Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:25 PM UTC

PDB ID	:	4KT0 / pdb_00004kt0
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

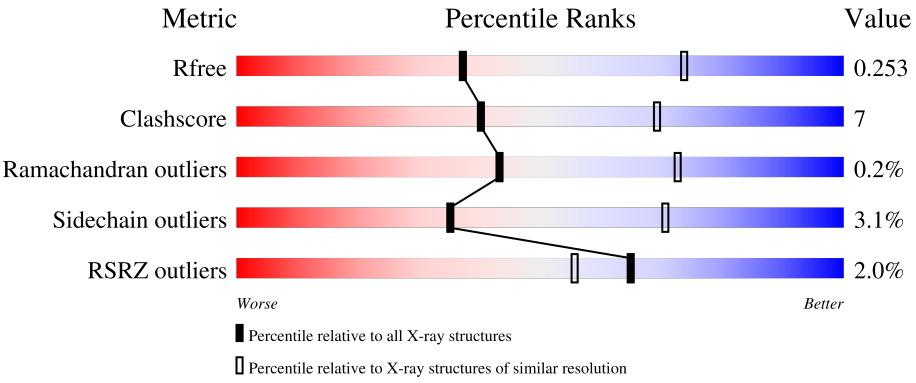
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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 <=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	89% 9% ·
2	B	731	89% 10% ·
3	C	81	4% 93% 5% ··
4	D	141	3% 89% 9% ··
5	E	74	78% 12% · 8%

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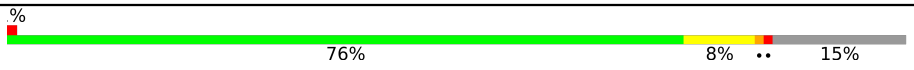
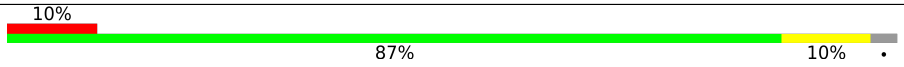
Mol	Chain	Length	Quality of chain
6	F	165	
7	J	40	
8	K	128	
9	M	31	

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	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	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	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	1215	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	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1228	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

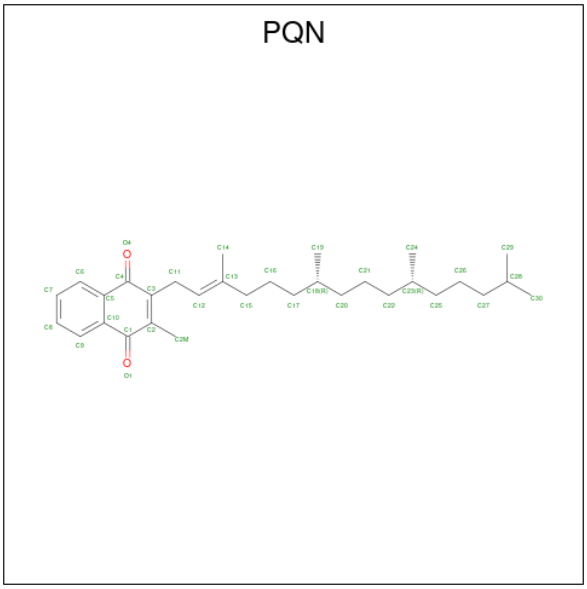
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

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.

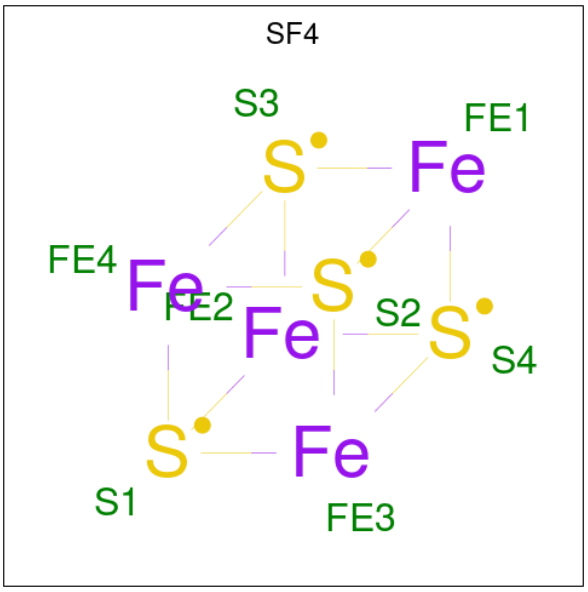
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	30	Total	C	N	O	0	0	0
			214	142	34	38			

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



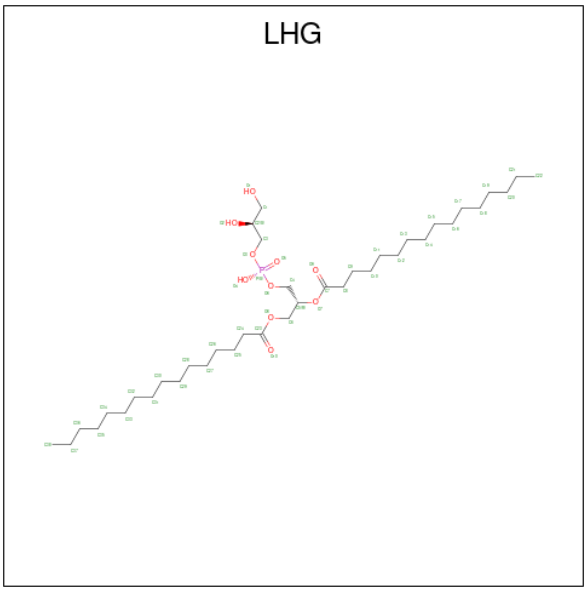
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			33	31	2		
10	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



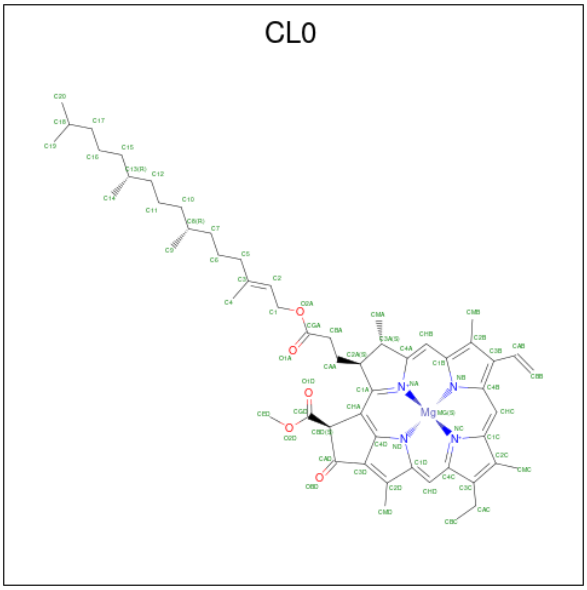
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Fe S 8 4 4	0	0
11	C	1	Total Fe S 8 4 4	0	0
11	C	1	Total Fe S 8 4 4	0	0

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



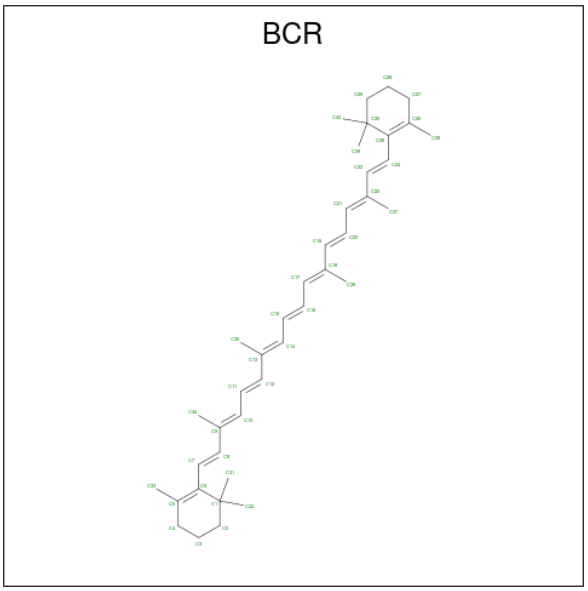
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			36	25	10	1		
12	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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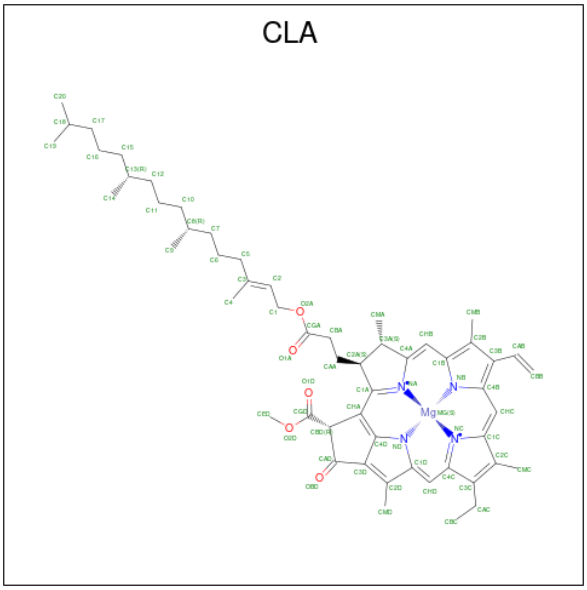
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C Mg N O 52 42 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0

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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
			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
			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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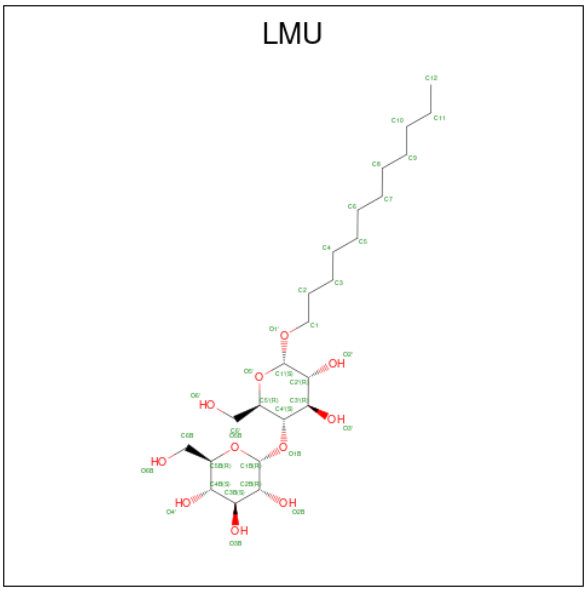
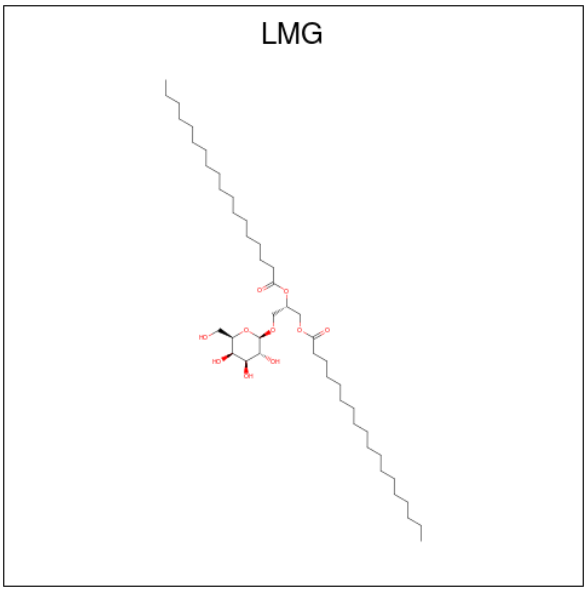
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
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 (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

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

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

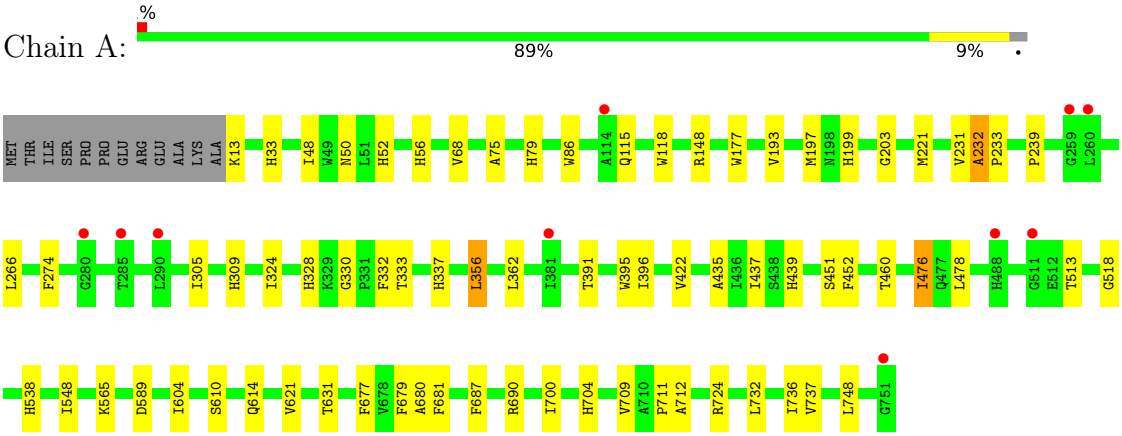
- Molecule 19 is water.

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

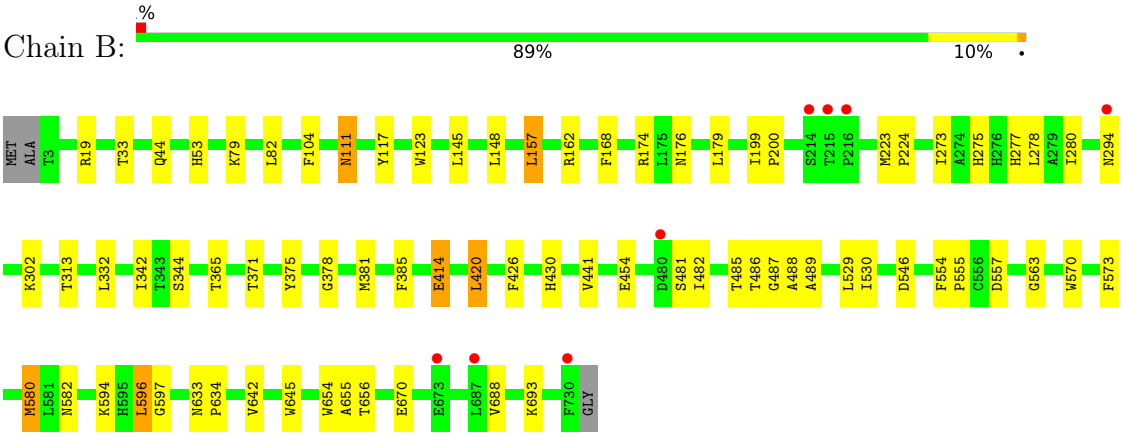
3 Residue-property plots (i)

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

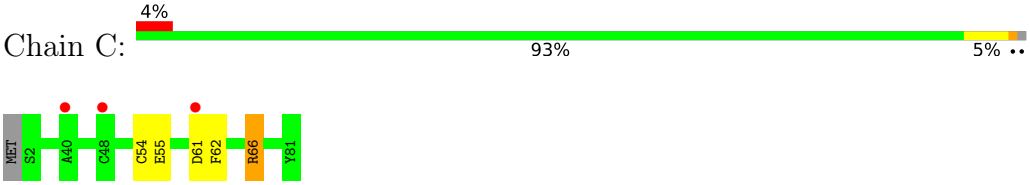
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

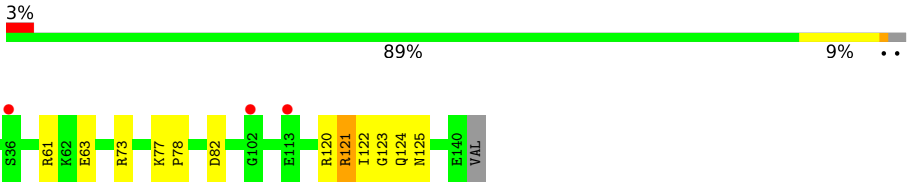


• Molecule 3: Photosystem I iron-sulfur center



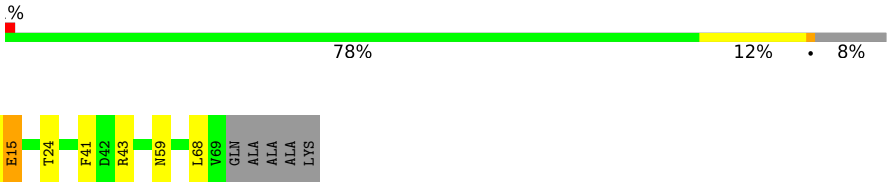
• Molecule 4: Photosystem I subunit II

Chain D:



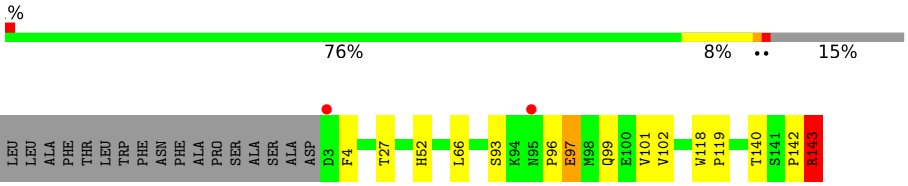
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



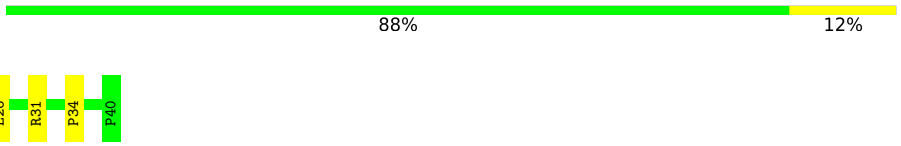
• Molecule 6: Photosystem I subunit III

Chain F:



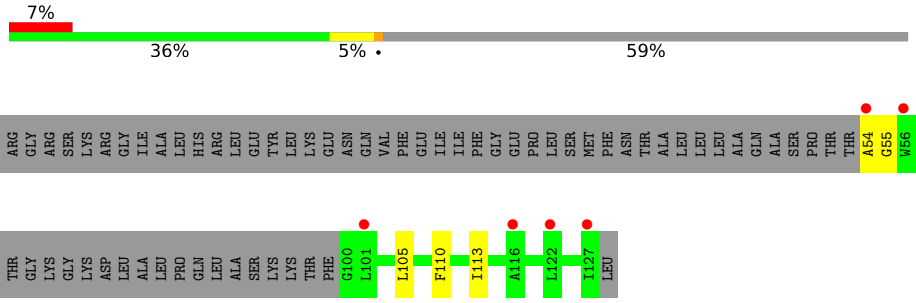
• Molecule 7: Photosystem I reaction center subunit IX

Chain J:



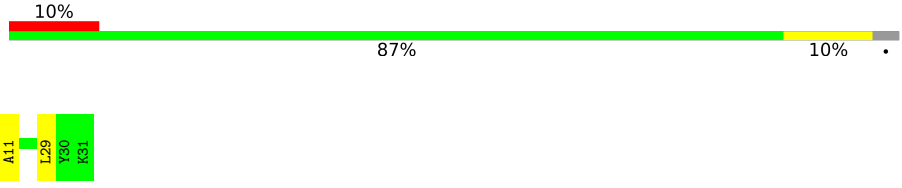
• Molecule 8: Photosystem I reaction center subunit PsaK

Chain K:



• Molecule 9: Photosystem I reaction center subunit XII

Chain M:



4 Data and refinement statistics (i)

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 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-2.80) 84.3 (29.98-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.245 0.207 , 0.253	Depositor DCC
R_{free} test set	5715 reflections (4.85%)	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)	0.28 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CLA, LMU, LMG, SF4, CL0, LHG, BCR, CL, PQN

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	0.30	0/5985	0.65	0/8158
2	B	0.31	0/5976	0.65	0/8173
3	C	0.33	0/610	0.65	0/826
4	D	0.29	0/1099	0.60	0/1482
5	E	0.29	0/542	0.69	0/733
6	F	0.33	0/1129	0.69	0/1535
7	J	0.31	0/328	0.65	0/443
8	K	0.36	0/371	0.75	0/499
9	M	0.30	0/217	0.68	0/295
All	All	0.31	0/16257	0.65	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5646	67	0
2	B	5765	0	5544	62	0
3	C	600	0	581	5	0
4	D	1075	0	1069	8	0
5	E	533	0	517	9	0
6	F	1099	0	1096	8	0
7	J	319	0	328	5	0
8	K	366	0	376	7	0
9	M	214	0	213	2	0
10	A	33	0	46	0	0
10	B	33	0	46	2	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	10	0
14	A	240	0	294	21	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	76	0
15	B	2365	0	2272	69	0
15	F	175	0	177	4	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	4	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	289	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 7.

