



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:19 PM BST

PDB ID : 4KT0
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-05-19
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

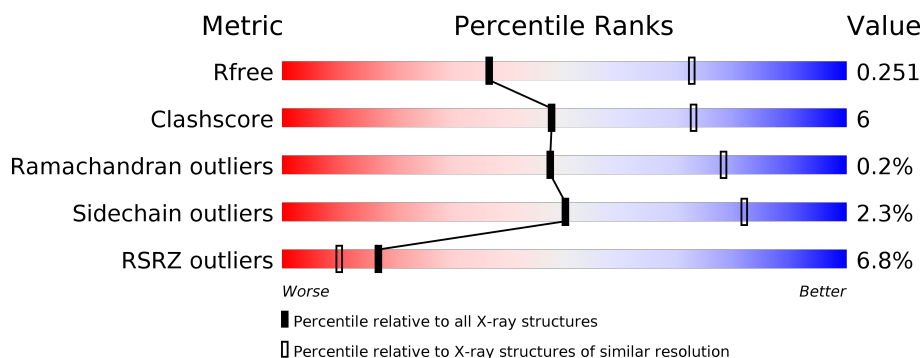
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	751	<div> <div>8%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	731	<div> <div>3%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
3	C	81	<div> <div>94%</div> <div>.</div> <div>..</div> </div>
4	D	141	<div> <div>16%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
5	E	74	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>.</div> <div>8%</div> </div>
6	F	165	<div> <div>2%</div> <div>78%</div> <div>7%</div> <div>..</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
7	J	40	
8	K	128	
9	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
13	CL0	A	1011	X	-	-	-
13	CL0	A	1108	X	-	-	-
15	CLA	A	1012	X	-	-	-
15	CLA	A	1022	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1801	X	-	-	-
15	CLA	B	1013	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1139	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1410	X	-	-	-
15	CLA	J	1302	X	-	-	-
15	CLA	J	1303	X	-	-	-
15	CLA	K	1401	X	-	-	-
15	CLA	K	1402	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5787	3791	984	985	27			

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

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

- 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 subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	681	187	204	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1099	711	183	200	5			

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

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

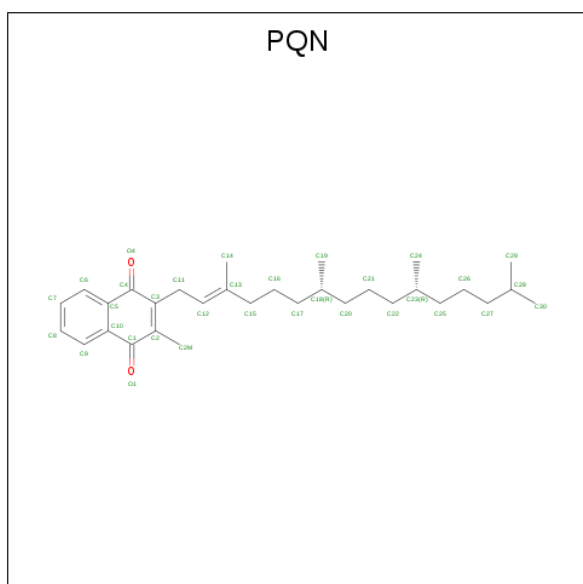
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	53	Total	C	N	O	S	0	0	0
			366	242	56	63	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	30	Total	C	N	O	0	0	0
			214	142	34	38			

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



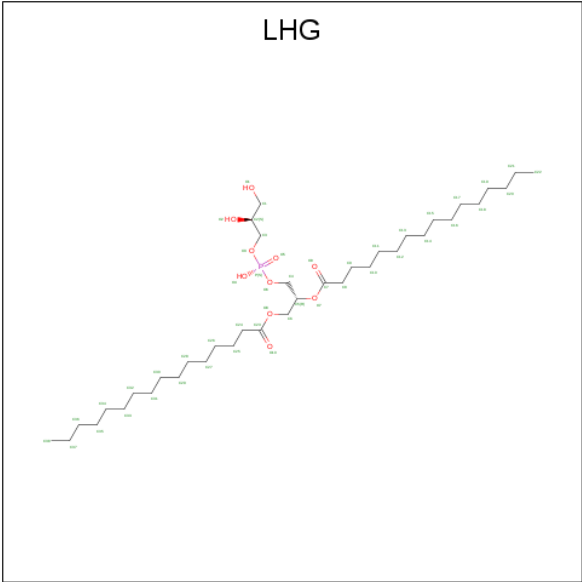
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			33	31	2		
10	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



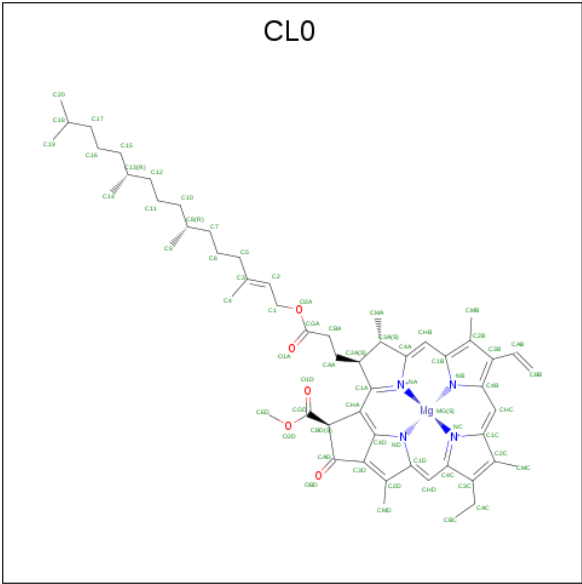
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



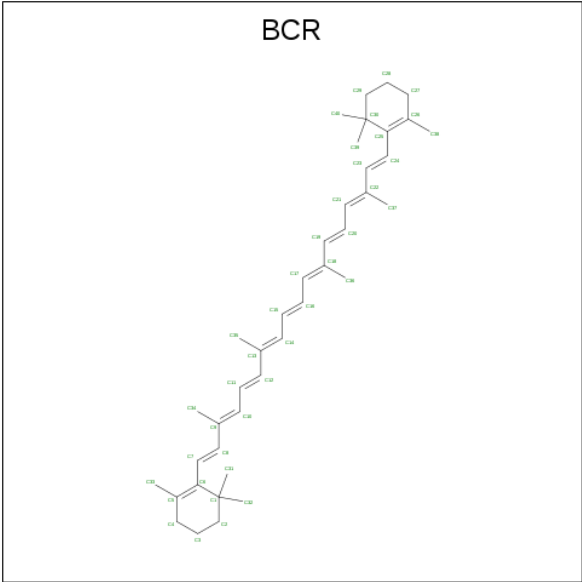
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			36	25	10	1		
12	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



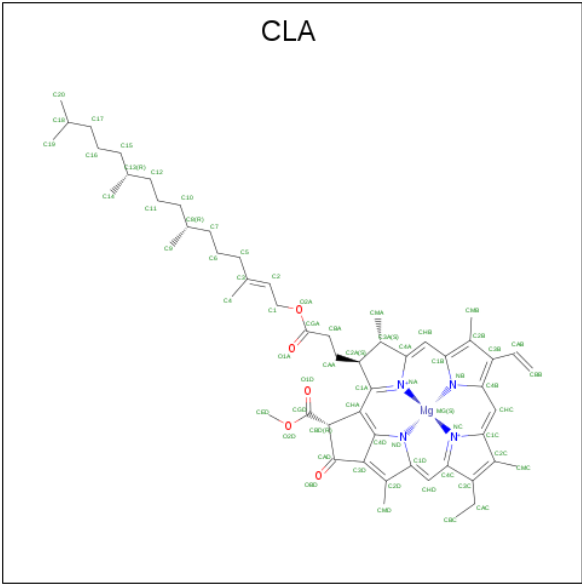
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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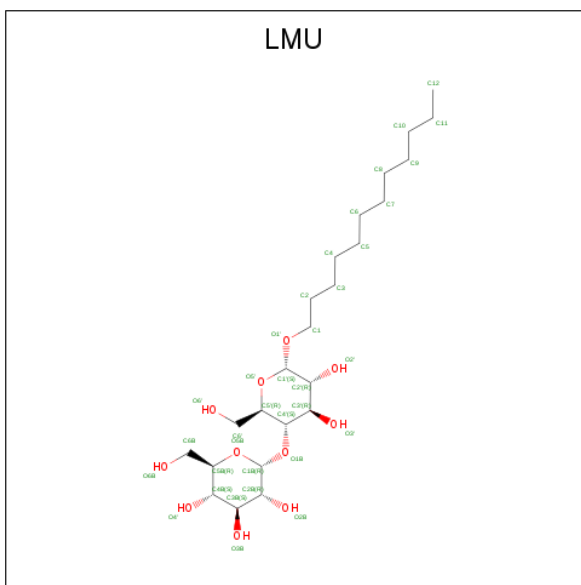
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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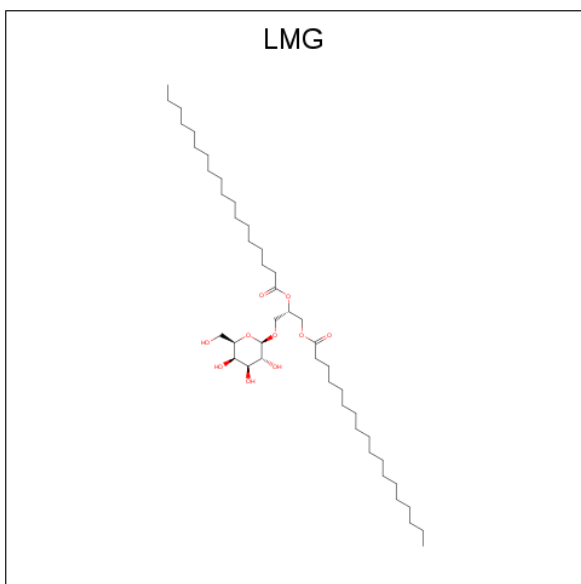
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total 35	C 24	O 11	0	0
16	J	1	Total 35	C 24	O 11	0	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

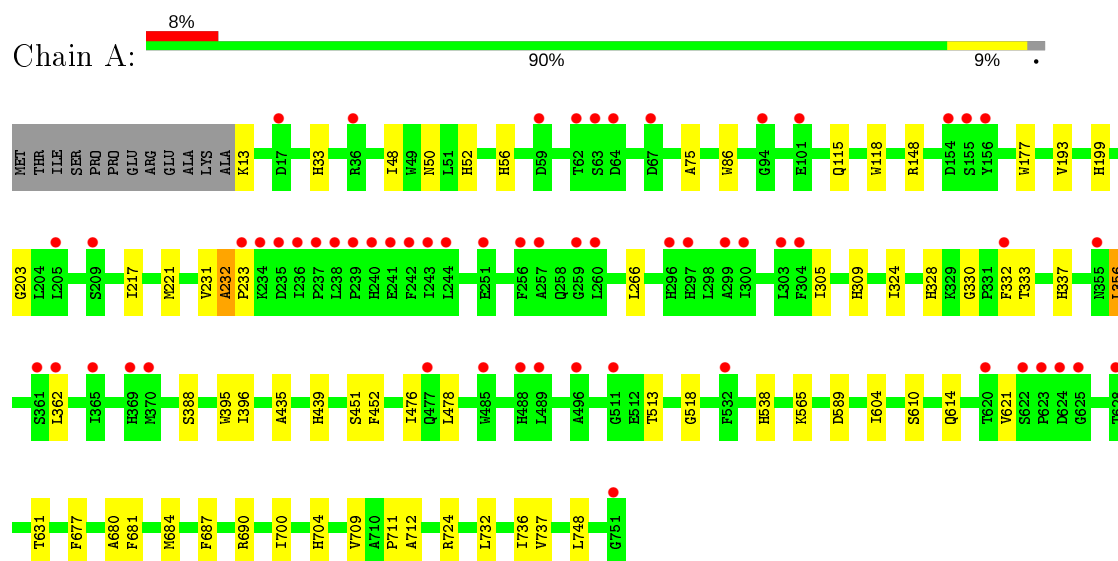
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	10	Total	O	0	0
			10	10		
19	B	15	Total	O	0	0
			15	15		
19	C	3	Total	O	0	0
			3	3		
19	F	1	Total	O	0	0
			1	1		

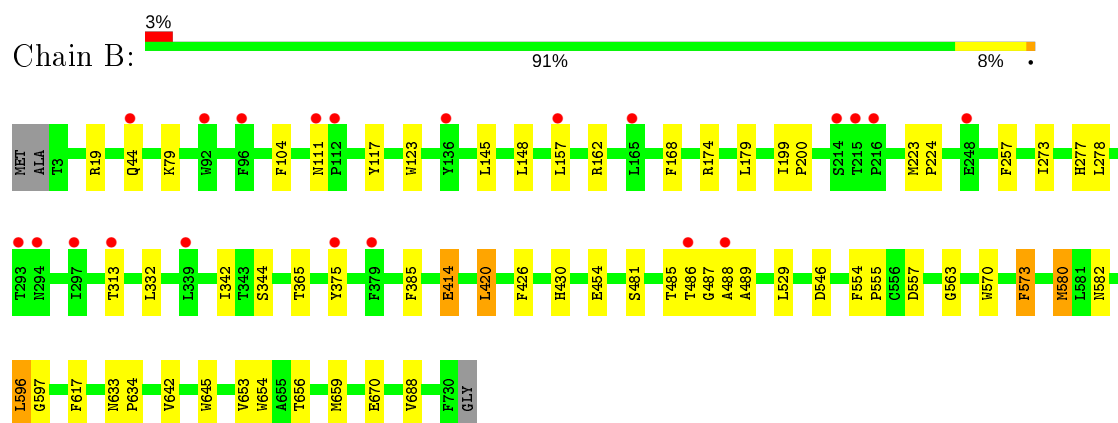
3 Residue-property plots [i](#)

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

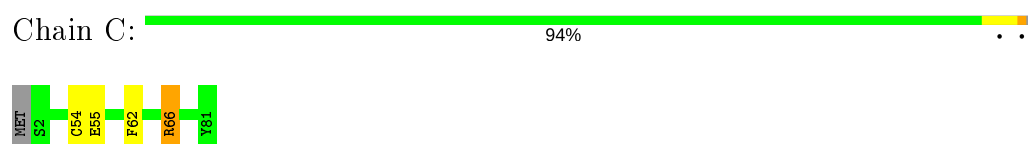
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



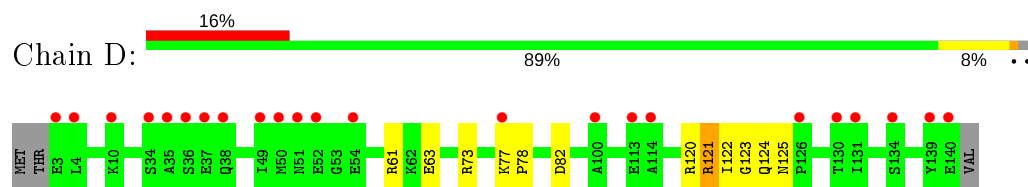
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



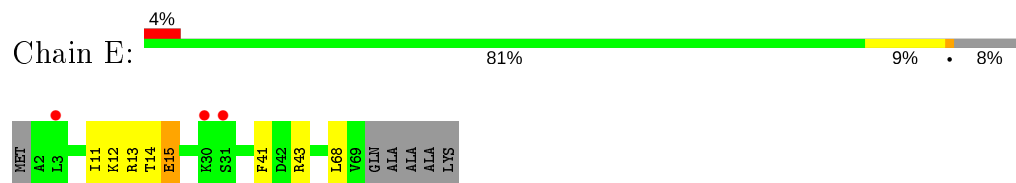
- Molecule 3: Photosystem I iron-sulfur center



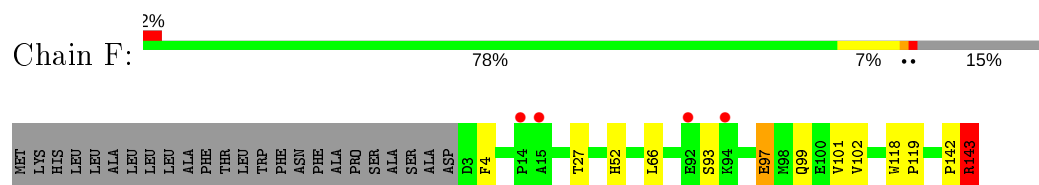
- Molecule 4: Photosystem I subunit II



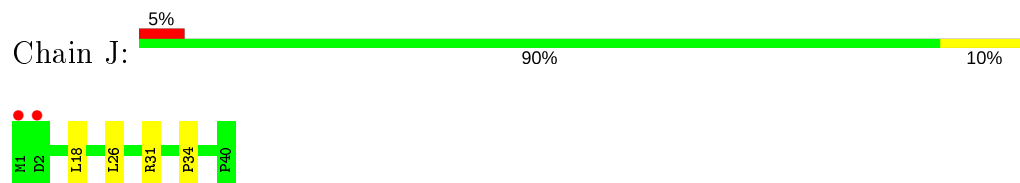
- Molecule 5: Photosystem I reaction center subunit IV



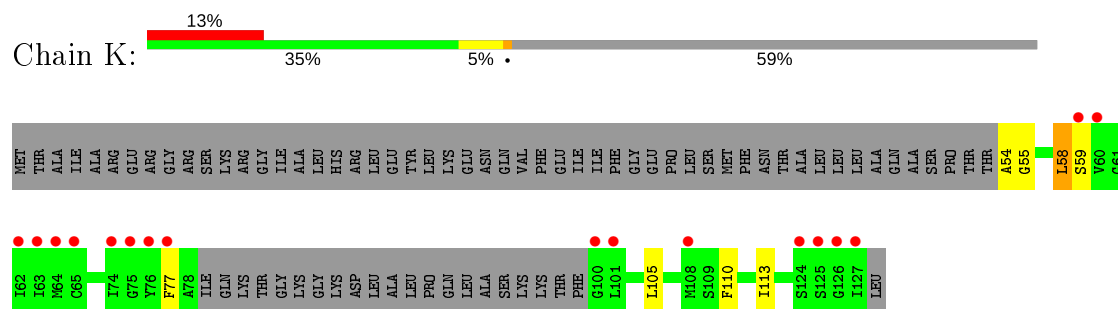
- Molecule 6: Photosystem I subunit III



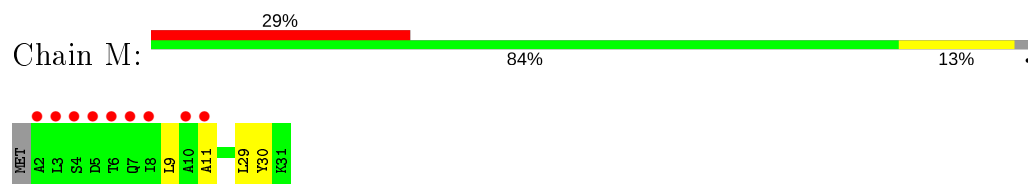
- Molecule 7: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit PsaK



- Molecule 9: 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, α , β , γ	120.18Å 173.31Å 179.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.80 48.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-2.80) 79.2 (48.55-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.245 0.203 , 0.251	Depositor DCC
R_{free} test set	5715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22051	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CL, SF4, LMU, PQN, CLA, CL0, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/5985	0.38	0/8158
2	B	0.23	0/5976	0.40	0/8173
3	C	0.24	0/610	0.45	0/826
4	D	0.23	0/1099	0.40	0/1482
5	E	0.24	0/542	0.45	0/733
6	F	0.23	0/1129	0.40	0/1535
7	J	0.26	0/328	0.38	0/443
8	K	0.25	0/371	0.39	0/499
9	M	0.22	0/217	0.35	0/295
All	All	0.23	0/16257	0.39	0/22144

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
6	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	121	ARG	Sidechain
6	F	143	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5646	60	0
2	B	5765	0	5544	56	0
3	C	600	0	581	4	0
4	D	1075	0	1069	7	0
5	E	533	0	517	8	0
6	F	1099	0	1096	7	0
7	J	319	0	328	4	0
8	K	366	0	376	7	0
9	M	214	0	213	2	0
10	A	33	0	46	1	0
10	B	33	0	46	3	0
11	A	8	0	0	0	0
11	C	16	0	0	0	0
12	A	134	0	190	18	0
12	B	49	0	74	2	0
13	A	110	0	105	12	0
14	A	240	0	294	17	0
14	B	320	0	390	26	0
14	F	80	0	97	8	0
14	J	40	0	49	3	0
15	A	2352	0	2285	69	0
15	B	2365	0	2272	58	0
15	F	175	0	177	3	0
15	J	91	0	66	2	0
15	K	92	0	66	2	0
16	B	35	0	46	0	0
16	J	35	0	46	2	0
17	B	55	0	86	2	0
18	B	1	0	0	0	0
19	A	10	0	0	5	0
19	B	15	0	0	6	0
19	C	3	0	0	0	0
19	F	1	0	0	1	0
All	All	22051	0	21705	267	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (267) 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)
13:A:1011:CL0:CMA	19:A:9109:HOH:O	1.91	1.19
13:A:1011:CL0:H6	19:A:9109:HOH:O	1.48	1.11
14:B:4004:BCR:H403	14:B:4004:BCR:H23C	1.51	0.92
13:A:1011:CL0:H71	19:A:9109:HOH:O	1.71	0.88
15:A:1110:CLA:HBD	15:A:1110:CLA:HBA1	1.57	0.86
12:A:5005:LHG:H251	12:A:5005:LHG:C8	2.11	0.81
1:A:395:TRP:CD1	15:A:1126:CLA:HAB	2.16	0.80
7:J:31:ARG:NH2	15:J:1302:CLA:O1D	2.15	0.80
14:A:4008:BCR:HC8	15:A:1124:CLA:HAB	1.61	0.80
1:A:604:ILE:HD11	13:A:1011:CL0:H35	1.66	0.78
2:B:123:TRP:CZ2	15:B:1210:CLA:H201	2.18	0.78
12:A:5005:LHG:HC81	12:A:5005:LHG:H251	1.66	0.78
15:J:1302:CLA:HBB1	15:J:1302:CLA:HHC	1.66	0.77
15:A:1113:CLA:HHC	15:A:1113:CLA:HBB1	1.67	0.76
1:A:538:HIS:ND1	15:A:1135:CLA:HAB	2.01	0.75
14:A:4003:BCR:H14C	15:A:1103:CLA:H201	1.69	0.74
1:A:13:LYS:HB2	15:A:1110:CLA:HAA1	1.69	0.74
15:A:1128:CLA:HHC	15:A:1128:CLA:HBB1	1.70	0.73
2:B:582:ASN:OD1	19:B:9102:HOH:O	2.05	0.73
1:A:332:PHE:HB2	12:A:5003:LHG:HC41	1.71	0.73
13:A:1011:CL0:C2A	19:A:9109:HOH:O	2.33	0.72
15:A:1101:CLA:H203	15:A:1126:CLA:H202	1.73	0.70
14:A:4008:BCR:C8	15:A:1124:CLA:HAB	2.21	0.70
2:B:656:THR:HA	15:B:1023:CLA:HAB	1.72	0.70
15:B:1203:CLA:HHB	15:B:1226:CLA:HAB	1.74	0.70
15:B:1227:CLA:HAB	15:B:1236:CLA:HBB2	1.73	0.69
1:A:330:GLY:HA3	12:A:5003:LHG:HC32	1.75	0.69
15:A:1110:CLA:CBD	15:A:1110:CLA:HBA1	2.23	0.69
15:A:1131:CLA:HBB1	15:A:1131:CLA:HHC	1.74	0.69
15:A:1101:CLA:HBB1	15:A:1101:CLA:HHC	1.74	0.69
19:B:9105:HOH:O	14:F:4015:BCR:HC32	1.94	0.68
1:A:737:VAL:HG22	14:B:4011:BCR:HC21	1.76	0.68
14:A:4001:BCR:H23C	8:K:110:PHE:HB2	1.75	0.68
5:E:13:ARG:O	5:E:14:THR:HB	1.93	0.67
1:A:476:ILE:HD12	12:A:5005:LHG:HC81	1.75	0.67
1:A:435:ALA:O	1:A:439:HIS:ND1	2.27	0.66
15:A:1110:CLA:HMB3	15:A:1118:CLA:C3D	2.25	0.66
15:A:1131:CLA:CBB	12:A:5005:LHG:H281	2.26	0.65
15:B:1220:CLA:HMD2	15:B:1221:CLA:HAB	1.76	0.65
14:A:4001:BCR:H24C	15:A:1120:CLA:HMD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1012:CLA:H42	14:B:4011:BCR:H362	1.77	0.65
15:A:1107:CLA:HBB1	15:A:1107:CLA:HHC	1.79	0.64
2:B:332:LEU:HD11	15:B:1226:CLA:HBB1	1.79	0.64
1:A:677:PHE:CG	14:B:4011:BCR:H363	2.33	0.64
1:A:231:VAL:O	1:A:232:ALA:HB3	1.97	0.64
15:A:1022:CLA:H202	14:B:4017:BCR:H343	1.80	0.63
16:J:1304:LMU:H82	16:J:1304:LMU:H41	1.80	0.63
13:A:1108:CL0:H15	13:A:1108:CL0:H2	1.81	0.63
13:A:1011:CL0:H5	19:A:9109:HOH:O	1.79	0.62
1:A:604:ILE:CD1	13:A:1011:CL0:H35	2.29	0.62
12:A:5005:LHG:HC82	12:A:5005:LHG:H251	1.82	0.62
12:B:5004:LHG:H202	14:B:4009:BCR:H353	1.82	0.62
15:B:1229:CLA:H192	14:F:4016:BCR:H19C	1.81	0.61
1:A:680:ALA:C	15:B:1013:CLA:HAB	2.20	0.61
2:B:430:HIS:HB2	14:F:4015:BCR:HC22	1.83	0.61
12:A:5005:LHG:HC82	12:A:5005:LHG:O10	2.00	0.61
15:B:1231:CLA:HHC	15:B:1231:CLA:HBB1	1.83	0.60
4:D:120:ARG:NH1	4:D:125:ASN:OD1	2.33	0.60
2:B:570:TRP:NE1	17:B:5002:LMG:O10	2.34	0.60
1:A:118:TRP:HB3	14:J:4013:BCR:HC21	1.84	0.60
1:A:589:ASP:OD1	1:A:724:ARG:NH1	2.34	0.60
15:B:1235:CLA:HBC2	14:F:4015:BCR:HC7	1.82	0.59
15:A:1110:CLA:HMB3	15:A:1118:CLA:CAD	2.32	0.59
15:B:1227:CLA:HAB	15:B:1236:CLA:CBB	2.31	0.59
15:F:1139:CLA:HHC	15:F:1139:CLA:HBB1	1.85	0.59
15:B:1205:CLA:CGA	15:B:1205:CLA:C1A	2.81	0.59
2:B:486:THR:N	2:B:487:GLY:CA	2.66	0.58
15:A:1102:CLA:H202	15:A:1105:CLA:H92	1.85	0.58
2:B:481:SER:O	2:B:485:THR:HG23	2.04	0.58
2:B:375:TYR:CD1	15:B:1224:CLA:HAB	2.39	0.58
15:A:1104:CLA:HBB1	15:A:1104:CLA:HHC	1.86	0.57
15:A:1110:CLA:HHC	15:A:1110:CLA:HBB1	1.86	0.57
14:J:4013:BCR:H23C	14:J:4013:BCR:H392	1.86	0.57
4:D:123:GLY:HA3	5:E:15:GLU:HG2	1.87	0.57
4:D:121:ARG:NH1	4:D:124:GLN:HG3	2.20	0.57
2:B:486:THR:N	2:B:487:GLY:HA2	2.19	0.56
14:A:4002:BCR:H342	15:A:1112:CLA:CHB	2.36	0.56
2:B:597:GLY:HA3	19:B:9112:HOH:O	2.05	0.55
2:B:656:THR:CA	15:B:1023:CLA:HAB	2.36	0.55
15:B:1231:CLA:C4C	15:B:1232:CLA:HAB	2.37	0.55
1:A:677:PHE:CD2	14:B:4011:BCR:H363	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1218:CLA:HHC	15:B:1218:CLA:HBB1	1.89	0.55
1:A:736:ILE:HG22	14:B:4011:BCR:HC31	1.88	0.55
15:A:1122:CLA:HHC	15:A:1122:CLA:HBB1	1.89	0.54
5:E:12:LYS:O	5:E:12:LYS:HD3	2.07	0.54
5:E:14:THR:O	5:E:14:THR:HG22	2.07	0.54
2:B:385:PHE:CZ	14:B:4010:BCR:H373	2.42	0.54
15:A:1106:CLA:HAB	15:A:1126:CLA:H142	1.90	0.54
1:A:217:ILE:HA	1:A:221:MET:HE2	1.90	0.53
9:M:9:LEU:O	9:M:11:ALA:N	2.37	0.53
15:A:1101:CLA:H203	15:A:1126:CLA:C20	2.36	0.53
15:A:1110:CLA:CHA	15:A:1110:CLA:HBA1	2.39	0.53
15:B:1230:CLA:OBD	19:B:9106:HOH:O	2.18	0.53
2:B:645:TRP:CZ3	14:B:4017:BCR:HC41	2.44	0.53
14:A:4003:BCR:H14C	15:A:1103:CLA:C20	2.38	0.53
2:B:385:PHE:CE2	14:B:4010:BCR:H373	2.44	0.53
2:B:19:ARG:HD2	19:B:9108:HOH:O	2.09	0.53
2:B:168:PHE:O	2:B:174:ARG:NH2	2.42	0.52
2:B:557:ASP:OD2	3:C:66:ARG:NH2	2.42	0.52
14:B:4014:BCR:HC41	15:B:1229:CLA:HBB2	1.91	0.52
15:A:1110:CLA:CBB	15:A:1110:CLA:HHC	2.40	0.52
1:A:395:TRP:NE1	15:A:1126:CLA:HAB	2.23	0.52
1:A:395:TRP:HD1	15:A:1126:CLA:HAB	1.73	0.52
1:A:56:HIS:CG	15:A:1103:CLA:HAB	2.45	0.52
10:B:2002:PQN:H302	17:B:5002:LMG:H192	1.92	0.52
4:D:61:ARG:NH2	4:D:63:GLU:OE1	2.43	0.52
2:B:385:PHE:HZ	15:B:1222:CLA:HAB	1.75	0.52
10:B:2002:PQN:H303	15:B:1239:CLA:O1A	2.11	0.51
2:B:554:PHE:HB2	2:B:555:PRO:HD2	1.92	0.51
13:A:1108:CL0:H27	15:A:1110:CLA:HMD1	1.93	0.51
1:A:711:PRO:HB2	19:F:9301:HOH:O	2.09	0.51
15:B:1229:CLA:HAB	15:B:1230:CLA:C2B	2.40	0.51
2:B:430:HIS:CG	14:F:4015:BCR:HC42	2.46	0.51
1:A:362:LEU:CD2	15:A:1127:CLA:H202	2.41	0.51
2:B:44:GLN:OE1	2:B:162:ARG:NH1	2.42	0.51
1:A:305:ILE:HG21	14:A:4001:BCR:H14C	1.93	0.51
15:B:1212:CLA:HAB	15:B:1211:CLA:CMC	2.40	0.51
8:K:58:LEU:N	8:K:58:LEU:CD1	2.73	0.51
1:A:681:PHE:HA	15:B:1013:CLA:HAB	1.92	0.50
1:A:324:ILE:O	1:A:328:HIS:ND1	2.36	0.50
1:A:231:VAL:O	1:A:232:ALA:CB	2.58	0.50
14:A:4002:BCR:HC41	15:A:1103:CLA:H122	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:PHE:CZ	14:F:4015:BCR:HC41	2.47	0.50
2:B:123:TRP:CE2	15:B:1210:CLA:H201	2.46	0.49
13:A:1108:CL0:OBD	15:A:1110:CLA:H71	2.13	0.49
1:A:33:HIS:NE2	15:A:1109:CLA:O1A	2.32	0.49
2:B:454:GLU:OE2	6:F:52:HIS:ND1	2.41	0.49
2:B:642:VAL:HG22	15:B:1206:CLA:HHD	1.95	0.49
8:K:58:LEU:HD13	8:K:58:LEU:H	1.78	0.48
1:A:75:ALA:HB1	15:A:1103:CLA:HBB1	1.95	0.48
14:A:4007:BCR:H15C	14:A:4007:BCR:H351	1.70	0.48
1:A:333:THR:OG1	12:A:5003:LHG:HC2	2.13	0.48
12:A:5005:LHG:HC82	12:A:5005:LHG:C23	2.43	0.48
1:A:684:MET:HE2	10:A:2001:PQN:H2M3	1.95	0.48
2:B:420:LEU:HD22	2:B:529:LEU:HB2	1.94	0.48
15:B:1235:CLA:H122	14:F:4016:BCR:H23C	1.95	0.48
15:A:1133:CLA:HHC	15:A:1133:CLA:HBB1	1.95	0.48
1:A:396:ILE:HD12	15:A:1127:CLA:HAB	1.94	0.48
14:A:4008:BCR:H371	14:A:4008:BCR:H24C	1.73	0.47
14:B:4006:BCR:H403	14:B:4006:BCR:C23	2.44	0.47
1:A:690:ARG:NH1	2:B:563:GLY:O	2.46	0.47
5:E:11:ILE:N	5:E:11:ILE:HD12	2.30	0.47
1:A:330:GLY:CA	12:A:5003:LHG:HC32	2.44	0.47
12:A:5005:LHG:H262	12:A:5005:LHG:H112	1.95	0.47
2:B:179:LEU:CD2	15:B:1216:CLA:HAB	2.44	0.47
1:A:610:SER:OG	1:A:614:GLN:NE2	2.47	0.47
15:A:1022:CLA:CAD	15:B:1021:CLA:HMB3	2.44	0.47
15:B:1215:CLA:H3A	15:B:1215:CLA:CGA	2.44	0.47
15:B:1235:CLA:C1A	15:B:1235:CLA:CGA	2.93	0.47
2:B:633:ASN:HB2	2:B:634:PRO:CD	2.44	0.47
15:A:1119:CLA:HMB2	15:A:1123:CLA:HMA3	1.97	0.47
15:B:1224:CLA:H3A	15:B:1224:CLA:CGA	2.45	0.47
2:B:486:THR:OG1	2:B:487:GLY:HA2	2.13	0.47
13:A:1011:CL0:H13	15:A:1012:CLA:HMD1	1.97	0.47
1:A:687:PHE:HB2	15:B:1013:CLA:HBC2	1.97	0.47
8:K:58:LEU:HD13	8:K:58:LEU:N	2.29	0.47
15:B:1013:CLA:CGA	15:B:1013:CLA:H3A	2.46	0.46
14:B:4010:BCR:H351	14:B:4010:BCR:H15C	1.69	0.46
14:A:4003:BCR:H24C	15:A:1127:CLA:H2	1.97	0.46
1:A:712:ALA:HB1	6:F:97:GLU:OE1	2.15	0.46
8:K:54:ALA:O	8:K:58:LEU:HD22	2.14	0.46
1:A:199:HIS:O	1:A:203:GLY:N	2.48	0.46
2:B:111:ASN:N	2:B:111:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:HA	15:A:1105:CLA:HBB2	1.98	0.46
15:A:1137:CLA:HAB	15:A:1129:CLA:CBB	2.45	0.46
2:B:273:ILE:O	2:B:277:HIS:ND1	2.43	0.46
14:J:4013:BCR:H15C	14:J:4013:BCR:H351	1.67	0.46
15:A:1022:CLA:H171	14:B:4017:BCR:H343	1.96	0.46
15:B:1203:CLA:OBD	15:B:1201:CLA:HHC	2.16	0.46
14:B:4017:BCR:H15C	14:B:4017:BCR:H351	1.68	0.46
1:A:681:PHE:N	15:B:1013:CLA:HAB	2.30	0.45
15:B:1215:CLA:HBB2	15:B:1221:CLA:H201	1.99	0.45
2:B:199:ILE:HB	2:B:200:PRO:HD3	1.99	0.45
1:A:362:LEU:HD22	15:A:1127:CLA:H202	1.97	0.45
15:A:1114:CLA:HBB1	15:A:1114:CLA:HHC	1.97	0.45
2:B:546:ASP:OD2	3:C:66:ARG:NH1	2.48	0.45
2:B:688:VAL:HG11	15:B:1237:CLA:HAB	1.99	0.45
15:A:1110:CLA:C3C	15:A:1111:CLA:HBB2	2.47	0.45
1:A:305:ILE:O	1:A:309:HIS:ND1	2.45	0.45
15:B:1236:CLA:HHC	15:B:1236:CLA:HBB1	1.99	0.45
14:B:4010:BCR:C23	14:B:4010:BCR:H403	2.46	0.45
1:A:565:LYS:NZ	2:B:670:GLU:OE2	2.44	0.45
1:A:476:ILE:CD1	12:A:5005:LHG:HC81	2.45	0.45
14:B:4010:BCR:H14C	15:B:1222:CLA:HMA1	1.99	0.45
5:E:13:ARG:O	5:E:14:THR:CB	2.59	0.45
2:B:573:PHE:CE2	15:B:1226:CLA:HMD2	2.52	0.45
2:B:104:PHE:CZ	2:B:642:VAL:HG23	2.52	0.44
14:B:4005:BCR:H351	14:B:4005:BCR:H15C	1.74	0.44
2:B:656:THR:N	15:B:1023:CLA:HAB	2.32	0.44
15:B:1212:CLA:HAB	15:B:1211:CLA:HMC3	1.99	0.44
15:A:1110:CLA:CGA	15:A:1110:CLA:C1A	2.95	0.44
14:A:4008:BCR:H15C	14:A:4008:BCR:H351	1.63	0.44
14:A:4012:BCR:C8	14:A:4012:BCR:H331	2.45	0.44
1:A:700:ILE:O	1:A:704:HIS:ND1	2.46	0.44
1:A:193:VAL:CG1	15:A:1123:CLA:HHD	2.48	0.44
8:K:54:ALA:HB3	15:K:1402:CLA:C1	2.48	0.44
1:A:680:ALA:O	15:B:1013:CLA:HAB	2.17	0.44
16:J:1304:LMU:H101	16:J:1304:LMU:H71	1.82	0.44
14:A:4002:BCR:H24C	14:A:4002:BCR:H371	1.72	0.44
14:B:4011:BCR:H392	14:B:4011:BCR:H23C	2.00	0.44
15:A:1106:CLA:H43	15:A:1126:CLA:HMD2	2.00	0.43
15:A:1801:CLA:HAB	15:A:1122:CLA:HHB	2.00	0.43
1:A:337:HIS:CE1	12:A:5003:LHG:HC12	2.53	0.43
15:B:1215:CLA:HBB1	15:B:1215:CLA:HHC	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1122:CLA:HBB1	15:A:1129:CLA:HMD2	2.00	0.43
2:B:117:TYR:HA	2:B:365:THR:HG22	2.01	0.43
2:B:426:PHE:CE1	14:F:4015:BCR:HC41	2.53	0.43
2:B:645:TRP:CE3	14:B:4017:BCR:HC41	2.54	0.43
5:E:11:ILE:HD11	5:E:41:PHE:HE1	1.82	0.43
14:A:4008:BCR:HC8	15:A:1124:CLA:CAB	2.42	0.43
5:E:14:THR:O	6:F:142:PRO:HG3	2.19	0.43
2:B:278:LEU:HG	15:B:1213:CLA:HAB	2.01	0.43
14:B:4014:BCR:HC8	15:B:1229:CLA:HBB1	2.01	0.43
15:A:1114:CLA:HHC	15:A:1114:CLA:CBB	2.49	0.42
15:A:1110:CLA:HMB3	15:A:1118:CLA:C4D	2.48	0.42
4:D:77:LYS:HB2	4:D:78:PRO:HD3	2.01	0.42
15:B:1222:CLA:H3A	15:B:1222:CLA:HBA2	1.88	0.42
14:A:4012:BCR:HC7	7:J:26:LEU:HD13	2.01	0.42
15:B:1215:CLA:HHC	15:B:1215:CLA:CBB	2.49	0.42
12:A:5003:LHG:H282	15:A:1122:CLA:H202	2.02	0.42
1:A:681:PHE:HA	15:B:1013:CLA:CAB	2.49	0.42
2:B:654:TRP:CE3	15:B:1021:CLA:HMA1	2.55	0.42
2:B:596:LEU:HD12	2:B:596:LEU:HA	1.81	0.42
1:A:177:TRP:HB2	15:A:1109:CLA:HMC3	2.01	0.42
1:A:356:LEU:HD11	15:A:1128:CLA:CBB	2.50	0.42
1:A:48:ILE:O	1:A:52:HIS:ND1	2.51	0.42
15:B:1235:CLA:HAB	19:B:9105:HOH:O	2.19	0.42
2:B:223:MET:N	2:B:224:PRO:CD	2.83	0.42
14:B:4004:BCR:H351	14:B:4004:BCR:H15C	1.67	0.42
6:F:93:SER:OG	6:F:99:GLN:NE2	2.53	0.42
1:A:518:GLY:O	1:A:621:VAL:N	2.52	0.42
1:A:737:VAL:HG22	14:B:4011:BCR:H323	2.01	0.42
2:B:488:ALA:O	2:B:489:ALA:HB3	2.19	0.42
15:A:1138:CLA:H203	15:F:1139:CLA:H62	2.02	0.41
1:A:337:HIS:HE1	12:A:5003:LHG:HC12	1.83	0.41
2:B:313:THR:OG1	12:B:5004:LHG:HC11	2.19	0.41
6:F:118:TRP:N	6:F:119:PRO:CD	2.83	0.41
1:A:50:ASN:ND2	12:A:5001:LHG:HC12	2.35	0.41
15:A:1121:CLA:HHC	15:A:1121:CLA:CBB	2.50	0.41
3:C:62:PHE:HD2	4:D:122:ILE:HG21	1.85	0.41
15:F:1139:CLA:H41	7:J:18:LEU:HD22	2.02	0.41
1:A:604:ILE:HD11	13:A:1011:CL0:C4	2.45	0.41
2:B:385:PHE:CZ	15:B:1222:CLA:HAB	2.53	0.41
6:F:27:THR:HG21	7:J:34:PRO:HG3	2.03	0.41
15:K:1401:CLA:HHC	15:K:1401:CLA:CBB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:ILE:HG21	15:B:1221:CLA:H41	2.02	0.41
15:B:1216:CLA:HMB2	15:B:1221:CLA:HMA3	2.03	0.41
14:B:4017:BCR:H24C	14:B:4017:BCR:H371	1.78	0.41
2:B:414:GLU:OE2	6:F:143:ARG:NH2	2.54	0.41
2:B:580:MET:HB3	2:B:580:MET:HE2	1.92	0.41
15:A:1121:CLA:HBB1	15:A:1121:CLA:HHC	2.02	0.41
2:B:157:LEU:HD11	9:M:29:LEU:HD12	2.03	0.41
4:D:120:ARG:HG2	4:D:124:GLN:HB2	2.01	0.41
1:A:451:SER:OG	1:A:452:PHE:N	2.54	0.41
2:B:653:VAL:HG22	15:B:1239:CLA:HMB3	2.03	0.41
3:C:54:CYS:SG	3:C:55:GLU:N	2.94	0.41
8:K:55:GLY:O	8:K:59:SER:OG	2.30	0.41
15:A:1102:CLA:HMA2	15:A:1109:CLA:HMD2	2.02	0.40
15:B:1231:CLA:CBB	15:B:1231:CLA:HHC	2.51	0.40
15:A:1133:CLA:HHC	15:A:1133:CLA:CBB	2.51	0.40
1:A:681:PHE:CA	15:B:1013:CLA:HAB	2.50	0.40
2:B:659:MET:HE2	10:B:2002:PQN:H2M3	2.02	0.40
15:A:1102:CLA:HMB1	15:A:1102:CLA:HBB1	2.04	0.40
12:A:5005:LHG:HC2	12:A:5005:LHG:O4	2.22	0.40
14:B:4004:BCR:H321	14:B:4004:BCR:HC8	2.03	0.40
1:A:388:SER:HB3	15:A:1126:CLA:HMA1	2.04	0.40
15:B:1218:CLA:CBB	15:B:1218:CLA:HHC	2.50	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	737/751 (98%)	694 (94%)	40 (5%)	3 (0%)	34	66
2	B	726/731 (99%)	695 (96%)	31 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	136/141 (96%)	123 (90%)	13 (10%)	0	100	100
5	E	66/74 (89%)	57 (86%)	9 (14%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
7	J	38/40 (95%)	38 (100%)	0	0	100	100
8	K	49/128 (38%)	46 (94%)	3 (6%)	0	100	100
9	M	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
All	All	1997/2142 (93%)	1887 (94%)	107 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	232	ALA
1	A	233	PRO

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	593/603 (98%)	584 (98%)	9 (2%)	65	89
2	B	582/583 (100%)	571 (98%)	11 (2%)	57	85
3	C	68/69 (99%)	67 (98%)	1 (2%)	65	89
4	D	112/116 (97%)	110 (98%)	2 (2%)	59	86
5	E	57/60 (95%)	54 (95%)	3 (5%)	22	54
6	F	118/137 (86%)	112 (95%)	6 (5%)	24	55
7	J	35/35 (100%)	35 (100%)	0	100	100
8	K	37/100 (37%)	33 (89%)	4 (11%)	6	19
9	M	19/25 (76%)	18 (95%)	1 (5%)	22	54
All	All	1621/1728 (94%)	1584 (98%)	37 (2%)	50	82

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	266	LEU
1	A	356	LEU
1	A	478	LEU
1	A	513	THR
1	A	631	THR
1	A	709	VAL
1	A	732	LEU
1	A	748	LEU
2	B	79	LYS
2	B	145	LEU
2	B	148	LEU
2	B	257	PHE
2	B	344	SER
2	B	414	GLU
2	B	420	LEU
2	B	573	PHE
2	B	580	MET
2	B	596	LEU
2	B	617	PHE
3	C	66	ARG
4	D	73	ARG
4	D	82	ASP
5	E	15	GLU
5	E	43	ARG
5	E	68	LEU
6	F	4	PHE
6	F	66	LEU
6	F	97	GLU
6	F	101	VAL
6	F	102	VAL
6	F	143	ARG
8	K	58	LEU
8	K	77	PHE
8	K	105	LEU
8	K	113	ILE
9	M	30	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	441	ASN
1	A	538	HIS
1	A	614	GLN
2	B	34	HIS
2	B	114	ASN
4	D	81	GLN
4	D	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 1 is monoatomic - leaving 121 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	$\# Z > 2$
15	CLA	B	1213	-	44,58,73	2.73	16 (36%)	49,95,113	2.38	13 (26%)
14	BCR	A	4008	-	41,41,41	2.74	7 (17%)	56,56,56	6.78	24 (42%)
14	BCR	B	4004	-	41,41,41	2.76	6 (14%)	56,56,56	6.37	26 (46%)
15	CLA	A	1118	-	40,54,73	2.87	14 (35%)	44,90,113	2.39	12 (27%)
15	CLA	B	1204	-	40,54,73	2.89	15 (37%)	44,90,113	2.38	13 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LHG	A	5005	-	35,35,48	1.08	2 (5%)	38,41,54	1.14	4 (10%)
15	CLA	B	1227	-	36,53,73	2.82	15 (41%)	39,89,113	2.48	11 (28%)
15	CLA	A	1022	19	59,73,73	2.35	16 (27%)	67,113,113	2.18	15 (22%)
15	CLA	J	1302	7	36,53,73	2.86	15 (41%)	39,89,113	2.39	10 (25%)
15	CLA	B	1207	-	40,54,73	2.89	15 (37%)	44,90,113	2.39	13 (29%)
15	CLA	F	1410	6	59,73,73	2.34	16 (27%)	67,113,113	2.17	15 (22%)
15	CLA	A	1134	1	40,54,73	2.91	16 (40%)	44,90,113	2.26	11 (25%)
15	CLA	A	1114	-	43,57,73	2.75	15 (34%)	46,93,113	2.46	14 (30%)
15	CLA	A	1110	-	48,62,73	2.55	15 (31%)	53,99,113	2.32	15 (28%)
15	CLA	B	1220	-	50,64,73	2.61	16 (32%)	56,102,113	2.23	16 (28%)
15	CLA	B	1240	12	36,53,73	2.90	15 (41%)	39,89,113	2.30	11 (28%)
15	CLA	B	1225	-	59,73,73	2.33	16 (27%)	67,113,113	2.20	16 (23%)
15	CLA	A	1128	-	59,73,73	2.30	15 (25%)	67,113,113	2.24	18 (26%)
10	PQN	B	2002	-	34,34,34	1.59	2 (5%)	42,45,45	1.13	4 (9%)
15	CLA	A	1105	-	59,73,73	2.35	16 (27%)	67,113,113	2.12	15 (22%)
14	BCR	B	4017	-	41,41,41	2.73	6 (14%)	56,56,56	6.59	25 (44%)
15	CLA	B	1209	-	36,53,73	2.87	14 (38%)	39,89,113	2.45	12 (30%)
15	CLA	B	1234	-	59,73,73	2.34	15 (25%)	67,113,113	2.13	16 (23%)
15	CLA	A	1124	-	49,63,73	2.58	16 (32%)	55,101,113	2.29	16 (29%)
15	CLA	A	1121	-	40,54,73	2.91	16 (40%)	44,90,113	2.37	12 (27%)
15	CLA	A	1104	-	59,73,73	2.30	15 (25%)	67,113,113	2.14	15 (22%)
15	CLA	B	1203	-	59,73,73	2.31	15 (25%)	67,113,113	2.16	13 (19%)
15	CLA	B	1217	-	41,55,73	2.77	16 (39%)	45,91,113	2.48	13 (28%)
15	CLA	B	1218	-	45,59,73	2.68	16 (35%)	50,96,113	2.63	17 (34%)
15	CLA	B	1201	-	40,54,73	2.89	16 (40%)	44,90,113	2.43	13 (29%)
12	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
16	LMU	B	1301	-	36,36,36	0.44	0	47,47,47	0.88	4 (8%)
11	SF4	C	3002	3	0,12,12	0.00	-	-	-	-
14	BCR	B	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.76	25 (44%)
15	CLA	A	1137	-	44,58,73	2.72	16 (36%)	49,95,113	2.47	13 (26%)
14	BCR	B	4005	-	41,41,41	2.75	6 (14%)	56,56,56	6.44	23 (41%)
15	CLA	B	1232	-	36,53,73	2.84	15 (41%)	39,89,113	2.37	10 (25%)
15	CLA	A	1138	-	59,73,73	2.39	15 (25%)	67,113,113	2.03	17 (25%)
15	CLA	B	1222	-	50,64,73	2.53	16 (32%)	56,102,113	2.39	16 (28%)
15	CLA	A	1101	-	59,73,73	2.34	15 (25%)	67,113,113	2.26	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1115	-	40,54,73	2.89	15 (37%)	44,90,113	2.34	13 (29%)
15	CLA	A	1123	-	59,73,73	2.35	15 (25%)	67,113,113	2.21	17 (25%)
15	CLA	F	1139	19	59,73,73	2.32	16 (27%)	67,113,113	2.11	12 (17%)
15	CLA	B	1224	-	59,73,73	2.34	15 (25%)	67,113,113	2.12	13 (19%)
15	CLA	B	1205	-	49,63,73	2.55	15 (30%)	55,101,113	2.48	15 (27%)
14	BCR	F	4015	-	41,41,41	2.76	7 (17%)	56,56,56	6.64	26 (46%)
15	CLA	A	1126	-	59,73,73	2.34	16 (27%)	67,113,113	2.15	20 (29%)
15	CLA	A	1801	12	46,60,73	2.68	16 (34%)	51,97,113	2.53	18 (35%)
15	CLA	B	1236	-	44,58,73	2.70	15 (34%)	49,95,113	2.39	15 (30%)
15	CLA	B	1212	-	36,53,73	2.88	15 (41%)	39,89,113	2.41	10 (25%)
15	CLA	B	1238	19	38,52,73	2.79	15 (39%)	40,87,113	2.24	10 (25%)
15	CLA	A	1120	-	43,57,73	2.75	15 (34%)	46,93,113	2.53	15 (32%)
14	BCR	F	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.73	23 (41%)
14	BCR	B	4011	-	41,41,41	2.77	6 (14%)	56,56,56	6.73	23 (41%)
15	CLA	B	1219	-	49,63,73	2.61	16 (32%)	55,101,113	2.39	15 (27%)
14	BCR	B	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.67	21 (37%)
15	CLA	A	1116	-	48,62,73	2.60	16 (33%)	53,99,113	2.38	17 (32%)
15	CLA	A	1122	-	59,73,73	2.34	16 (27%)	67,113,113	2.06	16 (23%)
17	LMG	B	5002	-	55,55,55	0.91	2 (3%)	63,63,63	0.98	2 (3%)
15	CLA	A	1127	-	59,73,73	2.34	16 (27%)	67,113,113	2.22	17 (25%)
15	CLA	A	1107	1	44,58,73	2.69	16 (36%)	49,95,113	2.42	18 (36%)
15	CLA	B	1023	-	59,73,73	2.31	15 (25%)	67,113,113	2.06	17 (25%)
14	BCR	B	4006	-	41,41,41	2.84	6 (14%)	56,56,56	6.69	24 (42%)
15	CLA	A	1135	-	49,63,73	2.58	15 (30%)	55,101,113	2.38	16 (29%)
14	BCR	J	4013	-	41,41,41	2.73	6 (14%)	56,56,56	6.62	28 (50%)
15	CLA	A	1119	-	58,72,73	2.37	16 (27%)	65,111,113	2.11	15 (23%)
15	CLA	B	1239	-	40,54,73	2.90	15 (37%)	44,90,113	2.49	12 (27%)
15	CLA	B	1230	-	59,73,73	2.32	15 (25%)	67,113,113	2.29	16 (23%)
15	CLA	K	1401	-	40,54,73	2.90	15 (37%)	44,90,113	2.38	14 (31%)
14	BCR	A	4012	-	41,41,41	2.81	6 (14%)	56,56,56	6.21	24 (42%)
15	CLA	B	1228	-	59,73,73	2.36	16 (27%)	67,113,113	1.98	13 (19%)
15	CLA	B	1214	-	59,73,73	2.34	16 (27%)	67,113,113	2.14	17 (25%)
15	CLA	A	1133	-	40,54,73	2.89	15 (37%)	44,90,113	2.38	12 (27%)
15	CLA	A	1117	-	59,73,73	2.36	16 (27%)	67,113,113	2.04	15 (22%)
15	CLA	J	1303	-	40,54,73	2.92	16 (40%)	44,90,113	2.38	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1208	-	36,53,73	2.89	14 (38%)	39,89,113	2.31	9 (23%)
15	CLA	A	1131	-	49,63,73	2.59	15 (30%)	55,101,113	2.39	16 (29%)
10	PQN	A	2001	-	34,34,34	1.60	2 (5%)	42,45,45	1.05	4 (9%)
15	CLA	A	1111	-	54,68,73	2.44	15 (27%)	61,107,113	2.16	15 (24%)
15	CLA	A	1136	-	59,73,73	2.33	15 (25%)	67,113,113	2.21	16 (23%)
15	CLA	B	1226	-	59,73,73	2.32	15 (25%)	67,113,113	2.22	14 (20%)
15	CLA	B	1221	-	59,73,73	2.34	16 (27%)	67,113,113	2.24	14 (20%)
15	CLA	B	1202	-	59,73,73	2.35	16 (27%)	67,113,113	2.14	14 (20%)
14	BCR	A	4003	-	41,41,41	2.74	6 (14%)	56,56,56	6.51	25 (44%)
14	BCR	B	4010	-	41,41,41	2.73	6 (14%)	56,56,56	6.65	23 (41%)
13	CL0	A	1108	-	36,53,73	2.86	15 (41%)	39,89,113	2.49	14 (35%)
15	CLA	A	1102	15	59,73,73	2.36	16 (27%)	67,113,113	2.12	15 (22%)
15	CLA	B	1211	-	40,54,73	2.89	16 (40%)	44,90,113	2.35	13 (29%)
15	CLA	B	1021	-	59,73,73	2.34	16 (27%)	67,113,113	2.27	21 (31%)
12	LHG	A	5003	15	48,48,48	0.95	2 (4%)	51,54,54	1.09	4 (7%)
15	CLA	B	1235	-	59,73,73	2.33	15 (25%)	67,113,113	2.12	15 (22%)
15	CLA	A	1112	-	36,53,73	2.87	15 (41%)	39,89,113	2.38	11 (28%)
15	CLA	B	1216	-	59,73,73	2.35	16 (27%)	67,113,113	2.00	15 (22%)
14	BCR	A	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.49	25 (44%)
11	SF4	C	3003	3	0,12,12	0.00	-	-	-	-
15	CLA	A	1132	-	56,70,73	2.39	16 (28%)	63,109,113	2.22	14 (22%)
15	CLA	A	1113	-	36,53,73	2.87	14 (38%)	39,89,113	2.32	12 (30%)
15	CLA	B	1206	2	40,54,73	2.91	16 (40%)	44,90,113	2.35	15 (34%)
15	CLA	A	1140	-	59,73,73	2.34	15 (25%)	67,113,113	2.06	14 (20%)
15	CLA	A	1012	19	59,73,73	2.37	16 (27%)	67,113,113	2.30	17 (25%)
15	CLA	A	1125	-	46,60,73	2.62	15 (32%)	51,97,113	2.51	18 (35%)
15	CLA	B	1237	19	49,63,73	2.57	16 (32%)	55,101,113	2.32	15 (27%)
14	BCR	A	4007	-	41,41,41	2.73	6 (14%)	56,56,56	6.72	25 (44%)
15	CLA	A	1129	-	40,54,73	2.87	15 (37%)	44,90,113	2.44	14 (31%)
12	LHG	B	5004	15	48,48,48	0.94	2 (4%)	51,54,54	1.14	4 (7%)
15	CLA	B	1013	-	59,73,73	2.32	14 (23%)	67,113,113	2.22	19 (28%)
15	CLA	B	1223	-	59,73,73	2.33	15 (25%)	67,113,113	2.17	15 (22%)
13	CL0	A	1011	-	59,73,73	2.30	14 (23%)	67,113,113	2.26	15 (22%)
16	LMU	J	1304	-	36,36,36	0.42	0	47,47,47	0.63	1 (2%)
15	CLA	A	1109	15	59,73,73	2.36	15 (25%)	67,113,113	2.20	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1229	-	59,73,73	2.33	15 (25%)	67,113,113	2.12	13 (19%)
15	CLA	B	1231	-	59,73,73	2.33	15 (25%)	67,113,113	2.16	15 (22%)
14	BCR	A	4001	-	41,41,41	2.77	6 (14%)	56,56,56	6.28	25 (44%)
15	CLA	F	1301	-	36,53,73	2.86	15 (41%)	39,89,113	2.32	10 (25%)
11	SF4	A	3001	1,2	0,12,12	0.00	-	-		
15	CLA	K	1402	-	40,54,73	2.90	16 (40%)	44,90,113	2.33	12 (27%)
15	CLA	A	1103	-	59,73,73	2.32	15 (25%)	67,113,113	2.10	16 (23%)
15	CLA	A	1106	1	59,73,73	2.35	16 (27%)	67,113,113	2.20	15 (22%)
15	CLA	A	1130	-	49,63,73	2.58	16 (32%)	55,101,113	2.22	14 (25%)
15	CLA	B	1215	-	59,73,73	2.36	15 (25%)	67,113,113	2.30	18 (26%)
15	CLA	B	1210	-	59,73,73	2.34	15 (25%)	67,113,113	2.09	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1213	-	2/2/17/25	7/19/117/135	-
14	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
14	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1118	-	3/3/16/25	9/15/113/135	-
15	CLA	B	1204	-	3/3/16/25	5/15/113/135	-
12	LHG	A	5005	-	-	25/40/40/53	-
15	CLA	B	1227	-	2/2/16/25	2/11/111/135	-
15	CLA	A	1022	19	2/2/20/25	9/37/135/135	-
15	CLA	J	1302	7	3/3/16/25	4/11/111/135	-
15	CLA	B	1207	-	3/3/16/25	9/15/113/135	-
15	CLA	F	1410	6	2/2/20/25	17/37/135/135	-
15	CLA	A	1134	1	3/3/16/25	7/15/113/135	-
15	CLA	A	1114	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1110	-	3/3/17/25	11/24/122/135	-
15	CLA	B	1220	-	3/3/18/25	9/27/125/135	-
15	CLA	B	1240	12	3/3/16/25	5/11/111/135	-
15	CLA	B	1225	-	3/3/20/25	16/37/135/135	-
15	CLA	A	1128	-	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	A	1105	-	3/3/20/25	11/37/135/135	-
14	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1209	-	3/3/16/25	5/11/111/135	-
14	BCR	B	4011	-	-	15/29/63/63	0/2/2/2
15	CLA	B	1234	-	3/3/20/25	16/37/135/135	-
15	CLA	A	1124	-	3/3/18/25	7/25/123/135	-
15	CLA	A	1121	-	3/3/16/25	7/15/113/135	-
15	CLA	A	1104	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1203	-	2/2/20/25	13/37/135/135	-
15	CLA	B	1217	-	3/3/16/25	7/16/114/135	-
15	CLA	B	1218	-	3/3/17/25	11/21/119/135	-
12	LHG	A	5001	-	-	29/53/53/53	-
16	LMU	B	1301	-	-	15/21/61/61	0/2/2/2
11	SF4	C	3002	3	-	-	0/6/5/5
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1137	-	3/3/17/25	9/19/117/135	-
14	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1232	-	3/3/16/25	4/11/111/135	-
15	CLA	A	1138	-	3/3/20/25	7/37/135/135	-
15	CLA	B	1222	-	2/2/18/25	10/27/125/135	-
15	CLA	A	1101	-	3/3/20/25	14/37/135/135	-
15	CLA	A	1115	-	3/3/16/25	7/15/113/135	-
15	CLA	A	1123	-	3/3/20/25	14/37/135/135	-
15	CLA	F	1139	19	3/3/20/25	12/37/135/135	-
15	CLA	B	1224	-	3/3/20/25	13/37/135/135	-
15	CLA	B	1205	-	3/3/18/25	10/25/123/135	-
14	BCR	F	4015	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1126	-	1/1/20/25	9/37/135/135	-
15	CLA	A	1801	12	3/3/17/25	11/22/120/135	-
15	CLA	B	1236	-	2/2/17/25	5/19/117/135	-
15	CLA	B	1212	-	3/3/16/25	5/11/111/135	-
15	CLA	B	1238	19	3/3/15/25	4/11/110/135	-
15	CLA	A	1120	-	3/3/16/25	8/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
15	CLA	B	1228	-	3/3/20/25	18/37/135/135	-
15	CLA	B	1219	-	3/3/18/25	9/25/123/135	-
14	BCR	B	4014	-	-	14/29/63/63	0/2/2/2
15	CLA	A	1116	-	3/3/17/25	7/24/122/135	-
15	CLA	A	1122	-	3/3/20/25	20/37/135/135	-
17	LMG	B	5002	-	-	30/50/70/70	0/1/1/1
15	CLA	A	1127	-	3/3/20/25	18/37/135/135	-
15	CLA	A	1107	1	2/2/17/25	6/19/117/135	-
15	CLA	B	1023	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1237	19	3/3/18/25	10/25/123/135	-
15	CLA	A	1135	-	3/3/18/25	11/25/123/135	-
14	BCR	J	4013	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1119	-	2/2/19/25	15/35/133/135	-
15	CLA	B	1239	-	3/3/16/25	8/15/113/135	-
15	CLA	B	1230	-	3/3/20/25	16/37/135/135	-
15	CLA	K	1401	-	3/3/16/25	12/15/113/135	-
14	BCR	A	4012	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1201	-	3/3/16/25	5/15/113/135	-
15	CLA	B	1214	-	2/2/20/25	12/37/135/135	-
15	CLA	A	1133	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1117	-	3/3/20/25	15/37/135/135	-
15	CLA	J	1303	-	3/3/16/25	5/15/113/135	-
15	CLA	B	1208	-	3/3/16/25	4/11/111/135	-
15	CLA	A	1131	-	3/3/18/25	12/25/123/135	-
10	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
15	CLA	A	1111	-	3/3/19/25	13/31/129/135	-
15	CLA	A	1136	-	3/3/20/25	18/37/135/135	-
15	CLA	B	1226	-	3/3/20/25	14/37/135/135	-
15	CLA	B	1221	-	3/3/20/25	8/37/135/135	-
15	CLA	B	1202	-	3/3/20/25	21/37/135/135	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
13	CL0	A	1108	-	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1102	15	3/3/20/25	14/37/135/135	-
15	CLA	B	1211	-	3/3/16/25	8/15/113/135	-
15	CLA	B	1021	-	3/3/20/25	23/37/135/135	-
12	LHG	A	5003	15	-	24/53/53/53	-
15	CLA	B	1235	-	3/3/20/25	14/37/135/135	-
15	CLA	A	1112	-	3/3/16/25	5/11/111/135	-
15	CLA	B	1216	-	2/2/20/25	12/37/135/135	-
14	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
11	SF4	C	3003	3	-	-	0/6/5/5
15	CLA	A	1132	-	3/3/19/25	14/34/132/135	-
15	CLA	A	1113	-	3/3/16/25	4/11/111/135	-
15	CLA	B	1206	2	3/3/16/25	6/15/113/135	-
15	CLA	A	1140	-	3/3/20/25	15/37/135/135	-
15	CLA	A	1012	19	2/2/20/25	16/37/135/135	-
15	CLA	A	1125	-	2/2/17/25	4/22/120/135	-
14	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	6/29/63/63	0/2/2/2
15	CLA	A	1129	-	3/3/16/25	11/15/113/135	-
12	LHG	B	5004	15	-	21/53/53/53	-
15	CLA	B	1013	-	2/2/20/25	16/37/135/135	-
15	CLA	B	1223	-	3/3/20/25	19/37/135/135	-
13	CL0	A	1011	-	3/3/20/25	4/37/135/135	-
16	LMU	J	1304	-	-	10/21/61/61	0/2/2/2
15	CLA	A	1109	15	2/2/20/25	14/37/135/135	-
15	CLA	B	1229	-	3/3/20/25	20/37/135/135	-
15	CLA	B	1231	-	3/3/20/25	13/37/135/135	-
14	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	F	1301	-	3/3/16/25	2/11/111/135	-
11	SF4	A	3001	1,2	-	-	0/6/5/5
15	CLA	K	1402	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1103	-	3/3/20/25	17/37/135/135	-
15	CLA	A	1106	1	3/3/20/25	15/37/135/135	-
15	CLA	A	1130	-	3/3/18/25	10/25/123/135	-
15	CLA	B	1215	-	2/2/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1210	-	3/3/20/25	17/37/135/135	-

