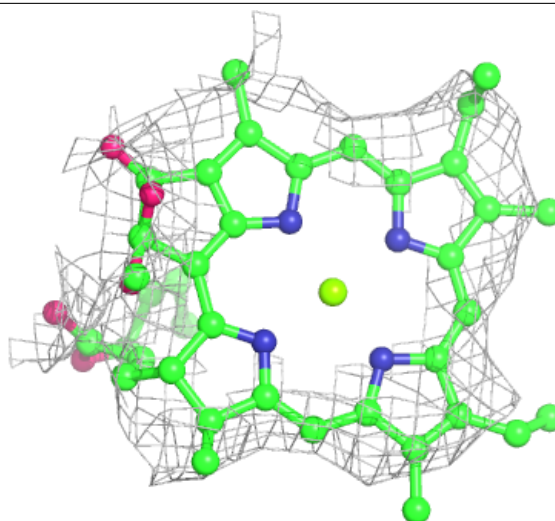
**Electron density around CLA B 1215:**

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



**Electron density around CLA B 1238:**

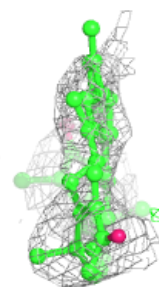
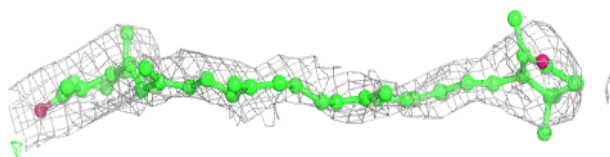
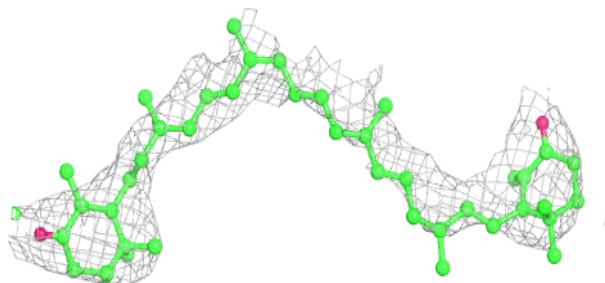
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



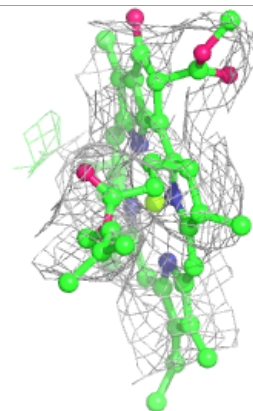
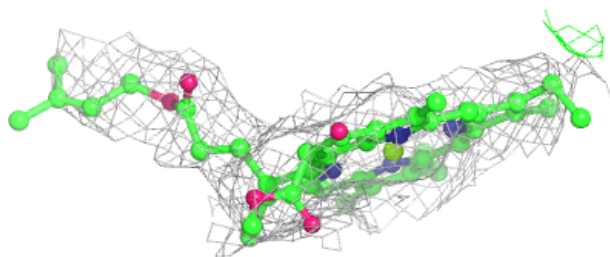
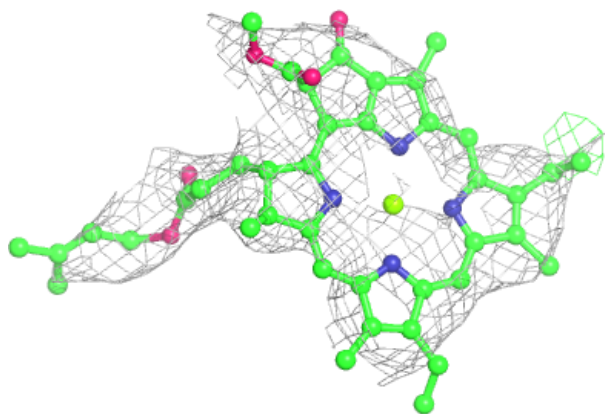


**Electron density around 45D B 4011:**

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

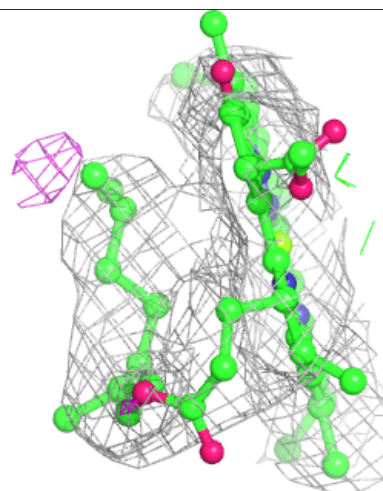
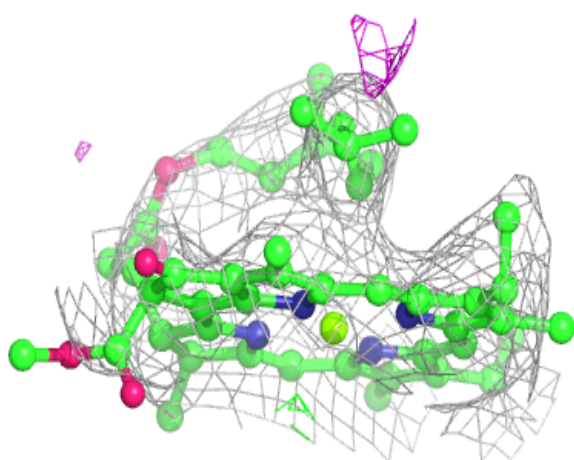
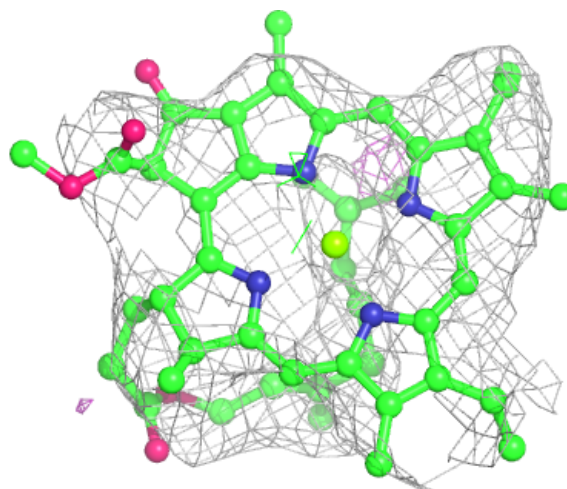
**Electron density around CLA B 1222:**

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



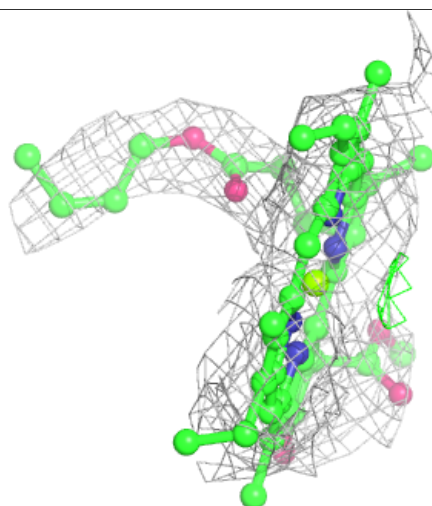
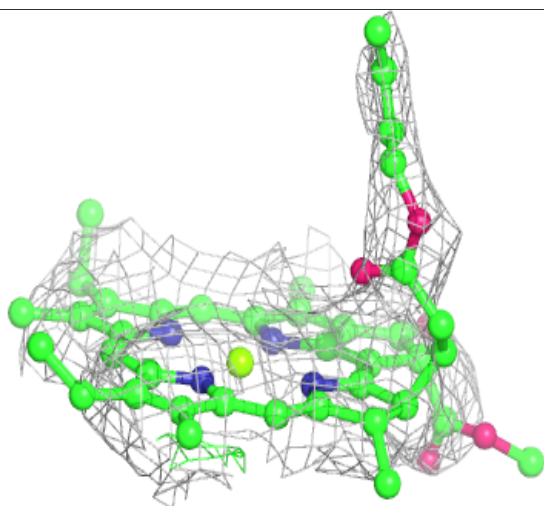
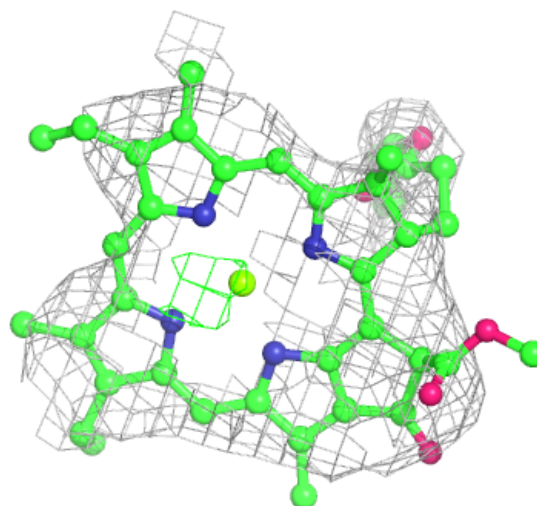
**Electron density around CLA B 1224:**