All (289) 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:H4	19:A:9109:HOH:O	1.32	1.23
13:A:1011:CL0:CMA	19:A:9109:HOH:O	1.91	1.06
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:HBA1	15:A:1110:CLA:HBD	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:H251	12:A:5005:LHG:HC81	1.66	0.78
15:J:1302:CLA:HHC	15:J:1302:CLA:HBB1	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
1:A:221:MET:HE1	1:A:274:PHE:HB2	1.69	0.74
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
14:A:4008:BCR:C8	15:A:1124:CLA:HAB	2.21	0.70
15:A:1101:CLA:H203	15:A:1126:CLA:H202	1.73	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:HBA1	15:A:1110:CLA:CBD	2.23	0.69
15:A:1131:CLA:HHC	15:A:1131:CLA:HBB1	1.74	0.69
15:A:1101:CLA:HHC	15:A:1101:CLA:HBB1	1.74	0.69
15:B:1240:CLA:HAB	15:B:1220:CLA:HMB1	1.73	0.68
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:680:ALA:C	15:B:1013:CLA:HAB	2.20	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
1:A:239:PRO:HB2	15:A:1112:CLA:HMD1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1131:CLA:CBB	12:A:5005:LHG:H281	2.26	0.65
15:A:1801:CLA:HAB	15:A:1122:CLA:HMB1	1.79	0.65
15:A:1012:CLA:H42	14:B:4011:BCR:H362	1.77	0.65
15:A:1107:CLA:HHC	15:A:1107:CLA:HBB1	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:H41	16:J:1304:LMU:H82	1.80	0.63
13:A:1108:CL0:H15	13:A:1108:CL0:H2	1.81	0.63
1:A:604:ILE:CD1	13:A:1011:CL0:H35	2.29	0.62
12:A:5005:LHG:H251	12:A:5005:LHG:HC82	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
2:B:430:HIS:HB2	14:F:4015:BCR:HC22	1.83	0.61
1:A:79:HIS:CE1	15:A:1103:CLA:HMA2	2.36	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
15:B:1216:CLA:HMB2	15:B:1221:CLA:CED	2.31	0.60
15:A:1110:CLA:HMB1	15:A:1118:CLA:C4D	2.32	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
2:B:530:ILE:HG12	15:B:1013:CLA:HMD3	1.83	0.59
1:A:679:PHE:CD1	13:A:1011:CL0:H6	2.37	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:C1A	15:B:1205:CLA:CGA	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:B:1013:CLA:HMA2	15:B:1013:CLA:H2	1.85	0.58
15:A:1104:CLA:HHC	15:A:1104:CLA:HBB1	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
15:B:1220:CLA:HMD3	15:B:1221:CLA:HHC	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:THR:N	2:B:487:GLY:HA2	2.19	0.56
2:B:176:ASN:HB3	15:B:1217:CLA:HMD2	1.88	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
1:A:677:PHE:CD2	14:B:4011:BCR:H363	2.41	0.55
15:B:1231:CLA:C4C	15:B:1232:CLA:HAB	2.37	0.55
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
14:A:4012:BCR:C8	15:A:1107:CLA:HMB3	2.37	0.55
2:B:275:HIS:HB3	15:B:1214:CLA:HMB2	1.89	0.54
15:A:1119:CLA:HMB2	15:A:1123:CLA:CED	2.37	0.54
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:HG22	5:E:14:THR:O	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
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:HBA1	15:A:1110:CLA:CHA	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
1:A:700:ILE:HD13	15:A:1138:CLA:HMD2	1.91	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
15:B:1212:CLA:HAB	15:B:1211:CLA:HMC1	1.91	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
1:A:395:TRP:NE1	15:A:1126:CLA:HAB	2.23	0.52
15:A:1110:CLA:HHC	15:A:1110:CLA:CBB	2.40	0.52
1:A:56:HIS:CG	15:A:1103:CLA:HAB	2.45	0.52
1:A:395:TRP:HD1	15:A:1126:CLA:HAB	1.73	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
2:B:554:PHE:HB2	2:B:555:PRO:HD2	1.92	0.51
10:B:2002:PQN:H303	15:B:1239:CLA:O1A	2.11	0.51
1:A:711:PRO:HB2	19:F:9301:HOH:O	2.09	0.51
15:B:1228:CLA:HBC2	15:B:1236:CLA:HMC2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	8:K:58:LEU:N	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
15:A:1104:CLA:HMB1	15:A:1128:CLA:HBB2	1.94	0.50
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
1:A:33:HIS:NE2	15:A:1109:CLA:O1A	2.32	0.49
13:A:1108:CL0:OBD	15:A:1110:CLA:H71	2.13	0.49
2:B:454:GLU:OE2	6:F:52:HIS:ND1	2.41	0.49
15:A:1122:CLA:HMD3	15:A:1123:CLA:HHC	1.95	0.49
2:B:642:VAL:HG22	15:B:1206:CLA:HHD	1.95	0.49
14:A:4012:BCR:C9	15:A:1107:CLA:HMB3	2.42	0.49
2:B:53:HIS:CE1	15:B:1202:CLA:HMA2	2.47	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
1:A:333:THR:OG1	12:A:5003:LHG:HC2	2.13	0.48
14:A:4007:BCR:H351	14:A:4007:BCR:H15C	1.70	0.48
12:A:5005:LHG:HC82	12:A:5005:LHG:C23	2.43	0.48
2:B:420:LEU:HD22	2:B:529:LEU:HB2	1.94	0.48
14:A:4001:BCR:H24C	15:A:1120:CLA:HMD2	1.95	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
2:B:371:THR:HB	15:B:1224:CLA:HMB2	1.95	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:HD12	5:E:11:ILE:N	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:460:THR:HG23	15:B:1206:CLA:HMC3	1.96	0.47
1:A:610:SER:OG	1:A:614:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:ASN:HB2	2:B:634:PRO:CD	2.44	0.47
15:B:1215:CLA:CGA	15:B:1215:CLA:H3A	2.44	0.47
15:B:1235:CLA:C1A	15:B:1235:CLA:CGA	2.93	0.47
2:B:486:THR:OG1	2:B:487:GLY:HA2	2.13	0.47
15:B:1224:CLA:CGA	15:B:1224:CLA:H3A	2.45	0.47
1:A:687:PHE:HB2	15:B:1013:CLA:HBC2	1.97	0.47
8:K:58:LEU:N	8:K:58:LEU:HD13	2.29	0.47
15:B:1013:CLA:CGA	15:B:1013:CLA:H3A	2.46	0.46
14:A:4012:BCR:HC8	15:A:1107:CLA:HMB3	1.97	0.46
14:B:4010:BCR:H15C	14:B:4010:BCR:H351	1.69	0.46
1:A:197:MET:HE2	15:A:1119:CLA:HMA2	1.96	0.46
1:A:712:ALA:HB1	6:F:97:GLU:OE1	2.15	0.46
14:A:4003:BCR:H24C	15:A:1127:CLA:H2	1.97	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:OD1	2:B:111:ASN:N	2.49	0.46
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:H351	14:J:4013:BCR:H15C	1.67	0.46
15:A:1022:CLA:H171	14:B:4017:BCR:H343	1.96	0.46
14:B:4017:BCR:H351	14:B:4017:BCR:H15C	1.68	0.46
15:B:1203:CLA:OBD	15:B:1201:CLA:HHC	2.16	0.46
1:A:681:PHE:N	15:B:1013:CLA:HAB	2.30	0.45
15:A:1102:CLA:HMB1	15:A:1102:CLA:HBB1	1.98	0.45
2:B:199:ILE:HB	2:B:200:PRO:HD3	1.99	0.45
15:B:1215:CLA:HBB2	15:B:1221:CLA:H201	1.99	0.45
1:A:362:LEU:HD22	15:A:1127:CLA:H202	1.97	0.45
15:A:1114:CLA:HHC	15:A:1114:CLA:HBB1	1.97	0.45
15:A:1132:CLA:HMC3	15:B:1023:CLA:H122	1.99	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
14:B:4010:BCR:C23	14:B:4010:BCR:H403	2.46	0.45
15:B:1236:CLA:HHC	15:B:1236:CLA:HBB1	1.99	0.45
1:A:476:ILE:CD1	12:A:5005:LHG:HC81	2.45	0.45
5:E:13:ARG:O	5:E:14:THR:CB	2.59	0.45
15:A:1125:CLA:HMB1	15:A:1133:CLA:HBA1	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:THR:N	15:B:1023:CLA:HAB	2.32	0.44
1:A:391:THR:OG1	15:A:1126:CLA:HMB2	2.16	0.44
1:A:700:ILE:O	1:A:704:HIS:ND1	2.46	0.44
14:A:4008:BCR:H351	14:A:4008:BCR:H15C	1.63	0.44
14:A:4012:BCR:C8	14:A:4012:BCR:H331	2.45	0.44
15:A:1110:CLA:C1A	15:A:1110:CLA:CGA	2.95	0.44
1:A:193:VAL:CG1	15:A:1123:CLA:HHD	2.48	0.44
15:B:1231:CLA:O2A	15:B:1232:CLA:HMB1	2.17	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:H23C	14:B:4011:BCR:H392	2.00	0.44
15:F:1301:CLA:HMB1	7:J:26:LEU:HD21	1.99	0.44
1:A:337:HIS:CE1	12:A:5003:LHG:HC12	2.53	0.43
15:A:1801:CLA:HAB	15:A:1122:CLA:HHB	2.00	0.43
15:B:1215:CLA:HHC	15:B:1215:CLA:HBB1	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
2:B:655:ALA:C	15:B:1023:CLA:HAB	2.43	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
1:A:177:TRP:HB2	15:A:1109:CLA:HMC2	2.01	0.43
2:B:278:LEU:HG	15:B:1213:CLA:HAB	2.01	0.43
2:B:378:GLY:C	2:B:580:MET:SD	3.01	0.43
6:F:96:PRO:O	6:F:97:GLU:C	2.61	0.43
2:B:654:TRP:CD2	15:B:1021:CLA:HMA2	2.54	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
4:D:77:LYS:HB2	4:D:78:PRO:HD3	2.01	0.42
15:B:1222:CLA:HBA2	15:B:1222:CLA:H3A	1.88	0.42
14:A:4012:BCR:HC7	7:J:26:LEU:HD13	2.01	0.42
2:B:693:LYS:NZ	4:D:25:GLU:OE2	2.50	0.42
15:B:1215:CLA:HHC	15:B:1215:CLA:CBB	2.49	0.42
1:A:681:PHE:HA	15:B:1013:CLA:CAB	2.49	0.42
12:A:5003:LHG:H282	15:A:1122:CLA:H202	2.02	0.42
2:B:596:LEU:HA	2:B:596:LEU:HD12	1.81	0.42
1:A:356:LEU:HD11	15:A:1128:CLA:CBB	2.50	0.42
14:A:4007:BCR:H362	15:A:1122:CLA:HMB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:B:1235:CLA:HMA2	15:B:1236:CLA:CED	2.49	0.42
2:B:223:MET:N	2:B:224:PRO:CD	2.83	0.42
2:B:381:MET:HE1	14:B:4010:BCR:H361	2.01	0.42
2:B:580:MET:HE2	2:B:580:MET:HB3	1.91	0.42
14:B:4004:BCR:H15C	14:B:4004:BCR:H351	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
1:A:193:VAL:HG13	15:A:1123:CLA:HMD1	2.01	0.41
1:A:337:HIS:HE1	12:A:5003:LHG:HC12	1.83	0.41
15:A:1138:CLA:H203	15:F:1139:CLA:H62	2.02	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:CBB	15:A:1121:CLA:HHC	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
3:C:61:ASP:HB2	5:E:59:ASN:CG	2.46	0.41
6:F:27:THR:HG21	7:J:34:PRO:HG3	2.03	0.41
15:K:1401:CLA:CBB	15:K:1401:CLA:HHC	2.51	0.41
2:B:342:ILE:HG21	15:B:1221:CLA:H41	2.02	0.41
2:B:414:GLU:OE2	6:F:143:ARG:NH2	2.54	0.41
14:B:4017:BCR:H371	14:B:4017:BCR:H24C	1.78	0.41
15:A:1121:CLA:HHC	15:A:1121:CLA:HBB1	2.02	0.41
2:B:157:LEU:HD11	9:M:29:LEU:HD12	2.03	0.41
1:A:451:SER:OG	1:A:452:PHE:N	2.54	0.41
3:C:54:CYS:SG	3:C:55:GLU:N	2.94	0.41
4:D:120:ARG:HG2	4:D:124:GLN:HB2	2.01	0.41
8:K:55:GLY:O	8:K:59:SER:OG	2.30	0.41
1:A:565:LYS:NZ	2:B:670:GLU:OE2	2.44	0.40
15:B:1231:CLA:HHC	15:B:1231:CLA:CBB	2.51	0.40
1:A:681:PHE:CA	15:B:1013:CLA:HAB	2.50	0.40
15:A:1133:CLA:HHC	15:A:1133:CLA:CBB	2.51	0.40
15:A:1110:CLA:CMB	15:A:1118:CLA:C3D	2.99	0.40
12:A:5005:LHG:HC2	12:A:5005:LHG:O4	2.22	0.40
14:B:4004:BCR:HC8	14:B:4004:BCR:H321	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1221:CLA:H12	15:B:1221:CLA:HMA3	2.03	0.40
1:A:548:ILE:HG12	15:B:1023:CLA:HMD3	2.04	0.40
15:B:1218:CLA:HHC	15:B:1218:CLA:CBB	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	694 (94%)	40 (5%)	3 (0%)	30	60
2	B	726/731 (99%)	695 (96%)	31 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
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%)	43	72

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	580 (98%)	13 (2%)	45	78
2	B	582/583 (100%)	563 (97%)	19 (3%)	33	69
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	84
4	D	112/116 (97%)	110 (98%)	2 (2%)	51	82
5	E	57/60 (95%)	53 (93%)	4 (7%)	14	40
6	F	118/137 (86%)	111 (94%)	7 (6%)	18	48
7	J	35/35 (100%)	34 (97%)	1 (3%)	37	73
8	K	37/100 (37%)	34 (92%)	3 (8%)	11	33
9	M	19/25 (76%)	19 (100%)	0	100	100
All	All	1621/1728 (94%)	1571 (97%)	50 (3%)	35	70

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	148	ARG
1	A	266	LEU
1	A	356	LEU
1	A	422	VAL
1	A	437	ILE
1	A	476	ILE
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	33	THR
2	B	79	LYS
2	B	82	LEU
2	B	111	ASN
2	B	145	LEU

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Mol	Chain	Res	Type
2	B	148	LEU
2	B	157	LEU
2	B	280	ILE
2	B	294	ASN
2	B	302	LYS
2	B	344	SER
2	B	414	GLU
2	B	420	LEU
2	B	441	VAL
2	B	482	ILE
2	B	573	PHE
2	B	580	MET
2	B	594	LYS
2	B	596	LEU
3	C	66	ARG
4	D	73	ARG
4	D	82	ASP
5	E	15	GLU
5	E	24	THR
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	140	THR
6	F	143	ARG
7	J	14	MET
8	K	58	LEU
8	K	105	LEU
8	K	113	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	54	ASN
1	A	79	HIS
1	A	138	GLN
1	A	441	ASN
1	A	484	GLN