All (1533) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1123	CLA	MG-NA	9.66	2.29	2.06
13	A	1108	CL0	MG-NA	9.62	2.29	2.06
15	B	1220	CLA	MG-NA	9.61	2.29	2.06
15	A	1138	CLA	MG-NA	9.59	2.29	2.06
15	B	1221	CLA	MG-NA	9.58	2.29	2.06
15	B	1240	CLA	MG-NA	9.56	2.29	2.06
15	A	1120	CLA	MG-NA	9.56	2.29	2.06
15	A	1801	CLA	MG-NA	9.56	2.29	2.06
15	A	1135	CLA	MG-NA	9.55	2.29	2.06
15	A	1125	CLA	MG-NA	9.52	2.28	2.06
15	J	1303	CLA	MG-NA	9.52	2.28	2.06
15	B	1236	CLA	MG-NA	9.51	2.28	2.06
15	B	1238	CLA	MG-NA	9.51	2.28	2.06
15	A	1117	CLA	MG-NA	9.50	2.28	2.06
15	B	1223	CLA	MG-NA	9.50	2.28	2.06
15	J	1302	CLA	MG-NA	9.50	2.28	2.06
15	B	1206	CLA	MG-NA	9.49	2.28	2.06
15	A	1112	CLA	MG-NA	9.48	2.28	2.06
15	B	1237	CLA	MG-NA	9.48	2.28	2.06
15	A	1134	CLA	MG-NA	9.48	2.28	2.06
15	B	1209	CLA	MG-NA	9.48	2.28	2.06
15	A	1131	CLA	MG-NA	9.48	2.28	2.06
15	F	1410	CLA	MG-NA	9.47	2.28	2.06
15	A	1101	CLA	MG-NA	9.47	2.28	2.06
15	A	1113	CLA	MG-NA	9.47	2.28	2.06
15	B	1229	CLA	MG-NA	9.47	2.28	2.06
15	A	1130	CLA	MG-NA	9.47	2.28	2.06
15	A	1119	CLA	MG-NA	9.47	2.28	2.06
15	A	1124	CLA	MG-NA	9.46	2.28	2.06
15	A	1114	CLA	MG-NA	9.46	2.28	2.06
15	A	1137	CLA	MG-NA	9.46	2.28	2.06
15	A	1121	CLA	MG-NA	9.46	2.28	2.06
15	B	1212	CLA	MG-NA	9.45	2.28	2.06
15	B	1021	CLA	MG-NA	9.45	2.28	2.06
15	B	1239	CLA	MG-NA	9.45	2.28	2.06
15	A	1012	CLA	MG-NA	9.45	2.28	2.06
15	B	1217	CLA	MG-NA	9.45	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1210	CLA	MG-NA	9.43	2.28	2.06
15	B	1232	CLA	MG-NA	9.43	2.28	2.06
15	B	1213	CLA	MG-NA	9.43	2.28	2.06
15	B	1215	CLA	MG-NA	9.42	2.28	2.06
15	F	1301	CLA	MG-NA	9.42	2.28	2.06
15	A	1110	CLA	MG-NA	9.42	2.28	2.06
15	K	1402	CLA	MG-NA	9.42	2.28	2.06
15	A	1122	CLA	MG-NA	9.41	2.28	2.06
15	F	1139	CLA	MG-NA	9.40	2.28	2.06
15	A	1132	CLA	MG-NA	9.40	2.28	2.06
15	A	1105	CLA	MG-NA	9.40	2.28	2.06
15	B	1214	CLA	MG-NA	9.40	2.28	2.06
15	B	1207	CLA	MG-NA	9.40	2.28	2.06
15	B	1205	CLA	MG-NA	9.39	2.28	2.06
15	B	1234	CLA	MG-NA	9.39	2.28	2.06
15	A	1116	CLA	MG-NA	9.39	2.28	2.06
15	B	1216	CLA	MG-NA	9.39	2.28	2.06
15	A	1133	CLA	MG-NA	9.38	2.28	2.06
15	B	1204	CLA	MG-NA	9.38	2.28	2.06
15	A	1140	CLA	MG-NA	9.38	2.28	2.06
15	B	1225	CLA	MG-NA	9.37	2.28	2.06
15	B	1226	CLA	MG-NA	9.36	2.28	2.06
15	B	1201	CLA	MG-NA	9.36	2.28	2.06
15	K	1401	CLA	MG-NA	9.36	2.28	2.06
15	A	1022	CLA	MG-NA	9.36	2.28	2.06
15	A	1127	CLA	MG-NA	9.36	2.28	2.06
15	B	1203	CLA	MG-NA	9.35	2.28	2.06
15	B	1224	CLA	MG-NA	9.35	2.28	2.06
15	A	1126	CLA	MG-NA	9.35	2.28	2.06
15	B	1211	CLA	MG-NA	9.34	2.28	2.06
15	A	1129	CLA	MG-NA	9.34	2.28	2.06
15	A	1102	CLA	MG-NA	9.33	2.28	2.06
15	B	1218	CLA	MG-NA	9.32	2.28	2.06
15	B	1231	CLA	MG-NA	9.31	2.28	2.06
15	A	1111	CLA	MG-NA	9.31	2.28	2.06
15	A	1115	CLA	MG-NA	9.30	2.28	2.06
15	A	1103	CLA	MG-NA	9.30	2.28	2.06
15	B	1219	CLA	MG-NA	9.30	2.28	2.06
13	A	1011	CL0	MG-NA	9.30	2.28	2.06
15	A	1118	CLA	MG-NA	9.29	2.28	2.06
15	A	1104	CLA	MG-NA	9.29	2.28	2.06
15	B	1208	CLA	MG-NA	9.28	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1202	CLA	MG-NA	9.28	2.28	2.06
15	B	1228	CLA	MG-NA	9.28	2.28	2.06
15	A	1106	CLA	MG-NA	9.27	2.28	2.06
15	B	1227	CLA	MG-NA	9.25	2.28	2.06
15	A	1136	CLA	MG-NA	9.25	2.28	2.06
15	A	1109	CLA	MG-NA	9.25	2.28	2.06
15	B	1023	CLA	MG-NA	9.24	2.28	2.06
15	B	1222	CLA	MG-NA	9.23	2.28	2.06
15	A	1128	CLA	MG-NA	9.21	2.28	2.06
15	B	1235	CLA	MG-NA	9.21	2.28	2.06
15	A	1107	CLA	MG-NA	9.20	2.28	2.06
15	B	1230	CLA	MG-NA	9.19	2.28	2.06
15	B	1013	CLA	MG-NA	9.07	2.27	2.06
14	B	4009	BCR	C8-C9	-8.25	1.28	1.45
14	A	4012	BCR	C11-C10	-8.20	1.18	1.43
14	F	4015	BCR	C8-C9	-8.20	1.28	1.45
14	B	4014	BCR	C8-C9	-8.19	1.28	1.45
14	F	4016	BCR	C8-C9	-8.18	1.28	1.45
14	B	4006	BCR	C11-C10	-8.17	1.18	1.43
14	A	4012	BCR	C8-C9	-8.15	1.28	1.45
14	B	4005	BCR	C8-C9	-8.14	1.28	1.45
14	J	4013	BCR	C8-C9	-8.13	1.28	1.45
14	B	4006	BCR	C8-C9	-8.08	1.28	1.45
14	F	4016	BCR	C11-C10	-8.08	1.18	1.43
14	A	4003	BCR	C8-C9	-8.08	1.28	1.45
14	B	4004	BCR	C11-C10	-8.04	1.18	1.43
14	B	4011	BCR	C8-C9	-8.03	1.28	1.45
14	A	4008	BCR	C8-C9	-8.02	1.28	1.45
14	A	4001	BCR	C8-C9	-8.02	1.28	1.45
14	B	4010	BCR	C11-C10	-8.01	1.18	1.43
14	B	4011	BCR	C11-C10	-7.98	1.18	1.43
14	B	4006	BCR	C10-C9	-7.98	1.25	1.35
14	A	4002	BCR	C8-C9	-7.96	1.28	1.45
14	A	4002	BCR	C11-C10	-7.95	1.18	1.43
14	B	4004	BCR	C8-C9	-7.94	1.28	1.45
14	B	4014	BCR	C11-C10	-7.94	1.18	1.43
14	B	4009	BCR	C11-C10	-7.93	1.18	1.43
14	A	4007	BCR	C8-C9	-7.92	1.28	1.45
14	B	4005	BCR	C11-C10	-7.92	1.18	1.43
14	B	4017	BCR	C8-C9	-7.92	1.28	1.45
14	F	4015	BCR	C11-C10	-7.90	1.19	1.43
14	B	4017	BCR	C11-C10	-7.90	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4003	BCR	C11-C10	-7.89	1.19	1.43
14	B	4010	BCR	C8-C9	-7.88	1.29	1.45
14	A	4007	BCR	C11-C10	-7.87	1.19	1.43
14	A	4001	BCR	C11-C10	-7.86	1.19	1.43
14	A	4008	BCR	C11-C10	-7.83	1.19	1.43
14	J	4013	BCR	C11-C10	-7.82	1.19	1.43
14	A	4001	BCR	C10-C9	-7.70	1.25	1.35
10	A	2001	PQN	C3-C2	7.67	1.49	1.35
10	B	2002	PQN	C3-C2	7.60	1.49	1.35
14	A	4012	BCR	C10-C9	-7.39	1.26	1.35
14	B	4004	BCR	C10-C9	-7.36	1.26	1.35
14	B	4017	BCR	C20-C21	-7.36	1.20	1.43
14	B	4011	BCR	C20-C21	-7.35	1.20	1.43
14	A	4002	BCR	C20-C21	-7.32	1.20	1.43
14	A	4012	BCR	C20-C21	-7.32	1.20	1.43
14	A	4008	BCR	C20-C21	-7.31	1.20	1.43
14	B	4006	BCR	C20-C21	-7.31	1.20	1.43
14	A	4012	BCR	C16-C17	-7.29	1.20	1.43
14	A	4002	BCR	C10-C9	-7.28	1.26	1.35
14	F	4015	BCR	C20-C21	-7.27	1.20	1.43
14	B	4006	BCR	C16-C17	-7.27	1.20	1.43
14	B	4009	BCR	C20-C21	-7.25	1.21	1.43
14	B	4010	BCR	C10-C9	-7.24	1.26	1.35
14	B	4005	BCR	C20-C21	-7.23	1.21	1.43
14	A	4001	BCR	C20-C21	-7.23	1.21	1.43
14	A	4007	BCR	C20-C21	-7.23	1.21	1.43
14	J	4013	BCR	C20-C21	-7.23	1.21	1.43
14	F	4016	BCR	C20-C21	-7.22	1.21	1.43
14	A	4003	BCR	C20-C21	-7.21	1.21	1.43
14	A	4008	BCR	C16-C17	-7.21	1.21	1.43
14	A	4002	BCR	C16-C17	-7.21	1.21	1.43
14	B	4009	BCR	C16-C17	-7.21	1.21	1.43
14	B	4005	BCR	C10-C9	-7.20	1.26	1.35
14	B	4014	BCR	C10-C9	-7.20	1.26	1.35
14	A	4001	BCR	C16-C17	-7.20	1.21	1.43
14	B	4011	BCR	C10-C9	-7.20	1.26	1.35
14	B	4004	BCR	C20-C21	-7.20	1.21	1.43
14	B	4011	BCR	C16-C17	-7.19	1.21	1.43
14	A	4003	BCR	C16-C17	-7.18	1.21	1.43
14	B	4005	BCR	C16-C17	-7.18	1.21	1.43
14	B	4014	BCR	C20-C21	-7.17	1.21	1.43
14	B	4010	BCR	C20-C21	-7.17	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	4015	BCR	C16-C17	-7.16	1.21	1.43
14	B	4004	BCR	C16-C17	-7.15	1.21	1.43
14	A	4007	BCR	C10-C9	-7.14	1.26	1.35
14	B	4017	BCR	C16-C17	-7.14	1.21	1.43
14	A	4003	BCR	C10-C9	-7.14	1.26	1.35
14	J	4013	BCR	C16-C17	-7.13	1.21	1.43
14	F	4015	BCR	C10-C9	-7.13	1.26	1.35
14	B	4014	BCR	C16-C17	-7.13	1.21	1.43
14	F	4016	BCR	C16-C17	-7.10	1.21	1.43
14	A	4007	BCR	C16-C17	-7.09	1.21	1.43
14	J	4013	BCR	C10-C9	-7.05	1.26	1.35
14	B	4010	BCR	C16-C17	-7.03	1.21	1.43
14	B	4017	BCR	C10-C9	-7.00	1.26	1.35
14	B	4009	BCR	C10-C9	-7.00	1.26	1.35
14	A	4008	BCR	C10-C9	-6.94	1.26	1.35
14	F	4016	BCR	C10-C9	-6.90	1.26	1.35
15	A	1118	CLA	O2A-C1	6.55	1.60	1.45
15	A	1129	CLA	O2A-C1	6.51	1.60	1.45
15	A	1134	CLA	O2A-C1	6.49	1.60	1.45
15	K	1401	CLA	O2A-C1	6.47	1.60	1.45
15	B	1239	CLA	O2A-C1	6.46	1.60	1.45
15	B	1201	CLA	O2A-C1	6.45	1.60	1.45
15	B	1206	CLA	O2A-C1	6.45	1.60	1.45
15	K	1402	CLA	O2A-C1	6.44	1.60	1.45
15	J	1303	CLA	O2A-C1	6.44	1.60	1.45
15	B	1211	CLA	O2A-C1	6.44	1.60	1.45
15	A	1115	CLA	O2A-C1	6.43	1.60	1.45
15	A	1121	CLA	O2A-C1	6.43	1.60	1.45
15	A	1133	CLA	O2A-C1	6.41	1.60	1.45
15	B	1207	CLA	O2A-C1	6.39	1.60	1.45
15	B	1204	CLA	O2A-C1	6.38	1.60	1.45
15	A	1138	CLA	CHC-C1C	5.73	1.49	1.35
15	B	1228	CLA	CHC-C1C	5.58	1.49	1.35
15	A	1126	CLA	CHC-C1C	5.54	1.49	1.35
15	B	1236	CLA	CHC-C1C	5.53	1.49	1.35
15	B	1235	CLA	CHC-C1C	5.51	1.49	1.35
15	A	1125	CLA	CHC-C1C	5.49	1.49	1.35
15	A	1106	CLA	O2A-C1	5.48	1.61	1.46
15	A	1012	CLA	O2A-C1	5.47	1.61	1.46
15	A	1101	CLA	CHC-C1C	5.47	1.49	1.35
15	A	1112	CLA	CHC-C1C	5.47	1.49	1.35
15	A	1122	CLA	CHC-C1C	5.46	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1130	CLA	CHC-C1C	5.45	1.48	1.35
15	A	1107	CLA	CHC-C1C	5.44	1.48	1.35
15	B	1224	CLA	O2A-C1	5.44	1.61	1.46
15	B	1219	CLA	C3B-C2B	5.42	1.47	1.40
15	A	1109	CLA	O2A-C1	5.42	1.61	1.46
15	A	1111	CLA	CHC-C1C	5.41	1.48	1.35
15	A	1115	CLA	CHC-C1C	5.41	1.48	1.35
15	A	1140	CLA	CHC-C1C	5.41	1.48	1.35
15	B	1215	CLA	O2A-C1	5.40	1.61	1.46
15	B	1220	CLA	CHC-C1C	5.39	1.48	1.35
15	B	1230	CLA	CHC-C1C	5.39	1.48	1.35
15	A	1103	CLA	CHC-C1C	5.39	1.48	1.35
15	B	1223	CLA	CHC-C1C	5.38	1.48	1.35
15	A	1134	CLA	CHC-C1C	5.38	1.48	1.35
15	A	1117	CLA	CHC-C1C	5.37	1.48	1.35
15	B	1240	CLA	CHC-C1C	5.36	1.48	1.35
15	A	1117	CLA	O2A-C1	5.35	1.61	1.46
15	A	1106	CLA	CHC-C1C	5.35	1.48	1.35
15	A	1109	CLA	CHC-C1C	5.35	1.48	1.35
15	B	1214	CLA	CHC-C1C	5.35	1.48	1.35
15	A	1022	CLA	CHC-C1C	5.33	1.48	1.35
15	J	1303	CLA	CHC-C1C	5.33	1.48	1.35
15	F	1301	CLA	CHC-C1C	5.33	1.48	1.35
15	B	1013	CLA	CHC-C1C	5.33	1.48	1.35
15	B	1234	CLA	O2A-C1	5.33	1.61	1.46
13	A	1108	CL0	CHC-C1C	5.32	1.48	1.35
15	A	1127	CLA	CHC-C1C	5.32	1.48	1.35
15	B	1013	CLA	O2D-CGD	5.32	1.46	1.33
15	B	1220	CLA	O2A-C1	5.32	1.61	1.46
15	B	1217	CLA	CHC-C1C	5.32	1.48	1.35
15	A	1132	CLA	CHC-C1C	5.32	1.48	1.35
15	B	1210	CLA	CHC-C1C	5.31	1.48	1.35
15	B	1202	CLA	CHC-C1C	5.31	1.48	1.35
15	B	1213	CLA	CHC-C1C	5.31	1.48	1.35
15	A	1138	CLA	O2D-CGD	5.30	1.46	1.33
15	B	1211	CLA	CHC-C1C	5.30	1.48	1.35
15	A	1119	CLA	CHC-C1C	5.30	1.48	1.35
15	B	1226	CLA	CHC-C1C	5.30	1.48	1.35
15	A	1131	CLA	O2A-C1	5.29	1.61	1.46
15	A	1102	CLA	CHC-C1C	5.29	1.48	1.35
15	A	1801	CLA	CHC-C1C	5.29	1.48	1.35
15	B	1231	CLA	O2A-C1	5.29	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1225	CLA	CHC-C1C	5.29	1.48	1.35
15	K	1401	CLA	CHC-C1C	5.29	1.48	1.35
15	K	1402	CLA	CHC-C1C	5.29	1.48	1.35
15	F	1139	CLA	O2D-CGD	5.29	1.46	1.33
15	F	1410	CLA	CHC-C1C	5.29	1.48	1.35
15	A	1012	CLA	CHC-C1C	5.29	1.48	1.35
15	B	1212	CLA	CHC-C1C	5.28	1.48	1.35
15	A	1012	CLA	O2D-CGD	5.28	1.46	1.33
15	A	1119	CLA	O2D-CGD	5.28	1.46	1.33
15	A	1104	CLA	CHC-C1C	5.28	1.48	1.35
15	K	1401	CLA	O2D-CGD	5.28	1.46	1.33
15	A	1103	CLA	O2D-CGD	5.28	1.46	1.33
15	A	1114	CLA	CHC-C1C	5.28	1.48	1.35
15	A	1116	CLA	CHC-C1C	5.28	1.48	1.35
15	A	1135	CLA	O2A-C1	5.27	1.61	1.46
15	A	1119	CLA	O2A-C1	5.27	1.61	1.46
15	A	1125	CLA	O2A-C1	5.27	1.61	1.46
15	B	1235	CLA	O2D-CGD	5.27	1.46	1.33
15	A	1116	CLA	O2A-C1	5.27	1.61	1.46
15	B	1207	CLA	CHC-C1C	5.27	1.48	1.35
15	A	1124	CLA	CHC-C1C	5.27	1.48	1.35
15	A	1129	CLA	CHC-C1C	5.27	1.48	1.35
15	B	1013	CLA	O2A-C1	5.27	1.61	1.46
15	B	1229	CLA	CHC-C1C	5.27	1.48	1.35
15	A	1138	CLA	O2A-C1	5.27	1.61	1.46
15	A	1121	CLA	O2D-CGD	5.27	1.46	1.33
15	A	1136	CLA	O2D-CGD	5.27	1.46	1.33
15	B	1023	CLA	CHC-C1C	5.27	1.48	1.35
15	A	1109	CLA	O2D-CGD	5.26	1.46	1.33
15	B	1208	CLA	CHC-C1C	5.26	1.48	1.35
15	A	1113	CLA	CHC-C1C	5.26	1.48	1.35
15	B	1021	CLA	CHC-C1C	5.26	1.48	1.35
15	B	1203	CLA	O2D-CGD	5.26	1.46	1.33
15	B	1205	CLA	O2A-C1	5.26	1.61	1.46
15	B	1219	CLA	CHC-C1C	5.26	1.48	1.35
15	B	1201	CLA	CHC-C1C	5.26	1.48	1.35
15	A	1120	CLA	O2D-CGD	5.26	1.46	1.33
15	B	1213	CLA	O2A-C1	5.25	1.60	1.46
15	F	1301	CLA	O2D-CGD	5.25	1.46	1.33
15	A	1137	CLA	CHC-C1C	5.25	1.48	1.35
15	A	1136	CLA	O2A-C1	5.25	1.60	1.46
15	B	1218	CLA	CHC-C1C	5.25	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1209	CLA	CHC-C1C	5.25	1.48	1.35
15	A	1127	CLA	O2D-CGD	5.25	1.46	1.33
15	B	1202	CLA	O2D-CGD	5.25	1.46	1.33
15	A	1102	CLA	O2A-C1	5.25	1.60	1.46
15	A	1133	CLA	CHC-C1C	5.24	1.48	1.35
15	B	1237	CLA	CHC-C1C	5.24	1.48	1.35
15	B	1227	CLA	O2D-CGD	5.24	1.46	1.33
15	B	1235	CLA	O2A-C1	5.24	1.60	1.46
15	B	1232	CLA	O2D-CGD	5.24	1.46	1.33
15	B	1021	CLA	O2D-CGD	5.24	1.46	1.33
15	B	1219	CLA	O2D-CGD	5.23	1.46	1.33
15	B	1208	CLA	O2D-CGD	5.23	1.46	1.33
15	B	1216	CLA	CHC-C1C	5.23	1.48	1.35
15	J	1303	CLA	O2D-CGD	5.23	1.46	1.33
15	A	1117	CLA	O2D-CGD	5.23	1.46	1.33
13	A	1108	CL0	O2D-CGD	5.23	1.46	1.33
15	A	1131	CLA	O2D-CGD	5.23	1.45	1.33
15	K	1402	CLA	O2D-CGD	5.23	1.45	1.33
15	B	1224	CLA	CHC-C1C	5.22	1.48	1.35
15	B	1240	CLA	O2D-CGD	5.22	1.45	1.33
15	B	1237	CLA	O2D-CGD	5.22	1.45	1.33
15	B	1234	CLA	CHC-C1C	5.22	1.48	1.35
15	B	1218	CLA	O2A-C1	5.22	1.60	1.46
15	A	1120	CLA	CHC-C1C	5.22	1.48	1.35
15	B	1204	CLA	CHC-C1C	5.22	1.48	1.35
15	A	1121	CLA	CHC-C1C	5.22	1.48	1.35
15	F	1139	CLA	CHC-C1C	5.21	1.48	1.35
15	A	1022	CLA	O2D-CGD	5.21	1.45	1.33
15	J	1302	CLA	CHC-C1C	5.21	1.48	1.35
15	A	1118	CLA	CHC-C1C	5.21	1.48	1.35
15	B	1216	CLA	O2D-CGD	5.21	1.45	1.33
15	B	1218	CLA	O2D-CGD	5.21	1.45	1.33
15	B	1227	CLA	CHC-C1C	5.21	1.48	1.35
15	B	1215	CLA	O2D-CGD	5.21	1.45	1.33
15	A	1105	CLA	O2A-C1	5.20	1.60	1.46
13	A	1011	CL0	O2A-C1	5.20	1.60	1.46
15	A	1112	CLA	O2D-CGD	5.20	1.45	1.33
15	A	1123	CLA	CHC-C1C	5.20	1.48	1.35
15	A	1124	CLA	O2D-CGD	5.19	1.45	1.33
15	B	1205	CLA	O2D-CGD	5.19	1.45	1.33
15	A	1801	CLA	O2D-CGD	5.19	1.45	1.33
15	A	1133	CLA	O2D-CGD	5.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1135	CLA	CHC-C1C	5.19	1.48	1.35
15	B	1207	CLA	O2D-CGD	5.19	1.45	1.33
15	B	1226	CLA	O2A-C1	5.18	1.60	1.46
15	B	1220	CLA	O2D-CGD	5.18	1.45	1.33
13	A	1011	CL0	O2D-CGD	5.18	1.45	1.33
15	A	1130	CLA	O2A-C1	5.18	1.60	1.46
15	A	1116	CLA	O2D-CGD	5.18	1.45	1.33
15	B	1212	CLA	O2D-CGD	5.18	1.45	1.33
15	B	1214	CLA	O2D-CGD	5.18	1.45	1.33
15	B	1236	CLA	O2A-C1	5.18	1.60	1.46
15	A	1122	CLA	O2D-CGD	5.18	1.45	1.33
15	B	1230	CLA	O2D-CGD	5.18	1.45	1.33
15	A	1105	CLA	CHC-C1C	5.17	1.48	1.35
15	B	1228	CLA	O2D-CGD	5.17	1.45	1.33
15	B	1206	CLA	O2D-CGD	5.17	1.45	1.33
15	A	1107	CLA	O2D-CGD	5.17	1.45	1.33
15	A	1118	CLA	O2D-CGD	5.17	1.45	1.33
15	A	1128	CLA	O2A-C1	5.17	1.60	1.46
15	A	1114	CLA	O2D-CGD	5.17	1.45	1.33
15	B	1206	CLA	CHC-C1C	5.17	1.48	1.35
15	A	1136	CLA	CHC-C1C	5.17	1.48	1.35
15	A	1124	CLA	O2A-C1	5.17	1.60	1.46
15	B	1221	CLA	CHC-C1C	5.17	1.48	1.35
15	A	1131	CLA	CHC-C1C	5.17	1.48	1.35
15	B	1219	CLA	O2A-C1	5.17	1.60	1.46
15	B	1209	CLA	O2D-CGD	5.17	1.45	1.33
15	A	1120	CLA	O2A-C1	5.17	1.60	1.46
15	A	1115	CLA	O2D-CGD	5.16	1.45	1.33
15	A	1105	CLA	O2D-CGD	5.16	1.45	1.33
15	B	1221	CLA	O2A-C1	5.16	1.60	1.46
15	A	1106	CLA	O2D-CGD	5.16	1.45	1.33
15	A	1801	CLA	O2A-C1	5.16	1.60	1.46
15	B	1205	CLA	CHC-C1C	5.16	1.48	1.35
15	A	1126	CLA	O2D-CGD	5.16	1.45	1.33
15	A	1129	CLA	O2D-CGD	5.16	1.45	1.33
15	A	1114	CLA	O2A-C1	5.16	1.60	1.46
15	B	1211	CLA	O2D-CGD	5.15	1.45	1.33
15	B	1222	CLA	CHC-C1C	5.15	1.48	1.35
15	A	1111	CLA	O2A-C1	5.15	1.60	1.46
15	B	1238	CLA	CHC-C1C	5.15	1.48	1.35
15	A	1113	CLA	O2D-CGD	5.15	1.45	1.33
15	B	1224	CLA	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1201	CLA	O2D-CGD	5.14	1.45	1.33
15	A	1132	CLA	O2D-CGD	5.14	1.45	1.33
15	F	1410	CLA	O2A-C1	5.14	1.60	1.46
15	B	1239	CLA	O2D-CGD	5.14	1.45	1.33
15	B	1204	CLA	O2D-CGD	5.14	1.45	1.33
15	A	1128	CLA	O2D-CGD	5.14	1.45	1.33
15	B	1223	CLA	O2A-C1	5.14	1.60	1.46
15	B	1221	CLA	O2D-CGD	5.14	1.45	1.33
15	A	1137	CLA	O2A-C1	5.14	1.60	1.46
15	A	1127	CLA	O2A-C1	5.14	1.60	1.46
15	A	1140	CLA	O2D-CGD	5.13	1.45	1.33
15	F	1410	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1213	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1023	CLA	O2D-CGD	5.13	1.45	1.33
15	J	1302	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1237	CLA	O2A-C1	5.13	1.60	1.46
15	B	1238	CLA	O2D-CGD	5.12	1.45	1.33
15	B	1216	CLA	O2A-C1	5.12	1.60	1.46
15	A	1110	CLA	CHC-C1C	5.11	1.48	1.35
15	A	1130	CLA	O2D-CGD	5.11	1.45	1.33
15	B	1228	CLA	O2A-C1	5.11	1.60	1.46
15	A	1111	CLA	O2D-CGD	5.11	1.45	1.33
15	B	1223	CLA	O2D-CGD	5.11	1.45	1.33
15	B	1217	CLA	O2D-CGD	5.11	1.45	1.33
13	A	1011	CL0	CHC-C1C	5.10	1.48	1.35
15	A	1137	CLA	O2D-CGD	5.10	1.45	1.33
15	B	1222	CLA	O2D-CGD	5.10	1.45	1.33
15	B	1228	CLA	C3B-C2B	5.10	1.47	1.40
15	A	1102	CLA	O2D-CGD	5.10	1.45	1.33
15	B	1232	CLA	CHC-C1C	5.09	1.48	1.35
15	A	1123	CLA	O2D-CGD	5.09	1.45	1.33
15	B	1215	CLA	CHC-C1C	5.09	1.48	1.35
15	B	1225	CLA	O2D-CGD	5.09	1.45	1.33
15	B	1021	CLA	O2A-C1	5.09	1.60	1.46
15	A	1107	CLA	O2A-C1	5.08	1.60	1.46
15	B	1202	CLA	O2A-C1	5.08	1.60	1.46
15	B	1236	CLA	O2D-CGD	5.08	1.45	1.33
15	B	1229	CLA	O2A-C1	5.08	1.60	1.46
15	B	1222	CLA	O2A-C1	5.08	1.60	1.46
15	A	1022	CLA	O2A-C1	5.07	1.60	1.46
15	A	1126	CLA	O2A-C1	5.07	1.60	1.46
15	A	1101	CLA	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1140	CLA	O2A-C1	5.07	1.60	1.46
15	A	1110	CLA	O2D-CGD	5.06	1.45	1.33
15	A	1125	CLA	O2D-CGD	5.06	1.45	1.33
15	B	1239	CLA	CHC-C1C	5.06	1.47	1.35
15	B	1231	CLA	CHC-C1C	5.06	1.47	1.35
15	A	1132	CLA	O2A-C1	5.06	1.60	1.46
15	B	1214	CLA	O2A-C1	5.06	1.60	1.46
15	B	1210	CLA	O2D-CGD	5.06	1.45	1.33
15	A	1135	CLA	O2D-CGD	5.05	1.45	1.33
15	B	1208	CLA	C3B-C2B	5.05	1.47	1.40
15	B	1229	CLA	O2D-CGD	5.05	1.45	1.33
15	B	1231	CLA	O2D-CGD	5.04	1.45	1.33
15	B	1023	CLA	O2A-C1	5.04	1.60	1.46
15	A	1122	CLA	O2A-C1	5.03	1.60	1.46
15	A	1123	CLA	O2A-C1	5.03	1.60	1.46
15	A	1110	CLA	O2A-C1	5.03	1.60	1.46
15	B	1226	CLA	O2D-CGD	5.03	1.45	1.33
15	A	1104	CLA	O2A-C1	5.02	1.60	1.46
15	B	1210	CLA	O2A-C1	5.02	1.60	1.46
15	B	1203	CLA	CHC-C1C	5.02	1.47	1.35
15	A	1128	CLA	CHC-C1C	5.01	1.47	1.35
15	A	1134	CLA	O2D-CGD	5.01	1.45	1.33
15	A	1104	CLA	O2D-CGD	5.00	1.45	1.33
15	B	1220	CLA	C3B-C2B	4.99	1.47	1.40
15	A	1101	CLA	O2A-C1	4.99	1.60	1.46
15	B	1225	CLA	O2A-C1	4.98	1.60	1.46
15	B	1229	CLA	OBD-CAD	4.98	1.29	1.22
15	A	1801	CLA	C3C-C2C	4.98	1.47	1.36
15	B	1203	CLA	O2A-C1	4.97	1.60	1.46
15	A	1124	CLA	OBD-CAD	4.95	1.29	1.22
15	A	1103	CLA	O2A-C1	4.95	1.60	1.46
15	B	1222	CLA	OBD-CAD	4.94	1.29	1.22
15	B	1230	CLA	O2A-C1	4.93	1.60	1.46
15	A	1102	CLA	C3B-C2B	4.91	1.47	1.40
15	A	1138	CLA	OBD-CAD	4.91	1.29	1.22
15	B	1202	CLA	OBD-CAD	4.91	1.29	1.22
15	A	1102	CLA	OBD-CAD	4.90	1.29	1.22
15	A	1022	CLA	OBD-CAD	4.90	1.29	1.22
15	A	1115	CLA	C3B-C2B	4.90	1.47	1.40
15	B	1218	CLA	OBD-CAD	4.90	1.29	1.22
15	B	1225	CLA	OBD-CAD	4.88	1.29	1.22
15	A	1101	CLA	OBD-CAD	4.88	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1120	CLA	OBD-CAD	4.86	1.29	1.22
15	F	1139	CLA	O2A-C1	4.86	1.59	1.46
15	B	1210	CLA	C3B-C2B	4.85	1.47	1.40
15	K	1401	CLA	OBD-CAD	4.85	1.29	1.22
15	B	1207	CLA	OBD-CAD	4.84	1.29	1.22
15	B	1021	CLA	OBD-CAD	4.84	1.29	1.22
15	B	1234	CLA	O2D-CGD	4.84	1.45	1.33
15	A	1137	CLA	C3B-C2B	4.84	1.47	1.40
15	B	1215	CLA	OBD-CAD	4.83	1.29	1.22
15	B	1239	CLA	OBD-CAD	4.83	1.29	1.22
15	B	1213	CLA	OBD-CAD	4.83	1.29	1.22
15	B	1224	CLA	OBD-CAD	4.83	1.29	1.22
15	B	1216	CLA	OBD-CAD	4.83	1.29	1.22
15	A	1022	CLA	C3D-C2D	4.83	1.48	1.39
15	B	1219	CLA	OBD-CAD	4.83	1.29	1.22
15	A	1140	CLA	OBD-CAD	4.82	1.29	1.22
15	B	1209	CLA	OBD-CAD	4.82	1.29	1.22
15	B	1214	CLA	OBD-CAD	4.82	1.29	1.22
15	B	1204	CLA	OBD-CAD	4.81	1.29	1.22
15	A	1116	CLA	OBD-CAD	4.81	1.29	1.22
15	A	1117	CLA	OBD-CAD	4.81	1.29	1.22
15	B	1220	CLA	OBD-CAD	4.81	1.29	1.22
15	A	1012	CLA	C3D-C2D	4.81	1.48	1.39
15	B	1205	CLA	OBD-CAD	4.81	1.29	1.22
15	B	1212	CLA	OBD-CAD	4.81	1.29	1.22
15	A	1106	CLA	OBD-CAD	4.80	1.29	1.22
15	B	1201	CLA	OBD-CAD	4.80	1.29	1.22
15	A	1127	CLA	C3B-C2B	4.80	1.47	1.40
15	A	1131	CLA	C3B-C2B	4.80	1.47	1.40
15	B	1226	CLA	OBD-CAD	4.80	1.29	1.22
15	B	1217	CLA	OBD-CAD	4.80	1.29	1.22
15	A	1134	CLA	OBD-CAD	4.79	1.29	1.22
15	B	1228	CLA	C3C-C2C	4.79	1.46	1.36
15	B	1240	CLA	OBD-CAD	4.79	1.29	1.22
15	A	1130	CLA	C3C-C2C	4.79	1.46	1.36
15	B	1208	CLA	C3C-C2C	4.79	1.46	1.36
15	A	1114	CLA	OBD-CAD	4.79	1.29	1.22
15	A	1112	CLA	OBD-CAD	4.79	1.29	1.22
15	A	1131	CLA	OBD-CAD	4.79	1.29	1.22
15	A	1111	CLA	OBD-CAD	4.79	1.29	1.22
15	J	1302	CLA	OBD-CAD	4.79	1.29	1.22
15	F	1410	CLA	OBD-CAD	4.78	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1118	CLA	OBD-CAD	4.78	1.29	1.22
15	F	1301	CLA	OBD-CAD	4.77	1.29	1.22
15	K	1402	CLA	OBD-CAD	4.77	1.29	1.22
15	B	1232	CLA	OBD-CAD	4.77	1.29	1.22
15	B	1230	CLA	OBD-CAD	4.77	1.29	1.22
15	B	1220	CLA	C3C-C2C	4.77	1.46	1.36
15	A	1012	CLA	OBD-CAD	4.77	1.29	1.22
15	A	1133	CLA	OBD-CAD	4.76	1.29	1.22
15	A	1801	CLA	OBD-CAD	4.76	1.29	1.22
15	A	1122	CLA	OBD-CAD	4.76	1.29	1.22
15	B	1222	CLA	C3C-C2C	4.76	1.46	1.36
13	A	1108	CL0	C3B-C2B	4.76	1.47	1.40
15	J	1303	CLA	OBD-CAD	4.76	1.29	1.22
15	A	1115	CLA	OBD-CAD	4.75	1.28	1.22
15	B	1231	CLA	OBD-CAD	4.75	1.28	1.22
15	A	1103	CLA	OBD-CAD	4.75	1.28	1.22
15	B	1212	CLA	C3B-C2B	4.75	1.47	1.40
15	B	1206	CLA	OBD-CAD	4.75	1.28	1.22
15	B	1208	CLA	OBD-CAD	4.75	1.28	1.22
15	A	1126	CLA	OBD-CAD	4.75	1.28	1.22
15	B	1221	CLA	C3B-C2B	4.75	1.47	1.40
15	B	1023	CLA	OBD-CAD	4.75	1.28	1.22
15	A	1135	CLA	OBD-CAD	4.75	1.28	1.22
15	B	1227	CLA	C3C-C2C	4.75	1.46	1.36
15	A	1128	CLA	OBD-CAD	4.74	1.28	1.22
15	B	1203	CLA	OBD-CAD	4.74	1.28	1.22
15	A	1136	CLA	C3B-C2B	4.74	1.46	1.40
10	B	2002	PQN	C10-C5	4.74	1.48	1.40
15	B	1234	CLA	C3B-C2B	4.74	1.46	1.40
15	B	1223	CLA	C3C-C2C	4.74	1.46	1.36
15	B	1240	CLA	C3C-C2C	4.74	1.46	1.36
15	A	1105	CLA	OBD-CAD	4.74	1.28	1.22
10	A	2001	PQN	C10-C5	4.73	1.48	1.40
15	B	1213	CLA	C3B-C2B	4.73	1.46	1.40
15	A	1123	CLA	OBD-CAD	4.73	1.28	1.22
15	A	1104	CLA	OBD-CAD	4.73	1.28	1.22
15	B	1238	CLA	OBD-CAD	4.73	1.28	1.22
15	A	1137	CLA	OBD-CAD	4.73	1.28	1.22
15	B	1234	CLA	OBD-CAD	4.73	1.28	1.22
15	B	1210	CLA	OBD-CAD	4.73	1.28	1.22
15	B	1013	CLA	OBD-CAD	4.72	1.28	1.22
15	A	1109	CLA	C3C-C2C	4.72	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1202	CLA	C3C-C2C	4.72	1.46	1.36
15	B	1230	CLA	C3B-C2B	4.72	1.46	1.40
15	A	1116	CLA	C3C-C2C	4.71	1.46	1.36
15	A	1107	CLA	OBD-CAD	4.71	1.28	1.22
15	A	1022	CLA	C3C-C2C	4.71	1.46	1.36
15	A	1132	CLA	OBD-CAD	4.71	1.28	1.22
15	B	1013	CLA	C3C-C2C	4.71	1.46	1.36
15	A	1119	CLA	OBD-CAD	4.71	1.28	1.22
15	A	1113	CLA	OBD-CAD	4.71	1.28	1.22
15	A	1107	CLA	C3C-C2C	4.71	1.46	1.36
15	B	1202	CLA	C3B-C2B	4.70	1.46	1.40
15	A	1122	CLA	C3C-C2C	4.70	1.46	1.36
15	J	1303	CLA	C3C-C2C	4.70	1.46	1.36
15	A	1140	CLA	C3B-C2B	4.70	1.46	1.40
15	A	1138	CLA	C3C-C2C	4.70	1.46	1.36
15	J	1302	CLA	C3B-C2B	4.70	1.46	1.40
15	A	1109	CLA	OBD-CAD	4.69	1.28	1.22
15	B	1201	CLA	C3B-C2B	4.69	1.46	1.40
15	A	1137	CLA	C3C-C2C	4.69	1.46	1.36
15	B	1235	CLA	C3C-C2C	4.69	1.46	1.36
15	B	1232	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1212	CLA	C3C-C2C	4.68	1.46	1.36
13	A	1011	CL0	OBD-CAD	4.68	1.28	1.22
15	A	1113	CLA	C3B-C2B	4.68	1.46	1.40
15	A	1136	CLA	OBD-CAD	4.68	1.28	1.22
15	B	1211	CLA	OBD-CAD	4.68	1.28	1.22
15	A	1127	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1211	CLA	C3B-C2B	4.68	1.46	1.40
15	B	1021	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1239	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1226	CLA	C3C-C2C	4.68	1.46	1.36
15	A	1130	CLA	OBD-CAD	4.68	1.28	1.22
15	A	1124	CLA	C3C-C2C	4.68	1.46	1.36
15	A	1140	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1238	CLA	C3B-C2B	4.67	1.46	1.40
15	A	1132	CLA	C3C-C2C	4.67	1.46	1.36
15	B	1216	CLA	C3C-C2C	4.67	1.46	1.36
15	B	1231	CLA	C3B-C2B	4.67	1.46	1.40
15	B	1229	CLA	C3C-C2C	4.67	1.46	1.36
15	B	1234	CLA	C3C-C2C	4.67	1.46	1.36
15	F	1139	CLA	OBD-CAD	4.67	1.28	1.22
15	A	1121	CLA	OBD-CAD	4.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1134	CLA	C3B-C2B	4.66	1.46	1.40
15	A	1012	CLA	C3C-C2C	4.66	1.46	1.36
15	B	1236	CLA	OBD-CAD	4.66	1.28	1.22
15	B	1220	CLA	C3D-C2D	4.66	1.47	1.39
15	B	1217	CLA	C3C-C2C	4.66	1.46	1.36
15	A	1119	CLA	C3C-C2C	4.66	1.46	1.36
15	A	1105	CLA	C3C-C2C	4.66	1.46	1.36
15	B	1237	CLA	C3B-C2B	4.65	1.46	1.40
15	B	1237	CLA	OBD-CAD	4.65	1.28	1.22
15	B	1214	CLA	C3C-C2C	4.65	1.46	1.36
15	B	1231	CLA	C3C-C2C	4.65	1.46	1.36
15	A	1102	CLA	C3D-C2D	4.65	1.47	1.39
15	A	1135	CLA	C3B-C2B	4.65	1.46	1.40
15	A	1114	CLA	C3C-C2C	4.65	1.46	1.36
15	F	1139	CLA	C3C-C2C	4.65	1.46	1.36
15	A	1134	CLA	C3C-C2C	4.65	1.46	1.36
15	A	1102	CLA	C3C-C2C	4.65	1.46	1.36
15	A	1112	CLA	C3C-C2C	4.64	1.46	1.36
15	A	1103	CLA	C3B-C2B	4.64	1.46	1.40
15	A	1129	CLA	C3C-C2C	4.64	1.46	1.36
15	A	1117	CLA	C3C-C2C	4.64	1.46	1.36
13	A	1108	CL0	OBD-CAD	4.64	1.28	1.22
15	F	1301	CLA	C3C-C2C	4.64	1.46	1.36
15	B	1225	CLA	C3B-C2B	4.64	1.46	1.40
15	A	1123	CLA	C3B-C2B	4.64	1.46	1.40
15	K	1402	CLA	C3C-C2C	4.64	1.46	1.36
15	A	1104	CLA	C3C-C2C	4.64	1.46	1.36
15	A	1110	CLA	OBD-CAD	4.63	1.28	1.22
15	B	1219	CLA	C3C-C2C	4.63	1.46	1.36
15	A	1121	CLA	C3C-C2C	4.63	1.46	1.36
15	B	1218	CLA	C3C-C2C	4.63	1.46	1.36
15	A	1111	CLA	C3B-C2B	4.62	1.46	1.40
15	A	1120	CLA	C3C-C2C	4.62	1.46	1.36
15	B	1224	CLA	C3B-C2B	4.62	1.46	1.40
15	A	1114	CLA	C3B-C2B	4.62	1.46	1.40
15	B	1221	CLA	OBD-CAD	4.62	1.28	1.22
15	A	1126	CLA	C3C-C2C	4.62	1.46	1.36
15	B	1203	CLA	C3C-C2C	4.62	1.46	1.36
15	A	1135	CLA	C3C-C2C	4.61	1.46	1.36
15	F	1139	CLA	C3B-C2B	4.61	1.46	1.40
15	F	1410	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1207	CLA	C3C-C2C	4.60	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1213	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1235	CLA	OBD-CAD	4.60	1.28	1.22
15	B	1209	CLA	C3C-C2C	4.60	1.46	1.36
15	A	1117	CLA	C3D-C2D	4.60	1.47	1.39
15	B	1238	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1215	CLA	C3C-C2C	4.59	1.46	1.36
15	A	1120	CLA	C3B-C2B	4.59	1.46	1.40
15	J	1303	CLA	C3B-C2B	4.59	1.46	1.40
15	B	1204	CLA	C3C-C2C	4.59	1.46	1.36
15	K	1401	CLA	C3C-C2C	4.59	1.46	1.36
15	K	1402	CLA	C3B-C2B	4.58	1.46	1.40
15	B	1207	CLA	C3B-C2B	4.58	1.46	1.40
15	B	1205	CLA	C3C-C2C	4.58	1.46	1.36
13	A	1011	CL0	C3C-C2C	4.58	1.46	1.36
15	A	1128	CLA	C3C-C2C	4.58	1.46	1.36
15	B	1222	CLA	C3B-C2B	4.58	1.46	1.40
15	A	1118	CLA	C3B-C2B	4.58	1.46	1.40
15	B	1206	CLA	C3B-C2B	4.58	1.46	1.40
15	A	1113	CLA	C3C-C2C	4.58	1.46	1.36
15	K	1401	CLA	C3B-C2B	4.57	1.46	1.40
15	F	1301	CLA	C3B-C2B	4.57	1.46	1.40
15	B	1209	CLA	C3B-C2B	4.57	1.46	1.40
15	B	1218	CLA	C3B-C2B	4.57	1.46	1.40
15	A	1131	CLA	C3C-C2C	4.57	1.46	1.36
15	B	1206	CLA	C3C-C2C	4.57	1.46	1.36
15	A	1106	CLA	C3C-C2C	4.57	1.46	1.36
15	B	1215	CLA	C3B-C2B	4.57	1.46	1.40
15	B	1201	CLA	C3C-C2C	4.57	1.46	1.36
15	A	1101	CLA	C3C-C2C	4.57	1.46	1.36
15	B	1216	CLA	C3B-C2B	4.57	1.46	1.40
15	J	1302	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1109	CLA	C3B-C2B	4.56	1.46	1.40
15	B	1224	CLA	C3C-C2C	4.56	1.46	1.36
15	B	1221	CLA	C3C-C2C	4.56	1.46	1.36
15	B	1239	CLA	C3B-C2B	4.56	1.46	1.40
15	B	1223	CLA	C3B-C2B	4.56	1.46	1.40
15	A	1801	CLA	C3B-C2B	4.56	1.46	1.40
15	B	1211	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1136	CLA	C3C-C2C	4.55	1.46	1.36
15	B	1023	CLA	C3C-C2C	4.55	1.46	1.36
15	B	1240	CLA	C3B-C2B	4.55	1.46	1.40
15	A	1125	CLA	C3C-C2C	4.55	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	CLA	C3C-C2C	4.54	1.46	1.36
15	B	1225	CLA	C3C-C2C	4.54	1.46	1.36
15	B	1230	CLA	C3C-C2C	4.54	1.46	1.36
15	A	1133	CLA	C3C-C2C	4.54	1.46	1.36
15	B	1013	CLA	C3D-C2D	4.53	1.47	1.39
15	A	1107	CLA	C3B-C2B	4.53	1.46	1.40
15	A	1115	CLA	C3C-C2C	4.53	1.46	1.36
15	B	1222	CLA	C3D-C2D	4.53	1.47	1.39
15	B	1227	CLA	OBD-CAD	4.52	1.28	1.22
15	A	1121	CLA	C3B-C2B	4.52	1.46	1.40
15	A	1132	CLA	C3B-C2B	4.52	1.46	1.40
15	A	1118	CLA	C3C-C2C	4.52	1.46	1.36
15	B	1214	CLA	C3D-C2D	4.52	1.47	1.39
15	A	1101	CLA	C3B-C2B	4.51	1.46	1.40
15	A	1125	CLA	OBD-CAD	4.51	1.28	1.22
15	B	1217	CLA	C3B-C2B	4.50	1.46	1.40
15	B	1013	CLA	C3B-C2B	4.50	1.46	1.40
15	B	1228	CLA	OBD-CAD	4.50	1.28	1.22
15	B	1232	CLA	C3D-C2D	4.50	1.47	1.39
15	B	1210	CLA	C3C-C2C	4.50	1.46	1.36
15	A	1106	CLA	C3D-C2D	4.49	1.47	1.39
15	B	1236	CLA	C3C-C2C	4.49	1.46	1.36
15	A	1138	CLA	C3D-C2D	4.49	1.47	1.39
15	B	1215	CLA	C3D-C2D	4.49	1.47	1.39
15	A	1129	CLA	C3B-C2B	4.49	1.46	1.40
15	A	1110	CLA	C3C-C2C	4.49	1.46	1.36
15	B	1238	CLA	C3D-C2D	4.49	1.47	1.39
15	A	1123	CLA	C3C-C2C	4.49	1.46	1.36
15	A	1127	CLA	OBD-CAD	4.48	1.28	1.22
15	B	1235	CLA	C3B-C2B	4.48	1.46	1.40
15	B	1204	CLA	C3B-C2B	4.48	1.46	1.40
15	A	1106	CLA	C3B-C2B	4.48	1.46	1.40
15	A	1112	CLA	C3B-C2B	4.47	1.46	1.40
15	B	1216	CLA	C3D-C2D	4.47	1.47	1.39
15	A	1111	CLA	C3C-C2C	4.46	1.46	1.36
15	B	1023	CLA	C3D-C2D	4.46	1.47	1.39
15	A	1103	CLA	C3C-C2C	4.46	1.46	1.36
15	A	1138	CLA	C3B-C2B	4.46	1.46	1.40
15	B	1214	CLA	C3B-C2B	4.46	1.46	1.40
15	A	1110	CLA	C3B-C2B	4.46	1.46	1.40
15	A	1130	CLA	C3B-C2B	4.46	1.46	1.40
15	F	1410	CLA	C3B-C2B	4.45	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1125	CLA	C3B-C2B	4.45	1.46	1.40
15	F	1301	CLA	C3D-C2D	4.45	1.47	1.39
15	A	1119	CLA	C3D-C2D	4.45	1.47	1.39
15	A	1124	CLA	C3D-C2D	4.44	1.47	1.39
15	B	1226	CLA	C3B-C2B	4.44	1.46	1.40
15	B	1217	CLA	C3D-C2D	4.43	1.47	1.39
15	B	1205	CLA	C3B-C2B	4.43	1.46	1.40
15	A	1116	CLA	C3B-C2B	4.43	1.46	1.40
15	B	1213	CLA	C3D-C2D	4.43	1.47	1.39
15	A	1109	CLA	C3D-C2D	4.43	1.47	1.39
15	A	1133	CLA	C3B-C2B	4.43	1.46	1.40
15	B	1203	CLA	C3B-C2B	4.42	1.46	1.40
15	B	1212	CLA	C3D-C2D	4.41	1.47	1.39
15	A	1128	CLA	C3D-C2D	4.41	1.47	1.39
15	A	1124	CLA	C3B-C2B	4.41	1.46	1.40
15	B	1208	CLA	C3D-C2D	4.41	1.47	1.39
15	B	1210	CLA	C3D-C2D	4.40	1.47	1.39
15	B	1211	CLA	C3D-C2D	4.40	1.47	1.39
15	A	1112	CLA	C3D-C2D	4.40	1.47	1.39
15	A	1126	CLA	C3B-C2B	4.40	1.46	1.40
13	A	1108	CL0	C3C-C2C	4.40	1.46	1.36
15	B	1235	CLA	C3D-C2D	4.40	1.47	1.39
15	B	1218	CLA	C3D-C2D	4.39	1.47	1.39
15	A	1133	CLA	C3D-C2D	4.39	1.47	1.39
15	A	1105	CLA	C3D-C2D	4.39	1.47	1.39
15	F	1410	CLA	C3D-C2D	4.38	1.47	1.39
15	A	1130	CLA	C3D-C2D	4.38	1.47	1.39
15	B	1201	CLA	C3D-C2D	4.38	1.47	1.39
15	A	1111	CLA	C3D-C2D	4.38	1.47	1.39
15	A	1117	CLA	C3B-C2B	4.37	1.46	1.40
15	B	1229	CLA	C3B-C2B	4.37	1.46	1.40
15	A	1129	CLA	OBD-CAD	4.37	1.28	1.22
15	B	1221	CLA	C3D-C2D	4.36	1.47	1.39
15	B	1240	CLA	C3D-C2D	4.36	1.47	1.39
15	A	1104	CLA	C3D-C2D	4.36	1.47	1.39
15	A	1132	CLA	C3D-C2D	4.36	1.47	1.39
15	A	1119	CLA	C3B-C2B	4.36	1.46	1.40
15	A	1101	CLA	C3D-C2D	4.36	1.47	1.39
15	B	1219	CLA	C3D-C2D	4.35	1.47	1.39
15	A	1104	CLA	C3B-C2B	4.35	1.46	1.40
15	B	1023	CLA	C3B-C2B	4.35	1.46	1.40
15	B	1021	CLA	C3D-C2D	4.34	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1206	CLA	C3D-C2D	4.34	1.47	1.39
12	A	5003	LHG	O8-C23	4.34	1.46	1.33
15	A	1012	CLA	C3B-C2B	4.34	1.46	1.40
15	B	1204	CLA	C3D-C2D	4.34	1.47	1.39
15	A	1114	CLA	C3D-C2D	4.34	1.47	1.39
15	A	1127	CLA	C3D-C2D	4.34	1.47	1.39
15	A	1135	CLA	C3D-C2D	4.33	1.47	1.39
15	A	1115	CLA	C3D-C2D	4.33	1.47	1.39
15	B	1236	CLA	C3B-C2B	4.33	1.46	1.40
15	A	1116	CLA	C3D-C2D	4.33	1.47	1.39
15	B	1205	CLA	C3D-C2D	4.33	1.47	1.39
15	B	1217	CLA	O2A-C1	4.33	1.60	1.46
15	A	1121	CLA	C3D-C2D	4.33	1.47	1.39
15	A	1122	CLA	C3B-C2B	4.32	1.46	1.40
15	A	1105	CLA	C3B-C2B	4.32	1.46	1.40
15	B	1224	CLA	C3D-C2D	4.32	1.47	1.39
15	B	1229	CLA	C3D-C2D	4.32	1.47	1.39
15	B	1209	CLA	C3D-C2D	4.31	1.47	1.39
15	A	1801	CLA	C3D-C2D	4.31	1.47	1.39
17	B	5002	LMG	O8-C28	4.31	1.45	1.33
15	B	1227	CLA	C3D-C2D	4.31	1.47	1.39
15	A	1118	CLA	C3D-C2D	4.31	1.47	1.39
15	B	1202	CLA	C3D-C2D	4.31	1.47	1.39
15	A	1022	CLA	C3B-C2B	4.31	1.46	1.40
15	A	1110	CLA	C3D-C2D	4.31	1.47	1.39
15	B	1223	CLA	C3D-C2D	4.31	1.47	1.39
15	A	1131	CLA	C3D-C2D	4.31	1.47	1.39
15	A	1113	CLA	C3D-C2D	4.31	1.47	1.39
15	B	1223	CLA	OBD-CAD	4.30	1.28	1.22
13	A	1011	CL0	C3D-C2D	4.29	1.47	1.39
15	B	1236	CLA	C3D-C2D	4.29	1.47	1.39
15	B	1228	CLA	C3D-C2D	4.29	1.47	1.39
15	B	1239	CLA	C3D-C2D	4.28	1.47	1.39
15	A	1123	CLA	C3D-C2D	4.28	1.47	1.39
15	B	1225	CLA	C3D-C2D	4.28	1.47	1.39
15	B	1234	CLA	C3D-C2D	4.27	1.47	1.39
15	B	1207	CLA	C3D-C2D	4.26	1.47	1.39
15	J	1302	CLA	C3D-C2D	4.26	1.47	1.39
15	B	1203	CLA	C3D-C2D	4.26	1.47	1.39
13	A	1011	CL0	C3B-C2B	4.26	1.46	1.40
15	B	1231	CLA	C3D-C2D	4.26	1.47	1.39
15	J	1303	CLA	C3D-C2D	4.24	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1136	CLA	C3D-C2D	4.24	1.47	1.39
15	K	1402	CLA	C3D-C2D	4.23	1.47	1.39
15	A	1140	CLA	C3D-C2D	4.23	1.47	1.39
15	A	1134	CLA	C3D-C2D	4.22	1.47	1.39
15	B	1021	CLA	C3B-C2B	4.22	1.46	1.40
15	B	1226	CLA	C3D-C2D	4.22	1.47	1.39
15	A	1120	CLA	C3D-C2D	4.21	1.47	1.39
12	A	5005	LHG	O8-C23	4.21	1.45	1.33
15	A	1129	CLA	C3D-C2D	4.20	1.47	1.39
12	B	5004	LHG	O8-C23	4.20	1.45	1.33
15	A	1137	CLA	C3D-C2D	4.20	1.47	1.39
15	A	1128	CLA	C3B-C2B	4.19	1.46	1.40
15	B	1230	CLA	C3D-C2D	4.19	1.46	1.39
15	A	1103	CLA	C3D-C2D	4.18	1.46	1.39
15	B	1237	CLA	C3D-C2D	4.18	1.46	1.39
15	K	1401	CLA	C3D-C2D	4.17	1.46	1.39
17	B	5002	LMG	O7-C10	4.16	1.46	1.34
12	A	5001	LHG	O8-C23	4.15	1.45	1.33
15	A	1122	CLA	C3D-C2D	4.15	1.46	1.39
12	B	5004	LHG	O7-C7	4.12	1.45	1.34
12	A	5001	LHG	O7-C7	4.11	1.45	1.34
15	B	1232	CLA	C3B-C2B	4.10	1.46	1.40
15	A	1126	CLA	C3D-C2D	4.10	1.46	1.39
12	A	5003	LHG	O7-C7	4.06	1.45	1.34
15	B	1227	CLA	C3B-C2B	4.06	1.46	1.40
15	A	1107	CLA	C3D-C2D	4.04	1.46	1.39
15	A	1012	CLA	MG-NC	4.03	2.15	2.06
12	A	5005	LHG	O7-C7	4.00	1.45	1.34
15	A	1125	CLA	C3D-C2D	4.00	1.46	1.39
15	F	1139	CLA	C3D-C2D	3.98	1.46	1.39
13	A	1108	CL0	C3D-C2D	3.96	1.46	1.39
15	A	1123	CLA	MG-NC	3.90	2.15	2.06
15	A	1801	CLA	MG-NC	3.87	2.15	2.06
13	A	1108	CL0	MG-NC	3.87	2.15	2.06
15	A	1137	CLA	MG-NC	3.86	2.15	2.06
15	B	1221	CLA	MG-NC	3.85	2.15	2.06
15	A	1121	CLA	MG-NC	3.84	2.15	2.06
15	B	1240	CLA	MG-NC	3.83	2.15	2.06
15	J	1303	CLA	MG-NC	3.83	2.15	2.06
15	B	1215	CLA	MG-NC	3.82	2.15	2.06
15	F	1410	CLA	MG-NC	3.81	2.15	2.06
15	B	1232	CLA	MG-NC	3.79	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1223	CLA	MG-NC	3.79	2.15	2.06
15	B	1227	CLA	MG-NC	3.79	2.15	2.06
15	A	1116	CLA	MG-NC	3.79	2.15	2.06
15	A	1124	CLA	MG-NC	3.79	2.15	2.06
15	A	1135	CLA	MG-NC	3.78	2.15	2.06
15	A	1134	CLA	MG-NC	3.78	2.15	2.06
15	F	1139	CLA	MG-NC	3.77	2.15	2.06
15	B	1021	CLA	MG-NC	3.77	2.15	2.06
15	A	1114	CLA	MG-NC	3.77	2.15	2.06
15	A	1022	CLA	MG-NC	3.77	2.15	2.06
15	B	1217	CLA	MG-NC	3.77	2.15	2.06
15	J	1302	CLA	MG-NC	3.77	2.15	2.06
15	A	1131	CLA	MG-NC	3.76	2.15	2.06
15	B	1206	CLA	MG-NC	3.76	2.15	2.06
15	B	1225	CLA	MG-NC	3.76	2.15	2.06
15	B	1238	CLA	MG-NC	3.75	2.15	2.06
15	A	1119	CLA	MG-NC	3.75	2.15	2.06
15	B	1209	CLA	MG-NC	3.75	2.15	2.06
15	A	1113	CLA	MG-NC	3.75	2.15	2.06
15	A	1127	CLA	MG-NC	3.74	2.15	2.06
15	B	1216	CLA	MG-NC	3.73	2.15	2.06
15	A	1105	CLA	MG-NC	3.73	2.15	2.06
15	A	1126	CLA	C1D-C2D	3.73	1.51	1.42
15	B	1205	CLA	MG-NC	3.73	2.15	2.06
15	A	1120	CLA	MG-NC	3.72	2.15	2.06
15	A	1112	CLA	MG-NC	3.72	2.15	2.06
15	F	1301	CLA	MG-NC	3.72	2.15	2.06
15	B	1207	CLA	MG-NC	3.72	2.15	2.06
15	B	1219	CLA	MG-NC	3.72	2.15	2.06
15	K	1401	CLA	MG-NC	3.71	2.15	2.06
15	B	1234	CLA	MG-NC	3.71	2.15	2.06
15	B	1212	CLA	MG-NC	3.71	2.15	2.06
15	A	1133	CLA	MG-NC	3.71	2.15	2.06
15	B	1213	CLA	MG-NC	3.71	2.15	2.06
15	B	1220	CLA	MG-NC	3.70	2.15	2.06
15	K	1402	CLA	MG-NC	3.70	2.15	2.06
15	B	1237	CLA	MG-NC	3.70	2.15	2.06
15	B	1239	CLA	MG-NC	3.70	2.15	2.06
15	A	1130	CLA	MG-NC	3.70	2.15	2.06
15	B	1210	CLA	MG-NC	3.69	2.15	2.06
13	A	1011	CL0	MG-NC	3.69	2.15	2.06
15	A	1125	CLA	MG-NC	3.69	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1132	CLA	MG-NC	3.68	2.15	2.06
15	A	1111	CLA	MG-NC	3.68	2.15	2.06
15	B	1201	CLA	MG-NC	3.67	2.15	2.06
15	B	1211	CLA	MG-NC	3.67	2.15	2.06
15	A	1117	CLA	MG-NC	3.65	2.15	2.06
15	B	1202	CLA	MG-NC	3.65	2.14	2.06
15	A	1129	CLA	MG-NC	3.65	2.14	2.06
15	B	1230	CLA	MG-NC	3.65	2.14	2.06
15	A	1136	CLA	MG-NC	3.65	2.14	2.06
15	B	1231	CLA	MG-NC	3.65	2.14	2.06
15	B	1229	CLA	MG-NC	3.64	2.14	2.06
15	B	1203	CLA	MG-NC	3.64	2.14	2.06
15	A	1128	CLA	MG-NC	3.64	2.14	2.06
15	B	1214	CLA	MG-NC	3.64	2.14	2.06
15	B	1224	CLA	MG-NC	3.63	2.14	2.06
15	A	1110	CLA	MG-NC	3.63	2.14	2.06
15	B	1218	CLA	MG-NC	3.63	2.14	2.06
15	A	1101	CLA	MG-NC	3.63	2.14	2.06
15	B	1235	CLA	MG-NC	3.63	2.14	2.06
15	A	1102	CLA	MG-NC	3.62	2.14	2.06
15	B	1226	CLA	MG-NC	3.62	2.14	2.06
15	B	1208	CLA	MG-NC	3.62	2.14	2.06
15	A	1140	CLA	MG-NC	3.62	2.14	2.06
15	A	1115	CLA	MG-NC	3.61	2.14	2.06
15	B	1204	CLA	MG-NC	3.61	2.14	2.06
15	A	1122	CLA	C1D-C2D	3.61	1.50	1.42
15	A	1109	CLA	MG-NC	3.61	2.14	2.06
15	A	1138	CLA	MG-NC	3.61	2.14	2.06
15	B	1222	CLA	MG-NC	3.60	2.14	2.06
15	A	1103	CLA	MG-NC	3.60	2.14	2.06
15	B	1236	CLA	MG-NC	3.58	2.14	2.06
15	A	1122	CLA	MG-NC	3.57	2.14	2.06
15	B	1228	CLA	MG-NC	3.57	2.14	2.06
15	B	1204	CLA	C1D-C2D	3.57	1.50	1.42
15	A	1129	CLA	C1D-C2D	3.57	1.50	1.42
15	A	1106	CLA	MG-NC	3.56	2.14	2.06
15	A	1109	CLA	C1D-C2D	3.55	1.50	1.42
15	B	1208	CLA	C1D-C2D	3.54	1.50	1.42
15	B	1213	CLA	C1D-C2D	3.53	1.50	1.42
15	B	1206	CLA	C1D-C2D	3.52	1.50	1.42
15	A	1107	CLA	MG-NC	3.52	2.14	2.06
15	A	1104	CLA	MG-NC	3.52	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1023	CLA	MG-NC	3.52	2.14	2.06
15	A	1126	CLA	MG-NC	3.52	2.14	2.06
15	B	1237	CLA	C1D-C2D	3.51	1.50	1.42
15	A	1107	CLA	C1D-C2D	3.50	1.50	1.42
15	A	1106	CLA	C1D-C2D	3.49	1.50	1.42
15	B	1231	CLA	C1D-C2D	3.49	1.50	1.42
15	A	1105	CLA	C1D-C2D	3.49	1.50	1.42
15	A	1120	CLA	C1D-C2D	3.49	1.50	1.42
15	A	1130	CLA	C1D-C2D	3.48	1.50	1.42
14	A	4012	BCR	C11-C12	-3.48	1.25	1.34
15	B	1219	CLA	C1D-C2D	3.48	1.50	1.42
15	B	1214	CLA	C1D-C2D	3.47	1.50	1.42
15	A	1124	CLA	C1D-C2D	3.47	1.50	1.42
15	B	1228	CLA	C1D-C2D	3.47	1.50	1.42
15	B	1209	CLA	C1D-C2D	3.47	1.50	1.42
15	A	1136	CLA	C1D-C2D	3.46	1.50	1.42
15	A	1118	CLA	MG-NC	3.46	2.14	2.06
15	A	1123	CLA	C1D-C2D	3.46	1.50	1.42
15	B	1013	CLA	MG-NC	3.46	2.14	2.06
15	A	1114	CLA	C1D-C2D	3.46	1.50	1.42
15	B	1202	CLA	C1D-C2D	3.46	1.50	1.42
15	B	1216	CLA	C1D-C2D	3.46	1.50	1.42
15	B	1239	CLA	C1D-C2D	3.45	1.50	1.42
15	B	1220	CLA	C1D-C2D	3.45	1.50	1.42
15	A	1134	CLA	C1D-C2D	3.44	1.50	1.42
15	A	1116	CLA	C1D-C2D	3.44	1.50	1.42
15	B	1215	CLA	C1D-C2D	3.43	1.50	1.42
15	B	1203	CLA	C1D-C2D	3.42	1.50	1.42
15	A	1103	CLA	C1D-C2D	3.42	1.50	1.42
15	A	1131	CLA	C1D-C2D	3.42	1.50	1.42
15	B	1236	CLA	C1D-C2D	3.42	1.50	1.42
15	B	1207	CLA	C1D-C2D	3.41	1.50	1.42
15	A	1111	CLA	C1D-C2D	3.41	1.50	1.42
15	B	1224	CLA	C1D-C2D	3.41	1.50	1.42
15	A	1104	CLA	C1D-C2D	3.41	1.50	1.42
15	K	1402	CLA	C1D-C2D	3.41	1.50	1.42
15	B	1240	CLA	C1D-C2D	3.41	1.50	1.42
15	A	1121	CLA	C1D-C2D	3.41	1.50	1.42
15	B	1230	CLA	C1D-C2D	3.41	1.50	1.42
15	A	1138	CLA	C1D-C2D	3.41	1.50	1.42
14	B	4006	BCR	C11-C12	-3.40	1.25	1.34
15	A	1133	CLA	C1D-C2D	3.40	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1102	CLA	C1D-C2D	3.40	1.50	1.42
15	B	1023	CLA	C1D-C2D	3.40	1.50	1.42
15	A	1117	CLA	C1D-C2D	3.40	1.50	1.42
15	F	1410	CLA	C1D-C2D	3.40	1.50	1.42
15	A	1119	CLA	C1D-C2D	3.39	1.50	1.42
15	B	1238	CLA	C1D-C2D	3.39	1.50	1.42
15	B	1227	CLA	C1D-C2D	3.38	1.50	1.42
15	A	1112	CLA	C1D-C2D	3.37	1.50	1.42
15	J	1303	CLA	C1D-C2D	3.37	1.50	1.42
15	K	1401	CLA	C1D-C2D	3.36	1.50	1.42
15	J	1302	CLA	C1D-C2D	3.36	1.50	1.42
15	A	1113	CLA	C1D-C2D	3.36	1.50	1.42
14	F	4016	BCR	C11-C12	-3.36	1.25	1.34
15	A	1135	CLA	C1D-C2D	3.35	1.50	1.42
15	B	1210	CLA	C1D-C2D	3.35	1.50	1.42
15	B	1232	CLA	C1D-C2D	3.34	1.50	1.42
14	B	4004	BCR	C11-C12	-3.33	1.26	1.34
15	B	1234	CLA	C1D-C2D	3.33	1.50	1.42
15	B	1201	CLA	C1D-C2D	3.33	1.50	1.42
15	A	1118	CLA	C1D-C2D	3.32	1.50	1.42
15	A	1801	CLA	C1D-C2D	3.32	1.50	1.42
15	A	1132	CLA	C1D-C2D	3.31	1.50	1.42
15	B	1217	CLA	C1D-C2D	3.31	1.50	1.42
15	B	1218	CLA	C1D-C2D	3.30	1.50	1.42
15	A	1110	CLA	C1D-C2D	3.29	1.50	1.42
15	B	1212	CLA	C1D-C2D	3.28	1.50	1.42
14	B	4010	BCR	C11-C12	-3.28	1.26	1.34
15	A	1137	CLA	C1D-C2D	3.28	1.50	1.42
15	B	1225	CLA	C1D-C2D	3.27	1.50	1.42
15	B	1235	CLA	C1D-C2D	3.27	1.50	1.42
15	A	1022	CLA	C1D-C2D	3.26	1.50	1.42
15	A	1140	CLA	C1D-C2D	3.26	1.50	1.42
15	F	1139	CLA	C1D-C2D	3.26	1.50	1.42
15	B	1222	CLA	C1D-C2D	3.26	1.49	1.42
15	F	1301	CLA	C1D-C2D	3.26	1.49	1.42
15	B	1226	CLA	C1D-C2D	3.26	1.49	1.42
15	B	1211	CLA	C1D-C2D	3.23	1.49	1.42
15	A	1115	CLA	C1D-C2D	3.22	1.49	1.42
15	A	1101	CLA	C1D-C2D	3.22	1.49	1.42
15	B	1021	CLA	C1D-C2D	3.21	1.49	1.42
15	B	1013	CLA	C1D-C2D	3.21	1.49	1.42
15	B	1229	CLA	C1D-C2D	3.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4014	BCR	C11-C12	-3.20	1.26	1.34
14	B	4011	BCR	C11-C12	-3.20	1.26	1.34
14	B	4005	BCR	C11-C12	-3.20	1.26	1.34
13	A	1108	CL0	C1D-C2D	3.19	1.49	1.42
15	B	1223	CLA	C1D-C2D	3.17	1.49	1.42
14	A	4002	BCR	C11-C12	-3.15	1.26	1.34
15	A	1127	CLA	C1D-C2D	3.13	1.49	1.42
14	A	4003	BCR	C11-C12	-3.12	1.26	1.34
15	B	1221	CLA	C1D-C2D	3.11	1.49	1.42
15	A	1125	CLA	C1D-C2D	3.10	1.49	1.42
15	B	1205	CLA	C1D-C2D	3.10	1.49	1.42
14	B	4017	BCR	C11-C12	-3.10	1.26	1.34
14	A	4007	BCR	C11-C12	-3.08	1.26	1.34
14	F	4015	BCR	C11-C12	-3.07	1.26	1.34
13	A	1011	CL0	C1D-C2D	3.07	1.49	1.42
14	B	4009	BCR	C11-C12	-3.06	1.26	1.34
15	A	1128	CLA	C1D-C2D	3.06	1.49	1.42
15	A	1138	CLA	C4B-CHC	3.05	1.49	1.41
14	A	4008	BCR	C11-C12	-3.05	1.26	1.34
14	J	4013	BCR	C11-C12	-3.05	1.26	1.34
15	A	1012	CLA	C1D-C2D	3.04	1.49	1.42
15	B	1236	CLA	C4B-CHC	2.96	1.49	1.41
15	A	1125	CLA	C4B-CHC	2.96	1.49	1.41
15	B	1228	CLA	C4B-CHC	2.93	1.49	1.41
15	A	1101	CLA	C4B-CHC	2.92	1.49	1.41
15	A	1126	CLA	C4B-CHC	2.89	1.49	1.41
15	A	1122	CLA	C4B-CHC	2.89	1.49	1.41
15	B	1230	CLA	C4B-CHC	2.87	1.49	1.41
14	A	4001	BCR	C11-C12	-2.86	1.27	1.34
15	B	1235	CLA	C4B-CHC	2.86	1.48	1.41
15	A	1107	CLA	C4B-CHC	2.86	1.48	1.41
15	A	1112	CLA	C4B-CHC	2.85	1.48	1.41
15	B	1223	CLA	C4B-CHC	2.84	1.48	1.41
13	A	1108	CL0	C1B-CHB	2.84	1.48	1.41
15	B	1220	CLA	C4B-CHC	2.84	1.48	1.41
15	A	1140	CLA	C4B-CHC	2.83	1.48	1.41
15	A	1130	CLA	C4B-CHC	2.82	1.48	1.41
15	B	1239	CLA	C1B-CHB	2.80	1.48	1.41
15	A	1128	CLA	C1C-NC	-2.80	1.33	1.37
15	B	1213	CLA	C4B-CHC	2.80	1.48	1.41
15	B	1229	CLA	C1B-CHB	2.79	1.48	1.41
15	A	1134	CLA	C4B-CHC	2.79	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1221	CLA	C1B-CHB	2.78	1.48	1.41
15	A	1104	CLA	C4B-CHC	2.78	1.48	1.41
15	B	1240	CLA	C4B-CHC	2.77	1.48	1.41
15	A	1131	CLA	C1B-CHB	2.77	1.48	1.41
15	F	1410	CLA	C4B-CHC	2.77	1.48	1.41
15	A	1136	CLA	C1B-CHB	2.77	1.48	1.41
15	A	1115	CLA	C4B-CHC	2.77	1.48	1.41
15	F	1301	CLA	C4B-CHC	2.77	1.48	1.41
15	A	1022	CLA	C4B-CHC	2.76	1.48	1.41
15	B	1211	CLA	C4B-CHC	2.76	1.48	1.41
15	A	1103	CLA	C4B-CHC	2.76	1.48	1.41
15	A	1132	CLA	C4B-CHC	2.76	1.48	1.41
13	A	1108	CL0	C4B-CHC	2.76	1.48	1.41
15	K	1402	CLA	C1B-CHB	2.76	1.48	1.41
15	A	1127	CLA	C4B-CHC	2.75	1.48	1.41
15	J	1303	CLA	C1B-CHB	2.75	1.48	1.41
15	A	1132	CLA	C1B-CHB	2.75	1.48	1.41
15	A	1109	CLA	C4B-CHC	2.75	1.48	1.41
15	B	1225	CLA	C4B-CHC	2.75	1.48	1.41
15	A	1137	CLA	C1B-CHB	2.75	1.48	1.41
15	B	1013	CLA	C4B-CHC	2.75	1.48	1.41
15	J	1303	CLA	C4B-CHC	2.74	1.48	1.41
15	B	1202	CLA	C4B-CHC	2.74	1.48	1.41
15	A	1119	CLA	C4B-CHC	2.74	1.48	1.41
15	B	1237	CLA	C1B-CHB	2.73	1.48	1.41
15	F	1139	CLA	C4B-CHC	2.73	1.48	1.41
15	A	1111	CLA	C4B-CHC	2.73	1.48	1.41
15	B	1212	CLA	C1B-CHB	2.73	1.48	1.41
15	A	1117	CLA	C4B-CHC	2.73	1.48	1.41
15	B	1213	CLA	C1B-CHB	2.73	1.48	1.41
15	B	1234	CLA	C1B-CHB	2.73	1.48	1.41
15	B	1214	CLA	C4B-CHC	2.73	1.48	1.41
15	B	1231	CLA	C1C-NC	-2.72	1.33	1.37
15	K	1401	CLA	C4B-CHC	2.72	1.48	1.41
15	A	1121	CLA	C1B-CHB	2.72	1.48	1.41
15	A	1135	CLA	C1B-CHB	2.72	1.48	1.41
15	A	1115	CLA	C1B-CHB	2.72	1.48	1.41
15	J	1302	CLA	C4B-CHC	2.72	1.48	1.41
15	B	1205	CLA	C1B-CHB	2.72	1.48	1.41
15	A	1801	CLA	C4B-CHC	2.72	1.48	1.41
15	B	1238	CLA	C1B-CHB	2.72	1.48	1.41
15	A	1113	CLA	C4B-CHC	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1114	CLA	C4B-CHC	2.72	1.48	1.41
15	A	1012	CLA	C4B-CHC	2.72	1.48	1.41
15	B	1229	CLA	C4B-CHC	2.72	1.48	1.41
15	F	1139	CLA	C1B-CHB	2.71	1.48	1.41
15	B	1237	CLA	C4B-CHC	2.71	1.48	1.41
15	B	1218	CLA	C4B-CHC	2.71	1.48	1.41
15	A	1801	CLA	C1B-CHB	2.71	1.48	1.41
15	A	1127	CLA	C1B-CHB	2.71	1.48	1.41
15	A	1114	CLA	C1B-CHB	2.71	1.48	1.41
15	B	1212	CLA	C4B-CHC	2.71	1.48	1.41
15	A	1118	CLA	C1B-CHB	2.71	1.48	1.41
15	B	1208	CLA	C1B-CHB	2.71	1.48	1.41
15	B	1215	CLA	C1B-CHB	2.70	1.48	1.41
15	A	1116	CLA	C4B-CHC	2.70	1.48	1.41
15	A	1140	CLA	C1B-CHB	2.70	1.48	1.41
15	B	1201	CLA	C4B-CHC	2.70	1.48	1.41
15	A	1123	CLA	C1B-CHB	2.70	1.48	1.41
15	A	1129	CLA	C1B-CHB	2.70	1.48	1.41
15	B	1207	CLA	C4B-CHC	2.70	1.48	1.41
15	B	1226	CLA	C1B-CHB	2.70	1.48	1.41
15	B	1217	CLA	C4B-CHC	2.70	1.48	1.41
15	J	1302	CLA	C1B-CHB	2.69	1.48	1.41
15	A	1107	CLA	C1C-NC	-2.69	1.33	1.37
15	B	1219	CLA	C1B-CHB	2.69	1.48	1.41
15	B	1211	CLA	C1B-CHB	2.69	1.48	1.41
15	B	1203	CLA	C1B-CHB	2.69	1.48	1.41
15	A	1137	CLA	C4B-CHC	2.69	1.48	1.41
15	A	1124	CLA	C4B-CHC	2.68	1.48	1.41
15	A	1102	CLA	C4B-CHC	2.68	1.48	1.41
15	A	1121	CLA	C4B-CHC	2.68	1.48	1.41
15	B	1221	CLA	C4B-CHC	2.68	1.48	1.41
15	B	1226	CLA	C4B-CHC	2.68	1.48	1.41
15	A	1133	CLA	C4B-CHC	2.68	1.48	1.41
15	B	1216	CLA	C4B-CHC	2.67	1.48	1.41
15	K	1402	CLA	C4B-CHC	2.67	1.48	1.41
15	B	1224	CLA	C4B-CHC	2.67	1.48	1.41
15	B	1208	CLA	C4B-CHC	2.67	1.48	1.41
15	B	1021	CLA	C4B-CHC	2.67	1.48	1.41
15	B	1238	CLA	C4B-CHC	2.67	1.48	1.41
15	A	1103	CLA	C1B-CHB	2.67	1.48	1.41
15	B	1240	CLA	C1B-CHB	2.67	1.48	1.41
15	B	1205	CLA	C4B-CHC	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1232	CLA	C1B-CHB	2.66	1.48	1.41
15	A	1129	CLA	C4B-CHC	2.65	1.48	1.41
15	B	1231	CLA	C1B-CHB	2.65	1.48	1.41
15	A	1105	CLA	C4B-CHC	2.65	1.48	1.41
15	A	1126	CLA	CHD-C4C	2.65	1.48	1.41
15	A	1133	CLA	C1B-CHB	2.65	1.48	1.41
15	A	1106	CLA	C4B-CHC	2.65	1.48	1.41
15	B	1201	CLA	C1B-CHB	2.64	1.48	1.41
15	B	1204	CLA	C1B-CHB	2.64	1.48	1.41
15	A	1109	CLA	C1B-CHB	2.63	1.48	1.41
15	B	1210	CLA	C4B-CHC	2.63	1.48	1.41
15	B	1207	CLA	C1B-CHB	2.63	1.48	1.41
15	B	1219	CLA	C4B-CHC	2.63	1.48	1.41
15	B	1217	CLA	C1B-CHB	2.63	1.48	1.41
15	A	1131	CLA	C4B-CHC	2.63	1.48	1.41
15	A	1120	CLA	C4B-CHC	2.63	1.48	1.41
15	A	1118	CLA	C4B-CHC	2.63	1.48	1.41
15	A	1134	CLA	C1B-CHB	2.63	1.48	1.41
15	B	1023	CLA	C4B-CHC	2.63	1.48	1.41
15	A	1116	CLA	C1B-CHB	2.63	1.48	1.41
15	A	1135	CLA	C4B-CHC	2.63	1.48	1.41
15	B	1230	CLA	C1B-CHB	2.63	1.48	1.41
15	A	1113	CLA	C1B-CHB	2.63	1.48	1.41
15	F	1410	CLA	C1B-CHB	2.62	1.48	1.41
15	B	1202	CLA	C1B-CHB	2.62	1.48	1.41
15	B	1204	CLA	C4B-CHC	2.62	1.48	1.41
15	A	1120	CLA	C1B-CHB	2.62	1.48	1.41
15	K	1401	CLA	C1B-CHB	2.62	1.48	1.41
15	B	1206	CLA	C4B-CHC	2.61	1.48	1.41
15	A	1105	CLA	C1B-CHB	2.60	1.48	1.41
15	A	1136	CLA	C4B-CHC	2.60	1.48	1.41
15	A	1110	CLA	C4B-CHC	2.60	1.48	1.41
15	B	1214	CLA	CHD-C4C	2.60	1.48	1.41
15	B	1208	CLA	CHD-C4C	2.60	1.48	1.41
15	B	1209	CLA	C4B-CHC	2.60	1.48	1.41
15	A	1128	CLA	C1B-CHB	2.60	1.48	1.41
15	B	1215	CLA	C4B-CHC	2.60	1.48	1.41
15	B	1235	CLA	C1B-CHB	2.60	1.48	1.41
15	B	1232	CLA	C4B-CHC	2.60	1.48	1.41
15	A	1130	CLA	CHD-C4C	2.60	1.48	1.41
15	B	1227	CLA	C4B-CHC	2.59	1.48	1.41
15	B	1218	CLA	C1B-CHB	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1222	CLA	C4B-CHC	2.59	1.48	1.41
15	A	1012	CLA	C1B-CHB	2.59	1.48	1.41
15	B	1216	CLA	C1B-CHB	2.59	1.48	1.41
15	B	1239	CLA	CHD-C4C	2.59	1.48	1.41
15	B	1234	CLA	C4B-CHC	2.59	1.48	1.41
15	B	1228	CLA	C1B-CHB	2.58	1.48	1.41
15	B	1223	CLA	C1B-CHB	2.58	1.48	1.41
15	B	1220	CLA	C1B-CHB	2.58	1.48	1.41
15	A	1125	CLA	C1B-CHB	2.58	1.48	1.41
15	B	1209	CLA	C1B-CHB	2.57	1.48	1.41
15	B	1220	CLA	CHD-C4C	2.57	1.48	1.41
15	A	1122	CLA	CHD-C4C	2.57	1.48	1.41
15	A	1123	CLA	C4C-C3C	2.57	1.49	1.45
15	B	1219	CLA	CHD-C4C	2.57	1.48	1.41
15	A	1106	CLA	CHD-C4C	2.57	1.48	1.41
15	A	1122	CLA	C1B-CHB	2.57	1.48	1.41
15	B	1222	CLA	C1B-CHB	2.56	1.48	1.41
15	B	1206	CLA	CHD-C4C	2.56	1.48	1.41
15	A	1110	CLA	C1B-CHB	2.56	1.48	1.41
15	B	1203	CLA	C4B-CHC	2.56	1.48	1.41
15	B	1021	CLA	C1B-CHB	2.56	1.48	1.41
15	B	1213	CLA	CHD-C4C	2.55	1.48	1.41
15	A	1123	CLA	C4B-CHC	2.55	1.48	1.41
15	B	1206	CLA	C1B-CHB	2.55	1.48	1.41
15	B	1227	CLA	C1B-CHB	2.54	1.48	1.41
15	A	1112	CLA	C1B-CHB	2.54	1.48	1.41
15	B	1231	CLA	C4B-CHC	2.54	1.48	1.41
15	A	1117	CLA	CHD-C4C	2.54	1.48	1.41
15	A	1102	CLA	C1B-CHB	2.54	1.48	1.41
15	A	1110	CLA	C1C-NC	-2.54	1.34	1.37
15	B	1225	CLA	C1B-CHB	2.53	1.48	1.41
15	B	1215	CLA	CHD-C4C	2.53	1.48	1.41
15	A	1109	CLA	CHD-C4C	2.53	1.48	1.41
15	B	1204	CLA	CHD-C4C	2.53	1.48	1.41
15	B	1216	CLA	CHD-C4C	2.53	1.48	1.41
13	A	1011	CL0	C4B-CHC	2.53	1.48	1.41
15	A	1022	CLA	C1B-CHB	2.52	1.48	1.41
15	A	1120	CLA	CHD-C4C	2.52	1.48	1.41
15	A	1135	CLA	CHD-C4C	2.52	1.48	1.41
15	A	1128	CLA	C4B-CHC	2.51	1.48	1.41
15	B	1023	CLA	C1B-CHB	2.51	1.48	1.41
15	A	1114	CLA	CHD-C4C	2.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1231	CLA	CHD-C4C	2.51	1.48	1.41
15	A	1124	CLA	CHD-C4C	2.51	1.48	1.41
15	B	1236	CLA	C1C-C2C	2.51	1.49	1.44
15	B	1227	CLA	CHD-C4C	2.51	1.48	1.41
15	A	1111	CLA	C1B-CHB	2.51	1.48	1.41
15	A	1123	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1119	CLA	C1B-CHB	2.50	1.47	1.41
15	B	1210	CLA	C1B-CHB	2.50	1.47	1.41
15	B	1237	CLA	CHD-C4C	2.50	1.48	1.41
15	B	1224	CLA	C1B-CHB	2.50	1.47	1.41
15	B	1224	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1119	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1102	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1105	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1107	CLA	CHD-C4C	2.50	1.48	1.41
15	A	1121	CLA	CHD-C4C	2.49	1.48	1.41
15	F	1139	CLA	C1C-NC	-2.49	1.34	1.37
15	B	1239	CLA	C4B-CHC	2.49	1.47	1.41
15	B	1236	CLA	C1B-CHB	2.49	1.47	1.41
15	B	1234	CLA	C1C-NC	-2.49	1.34	1.37
15	B	1203	CLA	CHD-C4C	2.49	1.48	1.41
15	B	1240	CLA	CHD-C4C	2.49	1.48	1.41
15	B	1218	CLA	CHD-C4C	2.49	1.48	1.41
15	F	1301	CLA	C1B-CHB	2.49	1.47	1.41
15	A	1116	CLA	CHD-C4C	2.48	1.48	1.41
15	A	1104	CLA	C1B-CHB	2.48	1.47	1.41
15	F	1410	CLA	CHD-C4C	2.48	1.48	1.41
15	A	1133	CLA	CHD-C4C	2.48	1.48	1.41
15	A	1117	CLA	C1B-CHB	2.47	1.47	1.41
15	A	1115	CLA	C1C-NC	-2.47	1.34	1.37
15	A	1103	CLA	CHD-C4C	2.47	1.48	1.41
15	B	1023	CLA	C1C-NC	-2.47	1.34	1.37
15	A	1138	CLA	CHD-C4C	2.47	1.48	1.41
15	B	1210	CLA	CHD-C4C	2.47	1.48	1.41
15	A	1131	CLA	C1C-NC	-2.47	1.34	1.37
15	B	1217	CLA	CHD-C4C	2.47	1.48	1.41
15	B	1209	CLA	C4C-C3C	2.47	1.49	1.45
15	A	1138	CLA	C1B-CHB	2.46	1.47	1.41
15	B	1209	CLA	CHD-C4C	2.46	1.48	1.41
15	B	1013	CLA	C1C-NC	-2.46	1.34	1.37
15	A	1129	CLA	CHD-C4C	2.46	1.48	1.41
15	A	1113	CLA	CHD-C4C	2.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1138	CLA	C1C-C2C	2.46	1.49	1.44
15	A	1801	CLA	C1C-NC	-2.46	1.34	1.37
15	B	1239	CLA	C1C-NC	-2.45	1.34	1.37
15	B	1238	CLA	CHD-C4C	2.45	1.48	1.41
15	A	1022	CLA	CHD-C4C	2.45	1.48	1.41
15	B	1228	CLA	CHD-C4C	2.45	1.48	1.41
15	A	1106	CLA	C1C-NC	-2.45	1.34	1.37
15	A	1101	CLA	C1B-CHB	2.45	1.47	1.41
15	B	1215	CLA	C1C-NC	-2.45	1.34	1.37
15	K	1401	CLA	CHD-C4C	2.45	1.48	1.41
15	A	1106	CLA	C1B-CHB	2.45	1.47	1.41
15	A	1126	CLA	C1B-CHB	2.44	1.47	1.41
15	B	1207	CLA	CHD-C4C	2.44	1.48	1.41
15	B	1222	CLA	C1C-NC	-2.44	1.34	1.37
15	A	1136	CLA	CHD-C4C	2.44	1.48	1.41
15	A	1114	CLA	C4C-C3C	2.44	1.49	1.45
15	B	1236	CLA	CHD-C4C	2.44	1.48	1.41
13	A	1011	CL0	C1B-CHB	2.44	1.47	1.41
15	A	1131	CLA	CHD-C4C	2.43	1.48	1.41
15	B	1234	CLA	CHD-C4C	2.43	1.48	1.41
15	B	1211	CLA	CHD-C4C	2.43	1.48	1.41
15	B	1232	CLA	CHD-C4C	2.43	1.48	1.41
15	B	1239	CLA	C4C-C3C	2.43	1.49	1.45
15	B	1202	CLA	CHD-C4C	2.43	1.48	1.41
15	A	1801	CLA	CHD-C4C	2.43	1.48	1.41
15	B	1206	CLA	C4C-C3C	2.42	1.49	1.45
15	A	1104	CLA	CHD-C4C	2.42	1.48	1.41
15	B	1021	CLA	CHD-C4C	2.42	1.48	1.41
15	B	1023	CLA	CHD-C4C	2.42	1.48	1.41
15	B	1208	CLA	C1C-NC	-2.42	1.34	1.37
15	A	1110	CLA	CHD-C4C	2.42	1.48	1.41
15	J	1302	CLA	CHD-C4C	2.42	1.48	1.41
15	B	1212	CLA	CHD-C4C	2.42	1.48	1.41
15	A	1134	CLA	CHD-C4C	2.42	1.48	1.41
15	A	1140	CLA	C1C-NC	-2.42	1.34	1.37
15	B	1222	CLA	CHD-C4C	2.42	1.48	1.41
15	B	1203	CLA	C1C-NC	-2.42	1.34	1.37
15	B	1211	CLA	C1C-NC	-2.42	1.34	1.37
15	K	1402	CLA	CHD-C4C	2.41	1.48	1.41
15	A	1113	CLA	C1C-NC	-2.41	1.34	1.37
15	A	1137	CLA	CHD-C4C	2.41	1.48	1.41
15	F	1139	CLA	CHD-C4C	2.41	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1102	CLA	C1C-NC	-2.41	1.34	1.37
15	K	1401	CLA	C1C-NC	-2.41	1.34	1.37
15	A	1103	CLA	C1C-NC	-2.41	1.34	1.37
15	B	1013	CLA	C1B-CHB	2.41	1.47	1.41
13	A	1011	CL0	C1C-NC	-2.41	1.34	1.37
15	A	1112	CLA	CHD-C4C	2.41	1.48	1.41
15	A	1107	CLA	C1B-CHB	2.41	1.47	1.41
15	A	1111	CLA	CHD-C4C	2.41	1.48	1.41
15	A	1105	CLA	C1C-NC	-2.41	1.34	1.37
15	B	1201	CLA	CHD-C4C	2.40	1.48	1.41
15	B	1210	CLA	C1C-NC	-2.40	1.34	1.37
15	B	1229	CLA	C1C-NC	-2.40	1.34	1.37
15	B	1214	CLA	C1B-CHB	2.40	1.47	1.41
15	A	1121	CLA	C1C-NC	-2.40	1.34	1.37
15	B	1216	CLA	C4C-C3C	2.40	1.49	1.45
15	B	1226	CLA	CHD-C4C	2.40	1.48	1.41
15	F	1301	CLA	CHD-C4C	2.40	1.48	1.41
15	J	1303	CLA	CHD-C4C	2.40	1.48	1.41
15	A	1012	CLA	CHD-C4C	2.40	1.48	1.41
15	B	1225	CLA	CHD-C4C	2.39	1.48	1.41
15	B	1218	CLA	C1C-NC	-2.39	1.34	1.37
15	B	1205	CLA	C1C-NC	-2.39	1.34	1.37
15	J	1302	CLA	C1C-NC	-2.39	1.34	1.37
15	A	1111	CLA	C1C-NC	-2.39	1.34	1.37
15	B	1238	CLA	C1C-NC	-2.39	1.34	1.37
15	A	1109	CLA	C1C-NC	-2.38	1.34	1.37
15	B	1212	CLA	C1C-NC	-2.38	1.34	1.37
15	A	1140	CLA	CHD-C4C	2.38	1.47	1.41
15	A	1133	CLA	C4C-C3C	2.38	1.49	1.45
15	A	1101	CLA	C1C-NC	-2.37	1.34	1.37
15	A	1135	CLA	C1C-NC	-2.37	1.34	1.37
15	A	1105	CLA	C4C-C3C	2.37	1.49	1.45
15	B	1227	CLA	C1C-NC	-2.37	1.34	1.37
15	A	1116	CLA	C1C-NC	-2.37	1.34	1.37
15	B	1202	CLA	C1C-NC	-2.37	1.34	1.37
15	A	1118	CLA	CHD-C4C	2.36	1.47	1.41
15	A	1116	CLA	C4C-C3C	2.36	1.49	1.45
15	A	1122	CLA	C1C-NC	-2.36	1.34	1.37
15	A	1130	CLA	C1B-CHB	2.36	1.47	1.41
15	A	1136	CLA	C1C-NC	-2.36	1.34	1.37
15	A	1101	CLA	CHD-C4C	2.36	1.47	1.41
15	B	1235	CLA	C1C-C2C	2.36	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1223	CLA	C1C-C2C	2.35	1.49	1.44
15	J	1303	CLA	C1C-NC	-2.35	1.34	1.37
15	A	1120	CLA	C1C-NC	-2.35	1.34	1.37
15	A	1124	CLA	C1B-CHB	2.35	1.47	1.41
15	B	1206	CLA	C1C-NC	-2.35	1.34	1.37
15	B	1216	CLA	C1C-NC	-2.35	1.34	1.37
15	A	1125	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1223	CLA	CHD-C4C	2.34	1.47	1.41
15	B	1229	CLA	CHD-C4C	2.34	1.47	1.41
15	K	1402	CLA	C1C-NC	-2.34	1.34	1.37
15	A	1133	CLA	C1C-NC	-2.34	1.34	1.37
15	A	1132	CLA	CHD-C4C	2.33	1.47	1.41
15	B	1232	CLA	C1C-NC	-2.33	1.34	1.37
15	A	1113	CLA	C4C-C3C	2.33	1.49	1.45
15	B	1204	CLA	C4C-C3C	2.33	1.49	1.45
15	A	1127	CLA	C1C-NC	-2.33	1.34	1.37
13	A	1011	CL0	CHD-C4C	2.33	1.47	1.41
15	B	1207	CLA	C1C-NC	-2.33	1.34	1.37
15	A	1137	CLA	C1C-NC	-2.33	1.34	1.37
15	A	1104	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1128	CLA	CHD-C4C	2.32	1.47	1.41
15	B	1230	CLA	C1C-NC	-2.32	1.34	1.37
15	B	1201	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1125	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1137	CLA	C4C-C3C	2.32	1.49	1.45
15	A	1120	CLA	C4C-C3C	2.32	1.49	1.45
15	A	1134	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1127	CLA	CHD-C4C	2.32	1.47	1.41
15	J	1303	CLA	C4C-C3C	2.32	1.49	1.45
15	A	1114	CLA	C1C-NC	-2.32	1.34	1.37
15	B	1215	CLA	C4C-C3C	2.31	1.49	1.45
15	B	1221	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1123	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1124	CLA	C1C-NC	-2.31	1.34	1.37
15	B	1235	CLA	CHD-C4C	2.31	1.47	1.41
15	B	1204	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1132	CLA	C1C-NC	-2.31	1.34	1.37
15	B	1237	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1131	CLA	C4C-C3C	2.31	1.49	1.45
15	A	1118	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1119	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1121	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1240	CLA	C4C-C3C	2.30	1.49	1.45
15	B	1224	CLA	C1C-NC	-2.30	1.34	1.37
15	A	1117	CLA	C1C-NC	-2.30	1.34	1.37
15	B	1013	CLA	CHD-C4C	2.30	1.47	1.41
15	K	1401	CLA	C4C-C3C	2.30	1.49	1.45
15	B	1227	CLA	C4C-C3C	2.29	1.49	1.45
15	A	1135	CLA	C4C-C3C	2.29	1.49	1.45
15	B	1214	CLA	C4C-C3C	2.29	1.49	1.45
15	B	1230	CLA	CHD-C4C	2.29	1.47	1.41
15	B	1209	CLA	C1C-NC	-2.29	1.34	1.37
15	F	1139	CLA	C1C-C2C	2.29	1.49	1.44
15	B	1207	CLA	C4C-C3C	2.28	1.49	1.45
13	A	1108	CL0	CHD-C4C	2.28	1.47	1.41
15	B	1021	CLA	C1C-NC	-2.28	1.34	1.37
15	B	1217	CLA	C1C-NC	-2.28	1.34	1.37
15	A	1104	CLA	C1C-C2C	2.28	1.49	1.44
15	B	1205	CLA	CHD-C4C	2.28	1.47	1.41
15	A	1115	CLA	CHD-C4C	2.27	1.47	1.41
15	B	1237	CLA	C4C-C3C	2.27	1.49	1.45
15	F	1301	CLA	C1C-NC	-2.27	1.34	1.37
15	B	1213	CLA	C1C-NC	-2.27	1.34	1.37
15	F	1410	CLA	C1C-NC	-2.27	1.34	1.37
15	B	1208	CLA	C4C-C3C	2.27	1.48	1.45
15	B	1235	CLA	C1C-NC	-2.27	1.34	1.37
15	A	1022	CLA	C1C-NC	-2.26	1.34	1.37
15	A	1119	CLA	C4C-C3C	2.26	1.48	1.45
15	A	1130	CLA	C1C-NC	-2.26	1.34	1.37
15	B	1203	CLA	C4C-C3C	2.26	1.48	1.45
15	B	1228	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1134	CLA	C4C-C3C	2.25	1.48	1.45
15	A	1111	CLA	C4C-C3C	2.25	1.48	1.45
15	A	1126	CLA	C1C-NC	-2.25	1.34	1.37
15	B	1220	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1124	CLA	C4C-C3C	2.25	1.48	1.45
15	B	1220	CLA	C4C-C3C	2.25	1.48	1.45
15	A	1109	CLA	C1C-C2C	2.25	1.48	1.44
15	A	1012	CLA	C4C-C3C	2.25	1.48	1.45
15	A	1129	CLA	C4C-C3C	2.24	1.48	1.45
15	B	1210	CLA	C4C-C3C	2.24	1.48	1.45
15	A	1130	CLA	C1C-C2C	2.24	1.48	1.44
15	B	1232	CLA	C4C-C3C	2.24	1.48	1.45
15	B	1219	CLA	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1220	CLA	C1C-C2C	2.24	1.48	1.44
15	B	1240	CLA	C1C-NC	-2.24	1.34	1.37
15	A	1136	CLA	C4C-C3C	2.24	1.48	1.45
15	F	1301	CLA	C1C-C2C	2.23	1.48	1.44
15	B	1023	CLA	C4C-C3C	2.23	1.48	1.45
15	A	1138	CLA	C1C-NC	-2.22	1.34	1.37
15	B	1221	CLA	CHD-C4C	2.22	1.47	1.41
15	B	1219	CLA	C1C-NC	-2.22	1.34	1.37
15	B	1225	CLA	C1C-NC	-2.22	1.34	1.37
15	K	1402	CLA	C4C-C3C	2.22	1.48	1.45
15	A	1122	CLA	C1C-C2C	2.22	1.48	1.44
15	A	1012	CLA	C1C-C2C	2.21	1.48	1.44
15	A	1140	CLA	C1C-C2C	2.21	1.48	1.44
15	B	1223	CLA	C1C-NC	-2.20	1.34	1.37
15	B	1213	CLA	C4C-C3C	2.20	1.48	1.45
15	J	1302	CLA	C4C-C3C	2.20	1.48	1.45
15	B	1214	CLA	C1C-NC	-2.20	1.34	1.37
15	A	1125	CLA	CHD-C4C	2.20	1.47	1.41
15	B	1217	CLA	C4C-C3C	2.20	1.48	1.45
15	A	1022	CLA	C1C-C2C	2.20	1.48	1.44
15	A	1129	CLA	C1C-NC	-2.20	1.34	1.37
13	A	1108	CL0	C1C-C2C	2.19	1.48	1.44
15	B	1238	CLA	C4C-C3C	2.19	1.48	1.45
15	A	1107	CLA	C4C-C3C	2.18	1.48	1.45
15	B	1218	CLA	C4C-C3C	2.18	1.48	1.45
15	B	1202	CLA	C4C-C3C	2.18	1.48	1.45
15	B	1230	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1201	CLA	C4C-C3C	2.17	1.48	1.45
15	A	1110	CLA	C4C-C3C	2.17	1.48	1.45
15	A	1130	CLA	C4C-C3C	2.17	1.48	1.45
15	A	1126	CLA	C4C-C3C	2.17	1.48	1.45
14	A	4008	BCR	C30-C25	-2.17	1.50	1.53
15	B	1240	CLA	C1C-C2C	2.17	1.48	1.44
15	B	1021	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1102	CLA	C4C-C3C	2.17	1.48	1.45
15	A	1801	CLA	C4C-C3C	2.16	1.48	1.45
15	B	1221	CLA	C4C-C3C	2.16	1.48	1.45
15	B	1228	CLA	C1C-C2C	2.16	1.48	1.44
15	A	1117	CLA	C4C-C3C	2.15	1.48	1.45
15	B	1213	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1021	CLA	C4C-C3C	2.15	1.48	1.45
15	A	1101	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1108	CL0	C1C-NC	-2.15	1.34	1.37
15	F	1410	CLA	C1C-C2C	2.15	1.48	1.44
15	A	1112	CLA	C4C-C3C	2.15	1.48	1.45
15	A	1112	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1217	CLA	C1C-C2C	2.14	1.48	1.44
15	A	1112	CLA	C1C-NC	-2.14	1.34	1.37
15	B	1227	CLA	C1C-C2C	2.14	1.48	1.44
15	A	1126	CLA	C1C-C2C	2.14	1.48	1.44
15	B	1236	CLA	C1C-NC	-2.13	1.34	1.37
15	B	1229	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1012	CLA	C1C-NC	-2.13	1.34	1.37
15	B	1228	CLA	C4C-C3C	2.13	1.48	1.45
15	B	1225	CLA	C1C-C2C	2.12	1.48	1.44
14	F	4015	BCR	C30-C25	-2.12	1.50	1.53
15	A	1106	CLA	C4C-C3C	2.12	1.48	1.45
15	A	1119	CLA	C1C-C2C	2.12	1.48	1.44
15	B	1219	CLA	C1C-C2C	2.12	1.48	1.44
15	B	1212	CLA	C1C-C2C	2.12	1.48	1.44
15	A	1103	CLA	C4C-C3C	2.11	1.48	1.45
15	F	1410	CLA	C4C-C3C	2.11	1.48	1.45
15	B	1226	CLA	C1C-NC	-2.11	1.34	1.37
15	B	1225	CLA	C4C-C3C	2.11	1.48	1.45
15	B	1221	CLA	C1C-C2C	2.11	1.48	1.44
15	B	1211	CLA	C1C-C2C	2.11	1.48	1.44
15	A	1801	CLA	C1C-C2C	2.11	1.48	1.44
15	B	1212	CLA	C4C-C3C	2.10	1.48	1.45
15	A	1127	CLA	C4C-C3C	2.10	1.48	1.45
15	F	1139	CLA	C4C-C3C	2.10	1.48	1.45
15	B	1234	CLA	C4C-C3C	2.10	1.48	1.45
15	A	1122	CLA	C4C-C3C	2.10	1.48	1.45
15	J	1303	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1237	CLA	C1C-C2C	2.09	1.48	1.44
14	B	4009	BCR	C30-C25	-2.08	1.50	1.53
15	A	1127	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1132	CLA	C4C-C3C	2.08	1.48	1.45
15	A	1107	CLA	C1C-C2C	2.08	1.48	1.44
15	B	1222	CLA	C4C-C3C	2.08	1.48	1.45
15	B	1231	CLA	C4C-C3C	2.08	1.48	1.45
15	A	1022	CLA	C4C-C3C	2.08	1.48	1.45
15	A	1105	CLA	C1C-C2C	2.07	1.48	1.44
15	A	1134	CLA	C1C-C2C	2.07	1.48	1.44
15	B	1214	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1121	CLA	C1C-C2C	2.07	1.48	1.44
15	A	1124	CLA	C1C-C2C	2.06	1.48	1.44
15	B	1201	CLA	C1C-C2C	2.06	1.48	1.44
15	A	1106	CLA	C1C-C2C	2.06	1.48	1.44
15	A	1117	CLA	C1C-C2C	2.05	1.48	1.44
15	B	1218	CLA	C1C-C2C	2.05	1.48	1.44
15	A	1102	CLA	C1C-C2C	2.05	1.48	1.44
15	K	1402	CLA	C1C-C2C	2.04	1.48	1.44
15	J	1302	CLA	C1C-C2C	2.04	1.48	1.44
15	B	1222	CLA	C1C-C2C	2.03	1.48	1.44
15	B	1202	CLA	C1C-C2C	2.03	1.48	1.44
15	A	1128	CLA	C4C-C3C	2.03	1.48	1.45
15	A	1137	CLA	C1C-C2C	2.03	1.48	1.44
13	A	1108	CL0	C4C-C3C	2.03	1.48	1.45
15	B	1226	CLA	C4C-C3C	2.03	1.48	1.45
15	B	1211	CLA	C4C-C3C	2.03	1.48	1.45
15	A	1116	CLA	C1C-C2C	2.02	1.48	1.44
15	A	1132	CLA	C1C-C2C	2.02	1.48	1.44
15	B	1238	CLA	C1C-C2C	2.02	1.48	1.44
15	B	1216	CLA	C1C-C2C	2.02	1.48	1.44
15	B	1232	CLA	C1C-C2C	2.01	1.48	1.44
15	F	1301	CLA	C4C-C3C	2.01	1.48	1.45
15	B	1205	CLA	C4C-C3C	2.01	1.48	1.45
15	B	1224	CLA	C4C-C3C	2.01	1.48	1.45
15	B	1206	CLA	C1C-C2C	2.00	1.48	1.44
15	A	1115	CLA	C4C-C3C	2.00	1.48	1.45