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



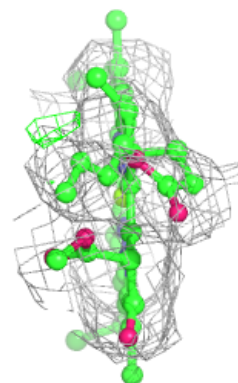
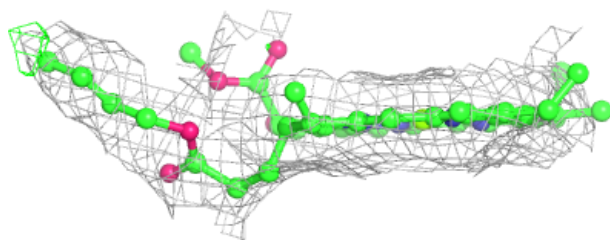
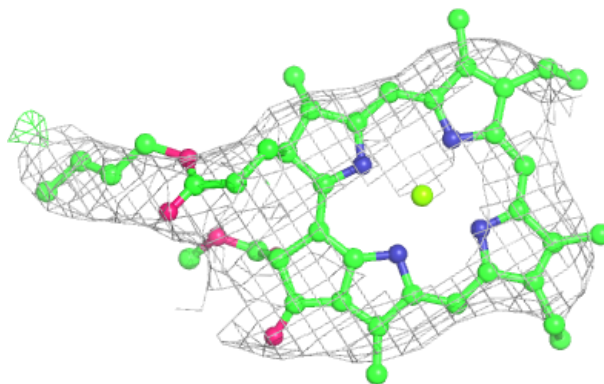
**Electron density around CLA B 1225:**

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



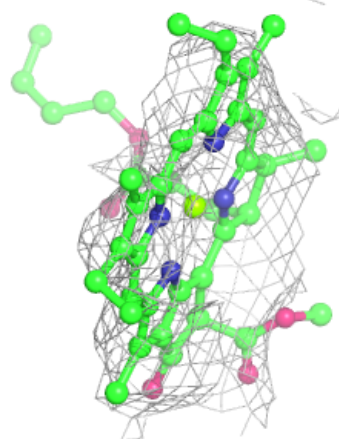
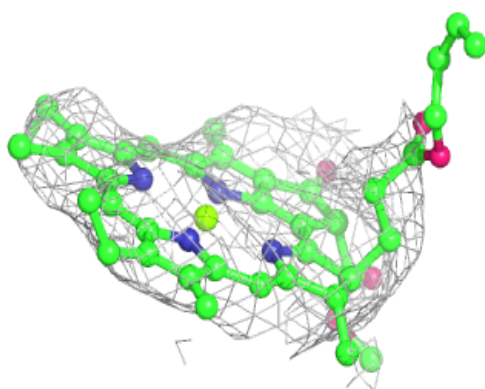
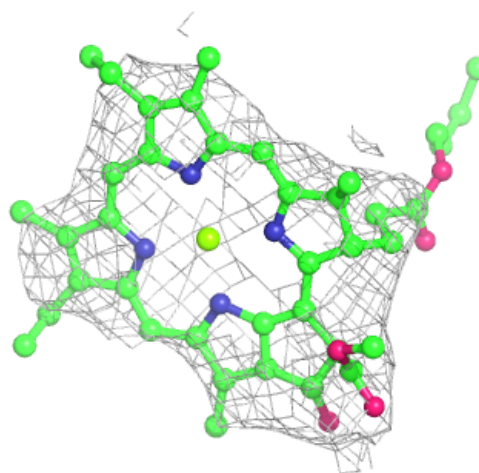
**Electron density around CLA A 1101:**

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



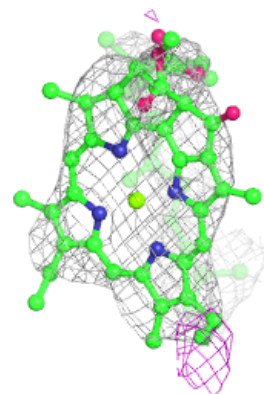
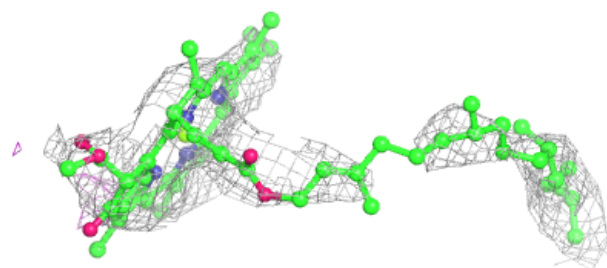
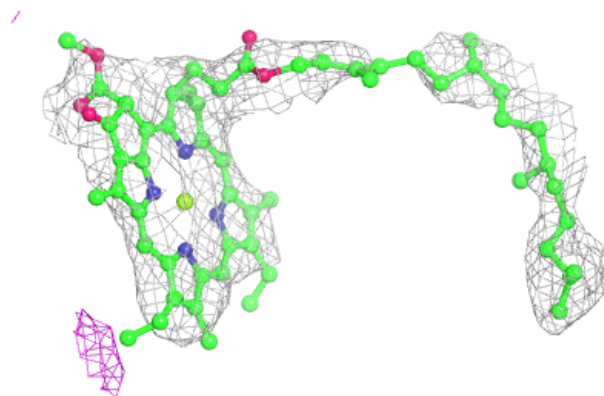
**Electron density around CLA B 1227:**

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

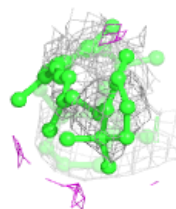
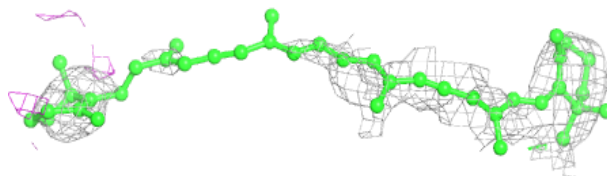
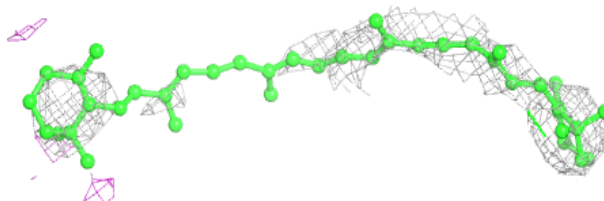


**Electron density around CLA A 1140:**

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

**Electron density around BCR F 4014:**

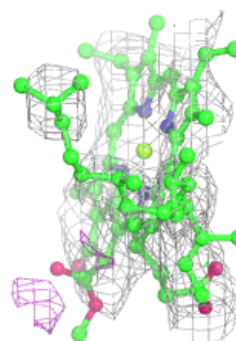
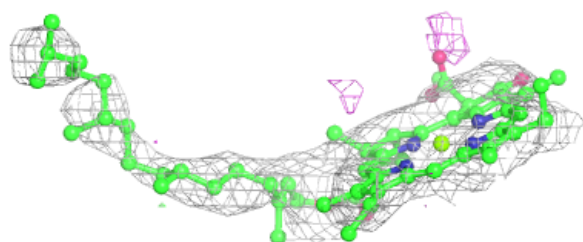
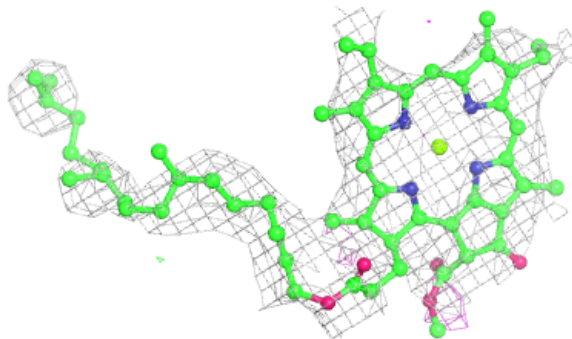
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