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Mol	Chain	Res	Type
1	A	614	GLN
1	A	714	GLN
2	B	34	HIS
2	B	53	HIS
2	B	102	ASN
2	B	114	ASN
2	B	133	GLN
2	B	308	HIS
2	B	319	ASN
2	B	366	GLN
2	B	624	ASN
2	B	638	ASN
4	D	51	ASN
4	D	81	GLN
4	D	95	GLN
6	F	99	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 oligosaccharides 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	A	1102	15	69,73,73	2.38	22 (31%)	82,113,113	2.43	24 (29%)
15	CLA	B	1204	-	50,54,73	2.83	22 (44%)	59,90,113	2.77	21 (35%)
15	CLA	A	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.74	23 (39%)
15	CLA	B	1225	-	69,73,73	2.36	23 (33%)	82,113,113	2.45	25 (30%)
15	CLA	A	1116	-	58,62,73	2.59	21 (36%)	68,99,113	2.69	26 (38%)
15	CLA	B	1021	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	29 (35%)
15	CLA	B	1216	-	69,73,73	2.37	22 (31%)	82,113,113	2.35	24 (29%)
15	CLA	J	1302	7	49,53,73	2.69	21 (42%)	58,89,113	2.76	22 (37%)
12	LHG	B	5004	15	48,48,48	0.94	2 (4%)	51,54,54	1.15	4 (7%)
15	CLA	B	1239	-	50,54,73	2.84	21 (42%)	59,90,113	2.79	23 (38%)
15	CLA	A	1126	-	69,73,73	2.38	23 (33%)	82,113,113	2.55	28 (34%)
15	CLA	B	1234	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	25 (30%)
15	CLA	A	1135	-	59,63,73	2.57	21 (35%)	70,101,113	2.64	25 (35%)
14	BCR	A	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.41	25 (44%)
15	CLA	A	1109	15	69,73,73	2.38	22 (31%)	82,113,113	2.53	26 (31%)
15	CLA	A	1122	-	69,73,73	2.38	22 (31%)	82,113,113	2.46	26 (31%)
15	CLA	B	1222	-	60,64,73	2.52	21 (35%)	71,102,113	2.70	23 (32%)
14	BCR	B	4014	-	41,41,41	2.58	6 (14%)	56,56,56	6.83	19 (33%)
15	CLA	B	1240	12	49,53,73	2.72	22 (44%)	58,89,113	2.72	22 (37%)
15	CLA	A	1112	-	49,53,73	2.70	22 (44%)	58,89,113	2.78	22 (37%)
15	CLA	B	1205	-	59,63,73	2.54	21 (35%)	70,101,113	2.67	24 (34%)
15	CLA	A	1105	-	69,73,73	2.37	22 (31%)	82,113,113	2.47	25 (30%)
15	CLA	A	1127	-	69,73,73	2.37	23 (33%)	82,113,113	2.42	24 (29%)
15	CLA	A	1128	-	69,73,73	2.33	21 (30%)	82,113,113	2.44	27 (32%)
15	CLA	B	1202	-	69,73,73	2.36	22 (31%)	82,113,113	2.48	23 (28%)
15	CLA	B	1217	-	51,55,73	2.72	23 (45%)	60,91,113	2.78	22 (36%)
15	CLA	A	1117	-	69,73,73	2.39	22 (31%)	82,113,113	2.38	26 (31%)
15	CLA	B	1214	-	69,73,73	2.37	22 (31%)	82,113,113	2.45	25 (30%)
14	BCR	A	4003	-	41,41,41	2.57	6 (14%)	56,56,56	6.66	25 (44%)
15	CLA	B	1228	-	69,73,73	2.38	23 (33%)	82,113,113	2.38	23 (28%)
14	BCR	B	4011	-	41,41,41	2.59	6 (14%)	56,56,56	6.87	25 (44%)
15	CLA	A	1131	-	59,63,73	2.57	22 (37%)	70,101,113	2.69	26 (37%)
15	CLA	A	1124	-	59,63,73	2.57	22 (37%)	70,101,113	2.60	26 (37%)
14	BCR	B	4010	-	41,41,41	2.56	6 (14%)	56,56,56	6.80	23 (41%)
15	CLA	B	1231	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	B	1215	-	69,73,73	2.38	22 (31%)	82,113,113	2.53	26 (31%)
15	CLA	B	1223	-	69,73,73	2.36	22 (31%)	82,113,113	2.46	25 (30%)
15	CLA	B	1206	2	50,54,73	2.84	22 (44%)	59,90,113	2.71	23 (38%)
14	BCR	B	4004	-	41,41,41	2.58	6 (14%)	56,56,56	6.52	27 (48%)
10	PQN	B	2002	-	34,34,34	1.62	2 (5%)	43,45,45	1.15	4 (9%)
15	CLA	B	1210	-	69,73,73	2.35	22 (31%)	82,113,113	2.41	25 (30%)
15	CLA	B	1224	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	23 (28%)
15	CLA	B	1218	-	55,59,73	2.65	22 (40%)	64,96,113	2.82	27 (42%)
15	CLA	A	1012	19	69,73,73	2.39	22 (31%)	82,113,113	2.42	24 (29%)
15	CLA	A	1132	-	66,70,73	2.40	21 (31%)	78,109,113	2.57	24 (30%)
15	CLA	B	1213	-	54,58,73	2.69	22 (40%)	64,95,113	2.70	22 (34%)
12	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
14	BCR	B	4006	-	41,41,41	2.64	6 (14%)	56,56,56	6.84	24 (42%)
15	CLA	A	1136	-	69,73,73	2.35	21 (30%)	82,113,113	2.54	26 (31%)
14	BCR	B	4017	-	41,41,41	2.57	7 (17%)	56,56,56	6.74	25 (44%)
15	CLA	B	1211	-	50,54,73	2.83	22 (44%)	59,90,113	2.70	22 (37%)
15	CLA	B	1220	-	60,64,73	2.58	23 (38%)	71,102,113	2.52	25 (35%)
15	CLA	A	1138	-	69,73,73	2.41	22 (31%)	82,113,113	2.41	26 (31%)
15	CLA	B	1209	-	49,53,73	2.70	21 (42%)	58,89,113	2.79	24 (41%)
15	CLA	A	1101	-	69,73,73	2.36	23 (33%)	82,113,113	2.50	29 (35%)
15	CLA	B	1226	-	69,73,73	2.35	22 (31%)	82,113,113	2.48	23 (28%)
15	CLA	A	1110	-	58,62,73	2.55	21 (36%)	68,99,113	2.66	24 (35%)
15	CLA	B	1230	-	69,73,73	2.34	22 (31%)	82,113,113	2.57	26 (31%)
15	CLA	J	1303	-	50,54,73	2.85	23 (46%)	59,90,113	2.76	22 (37%)
15	CLA	A	1111	-	64,68,73	2.45	22 (34%)	76,107,113	2.51	24 (31%)
14	BCR	A	4002	-	41,41,41	2.58	7 (17%)	56,56,56	6.64	25 (44%)
16	LMU	J	1304	-	36,36,36	0.43	0	47,47,47	0.65	1 (2%)
11	SF4	C	3002	3	0,12,12	-	-	-		
15	CLA	A	1125	-	56,60,73	2.61	22 (39%)	65,97,113	2.81	27 (41%)
15	CLA	B	1235	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	25 (30%)
15	CLA	B	1219	-	59,63,73	2.57	23 (38%)	70,101,113	2.65	25 (35%)
12	LHG	A	5005	-	35,35,48	1.08	2 (5%)	38,41,54	1.16	4 (10%)
15	CLA	B	1229	-	69,73,73	2.34	22 (31%)	82,113,113	2.49	23 (28%)
15	CLA	B	1201	-	50,54,73	2.83	22 (44%)	59,90,113	2.74	22 (37%)
14	BCR	F	4016	-	41,41,41	2.57	6 (14%)	56,56,56	6.89	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	A	1107	1	54,58,73	2.67	23 (42%)	64,95,113	2.77	29 (45%)
15	CLA	A	1022	19	69,73,73	2.37	23 (33%)	82,113,113	2.39	22 (26%)
15	CLA	A	1133	-	50,54,73	2.83	22 (44%)	59,90,113	2.71	21 (35%)
15	CLA	B	1227	-	49,53,73	2.68	21 (42%)	58,89,113	2.85	22 (37%)
16	LMU	B	1301	-	36,36,36	0.45	0	47,47,47	0.90	4 (8%)
14	BCR	A	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.87	24 (42%)
15	CLA	A	1130	-	59,63,73	2.58	23 (38%)	70,101,113	2.56	23 (32%)
14	BCR	B	4005	-	41,41,41	2.58	6 (14%)	56,56,56	6.60	24 (42%)
15	CLA	A	1140	-	69,73,73	2.36	22 (31%)	82,113,113	2.41	23 (28%)
11	SF4	A	3001	1,2	0,12,12	-	-	-		
14	BCR	B	4009	-	41,41,41	2.59	7 (17%)	56,56,56	6.91	25 (44%)
10	PQN	A	2001	-	34,34,34	1.63	2 (5%)	43,45,45	1.08	4 (9%)
14	BCR	F	4015	-	41,41,41	2.59	7 (17%)	56,56,56	6.80	24 (42%)
15	CLA	B	1236	-	54,58,73	2.68	22 (40%)	64,95,113	2.75	25 (39%)
15	CLA	B	1212	-	49,53,73	2.70	22 (44%)	58,89,113	2.78	21 (36%)
15	CLA	F	1139	19	69,73,73	2.35	22 (31%)	82,113,113	2.42	24 (29%)
13	CL0	A	1011	-	58,73,73	3.17	17 (29%)	60,113,113	2.62	17 (28%)
14	BCR	A	4012	-	41,41,41	2.62	6 (14%)	56,56,56	6.35	23 (41%)
15	CLA	B	1221	-	69,73,73	2.36	23 (33%)	82,113,113	2.50	21 (25%)
11	SF4	C	3003	3	0,12,12	-	-	-		
15	CLA	A	1115	-	50,54,73	2.81	22 (44%)	59,90,113	2.71	21 (35%)
15	CLA	A	1129	-	50,54,73	2.83	22 (44%)	59,90,113	2.79	23 (38%)
15	CLA	B	1237	19	59,63,73	2.56	23 (38%)	70,101,113	2.64	24 (34%)
15	CLA	B	1238	19	47,52,73	2.75	21 (44%)	55,87,113	2.67	19 (34%)
14	BCR	A	4008	-	41,41,41	2.57	7 (17%)	56,56,56	6.95	24 (42%)
15	CLA	K	1402	-	50,54,73	2.83	21 (42%)	59,90,113	2.75	22 (37%)
15	CLA	A	1120	-	53,57,73	2.71	22 (41%)	61,93,113	2.81	24 (39%)
15	CLA	K	1401	-	50,54,73	2.83	22 (44%)	59,90,113	2.78	23 (38%)
15	CLA	A	1123	-	69,73,73	2.37	21 (30%)	82,113,113	2.47	25 (30%)
15	CLA	A	1801	12	56,60,73	2.65	23 (41%)	65,97,113	2.75	25 (38%)
15	CLA	A	1137	-	54,58,73	2.68	21 (38%)	64,95,113	2.73	22 (34%)
15	CLA	F	1410	6	69,73,73	2.37	23 (33%)	82,113,113	2.49	24 (29%)
15	CLA	A	1134	1	50,54,73	2.84	22 (44%)	59,90,113	2.70	20 (33%)
15	CLA	B	1208	-	49,53,73	2.71	21 (42%)	58,89,113	2.72	19 (32%)
15	CLA	B	1023	-	69,73,73	2.34	22 (31%)	82,113,113	2.41	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	A	1118	-	50,54,73	2.80	20 (40%)	59,90,113	2.79	21 (35%)
17	LMG	B	5002	-	55,55,55	0.92	2 (3%)	63,63,63	0.98	2 (3%)
15	CLA	A	1106	1	69,73,73	2.38	22 (31%)	82,113,113	2.52	24 (29%)
15	CLA	A	1104	-	69,73,73	2.33	21 (30%)	82,113,113	2.50	25 (30%)
15	CLA	B	1232	-	49,53,73	2.69	20 (40%)	58,89,113	2.72	21 (36%)
15	CLA	B	1203	-	69,73,73	2.35	21 (30%)	82,113,113	2.46	23 (28%)
15	CLA	F	1301	-	49,53,73	2.69	22 (44%)	58,89,113	2.72	20 (34%)
15	CLA	B	1207	-	50,54,73	2.83	22 (44%)	59,90,113	2.76	22 (37%)
13	CL0	A	1108	-	38,53,73	3.87	15 (39%)	36,89,113	3.13	15 (41%)
15	CLA	A	1114	-	53,57,73	2.71	22 (41%)	61,93,113	2.80	24 (39%)
15	CLA	B	1013	-	69,73,73	2.35	21 (30%)	82,113,113	2.53	28 (34%)
15	CLA	A	1103	-	69,73,73	2.36	22 (31%)	82,113,113	2.42	24 (29%)
15	CLA	A	1119	-	68,72,73	2.40	23 (33%)	80,111,113	2.42	25 (31%)
12	LHG	A	5003	15	48,48,48	0.95	2 (4%)	51,54,54	1.11	4 (7%)
14	BCR	J	4013	-	41,41,41	2.57	7 (17%)	56,56,56	6.78	26 (46%)
15	CLA	A	1121	-	50,54,73	2.85	22 (44%)	59,90,113	2.72	21 (35%)

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	A	1102	15	1/1/15/20	13/39/115/115	-
15	CLA	B	1204	-	1/1/11/20	5/17/93/115	-
15	CLA	A	1113	-	1/1/11/20	4/15/91/115	-
15	CLA	B	1225	-	1/1/15/20	16/39/115/115	-
15	CLA	A	1116	-	1/1/12/20	9/26/102/115	-
15	CLA	B	1021	-	1/1/15/20	23/39/115/115	-
15	CLA	B	1216	-	-	13/39/115/115	-
15	CLA	J	1302	7	1/1/11/20	4/15/91/115	-
12	LHG	B	5004	15	-	21/53/53/53	-
15	CLA	B	1239	-	1/1/11/20	8/17/93/115	-
15	CLA	A	1126	-	-	11/39/115/115	-
15	CLA	B	1234	-	1/1/15/20	12/39/115/115	-
15	CLA	A	1135	-	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1122	-	1/1/15/20	18/39/115/115	-
14	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1109	15	-	11/39/115/115	-
15	CLA	B	1222	-	-	11/29/105/115	-
14	BCR	B	4014	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1240	12	1/1/11/20	6/15/91/115	-
15	CLA	A	1112	-	1/1/11/20	6/15/91/115	-
15	CLA	B	1205	-	1/1/13/20	13/27/103/115	-
15	CLA	A	1105	-	1/1/15/20	13/39/115/115	-
15	CLA	A	1127	-	1/1/15/20	17/39/115/115	-
15	CLA	A	1128	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1202	-	1/1/15/20	21/39/115/115	-
15	CLA	B	1217	-	1/1/11/20	9/18/94/115	-
15	CLA	A	1117	-	1/1/15/20	17/39/115/115	-
15	CLA	B	1214	-	-	13/39/115/115	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1228	-	1/1/15/20	18/39/115/115	-
14	BCR	B	4011	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1131	-	1/1/13/20	10/27/103/115	-
15	CLA	A	1124	-	1/1/13/20	9/27/103/115	-
15	CLA	B	1231	-	1/1/15/20	13/39/115/115	-
14	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1215	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1223	-	1/1/15/20	18/39/115/115	-
15	CLA	B	1206	2	1/1/11/20	8/17/93/115	-
15	CLA	B	1210	-	1/1/15/20	17/39/115/115	-
10	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1224	-	1/1/15/20	14/39/115/115	-
15	CLA	B	1218	-	1/1/12/20	10/23/99/115	-
15	CLA	A	1012	19	1/1/15/20	14/39/115/115	-
15	CLA	A	1132	-	1/1/14/20	16/36/112/115	-
15	CLA	B	1213	-	-	9/21/97/115	-
12	LHG	A	5001	-	-	28/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1136	-	1/1/15/20	16/39/115/115	-
14	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1211	-	1/1/11/20	9/17/93/115	-
15	CLA	B	1220	-	1/1/13/20	7/29/105/115	-
15	CLA	A	1138	-	1/1/15/20	5/39/115/115	-
15	CLA	B	1209	-	1/1/11/20	8/15/91/115	-
15	CLA	A	1101	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
15	CLA	A	1110	-	1/1/12/20	10/26/102/115	-
15	CLA	B	1230	-	1/1/15/20	15/39/115/115	-
15	CLA	J	1303	-	1/1/11/20	5/17/93/115	-
15	CLA	A	1111	-	1/1/14/20	14/33/109/115	-
14	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
16	LMU	J	1304	-	-	10/21/61/61	0/2/2/2
11	SF4	C	3002	3	-	-	0/6/5/5
15	CLA	A	1125	-	1/1/12/20	5/24/100/115	-
15	CLA	B	1235	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1219	-	1/1/13/20	9/27/103/115	-
12	LHG	A	5005	-	-	24/40/40/53	-
15	CLA	B	1229	-	1/1/15/20	21/39/115/115	-
15	CLA	B	1201	-	1/1/11/20	4/17/93/115	-
14	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1107	1	-	6/21/97/115	-
15	CLA	A	1022	19	1/1/15/20	11/39/115/115	-
15	CLA	A	1133	-	1/1/11/20	6/17/93/115	-
15	CLA	B	1227	-	-	4/15/91/115	-
16	LMU	B	1301	-	-	15/21/61/61	0/2/2/2
14	BCR	A	4007	-	-	6/29/63/63	0/2/2/2
15	CLA	A	1130	-	1/1/13/20	11/27/103/115	-
15	CLA	A	1140	-	1/1/15/20	16/39/115/115	-
14	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
11	SF4	A	3001	1,2	-	-	0/6/5/5
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
14	BCR	F	4015	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1236	-	1/1/12/20	5/21/97/115	-
15	CLA	B	1212	-	1/1/11/20	8/15/91/115	-
15	CLA	F	1139	19	1/1/15/20	12/39/115/115	-
13	CL0	A	1011	-	3/3/20/25	6/37/135/135	-
15	CLA	B	1221	-	1/1/15/20	9/39/115/115	-
14	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1115	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1129	-	1/1/11/20	12/17/93/115	-
11	SF4	C	3003	3	-	-	0/6/5/5
15	CLA	B	1237	19	1/1/13/20	10/27/103/115	-
15	CLA	B	1238	19	1/1/10/20	4/14/90/115	-
14	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
15	CLA	K	1402	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1120	-	1/1/11/20	10/20/96/115	-
15	CLA	K	1401	-	1/1/11/20	10/17/93/115	-
15	CLA	A	1123	-	1/1/15/20	18/39/115/115	-
15	CLA	A	1801	12	1/1/12/20	11/24/100/115	-
15	CLA	A	1137	-	1/1/12/20	7/21/97/115	-
15	CLA	F	1410	6	1/1/15/20	19/39/115/115	-
15	CLA	A	1134	1	1/1/11/20	7/17/93/115	-
15	CLA	B	1208	-	1/1/11/20	3/15/91/115	-
15	CLA	B	1023	-	1/1/15/20	13/39/115/115	-
15	CLA	A	1118	-	1/1/11/20	9/17/93/115	-
17	LMG	B	5002	-	-	30/50/70/70	0/1/1/1
15	CLA	A	1106	1	1/1/15/20	16/39/115/115	-
15	CLA	A	1104	-	1/1/15/20	12/39/115/115	-
15	CLA	B	1232	-	1/1/11/20	8/15/91/115	-
15	CLA	B	1203	-	1/1/15/20	11/39/115/115	-
15	CLA	F	1301	-	1/1/11/20	6/15/91/115	-
15	CLA	B	1207	-	1/1/11/20	8/17/93/115	-
13	CL0	A	1108	-	3/3/16/25	5/13/111/135	-
15	CLA	A	1114	-	1/1/11/20	7/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1013	-	-	17/39/115/115	-
15	CLA	A	1103	-	1/1/15/20	17/39/115/115	-
15	CLA	A	1119	-	-	13/37/113/115	-
12	LHG	A	5003	15	-	24/53/53/53	-
14	BCR	J	4013	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1121	-	1/1/11/20	7/17/93/115	-