All (1779) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4009	BCR	C16-C17-C18	26.76	165.49	127.31
14	F	4016	BCR	C20-C21-C22	25.34	163.47	127.31
14	B	4006	BCR	C20-C21-C22	23.95	161.49	127.31
14	A	4008	BCR	C20-C21-C22	23.24	160.48	127.31
14	A	4007	BCR	C20-C21-C22	23.24	160.48	127.31
14	B	4014	BCR	C16-C17-C18	23.08	160.24	127.31
14	B	4010	BCR	C20-C21-C22	23.05	160.21	127.31
14	F	4015	BCR	C20-C21-C22	22.19	158.97	127.31
14	A	4008	BCR	C16-C17-C18	22.18	158.97	127.31
14	A	4007	BCR	C16-C17-C18	21.89	158.55	127.31
14	J	4013	BCR	C20-C21-C22	21.86	158.50	127.31
14	F	4015	BCR	C16-C17-C18	21.82	158.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4011	BCR	C16-C17-C18	21.81	158.44	127.31
14	A	4003	BCR	C16-C17-C18	21.27	157.67	127.31
14	B	4010	BCR	C16-C17-C18	21.18	157.54	127.31
14	A	4002	BCR	C20-C21-C22	21.06	157.36	127.31
14	B	4017	BCR	C20-C21-C22	20.96	157.23	127.31
14	A	4002	BCR	C15-C16-C17	20.77	166.01	123.47
14	F	4016	BCR	C16-C17-C18	20.67	156.80	127.31
14	F	4016	BCR	C15-C16-C17	20.66	165.79	123.47
14	B	4005	BCR	C15-C16-C17	20.53	165.52	123.47
14	J	4013	BCR	C16-C17-C18	20.52	156.59	127.31
14	B	4006	BCR	C16-C17-C18	20.44	156.48	127.31
14	B	4005	BCR	C20-C21-C22	20.30	156.28	127.31
14	B	4017	BCR	C15-C16-C17	20.25	164.95	123.47
14	A	4001	BCR	C20-C21-C22	20.21	156.15	127.31
14	A	4012	BCR	C15-C16-C17	20.18	164.81	123.47
14	B	4009	BCR	C20-C21-C22	20.15	156.06	127.31
14	A	4003	BCR	C15-C16-C17	20.05	164.55	123.47
14	B	4004	BCR	C15-C16-C17	20.03	164.51	123.47
14	B	4017	BCR	C16-C17-C18	19.95	155.78	127.31
14	A	4001	BCR	C15-C16-C17	19.77	163.98	123.47
14	A	4003	BCR	C20-C21-C22	19.77	155.53	127.31
14	B	4014	BCR	C20-C21-C22	19.74	155.48	127.31
14	B	4006	BCR	C15-C16-C17	19.72	163.88	123.47
14	B	4004	BCR	C20-C21-C22	19.68	155.40	127.31
14	A	4012	BCR	C16-C17-C18	19.42	155.03	127.31
14	J	4013	BCR	C15-C16-C17	19.42	163.25	123.47
14	A	4001	BCR	C16-C17-C18	19.37	154.96	127.31
14	B	4011	BCR	C15-C16-C17	19.34	163.09	123.47
14	B	4011	BCR	C20-C21-C22	19.33	154.90	127.31
14	A	4007	BCR	C15-C16-C17	19.28	162.96	123.47
14	B	4005	BCR	C16-C17-C18	19.09	154.56	127.31
14	B	4010	BCR	C15-C16-C17	19.05	162.50	123.47
14	A	4002	BCR	C16-C17-C18	18.98	154.39	127.31
14	A	4012	BCR	C20-C21-C22	18.89	154.26	127.31
14	A	4008	BCR	C15-C16-C17	18.81	162.01	123.47
14	B	4014	BCR	C15-C16-C17	18.60	161.57	123.47
14	B	4004	BCR	C16-C17-C18	18.40	153.56	127.31
14	F	4015	BCR	C15-C16-C17	17.76	159.85	123.47
14	F	4015	BCR	C10-C11-C12	17.46	177.72	123.22
14	B	4005	BCR	C10-C11-C12	17.29	177.17	123.22
14	B	4014	BCR	C10-C11-C12	17.27	177.11	123.22
14	J	4013	BCR	C10-C11-C12	17.27	177.10	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4008	BCR	C10-C11-C12	17.20	176.90	123.22
14	B	4017	BCR	C10-C11-C12	17.20	176.89	123.22
14	B	4006	BCR	C10-C11-C12	17.18	176.83	123.22
14	A	4002	BCR	C10-C11-C12	17.12	176.64	123.22
14	B	4011	BCR	C11-C10-C9	17.11	151.74	127.31
14	A	4007	BCR	C10-C11-C12	16.95	176.12	123.22
14	B	4010	BCR	C10-C11-C12	16.92	176.01	123.22
14	B	4004	BCR	C10-C11-C12	16.77	175.56	123.22
14	F	4016	BCR	C10-C11-C12	16.69	175.29	123.22
14	A	4003	BCR	C10-C11-C12	16.58	174.95	123.22
14	B	4009	BCR	C16-C15-C14	16.51	157.29	123.47
14	B	4009	BCR	C15-C16-C17	15.93	156.10	123.47
14	B	4011	BCR	C10-C11-C12	15.59	171.87	123.22
14	A	4012	BCR	C10-C11-C12	15.32	171.03	123.22
14	B	4009	BCR	C10-C11-C12	15.19	170.63	123.22
14	F	4015	BCR	C16-C15-C14	15.03	154.25	123.47
14	B	4014	BCR	C16-C15-C14	15.02	154.24	123.47
14	A	4001	BCR	C10-C11-C12	14.94	169.83	123.22
14	B	4017	BCR	C11-C10-C9	13.93	147.18	127.31
14	A	4008	BCR	C16-C15-C14	13.91	151.97	123.47
14	B	4004	BCR	C21-C20-C19	13.76	166.17	123.22
14	B	4014	BCR	C11-C10-C9	13.62	146.75	127.31
14	J	4013	BCR	C16-C15-C14	13.62	151.38	123.47
14	B	4010	BCR	C16-C15-C14	13.61	151.35	123.47
14	A	4001	BCR	C21-C20-C19	13.59	165.64	123.22
14	A	4003	BCR	C16-C15-C14	13.54	151.22	123.47
14	B	4004	BCR	C16-C15-C14	13.49	151.10	123.47
14	A	4012	BCR	C21-C20-C19	13.45	165.18	123.22
14	B	4014	BCR	C21-C20-C19	13.36	164.92	123.22
14	A	4007	BCR	C16-C15-C14	13.33	150.78	123.47
14	B	4006	BCR	C11-C10-C9	13.32	146.32	127.31
14	A	4003	BCR	C21-C20-C19	13.32	164.79	123.22
14	B	4010	BCR	C11-C10-C9	13.32	146.32	127.31
14	B	4005	BCR	C21-C20-C19	13.29	164.70	123.22
14	A	4008	BCR	C11-C10-C9	13.24	146.20	127.31
14	B	4009	BCR	C21-C20-C19	13.17	164.32	123.22
14	B	4017	BCR	C21-C20-C19	13.13	164.19	123.22
14	A	4001	BCR	C16-C15-C14	13.13	150.36	123.47
14	B	4011	BCR	C16-C15-C14	13.09	150.29	123.47
14	J	4013	BCR	C11-C10-C9	13.07	145.96	127.31
14	A	4007	BCR	C11-C10-C9	13.06	145.94	127.31
14	A	4002	BCR	C21-C20-C19	12.98	163.73	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4017	BCR	C16-C15-C14	12.91	149.93	123.47
14	B	4005	BCR	C11-C10-C9	12.80	145.57	127.31
14	B	4011	BCR	C21-C20-C19	12.65	162.71	123.22
14	A	4002	BCR	C11-C10-C9	12.56	145.23	127.31
14	B	4006	BCR	C16-C15-C14	12.53	149.13	123.47
14	B	4004	BCR	C11-C10-C9	12.52	145.18	127.31
14	F	4016	BCR	C21-C20-C19	12.52	162.28	123.22
14	B	4005	BCR	C16-C15-C14	12.41	148.90	123.47
14	F	4015	BCR	C21-C20-C19	12.40	161.92	123.22
14	B	4011	BCR	C11-C12-C13	12.32	161.04	126.42
14	A	4008	BCR	C21-C20-C19	12.27	161.50	123.22
14	F	4016	BCR	C16-C15-C14	12.19	148.45	123.47
14	A	4007	BCR	C21-C20-C19	12.14	161.09	123.22
14	B	4010	BCR	C21-C20-C19	12.10	160.97	123.22
14	F	4015	BCR	C11-C10-C9	12.03	144.48	127.31
14	A	4012	BCR	C16-C15-C14	12.00	148.06	123.47
14	B	4006	BCR	C21-C20-C19	11.94	160.47	123.22
14	A	4002	BCR	C16-C15-C14	11.90	147.85	123.47
14	J	4013	BCR	C21-C20-C19	11.72	159.80	123.22
14	F	4016	BCR	C11-C10-C9	11.58	143.84	127.31
14	B	4009	BCR	C11-C10-C9	11.57	143.82	127.31
14	A	4003	BCR	C11-C10-C9	11.50	143.73	127.31
14	A	4002	BCR	C11-C12-C13	11.48	158.66	126.42
14	A	4007	BCR	C11-C12-C13	11.33	158.23	126.42
14	B	4005	BCR	C11-C12-C13	11.10	157.59	126.42
14	J	4013	BCR	C11-C12-C13	10.97	157.25	126.42
14	A	4008	BCR	C11-C12-C13	10.97	157.22	126.42
14	F	4015	BCR	C11-C12-C13	10.91	157.06	126.42
14	A	4012	BCR	C11-C12-C13	10.89	157.01	126.42
14	B	4010	BCR	C11-C12-C13	10.84	156.85	126.42
14	B	4006	BCR	C11-C12-C13	10.83	156.85	126.42
14	B	4004	BCR	C11-C12-C13	10.73	156.54	126.42
14	A	4012	BCR	C11-C10-C9	10.60	142.44	127.31
14	B	4017	BCR	C11-C12-C13	10.53	155.99	126.42
14	A	4003	BCR	C11-C12-C13	10.50	155.91	126.42
14	A	4001	BCR	C11-C10-C9	10.42	142.18	127.31
14	B	4014	BCR	C11-C12-C13	10.38	155.58	126.42
14	A	4001	BCR	C11-C12-C13	9.64	153.49	126.42
14	B	4009	BCR	C11-C12-C13	9.51	153.13	126.42
14	F	4016	BCR	C11-C12-C13	8.85	151.27	126.42
14	F	4016	BCR	C20-C19-C18	8.60	150.57	126.42
14	A	4007	BCR	C20-C19-C18	8.60	150.57	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4008	BCR	C20-C19-C18	8.50	150.30	126.42
14	B	4010	BCR	C20-C19-C18	8.49	150.28	126.42
14	B	4006	BCR	C20-C19-C18	8.02	148.96	126.42
14	J	4013	BCR	C20-C19-C18	7.99	148.86	126.42
14	B	4011	BCR	C20-C19-C18	7.93	148.69	126.42
14	F	4015	BCR	C20-C19-C18	7.57	147.67	126.42
14	B	4014	BCR	C20-C19-C18	7.32	146.97	126.42
15	B	1215	CLA	C2C-C1C-NC	6.92	116.45	109.97
15	B	1239	CLA	C2C-C1C-NC	6.91	116.45	109.97
14	A	4003	BCR	C20-C19-C18	6.89	145.77	126.42
15	B	1221	CLA	C4A-NA-C1A	6.87	109.79	106.71
13	A	1011	CL0	C2C-C1C-NC	6.84	116.38	109.97
15	A	1136	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	A	1135	CLA	C2C-C1C-NC	6.80	116.35	109.97
15	B	1222	CLA	O2D-CGD-CBD	6.80	123.35	111.27
15	B	1207	CLA	C2C-C1C-NC	6.79	116.33	109.97
15	B	1203	CLA	C2C-C1C-NC	6.78	116.33	109.97
15	A	1131	CLA	C2C-C1C-NC	6.78	116.32	109.97
15	A	1128	CLA	C2C-C1C-NC	6.75	116.30	109.97
15	A	1123	CLA	C2C-C1C-NC	6.72	116.27	109.97
15	A	1136	CLA	C2C-C1C-NC	6.71	116.26	109.97
15	B	1205	CLA	O2D-CGD-CBD	6.70	123.18	111.27
15	A	1137	CLA	C2C-C1C-NC	6.69	116.24	109.97
14	B	4009	BCR	C20-C19-C18	6.68	145.19	126.42
14	B	4017	BCR	C20-C19-C18	6.68	145.18	126.42
15	B	1231	CLA	C2C-C1C-NC	6.68	116.23	109.97
14	A	4002	BCR	C20-C19-C18	6.67	145.15	126.42
15	A	1801	CLA	C2C-C1C-NC	6.66	116.21	109.97
15	A	1133	CLA	C2C-C1C-NC	6.66	116.21	109.97
15	B	1222	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	B	1232	CLA	C2C-C1C-NC	6.66	116.21	109.97
15	B	1021	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	A	4012	BCR	C20-C19-C18	6.65	145.10	126.42
14	B	4005	BCR	C20-C19-C18	6.65	145.09	126.42
15	B	1226	CLA	O2D-CGD-CBD	6.65	123.08	111.27
15	J	1302	CLA	C2C-C1C-NC	6.65	116.20	109.97
15	B	1209	CLA	C2C-C1C-NC	6.62	116.17	109.97
15	B	1205	CLA	C4A-NA-C1A	6.62	109.68	106.71
15	B	1229	CLA	C4A-NA-C1A	6.62	109.68	106.71
15	A	1118	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	A	1011	CL0	C4A-NA-C1A	6.60	109.67	106.71
15	A	1120	CLA	C2C-C1C-NC	6.59	116.15	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1221	CLA	C2C-C1C-NC	6.59	116.14	109.97
15	A	1113	CLA	C2C-C1C-NC	6.58	116.14	109.97
15	A	1105	CLA	C2C-C1C-NC	6.57	116.13	109.97
15	B	1227	CLA	C2C-C1C-NC	6.57	116.13	109.97
15	B	1205	CLA	C2C-C1C-NC	6.57	116.12	109.97
15	A	1012	CLA	C2C-C1C-NC	6.55	116.10	109.97
15	B	1204	CLA	C2C-C1C-NC	6.53	116.09	109.97
15	J	1303	CLA	C2C-C1C-NC	6.52	116.08	109.97
14	A	4001	BCR	C20-C19-C18	6.49	144.66	126.42
15	B	1222	CLA	C2C-C1C-NC	6.49	116.05	109.97
15	A	1110	CLA	C2C-C1C-NC	6.48	116.05	109.97
15	B	1225	CLA	C2C-C1C-NC	6.48	116.04	109.97
15	A	1114	CLA	C2C-C1C-NC	6.47	116.04	109.97
15	B	1226	CLA	C2C-C1C-NC	6.47	116.04	109.97
15	B	1203	CLA	C4A-NA-C1A	6.47	109.61	106.71
15	A	1116	CLA	C2C-C1C-NC	6.46	116.03	109.97
15	A	1127	CLA	C2C-C1C-NC	6.46	116.03	109.97
15	K	1402	CLA	C2C-C1C-NC	6.46	116.02	109.97
15	B	1238	CLA	C2C-C1C-NC	6.46	116.02	109.97
15	A	1106	CLA	O2D-CGD-CBD	6.44	122.71	111.27
15	A	1121	CLA	C2C-C1C-NC	6.44	116.00	109.97
15	A	1129	CLA	C2C-C1C-NC	6.42	115.99	109.97
15	B	1234	CLA	C2C-C1C-NC	6.41	115.98	109.97
15	A	1801	CLA	C4A-NA-C1A	6.40	109.58	106.71
15	K	1401	CLA	C2C-C1C-NC	6.39	115.96	109.97
15	A	1118	CLA	C2C-C1C-NC	6.38	115.95	109.97
15	A	1124	CLA	C2C-C1C-NC	6.37	115.94	109.97
15	B	1206	CLA	C2C-C1C-NC	6.37	115.94	109.97
15	B	1239	CLA	C4A-NA-C1A	6.35	109.56	106.71
15	A	1022	CLA	C2C-C1C-NC	6.35	115.92	109.97
15	A	1012	CLA	C4A-NA-C1A	6.34	109.56	106.71
15	B	1229	CLA	C2C-C1C-NC	6.33	115.90	109.97
15	B	1217	CLA	C2C-C1C-NC	6.32	115.89	109.97
15	B	1212	CLA	C2C-C1C-NC	6.32	115.89	109.97
15	B	1201	CLA	C2C-C1C-NC	6.30	115.88	109.97
15	B	1216	CLA	C2C-C1C-NC	6.30	115.88	109.97
15	B	1224	CLA	C2C-C1C-NC	6.30	115.88	109.97
14	B	4004	BCR	C20-C19-C18	6.30	144.12	126.42
15	B	1219	CLA	C2C-C1C-NC	6.30	115.87	109.97
15	A	1128	CLA	O2D-CGD-CBD	6.30	122.46	111.27
15	B	1218	CLA	C2C-C1C-NC	6.29	115.87	109.97
13	A	1108	CL0	C2C-C1C-NC	6.29	115.87	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	1139	CLA	C2C-C1C-NC	6.29	115.86	109.97
15	B	1237	CLA	C2C-C1C-NC	6.29	115.86	109.97
15	B	1023	CLA	C2C-C1C-NC	6.27	115.85	109.97
15	A	1134	CLA	C2C-C1C-NC	6.27	115.84	109.97
15	F	1410	CLA	C2C-C1C-NC	6.27	115.84	109.97
15	B	1208	CLA	C2C-C1C-NC	6.25	115.83	109.97
15	B	1240	CLA	C2C-C1C-NC	6.24	115.81	109.97
15	B	1021	CLA	C2C-C1C-NC	6.23	115.81	109.97
15	A	1132	CLA	C4A-NA-C1A	6.22	109.50	106.71
15	B	1202	CLA	C2C-C1C-NC	6.21	115.79	109.97
15	B	1234	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	A	1108	CL0	C4A-NA-C1A	6.20	109.49	106.71
15	K	1402	CLA	C4A-NA-C1A	6.19	109.49	106.71
15	A	1119	CLA	C2C-C1C-NC	6.19	115.77	109.97
15	A	1112	CLA	C2C-C1C-NC	6.18	115.76	109.97
15	A	1123	CLA	O2D-CGD-CBD	6.18	122.25	111.27
15	B	1230	CLA	C2C-C1C-NC	6.18	115.76	109.97
15	A	1132	CLA	C2C-C1C-NC	6.18	115.76	109.97
15	A	1115	CLA	C4A-NA-C1A	6.17	109.48	106.71
15	B	1226	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	B	4009	BCR	C15-C14-C13	-6.15	118.53	127.31
15	B	1235	CLA	C4A-NA-C1A	6.14	109.47	106.71
15	A	1102	CLA	C2C-C1C-NC	6.14	115.72	109.97
15	B	1201	CLA	O2D-CGD-CBD	6.14	122.17	111.27
15	B	1013	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	B	1213	CLA	C2C-C1C-NC	6.12	115.70	109.97
15	A	1106	CLA	C2C-C1C-NC	6.12	115.70	109.97
15	F	1139	CLA	C4A-NA-C1A	6.12	109.46	106.71
15	A	1123	CLA	C4A-NA-C1A	6.11	109.45	106.71
15	A	1101	CLA	O2D-CGD-CBD	6.10	122.10	111.27
15	B	1231	CLA	C4A-NA-C1A	6.08	109.44	106.71
15	A	1128	CLA	C4A-NA-C1A	6.08	109.44	106.71
15	F	1301	CLA	C2C-C1C-NC	6.07	115.66	109.97
15	B	1201	CLA	C4A-NA-C1A	6.05	109.43	106.71
15	A	1115	CLA	C2C-C1C-NC	6.05	115.64	109.97
15	B	1223	CLA	C2C-C1C-NC	6.05	115.64	109.97
15	A	1120	CLA	C4A-NA-C1A	6.02	109.41	106.71
15	B	1214	CLA	C2C-C1C-NC	6.01	115.60	109.97
15	A	1125	CLA	O2D-CGD-CBD	6.01	121.94	111.27
15	B	1209	CLA	C4A-NA-C1A	6.00	109.40	106.71
15	A	1140	CLA	C4A-NA-C1A	5.99	109.40	106.71
15	A	1117	CLA	C2C-C1C-NC	5.99	115.58	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1211	CLA	C2C-C1C-NC	5.99	115.58	109.97
15	A	1137	CLA	C4A-NA-C1A	5.98	109.40	106.71
15	A	1104	CLA	C2C-C1C-NC	5.98	115.58	109.97
15	B	1212	CLA	C4A-NA-C1A	5.97	109.39	106.71
15	J	1303	CLA	C4A-NA-C1A	5.97	109.39	106.71
15	B	1023	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	B	1207	CLA	C4A-NA-C1A	5.94	109.38	106.71
15	B	1237	CLA	C4A-NA-C1A	5.94	109.38	106.71
15	B	1227	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	A	1133	CLA	C4A-NA-C1A	5.91	109.36	106.71
15	B	1013	CLA	C2C-C1C-NC	5.90	115.50	109.97
15	B	1230	CLA	C4A-NA-C1A	5.90	109.36	106.71
15	A	1111	CLA	C2C-C1C-NC	5.89	115.49	109.97
15	B	1210	CLA	C2C-C1C-NC	5.89	115.49	109.97
15	B	1232	CLA	C4A-NA-C1A	5.89	109.35	106.71
15	B	1220	CLA	C2C-C1C-NC	5.88	115.48	109.97
15	A	1127	CLA	C4A-NA-C1A	5.88	109.35	106.71
15	A	1106	CLA	C4A-NA-C1A	5.87	109.35	106.71
15	A	1131	CLA	O2D-CGD-CBD	5.87	121.70	111.27
15	B	1204	CLA	C4A-NA-C1A	5.85	109.34	106.71
15	B	1227	CLA	O2D-CGD-CBD	5.85	121.66	111.27
15	B	1202	CLA	C4A-NA-C1A	5.85	109.33	106.71
15	A	1130	CLA	C2C-C1C-NC	5.83	115.43	109.97
15	A	1140	CLA	C2C-C1C-NC	5.83	115.43	109.97
15	A	1101	CLA	C2C-C1C-NC	5.83	115.43	109.97
15	J	1302	CLA	C4A-NA-C1A	5.81	109.32	106.71
15	A	1102	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	B	1211	CLA	O2D-CGD-CBD	5.79	121.55	111.27
15	A	1103	CLA	C2C-C1C-NC	5.78	115.39	109.97
15	B	1218	CLA	C4-C3-C5	5.78	122.60	115.98
15	B	1221	CLA	O2D-CGD-CBD	5.78	121.54	111.27
15	K	1401	CLA	C4A-NA-C1A	5.77	109.30	106.71
15	A	1112	CLA	C4A-NA-C1A	5.76	109.30	106.71
15	B	1235	CLA	C2C-C1C-NC	5.76	115.37	109.97
15	A	1129	CLA	C4A-NA-C1A	5.76	109.30	106.71
15	B	1013	CLA	O2A-C1-C2	5.75	123.76	108.64
15	A	1131	CLA	C4A-NA-C1A	5.75	109.29	106.71
15	A	1132	CLA	O2D-CGD-CBD	5.74	121.46	111.27
15	B	1212	CLA	O2D-CGD-CBD	5.73	121.45	111.27
13	A	1011	CL0	C1C-C2C-C3C	-5.73	100.94	106.96
15	A	1109	CLA	C2C-C1C-NC	5.72	115.33	109.97
15	A	1103	CLA	C4A-NA-C1A	5.72	109.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1126	CLA	C4A-NA-C1A	5.72	109.28	106.71
15	B	1228	CLA	C2C-C1C-NC	5.70	115.31	109.97
15	A	1122	CLA	C2C-C1C-NC	5.69	115.30	109.97
13	A	1011	CL0	O2D-CGD-CBD	5.69	121.38	111.27
13	A	1108	CL0	C4D-C3D-CAD	5.68	111.64	108.47
15	A	1126	CLA	O2D-CGD-CBD	5.68	121.36	111.27
15	A	1104	CLA	C1C-C2C-C3C	-5.67	100.99	106.96
14	B	4011	BCR	C34-C9-C10	-5.67	114.98	122.92
15	A	1102	CLA	O2D-CGD-CBD	5.66	121.32	111.27
15	A	1137	CLA	O2D-CGD-CBD	5.64	121.29	111.27
15	B	1219	CLA	C4A-NA-C1A	5.63	109.24	106.71
15	B	1225	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	A	1107	CLA	C2C-C1C-NC	5.61	115.23	109.97
15	A	1111	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	B	1224	CLA	O2D-CGD-CBD	5.61	121.24	111.27
15	A	1118	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
15	B	1210	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	B	1223	CLA	C4A-NA-C1A	5.60	109.22	106.71
15	B	1211	CLA	C4A-NA-C1A	5.59	109.22	106.71
15	A	1134	CLA	C4A-NA-C1A	5.59	109.22	106.71
15	B	1240	CLA	C4A-NA-C1A	5.58	109.21	106.71
15	A	1135	CLA	C4A-NA-C1A	5.57	109.21	106.71
15	A	1121	CLA	C4A-NA-C1A	5.57	109.21	106.71
15	B	1231	CLA	C1C-C2C-C3C	-5.57	101.10	106.96
15	B	1217	CLA	C4A-NA-C1A	5.57	109.21	106.71
15	B	1217	CLA	O2D-CGD-CBD	5.56	121.16	111.27
15	A	1125	CLA	C4A-NA-C1A	5.56	109.21	106.71
15	A	1116	CLA	C4A-NA-C1A	5.56	109.20	106.71
15	A	1126	CLA	C4D-C3D-CAD	5.56	111.57	108.47
14	J	4013	BCR	C7-C8-C9	-5.55	117.84	126.23
15	A	1101	CLA	CAA-C2A-C3A	-5.55	97.58	112.78
15	A	1130	CLA	O2D-CGD-CBD	5.54	121.11	111.27
15	A	1103	CLA	C4D-C3D-CAD	5.54	111.56	108.47
15	B	1208	CLA	C4A-NA-C1A	5.54	109.19	106.71
15	B	1203	CLA	C1C-C2C-C3C	-5.53	101.15	106.96
15	F	1139	CLA	C4D-C3D-CAD	5.53	111.55	108.47
15	A	1012	CLA	O2A-C1-C2	5.52	123.15	108.64
15	B	1215	CLA	O2A-C1-C2	5.52	123.14	108.64
15	B	1215	CLA	C1C-C2C-C3C	-5.52	101.16	106.96
15	A	1125	CLA	C4D-C3D-CAD	5.52	111.55	108.47
15	B	1218	CLA	C4A-NA-C1A	5.51	109.18	106.71
15	B	1236	CLA	C2C-C1C-NC	5.51	115.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1109	CLA	C4A-NA-C1A	5.50	109.18	106.71
15	B	1232	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
15	A	1104	CLA	C4A-NA-C1A	5.49	109.18	106.71
15	A	1116	CLA	O2D-CGD-CBD	5.49	121.03	111.27
15	A	1101	CLA	C4A-NA-C1A	5.49	109.17	106.71
15	A	1135	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
15	B	1229	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
15	B	1209	CLA	O2D-CGD-CBD	5.46	120.98	111.27
15	B	1239	CLA	C1C-C2C-C3C	-5.46	101.21	106.96
15	A	1105	CLA	O2D-CGD-CBD	5.46	120.97	111.27
15	B	1235	CLA	O2D-CGD-CBD	5.46	120.97	111.27
15	B	1013	CLA	O2A-CGA-O1A	-5.45	109.84	123.59
15	F	1301	CLA	C4A-NA-C1A	5.45	109.15	106.71
15	B	1234	CLA	O2D-CGD-CBD	5.44	120.94	111.27
15	A	1131	CLA	C1C-C2C-C3C	-5.44	101.23	106.96
15	B	1226	CLA	C1C-C2C-C3C	-5.44	101.23	106.96
15	B	1219	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
15	F	1410	CLA	O2D-CGD-CBD	5.44	120.93	111.27
15	A	1801	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
15	B	1202	CLA	O2D-CGD-CBD	5.44	120.93	111.27
15	B	1207	CLA	C1C-C2C-C3C	-5.43	101.25	106.96
15	A	1125	CLA	C2C-C1C-NC	5.42	115.05	109.97
13	A	1108	CL0	C1C-C2C-C3C	-5.42	101.25	106.96
15	B	1227	CLA	C1C-C2C-C3C	-5.42	101.25	106.96
15	B	1224	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
15	A	1124	CLA	C4A-NA-C1A	5.42	109.14	106.71
15	J	1302	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
15	A	1126	CLA	C2C-C1C-NC	5.42	115.05	109.97
15	A	1114	CLA	C4A-NA-C1A	5.42	109.14	106.71
15	B	1215	CLA	C4A-NA-C1A	5.41	109.14	106.71
15	A	1133	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
15	A	1113	CLA	C4A-NA-C1A	5.41	109.14	106.71
15	B	1230	CLA	C4-C3-C5	5.41	124.37	115.27
15	A	1128	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
15	B	1204	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
15	A	1801	CLA	C4D-C3D-CAD	5.40	111.48	108.47
15	B	1206	CLA	C4A-NA-C1A	5.39	109.13	106.71
15	A	1119	CLA	O2A-CGA-O1A	-5.39	109.98	123.59
15	B	1222	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
15	B	1236	CLA	O2D-CGD-CBD	5.39	120.84	111.27
15	B	1214	CLA	O2D-CGD-CBD	5.39	120.84	111.27
15	A	1022	CLA	C1C-C2C-C3C	-5.39	101.30	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1221	CLA	O2A-CGA-O1A	-5.38	110.00	123.59
15	A	1105	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	A	1120	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	B	1238	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	B	1205	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	B	1205	CLA	O2A-CGA-O1A	-5.38	110.02	123.59
15	B	1213	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	B	1215	CLA	O2D-CGD-CBD	5.38	120.82	111.27
15	A	1118	CLA	O2D-CGD-CBD	5.37	120.81	111.27
15	A	1105	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	B	1238	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	A	1106	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
15	A	1136	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
15	A	1112	CLA	O2D-CGD-CBD	5.36	120.80	111.27
15	A	1114	CLA	O2D-CGD-CBD	5.36	120.79	111.27
15	A	1137	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
15	B	1230	CLA	O2D-CGD-CBD	5.35	120.78	111.27
15	A	1120	CLA	C4D-C3D-CAD	5.35	111.45	108.47
15	B	1221	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
15	A	1129	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
15	B	1235	CLA	O2A-CGA-O1A	-5.34	110.11	123.59
15	F	1139	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
15	B	1203	CLA	O2A-C1-C2	5.33	122.65	108.64
15	B	1208	CLA	C1C-C2C-C3C	-5.33	101.36	106.96
15	A	1127	CLA	C1C-C2C-C3C	-5.33	101.36	106.96
15	A	1136	CLA	O2D-CGD-CBD	5.32	120.72	111.27
15	B	1206	CLA	C4D-C3D-CAD	5.32	111.44	108.47
15	F	1410	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	B	1224	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	A	1124	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
15	B	1218	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
15	B	1223	CLA	O2D-CGD-CBD	5.32	120.72	111.27
15	B	1212	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
15	B	1021	CLA	C4D-C3D-CAD	5.32	111.44	108.47
15	B	1225	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
15	B	1202	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
15	K	1402	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
15	B	1213	CLA	C4A-NA-C1A	5.30	109.09	106.71
15	B	1239	CLA	O2D-CGD-CBD	5.30	120.68	111.27
15	A	1138	CLA	C4A-NA-C1A	5.29	109.09	106.71
15	A	1110	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
15	B	1236	CLA	C1C-C2C-C3C	-5.28	101.41	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1136	CLA	O2A-CGA-O1A	-5.28	110.28	123.59
15	B	1201	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
15	A	1127	CLA	C4D-C3D-CAD	5.27	111.41	108.47
15	F	1410	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
15	A	1109	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
15	B	1206	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
15	A	1132	CLA	O2A-CGA-O1A	-5.26	110.31	123.59
15	A	1113	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
15	A	1123	CLA	C4D-C3D-CAD	5.26	111.40	108.47
15	B	1217	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
15	A	1121	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
15	B	1209	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
15	B	1021	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
15	B	1218	CLA	O2D-CGD-CBD	5.25	120.60	111.27
15	A	1114	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
15	B	1216	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
15	A	1101	CLA	C4D-C3D-CAD	5.25	111.39	108.47
15	B	1013	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
15	B	1219	CLA	O2D-CGD-CBD	5.23	120.56	111.27
15	B	1235	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
15	B	1237	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
15	B	1207	CLA	O2D-CGD-CBD	5.23	120.55	111.27
15	A	1116	CLA	C1C-C2C-C3C	-5.22	101.46	106.96
15	A	1140	CLA	O2D-CGD-CBD	5.22	120.55	111.27
15	A	1801	CLA	O2A-CGA-O1A	-5.22	110.41	123.59
15	A	1129	CLA	O2D-CGD-CBD	5.22	120.54	111.27
15	B	1218	CLA	C4D-C3D-CAD	5.21	111.38	108.47
15	F	1301	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
15	B	1234	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
15	B	1230	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
15	B	1213	CLA	O2D-CGD-CBD	5.20	120.51	111.27
15	J	1303	CLA	C4D-C3D-CAD	5.20	111.37	108.47
15	A	1119	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
15	B	1202	CLA	O2A-CGA-O1A	-5.20	110.48	123.59
15	B	1214	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
15	A	1107	CLA	O2D-CGD-CBD	5.20	120.50	111.27
15	B	1210	CLA	O2A-CGA-O1A	-5.19	110.49	123.59
15	A	1102	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
14	B	4017	BCR	C24-C23-C22	-5.19	118.39	126.23
15	B	1239	CLA	C4D-C3D-CAD	5.19	111.36	108.47
15	B	1223	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
14	F	4016	BCR	C38-C26-C25	-5.19	118.70	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1012	CLA	O2D-CGD-CBD	5.19	120.48	111.27
15	A	1112	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
15	A	1129	CLA	C4D-C3D-CAD	5.18	111.36	108.47
15	K	1401	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
15	B	1231	CLA	O2A-CGA-O1A	-5.17	110.55	123.59
15	A	1134	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
15	B	1237	CLA	C4D-C3D-CAD	5.16	111.35	108.47
15	J	1303	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
15	A	1123	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
15	A	1117	CLA	C4A-NA-C1A	5.15	109.02	106.71
15	A	1012	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
15	A	1121	CLA	C4D-C3D-CAD	5.13	111.33	108.47
15	F	1410	CLA	C4-C3-C5	5.13	123.90	115.27
15	A	1102	CLA	O2A-CGA-O1A	-5.12	110.67	123.59
15	B	1240	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
15	A	1130	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
15	A	1116	CLA	C4D-C3D-CAD	5.11	111.32	108.47
15	A	1107	CLA	C4D-C3D-CAD	5.10	111.31	108.47
15	B	1023	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
15	B	1211	CLA	C1C-C2C-C3C	-5.09	101.60	106.96
15	A	1103	CLA	O2D-CGD-CBD	5.09	120.31	111.27
15	A	1131	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
15	A	1122	CLA	C4D-C3D-CAD	5.09	111.31	108.47
15	A	1111	CLA	O2A-CGA-O1A	-5.09	110.76	123.59
15	A	1122	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
15	B	1220	CLA	O2A-C1-C2	5.08	121.99	108.64
15	B	1230	CLA	O2A-CGA-O1A	-5.08	110.77	123.59
15	B	1220	CLA	C1C-C2C-C3C	-5.07	101.62	106.96
15	A	1115	CLA	O2D-CGD-CBD	5.07	120.27	111.27
15	A	1135	CLA	O2A-CGA-O1A	-5.07	110.81	123.59
15	J	1302	CLA	C4D-C3D-CAD	5.06	111.29	108.47
15	B	1209	CLA	C4D-C3D-CAD	5.06	111.29	108.47
15	B	1021	CLA	O2A-CGA-O1A	-5.06	110.83	123.59
15	A	1135	CLA	O2A-C1-C2	5.06	121.93	108.64
15	A	1133	CLA	O2D-CGD-CBD	5.06	120.26	111.27
15	A	1132	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
15	B	1204	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	A	1140	CLA	C1C-C2C-C3C	-5.05	101.64	106.96
15	A	1124	CLA	O2A-C1-C2	5.05	121.92	108.64
15	A	1103	CLA	C1C-C2C-C3C	-5.05	101.65	106.96
14	A	4012	BCR	C38-C26-C25	-5.05	118.86	124.53
15	F	1301	CLA	O2D-CGD-CBD	5.04	120.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1117	CLA	C1C-C2C-C3C	-5.04	101.65	106.96
15	A	1022	CLA	O2D-CGD-CBD	5.04	120.22	111.27
14	A	4001	BCR	C7-C8-C9	-5.03	118.63	126.23
15	A	1105	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
15	B	1218	CLA	O2A-C1-C2	5.03	121.86	108.64
15	B	1229	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	B	1205	CLA	C4D-C3D-CAD	5.03	111.27	108.47
15	A	1104	CLA	O2A-CGA-O1A	-5.03	110.91	123.59
15	A	1104	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	A	1107	CLA	O2A-CGA-O1A	-5.02	110.92	123.59
15	A	1128	CLA	C4D-C3D-CAD	5.02	111.27	108.47
15	A	1127	CLA	O2A-C1-C2	5.02	121.82	108.64
15	A	1109	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
15	K	1401	CLA	C4D-C3D-CAD	5.01	111.26	108.47
15	B	1218	CLA	O2A-CGA-O1A	-5.01	110.96	123.59
15	A	1109	CLA	C4D-C3D-CAD	5.00	111.26	108.47
15	A	1105	CLA	O2A-C1-C2	4.99	121.75	108.64
14	B	4006	BCR	C38-C26-C25	-4.99	118.92	124.53
15	B	1226	CLA	O2A-CGA-O1A	-4.99	111.00	123.59
15	A	1110	CLA	C4A-NA-C1A	4.99	108.95	106.71
15	B	1214	CLA	O2A-CGA-O1A	-4.98	111.01	123.59
15	A	1121	CLA	O2D-CGD-CBD	4.98	120.11	111.27
15	A	1109	CLA	C4-C3-C5	4.97	123.63	115.27
15	A	1111	CLA	O2D-CGD-CBD	4.96	120.09	111.27
15	A	1022	CLA	C4A-NA-C1A	4.96	108.94	106.71
15	A	1123	CLA	O2A-CGA-O1A	-4.95	111.09	123.59
15	J	1303	CLA	O2D-CGD-CBD	4.95	120.06	111.27
15	A	1134	CLA	C4D-C3D-CAD	4.94	111.23	108.47
15	A	1101	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
15	B	1237	CLA	O2D-CGD-CBD	4.94	120.05	111.27
15	B	1228	CLA	C1C-C2C-C3C	-4.93	101.77	106.96
15	B	1225	CLA	O2D-CGD-CBD	4.92	120.01	111.27
15	A	1022	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
15	B	1204	CLA	C4D-C3D-CAD	4.92	111.21	108.47
15	A	1119	CLA	C4A-NA-C1A	4.91	108.92	106.71
15	K	1401	CLA	O2D-CGD-CBD	4.91	119.99	111.27
15	A	1130	CLA	O2A-CGA-O1A	-4.91	111.20	123.59
15	B	1228	CLA	C4A-NA-C1A	4.91	108.91	106.71
15	A	1122	CLA	O2D-CGD-CBD	4.90	119.98	111.27
14	A	4003	BCR	C7-C8-C9	-4.90	118.83	126.23
15	A	1119	CLA	O2D-CGD-CBD	4.90	119.97	111.27
15	A	1110	CLA	O2A-C1-C2	4.89	121.49	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1137	CLA	C4D-C3D-CAD	4.89	111.20	108.47
15	B	1219	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
13	A	1011	CL0	O2A-CGA-O1A	-4.88	111.27	123.59
15	B	1225	CLA	C4-C3-C5	4.88	123.49	115.27
15	B	1210	CLA	O2D-CGD-CBD	4.88	119.94	111.27
15	B	1217	CLA	O2A-CGA-O1A	-4.88	111.28	123.59
15	A	1126	CLA	C1C-C2C-C3C	-4.87	101.83	106.96
15	A	1138	CLA	C2C-C1C-NC	4.87	114.53	109.97
15	A	1110	CLA	O2A-CGA-O1A	-4.86	111.32	123.59
15	A	1140	CLA	O2A-CGA-O1A	-4.86	111.33	123.59
15	B	1231	CLA	O2A-C1-C2	4.86	121.41	108.64
15	A	1111	CLA	C1C-C2C-C3C	-4.86	101.85	106.96
15	B	1234	CLA	O2A-C1-C2	4.86	121.40	108.64
15	B	1238	CLA	O2D-CGD-CBD	4.86	119.90	111.27
15	J	1302	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	B	1236	CLA	O2A-CGA-O1A	-4.85	111.34	123.59
15	A	1137	CLA	O2A-CGA-O1A	-4.85	111.35	123.59
15	B	1216	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	A	1109	CLA	O2A-C1-C2	4.85	121.37	108.64
15	A	1120	CLA	O2A-C1-C2	4.84	120.29	108.97
15	A	1124	CLA	C4D-C3D-CAD	4.84	111.17	108.47
15	A	1117	CLA	O2D-CGD-CBD	4.84	119.87	111.27
15	B	1224	CLA	C4D-C3D-CAD	4.84	111.17	108.47
15	B	1220	CLA	O2D-CGD-CBD	4.84	119.86	111.27
15	B	1215	CLA	C4-C3-C5	4.83	123.40	115.27
15	A	1127	CLA	O2D-CGD-CBD	4.83	119.85	111.27
15	A	1115	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
15	B	1203	CLA	C4D-C3D-CAD	4.83	111.16	108.47
15	B	1208	CLA	O2D-CGD-CBD	4.83	119.84	111.27
15	K	1402	CLA	C4D-C3D-CAD	4.82	111.16	108.47
15	B	1220	CLA	O2A-CGA-O1A	-4.82	111.42	123.59
15	B	1228	CLA	O2A-CGA-O1A	-4.82	111.42	123.59
15	A	1136	CLA	C4D-C3D-CAD	4.82	111.16	108.47
15	B	1202	CLA	C4D-C3D-CAD	4.82	111.16	108.47
15	B	1230	CLA	C4D-C3D-CAD	4.81	111.16	108.47
15	A	1112	CLA	C4D-C3D-CAD	4.81	111.15	108.47
15	A	1140	CLA	C4D-C3D-CAD	4.81	111.15	108.47
15	A	1122	CLA	C4A-NA-C1A	4.81	108.87	106.71
15	A	1119	CLA	O2A-C1-C2	4.81	120.21	108.97
15	A	1107	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
15	A	1117	CLA	O2A-C1-C2	4.80	121.24	108.64
15	B	1219	CLA	C4D-C3D-CAD	4.79	111.14	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1128	CLA	O2A-CGA-O1A	-4.79	111.51	123.59
15	B	1203	CLA	O2D-CGD-CBD	4.79	119.77	111.27
15	B	1216	CLA	C4A-NA-C1A	4.78	108.86	106.71
14	A	4003	BCR	C38-C26-C25	-4.78	119.16	124.53
14	A	4008	BCR	C33-C5-C6	-4.78	119.16	124.53
15	B	1227	CLA	C4D-C3D-CAD	4.78	111.14	108.47
15	B	1207	CLA	C4D-C3D-CAD	4.77	111.13	108.47
15	A	1120	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
15	B	1213	CLA	O2A-C1-C2	4.77	121.16	108.64
15	A	1012	CLA	O2A-CGA-O1A	-4.76	111.57	123.59
15	B	1226	CLA	O2A-C1-C2	4.75	121.13	108.64
13	A	1011	CL0	C4D-C3D-CAD	4.75	111.12	108.47
15	B	1219	CLA	O2A-C1-C2	4.74	121.10	108.64
15	A	1122	CLA	O2A-CGA-O1A	-4.74	111.63	123.59
15	F	1139	CLA	O2D-CGD-CBD	4.74	119.69	111.27
15	A	1114	CLA	O2A-CGA-O1A	-4.74	111.64	123.59
15	A	1138	CLA	O2D-CGD-CBD	4.73	119.68	111.27
15	B	1234	CLA	O2A-CGA-O1A	-4.73	111.64	123.59
15	F	1410	CLA	O2A-CGA-O1A	-4.73	111.65	123.59
14	A	4002	BCR	C24-C23-C22	-4.73	119.08	126.23
15	A	1115	CLA	C4D-C3D-CAD	4.73	111.11	108.47
15	B	1210	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
15	B	1217	CLA	C4D-C3D-CAD	4.73	111.11	108.47
15	B	1229	CLA	C4D-C3D-CAD	4.73	111.11	108.47
15	B	1023	CLA	O2A-CGA-O1A	-4.72	111.68	123.59
15	B	1236	CLA	C4D-C3D-CAD	4.72	111.10	108.47
14	J	4013	BCR	C3-C4-C5	-4.72	105.66	114.08
15	A	1120	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	A	1125	CLA	OBD-CAD-C3D	-4.71	120.16	127.98
15	B	1228	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	A	1116	CLA	O2A-CGA-O1A	-4.71	111.71	123.59
15	B	1240	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	A	1113	CLA	O2D-CGD-CBD	4.71	119.63	111.27
15	B	1223	CLA	C4D-C3D-CAD	4.70	111.09	108.47
15	A	1124	CLA	O2D-CGD-CBD	4.70	119.62	111.27
15	A	1107	CLA	C4A-NA-C1A	4.70	108.82	106.71
15	A	1106	CLA	O2A-C1-C2	4.69	120.97	108.64
15	B	1231	CLA	O2D-CGD-CBD	4.69	119.60	111.27
15	B	1215	CLA	O2A-CGA-O1A	-4.69	111.77	123.59
15	B	1214	CLA	C4D-C3D-CAD	4.68	111.08	108.47
15	B	1206	CLA	O2D-CGD-CBD	4.67	119.57	111.27
15	B	1214	CLA	C4A-NA-C1A	4.67	108.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1135	CLA	O2D-CGD-CBD	4.67	119.57	111.27
15	B	1225	CLA	C4D-C3D-CAD	4.67	111.07	108.47
15	A	1114	CLA	O2A-C1-C2	4.67	119.89	108.97
15	A	1110	CLA	O2D-CGD-CBD	4.66	119.55	111.27
14	B	4014	BCR	C7-C8-C9	-4.66	119.19	126.23
15	B	1221	CLA	O2A-CGA-CBA	4.66	126.52	111.91
15	A	1801	CLA	O2D-CGD-CBD	4.65	119.53	111.27
15	A	1114	CLA	C4D-C3D-CAD	4.65	111.06	108.47
15	B	1023	CLA	O2D-CGD-CBD	4.65	119.53	111.27
15	A	1125	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
15	A	1127	CLA	O2A-CGA-O1A	-4.64	111.88	123.59
15	A	1133	CLA	C4D-C3D-CAD	4.64	111.06	108.47
15	B	1224	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
15	B	1237	CLA	O2A-CGA-O1A	-4.64	111.89	123.59
13	A	1011	CL0	O2A-C1-C2	4.64	120.82	108.64
15	B	1226	CLA	C4D-C3D-CAD	4.63	111.05	108.47
15	A	1117	CLA	O2A-CGA-O1A	-4.62	111.92	123.59
15	B	1212	CLA	C4D-C3D-CAD	4.62	111.05	108.47
15	B	1021	CLA	O2D-CGD-CBD	4.61	119.46	111.27
15	A	1131	CLA	O2A-C1-C2	4.60	120.74	108.64
15	B	1223	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
15	F	1301	CLA	C4D-C3D-CAD	4.60	111.03	108.47
15	A	1125	CLA	O2A-CGA-O1A	-4.60	111.99	123.59
14	B	4009	BCR	C24-C23-C22	-4.59	119.30	126.23
14	B	4009	BCR	C7-C8-C9	-4.59	119.30	126.23
12	B	5004	LHG	O7-C7-C8	4.58	121.38	111.50
15	B	1223	CLA	O2A-C1-C2	4.58	120.67	108.64
14	B	4009	BCR	C33-C5-C6	-4.57	119.40	124.53
15	B	1232	CLA	C4D-C3D-CAD	4.56	111.02	108.47
15	A	1138	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
15	A	1136	CLA	O2A-CGA-CBA	4.55	126.17	111.91
14	B	4004	BCR	C33-C5-C6	-4.54	119.43	124.53
15	A	1138	CLA	C4D-C3D-CAD	4.54	111.00	108.47
15	A	1113	CLA	C4D-C3D-CAD	4.53	111.00	108.47
14	B	4014	BCR	C33-C5-C6	-4.53	119.44	124.53
15	B	1225	CLA	O2A-CGA-O1A	-4.53	112.16	123.59
15	A	1111	CLA	O2A-C1-C2	4.53	120.54	108.64
15	K	1402	CLA	O2D-CGD-CBD	4.53	119.31	111.27
15	A	1109	CLA	O2D-CGD-CBD	4.52	119.30	111.27
15	A	1118	CLA	C4D-C3D-CAD	4.52	110.99	108.47
14	F	4015	BCR	C24-C23-C22	-4.51	119.42	126.23
15	A	1126	CLA	O2A-CGA-O1A	-4.51	112.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4008	BCR	C24-C23-C22	-4.50	119.43	126.23
15	A	1132	CLA	C4D-C3D-CAD	4.50	110.98	108.47
12	A	5003	LHG	O7-C7-C8	4.50	121.21	111.50
15	B	1211	CLA	C4D-C3D-CAD	4.50	110.98	108.47
15	B	1229	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
15	A	1122	CLA	C4-C3-C5	4.49	122.83	115.27
15	A	1022	CLA	OBD-CAD-CBD	-4.49	119.48	125.89
15	A	1106	CLA	O2A-CGA-O1A	-4.49	112.27	123.59
14	B	4014	BCR	C24-C23-C22	-4.49	119.46	126.23
14	B	4014	BCR	C38-C26-C25	-4.48	119.49	124.53
15	B	1236	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	B	1213	CLA	C4D-C3D-CAD	4.48	110.97	108.47
15	B	1240	CLA	C4D-C3D-CAD	4.47	110.96	108.47
15	B	1203	CLA	O2A-CGA-O1A	-4.46	112.33	123.59
14	B	4011	BCR	C24-C23-C22	-4.46	119.49	126.23
14	F	4015	BCR	C33-C5-C6	-4.46	119.52	124.53
15	B	1201	CLA	C4D-C3D-CAD	4.46	110.96	108.47
15	A	1131	CLA	O2A-CGA-CBA	4.46	125.89	111.91
15	B	1232	CLA	O2D-CGD-CBD	4.45	119.18	111.27
15	A	1132	CLA	O2A-CGA-CBA	4.45	125.86	111.91
14	A	4012	BCR	C24-C23-C22	-4.44	119.53	126.23
15	B	1213	CLA	O2A-CGA-O1A	-4.44	112.39	123.59
15	B	1220	CLA	C4A-NA-C1A	4.44	108.70	106.71
15	A	1131	CLA	C4D-C3D-CAD	4.43	110.94	108.47
15	A	1111	CLA	C4D-C3D-CAD	4.43	110.94	108.47
15	B	1228	CLA	C4D-C3D-CAD	4.43	110.94	108.47
15	A	1103	CLA	O2A-C1-C2	4.42	120.26	108.64
15	B	1231	CLA	C4D-C3D-CAD	4.42	110.94	108.47
15	B	1222	CLA	O2A-CGA-O1A	-4.42	112.44	123.59
15	A	1125	CLA	O2A-C1-C2	4.41	120.22	108.64
15	B	1224	CLA	O2A-CGA-CBA	4.40	125.72	111.91
15	B	1216	CLA	O2A-CGA-O1A	-4.40	112.48	123.59
15	B	1013	CLA	O2D-CGD-CBD	4.40	119.08	111.27
14	B	4017	BCR	C33-C5-C6	-4.40	119.59	124.53
15	A	1138	CLA	O2A-CGA-O1A	-4.39	112.52	123.59
15	B	1210	CLA	C4D-C3D-CAD	4.39	110.92	108.47
15	A	1119	CLA	C4D-C3D-CAD	4.38	110.92	108.47
15	A	1106	CLA	C4D-C3D-CAD	4.38	110.91	108.47
15	B	1230	CLA	O2A-C1-C2	4.38	120.14	108.64
15	A	1105	CLA	C4D-C3D-CAD	4.37	110.91	108.47
15	F	1410	CLA	C4D-C3D-CAD	4.37	110.91	108.47
15	A	1128	CLA	O2A-C1-C2	4.37	120.12	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1236	CLA	O2A-C1-C2	4.35	120.06	108.64
15	B	1023	CLA	O2A-C1-C2	4.34	120.04	108.64
15	F	1139	CLA	O2A-CGA-O1A	-4.34	112.64	123.59
15	A	1135	CLA	C4D-C3D-CAD	4.33	110.88	108.47
15	A	1022	CLA	OBD-CAD-C3D	-4.32	120.81	127.98
15	A	1130	CLA	O2A-C1-C2	4.31	119.97	108.64
15	B	1222	CLA	C4D-C3D-CAD	4.31	110.87	108.47
15	B	1236	CLA	CMC-C2C-C1C	4.31	131.60	125.04
15	A	1101	CLA	O2A-CGA-O1A	-4.31	112.72	123.59
15	B	1218	CLA	O2A-CGA-CBA	4.30	125.39	111.91
15	B	1023	CLA	C4D-C3D-CAD	4.29	110.86	108.47
15	A	1801	CLA	O2A-CGA-CBA	4.29	125.38	111.91
15	A	1104	CLA	O2A-CGA-CBA	4.29	125.38	111.91
15	A	1022	CLA	O2A-C1-C2	4.28	119.90	108.64
15	B	1215	CLA	C4D-C3D-CAD	4.28	110.86	108.47
15	B	1208	CLA	C4D-C3D-CAD	4.28	110.86	108.47
15	A	1130	CLA	C4D-C3D-CAD	4.28	110.85	108.47
15	B	1221	CLA	C4D-C3D-CAD	4.26	110.84	108.47
15	A	1012	CLA	C4D-C3D-CAD	4.26	110.84	108.47
15	A	1126	CLA	O2A-C1-C2	4.26	119.82	108.64
15	B	1234	CLA	C4D-C3D-CAD	4.26	110.84	108.47
15	B	1021	CLA	O2A-C1-C2	4.26	119.82	108.64
15	A	1111	CLA	O2A-CGA-CBA	4.25	125.23	111.91
15	A	1104	CLA	O2A-C1-C2	4.24	119.79	108.64
15	B	1013	CLA	O2A-CGA-CBA	4.24	125.22	111.91
15	B	1210	CLA	O2A-C1-C2	4.24	119.78	108.64
15	B	1214	CLA	C4-C3-C5	4.23	122.39	115.27
15	A	1137	CLA	O2A-C1-C2	4.23	119.76	108.64
15	B	1230	CLA	O2A-CGA-CBA	4.23	125.19	111.91
15	A	1102	CLA	O2A-C1-C2	4.23	119.75	108.64
15	B	1216	CLA	C4D-C3D-CAD	4.23	110.83	108.47
15	A	1132	CLA	O2A-C1-C2	4.22	119.74	108.64
15	B	1013	CLA	C4D-C3D-CAD	4.22	110.83	108.47
15	F	1410	CLA	O2A-C1-C2	4.22	119.73	108.64
15	A	1119	CLA	O2A-CGA-CBA	4.21	125.11	111.91
15	A	1103	CLA	O2A-CGA-O1A	-4.21	112.98	123.59
14	B	4010	BCR	C33-C5-C6	-4.20	119.81	124.53
14	A	4001	BCR	C33-C5-C6	-4.20	119.81	124.53
15	A	1130	CLA	C4A-NA-C1A	4.19	108.59	106.71
14	A	4003	BCR	C24-C23-C22	-4.18	119.92	126.23
14	B	4004	BCR	C38-C26-C25	-4.17	119.84	124.53
15	A	1012	CLA	OBD-CAD-CBD	-4.17	119.93	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4011	BCR	C33-C5-C6	-4.17	119.84	124.53
15	B	1021	CLA	O2A-CGA-CBA	4.17	125.00	111.91
15	B	1231	CLA	O2A-CGA-CBA	4.16	124.98	111.91
15	B	1210	CLA	O2A-CGA-CBA	4.16	124.96	111.91
15	B	1235	CLA	O2A-CGA-CBA	4.16	124.95	111.91
15	B	1219	CLA	CMB-C2B-C3B	4.15	132.45	124.68
15	A	1117	CLA	C4D-C3D-CAD	4.15	110.78	108.47
15	B	1214	CLA	O2A-CGA-CBA	4.15	124.92	111.91
14	F	4015	BCR	C7-C8-C9	-4.14	119.97	126.23
15	A	1104	CLA	C4D-C3D-CAD	4.13	110.78	108.47
14	B	4017	BCR	C7-C8-C9	-4.13	119.99	126.23
15	B	1220	CLA	C4D-C3D-CAD	4.13	110.77	108.47
15	B	1238	CLA	C4D-C3D-CAD	4.12	110.77	108.47
15	B	1239	CLA	O2A-CGA-O1A	-4.12	110.21	123.14
14	A	4012	BCR	C33-C5-C6	-4.12	119.90	124.53
15	B	1235	CLA	C4D-C3D-CAD	4.12	110.77	108.47
15	A	1102	CLA	O2A-CGA-CBA	4.11	124.81	111.91
15	A	1116	CLA	O2A-CGA-CBA	4.11	124.79	111.91
14	F	4015	BCR	C15-C14-C13	-4.10	121.45	127.31
15	A	1124	CLA	O2A-CGA-O1A	-4.09	113.26	123.59
14	B	4011	BCR	C38-C26-C25	-4.08	119.94	124.53
15	A	1121	CLA	O2A-CGA-O1A	-4.08	110.35	123.14
15	A	1134	CLA	O2D-CGD-CBD	4.08	118.52	111.27
15	A	1120	CLA	O2A-CGA-CBA	4.08	124.71	111.91
15	B	1229	CLA	O2A-C1-C2	4.07	119.32	108.64
15	A	1109	CLA	O2A-CGA-CBA	4.07	124.67	111.91
15	B	1224	CLA	O2A-C1-C2	4.06	119.31	108.64
15	B	1013	CLA	C1-O2A-CGA	4.06	127.10	116.44
15	B	1217	CLA	O2A-CGA-CBA	4.06	124.65	111.91
14	A	4003	BCR	C33-C5-C6	-4.06	119.97	124.53
15	A	1130	CLA	O2A-CGA-CBA	4.05	124.63	111.91
13	A	1108	CL0	CMC-C2C-C1C	4.05	131.21	125.04
12	A	5001	LHG	O7-C7-C8	4.05	120.23	111.50
14	A	4002	BCR	C33-C5-C6	-4.04	119.99	124.53
10	B	2002	PQN	C14-C13-C15	4.04	122.06	115.27
15	A	1116	CLA	O2A-C1-C2	4.04	119.25	108.64
14	B	4011	BCR	C7-C8-C9	-4.03	120.15	126.23
15	A	1101	CLA	O2A-C1-C2	4.02	119.20	108.64
14	B	4006	BCR	C34-C9-C10	-4.02	117.30	122.92
15	A	1110	CLA	C4D-C3D-CAD	4.02	110.71	108.47
14	F	4016	BCR	C33-C5-C6	-4.01	120.02	124.53
14	A	4012	BCR	C37-C22-C21	-4.00	117.31	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4003	BCR	C34-C9-C10	-4.00	117.32	122.92
17	B	5002	LMG	O7-C10-C11	4.00	120.11	111.50
15	A	1107	CLA	O2A-CGA-CBA	3.99	124.42	111.91
15	A	1135	CLA	O2A-CGA-CBA	3.98	124.41	111.91
15	A	1801	CLA	O2A-C1-C2	3.98	119.10	108.64
14	B	4010	BCR	C38-C26-C25	-3.98	120.06	124.53
15	B	1205	CLA	O2A-CGA-CBA	3.98	124.39	111.91
15	B	1202	CLA	O2A-CGA-CBA	3.97	124.35	111.91
14	B	4005	BCR	C33-C5-C6	-3.96	120.08	124.53
15	B	1225	CLA	O2A-C1-C2	3.96	119.04	108.64
15	A	1138	CLA	O2A-C1-C2	3.96	119.04	108.64
15	A	1137	CLA	O2A-CGA-CBA	3.95	124.32	111.91
15	B	1204	CLA	O2A-CGA-O1A	-3.95	110.77	123.14
15	B	1223	CLA	O2A-CGA-CBA	3.92	124.22	111.91
15	B	1205	CLA	O2A-C1-C2	3.92	118.94	108.64
15	B	1219	CLA	O2A-CGA-CBA	3.92	124.20	111.91
15	A	1110	CLA	O2A-CGA-CBA	3.91	124.17	111.91
12	A	5005	LHG	O7-C7-C8	3.90	119.91	111.50
15	J	1303	CLA	O2A-CGA-O1A	-3.90	110.91	123.14
15	B	1226	CLA	O2A-CGA-CBA	3.90	124.15	111.91
14	B	4004	BCR	C19-C18-C17	3.90	124.92	118.94
15	B	1215	CLA	O2A-CGA-CBA	3.90	124.14	111.91
15	A	1115	CLA	O2A-CGA-O1A	-3.89	110.93	123.14
15	A	1117	CLA	O2A-CGA-CBA	3.89	124.10	111.91
15	B	1236	CLA	O2A-CGA-CBA	3.88	124.09	111.91
15	A	1127	CLA	O2A-CGA-CBA	3.88	124.08	111.91
15	B	1234	CLA	O2A-CGA-CBA	3.88	124.08	111.91
15	B	1201	CLA	O2A-CGA-O1A	-3.88	110.99	123.14
15	A	1133	CLA	O2A-CGA-O1A	-3.88	110.99	123.14
15	A	1140	CLA	O2A-CGA-CBA	3.87	124.07	111.91
15	B	1202	CLA	O2A-C1-C2	3.87	118.79	108.64
14	B	4014	BCR	C37-C22-C21	-3.86	117.51	122.92
15	K	1401	CLA	O2A-CGA-O1A	-3.86	111.03	123.14
15	B	1211	CLA	O2A-CGA-O1A	-3.86	111.04	123.14
15	B	1207	CLA	O2A-CGA-O1A	-3.86	111.06	123.14
13	A	1011	CL0	O2A-CGA-CBA	3.85	124.00	111.91
15	A	1118	CLA	O2A-CGA-O1A	-3.85	111.07	123.14
14	A	4001	BCR	C24-C23-C22	-3.85	120.42	126.23
14	B	4011	BCR	C37-C22-C21	-3.85	117.53	122.92
15	B	1228	CLA	CMB-C2B-C3B	3.84	131.87	124.68
14	A	4001	BCR	C36-C18-C17	-3.83	117.56	122.92
15	A	1140	CLA	O2A-C1-C2	3.83	118.69	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1129	CLA	O2A-CGA-O1A	-3.83	111.15	123.14
13	A	1108	CL0	O2D-CGD-CBD	3.82	118.06	111.27
14	A	4001	BCR	C38-C26-C25	-3.82	120.24	124.53
15	K	1402	CLA	O2A-CGA-O1A	-3.81	111.19	123.14
15	F	1139	CLA	O2A-C1-C2	3.81	118.64	108.64
15	B	1228	CLA	O2A-C1-C2	3.80	118.63	108.64
15	A	1114	CLA	O2A-CGA-CBA	3.79	123.80	111.91
15	A	1125	CLA	O2A-CGA-CBA	3.79	123.80	111.91
14	B	4004	BCR	C36-C18-C17	-3.79	117.62	122.92
14	A	4007	BCR	C38-C26-C25	-3.79	120.28	124.53
15	A	1127	CLA	C4-C3-C5	3.77	121.62	115.27
15	B	1220	CLA	O2A-CGA-CBA	3.76	123.72	111.91
15	A	1102	CLA	C4D-C3D-CAD	3.76	110.56	108.47
15	B	1228	CLA	O2A-CGA-CBA	3.76	123.70	111.91
15	B	1023	CLA	O2A-CGA-CBA	3.75	123.69	111.91
14	B	4006	BCR	C33-C5-C6	-3.75	120.32	124.53
14	A	4008	BCR	C7-C8-C9	-3.74	120.58	126.23
15	A	1123	CLA	O2A-C1-C2	3.73	118.45	108.64
14	B	4009	BCR	C34-C9-C10	-3.73	117.69	122.92
15	A	1022	CLA	O2A-CGA-CBA	3.73	123.61	111.91
15	B	1229	CLA	O2A-CGA-CBA	3.72	123.59	111.91
15	B	1235	CLA	O2A-C1-C2	3.72	118.41	108.64
14	B	4005	BCR	C7-C8-C9	-3.70	120.64	126.23
15	B	1237	CLA	O2A-C1-C2	3.70	118.37	108.64
14	A	4008	BCR	C38-C26-C27	3.70	120.73	113.62
15	A	1124	CLA	C1-O2A-CGA	3.70	126.16	116.44
15	B	1220	CLA	CMB-C2B-C3B	3.69	131.59	124.68
15	B	1213	CLA	O2A-CGA-CBA	3.68	123.47	111.91
14	A	4001	BCR	C37-C22-C21	-3.68	117.77	122.92
14	B	4005	BCR	C24-C23-C22	-3.67	120.70	126.23
15	B	1206	CLA	O2A-CGA-O1A	-3.66	111.66	123.14
15	A	1012	CLA	O2A-CGA-CBA	3.66	123.39	111.91
15	A	1134	CLA	O2A-CGA-O1A	-3.66	111.68	123.14
15	A	1123	CLA	O2A-CGA-CBA	3.64	123.34	111.91
15	A	1122	CLA	O2A-C1-C2	3.64	118.21	108.64
15	A	1128	CLA	O2A-CGA-CBA	3.64	123.33	111.91
15	A	1123	CLA	CAC-C3C-C4C	3.63	129.52	124.81
15	A	1106	CLA	O2A-CGA-CBA	3.63	123.30	111.91
15	A	1105	CLA	O2A-CGA-CBA	3.62	123.28	111.91
14	A	4003	BCR	C37-C22-C21	-3.62	117.85	122.92
15	F	1410	CLA	O2A-CGA-CBA	3.60	123.22	111.91
15	A	1138	CLA	CMC-C2C-C1C	3.60	130.52	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	O2A-CGA-CBA	3.59	123.18	111.91
15	B	1208	CLA	CMB-C2B-C3B	3.59	131.39	124.68
15	B	1214	CLA	C4-C3-C2	-3.59	114.48	123.68
15	B	1237	CLA	O2A-CGA-CBA	3.58	123.15	111.91
14	A	4012	BCR	C36-C18-C17	-3.57	117.92	122.92
15	A	1107	CLA	O2A-C1-C2	3.57	118.01	108.64
14	B	4005	BCR	C36-C18-C17	-3.57	117.92	122.92
15	B	1237	CLA	C4-C3-C5	3.56	121.25	115.27
15	A	1022	CLA	C4D-C3D-CAD	3.55	110.45	108.47
14	A	4001	BCR	C19-C18-C17	3.55	124.39	118.94
15	B	1214	CLA	O2A-C1-C2	3.55	117.95	108.64
15	A	1126	CLA	O2A-CGA-CBA	3.54	123.01	111.91
15	A	1119	CLA	CMB-C2B-C3B	3.54	131.29	124.68
14	B	4017	BCR	C3-C4-C5	-3.53	107.77	114.08
14	F	4016	BCR	C35-C13-C14	-3.53	117.98	122.92
14	A	4002	BCR	C38-C26-C27	3.52	120.38	113.62
15	B	1210	CLA	CMB-C2B-C3B	3.52	131.26	124.68
15	A	1104	CLA	CMC-C2C-C1C	3.50	130.38	125.04
14	B	4009	BCR	C36-C18-C17	-3.50	118.02	122.92
14	B	4009	BCR	C19-C18-C17	3.50	124.31	118.94
15	A	1106	CLA	C1-O2A-CGA	3.49	125.60	116.44
14	B	4005	BCR	C19-C18-C17	3.48	124.28	118.94
15	F	1139	CLA	O2A-CGA-CBA	3.47	122.79	111.91
14	F	4016	BCR	C12-C13-C14	3.46	124.26	118.94
14	A	4007	BCR	C38-C26-C27	3.46	120.26	113.62
15	B	1221	CLA	O2A-C1-C2	3.46	117.72	108.64
14	B	4004	BCR	C37-C22-C21	-3.45	118.08	122.92
15	A	1102	CLA	CMB-C2B-C3B	3.44	131.12	124.68
15	B	1220	CLA	C1-O2A-CGA	3.43	125.44	116.44
14	A	4001	BCR	C34-C9-C10	-3.43	118.12	122.92
14	B	4017	BCR	C19-C18-C17	3.43	124.20	118.94
15	A	1012	CLA	OBD-CAD-C3D	-3.43	122.29	127.98
14	B	4017	BCR	C34-C9-C10	-3.42	118.14	122.92
14	B	4011	BCR	C33-C5-C4	3.41	120.16	113.62
15	A	1125	CLA	CMC-C2C-C1C	3.40	130.21	125.04
15	B	1211	CLA	CMC-C2C-C1C	3.40	130.21	125.04
14	B	4005	BCR	C37-C22-C21	-3.39	118.18	122.92
15	A	1135	CLA	C4-C3-C5	3.39	120.97	115.27
14	A	4002	BCR	C19-C18-C17	3.38	124.12	118.94
15	A	1121	CLA	O2A-CGA-CBA	3.37	125.56	112.23
15	A	1104	CLA	C1-C2-C3	-3.37	120.22	126.04
14	B	4017	BCR	C36-C18-C17	-3.36	118.21	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1225	CLA	O2A-CGA-CBA	3.36	122.46	111.91
15	A	1138	CLA	CED-O2D-CGD	3.35	123.53	115.94
15	A	1125	CLA	C3C-C4C-NC	3.34	114.32	110.57
15	B	1216	CLA	O2A-C1-C2	3.34	117.42	108.64
15	B	1216	CLA	O2A-CGA-CBA	3.34	122.40	111.91
15	B	1216	CLA	CMB-C2B-C3B	3.34	130.93	124.68
15	K	1401	CLA	O2A-CGA-CBA	3.34	125.44	112.23
15	B	1235	CLA	CMC-C2C-C1C	3.34	130.13	125.04
15	A	1101	CLA	O2A-CGA-CBA	3.34	122.37	111.91
14	A	4008	BCR	C27-C26-C25	-3.33	117.89	122.73
15	B	1203	CLA	O2A-CGA-CBA	3.33	122.35	111.91
15	A	1122	CLA	C4-C3-C2	-3.33	115.15	123.68
14	F	4015	BCR	C38-C26-C25	-3.32	120.80	124.53
14	F	4016	BCR	C3-C4-C5	-3.32	108.14	114.08
14	B	4005	BCR	C38-C26-C25	-3.32	120.80	124.53
15	B	1223	CLA	C1-C2-C3	-3.32	120.30	126.04
14	A	4002	BCR	C36-C18-C17	-3.31	118.28	122.92
14	A	4002	BCR	C38-C26-C25	-3.31	120.81	124.53
14	A	4002	BCR	C34-C9-C10	-3.31	118.28	122.92
14	B	4006	BCR	C36-C18-C17	-3.31	118.29	122.92
15	A	1130	CLA	CMB-C2B-C3B	3.30	130.86	124.68
12	B	5004	LHG	C5-O7-C7	-3.30	109.66	117.79
14	B	4011	BCR	C8-C9-C10	3.29	124.00	118.94
15	B	1229	CLA	C1-C2-C3	-3.29	120.36	126.04
14	B	4009	BCR	C38-C26-C25	-3.28	120.85	124.53
15	B	1239	CLA	O2A-CGA-CBA	3.27	125.16	112.23
14	B	4011	BCR	C23-C22-C21	3.27	123.96	118.94
14	B	4009	BCR	C38-C26-C27	3.26	119.88	113.62
14	J	4013	BCR	C30-C25-C26	-3.25	118.03	122.61
14	A	4007	BCR	C33-C5-C6	-3.24	120.89	124.53
14	B	4010	BCR	C24-C23-C22	-3.24	121.34	126.23
15	A	1123	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	A	1138	CLA	CMB-C2B-C3B	3.23	130.72	124.68
15	A	1012	CLA	C1-O2A-CGA	3.23	124.91	116.44
14	A	4012	BCR	C7-C8-C9	-3.22	121.36	126.23
15	F	1410	CLA	CMC-C2C-C1C	3.22	129.94	125.04
15	A	1136	CLA	O2A-C1-C2	3.22	117.09	108.64
15	B	1021	CLA	CMA-C3A-C4A	-3.21	103.13	111.77
15	A	1122	CLA	O2A-CGA-CBA	3.21	121.97	111.91
14	B	4014	BCR	C23-C22-C21	3.20	123.84	118.94
15	B	1226	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
15	B	1222	CLA	O2D-CGD-O1D	-3.19	117.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1012	CLA	C3C-C4C-NC	3.19	114.15	110.57
15	A	1110	CLA	C1-C2-C3	-3.19	120.53	126.04
15	B	1225	CLA	CMC-C2C-C1C	3.19	129.89	125.04
15	B	1230	CLA	CMC-C2C-C1C	3.18	129.88	125.04
14	B	4006	BCR	C7-C8-C9	-3.18	121.44	126.23
15	B	1237	CLA	CMC-C2C-C1C	3.17	129.87	125.04
15	B	1222	CLA	C1-O2A-CGA	3.17	124.76	116.44
14	J	4013	BCR	C33-C5-C4	3.15	119.67	113.62
14	A	4007	BCR	C24-C23-C22	-3.15	121.47	126.23
14	J	4013	BCR	C38-C26-C27	3.15	119.66	113.62
15	B	1223	CLA	OBD-CAD-C3D	-3.13	122.78	127.98
12	A	5003	LHG	C5-O7-C7	-3.13	110.09	117.79
15	B	1213	CLA	CMC-C2C-C1C	3.13	129.80	125.04
15	J	1303	CLA	O2A-CGA-CBA	3.12	124.58	112.23
14	B	4009	BCR	C3-C4-C5	-3.12	108.50	114.08
15	A	1122	CLA	CMC-C2C-C1C	3.12	129.79	125.04
14	A	4003	BCR	C33-C5-C4	3.12	119.61	113.62
15	A	1115	CLA	O2A-CGA-CBA	3.12	124.56	112.23
15	B	1205	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	B	4010	BCR	C36-C18-C17	-3.12	118.56	122.92
15	A	1107	CLA	CAA-C2A-C1A	-3.11	101.78	111.97
15	F	1139	CLA	CMC-C2C-C1C	3.11	129.77	125.04
15	F	1410	CLA	C4-C3-C2	-3.11	115.71	123.68
15	A	1109	CLA	CMC-C2C-C1C	3.10	129.76	125.04
14	F	4015	BCR	C38-C26-C27	3.10	119.56	113.62
14	B	4006	BCR	C33-C5-C4	3.09	119.56	113.62
15	B	1204	CLA	O2A-CGA-CBA	3.08	124.42	112.23
14	A	4002	BCR	C7-C8-C9	-3.08	121.58	126.23
14	J	4013	BCR	C36-C18-C17	-3.08	118.61	122.92
15	F	1301	CLA	CMC-C2C-C1C	3.08	129.73	125.04
15	A	1126	CLA	CMB-C2B-C3B	3.08	130.44	124.68
15	B	1202	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
14	A	4001	BCR	C3-C4-C5	-3.08	108.58	114.08
15	B	1223	CLA	C3C-C4C-NC	3.08	114.02	110.57
15	B	1217	CLA	O2A-C1-C2	3.07	119.70	108.42
15	A	1106	CLA	CMC-C2C-C1C	3.06	129.71	125.04
15	B	1223	CLA	CMC-C2C-C1C	3.06	129.70	125.04
14	A	4003	BCR	C36-C18-C17	-3.06	118.64	122.92
15	B	1221	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	B	4009	BCR	C37-C22-C21	-3.06	118.64	122.92
15	A	1128	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	A	4007	BCR	C3-C4-C5	-3.05	108.62	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1230	CLA	C3C-C4C-NC	3.05	114.00	110.57
15	A	1134	CLA	O2A-CGA-CBA	3.05	124.30	112.23
14	A	4012	BCR	C19-C18-C17	3.05	123.62	118.94
14	B	4011	BCR	C38-C26-C27	3.05	119.47	113.62
15	B	1201	CLA	CMC-C2C-C1C	3.04	129.68	125.04
15	K	1402	CLA	O2A-CGA-CBA	3.04	124.26	112.23
15	A	1132	CLA	C1-C2-C3	-3.04	120.78	126.04
14	A	4008	BCR	C30-C25-C26	-3.03	118.34	122.61
14	J	4013	BCR	C38-C26-C25	-3.03	121.13	124.53
15	B	1215	CLA	C1-O2A-CGA	3.03	124.38	116.44
15	A	1101	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
14	A	4001	BCR	C38-C26-C27	3.02	119.42	113.62
15	A	1105	CLA	CMC-C2C-C1C	3.02	129.64	125.04
15	B	1217	CLA	CMC-C2C-C1C	3.02	129.64	125.04
15	A	1022	CLA	CMC-C2C-C1C	3.02	129.63	125.04
15	A	1106	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
15	A	1801	CLA	C3C-C4C-NC	3.01	113.95	110.57
15	A	1112	CLA	CMC-C2C-C1C	3.01	129.63	125.04
15	A	1103	CLA	O2A-CGA-CBA	3.01	121.36	111.91
15	A	1125	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	B	1237	CLA	C4-C3-C2	-3.00	115.98	123.68
15	B	1214	CLA	CMB-C2B-C3B	3.00	130.29	124.68
15	A	1126	CLA	CMC-C2C-C1C	3.00	129.61	125.04
10	A	2001	PQN	C14-C13-C15	3.00	120.31	115.27
14	B	4010	BCR	C3-C4-C5	-2.99	108.73	114.08
15	B	1221	CLA	C3C-C4C-NC	2.99	113.93	110.57
15	A	1107	CLA	CMB-C2B-C3B	2.99	130.26	124.68
15	A	1127	CLA	CMB-C2B-C3B	2.99	130.26	124.68
15	B	1230	CLA	C4-C3-C2	-2.98	116.03	123.68
15	B	1211	CLA	O2A-CGA-CBA	2.98	123.99	112.23
15	A	1129	CLA	O2A-CGA-CBA	2.97	123.96	112.23
14	J	4013	BCR	C15-C14-C13	-2.96	123.08	127.31
15	A	1109	CLA	C1-O2A-CGA	2.96	124.22	116.44
15	B	1214	CLA	CMC-C2C-C1C	2.96	129.55	125.04
15	A	1118	CLA	O2A-CGA-CBA	2.96	123.94	112.23
13	A	1011	CL0	CHB-C4A-NA	2.96	128.61	124.51
15	A	1012	CLA	C4-C3-C5	2.96	120.25	115.27
13	A	1011	CL0	CMC-C2C-C1C	2.96	129.54	125.04
15	B	1231	CLA	C4-C3-C5	2.96	120.25	115.27
14	B	4004	BCR	C7-C8-C9	-2.96	121.77	126.23
15	A	1130	CLA	CMC-C2C-C1C	2.96	129.54	125.04
15	B	1219	CLA	CMC-C2C-C1C	2.95	129.53	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1201	CLA	O2A-CGA-CBA	2.95	123.89	112.23
15	B	1220	CLA	CMC-C2C-C1C	2.95	129.53	125.04
15	B	1229	CLA	CMC-C2C-C1C	2.94	129.52	125.04
15	B	1219	CLA	C4-C3-C5	2.94	120.22	115.27
15	A	1129	CLA	OBD-CAD-C3D	-2.94	123.10	127.98
15	B	1216	CLA	C1-O2A-CGA	2.94	124.15	116.44
14	J	4013	BCR	C37-C22-C21	-2.93	118.81	122.92
13	A	1011	CL0	O2D-CGD-O1D	-2.93	118.10	123.84
15	B	1210	CLA	CMC-C2C-C1C	2.93	129.50	125.04
15	B	1224	CLA	CMB-C2B-C3B	2.93	130.16	124.68
15	B	1223	CLA	CMB-C2B-C3B	2.92	130.15	124.68
15	A	1127	CLA	C3C-C4C-NC	2.92	113.85	110.57
14	A	4001	BCR	C30-C25-C26	-2.92	118.50	122.61
15	A	1101	CLA	CMC-C2C-C1C	2.92	129.48	125.04
15	B	1238	CLA	CMC-C2C-C1C	2.92	129.48	125.04
14	B	4017	BCR	C38-C26-C27	2.91	119.21	113.62
15	B	1221	CLA	CMB-C2B-C3B	2.91	130.13	124.68
14	F	4016	BCR	C36-C18-C17	-2.91	118.84	122.92
15	B	1210	CLA	CAC-C3C-C4C	2.91	128.59	124.81
14	B	4004	BCR	C33-C5-C4	2.91	119.20	113.62
15	A	1115	CLA	C3C-C4C-NC	2.91	113.83	110.57
15	A	1121	CLA	CMC-C2C-C1C	2.90	129.46	125.04
15	A	1131	CLA	CMC-C2C-C1C	2.90	129.46	125.04
14	A	4012	BCR	C23-C22-C21	2.90	123.39	118.94
15	A	1133	CLA	O2A-CGA-CBA	2.90	123.69	112.23
15	B	1206	CLA	CMC-C2C-C1C	2.90	129.45	125.04
15	B	1227	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	B	1224	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	J	1302	CLA	CMC-C2C-C1C	2.90	129.45	125.04
15	A	1132	CLA	C4-C3-C5	2.89	120.14	115.27
14	A	4012	BCR	C34-C9-C10	-2.88	118.89	122.92
15	B	1207	CLA	O2A-CGA-CBA	2.88	123.62	112.23
14	A	4002	BCR	C34-C9-C8	2.88	122.61	118.08
15	A	1117	CLA	C1-O2A-CGA	2.88	123.99	116.44
15	B	1021	CLA	CMC-C2C-C1C	2.88	129.42	125.04
15	B	1201	CLA	CMB-C2B-C3B	2.87	130.06	124.68
14	B	4011	BCR	C28-C27-C26	-2.87	108.94	114.08
15	A	1125	CLA	C1-O2A-CGA	2.87	123.97	116.44
15	A	1127	CLA	OBD-CAD-C3D	-2.87	123.22	127.98
14	B	4006	BCR	C3-C4-C5	-2.86	108.96	114.08
14	A	4003	BCR	C23-C22-C21	2.86	123.33	118.94
15	A	1801	CLA	C6-C5-C3	-2.86	109.94	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	4013	BCR	C34-C9-C10	-2.86	118.92	122.92
15	A	1107	CLA	C1-C2-C3	-2.86	122.13	126.75
15	J	1303	CLA	C3C-C4C-NC	2.86	113.78	110.57
14	B	4017	BCR	C33-C5-C4	2.85	119.10	113.62
15	B	1211	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	A	1140	CLA	CMC-C2C-C1C	2.85	129.38	125.04
15	B	1212	CLA	CMC-C2C-C1C	2.85	129.38	125.04
15	A	1012	CLA	CMC-C2C-C1C	2.85	129.37	125.04
15	A	1127	CLA	CMC-C2C-C1C	2.84	129.37	125.04
15	A	1134	CLA	CMC-C2C-C1C	2.84	129.37	125.04
15	B	1222	CLA	O2A-CGA-CBA	2.84	120.83	111.91
15	A	1102	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	A	1134	CLA	CMB-C2B-C3B	2.84	129.98	124.68
15	A	1101	CLA	C3C-C4C-NC	2.83	113.75	110.57
15	A	1123	CLA	CMC-C2C-C1C	2.83	129.35	125.04
15	B	1206	CLA	O2A-CGA-CBA	2.83	123.42	112.23
15	A	1124	CLA	O2A-CGA-CBA	2.83	120.79	111.91
15	A	1138	CLA	C1-C2-C3	-2.83	121.15	126.04
15	B	1235	CLA	C3C-C4C-NC	2.83	113.74	110.57
15	A	1118	CLA	CMC-C2C-C1C	2.82	129.34	125.04
14	B	4006	BCR	C34-C9-C8	2.82	122.53	118.08
15	B	1205	CLA	C3C-C4C-NC	2.82	113.73	110.57
15	A	1111	CLA	CAC-C3C-C4C	2.82	128.47	124.81
15	B	1225	CLA	C3C-C4C-NC	2.82	113.73	110.57
14	F	4016	BCR	C8-C7-C6	-2.82	119.29	127.20
14	B	4004	BCR	C38-C26-C27	2.82	119.02	113.62
15	A	1132	CLA	C3C-C4C-NC	2.81	113.72	110.57
15	B	1201	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
15	B	1229	CLA	C3C-C4C-NC	2.81	113.72	110.57
15	A	1102	CLA	CMC-C2C-C1C	2.80	129.31	125.04
14	A	4008	BCR	C38-C26-C25	-2.80	121.38	124.53
15	K	1402	CLA	CMC-C2C-C1C	2.80	129.30	125.04
15	A	1136	CLA	C1-O2A-CGA	2.80	123.79	116.44
14	B	4010	BCR	C34-C9-C10	-2.80	119.01	122.92
15	A	1137	CLA	CMB-C2B-C3B	2.79	129.90	124.68
15	A	1124	CLA	CMC-C2C-C1C	2.78	129.28	125.04
15	B	1209	CLA	CMB-C2B-C3B	2.78	129.88	124.68
15	A	1111	CLA	CMC-C2C-C1C	2.78	129.28	125.04
15	B	1221	CLA	CMC-C2C-C1C	2.78	129.27	125.04
15	A	1113	CLA	CMC-C2C-C1C	2.78	129.27	125.04
15	B	1225	CLA	CMB-C2B-C3B	2.78	129.88	124.68
15	A	1138	CLA	C4-C3-C5	2.78	119.95	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1117	CLA	CMC-C2C-C1C	2.78	129.27	125.04
14	B	4017	BCR	C37-C22-C21	-2.78	119.03	122.92
14	A	4008	BCR	C33-C5-C4	2.78	118.95	113.62
15	B	1205	CLA	CMC-C2C-C1C	2.77	129.26	125.04
15	A	1110	CLA	CMC-C2C-C1C	2.77	129.26	125.04
14	A	4002	BCR	C3-C4-C5	-2.77	109.13	114.08
15	B	1204	CLA	CMC-C2C-C1C	2.77	129.26	125.04
15	B	1218	CLA	CMC-C2C-C1C	2.77	129.26	125.04
14	F	4016	BCR	C23-C24-C25	-2.77	119.43	127.20
15	A	1133	CLA	CMC-C2C-C1C	2.77	129.25	125.04
15	A	1126	CLA	CMD-C2D-C3D	-2.76	119.51	124.68
15	B	1222	CLA	C3C-C4C-NC	2.76	113.66	110.57
10	B	2002	PQN	C2M-C2-C3	-2.76	119.91	124.40
14	F	4016	BCR	C34-C9-C10	-2.75	119.06	122.92
15	A	1104	CLA	C4-C3-C5	2.75	119.90	115.27
15	B	1240	CLA	CMC-C2C-C1C	2.75	129.22	125.04
15	B	1209	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
14	B	4004	BCR	C34-C9-C10	-2.74	119.08	122.92
15	B	1215	CLA	CMC-C2C-C1C	2.74	129.21	125.04
14	B	4014	BCR	C15-C14-C13	-2.74	123.40	127.31
15	B	1223	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
14	B	4010	BCR	C34-C9-C8	2.74	122.39	118.08
15	B	1206	CLA	CAC-C3C-C4C	2.73	128.36	124.81
13	A	1011	CL0	C3C-C4C-NC	2.73	113.64	110.57
15	A	1103	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	A	1101	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	A	1135	CLA	C4-C3-C2	-2.73	116.68	123.68
15	B	1225	CLA	C5-C3-C2	-2.73	115.59	121.12
14	B	4005	BCR	C3-C4-C5	-2.73	109.20	114.08
15	A	1115	CLA	CMC-C2C-C1C	2.73	129.19	125.04
15	A	1022	CLA	C3C-C4C-NC	2.73	113.63	110.57
15	B	1224	CLA	CMC-C2C-C1C	2.72	129.19	125.04
15	F	1301	CLA	C3C-C4C-NC	2.72	113.62	110.57
15	A	1129	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	B	1235	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	A	1119	CLA	CMC-C2C-C1C	2.72	129.18	125.04
15	B	1215	CLA	C4-C3-C2	-2.72	116.70	123.68
15	B	1013	CLA	CMB-C2B-C3B	2.72	129.76	124.68
15	B	1215	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	A	1137	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	A	1135	CLA	CMC-C2C-C1C	2.72	129.18	125.04
15	A	1137	CLA	C3C-C4C-NC	2.72	113.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1240	CLA	CMB-C2B-C3B	2.71	129.76	124.68
15	A	1131	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	B	1212	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	A	1112	CLA	C3C-C4C-NC	2.71	113.61	110.57
14	B	4004	BCR	C23-C22-C21	2.71	123.10	118.94
15	B	1236	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	B	1209	CLA	CAC-C3C-C4C	2.70	128.32	124.81
14	A	4002	BCR	C27-C26-C25	-2.70	118.81	122.73
14	J	4013	BCR	C33-C5-C6	-2.70	121.50	124.53
15	B	1240	CLA	C3C-C4C-NC	2.70	113.60	110.57
15	B	1217	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
15	A	1125	CLA	CMB-C2B-C3B	2.70	129.72	124.68
15	B	1220	CLA	CED-O2D-CGD	2.70	122.03	115.94
15	A	1140	CLA	C3C-C4C-NC	2.69	113.59	110.57
15	A	1107	CLA	CMC-C2C-C1C	2.69	129.14	125.04
15	B	1223	CLA	C4-C3-C5	2.69	119.80	115.27
15	A	1129	CLA	CMC-C2C-C1C	2.69	129.13	125.04
14	A	4008	BCR	C3-C4-C5	-2.69	109.28	114.08
14	J	4013	BCR	C4-C5-C6	-2.69	118.83	122.73
15	B	1236	CLA	CMB-C2B-C3B	2.68	129.70	124.68
15	A	1116	CLA	CMC-C2C-C1C	2.68	129.12	125.04
15	A	1128	CLA	C3C-C4C-NC	2.68	113.58	110.57
15	B	1234	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	A	4003	BCR	C3-C4-C5	-2.68	109.29	114.08
15	J	1303	CLA	CMC-C2C-C1C	2.68	129.12	125.04
15	A	1118	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
15	B	1227	CLA	C3C-C4C-NC	2.68	113.57	110.57
15	B	1202	CLA	C1-C2-C3	-2.68	121.42	126.04
15	F	1139	CLA	C3C-C4C-NC	2.68	113.57	110.57
14	A	4012	BCR	C3-C4-C5	-2.67	109.31	114.08
14	A	4008	BCR	C15-C14-C13	-2.67	123.50	127.31
15	A	1135	CLA	CMB-C2B-C3B	2.67	129.67	124.68
15	B	1222	CLA	C4-C3-C5	2.67	119.76	115.27
12	A	5001	LHG	C5-O7-C7	-2.67	111.23	117.79
15	A	1022	CLA	C4-C3-C5	2.66	119.75	115.27
15	B	1222	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
15	B	1228	CLA	CMC-C2C-C1C	2.66	129.09	125.04
15	B	1232	CLA	OBD-CAD-C3D	-2.66	123.56	127.98
14	F	4016	BCR	C38-C26-C27	2.66	118.72	113.62
12	A	5005	LHG	O8-C23-C24	2.66	120.25	111.91
15	A	1120	CLA	CMC-C2C-C1C	2.66	129.09	125.04
15	B	1207	CLA	O2D-CGD-O1D	-2.66	118.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1135	CLA	C1-O2A-CGA	2.66	123.41	116.44
14	B	4005	BCR	C23-C22-C21	2.66	123.02	118.94
15	K	1401	CLA	CMC-C2C-C1C	2.65	129.08	125.04
15	A	1801	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
15	B	1215	CLA	C1-C2-C3	-2.65	121.45	126.04
14	A	4007	BCR	C23-C24-C25	-2.65	119.75	127.20
14	F	4016	BCR	C34-C9-C8	2.65	122.25	118.08
15	J	1302	CLA	C3C-C4C-NC	2.65	113.54	110.57
15	A	1114	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
15	B	1207	CLA	C3C-C4C-NC	2.65	113.54	110.57
15	B	1021	CLA	C3C-C4C-NC	2.64	113.53	110.57
15	A	1110	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	A	1111	CLA	CMB-C2B-C3B	2.64	129.62	124.68
15	B	1205	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
15	A	1105	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
14	A	4007	BCR	C7-C8-C9	-2.64	122.25	126.23
15	A	1138	CLA	C1-O2A-CGA	2.64	123.37	116.44
15	A	1126	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	B	1203	CLA	C1-O2A-CGA	2.64	123.36	116.44
15	A	1130	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
15	A	1114	CLA	CMC-C2C-C1C	2.64	129.05	125.04
15	B	1205	CLA	C1-C2-C3	-2.63	121.49	126.04
15	F	1301	CLA	CMB-C2B-C3B	2.63	129.61	124.68
15	A	1136	CLA	CMC-C2C-C1C	2.63	129.05	125.04
15	B	1216	CLA	CMC-C2C-C1C	2.63	129.05	125.04
14	J	4013	BCR	C23-C24-C25	-2.63	119.81	127.20
15	B	1234	CLA	C1-O2A-CGA	2.63	123.35	116.44
12	B	5004	LHG	O8-C23-C24	2.63	120.16	111.91
15	A	1103	CLA	CMC-C2C-C1C	2.63	129.04	125.04
15	B	1013	CLA	C3C-C4C-NC	2.63	113.52	110.57
14	B	4006	BCR	C24-C23-C22	-2.62	122.27	126.23
13	A	1108	CL0	C3C-C4C-NC	2.62	113.51	110.57
15	A	1134	CLA	C3C-C4C-NC	2.62	113.51	110.57
15	B	1226	CLA	C3C-C4C-NC	2.62	113.51	110.57
15	K	1402	CLA	C3C-C4C-NC	2.61	113.50	110.57
14	A	4003	BCR	C15-C14-C13	-2.61	123.58	127.31
15	B	1212	CLA	C3C-C4C-NC	2.61	113.50	110.57
15	B	1236	CLA	C3C-C4C-NC	2.61	113.50	110.57
15	A	1140	CLA	CMB-C2B-C3B	2.61	129.56	124.68
14	A	4007	BCR	C34-C9-C10	-2.61	119.27	122.92
15	B	1227	CLA	CMC-C2C-C1C	2.61	129.01	125.04
14	B	4017	BCR	C27-C26-C25	-2.61	118.95	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1213	CLA	C1-O2A-CGA	2.60	123.28	116.44
15	B	1207	CLA	CMC-C2C-C1C	2.60	129.00	125.04
15	A	1117	CLA	CMB-C2B-C3B	2.60	129.54	124.68
15	A	1132	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
15	B	1226	CLA	CMC-C2C-C1C	2.60	129.00	125.04
15	A	1131	CLA	CAC-C3C-C4C	2.60	128.18	124.81
15	B	1232	CLA	C3C-C4C-NC	2.60	113.48	110.57
15	A	1103	CLA	C1-O2A-CGA	2.60	123.26	116.44
15	A	1022	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	B	1023	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	A	1124	CLA	CMB-C2B-C3B	2.59	129.53	124.68
14	B	4014	BCR	C34-C9-C10	-2.59	119.29	122.92
15	A	1115	CLA	CMB-C2B-C3B	2.59	129.53	124.68
15	A	1113	CLA	C3C-C4C-NC	2.59	113.48	110.57
15	B	1232	CLA	CMC-C2C-C1C	2.59	128.98	125.04
15	B	1236	CLA	C1-C2-C3	-2.59	122.56	126.75
15	A	1101	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	B	1213	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
17	B	5002	LMG	O8-C28-C29	2.58	120.02	111.91
15	B	1217	CLA	C3C-C4C-NC	2.57	113.46	110.57
15	A	1135	CLA	C3C-C4C-NC	2.57	113.46	110.57
15	A	1012	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	B	1239	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	B	4011	BCR	C3-C4-C5	-2.57	109.49	114.08
15	A	1102	CLA	C4-C3-C5	2.57	119.59	115.27
15	B	1203	CLA	CMC-C2C-C1C	2.57	128.95	125.04
14	A	4002	BCR	C30-C25-C26	-2.56	119.00	122.61
15	F	1410	CLA	C3C-C4C-NC	2.56	113.45	110.57
15	A	1116	CLA	C1-O2A-CGA	2.56	123.17	116.44
15	B	1230	CLA	CMB-C2B-C3B	2.56	129.47	124.68
14	A	4008	BCR	C23-C24-C25	-2.56	120.02	127.20
15	A	1012	CLA	CMB-C2B-C3B	2.56	129.46	124.68
15	A	1140	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	A	1116	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	B	1219	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	B	1234	CLA	C3C-C4C-NC	2.56	113.44	110.57
15	B	1209	CLA	CMC-C2C-C1C	2.56	128.93	125.04
15	B	1218	CLA	OBD-CAD-C3D	-2.55	123.74	127.98
15	A	1136	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
14	A	4007	BCR	C33-C5-C4	2.55	118.52	113.62
14	B	4011	BCR	C1-C6-C5	-2.55	119.02	122.61
15	B	1212	CLA	CMB-C2B-C3B	2.55	129.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2001	PQN	C2M-C2-C3	-2.55	120.24	124.40
15	J	1302	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
14	B	4009	BCR	C33-C5-C4	2.55	118.51	113.62
15	B	1224	CLA	C1-O2A-CGA	2.55	123.13	116.44
15	A	1109	CLA	CMB-C2B-C3B	2.55	129.44	124.68
14	F	4015	BCR	C36-C18-C17	-2.54	119.36	122.92
15	A	1116	CLA	C3C-C4C-NC	2.54	113.42	110.57
15	A	1112	CLA	CMB-C2B-C3B	2.54	129.43	124.68
14	A	4003	BCR	C38-C26-C27	2.54	118.49	113.62
15	A	1121	CLA	C3C-C4C-NC	2.54	113.42	110.57
15	A	1136	CLA	C3C-C4C-NC	2.54	113.42	110.57
15	B	1228	CLA	C3C-C4C-NC	2.54	113.42	110.57
14	B	4010	BCR	C30-C25-C26	-2.53	119.05	122.61
15	B	1206	CLA	CMB-C2B-C3B	2.53	129.41	124.68
15	B	1013	CLA	C1-C2-C3	-2.53	121.67	126.04
15	B	1215	CLA	C3C-C4C-NC	2.53	113.40	110.57
15	A	1022	CLA	CMB-C2B-C3B	2.52	129.40	124.68
15	A	1801	CLA	CMB-C2B-C3B	2.52	129.40	124.68
15	B	1222	CLA	CHB-C4A-NA	2.52	128.00	124.51
15	B	1226	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
15	B	1218	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	J	4013	BCR	C2-C1-C6	2.52	114.36	110.48
15	B	1013	CLA	CED-O2D-CGD	2.52	121.63	115.94
15	A	1128	CLA	C1-O2A-CGA	2.51	123.04	116.44
15	A	1119	CLA	C3C-C4C-NC	2.51	113.39	110.57
15	F	1410	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
15	A	1106	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
15	A	1110	CLA	CMB-C2B-C3B	2.51	129.37	124.68
15	B	1218	CLA	C1-O2A-CGA	2.51	123.03	116.44
15	B	1226	CLA	CMB-C2B-C3B	2.51	129.37	124.68
15	B	1235	CLA	CMB-C2B-C3B	2.51	129.37	124.68
15	B	1237	CLA	CMB-C2B-C3B	2.50	129.36	124.68
15	A	1110	CLA	C3C-C4C-NC	2.50	113.38	110.57
14	A	4002	BCR	C35-C13-C12	2.50	122.02	118.08
15	A	1137	CLA	CMC-C2C-C1C	2.50	128.85	125.04
14	B	4010	BCR	C33-C5-C4	2.50	118.42	113.62
15	A	1133	CLA	CAC-C3C-C4C	2.50	128.05	124.81
14	A	4007	BCR	C36-C18-C17	-2.50	119.43	122.92
15	B	1230	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
15	A	1127	CLA	C1-O2A-CGA	2.49	122.99	116.44
14	B	4006	BCR	C37-C22-C21	-2.49	119.43	122.92
15	A	1131	CLA	C3C-C4C-NC	2.49	113.37	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1211	CLA	C3C-C4C-NC	2.49	113.37	110.57
15	B	1213	CLA	CMB-C2B-C3B	2.49	129.34	124.68
15	B	1237	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	B	1021	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	A	1110	CLA	C4-C3-C5	2.49	119.45	115.27
15	B	1214	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	B	1201	CLA	C3C-C4C-NC	2.49	113.36	110.57
15	B	1221	CLA	C4-C3-C2	-2.48	117.31	123.68
15	A	1133	CLA	C3C-C4C-NC	2.48	113.36	110.57
15	B	1218	CLA	C4-C3-C2	-2.48	117.31	123.68
15	A	1115	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	A	1105	CLA	C3C-C4C-NC	2.48	113.35	110.57
13	A	1108	CL0	CAC-C3C-C4C	2.48	128.03	124.81
15	B	1231	CLA	CED-O2D-CGD	2.48	121.54	115.94
15	A	1129	CLA	C3C-C4C-NC	2.48	113.35	110.57
15	A	1109	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
15	K	1401	CLA	C3C-C4C-NC	2.48	113.35	110.57
15	A	1107	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
14	A	4002	BCR	C37-C22-C21	-2.47	119.46	122.92
15	A	1133	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
15	B	1234	CLA	C5-C3-C2	2.47	126.12	121.12
15	B	1229	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
12	A	5003	LHG	O8-C23-C24	2.47	119.65	111.91
14	A	4001	BCR	C15-C14-C13	-2.47	123.79	127.31
15	A	1113	CLA	CMB-C2B-C3B	2.46	129.29	124.68
15	B	1238	CLA	C3C-C4C-NC	2.46	113.33	110.57
15	A	1101	CLA	CBA-CAA-C2A	2.46	121.13	113.86
14	A	4012	BCR	C38-C26-C27	2.46	118.34	113.62
15	A	1122	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	B	1234	CLA	CMC-C2C-C1C	2.46	128.78	125.04
14	B	4010	BCR	C38-C26-C27	2.46	118.34	113.62
14	F	4015	BCR	C35-C13-C14	-2.46	119.48	122.92
14	B	4009	BCR	C30-C25-C26	-2.46	119.16	122.61
15	B	1219	CLA	C4-C3-C2	-2.46	117.38	123.68
15	B	1231	CLA	CMB-C2B-C3B	2.45	129.27	124.68
15	B	1208	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
14	B	4004	BCR	C1-C6-C5	-2.45	119.16	122.61
15	B	1211	CLA	CMB-C2B-C3B	2.45	129.26	124.68
15	B	1216	CLA	C4-C3-C5	2.45	119.39	115.27
14	B	4005	BCR	C34-C9-C10	-2.45	119.49	122.92
15	A	1106	CLA	CMB-C2B-C3B	2.45	129.26	124.68
14	A	4007	BCR	C28-C27-C26	-2.45	109.71	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1225	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
15	A	1112	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
15	B	1013	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
15	B	1201	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
15	B	1238	CLA	CMB-C2B-C3B	2.45	129.25	124.68
15	B	1202	CLA	C3C-C4C-NC	2.44	113.31	110.57
15	B	1222	CLA	CMB-C2B-C3B	2.44	129.25	124.68
15	B	1234	CLA	CMB-C2B-C3B	2.44	129.24	124.68
15	A	1130	CLA	C3C-C4C-NC	2.44	113.30	110.57
15	B	1210	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	B	1220	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
12	A	5005	LHG	C5-O7-C7	-2.43	111.80	117.79
13	A	1011	CL0	C1-O2A-CGA	2.43	122.83	116.44
15	A	1132	CLA	CMC-C2C-C1C	2.43	128.75	125.04
14	A	4003	BCR	C19-C18-C17	2.43	122.67	118.94
14	B	4017	BCR	C30-C25-C26	-2.43	119.19	122.61
15	A	1114	CLA	CAC-C3C-C4C	2.43	127.96	124.81
15	F	1301	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
15	A	1124	CLA	C3C-C4C-NC	2.43	113.30	110.57
15	A	1125	CLA	CHD-C4C-C3C	-2.43	121.27	124.84
14	J	4013	BCR	C27-C26-C25	-2.43	119.21	122.73
10	A	2001	PQN	C11-C12-C13	-2.43	122.75	126.79
15	B	1202	CLA	CMB-C2B-C3B	2.43	129.22	124.68
15	A	1121	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
15	B	1231	CLA	C3C-C4C-NC	2.43	113.29	110.57
15	B	1204	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	A	4008	BCR	C34-C9-C10	-2.42	119.53	122.92
15	A	1104	CLA	CMB-C2B-C3B	2.42	129.21	124.68
15	B	1202	CLA	CMC-C2C-C1C	2.42	128.73	125.04
15	B	1216	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	B	4011	BCR	C35-C13-C12	2.41	121.88	118.08
15	A	1117	CLA	C3C-C4C-NC	2.41	113.28	110.57
15	B	1203	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
15	B	1222	CLA	CMC-C2C-C1C	2.41	128.71	125.04
15	A	1119	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	A	1127	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	A	1120	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	A	1104	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	A	1122	CLA	CMB-C2B-C3B	2.41	129.18	124.68
15	B	1234	CLA	C4-C3-C2	-2.41	117.50	123.68
14	B	4017	BCR	C38-C26-C25	-2.40	121.83	124.53
15	B	1209	CLA	C3C-C4C-NC	2.40	113.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1217	CLA	CMB-C2B-C3B	2.40	129.17	124.68
15	B	1220	CLA	C3C-C4C-NC	2.40	113.27	110.57
15	A	1123	CLA	CMB-C2B-C3B	2.40	129.17	124.68
15	B	1013	CLA	CMC-C2C-C1C	2.40	128.69	125.04
15	A	1114	CLA	CMB-C2B-C3B	2.40	129.17	124.68
14	B	4010	BCR	C37-C22-C21	-2.40	119.56	122.92
15	A	1102	CLA	C3C-C4C-NC	2.40	113.26	110.57
15	B	1231	CLA	C4-C3-C2	-2.40	117.53	123.68
15	B	1222	CLA	O2A-C1-C2	2.40	114.93	108.64
15	A	1105	CLA	C1-O2A-CGA	2.39	122.72	116.44
15	B	1225	CLA	CBA-CAA-C2A	2.39	120.93	113.86
14	B	4009	BCR	C8-C9-C10	2.39	122.61	118.94
13	A	1108	CL0	CED-O2D-CGD	2.39	121.35	115.94
15	A	1123	CLA	C3C-C4C-NC	2.39	113.25	110.57
15	A	1133	CLA	CMB-C2B-C3B	2.39	129.14	124.68
15	A	1801	CLA	OBD-CAD-C3D	-2.39	124.02	127.98
15	A	1105	CLA	CAC-C3C-C4C	2.39	127.91	124.81
14	B	4009	BCR	C27-C26-C25	-2.38	119.28	122.73
14	A	4012	BCR	C8-C7-C6	-2.38	120.52	127.20
15	B	1237	CLA	CAC-C3C-C4C	2.38	127.89	124.81
15	A	1114	CLA	C3C-C4C-NC	2.38	113.24	110.57
15	A	1120	CLA	C3C-C4C-NC	2.38	113.24	110.57
15	A	1117	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	F	1410	CLA	CMB-C2B-C3B	2.37	129.12	124.68
15	A	1120	CLA	CMB-C2B-C3B	2.37	129.12	124.68
15	A	1110	CLA	CAC-C3C-C4C	2.37	127.89	124.81
15	B	1239	CLA	CAC-C3C-C4C	2.37	127.89	124.81
15	J	1303	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	B	1210	CLA	C3C-C4C-NC	2.37	113.23	110.57
15	B	1237	CLA	C3C-C4C-NC	2.37	113.23	110.57
15	B	1204	CLA	CMB-C2B-C3B	2.37	129.11	124.68
15	A	1118	CLA	C3C-C4C-NC	2.36	113.22	110.57
15	F	1139	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
14	B	4017	BCR	C34-C9-C8	2.36	121.80	118.08
14	F	4015	BCR	C8-C7-C6	-2.36	120.58	127.20
14	A	4002	BCR	C23-C24-C25	-2.36	120.58	127.20
15	B	1228	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
14	B	4014	BCR	C36-C18-C17	-2.36	119.62	122.92
14	A	4001	BCR	C33-C5-C4	2.35	118.14	113.62
15	A	1128	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
15	B	1021	CLA	CMA-C3A-C2A	-2.35	104.34	113.83
15	A	1113	CLA	CAC-C3C-C4C	2.35	127.86	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	1304	LMU	C1B-O1B-C4'	-2.35	112.15	117.96
15	A	1104	CLA	C3C-C4C-NC	2.35	113.21	110.57
15	B	1021	CLA	CBA-CAA-C2A	2.35	120.80	113.86
15	A	1138	CLA	C3C-C4C-NC	2.35	113.20	110.57
15	K	1401	CLA	CMB-C2B-C3B	2.35	129.07	124.68
15	K	1401	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
14	A	4003	BCR	C28-C27-C26	-2.35	109.89	114.08
15	A	1103	CLA	CMB-C2B-C3B	2.34	129.06	124.68
15	B	1240	CLA	CAA-CBA-CGA	-2.34	108.56	113.59
14	A	4008	BCR	C36-C18-C17	-2.34	119.64	122.92
15	A	1107	CLA	C3C-C4C-NC	2.34	113.19	110.57
14	A	4007	BCR	C30-C25-C26	-2.34	119.32	122.61
15	B	1218	CLA	C3C-C4C-NC	2.34	113.19	110.57
15	B	1239	CLA	CMC-C2C-C1C	2.33	128.59	125.04
15	A	1103	CLA	CHB-C4A-NA	2.33	127.74	124.51
15	A	1101	CLA	C1-O2A-CGA	2.33	122.56	116.44
15	B	1203	CLA	C3C-C4C-NC	2.33	113.18	110.57
15	A	1123	CLA	OBD-CAD-C3D	-2.33	124.12	127.98
15	B	1218	CLA	CMB-C2B-C3B	2.33	129.03	124.68
15	B	1023	CLA	CMC-C2C-C1C	2.33	128.58	125.04
15	A	1111	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
15	B	1215	CLA	CMB-C2B-C3B	2.33	129.03	124.68
13	A	1011	CL0	CMA-C3A-C4A	-2.33	105.52	111.77
15	B	1235	CLA	C4-C3-C5	2.32	119.18	115.27
16	B	1301	LMU	C1B-O1B-C4'	-2.32	112.22	117.96
14	F	4015	BCR	C3-C4-C5	-2.32	109.94	114.08
15	A	1107	CLA	C5-C3-C4	2.31	119.71	114.60
10	A	2001	PQN	C2M-C2-C1	2.31	120.10	116.27
15	A	1107	CLA	CAA-CBA-CGA	-2.31	106.50	113.25
15	A	1012	CLA	CHB-C4A-NA	2.31	127.70	124.51
14	B	4004	BCR	C15-C14-C13	-2.31	124.02	127.31
15	A	1131	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
14	A	4001	BCR	C23-C22-C21	2.31	122.48	118.94
15	K	1401	CLA	CAC-C3C-C4C	2.30	127.80	124.81
15	B	1206	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	F	4015	BCR	C30-C25-C26	-2.30	119.37	122.61
14	F	4015	BCR	C19-C18-C17	2.30	122.47	118.94
15	B	1218	CLA	C1-C2-C3	-2.30	122.07	126.04
15	A	1112	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	A	1132	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
15	A	1113	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
14	B	4006	BCR	C23-C24-C25	-2.30	120.76	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4016	BCR	C33-C5-C4	2.30	118.03	113.62
14	F	4016	BCR	C7-C6-C5	-2.29	115.91	121.46
15	A	1136	CLA	CAC-C3C-C4C	2.29	127.78	124.81
15	B	1208	CLA	CMC-C2C-C1C	2.29	128.52	125.04
15	B	1021	CLA	C1-O2A-CGA	2.29	122.44	116.44
10	B	2002	PQN	C2M-C2-C1	2.29	120.06	116.27
15	B	1227	CLA	OBD-CAD-C3D	-2.29	124.19	127.98
15	A	1104	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
15	A	1124	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
15	A	1117	CLA	C4-C3-C5	2.28	119.11	115.27
14	J	4013	BCR	C19-C18-C17	2.28	122.44	118.94
15	B	1216	CLA	C3C-C4C-NC	2.28	113.13	110.57
15	K	1402	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
15	A	1125	CLA	C6-C5-C3	-2.28	110.89	114.62
15	A	1109	CLA	C3C-C4C-NC	2.28	113.13	110.57
15	A	1124	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	A	1127	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
15	A	1119	CLA	C1-O2A-CGA	2.28	122.42	116.44
15	A	1129	CLA	CMB-C2B-C3B	2.27	128.93	124.68
15	B	1239	CLA	C3C-C4C-NC	2.27	113.12	110.57
15	A	1101	CLA	C4-C3-C2	-2.27	117.84	123.68
15	B	1240	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
15	B	1232	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
14	B	4005	BCR	C38-C26-C27	2.27	117.98	113.62
15	A	1128	CLA	OBD-CAD-C3D	-2.27	124.22	127.98
15	B	1023	CLA	C4-C3-C5	2.27	119.08	115.27
15	A	1138	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
15	B	1207	CLA	CMB-C2B-C3B	2.27	128.92	124.68
15	A	1121	CLA	CAC-C3C-C4C	2.27	127.75	124.81
14	A	4008	BCR	C28-C27-C26	-2.26	110.04	114.08
15	A	1111	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	B	1023	CLA	CMB-C2B-C3B	2.26	128.91	124.68
14	B	4014	BCR	C38-C26-C27	2.26	117.96	113.62
15	A	1105	CLA	CMB-C2B-C3B	2.26	128.90	124.68
15	F	1301	CLA	CHB-C4A-NA	2.26	127.63	124.51
15	A	1128	CLA	CMB-C2B-C3B	2.26	128.90	124.68
14	B	4004	BCR	C30-C25-C26	-2.26	119.44	122.61
14	B	4005	BCR	C33-C5-C4	2.26	117.95	113.62
15	B	1023	CLA	C3C-C4C-NC	2.26	113.10	110.57
15	A	1140	CLA	C4-C3-C5	2.25	119.06	115.27
14	A	4007	BCR	C27-C26-C25	-2.25	119.46	122.73
15	A	1111	CLA	C3C-C4C-NC	2.25	113.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	2002	PQN	C11-C12-C13	-2.25	123.05	126.79
15	A	1801	CLA	C1-O2A-CGA	2.25	122.34	116.44
14	A	4007	BCR	C34-C9-C8	2.25	121.61	118.08
15	B	1023	CLA	OBD-CAD-C3D	-2.24	124.25	127.98
15	A	1119	CLA	CED-O2D-CGD	2.24	121.01	115.94
15	A	1103	CLA	CED-O2D-CGD	2.24	121.01	115.94
15	B	1204	CLA	CAC-C3C-C4C	2.24	127.72	124.81
15	B	1202	CLA	CHB-C4A-NA	2.24	127.61	124.51
15	B	1215	CLA	CAC-C3C-C4C	2.24	127.72	124.81
15	B	1013	CLA	CHB-C4A-NA	2.24	127.61	124.51
14	F	4015	BCR	C23-C24-C25	-2.24	120.92	127.20
15	A	1130	CLA	C1-O2A-CGA	2.24	122.31	116.44
15	B	1021	CLA	CED-O2D-CGD	2.24	120.99	115.94
15	A	1126	CLA	C1-C2-C3	-2.24	122.18	126.04
15	B	1231	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
14	A	4002	BCR	C33-C5-C4	2.23	117.91	113.62
15	A	1126	CLA	CAC-C3C-C4C	2.23	127.71	124.81
15	A	1122	CLA	C3C-C4C-NC	2.23	113.08	110.57
15	B	1213	CLA	C3C-C4C-NC	2.23	113.07	110.57
15	A	1126	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
15	B	1021	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	A	1116	CLA	CAC-C3C-C4C	2.23	127.70	124.81
14	F	4015	BCR	C37-C22-C21	-2.23	119.80	122.92
15	B	1206	CLA	OBD-CAD-C3D	-2.23	124.29	127.98
15	A	1109	CLA	C1-C2-C3	-2.22	122.20	126.04
15	A	1135	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
12	B	5004	LHG	O7-C7-O9	-2.22	118.34	123.70
13	A	1108	CL0	CGD-CBD-CAD	-2.22	103.55	110.73
15	A	1106	CLA	C3C-C4C-NC	2.22	113.06	110.57
14	A	4001	BCR	C30-C25-C24	2.22	122.05	115.78
12	A	5001	LHG	O8-C23-C24	2.21	118.86	111.91
15	B	1238	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
15	A	1801	CLA	CAC-C3C-C2C	2.21	131.31	127.53
15	A	1116	CLA	C4-C3-C5	2.21	118.99	115.27
15	A	1101	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
14	A	4007	BCR	C37-C22-C21	-2.21	119.83	122.92
15	A	1103	CLA	CAC-C3C-C4C	2.21	127.67	124.81
15	B	1227	CLA	CHB-C4A-NA	2.20	127.56	124.51
15	A	1111	CLA	C1-O2A-CGA	2.20	122.23	116.44
15	A	1127	CLA	CED-O2D-CGD	2.20	120.92	115.94
15	A	1801	CLA	C1-C2-C3	-2.20	122.23	126.04
15	B	1228	CLA	CED-O2D-CGD	2.20	120.92	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1206	CLA	C3C-C4C-NC	2.20	113.04	110.57
15	A	1109	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
14	F	4015	BCR	C32-C1-C6	-2.19	106.74	110.30
14	B	4006	BCR	C15-C14-C13	-2.19	124.18	127.31
15	A	1131	CLA	C1-C2-C3	-2.19	122.25	126.04
15	B	1219	CLA	C3C-C4C-NC	2.19	113.03	110.57
15	B	1212	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
14	A	4003	BCR	C8-C9-C10	2.19	122.30	118.94
15	A	1126	CLA	C4-C3-C5	2.19	118.95	115.27
15	B	1231	CLA	CMC-C2C-C1C	2.19	128.37	125.04
15	B	1224	CLA	C3C-C4C-NC	2.18	113.02	110.57
15	A	1109	CLA	C4-C3-C2	-2.18	118.07	123.68
15	B	1211	CLA	CAC-C3C-C4C	2.18	127.64	124.81
15	J	1302	CLA	CMB-C2B-C3B	2.18	128.76	124.68
15	B	1021	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
14	B	4004	BCR	C35-C13-C14	-2.18	119.87	122.92
15	B	1219	CLA	C1-O2A-CGA	2.18	122.16	116.44
15	B	1201	CLA	CAC-C3C-C4C	2.18	127.63	124.81
15	B	1235	CLA	C1-O2A-CGA	2.18	122.15	116.44
14	A	4001	BCR	C31-C1-C6	-2.18	106.77	110.30
15	A	1128	CLA	C1-C2-C3	-2.17	122.28	126.04
15	B	1232	CLA	CMB-C2B-C3B	2.17	128.74	124.68
14	B	4005	BCR	C23-C24-C25	-2.17	121.10	127.20
15	B	1023	CLA	CAC-C3C-C4C	2.17	127.62	124.81
13	A	1108	CL0	CHB-C4A-NA	2.17	127.51	124.51
15	B	1236	CLA	C1-O2A-CGA	2.16	122.12	116.44
15	B	1205	CLA	CMB-C2B-C3B	2.16	128.72	124.68
15	B	1021	CLA	C4-C3-C5	2.16	118.90	115.27
15	B	1013	CLA	C4-C3-C5	2.16	118.90	115.27
15	B	1021	CLA	CMB-C2B-C3B	2.16	128.72	124.68
15	B	1214	CLA	C3C-C4C-NC	2.16	112.99	110.57
15	K	1401	CLA	CHB-C4A-NA	2.16	127.49	124.51
15	B	1221	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	B	1208	CLA	C3C-C4C-NC	2.15	112.99	110.57
15	A	1102	CLA	C1-O2A-CGA	2.15	122.09	116.44
15	K	1401	CLA	CED-O2D-CGD	2.15	120.81	115.94
15	A	1118	CLA	CMB-C2B-C3B	2.15	128.71	124.68
14	J	4013	BCR	C35-C13-C14	-2.15	119.91	122.92
15	F	1139	CLA	C4-C3-C2	-2.15	118.16	123.68
15	A	1102	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	A	1125	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
14	F	4016	BCR	C7-C8-C9	-2.15	122.99	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1135	CLA	CED-O2D-CGD	2.14	120.79	115.94
12	A	5003	LHG	O7-C7-O9	-2.14	118.52	123.70
14	B	4014	BCR	C33-C5-C4	2.14	117.73	113.62
13	A	1011	CL0	CMB-C2B-C3B	2.14	128.68	124.68
15	B	1207	CLA	CHB-C4A-NA	2.14	127.47	124.51
15	A	1123	CLA	C4-C3-C5	2.14	118.87	115.27
15	B	1205	CLA	C4-C3-C5	2.13	118.86	115.27
14	A	4012	BCR	C33-C5-C4	2.13	117.71	113.62
13	A	1108	CL0	OBD-CAD-C3D	-2.13	124.44	127.98
14	F	4015	BCR	C27-C26-C25	-2.13	119.64	122.73
15	A	1131	CLA	CED-O2D-CGD	2.13	120.75	115.94
15	A	1116	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
15	F	1410	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
15	B	1204	CLA	C3C-C4C-NC	2.13	112.96	110.57
15	B	1206	CLA	CHB-C4A-NA	2.13	127.45	124.51
15	A	1122	CLA	CMD-C2D-C3D	-2.13	120.70	124.68
15	A	1128	CLA	CMC-C2C-C1C	2.12	128.27	125.04
15	A	1118	CLA	CHB-C4A-NA	2.12	127.45	124.51
15	A	1136	CLA	CMB-C2B-C3B	2.12	128.65	124.68
15	A	1126	CLA	CHB-C4A-NA	2.12	127.44	124.51
15	B	1203	CLA	C1-C2-C3	-2.12	122.38	126.04
14	B	4004	BCR	C23-C24-C25	-2.12	121.25	127.20
15	A	1112	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
15	B	1214	CLA	OBD-CAD-C3D	-2.12	124.47	127.98
15	A	1107	CLA	CAC-C3C-C4C	2.12	127.56	124.81
14	B	4006	BCR	C19-C18-C17	2.12	122.19	118.94
15	B	1230	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
15	B	1227	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
15	J	1302	CLA	CAC-C3C-C4C	2.11	127.55	124.81
14	F	4015	BCR	C33-C5-C4	2.11	117.67	113.62
15	A	1131	CLA	CMB-C2B-C3B	2.11	128.63	124.68
14	A	4003	BCR	C23-C24-C25	-2.11	121.28	127.20
15	A	1116	CLA	CMB-C2B-C3B	2.11	128.62	124.68
15	A	1124	CLA	CED-O2D-CGD	2.11	120.70	115.94
14	B	4010	BCR	C7-C8-C9	-2.11	123.05	126.23
13	A	1108	CL0	O2D-CGD-O1D	-2.10	119.72	123.84
15	A	1137	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
16	B	1301	LMU	O5'-C5'-C4'	2.10	114.19	109.75
15	B	1214	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
15	B	1211	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
15	B	1023	CLA	CHB-C4A-NA	2.10	127.42	124.51
15	B	1235	CLA	CHB-C4A-NA	2.10	127.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	1402	CLA	CMB-C2B-C3B	2.09	128.60	124.68
14	B	4004	BCR	C3-C4-C5	-2.09	110.34	114.08
15	A	1130	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
15	A	1119	CLA	CAC-C3C-C4C	2.09	127.52	124.81
14	B	4014	BCR	C3-C4-C5	-2.09	110.35	114.08
15	B	1210	CLA	C16-C15-C13	-2.09	109.17	115.92
15	B	1209	CLA	CHB-C4A-NA	2.09	127.40	124.51
15	B	1021	CLA	C11-C12-C13	-2.09	109.17	115.92
15	A	1115	CLA	CAC-C3C-C4C	2.09	127.52	124.81
14	B	4005	BCR	C35-C13-C12	2.09	121.36	118.08
15	A	1115	CLA	OBD-CAD-C3D	-2.09	124.52	127.98
16	B	1301	LMU	C1'-O5'-C5'	2.08	117.78	113.69
15	A	1123	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
15	B	1216	CLA	CAC-C3C-C4C	2.08	127.51	124.81
15	B	1214	CLA	CHB-C4A-NA	2.08	127.39	124.51
16	B	1301	LMU	O1'-C1'-C2'	-2.08	105.06	108.30
15	A	1128	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
15	B	1230	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
14	B	4004	BCR	C24-C23-C22	-2.06	123.11	126.23
14	J	4013	BCR	C35-C13-C12	2.06	121.33	118.08
13	A	1108	CL0	CMB-C2B-C3B	2.06	128.53	124.68
15	A	1122	CLA	CED-O2D-CGD	2.06	120.59	115.94
14	B	4017	BCR	C31-C1-C6	-2.06	106.96	110.30
15	B	1013	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
14	J	4013	BCR	C23-C22-C21	2.06	122.10	118.94
15	B	1225	CLA	C1-O2A-CGA	2.06	121.84	116.44
15	B	1217	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
15	B	1236	CLA	CHD-C4C-C3C	-2.06	121.82	124.84
15	B	1239	CLA	CHC-C1C-C2C	-2.06	121.04	126.72
15	A	1121	CLA	CMB-C2B-C3B	2.05	128.52	124.68
14	A	4012	BCR	C35-C13-C12	2.05	121.31	118.08
15	A	1129	CLA	CAC-C3C-C4C	2.05	127.47	124.81
15	A	1128	CLA	CHB-C4A-NA	2.05	127.35	124.51
15	A	1801	CLA	CHB-C4A-NA	2.05	127.35	124.51
15	A	1801	CLA	C4-C3-C2	-2.05	118.42	123.68
14	B	4010	BCR	C8-C7-C6	-2.05	121.45	127.20
15	A	1125	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
15	A	1123	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
15	A	1116	CLA	CHB-C4A-NA	2.05	127.34	124.51
15	A	1113	CLA	CHB-C4A-NA	2.05	127.34	124.51
14	B	4006	BCR	C38-C26-C27	2.05	117.55	113.62
15	B	1204	CLA	CHB-C4A-NA	2.04	127.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4008	BCR	C37-C22-C21	-2.04	120.06	122.92
14	B	4006	BCR	C29-C28-C27	2.04	115.94	111.38
15	A	1113	CLA	CAA-CBA-CGA	-2.04	109.20	113.59
14	A	4007	BCR	C35-C13-C12	2.04	121.29	118.08
14	B	4010	BCR	C19-C18-C17	2.04	122.07	118.94
15	A	1124	CLA	C1-C2-C3	-2.04	122.51	126.04
15	A	1117	CLA	C1-C2-C3	-2.04	122.52	126.04
15	A	1126	CLA	C6-C5-C3	-2.04	108.11	113.45
14	B	4017	BCR	C15-C14-C13	-2.04	124.40	127.31
15	B	1023	CLA	C1-O2A-CGA	2.04	121.78	116.44
15	B	1220	CLA	C4-C3-C5	2.03	118.69	115.27
15	A	1140	CLA	C1-C2-C3	-2.03	122.53	126.04
15	J	1303	CLA	CHB-C4A-NA	2.03	127.32	124.51
15	A	1120	CLA	CED-O2D-CGD	2.03	120.53	115.94
15	A	1120	CLA	CHB-C4A-NA	2.03	127.32	124.51
15	A	1138	CLA	CHB-C4A-NA	2.03	127.32	124.51
15	A	1126	CLA	C3C-C4C-NC	2.03	112.84	110.57
15	A	1103	CLA	C3C-C4C-NC	2.03	112.84	110.57
15	A	1136	CLA	CED-O2D-CGD	2.03	120.52	115.94
15	B	1238	CLA	CAC-C3C-C4C	2.03	127.44	124.81
15	B	1209	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
14	B	4009	BCR	C23-C24-C25	-2.02	121.52	127.20
15	A	1129	CLA	CHB-C4A-NA	2.02	127.31	124.51
15	A	1109	CLA	CED-O2D-CGD	2.02	120.51	115.94
15	B	1240	CLA	CAC-C3C-C4C	2.02	127.43	124.81
15	A	1105	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
15	A	1114	CLA	C1-O2A-CGA	2.02	121.74	116.44
15	B	1229	CLA	CMB-C2B-C3B	2.02	128.45	124.68
15	B	1220	CLA	CAC-C3C-C4C	2.02	127.43	124.81
12	A	5005	LHG	O7-C7-O9	-2.02	118.83	123.70
14	A	4012	BCR	C34-C9-C8	2.01	121.25	118.08
15	B	1206	CLA	CED-O2D-CGD	2.01	120.49	115.94
15	A	1126	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
15	J	1303	CLA	CAC-C3C-C4C	2.01	127.42	124.81
15	B	1207	CLA	CAC-C3C-C4C	2.01	127.42	124.81
15	A	1136	CLA	CHB-C4A-NA	2.01	127.29	124.51
15	B	1226	CLA	CHB-C4A-NA	2.01	127.29	124.51
15	A	1134	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
15	A	1120	CLA	CAC-C3C-C4C	2.01	127.41	124.81
15	A	1106	CLA	CHB-C4A-NA	2.01	127.29	124.51
15	A	1107	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
15	K	1402	CLA	CAC-C3C-C4C	2.00	127.41	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1215	CLA	OBD-CAD-C3D	-2.00	124.66	127.98
15	B	1013	CLA	OBD-CAD-C3D	-2.00	124.66	127.98
15	B	1234	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (258) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	B	1213	CLA	NC
15	B	1213	CLA	NA
15	A	1118	CLA	NC
15	A	1118	CLA	ND
15	A	1118	CLA	NA
15	B	1204	CLA	NC
15	B	1204	CLA	ND
15	B	1204	CLA	NA
15	B	1227	CLA	NC
15	B	1227	CLA	NA
15	A	1022	CLA	ND
15	A	1022	CLA	NA
15	J	1302	CLA	NC
15	J	1302	CLA	ND
15	J	1302	CLA	NA
15	B	1207	CLA	NC
15	B	1207	CLA	ND
15	B	1207	CLA	NA
15	F	1410	CLA	ND
15	F	1410	CLA	NA
15	A	1134	CLA	NC
15	A	1134	CLA	ND
15	A	1134	CLA	NA
15	A	1114	CLA	NC
15	A	1114	CLA	ND
15	A	1114	CLA	NA
15	A	1110	CLA	NC
15	A	1110	CLA	ND
15	A	1110	CLA	NA
15	B	1220	CLA	NC
15	B	1220	CLA	ND
15	B	1220	CLA	NA
15	B	1240	CLA	NC
15	B	1240	CLA	ND
15	B	1240	CLA	NA

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Mol	Chain	Res	Type	Atom
15	B	1225	CLA	NC
15	B	1225	CLA	ND
15	B	1225	CLA	NA
15	A	1128	CLA	NC
15	A	1128	CLA	ND
15	A	1128	CLA	NA
15	A	1105	CLA	NC
15	A	1105	CLA	ND
15	A	1105	CLA	NA
15	B	1209	CLA	NC
15	B	1209	CLA	ND
15	B	1209	CLA	NA
15	B	1234	CLA	NC
15	B	1234	CLA	ND
15	B	1234	CLA	NA
15	A	1124	CLA	NC
15	A	1124	CLA	ND
15	A	1124	CLA	NA
15	A	1121	CLA	NC
15	A	1121	CLA	ND
15	A	1121	CLA	NA
15	A	1104	CLA	NC
15	A	1104	CLA	ND
15	A	1104	CLA	NA
15	B	1203	CLA	ND
15	B	1203	CLA	NA
15	B	1217	CLA	NC
15	B	1217	CLA	ND
15	B	1217	CLA	NA
15	B	1218	CLA	NC
15	B	1218	CLA	ND
15	B	1218	CLA	NA
15	B	1201	CLA	NC
15	B	1201	CLA	ND
15	B	1201	CLA	NA
15	A	1137	CLA	NC
15	A	1137	CLA	NA
15	A	1137	CLA	ND
15	B	1232	CLA	NC
15	B	1232	CLA	ND
15	B	1232	CLA	NA
15	A	1138	CLA	NC

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Mol	Chain	Res	Type	Atom
15	A	1138	CLA	ND
15	A	1138	CLA	NA
15	B	1222	CLA	NC
15	B	1222	CLA	NA
15	A	1101	CLA	NC
15	A	1101	CLA	ND
15	A	1101	CLA	NA
15	A	1115	CLA	NC
15	A	1115	CLA	ND
15	A	1115	CLA	NA
15	A	1123	CLA	NC
15	A	1123	CLA	ND
15	A	1123	CLA	NA
15	F	1139	CLA	NC
15	F	1139	CLA	ND
15	F	1139	CLA	NA
15	B	1224	CLA	NC
15	B	1224	CLA	NA
15	B	1224	CLA	ND
15	B	1205	CLA	NC
15	B	1205	CLA	ND
15	B	1205	CLA	NA
15	A	1126	CLA	NA
15	A	1801	CLA	NC
15	A	1801	CLA	ND
15	A	1801	CLA	NA
15	B	1236	CLA	ND
15	B	1236	CLA	NA
15	B	1212	CLA	NC
15	B	1212	CLA	ND
15	B	1212	CLA	NA
15	B	1238	CLA	NC
15	B	1238	CLA	ND
15	B	1238	CLA	NA
15	A	1120	CLA	NC
15	A	1120	CLA	ND
15	A	1120	CLA	NA
15	B	1219	CLA	NC
15	B	1219	CLA	ND
15	B	1219	CLA	NA
15	A	1116	CLA	NC
15	A	1116	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1116	CLA	NA
15	A	1122	CLA	NC
15	A	1122	CLA	ND
15	A	1122	CLA	NA
15	A	1127	CLA	NC
15	A	1127	CLA	ND
15	A	1127	CLA	NA
15	A	1107	CLA	NC
15	A	1107	CLA	NA
15	B	1023	CLA	NC
15	B	1023	CLA	ND
15	B	1023	CLA	NA
15	A	1135	CLA	NC
15	A	1135	CLA	ND
15	A	1135	CLA	NA
15	A	1119	CLA	NC
15	A	1119	CLA	NA
15	B	1239	CLA	NC
15	B	1239	CLA	ND
15	B	1239	CLA	NA
15	B	1230	CLA	NC
15	B	1230	CLA	ND
15	B	1230	CLA	NA
15	K	1401	CLA	NC
15	K	1401	CLA	NA
15	K	1401	CLA	ND
15	B	1228	CLA	NC
15	B	1228	CLA	ND
15	B	1228	CLA	NA
15	B	1214	CLA	NC
15	B	1214	CLA	NA
15	A	1133	CLA	NC
15	A	1133	CLA	ND
15	A	1133	CLA	NA
15	A	1117	CLA	NC
15	A	1117	CLA	ND
15	A	1117	CLA	NA
15	J	1303	CLA	NC
15	J	1303	CLA	NA
15	J	1303	CLA	ND
15	B	1208	CLA	NC
15	B	1208	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1208	CLA	NA
15	A	1131	CLA	NC
15	A	1131	CLA	NA
15	A	1131	CLA	ND
15	A	1111	CLA	NC
15	A	1111	CLA	ND
15	A	1111	CLA	NA
15	A	1136	CLA	NC
15	A	1136	CLA	ND
15	A	1136	CLA	NA
15	B	1226	CLA	NC
15	B	1226	CLA	ND
15	B	1226	CLA	NA
15	B	1221	CLA	NC
15	B	1221	CLA	NA
15	B	1221	CLA	ND
15	B	1202	CLA	NC
15	B	1202	CLA	NA
15	B	1202	CLA	ND
13	A	1108	CL0	NC
13	A	1108	CL0	ND
13	A	1108	CL0	NA
15	A	1102	CLA	NC
15	A	1102	CLA	ND
15	A	1102	CLA	NA
15	B	1211	CLA	NC
15	B	1211	CLA	ND
15	B	1211	CLA	NA
15	B	1021	CLA	NC
15	B	1021	CLA	ND
15	B	1021	CLA	NA
15	B	1235	CLA	NC
15	B	1235	CLA	ND
15	B	1235	CLA	NA
15	A	1112	CLA	NC
15	A	1112	CLA	ND
15	A	1112	CLA	NA
15	B	1216	CLA	NC
15	B	1216	CLA	NA
15	A	1132	CLA	NC
15	A	1132	CLA	ND
15	A	1132	CLA	NA

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Mol	Chain	Res	Type	Atom
15	A	1113	CLA	NC
15	A	1113	CLA	ND
15	A	1113	CLA	NA
15	B	1206	CLA	NC
15	B	1206	CLA	ND
15	B	1206	CLA	NA
15	A	1140	CLA	NC
15	A	1140	CLA	ND
15	A	1140	CLA	NA
15	A	1012	CLA	ND
15	A	1012	CLA	NA
15	A	1125	CLA	ND
15	A	1125	CLA	NA
15	B	1237	CLA	NC
15	B	1237	CLA	ND
15	B	1237	CLA	NA
15	A	1129	CLA	NC
15	A	1129	CLA	ND
15	A	1129	CLA	NA
15	B	1013	CLA	NC
15	B	1013	CLA	NA
15	B	1223	CLA	NC
15	B	1223	CLA	ND
15	B	1223	CLA	NA
13	A	1011	CL0	NC
13	A	1011	CL0	ND
13	A	1011	CL0	NA
15	A	1109	CLA	NC
15	A	1109	CLA	NA
15	B	1229	CLA	NC
15	B	1229	CLA	ND
15	B	1229	CLA	NA
15	B	1231	CLA	NC
15	B	1231	CLA	ND
15	B	1231	CLA	NA
15	F	1301	CLA	NC
15	F	1301	CLA	ND
15	F	1301	CLA	NA
15	K	1402	CLA	NC
15	K	1402	CLA	NA
15	K	1402	CLA	ND
15	A	1103	CLA	NC

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Mol	Chain	Res	Type	Atom
15	A	1103	CLA	NA
15	A	1103	CLA	ND
15	A	1106	CLA	NC
15	A	1106	CLA	ND
15	A	1106	CLA	NA
15	A	1130	CLA	NC
15	A	1130	CLA	ND
15	A	1130	CLA	NA
15	B	1215	CLA	ND
15	B	1215	CLA	NA
15	B	1210	CLA	NC
15	B	1210	CLA	ND
15	B	1210	CLA	NA

All (1338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
14	B	4004	BCR	C1-C6-C7-C8
14	B	4004	BCR	C5-C6-C7-C8
14	B	4004	BCR	C7-C8-C9-C10
14	B	4004	BCR	C21-C22-C23-C24
14	B	4004	BCR	C37-C22-C23-C24
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	B	1204	CLA	CHA-CBD-CGD-O2D
12	A	5005	LHG	O1-C1-C2-C3
12	A	5005	LHG	C2-C3-O3-P
12	A	5005	LHG	C3-O3-P-O4
12	A	5005	LHG	C3-O3-P-O5
15	A	1022	CLA	C2-C1-O2A-CGA
15	A	1022	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	C1A-C2A-CAA-CBA
15	J	1302	CLA	C3A-C2A-CAA-CBA
15	B	1207	CLA	CBD-CGD-O2D-CED
15	F	1410	CLA	C2-C3-C5-C6
15	F	1410	CLA	C4-C3-C5-C6
15	A	1134	CLA	CBA-CGA-O2A-C1
15	A	1134	CLA	CBD-CGD-O2D-CED
15	A	1110	CLA	C1A-C2A-CAA-CBA
15	B	1220	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1220	CLA	CHA-CBD-CGD-O1D
15	B	1220	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1225	CLA	C3A-C2A-CAA-CBA
15	B	1225	CLA	CHA-CBD-CGD-O1D
15	B	1225	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1105	CLA	CBD-CGD-O2D-CED
14	B	4017	BCR	C7-C8-C9-C10
14	B	4017	BCR	C7-C8-C9-C34
14	B	4017	BCR	C11-C10-C9-C8
14	B	4017	BCR	C11-C10-C9-C34
14	B	4017	BCR	C10-C11-C12-C13
15	A	1124	CLA	C1A-C2A-CAA-CBA
15	A	1124	CLA	C3A-C2A-CAA-CBA
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	A	1104	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	CBD-CGD-O2D-CED
15	B	1218	CLA	C2-C3-C5-C6
15	B	1218	CLA	C4-C3-C5-C6
12	A	5001	LHG	C1-C2-C3-O3
14	B	4009	BCR	C11-C10-C9-C8
14	B	4009	BCR	C11-C10-C9-C34
14	B	4009	BCR	C10-C11-C12-C13
15	A	1137	CLA	C2-C1-O2A-CGA
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C34
14	B	4005	BCR	C21-C22-C23-C24
15	A	1138	CLA	CHA-CBD-CGD-O1D
15	B	1222	CLA	C1A-C2A-CAA-CBA
15	B	1222	CLA	C3A-C2A-CAA-CBA
15	A	1115	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	C1A-C2A-CAA-CBA
15	A	1123	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1123	CLA	C2-C1-O2A-CGA
15	F	1139	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1224	CLA	CBD-CGD-O2D-CED
14	F	4015	BCR	C17-C18-C19-C20
14	F	4015	BCR	C36-C18-C19-C20
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1801	CLA	CBA-CGA-O2A-C1
15	A	1801	CLA	O1A-CGA-O2A-C1
15	A	1801	CLA	CAD-CBD-CGD-O1D
15	A	1801	CLA	CAD-CBD-CGD-O2D
15	B	1236	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	A	1120	CLA	C3A-C2A-CAA-CBA
15	A	1120	CLA	CBD-CGD-O2D-CED
14	F	4016	BCR	C5-C6-C7-C8
14	F	4016	BCR	C7-C8-C9-C10
14	F	4016	BCR	C7-C8-C9-C34
14	F	4016	BCR	C11-C10-C9-C34
14	F	4016	BCR	C10-C11-C12-C13
14	F	4016	BCR	C19-C20-C21-C22
14	F	4016	BCR	C21-C22-C23-C24
14	F	4016	BCR	C37-C22-C23-C24
14	B	4011	BCR	C7-C8-C9-C10
14	B	4011	BCR	C7-C8-C9-C34
14	B	4011	BCR	C36-C18-C19-C20
14	B	4011	BCR	C23-C24-C25-C26
14	B	4011	BCR	C23-C24-C25-C30
15	B	1219	CLA	C2-C1-O2A-CGA
14	B	4014	BCR	C7-C8-C9-C10
14	B	4014	BCR	C7-C8-C9-C34
14	B	4014	BCR	C11-C10-C9-C8
14	B	4014	BCR	C11-C10-C9-C34
14	B	4014	BCR	C10-C11-C12-C13
14	B	4014	BCR	C37-C22-C23-C24
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1122	CLA	CHA-CBD-CGD-O1D
15	A	1122	CLA	CHA-CBD-CGD-O2D
15	A	1127	CLA	C2-C3-C5-C6
15	A	1127	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B	1023	CLA	CBD-CGD-O2D-CED
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C21-C22-C23-C24
14	B	4006	BCR	C37-C22-C23-C24
14	B	4006	BCR	C23-C24-C25-C26
14	B	4006	BCR	C23-C24-C25-C30
15	A	1135	CLA	CHA-CBD-CGD-O1D
15	A	1135	CLA	CHA-CBD-CGD-O2D
15	A	1135	CLA	CBD-CGD-O2D-CED
14	J	4013	BCR	C11-C10-C9-C8
14	J	4013	BCR	C11-C10-C9-C34
14	J	4013	BCR	C21-C22-C23-C24
14	J	4013	BCR	C37-C22-C23-C24
14	J	4013	BCR	C23-C24-C25-C26
14	J	4013	BCR	C23-C24-C25-C30
15	A	1119	CLA	CHA-CBD-CGD-O1D
15	B	1239	CLA	C3A-C2A-CAA-CBA
15	B	1239	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	K	1401	CLA	C3A-C2A-CAA-CBA
15	K	1401	CLA	CBA-CGA-O2A-C1
15	K	1401	CLA	CHA-CBD-CGD-O1D
15	K	1401	CLA	CHA-CBD-CGD-O2D
15	K	1401	CLA	CAD-CBD-CGD-O1D
15	K	1401	CLA	CAD-CBD-CGD-O2D
14	A	4012	BCR	C7-C8-C9-C10
14	A	4012	BCR	C7-C8-C9-C34
14	A	4012	BCR	C10-C11-C12-C13
14	A	4012	BCR	C37-C22-C23-C24
15	B	1228	CLA	C2-C1-O2A-CGA
15	A	1133	CLA	C1A-C2A-CAA-CBA
15	A	1133	CLA	C3A-C2A-CAA-CBA
15	A	1133	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	C2-C1-O2A-CGA
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	B	1202	CLA	CHA-CBD-CGD-O1D
15	B	1202	CLA	CAD-CBD-CGD-O1D
15	B	1202	CLA	CAD-CBD-CGD-O2D
14	A	4003	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	A	4003	BCR	C7-C8-C9-C34
14	A	4003	BCR	C11-C10-C9-C8
14	A	4003	BCR	C11-C10-C9-C34
14	A	4003	BCR	C15-C16-C17-C18
14	A	4003	BCR	C36-C18-C19-C20
14	B	4010	BCR	C17-C18-C19-C20
14	B	4010	BCR	C36-C18-C19-C20
14	B	4010	BCR	C23-C24-C25-C26
14	B	4010	BCR	C23-C24-C25-C30
13	A	1108	CL0	CBD-CGD-O2D-CED
15	A	1102	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	C1A-C2A-CAA-CBA
15	B	1021	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	O1D-CGD-O2D-CED
15	B	1021	CLA	C6-C7-C8-C9
12	A	5003	LHG	C1-C2-C3-O3
15	B	1235	CLA	CHA-CBD-CGD-O1D
15	B	1235	CLA	CHA-CBD-CGD-O2D
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C3A-C2A-CAA-CBA
15	A	1112	CLA	CBD-CGD-O2D-CED
14	A	4002	BCR	C7-C8-C9-C10
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C11-C10-C9-C34
15	A	1132	CLA	C11-C10-C8-C7
15	A	1113	CLA	CHA-CBD-CGD-O1D
15	A	1113	CLA	CHA-CBD-CGD-O2D
15	A	1113	CLA	CBD-CGD-O2D-CED
15	B	1206	CLA	CBA-CGA-O2A-C1
15	B	1206	CLA	CBD-CGD-O2D-CED
15	A	1012	CLA	CHA-CBD-CGD-O1D
15	A	1012	CLA	CHA-CBD-CGD-O2D
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	CAD-CBD-CGD-O2D
15	A	1012	CLA	O2A-C1-C2-C3
15	B	1237	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C3A-C2A-CAA-CBA
15	B	1237	CLA	CBD-CGD-O2D-CED
14	A	4007	BCR	C7-C8-C9-C10
14	A	4007	BCR	C7-C8-C9-C34
15	A	1129	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	CBA-CGA-O2A-C1
12	B	5004	LHG	O1-C1-C2-C3
12	B	5004	LHG	C3-O3-P-O4
12	B	5004	LHG	C3-O3-P-O5
12	B	5004	LHG	C3-O3-P-O6
15	B	1013	CLA	C2-C1-O2A-CGA
15	A	1109	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	C1A-C2A-CAA-CBA
15	B	1231	CLA	CBD-CGD-O2D-CED
14	A	4001	BCR	C7-C8-C9-C10
14	A	4001	BCR	C7-C8-C9-C34
14	A	4001	BCR	C11-C10-C9-C8
14	A	4001	BCR	C11-C10-C9-C34
14	A	4001	BCR	C21-C22-C23-C24
14	A	4001	BCR	C37-C22-C23-C24
14	A	4001	BCR	C23-C24-C25-C26
15	F	1301	CLA	CBD-CGD-O2D-CED
15	A	1103	CLA	CHA-CBD-CGD-O1D
15	A	1103	CLA	CHA-CBD-CGD-O2D
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1215	CLA	CBD-CGD-O2D-CED
15	B	1215	CLA	C4-C3-C5-C6
15	B	1215	CLA	C11-C12-C13-C14
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	A	1134	CLA	O1D-CGD-O2D-CED
15	A	1124	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	B	1238	CLA	O1D-CGD-O2D-CED
15	J	1303	CLA	O1D-CGD-O2D-CED
15	B	1208	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	A	1109	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	B	1240	CLA	O1D-CGD-O2D-CED
15	B	1232	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1117	CLA	O1D-CGD-O2D-CED
15	B	1231	CLA	O1D-CGD-O2D-CED
15	K	1402	CLA	O1D-CGD-O2D-CED
15	A	1118	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	CBD-CGD-O2D-CED
15	F	1410	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	B	1240	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBD-CGD-O2D-CED
15	B	1203	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	CBD-CGD-O2D-CED
15	B	1205	CLA	CBD-CGD-O2D-CED
15	B	1219	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CBD-CGD-O2D-CED
15	K	1401	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	J	1303	CLA	CBD-CGD-O2D-CED
15	B	1208	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
15	A	1111	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	CBD-CGD-O2D-CED
15	B	1223	CLA	CBD-CGD-O2D-CED
15	K	1402	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CBD-CGD-O2D-CED
15	B	1210	CLA	CBD-CGD-O2D-CED
15	F	1410	CLA	O1A-CGA-O2A-C1
15	A	1110	CLA	O1A-CGA-O2A-C1
15	B	1013	CLA	O1A-CGA-O2A-C1
15	A	1134	CLA	O1A-CGA-O2A-C1
15	A	1115	CLA	O1A-CGA-O2A-C1
15	K	1401	CLA	O1A-CGA-O2A-C1
15	A	1133	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1206	CLA	O1A-CGA-O2A-C1
15	A	1129	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	O1D-CGD-O2D-CED
15	A	1131	CLA	O1D-CGD-O2D-CED
15	B	1211	CLA	CBA-CGA-O2A-C1
15	A	1801	CLA	C4C-C3C-CAC-CBC
12	A	5005	LHG	C5-C6-O8-C23
15	A	1022	CLA	O1D-CGD-O2D-CED
15	F	1410	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	B	1218	CLA	O1D-CGD-O2D-CED
15	A	1120	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	O1D-CGD-O2D-CED
15	B	1239	CLA	O1D-CGD-O2D-CED
15	A	1111	CLA	O1D-CGD-O2D-CED
13	A	1108	CL0	O1D-CGD-O2D-CED
15	A	1110	CLA	CBA-CGA-O2A-C1
15	B	1213	CLA	CBD-CGD-O2D-CED
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1220	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CBD-CGD-O2D-CED
15	B	1201	CLA	CBD-CGD-O2D-CED
15	A	1801	CLA	CBD-CGD-O2D-CED
15	B	1212	CLA	CBD-CGD-O2D-CED
15	A	1122	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	CBD-CGD-O2D-CED
15	B	1214	CLA	CBD-CGD-O2D-CED
15	A	1136	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	CBD-CGD-O2D-CED
15	A	1125	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	CBD-CGD-O2D-CED
15	B	1013	CLA	CBD-CGD-O2D-CED
15	A	1106	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	O1A-CGA-O2A-C1
15	A	1102	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	O1A-CGA-O2A-C1
15	A	1132	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1237	CLA	O1A-CGA-O2A-C1
15	A	1109	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	O1A-CGA-O2A-C1
15	B	1225	CLA	O1D-CGD-O2D-CED
15	B	1236	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	B	1215	CLA	O1D-CGD-O2D-CED
15	B	1207	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1128	CLA	CBD-CGD-O2D-CED
15	A	1102	CLA	CBD-CGD-O2D-CED
15	F	1139	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	O1D-CGD-O2D-CED
15	B	1210	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	CBA-CGA-O2A-C1
15	K	1402	CLA	CBA-CGA-O2A-C1
15	B	1217	CLA	C2-C1-O2A-CGA
15	B	1205	CLA	C3-C5-C6-C7
15	A	1126	CLA	C3-C5-C6-C7
15	A	1131	CLA	C3-C5-C6-C7
15	A	1136	CLA	C3-C5-C6-C7
15	A	1132	CLA	C3-C5-C6-C7
15	A	1012	CLA	C3-C5-C6-C7
15	F	1410	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	CBA-CGA-O2A-C1
15	A	1119	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	CBA-CGA-O2A-C1
15	B	1237	CLA	CBA-CGA-O2A-C1
15	B	1013	CLA	CBA-CGA-O2A-C1
15	A	1109	CLA	CBA-CGA-O2A-C1
15	B	1210	CLA	CBA-CGA-O2A-C1
15	A	1801	CLA	C2C-C3C-CAC-CBC
15	B	1219	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1103	CLA	CBD-CGD-O2D-CED
16	B	1301	LMU	O5B-C5B-C6B-O6B
17	B	5002	LMG	O6-C5-C6-O5
15	B	1214	CLA	C4-C3-C5-C6
16	J	1304	LMU	C4B-C5B-C6B-O6B
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	C2A-CAA-CBA-CGA
15	B	1219	CLA	C2A-CAA-CBA-CGA
15	A	1119	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	C2A-CAA-CBA-CGA
15	A	1119	CLA	O1D-CGD-O2D-CED
15	K	1402	CLA	O1A-CGA-O2A-C1
15	A	1128	CLA	C3-C5-C6-C7
15	B	1226	CLA	C3-C5-C6-C7
15	A	1130	CLA	C3-C5-C6-C7
15	B	1210	CLA	C3-C5-C6-C7
15	B	1226	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	CBA-CGA-O2A-C1
15	A	1102	CLA	CBA-CGA-O2A-C1
15	A	1132	CLA	CBA-CGA-O2A-C1
15	A	1130	CLA	CBA-CGA-O2A-C1
15	A	1118	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1115	CLA	O1D-CGD-O2D-CED
15	K	1401	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	A	1116	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	A	1104	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	O1A-CGA-O2A-C1
15	B	1221	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	C2A-CAA-CBA-CGA
15	A	1138	CLA	O1D-CGD-O2D-CED
14	A	4008	BCR	C19-C20-C21-C22
14	B	4009	BCR	C9-C10-C11-C12
14	B	4014	BCR	C15-C16-C17-C18
14	A	4007	BCR	C19-C20-C21-C22
15	B	1204	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1235	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1229	CLA	CBD-CGD-O2D-CED
12	A	5001	LHG	O2-C2-C3-O3
12	A	5003	LHG	O2-C2-C3-O3
15	B	1203	CLA	C3-C5-C6-C7
15	B	1216	CLA	C3-C5-C6-C7
15	A	1123	CLA	CBA-CGA-O2A-C1
17	B	5002	LMG	C29-C28-O8-C9
15	B	1228	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	O1A-CGA-O2A-C1
15	B	1210	CLA	O1A-CGA-O2A-C1
15	A	1133	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	CBA-CGA-O2A-C1
15	B	1239	CLA	CBA-CGA-O2A-C1
17	B	5002	LMG	C4-C5-C6-O5
15	B	1228	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	O1D-CGD-O2D-CED
15	B	1226	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	C3-C5-C6-C7
15	A	1127	CLA	C3-C5-C6-C7
15	B	1219	CLA	CBA-CGA-O2A-C1
16	J	1304	LMU	O5B-C5B-C6B-O6B
15	B	1225	CLA	C4-C3-C5-C6
15	B	1230	CLA	C4-C3-C5-C6
15	A	1109	CLA	C4-C3-C5-C6
16	B	1301	LMU	C4B-C5B-C6B-O6B
15	B	1225	CLA	C2-C3-C5-C6
15	B	1230	CLA	C2-C3-C5-C6
15	A	1109	CLA	C2-C3-C5-C6
15	B	1215	CLA	C2-C3-C5-C6
15	A	1137	CLA	CBD-CGD-O2D-CED
15	A	1801	CLA	C2A-CAA-CBA-CGA
15	A	1111	CLA	C2A-CAA-CBA-CGA
15	A	1801	CLA	O1D-CGD-O2D-CED
16	B	1301	LMU	O5'-C5'-C6'-O6'
17	B	5002	LMG	O10-C28-O8-C9
15	B	1230	CLA	O1D-CGD-O2D-CED
15	B	1220	CLA	O1D-CGD-O2D-CED
15	B	1223	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	O1D-CGD-O2D-CED
15	B	1213	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1201	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	O1D-CGD-O2D-CED
15	B	1212	CLA	O1D-CGD-O2D-CED
15	A	1106	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	B	1218	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	B	1218	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	CBA-CGA-O2A-C1
15	A	1140	CLA	CBA-CGA-O2A-C1
14	B	4017	BCR	C9-C10-C11-C12
10	A	2001	PQN	C18-C20-C21-C22
15	B	1216	CLA	C15-C16-C17-C18
15	A	1012	CLA	C5-C6-C7-C8
15	B	1214	CLA	C2-C3-C5-C6
15	A	1128	CLA	C6-C7-C8-C9
15	A	1105	CLA	C11-C10-C8-C9
15	A	1105	CLA	C11-C12-C13-C14
15	B	1234	CLA	C14-C13-C15-C16
15	B	1203	CLA	C14-C13-C15-C16
15	B	1013	CLA	C14-C13-C15-C16
15	A	1106	CLA	C14-C13-C15-C16
15	A	1129	CLA	O1D-CGD-O2D-CED
10	B	2002	PQN	C15-C16-C17-C18
15	B	1228	CLA	C10-C11-C12-C13
15	B	1210	CLA	C8-C10-C11-C12
15	A	1126	CLA	C2A-CAA-CBA-CGA
14	A	4008	BCR	C7-C8-C9-C34
14	B	4004	BCR	C7-C8-C9-C34
14	B	4009	BCR	C7-C8-C9-C34
14	B	4005	BCR	C7-C8-C9-C34
14	B	4005	BCR	C37-C22-C23-C24
14	F	4015	BCR	C37-C22-C23-C24
14	B	4011	BCR	C37-C22-C23-C24
14	J	4013	BCR	C7-C8-C9-C34
14	A	4003	BCR	C37-C22-C23-C24
14	A	4008	BCR	C7-C8-C9-C10
14	B	4009	BCR	C7-C8-C9-C10
14	B	4005	BCR	C7-C8-C9-C10
14	B	4011	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	J	4013	BCR	C7-C8-C9-C10
14	A	4012	BCR	C21-C22-C23-C24
14	A	4003	BCR	C17-C18-C19-C20
14	A	4007	BCR	C21-C22-C23-C24
15	A	1122	CLA	O1D-CGD-O2D-CED
15	B	1235	CLA	O1A-CGA-O2A-C1
15	A	1140	CLA	O1A-CGA-O2A-C1
15	B	1225	CLA	C5-C6-C7-C8
15	F	1410	CLA	C10-C11-C12-C13
15	B	1234	CLA	C8-C10-C11-C12
15	B	1203	CLA	C10-C11-C12-C13
15	A	1126	CLA	C10-C11-C12-C13
15	A	1122	CLA	C10-C11-C12-C13
15	A	1127	CLA	C8-C10-C11-C12
15	B	1221	CLA	C5-C6-C7-C8
15	B	1220	CLA	C5-C6-C7-C8
15	B	1225	CLA	C13-C15-C16-C17
10	B	2002	PQN	C18-C20-C21-C22
15	A	1104	CLA	C15-C16-C17-C18
15	B	1224	CLA	C8-C10-C11-C12
15	B	1224	CLA	C15-C16-C17-C18
15	A	1126	CLA	C13-C15-C16-C17
15	B	1023	CLA	C8-C10-C11-C12
15	B	1023	CLA	C15-C16-C17-C18
15	A	1119	CLA	C13-C15-C16-C17
15	B	1226	CLA	C8-C10-C11-C12
15	B	1226	CLA	C13-C15-C16-C17
15	B	1216	CLA	C13-C15-C16-C17
15	B	1229	CLA	C8-C10-C11-C12
15	B	1210	CLA	C5-C6-C7-C8
16	B	1301	LMU	C4'-C5'-C6'-O6'
15	B	1239	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1D-CGD-O2D-CED
12	B	5004	LHG	C23-C24-C25-C26
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1127	CLA	C15-C16-C17-C18
15	A	1135	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	O1D-CGD-O2D-CED
15	B	1213	CLA	C2-C1-O2A-CGA
15	A	1104	CLA	C2-C1-O2A-CGA
15	B	1203	CLA	C2-C1-O2A-CGA
15	B	1218	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1214	CLA	C2-C1-O2A-CGA
15	A	1117	CLA	C2-C1-O2A-CGA
15	A	1103	CLA	C2-C1-O2A-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	C13-C15-C16-C17
15	B	1202	CLA	C15-C16-C17-C18
15	B	1021	CLA	C13-C15-C16-C17
15	B	1215	CLA	C5-C6-C7-C8
12	A	5005	LHG	C8-C7-O7-C5
15	A	1136	CLA	C8-C10-C11-C12
15	A	1102	CLA	C13-C15-C16-C17
15	B	1013	CLA	C10-C11-C12-C13
15	B	1220	CLA	C3-C5-C6-C7
15	B	1230	CLA	O1A-CGA-O2A-C1
14	B	4004	BCR	C19-C20-C21-C22
15	B	1222	CLA	CBA-CGA-O2A-C1
15	A	1128	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	O1D-CGD-O2D-CED
15	A	1102	CLA	O1D-CGD-O2D-CED
15	B	1013	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	O1D-CGD-O2D-CED
15	B	1207	CLA	CBA-CGA-O2A-C1
15	A	1101	CLA	C10-C11-C12-C13
16	B	1301	LMU	O1'-C1-C2-C3
14	B	4005	BCR	C10-C11-C12-C13
14	J	4013	BCR	C10-C11-C12-C13
15	A	1121	CLA	O1A-CGA-O2A-C1
15	A	1132	CLA	C13-C15-C16-C17
15	A	1105	CLA	C5-C6-C7-C8
15	B	1230	CLA	C13-C15-C16-C17
15	B	1202	CLA	C13-C15-C16-C17
15	B	1021	CLA	C8-C10-C11-C12
15	B	1223	CLA	C5-C6-C7-C8
15	A	1135	CLA	O1A-CGA-O2A-C1
16	J	1304	LMU	O1'-C1-C2-C3
15	B	1234	CLA	C10-C11-C12-C13
15	B	1234	CLA	C15-C16-C17-C18
15	A	1122	CLA	C8-C10-C11-C12
15	B	1235	CLA	C15-C16-C17-C18
15	A	1012	CLA	C15-C16-C17-C18
15	A	1117	CLA	C13-C15-C16-C17
15	B	1231	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	A	1103	CLA	C8-C10-C11-C12
12	A	5005	LHG	C3-O3-P-O6
12	A	5003	LHG	C3-O3-P-O6
12	A	5003	LHG	C4-O6-P-O3
15	B	1231	CLA	C3-C5-C6-C7
15	A	1132	CLA	O1D-CGD-O2D-CED
12	A	5005	LHG	O9-C7-O7-C5
15	A	1110	CLA	C4-C3-C5-C6
15	B	1224	CLA	C13-C15-C16-C17
15	A	1136	CLA	C2A-CAA-CBA-CGA
15	A	1117	CLA	C3-C5-C6-C7
15	F	1139	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	C15-C16-C17-C18
15	A	1109	CLA	C15-C16-C17-C18
14	A	4003	BCR	C13-C14-C15-C16
14	A	4001	BCR	C19-C20-C21-C22
17	B	5002	LMG	C32-C33-C34-C35
15	A	1104	CLA	C8-C10-C11-C12
15	F	1139	CLA	C8-C10-C11-C12
15	B	1021	CLA	C5-C6-C7-C8
14	B	4004	BCR	C11-C10-C9-C34
14	A	4012	BCR	C11-C10-C9-C34
17	B	5002	LMG	C23-C24-C25-C26
12	B	5004	LHG	C13-C14-C15-C16
15	B	1222	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	C16-C17-C18-C19
15	A	1126	CLA	C16-C17-C18-C20
15	B	1229	CLA	C16-C17-C18-C20
15	A	1122	CLA	CBA-CGA-O2A-C1
15	A	1131	CLA	CBA-CGA-O2A-C1
12	A	5005	LHG	C10-C11-C12-C13
17	B	5002	LMG	C14-C15-C16-C17
17	B	5002	LMG	C33-C34-C35-C36
12	A	5003	LHG	C11-C12-C13-C14
12	A	5003	LHG	C30-C31-C32-C33
15	B	1210	CLA	C15-C16-C17-C18
16	B	1301	LMU	C3-C4-C5-C6
16	B	1301	LMU	C6-C7-C8-C9
12	A	5005	LHG	C9-C10-C11-C12
14	B	4004	BCR	C11-C10-C9-C8
14	F	4016	BCR	C11-C10-C9-C8
14	A	4012	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	A	4002	BCR	C11-C10-C9-C8
15	A	1105	CLA	C15-C16-C17-C18
15	A	1132	CLA	C5-C6-C7-C8
15	B	1222	CLA	O1A-CGA-O2A-C1
15	A	1128	CLA	C16-C17-C18-C19
15	B	1235	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	C2-C3-C5-C6
15	A	1128	CLA	C11-C10-C8-C9
10	A	2001	PQN	C19-C18-C20-C21
15	A	1132	CLA	C11-C10-C8-C9
15	B	1229	CLA	O1D-CGD-O2D-CED
12	A	5003	LHG	C14-C15-C16-C17
12	A	5003	LHG	C33-C34-C35-C36
12	B	5004	LHG	C11-C12-C13-C14
16	J	1304	LMU	C6-C7-C8-C9
15	B	1021	CLA	C2A-CAA-CBA-CGA
15	A	1140	CLA	C2A-CAA-CBA-CGA
14	F	4015	BCR	C7-C8-C9-C34
14	A	4007	BCR	C37-C22-C23-C24
14	F	4015	BCR	C7-C8-C9-C10
14	B	4011	BCR	C17-C18-C19-C20
14	B	4014	BCR	C21-C22-C23-C24
15	A	1140	CLA	C3-C5-C6-C7
17	B	5002	LMG	O9-C10-O7-C8
15	A	1123	CLA	C10-C11-C12-C13
17	B	5002	LMG	C11-C10-O7-C8
16	B	1301	LMU	C2-C3-C4-C5
12	A	5003	LHG	C28-C29-C30-C31
15	A	1111	CLA	C11-C12-C13-C14
15	B	1223	CLA	C16-C17-C18-C19
15	B	1223	CLA	C16-C17-C18-C20
13	A	1011	CL0	C16-C17-C18-C19
15	A	1103	CLA	C16-C17-C18-C19
15	B	1204	CLA	O1D-CGD-O2D-CED
17	B	5002	LMG	C11-C12-C13-C14
15	A	1122	CLA	C5-C6-C7-C8
12	A	5005	LHG	C25-C26-C27-C28
13	A	1108	CL0	C2A-CAA-CBA-CGA
15	A	1127	CLA	CBA-CGA-O2A-C1
12	A	5001	LHG	C28-C29-C30-C31
15	A	1110	CLA	C3A-C2A-CAA-CBA
15	B	1234	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
15	A	1107	CLA	C3A-C2A-CAA-CBA
15	A	1131	CLA	C3A-C2A-CAA-CBA
15	B	1216	CLA	C8-C10-C11-C12
14	F	4015	BCR	C15-C16-C17-C18
16	B	1301	LMU	C2-C1-O1'-C1'
12	A	5003	LHG	C7-C8-C9-C10
15	A	1126	CLA	C16-C17-C18-C19
15	A	1111	CLA	C11-C12-C13-C15
15	B	1229	CLA	C16-C17-C18-C19
15	A	1103	CLA	C16-C17-C18-C20
12	A	5001	LHG	C31-C32-C33-C34
16	J	1304	LMU	C7-C8-C9-C10
15	A	1103	CLA	C10-C11-C12-C13
15	B	1228	CLA	C4-C3-C5-C6
15	B	1225	CLA	C2A-CAA-CBA-CGA
12	A	5005	LHG	O1-C1-C2-O2
12	B	5004	LHG	O1-C1-C2-O2
17	B	5002	LMG	C21-C22-C23-C24
15	F	1139	CLA	O1A-CGA-O2A-C1
15	B	1203	CLA	C16-C17-C18-C20
13	A	1011	CL0	C16-C17-C18-C20
12	A	5001	LHG	C11-C12-C13-C14
12	A	5001	LHG	C24-C25-C26-C27
12	A	5001	LHG	C25-C26-C27-C28
12	B	5004	LHG	C11-C10-C9-C8
12	B	5004	LHG	C9-C10-C11-C12
12	A	5001	LHG	C26-C27-C28-C29
15	A	1114	CLA	C2-C1-O2A-CGA
15	A	1101	CLA	C2-C1-O2A-CGA
15	A	1126	CLA	C2-C1-O2A-CGA
15	A	1135	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	C2-C1-O2A-CGA
15	A	1130	CLA	C2-C1-O2A-CGA
15	A	1124	CLA	C5-C6-C7-C8
15	A	1119	CLA	C8-C10-C11-C12
15	B	1223	CLA	C15-C16-C17-C18
15	B	1231	CLA	C8-C10-C11-C12
15	A	1127	CLA	O1A-CGA-O2A-C1
15	A	1131	CLA	O1A-CGA-O2A-C1
14	A	4008	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C5-C6-C7-C8
14	B	4017	BCR	C5-C6-C7-C8
14	B	4009	BCR	C1-C6-C7-C8
14	B	4009	BCR	C5-C6-C7-C8
14	B	4005	BCR	C1-C6-C7-C8
14	F	4015	BCR	C1-C6-C7-C8
14	F	4015	BCR	C5-C6-C7-C8
14	F	4016	BCR	C1-C6-C7-C8
14	F	4016	BCR	C23-C24-C25-C26
14	F	4016	BCR	C23-C24-C25-C30
14	A	4012	BCR	C23-C24-C25-C26
14	A	4012	BCR	C23-C24-C25-C30
15	B	1228	CLA	C3-C5-C6-C7
15	B	1021	CLA	C3-C5-C6-C7
14	A	4001	BCR	C23-C24-C25-C30
15	B	1234	CLA	CBA-CGA-O2A-C1
10	B	2002	PQN	C25-C26-C27-C28
15	A	1101	CLA	C8-C10-C11-C12
15	B	1224	CLA	C5-C6-C7-C8
15	B	1230	CLA	C8-C10-C11-C12
15	B	1228	CLA	C13-C15-C16-C17
15	A	1117	CLA	C10-C11-C12-C13
10	B	2002	PQN	C20-C21-C22-C23
15	B	1214	CLA	C8-C10-C11-C12
15	A	1136	CLA	C15-C16-C17-C18
15	B	1231	CLA	C4-C3-C5-C6
15	A	1128	CLA	C6-C7-C8-C10
15	A	1128	CLA	C11-C10-C8-C7
15	A	1105	CLA	C11-C10-C8-C7
15	B	1234	CLA	C12-C13-C15-C16
15	A	1123	CLA	C11-C10-C8-C7
15	A	1122	CLA	C11-C12-C13-C15
15	A	1119	CLA	C12-C13-C15-C16
10	A	2001	PQN	C21-C22-C23-C25
15	B	1021	CLA	C11-C10-C8-C7
15	B	1013	CLA	C6-C7-C8-C10
15	B	1223	CLA	C6-C7-C8-C10
15	A	1122	CLA	O1A-CGA-O2A-C1
14	B	4014	BCR	C9-C10-C11-C12
15	A	1110	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	C16-C17-C18-C19
15	A	1137	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1107	CLA	CBA-CGA-O2A-C1
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C15-C16-C17-C18
16	J	1304	LMU	C2-C3-C4-C5
15	B	1237	CLA	C5-C6-C7-C8
15	A	1128	CLA	CBA-CGA-O2A-C1
15	A	1122	CLA	C13-C15-C16-C17
15	B	1228	CLA	C15-C16-C17-C18
16	B	1301	LMU	C5-C6-C7-C8
15	B	1225	CLA	C10-C11-C12-C13
15	A	1122	CLA	C3-C5-C6-C7
16	B	1301	LMU	C2'-C1'-O1'-C1
17	B	5002	LMG	C2-C1-O1-C7
15	A	1128	CLA	C16-C17-C18-C20
15	A	1122	CLA	C2-C3-C5-C6
15	B	1228	CLA	C2-C3-C5-C6
15	A	1123	CLA	C11-C10-C8-C9
15	A	1119	CLA	C14-C13-C15-C16
15	B	1214	CLA	C11-C12-C13-C14
15	A	1117	CLA	C6-C7-C8-C9
10	A	2001	PQN	C21-C22-C23-C24
15	A	1136	CLA	C14-C13-C15-C16
15	B	1021	CLA	C11-C10-C8-C9
15	B	1013	CLA	C6-C7-C8-C9
15	B	1223	CLA	C6-C7-C8-C9
15	A	1137	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	C2A-CAA-CBA-CGA
14	B	4009	BCR	C37-C22-C23-C24
14	B	4010	BCR	C37-C22-C23-C24
15	A	1117	CLA	C8-C10-C11-C12
15	A	1103	CLA	C5-C6-C7-C8
14	B	4010	BCR	C21-C22-C23-C24
15	B	1234	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	B	1209	CLA	C1A-C2A-CAA-CBA
15	B	1217	CLA	C1A-C2A-CAA-CBA
15	B	1218	CLA	C1A-C2A-CAA-CBA
15	B	1212	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1122	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1107	CLA	C1A-C2A-CAA-CBA
15	B	1239	CLA	C1A-C2A-CAA-CBA
15	K	1401	CLA	C1A-C2A-CAA-CBA
15	A	1117	CLA	C1A-C2A-CAA-CBA
15	B	1208	CLA	C1A-C2A-CAA-CBA
15	A	1131	CLA	C1A-C2A-CAA-CBA
15	B	1226	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	A	1102	CLA	C1A-C2A-CAA-CBA
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	A	1129	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	B	1215	CLA	C1A-C2A-CAA-CBA
12	A	5003	LHG	C11-C10-C9-C8
14	B	4011	BCR	C19-C20-C21-C22
14	A	4001	BCR	C13-C14-C15-C16
14	A	4001	BCR	C15-C16-C17-C18
15	A	1128	CLA	C10-C11-C12-C13
15	B	1215	CLA	C15-C16-C17-C18
12	A	5001	LHG	O6-C4-C5-C6
12	A	5003	LHG	C23-C24-C25-C26
12	A	5005	LHG	C11-C12-C13-C14
15	B	1205	CLA	C4-C3-C5-C6
15	A	1135	CLA	C4-C3-C5-C6
15	A	1117	CLA	C15-C16-C17-C18
15	A	1128	CLA	O1A-CGA-O2A-C1
15	A	1137	CLA	O1A-CGA-O2A-C1
15	A	1107	CLA	O1A-CGA-O2A-C1
12	A	5001	LHG	C17-C18-C19-C20
15	A	1127	CLA	C2A-CAA-CBA-CGA
15	A	1127	CLA	C16-C17-C18-C19
17	B	5002	LMG	O1-C7-C8-C9
15	A	1012	CLA	C10-C11-C12-C13
12	B	5004	LHG	C26-C27-C28-C29
15	B	1231	CLA	C2C-C3C-CAC-CBC
15	A	1131	CLA	C5-C6-C7-C8
15	A	1106	CLA	C5-C6-C7-C8
15	B	1217	CLA	CAA-CBA-CGA-O2A
15	B	1228	CLA	CAA-CBA-CGA-O2A
15	A	1132	CLA	CAA-CBA-CGA-O2A
15	B	1215	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	A	5001	LHG	C29-C30-C31-C32
15	B	1207	CLA	C2C-C3C-CAC-CBC
15	A	1127	CLA	O1D-CGD-O2D-CED
15	A	1101	CLA	C16-C17-C18-C20
15	B	1213	CLA	CBA-CGA-O2A-C1
15	B	1203	CLA	C13-C15-C16-C17
15	B	1207	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	C2A-CAA-CBA-CGA
15	F	1139	CLA	C2-C1-O2A-CGA
15	B	1236	CLA	C2-C1-O2A-CGA
17	B	5002	LMG	C41-C42-C43-C44
12	B	5004	LHG	C28-C29-C30-C31
12	A	5005	LHG	O6-C4-C5-O7
12	A	5001	LHG	C35-C36-C37-C38
12	A	5005	LHG	O7-C5-C6-O8
15	A	1137	CLA	C2C-C3C-CAC-CBC
15	A	1105	CLA	C11-C12-C13-C15
15	A	1104	CLA	C11-C12-C13-C15
15	B	1203	CLA	C12-C13-C15-C16
15	F	1139	CLA	C12-C13-C15-C16
15	B	1224	CLA	C11-C12-C13-C15
15	B	1205	CLA	C2-C3-C5-C6
15	A	1117	CLA	C12-C13-C15-C16
15	A	1136	CLA	C12-C13-C15-C16
15	B	1226	CLA	C6-C7-C8-C10
15	B	1021	CLA	C6-C7-C8-C10
15	B	1215	CLA	C11-C10-C8-C7
15	A	1105	CLA	C3-C5-C6-C7
15	A	1104	CLA	C11-C12-C13-C14
15	A	1101	CLA	C11-C10-C8-C9
15	B	1023	CLA	C11-C10-C8-C9
15	B	1226	CLA	C6-C7-C8-C9
15	B	1202	CLA	C11-C12-C13-C14
15	A	1106	CLA	C11-C10-C8-C9
15	B	1215	CLA	C11-C10-C8-C9
14	A	4012	BCR	C19-C20-C21-C22
15	A	1110	CLA	C5-C6-C7-C8
10	A	2001	PQN	C25-C26-C27-C28
16	J	1304	LMU	C4-C5-C6-C7
15	A	1127	CLA	C16-C17-C18-C20
14	B	4014	BCR	C17-C18-C19-C20
15	B	1213	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	5004	LHG	C25-C26-C27-C28
17	B	5002	LMG	O6-C1-O1-C7
12	A	5005	LHG	O6-C4-C5-C6
15	B	1223	CLA	C3-C5-C6-C7
14	A	4008	BCR	C18-C19-C20-C21
15	A	1104	CLA	C13-C15-C16-C17
15	A	1122	CLA	C4-C3-C5-C6
17	B	5002	LMG	C31-C32-C33-C34
15	A	1118	CLA	C2A-CAA-CBA-CGA
15	B	1220	CLA	CBA-CGA-O2A-C1
15	F	1410	CLA	C3A-C2A-CAA-CBA
15	B	1209	CLA	C3A-C2A-CAA-CBA
15	B	1229	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA
14	A	4008	BCR	C9-C10-C11-C12
12	A	5005	LHG	C4-C5-C6-O8
12	B	5004	LHG	C35-C36-C37-C38
12	A	5003	LHG	C31-C32-C33-C34
15	B	1202	CLA	C4-C3-C5-C6
15	A	1135	CLA	C2-C3-C5-C6
15	B	1239	CLA	C2C-C3C-CAC-CBC
15	A	1111	CLA	C3-C5-C6-C7
15	B	1202	CLA	C10-C11-C12-C13
17	B	5002	LMG	C24-C25-C26-C27
15	A	1111	CLA	C8-C10-C11-C12
12	B	5004	LHG	O7-C5-C6-O8
15	A	1110	CLA	O1D-CGD-O2D-CED
14	J	4013	BCR	C19-C20-C21-C22
15	A	1022	CLA	C15-C16-C17-C18
15	B	1235	CLA	C8-C10-C11-C12
17	B	5002	LMG	C17-C18-C19-C20
17	B	5002	LMG	C40-C41-C42-C43
15	B	1210	CLA	C2-C1-O2A-CGA
15	A	1122	CLA	C14-C13-C15-C16
15	B	1021	CLA	C14-C13-C15-C16
15	B	1216	CLA	C6-C7-C8-C9
15	B	1210	CLA	C11-C12-C13-C14
12	A	5003	LHG	C2-C3-O3-P
15	B	1220	CLA	O1A-CGA-O2A-C1
17	B	5002	LMG	C13-C14-C15-C16
17	B	5002	LMG	C42-C43-C44-C45
14	B	4017	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	B	4011	BCR	C1-C6-C7-C8
14	B	4011	BCR	C5-C6-C7-C8
14	J	4013	BCR	C1-C6-C7-C8
14	J	4013	BCR	C5-C6-C7-C8
14	A	4012	BCR	C1-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C26
14	A	4003	BCR	C23-C24-C25-C30
14	A	4001	BCR	C1-C6-C7-C8
14	A	4001	BCR	C5-C6-C7-C8
15	B	1229	CLA	C13-C15-C16-C17
15	B	1231	CLA	C4C-C3C-CAC-CBC
14	B	4014	BCR	C36-C18-C19-C20
14	B	4009	BCR	C21-C22-C23-C24
14	F	4015	BCR	C21-C22-C23-C24
14	A	4003	BCR	C21-C22-C23-C24
15	A	1138	CLA	C5-C6-C7-C8
15	B	1202	CLA	C8-C10-C11-C12
15	A	1109	CLA	C5-C6-C7-C8
15	A	1106	CLA	C8-C10-C11-C12
15	B	1222	CLA	C6-C7-C8-C10
15	A	1101	CLA	C12-C13-C15-C16
15	A	1122	CLA	C12-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C7
15	A	1119	CLA	C11-C12-C13-C15
15	B	1230	CLA	C12-C13-C15-C16
10	A	2001	PQN	C17-C18-C20-C21
15	B	1202	CLA	C11-C12-C13-C15
15	B	1021	CLA	C12-C13-C15-C16
15	B	1235	CLA	C6-C7-C8-C10
15	B	1216	CLA	C6-C7-C8-C10
15	A	1106	CLA	C11-C10-C8-C7
15	B	1210	CLA	C11-C12-C13-C15
14	B	4009	BCR	C19-C20-C21-C22
14	B	4006	BCR	C19-C20-C21-C22
14	B	4010	BCR	C19-C20-C21-C22
15	B	1237	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	C2A-CAA-CBA-CGA
15	J	1303	CLA	C2C-C3C-CAC-CBC
15	A	1022	CLA	CBA-CGA-O2A-C1
15	B	1236	CLA	CBA-CGA-O2A-C1
12	B	5004	LHG	C34-C35-C36-C37
15	A	1121	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1201	CLA	CAD-CBD-CGD-O2D
15	B	1222	CLA	CAD-CBD-CGD-O2D
15	A	1120	CLA	CAD-CBD-CGD-O2D
17	B	5002	LMG	C9-C8-O7-C10
15	B	1230	CLA	CAD-CBD-CGD-O2D
15	B	1221	CLA	CAD-CBD-CGD-O2D
15	A	1140	CLA	CAD-CBD-CGD-O2D
15	B	1229	CLA	C15-C16-C17-C18
16	B	1301	LMU	C1-C2-C3-C4
15	A	1127	CLA	C10-C11-C12-C13
15	A	1119	CLA	C3-C5-C6-C7
17	B	5002	LMG	C7-C8-C9-O8
15	B	1236	CLA	O1A-CGA-O2A-C1
12	A	5003	LHG	O6-C4-C5-O7
15	A	1106	CLA	C10-C11-C12-C13
15	A	1122	CLA	C16-C17-C18-C19
15	A	1118	CLA	CHA-CBD-CGD-O1D
15	A	1118	CLA	CHA-CBD-CGD-O2D
15	A	1138	CLA	CHA-CBD-CGD-O2D
15	B	1205	CLA	CHA-CBD-CGD-O1D
15	B	1205	CLA	CHA-CBD-CGD-O2D
15	A	1119	CLA	CHA-CBD-CGD-O2D
15	A	1111	CLA	CHA-CBD-CGD-O1D
15	A	1136	CLA	CHA-CBD-CGD-O2D
15	B	1226	CLA	CHA-CBD-CGD-O1D
15	B	1226	CLA	CHA-CBD-CGD-O2D
15	B	1202	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1102	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CHA-CBD-CGD-O1D
15	B	1223	CLA	CHA-CBD-CGD-O1D
15	B	1223	CLA	CHA-CBD-CGD-O2D
14	B	4011	BCR	C11-C10-C9-C8
17	B	5002	LMG	O1-C7-C8-O7
15	B	1205	CLA	C6-C7-C8-C10
12	A	5001	LHG	O1-C1-C2-O2
15	B	1207	CLA	C4C-C3C-CAC-CBC
15	B	1235	CLA	C3-C5-C6-C7
15	B	1226	CLA	C15-C16-C17-C18
15	A	1123	CLA	C4-C3-C5-C6
15	A	1103	CLA	C4-C3-C5-C6
15	B	1231	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	A	1101	CLA	C14-C13-C15-C16
15	B	1230	CLA	C14-C13-C15-C16
15	B	1223	CLA	C14-C13-C15-C16
15	A	1109	CLA	C14-C13-C15-C16
15	A	1123	CLA	C8-C10-C11-C12
12	A	5003	LHG	C16-C17-C18-C19
15	A	1012	CLA	C2A-CAA-CBA-CGA
12	A	5001	LHG	O1-C1-C2-C3
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	A	1127	CLA	C13-C15-C16-C17
15	A	1105	CLA	C2-C1-O2A-CGA
15	B	1237	CLA	C2-C1-O2A-CGA
15	A	1109	CLA	C2-C1-O2A-CGA
12	A	5001	LHG	C11-C10-C9-C8
15	B	1237	CLA	C3-C5-C6-C7
12	A	5003	LHG	C3-O3-P-O5
12	A	5003	LHG	C4-O6-P-O5
15	A	1119	CLA	O2A-C1-C2-C3
16	B	1301	LMU	O5'-C1'-O1'-C1
17	B	5002	LMG	C36-C37-C38-C39
12	A	5005	LHG	C11-C10-C9-C8
15	A	1140	CLA	C16-C17-C18-C19
12	A	5001	LHG	C19-C20-C21-C22
15	A	1118	CLA	CAD-CBD-CGD-O1D
15	A	1111	CLA	CAD-CBD-CGD-O1D
15	A	1102	CLA	CAD-CBD-CGD-O1D
15	B	1211	CLA	CAD-CBD-CGD-O1D
15	A	1129	CLA	CAD-CBD-CGD-O1D
15	B	1223	CLA	CAD-CBD-CGD-O1D
15	B	1230	CLA	C5-C6-C7-C8
15	B	1216	CLA	C10-C11-C12-C13
17	B	5002	LMG	C38-C39-C40-C41
15	A	1022	CLA	O1A-CGA-O2A-C1
15	B	1013	CLA	C3-C5-C6-C7
12	B	5004	LHG	C33-C34-C35-C36
15	A	1136	CLA	C16-C17-C18-C20
15	F	1410	CLA	C6-C7-C8-C10
15	F	1410	CLA	C12-C13-C15-C16
12	A	5001	LHG	O6-C4-C5-O7
15	A	1138	CLA	C11-C10-C8-C7
15	B	1228	CLA	C11-C12-C13-C15
15	A	1117	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	B	1202	CLA	C2-C3-C5-C6
15	A	1102	CLA	C12-C13-C15-C16
15	B	1013	CLA	C12-C13-C15-C16
15	B	1229	CLA	C11-C10-C8-C7
15	B	1231	CLA	C6-C7-C8-C10
15	K	1402	CLA	CAA-CBA-CGA-O2A
12	A	5001	LHG	C8-C7-O7-C5
12	A	5003	LHG	C13-C14-C15-C16
12	B	5004	LHG	C4-C5-C6-O8
17	B	5002	LMG	O7-C8-C9-O8
17	B	5002	LMG	C15-C16-C17-C18
12	A	5005	LHG	C12-C13-C14-C15
15	B	1224	CLA	C4-C3-C5-C6
15	B	1234	CLA	C11-C10-C8-C9
15	B	1222	CLA	C6-C7-C8-C9
15	A	1122	CLA	C11-C12-C13-C14
15	A	1119	CLA	C11-C12-C13-C14
15	A	1117	CLA	C14-C13-C15-C16
15	B	1235	CLA	C6-C7-C8-C9
14	F	4016	BCR	C18-C19-C20-C21
14	J	4013	BCR	C18-C19-C20-C21
14	B	4010	BCR	C18-C19-C20-C21
14	A	4007	BCR	C18-C19-C20-C21
15	A	1137	CLA	C4C-C3C-CAC-CBC
12	A	5003	LHG	C24-C23-O8-C6
12	A	5005	LHG	O2-C2-C3-O3
15	B	1204	CLA	CBA-CGA-O2A-C1
14	B	4011	BCR	C11-C10-C9-C34
15	A	1123	CLA	C2-C3-C5-C6
15	A	1120	CLA	C1-C2-C3-C4
12	A	5003	LHG	O6-C4-C5-C6
12	A	5001	LHG	O9-C7-O7-C5
15	A	1110	CLA	C2-C1-O2A-CGA
15	A	1131	CLA	C2-C1-O2A-CGA
15	A	1102	CLA	C2-C1-O2A-CGA
15	B	1021	CLA	C2-C1-O2A-CGA
15	B	1216	CLA	C2-C1-O2A-CGA
15	B	1226	CLA	C5-C6-C7-C8
14	B	4004	BCR	C23-C24-C25-C26
14	A	4012	BCR	C5-C6-C7-C8
15	A	1103	CLA	C2-C3-C5-C6
15	B	1219	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1117	CLA	C5-C6-C7-C8
15	B	1239	CLA	C4C-C3C-CAC-CBC
15	J	1303	CLA	C4C-C3C-CAC-CBC
15	B	1202	CLA	C3-C5-C6-C7
15	J	1303	CLA	C2A-CAA-CBA-CGA
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	A	1101	CLA	C15-C16-C17-C18
12	A	5005	LHG	C4-O6-P-O3
12	A	5001	LHG	C3-O3-P-O6
15	B	1210	CLA	C10-C11-C12-C13
15	B	1234	CLA	C11-C10-C8-C7
15	A	1101	CLA	C11-C10-C8-C7
15	B	1223	CLA	C12-C13-C15-C16
12	A	5003	LHG	C9-C10-C11-C12
15	F	1410	CLA	C6-C7-C8-C9
15	F	1139	CLA	C14-C13-C15-C16
15	A	1012	CLA	C6-C7-C8-C9
15	B	1231	CLA	C6-C7-C8-C9
15	B	1228	CLA	CAA-CBA-CGA-O1A
12	A	5003	LHG	C10-C11-C12-C13
15	A	1116	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	C5-C6-C7-C8
15	B	1217	CLA	CAA-CBA-CGA-O1A
12	A	5001	LHG	C14-C15-C16-C17
15	B	1229	CLA	C5-C6-C7-C8
14	A	4002	BCR	C19-C20-C21-C22
12	A	5003	LHG	O10-C23-O8-C6
13	A	1011	CL0	O1A-CGA-O2A-C1
15	B	1225	CLA	C8-C10-C11-C12
15	A	1101	CLA	CAA-CBA-CGA-O2A
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	B	1225	CLA	C2-C1-O2A-CGA
15	B	1013	CLA	C2A-CAA-CBA-CGA
12	B	5004	LHG	C15-C16-C17-C18
15	A	1140	CLA	C3A-C2A-CAA-CBA
15	A	1140	CLA	C16-C17-C18-C20
15	B	1225	CLA	C15-C16-C17-C18
15	A	1136	CLA	C6-C7-C8-C9
15	A	1102	CLA	C14-C13-C15-C16
15	A	1103	CLA	C6-C7-C8-C9
15	A	1136	CLA	C16-C17-C18-C19
14	B	4009	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
14	F	4015	BCR	C11-C10-C9-C34
14	F	4016	BCR	C35-C13-C14-C15
14	B	4011	BCR	C16-C17-C18-C36
14	B	4006	BCR	C20-C21-C22-C37
15	F	1410	CLA	C2A-CAA-CBA-CGA
15	A	1114	CLA	C2C-C3C-CAC-CBC
14	B	4006	BCR	C7-C8-C9-C34
14	B	4014	BCR	C14-C15-C16-C17
15	F	1410	CLA	C1A-C2A-CAA-CBA
15	B	1232	CLA	C1A-C2A-CAA-CBA
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	B	1228	CLA	C1A-C2A-CAA-CBA
15	B	1223	CLA	C1A-C2A-CAA-CBA
15	F	1139	CLA	C6-C7-C8-C10
15	B	1224	CLA	C2-C3-C5-C6
15	B	1023	CLA	C12-C13-C15-C16
15	B	1221	CLA	C12-C13-C15-C16
15	A	1012	CLA	C11-C12-C13-C15
15	A	1106	CLA	C12-C13-C15-C16
15	B	1013	CLA	C13-C15-C16-C17
14	B	4004	BCR	C9-C10-C11-C12
15	B	1235	CLA	C5-C6-C7-C8
15	A	1114	CLA	C2A-CAA-CBA-CGA
15	A	1111	CLA	C10-C11-C12-C13
12	A	5005	LHG	C24-C25-C26-C27
12	B	5004	LHG	C31-C32-C33-C34
15	F	1410	CLA	C8-C10-C11-C12
15	A	1123	CLA	C5-C6-C7-C8
14	B	4009	BCR	C16-C17-C18-C19
14	F	4016	BCR	C12-C13-C14-C15
14	B	4011	BCR	C16-C17-C18-C19
14	B	4006	BCR	C20-C21-C22-C23
15	A	1116	CLA	CBA-CGA-O2A-C1
15	A	1101	CLA	C5-C6-C7-C8
12	A	5001	LHG	C15-C16-C17-C18
15	B	1230	CLA	C16-C17-C18-C20
15	B	1215	CLA	CAA-CBA-CGA-O1A
15	A	1022	CLA	C4-C3-C5-C6
16	J	1304	LMU	C9-C10-C11-C12
15	A	1116	CLA	C2-C1-O2A-CGA
15	B	1023	CLA	C10-C11-C12-C13
15	B	1218	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	B	4004	BCR	C23-C24-C25-C30
14	B	4014	BCR	C1-C6-C7-C8
12	A	5001	LHG	C12-C13-C14-C15
14	B	4006	BCR	C13-C14-C15-C16
15	B	1223	CLA	C4-C3-C5-C6
15	B	1223	CLA	C8-C10-C11-C12
15	B	1223	CLA	C13-C15-C16-C17
15	F	1139	CLA	C15-C16-C17-C18
15	A	1140	CLA	C10-C11-C12-C13
15	B	1234	CLA	C13-C15-C16-C17
10	A	2001	PQN	C23-C25-C26-C27
16	J	1304	LMU	O5B-C1B-O1B-C4'
15	A	1109	CLA	C12-C13-C15-C16
15	A	1012	CLA	C13-C15-C16-C17
16	J	1304	LMU	C2B-C1B-O1B-C4'
15	B	1229	CLA	C10-C11-C12-C13
12	A	5001	LHG	O8-C23-C24-C25
15	B	1021	CLA	CAA-CBA-CGA-O2A
13	A	1011	CL0	CBA-CGA-O2A-C1
15	A	1136	CLA	C4-C3-C5-C6
15	A	1132	CLA	C4-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	B	1013	CLA	C4-C3-C5-C6
15	A	1106	CLA	C16-C17-C18-C20
15	F	1410	CLA	C14-C13-C15-C16
15	A	1138	CLA	C11-C10-C8-C9
15	B	1023	CLA	C14-C13-C15-C16
15	B	1214	CLA	C6-C7-C8-C9
15	A	1117	CLA	C11-C12-C13-C14
15	B	1221	CLA	C14-C13-C15-C16
15	B	1229	CLA	C11-C10-C8-C9
15	F	1410	CLA	C15-C16-C17-C18
16	B	1301	LMU	C4-C5-C6-C7
15	B	1219	CLA	C3A-C2A-CAA-CBA
15	B	1223	CLA	C3A-C2A-CAA-CBA
15	B	1202	CLA	CAA-CBA-CGA-O2A
15	B	1210	CLA	CAA-CBA-CGA-O2A
15	A	1110	CLA	CAD-CBD-CGD-O2D
15	A	1124	CLA	CAD-CBD-CGD-O2D
15	B	1212	CLA	CAD-CBD-CGD-O2D
15	K	1402	CLA	CAD-CBD-CGD-O2D
15	B	1023	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	A	5001	LHG	O7-C7-C8-C9
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	B	1231	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	C4-C3-C5-C6
15	B	1234	CLA	C3-C5-C6-C7
15	A	1022	CLA	C2-C3-C5-C6
15	B	1229	CLA	O2A-C1-C2-C3
15	A	1131	CLA	C2C-C3C-CAC-CBC
15	K	1401	CLA	CAA-CBA-CGA-O2A
12	A	5001	LHG	C13-C14-C15-C16
15	A	1114	CLA	CHA-CBD-CGD-O1D
15	A	1114	CLA	CHA-CBD-CGD-O2D
15	B	1240	CLA	CHA-CBD-CGD-O1D
15	B	1240	CLA	CHA-CBD-CGD-O2D
15	B	1234	CLA	CHA-CBD-CGD-O1D
15	B	1234	CLA	CHA-CBD-CGD-O2D
15	A	1124	CLA	CHA-CBD-CGD-O1D
15	A	1104	CLA	CHA-CBD-CGD-O1D
15	A	1104	CLA	CHA-CBD-CGD-O2D
15	A	1801	CLA	CHA-CBD-CGD-O1D
15	A	1801	CLA	CHA-CBD-CGD-O2D
15	A	1127	CLA	CHA-CBD-CGD-O1D
15	A	1127	CLA	CHA-CBD-CGD-O2D
15	B	1023	CLA	CHA-CBD-CGD-O1D
15	B	1023	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	CHA-CBD-CGD-O1D
15	A	1131	CLA	CHA-CBD-CGD-O2D
15	A	1111	CLA	CHA-CBD-CGD-O2D
15	B	1211	CLA	CHA-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O2D
15	A	1112	CLA	CHA-CBD-CGD-O2D
15	A	1132	CLA	CHA-CBD-CGD-O1D
15	A	1132	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CHA-CBD-CGD-O2D
15	B	1013	CLA	CHA-CBD-CGD-O1D
15	B	1013	CLA	CHA-CBD-CGD-O2D
15	A	1109	CLA	CHA-CBD-CGD-O1D
15	A	1109	CLA	CHA-CBD-CGD-O2D
15	A	1134	CLA	CAA-CBA-CGA-O2A
10	A	2001	PQN	C20-C21-C22-C23
15	A	1136	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	B	1205	CLA	C5-C6-C7-C8
15	A	1120	CLA	CAA-CBA-CGA-O2A
15	A	1135	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	F	1139	CLA	C16-C17-C18-C20
15	A	1022	CLA	C13-C15-C16-C17
15	B	1207	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	A	1114	CLA	C4C-C3C-CAC-CBC
12	A	5001	LHG	C27-C28-C29-C30
15	F	1139	CLA	C6-C7-C8-C9
15	B	1228	CLA	C11-C12-C13-C14
15	A	1012	CLA	C11-C12-C13-C14
15	B	1229	CLA	C11-C12-C13-C14
14	B	4014	BCR	C19-C20-C21-C22
15	B	1222	CLA	C2C-C3C-CAC-CBC
12	A	5005	LHG	O8-C23-C24-C25
15	K	1401	CLA	CAA-CBA-CGA-O1A
12	B	5004	LHG	C19-C20-C21-C22
15	B	1210	CLA	CAA-CBA-CGA-O1A
15	A	1125	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	CAA-CBA-CGA-O1A
15	B	1231	CLA	CAA-CBA-CGA-O1A
14	A	4002	BCR	C11-C12-C13-C14
15	B	1228	CLA	C2C-C3C-CAC-CBC
15	B	1213	CLA	C1A-C2A-CAA-CBA
15	B	1207	CLA	C1A-C2A-CAA-CBA
15	A	1114	CLA	C1A-C2A-CAA-CBA
15	B	1219	CLA	C1A-C2A-CAA-CBA
15	B	1214	CLA	C1A-C2A-CAA-CBA
15	A	1140	CLA	C1A-C2A-CAA-CBA
15	A	1134	CLA	CAA-CBA-CGA-O1A
12	A	5001	LHG	O9-C7-C8-C9
15	B	1202	CLA	CAA-CBA-CGA-O1A
15	A	1128	CLA	C15-C16-C17-C18
12	A	5001	LHG	O10-C23-C24-C25
15	B	1206	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	A	1136	CLA	CAA-CBA-CGA-O1A
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	B	1234	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	A	5005	LHG	O10-C23-C24-C25
15	B	1201	CLA	CAA-CBA-CGA-O2A
15	B	1213	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	CAA-CBA-CGA-O2A
15	A	1123	CLA	C15-C16-C17-C18
14	B	4005	BCR	C19-C20-C21-C22
15	B	1240	CLA	CAD-CBD-CGD-O1D
15	B	1218	CLA	CAD-CBD-CGD-O1D
15	B	1224	CLA	CAD-CBD-CGD-O1D
15	A	1127	CLA	CAD-CBD-CGD-O1D
15	B	1023	CLA	CAD-CBD-CGD-O1D
15	B	1208	CLA	CAD-CBD-CGD-O1D
15	A	1109	CLA	CAD-CBD-CGD-O1D
15	B	1210	CLA	CAD-CBD-CGD-O1D
15	B	1203	CLA	O1A-CGA-O2A-C1
15	B	1207	CLA	CAA-CBA-CGA-O1A
12	A	5005	LHG	C26-C27-C28-C29
15	B	1205	CLA	CAA-CBA-CGA-O2A
15	B	1211	CLA	CAA-CBA-CGA-O2A
15	B	1229	CLA	CAA-CBA-CGA-O2A
16	B	1301	LMU	C7-C8-C9-C10
15	B	1203	CLA	CAA-CBA-CGA-O2A
15	A	1102	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	A	1120	CLA	CAA-CBA-CGA-O1A
15	A	1129	CLA	CAA-CBA-CGA-O1A
17	B	5002	LMG	C34-C35-C36-C37
13	A	1108	CL0	C2C-C3C-CAC-CBC
15	B	1225	CLA	C6-C7-C8-C10
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	B	1023	CLA	C11-C12-C13-C15
15	A	1012	CLA	C6-C7-C8-C10
15	B	1229	CLA	C11-C12-C13-C15
15	B	1215	CLA	C11-C12-C13-C15
15	B	1201	CLA	CAA-CBA-CGA-O1A
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	B	1211	CLA	CAA-CBA-CGA-O1A
15	B	1229	CLA	CAA-CBA-CGA-O1A
15	A	1127	CLA	CAA-CBA-CGA-O2A
15	B	1216	CLA	CAA-CBA-CGA-O2A
14	B	4006	BCR	C7-C8-C9-C10
15	A	1135	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	1230	CLA	C16-C17-C18-C19
15	A	1012	CLA	C8-C10-C11-C12
15	B	1212	CLA	C2C-C3C-CAC-CBC
15	B	1235	CLA	CAA-CBA-CGA-O1A
15	F	1410	CLA	C13-C15-C16-C17
15	A	1140	CLA	C5-C6-C7-C8
15	B	1224	CLA	O1A-CGA-O2A-C1
15	A	1128	CLA	CAA-CBA-CGA-O2A
15	B	1209	CLA	C2A-CAA-CBA-CGA
15	B	1228	CLA	C8-C10-C11-C12
15	B	1203	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