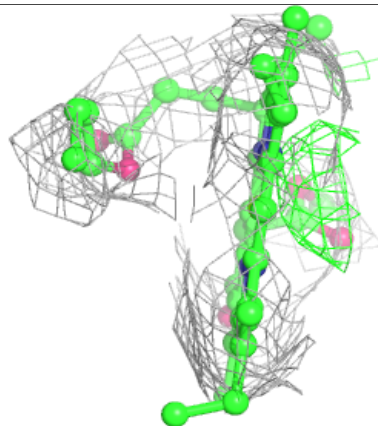
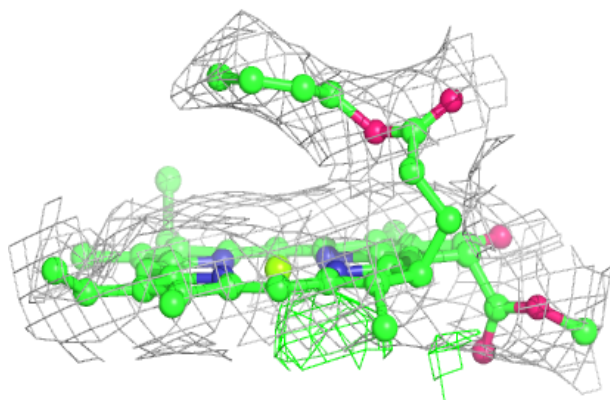
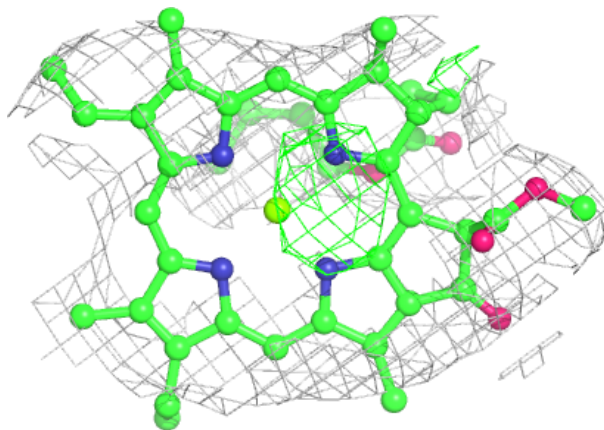


**Electron density around CLA A 1013:**

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

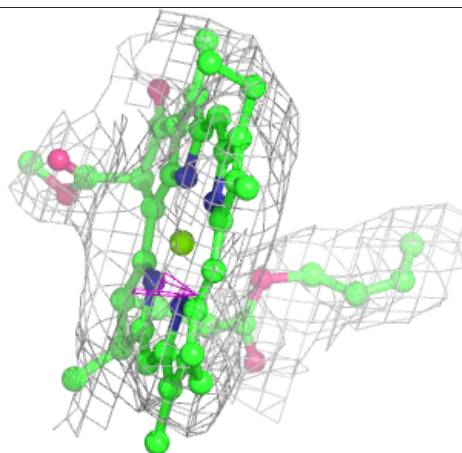
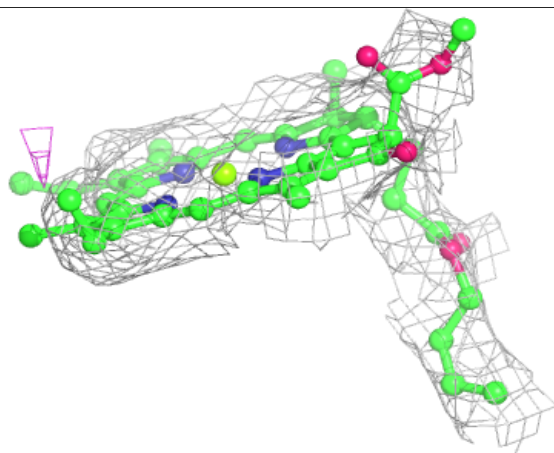
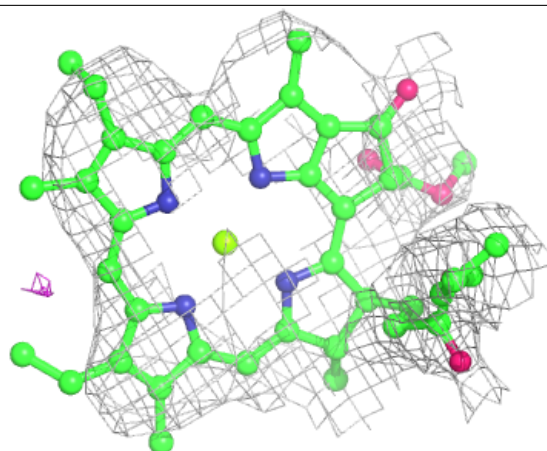
**Electron density around CLA B 1237:**

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

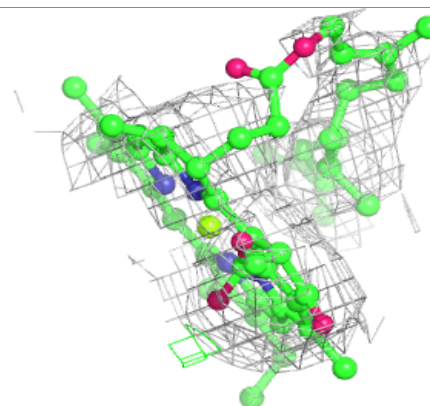
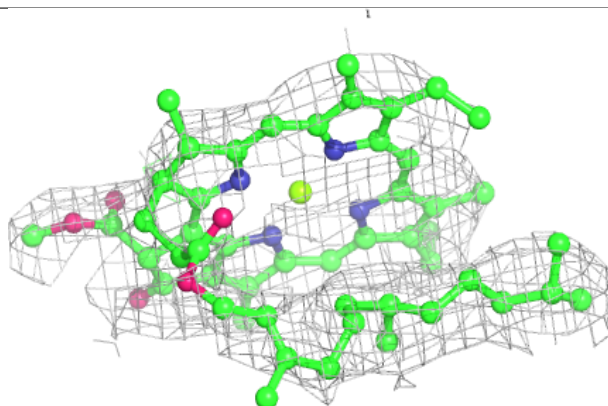
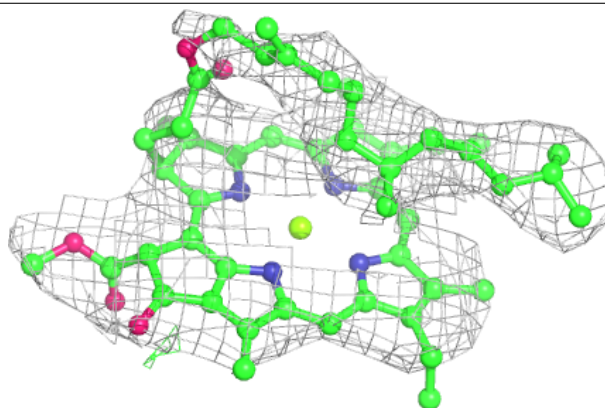


**Electron density around CLA B 1236:**

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

**Electron density around CLA B 1214:**

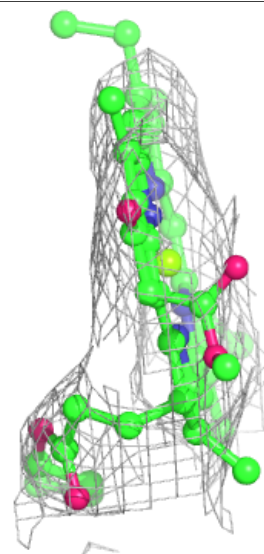
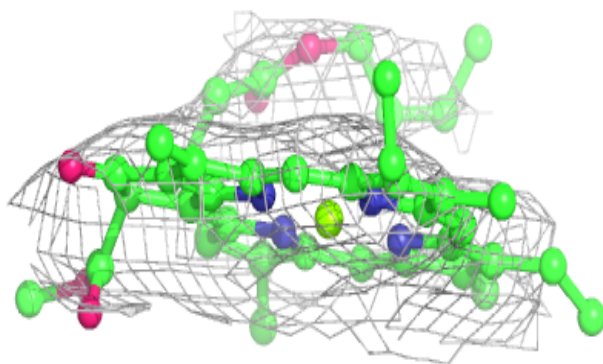
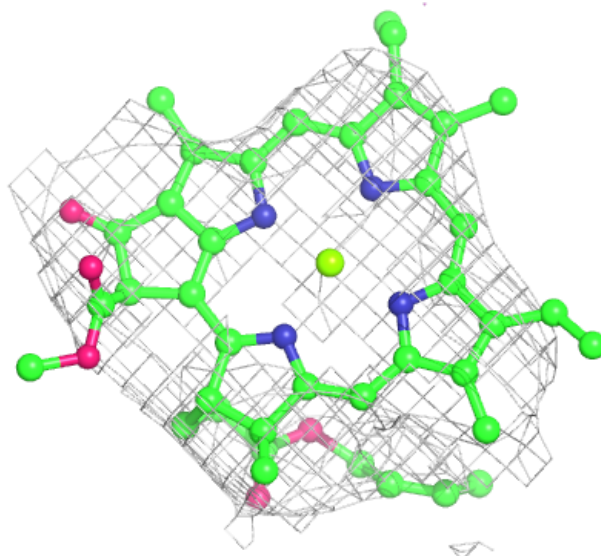
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