All (2125) 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
15	B	1220	CLA	MG-NA	9.61	2.29	2.06
13	A	1011	CL0	C1A-CHA	9.60	1.50	1.40
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1103	CLA	MG-NA	9.30	2.28	2.06
15	B	1219	CLA	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	1202	CLA	MG-NA	9.28	2.28	2.06
15	B	1208	CLA	MG-NA	9.28	2.28	2.06
15	B	1228	CLA	MG-NA	9.28	2.28	2.06
13	A	1108	CL0	C1A-CHA	9.28	1.50	1.40
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
13	A	1108	CL0	C1B-C2B	9.21	1.50	1.39
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
13	A	1108	CL0	C1D-C2D	8.98	1.49	1.39
13	A	1011	CL0	C1D-C2D	8.75	1.49	1.39
13	A	1011	CL0	C1B-C2B	8.66	1.49	1.39
14	B	4009	BCR	C8-C9	-8.28	1.28	1.46
14	F	4015	BCR	C8-C9	-8.23	1.28	1.46
14	B	4014	BCR	C8-C9	-8.22	1.28	1.46
14	F	4016	BCR	C8-C9	-8.22	1.28	1.46
14	A	4012	BCR	C8-C9	-8.18	1.28	1.46
14	B	4005	BCR	C8-C9	-8.17	1.28	1.46
14	J	4013	BCR	C8-C9	-8.16	1.28	1.46
13	A	1108	CL0	C3B-C4B	8.12	1.49	1.41
14	B	4006	BCR	C8-C9	-8.11	1.28	1.46
14	A	4003	BCR	C8-C9	-8.11	1.28	1.46
14	A	4012	BCR	C11-C10	-8.11	1.18	1.43
14	B	4006	BCR	C11-C10	-8.08	1.18	1.43
14	B	4011	BCR	C8-C9	-8.06	1.28	1.46
14	A	4008	BCR	C8-C9	-8.05	1.28	1.46
14	A	4001	BCR	C8-C9	-8.05	1.28	1.46
14	A	4002	BCR	C8-C9	-8.00	1.28	1.46
14	F	4016	BCR	C11-C10	-7.98	1.18	1.43
14	B	4004	BCR	C8-C9	-7.98	1.28	1.46
14	A	4007	BCR	C8-C9	-7.96	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4017	BCR	C8-C9	-7.95	1.28	1.46
14	B	4004	BCR	C11-C10	-7.95	1.18	1.43
14	B	4010	BCR	C11-C10	-7.92	1.18	1.43
14	B	4010	BCR	C8-C9	-7.91	1.29	1.46
14	B	4011	BCR	C11-C10	-7.89	1.18	1.43
14	A	4002	BCR	C11-C10	-7.86	1.18	1.43
14	B	4014	BCR	C11-C10	-7.84	1.18	1.43
14	B	4009	BCR	C11-C10	-7.84	1.18	1.43
14	B	4005	BCR	C11-C10	-7.83	1.18	1.43
10	A	2001	PQN	C3-C2	7.81	1.49	1.35
14	F	4015	BCR	C11-C10	-7.81	1.19	1.43
14	B	4017	BCR	C11-C10	-7.80	1.19	1.43
14	A	4003	BCR	C11-C10	-7.79	1.19	1.43
14	A	4007	BCR	C11-C10	-7.78	1.19	1.43
14	A	4001	BCR	C11-C10	-7.77	1.19	1.43
10	B	2002	PQN	C3-C2	7.75	1.49	1.35
14	A	4008	BCR	C11-C10	-7.74	1.19	1.43
14	J	4013	BCR	C11-C10	-7.72	1.19	1.43
13	A	1011	CL0	C3B-C4B	7.58	1.48	1.41
14	B	4017	BCR	C20-C21	-7.27	1.20	1.43
14	B	4011	BCR	C20-C21	-7.26	1.20	1.43
14	A	4002	BCR	C20-C21	-7.23	1.20	1.43
14	A	4012	BCR	C20-C21	-7.23	1.20	1.43
14	A	4008	BCR	C20-C21	-7.22	1.20	1.43
14	B	4006	BCR	C20-C21	-7.22	1.20	1.43
14	A	4012	BCR	C16-C17	-7.20	1.20	1.43
14	F	4015	BCR	C20-C21	-7.18	1.20	1.43
14	B	4006	BCR	C16-C17	-7.18	1.20	1.43
14	B	4009	BCR	C20-C21	-7.16	1.21	1.43
14	B	4005	BCR	C20-C21	-7.14	1.21	1.43
14	A	4001	BCR	C20-C21	-7.14	1.21	1.43
14	A	4007	BCR	C20-C21	-7.14	1.21	1.43
14	J	4013	BCR	C20-C21	-7.13	1.21	1.43
14	F	4016	BCR	C20-C21	-7.13	1.21	1.43
14	A	4003	BCR	C20-C21	-7.12	1.21	1.43
14	A	4008	BCR	C16-C17	-7.12	1.21	1.43
14	A	4002	BCR	C16-C17	-7.12	1.21	1.43
14	B	4009	BCR	C16-C17	-7.12	1.21	1.43
14	A	4001	BCR	C16-C17	-7.11	1.21	1.43
14	B	4004	BCR	C20-C21	-7.10	1.21	1.43
14	B	4011	BCR	C16-C17	-7.10	1.21	1.43
14	A	4003	BCR	C16-C17	-7.09	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4005	BCR	C16-C17	-7.09	1.21	1.43
14	B	4014	BCR	C20-C21	-7.08	1.21	1.43
14	B	4010	BCR	C20-C21	-7.08	1.21	1.43
14	F	4015	BCR	C16-C17	-7.07	1.21	1.43
14	B	4004	BCR	C16-C17	-7.06	1.21	1.43
14	B	4017	BCR	C16-C17	-7.05	1.21	1.43
14	J	4013	BCR	C16-C17	-7.04	1.21	1.43
14	B	4014	BCR	C16-C17	-7.04	1.21	1.43
14	F	4016	BCR	C16-C17	-7.01	1.21	1.43
14	A	4007	BCR	C16-C17	-7.00	1.21	1.43
14	B	4010	BCR	C16-C17	-6.94	1.21	1.43
15	A	1118	CLA	O2A-C1	6.93	1.60	1.45
15	A	1129	CLA	O2A-C1	6.90	1.60	1.45
15	A	1134	CLA	O2A-C1	6.87	1.60	1.45
15	K	1401	CLA	O2A-C1	6.86	1.60	1.45
15	B	1239	CLA	O2A-C1	6.85	1.60	1.45
15	B	1201	CLA	O2A-C1	6.83	1.60	1.45
15	B	1206	CLA	O2A-C1	6.83	1.60	1.45
15	K	1402	CLA	O2A-C1	6.83	1.60	1.45
15	J	1303	CLA	O2A-C1	6.82	1.60	1.45
15	B	1211	CLA	O2A-C1	6.82	1.60	1.45
15	A	1115	CLA	O2A-C1	6.81	1.60	1.45
15	A	1121	CLA	O2A-C1	6.81	1.60	1.45
15	A	1133	CLA	O2A-C1	6.79	1.60	1.45
15	B	1207	CLA	O2A-C1	6.77	1.60	1.45
15	B	1204	CLA	O2A-C1	6.76	1.60	1.45
15	A	1106	CLA	O2A-C1	5.75	1.61	1.46
15	A	1012	CLA	O2A-C1	5.74	1.61	1.46
13	A	1108	CL0	CHB-C1B	5.73	1.48	1.39
15	B	1224	CLA	O2A-C1	5.70	1.61	1.46
15	A	1109	CLA	O2A-C1	5.68	1.61	1.46
15	B	1215	CLA	O2A-C1	5.66	1.61	1.46
15	A	1117	CLA	O2A-C1	5.61	1.61	1.46
15	B	1234	CLA	O2A-C1	5.58	1.61	1.46
15	A	1138	CLA	CHC-C1C	5.58	1.49	1.38
13	A	1108	CL0	CHC-C4B	5.58	1.48	1.39
15	B	1220	CLA	O2A-C1	5.57	1.61	1.46
15	A	1131	CLA	O2A-C1	5.55	1.61	1.46
15	B	1231	CLA	O2A-C1	5.54	1.61	1.46
15	A	1135	CLA	O2A-C1	5.53	1.61	1.46
15	A	1119	CLA	O2A-C1	5.53	1.61	1.46
15	A	1125	CLA	O2A-C1	5.52	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1116	CLA	O2A-C1	5.52	1.61	1.46
15	B	1013	CLA	O2A-C1	5.52	1.61	1.46
15	A	1138	CLA	O2A-C1	5.52	1.61	1.46
15	B	1205	CLA	O2A-C1	5.51	1.61	1.46
15	B	1213	CLA	O2A-C1	5.51	1.60	1.46
15	A	1136	CLA	O2A-C1	5.50	1.60	1.46
15	A	1102	CLA	O2A-C1	5.50	1.60	1.46
15	B	1235	CLA	O2A-C1	5.49	1.60	1.46
15	B	1218	CLA	O2A-C1	5.47	1.60	1.46
15	A	1105	CLA	O2A-C1	5.45	1.60	1.46
13	A	1011	CL0	O2A-C1	5.45	1.60	1.46
15	B	1226	CLA	O2A-C1	5.43	1.60	1.46
15	A	1130	CLA	O2A-C1	5.43	1.60	1.46
15	B	1236	CLA	O2A-C1	5.42	1.60	1.46
15	A	1128	CLA	O2A-C1	5.42	1.60	1.46
15	A	1124	CLA	O2A-C1	5.42	1.60	1.46
15	B	1219	CLA	O2A-C1	5.42	1.60	1.46
15	A	1120	CLA	O2A-C1	5.42	1.60	1.46
15	B	1221	CLA	O2A-C1	5.41	1.60	1.46
15	A	1801	CLA	O2A-C1	5.41	1.60	1.46
15	A	1114	CLA	O2A-C1	5.40	1.60	1.46
15	A	1111	CLA	O2A-C1	5.40	1.60	1.46
15	F	1410	CLA	O2A-C1	5.39	1.60	1.46
15	B	1223	CLA	O2A-C1	5.39	1.60	1.46
15	A	1137	CLA	O2A-C1	5.39	1.60	1.46
15	B	1228	CLA	CHC-C1C	5.38	1.49	1.38
15	A	1127	CLA	O2A-C1	5.38	1.60	1.46
15	B	1237	CLA	O2A-C1	5.37	1.60	1.46
15	B	1216	CLA	O2A-C1	5.36	1.60	1.46
15	B	1228	CLA	O2A-C1	5.36	1.60	1.46
15	A	1126	CLA	CHC-C1C	5.34	1.49	1.38
15	B	1021	CLA	O2A-C1	5.33	1.60	1.46
15	A	1107	CLA	O2A-C1	5.33	1.60	1.46
15	B	1202	CLA	O2A-C1	5.32	1.60	1.46
15	B	1229	CLA	O2A-C1	5.32	1.60	1.46
15	B	1236	CLA	CHC-C1C	5.32	1.49	1.38
15	B	1222	CLA	O2A-C1	5.32	1.60	1.46
15	A	1022	CLA	O2A-C1	5.31	1.60	1.46
15	A	1126	CLA	O2A-C1	5.31	1.60	1.46
15	A	1140	CLA	O2A-C1	5.31	1.60	1.46
15	A	1132	CLA	O2A-C1	5.30	1.60	1.46
15	B	1214	CLA	O2A-C1	5.30	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1235	CLA	CHC-C1C	5.30	1.49	1.38
15	B	1023	CLA	O2A-C1	5.28	1.60	1.46
15	A	1122	CLA	O2A-C1	5.27	1.60	1.46
15	A	1125	CLA	CHC-C1C	5.27	1.49	1.38
15	A	1123	CLA	O2A-C1	5.27	1.60	1.46
15	B	1013	CLA	O2D-CGD	5.27	1.46	1.33
15	A	1110	CLA	O2A-C1	5.27	1.60	1.46
15	A	1104	CLA	O2A-C1	5.27	1.60	1.46
15	B	1210	CLA	O2A-C1	5.26	1.60	1.46
15	A	1138	CLA	O2D-CGD	5.25	1.46	1.33
15	A	1101	CLA	CHC-C1C	5.24	1.49	1.38
15	A	1112	CLA	CHC-C1C	5.24	1.49	1.38
15	F	1139	CLA	O2D-CGD	5.24	1.46	1.33
15	A	1012	CLA	O2D-CGD	5.23	1.46	1.33
15	A	1101	CLA	O2A-C1	5.23	1.60	1.46
15	A	1119	CLA	O2D-CGD	5.23	1.46	1.33
15	K	1401	CLA	O2D-CGD	5.23	1.46	1.33
15	A	1122	CLA	CHC-C1C	5.23	1.49	1.38
15	A	1103	CLA	O2D-CGD	5.23	1.46	1.33
15	B	1225	CLA	O2A-C1	5.22	1.60	1.46
15	B	1235	CLA	O2D-CGD	5.22	1.46	1.33
15	A	1130	CLA	CHC-C1C	5.22	1.48	1.38
15	A	1136	CLA	O2D-CGD	5.21	1.46	1.33
15	A	1121	CLA	O2D-CGD	5.21	1.46	1.33
15	B	1203	CLA	O2A-C1	5.21	1.60	1.46
15	A	1109	CLA	O2D-CGD	5.21	1.46	1.33
15	A	1107	CLA	CHC-C1C	5.21	1.48	1.38
15	B	1203	CLA	O2D-CGD	5.21	1.46	1.33
15	A	1120	CLA	O2D-CGD	5.20	1.46	1.33
15	F	1301	CLA	O2D-CGD	5.20	1.46	1.33
15	A	1127	CLA	O2D-CGD	5.19	1.46	1.33
15	B	1202	CLA	O2D-CGD	5.19	1.46	1.33
15	A	1103	CLA	O2A-C1	5.19	1.60	1.46
15	B	1227	CLA	O2D-CGD	5.19	1.46	1.33
15	B	1232	CLA	O2D-CGD	5.19	1.46	1.33
15	B	1021	CLA	O2D-CGD	5.19	1.46	1.33
15	B	1219	CLA	O2D-CGD	5.18	1.46	1.33
15	B	1208	CLA	O2D-CGD	5.18	1.46	1.33
13	A	1011	CL0	CHC-C4B	5.18	1.48	1.39
15	J	1303	CLA	O2D-CGD	5.18	1.46	1.33
15	A	1117	CLA	O2D-CGD	5.18	1.46	1.33
13	A	1108	CL0	O2D-CGD	5.18	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1111	CLA	CHC-C1C	5.17	1.48	1.38
15	A	1115	CLA	CHC-C1C	5.17	1.48	1.38
15	A	1131	CLA	O2D-CGD	5.17	1.45	1.33
15	K	1402	CLA	O2D-CGD	5.17	1.45	1.33
15	B	1240	CLA	O2D-CGD	5.17	1.45	1.33
15	B	1230	CLA	O2A-C1	5.17	1.60	1.46
15	B	1237	CLA	O2D-CGD	5.17	1.45	1.33
15	A	1140	CLA	CHC-C1C	5.17	1.48	1.38
15	A	1022	CLA	O2D-CGD	5.16	1.45	1.33
15	B	1216	CLA	O2D-CGD	5.16	1.45	1.33
15	B	1218	CLA	O2D-CGD	5.16	1.45	1.33
15	B	1215	CLA	O2D-CGD	5.15	1.45	1.33
15	A	1112	CLA	O2D-CGD	5.15	1.45	1.33
15	B	1220	CLA	CHC-C1C	5.15	1.48	1.38
15	B	1230	CLA	CHC-C1C	5.14	1.48	1.38
15	A	1124	CLA	O2D-CGD	5.14	1.45	1.33
15	A	1801	CLA	O2D-CGD	5.14	1.45	1.33
15	B	1205	CLA	O2D-CGD	5.14	1.45	1.33
15	A	1103	CLA	CHC-C1C	5.14	1.48	1.38
15	B	1223	CLA	CHC-C1C	5.14	1.48	1.38
15	A	1133	CLA	O2D-CGD	5.14	1.45	1.33
15	B	1207	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1220	CLA	O2D-CGD	5.13	1.45	1.33
13	A	1011	CL0	O2D-CGD	5.13	1.45	1.33
15	A	1116	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1212	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1214	CLA	O2D-CGD	5.13	1.45	1.33
15	A	1134	CLA	CHC-C1C	5.13	1.48	1.38
15	A	1122	CLA	O2D-CGD	5.13	1.45	1.33
15	B	1230	CLA	O2D-CGD	5.12	1.45	1.33
15	B	1228	CLA	O2D-CGD	5.12	1.45	1.33
15	B	1206	CLA	O2D-CGD	5.12	1.45	1.33
15	A	1107	CLA	O2D-CGD	5.12	1.45	1.33
15	A	1118	CLA	O2D-CGD	5.12	1.45	1.33
15	A	1114	CLA	O2D-CGD	5.12	1.45	1.33
15	B	1209	CLA	O2D-CGD	5.12	1.45	1.33
15	A	1115	CLA	O2D-CGD	5.11	1.45	1.33
15	A	1105	CLA	O2D-CGD	5.11	1.45	1.33
15	A	1117	CLA	CHC-C1C	5.11	1.48	1.38
15	A	1106	CLA	O2D-CGD	5.11	1.45	1.33
15	A	1126	CLA	O2D-CGD	5.10	1.45	1.33
15	A	1129	CLA	O2D-CGD	5.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1211	CLA	O2D-CGD	5.10	1.45	1.33
15	B	1240	CLA	CHC-C1C	5.10	1.48	1.38
15	A	1113	CLA	O2D-CGD	5.10	1.45	1.33
15	A	1106	CLA	CHC-C1C	5.10	1.48	1.38
15	B	1224	CLA	O2D-CGD	5.09	1.45	1.33
15	B	1201	CLA	O2D-CGD	5.09	1.45	1.33
15	A	1132	CLA	O2D-CGD	5.09	1.45	1.33
15	F	1139	CLA	O2A-C1	5.09	1.59	1.46
15	B	1239	CLA	O2D-CGD	5.09	1.45	1.33
15	B	1204	CLA	O2D-CGD	5.09	1.45	1.33
15	A	1128	CLA	O2D-CGD	5.09	1.45	1.33
15	B	1221	CLA	O2D-CGD	5.09	1.45	1.33
15	A	1109	CLA	CHC-C1C	5.09	1.48	1.38
15	B	1214	CLA	CHC-C1C	5.09	1.48	1.38
15	A	1140	CLA	O2D-CGD	5.08	1.45	1.33
15	F	1410	CLA	O2D-CGD	5.08	1.45	1.33
15	B	1213	CLA	O2D-CGD	5.08	1.45	1.33
15	B	1023	CLA	O2D-CGD	5.08	1.45	1.33
15	J	1302	CLA	O2D-CGD	5.08	1.45	1.33
15	A	1022	CLA	CHC-C1C	5.07	1.48	1.38
15	B	1238	CLA	O2D-CGD	5.07	1.45	1.33
15	J	1303	CLA	CHC-C1C	5.07	1.48	1.38
15	F	1301	CLA	CHC-C1C	5.07	1.48	1.38
15	B	1013	CLA	CHC-C1C	5.07	1.48	1.38
15	A	1130	CLA	O2D-CGD	5.06	1.45	1.33
15	A	1111	CLA	O2D-CGD	5.06	1.45	1.33
15	B	1223	CLA	O2D-CGD	5.06	1.45	1.33
15	A	1127	CLA	CHC-C1C	5.06	1.48	1.38
15	B	1217	CLA	O2D-CGD	5.05	1.45	1.33
15	A	1137	CLA	O2D-CGD	5.05	1.45	1.33
15	B	1222	CLA	O2D-CGD	5.05	1.45	1.33
15	A	1132	CLA	CHC-C1C	5.05	1.48	1.38
15	B	1217	CLA	CHC-C1C	5.05	1.48	1.38
15	B	1210	CLA	CHC-C1C	5.05	1.48	1.38
15	A	1102	CLA	O2D-CGD	5.05	1.45	1.33
15	B	1202	CLA	CHC-C1C	5.04	1.48	1.38
15	A	1123	CLA	O2D-CGD	5.04	1.45	1.33
15	B	1213	CLA	CHC-C1C	5.04	1.48	1.38
15	B	1225	CLA	O2D-CGD	5.04	1.45	1.33
15	B	1211	CLA	CHC-C1C	5.03	1.48	1.38
13	A	1011	CL0	CHB-C1B	5.03	1.47	1.39
15	A	1119	CLA	CHC-C1C	5.03	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1236	CLA	O2D-CGD	5.03	1.45	1.33
15	B	1226	CLA	CHC-C1C	5.03	1.48	1.38
15	A	1102	CLA	CHC-C1C	5.02	1.48	1.38
15	A	1801	CLA	CHC-C1C	5.02	1.48	1.38
15	B	1225	CLA	CHC-C1C	5.02	1.48	1.38
15	K	1401	CLA	CHC-C1C	5.02	1.48	1.38
15	A	1101	CLA	O2D-CGD	5.02	1.45	1.33
15	K	1402	CLA	CHC-C1C	5.01	1.48	1.38
15	A	1110	CLA	O2D-CGD	5.01	1.45	1.33
15	A	1125	CLA	O2D-CGD	5.01	1.45	1.33
15	F	1410	CLA	CHC-C1C	5.01	1.48	1.38
15	A	1012	CLA	CHC-C1C	5.01	1.48	1.38
15	B	1212	CLA	CHC-C1C	5.01	1.48	1.38
15	A	1104	CLA	CHC-C1C	5.01	1.48	1.38
15	B	1210	CLA	O2D-CGD	5.01	1.45	1.33
15	A	1114	CLA	CHC-C1C	5.00	1.48	1.38
15	A	1135	CLA	O2D-CGD	5.00	1.45	1.33
15	A	1116	CLA	CHC-C1C	5.00	1.48	1.38
15	B	1229	CLA	O2D-CGD	5.00	1.45	1.33
13	A	1011	CL0	OBD-CAD	4.99	1.28	1.22
15	B	1231	CLA	O2D-CGD	4.99	1.45	1.33
15	B	1207	CLA	CHC-C1C	4.99	1.48	1.38
15	A	1124	CLA	CHC-C1C	4.99	1.48	1.38
15	A	1129	CLA	CHC-C1C	4.99	1.48	1.38
15	B	1229	CLA	CHC-C1C	4.99	1.48	1.38
15	B	1023	CLA	CHC-C1C	4.99	1.48	1.38
15	B	1208	CLA	CHC-C1C	4.98	1.48	1.38
15	A	1113	CLA	CHC-C1C	4.98	1.48	1.38
15	B	1021	CLA	CHC-C1C	4.98	1.48	1.38
15	B	1226	CLA	O2D-CGD	4.98	1.45	1.33
15	B	1219	CLA	CHC-C1C	4.98	1.48	1.38
15	B	1201	CLA	CHC-C1C	4.97	1.48	1.38
15	A	1137	CLA	CHC-C1C	4.97	1.48	1.38
15	B	1218	CLA	CHC-C1C	4.96	1.48	1.38