91 monomers are involved in 200 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1213	CLA	1	0
14	A	4008	BCR	5	0
14	B	4004	BCR	3	0
15	A	1118	CLA	3	0
12	A	5005	LHG	10	0
15	B	1227	CLA	2	0
15	A	1022	CLA	3	0
15	J	1302	CLA	2	0
15	A	1114	CLA	2	0
15	A	1110	CLA	13	0
15	B	1220	CLA	1	0
15	A	1128	CLA	2	0
10	B	2002	PQN	3	0
15	A	1105	CLA	2	0
14	B	4017	BCR	6	0
15	A	1124	CLA	3	0
15	A	1121	CLA	2	0
15	A	1104	CLA	1	0
15	B	1203	CLA	2	0
15	B	1218	CLA	2	0
15	B	1201	CLA	1	0
12	A	5001	LHG	1	0
14	B	4009	BCR	1	0
15	A	1137	CLA	1	0
14	B	4005	BCR	1	0
15	B	1232	CLA	1	0

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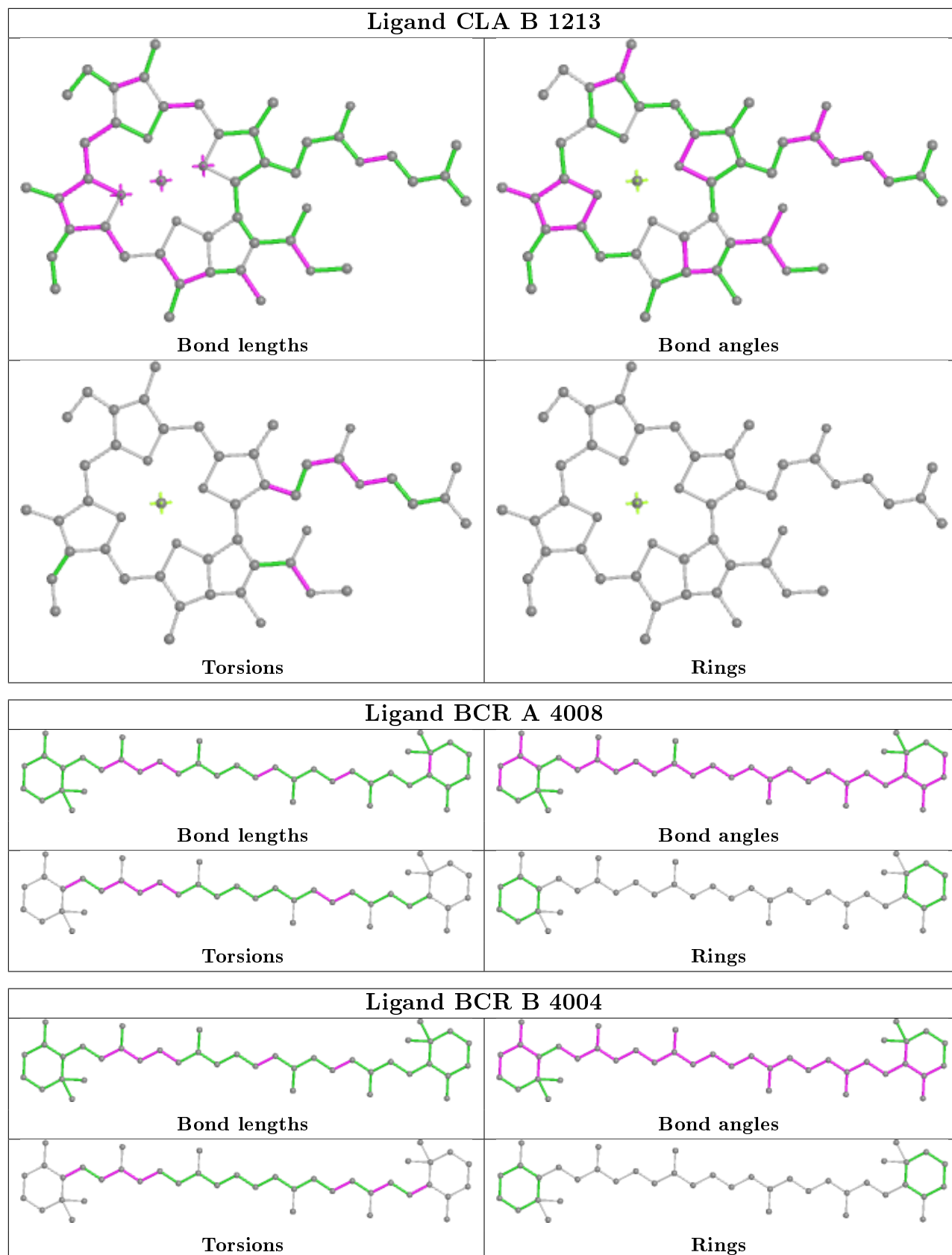
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1138	CLA	1	0
15	B	1222	CLA	4	0
15	A	1101	CLA	3	0
15	A	1123	CLA	2	0
15	F	1139	CLA	3	0
15	B	1224	CLA	2	0
15	B	1205	CLA	1	0
14	F	4015	BCR	6	0
15	A	1126	CLA	8	0
15	A	1801	CLA	1	0
15	B	1236	CLA	3	0
15	B	1212	CLA	2	0
15	A	1120	CLA	1	0
14	F	4016	BCR	2	0
14	B	4011	BCR	7	0
14	B	4014	BCR	2	0
15	A	1122	CLA	4	0
17	B	5002	LMG	2	0
15	A	1127	CLA	4	0
15	A	1107	CLA	1	0
15	B	1023	CLA	3	0
14	B	4006	BCR	1	0
15	A	1135	CLA	1	0
14	J	4013	BCR	3	0
15	A	1119	CLA	1	0
15	B	1239	CLA	2	0
15	B	1230	CLA	2	0
15	K	1401	CLA	1	0
14	A	4012	BCR	2	0
15	A	1133	CLA	2	0
15	A	1131	CLA	2	0
10	A	2001	PQN	1	0
15	A	1111	CLA	1	0
15	B	1226	CLA	3	0
15	B	1221	CLA	4	0
14	A	4003	BCR	3	0
14	B	4010	BCR	5	0
13	A	1108	CL0	3	0
15	A	1102	CLA	3	0
15	B	1211	CLA	2	0
15	B	1021	CLA	2	0
12	A	5003	LHG	7	0

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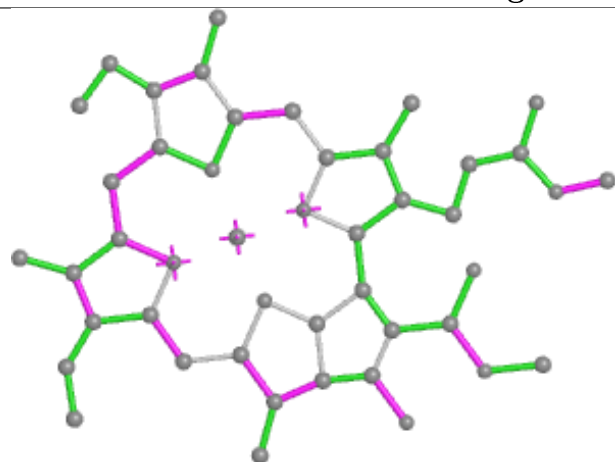
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1235	CLA	4	0
15	A	1112	CLA	1	0
15	B	1216	CLA	2	0
14	A	4002	BCR	3	0
15	A	1113	CLA	1	0
15	B	1206	CLA	1	0
15	A	1012	CLA	2	0
15	B	1237	CLA	1	0
14	A	4007	BCR	1	0
15	A	1129	CLA	2	0
12	B	5004	LHG	2	0
15	B	1013	CLA	8	0
13	A	1011	CL0	9	0
16	J	1304	LMU	2	0
15	A	1109	CLA	3	0
15	B	1229	CLA	4	0
15	B	1231	CLA	3	0
14	A	4001	BCR	3	0
15	K	1402	CLA	1	0
15	A	1103	CLA	5	0
15	A	1106	CLA	2	0
15	B	1215	CLA	4	0
15	B	1210	CLA	2	0

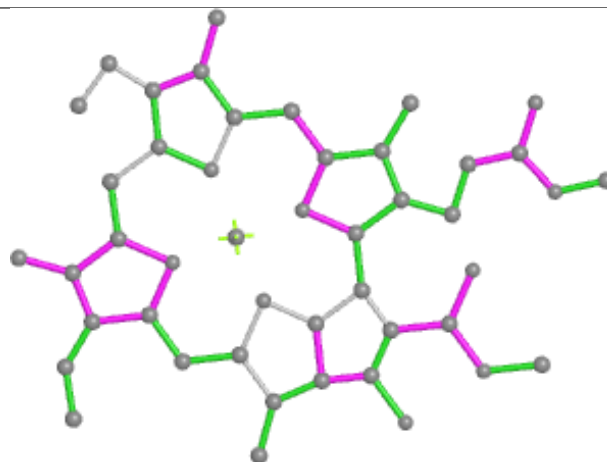
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



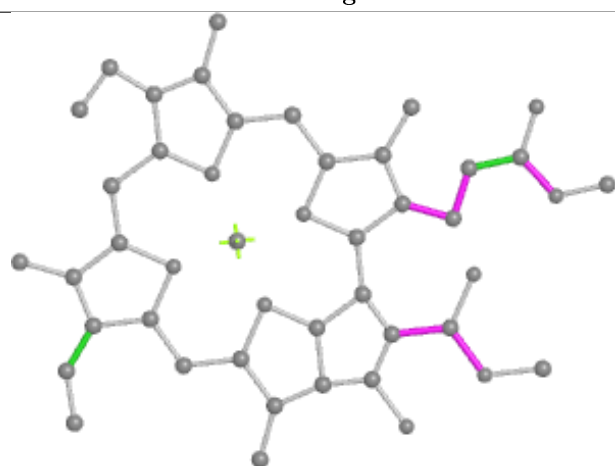
Ligand CLA A 1118



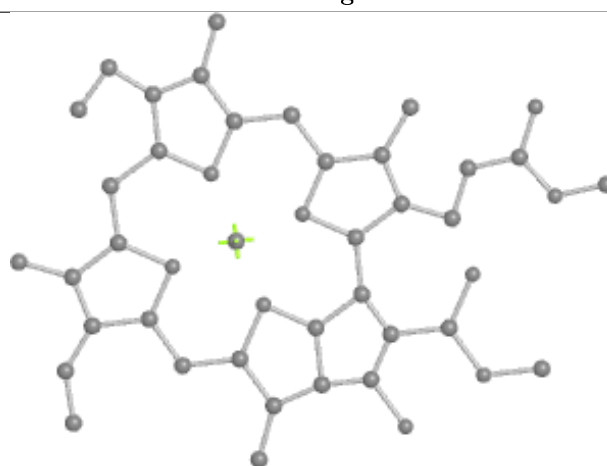
Bond lengths



Bond angles

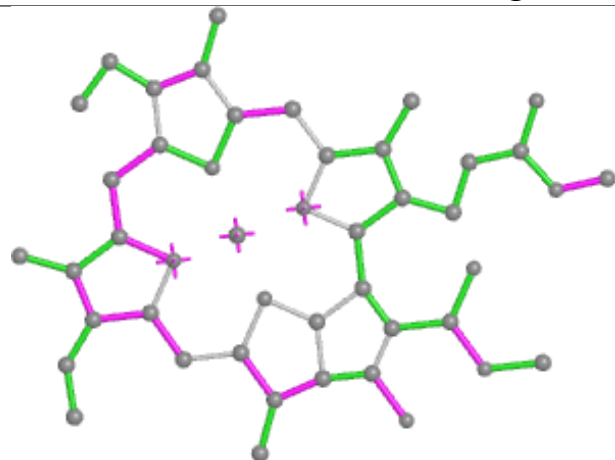


Torsions

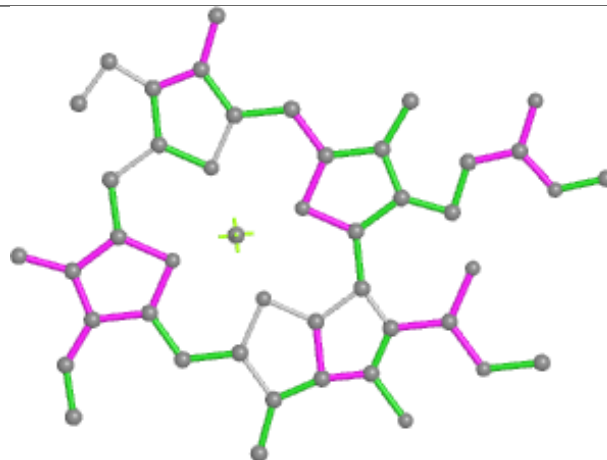


Rings

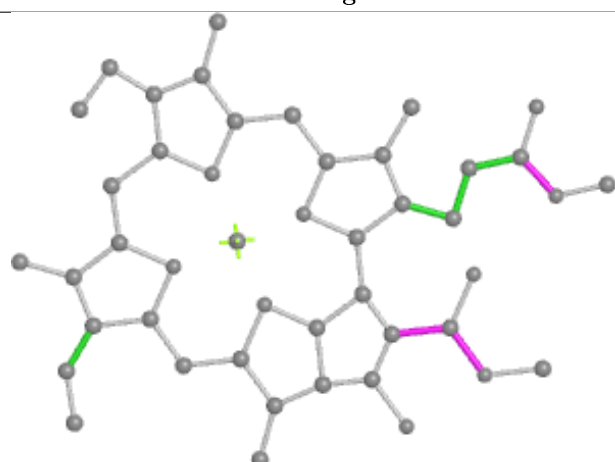
Ligand CLA B 1204



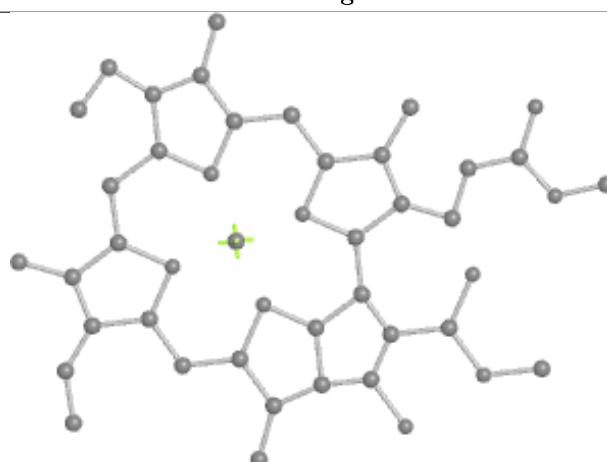
Bond lengths



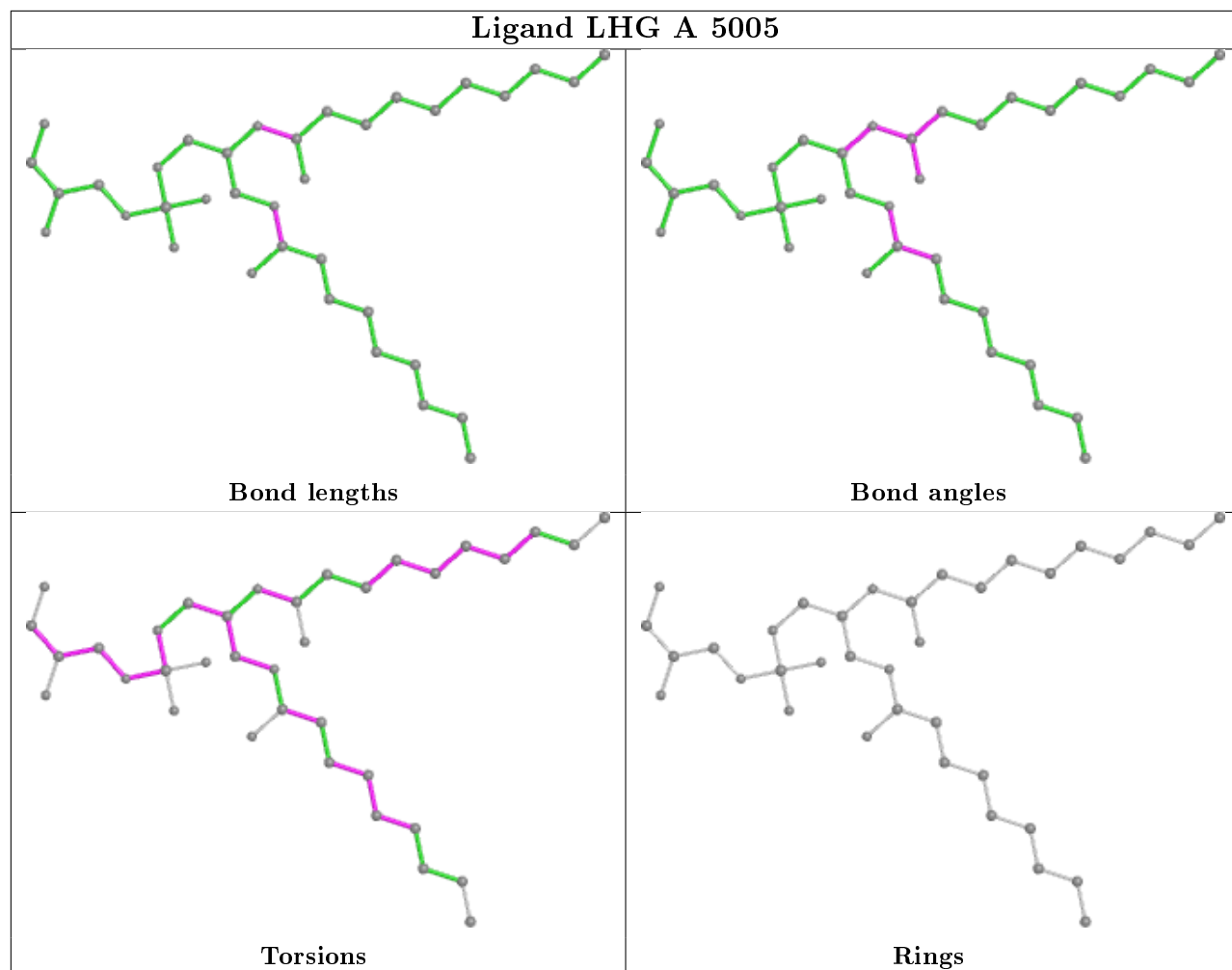
Bond angles



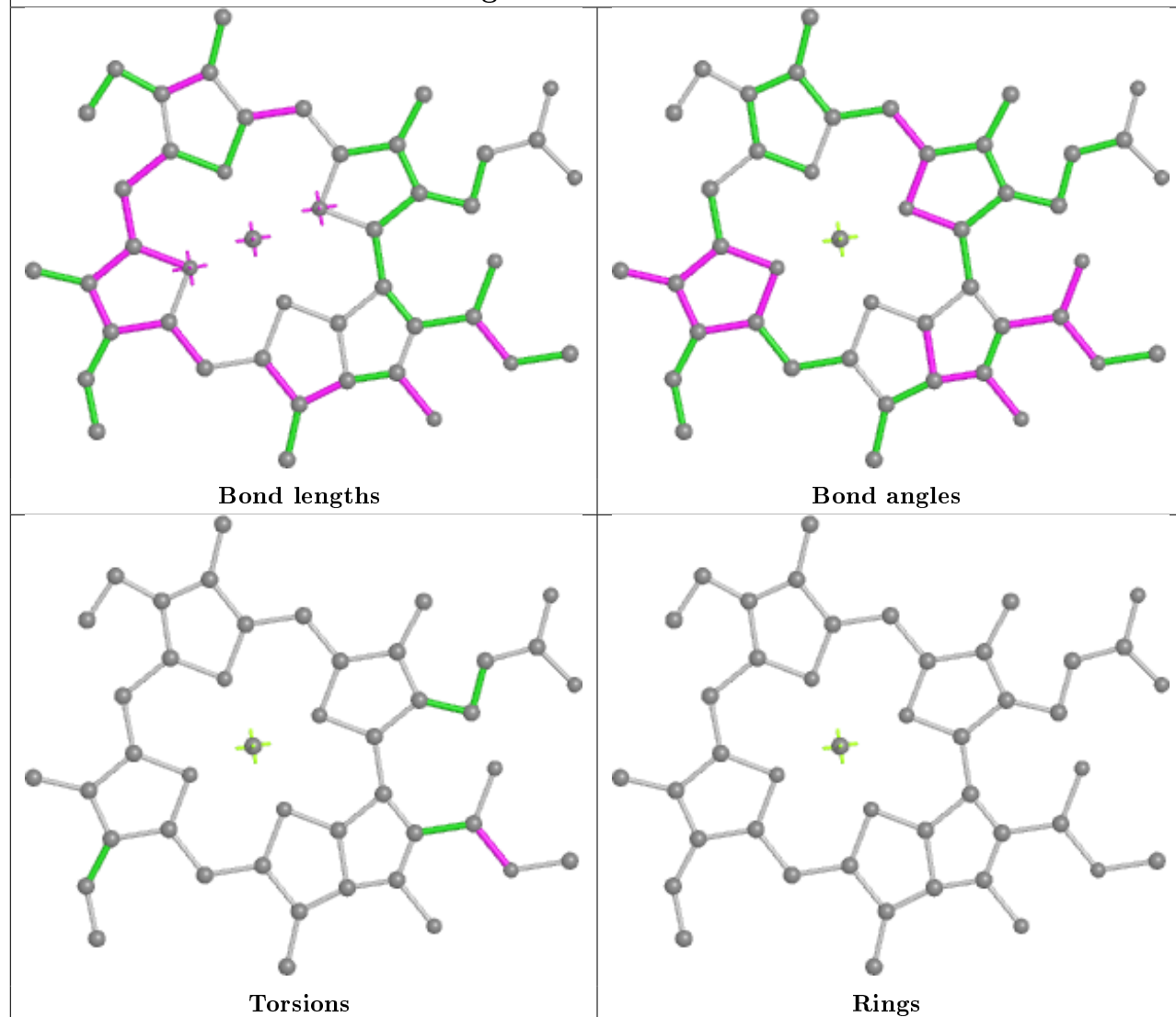
Torsions



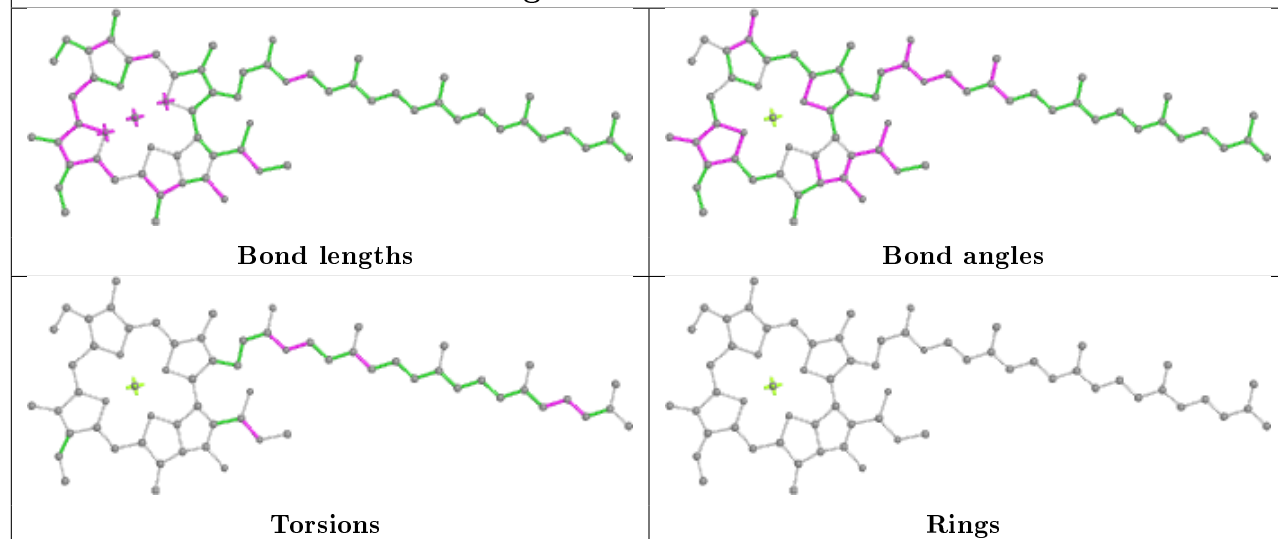
Rings

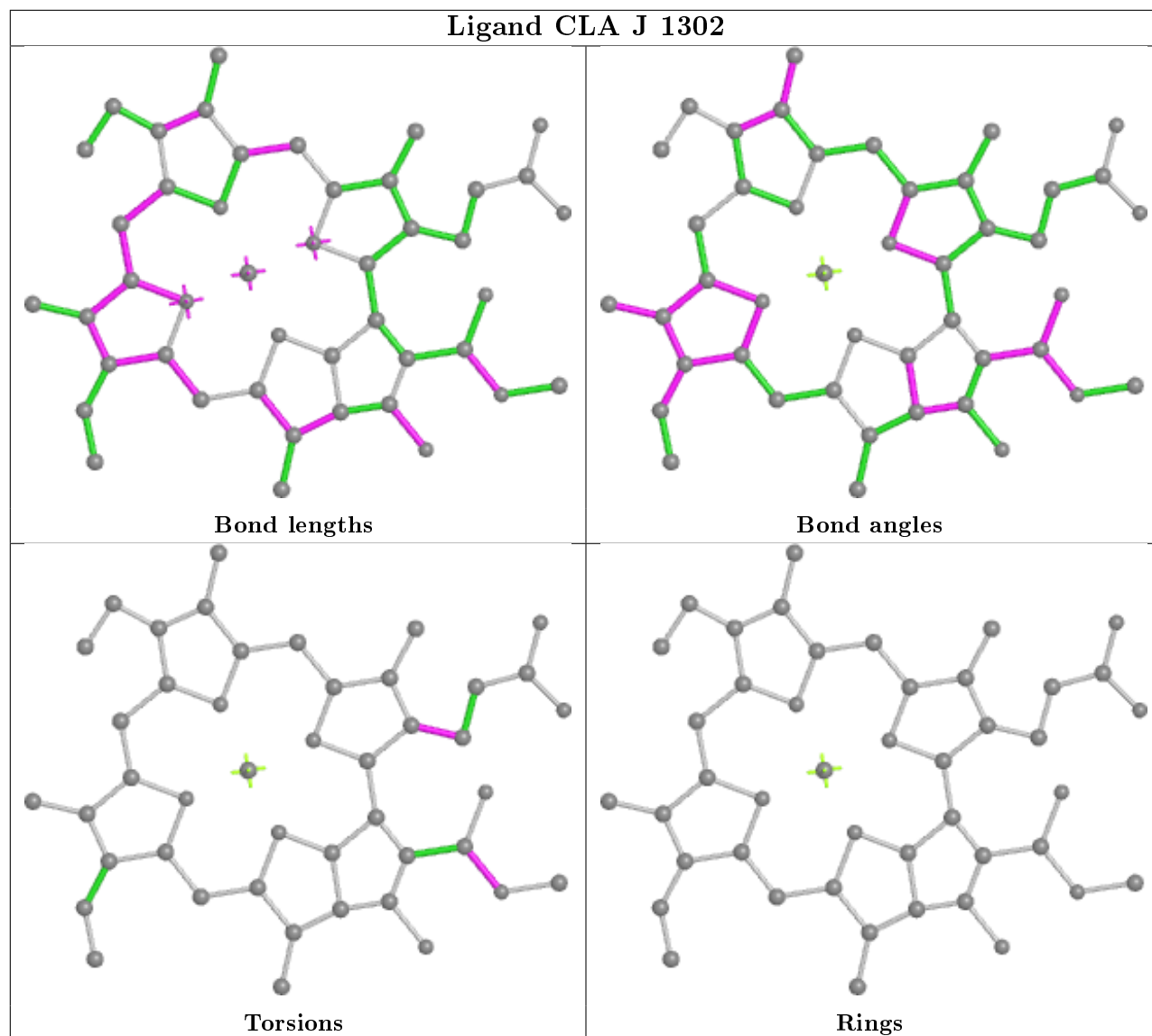


Ligand CLA B 1227

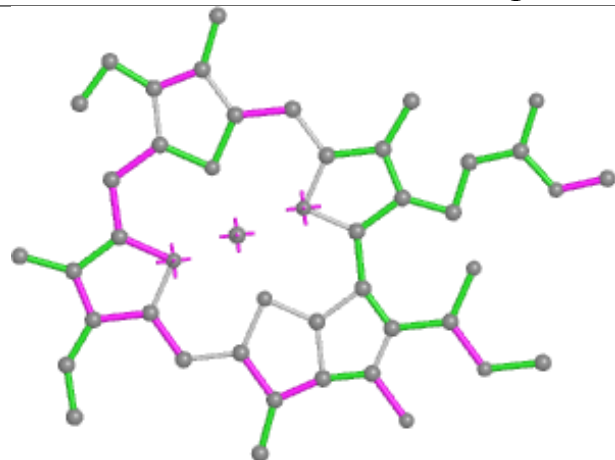


Ligand CLA A 1022

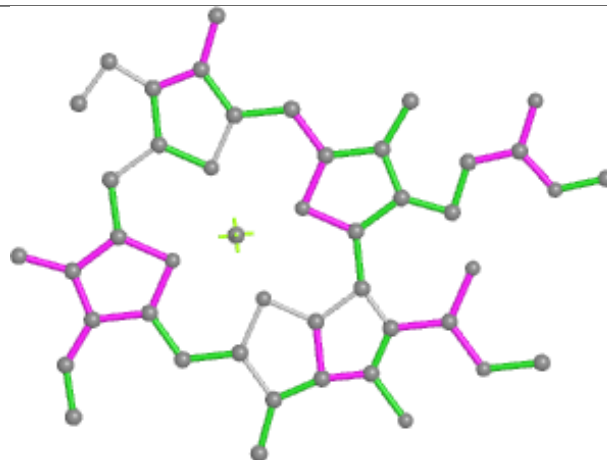




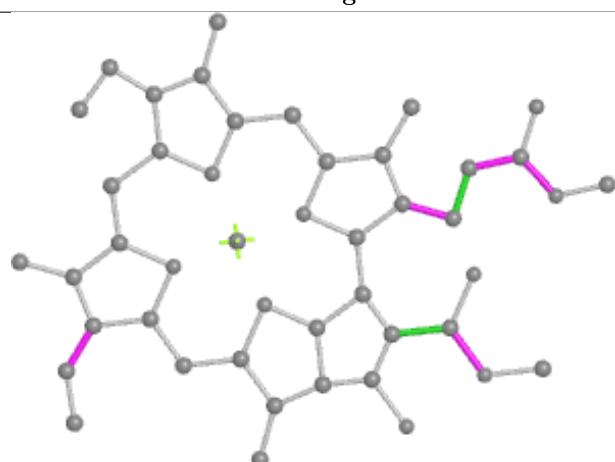
Ligand CLA B 1207



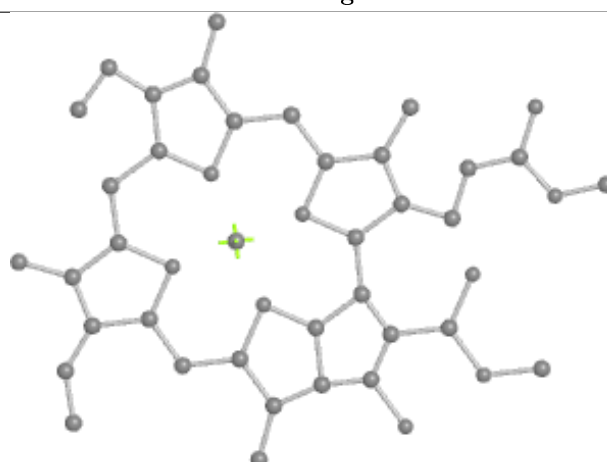
Bond lengths



Bond angles

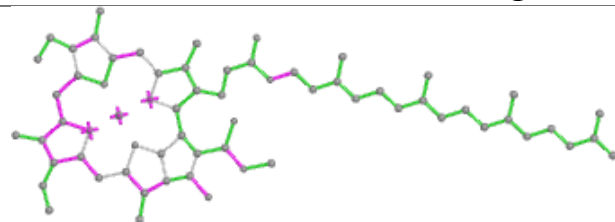


Torsions

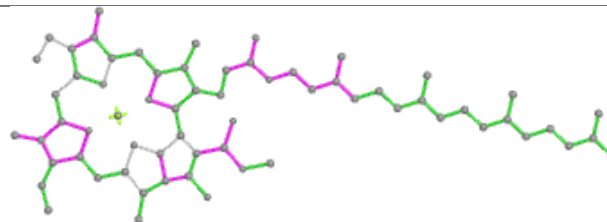


Rings

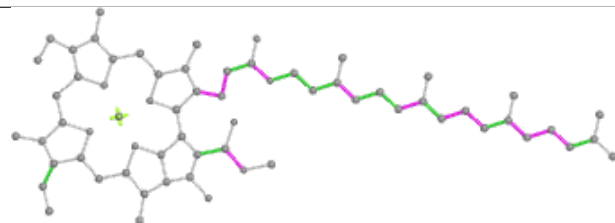
Ligand CLA F 1410



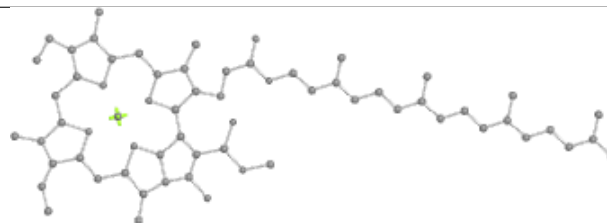
Bond lengths



Bond angles

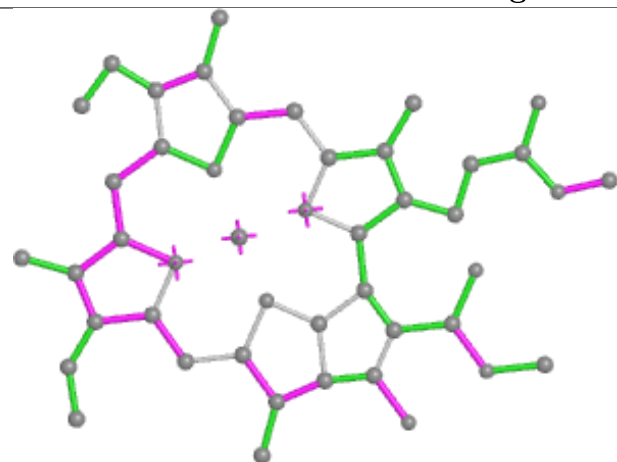


Torsions

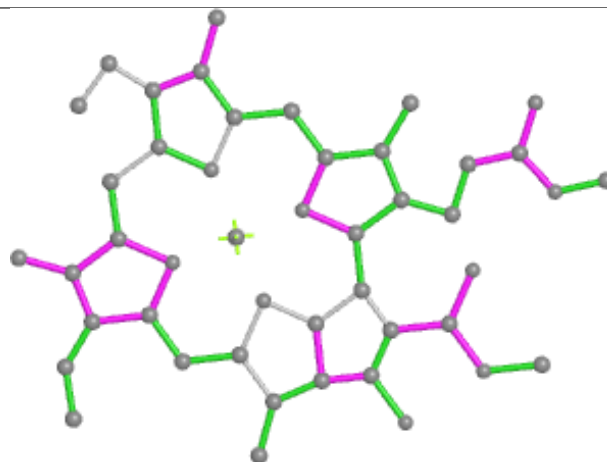


Rings

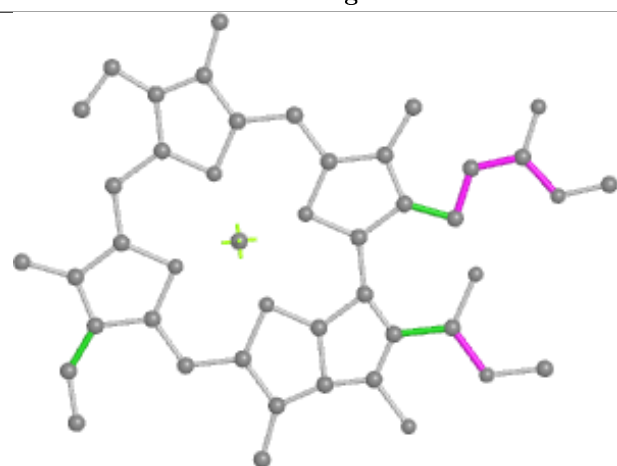
Ligand CLA A 1134



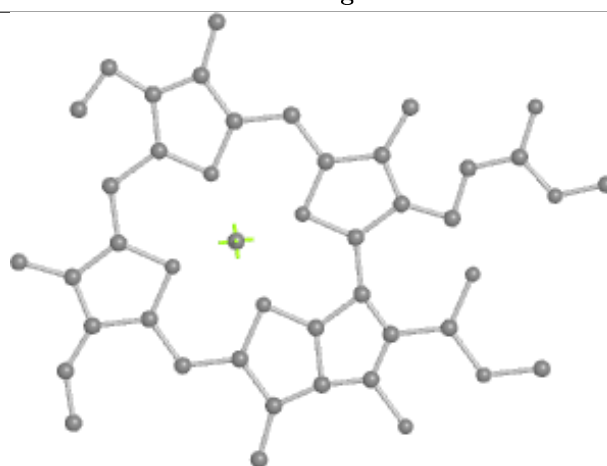
Bond lengths



Bond angles

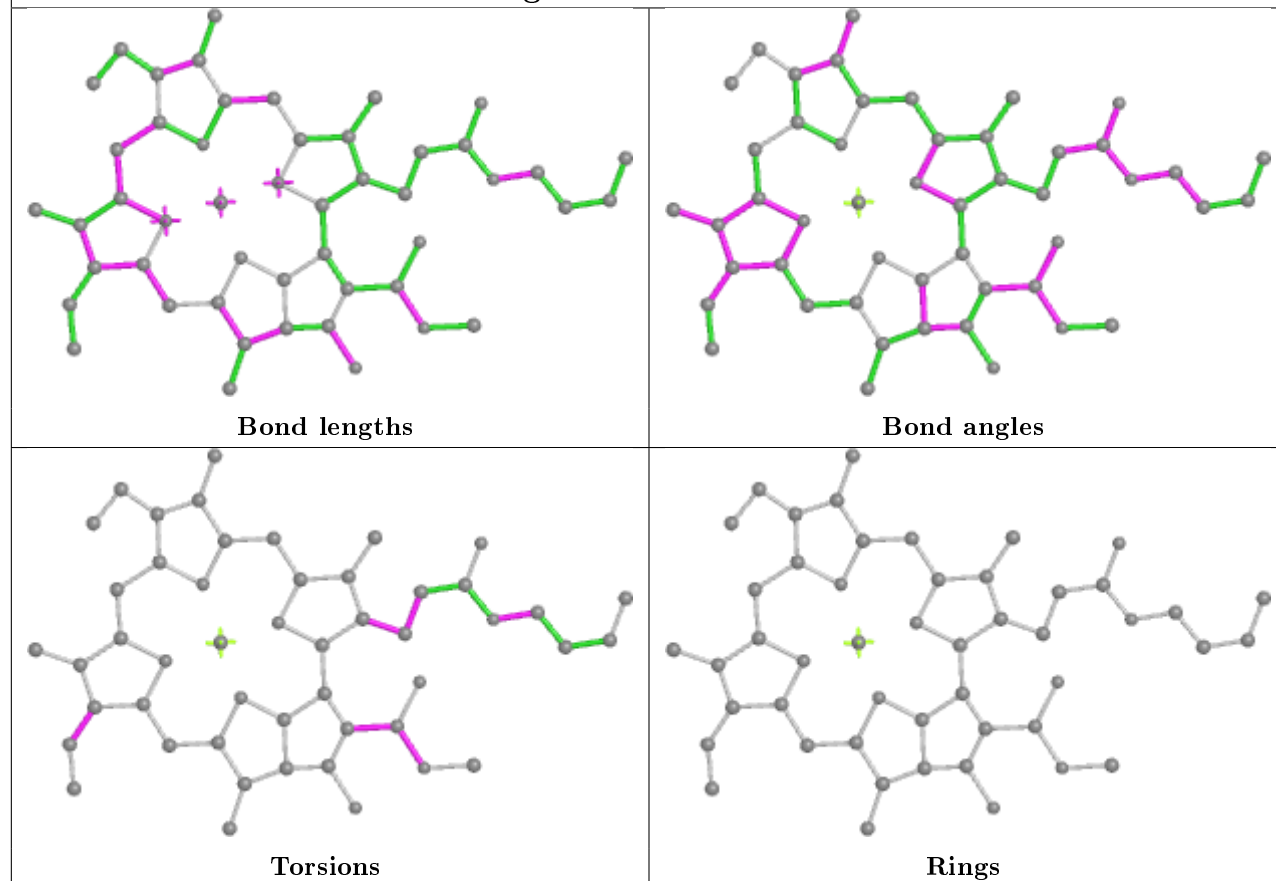


Torsions

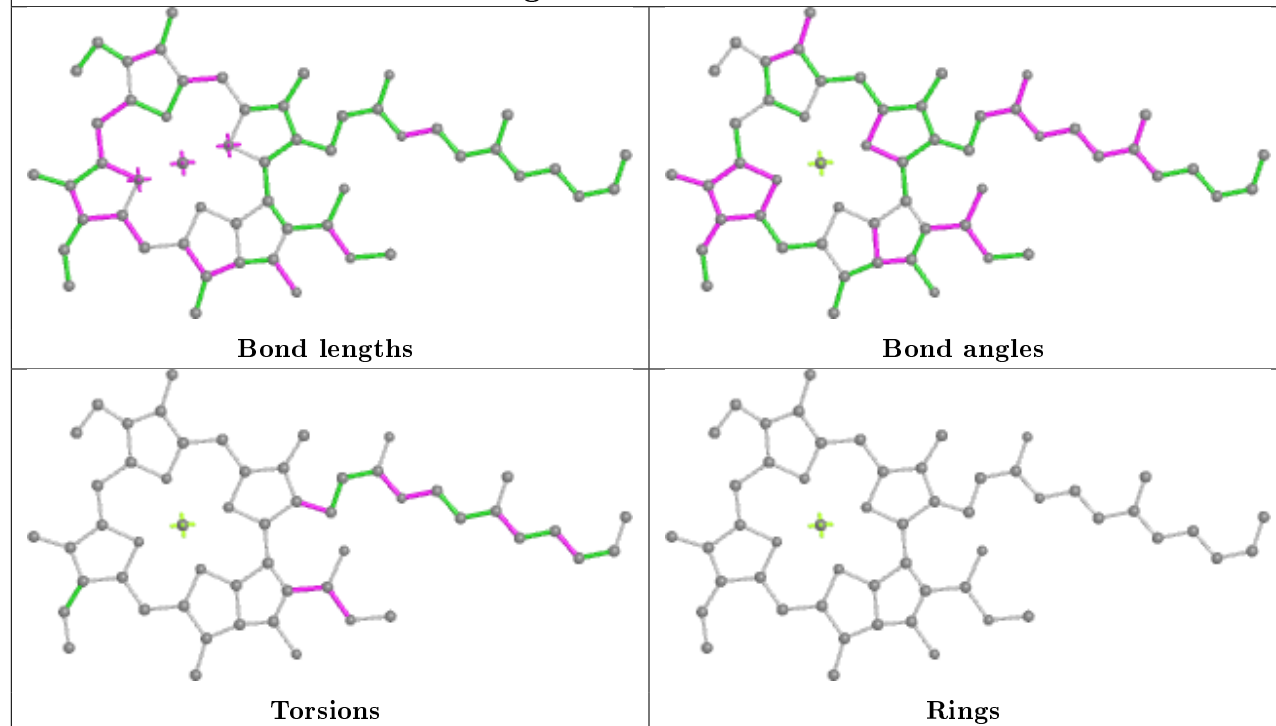


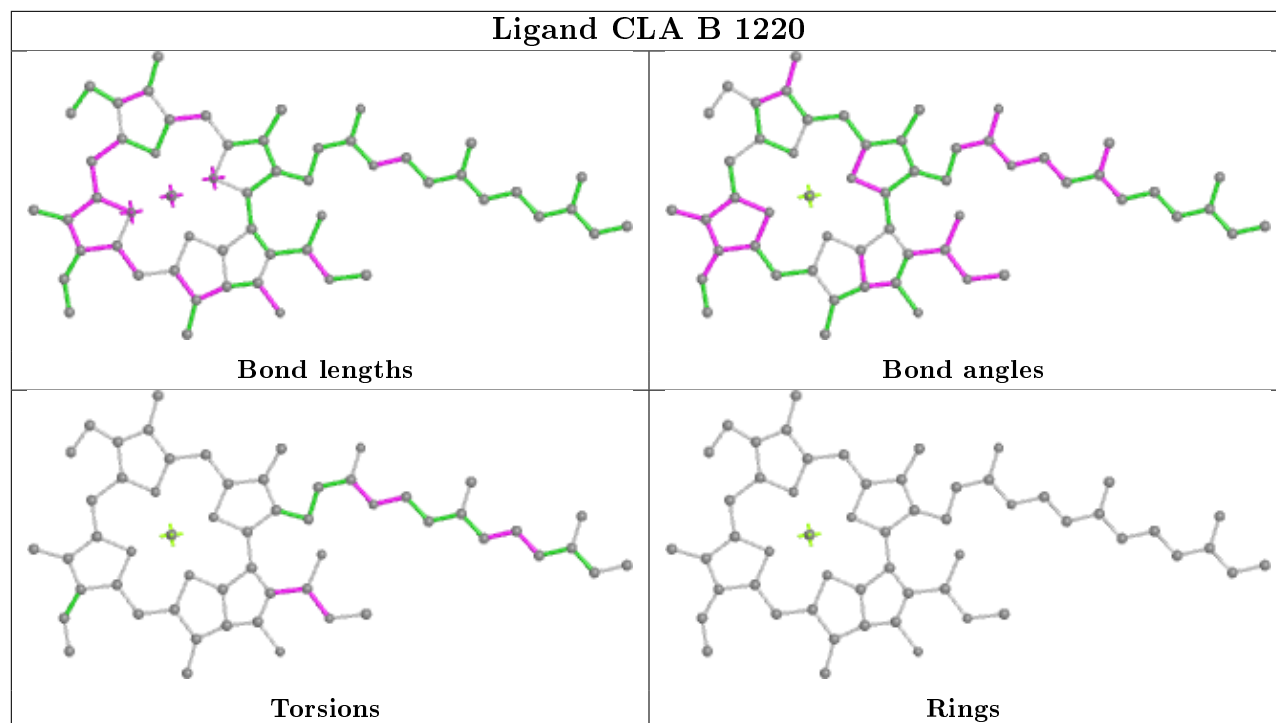
Rings

Ligand CLA A 1114

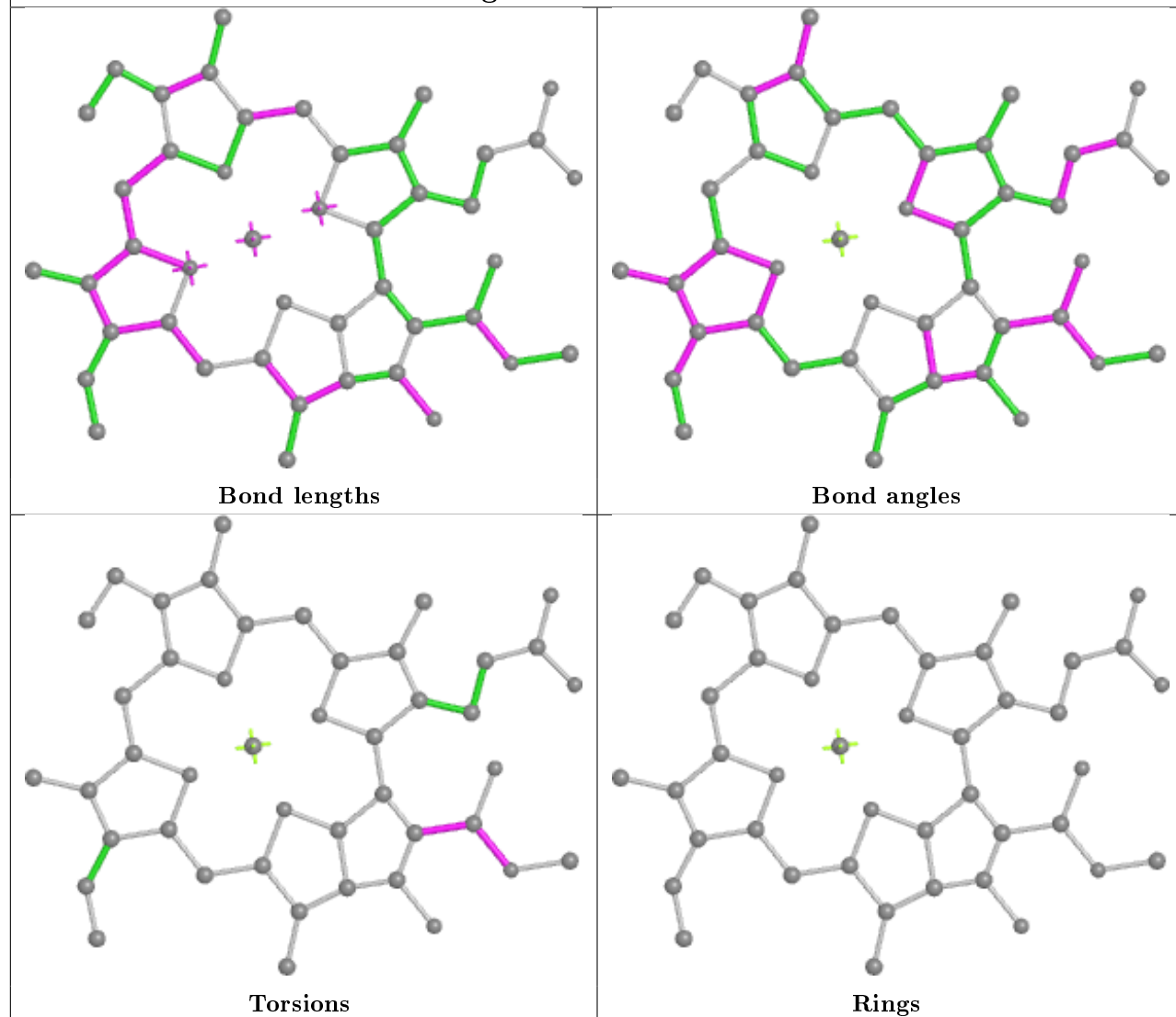


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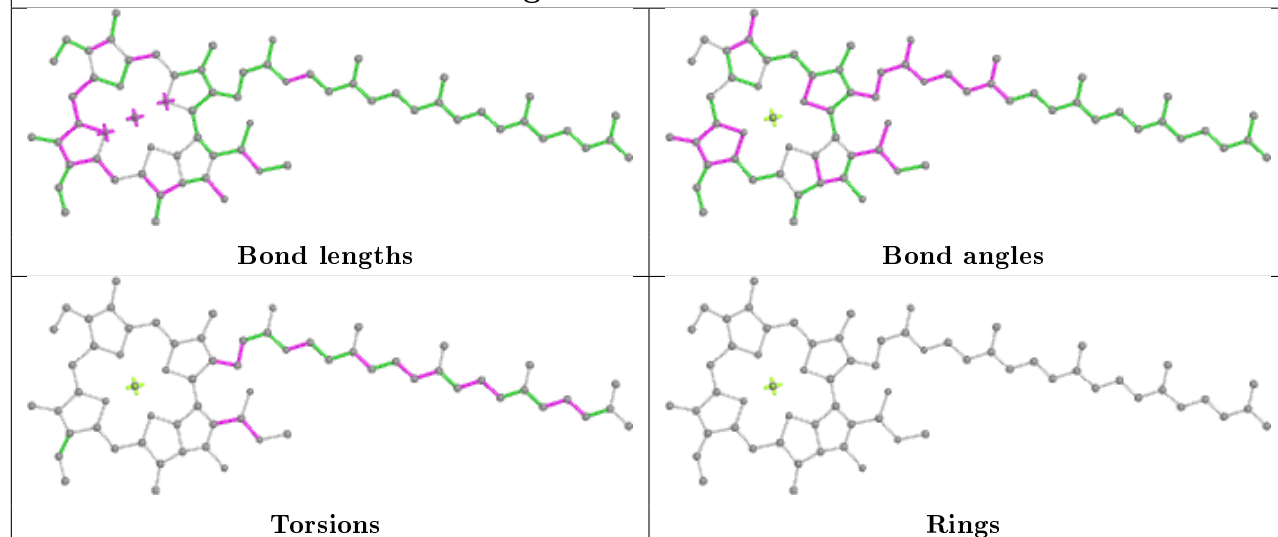




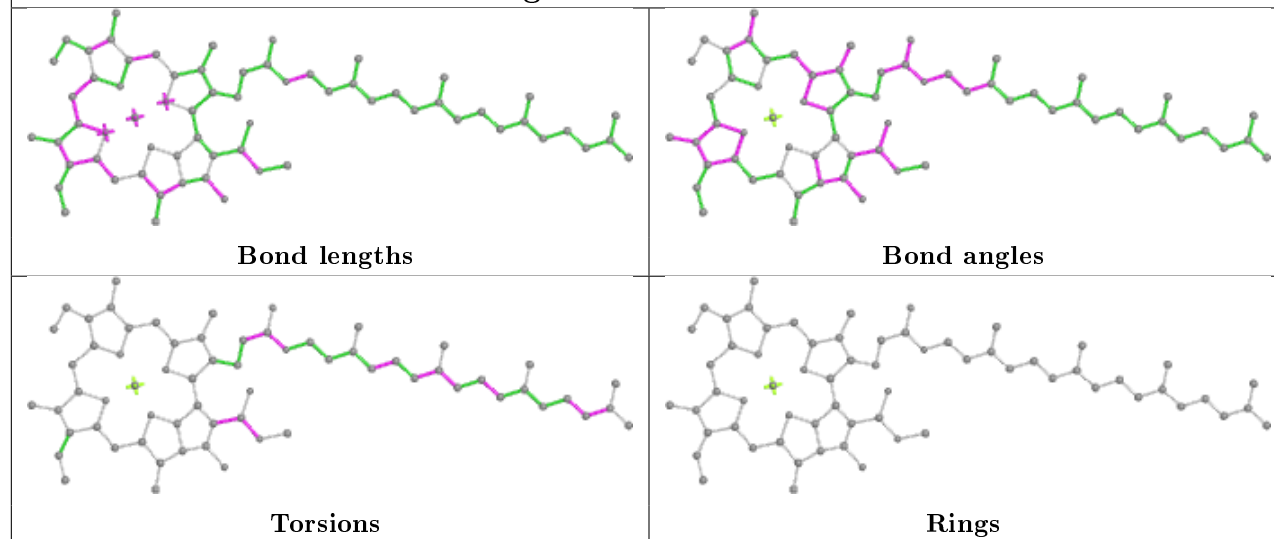
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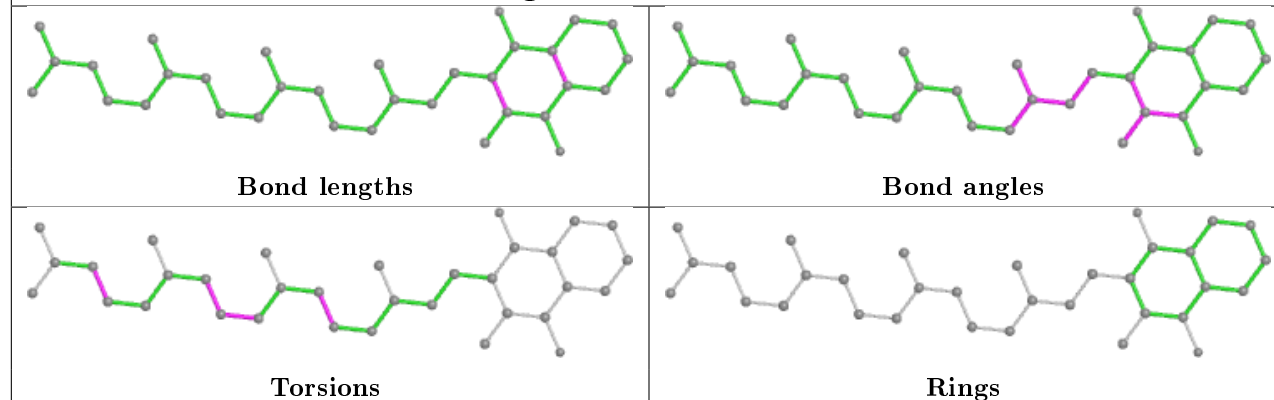
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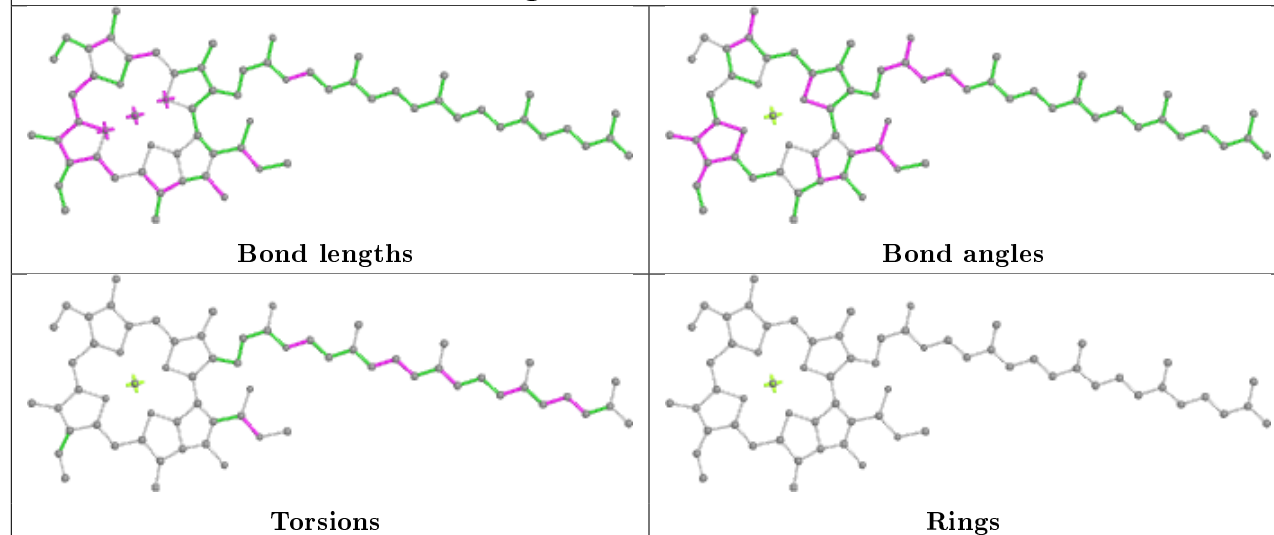
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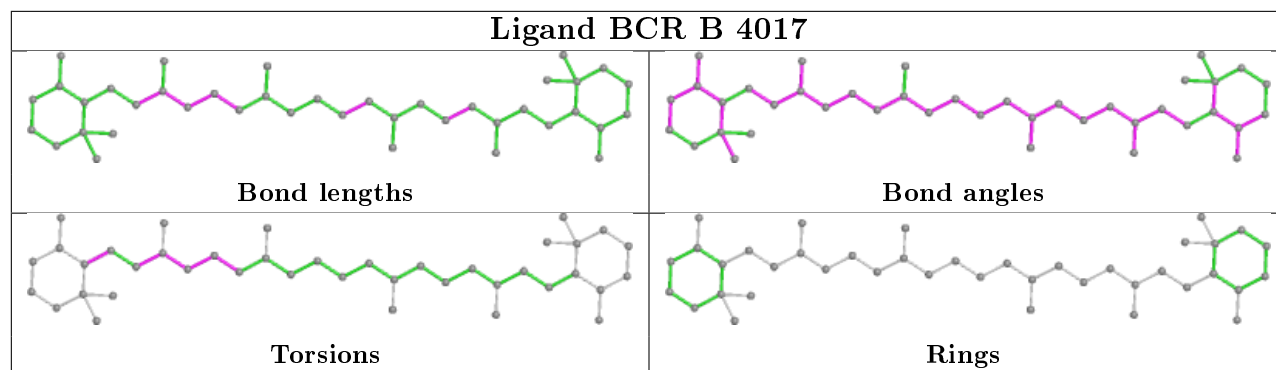
Ligand PQN B 2002



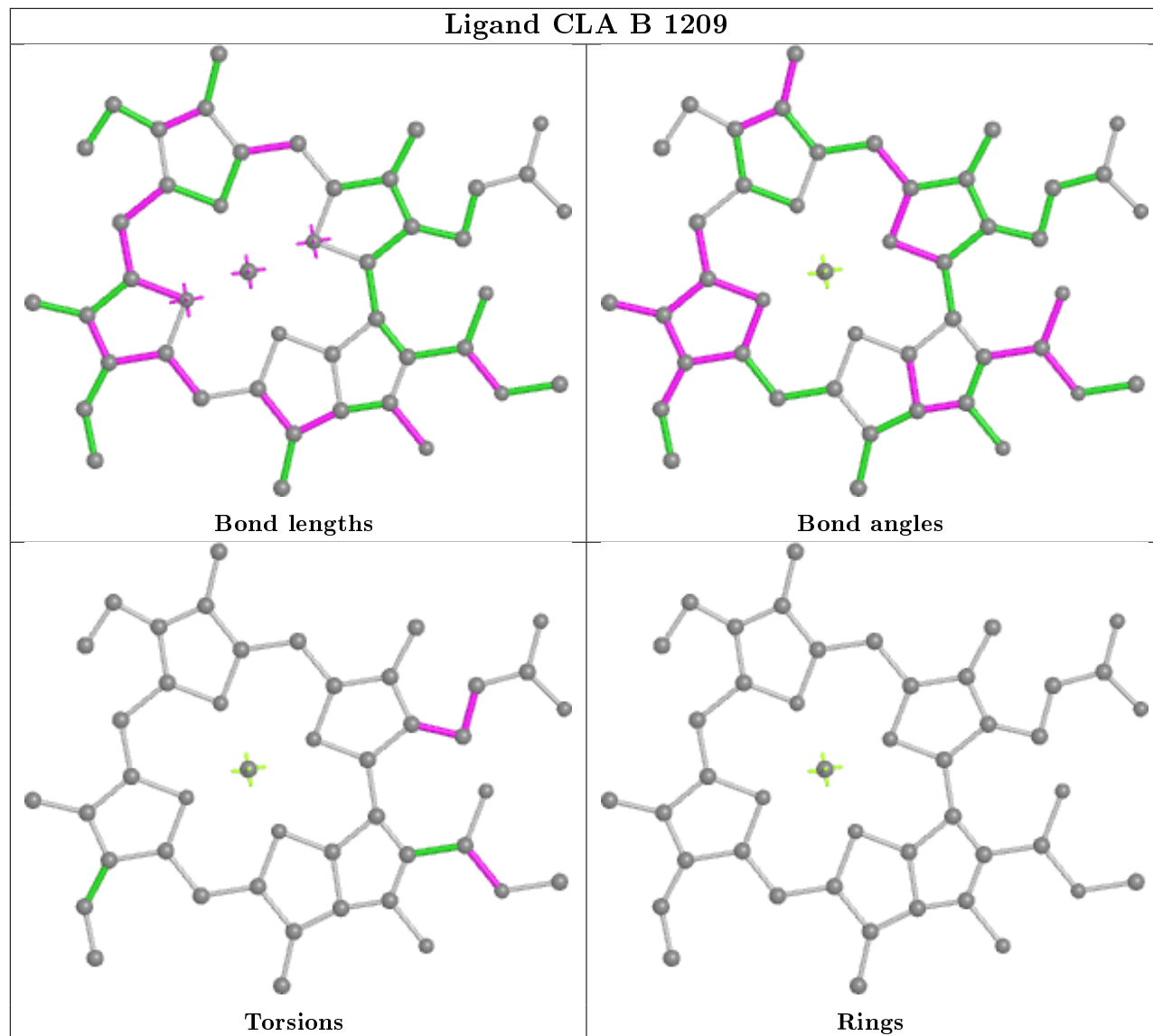
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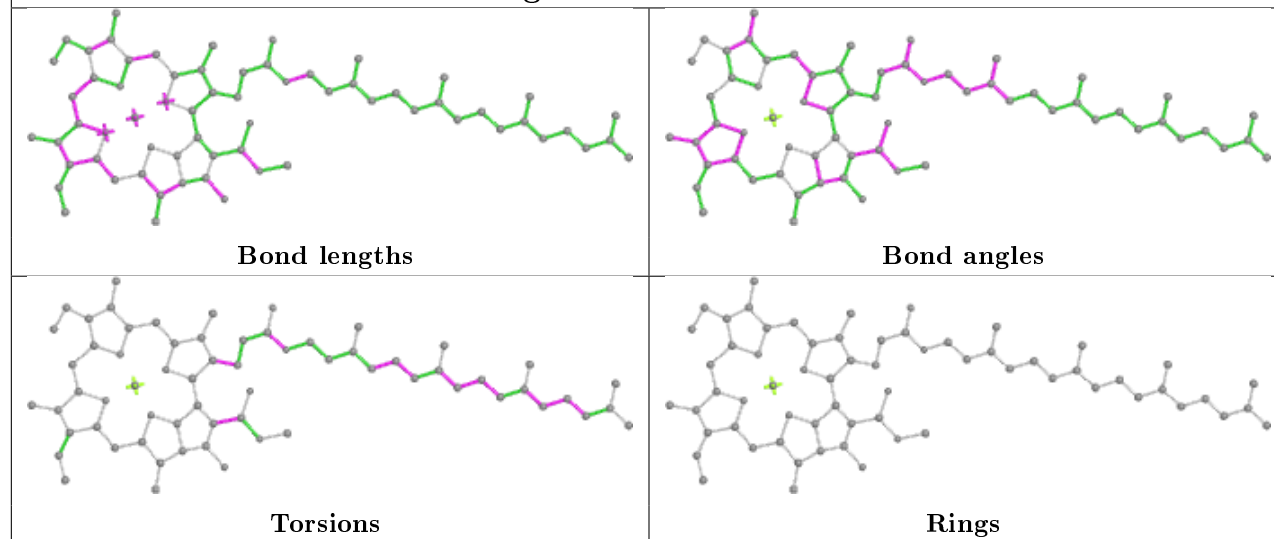
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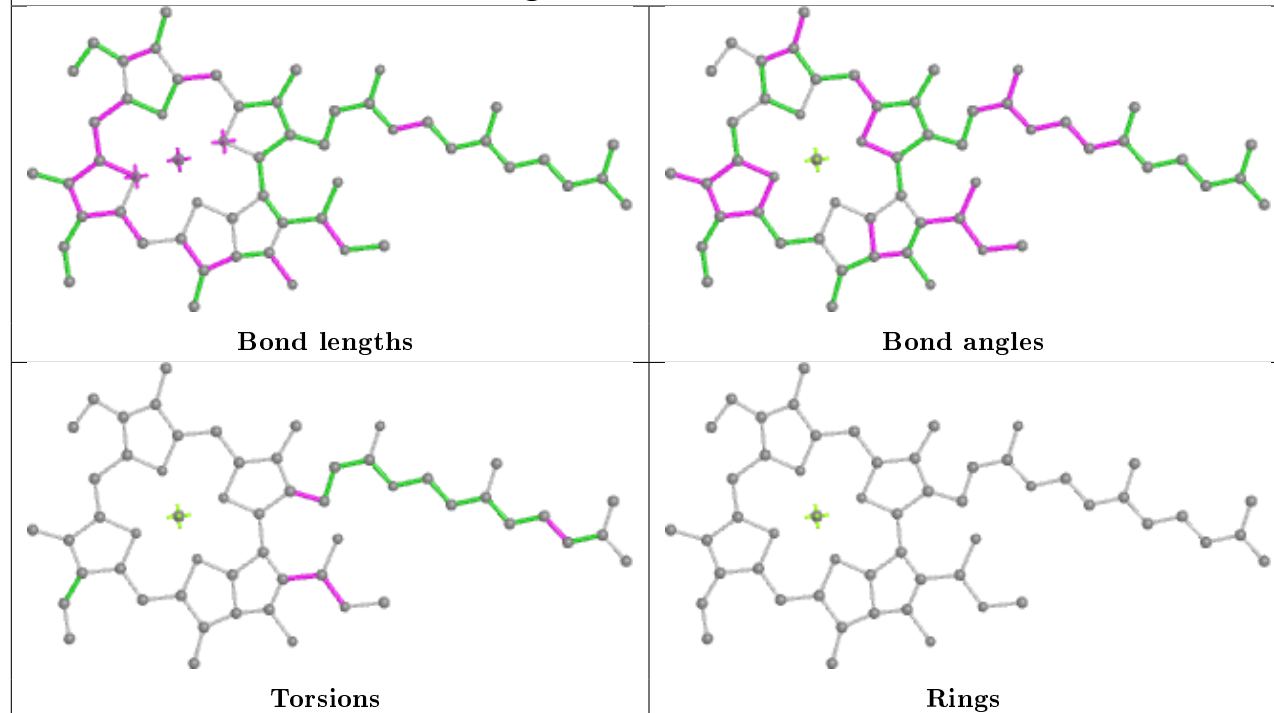
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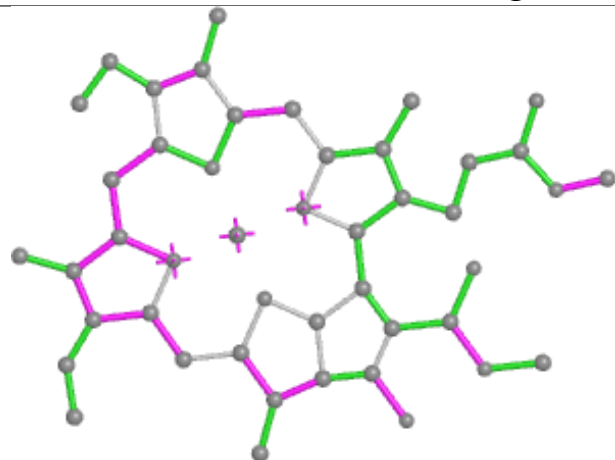
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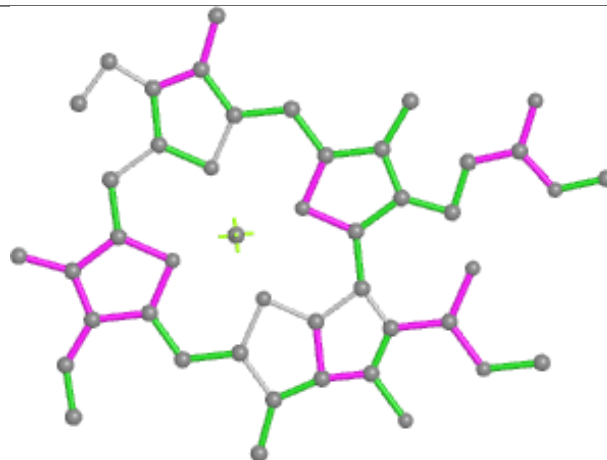
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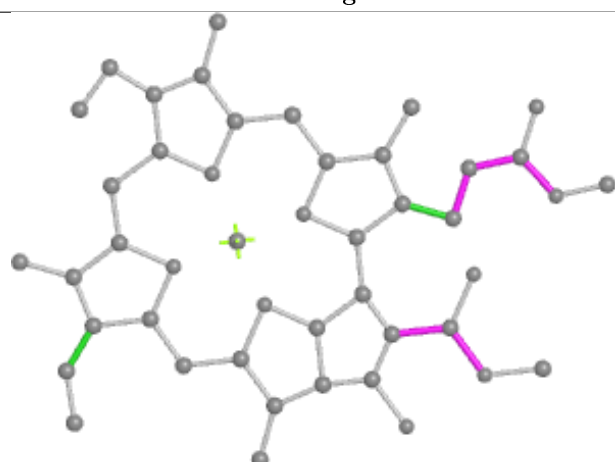
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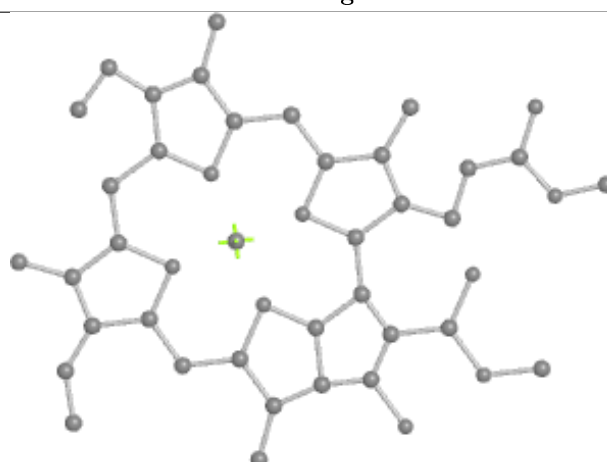
Bond lengths



Bond angles

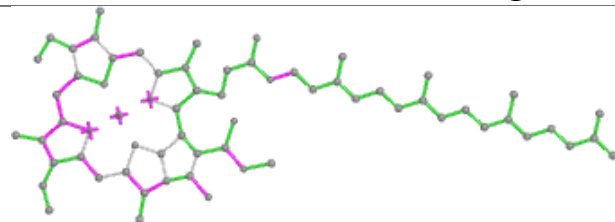


Torsions

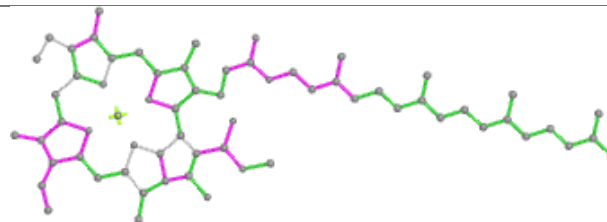


Rings

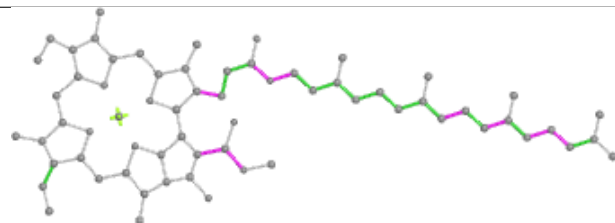
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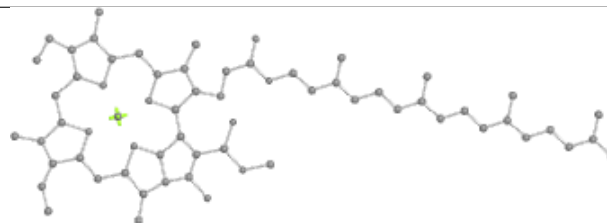
Bond lengths



Bond angles

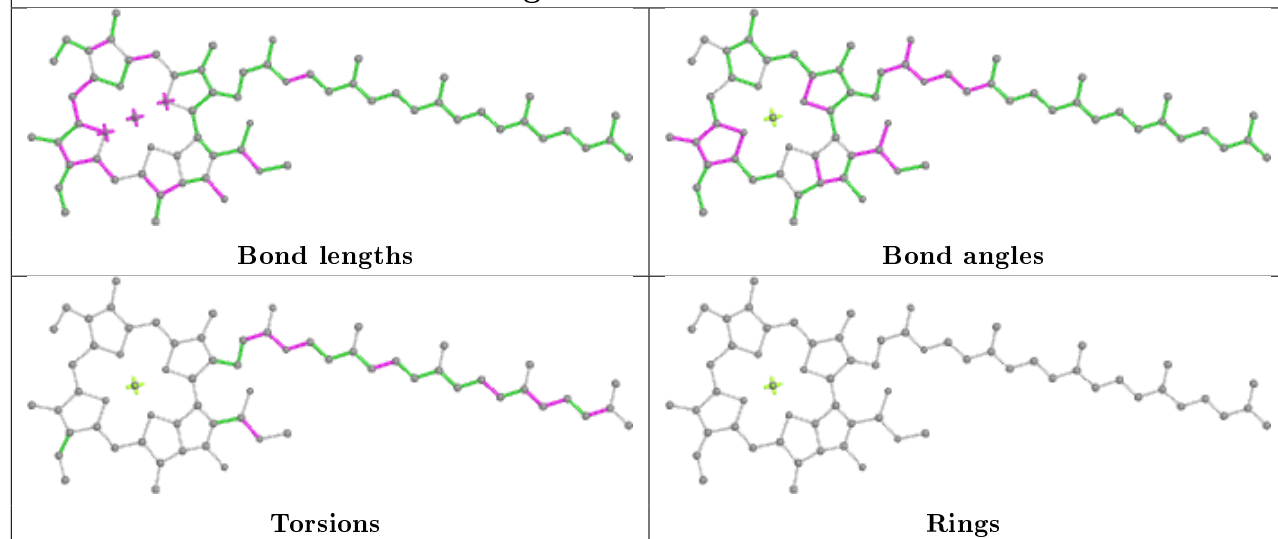


Torsions

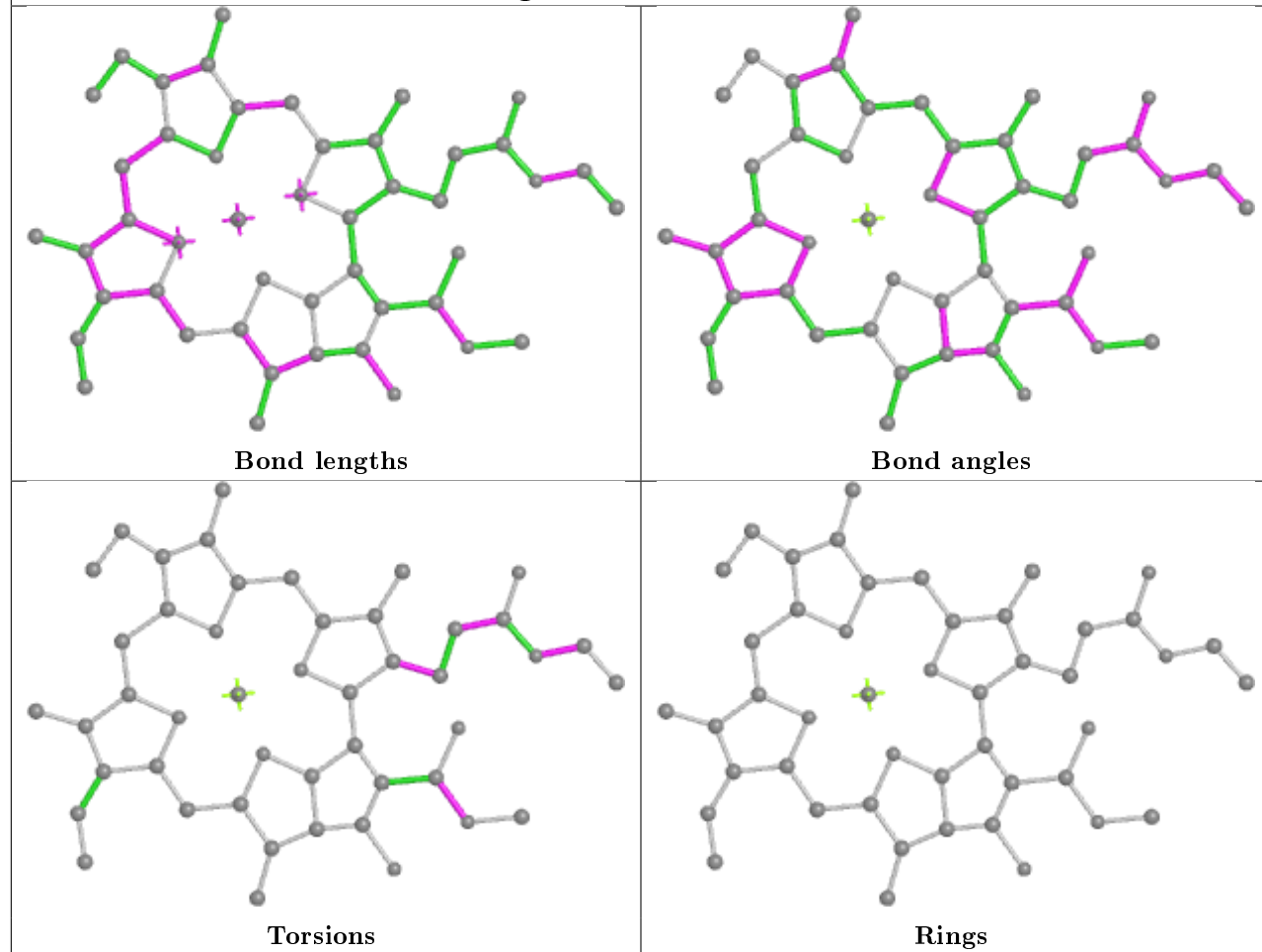


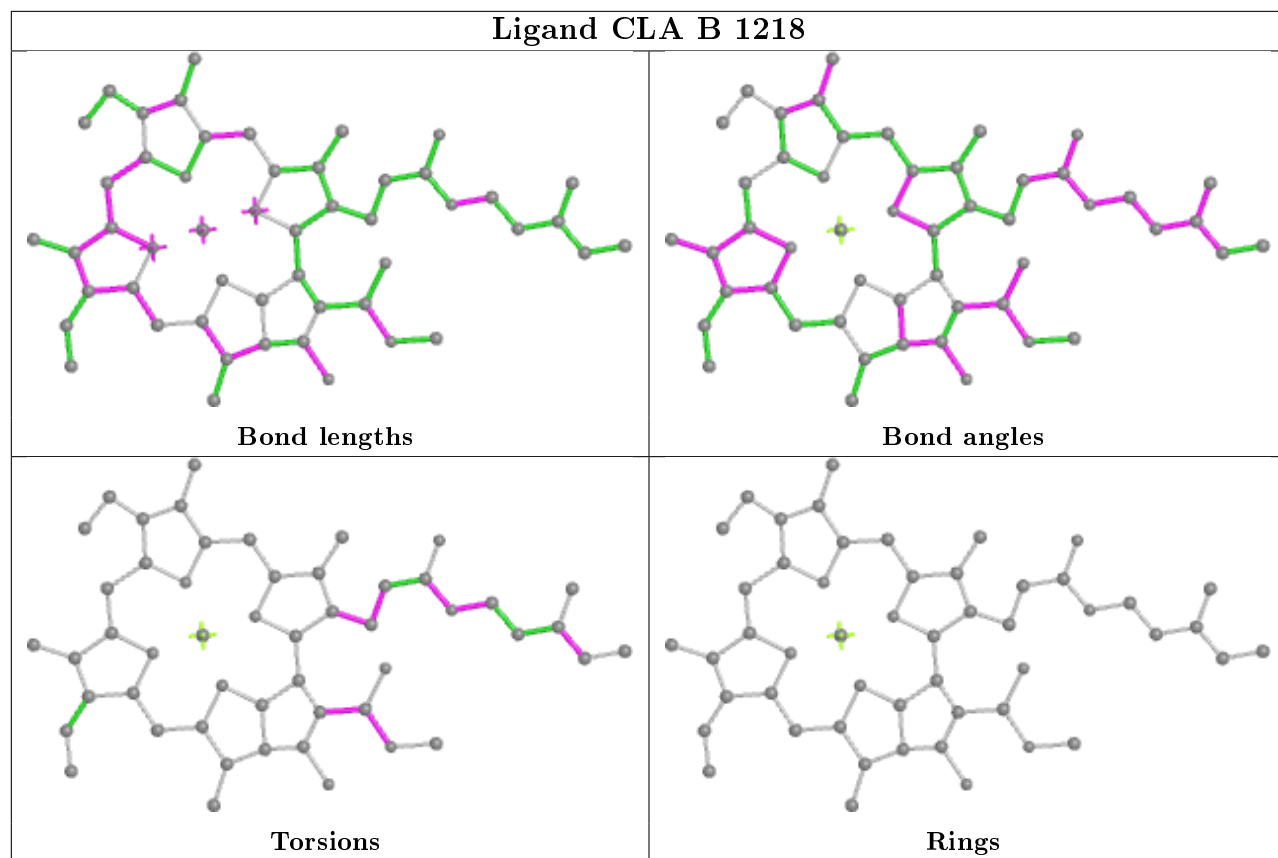
Rings

Ligand CLA B 1203

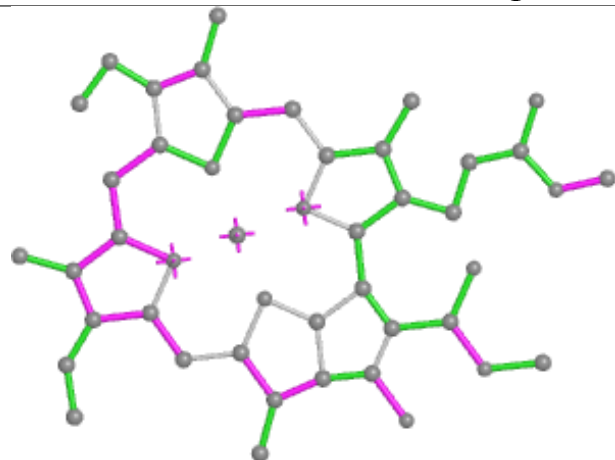


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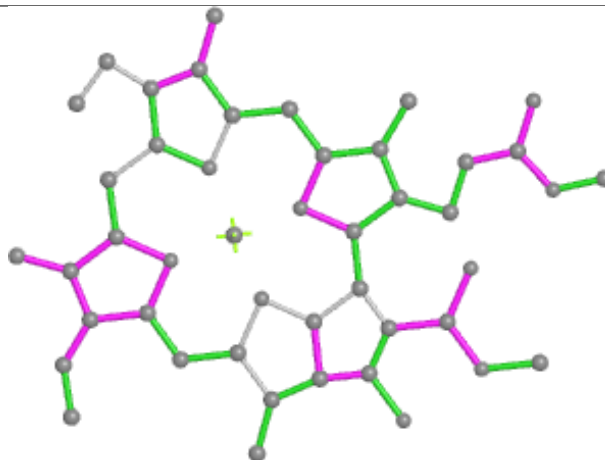




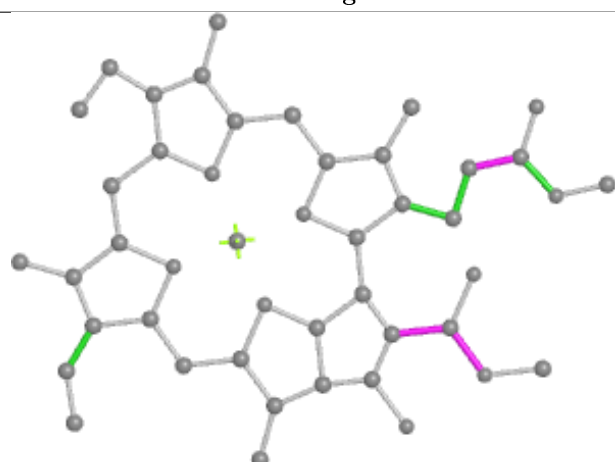
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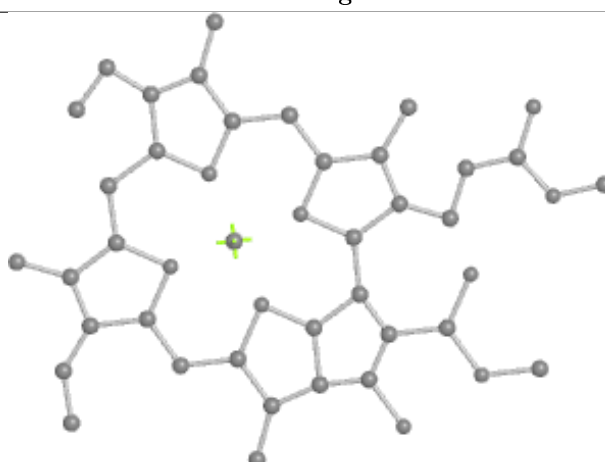
Bond lengths