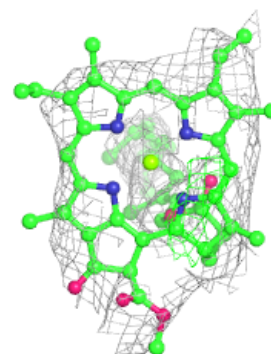
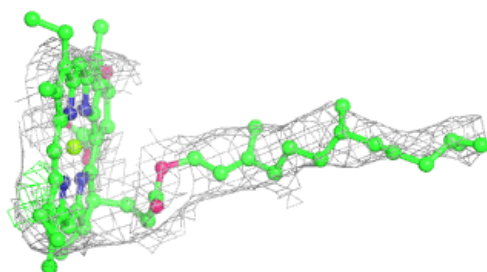
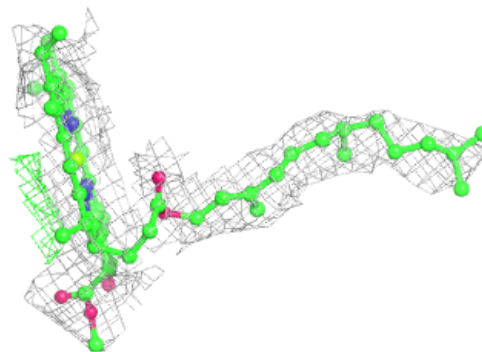
**Electron density around CLA A 1117:**

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



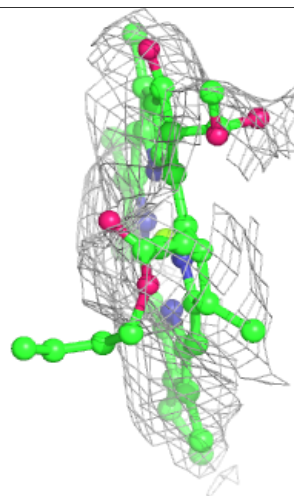
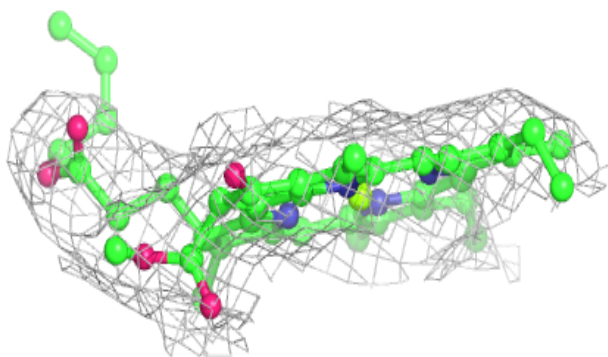
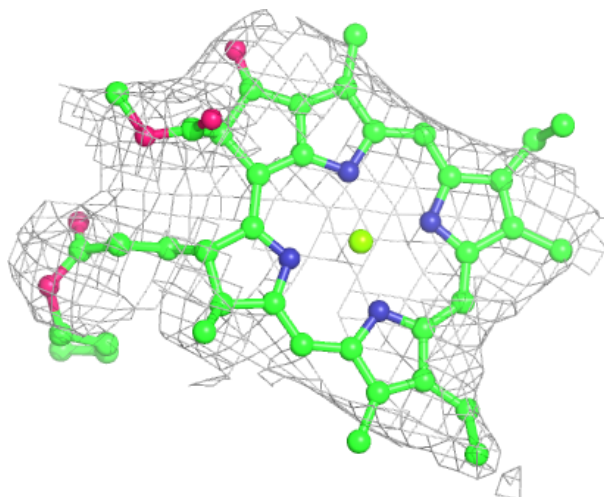
**Electron density around CLA A 1126:**

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



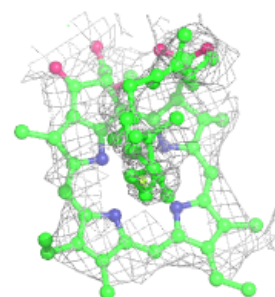
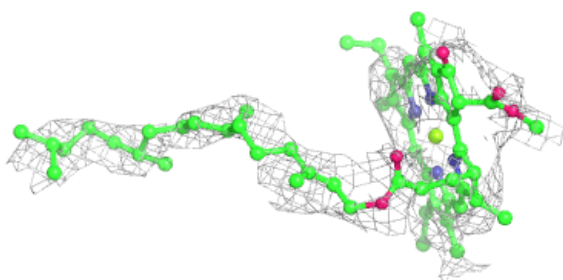
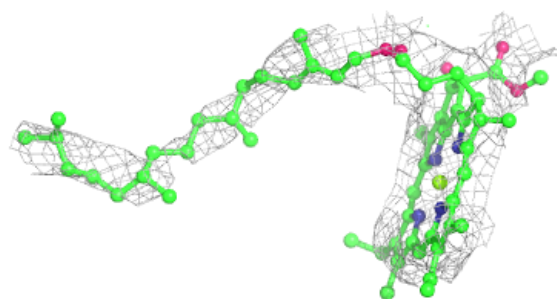
**Electron density around CLA B 1206:**

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



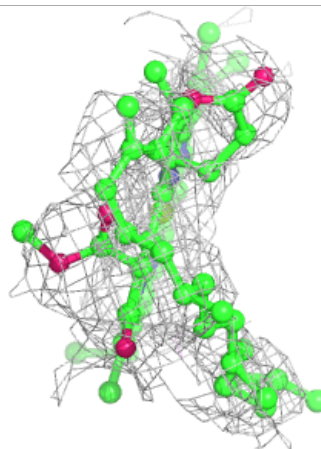
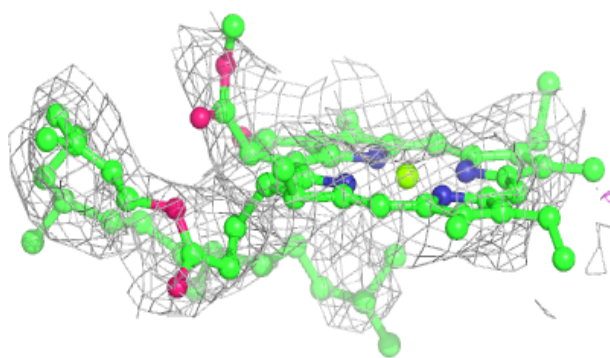
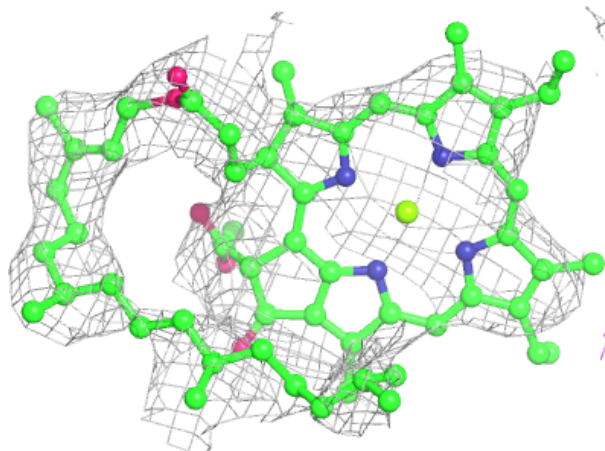
**Electron density around CLA A 1128:**