15	B	1209	CLA	CHC-C1C	4.96	1.48	1.38
15	A	1134	CLA	O2D-CGD	4.96	1.45	1.33
15	A	1133	CLA	CHC-C1C	4.96	1.48	1.38
15	A	1104	CLA	O2D-CGD	4.95	1.45	1.33
15	B	1237	CLA	CHC-C1C	4.95	1.48	1.38
13	A	1108	CL0	OBD-CAD	4.95	1.28	1.22
15	B	1216	CLA	CHC-C1C	4.94	1.48	1.38
15	B	1224	CLA	CHC-C1C	4.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1234	CLA	CHC-C1C	4.93	1.48	1.38
15	A	1120	CLA	CHC-C1C	4.93	1.48	1.38
15	B	1204	CLA	CHC-C1C	4.92	1.48	1.38
15	A	1121	CLA	CHC-C1C	4.92	1.48	1.38
15	F	1139	CLA	CHC-C1C	4.92	1.48	1.38
15	J	1302	CLA	CHC-C1C	4.91	1.48	1.38
15	A	1118	CLA	CHC-C1C	4.91	1.48	1.38
15	B	1227	CLA	CHC-C1C	4.91	1.48	1.38
15	A	1123	CLA	CHC-C1C	4.90	1.48	1.38
15	A	1801	CLA	C3C-C2C	4.89	1.47	1.36
15	A	1135	CLA	CHC-C1C	4.88	1.48	1.38
13	A	1108	CL0	C3B-C2B	4.87	1.47	1.40
15	A	1105	CLA	CHC-C1C	4.87	1.48	1.38
15	B	1206	CLA	CHC-C1C	4.86	1.48	1.38
15	A	1136	CLA	CHC-C1C	4.86	1.48	1.38
15	B	1221	CLA	CHC-C1C	4.86	1.48	1.38
15	A	1131	CLA	CHC-C1C	4.86	1.48	1.38
15	B	1205	CLA	CHC-C1C	4.84	1.48	1.38
15	B	1222	CLA	CHC-C1C	4.84	1.48	1.38
15	B	1238	CLA	CHC-C1C	4.84	1.48	1.38
10	B	2002	PQN	C10-C5	4.83	1.48	1.40
10	A	2001	PQN	C10-C5	4.82	1.48	1.40
13	A	1108	CL0	CHC-C1C	4.81	1.48	1.39
15	A	1130	CLA	CHD-C1D	4.81	1.47	1.38
15	B	1206	CLA	CHD-C1D	4.80	1.47	1.38
15	A	1123	CLA	CHD-C1D	4.79	1.47	1.38
15	A	1110	CLA	CHC-C1C	4.79	1.48	1.38
15	B	1234	CLA	O2D-CGD	4.79	1.45	1.33
15	A	1120	CLA	CHD-C1D	4.79	1.47	1.38
15	A	1126	CLA	CHD-C1D	4.76	1.47	1.38
15	B	1214	CLA	CHD-C1D	4.76	1.47	1.38
15	B	1232	CLA	CHC-C1C	4.76	1.48	1.38
15	B	1215	CLA	CHC-C1C	4.76	1.48	1.38
15	A	1116	CLA	CHD-C1D	4.76	1.47	1.38
15	B	1227	CLA	CHD-C1D	4.74	1.47	1.38
15	B	1204	CLA	CHD-C1D	4.73	1.47	1.38
15	B	1239	CLA	CHD-C1D	4.73	1.47	1.38
15	B	1239	CLA	CHC-C1C	4.72	1.47	1.38
15	B	1237	CLA	CHD-C1D	4.72	1.47	1.38
15	B	1231	CLA	CHC-C1C	4.72	1.47	1.38
15	B	1209	CLA	CHD-C1D	4.72	1.47	1.38
15	B	1203	CLA	CHD-C1D	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1216	CLA	CHD-C1D	4.71	1.47	1.38
15	A	1102	CLA	CHD-C1D	4.71	1.47	1.38
15	B	1208	CLA	CHD-C1D	4.70	1.47	1.38
15	B	1228	CLA	C3C-C2C	4.70	1.46	1.36
15	A	1130	CLA	C3C-C2C	4.70	1.46	1.36
15	A	1114	CLA	CHD-C1D	4.70	1.47	1.38
15	B	1208	CLA	C3C-C2C	4.70	1.46	1.36
15	A	1124	CLA	CHD-C1D	4.70	1.47	1.38
15	B	1220	CLA	CHD-C1D	4.69	1.47	1.38
15	B	1215	CLA	CHD-C1D	4.69	1.47	1.38
15	A	1105	CLA	CHD-C1D	4.69	1.47	1.38
15	A	1121	CLA	CHD-C1D	4.69	1.47	1.38
15	A	1117	CLA	CHD-C1D	4.69	1.47	1.38
15	B	1213	CLA	CHD-C1D	4.69	1.47	1.38
13	A	1011	CL0	CHD-C1D	4.69	1.47	1.39
15	A	1129	CLA	CHD-C1D	4.68	1.47	1.38
15	A	1106	CLA	CHD-C1D	4.68	1.47	1.38
15	A	1133	CLA	CHD-C1D	4.68	1.47	1.38
15	B	1220	CLA	C3C-C2C	4.68	1.46	1.36
15	B	1222	CLA	C3C-C2C	4.67	1.46	1.36
15	B	1203	CLA	CHC-C1C	4.66	1.47	1.38
15	A	1119	CLA	CHD-C1D	4.66	1.47	1.38
15	A	1103	CLA	CHD-C1D	4.66	1.47	1.38
15	A	1128	CLA	CHC-C1C	4.66	1.47	1.38
15	B	1227	CLA	C3C-C2C	4.66	1.46	1.36
15	A	1107	CLA	CHD-C1D	4.65	1.47	1.38
15	B	1232	CLA	CHD-C1D	4.65	1.47	1.38
15	B	1223	CLA	C3C-C2C	4.65	1.46	1.36
15	B	1021	CLA	CHD-C1D	4.65	1.47	1.38
15	B	1240	CLA	C3C-C2C	4.65	1.46	1.36
15	B	1201	CLA	CHD-C1D	4.65	1.47	1.38
15	B	1240	CLA	CHD-C1D	4.64	1.47	1.38
15	A	1138	CLA	CHD-C1D	4.64	1.47	1.38
15	B	1219	CLA	CHD-C1D	4.64	1.47	1.38
15	A	1109	CLA	C3C-C2C	4.63	1.46	1.36
15	B	1202	CLA	C3C-C2C	4.63	1.46	1.36
15	A	1122	CLA	CHD-C1D	4.63	1.47	1.38
15	K	1401	CLA	CHD-C1D	4.63	1.47	1.38
15	A	1109	CLA	CHD-C1D	4.63	1.47	1.38
15	A	1116	CLA	C3C-C2C	4.62	1.46	1.36
15	A	1022	CLA	C3C-C2C	4.62	1.46	1.36
15	A	1131	CLA	CHD-C1D	4.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1013	CLA	C3C-C2C	4.62	1.46	1.36
15	A	1107	CLA	C3C-C2C	4.62	1.46	1.36
15	A	1122	CLA	C3C-C2C	4.62	1.46	1.36
15	J	1303	CLA	C3C-C2C	4.61	1.46	1.36
15	B	1224	CLA	CHD-C1D	4.61	1.47	1.38
15	A	1137	CLA	CHD-C1D	4.61	1.47	1.38
15	B	1217	CLA	CHD-C1D	4.61	1.47	1.38
15	A	1138	CLA	C3C-C2C	4.61	1.46	1.36
15	B	1210	CLA	CHD-C1D	4.61	1.47	1.38
15	B	1023	CLA	CHD-C1D	4.60	1.47	1.38
15	B	1228	CLA	CHD-C1D	4.60	1.47	1.38
15	F	1410	CLA	CHD-C1D	4.60	1.47	1.38
15	A	1137	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1235	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1207	CLA	CHD-C1D	4.60	1.47	1.38
15	B	1212	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1232	CLA	C3C-C2C	4.60	1.46	1.36
15	B	1225	CLA	CHD-C1D	4.59	1.47	1.38
15	A	1127	CLA	C3C-C2C	4.59	1.46	1.36
15	A	1113	CLA	CHD-C1D	4.59	1.47	1.38
15	J	1303	CLA	CHD-C1D	4.59	1.47	1.38
15	F	1139	CLA	CHD-C1D	4.59	1.47	1.38
15	B	1021	CLA	C3C-C2C	4.59	1.46	1.36
15	B	1226	CLA	C3C-C2C	4.59	1.46	1.36
15	B	1239	CLA	C3C-C2C	4.59	1.46	1.36
15	A	1124	CLA	C3C-C2C	4.59	1.46	1.36
15	A	1140	CLA	C3C-C2C	4.59	1.46	1.36
15	A	1112	CLA	CHD-C1D	4.59	1.47	1.38
15	A	1132	CLA	C3C-C2C	4.59	1.46	1.36
15	B	1216	CLA	C3C-C2C	4.58	1.46	1.36
15	B	1218	CLA	CHD-C1D	4.58	1.47	1.38
15	B	1229	CLA	C3C-C2C	4.58	1.46	1.36
14	B	4006	BCR	C10-C9	-4.58	1.25	1.35
15	B	1234	CLA	C3C-C2C	4.58	1.46	1.36
15	A	1022	CLA	CHD-C1D	4.58	1.47	1.38
15	B	1217	CLA	O2A-C1	4.58	1.60	1.46
15	A	1135	CLA	CHD-C1D	4.58	1.47	1.38
15	A	1012	CLA	C3C-C2C	4.57	1.46	1.36
15	B	1226	CLA	CHD-C1D	4.57	1.47	1.38
15	B	1217	CLA	C3C-C2C	4.57	1.46	1.36
13	A	1011	CL0	C3D-C4D	-4.57	1.34	1.41
15	B	1211	CLA	CHD-C1D	4.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1119	CLA	C3C-C2C	4.57	1.46	1.36
15	A	1134	CLA	CHD-C1D	4.57	1.47	1.38
15	A	1105	CLA	C3C-C2C	4.57	1.46	1.36
15	B	1214	CLA	C3C-C2C	4.56	1.46	1.36
15	B	1231	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1136	CLA	CHD-C1D	4.56	1.47	1.38
15	A	1114	CLA	C3C-C2C	4.56	1.46	1.36
15	F	1139	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1134	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1102	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1112	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1801	CLA	CHD-C1D	4.56	1.47	1.38
15	B	1231	CLA	CHD-C1D	4.56	1.47	1.38
15	A	1129	CLA	C3C-C2C	4.56	1.46	1.36
15	A	1117	CLA	C3C-C2C	4.55	1.46	1.36
15	F	1301	CLA	C3C-C2C	4.55	1.46	1.36
15	F	1301	CLA	CHD-C1D	4.55	1.47	1.38
13	A	1108	CL0	C3D-C4D	-4.55	1.34	1.41
15	K	1402	CLA	C3C-C2C	4.55	1.46	1.36
15	A	1104	CLA	C3C-C2C	4.55	1.46	1.36
15	B	1219	CLA	C3C-C2C	4.54	1.46	1.36
15	A	1111	CLA	CHD-C1D	4.54	1.47	1.38
15	A	1121	CLA	C3C-C2C	4.54	1.46	1.36
15	B	1218	CLA	C3C-C2C	4.54	1.46	1.36
15	J	1302	CLA	CHD-C1D	4.53	1.47	1.38
15	K	1402	CLA	CHD-C1D	4.53	1.47	1.38
15	A	1120	CLA	C3C-C2C	4.53	1.46	1.36
15	B	1202	CLA	CHD-C1D	4.53	1.47	1.38
15	A	1126	CLA	C3C-C2C	4.53	1.46	1.36
15	A	1128	CLA	CHD-C1D	4.53	1.47	1.38
15	B	1238	CLA	CHD-C1D	4.53	1.47	1.38
15	B	1203	CLA	C3C-C2C	4.53	1.46	1.36
15	A	1135	CLA	C3C-C2C	4.53	1.46	1.36
13	A	1011	CL0	CHC-C1C	4.52	1.48	1.39
15	A	1101	CLA	CHD-C1D	4.52	1.47	1.38
15	F	1410	CLA	C3C-C2C	4.51	1.46	1.36
15	B	1207	CLA	C3C-C2C	4.51	1.46	1.36
15	B	1213	CLA	C3C-C2C	4.51	1.46	1.36
15	B	1209	CLA	C3C-C2C	4.51	1.46	1.36
15	B	1238	CLA	C3C-C2C	4.51	1.46	1.36
15	B	1215	CLA	C3C-C2C	4.50	1.46	1.36
15	A	1127	CLA	CHD-C1D	4.50	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1204	CLA	C3C-C2C	4.50	1.46	1.36
15	K	1401	CLA	C3C-C2C	4.50	1.46	1.36
15	B	1205	CLA	C3C-C2C	4.50	1.46	1.36
15	A	1128	CLA	C3C-C2C	4.49	1.46	1.36
15	B	1212	CLA	CHD-C1D	4.49	1.47	1.38
15	A	1113	CLA	C3C-C2C	4.49	1.46	1.36
15	B	1222	CLA	CHD-C1D	4.49	1.47	1.38
15	A	1138	CLA	CHC-C4B	4.48	1.49	1.39
13	A	1108	CL0	CHD-C1D	4.48	1.46	1.39
15	A	1131	CLA	C3C-C2C	4.48	1.46	1.36
15	B	1234	CLA	CHD-C1D	4.48	1.47	1.38
15	A	1110	CLA	CHD-C1D	4.48	1.47	1.38
15	A	1106	CLA	C3C-C2C	4.48	1.46	1.36
15	B	1206	CLA	C3C-C2C	4.48	1.46	1.36
15	A	1101	CLA	C3C-C2C	4.48	1.46	1.36
15	B	1201	CLA	C3C-C2C	4.48	1.46	1.36
15	J	1302	CLA	C3C-C2C	4.48	1.46	1.36
15	B	1230	CLA	CHD-C1D	4.47	1.47	1.38
15	B	1224	CLA	C3C-C2C	4.47	1.46	1.36
15	B	1221	CLA	C3C-C2C	4.47	1.46	1.36
15	B	1211	CLA	C3C-C2C	4.47	1.46	1.36
15	A	1136	CLA	C3C-C2C	4.47	1.46	1.36
15	B	1023	CLA	C3C-C2C	4.46	1.46	1.36
15	A	1125	CLA	C3C-C2C	4.46	1.46	1.36
15	A	1104	CLA	CHD-C1D	4.46	1.47	1.38
15	B	1237	CLA	C3C-C2C	4.46	1.46	1.36
15	B	1225	CLA	C3C-C2C	4.45	1.46	1.36
15	B	1230	CLA	C3C-C2C	4.45	1.46	1.36
15	A	1133	CLA	C3C-C2C	4.45	1.46	1.36
15	B	1205	CLA	CHD-C1D	4.45	1.47	1.38
15	A	1115	CLA	C3C-C2C	4.44	1.46	1.36
15	A	1140	CLA	CHD-C1D	4.44	1.47	1.38
15	A	1012	CLA	CHD-C1D	4.44	1.47	1.38
15	A	1118	CLA	CHD-C1D	4.44	1.47	1.38
15	B	1013	CLA	CHD-C1D	4.43	1.47	1.38
15	B	1236	CLA	CHD-C1D	4.43	1.47	1.38
15	A	1118	CLA	C3C-C2C	4.43	1.46	1.36
15	B	1221	CLA	CHD-C1D	4.43	1.47	1.38
14	A	4001	BCR	C10-C9	-4.42	1.25	1.35
15	A	1132	CLA	CHD-C1D	4.41	1.47	1.38
15	B	1210	CLA	C3C-C2C	4.41	1.46	1.36
15	B	1236	CLA	C3C-C2C	4.41	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1110	CLA	C3C-C2C	4.40	1.46	1.36
15	A	1127	CLA	C3D-C4D	-4.40	1.34	1.44
15	A	1123	CLA	C3C-C2C	4.40	1.46	1.36
15	A	1110	CLA	C3D-C4D	-4.39	1.34	1.44
13	A	1011	CL0	C3D-C2D	4.39	1.47	1.39
13	A	1011	CL0	CHD-C4C	4.38	1.47	1.39
15	A	1129	CLA	C3D-C4D	-4.38	1.34	1.44
15	A	1111	CLA	C3C-C2C	4.38	1.46	1.36
15	B	1236	CLA	CHC-C4B	4.37	1.49	1.39
15	A	1103	CLA	C3C-C2C	4.37	1.46	1.36
15	A	1125	CLA	CHC-C4B	4.37	1.49	1.39
15	B	1223	CLA	CHD-C1D	4.37	1.46	1.38
13	A	1011	CL0	C3B-C2B	4.36	1.46	1.40
15	B	1235	CLA	CHD-C1D	4.35	1.46	1.38
12	A	5003	LHG	O8-C23	4.35	1.46	1.33
15	B	1227	CLA	C3D-C4D	-4.34	1.34	1.44
15	A	1126	CLA	C3D-C4D	-4.33	1.34	1.44
15	A	1130	CLA	C3D-C4D	-4.33	1.34	1.44
15	B	1228	CLA	CHC-C4B	4.33	1.49	1.39
17	B	5002	LMG	O8-C28	4.32	1.45	1.33
15	A	1101	CLA	CHC-C4B	4.32	1.49	1.39
15	A	1107	CLA	C3D-C4D	-4.32	1.34	1.44
13	A	1108	CL0	CHD-C4C	4.31	1.47	1.39
15	A	1125	CLA	C3D-C4D	-4.31	1.34	1.44
15	B	1216	CLA	C3D-C4D	-4.30	1.34	1.44
15	A	1122	CLA	C3D-C4D	-4.30	1.34	1.44
15	A	1119	CLA	C3D-C4D	-4.29	1.34	1.44
15	A	1115	CLA	CHD-C1D	4.29	1.46	1.38
15	A	1126	CLA	CHC-C4B	4.29	1.49	1.39
15	A	1122	CLA	CHC-C4B	4.28	1.49	1.39
15	A	1022	CLA	C3D-C4D	-4.28	1.34	1.44
15	B	1229	CLA	CHD-C1D	4.28	1.46	1.38
15	B	1218	CLA	C3D-C4D	-4.27	1.34	1.44
15	B	1211	CLA	C3D-C4D	-4.27	1.34	1.44
15	B	1230	CLA	C3D-C4D	-4.27	1.34	1.44
15	F	1139	CLA	C3D-C4D	-4.27	1.34	1.44
15	B	1228	CLA	C3D-C4D	-4.26	1.34	1.44
15	B	1225	CLA	C3D-C4D	-4.26	1.34	1.44
15	B	1013	CLA	C3D-C4D	-4.26	1.34	1.44
15	B	1223	CLA	C3D-C4D	-4.26	1.34	1.44
15	B	1230	CLA	CHC-C4B	4.25	1.49	1.39
15	B	1235	CLA	CHC-C4B	4.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	CLA	C3D-C4D	-4.25	1.34	1.44
15	A	1107	CLA	CHC-C4B	4.24	1.48	1.39
15	B	1224	CLA	C3D-C4D	-4.24	1.34	1.44
14	A	4012	BCR	C10-C9	-4.24	1.26	1.35
15	B	1204	CLA	C3D-C4D	-4.24	1.34	1.44
15	B	1226	CLA	C3D-C4D	-4.24	1.34	1.44
15	A	1131	CLA	C3D-C4D	-4.24	1.34	1.44
15	A	1112	CLA	CHC-C4B	4.23	1.48	1.39
15	A	1128	CLA	C3D-C4D	-4.23	1.34	1.44
15	B	1208	CLA	C3D-C4D	-4.23	1.34	1.44
14	B	4004	BCR	C10-C9	-4.23	1.26	1.35
15	B	1203	CLA	C3D-C4D	-4.23	1.34	1.44
15	A	1103	CLA	C3D-C4D	-4.23	1.34	1.44
15	B	1223	CLA	CHC-C4B	4.23	1.48	1.39
15	A	1105	CLA	C3D-C4D	-4.23	1.34	1.44
15	B	1213	CLA	C3D-C4D	-4.23	1.34	1.44
15	B	1232	CLA	C3D-C4D	-4.22	1.34	1.44
15	B	1236	CLA	C3D-C4D	-4.22	1.34	1.44
15	B	1239	CLA	C3D-C4D	-4.22	1.34	1.44
15	B	1023	CLA	C3D-C4D	-4.22	1.34	1.44
12	A	5005	LHG	O8-C23	4.22	1.45	1.33
15	B	1220	CLA	CHC-C4B	4.22	1.48	1.39
15	B	1231	CLA	C3D-C4D	-4.22	1.34	1.44
15	A	1118	CLA	C3D-C4D	-4.22	1.34	1.44
15	A	1133	CLA	C3D-C4D	-4.22	1.34	1.44
15	A	1114	CLA	C3D-C4D	-4.21	1.34	1.44
15	A	1115	CLA	C3D-C4D	-4.21	1.34	1.44
15	B	1214	CLA	C3D-C4D	-4.21	1.34	1.44
15	B	1234	CLA	C3D-C4D	-4.21	1.34	1.44
15	A	1140	CLA	CHC-C4B	4.21	1.48	1.39
15	A	1109	CLA	C3D-C4D	-4.21	1.34	1.44
15	B	1235	CLA	C3D-C4D	-4.21	1.34	1.44
15	A	1121	CLA	C3D-C4D	-4.21	1.34	1.44
12	B	5004	LHG	O8-C23	4.21	1.45	1.33
15	A	1136	CLA	C3D-C4D	-4.21	1.34	1.44
15	K	1402	CLA	C3D-C4D	-4.21	1.34	1.44
15	A	1104	CLA	C3D-C4D	-4.21	1.34	1.44
15	A	1106	CLA	C3D-C4D	-4.20	1.34	1.44
15	A	1130	CLA	CHC-C4B	4.20	1.48	1.39
15	A	1135	CLA	C3D-C4D	-4.20	1.34	1.44
15	B	1205	CLA	C3D-C4D	-4.20	1.34	1.44
15	B	1238	CLA	C3D-C4D	-4.20	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1113	CLA	C3D-C4D	-4.19	1.34	1.44
15	A	1111	CLA	C3D-C4D	-4.19	1.34	1.44
15	A	1123	CLA	C3D-C4D	-4.19	1.34	1.44
15	B	1021	CLA	C3D-C4D	-4.19	1.34	1.44
15	A	1132	CLA	C3D-C4D	-4.19	1.34	1.44
15	B	1210	CLA	C3D-C4D	-4.18	1.34	1.44
15	F	1410	CLA	C3D-C4D	-4.18	1.34	1.44
15	A	1140	CLA	C3D-C4D	-4.18	1.34	1.44
15	A	1120	CLA	C3D-C4D	-4.18	1.34	1.44
14	A	4002	BCR	C10-C9	-4.18	1.26	1.35
15	A	1126	CLA	CHD-C4C	4.18	1.48	1.39
15	A	1137	CLA	C3D-C4D	-4.18	1.34	1.44
15	B	1212	CLA	C3D-C4D	-4.18	1.34	1.44
15	B	1201	CLA	C3D-C4D	-4.18	1.34	1.44