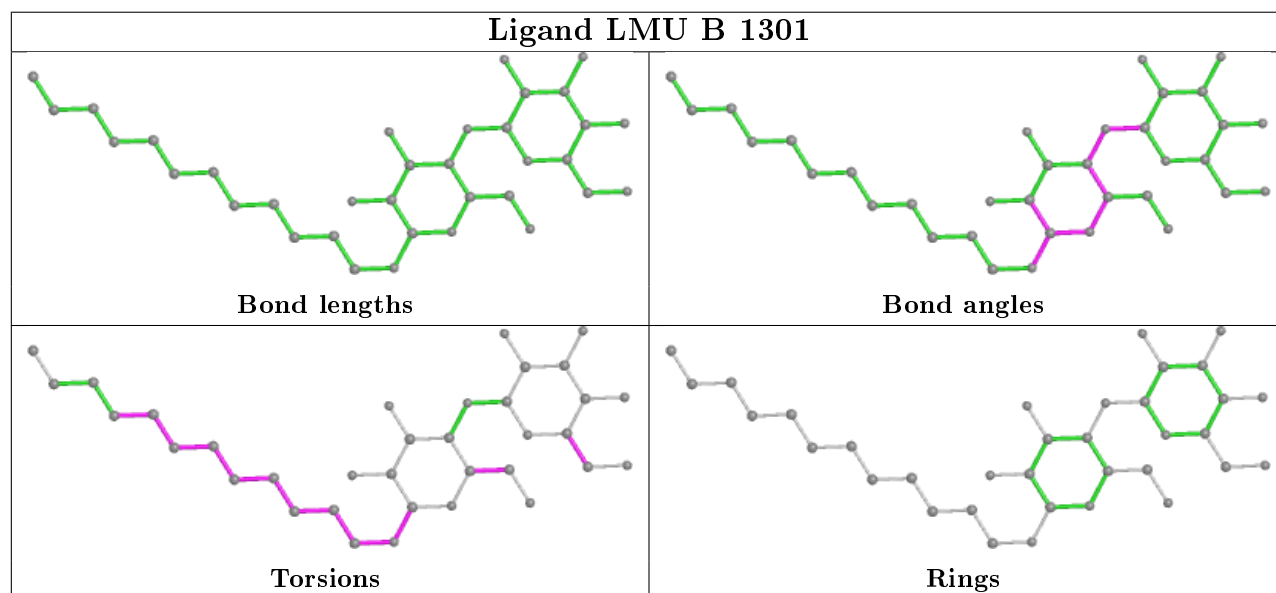
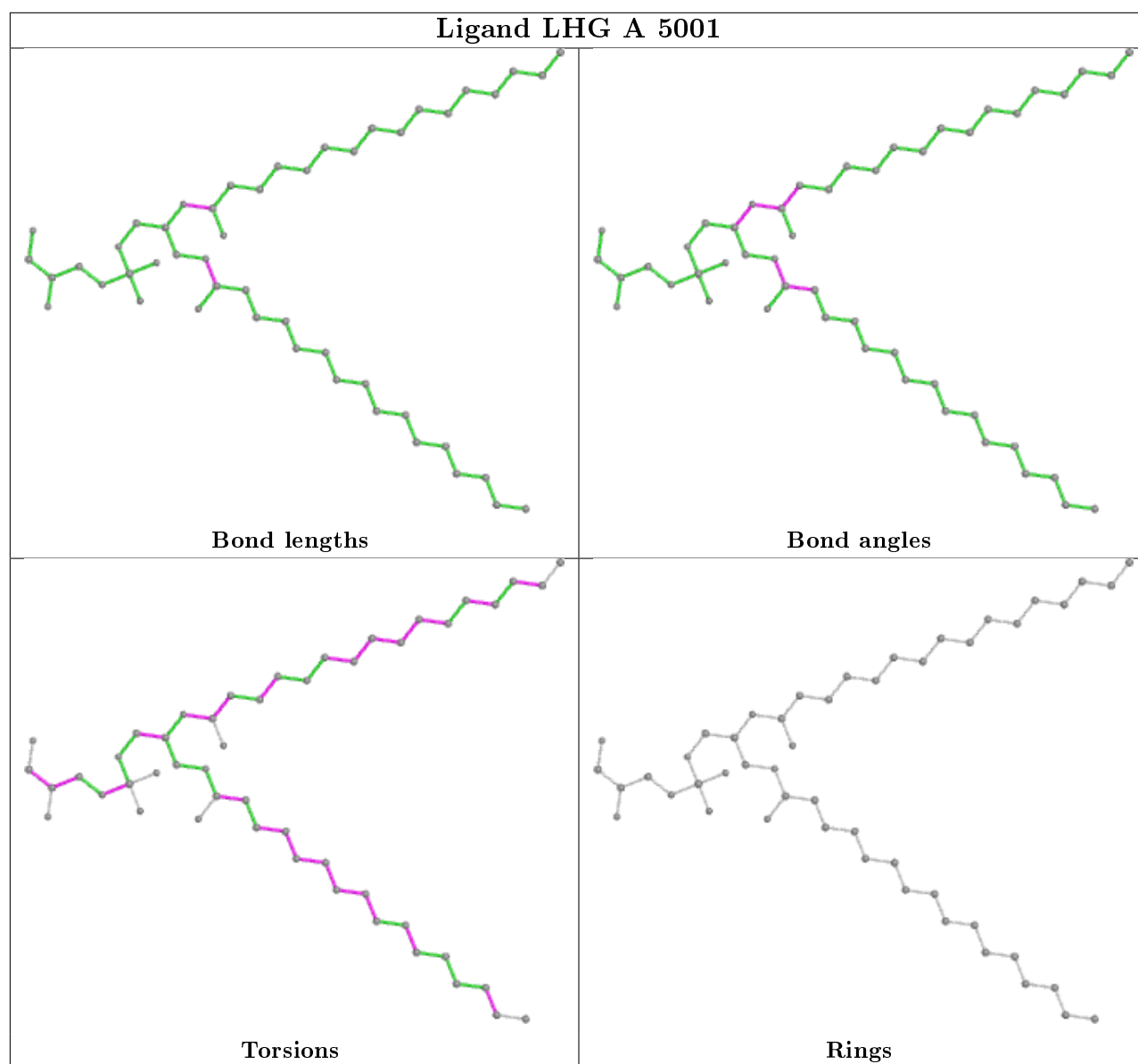
Bond angles



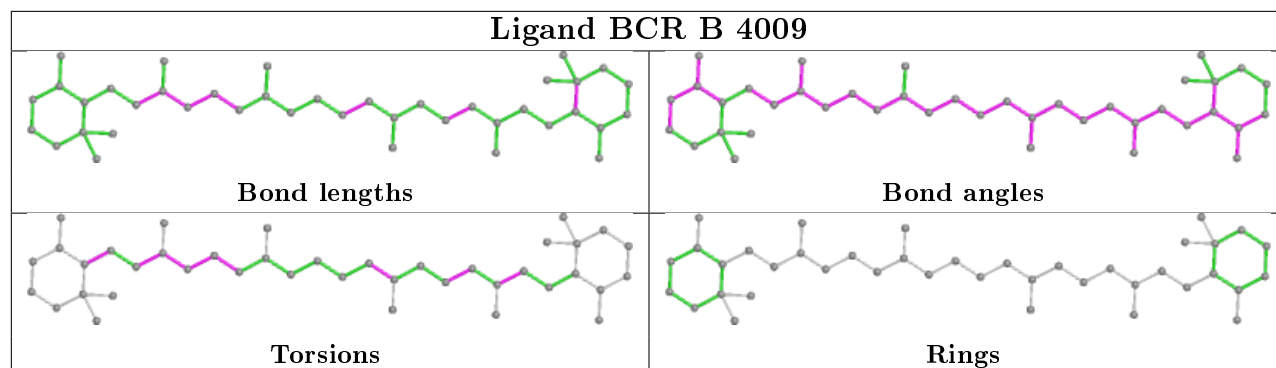
Torsions



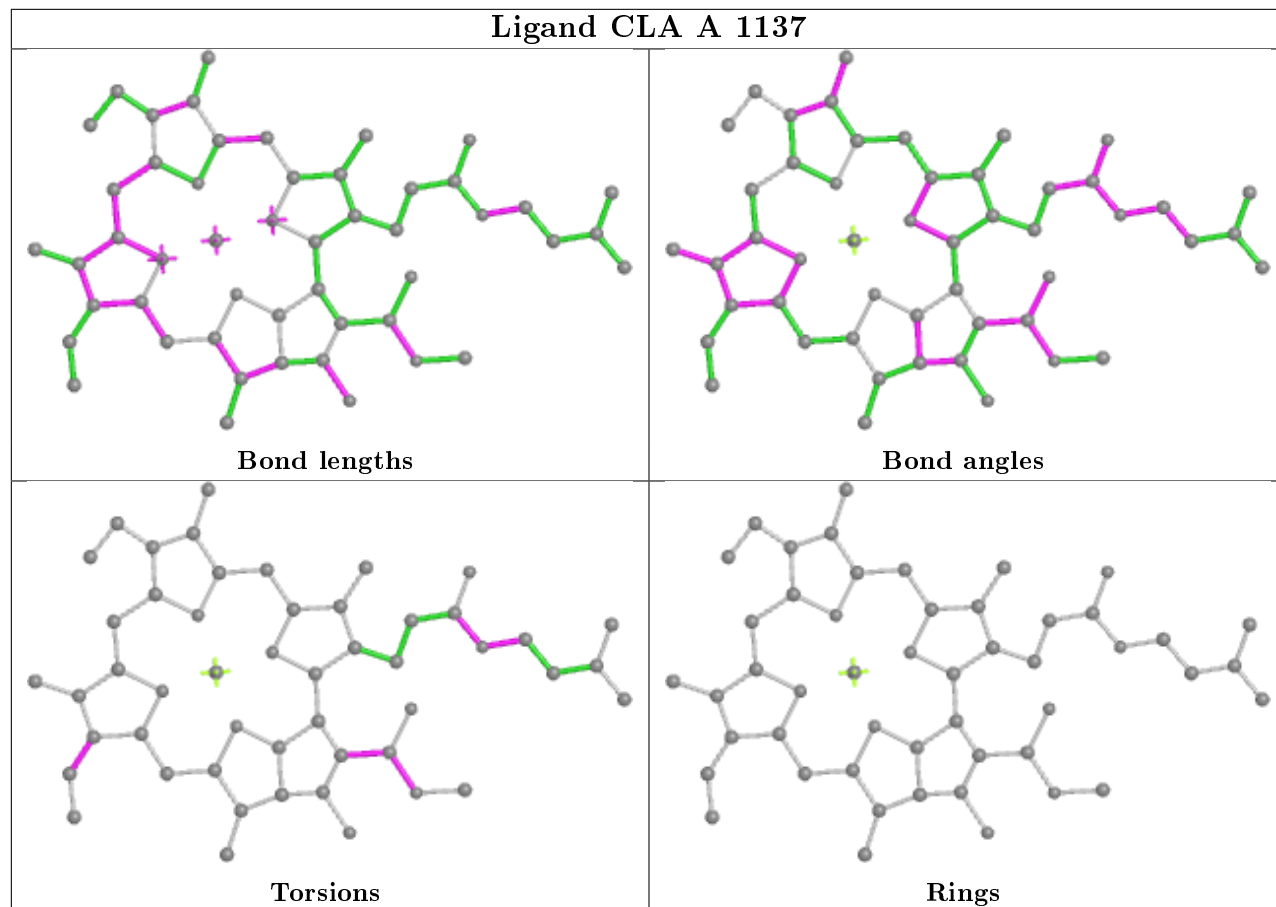
Rings



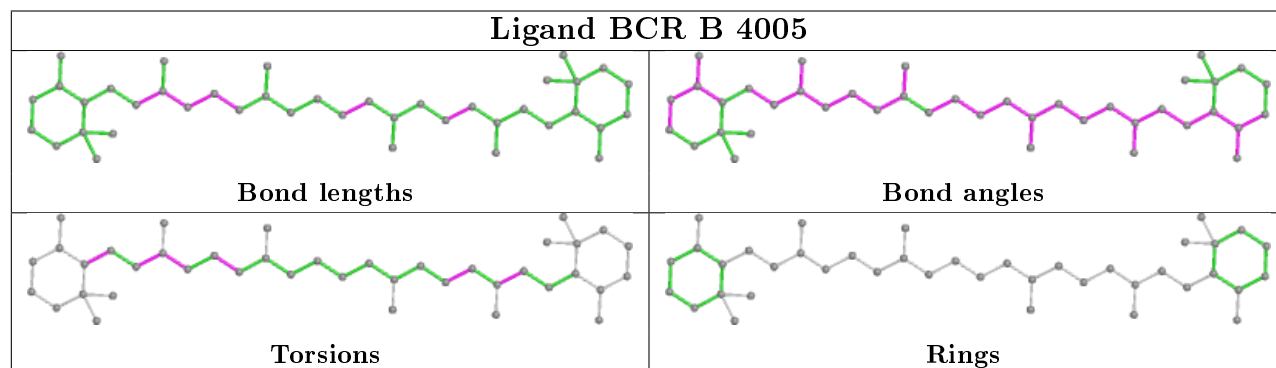
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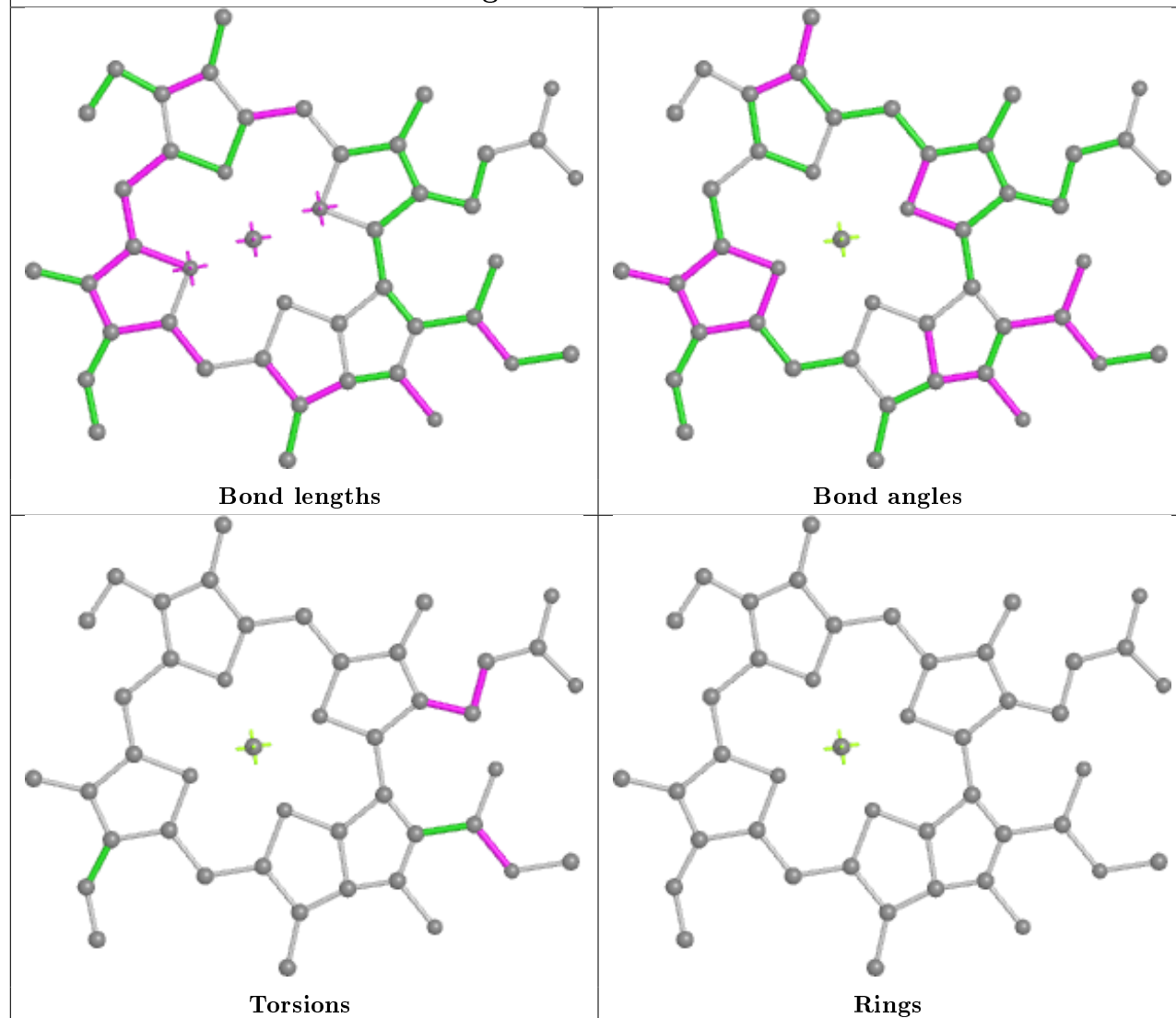
Ligand CLA A 1137



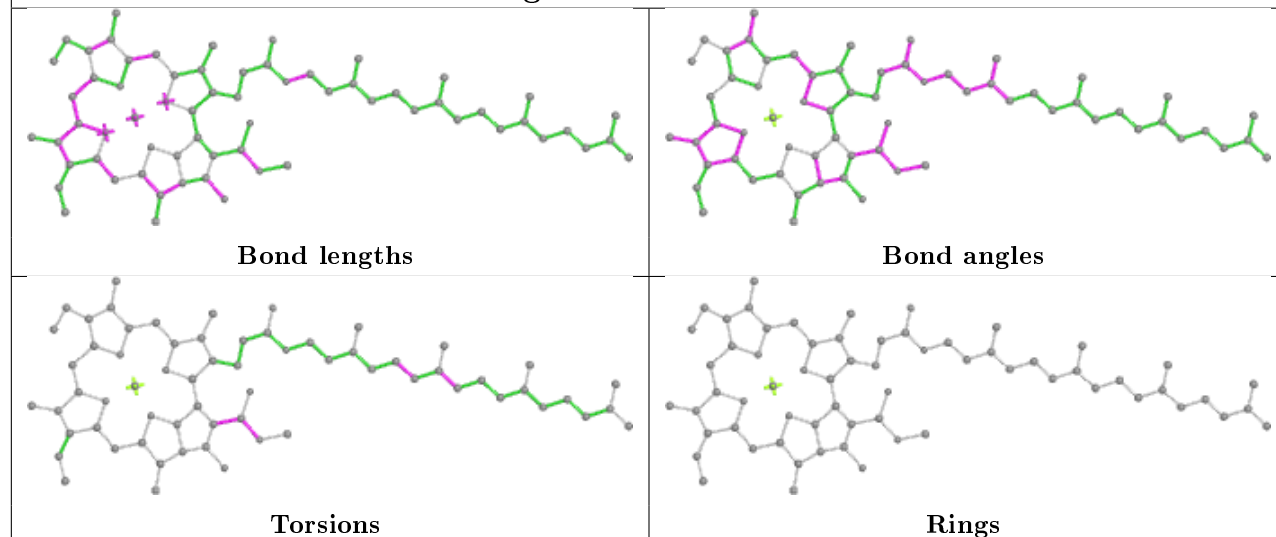
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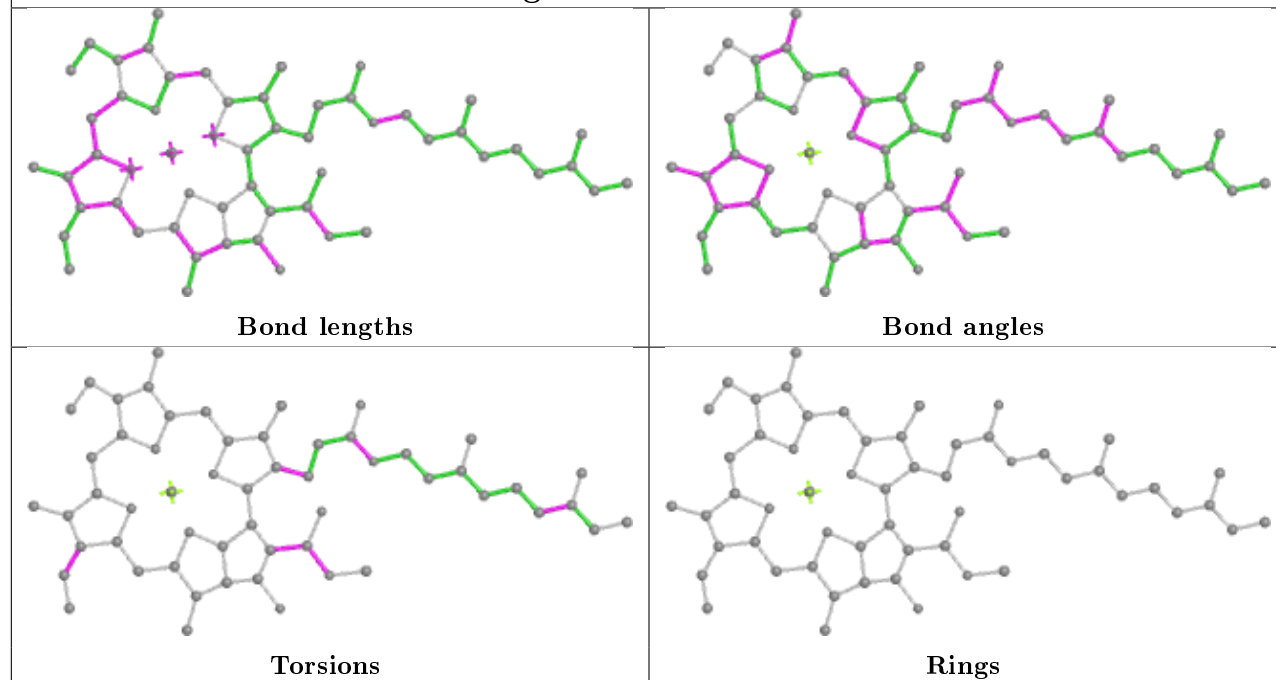
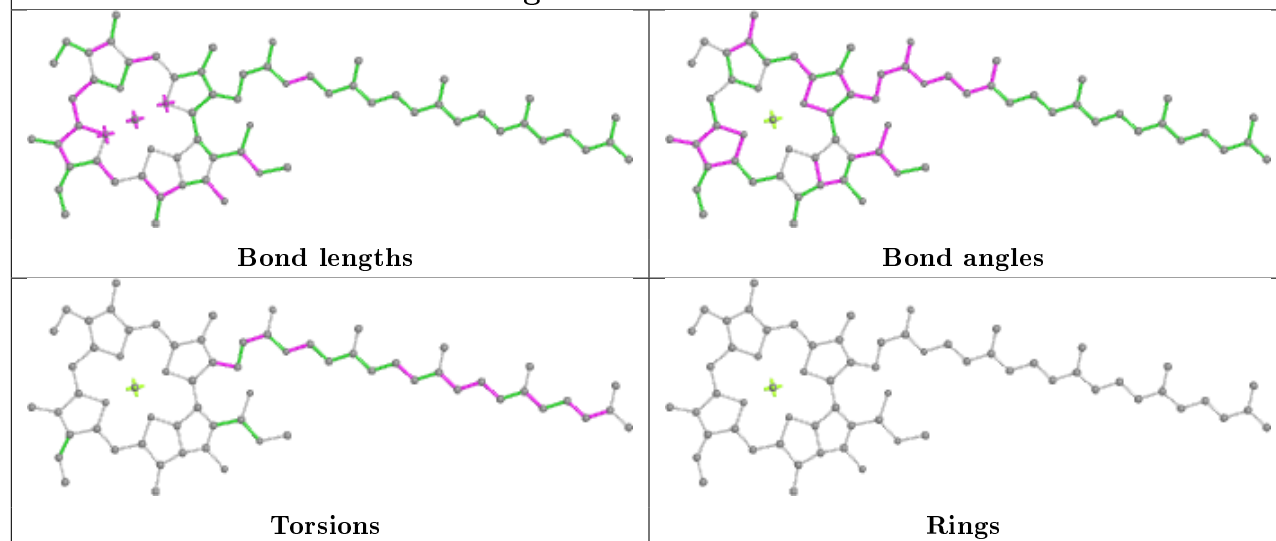


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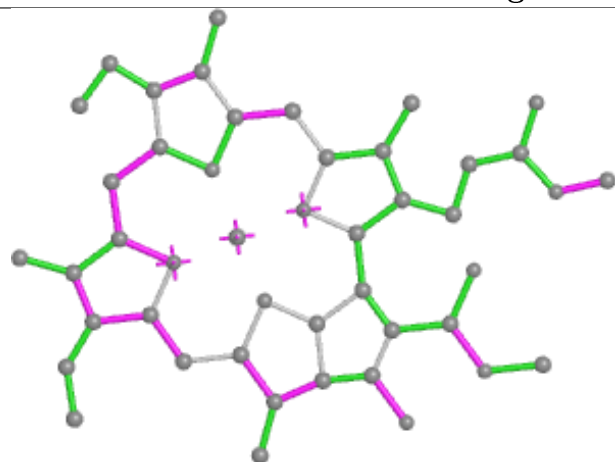


Ligand CLA A 1138

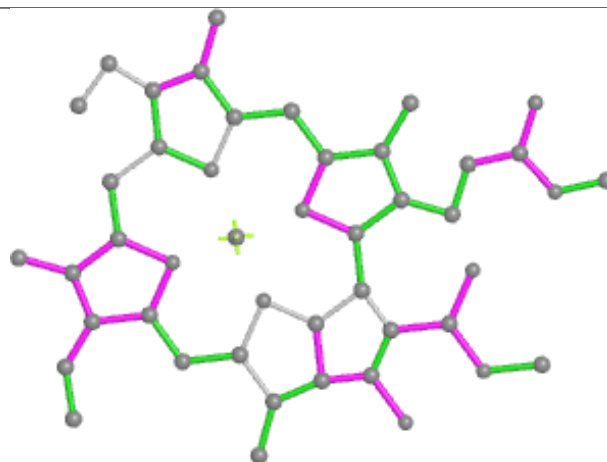


Ligand CLA B 1222**Ligand CLA A 1101**

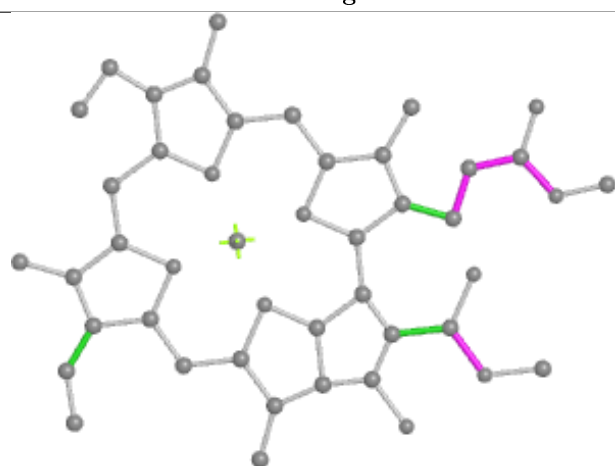
Ligand CLA A 1115



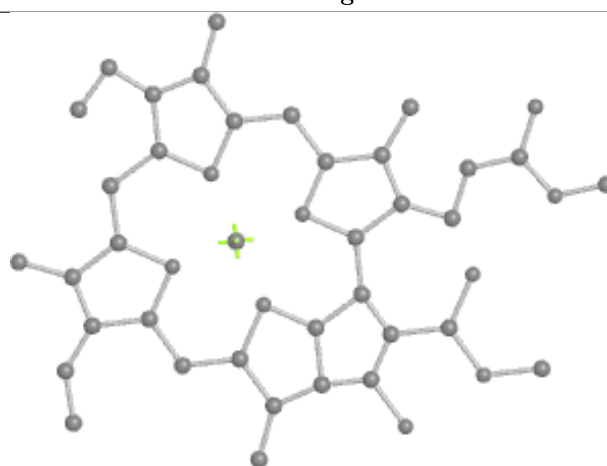
Bond lengths



Bond angles

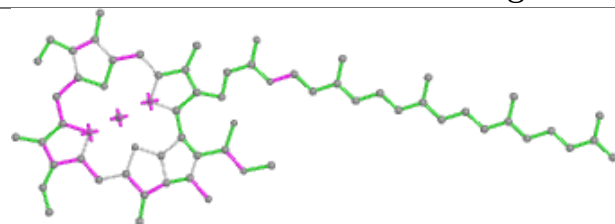


Torsions

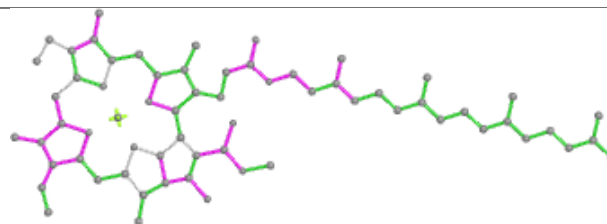


Rings

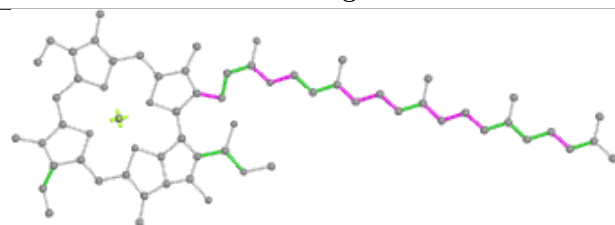
Ligand CLA A 1123



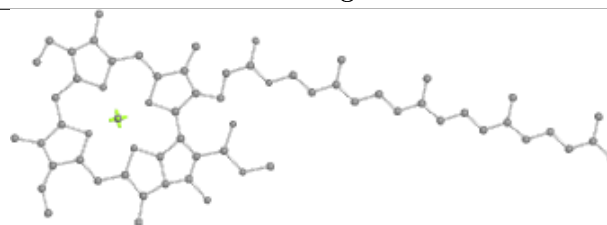
Bond lengths



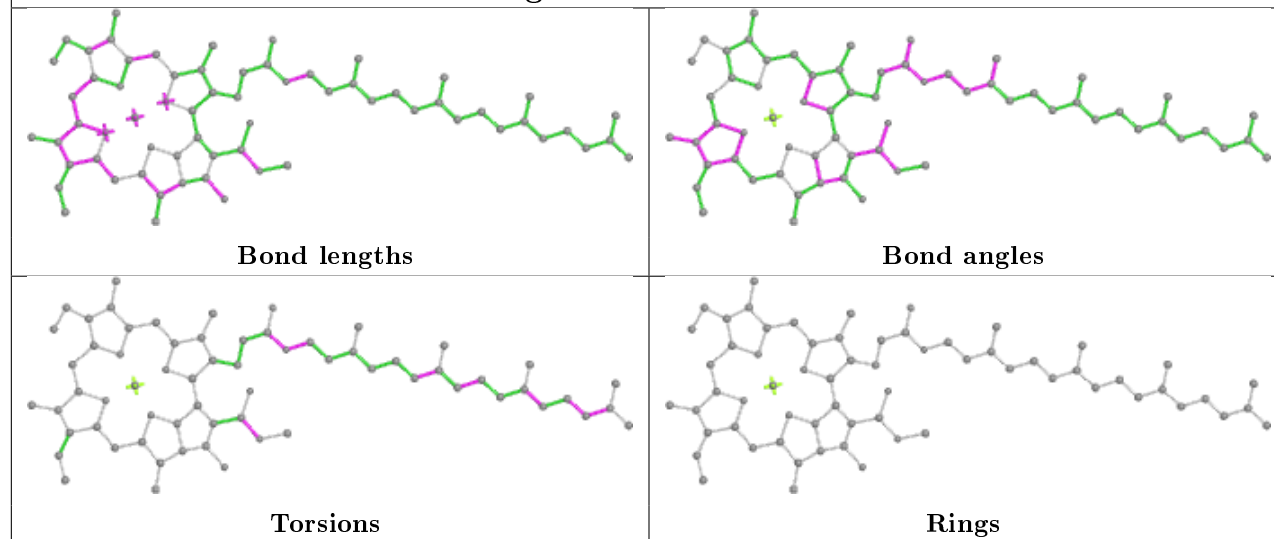
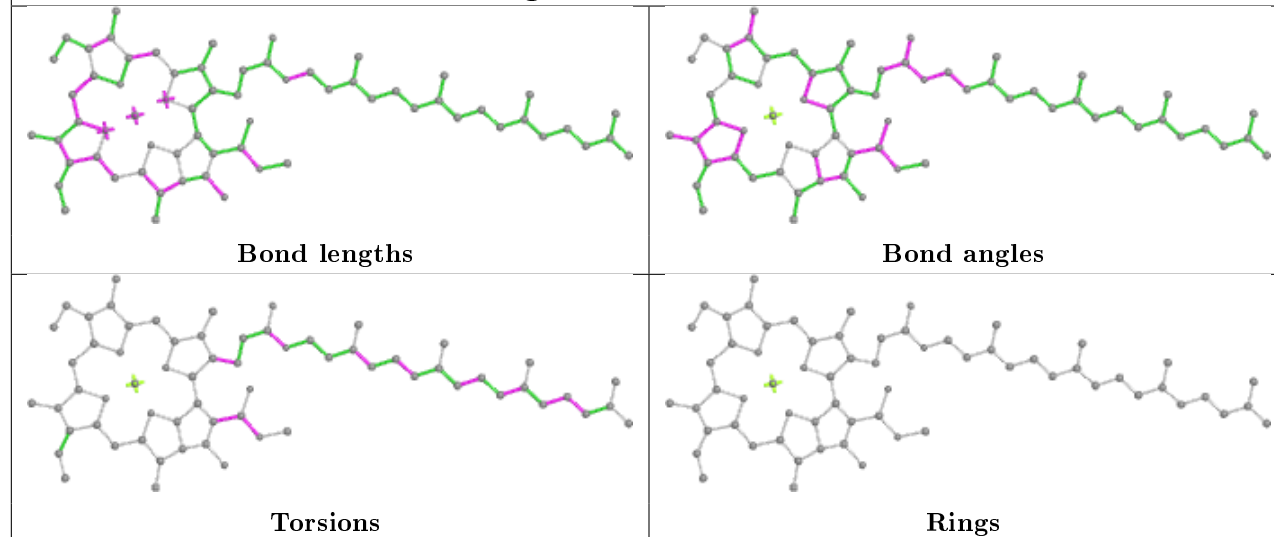
Bond angles

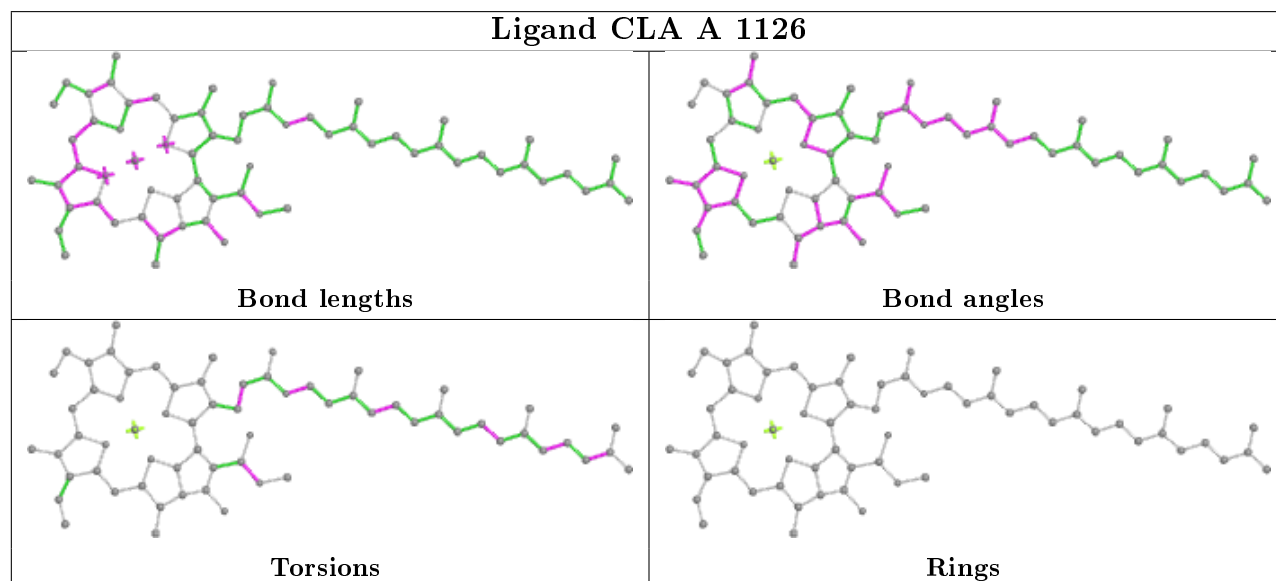
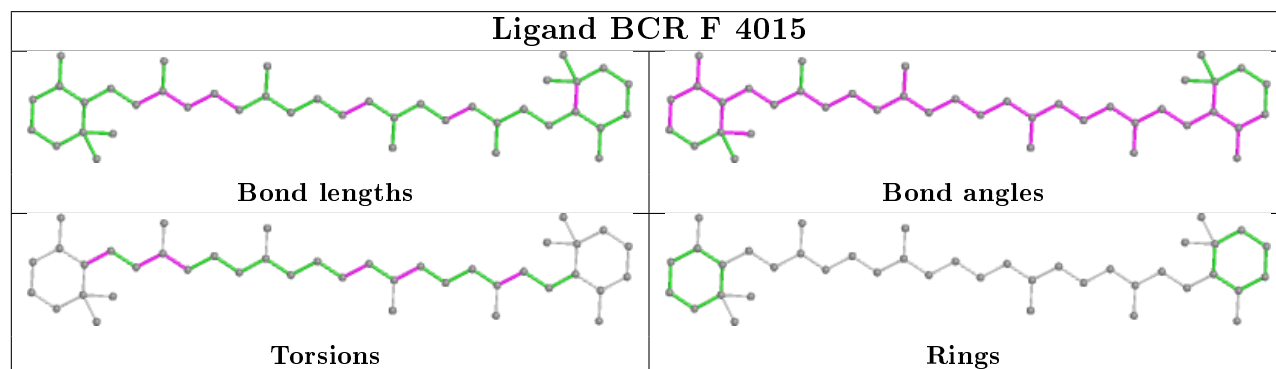
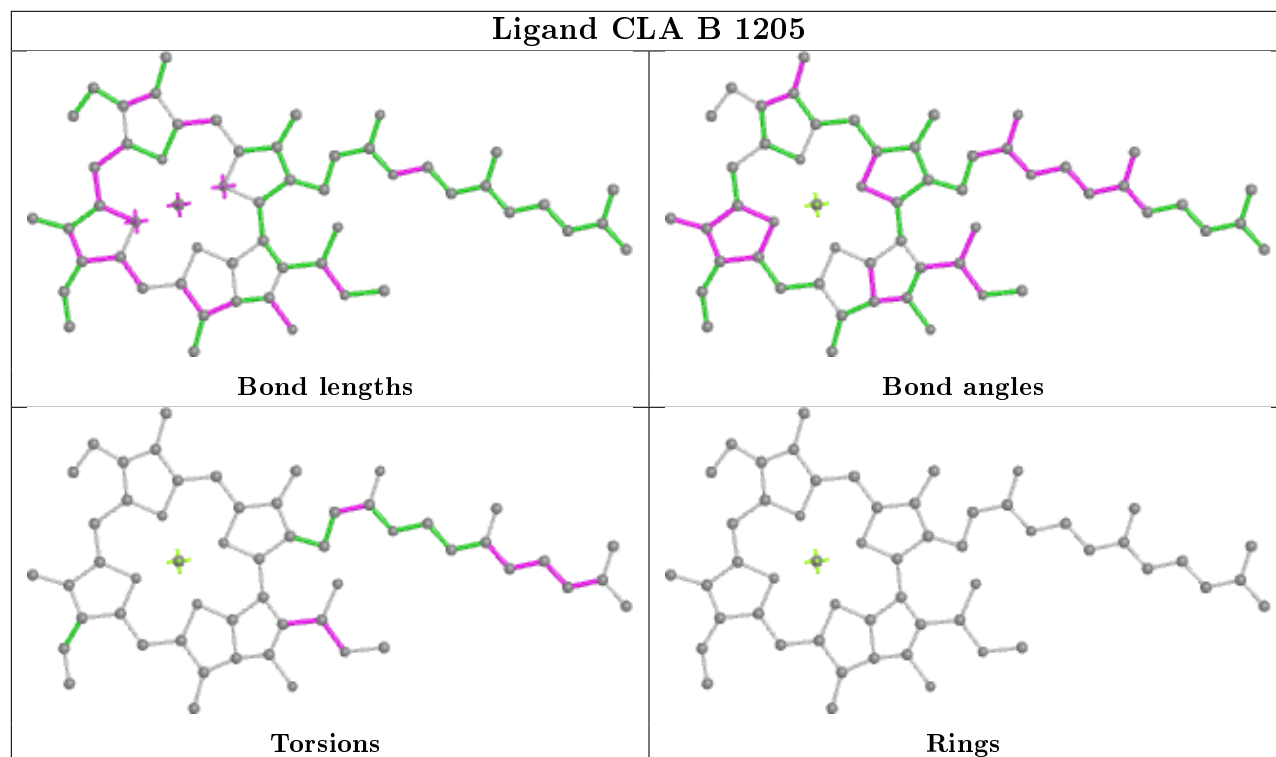


Torsions

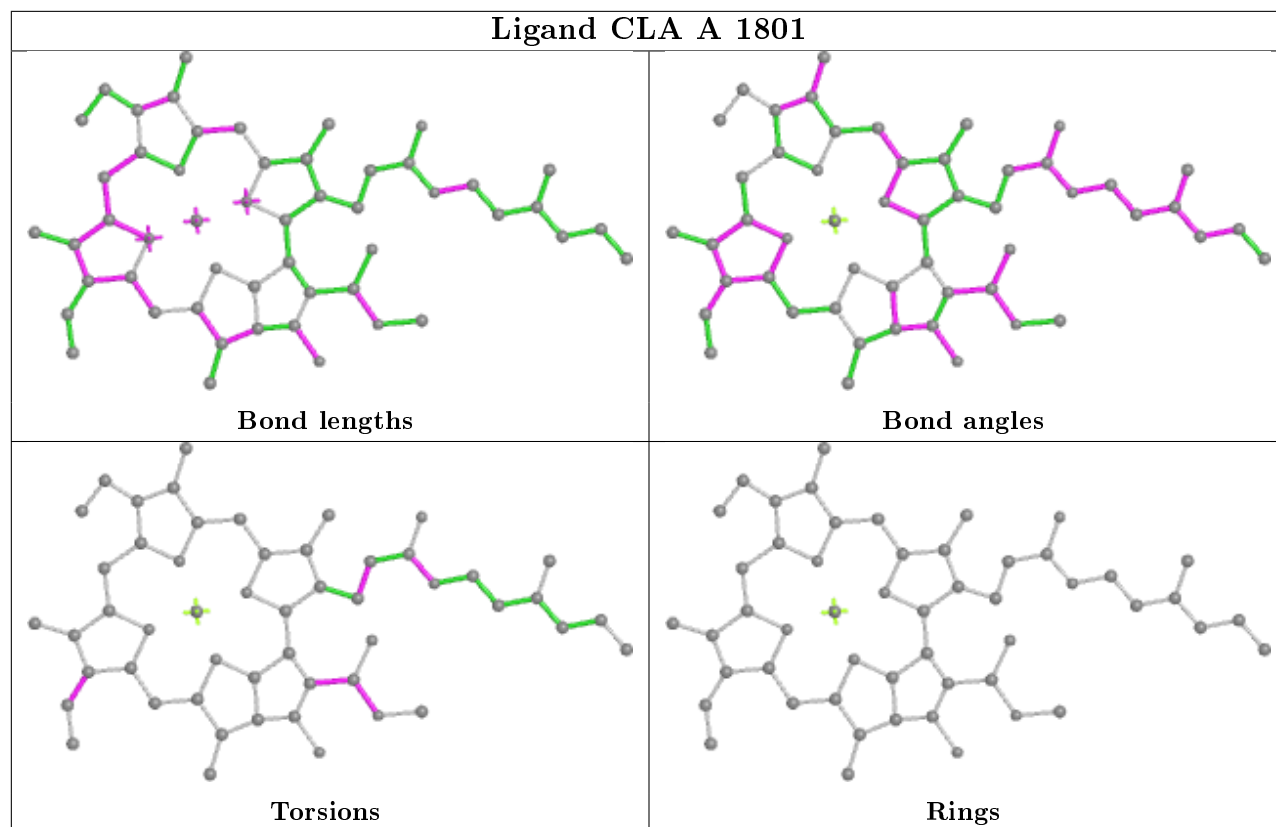


Rings

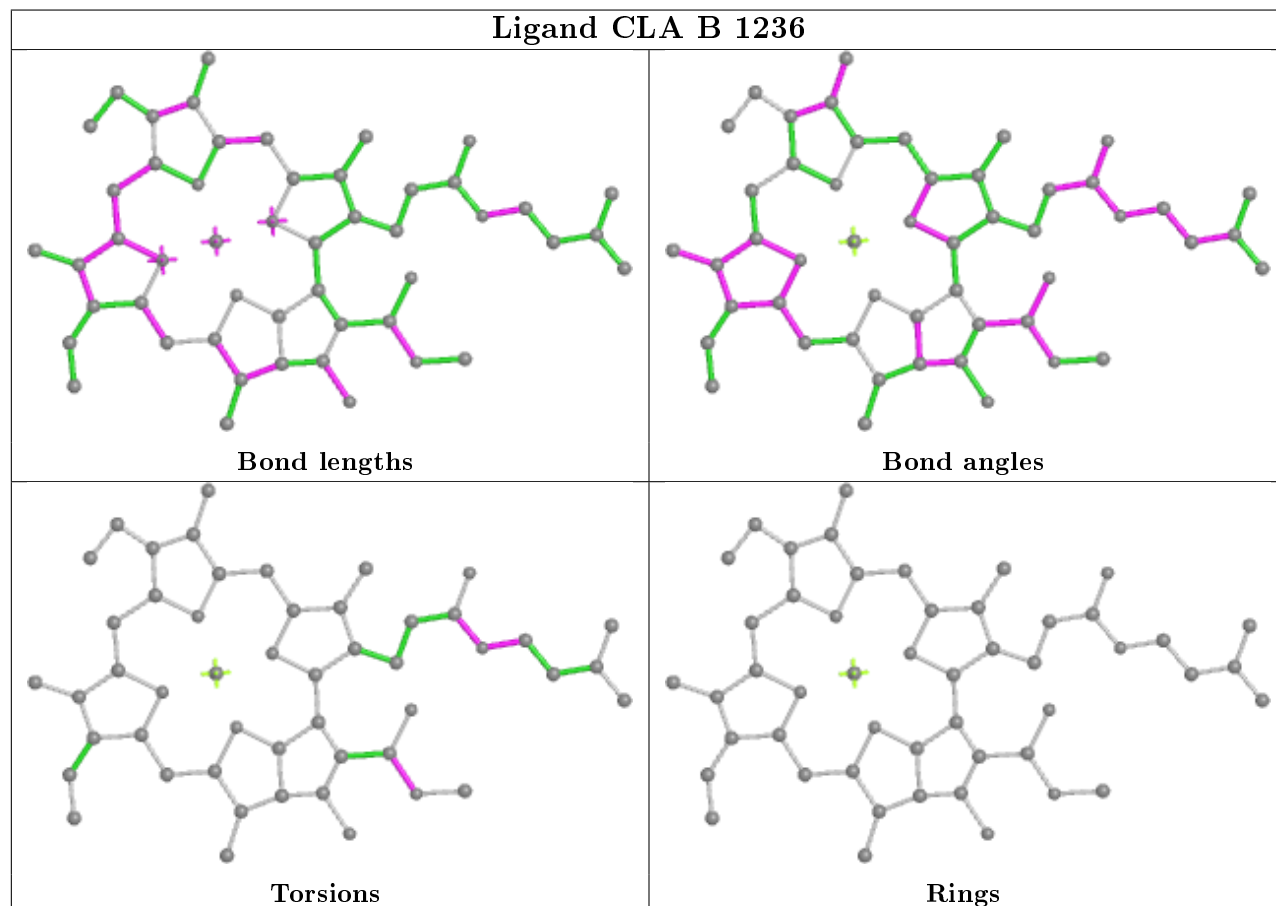
Ligand CLA F 1139**Ligand CLA B 1224**



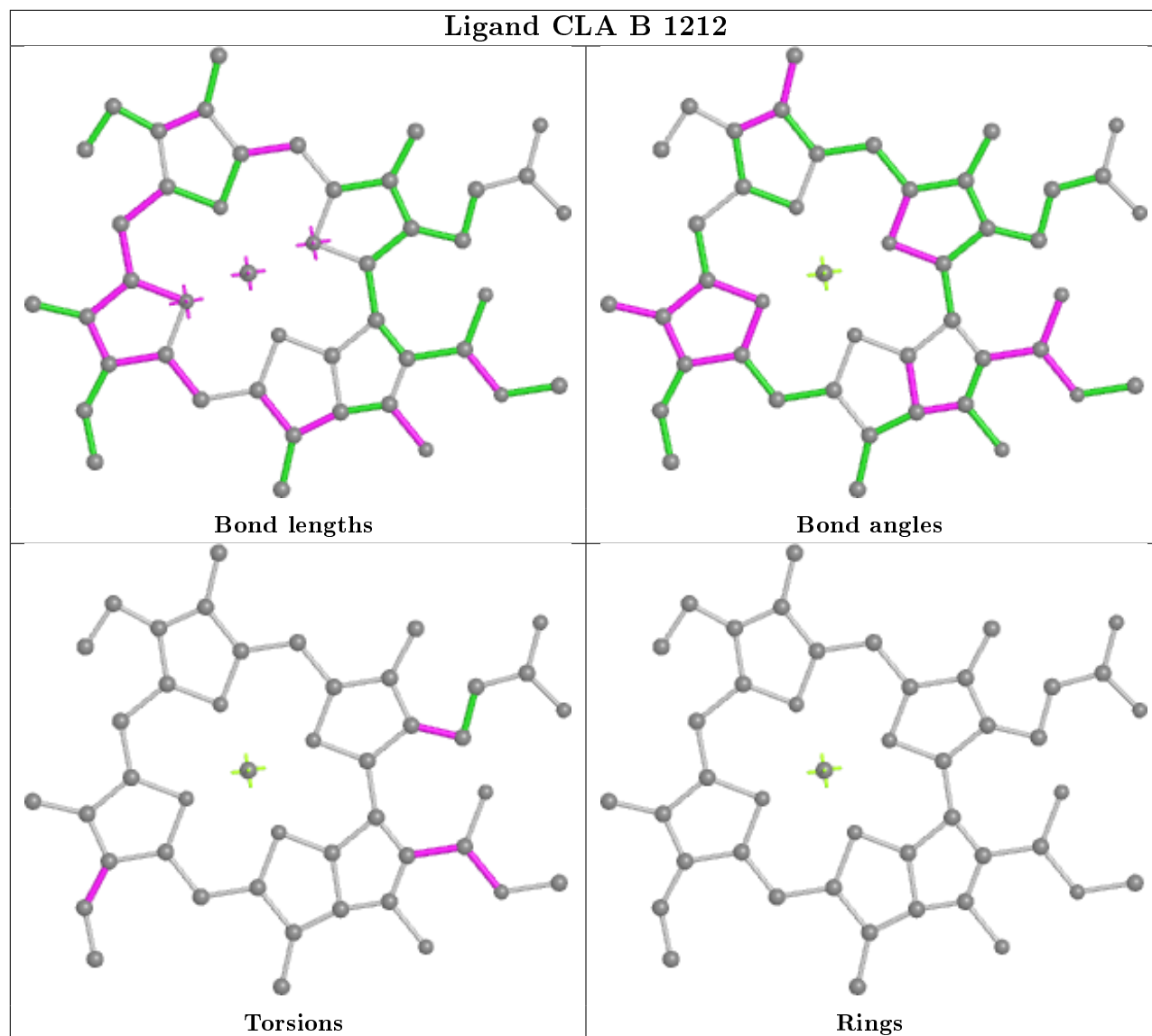
Ligand CLA A 1801



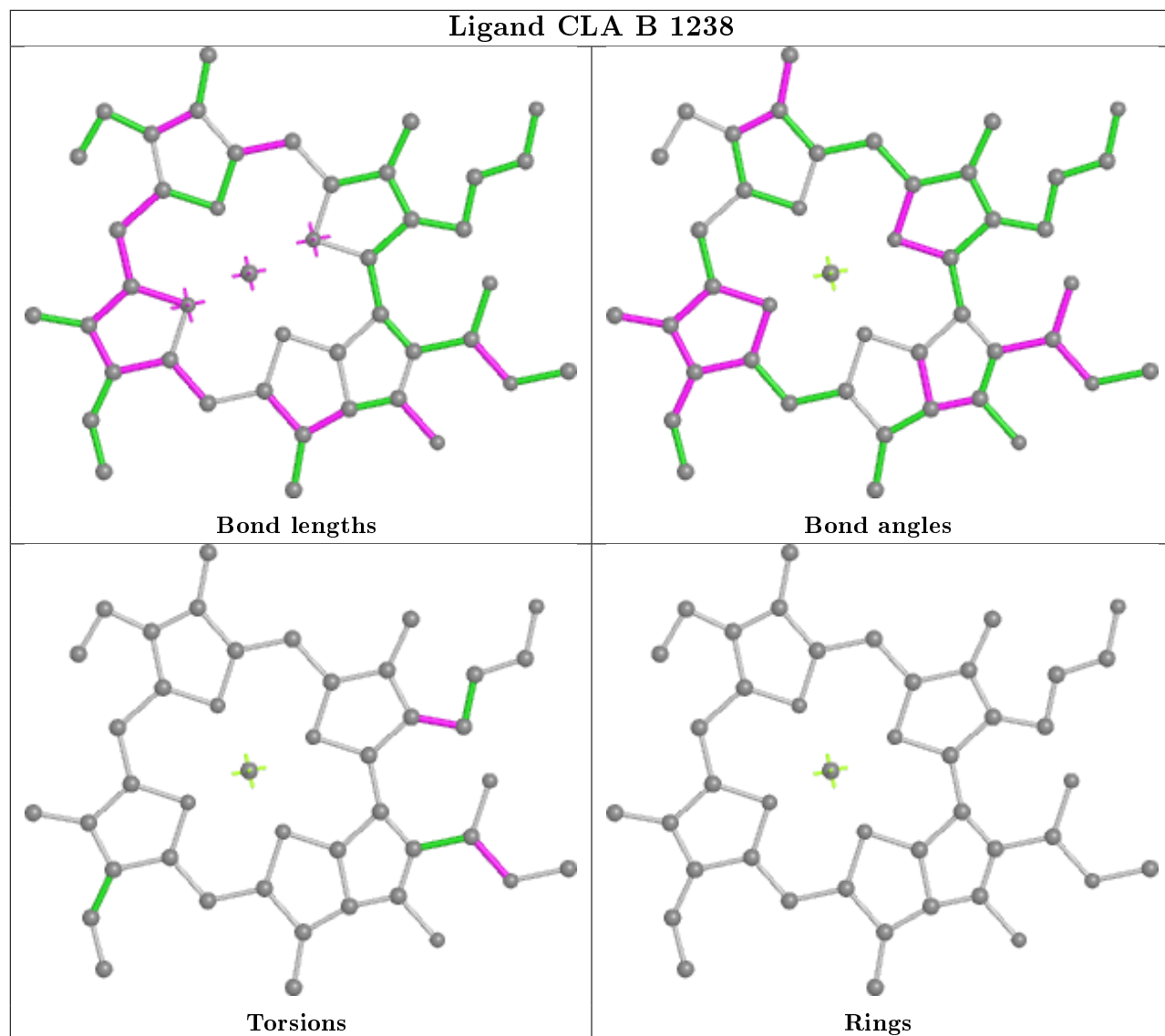
Ligand CLA B 1236

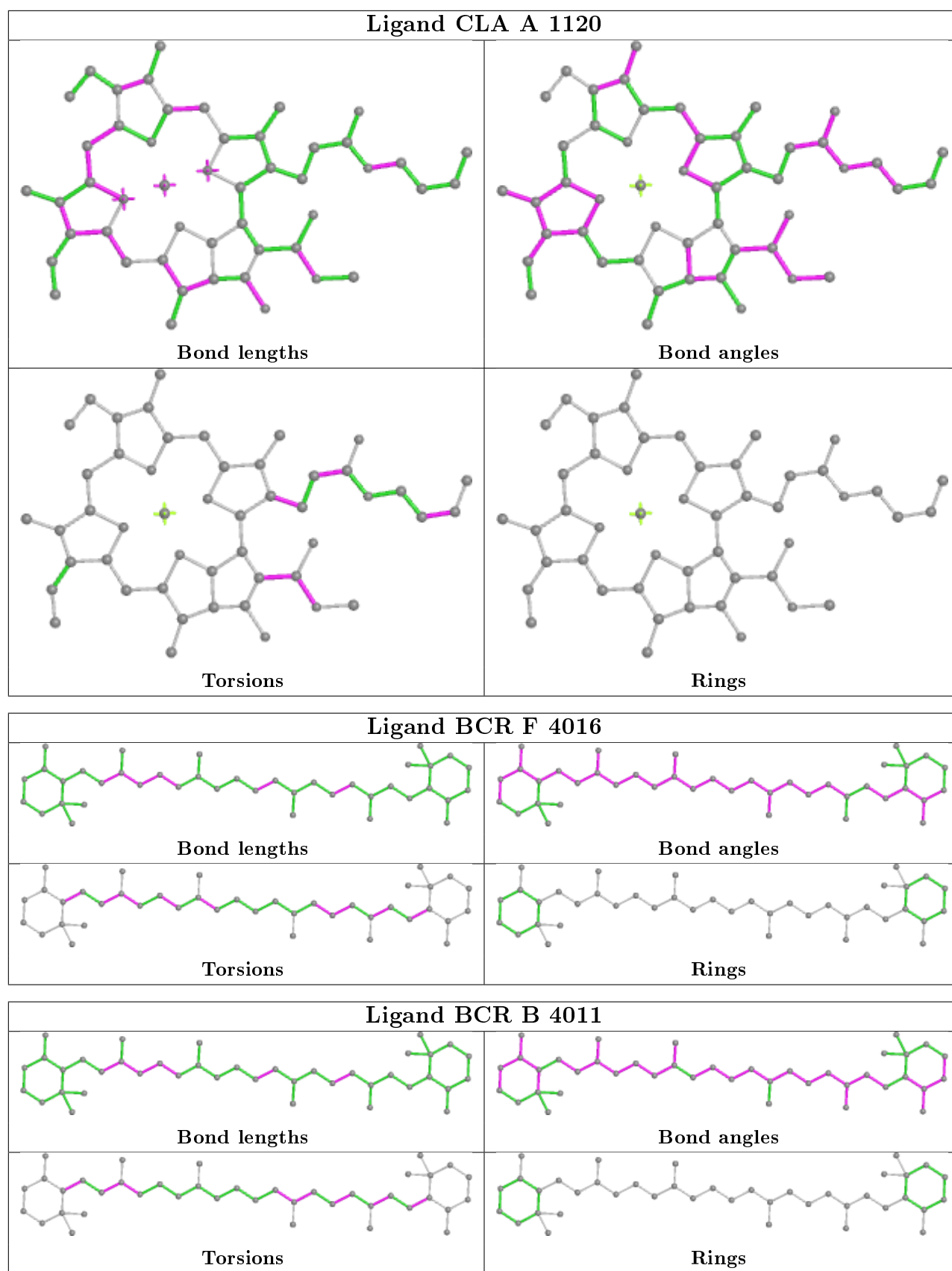


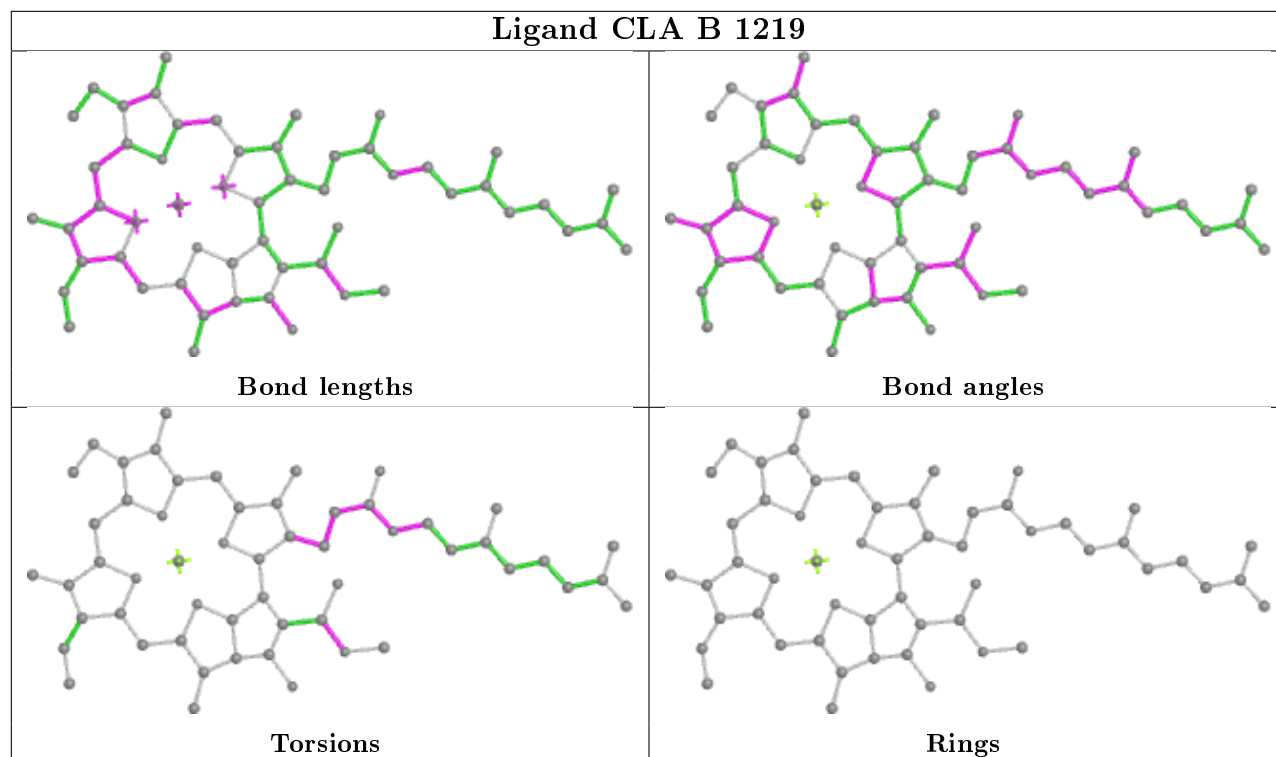
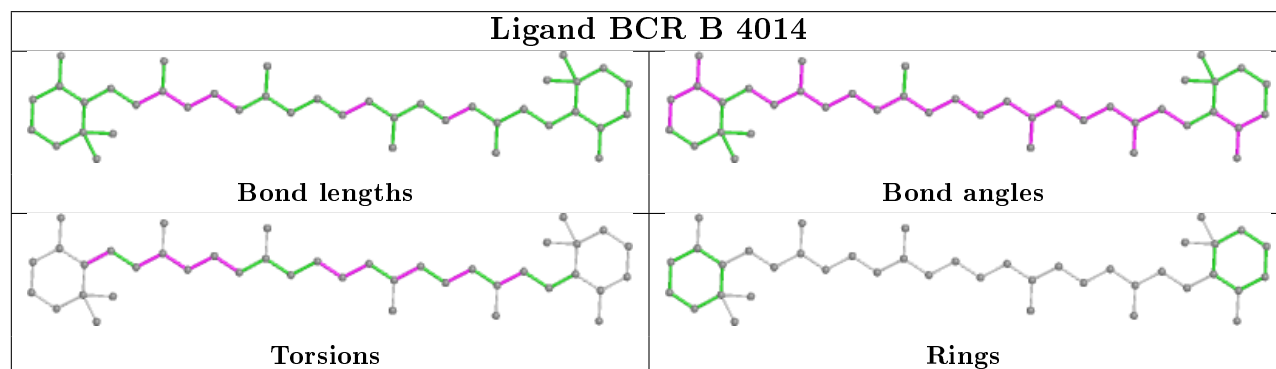
Ligand CLA B 1212



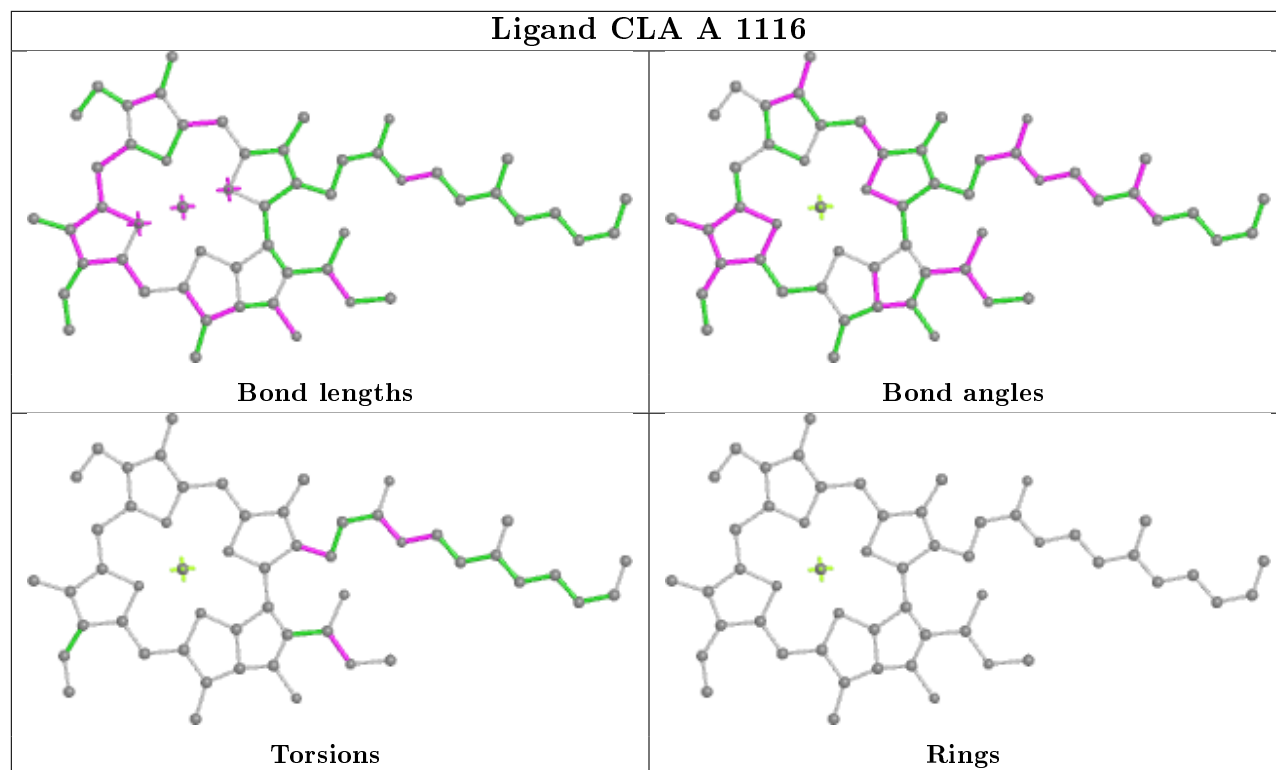
Ligand CLA B 1238



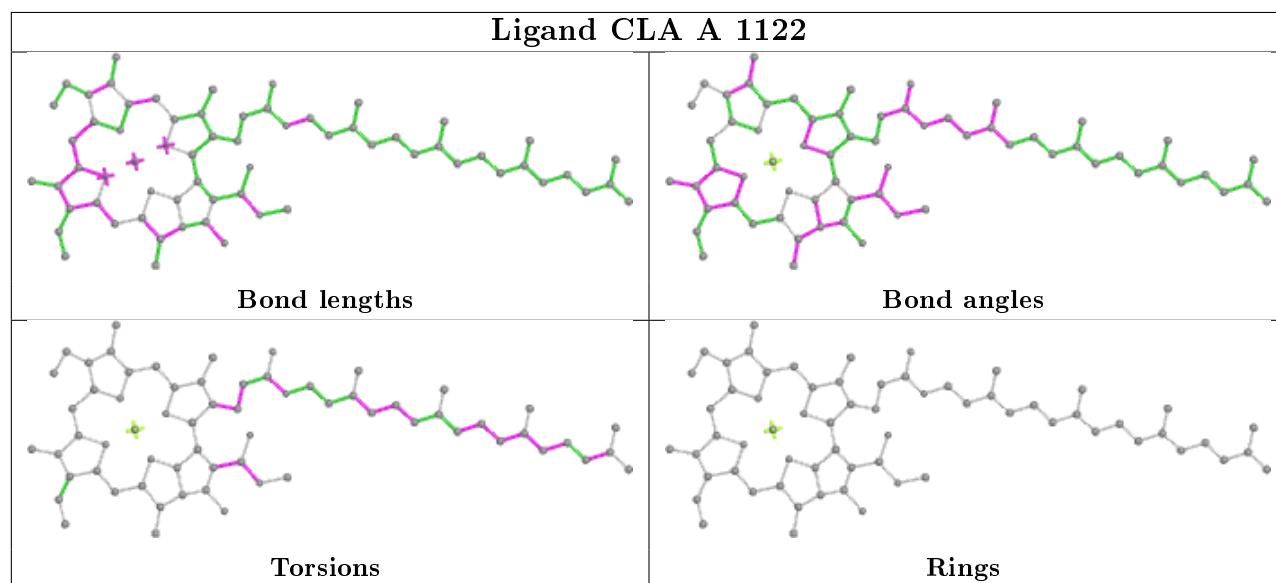


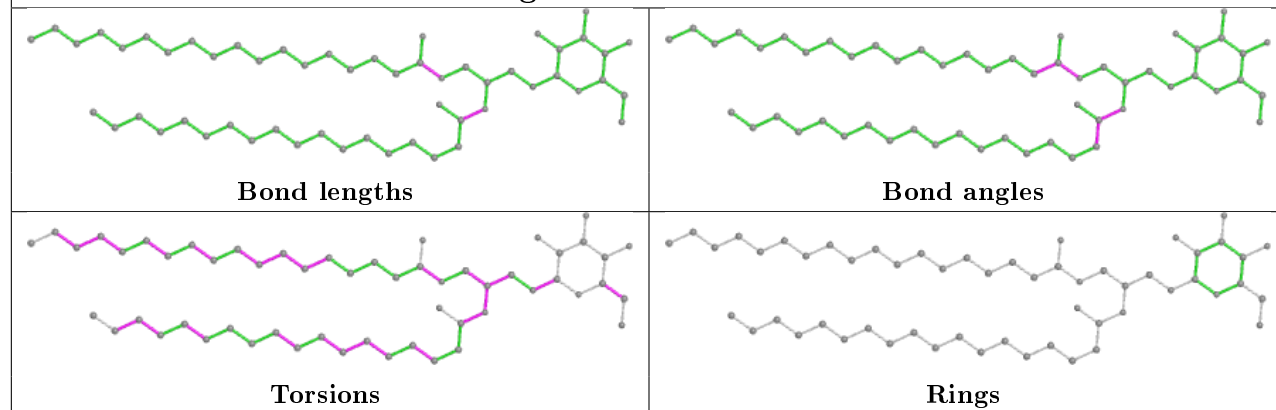
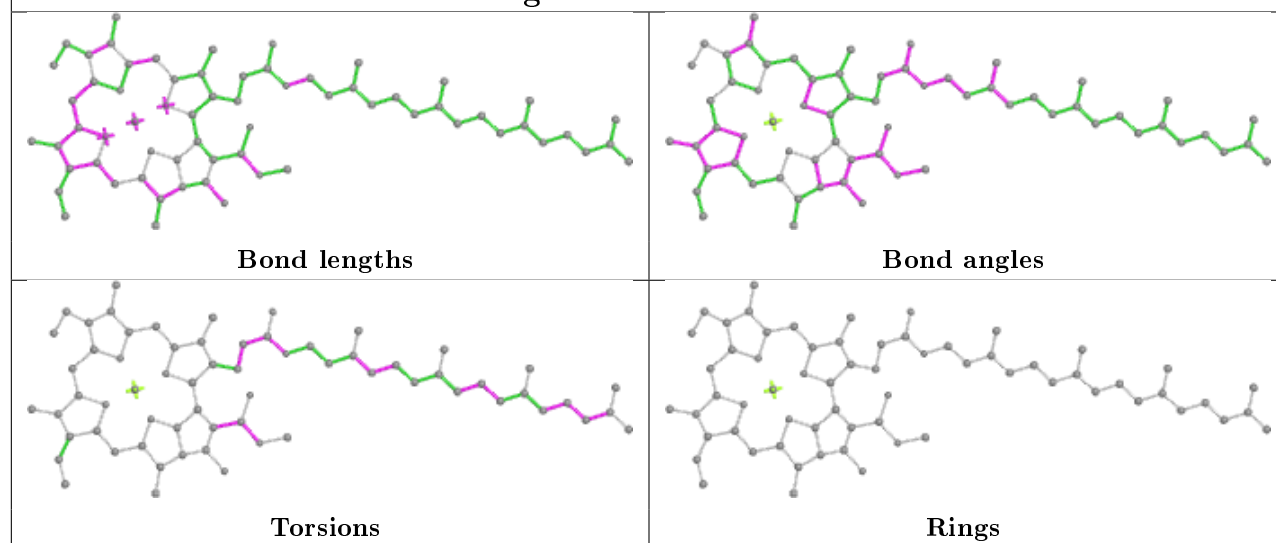
Ligand CLA B 1219**Ligand BCR B 4014**

Ligand CLA A 1116

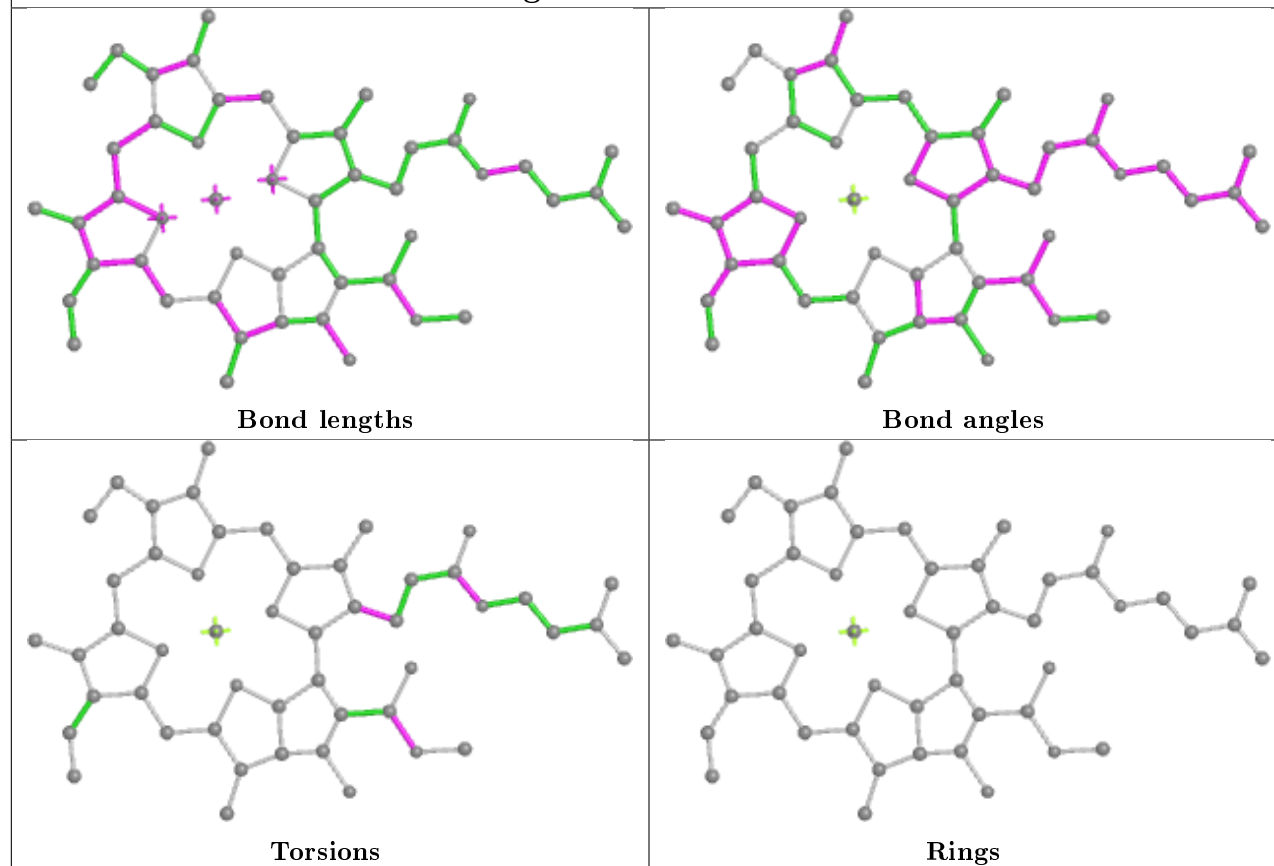


Ligand CLA A 1122

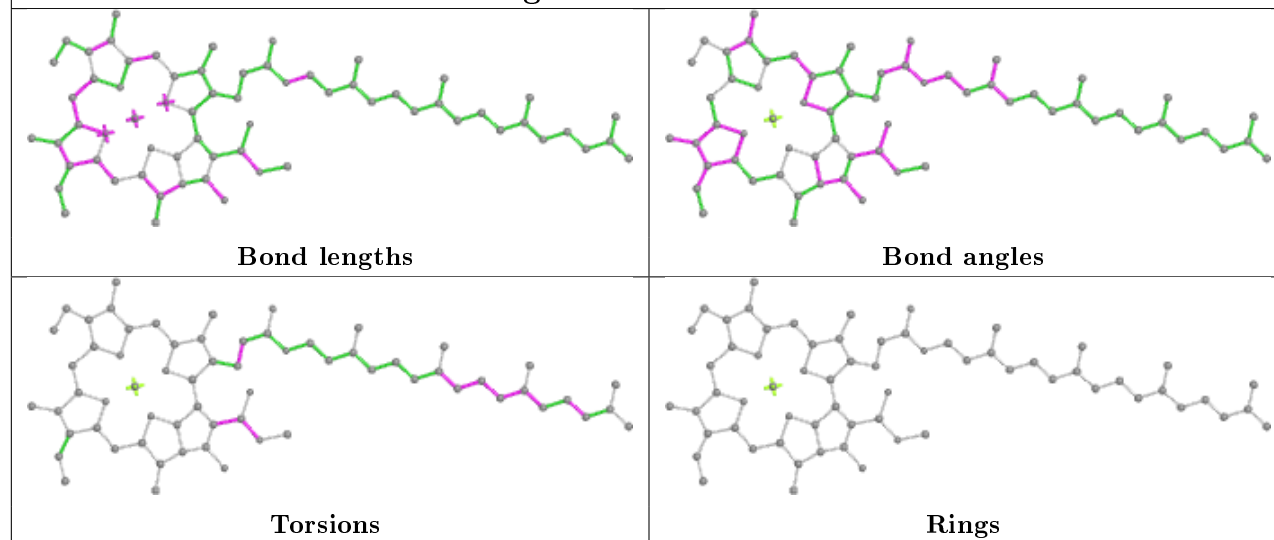


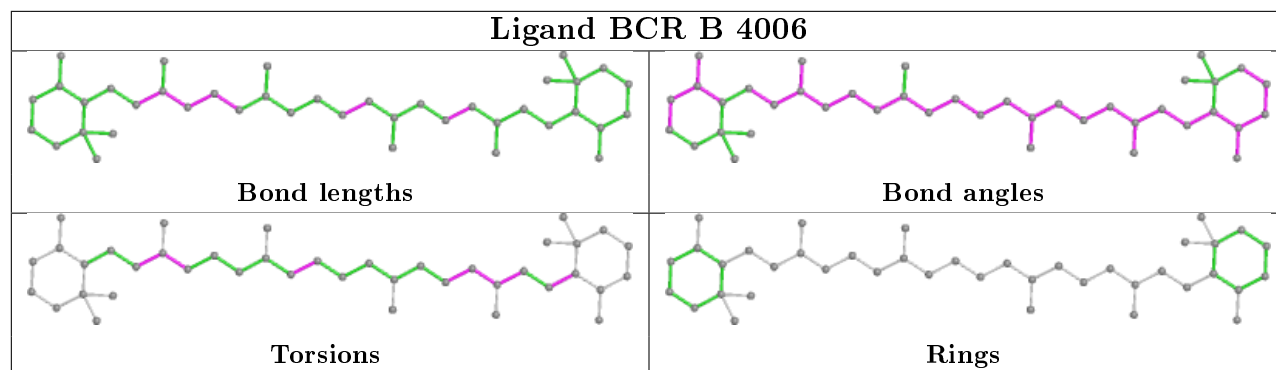
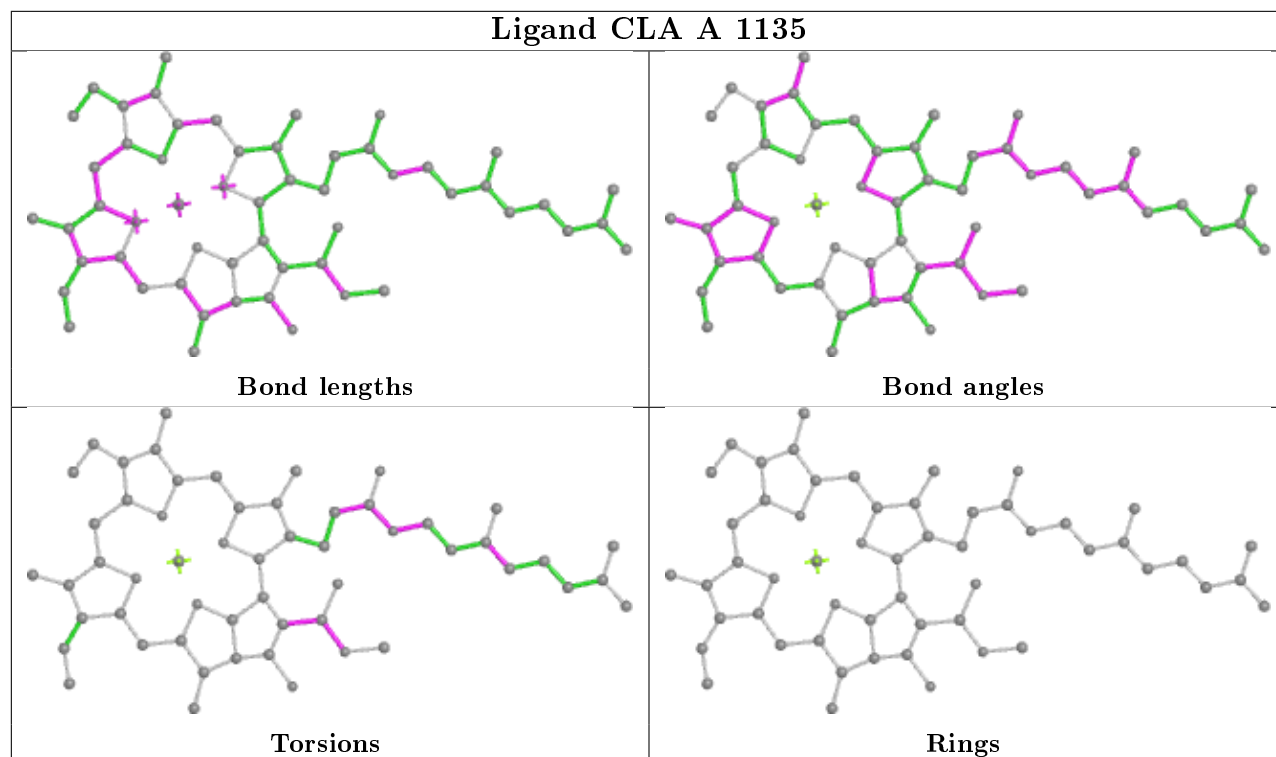
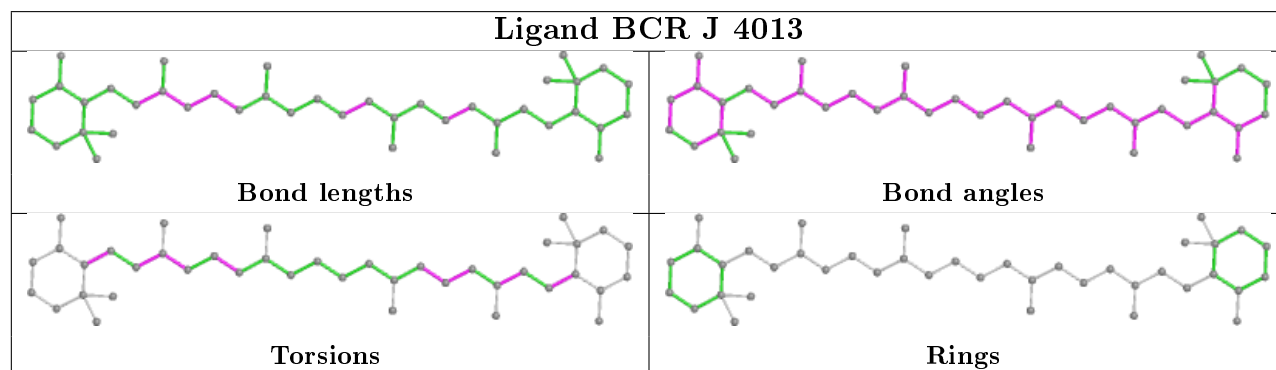
Ligand LMG B 5002**Ligand CLA A 1127**

Ligand CLA A 1107

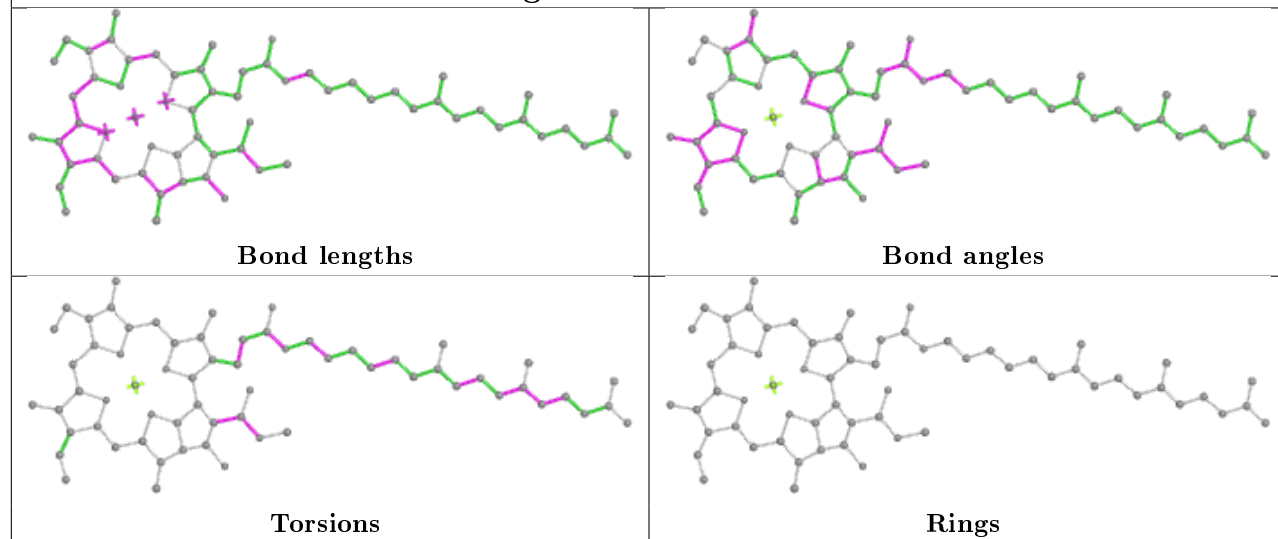


Ligand CLA B 1023

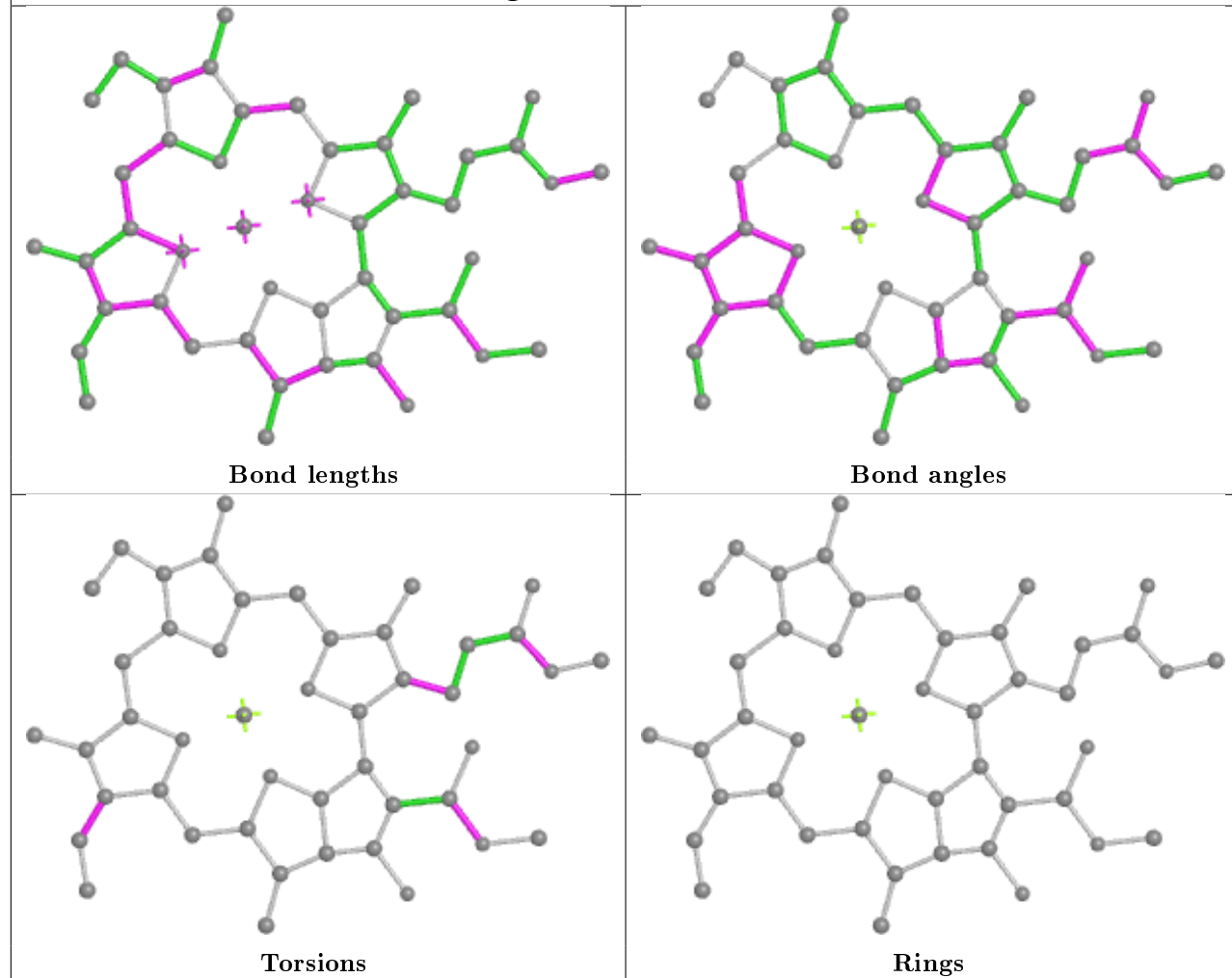


Ligand BCR B 4006**Ligand CLA A 1135****Ligand BCR J 4013**

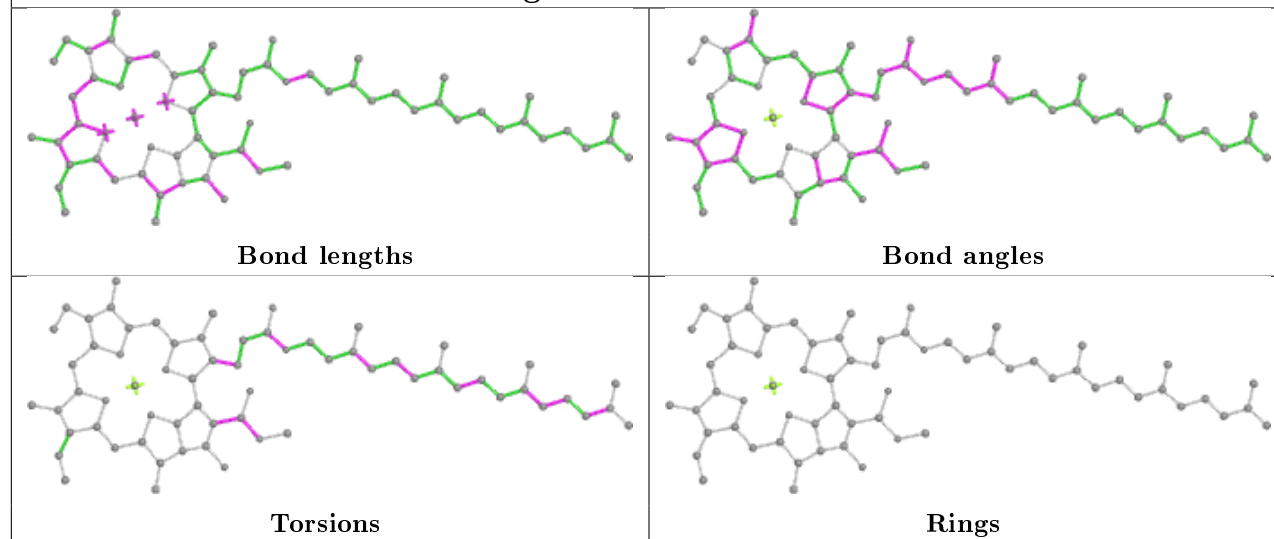
Ligand CLA A 1119



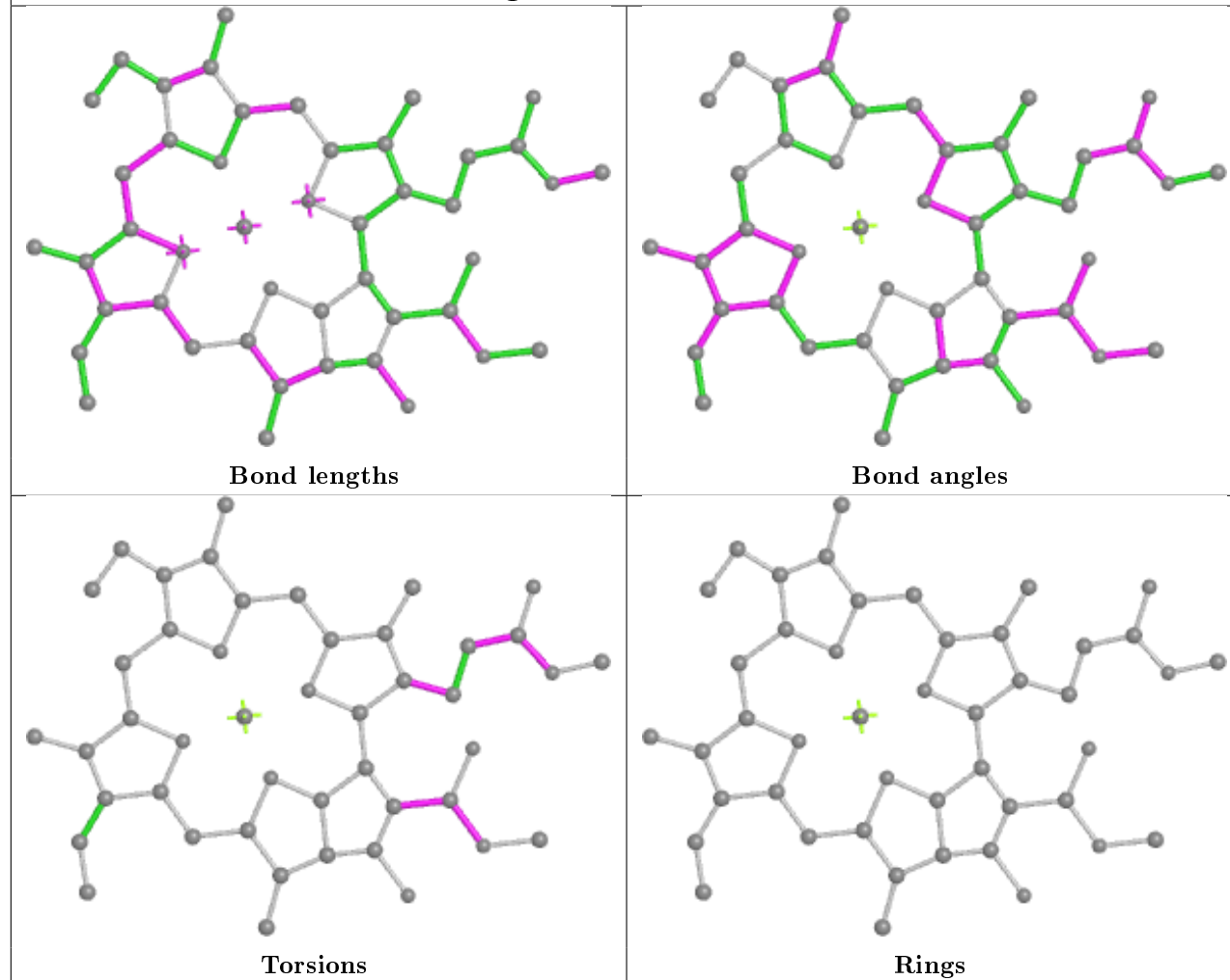
Ligand CLA B 1239

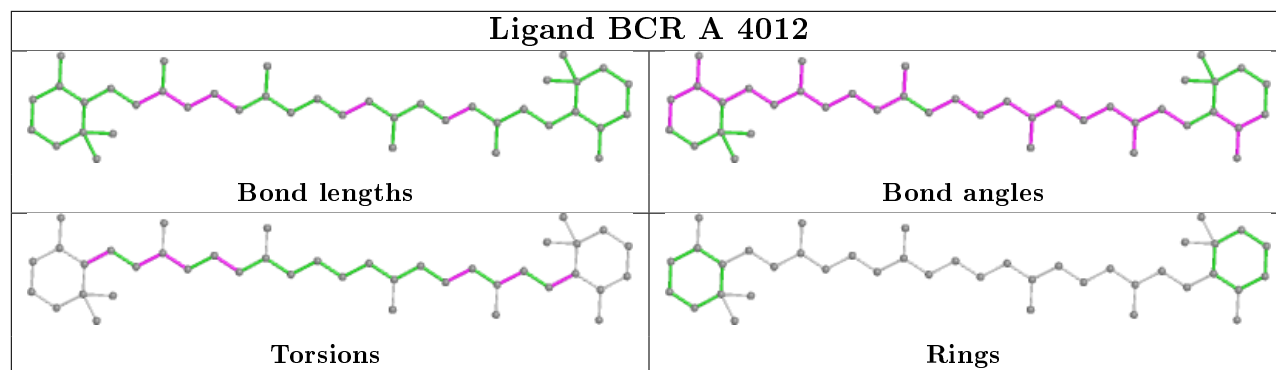
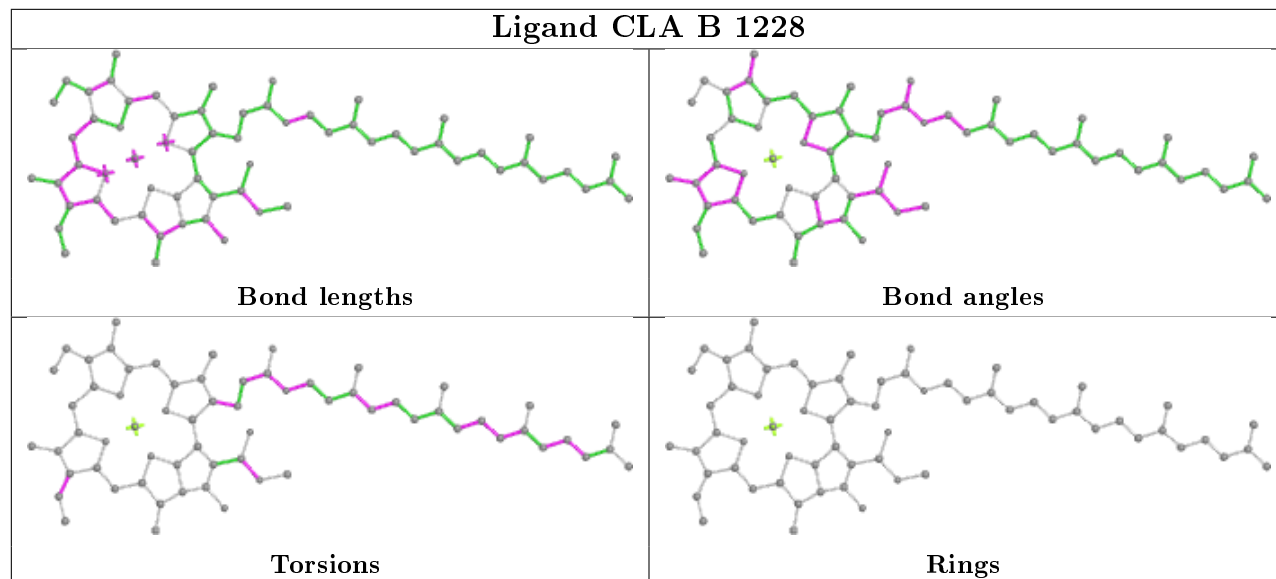
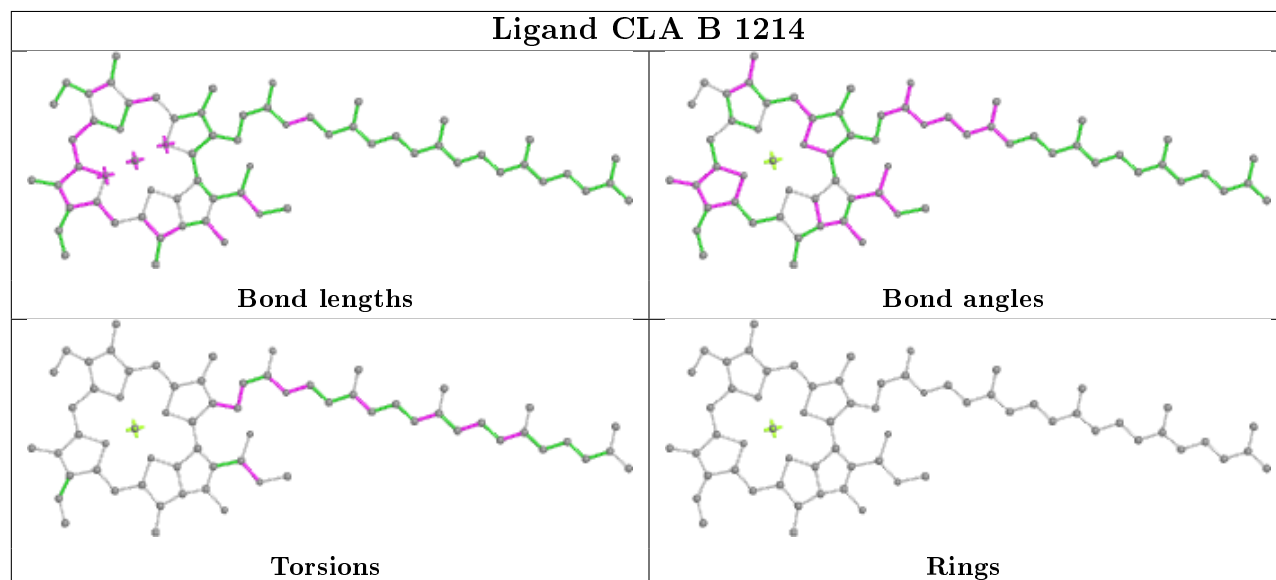


Ligand CLA B 1230

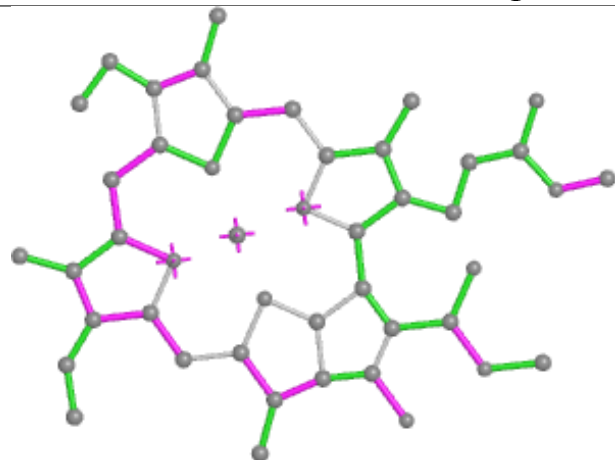


Ligand CLA K 1401

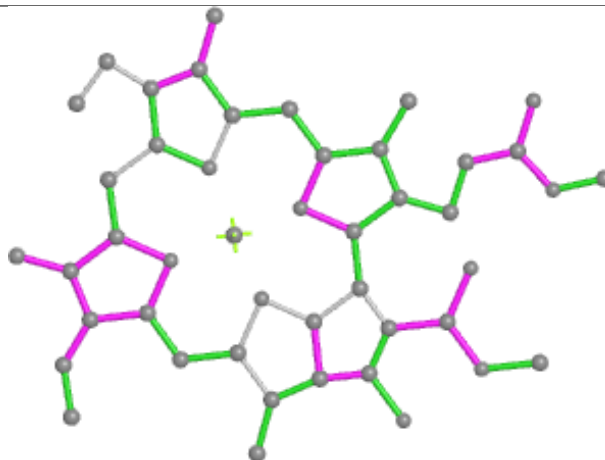


Ligand BCR A 4012**Ligand CLA B 1228****Ligand CLA B 1214**

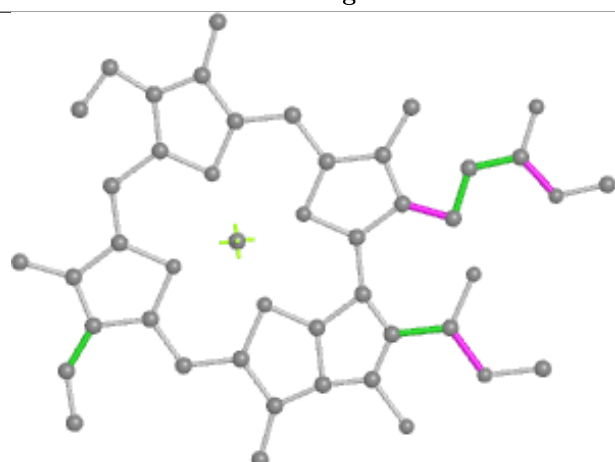
Ligand CLA A 1133



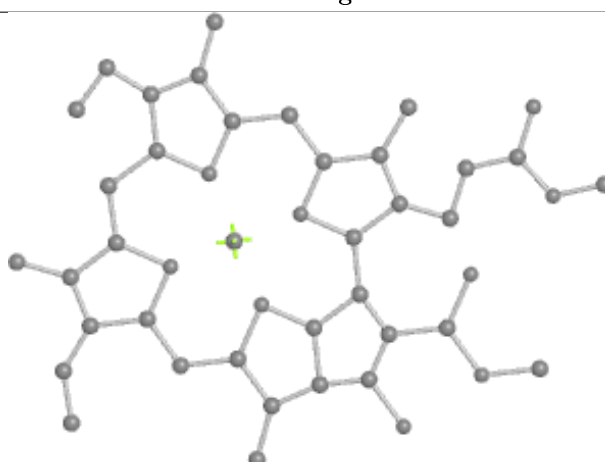
Bond lengths



Bond angles

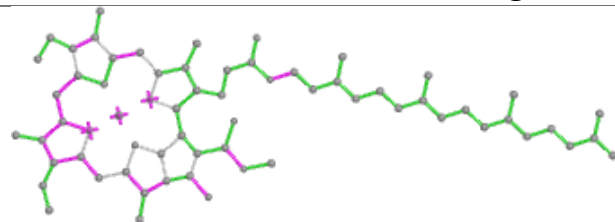


Torsions

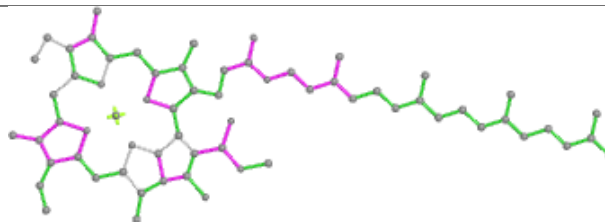


Rings

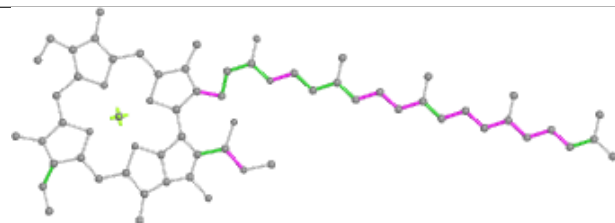
Ligand CLA A 1117



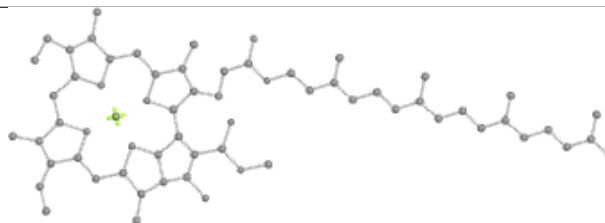
Bond lengths



Bond angles

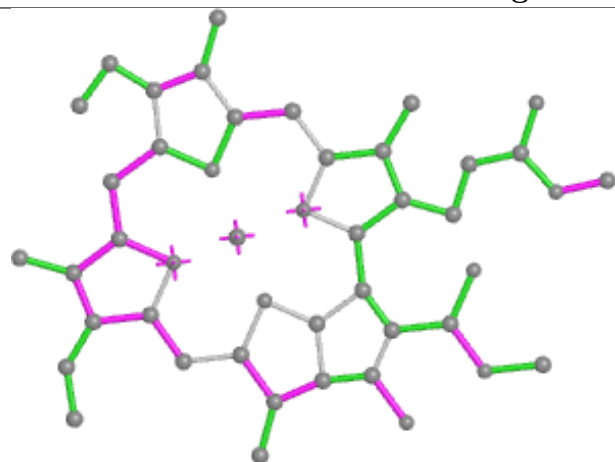


Torsions

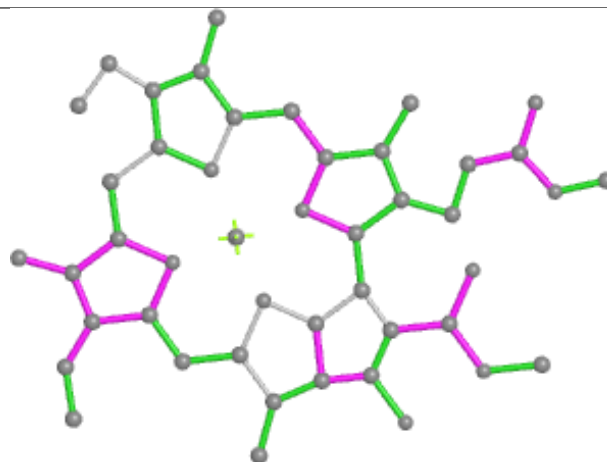


Rings

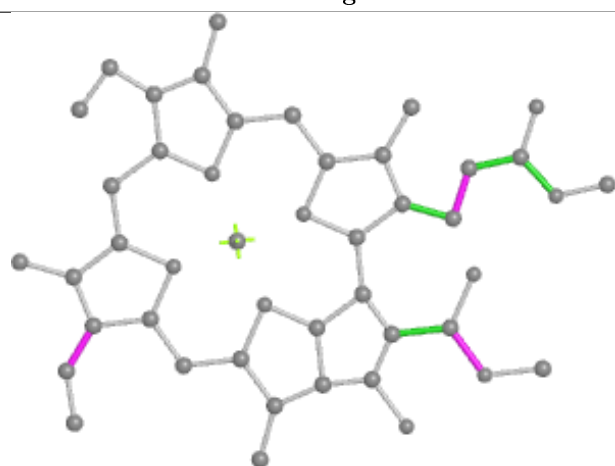
Ligand CLA J 1303



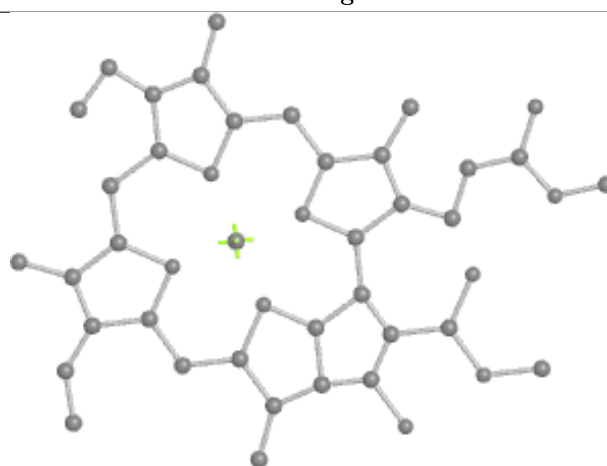
Bond lengths



Bond angles

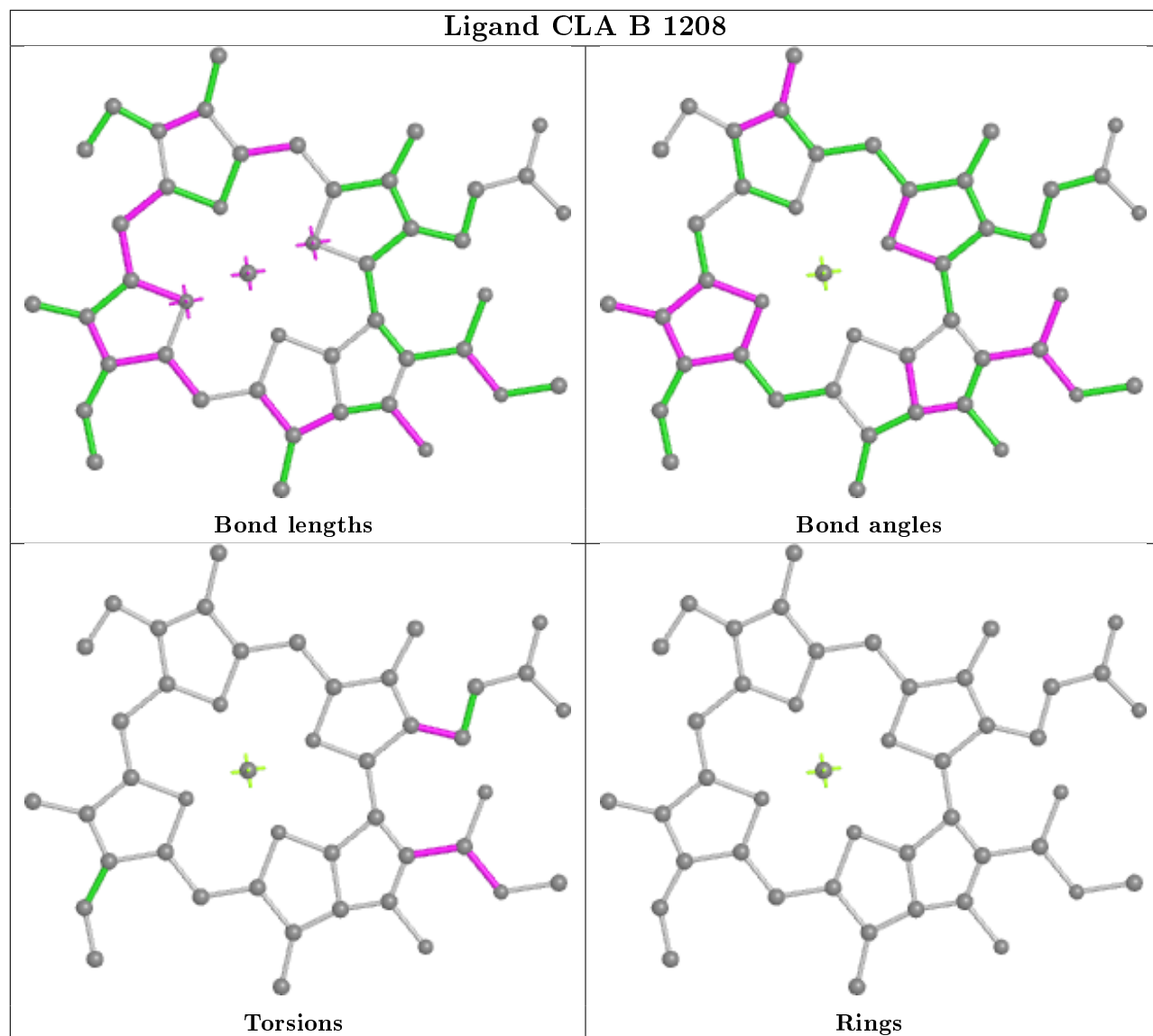


Torsions

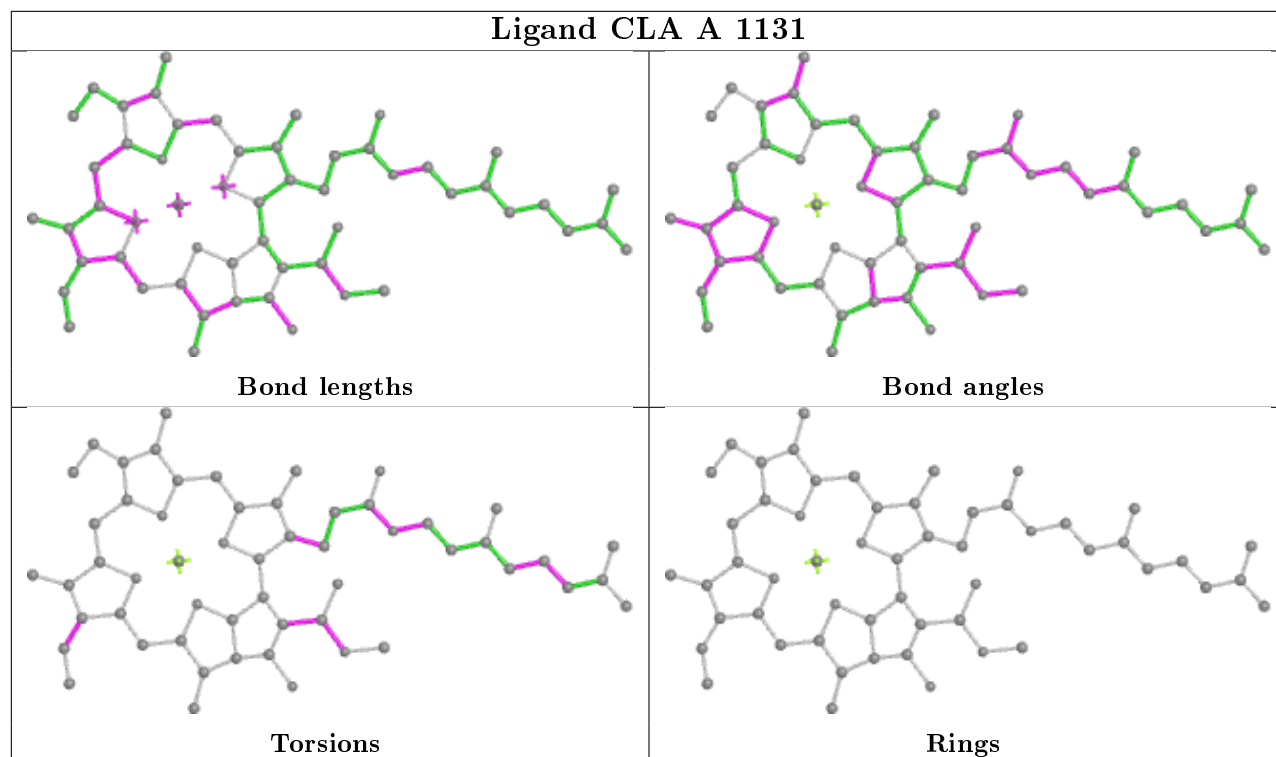


Rings

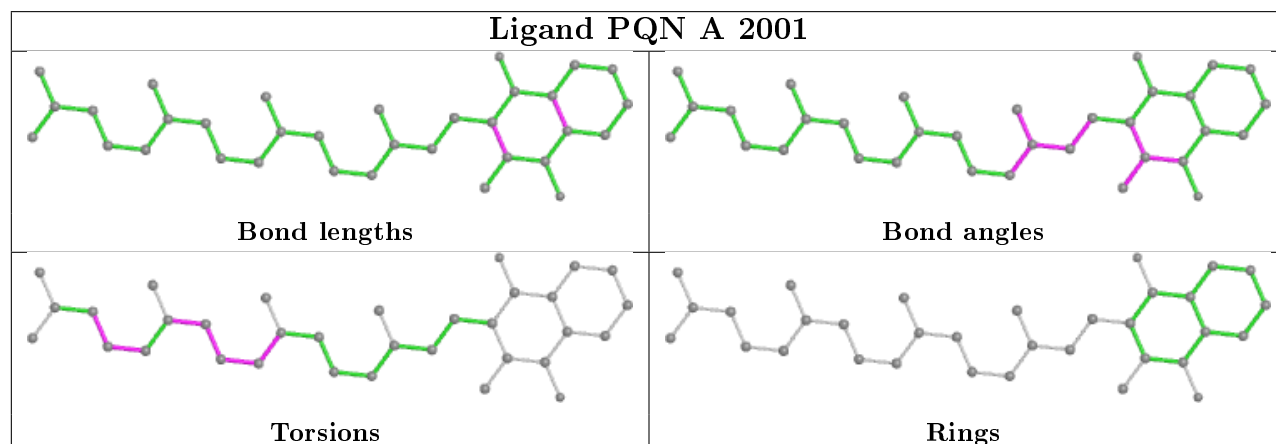
Ligand CLA B 1208

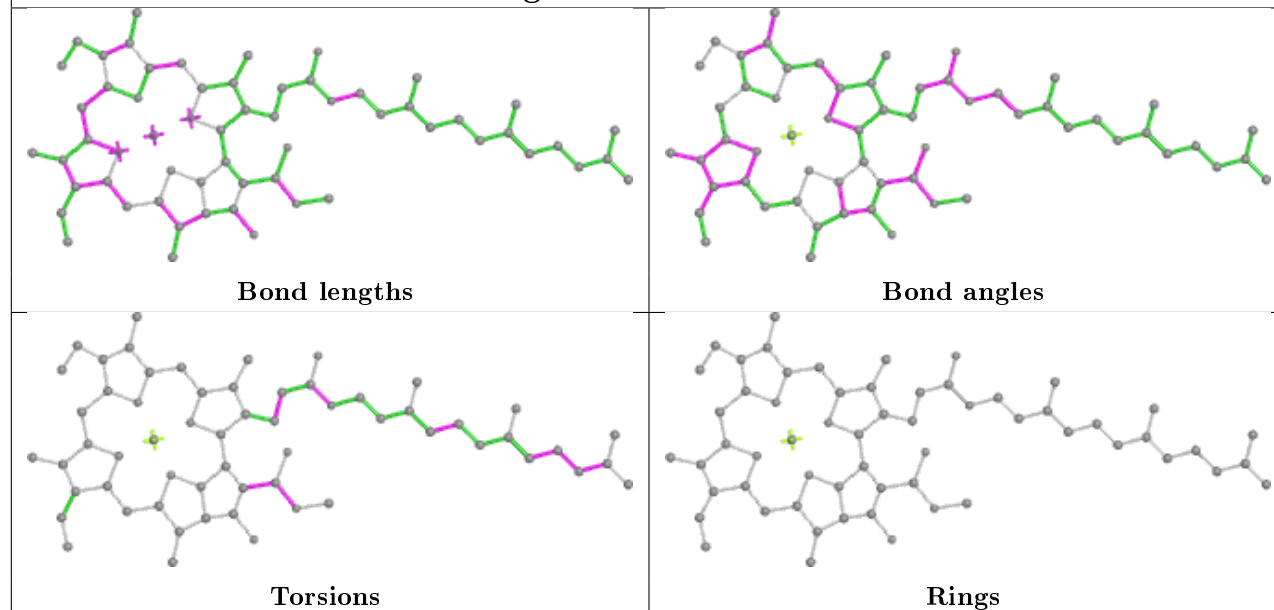
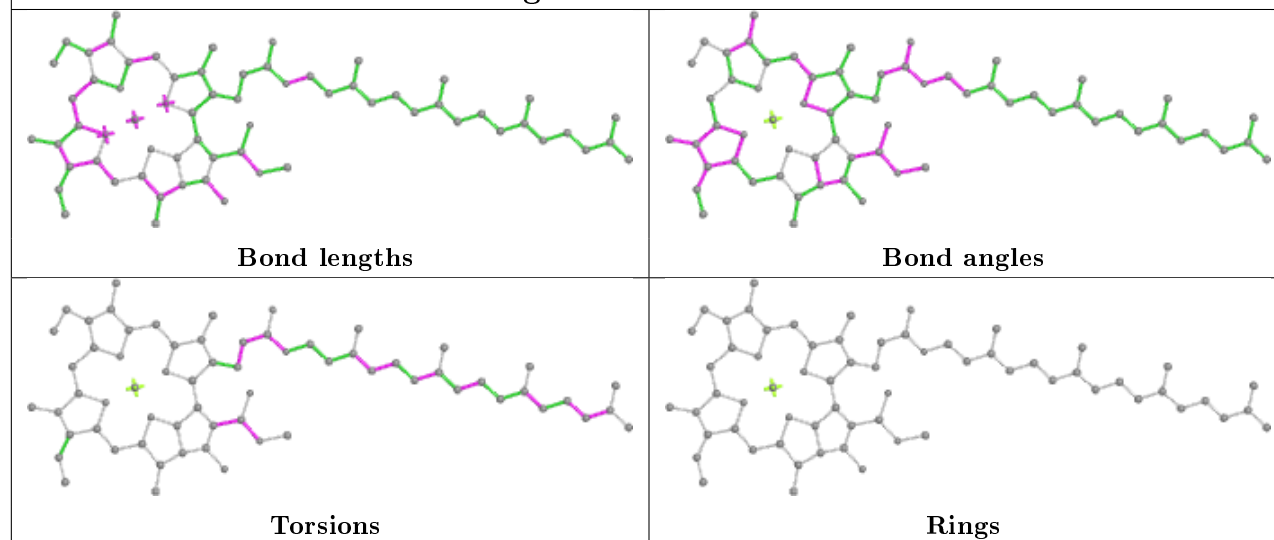