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



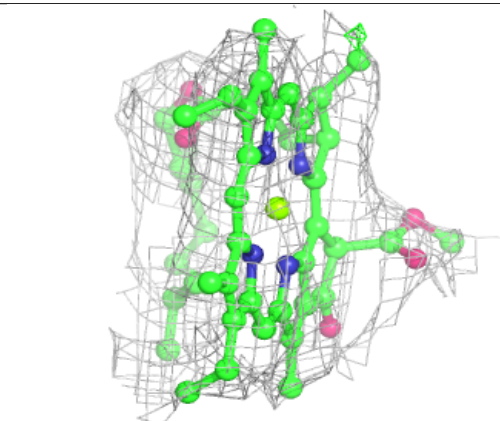
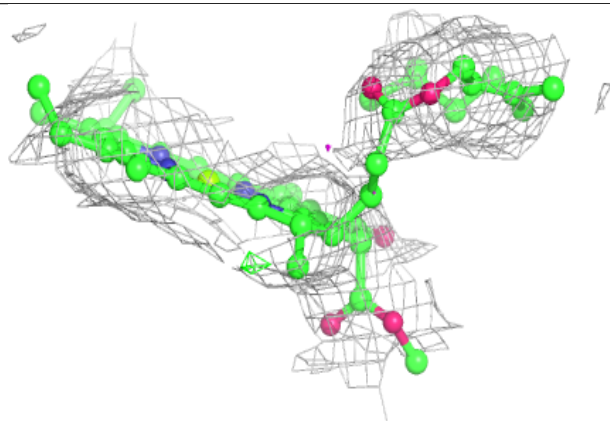
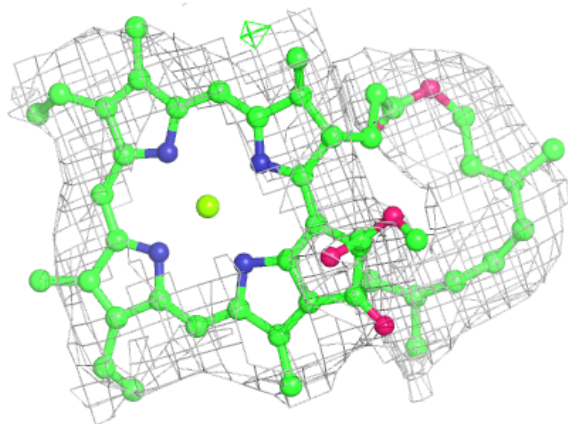
**Electron density around CLA B 1202:**

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

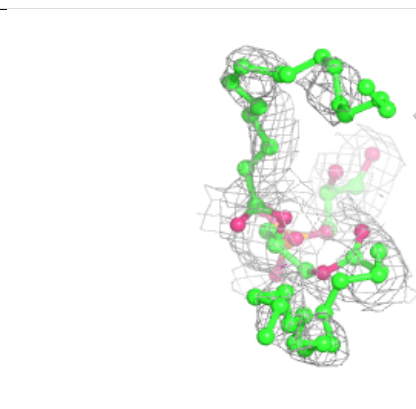
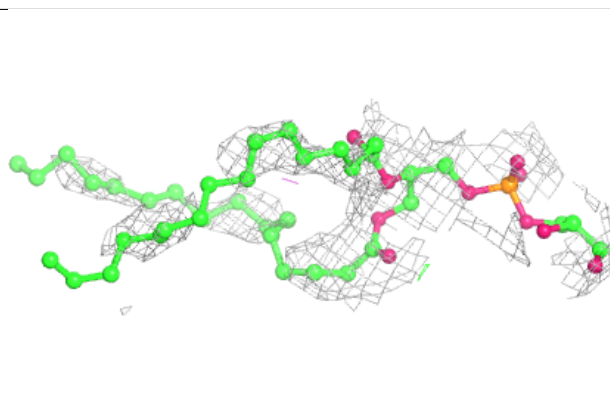
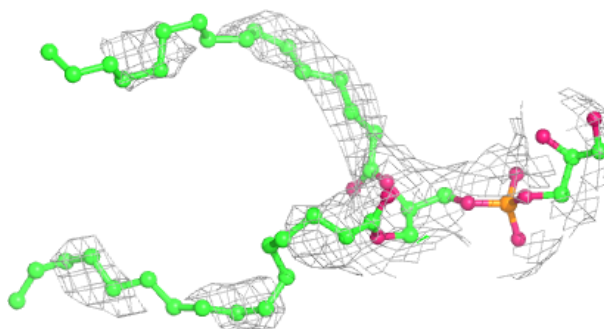


**Electron density around CLA B 1229:**

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

**Electron density around LHG A 5001:**

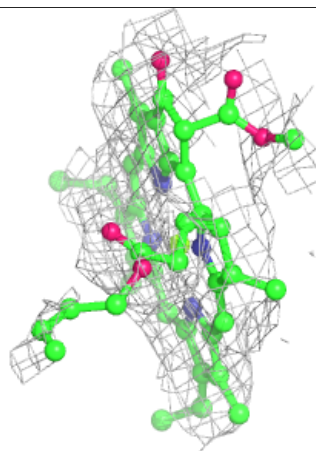
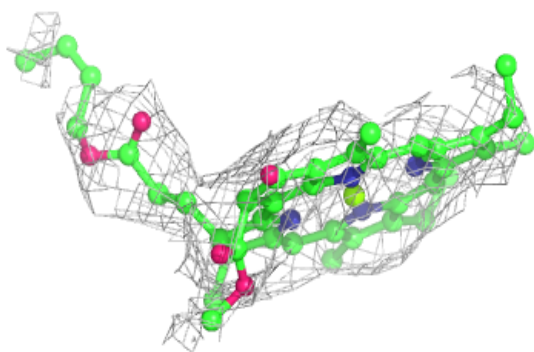
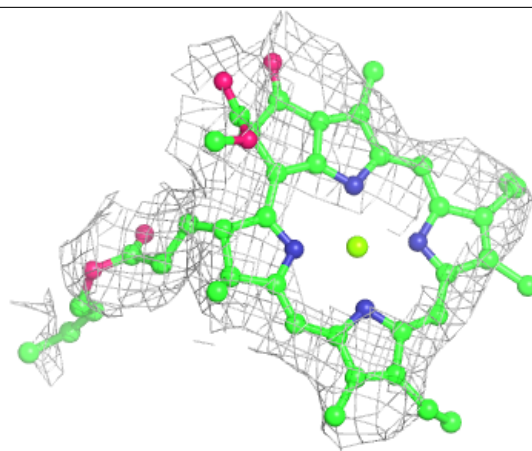
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





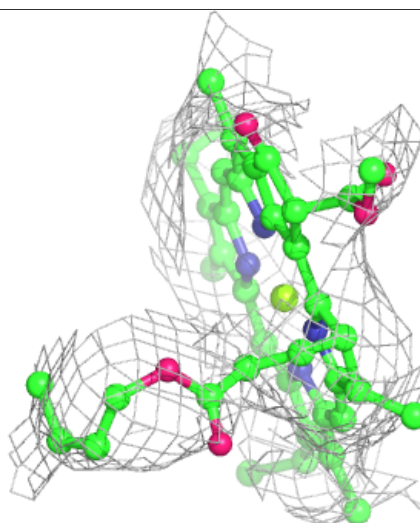
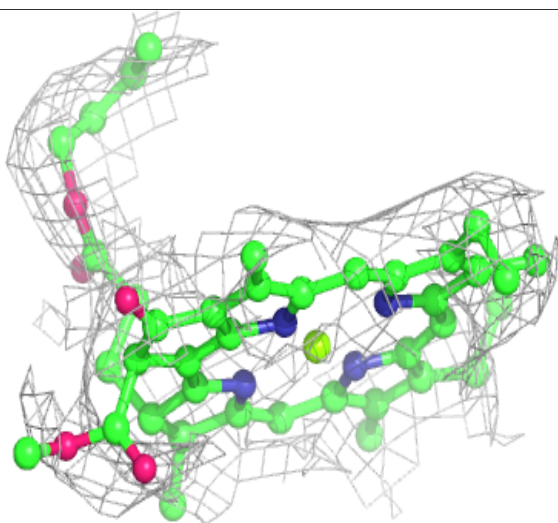
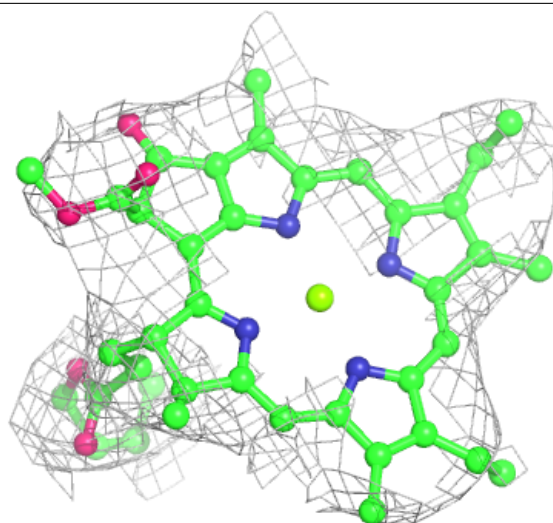
**Electron density around CLA B 1230:**