15	B	1206	CLA	C3D-C4D	-4.18	1.34	1.44
15	B	1239	CLA	CHB-C1B	4.17	1.48	1.39
15	A	1134	CLA	C3D-C4D	-4.17	1.34	1.44
15	B	1215	CLA	C3D-C4D	-4.17	1.34	1.44
15	K	1401	CLA	C3D-C4D	-4.17	1.34	1.44
15	B	1219	CLA	C3D-C4D	-4.17	1.34	1.44
15	B	1213	CLA	CHC-C4B	4.17	1.48	1.39
15	B	1207	CLA	C3D-C4D	-4.17	1.34	1.44
15	B	1229	CLA	CHB-C1B	4.17	1.48	1.39
15	J	1303	CLA	C3D-C4D	-4.17	1.34	1.44
15	A	1134	CLA	CHC-C4B	4.16	1.48	1.39
17	B	5002	LMG	O7-C10	4.16	1.46	1.34
15	B	1220	CLA	C3D-C4D	-4.16	1.34	1.44
12	A	5001	LHG	O8-C23	4.16	1.45	1.33
14	B	4010	BCR	C10-C9	-4.16	1.26	1.35
15	A	1116	CLA	C3D-C4D	-4.15	1.34	1.44
15	J	1302	CLA	C3D-C4D	-4.15	1.34	1.44
15	B	1221	CLA	CHB-C1B	4.15	1.48	1.39
15	A	1112	CLA	C3D-C4D	-4.15	1.34	1.44
15	B	1217	CLA	C3D-C4D	-4.15	1.34	1.44
15	A	1104	CLA	CHC-C4B	4.15	1.48	1.39
15	A	1117	CLA	C3D-C4D	-4.15	1.34	1.44
15	B	1209	CLA	C3D-C4D	-4.14	1.34	1.44
15	B	1240	CLA	C3D-C4D	-4.14	1.34	1.44
15	B	1240	CLA	CHC-C4B	4.14	1.48	1.39
15	A	1801	CLA	C3D-C4D	-4.14	1.34	1.44
15	A	1131	CLA	CHB-C1B	4.14	1.48	1.39
14	B	4005	BCR	C10-C9	-4.14	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4014	BCR	C10-C9	-4.14	1.26	1.35
15	F	1410	CLA	CHC-C4B	4.14	1.48	1.39
15	A	1136	CLA	CHB-C1B	4.13	1.48	1.39
15	A	1124	CLA	C3D-C4D	-4.13	1.34	1.44
14	B	4011	BCR	C10-C9	-4.13	1.26	1.35
15	A	1115	CLA	CHC-C4B	4.13	1.48	1.39
15	F	1301	CLA	CHC-C4B	4.13	1.48	1.39
15	B	1221	CLA	C3D-C4D	-4.13	1.34	1.44
15	B	1202	CLA	C3D-C4D	-4.12	1.34	1.44
15	A	1022	CLA	CHC-C4B	4.12	1.48	1.39
15	A	1103	CLA	CHC-C4B	4.12	1.48	1.39
15	B	1211	CLA	CHC-C4B	4.12	1.48	1.39
15	A	1132	CLA	CHC-C4B	4.12	1.48	1.39
12	B	5004	LHG	O7-C7	4.12	1.45	1.34
15	K	1402	CLA	CHB-C1B	4.12	1.48	1.39
15	A	1102	CLA	C3D-C4D	-4.12	1.34	1.44
15	B	1214	CLA	CHD-C4C	4.12	1.48	1.39
15	B	1208	CLA	CHD-C4C	4.12	1.48	1.39
15	A	1127	CLA	CHC-C4B	4.11	1.48	1.39
15	J	1303	CLA	CHB-C1B	4.11	1.48	1.39
15	F	1301	CLA	C3D-C4D	-4.11	1.34	1.44
12	A	5001	LHG	O7-C7	4.11	1.45	1.34
15	A	1109	CLA	CHC-C4B	4.11	1.48	1.39
15	A	1132	CLA	CHB-C1B	4.11	1.48	1.39
15	A	1137	CLA	CHB-C1B	4.11	1.48	1.39
15	B	1225	CLA	CHC-C4B	4.11	1.48	1.39
15	B	1013	CLA	CHC-C4B	4.11	1.48	1.39
15	A	1130	CLA	CHD-C4C	4.11	1.48	1.39
14	A	4007	BCR	C10-C9	-4.10	1.26	1.35
15	J	1303	CLA	CHC-C4B	4.10	1.48	1.39
14	A	4003	BCR	C10-C9	-4.10	1.26	1.35
15	B	1239	CLA	CHD-C4C	4.10	1.48	1.39
14	F	4015	BCR	C10-C9	-4.10	1.26	1.35
15	B	1202	CLA	CHC-C4B	4.09	1.48	1.39
15	A	1119	CLA	CHC-C4B	4.09	1.48	1.39
15	B	1237	CLA	CHB-C1B	4.09	1.48	1.39
15	F	1139	CLA	CHC-C4B	4.09	1.48	1.39
15	A	1111	CLA	CHC-C4B	4.09	1.48	1.39
15	A	1125	CLA	CHD-C1D	4.08	1.46	1.38
15	B	1212	CLA	CHB-C1B	4.08	1.48	1.39
15	A	1117	CLA	CHC-C4B	4.08	1.48	1.39
15	B	1213	CLA	CHB-C1B	4.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1101	CLA	C3D-C4D	-4.08	1.35	1.44
15	B	1234	CLA	CHB-C1B	4.08	1.48	1.39
15	B	1214	CLA	CHC-C4B	4.08	1.48	1.39
15	B	1220	CLA	CHD-C4C	4.08	1.48	1.39
15	B	1222	CLA	C3D-C4D	-4.08	1.35	1.44
15	K	1401	CLA	CHC-C4B	4.08	1.48	1.39
15	A	1122	CLA	CHD-C4C	4.08	1.48	1.39
15	A	1121	CLA	CHB-C1B	4.08	1.48	1.39
15	A	1135	CLA	CHB-C1B	4.08	1.48	1.39
15	A	1115	CLA	CHB-C1B	4.08	1.48	1.39
15	B	1219	CLA	CHD-C4C	4.07	1.48	1.39
15	B	1205	CLA	CHB-C1B	4.07	1.48	1.39
15	J	1302	CLA	CHC-C4B	4.07	1.48	1.39
15	A	1801	CLA	CHC-C4B	4.07	1.48	1.39
15	A	1106	CLA	CHD-C4C	4.07	1.48	1.39
15	A	1113	CLA	CHC-C4B	4.07	1.48	1.39
15	B	1238	CLA	CHB-C1B	4.07	1.48	1.39
15	A	1114	CLA	CHC-C4B	4.07	1.48	1.39
15	A	1138	CLA	C3D-C4D	-4.07	1.35	1.44
15	A	1012	CLA	CHC-C4B	4.07	1.48	1.39
15	B	1229	CLA	CHC-C4B	4.07	1.48	1.39
12	A	5003	LHG	O7-C7	4.07	1.45	1.34
15	F	1139	CLA	CHB-C1B	4.06	1.48	1.39
15	B	1237	CLA	CHC-C4B	4.06	1.48	1.39
15	B	1206	CLA	CHD-C4C	4.06	1.48	1.39
15	B	1218	CLA	CHC-C4B	4.06	1.48	1.39
15	A	1801	CLA	CHB-C1B	4.06	1.48	1.39
15	A	1127	CLA	CHB-C1B	4.06	1.48	1.39
15	A	1114	CLA	CHB-C1B	4.06	1.48	1.39
15	B	1212	CLA	CHC-C4B	4.06	1.48	1.39
15	B	1213	CLA	CHD-C4C	4.06	1.48	1.39
15	A	1118	CLA	CHB-C1B	4.06	1.48	1.39
15	B	1208	CLA	CHB-C1B	4.06	1.48	1.39
15	B	1215	CLA	CHB-C1B	4.05	1.48	1.39
15	A	1116	CLA	CHC-C4B	4.05	1.48	1.39
15	A	1140	CLA	CHB-C1B	4.05	1.48	1.39
15	B	1201	CLA	CHC-C4B	4.05	1.48	1.39
15	A	1123	CLA	CHB-C1B	4.05	1.48	1.39
15	A	1129	CLA	CHB-C1B	4.05	1.48	1.39
15	B	1207	CLA	CHC-C4B	4.05	1.48	1.39
14	J	4013	BCR	C10-C9	-4.05	1.26	1.35
15	B	1226	CLA	CHB-C1B	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1217	CLA	CHC-C4B	4.04	1.48	1.39
15	J	1302	CLA	CHB-C1B	4.04	1.48	1.39
15	A	1117	CLA	CHD-C4C	4.04	1.48	1.39
15	B	1219	CLA	CHB-C1B	4.03	1.48	1.39
15	A	1012	CLA	MG-NC	4.03	2.15	2.06
15	B	1211	CLA	CHB-C1B	4.03	1.48	1.39
13	A	1108	CL0	C3D-C2D	4.03	1.46	1.39
15	B	1203	CLA	CHB-C1B	4.03	1.48	1.39
15	A	1137	CLA	CHC-C4B	4.03	1.48	1.39
15	A	1124	CLA	CHC-C4B	4.03	1.48	1.39
15	B	1215	CLA	CHD-C4C	4.03	1.48	1.39
15	A	1102	CLA	CHC-C4B	4.03	1.48	1.39
15	A	1121	CLA	CHC-C4B	4.03	1.48	1.39
15	A	1109	CLA	CHD-C4C	4.03	1.48	1.39
15	B	1221	CLA	CHC-C4B	4.03	1.48	1.39
15	B	1204	CLA	CHD-C4C	4.02	1.48	1.39
15	B	1226	CLA	CHC-C4B	4.02	1.48	1.39
15	A	1133	CLA	CHC-C4B	4.02	1.48	1.39
15	B	1229	CLA	C3D-C4D	-4.02	1.35	1.44
14	B	4017	BCR	C10-C9	-4.02	1.26	1.35
15	B	1216	CLA	CHD-C4C	4.02	1.48	1.39
14	B	4009	BCR	C10-C9	-4.02	1.26	1.35
15	B	1216	CLA	CHC-C4B	4.02	1.48	1.39
15	K	1402	CLA	CHC-C4B	4.02	1.48	1.39
15	B	1021	CLA	CHC-C4B	4.01	1.48	1.39
15	B	1208	CLA	CHC-C4B	4.01	1.48	1.39
15	B	1224	CLA	CHC-C4B	4.01	1.48	1.39
15	A	1012	CLA	C3D-C4D	-4.01	1.35	1.44
15	A	1120	CLA	CHD-C4C	4.01	1.48	1.39
15	A	1103	CLA	CHB-C1B	4.01	1.48	1.39
15	B	1238	CLA	CHC-C4B	4.01	1.48	1.39
15	B	1240	CLA	CHB-C1B	4.01	1.48	1.39
15	A	1135	CLA	CHD-C4C	4.01	1.48	1.39
12	A	5005	LHG	O7-C7	4.00	1.45	1.34
15	A	1114	CLA	CHD-C4C	4.00	1.48	1.39
15	B	1231	CLA	CHD-C4C	4.00	1.48	1.39
15	A	1124	CLA	CHD-C4C	4.00	1.48	1.39
15	B	1205	CLA	CHC-C4B	4.00	1.48	1.39
15	B	1227	CLA	CHD-C4C	4.00	1.48	1.39
15	B	1232	CLA	CHB-C1B	3.99	1.48	1.39
15	A	1123	CLA	CHD-C4C	3.99	1.48	1.39
15	B	1237	CLA	CHD-C4C	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1129	CLA	CHC-C4B	3.99	1.48	1.39
15	B	1231	CLA	CHB-C1B	3.99	1.48	1.39
15	A	1105	CLA	CHC-C4B	3.99	1.48	1.39
15	A	1119	CLA	CHD-C4C	3.99	1.48	1.39
15	B	1224	CLA	CHD-C4C	3.99	1.48	1.39
14	A	4008	BCR	C10-C9	-3.99	1.26	1.35
15	A	1133	CLA	CHB-C1B	3.99	1.48	1.39
15	A	1102	CLA	CHD-C4C	3.98	1.48	1.39
15	A	1105	CLA	CHD-C4C	3.98	1.48	1.39
15	A	1107	CLA	CHD-C4C	3.98	1.48	1.39
15	A	1106	CLA	CHC-C4B	3.98	1.48	1.39
15	A	1121	CLA	CHD-C4C	3.98	1.48	1.39
15	B	1201	CLA	CHB-C1B	3.98	1.48	1.39
15	B	1203	CLA	CHD-C4C	3.97	1.48	1.39
15	B	1204	CLA	CHB-C1B	3.97	1.48	1.39
15	B	1240	CLA	CHD-C4C	3.97	1.48	1.39
15	B	1218	CLA	CHD-C4C	3.97	1.48	1.39
15	A	1109	CLA	CHB-C1B	3.97	1.48	1.39
15	A	1116	CLA	CHD-C4C	3.97	1.48	1.39
15	B	1210	CLA	CHC-C4B	3.97	1.48	1.39
15	B	1207	CLA	CHB-C1B	3.97	1.48	1.39
15	B	1219	CLA	CHC-C4B	3.97	1.48	1.39
14	F	4016	BCR	C10-C9	-3.96	1.26	1.35
15	A	1131	CLA	CHC-C4B	3.96	1.48	1.39
15	B	1217	CLA	CHB-C1B	3.96	1.48	1.39
15	A	1120	CLA	CHC-C4B	3.96	1.48	1.39
15	F	1410	CLA	CHD-C4C	3.96	1.48	1.39
15	A	1118	CLA	CHC-C4B	3.96	1.48	1.39
15	A	1134	CLA	CHB-C1B	3.96	1.48	1.39
15	B	1023	CLA	CHC-C4B	3.96	1.48	1.39
15	A	1116	CLA	CHB-C1B	3.96	1.48	1.39
15	A	1135	CLA	CHC-C4B	3.96	1.48	1.39
15	A	1113	CLA	CHB-C1B	3.96	1.48	1.39
15	B	1230	CLA	CHB-C1B	3.96	1.48	1.39
15	A	1133	CLA	CHD-C4C	3.96	1.48	1.39
15	F	1410	CLA	CHB-C1B	3.95	1.48	1.39
15	B	1202	CLA	CHB-C1B	3.95	1.48	1.39
15	A	1103	CLA	CHD-C4C	3.95	1.48	1.39
15	B	1204	CLA	CHC-C4B	3.95	1.48	1.39
15	A	1138	CLA	CHD-C4C	3.95	1.48	1.39
15	B	1210	CLA	CHD-C4C	3.95	1.48	1.39
15	B	1217	CLA	CHD-C4C	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1120	CLA	CHB-C1B	3.94	1.48	1.39
15	K	1401	CLA	CHB-C1B	3.94	1.48	1.39
15	B	1229	CLA	OBD-CAD	3.94	1.29	1.22
15	B	1206	CLA	CHC-C4B	3.94	1.48	1.39
15	B	1209	CLA	CHD-C4C	3.94	1.48	1.39
15	A	1129	CLA	CHD-C4C	3.94	1.48	1.39
15	A	1113	CLA	CHD-C4C	3.94	1.48	1.39
15	A	1105	CLA	CHB-C1B	3.93	1.48	1.39
15	A	1136	CLA	CHC-C4B	3.93	1.48	1.39
15	A	1110	CLA	CHC-C4B	3.93	1.48	1.39
15	B	1238	CLA	CHD-C4C	3.93	1.48	1.39
15	B	1209	CLA	CHC-C4B	3.93	1.48	1.39
15	A	1022	CLA	CHD-C4C	3.92	1.48	1.39
15	A	1128	CLA	CHB-C1B	3.92	1.48	1.39
15	B	1215	CLA	CHC-C4B	3.92	1.48	1.39
15	B	1228	CLA	CHD-C4C	3.92	1.48	1.39
15	B	1235	CLA	CHB-C1B	3.92	1.48	1.39
15	B	1232	CLA	CHC-C4B	3.92	1.48	1.39
15	K	1401	CLA	CHD-C4C	3.92	1.48	1.39
15	B	1227	CLA	CHC-C4B	3.92	1.48	1.39
15	B	1218	CLA	CHB-C1B	3.92	1.48	1.39
15	A	1124	CLA	OBD-CAD	3.92	1.29	1.22
15	B	1222	CLA	CHC-C4B	3.91	1.48	1.39
15	B	1207	CLA	CHD-C4C	3.91	1.48	1.39
15	A	1136	CLA	CHD-C4C	3.91	1.48	1.39
15	A	1012	CLA	CHB-C1B	3.91	1.48	1.39
15	B	1216	CLA	CHB-C1B	3.91	1.48	1.39
15	B	1234	CLA	CHC-C4B	3.91	1.48	1.39
15	B	1236	CLA	CHD-C4C	3.91	1.48	1.39
15	B	1222	CLA	OBD-CAD	3.91	1.29	1.22
15	B	1228	CLA	CHB-C1B	3.90	1.48	1.39
15	A	1123	CLA	MG-NC	3.90	2.15	2.06
15	B	1223	CLA	CHB-C1B	3.90	1.48	1.39
15	A	1131	CLA	CHD-C4C	3.90	1.48	1.39
15	B	1234	CLA	CHD-C4C	3.90	1.48	1.39
15	B	1211	CLA	CHD-C4C	3.90	1.48	1.39
15	B	1220	CLA	CHB-C1B	3.90	1.48	1.39
15	A	1125	CLA	CHB-C1B	3.90	1.48	1.39
15	B	1232	CLA	CHD-C4C	3.90	1.48	1.39
15	B	1202	CLA	CHD-C4C	3.90	1.48	1.39
15	A	1801	CLA	CHD-C4C	3.89	1.48	1.39
15	B	1209	CLA	CHB-C1B	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1104	CLA	CHD-C4C	3.89	1.48	1.39
15	B	1021	CLA	CHD-C4C	3.89	1.48	1.39
15	B	1023	CLA	CHD-C4C	3.89	1.48	1.39
15	A	1110	CLA	CHD-C4C	3.89	1.48	1.39
15	J	1302	CLA	CHD-C4C	3.89	1.48	1.39
15	B	1212	CLA	CHD-C4C	3.88	1.48	1.39
15	A	1138	CLA	OBD-CAD	3.88	1.29	1.22
15	A	1122	CLA	CHB-C1B	3.88	1.48	1.39
15	A	1134	CLA	CHD-C4C	3.88	1.48	1.39
15	B	1222	CLA	CHD-C4C	3.88	1.48	1.39
15	K	1402	CLA	CHD-C4C	3.88	1.48	1.39
15	B	1202	CLA	OBD-CAD	3.88	1.29	1.22
15	B	1222	CLA	CHB-C1B	3.88	1.48	1.39
15	A	1102	CLA	OBD-CAD	3.88	1.29	1.22
15	A	1137	CLA	CHD-C4C	3.88	1.48	1.39
15	A	1801	CLA	MG-NC	3.87	2.15	2.06
15	A	1022	CLA	OBD-CAD	3.87	1.29	1.22
15	A	1110	CLA	CHB-C1B	3.87	1.48	1.39
15	F	1139	CLA	CHD-C4C	3.87	1.48	1.39
15	B	1218	CLA	OBD-CAD	3.87	1.29	1.22
15	B	1021	CLA	CHB-C1B	3.87	1.48	1.39
15	B	1203	CLA	CHC-C4B	3.87	1.48	1.39
15	A	1112	CLA	CHD-C4C	3.87	1.48	1.39
15	A	1123	CLA	CHC-C4B	3.87	1.48	1.39
15	A	1111	CLA	CHD-C4C	3.87	1.48	1.39
15	B	1201	CLA	CHD-C4C	3.87	1.48	1.39
15	B	1206	CLA	CHB-C1B	3.86	1.48	1.39
15	B	1225	CLA	OBD-CAD	3.86	1.29	1.22
15	A	1137	CLA	MG-NC	3.86	2.15	2.06
15	B	1227	CLA	CHB-C1B	3.86	1.48	1.39
15	B	1226	CLA	CHD-C4C	3.86	1.48	1.39
15	F	1301	CLA	CHD-C4C	3.86	1.48	1.39
15	A	1101	CLA	OBD-CAD	3.85	1.29	1.22
15	A	1012	CLA	CHD-C4C	3.85	1.48	1.39
15	J	1303	CLA	CHD-C4C	3.85	1.48	1.39
15	B	1225	CLA	CHD-C4C	3.85	1.48	1.39
15	A	1112	CLA	CHB-C1B	3.85	1.48	1.39
15	B	1231	CLA	CHC-C4B	3.85	1.48	1.39
15	B	1221	CLA	MG-NC	3.85	2.15	2.06
15	A	1102	CLA	CHB-C1B	3.85	1.48	1.39
15	A	1121	CLA	MG-NC	3.84	2.15	2.06
15	A	1120	CLA	OBD-CAD	3.84	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1225	CLA	CHB-C1B	3.84	1.48	1.39
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	K	1401	CLA	OBD-CAD	3.83	1.29	1.22
15	A	1140	CLA	CHD-C4C	3.83	1.47	1.39
15	B	1207	CLA	OBD-CAD	3.83	1.29	1.22
15	B	1021	CLA	OBD-CAD	3.83	1.29	1.22
15	B	1215	CLA	MG-NC	3.82	2.15	2.06
15	A	1022	CLA	CHB-C1B	3.82	1.48	1.39
15	B	1215	CLA	OBD-CAD	3.82	1.29	1.22
15	A	1128	CLA	CHC-C4B	3.82	1.48	1.39
15	B	1023	CLA	CHB-C1B	3.82	1.48	1.39
15	B	1239	CLA	OBD-CAD	3.82	1.29	1.22
15	B	1213	CLA	OBD-CAD	3.82	1.29	1.22
15	B	1224	CLA	OBD-CAD	3.82	1.29	1.22
15	A	1118	CLA	CHD-C4C	3.81	1.47	1.39
15	B	1216	CLA	OBD-CAD	3.81	1.29	1.22
15	B	1219	CLA	OBD-CAD	3.81	1.29	1.22
15	A	1140	CLA	OBD-CAD	3.81	1.29	1.22
15	F	1410	CLA	MG-NC	3.81	2.15	2.06
15	A	1111	CLA	CHB-C1B	3.81	1.48	1.39
15	B	1209	CLA	OBD-CAD	3.81	1.29	1.22
15	A	1101	CLA	CHD-C4C	3.81	1.47	1.39
15	B	1214	CLA	OBD-CAD	3.81	1.29	1.22
15	A	1119	CLA	CHB-C1B	3.80	1.47	1.39
15	B	1210	CLA	CHB-C1B	3.80	1.47	1.39
15	A	1116	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1204	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1224	CLA	CHB-C1B	3.80	1.47	1.39
15	A	1117	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1220	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1205	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1212	CLA	OBD-CAD	3.80	1.29	1.22
15	A	1106	CLA	OBD-CAD	3.80	1.29	1.22
15	B	1239	CLA	CHC-C4B	3.79	1.47	1.39
15	B	1201	CLA	OBD-CAD	3.79	1.29	1.22
15	B	1236	CLA	CHB-C1B	3.79	1.47	1.39
15	B	1232	CLA	MG-NC	3.79	2.15	2.06
15	B	1223	CLA	CHD-C4C	3.79	1.47	1.39
15	B	1226	CLA	OBD-CAD	3.79	1.29	1.22
15	B	1217	CLA	OBD-CAD	3.79	1.29	1.22
15	B	1229	CLA	CHD-C4C	3.79	1.47	1.39