Ligand CLA A 1131

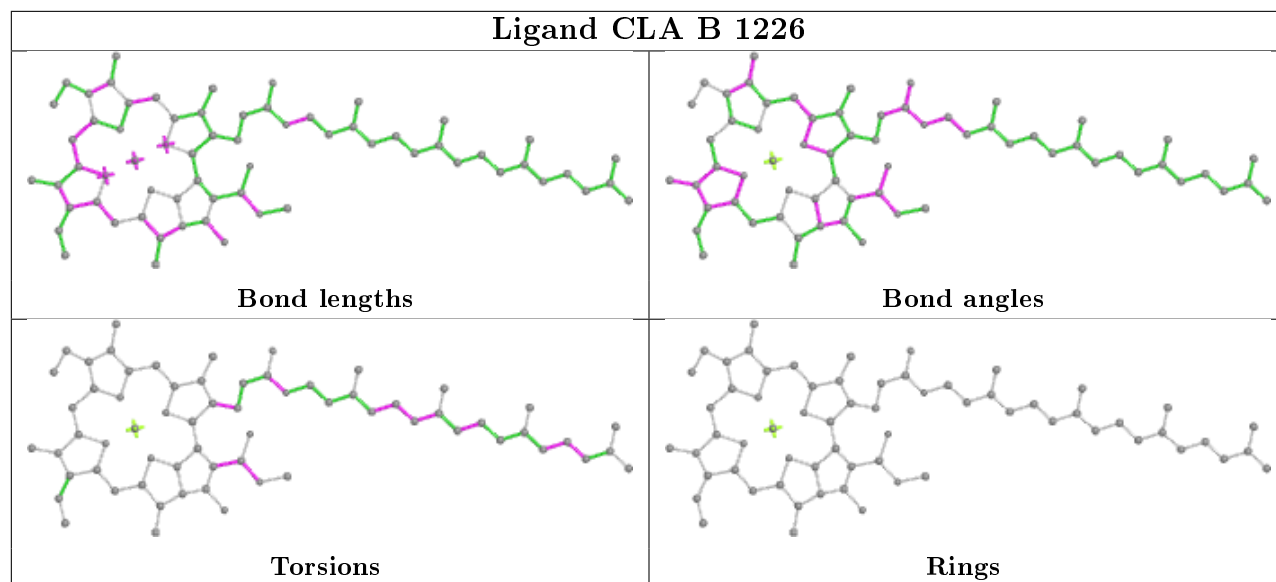


Ligand PQN A 2001

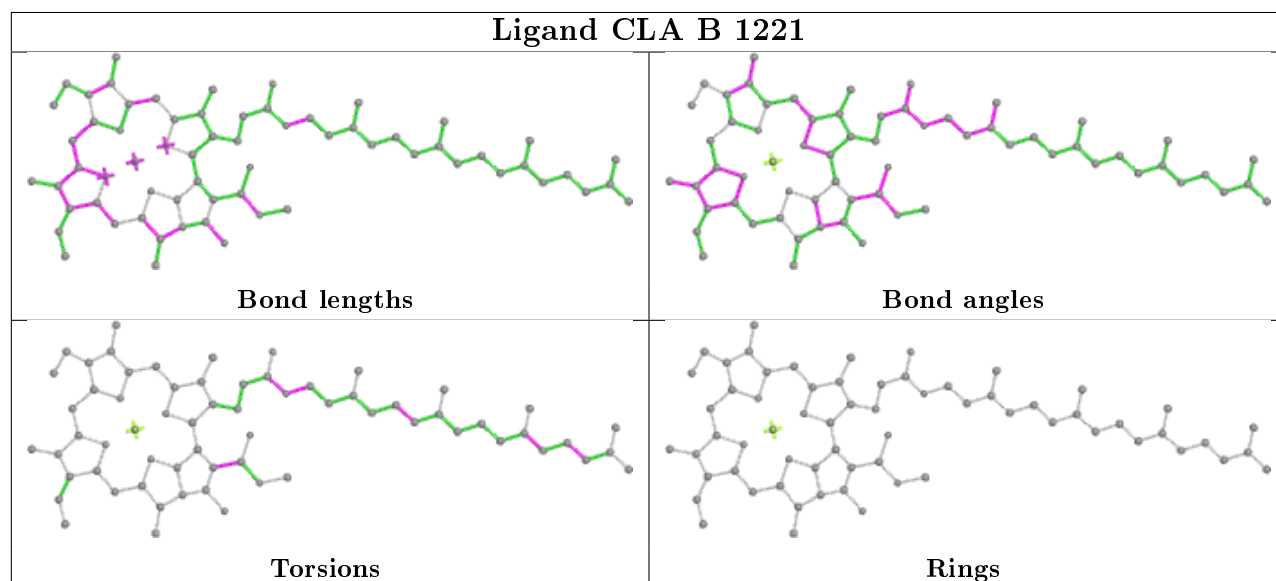


Ligand CLA A 1111**Ligand CLA A 1136**

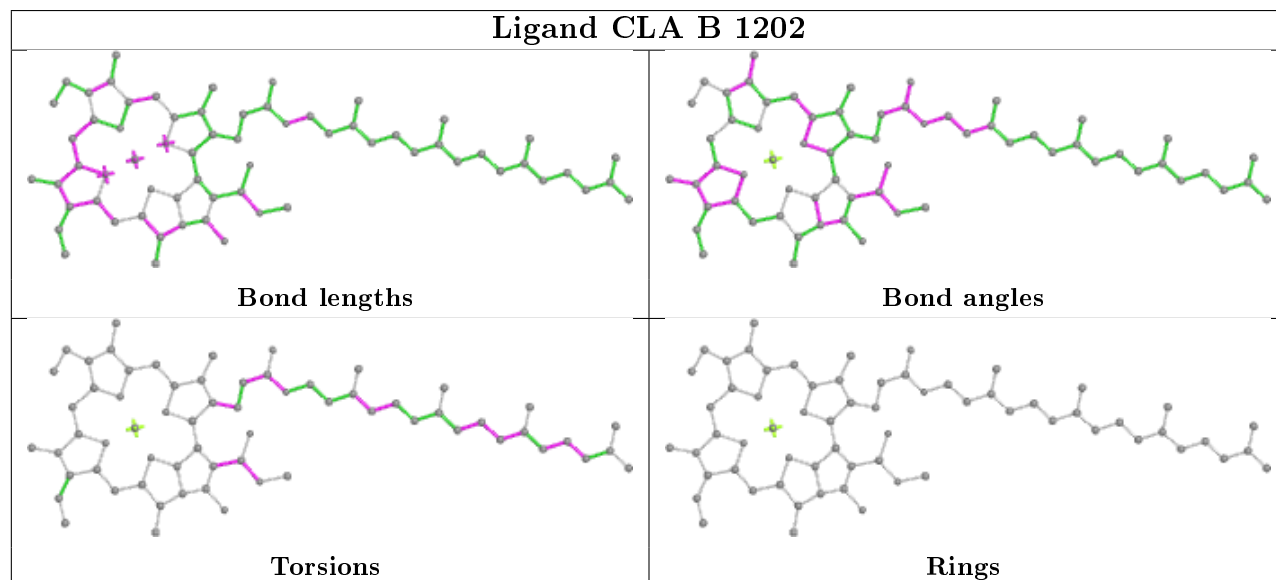
Ligand CLA B 1226

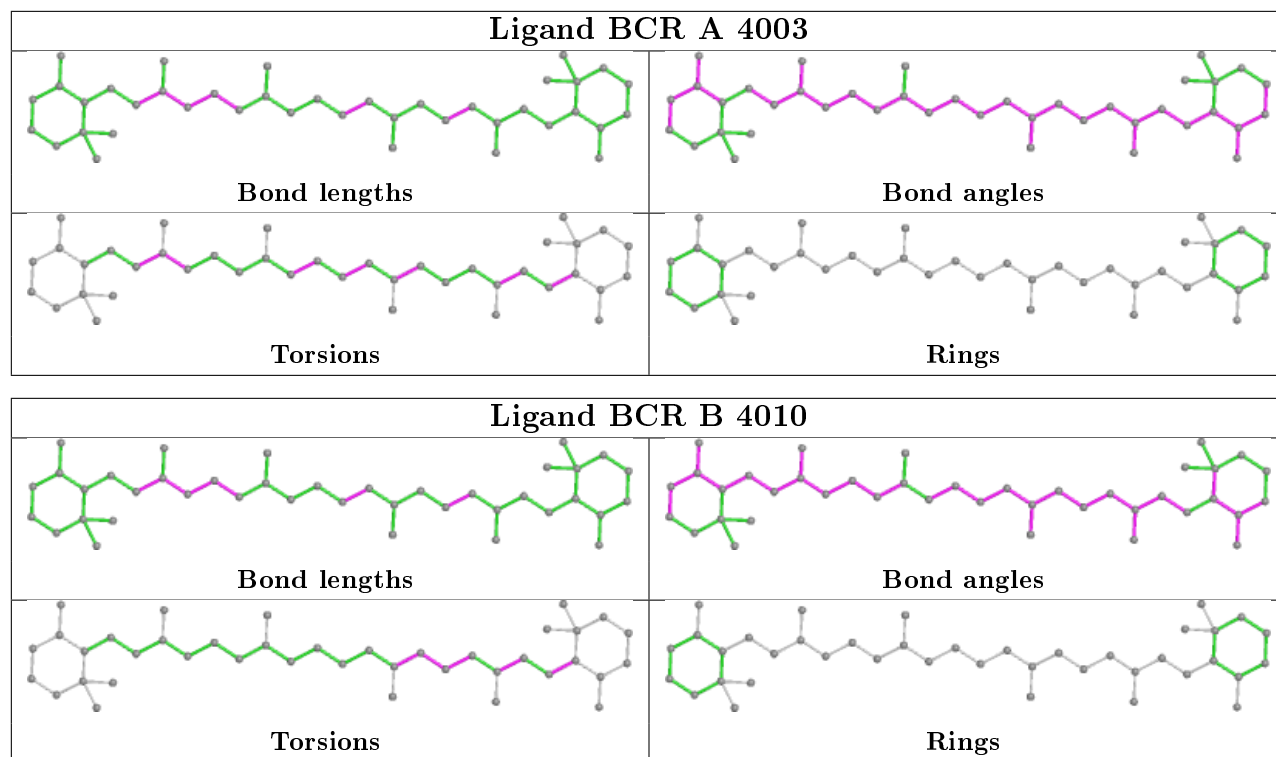


Ligand CLA B 1221

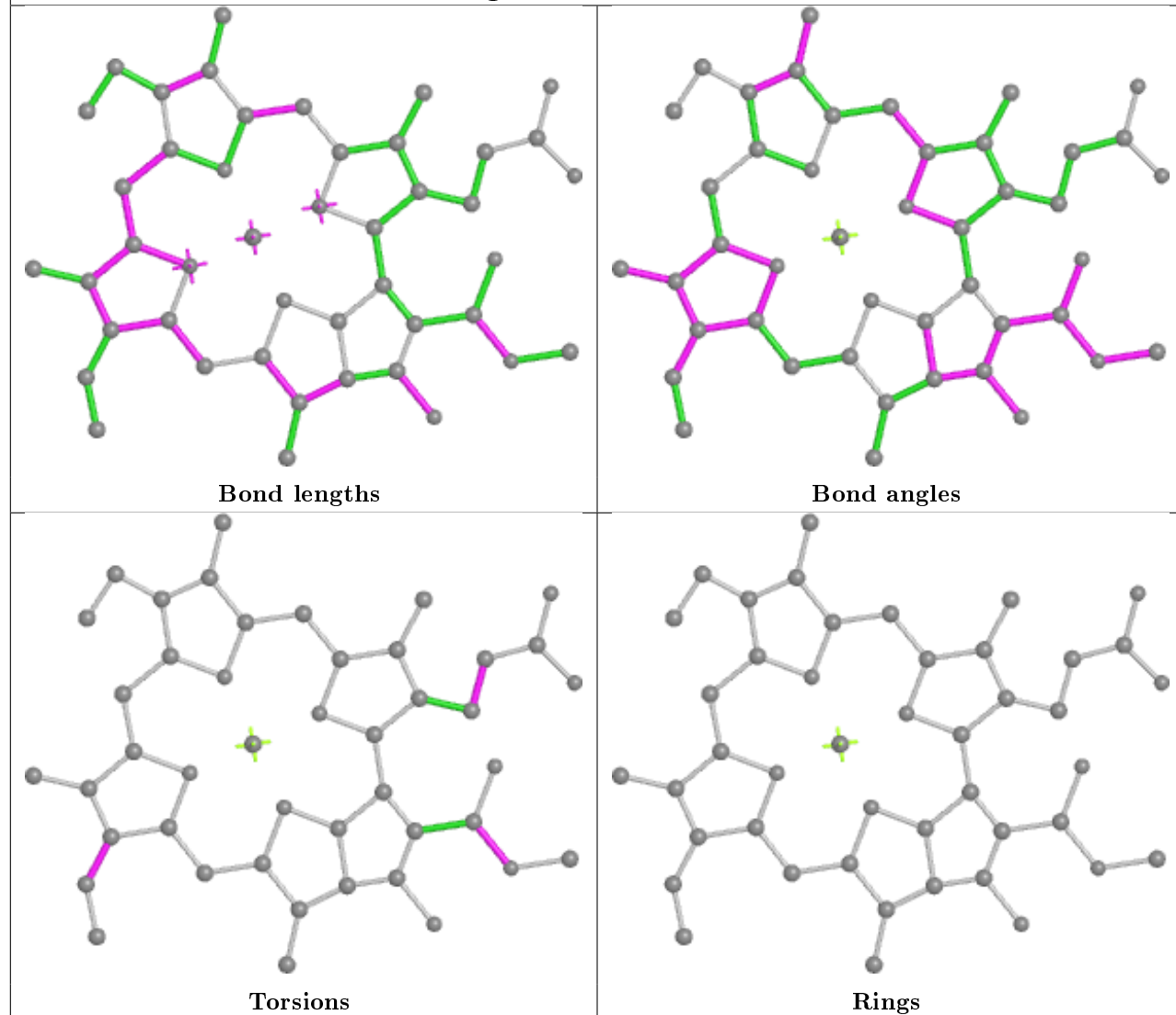


Ligand CLA B 1202

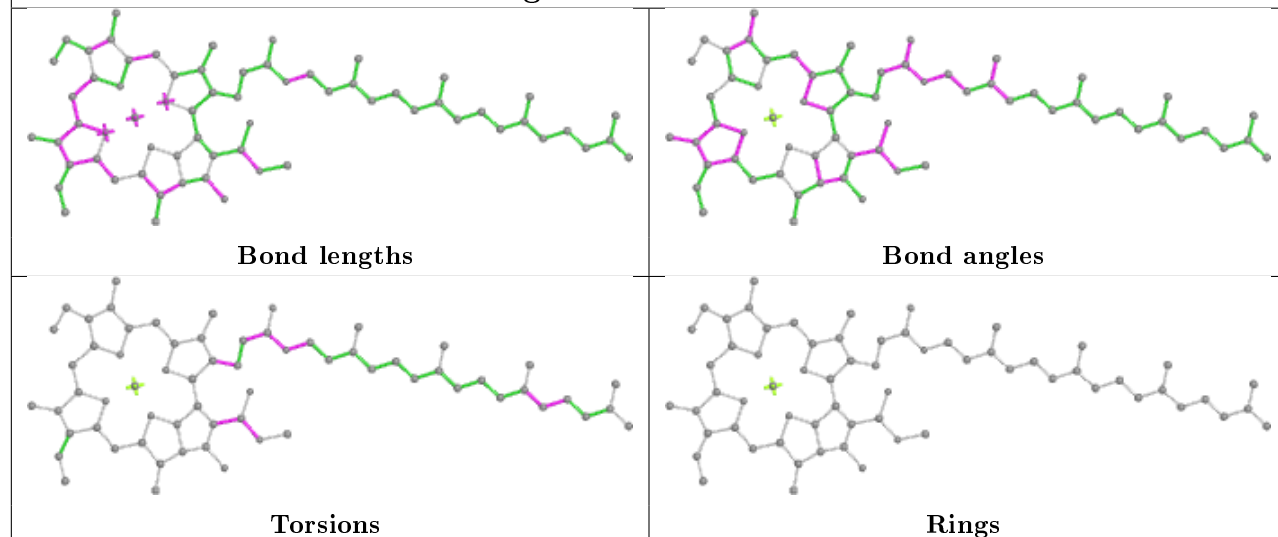




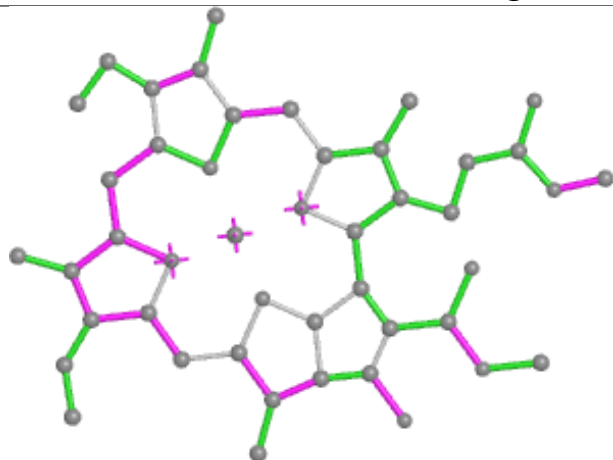
Ligand CL0 A 1108



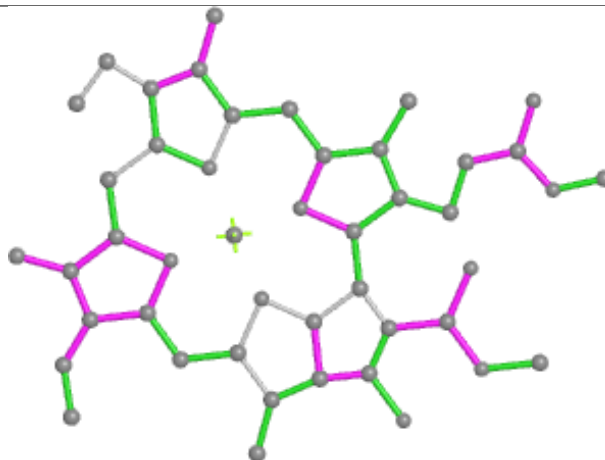
Ligand CLA A 1102



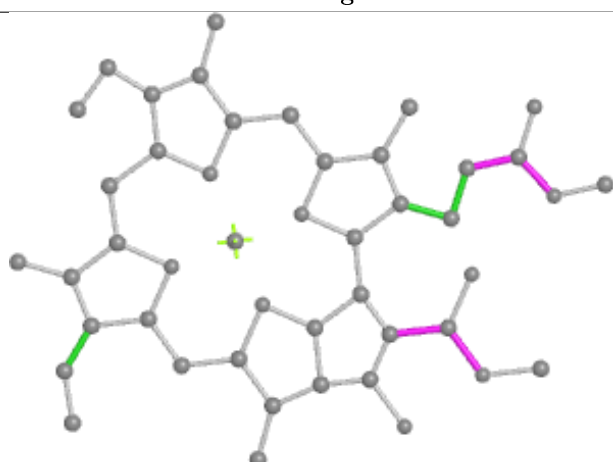
Ligand CLA B 1211



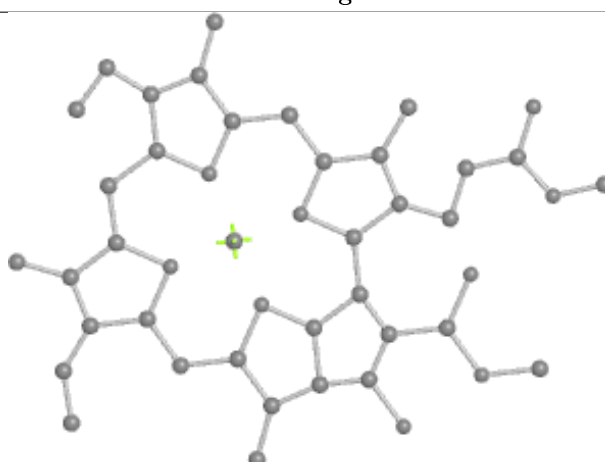
Bond lengths



Bond angles

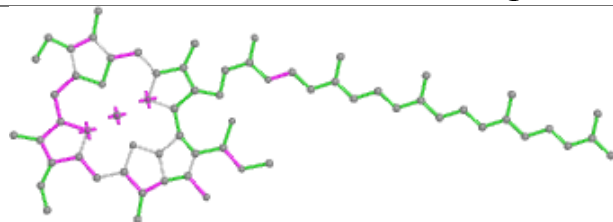


Torsions

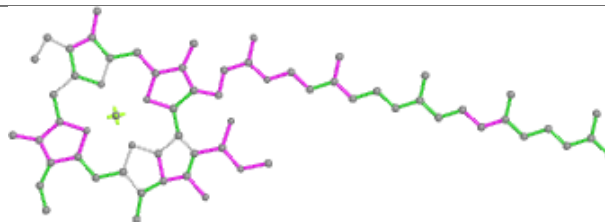


Rings

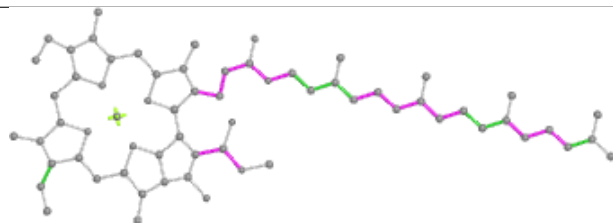
Ligand CLA B 1021



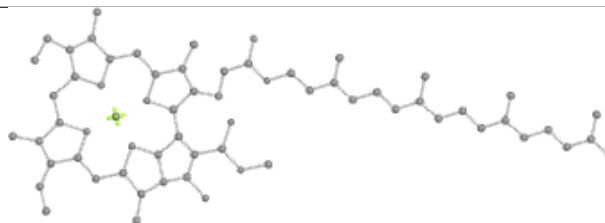
Bond lengths



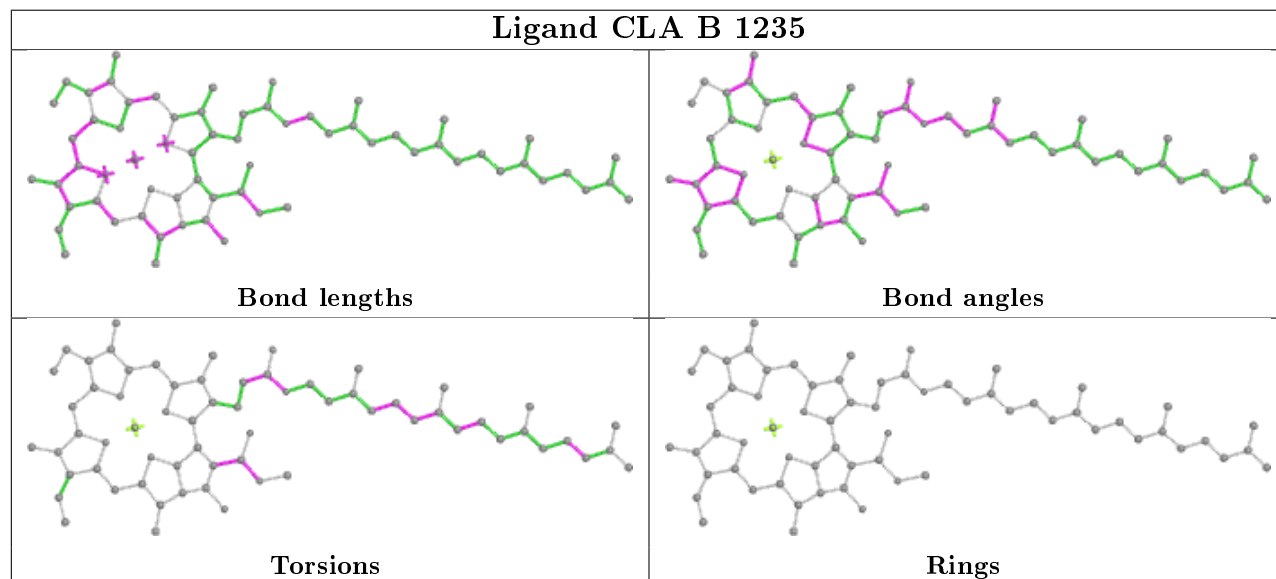
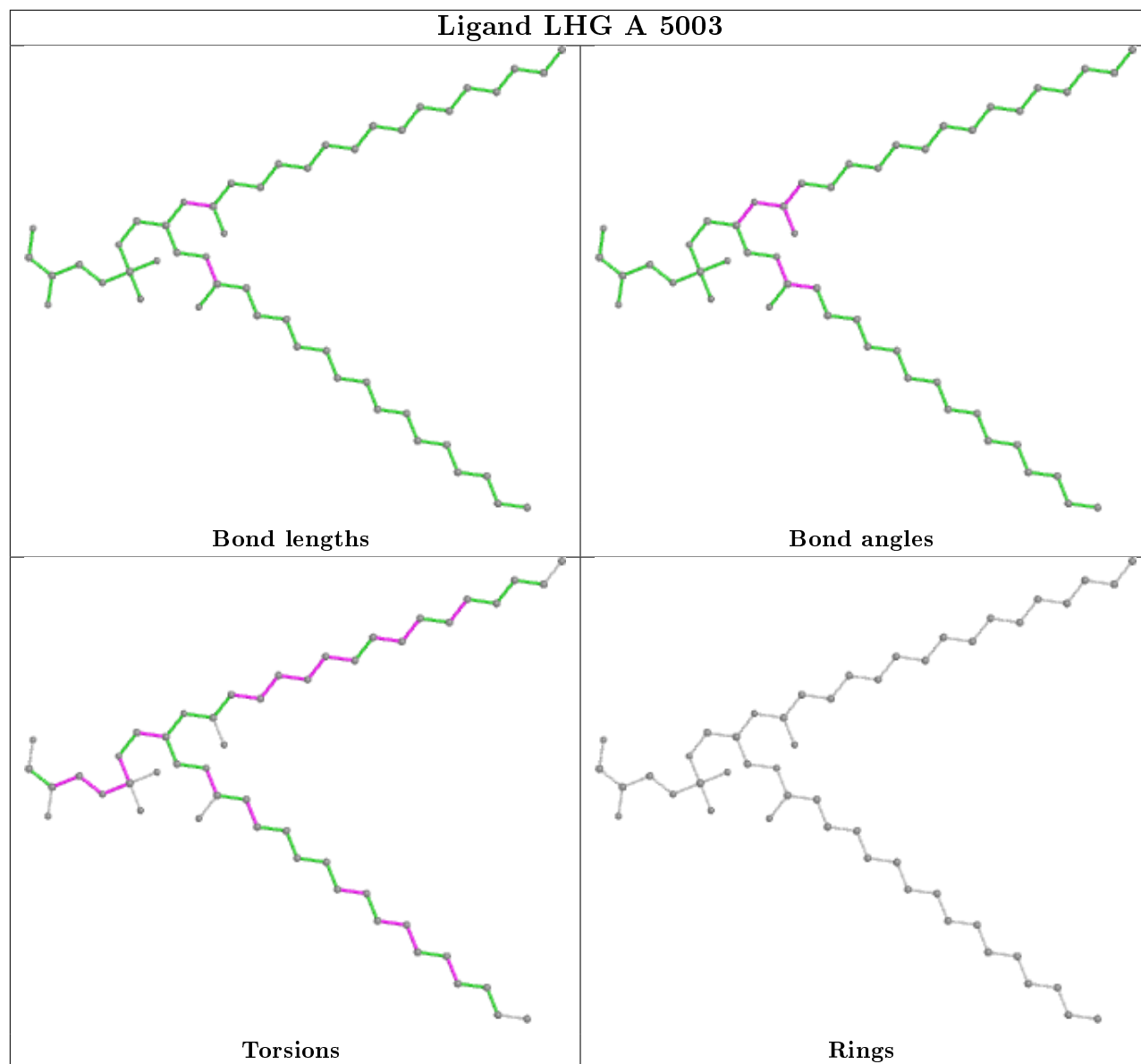
Bond angles



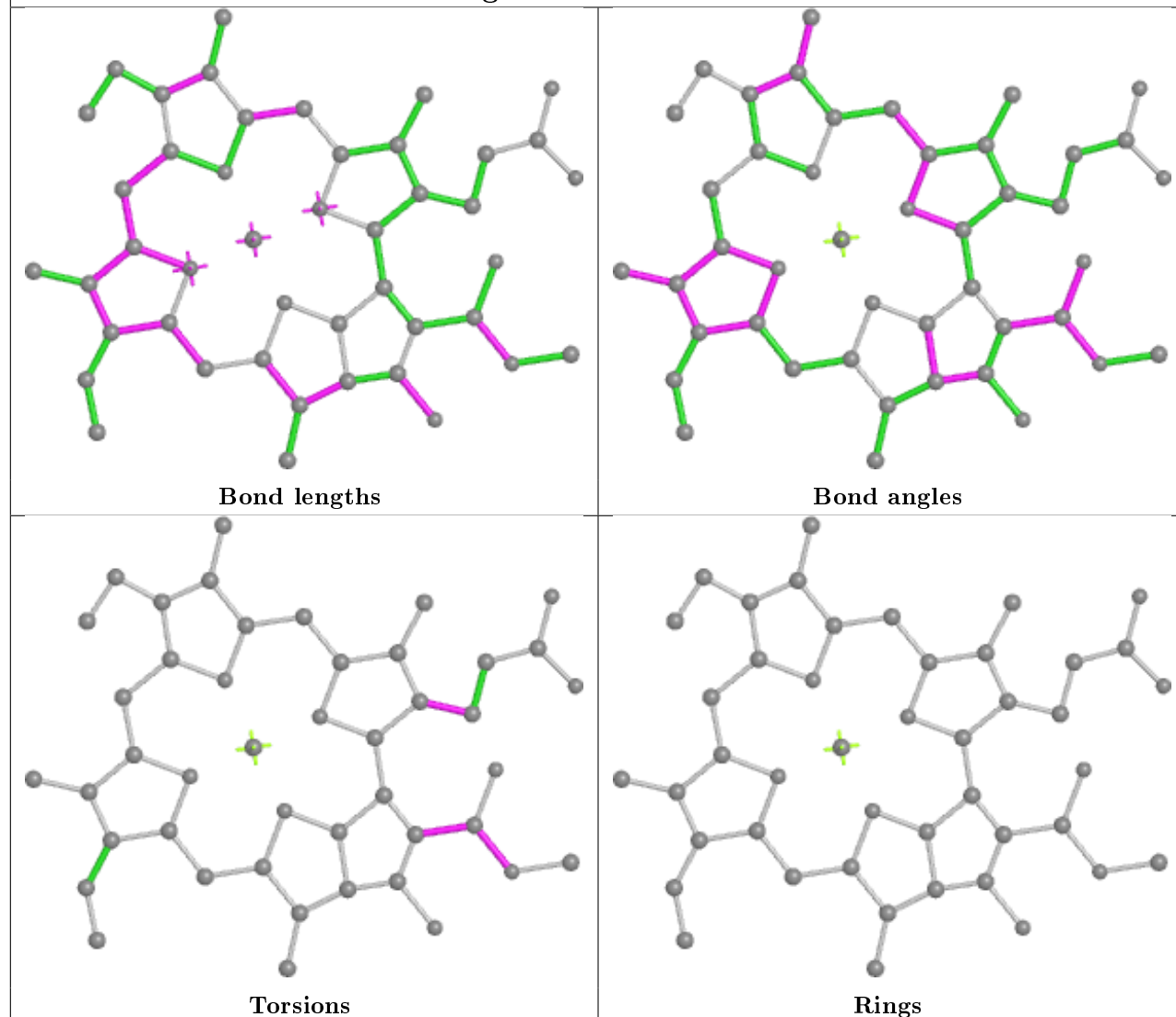
Torsions



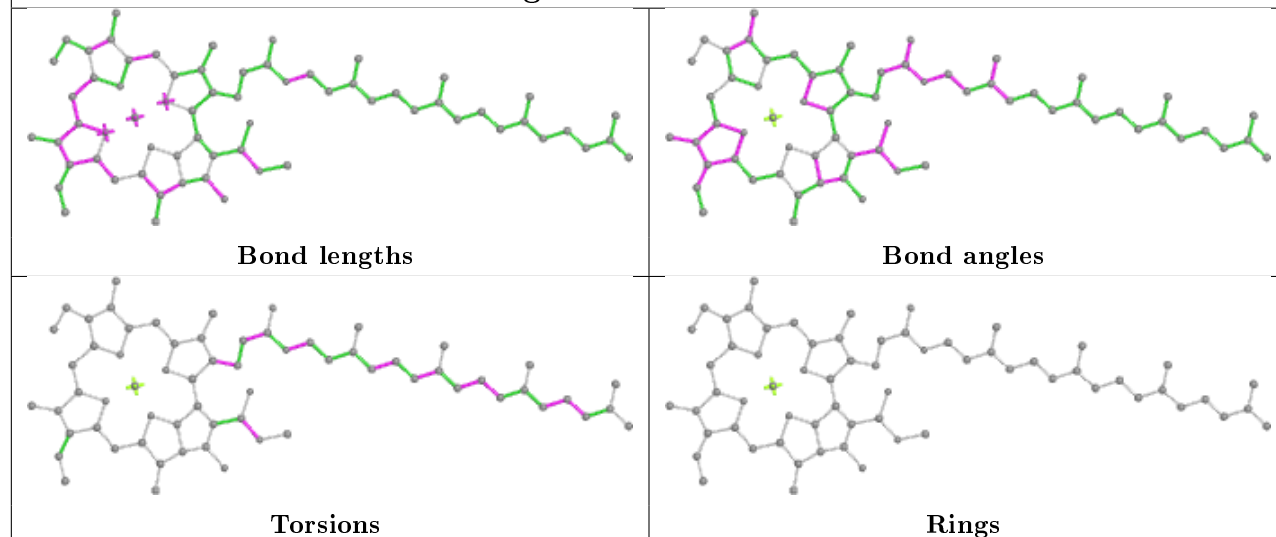
Rings

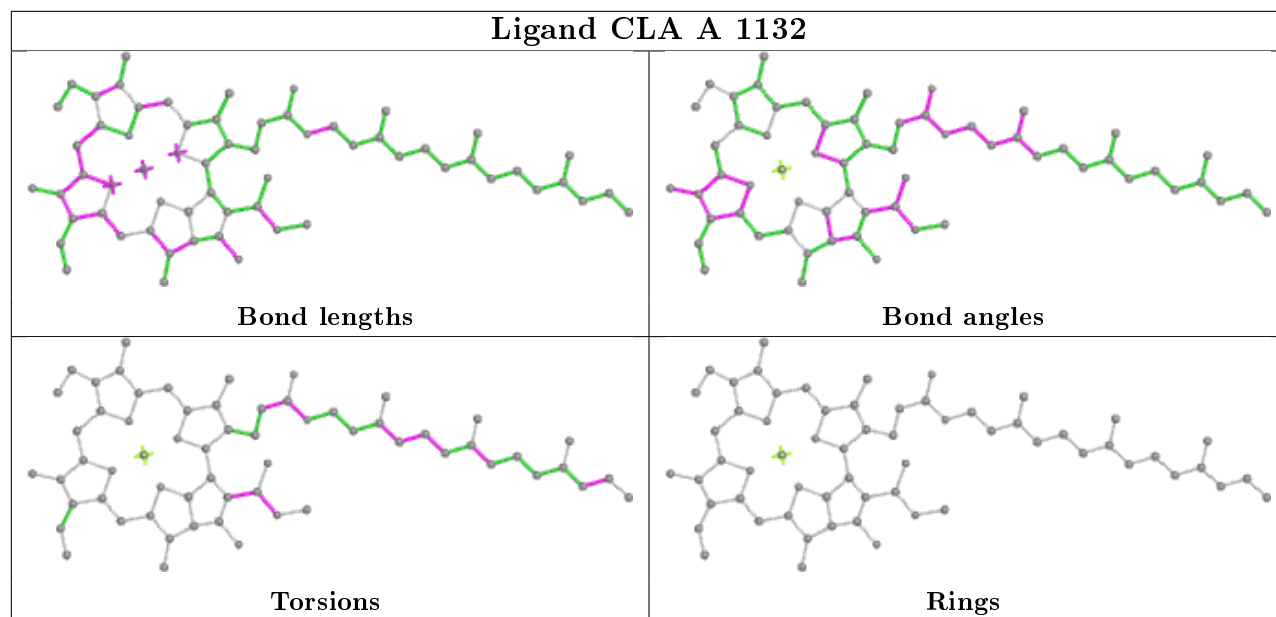
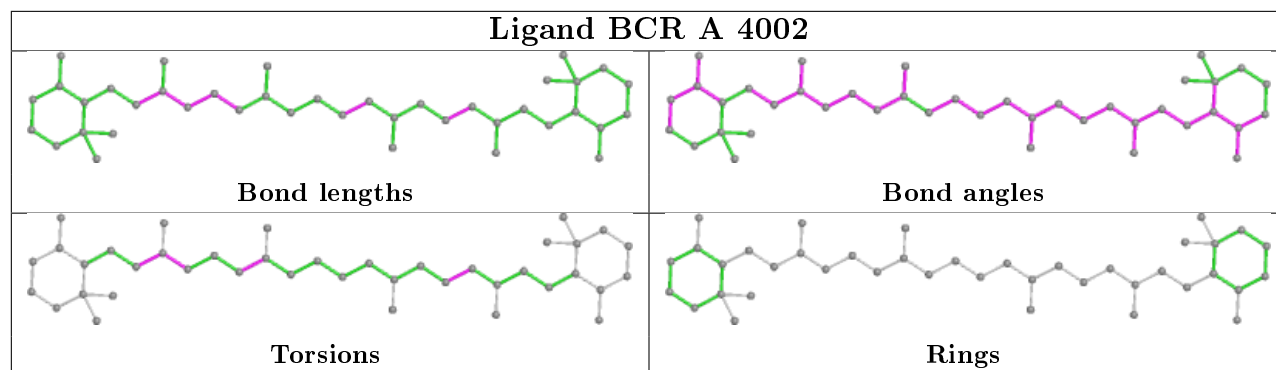


Ligand CLA A 1112

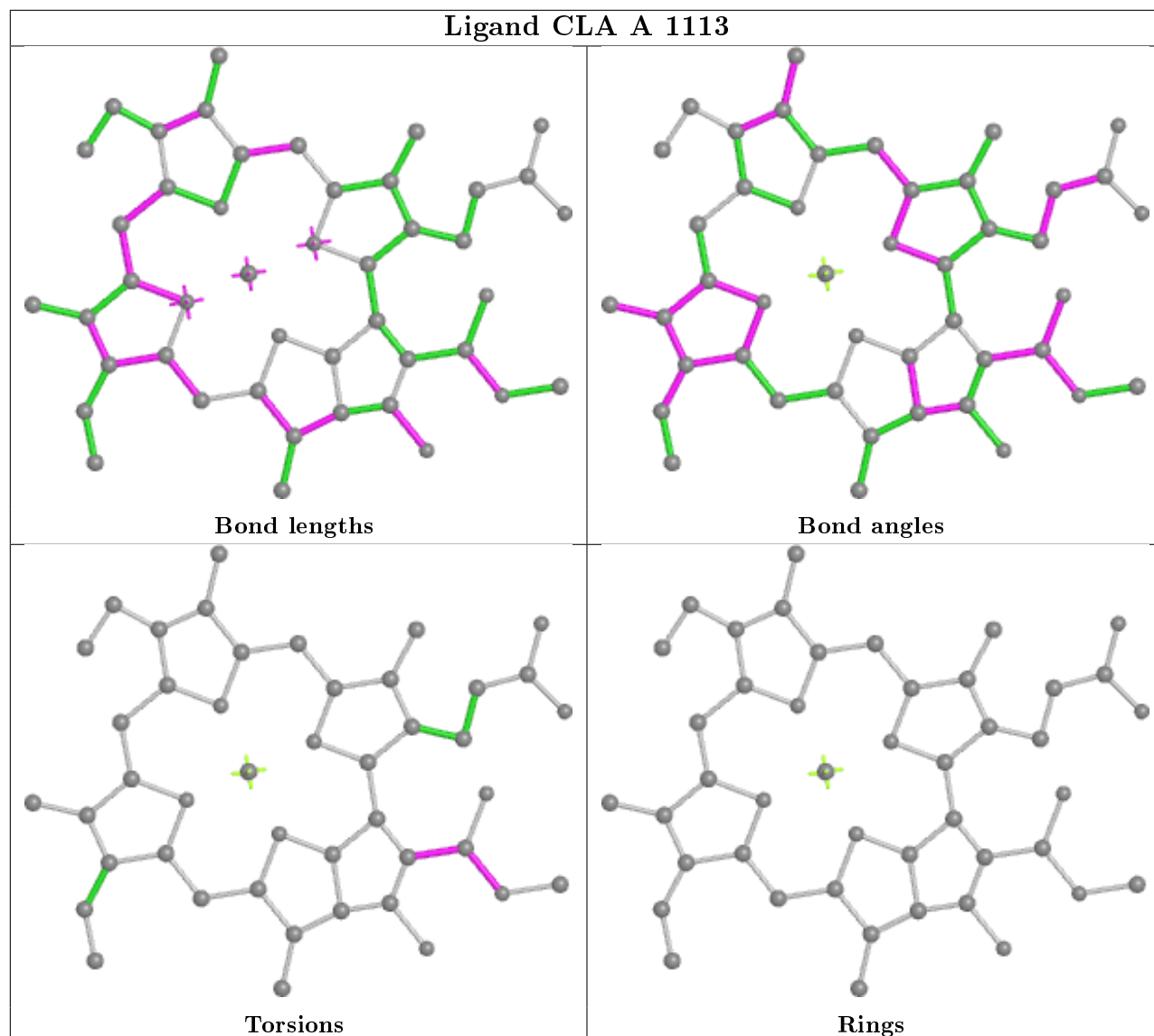


Ligand CLA B 1216

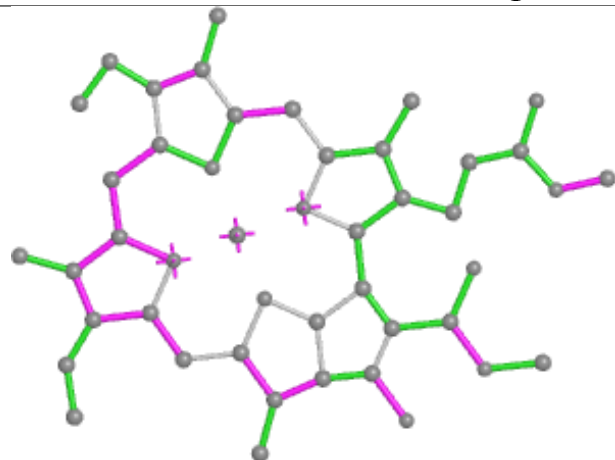




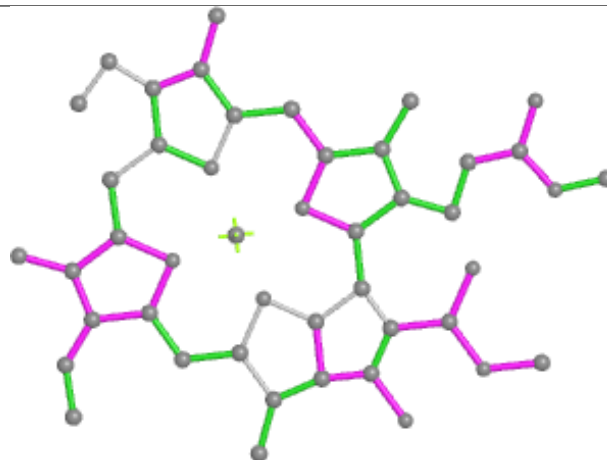
Ligand CLA A 1113



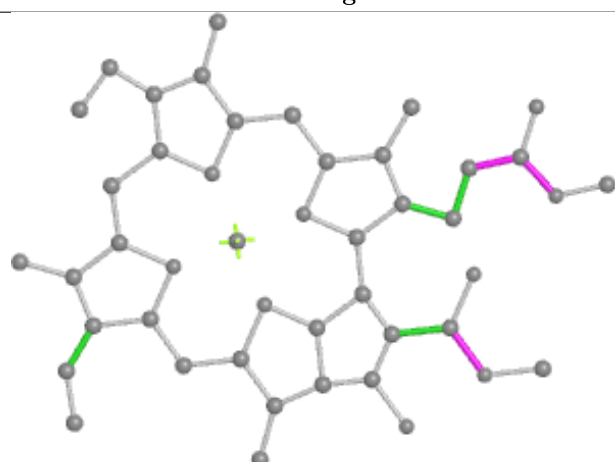
Ligand CLA B 1206



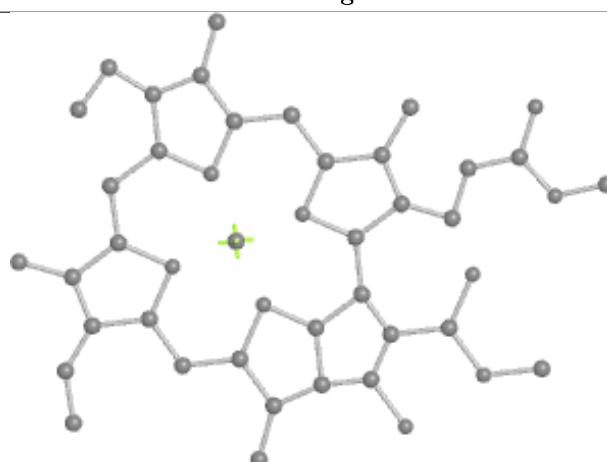
Bond lengths



Bond angles

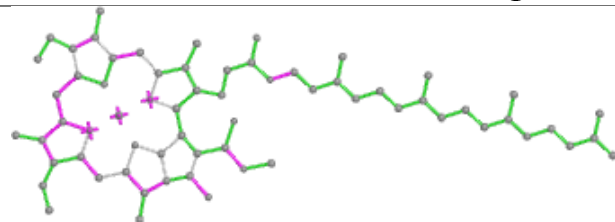


Torsions

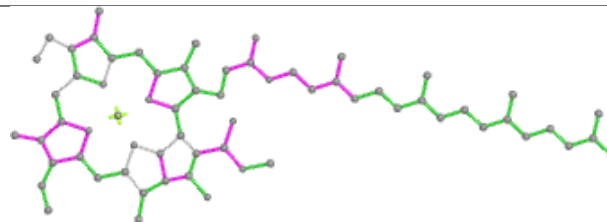


Rings

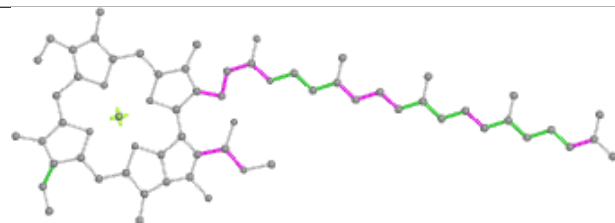
Ligand CLA A 1140



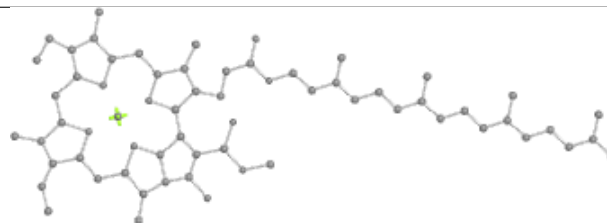
Bond lengths



Bond angles

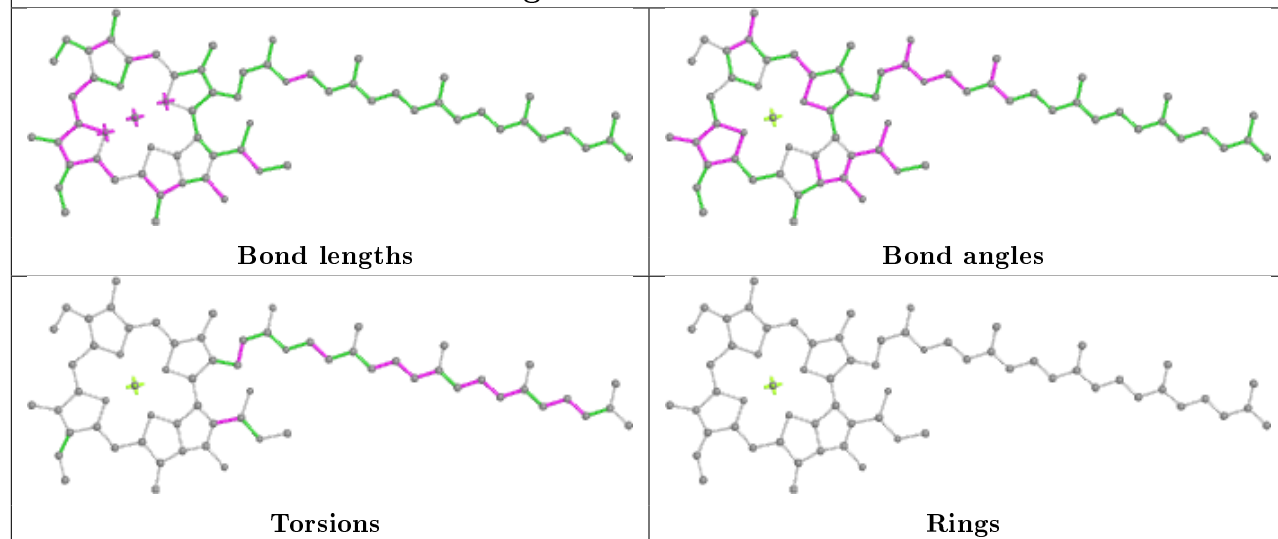


Torsions

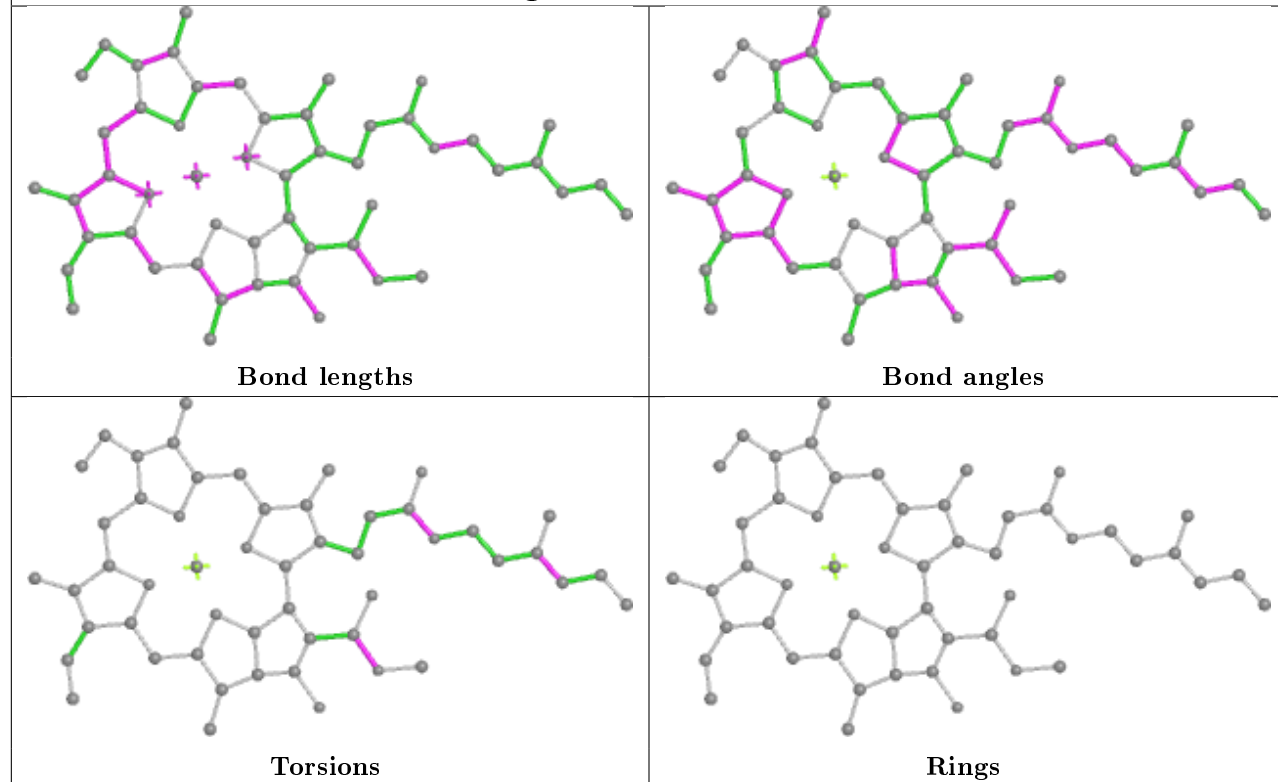


Rings

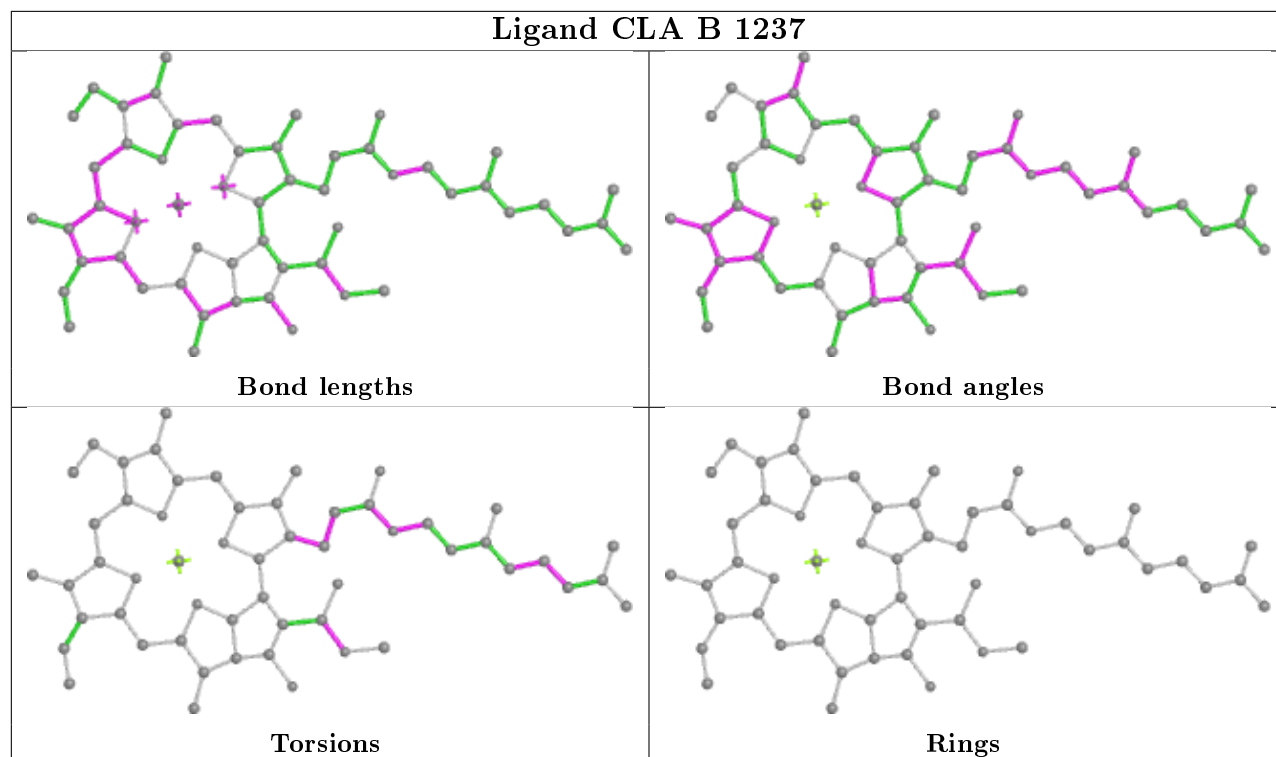
Ligand CLA A 1012



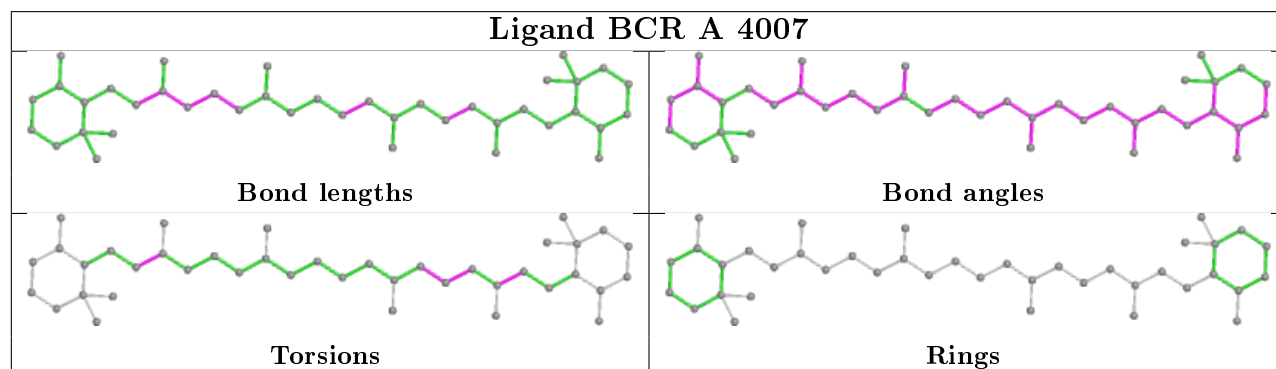
Ligand CLA A 1125



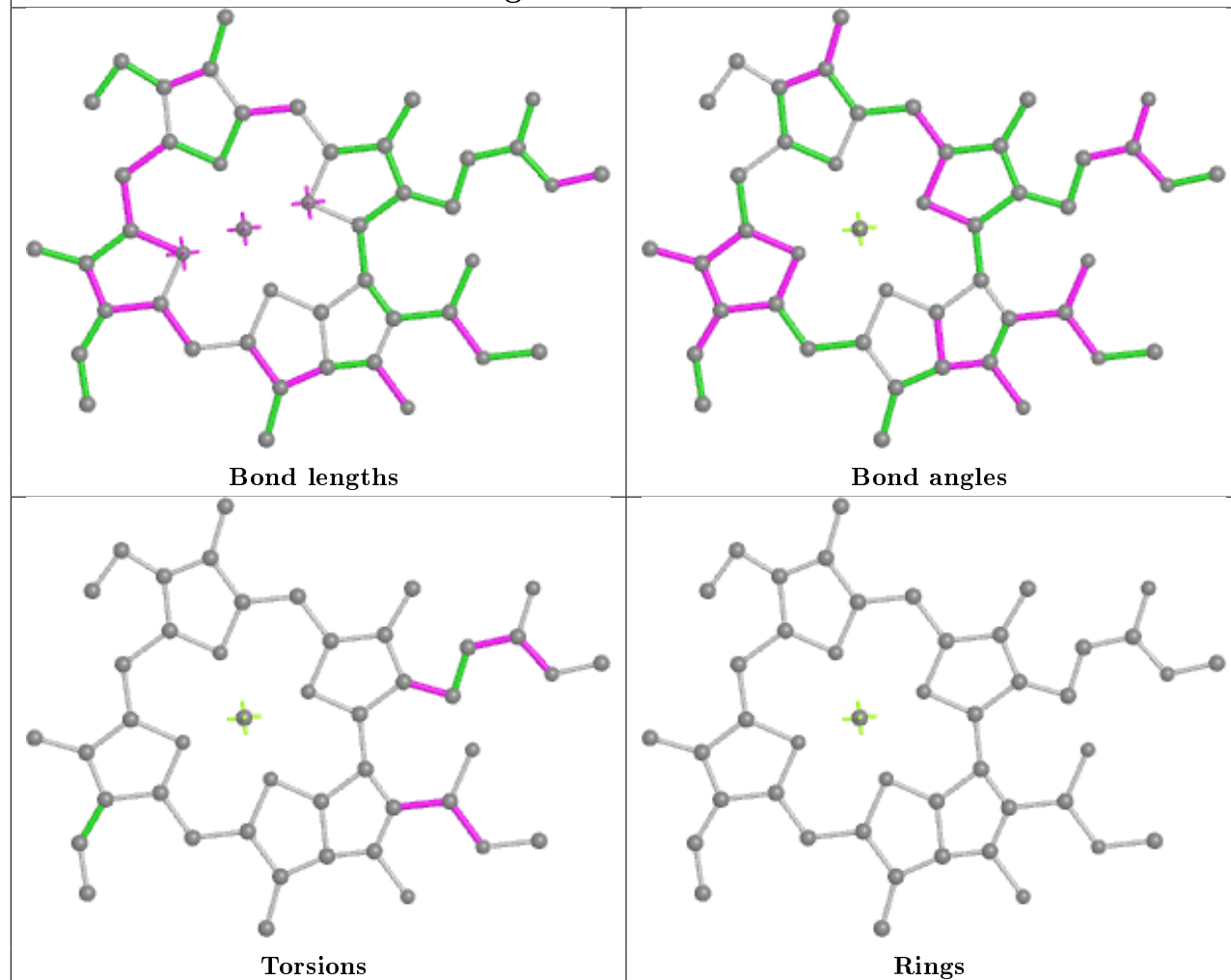
Ligand CLA B 1237

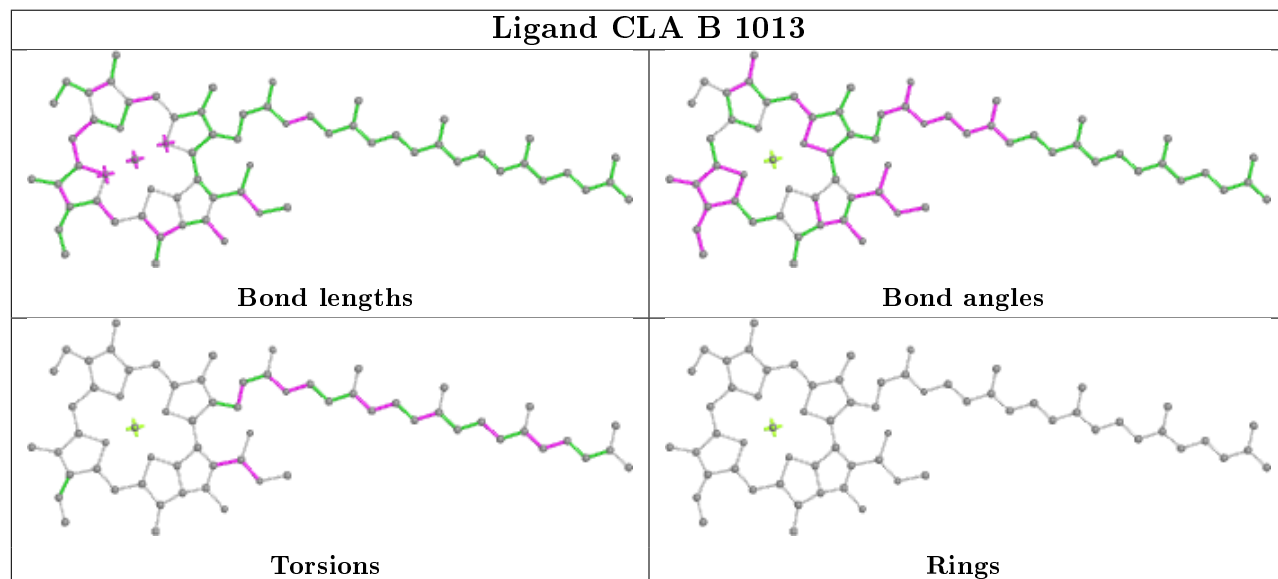
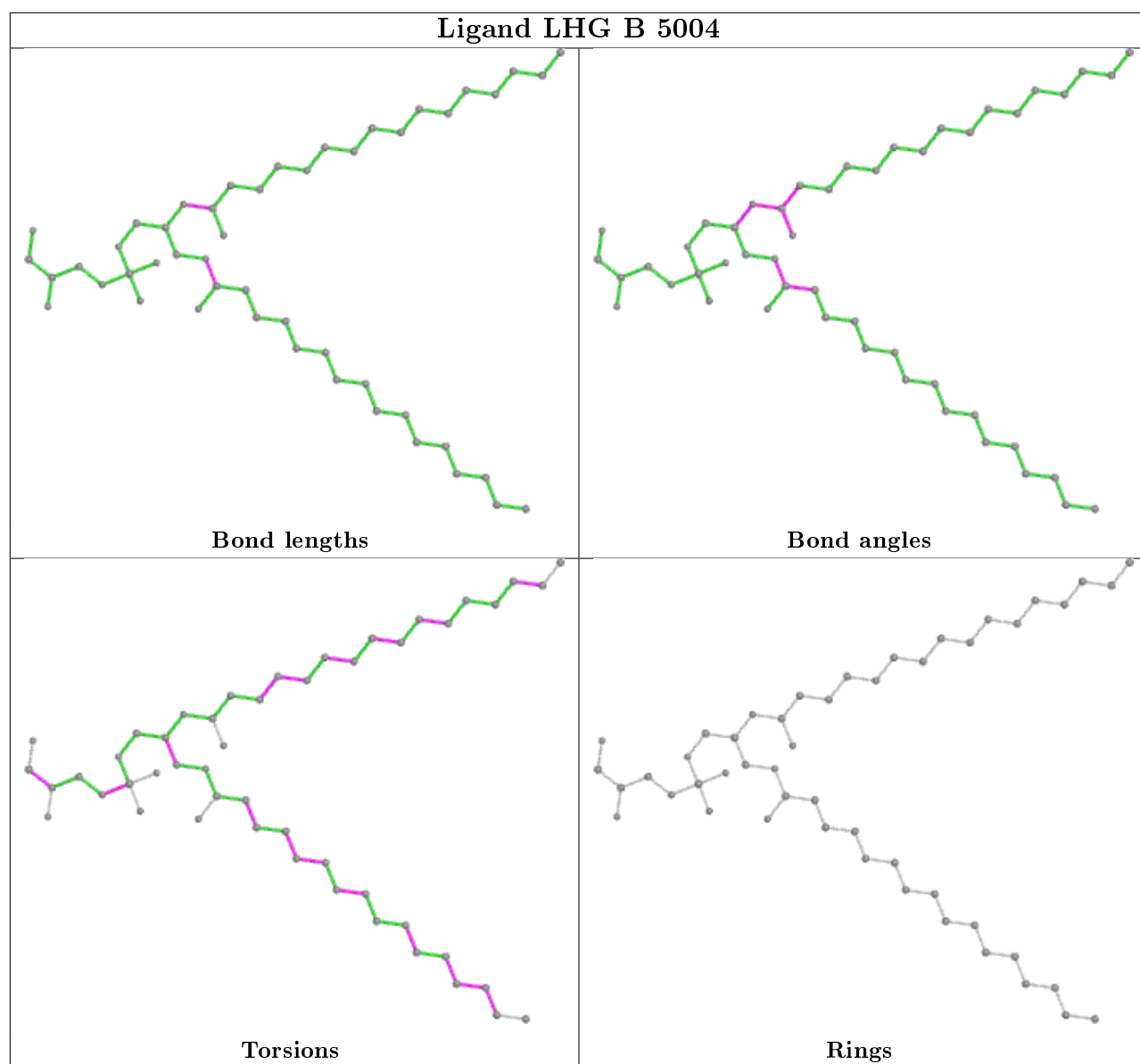


Ligand BCR A 4007

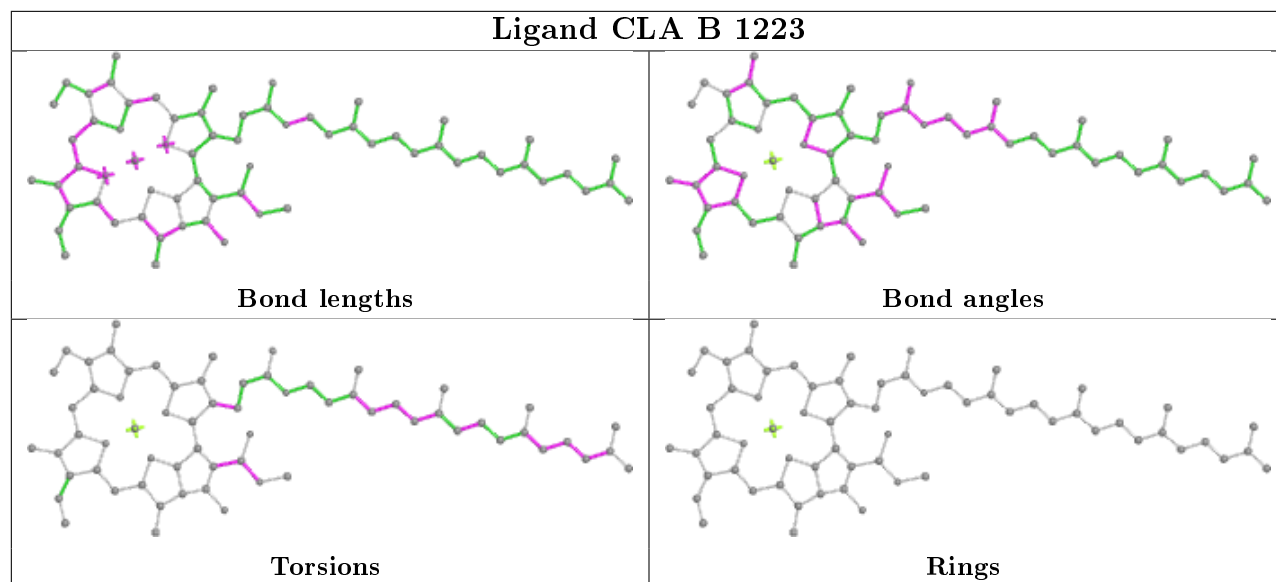


Ligand CLA A 1129

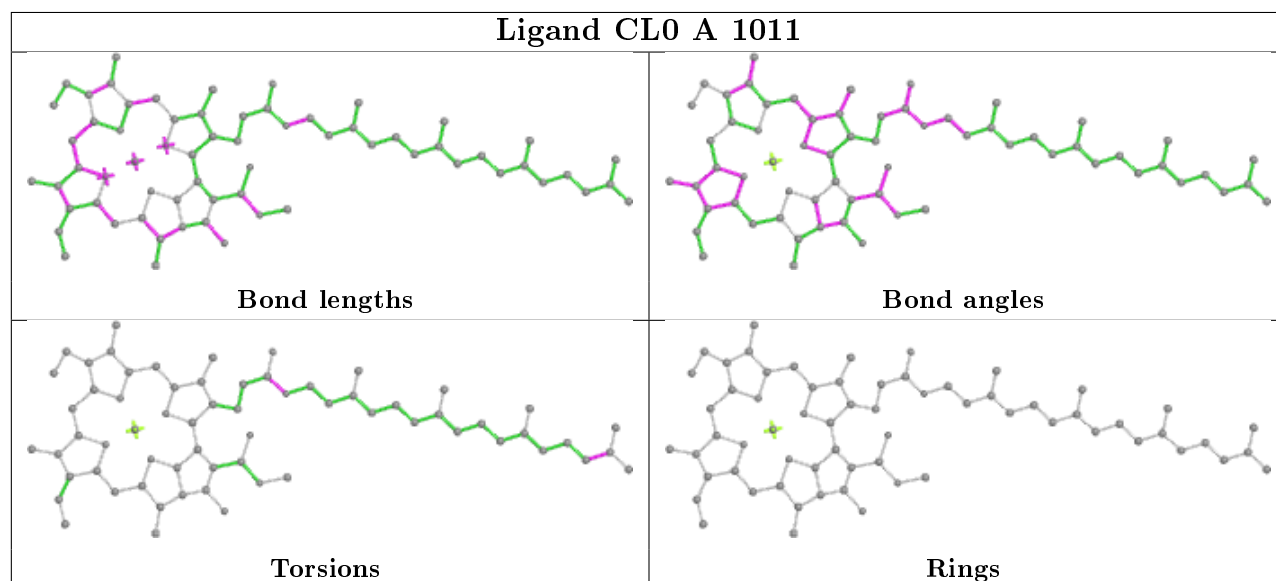




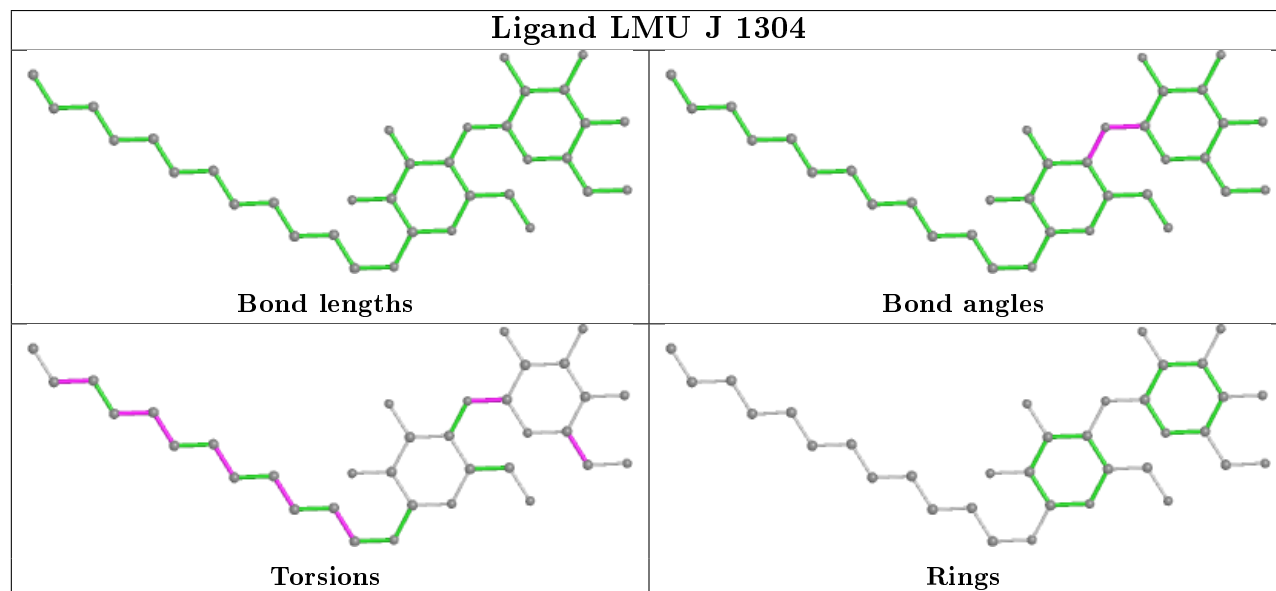
Ligand CLA B 1223



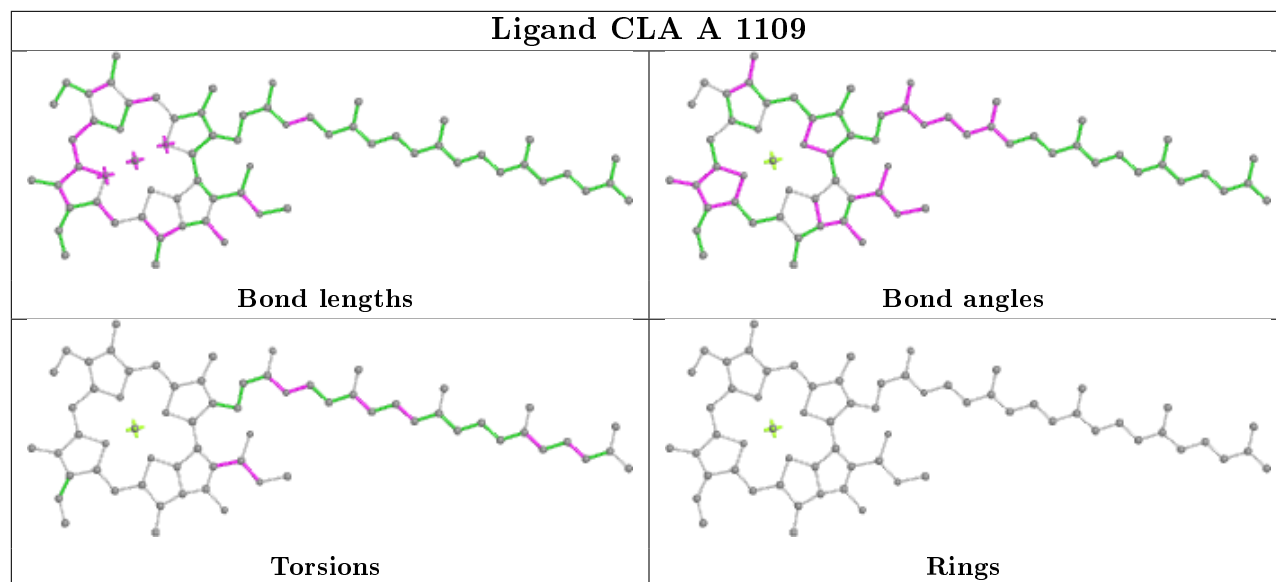
Ligand CL0 A 1011



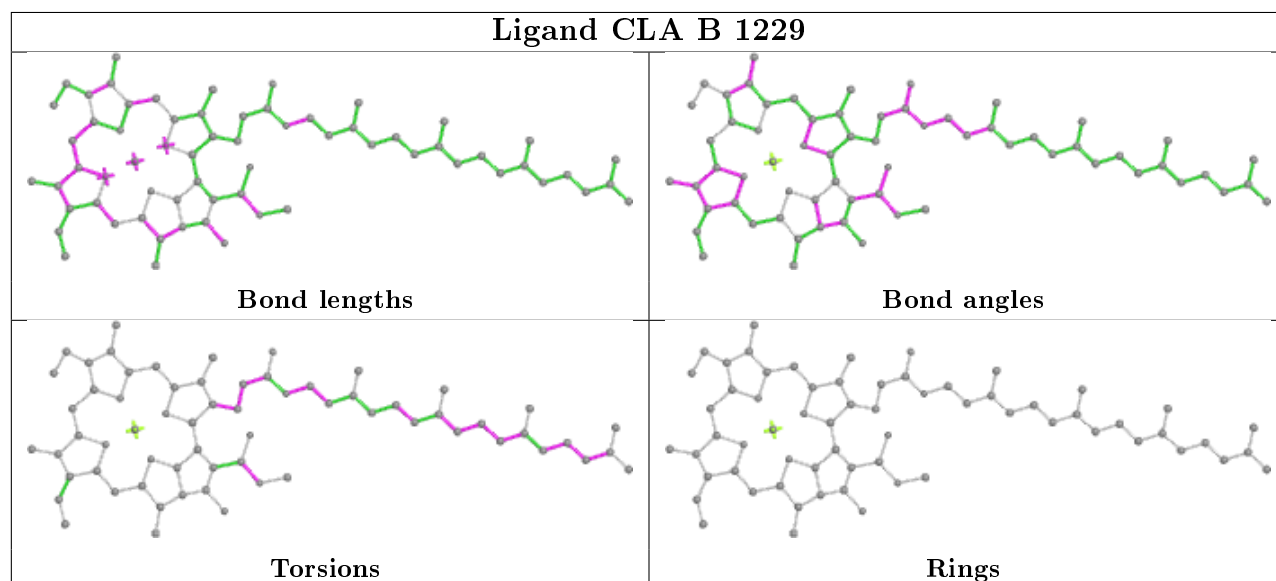
Ligand LMU J 1304



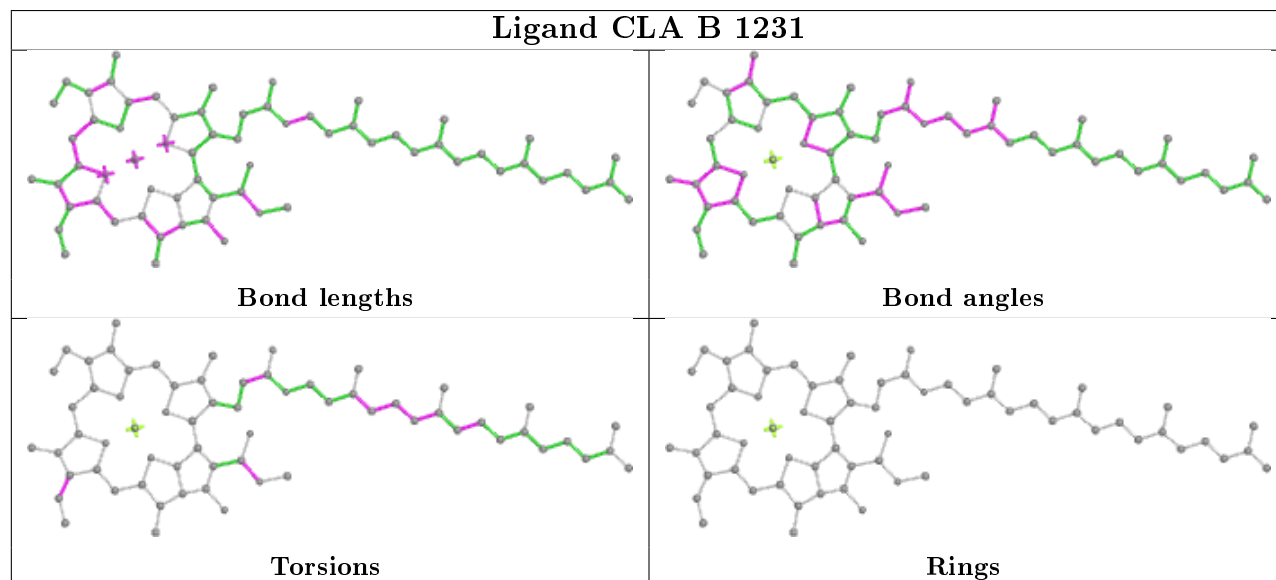
Ligand CLA A 1109



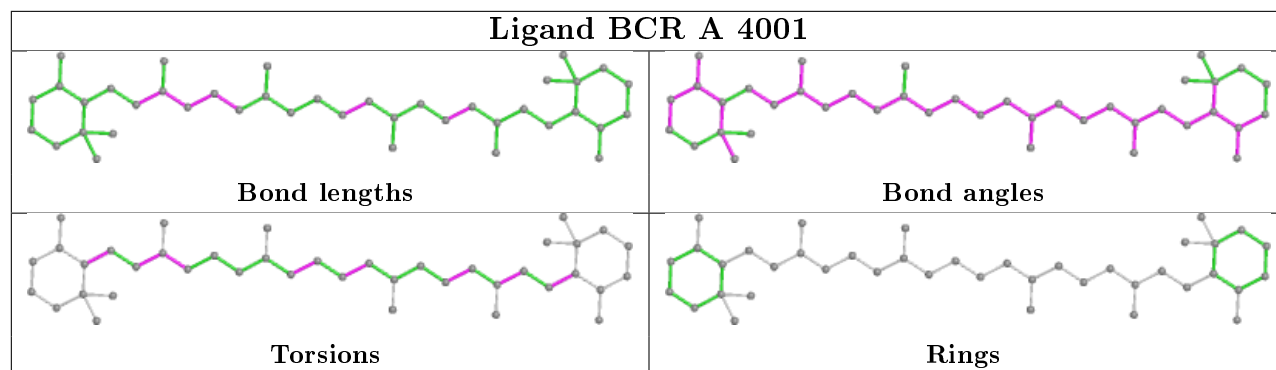
Ligand CLA B 1229



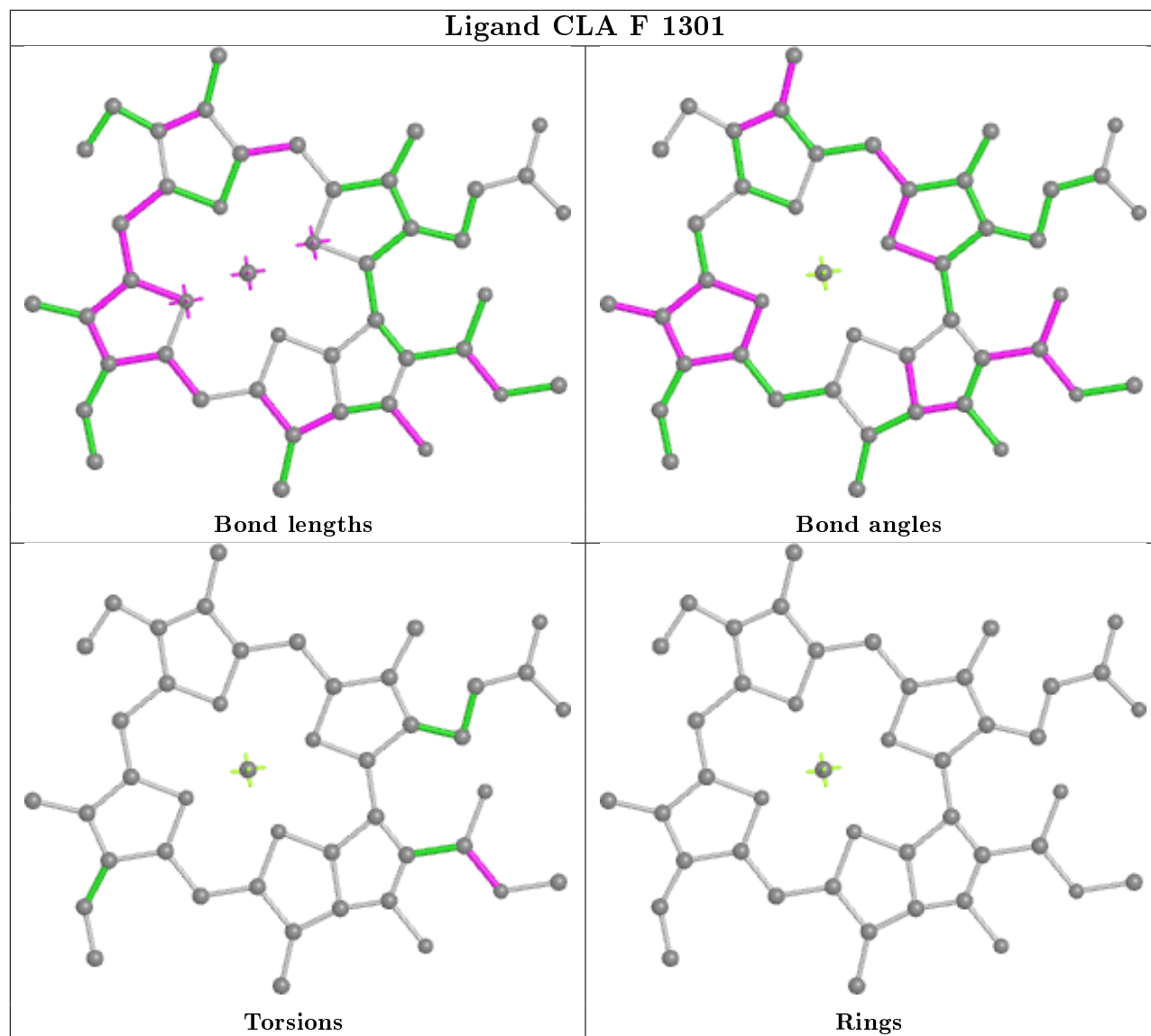
Ligand CLA B 1231



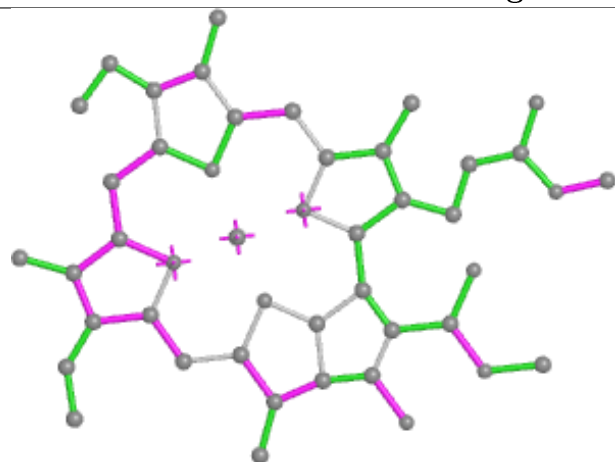
Ligand BCR A 4001



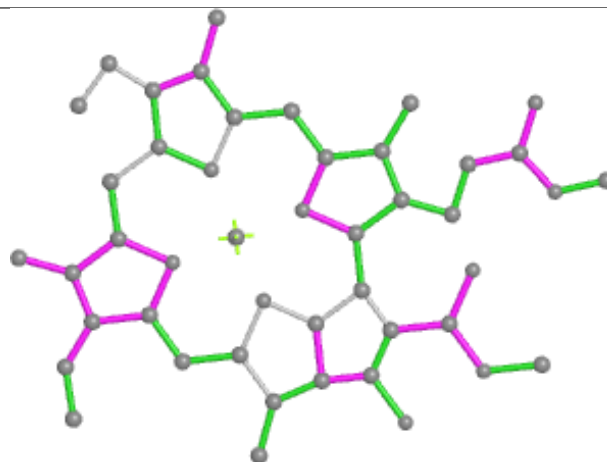
Ligand CLA F 1301



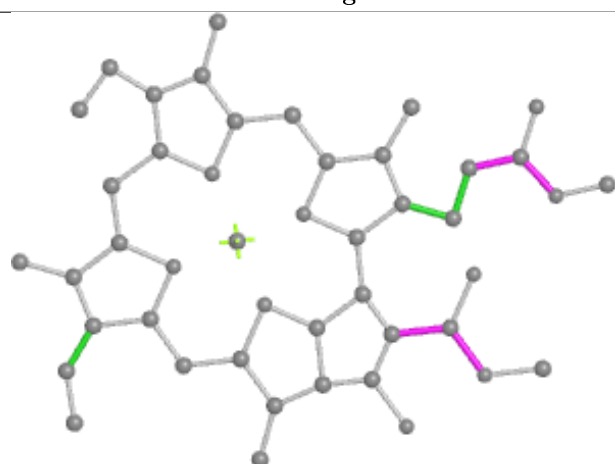
Ligand CLA K 1402



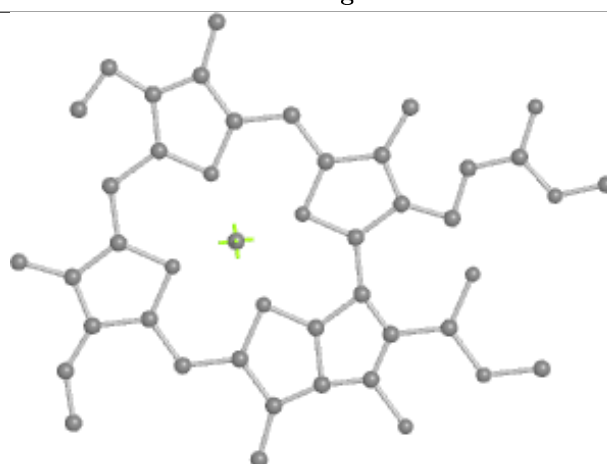
Bond lengths



Bond angles

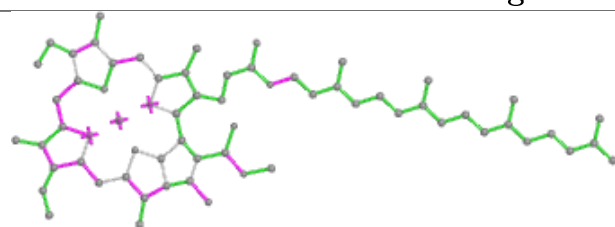


Torsions

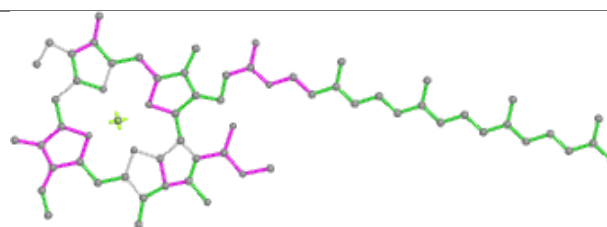


Rings

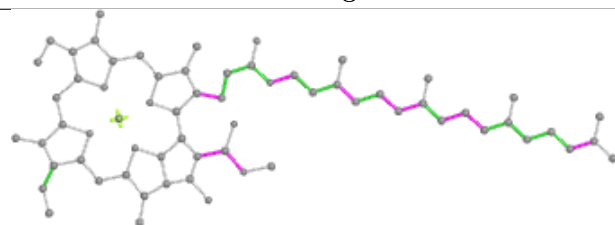
Ligand CLA A 1103



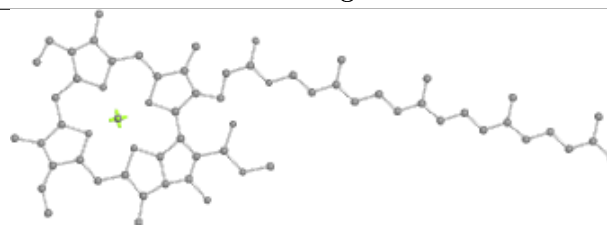
Bond lengths



Bond angles

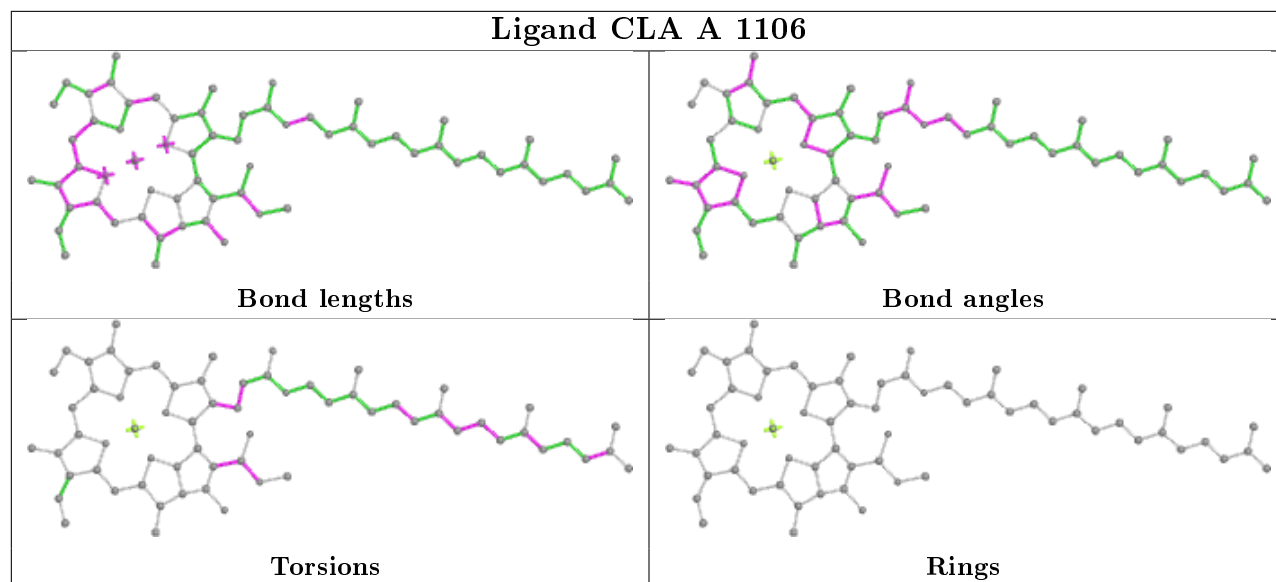


Torsions

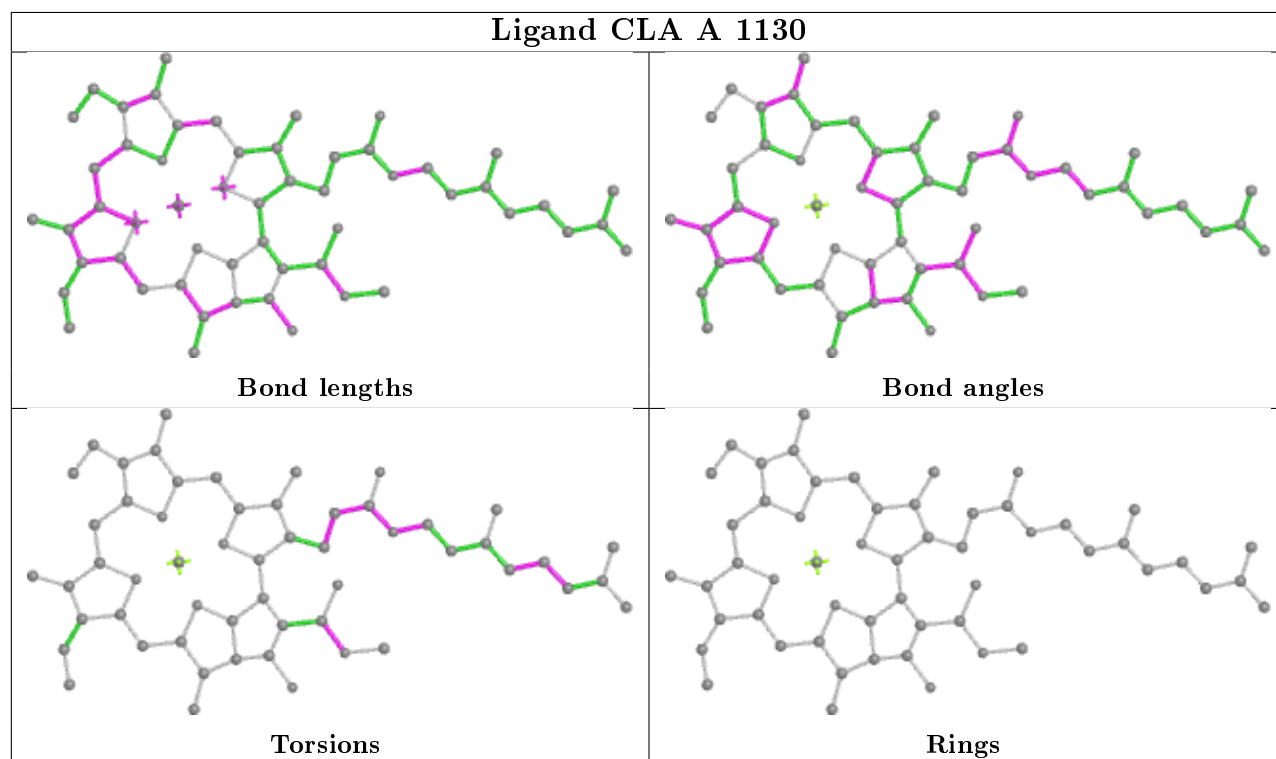


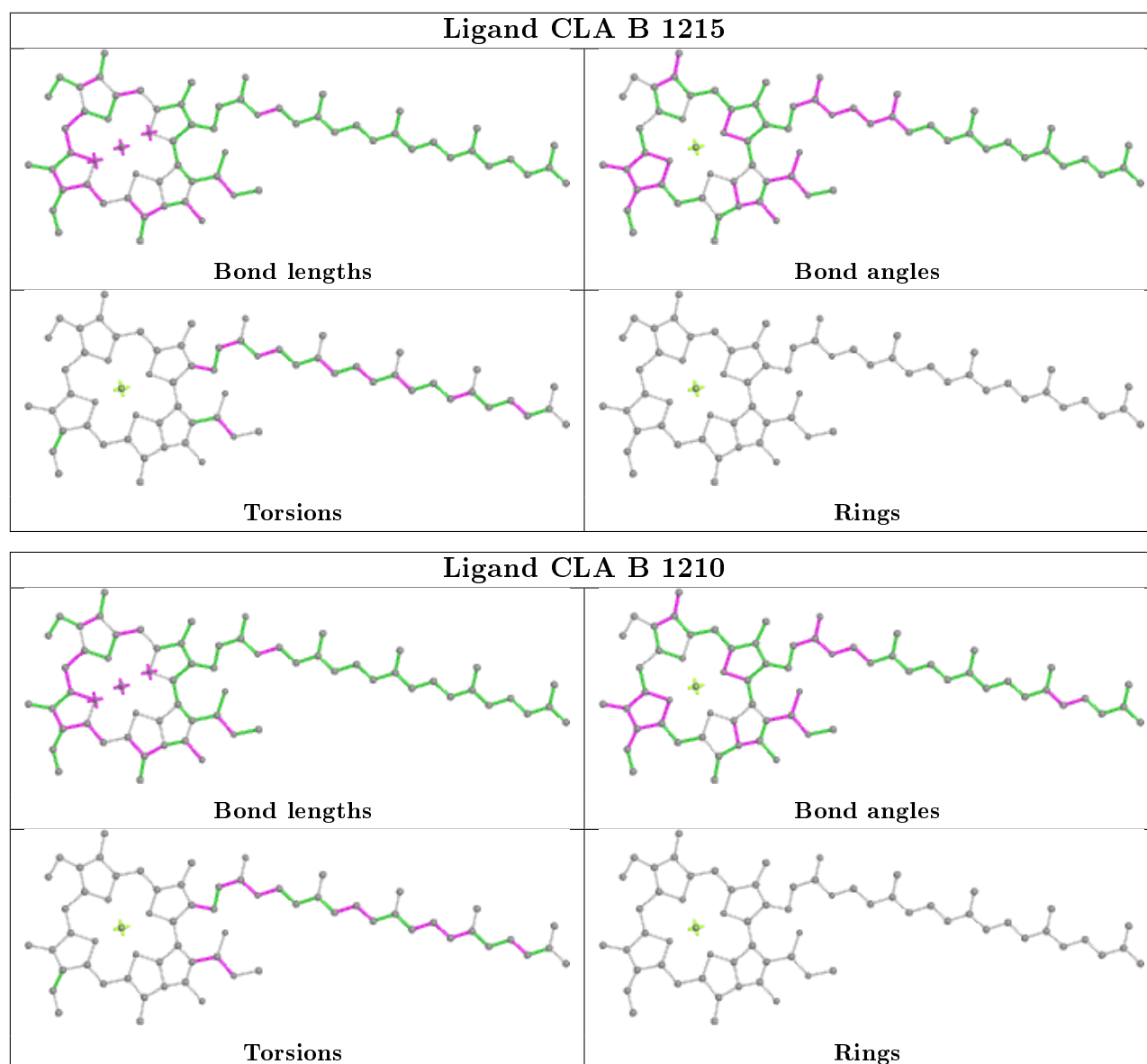
Rings

Ligand CLA A 1106



Ligand CLA A 1130





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	739/751 (98%)	0.20	58 (7%) 13 7	43, 90, 141, 226	0
2	B	728/731 (99%)	-0.09	21 (2%) 51 41	53, 83, 126, 179	0
3	C	80/81 (98%)	-0.30	0 100 100	60, 72, 95, 105	0
4	D	138/141 (97%)	0.46	23 (16%) 1 1	72, 90, 125, 161	0
5	E	68/74 (91%)	-0.00	3 (4%) 34 24	59, 75, 109, 138	0
6	F	141/165 (85%)	-0.26	4 (2%) 53 43	64, 82, 111, 169	0
7	J	40/40 (100%)	-0.45	2 (5%) 28 19	66, 76, 124, 149	0
8	K	53/128 (41%)	1.48	17 (32%) 0 0	134, 160, 207, 253	0
9	M	30/31 (96%)	1.98	9 (30%) 0 0	109, 132, 158, 172	0
All	All	2017/2142 (94%)	0.10	137 (6%) 17 10	43, 86, 145, 253	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	M	2	ALA	21.6
9	M	3	LEU	12.4
8	K	127	ILE	10.2
1	A	751	GLY	8.3
1	A	257	ALA	5.8
1	A	260	LEU	5.8
1	A	238	LEU	5.8
8	K	100	GLY	5.8
1	A	241	GLU	5.7
8	K	64	MET	5.6
8	K	60	VAL	5.5
9	M	4	SER	5.5
1	A	239	PRO	5.5
8	K	101	LEU	5.3
1	A	488	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
4	D	113	GLU	5.0
4	D	36	SER	4.9
2	B	96	PHE	4.8
8	K	126	GLY	4.7
1	A	485	TRP	4.7
9	M	6	THR	4.6
5	E	31	SER	4.6
4	D	52	GLU	4.5
1	A	511	GLY	4.4
1	A	235	ASP	4.2
1	A	237	PRO	4.2
1	A	256	PHE	4.2
4	D	130	THR	4.2
1	A	244	LEU	4.1
1	A	236	ILE	4.0
1	A	154	ASP	3.9
1	A	156	TYR	3.9
4	D	37	GLU	3.9
2	B	92	TRP	3.8
4	D	49	ILE	3.8
1	A	622	SER	3.8
1	A	233	PRO	3.8
6	F	94	LYS	3.7
1	A	304	PHE	3.7
2	B	216	PRO	3.7
2	B	111	ASN	3.6
2	B	214	SER	3.6
2	B	294	ASN	3.6
5	E	3	LEU	3.6
6	F	15	ALA	3.5
1	A	300	ILE	3.5
1	A	623	PRO	3.5
2	B	248	GLU	3.5
1	A	59	ASP	3.4
8	K	59	SER	3.4
1	A	240	HIS	3.4
8	K	108	MET	3.3
4	D	77	LYS	3.3
2	B	486	THR	3.2
9	M	8	ILE	3.1
1	A	234	LYS	3.1
1	A	620	THR	3.1

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Mol	Chain	Res	Type	RSRZ
9	M	7	GLN	3.1
2	B	165	LEU	3.1
1	A	361	SER	3.1
1	A	489	LEU	3.1
4	D	35	ALA	3.0
4	D	54	GLU	3.0
8	K	76	TYR	3.0
1	A	63	SER	3.0
2	B	215	THR	2.9
9	M	5	ASP	2.9
9	M	11	ALA	2.9
1	A	369	HIS	2.9
6	F	14	PRO	2.9
1	A	259	GLY	2.8
4	D	140	GLU	2.8
4	D	51	ASN	2.8
4	D	50	MET	2.7
8	K	125	SER	2.7
4	D	10	LYS	2.7
1	A	297	HIS	2.7
6	F	92	GLU	2.7
8	K	77	PHE	2.7
4	D	114	ALA	2.7
1	A	64	ASP	2.7
9	M	10	ALA	2.6
2	B	375	TYR	2.6
1	A	296	HIS	2.6
4	D	139	TYR	2.6
4	D	3	GLU	2.6
1	A	62	THR	2.6
2	B	297	ILE	2.6
4	D	134	SER	2.6
1	A	332	PHE	2.5
4	D	34	SER	2.5
8	K	63	ILE	2.5
2	B	157	LEU	2.5
8	K	75	GLY	2.5
1	A	242	PHE	2.5
2	B	136	TYR	2.5
2	B	313	THR	2.5
1	A	303	LEU	2.5
5	E	30	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	131	ILE	2.4
1	A	370	MET	2.4
1	A	624	ASP	2.4
1	A	365	ILE	2.4
2	B	293	THR	2.4
4	D	126	PRO	2.4
4	D	38	GLN	2.3
1	A	628	THR	2.3
2	B	488	ALA	2.3
1	A	205	LEU	2.3
1	A	155	SER	2.3
1	A	299	ALA	2.3
1	A	355	ASN	2.3
8	K	62	ILE	2.3
8	K	74	ILE	2.3
1	A	67	ASP	2.2
7	J	1	MET	2.2
1	A	101	GLU	2.2
1	A	243	ILE	2.2
1	A	625	GLY	2.2
1	A	362	LEU	2.2
1	A	532	PHE	2.2
2	B	44	GLN	2.2
1	A	251	GLU	2.2
4	D	4	LEU	2.2
7	J	2	ASP	2.2
4	D	100	ALA	2.2
1	A	94	GLY	2.1
2	B	379	PHE	2.1
2	B	112	PRO	2.1
8	K	124	SER	2.1
2	B	339	LEU	2.1
1	A	209	SER	2.1
1	A	496	ALA	2.1
1	A	17	ASP	2.0
1	A	477	GLN	2.0
8	K	65	CYS	2.0
1	A	36	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	BCR	B	4004	40/40	0.66	0.31	101,115,147,151	0
15	CLA	K	1401	46/65	0.67	0.34	120,155,169,173	0
14	BCR	A	4007	40/40	0.69	0.39	69,86,137,139	0
16	LMU	J	1304	35/35	0.69	0.26	91,159,172,173	0
14	BCR	A	4003	40/40	0.75	0.39	69,111,146,146	0
14	BCR	B	4009	40/40	0.77	0.27	72,103,147,151	0
15	CLA	K	1402	46/65	0.79	0.30	163,187,214,221	0
16	LMU	B	1301	35/35	0.82	0.21	120,136,148,154	0
14	BCR	A	4008	40/40	0.82	0.29	67,93,105,115	0
14	BCR	J	4013	40/40	0.82	0.29	78,97,112,121	0
15	CLA	B	1207	46/65	0.82	0.40	118,164,185,189	0
14	BCR	B	4005	40/40	0.83	0.27	73,93,125,128	0
15	CLA	A	1135	55/65	0.83	0.26	70,98,132,135	0
14	BCR	B	4006	40/40	0.84	0.22	86,109,141,142	0
12	LHG	A	5005	36/49	0.84	0.35	103,143,182,188	0
15	CLA	B	1212	45/65	0.84	0.19	101,117,128,143	0
17	LMG	B	5002	55/55	0.84	0.29	71,101,130,137	0
12	LHG	B	5004	49/49	0.85	0.24	59,88,99,106	0
15	CLA	A	1114	49/65	0.85	0.36	98,124,137,150	0
15	CLA	A	1133	46/65	0.85	0.29	86,103,118,128	0
14	BCR	A	4001	40/40	0.86	0.23	111,127,138,140	0
15	CLA	B	1210	65/65	0.86	0.26	75,95,108,120	0
13	CL0	A	1108	45/65	0.87	0.23	86,113,154,170	0
12	LHG	A	5003	49/49	0.87	0.30	91,121,142,143	0
15	CLA	J	1303	46/65	0.87	0.35	94,114,141,159	0
15	CLA	A	1110	54/65	0.87	0.22	96,121,150,154	0
15	CLA	A	1113	45/65	0.88	0.23	112,129,158,162	0
15	CLA	A	1118	46/65	0.88	0.22	99,113,135,154	0
15	CLA	A	1134	46/65	0.88	0.24	109,127,151,186	0
15	CLA	A	1111	60/65	0.88	0.24	78,96,107,112	0
15	CLA	A	1119	64/65	0.88	0.27	78,97,115,137	0
15	CLA	A	1124	55/65	0.88	0.27	61,92,120,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	B	1214	65/65	0.88	0.24	72,89,119,133	0
15	CLA	A	1116	54/65	0.89	0.37	84,113,130,141	0
15	CLA	B	1213	50/65	0.89	0.16	89,104,128,136	0
15	CLA	J	1302	45/65	0.89	0.30	82,93,138,150	0
15	CLA	B	1224	65/65	0.89	0.26	60,78,98,108	0
15	CLA	B	1216	65/65	0.89	0.18	67,91,106,118	0
11	SF4	C	3002	8/8	0.89	0.20	60,88,151,152	0
15	CLA	B	1221	65/65	0.90	0.19	68,79,105,125	0
15	CLA	A	1123	65/65	0.90	0.27	75,88,98,104	0
15	CLA	A	1105	65/65	0.90	0.21	70,96,111,120	0
15	CLA	B	1208	45/65	0.90	0.19	88,114,130,140	0
15	CLA	A	1112	45/65	0.90	0.18	89,115,127,130	0
15	CLA	A	1801	52/65	0.90	0.43	100,122,154,158	0
15	CLA	A	1103	65/65	0.90	0.24	61,80,108,118	0
15	CLA	A	1132	62/65	0.90	0.24	74,105,153,156	0
15	CLA	A	1129	46/65	0.91	0.21	76,92,115,151	0
15	CLA	B	1217	47/65	0.91	0.25	96,114,132,157	0
14	BCR	F	4015	40/40	0.91	0.22	52,73,107,111	0
15	CLA	B	1231	65/65	0.91	0.22	66,89,115,138	0
15	CLA	A	1128	65/65	0.91	0.20	54,74,90,101	0
10	PQN	B	2002	33/33	0.91	0.25	59,79,99,105	0
15	CLA	A	1120	49/65	0.91	0.19	101,116,140,156	0
15	CLA	B	1211	46/65	0.91	0.17	90,106,116,133	0
14	BCR	A	4002	40/40	0.92	0.21	88,109,128,130	0
15	CLA	B	1203	65/65	0.92	0.22	62,83,99,104	0
15	CLA	F	1410	65/65	0.92	0.23	69,96,135,147	0
15	CLA	B	1218	51/65	0.92	0.21	86,98,125,159	0
15	CLA	B	1232	45/65	0.92	0.17	72,89,109,115	0
14	BCR	B	4010	40/40	0.92	0.21	55,74,102,113	0
14	BCR	F	4016	40/40	0.92	0.16	59,72,89,94	0
15	CLA	A	1102	65/65	0.92	0.17	55,81,107,112	0
15	CLA	B	1228	65/65	0.92	0.18	54,74,105,114	0
15	CLA	B	1201	46/65	0.92	0.21	72,83,107,123	0
15	CLA	A	1022	65/65	0.92	0.25	53,78,96,103	0
15	CLA	B	1023	65/65	0.92	0.24	55,79,111,119	0
15	CLA	B	1222	56/65	0.93	0.21	52,66,101,108	0
15	CLA	A	1101	65/65	0.93	0.17	55,73,89,96	0
15	CLA	A	1136	65/65	0.93	0.26	78,105,139,142	0
15	CLA	B	1226	65/65	0.93	0.20	54,79,133,144	0
15	CLA	A	1125	52/65	0.93	0.29	76,98,124,133	0
15	CLA	B	1227	45/65	0.93	0.16	54,72,94,98	0
15	CLA	B	1202	65/65	0.93	0.20	67,82,99,106	0

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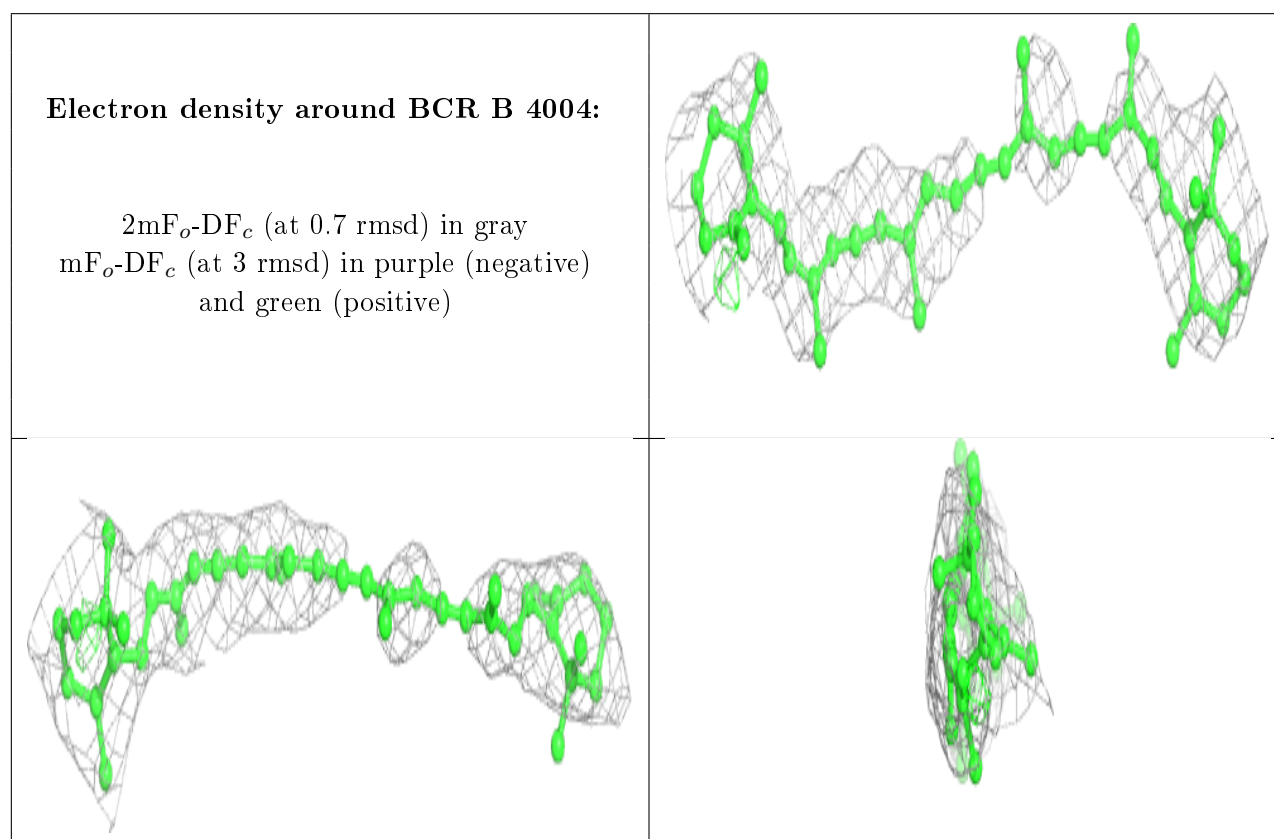
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	F	1139	65/65	0.93	0.22	47,58,90,98	0
15	CLA	B	1223	65/65	0.93	0.22	59,77,94,98	0
15	CLA	B	1219	55/65	0.93	0.19	74,86,119,142	0
15	CLA	A	1109	65/65	0.93	0.18	66,81,105,112	0
14	BCR	B	4014	40/40	0.93	0.19	46,62,88,89	0
15	CLA	B	1234	65/65	0.93	0.21	56,73,108,120	0
11	SF4	A	3001	8/8	0.93	0.23	50,62,210,290	0
15	CLA	A	1122	65/65	0.93	0.19	74,91,119,129	0
15	CLA	B	1240	45/65	0.93	0.30	71,83,124,151	0
15	CLA	A	1127	65/65	0.93	0.42	67,79,100,106	0
15	CLA	A	1131	55/65	0.94	0.26	78,107,126,140	0
10	PQN	A	2001	33/33	0.94	0.20	45,57,68,74	0
15	CLA	A	1138	65/65	0.94	0.22	47,55,69,77	0
15	CLA	B	1236	50/65	0.94	0.20	52,72,106,114	0
15	CLA	B	1237	55/65	0.94	0.19	71,82,117,132	0
15	CLA	B	1204	46/65	0.94	0.17	79,96,115,137	0
15	CLA	B	1238	44/65	0.94	0.13	68,80,92,111	0
15	CLA	B	1220	56/65	0.94	0.15	61,77,111,119	0
15	CLA	B	1013	65/65	0.94	0.22	46,53,77,89	0
15	CLA	A	1115	46/65	0.94	0.21	109,129,140,151	0
13	CL0	A	1011	65/65	0.94	0.20	51,69,81,99	0
14	BCR	B	4011	40/40	0.94	0.26	49,67,84,91	0
14	BCR	A	4012	40/40	0.94	0.18	55,77,87,91	0
15	CLA	A	1121	46/65	0.94	0.25	91,114,141,163	0
15	CLA	A	1137	50/65	0.94	0.18	72,94,128,134	0
15	CLA	F	1301	45/65	0.94	0.16	54,75,97,131	0
15	CLA	A	1104	65/65	0.94	0.23	58,72,83,96	0
15	CLA	B	1235	65/65	0.94	0.16	55,66,85,92	0
12	LHG	A	5001	49/49	0.94	0.20	49,70,91,100	0
15	CLA	A	1106	65/65	0.94	0.20	59,79,98,109	0
15	CLA	B	1215	65/65	0.94	0.31	72,85,104,106	0
15	CLA	A	1126	65/65	0.94	0.23	63,80,101,116	0
14	BCR	B	4017	40/40	0.95	0.18	70,87,101,104	0
15	CLA	A	1117	65/65	0.95	0.43	80,100,111,113	0
15	CLA	B	1206	46/65	0.95	0.18	78,100,119,149	0
18	CL	B	6000	1/1	0.95	0.12	82,82,82,82	0
15	CLA	A	1012	65/65	0.95	0.27	47,60,86,93	0
15	CLA	B	1230	65/65	0.95	0.17	53,68,118,125	0
15	CLA	B	1225	65/65	0.95	0.29	66,80,100,104	0
15	CLA	B	1021	65/65	0.95	0.26	49,69,80,84	0
15	CLA	A	1140	65/65	0.96	0.22	52,73,103,116	0
15	CLA	B	1239	46/65	0.96	0.21	62,78,107,141	0

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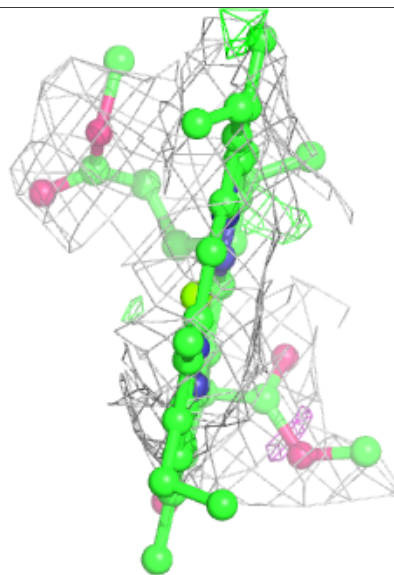
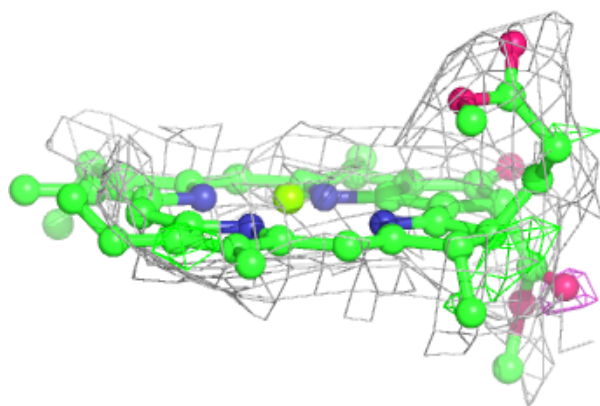
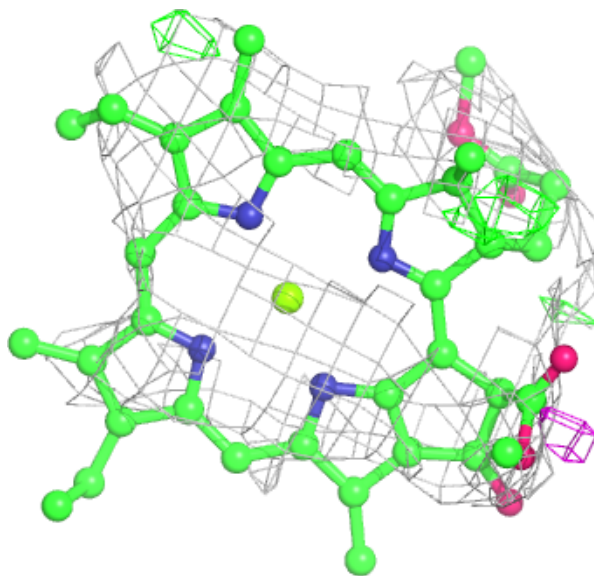
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	B	1229	65/65	0.96	0.17	50,62,86,107	0
15	CLA	A	1107	50/65	0.96	0.15	56,64,98,112	0
15	CLA	A	1130	55/65	0.96	0.20	82,106,133,139	0
15	CLA	B	1205	55/65	0.96	0.17	68,87,100,112	0
15	CLA	B	1209	45/65	0.96	0.19	102,113,134,148	0
11	SF4	C	3003	8/8	0.97	0.19	60,67,100,115	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.