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



**Electron density around CLA B 1232:**

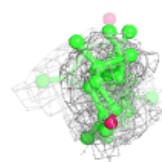
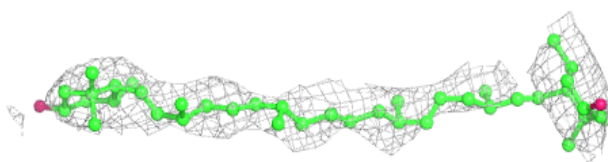
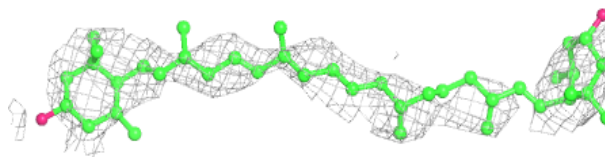
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



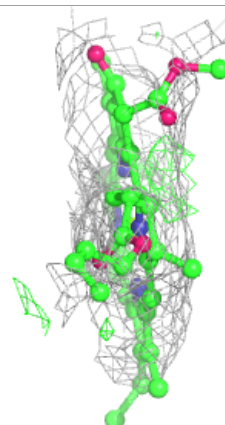
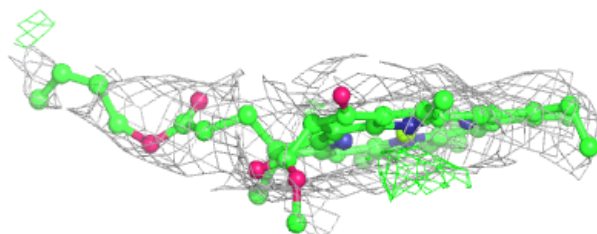
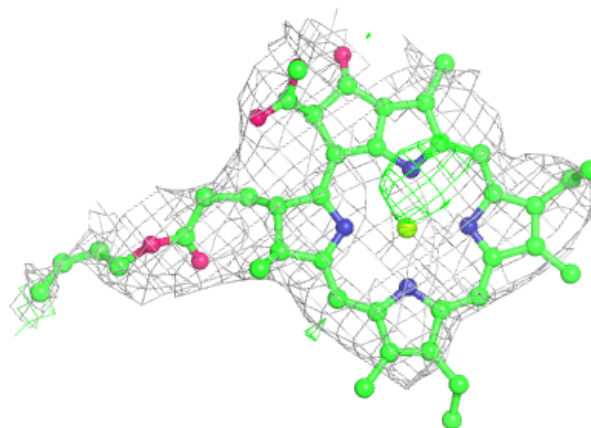


**Electron density around C7Z J 4015:**

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

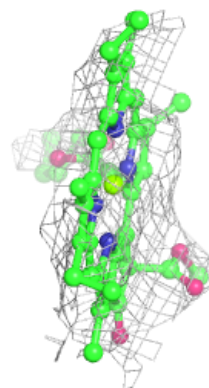
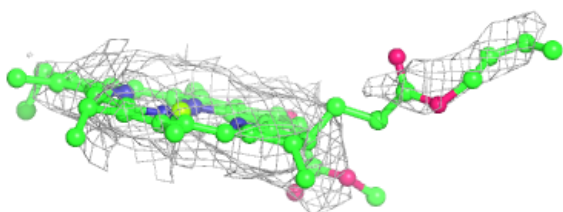
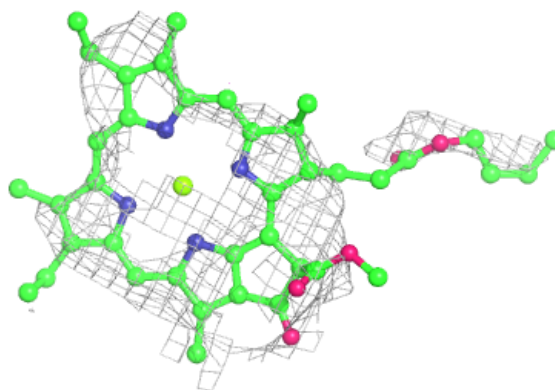
**Electron density around CLA A 1012:**

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



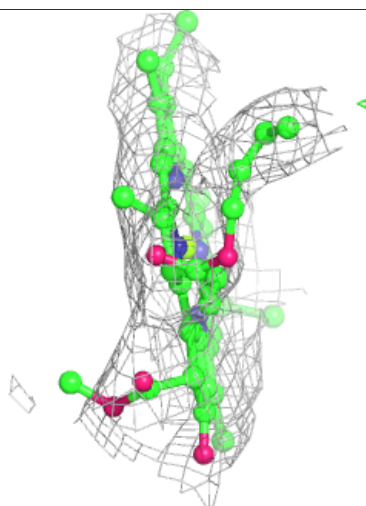
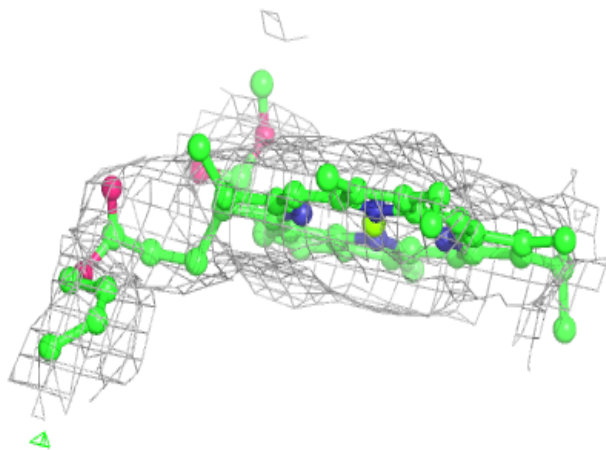
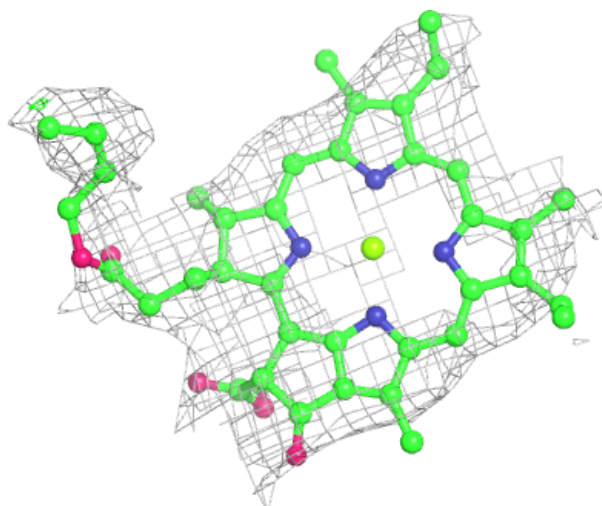
**Electron density around CLA B 1223:**

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



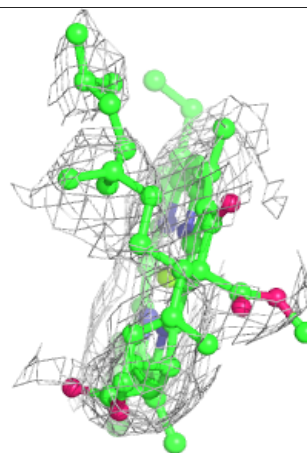
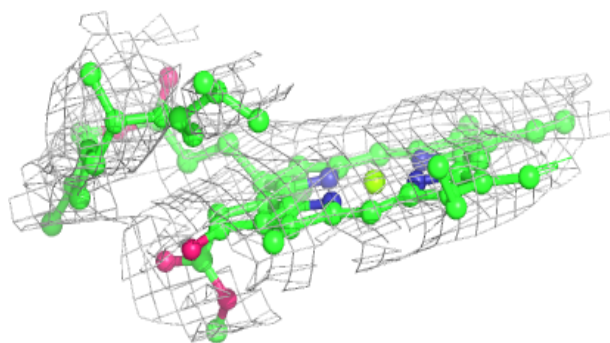
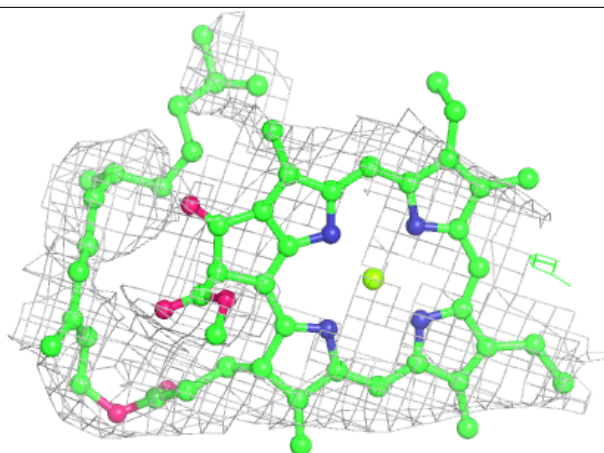
**Electron density around CLA B 1210:**