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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	1134	CLA	OBD-CAD	3.79	1.29	1.22
15	A	1116	CLA	MG-NC	3.79	2.15	2.06
15	F	1301	CLA	CHB-C1B	3.79	1.47	1.39
15	B	1240	CLA	OBD-CAD	3.79	1.29	1.22
15	A	1124	CLA	MG-NC	3.79	2.15	2.06
15	A	1114	CLA	OBD-CAD	3.78	1.29	1.22
15	A	1112	CLA	OBD-CAD	3.78	1.29	1.22
15	A	1111	CLA	OBD-CAD	3.78	1.29	1.22
15	A	1131	CLA	OBD-CAD	3.78	1.29	1.22
15	J	1302	CLA	OBD-CAD	3.78	1.29	1.22
15	A	1135	CLA	MG-NC	3.78	2.15	2.06
15	F	1410	CLA	OBD-CAD	3.78	1.29	1.22
15	A	1134	CLA	MG-NC	3.78	2.15	2.06
15	A	1132	CLA	CHD-C4C	3.78	1.47	1.39
15	A	1104	CLA	CHB-C1B	3.78	1.47	1.39
15	A	1118	CLA	OBD-CAD	3.77	1.29	1.22
15	B	1021	CLA	MG-NC	3.77	2.15	2.06
15	F	1139	CLA	MG-NC	3.77	2.15	2.06
15	F	1301	CLA	OBD-CAD	3.77	1.29	1.22
15	K	1402	CLA	OBD-CAD	3.77	1.29	1.22
15	A	1117	CLA	CHB-C1B	3.77	1.47	1.39
15	B	1230	CLA	OBD-CAD	3.77	1.29	1.22
15	B	1232	CLA	OBD-CAD	3.77	1.29	1.22
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	1012	CLA	OBD-CAD	3.77	1.29	1.22
15	A	1128	CLA	CHD-C4C	3.76	1.47	1.39
15	A	1131	CLA	MG-NC	3.76	2.15	2.06
15	A	1133	CLA	OBD-CAD	3.76	1.29	1.22
15	A	1801	CLA	OBD-CAD	3.76	1.29	1.22
15	A	1122	CLA	OBD-CAD	3.76	1.29	1.22
15	J	1303	CLA	OBD-CAD	3.76	1.29	1.22
15	B	1206	CLA	MG-NC	3.76	2.15	2.06
15	A	1127	CLA	CHD-C4C	3.76	1.47	1.39
15	A	1138	CLA	CHB-C1B	3.76	1.47	1.39
15	B	1225	CLA	MG-NC	3.76	2.15	2.06
15	A	1115	CLA	OBD-CAD	3.76	1.28	1.22
15	B	1231	CLA	OBD-CAD	3.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1103	CLA	OBD-CAD	3.75	1.28	1.22
15	B	1206	CLA	OBD-CAD	3.75	1.28	1.22
15	B	1208	CLA	OBD-CAD	3.75	1.28	1.22
15	A	1126	CLA	OBD-CAD	3.75	1.28	1.22
15	B	1023	CLA	OBD-CAD	3.75	1.28	1.22
15	A	1135	CLA	OBD-CAD	3.75	1.28	1.22
15	A	1119	CLA	MG-NC	3.75	2.15	2.06
15	B	1238	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	1128	CLA	OBD-CAD	3.75	1.28	1.22
15	B	1235	CLA	CHD-C4C	3.75	1.47	1.39
15	B	1203	CLA	OBD-CAD	3.75	1.28	1.22
15	A	1127	CLA	MG-NC	3.74	2.15	2.06
15	A	1105	CLA	OBD-CAD	3.74	1.28	1.22
15	A	1101	CLA	CHB-C1B	3.74	1.47	1.39
15	A	1123	CLA	OBD-CAD	3.74	1.28	1.22
15	A	1104	CLA	OBD-CAD	3.73	1.28	1.22
15	B	1238	CLA	OBD-CAD	3.73	1.28	1.22
15	A	1137	CLA	OBD-CAD	3.73	1.28	1.22
15	A	1106	CLA	CHB-C1B	3.73	1.47	1.39
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	B	1210	CLA	OBD-CAD	3.73	1.28	1.22
15	B	1234	CLA	OBD-CAD	3.73	1.28	1.22
15	A	1126	CLA	CHB-C1B	3.73	1.47	1.39
15	B	1013	CLA	OBD-CAD	3.73	1.28	1.22
15	B	1205	CLA	MG-NC	3.73	2.15	2.06
15	B	1013	CLA	CHD-C4C	3.73	1.47	1.39
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	A	1107	CLA	OBD-CAD	3.72	1.28	1.22
15	B	1230	CLA	CHD-C4C	3.72	1.47	1.39
15	B	1207	CLA	MG-NC	3.72	2.15	2.06
15	A	1132	CLA	OBD-CAD	3.72	1.28	1.22
15	B	1219	CLA	MG-NC	3.72	2.15	2.06
15	A	1119	CLA	OBD-CAD	3.72	1.28	1.22
15	A	1113	CLA	OBD-CAD	3.72	1.28	1.22
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	1205	CLA	CHD-C4C	3.71	1.47	1.39
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	A	1109	CLA	OBD-CAD	3.70	1.28	1.22
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	A	1115	CLA	CHD-C4C	3.70	1.47	1.39
15	A	1136	CLA	OBD-CAD	3.70	1.28	1.22
15	B	1211	CLA	OBD-CAD	3.70	1.28	1.22
15	A	1130	CLA	OBD-CAD	3.69	1.28	1.22
15	B	1210	CLA	MG-NC	3.69	2.15	2.06
15	B	1013	CLA	CHB-C1B	3.69	1.47	1.39
15	A	1125	CLA	MG-NC	3.69	2.15	2.06
15	F	1139	CLA	OBD-CAD	3.69	1.28	1.22
15	A	1121	CLA	OBD-CAD	3.68	1.28	1.22
15	A	1107	CLA	CHB-C1B	3.68	1.47	1.39
15	A	1132	CLA	MG-NC	3.68	2.15	2.06
15	B	1236	CLA	OBD-CAD	3.68	1.28	1.22
15	B	1214	CLA	CHB-C1B	3.68	1.47	1.39
15	A	1111	CLA	MG-NC	3.68	2.15	2.06
15	B	1237	CLA	OBD-CAD	3.67	1.28	1.22
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	1110	CLA	OBD-CAD	3.66	1.28	1.22
15	A	1117	CLA	MG-NC	3.65	2.15	2.06
15	A	1129	CLA	MG-NC	3.65	2.14	2.06
15	B	1202	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	1221	CLA	OBD-CAD	3.64	1.28	1.22
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	1221	CLA	CHD-C4C	3.64	1.47	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B	1235	CLA	OBD-CAD	3.63	1.28	1.22
15	A	1130	CLA	CHB-C1B	3.63	1.47	1.39
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	1124	CLA	CHB-C1B	3.61	1.47	1.39
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	1109	CLA	MG-NC	3.61	2.14	2.06
15	A	1138	CLA	MG-NC	3.61	2.14	2.06
15	A	1125	CLA	CHD-C4C	3.61	1.47	1.39
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	1227	CLA	OBD-CAD	3.57	1.28	1.22
15	A	1106	CLA	MG-NC	3.56	2.14	2.06
15	A	1125	CLA	OBD-CAD	3.55	1.28	1.22
15	B	1228	CLA	OBD-CAD	3.55	1.28	1.22
15	A	1127	CLA	OBD-CAD	3.54	1.28	1.22
15	A	1107	CLA	MG-NC	3.52	2.14	2.06
15	A	1104	CLA	MG-NC	3.52	2.14	2.06
15	B	1023	CLA	MG-NC	3.52	2.14	2.06
15	A	1126	CLA	MG-NC	3.52	2.14	2.06
14	A	4012	BCR	C11-C12	-3.47	1.25	1.34
15	A	1118	CLA	MG-NC	3.46	2.14	2.06
15	B	1013	CLA	MG-NC	3.46	2.14	2.06
15	A	1129	CLA	OBD-CAD	3.44	1.28	1.22
14	B	4006	BCR	C11-C12	-3.40	1.25	1.34
15	B	1223	CLA	OBD-CAD	3.39	1.28	1.22
14	F	4016	BCR	C11-C12	-3.35	1.25	1.34
15	A	1022	CLA	C3D-C2D	3.33	1.48	1.39
13	A	1011	CL0	CHB-C4A	-3.33	1.34	1.38
14	B	4004	BCR	C11-C12	-3.33	1.26	1.34
15	A	1012	CLA	C3D-C2D	3.32	1.48	1.39
14	B	4010	BCR	C11-C12	-3.28	1.26	1.34
15	B	1220	CLA	C3D-C2D	3.22	1.47	1.39
15	A	1102	CLA	C3D-C2D	3.22	1.47	1.39