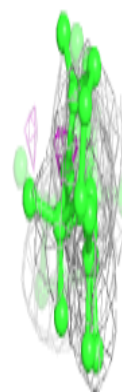
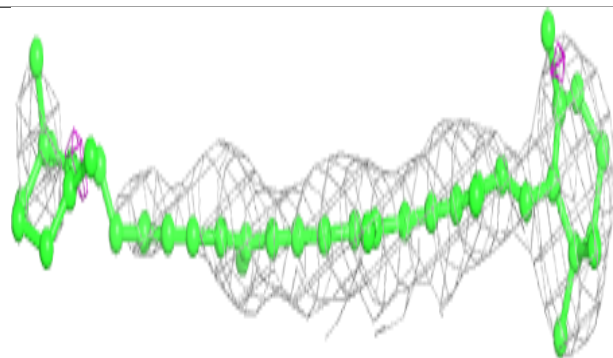
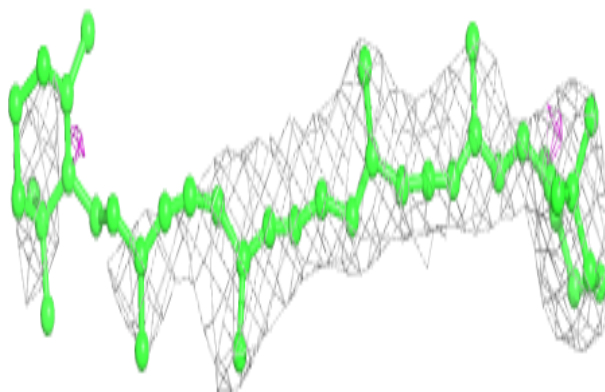
Electron density around CLA K 1401:

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

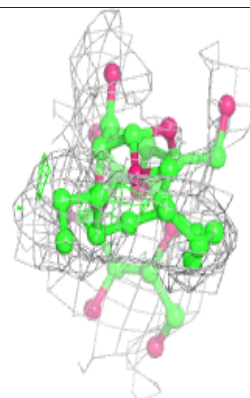
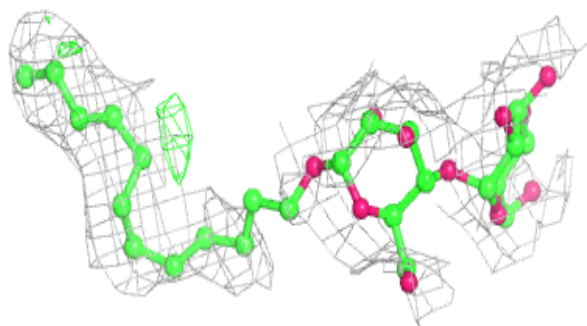
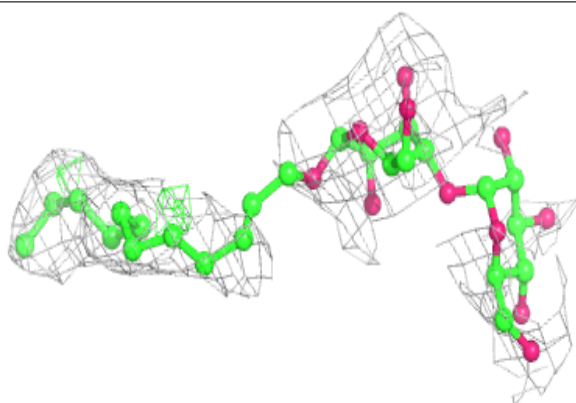


Electron density around BCR A 4007:

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

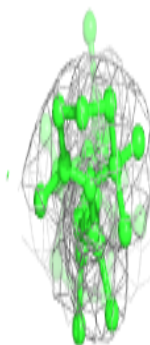
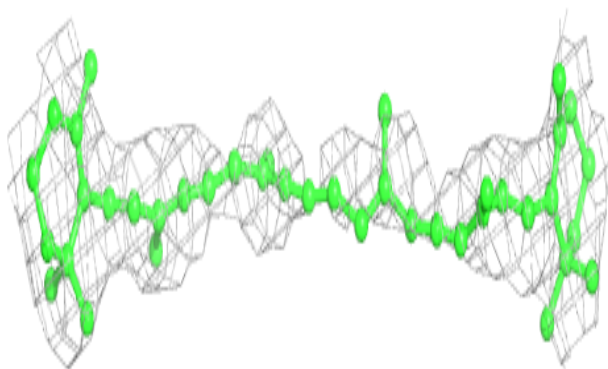
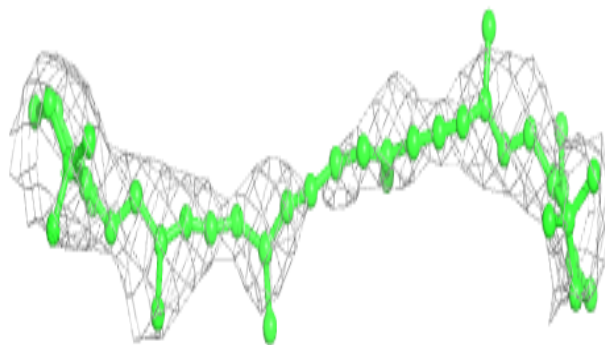
**Electron density around LMU J 1304:**

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

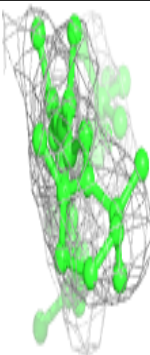
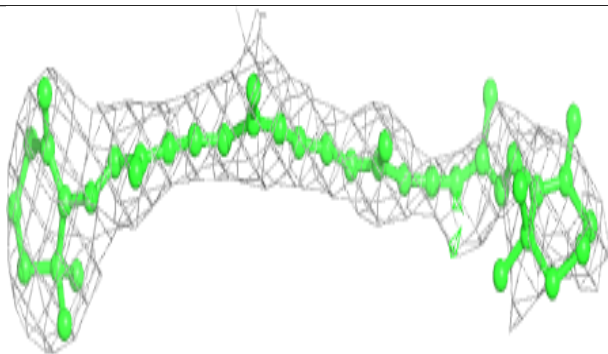
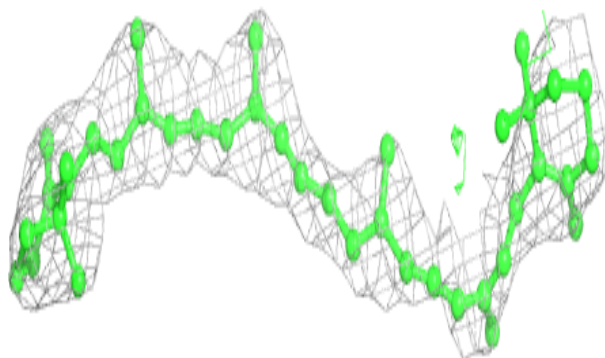


Electron density around BCR A 4003:

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

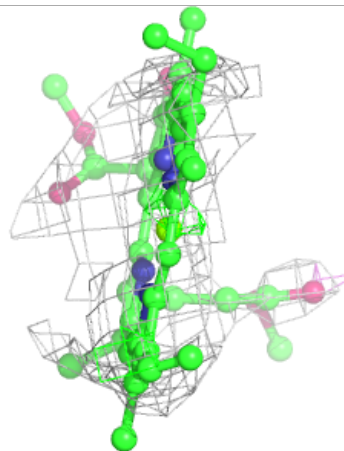
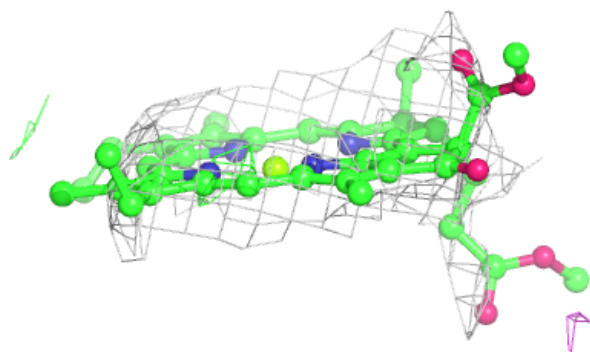
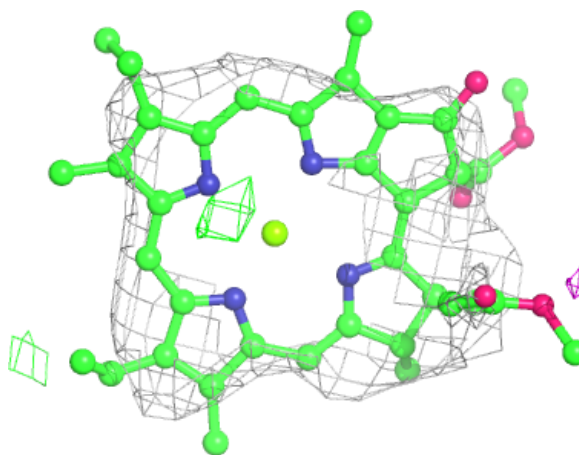
**Electron density around BCR B 4009:**

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



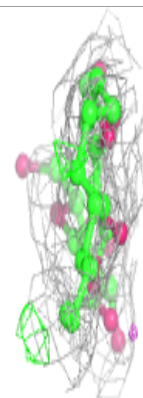
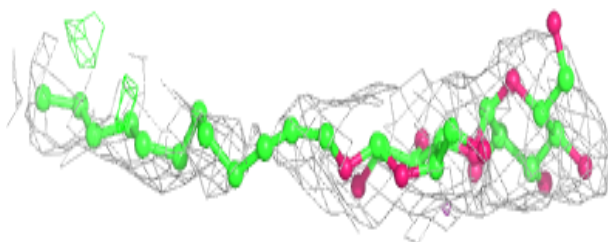
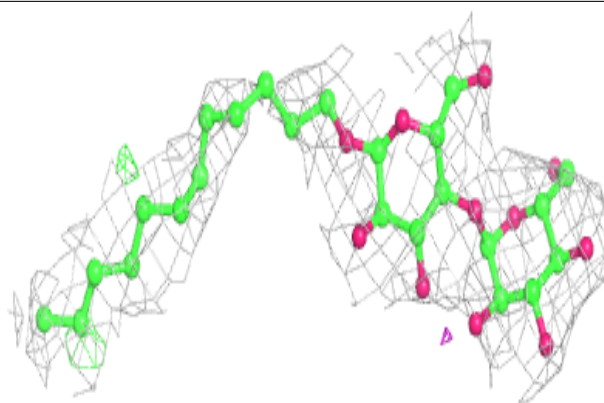
Electron density around CLA K 1402:

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

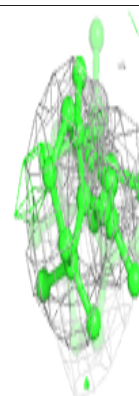
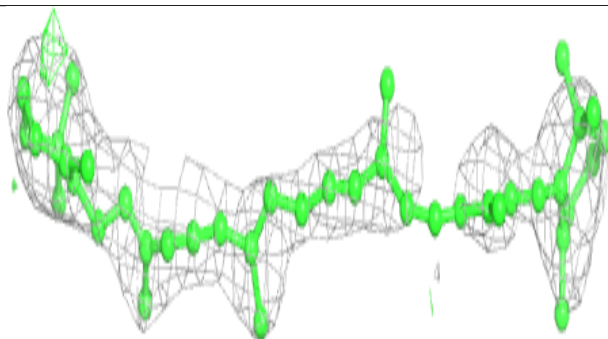
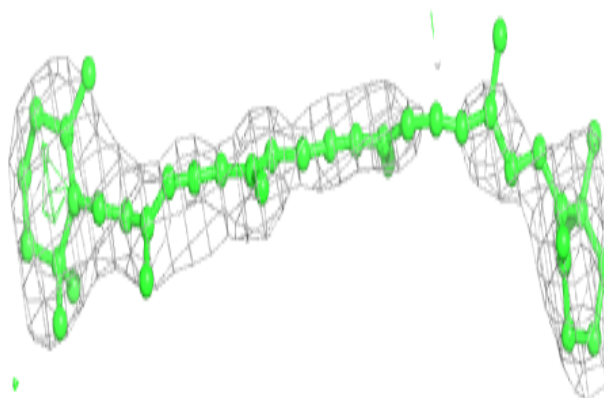


Electron density around LMU B 1301:

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

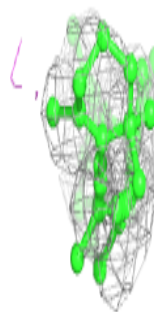
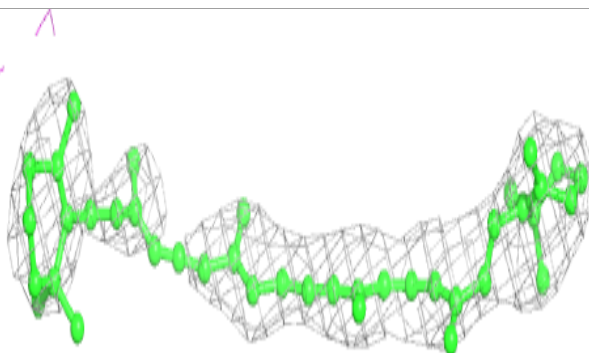
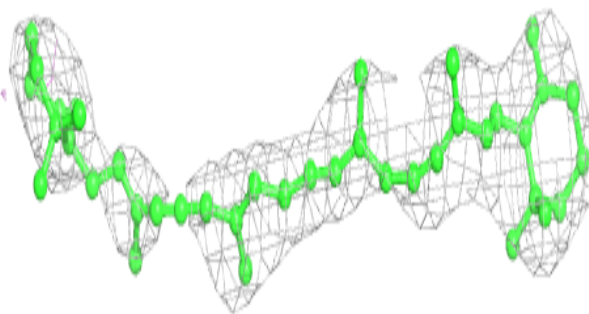
**Electron density around BCR A 4008:**

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



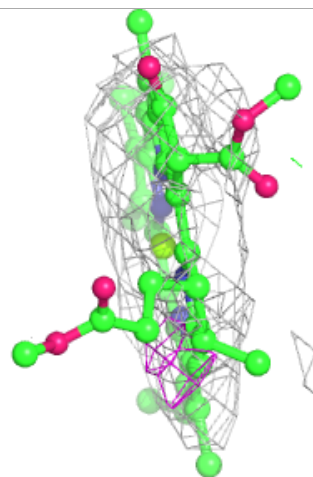
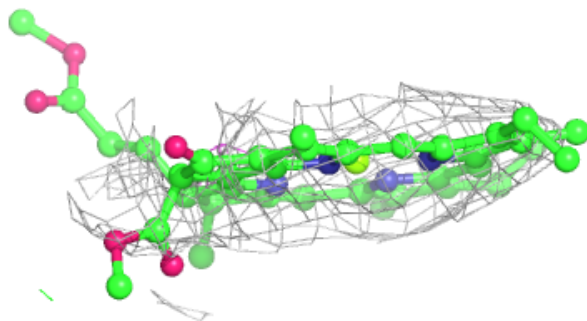
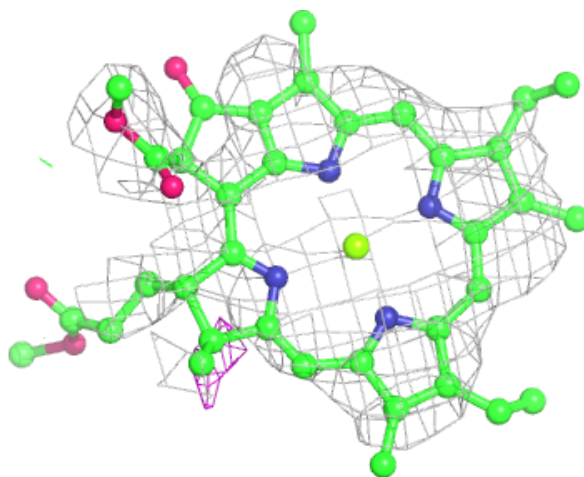
Electron density around BCR J 4013:

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



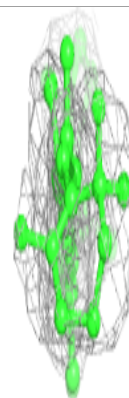
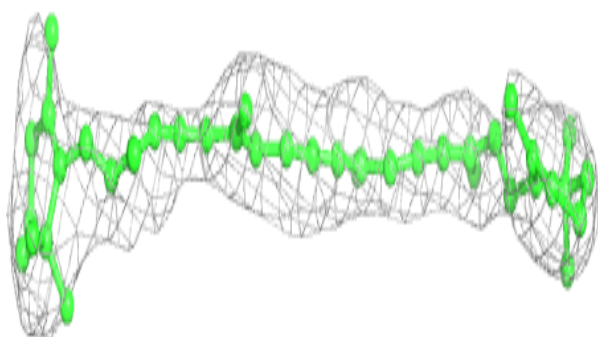
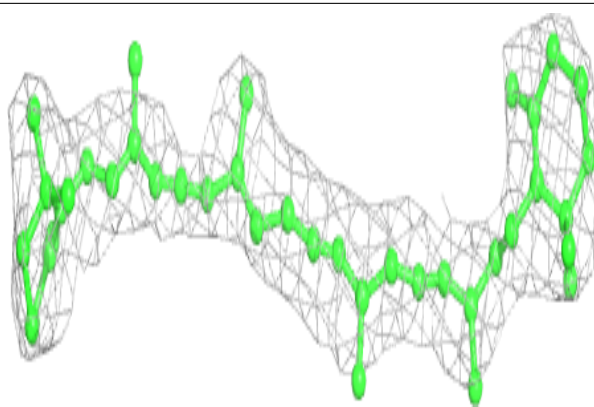
Electron density around CLA B 1207:

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

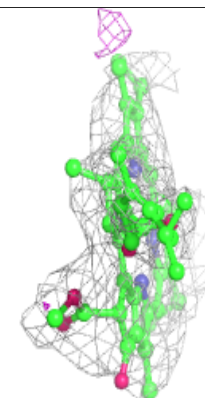
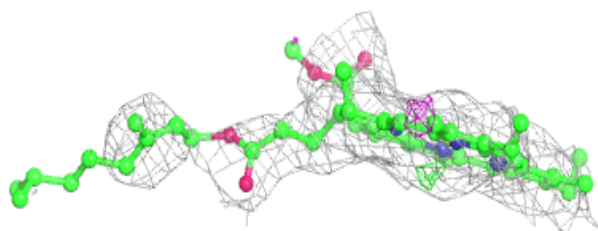
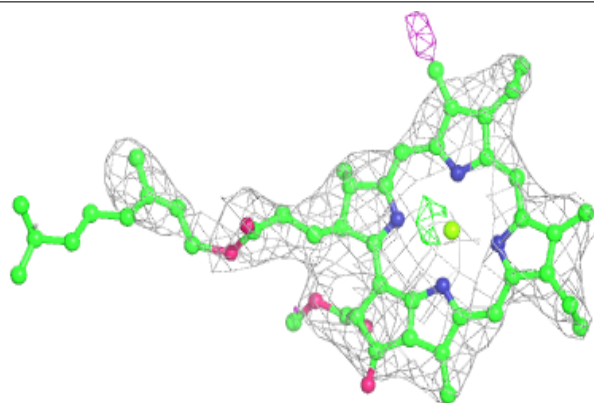


Electron density around BCR B 4005:

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

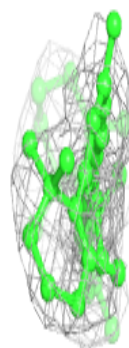
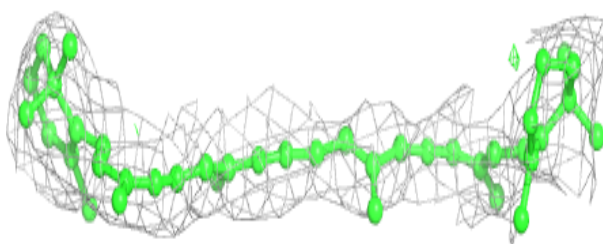
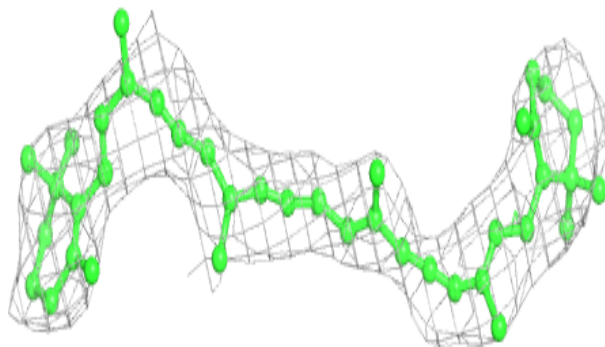
**Electron density around CLA A 1135:**

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

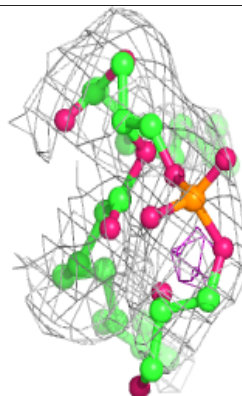
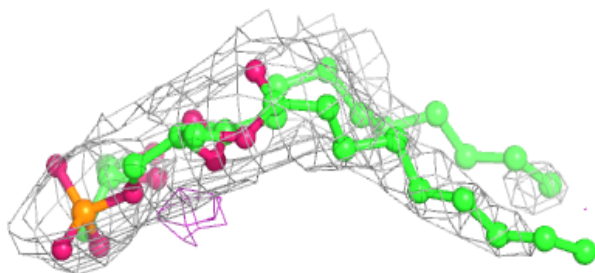
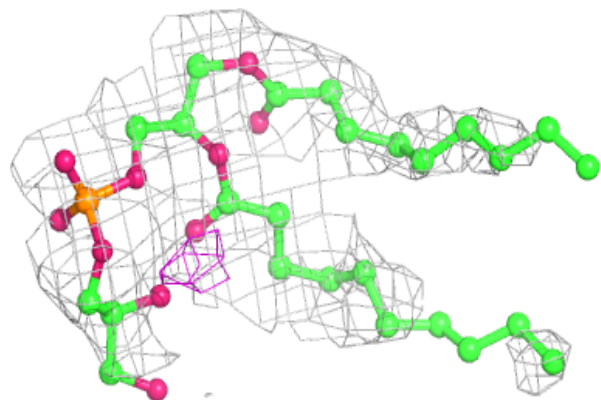


Electron density around BCR B 4006:

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

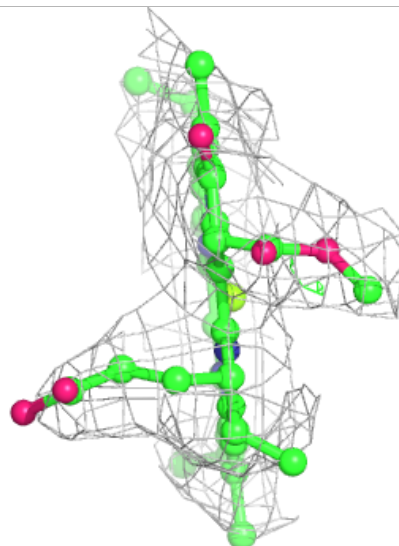
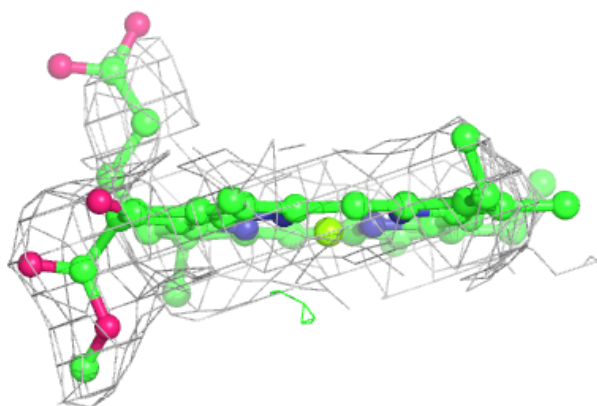
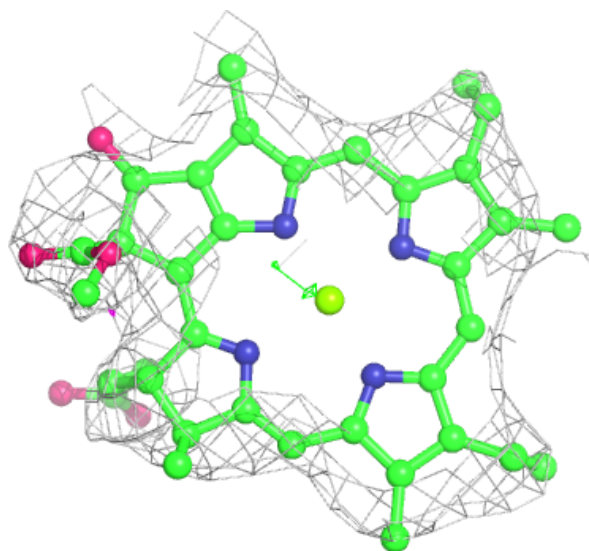
**Electron density around LHG A 5005:**

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



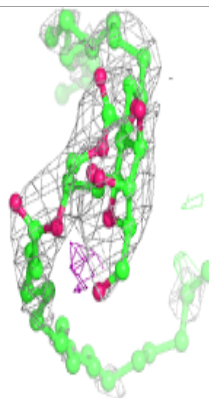
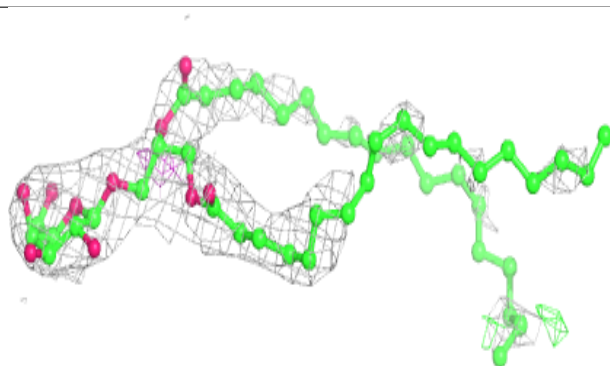
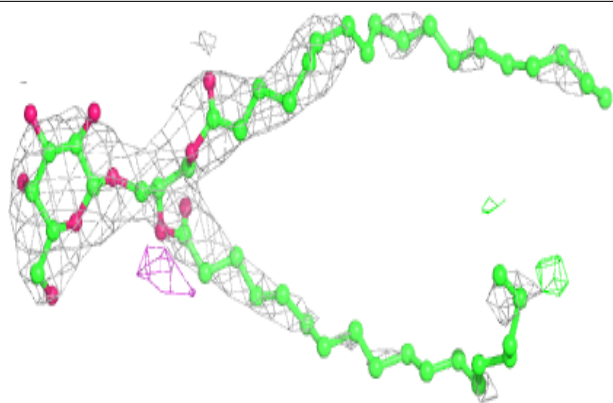
Electron density around CLA B 1212:

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



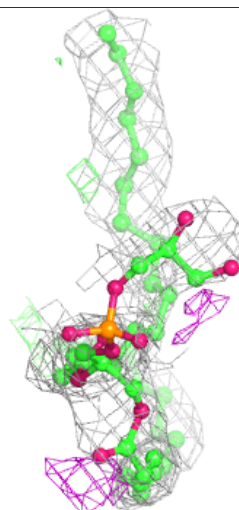
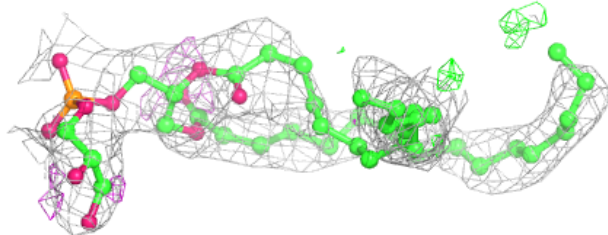
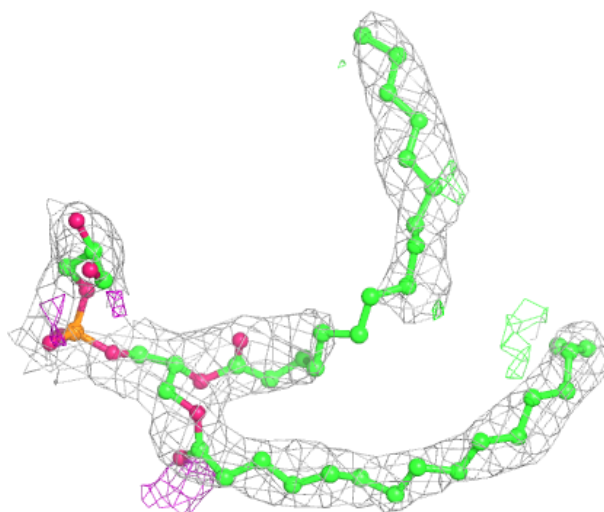
Electron density around LMG B 5002:

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



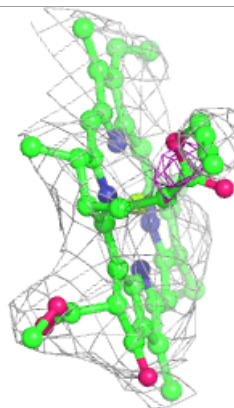
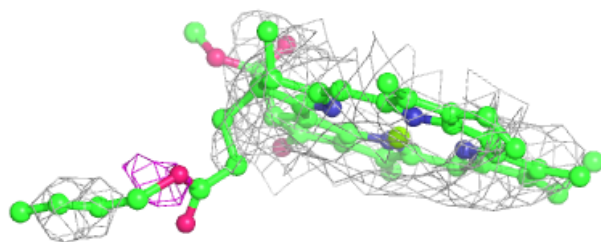
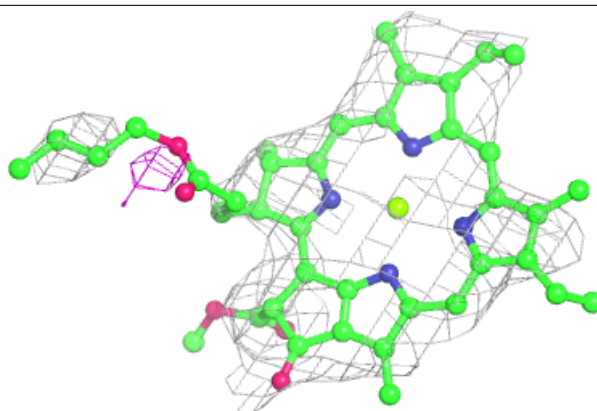
Electron density around LHG B 5004:

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



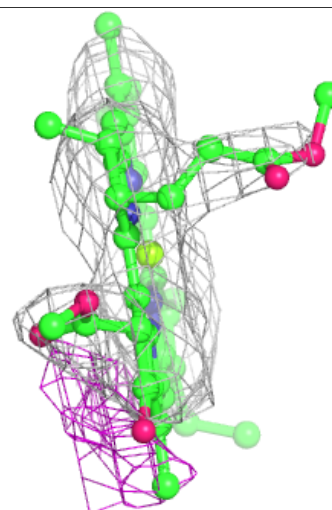
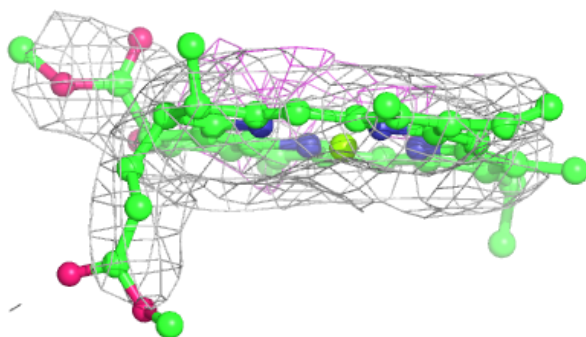
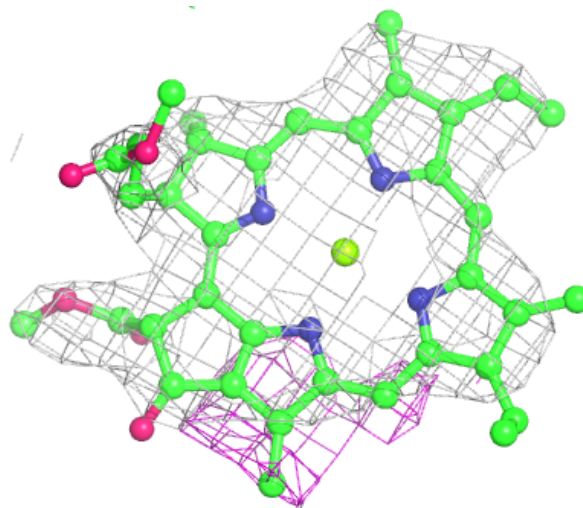
Electron density around CLA A 1114:

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



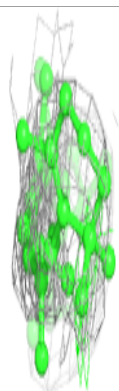
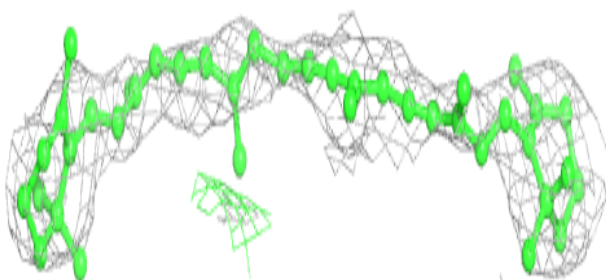
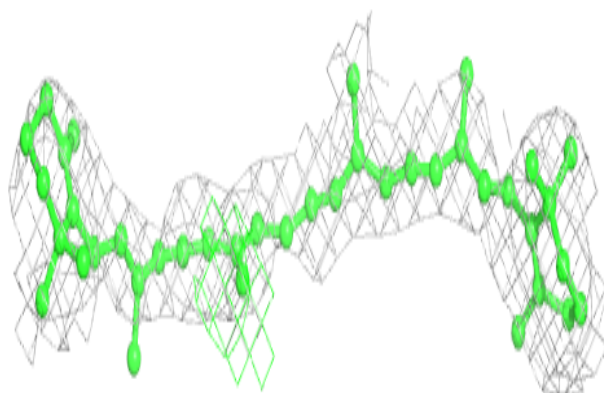
Electron density around CLA A 1133:

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

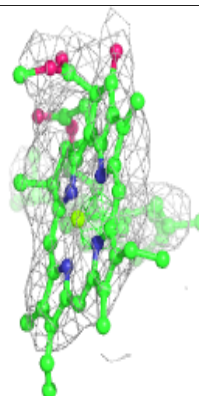
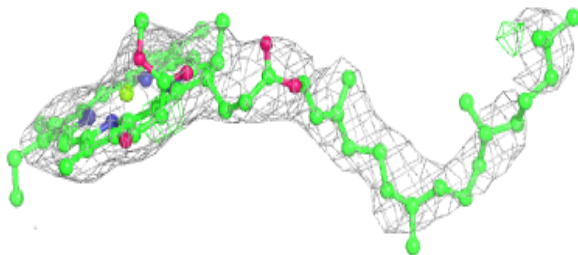
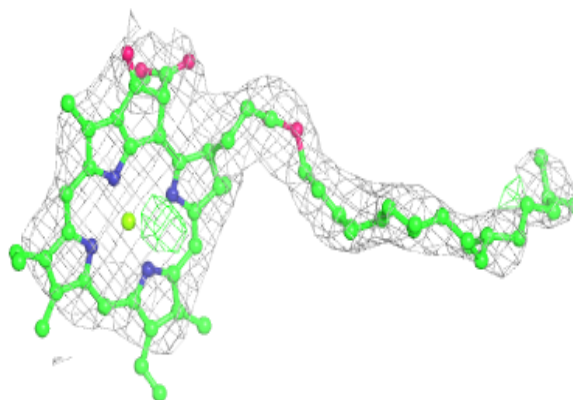


Electron density around BCR A 4001:

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

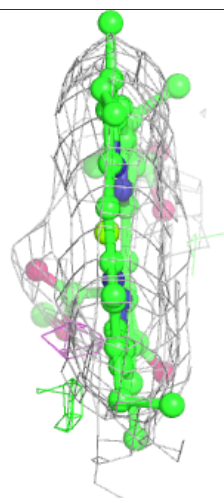
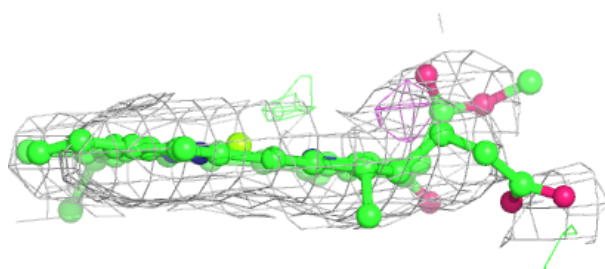
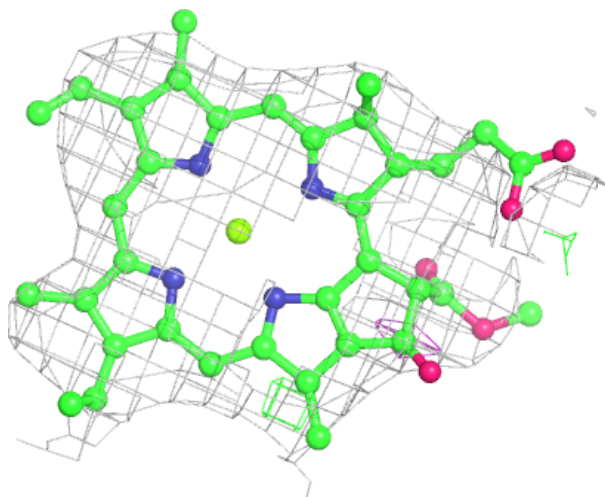
**Electron density around CLA B 1210:**

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



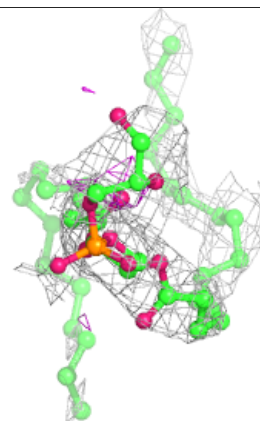
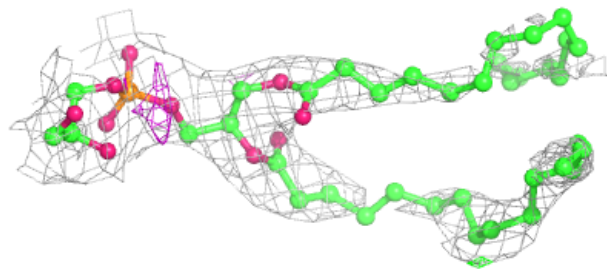
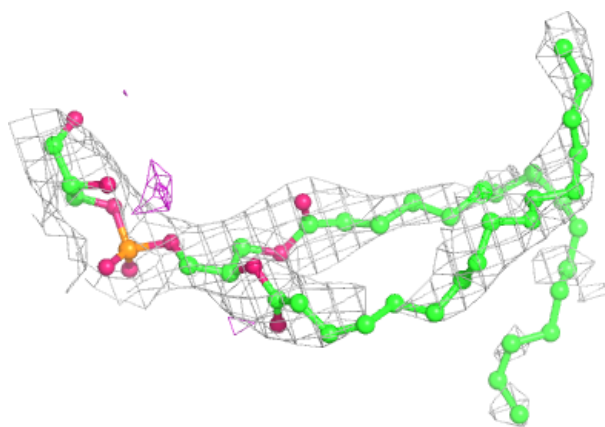
Electron density around CL0 A 1108:

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



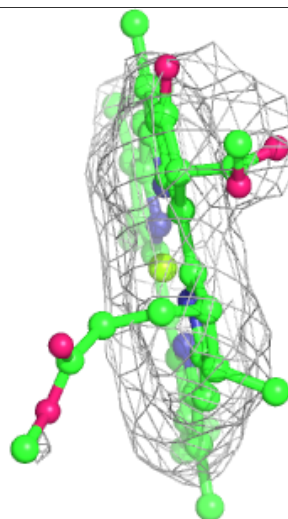
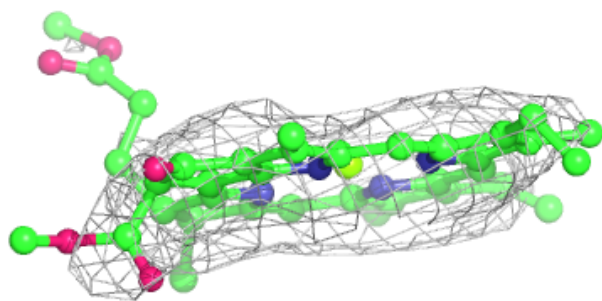
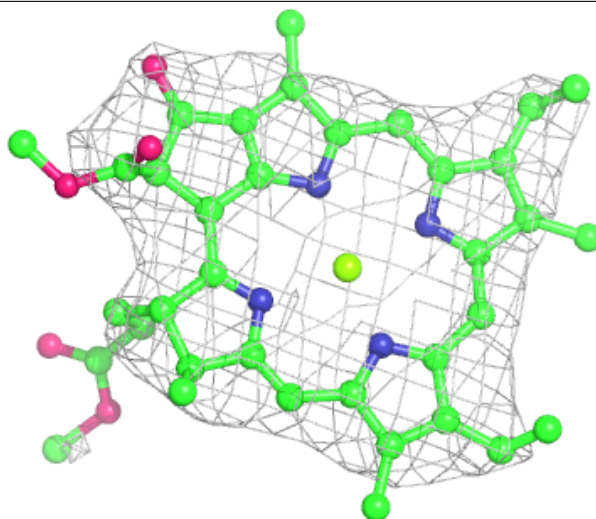
Electron density around LHG A 5003:

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



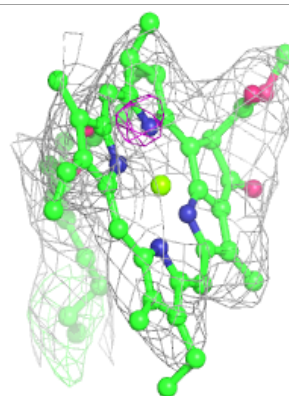
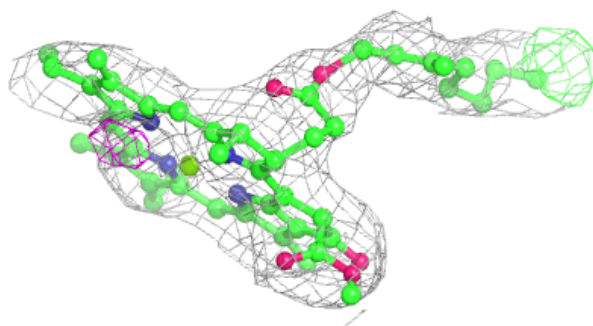
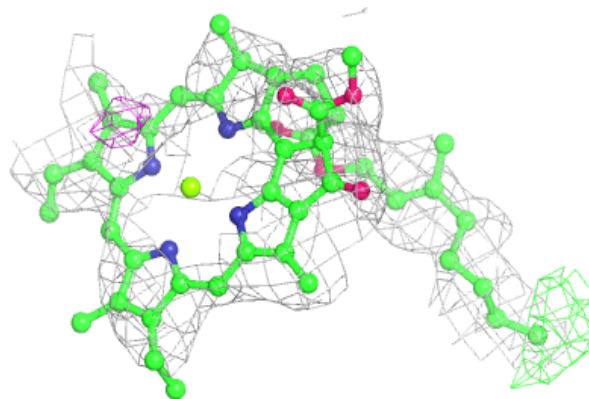
Electron density around CLA J 1303:

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



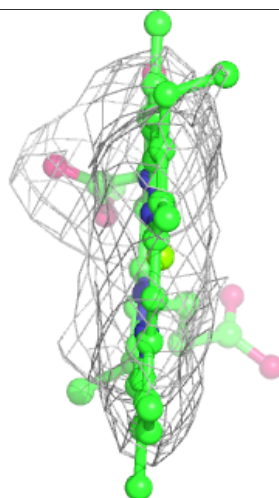
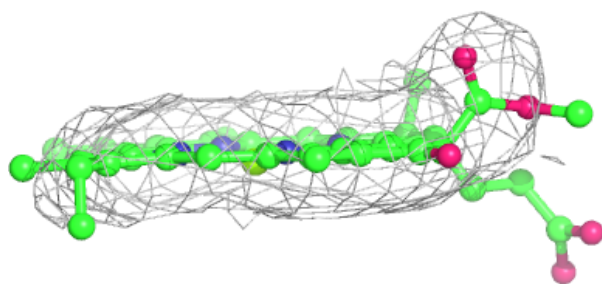
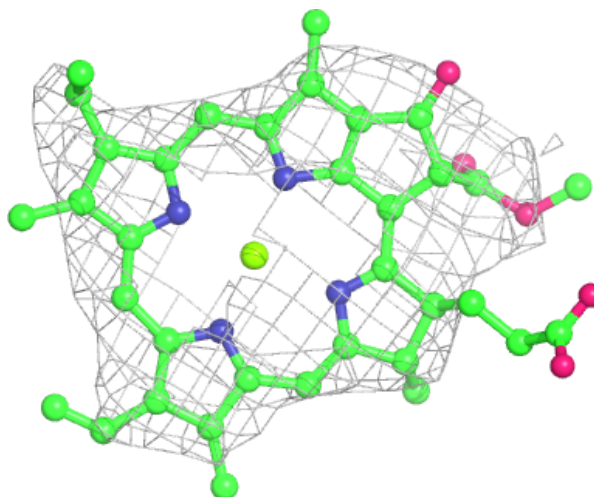
Electron density around CLA A 1110:

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



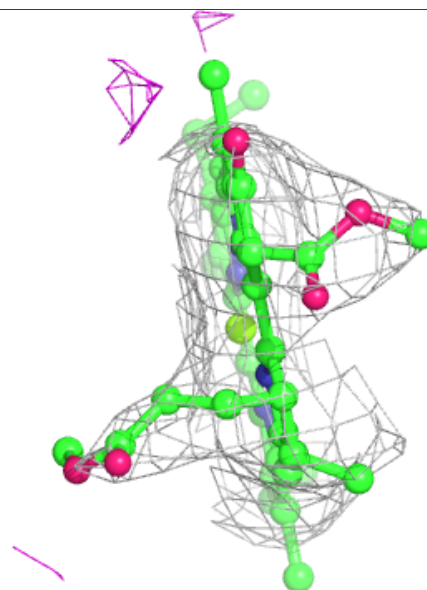
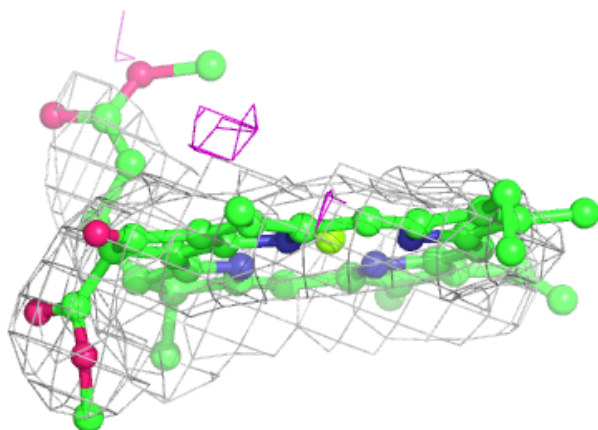
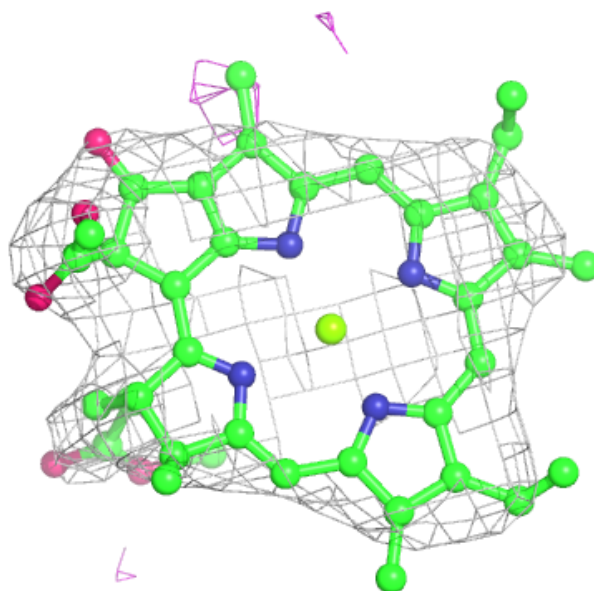
Electron density around CLA A 1113:

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



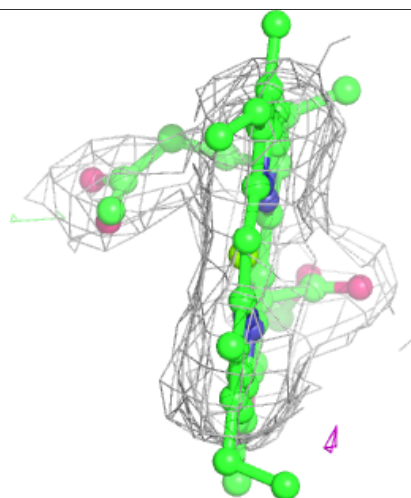
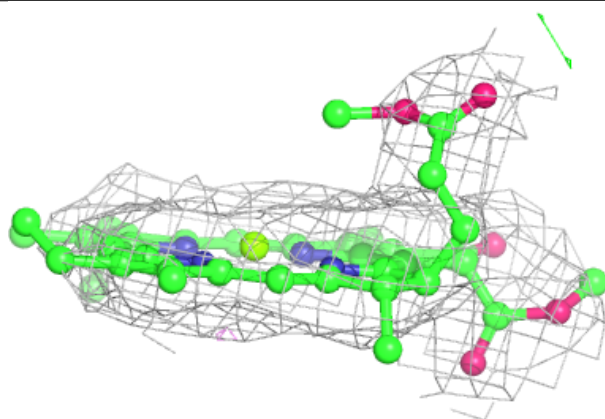
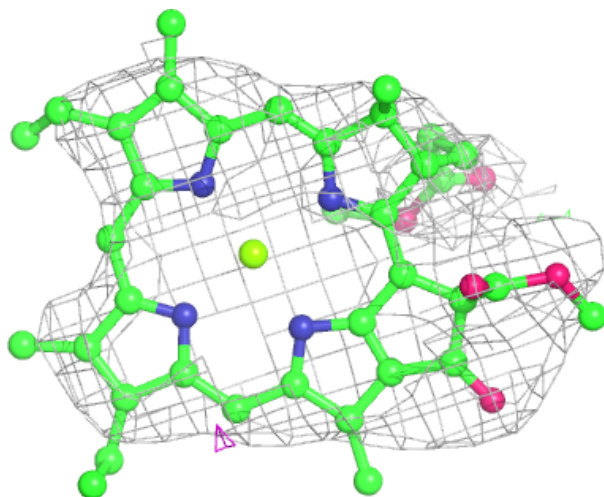
Electron density around CLA A 1118:

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



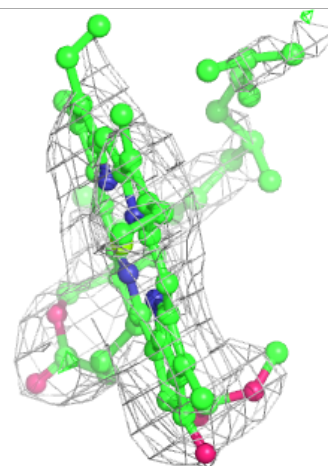
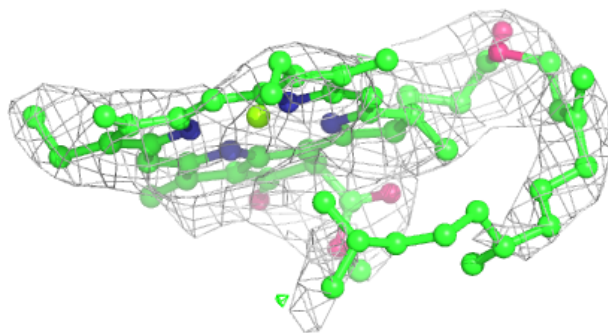
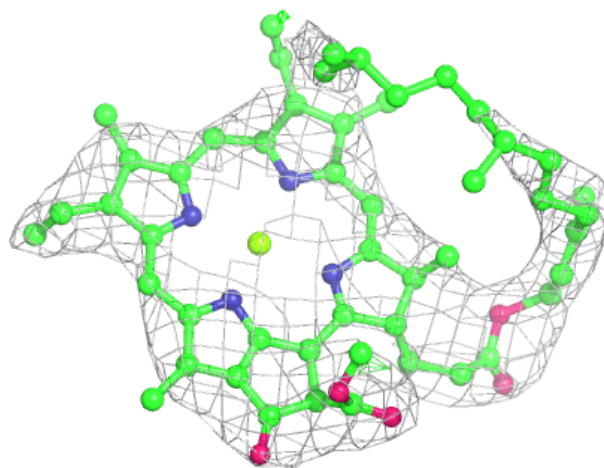
Electron density around CLA A 1134:

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



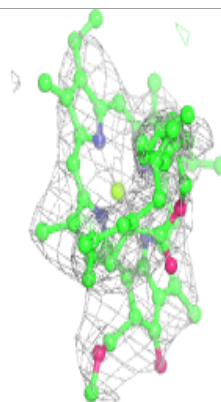
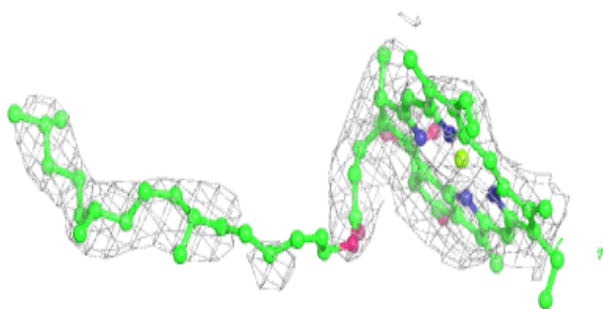
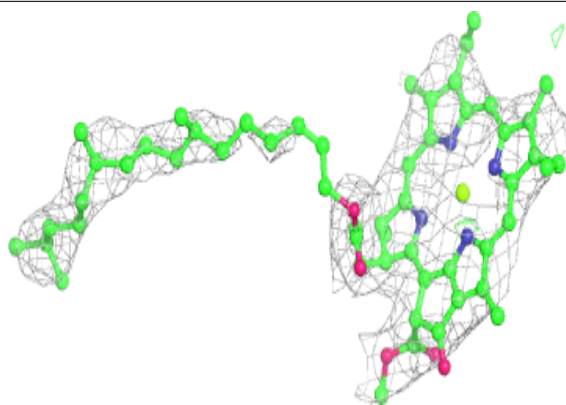
Electron density around CLA A 1111:

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

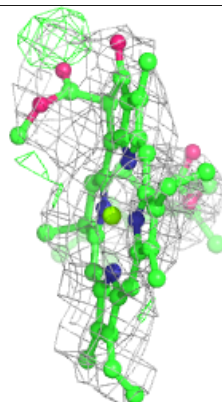
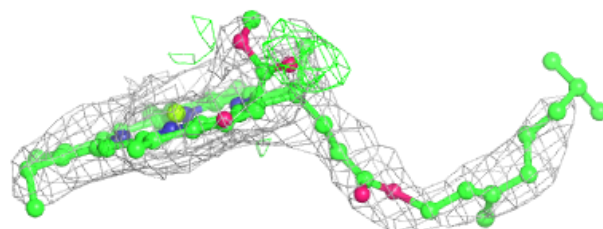
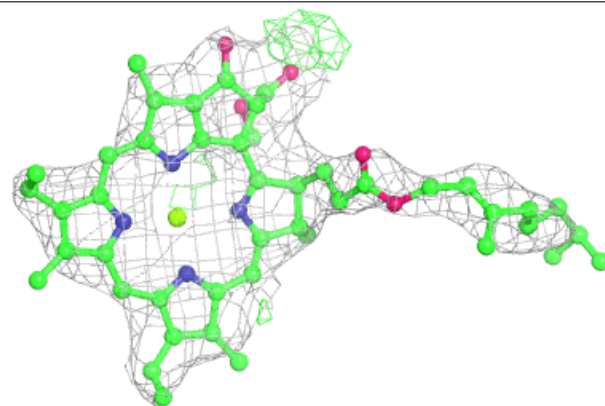


Electron density around CLA A 1119:

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

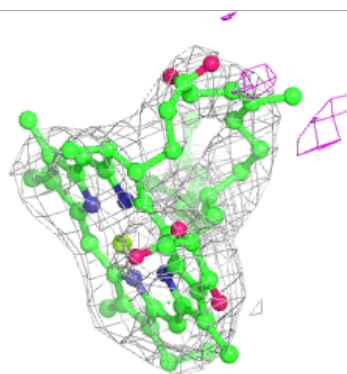
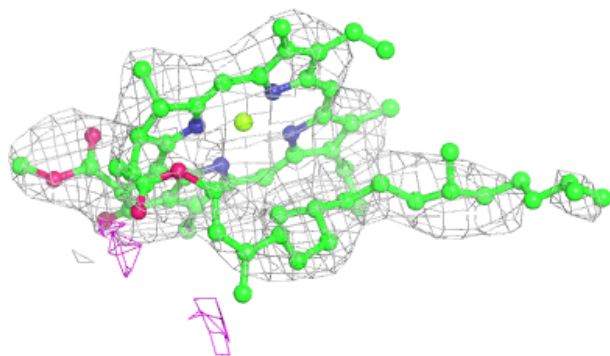
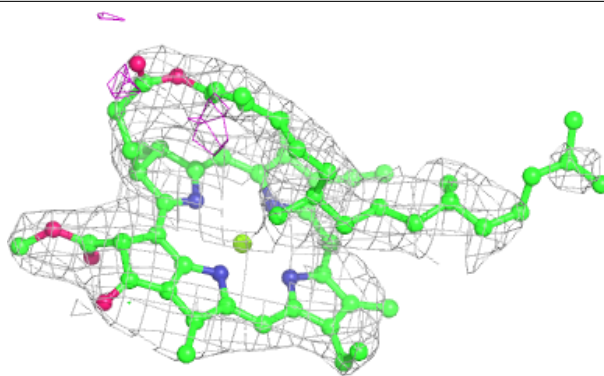
**Electron density around CLA A 1124:**

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

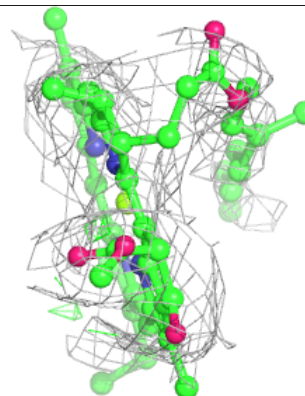
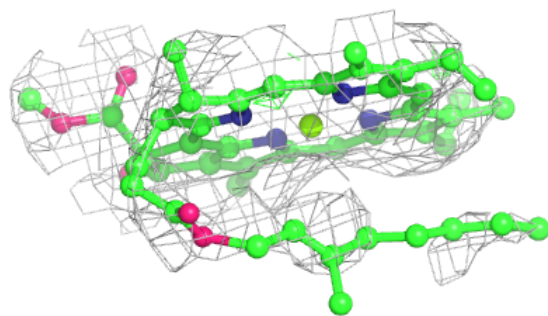
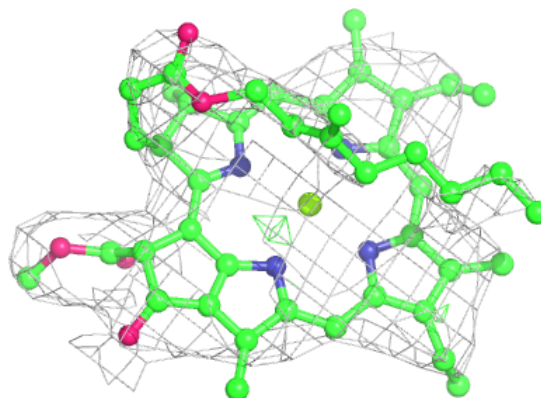


Electron density around CLA B 1214:

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

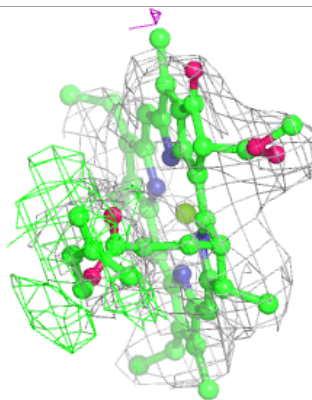
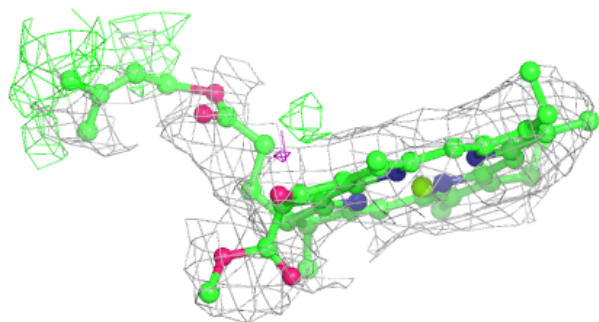
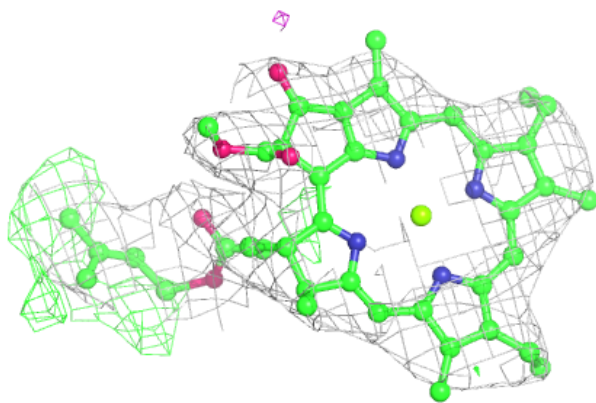
**Electron density around CLA A 1116:**

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



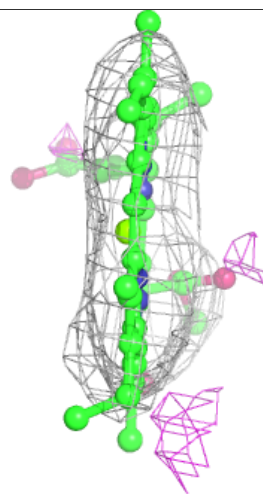
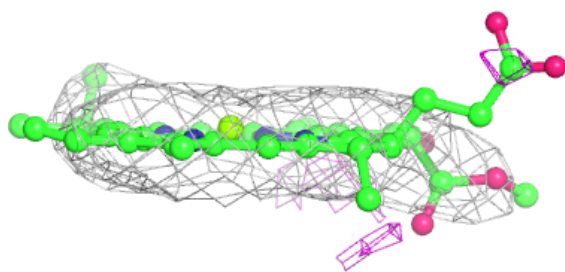
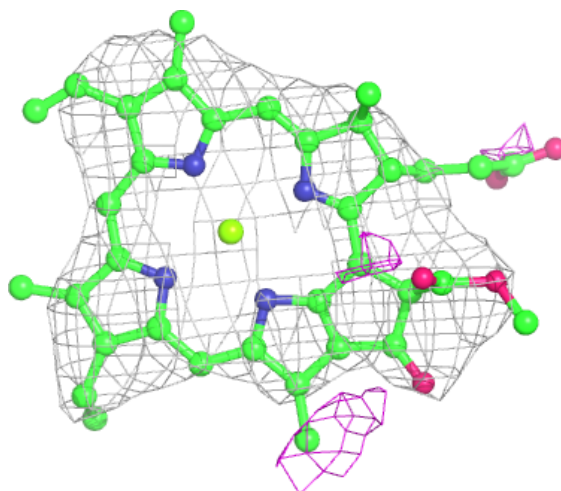
Electron density around CLA B 1213:

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



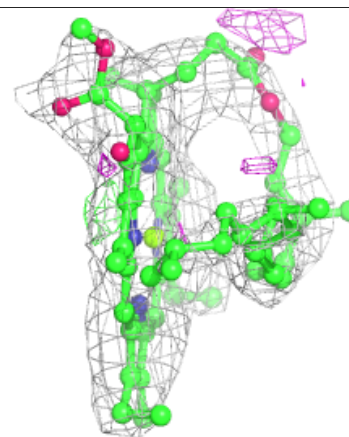
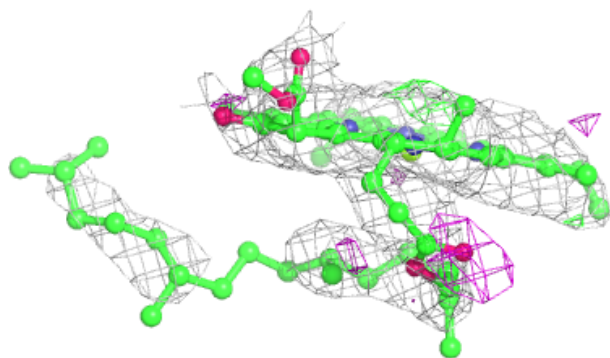
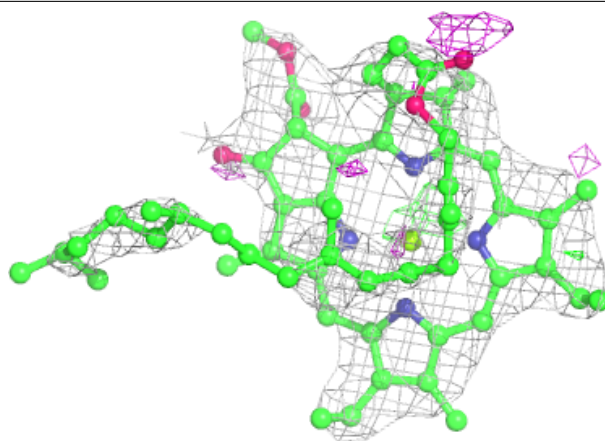
Electron density around CLA J 1302:

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



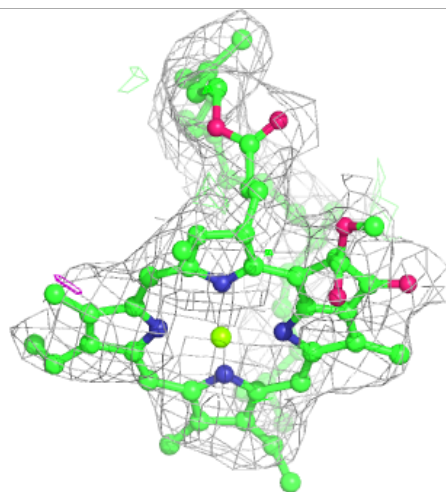
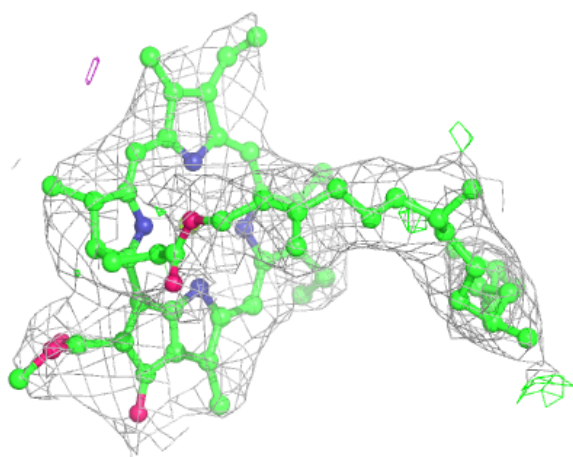
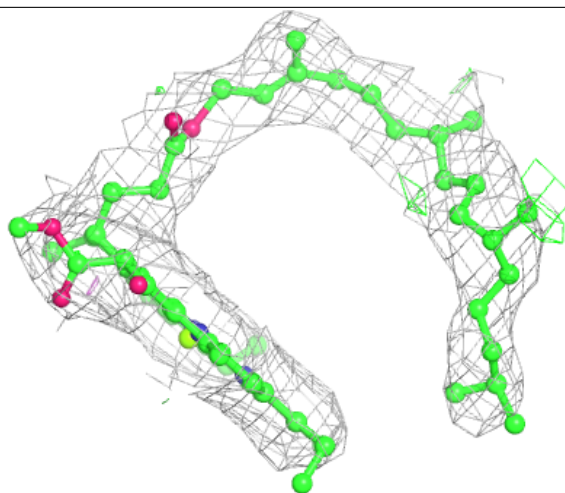
Electron density around CLA B 1224:

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



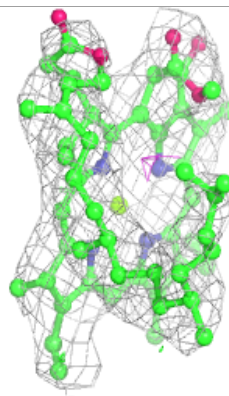
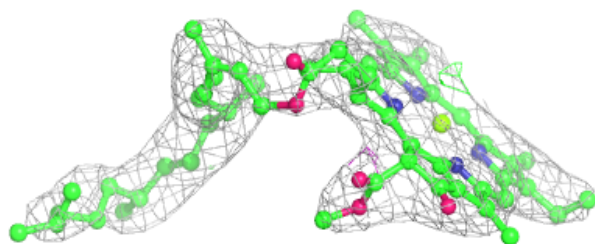
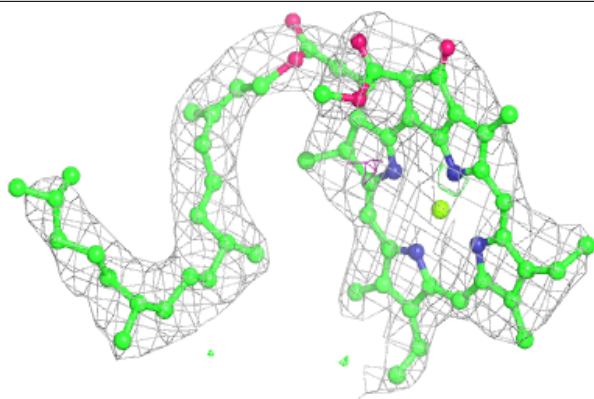
Electron density around CLA B 1216:

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



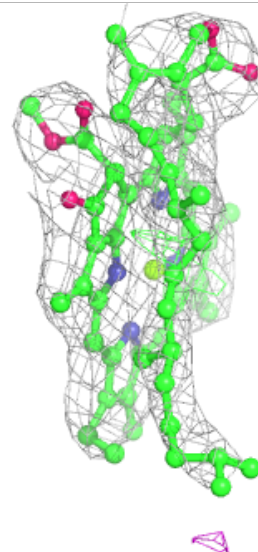
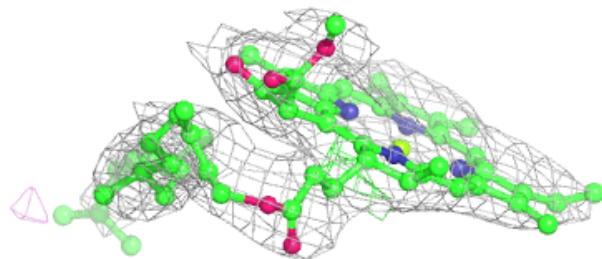
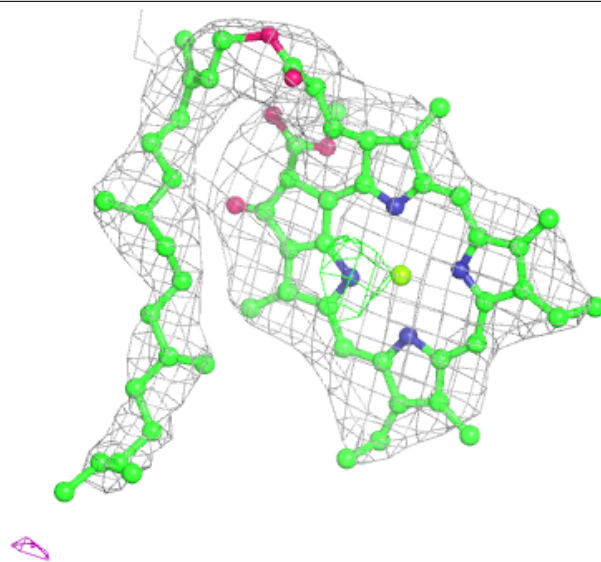
Electron density around CLA B 1221:

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



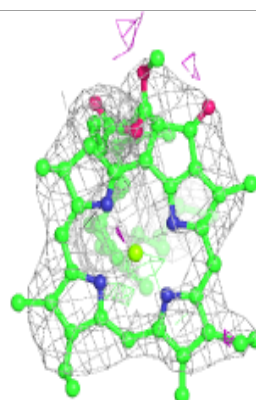
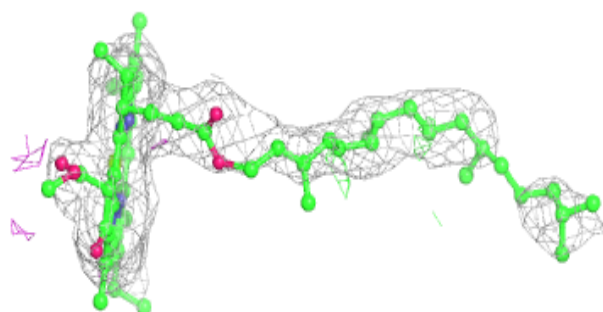
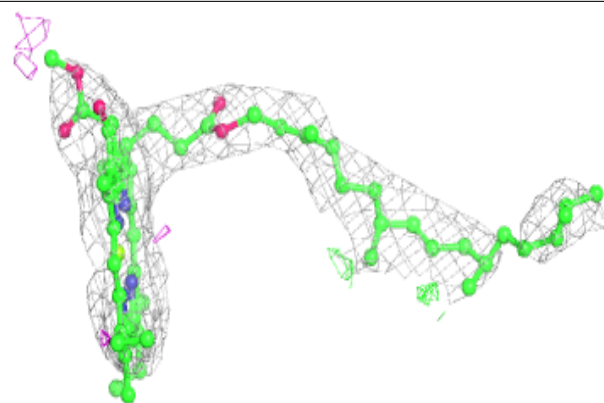
Electron density around CLA A 1123:

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

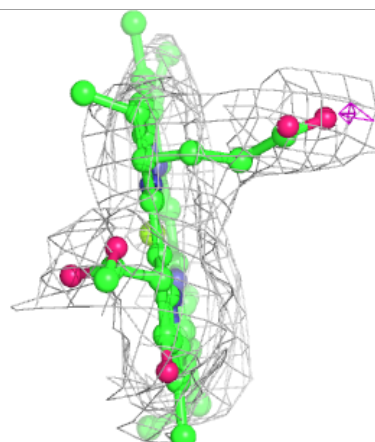
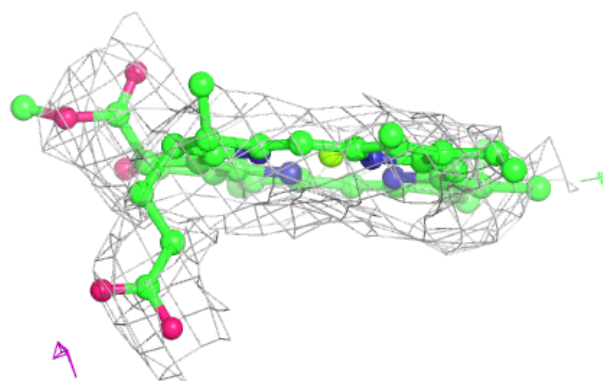
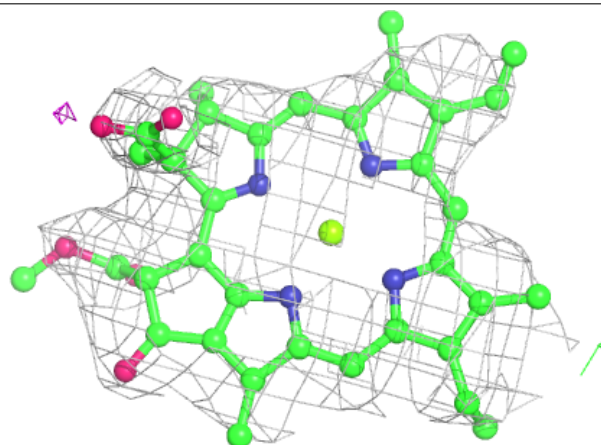


Electron density around CLA A 1105:

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

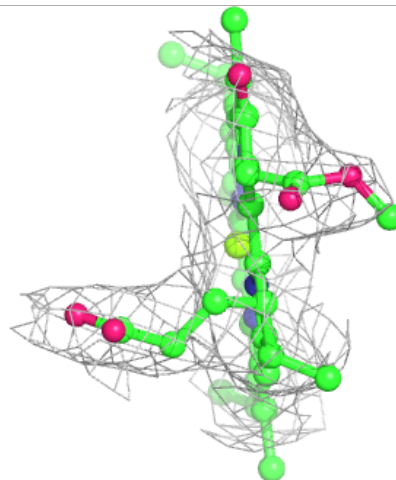
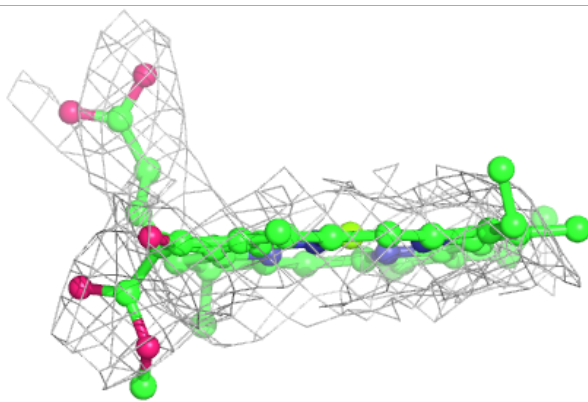
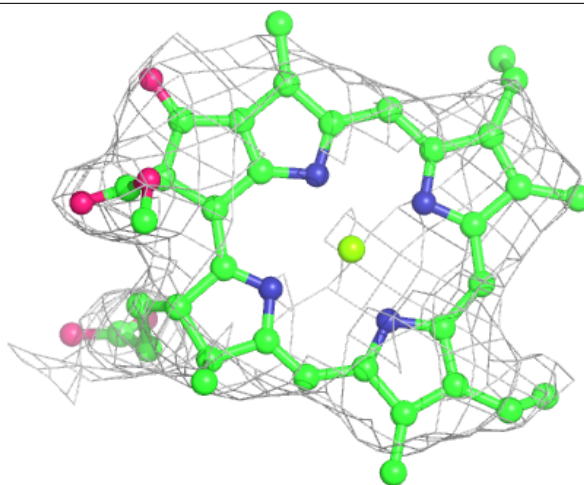
**Electron density around CLA B 1208:**

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



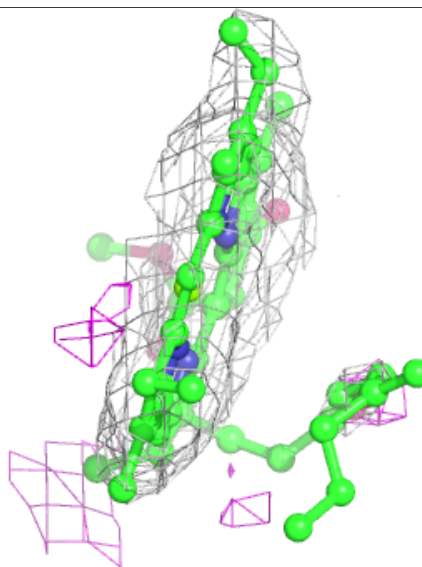
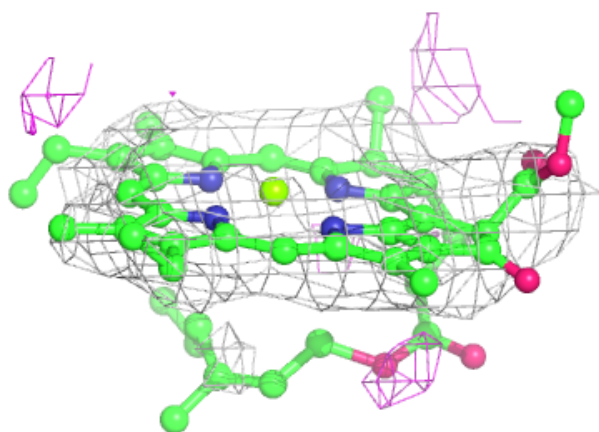
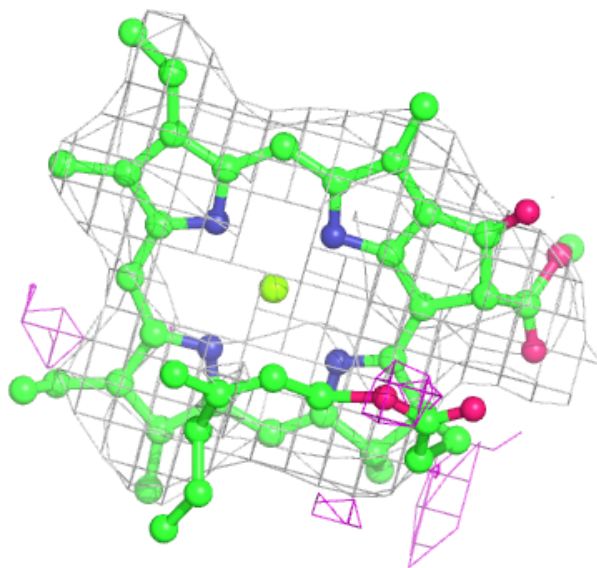
Electron density around CLA A 1112:

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



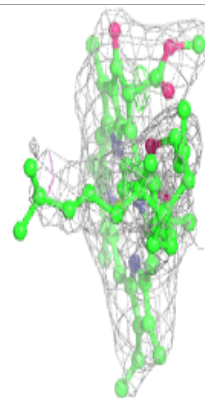
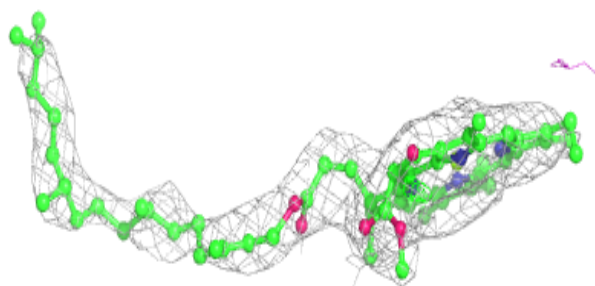
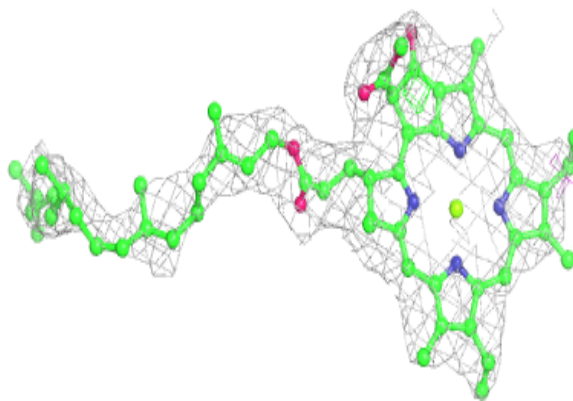
Electron density around CLA A 1801:

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

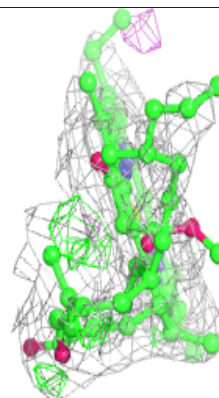
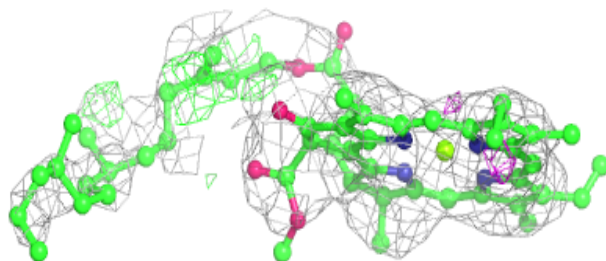
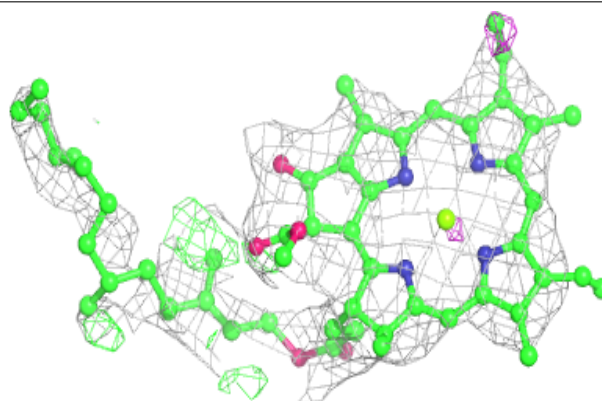


Electron density around CLA A 1103:

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

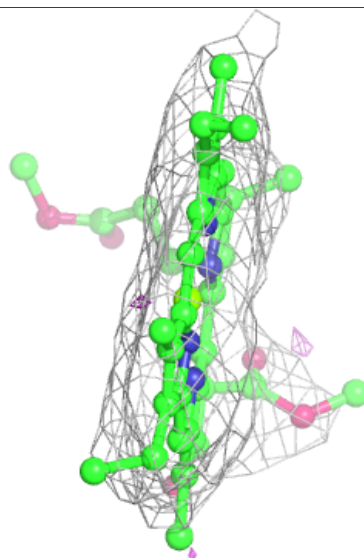
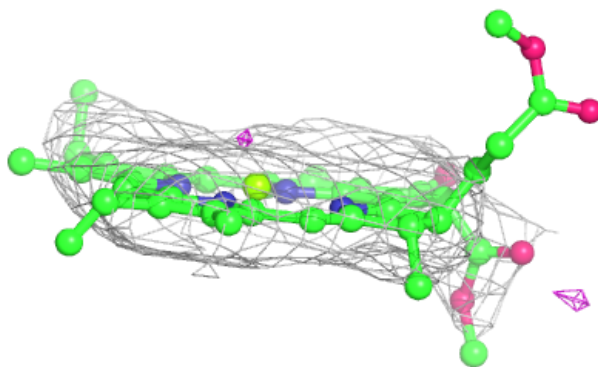
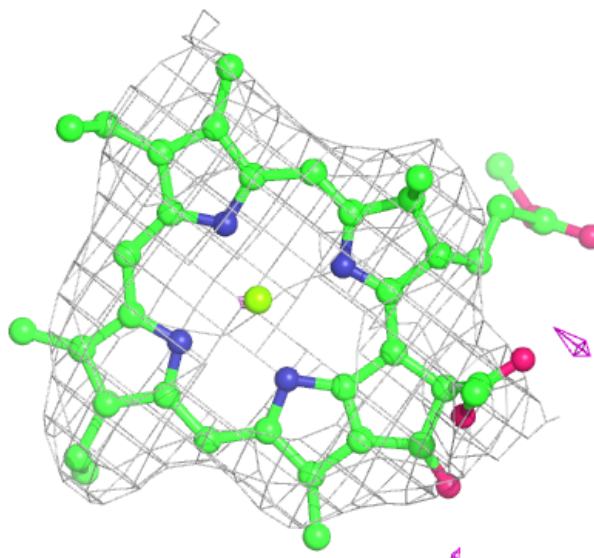
**Electron density around CLA A 1132:**

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



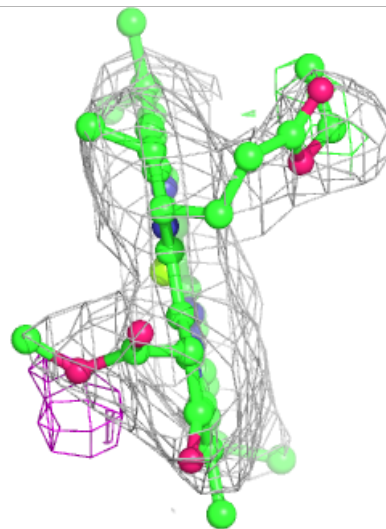
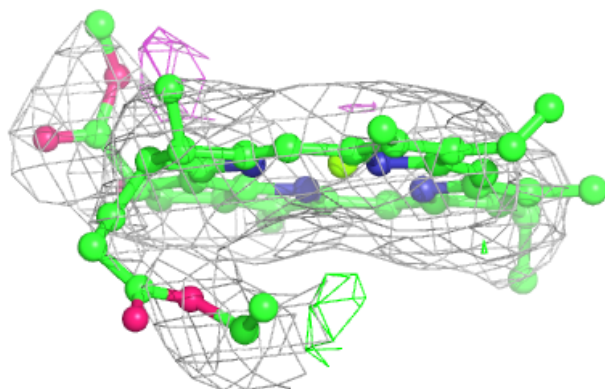
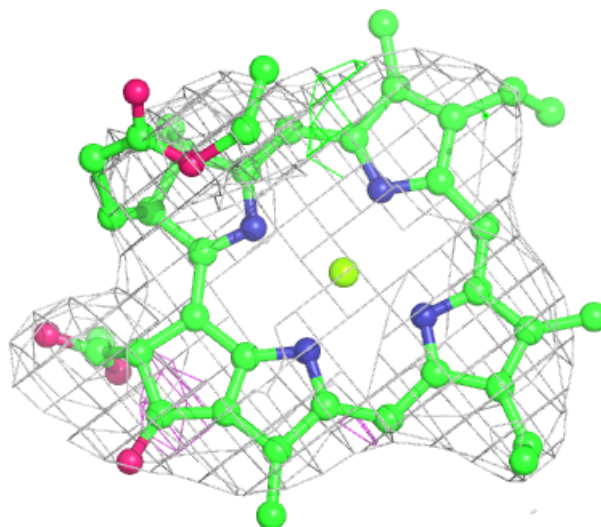
Electron density around CLA A 1129:

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



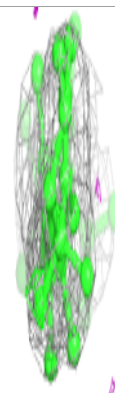
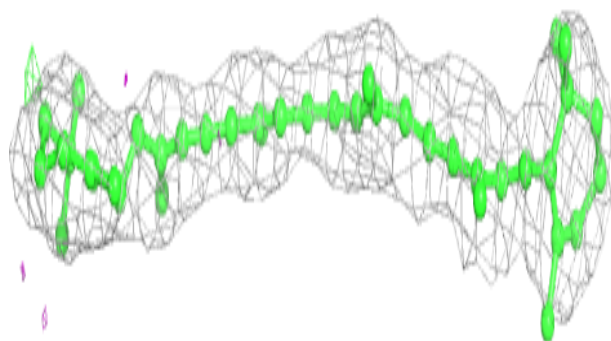
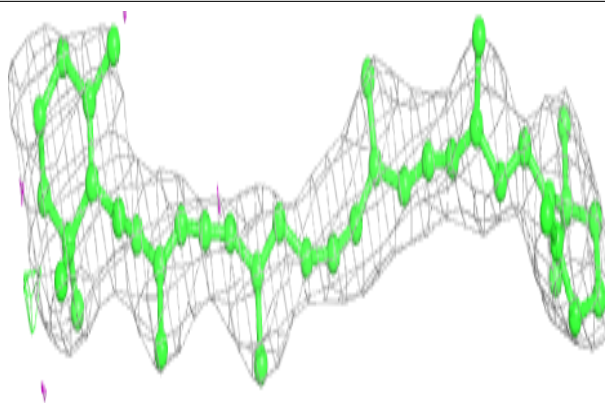
Electron density around CLA B 1217:

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

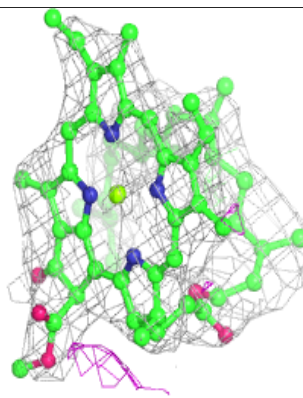
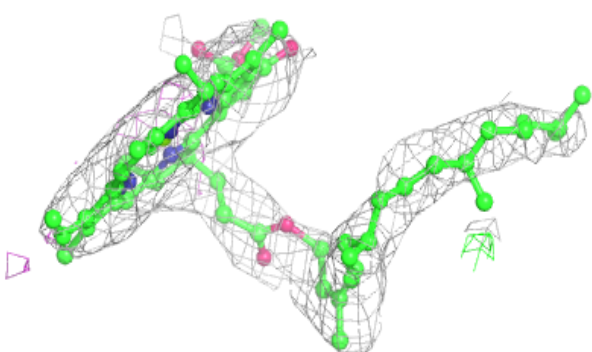
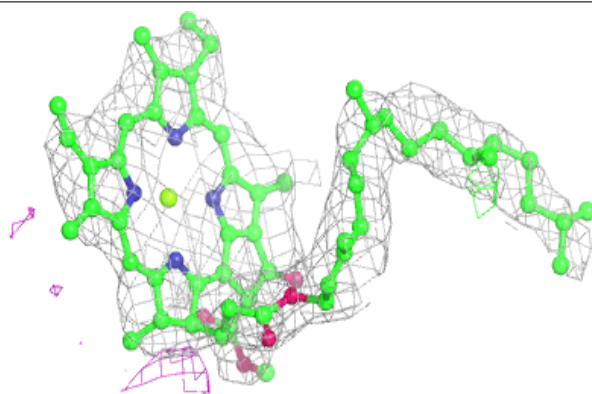


Electron density around BCR F 4015:

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

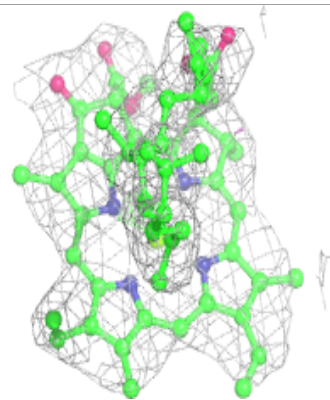
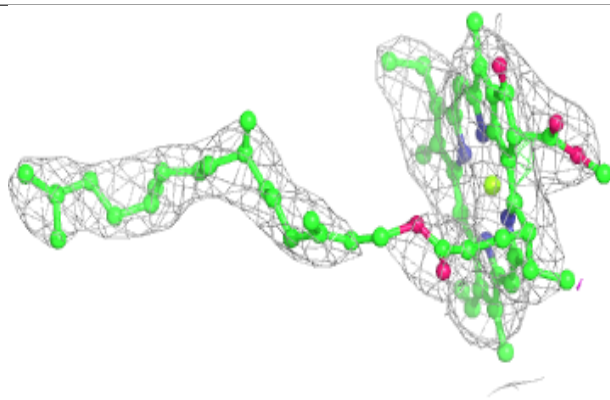
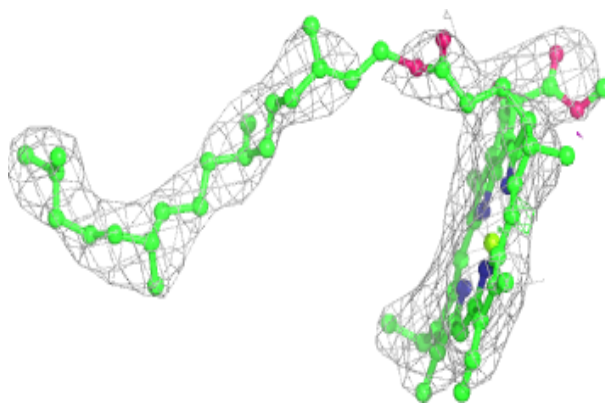
**Electron density around CLA B 1231:**

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

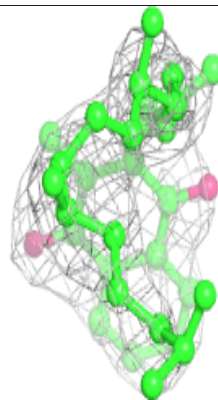
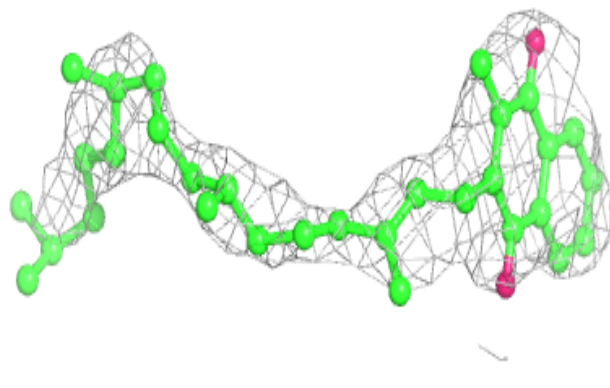
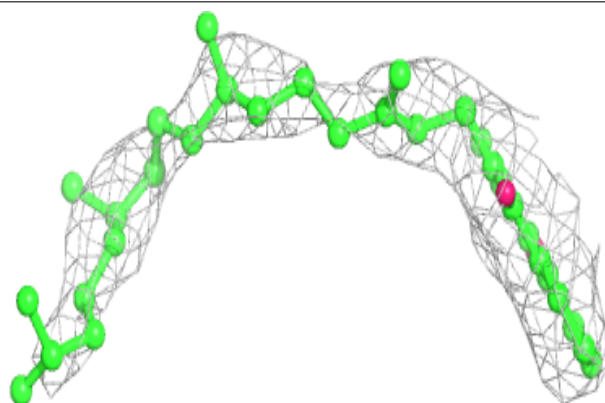


Electron density around CLA A 1128:

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

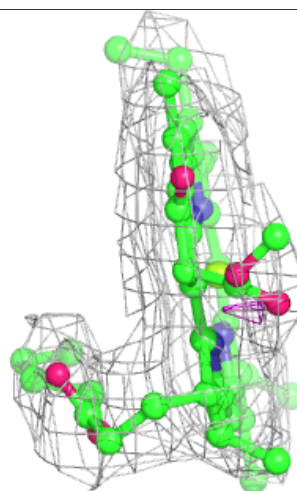
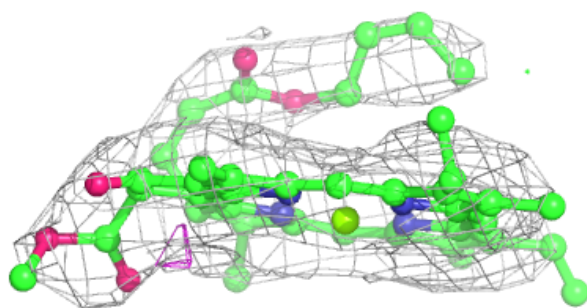
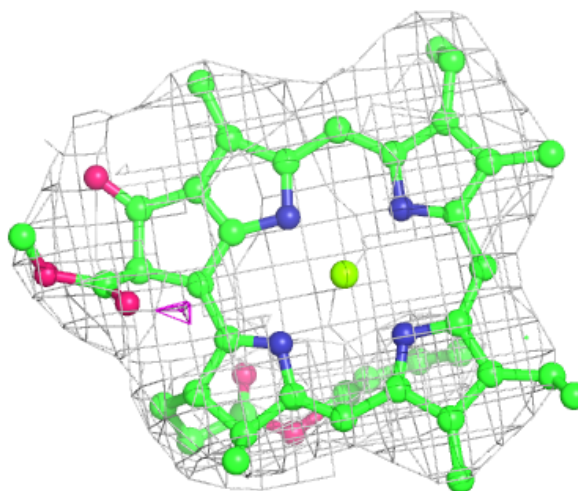
**Electron density around PQN B 2002:**

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



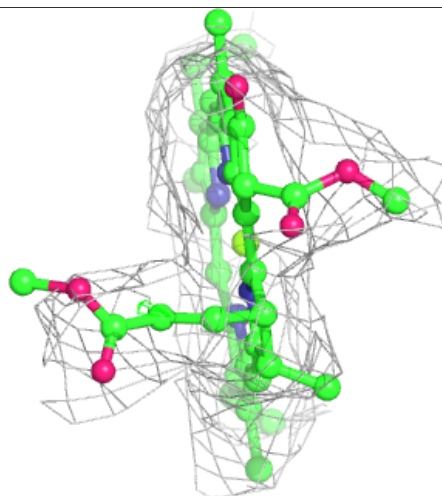
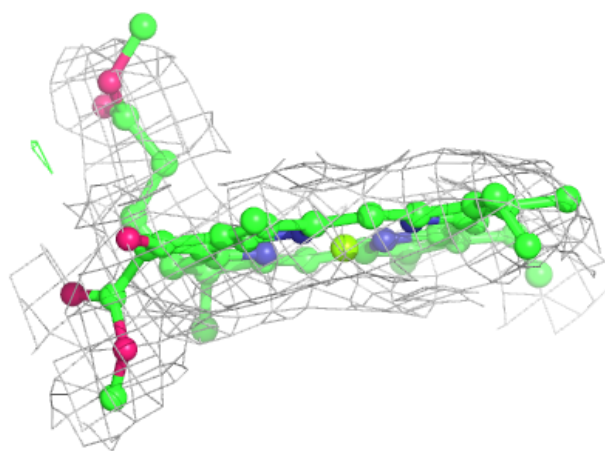
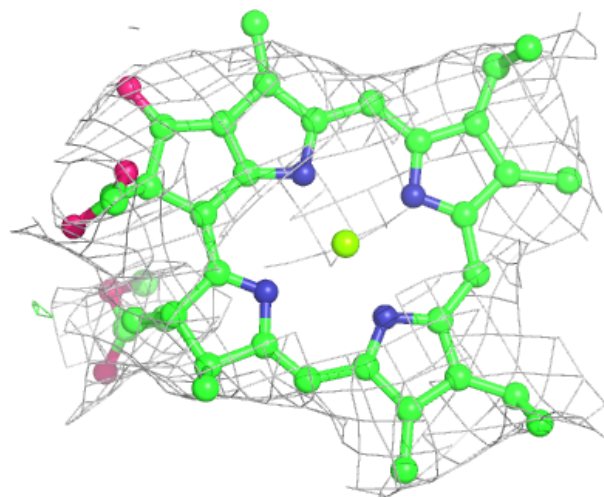
Electron density around CLA A 1120:

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



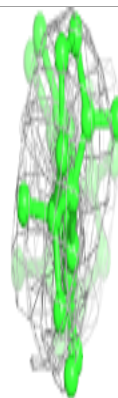
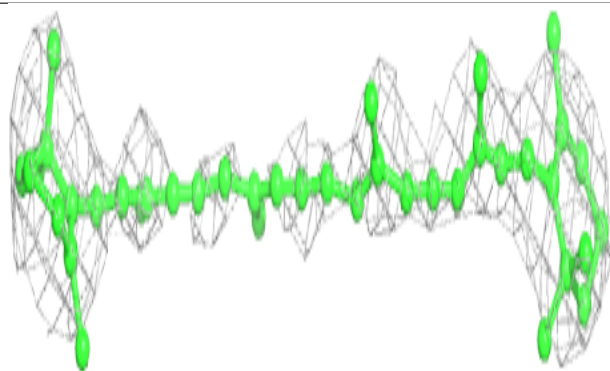
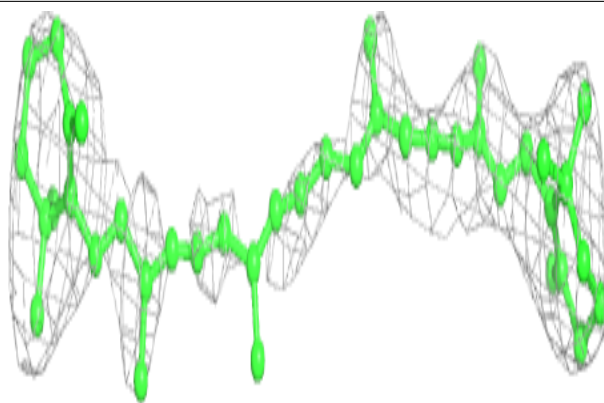
Electron density around CLA B 1211:

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



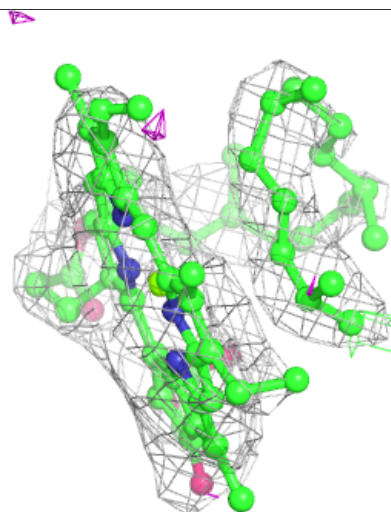
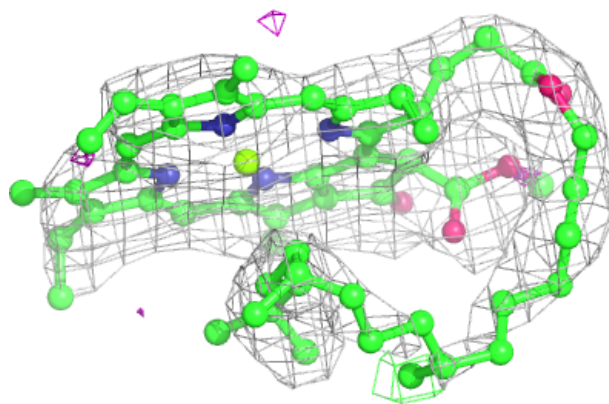
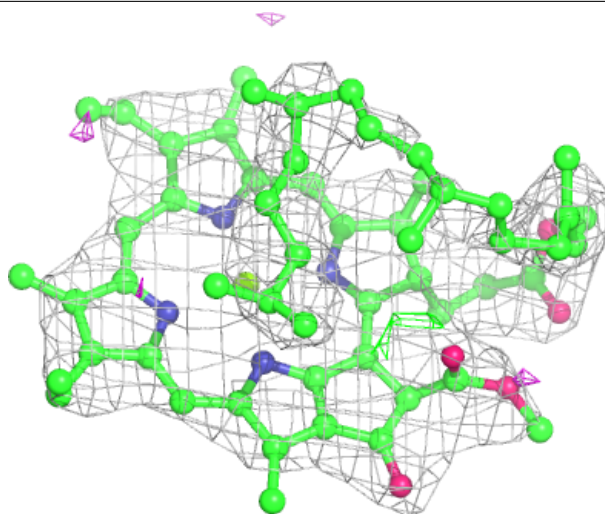
Electron density around BCR A 4002:

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



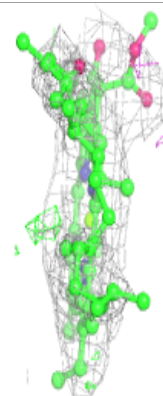
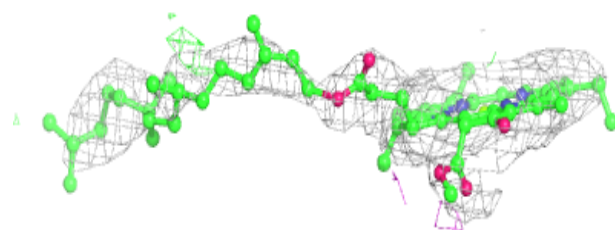
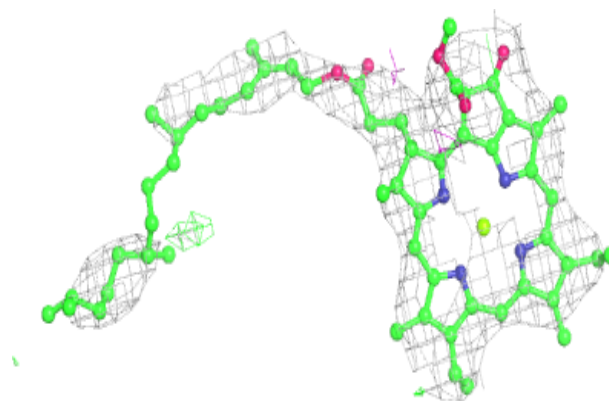
Electron density around CLA B 1203:

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



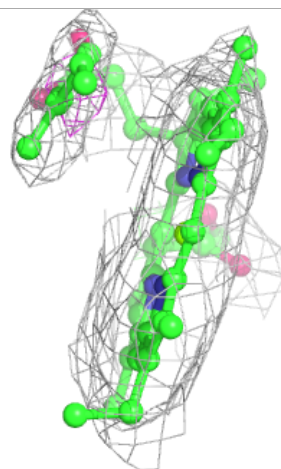
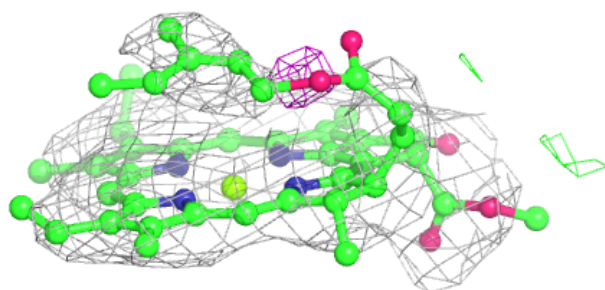
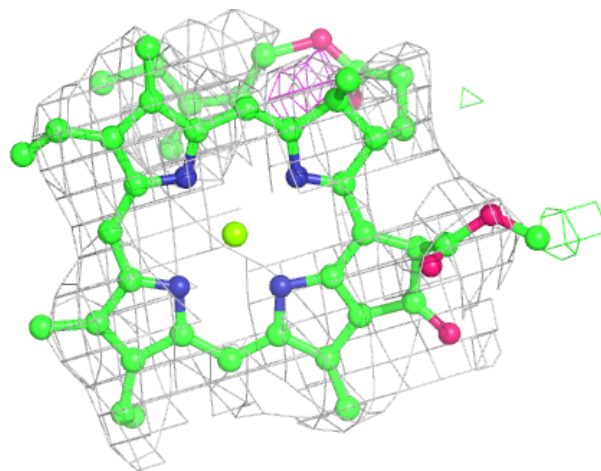
Electron density around CLA F 1410:

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



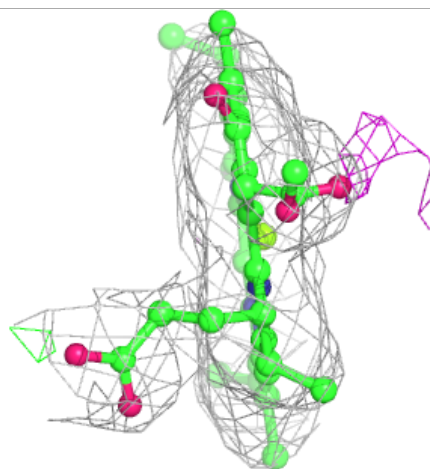
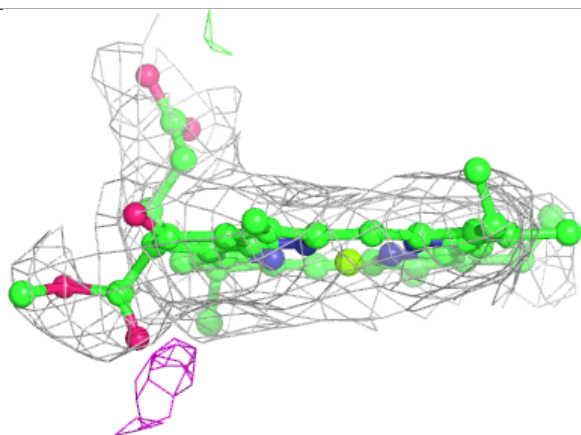
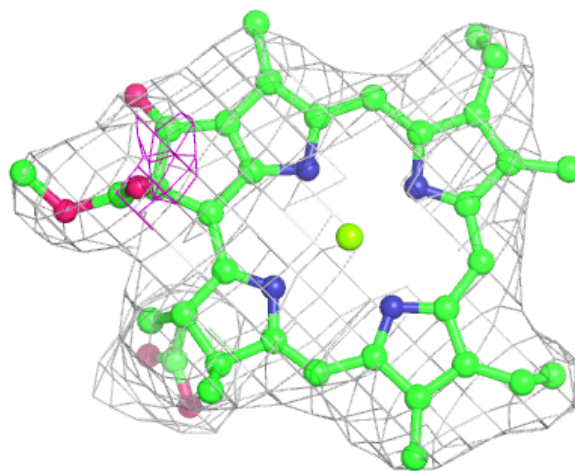
Electron density around CLA B 1218:

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



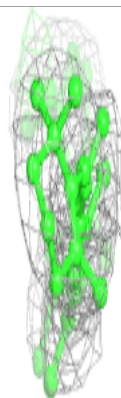
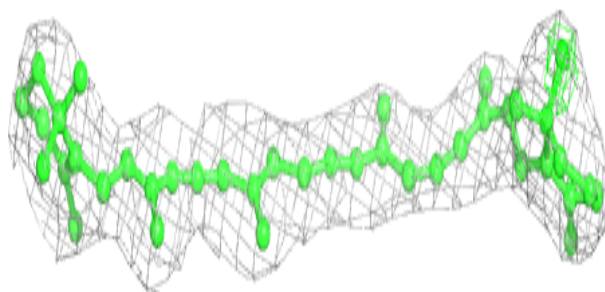
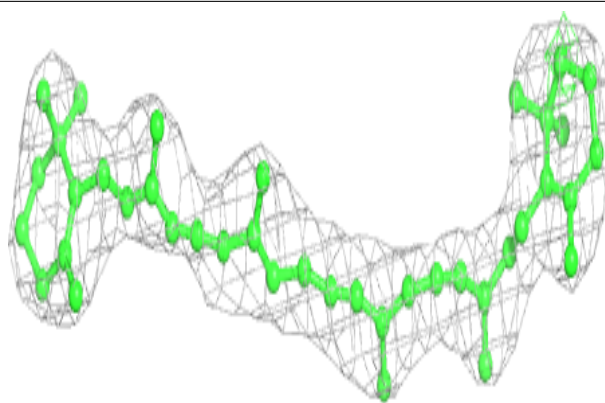
Electron density around CLA B 1232:

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

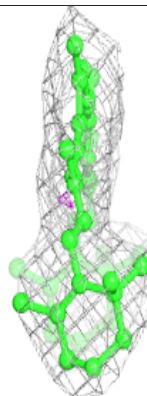
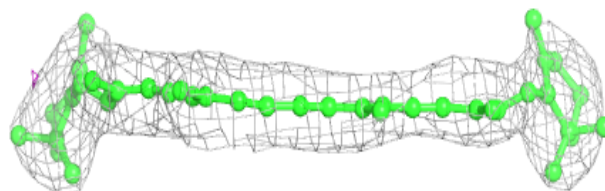
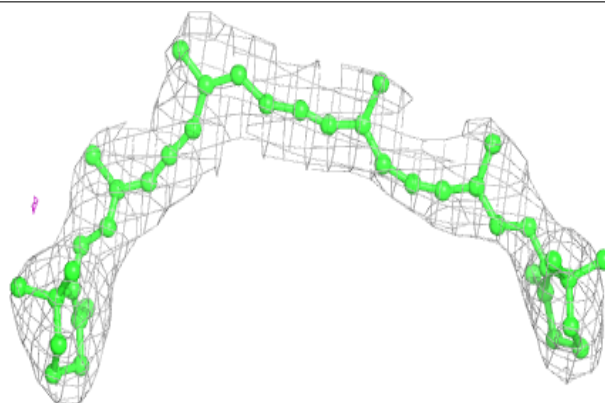


Electron density around BCR B 4010:

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

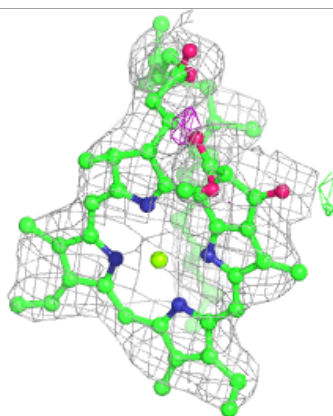
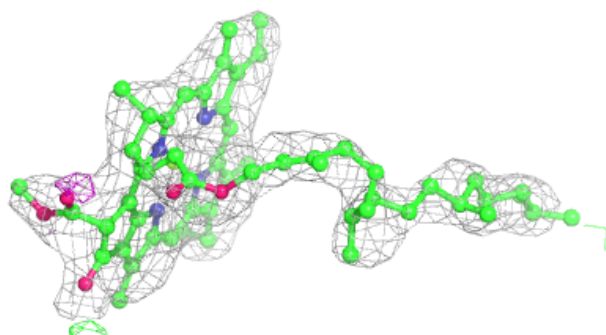
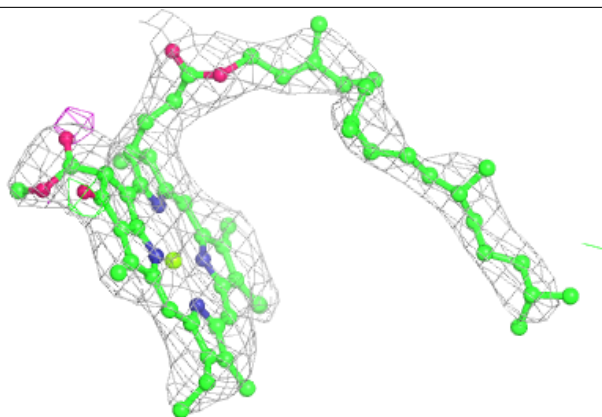
**Electron density around BCR F 4016:**

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



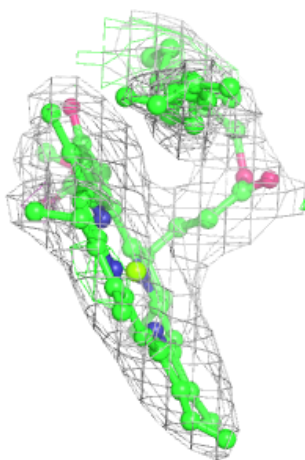
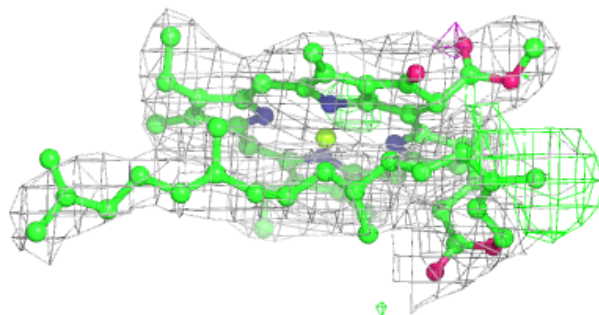
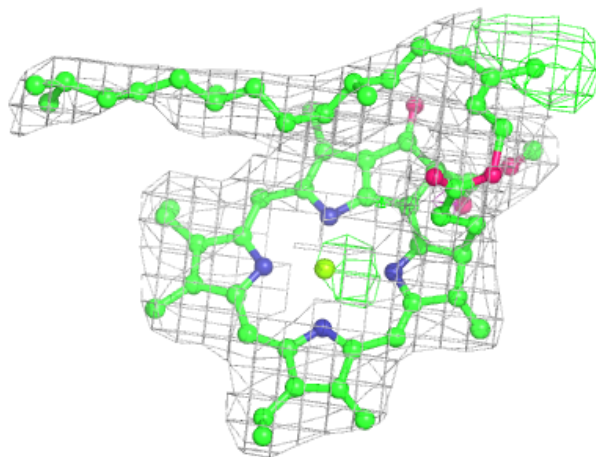
Electron density around CLA A 1102:

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



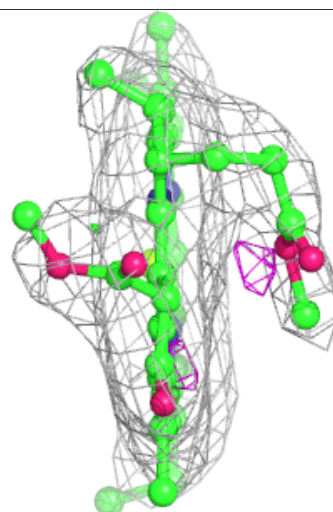
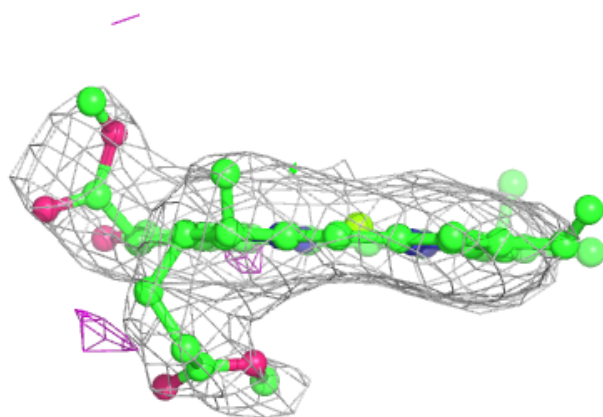
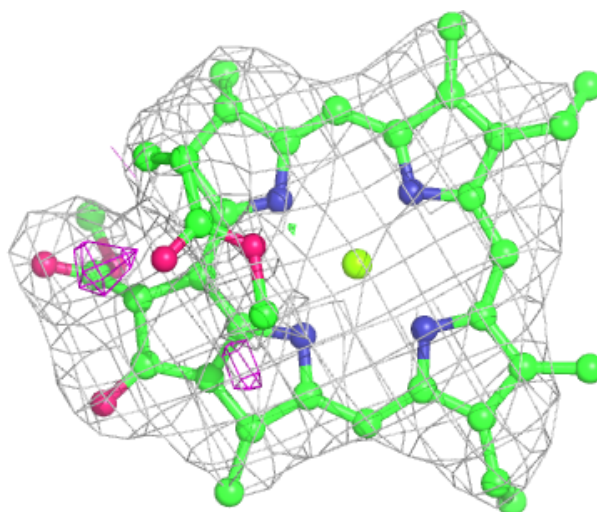
Electron density around CLA B 1228:

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



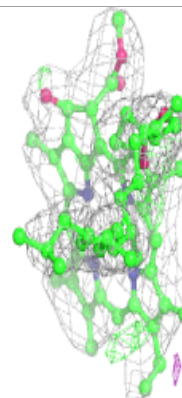
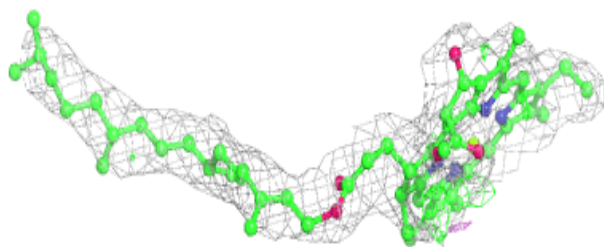
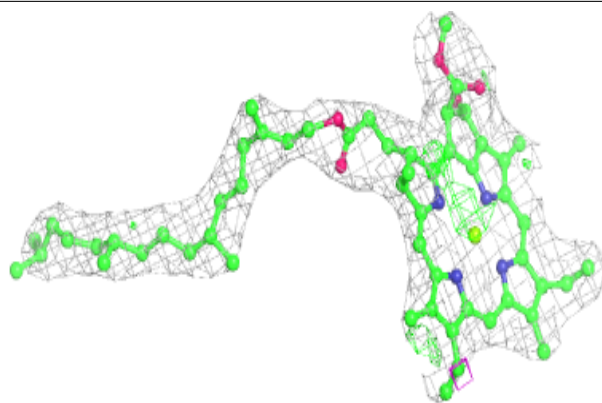
Electron density around CLA B 1201:

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

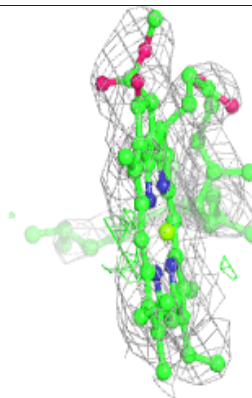
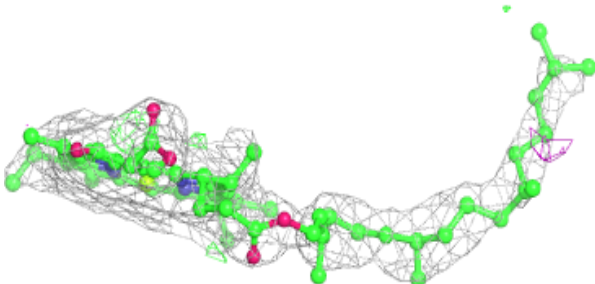
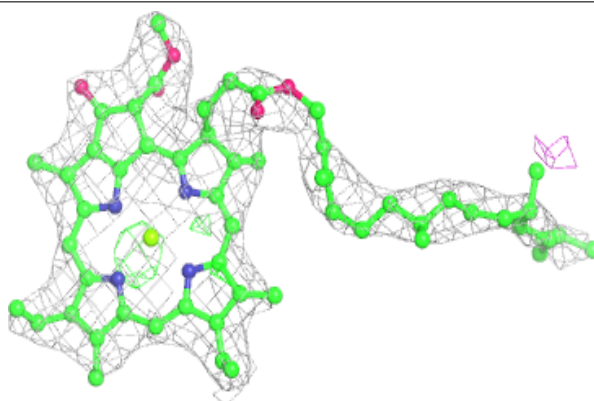


Electron density around CLA A 1022:

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

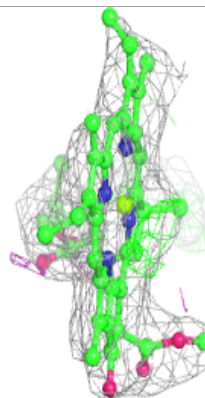
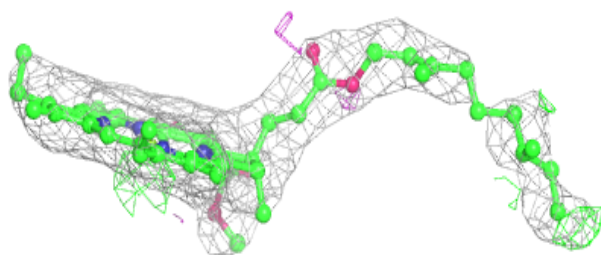
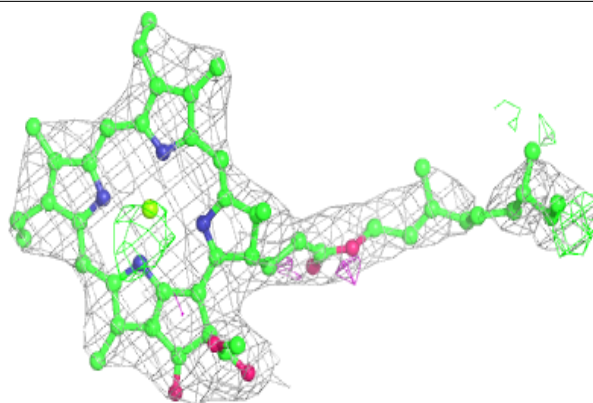
**Electron density around CLA B 1023:**

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

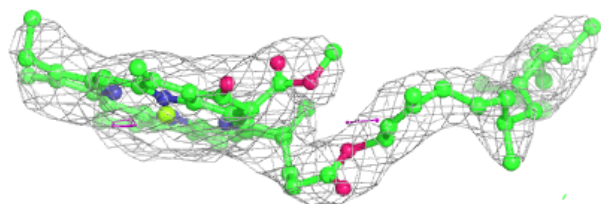
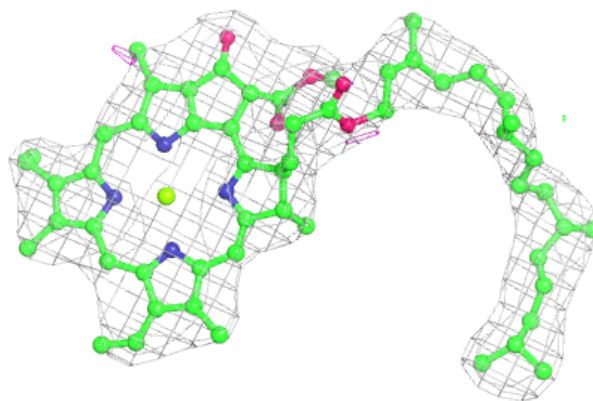


Electron density around CLA B 1222:

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

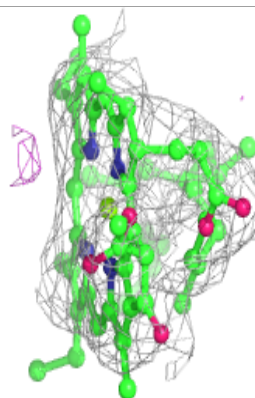
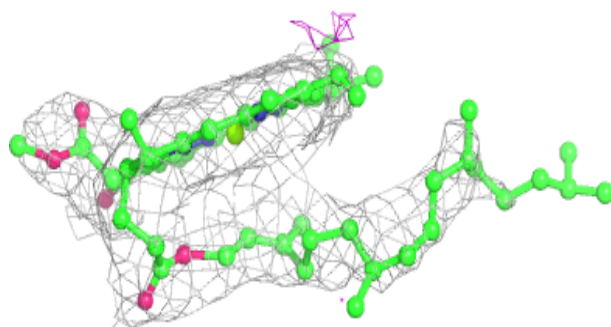
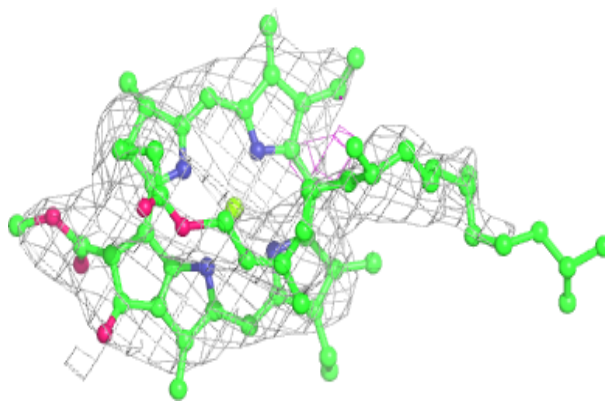
**Electron density around CLA A 1101:**

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

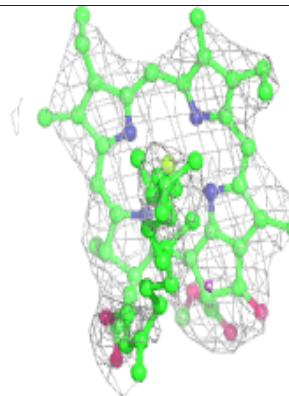
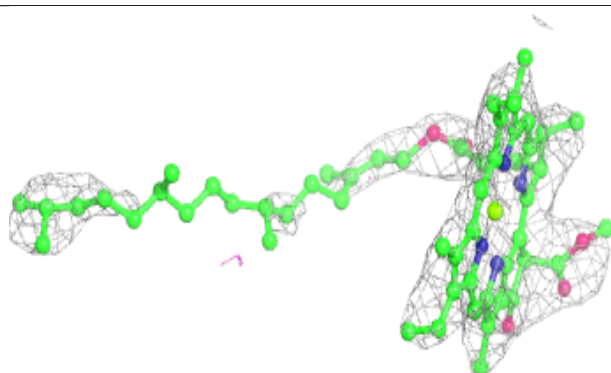
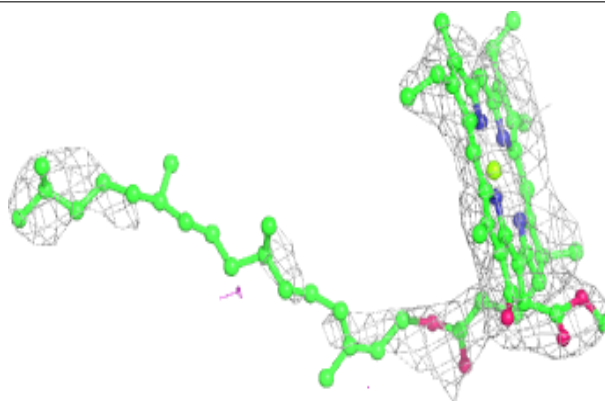


Electron density around CLA A 1136:

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

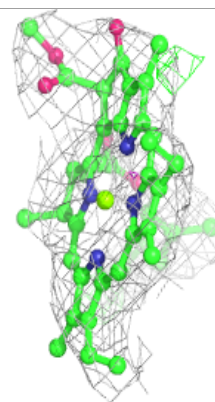
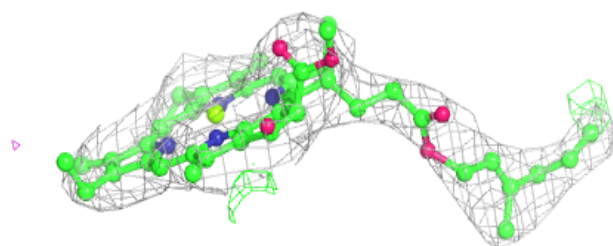
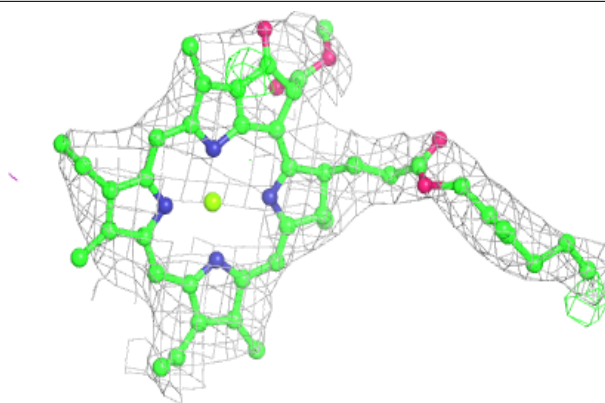
**Electron density around CLA B 1226:**

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



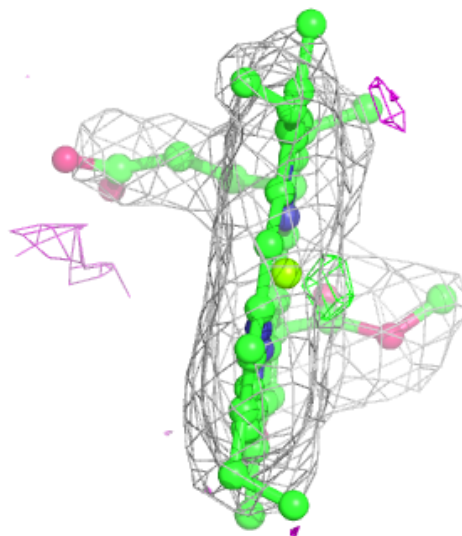
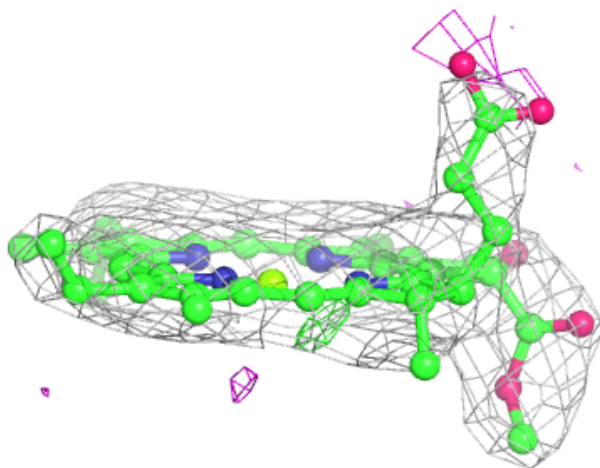
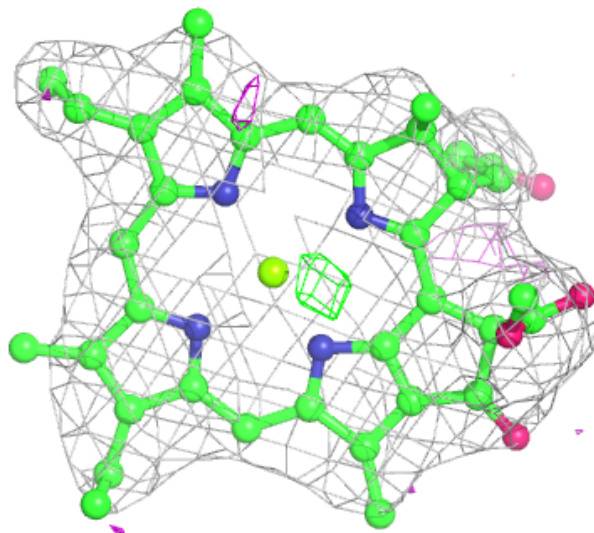
Electron density around CLA A 1125:

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



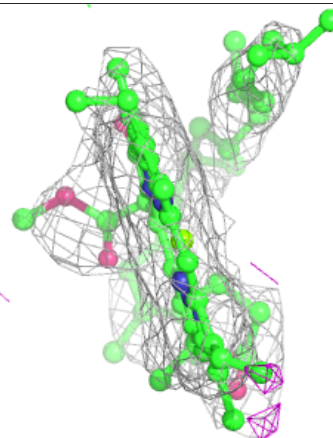
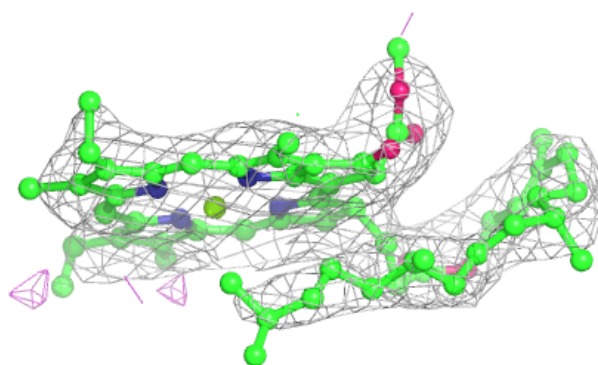
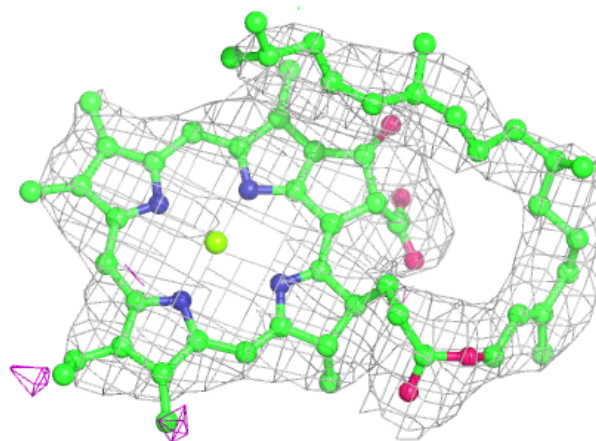
Electron density around CLA B 1227:

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

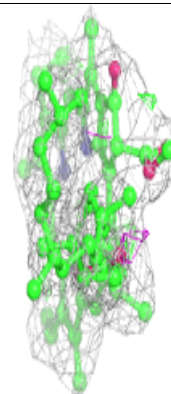
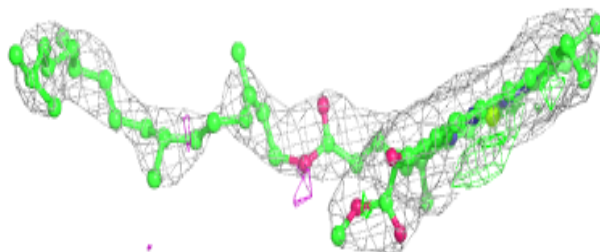
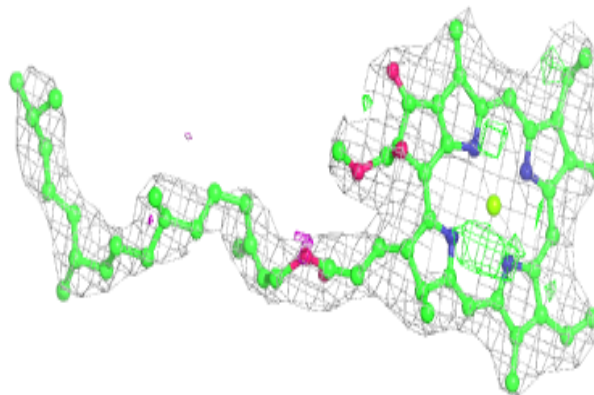


Electron density around CLA B 1202:

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

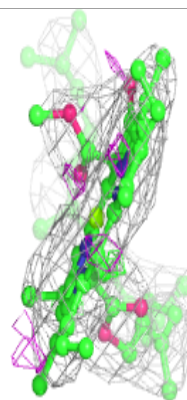
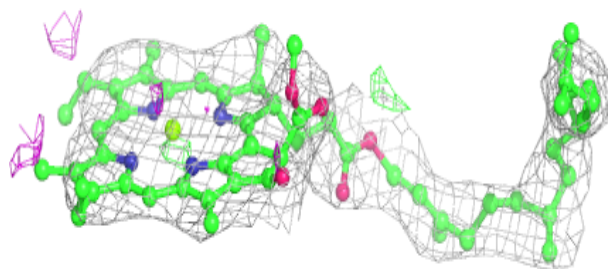
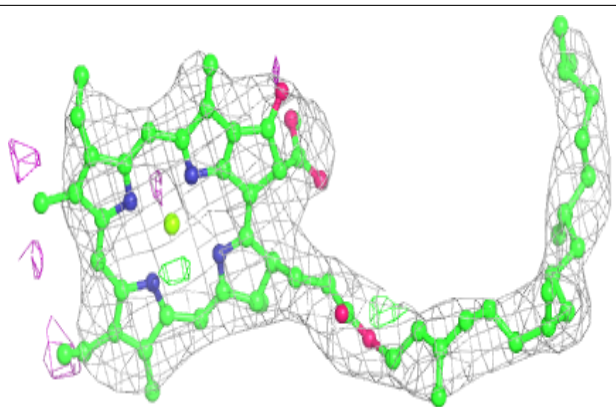
**Electron density around CLA F 1139:**

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



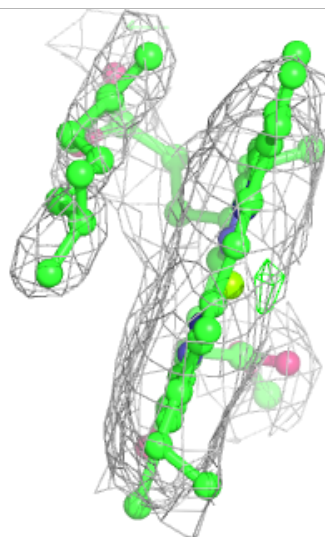
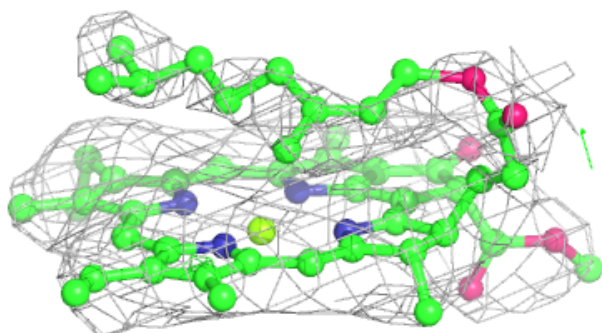
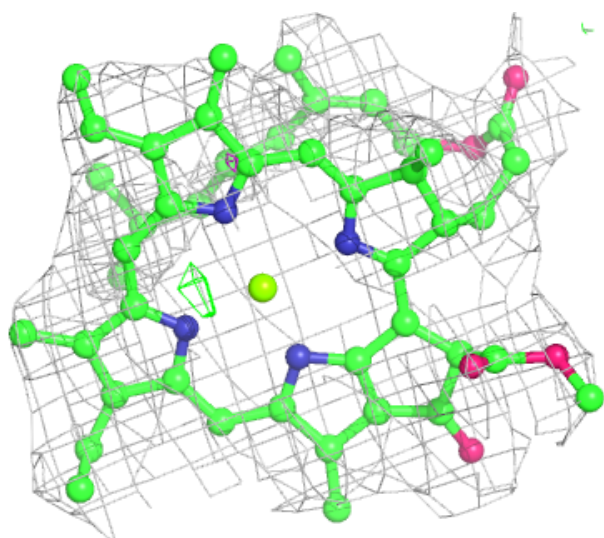
Electron density around CLA B 1223:

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



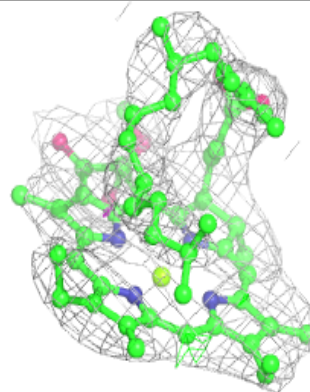
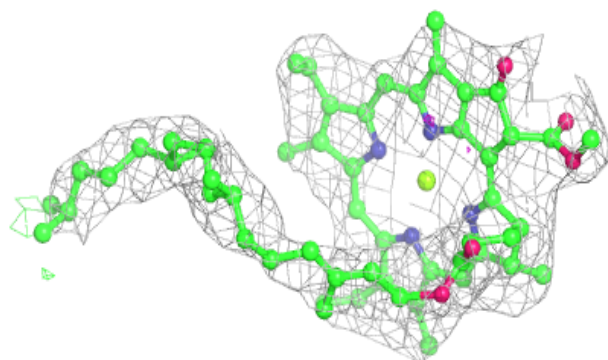
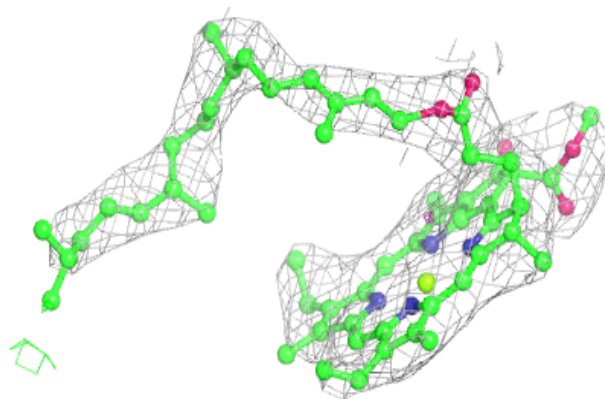
Electron density around CLA B 1219:

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

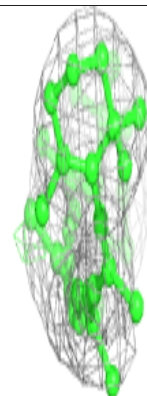
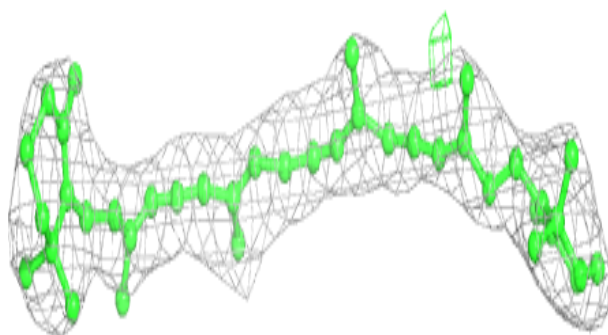
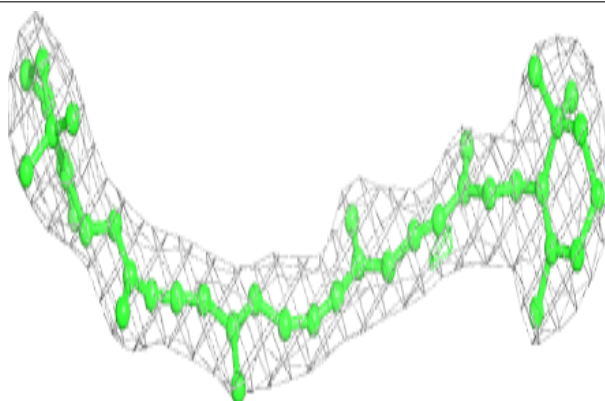


Electron density around CLA A 1109:

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

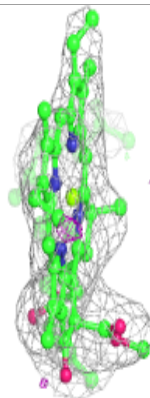
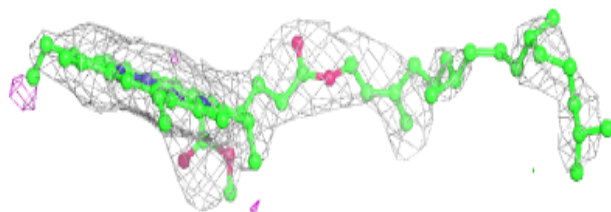
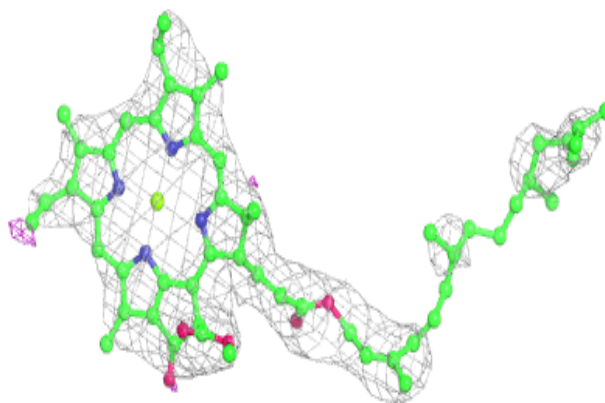
**Electron density around BCR B 4014:**

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

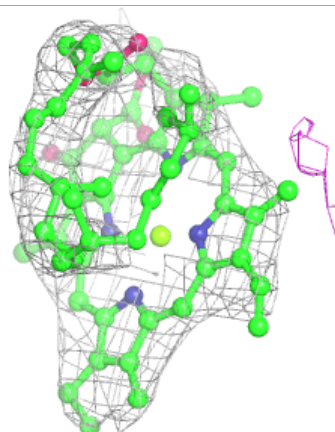
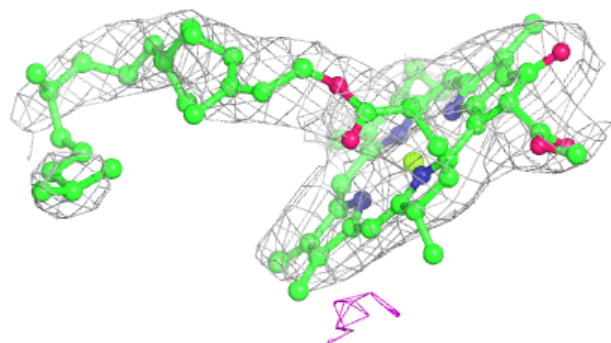
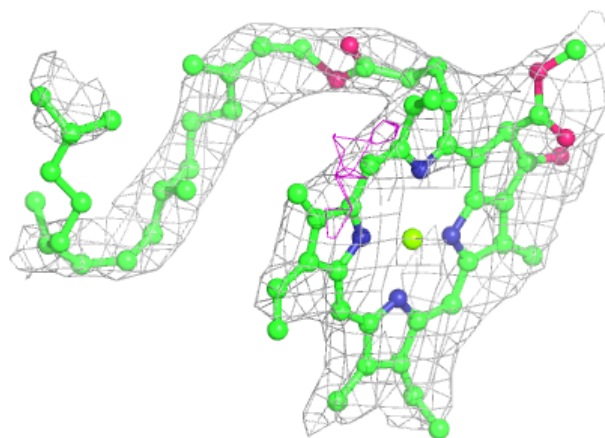


Electron density around CLA B 1234:

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

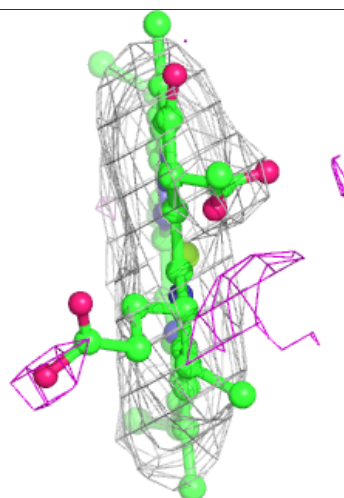
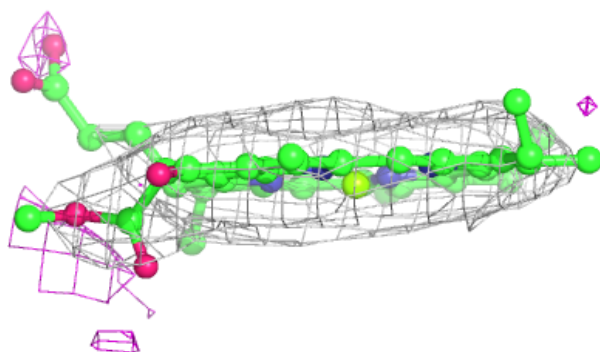
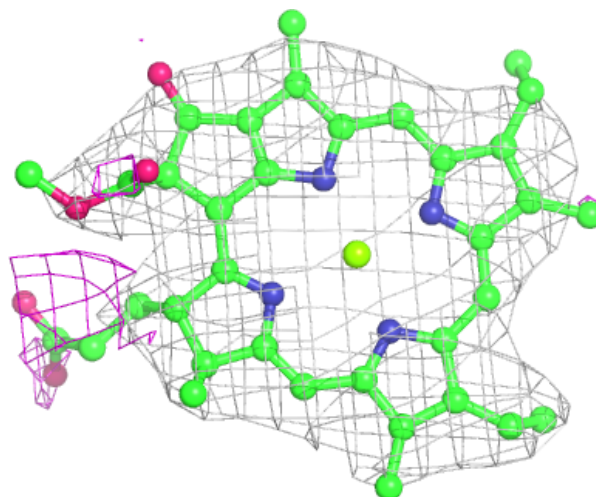
**Electron density around CLA A 1122:**

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



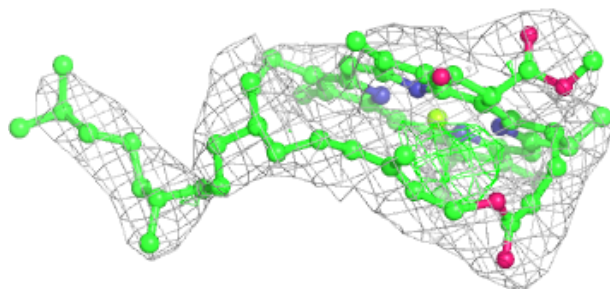
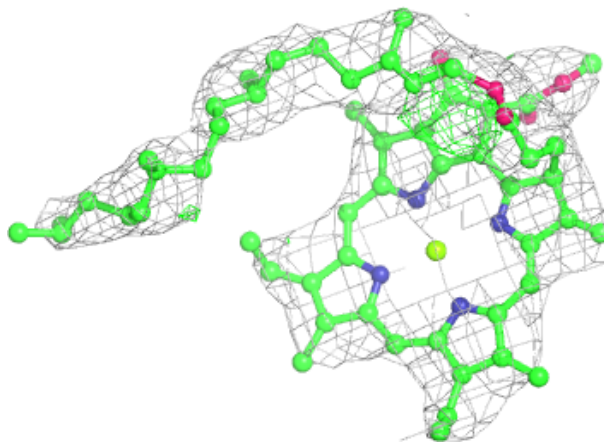
Electron density around CLA B 1240:

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



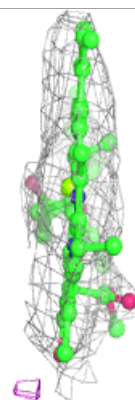
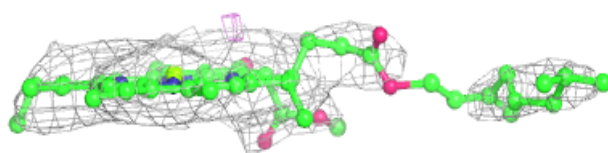
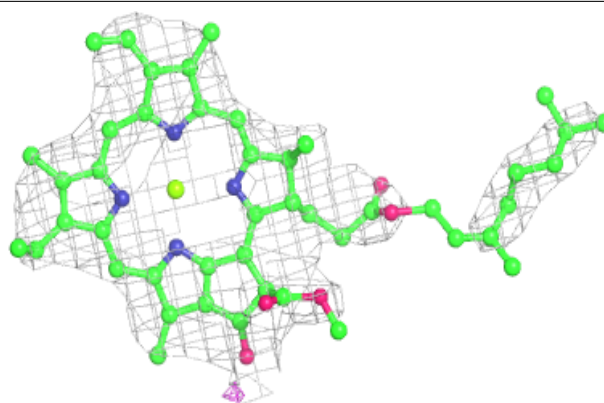
Electron density around CLA A 1127:

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

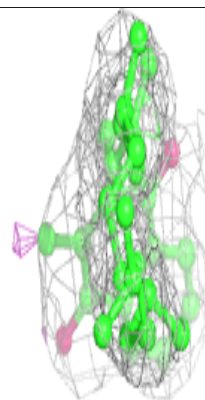
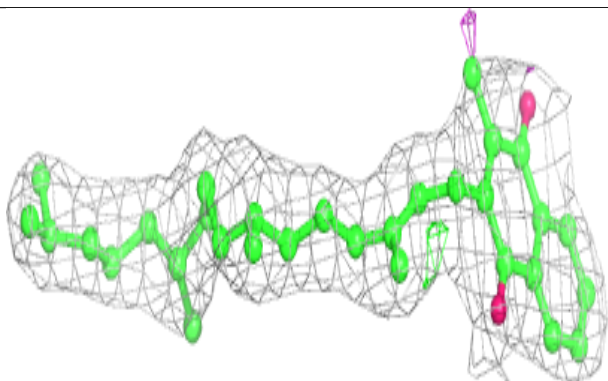
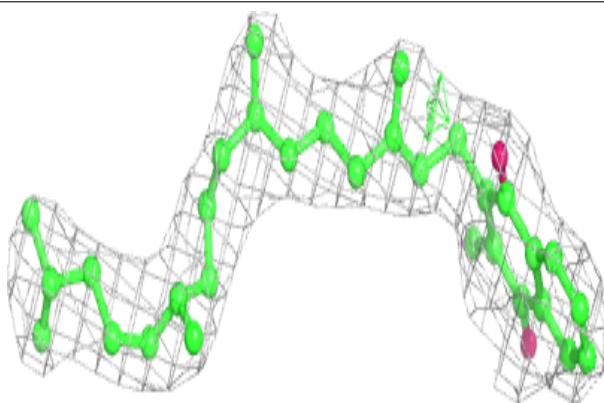


Electron density around CLA A 1131:

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

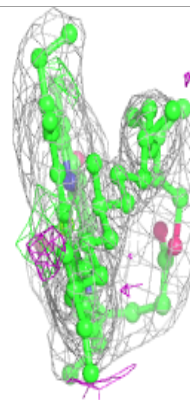
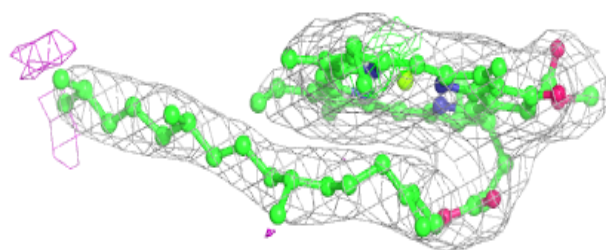
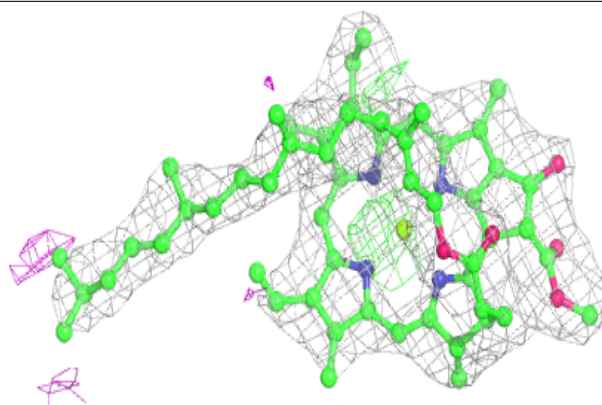
**Electron density around PQN A 2001:**

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



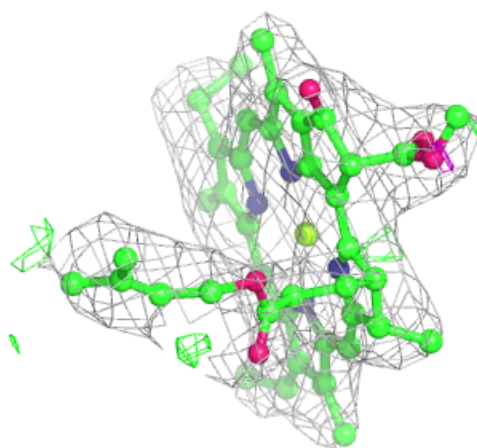
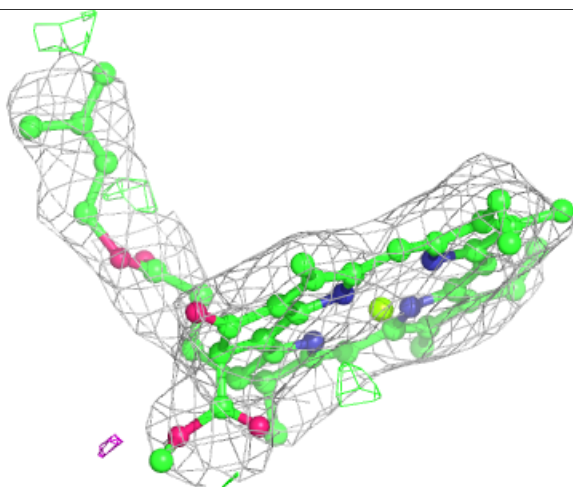
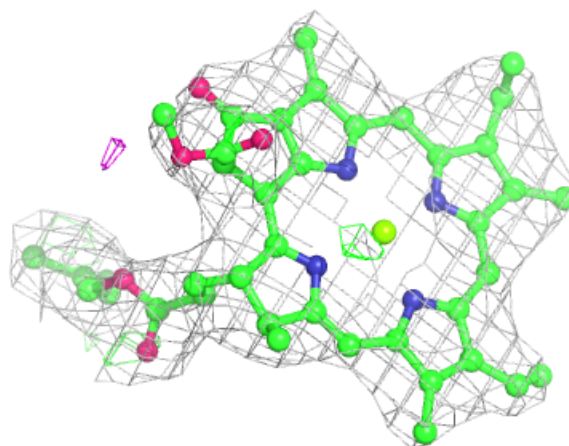
Electron density around CLA A 1138:

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



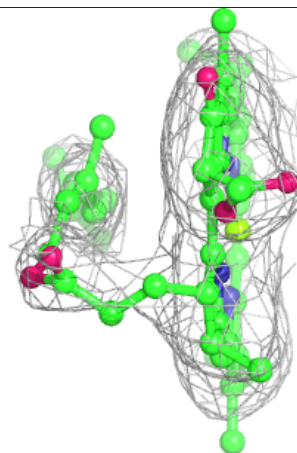
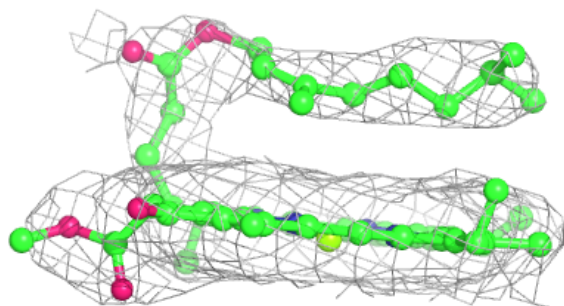
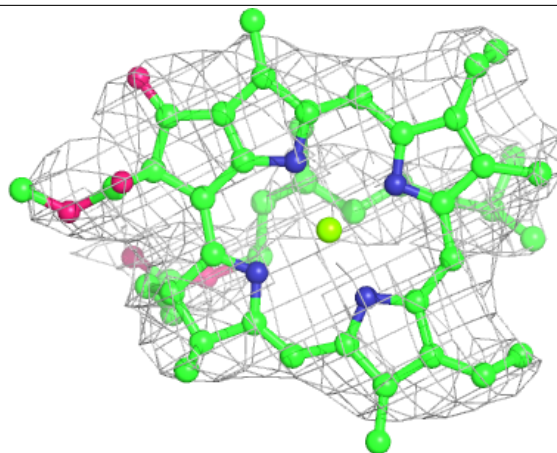
Electron density around CLA B 1236:

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



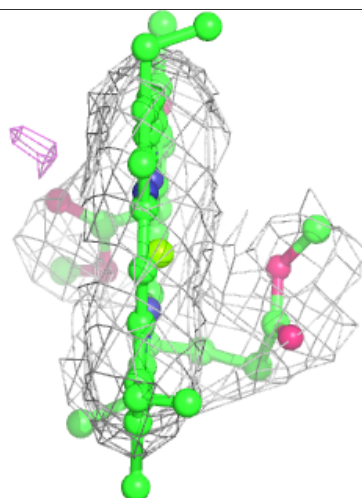
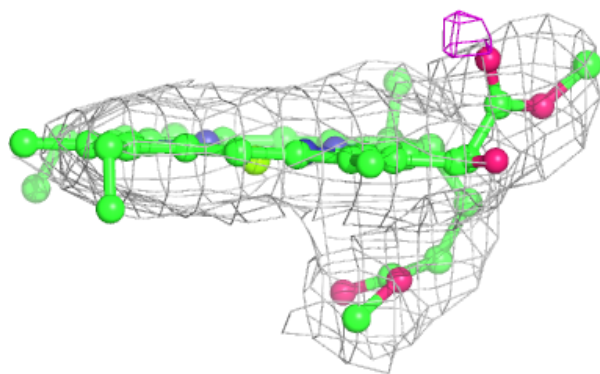
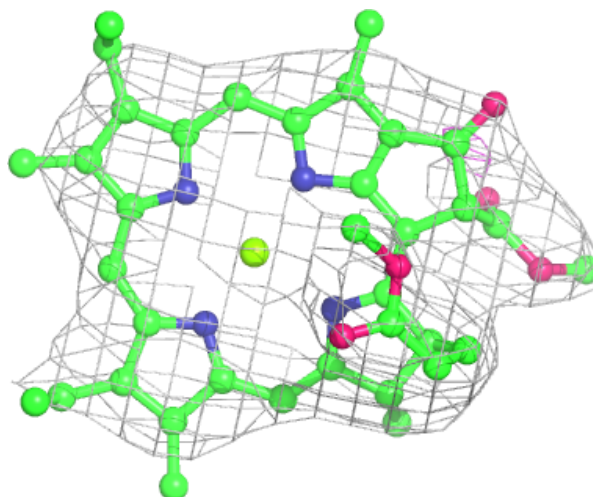
Electron density around CLA B 1237:

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



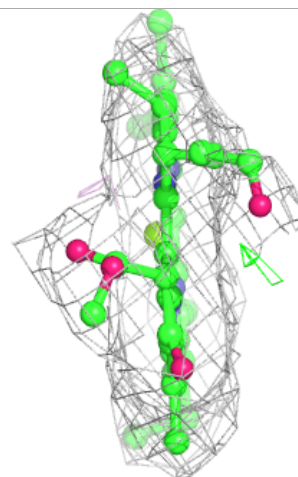
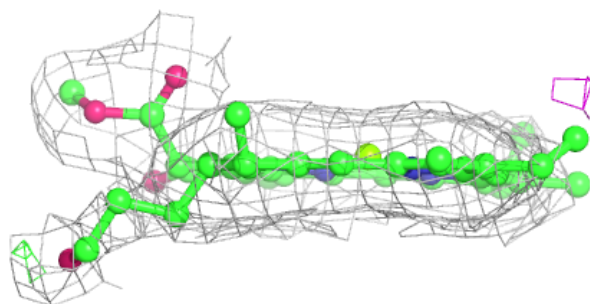
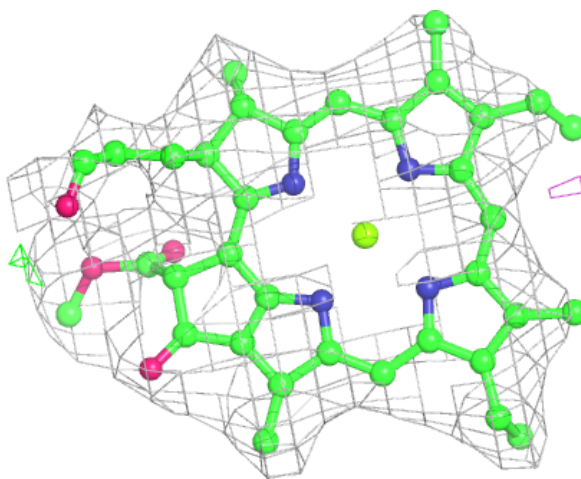
Electron density around CLA B 1204:

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



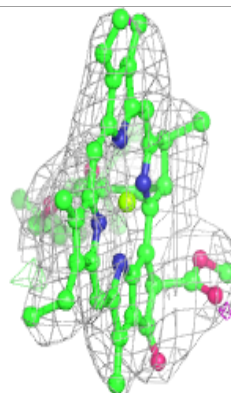
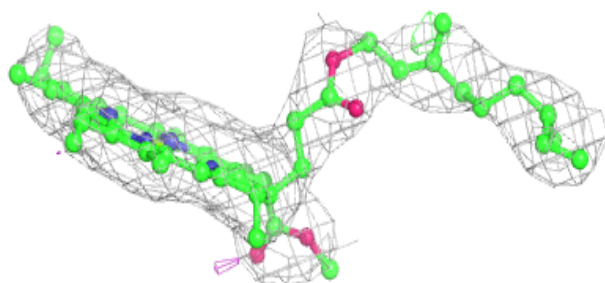
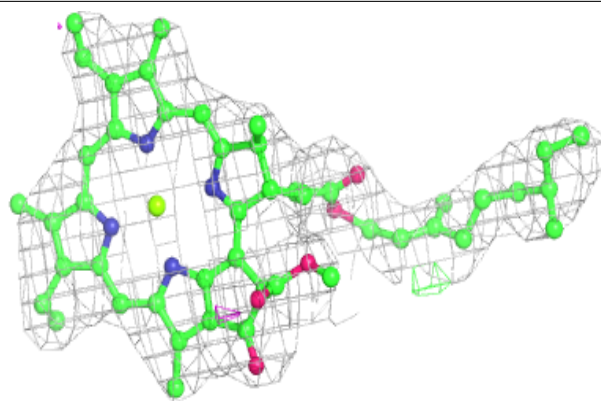
Electron density around CLA B 1238:

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

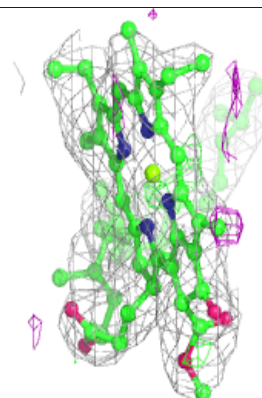
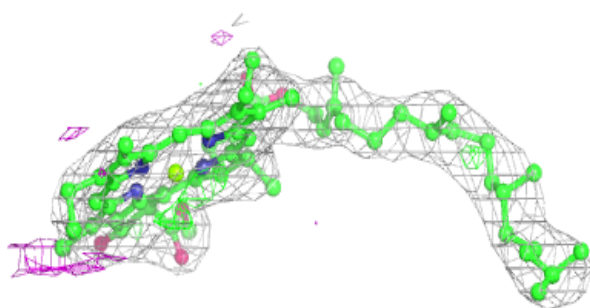
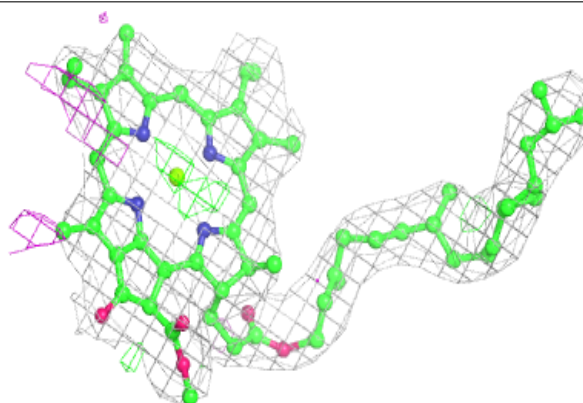


Electron density around CLA B 1220:

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

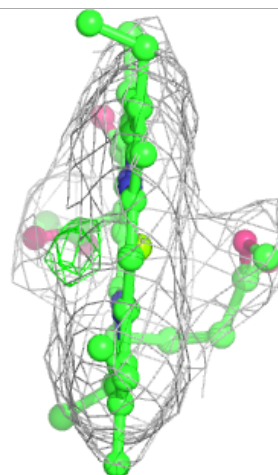
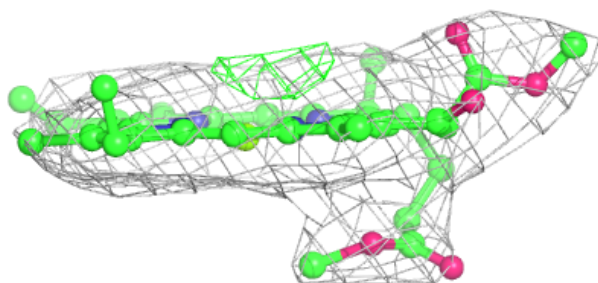
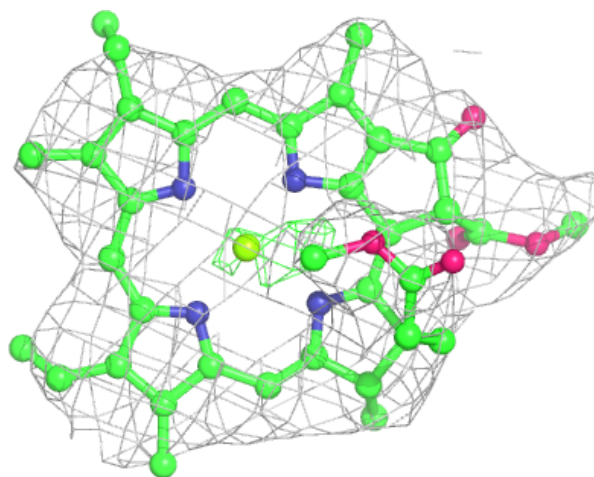
**Electron density around CLA B 1013:**

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



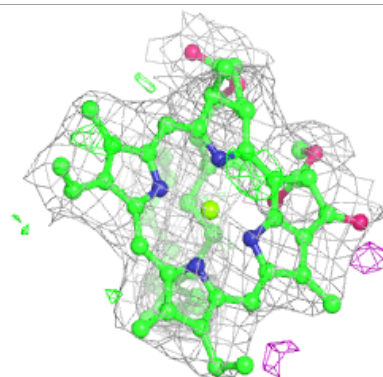
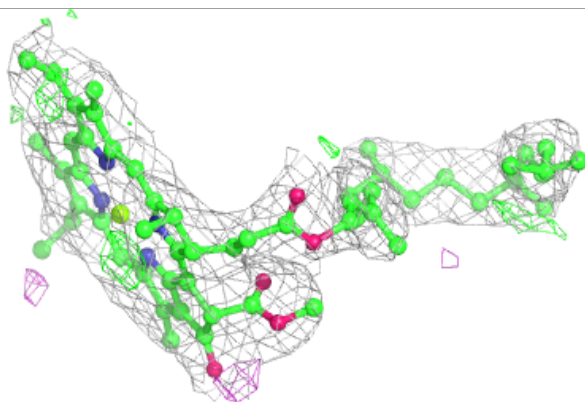
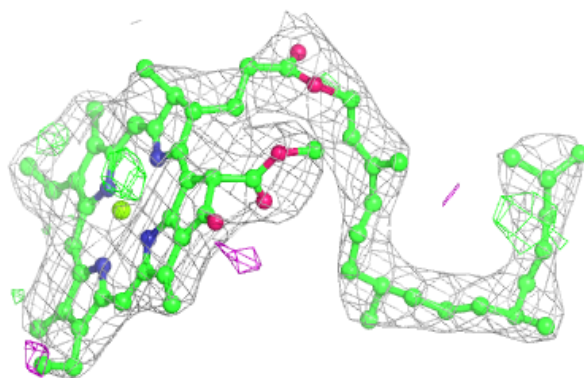
Electron density around CLA A 1115:

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

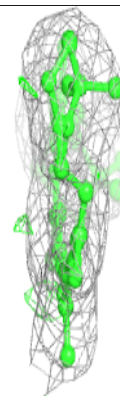
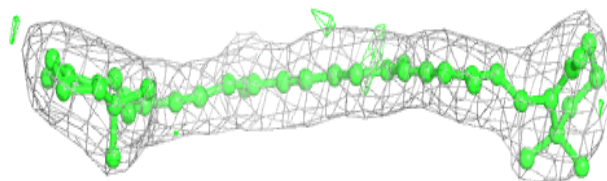
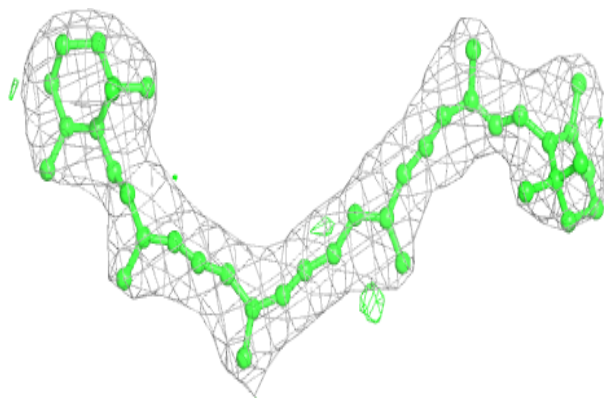


Electron density around CL0 A 1011:

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

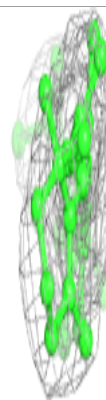
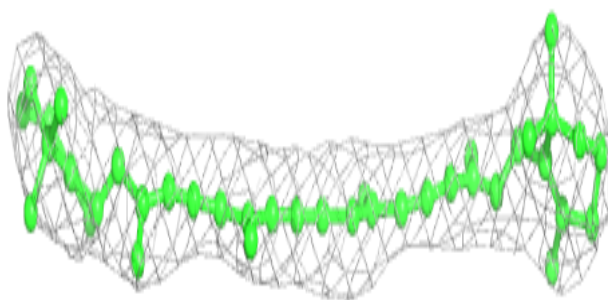
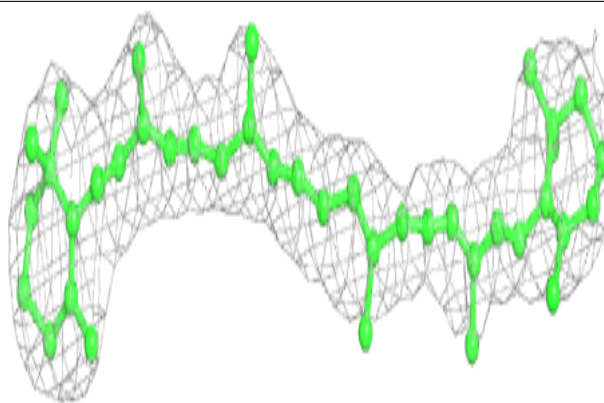
**Electron density around BCR B 4011:**

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



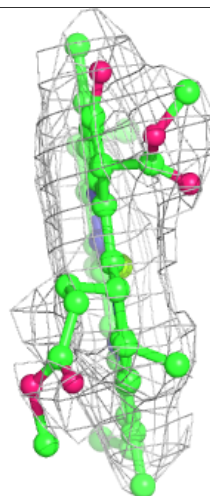
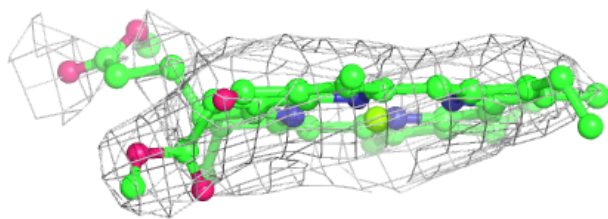
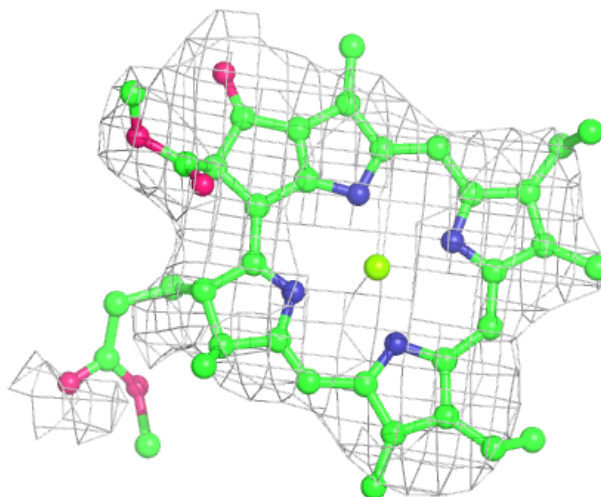
Electron density around BCR A 4012:

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



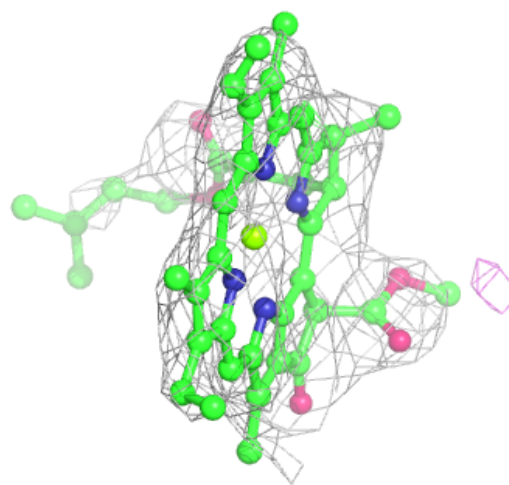
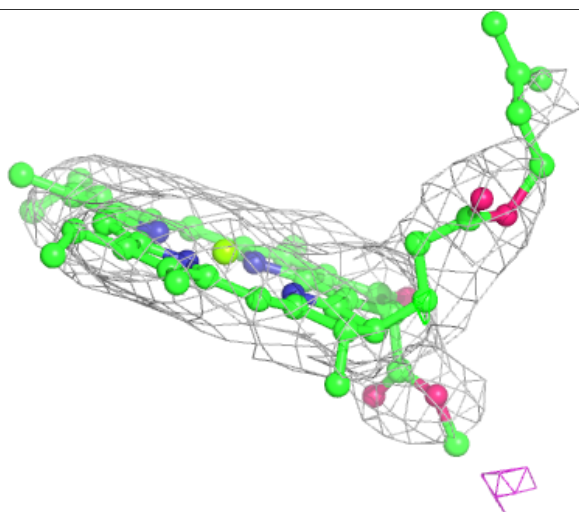
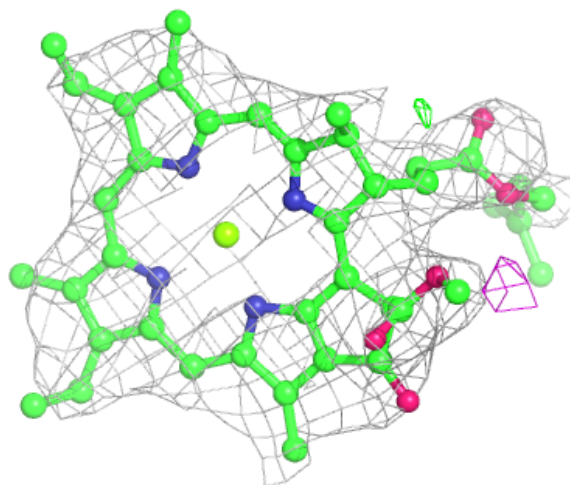
Electron density around CLA A 1121:

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



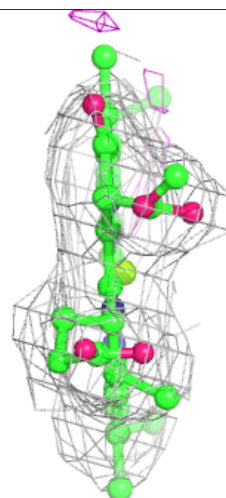
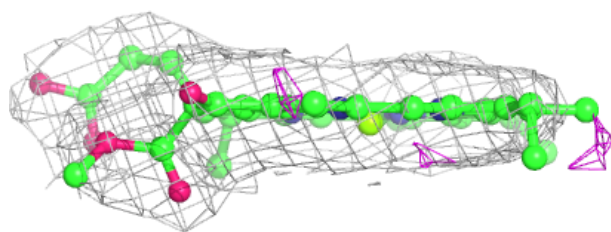
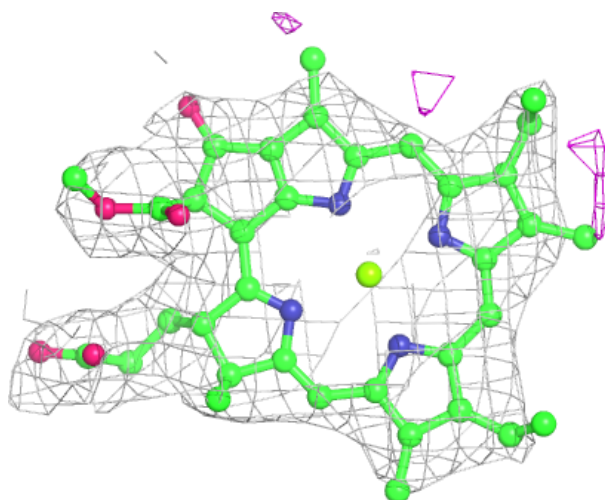
Electron density around CLA A 1137:

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



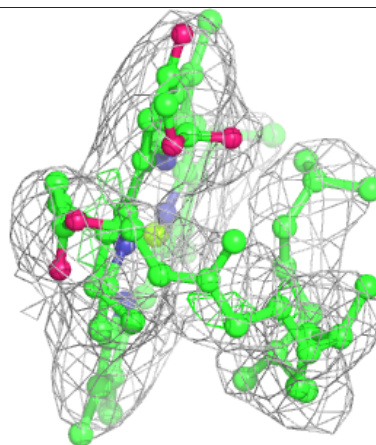
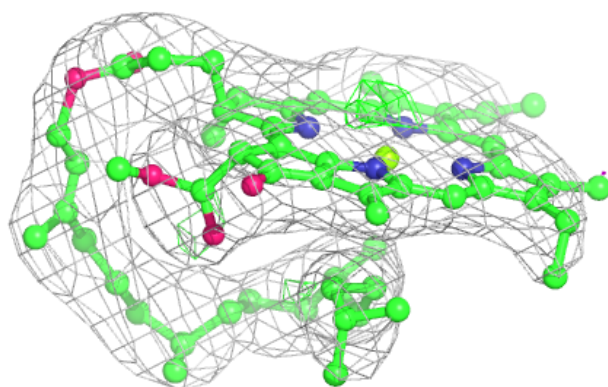
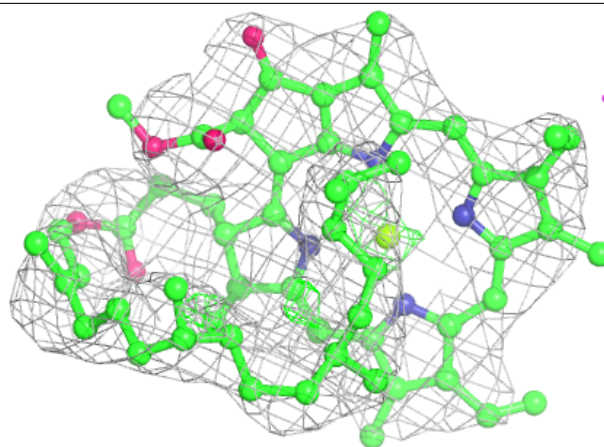
Electron density around CLA F 1301:

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

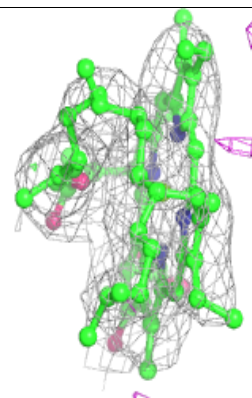
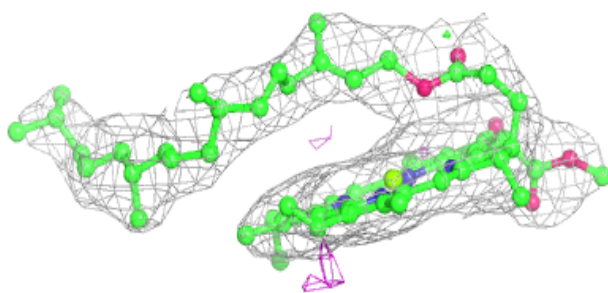
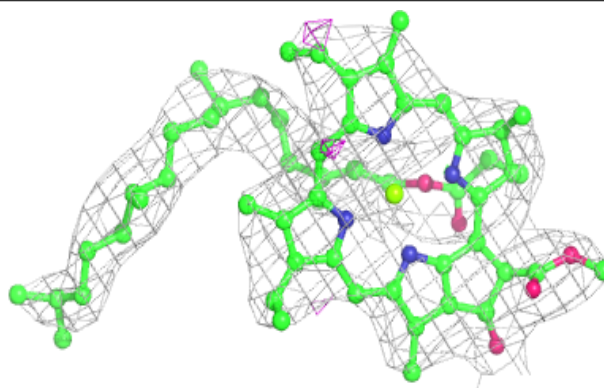


Electron density around CLA A 1104:

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

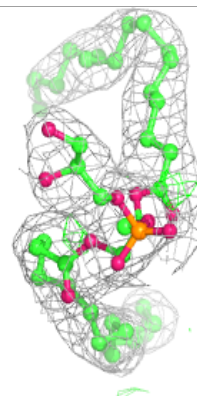
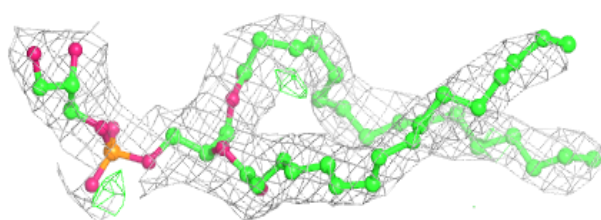
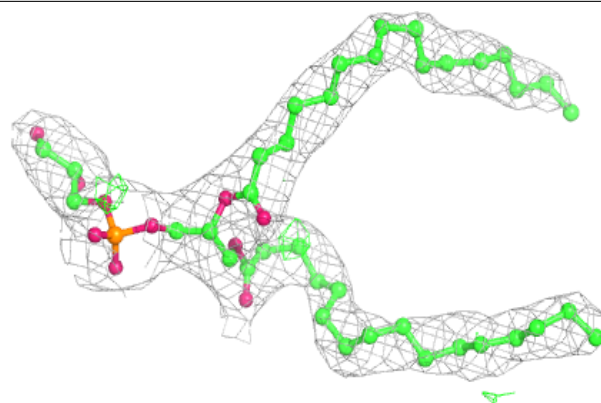
**Electron density around CLA B 1235:**

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

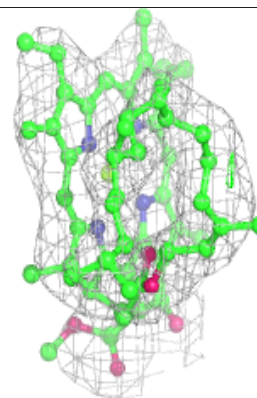
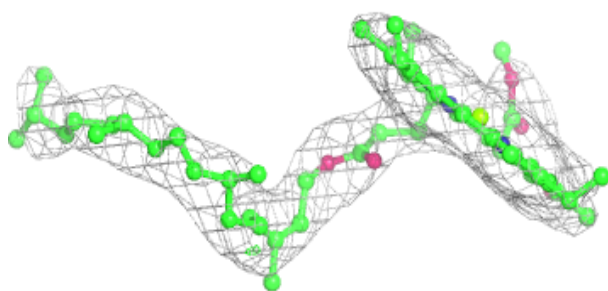
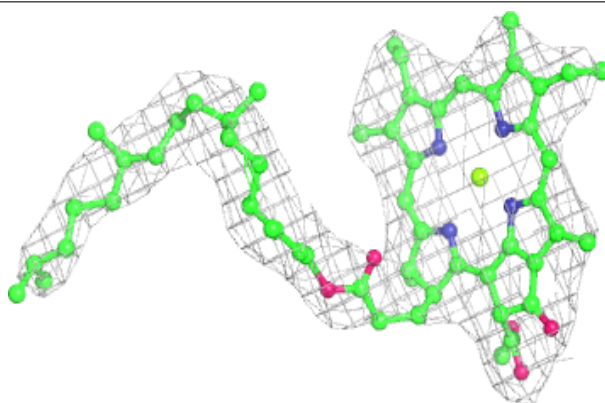


Electron density around LHG A 5001:

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

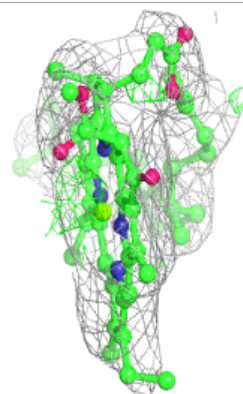
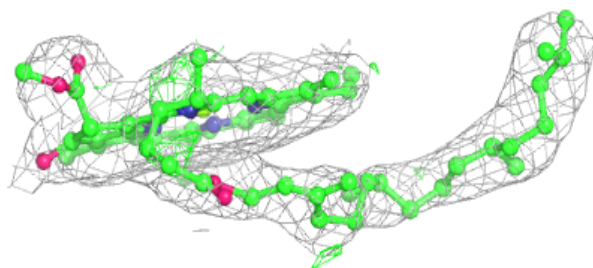
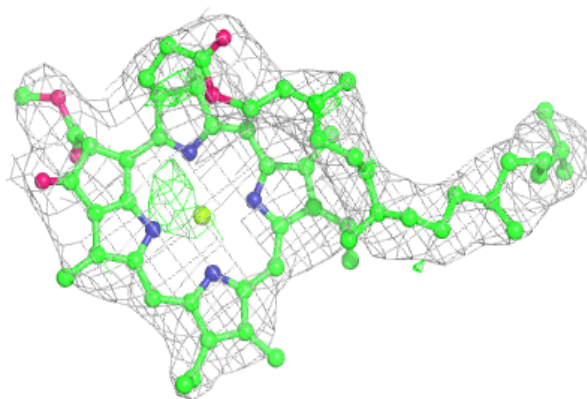
**Electron density around CLA A 1106:**

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

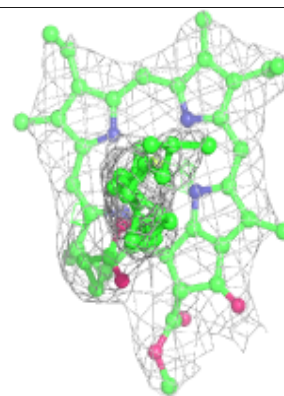
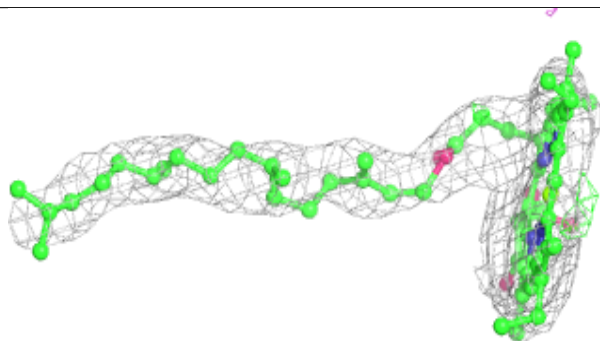
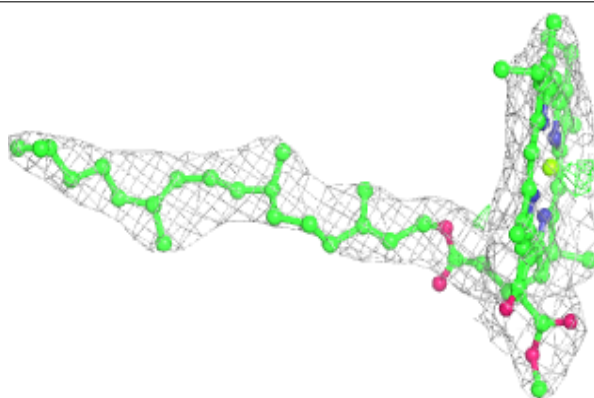


Electron density around CLA B 1215:

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

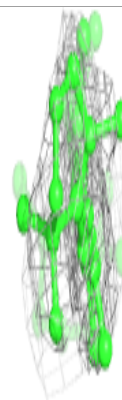
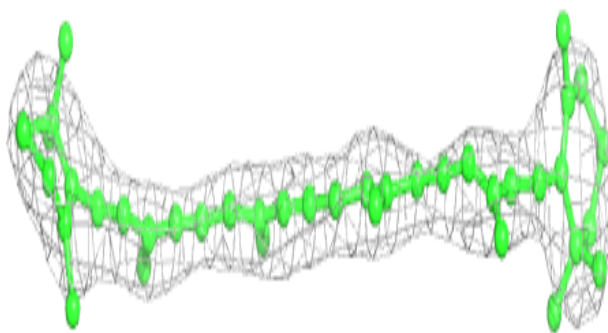
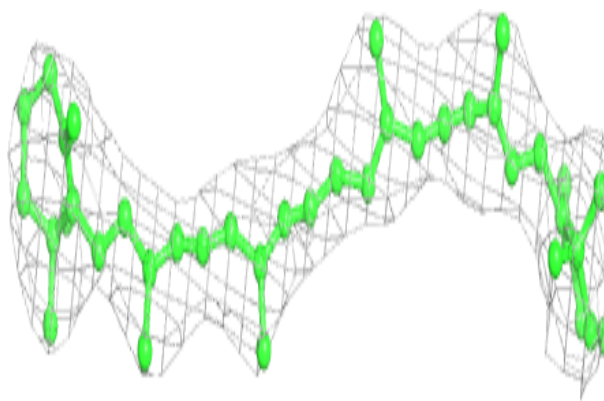
**Electron density around CLA A 1126:**

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

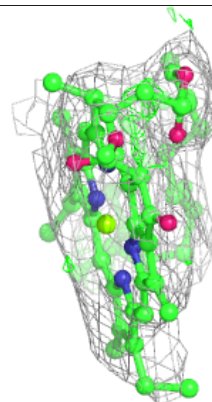
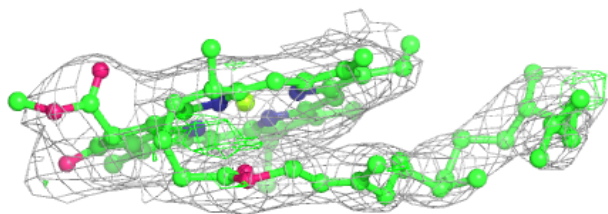
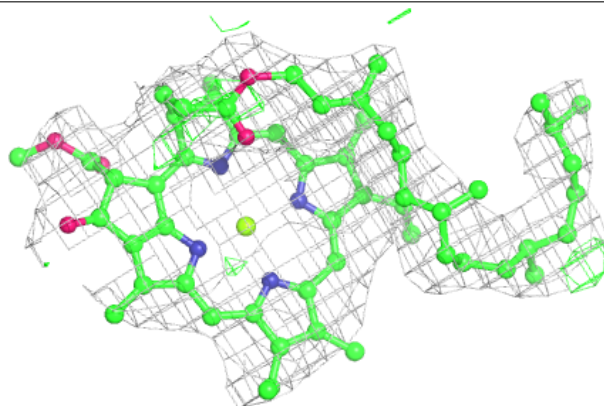


Electron density around BCR B 4017:

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

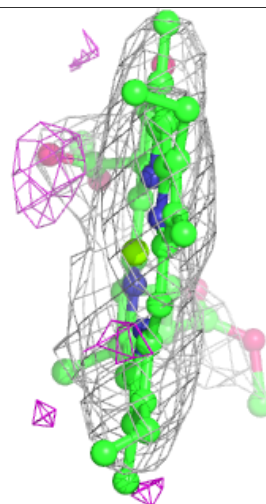
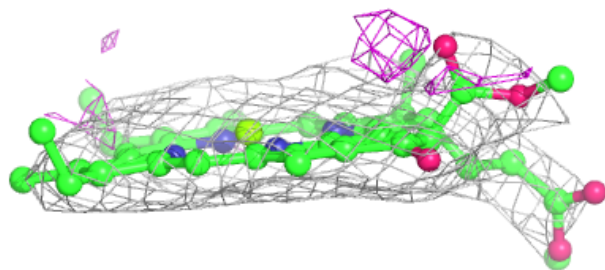
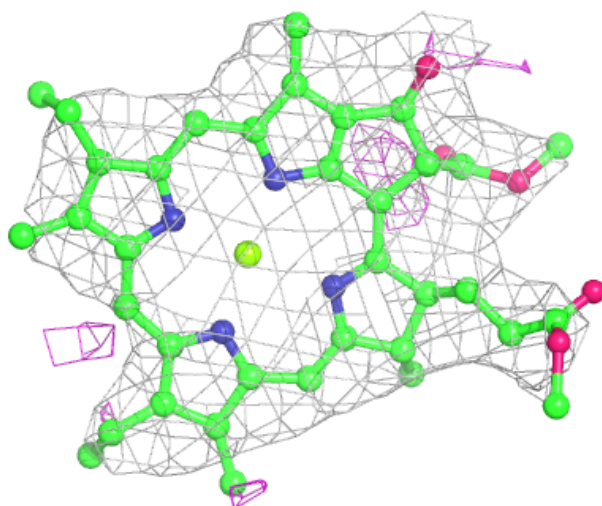
**Electron density around CLA A 1117:**

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



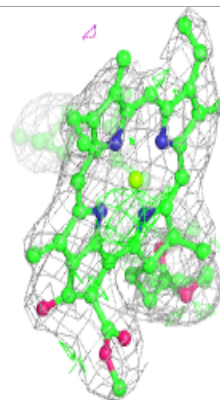
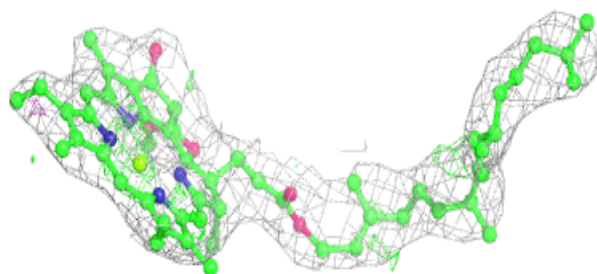
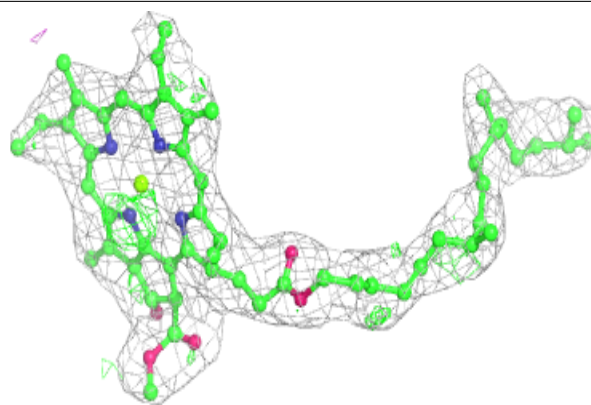
Electron density around CLA B 1206:

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

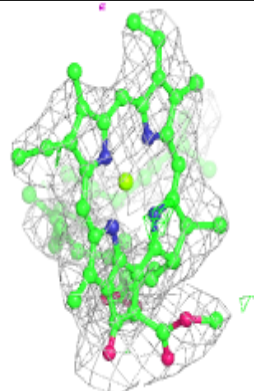
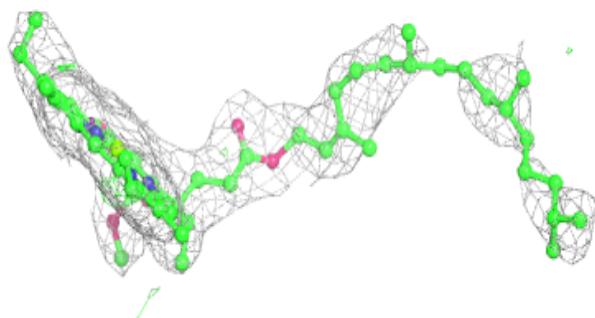
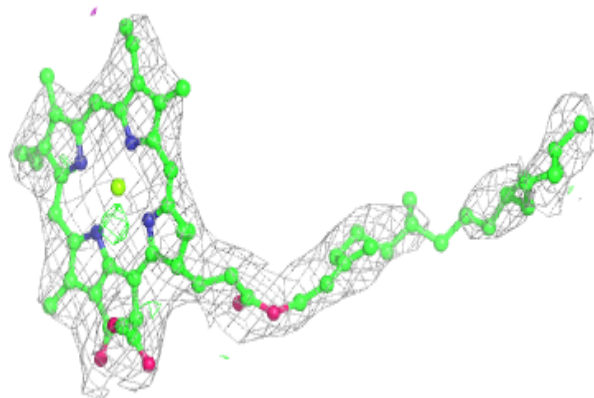


Electron density around CLA A 1012:

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

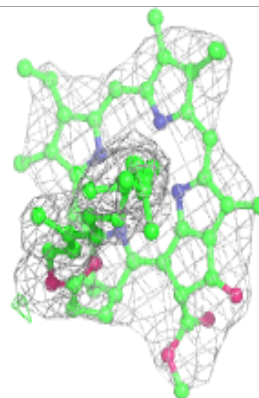
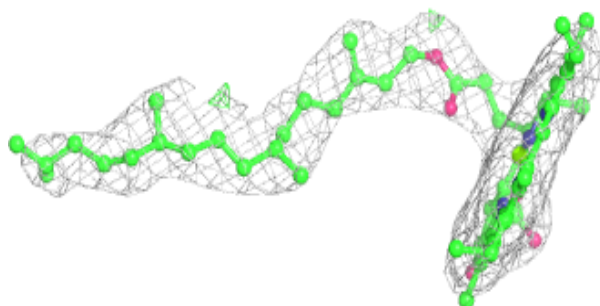
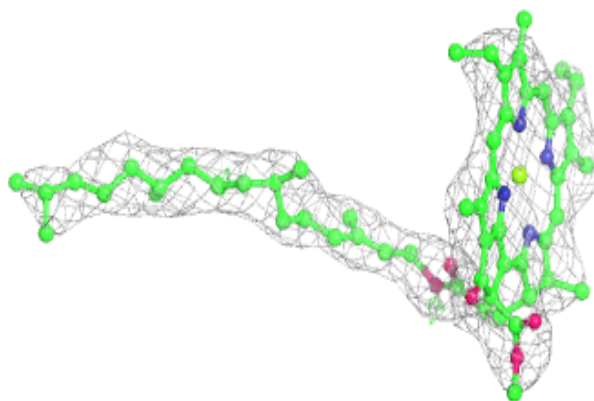
**Electron density around CLA B 1230:**

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

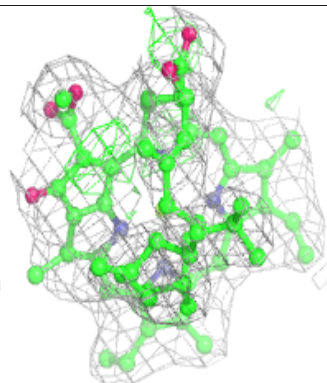
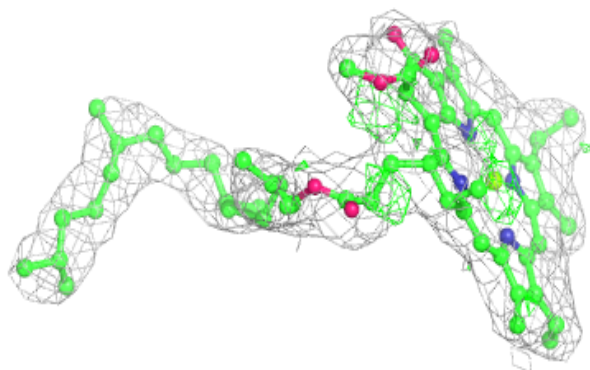
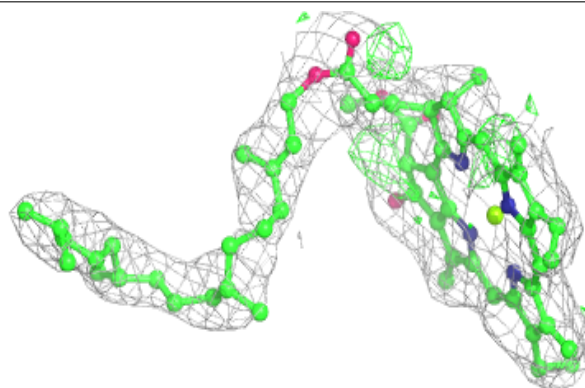


Electron density around CLA B 1225:

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

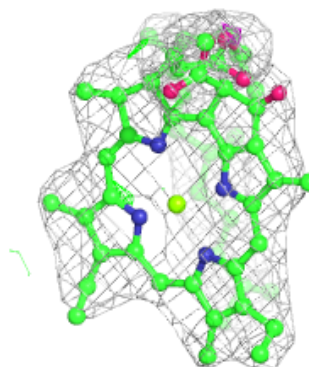
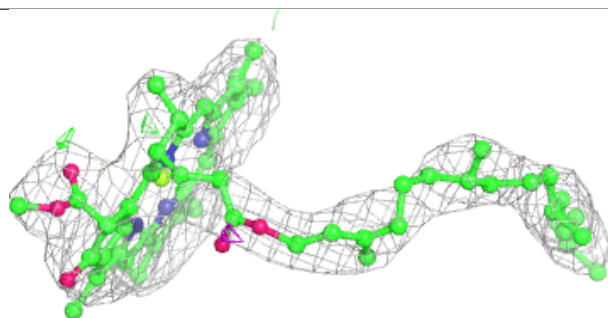
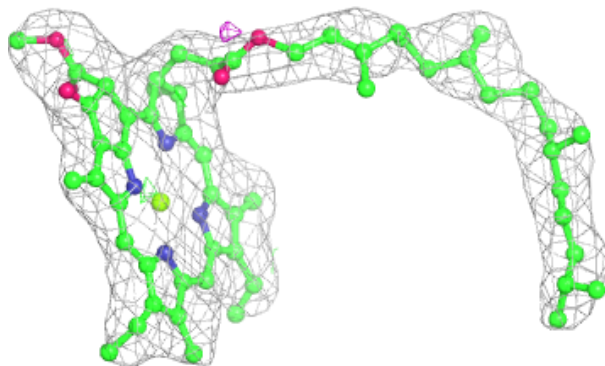
**Electron density around CLA B 1021:**

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



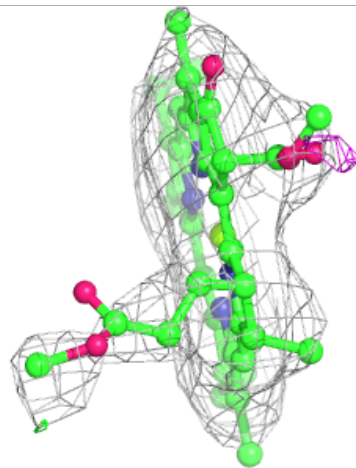
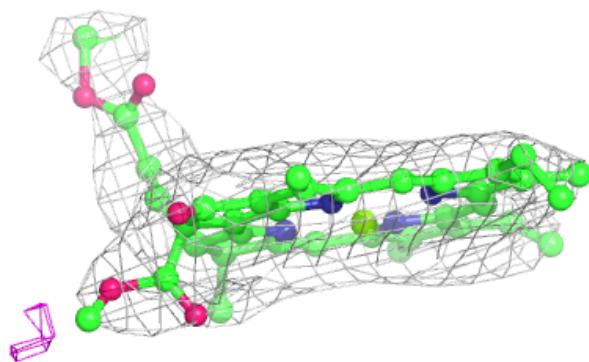
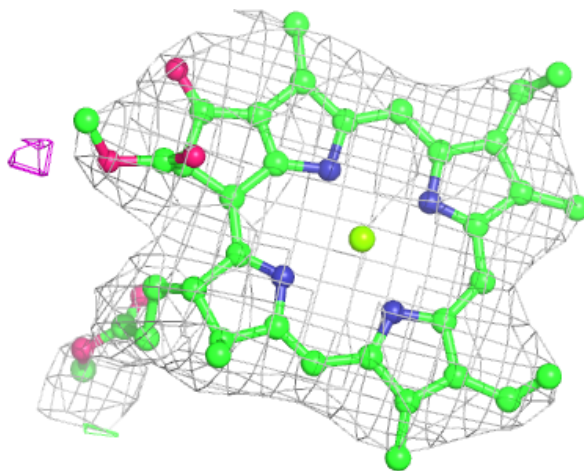
Electron density around CLA A 1140:

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



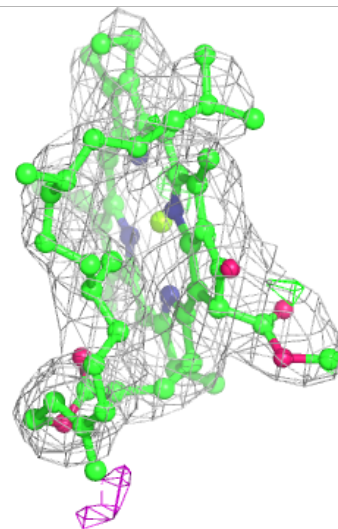
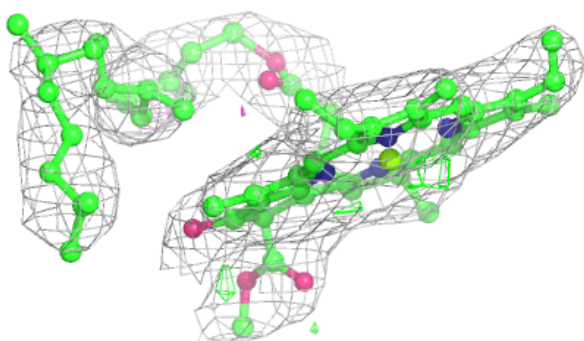
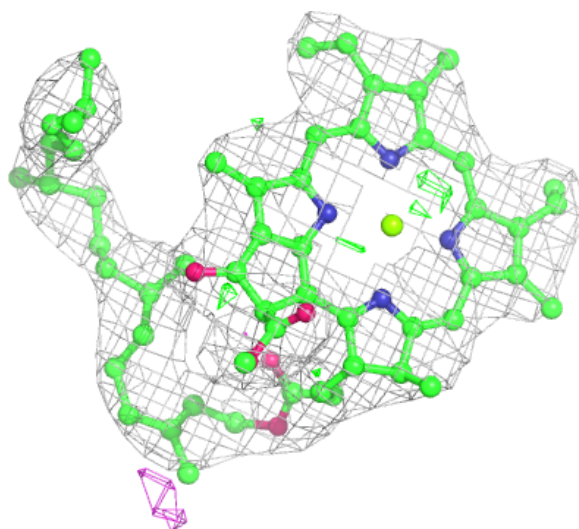
Electron density around CLA B 1239:

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



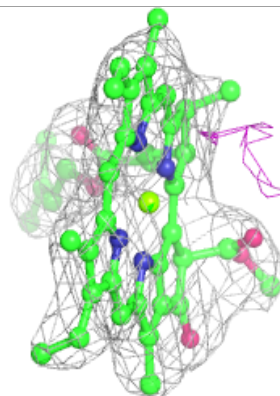
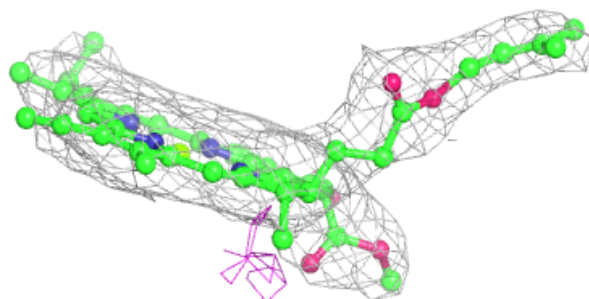
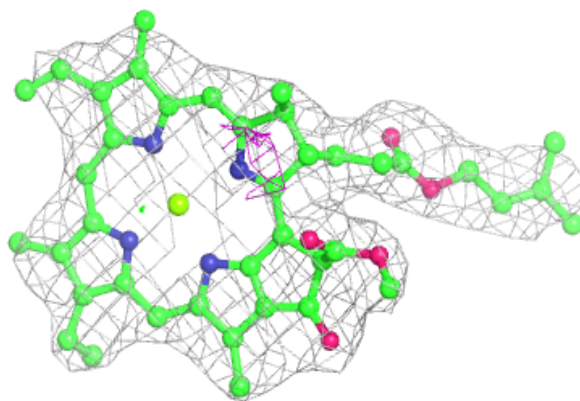
Electron density around CLA B 1229:

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



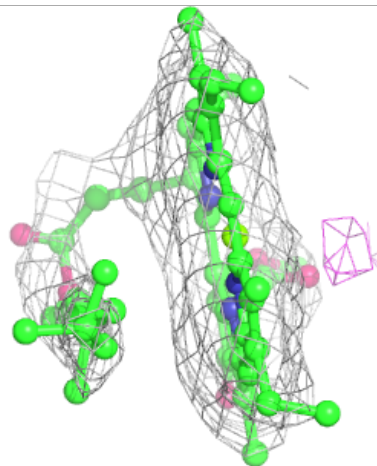
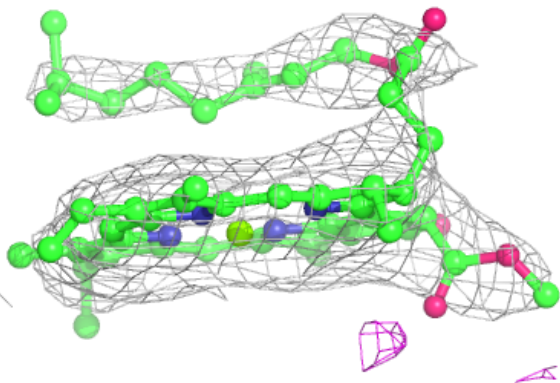
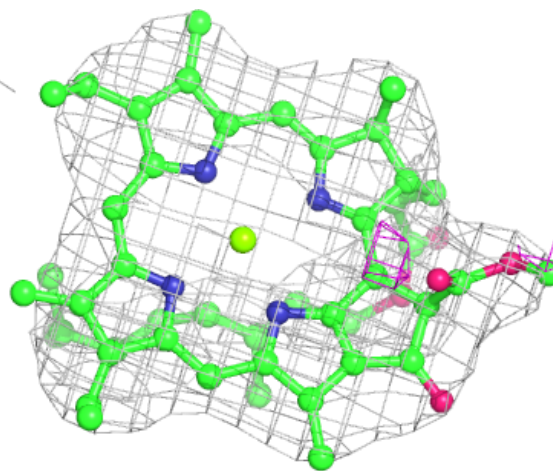
Electron density around CLA A 1107:

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



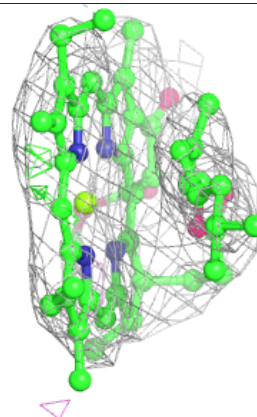
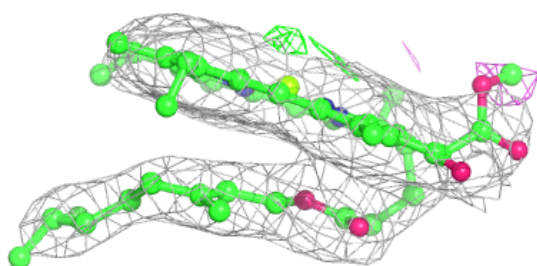
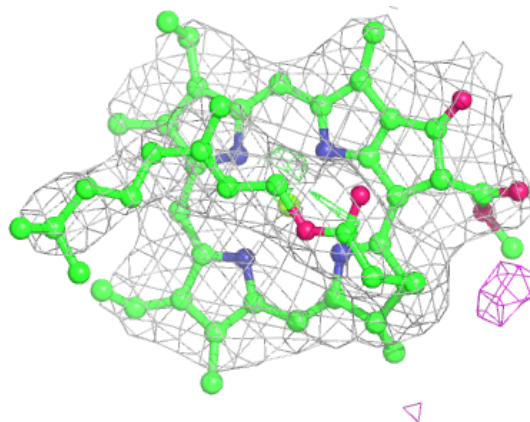
Electron density around CLA A 1130:

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



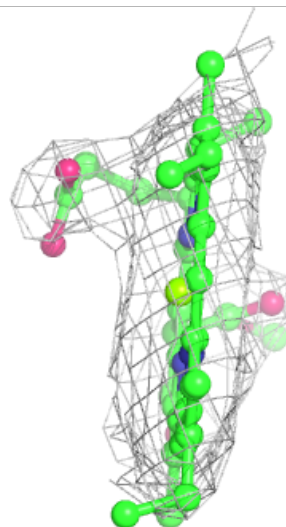
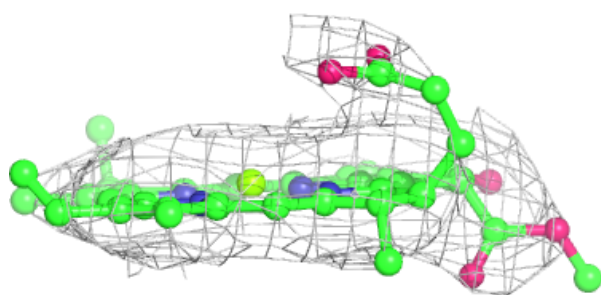
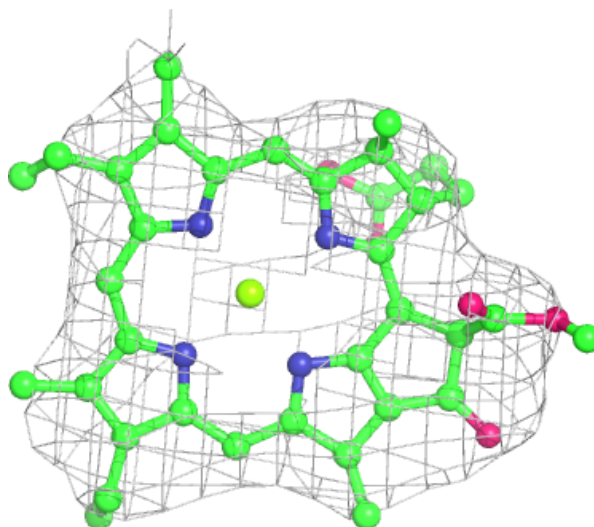
Electron density around CLA B 1205:

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



Electron density around CLA B 1209:

$2mF_o-DF_c$ (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.