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



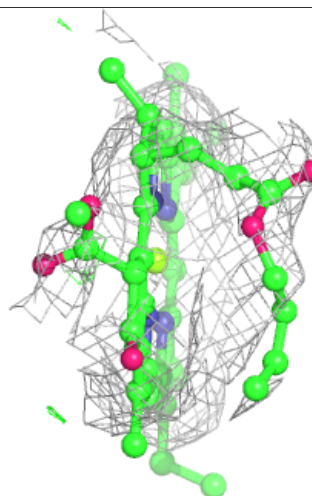
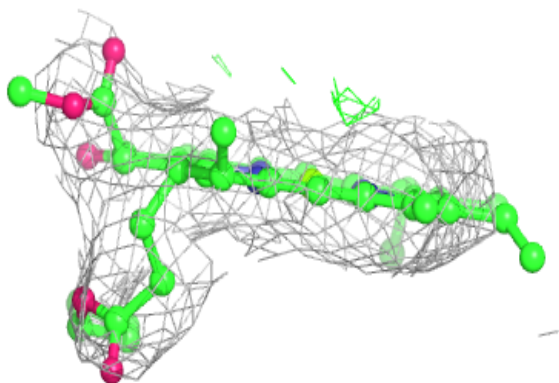
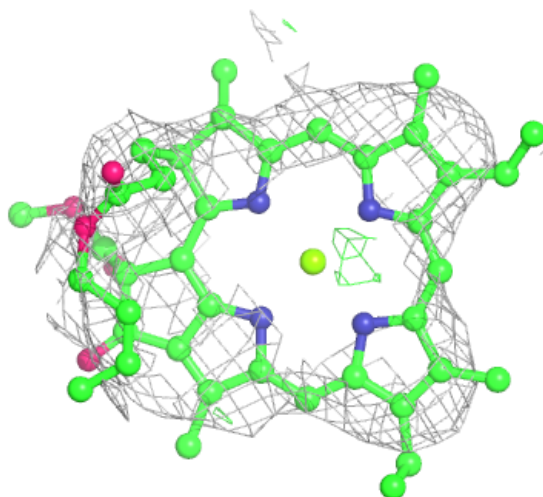
**Electron density around CLA A 1123:**

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



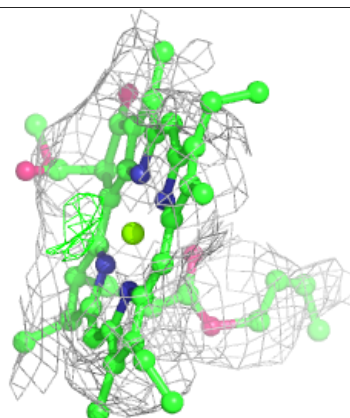
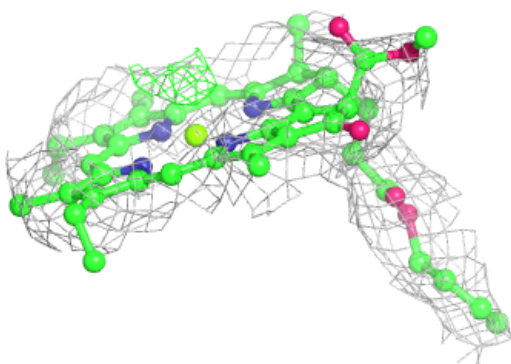
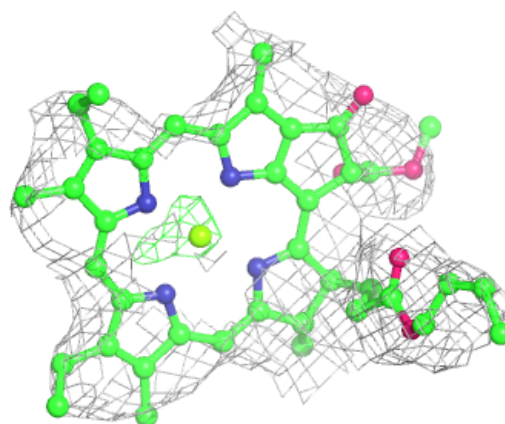
**Electron density around CLA A 1127:**

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

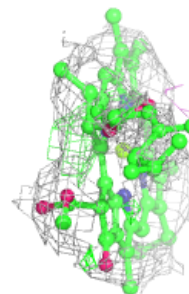
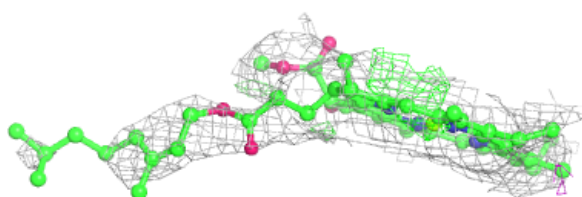
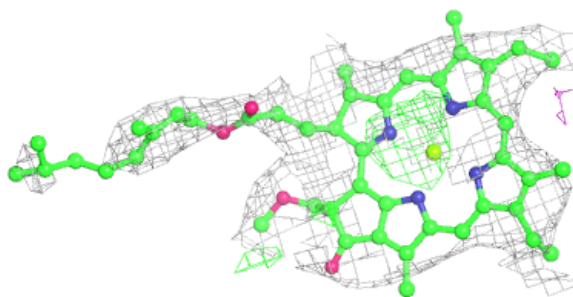


**Electron density around CLA B 1231:**

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

**Electron density around CLA A 1139:**

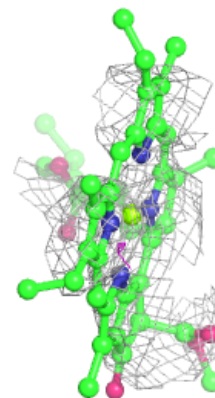
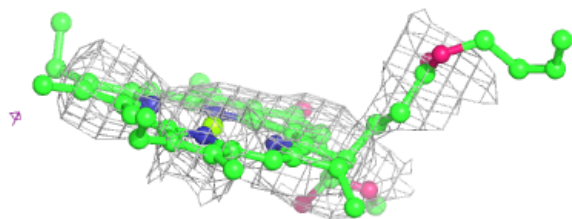
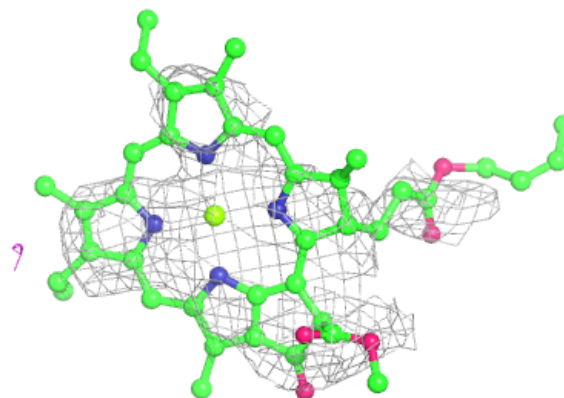
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





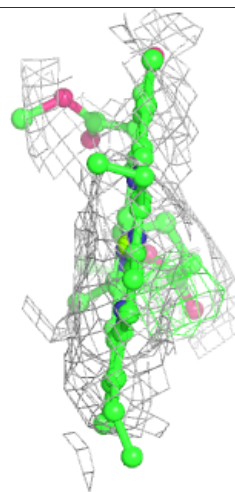
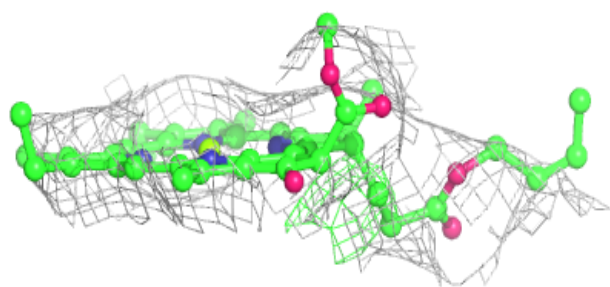
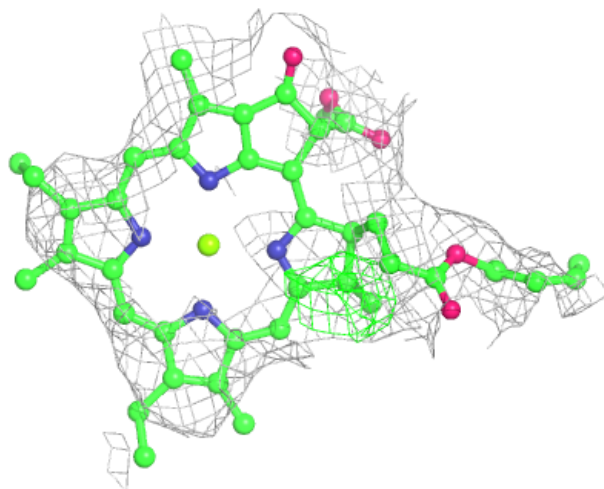
**Electron density around CLA A 1124:**

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



**Electron density around CLA A 1103:**

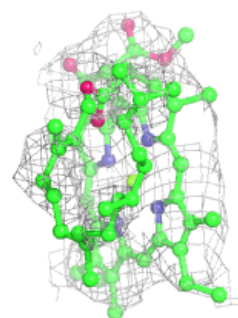
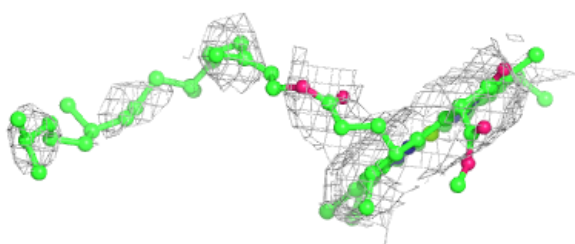
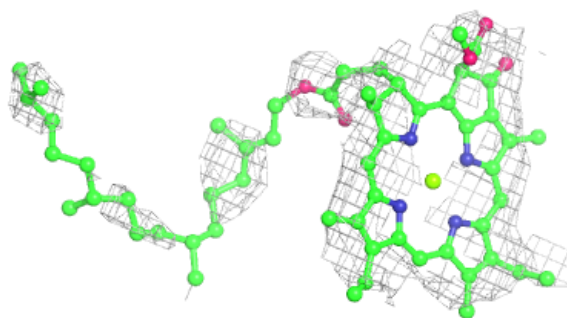
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





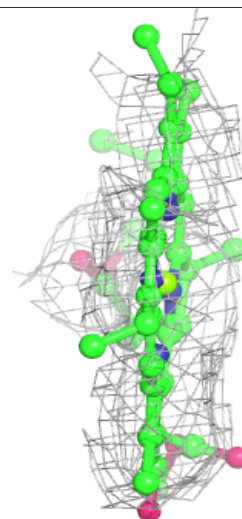
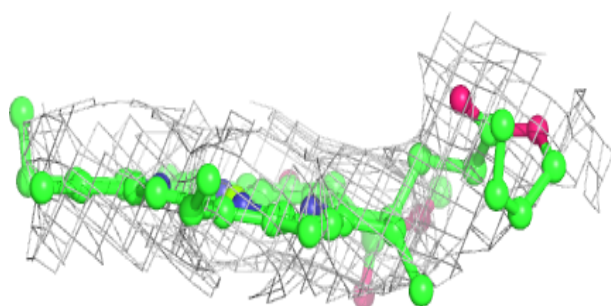
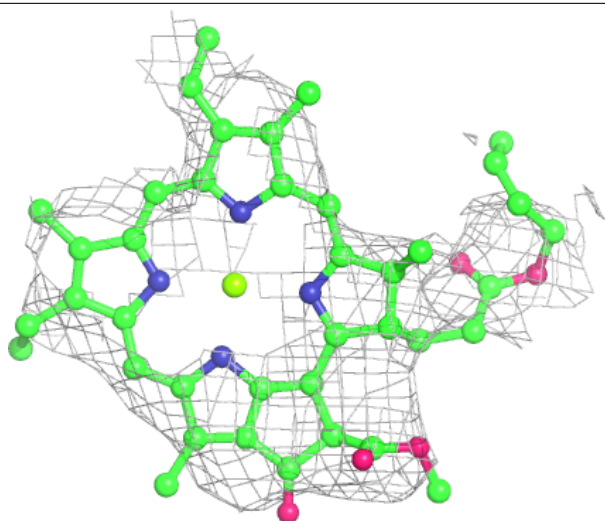
**Electron density around CLA A 1106:**

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



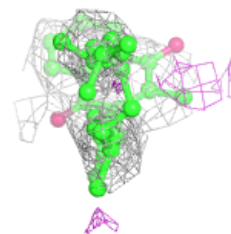
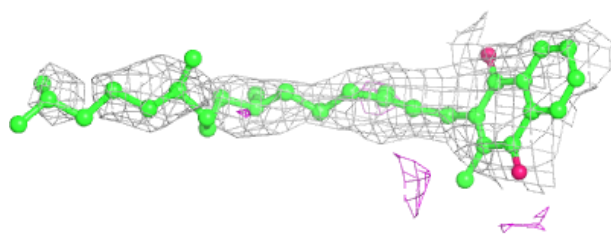
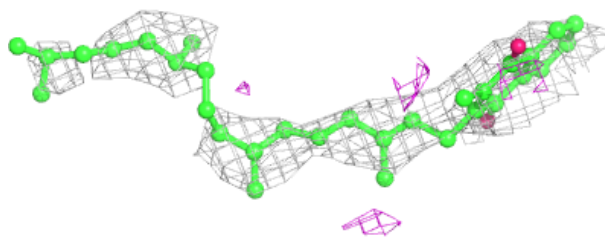
**Electron density around CLA B 1023:**

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



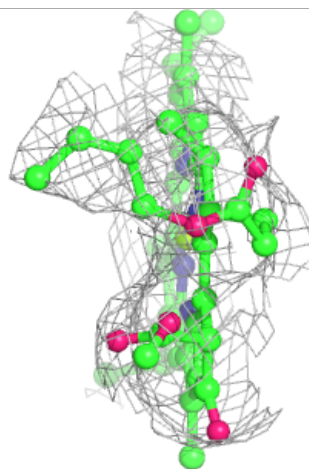
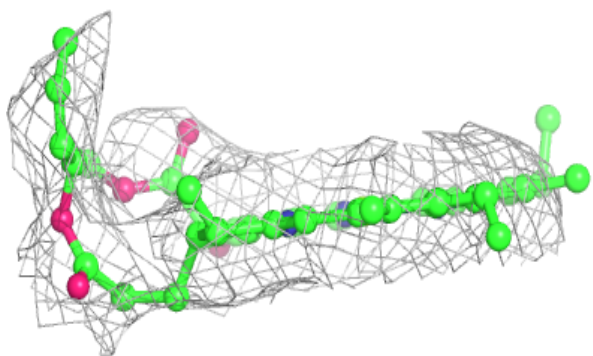
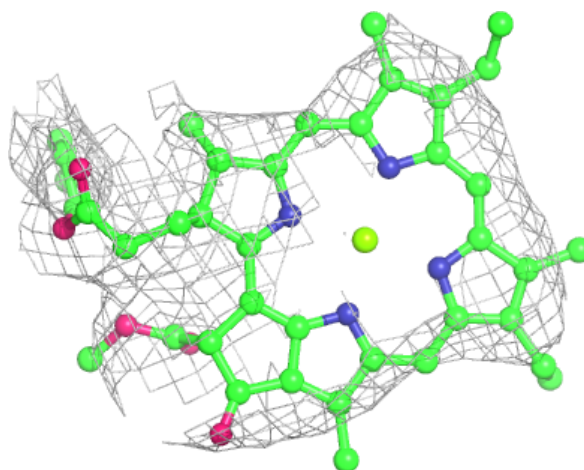
**Electron density around PQN A 2001:**

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



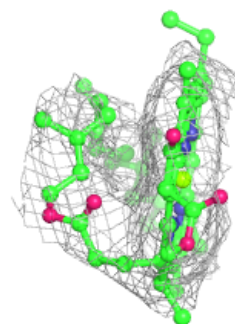
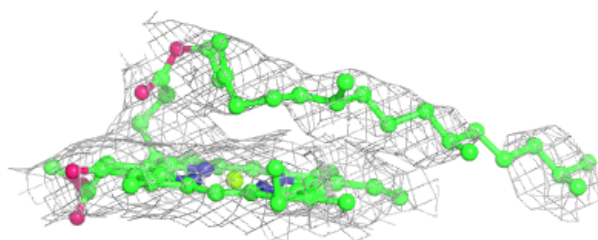
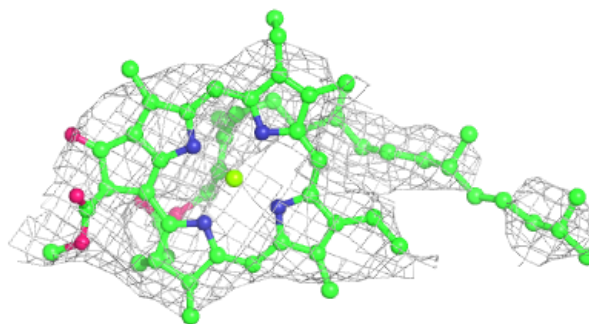
**Electron density around CLA A 1104:**

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



**Electron density around CLA A 1138:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.