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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
15	A	1117	CLA	C3D-C2D	3.18	1.47	1.39
14	A	4002	BCR	C11-C12	-3.15	1.26	1.34
15	B	1239	CLA	C1B-C2B	3.14	1.50	1.43
15	B	1013	CLA	C3D-C2D	3.14	1.47	1.39
15	B	1222	CLA	C3D-C2D	3.14	1.47	1.39
15	B	1214	CLA	C3D-C2D	3.13	1.47	1.39
15	B	1232	CLA	C3D-C2D	3.12	1.47	1.39
15	A	1106	CLA	C3D-C2D	3.12	1.47	1.39
14	A	4003	BCR	C11-C12	-3.12	1.26	1.34
15	A	1138	CLA	C3D-C2D	3.11	1.47	1.39
15	B	1215	CLA	C3D-C2D	3.11	1.47	1.39
15	B	1238	CLA	C3D-C2D	3.11	1.47	1.39
15	B	1216	CLA	C3D-C2D	3.10	1.47	1.39
14	B	4017	BCR	C11-C12	-3.10	1.26	1.34
15	B	1023	CLA	C3D-C2D	3.09	1.47	1.39
14	A	4007	BCR	C11-C12	-3.08	1.26	1.34
15	F	1301	CLA	C3D-C2D	3.08	1.47	1.39
15	A	1119	CLA	C3D-C2D	3.08	1.47	1.39
15	A	1124	CLA	C3D-C2D	3.08	1.47	1.39
15	B	1217	CLA	C3D-C2D	3.08	1.47	1.39
14	F	4015	BCR	C11-C12	-3.07	1.26	1.34
15	B	1213	CLA	C3D-C2D	3.07	1.47	1.39
15	A	1109	CLA	C3D-C2D	3.07	1.47	1.39
14	B	4009	BCR	C11-C12	-3.06	1.26	1.34
15	B	1212	CLA	C3D-C2D	3.06	1.47	1.39
15	A	1128	CLA	C3D-C2D	3.06	1.47	1.39
15	B	1208	CLA	C3D-C2D	3.06	1.47	1.39
15	B	1203	CLA	C1B-C2B	3.06	1.50	1.43
15	B	1210	CLA	C3D-C2D	3.06	1.47	1.39
15	A	1112	CLA	C3D-C2D	3.05	1.47	1.39
15	B	1211	CLA	C3D-C2D	3.05	1.47	1.39
14	A	4008	BCR	C11-C12	-3.05	1.26	1.34
15	B	1235	CLA	C3D-C2D	3.05	1.47	1.39
15	B	1218	CLA	C3D-C2D	3.05	1.47	1.39
15	A	1133	CLA	C3D-C2D	3.05	1.47	1.39
14	J	4013	BCR	C11-C12	-3.05	1.26	1.34
15	A	1105	CLA	C3D-C2D	3.04	1.47	1.39
15	F	1410	CLA	C3D-C2D	3.04	1.47	1.39
15	A	1136	CLA	C1B-C2B	3.04	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1130	CLA	C3D-C2D	3.04	1.47	1.39
15	B	1201	CLA	C3D-C2D	3.04	1.47	1.39
15	A	1111	CLA	C3D-C2D	3.04	1.47	1.39
15	B	1221	CLA	C3D-C2D	3.03	1.47	1.39
15	B	1240	CLA	C3D-C2D	3.03	1.47	1.39
15	A	1104	CLA	C3D-C2D	3.03	1.47	1.39
15	A	1132	CLA	C3D-C2D	3.03	1.47	1.39
15	A	1101	CLA	C3D-C2D	3.03	1.47	1.39
15	B	1219	CLA	C3D-C2D	3.02	1.47	1.39
15	A	1012	CLA	C1D-ND	-3.02	1.33	1.37
15	B	1021	CLA	C3D-C2D	3.02	1.47	1.39
15	K	1402	CLA	C1B-C2B	3.02	1.50	1.43
15	B	1206	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1114	CLA	C3D-C2D	3.01	1.47	1.39
15	B	1204	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1127	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1135	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1115	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1116	CLA	C3D-C2D	3.01	1.47	1.39
15	B	1205	CLA	C3D-C2D	3.01	1.47	1.39
15	A	1121	CLA	C3D-C2D	3.00	1.47	1.39
15	B	1224	CLA	C3D-C2D	3.00	1.47	1.39
15	B	1229	CLA	C3D-C2D	3.00	1.47	1.39
15	A	1801	CLA	C3D-C2D	3.00	1.47	1.39
15	B	1209	CLA	C3D-C2D	3.00	1.47	1.39
15	B	1227	CLA	C3D-C2D	3.00	1.47	1.39
15	A	1124	CLA	C4D-CHA	3.00	1.48	1.38
15	A	1118	CLA	C3D-C2D	3.00	1.47	1.39
15	B	1202	CLA	C3D-C2D	2.99	1.47	1.39
15	A	1110	CLA	C3D-C2D	2.99	1.47	1.39
15	B	1223	CLA	C3D-C2D	2.99	1.47	1.39
15	A	1113	CLA	C3D-C2D	2.99	1.47	1.39
15	A	1131	CLA	C3D-C2D	2.99	1.47	1.39
15	B	1013	CLA	C1D-ND	-2.99	1.33	1.37
15	B	1222	CLA	C1B-C2B	2.98	1.50	1.43
15	B	1221	CLA	C4D-CHA	2.98	1.48	1.38
15	B	1228	CLA	C3D-C2D	2.98	1.47	1.39
15	B	1236	CLA	C3D-C2D	2.98	1.47	1.39
15	B	1239	CLA	C3D-C2D	2.98	1.47	1.39
15	B	1234	CLA	C1B-C2B	2.98	1.50	1.43
15	A	1123	CLA	C3D-C2D	2.98	1.47	1.39
15	B	1225	CLA	C3D-C2D	2.97	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1234	CLA	C3D-C2D	2.97	1.47	1.39
15	B	1222	CLA	C4D-CHA	2.97	1.48	1.38
15	J	1303	CLA	C1B-C2B	2.97	1.50	1.43
15	B	1207	CLA	C3D-C2D	2.96	1.47	1.39
15	B	1203	CLA	C3D-C2D	2.96	1.47	1.39
15	J	1302	CLA	C3D-C2D	2.96	1.47	1.39
15	B	1219	CLA	C1B-C2B	2.96	1.50	1.43
15	A	1132	CLA	C1B-C2B	2.96	1.50	1.43
15	B	1231	CLA	C3D-C2D	2.96	1.47	1.39
15	J	1303	CLA	C3D-C2D	2.95	1.47	1.39
15	A	1136	CLA	C3D-C2D	2.95	1.47	1.39
15	A	1801	CLA	C4D-CHA	2.95	1.48	1.38
15	A	1102	CLA	C4D-CHA	2.94	1.48	1.38
15	A	1137	CLA	C1B-C2B	2.94	1.50	1.43
15	A	1120	CLA	C4D-CHA	2.94	1.48	1.38
15	B	1209	CLA	C4D-CHA	2.94	1.48	1.38
15	K	1402	CLA	C3D-C2D	2.94	1.47	1.39
15	A	1140	CLA	C3D-C2D	2.94	1.47	1.39
15	A	1123	CLA	C4D-CHA	2.94	1.48	1.38
15	A	1134	CLA	C3D-C2D	2.94	1.47	1.39
15	A	1118	CLA	C1B-C2B	2.93	1.50	1.43
15	B	1226	CLA	C3D-C2D	2.93	1.47	1.39
15	B	1205	CLA	C1B-C2B	2.93	1.50	1.43
15	A	1120	CLA	C3D-C2D	2.93	1.47	1.39
15	A	1116	CLA	C1B-C2B	2.93	1.50	1.43
15	A	1129	CLA	C3D-C2D	2.92	1.47	1.39
15	A	1101	CLA	C4D-CHA	2.92	1.48	1.38
15	A	1120	CLA	C1B-C2B	2.92	1.50	1.43
15	A	1137	CLA	C3D-C2D	2.92	1.47	1.39
15	B	1230	CLA	C3D-C2D	2.92	1.46	1.39
15	B	1227	CLA	C1B-C2B	2.91	1.50	1.43
15	B	1240	CLA	C4D-CHA	2.91	1.48	1.38
15	A	1128	CLA	C1D-ND	-2.91	1.34	1.37
15	A	1103	CLA	C3D-C2D	2.91	1.46	1.39
15	B	1215	CLA	C1B-C2B	2.91	1.50	1.43
15	A	1121	CLA	C1B-C2B	2.91	1.50	1.43
15	B	1211	CLA	C1B-C2B	2.91	1.50	1.43
15	J	1303	CLA	C4D-CHA	2.91	1.48	1.38
15	A	1105	CLA	C1B-C2B	2.91	1.50	1.43
15	B	1237	CLA	C3D-C2D	2.91	1.46	1.39
15	B	1203	CLA	C4D-CHA	2.91	1.48	1.38
15	B	1212	CLA	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1103	CLA	C1B-C2B	2.90	1.49	1.43
15	B	1207	CLA	C1B-C2B	2.90	1.49	1.43
15	A	1110	CLA	C1D-ND	-2.90	1.34	1.37
15	K	1401	CLA	C3D-C2D	2.90	1.46	1.39
15	B	1217	CLA	C1B-C2B	2.90	1.49	1.43
15	A	1022	CLA	C1D-ND	-2.90	1.34	1.37
15	K	1401	CLA	C1B-C2B	2.90	1.49	1.43
15	B	1201	CLA	C4D-CHA	2.89	1.48	1.38
15	B	1231	CLA	C1B-C2B	2.89	1.49	1.43
15	A	1117	CLA	C4D-CHA	2.89	1.48	1.38
15	B	1226	CLA	C4D-CHA	2.89	1.48	1.38
15	B	1210	CLA	C4D-CHA	2.89	1.48	1.38
15	A	1122	CLA	C3D-C2D	2.89	1.46	1.39
15	J	1302	CLA	C4D-CHA	2.89	1.48	1.38
15	A	1129	CLA	C1B-C2B	2.89	1.49	1.43
15	B	1208	CLA	C1B-C2B	2.88	1.49	1.43
15	B	1207	CLA	C4D-CHA	2.88	1.48	1.38
15	A	1012	CLA	C4D-CHA	2.88	1.48	1.38
15	A	1123	CLA	C1B-C2B	2.88	1.49	1.43
15	B	1206	CLA	C1B-C2B	2.88	1.49	1.43
15	B	1206	CLA	C4D-CHA	2.88	1.48	1.38
15	B	1232	CLA	C4D-CHA	2.87	1.48	1.38
15	A	1801	CLA	C1B-C2B	2.87	1.49	1.43
15	A	1112	CLA	C4D-CHA	2.87	1.48	1.38
15	B	1217	CLA	C4D-CHA	2.87	1.48	1.38
15	B	1202	CLA	C1B-C2B	2.87	1.49	1.43
15	A	1106	CLA	C4D-CHA	2.87	1.48	1.38
15	B	1213	CLA	C1B-C2B	2.87	1.49	1.43
15	A	1126	CLA	C1D-C2D	2.87	1.51	1.45
15	F	1301	CLA	C4D-CHA	2.87	1.48	1.38
14	A	4001	BCR	C11-C12	-2.87	1.27	1.34
15	B	1238	CLA	C1B-C2B	2.87	1.49	1.43
15	B	1225	CLA	C4D-CHA	2.87	1.48	1.38
15	A	1131	CLA	C1B-C2B	2.87	1.49	1.43
15	B	1239	CLA	C4D-CHA	2.86	1.48	1.38
15	B	1212	CLA	C1B-C2B	2.86	1.49	1.43
15	B	1229	CLA	C1B-C2B	2.86	1.49	1.43
15	B	1224	CLA	C4D-CHA	2.86	1.48	1.38
15	B	1205	CLA	C1D-ND	-2.86	1.34	1.37
15	B	1202	CLA	C4D-CHA	2.86	1.48	1.38
15	B	1227	CLA	C4D-CHA	2.86	1.48	1.38
15	A	1113	CLA	C4D-CHA	2.86	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1103	CLA	C4D-CHA	2.86	1.48	1.38
15	B	1236	CLA	C1D-ND	-2.86	1.34	1.37
15	B	1204	CLA	C1B-C2B	2.85	1.49	1.43
15	A	1126	CLA	C3D-C2D	2.85	1.46	1.39
15	A	1138	CLA	C4D-CHA	2.85	1.48	1.38
15	A	1135	CLA	C1B-C2B	2.85	1.49	1.43
15	B	1223	CLA	C4D-CHA	2.85	1.48	1.38
15	A	1119	CLA	C4D-CHA	2.85	1.48	1.38
15	A	1131	CLA	C4D-CHA	2.85	1.48	1.38
15	B	1021	CLA	C4D-CHA	2.84	1.48	1.38
15	A	1106	CLA	C1B-C2B	2.84	1.49	1.43
15	A	1114	CLA	C1B-C2B	2.84	1.49	1.43
15	A	1125	CLA	C4D-CHA	2.84	1.48	1.38
15	B	1237	CLA	C1B-C2B	2.84	1.49	1.43
15	B	1219	CLA	C4D-CHA	2.84	1.48	1.38
15	K	1402	CLA	C4D-CHA	2.84	1.48	1.38
15	K	1401	CLA	C4D-CHA	2.84	1.48	1.38
15	A	1109	CLA	C1B-C2B	2.84	1.49	1.43
15	A	1128	CLA	C4D-CHA	2.84	1.48	1.38
15	B	1221	CLA	C1B-C2B	2.83	1.49	1.43
15	A	1129	CLA	C4D-CHA	2.83	1.48	1.38
15	F	1410	CLA	C4D-CHA	2.83	1.48	1.38
15	A	1110	CLA	C1B-C2B	2.83	1.49	1.43
15	F	1410	CLA	C1B-C2B	2.83	1.49	1.43
15	B	1220	CLA	C4D-CHA	2.83	1.48	1.38
15	A	1111	CLA	C4D-CHA	2.83	1.48	1.38
15	F	1139	CLA	C1B-C2B	2.83	1.49	1.43
15	A	1134	CLA	C4D-CHA	2.83	1.48	1.38
15	B	1229	CLA	C4D-CHA	2.82	1.48	1.38
15	A	1133	CLA	C4D-CHA	2.82	1.48	1.38
15	A	1121	CLA	C4D-CHA	2.82	1.48	1.38
15	J	1302	CLA	C1B-C2B	2.82	1.49	1.43
15	A	1118	CLA	C4D-CHA	2.82	1.48	1.38
15	A	1102	CLA	C1B-C2B	2.82	1.49	1.43
15	B	1235	CLA	C4D-CHA	2.82	1.48	1.38
15	B	1237	CLA	C4D-CHA	2.81	1.48	1.38
15	A	1107	CLA	C3D-C2D	2.81	1.46	1.39
15	A	1132	CLA	C4D-CHA	2.81	1.48	1.38
15	B	1214	CLA	C4D-CHA	2.81	1.48	1.38
15	B	1201	CLA	C1B-C2B	2.81	1.49	1.43
15	B	1211	CLA	C4D-CHA	2.81	1.48	1.38
15	A	1105	CLA	C4D-CHA	2.81	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1215	CLA	C4D-CHA	2.81	1.48	1.38
15	A	1115	CLA	C1B-C2B	2.81	1.49	1.43
15	B	1240	CLA	C1B-C2B	2.81	1.49	1.43
15	A	1114	CLA	C4D-CHA	2.81	1.48	1.38
15	B	1238	CLA	C4D-CHA	2.81	1.48	1.38
15	A	1140	CLA	C1B-C2B	2.80	1.49	1.43
15	A	1127	CLA	C1D-ND	-2.80	1.34	1.37
15	A	1137	CLA	C4D-CHA	2.80	1.48	1.38
15	A	1135	CLA	C4D-CHA	2.80	1.48	1.38
15	B	1234	CLA	C4D-CHA	2.80	1.48	1.38
15	B	1231	CLA	C4D-CHA	2.80	1.48	1.38
15	B	1205	CLA	C4D-CHA	2.79	1.48	1.38
15	B	1223	CLA	C1D-ND	-2.79	1.34	1.37
15	A	1130	CLA	C4D-CHA	2.79	1.48	1.38
15	A	1125	CLA	C3D-C2D	2.79	1.46	1.39
15	B	1226	CLA	C1B-NB	-2.79	1.34	1.37
15	B	1208	CLA	C4D-CHA	2.79	1.48	1.38
15	B	1023	CLA	C1B-C2B	2.79	1.49	1.43
15	A	1116	CLA	C4D-CHA	2.79	1.47	1.38
15	B	1228	CLA	C4D-CHA	2.79	1.47	1.38
15	A	1119	CLA	C1D-ND	-2.79	1.34	1.37
15	B	1021	CLA	C1D-ND	-2.79	1.34	1.37
15	B	1213	CLA	C4D-CHA	2.78	1.47	1.38
15	A	1126	CLA	C4D-CHA	2.78	1.47	1.38
15	B	1216	CLA	C4D-CHA	2.78	1.47	1.38
15	B	1204	CLA	C4D-CHA	2.78	1.47	1.38
15	A	1127	CLA	C1B-NB	-2.78	1.34	1.37
15	A	1128	CLA	C1B-NB	-2.78	1.34	1.37
15	A	1111	CLA	C1B-C2B	2.78	1.49	1.43
15	F	1139	CLA	C3D-C2D	2.78	1.46	1.39
15	A	1140	CLA	C4D-CHA	2.78	1.47	1.38
15	B	1210	CLA	C1B-C2B	2.77	1.49	1.43
15	B	1225	CLA	C1B-NB	-2.77	1.34	1.37
15	A	1104	CLA	C4D-CHA	2.77	1.47	1.38
15	F	1301	CLA	C1D-ND	-2.77	1.34	1.37
15	A	1022	CLA	C4D-CHA	2.76	1.47	1.38
15	A	1130	CLA	C1D-ND	-2.76	1.34	1.37
15	A	1122	CLA	C4D-CHA	2.76	1.47	1.38
15	B	1232	CLA	C1B-C2B	2.76	1.49	1.43
15	A	1136	CLA	C4D-CHA	2.76	1.47	1.38
15	B	1218	CLA	C4D-CHA	2.75	1.47	1.38
15	A	1124	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1115	CLA	C1D-ND	-2.75	1.34	1.37
15	A	1104	CLA	C1D-ND	-2.75	1.34	1.37
15	B	1228	CLA	C1B-NB	-2.74	1.34	1.37
15	A	1012	CLA	C1B-C2B	2.74	1.49	1.43
15	A	1113	CLA	C1B-C2B	2.74	1.49	1.43
15	B	1209	CLA	C1B-C2B	2.73	1.49	1.43
15	A	1122	CLA	C1D-C2D	2.73	1.50	1.45
15	B	1236	CLA	C4D-CHA	2.73	1.47	1.38
15	F	1301	CLA	C1B-C2B	2.73	1.49	1.43
15	B	1230	CLA	C1B-C2B	2.73	1.49	1.43
15	B	1230	CLA	C4D-CHA	2.73	1.47	1.38
15	A	1140	CLA	C1D-ND	-2.73	1.34	1.37
15	B	1023	CLA	C4D-CHA	2.73	1.47	1.38
15	B	1221	CLA	C1B-NB	-2.73	1.34	1.37
15	B	1201	CLA	C1D-ND	-2.72	1.34	1.37
15	A	1110	CLA	C4D-CHA	2.72	1.47	1.38
15	B	1218	CLA	C1B-C2B	2.72	1.49	1.43
15	B	1234	CLA	C1D-ND	-2.72	1.34	1.37
15	A	1101	CLA	C1D-ND	-2.72	1.34	1.37
15	A	1109	CLA	C4D-CHA	2.72	1.47	1.38
15	A	1121	CLA	C1D-ND	-2.72	1.34	1.37
15	A	1134	CLA	C1B-C2B	2.72	1.49	1.43
15	B	1013	CLA	C4D-CHA	2.72	1.47	1.38
15	B	1217	CLA	C1D-ND	-2.71	1.34	1.37
15	B	1232	CLA	C1D-ND	-2.71	1.34	1.37
15	A	1115	CLA	C4D-CHA	2.71	1.47	1.38
15	B	1238	CLA	C1D-ND	-2.71	1.34	1.37
15	B	1013	CLA	C1B-C2B	2.71	1.49	1.43
15	A	1128	CLA	C1C-NC	-2.71	1.33	1.37
15	B	1220	CLA	C1D-ND	-2.70	1.34	1.37
15	B	1211	CLA	C1D-ND	-2.70	1.34	1.37
15	B	1209	CLA	C1B-NB	-2.70	1.34	1.37
15	B	1230	CLA	C1B-NB	-2.70	1.34	1.37
15	A	1117	CLA	C1D-ND	-2.70	1.34	1.37
15	B	1021	CLA	C1B-NB	-2.70	1.34	1.37
15	F	1139	CLA	C4D-CHA	2.69	1.47	1.38
15	F	1410	CLA	C1D-ND	-2.69	1.34	1.37
15	A	1127	CLA	C4D-CHA	2.69	1.47	1.38
15	A	1125	CLA	C1D-ND	-2.69	1.34	1.37
15	A	1127	CLA	C1B-C2B	2.68	1.49	1.43
15	A	1135	CLA	C1D-ND	-2.68	1.34	1.37
15	B	1212	CLA	C1D-ND	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1129	CLA	C1D-C2D	2.68	1.50	1.45
15	B	1204	CLA	C1D-C2D	2.68	1.50	1.45
15	A	1107	CLA	C4D-CHA	2.68	1.47	1.38
15	B	1023	CLA	C1D-ND	-2.68	1.34	1.37
15	F	1139	CLA	C1D-ND	-2.68	1.34	1.37
15	A	1112	CLA	C1B-C2B	2.68	1.49	1.43
15	B	1224	CLA	C1B-C2B	2.68	1.49	1.43
15	B	1229	CLA	C1D-ND	-2.68	1.34	1.37
13	A	1011	CL0	C3A-C2A	-2.68	1.52	1.54
15	A	1022	CLA	C1B-C2B	2.67	1.49	1.43
15	B	1225	CLA	C1D-ND	-2.67	1.34	1.37
15	A	1133	CLA	C1B-C2B	2.67	1.49	1.43
15	A	1109	CLA	C1D-C2D	2.67	1.50	1.45
15	B	1218	CLA	C1D-ND	-2.67	1.34	1.37
15	B	1226	CLA	C1B-C2B	2.66	1.49	1.43
15	B	1219	CLA	C1B-NB	-2.66	1.34	1.37
15	A	1104	CLA	C1B-C2B	2.66	1.49	1.43
15	B	1208	CLA	C1D-C2D	2.65	1.50	1.45
15	B	1224	CLA	C1B-NB	-2.65	1.34	1.37
15	B	1021	CLA	C1B-C2B	2.65	1.49	1.43
15	B	1225	CLA	C1B-C2B	2.65	1.49	1.43
15	B	1213	CLA	C1D-C2D	2.64	1.50	1.45
15	A	1102	CLA	C1D-ND	-2.64	1.34	1.37
15	B	1231	CLA	C1C-NC	-2.64	1.33	1.37
15	A	1138	CLA	C1D-ND	-2.64	1.34	1.37
15	A	1125	CLA	C1B-C2B	2.64	1.49	1.43
15	A	1012	CLA	C1B-NB	-2.63	1.34	1.37
15	B	1206	CLA	C1D-C2D	2.63	1.50	1.45
15	B	1213	CLA	C1D-ND	-2.63	1.34	1.37
15	B	1216	CLA	C1D-ND	-2.63	1.34	1.37
15	A	1801	CLA	C1D-ND	-2.63	1.34	1.37
15	B	1235	CLA	C1B-C2B	2.62	1.49	1.43
15	B	1210	CLA	C1B-NB	-2.62	1.34	1.37
15	B	1220	CLA	C1B-C2B	2.62	1.49	1.43
15	B	1237	CLA	C1D-C2D	2.61	1.50	1.45
15	A	1105	CLA	C1D-ND	-2.61	1.34	1.37
15	B	1230	CLA	C1D-ND	-2.61	1.34	1.37
15	B	1236	CLA	C1B-C2B	2.61	1.49	1.43
15	B	1208	CLA	C1D-ND	-2.61	1.34	1.37
15	A	1107	CLA	C1D-C2D	2.61	1.50	1.45
15	B	1222	CLA	C1D-ND	-2.61	1.34	1.37
15	A	1123	CLA	C4C-C3C	2.61	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1107	CLA	C1C-NC	-2.61	1.33	1.37
15	B	1214	CLA	C1B-NB	-2.60	1.34	1.37
15	B	1207	CLA	C1B-NB	-2.60	1.34	1.37
15	B	1223	CLA	C1B-C2B	2.60	1.49	1.43
15	A	1106	CLA	C1D-C2D	2.60	1.50	1.45
15	B	1231	CLA	C1D-C2D	2.60	1.50	1.45
15	A	1105	CLA	C1D-C2D	2.59	1.50	1.45
15	B	1240	CLA	C1D-ND	-2.59	1.34	1.37
15	A	1101	CLA	C1B-NB	-2.59	1.34	1.37
15	B	1013	CLA	C1B-NB	-2.59	1.34	1.37
15	B	1235	CLA	C1D-ND	-2.59	1.34	1.37
15	A	1120	CLA	C1D-C2D	2.59	1.50	1.45
15	B	1223	CLA	C1B-NB	-2.59	1.34	1.37
15	A	1107	CLA	C1D-ND	-2.59	1.34	1.37
15	A	1122	CLA	C1B-C2B	2.59	1.49	1.43
15	A	1106	CLA	C1D-ND	-2.59	1.34	1.37
15	A	1130	CLA	C1D-C2D	2.59	1.50	1.45
15	A	1118	CLA	C1D-ND	-2.59	1.34	1.37
15	B	1219	CLA	C1D-C2D	2.58	1.50	1.45
15	B	1227	CLA	C1D-ND	-2.58	1.34	1.37
15	A	1119	CLA	C1B-NB	-2.58	1.34	1.37
15	B	1214	CLA	C1D-C2D	2.58	1.50	1.45
15	A	1113	CLA	C1B-NB	-2.57	1.34	1.37
15	A	1118	CLA	C1B-NB	-2.57	1.34	1.37
15	A	1124	CLA	C1D-C2D	2.57	1.50	1.45
15	B	1214	CLA	C1D-ND	-2.57	1.34	1.37
15	B	1228	CLA	C1D-C2D	2.57	1.50	1.45
15	B	1228	CLA	C1B-C2B	2.57	1.49	1.43
15	A	1131	CLA	C1B-NB	-2.57	1.34	1.37
15	B	1023	CLA	C1B-NB	-2.57	1.34	1.37
15	B	1209	CLA	C1D-C2D	2.57	1.50	1.45
15	A	1117	CLA	C1B-C2B	2.57	1.49	1.43
15	A	1117	CLA	C1B-NB	-2.57	1.34	1.37
15	B	1226	CLA	C1D-ND	-2.56	1.34	1.37
15	A	1136	CLA	C1D-C2D	2.56	1.50	1.45
15	A	1128	CLA	C1B-C2B	2.56	1.49	1.43
15	F	1301	CLA	C1B-NB	-2.56	1.34	1.37
15	B	1202	CLA	C1B-NB	-2.56	1.34	1.37
15	A	1123	CLA	C1D-C2D	2.56	1.50	1.45
15	B	1215	CLA	C1D-ND	-2.56	1.34	1.37
15	A	1112	CLA	C1B-NB	-2.56	1.34	1.37
15	A	1114	CLA	C1D-C2D	2.56	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1202	CLA	C1D-C2D	2.55	1.50	1.45
15	B	1216	CLA	C1D-C2D	2.55	1.50	1.45
15	A	1109	CLA	C1D-ND	-2.55	1.34	1.37
15	A	1125	CLA	C1B-NB	-2.55	1.34	1.37
15	B	1206	CLA	C1B-NB	-2.55	1.34	1.37
15	B	1214	CLA	C1B-C2B	2.55	1.49	1.43
15	B	1239	CLA	C1D-C2D	2.55	1.50	1.45
15	A	1123	CLA	C1B-NB	-2.55	1.34	1.37
15	J	1302	CLA	C1B-NB	-2.55	1.34	1.37
15	A	1103	CLA	C1B-NB	-2.55	1.34	1.37
15	B	1220	CLA	C1D-C2D	2.55	1.50	1.45
15	B	1231	CLA	C1D-ND	-2.54	1.34	1.37
15	A	1134	CLA	C1D-C2D	2.54	1.50	1.45
15	A	1116	CLA	C1D-C2D	2.54	1.50	1.45
15	A	1129	CLA	C1B-NB	-2.54	1.34	1.37
15	A	1137	CLA	C1D-ND	-2.54	1.34	1.37
15	B	1210	CLA	C1D-ND	-2.54	1.34	1.37
15	A	1112	CLA	C1D-ND	-2.53	1.34	1.37
15	J	1302	CLA	C1D-ND	-2.53	1.34	1.37
15	A	1105	CLA	C4B-NB	-2.53	1.34	1.37
15	A	1111	CLA	C1B-NB	-2.53	1.34	1.37
15	B	1208	CLA	C1B-NB	-2.53	1.34	1.37
15	A	1102	CLA	C1B-NB	-2.52	1.34	1.37
15	B	1023	CLA	C4B-NB	-2.52	1.34	1.37
15	B	1215	CLA	C1D-C2D	2.52	1.50	1.45
15	B	1203	CLA	C1D-ND	-2.52	1.34	1.37
15	B	1203	CLA	C1D-C2D	2.52	1.50	1.45
15	A	1103	CLA	C1D-C2D	2.52	1.50	1.45
15	A	1130	CLA	C1B-NB	-2.52	1.34	1.37
15	B	1221	CLA	C1D-ND	-2.52	1.34	1.37
15	A	1131	CLA	C1D-C2D	2.51	1.50	1.45
15	B	1235	CLA	C1B-NB	-2.51	1.34	1.37
15	A	1133	CLA	C1D-ND	-2.51	1.34	1.37
15	B	1206	CLA	C1D-ND	-2.51	1.34	1.37
15	B	1236	CLA	C1D-C2D	2.51	1.50	1.45
15	B	1207	CLA	C1D-C2D	2.51	1.50	1.45
15	A	1111	CLA	C1D-C2D	2.51	1.50	1.45
15	B	1203	CLA	C1B-NB	-2.51	1.34	1.37
15	B	1224	CLA	C1D-C2D	2.50	1.50	1.45
15	B	1209	CLA	C4C-C3C	2.50	1.49	1.45
15	A	1104	CLA	C1D-C2D	2.50	1.50	1.45
15	K	1402	CLA	C1D-C2D	2.50	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1121	CLA	C1D-C2D	2.50	1.50	1.45
15	B	1240	CLA	C1D-C2D	2.50	1.50	1.45
15	B	1230	CLA	C1D-C2D	2.50	1.50	1.45
15	B	1218	CLA	C1B-NB	-2.50	1.34	1.37
15	A	1138	CLA	C1D-C2D	2.50	1.50	1.45
15	B	1222	CLA	C1B-NB	-2.50	1.34	1.37
15	A	1133	CLA	C1D-C2D	2.50	1.50	1.45
15	A	1101	CLA	C3B-C4B	2.50	1.50	1.42
15	B	1216	CLA	C1B-C2B	2.49	1.49	1.43
15	A	1102	CLA	C1D-C2D	2.49	1.50	1.45
15	B	1023	CLA	C1D-C2D	2.49	1.50	1.45
15	A	1113	CLA	C1D-ND	-2.49	1.34	1.37
15	A	1117	CLA	C1D-C2D	2.49	1.50	1.45
15	A	1132	CLA	C1D-ND	-2.49	1.34	1.37
15	B	1216	CLA	C1B-NB	-2.49	1.34	1.37
15	F	1410	CLA	C1D-C2D	2.49	1.50	1.45
15	A	1120	CLA	C1D-ND	-2.49	1.34	1.37
15	A	1122	CLA	C1B-NB	-2.49	1.34	1.37
15	A	1119	CLA	C1D-C2D	2.48	1.50	1.45
15	A	1137	CLA	C1B-NB	-2.48	1.34	1.37
15	B	1238	CLA	C1D-C2D	2.48	1.50	1.45
15	A	1122	CLA	C1D-ND	-2.48	1.34	1.37
15	A	1124	CLA	C1B-NB	-2.48	1.34	1.37
15	A	1114	CLA	C4C-C3C	2.48	1.49	1.45
15	B	1204	CLA	C1B-NB	-2.47	1.34	1.37
15	A	1124	CLA	C1D-ND	-2.47	1.34	1.37
15	A	1131	CLA	C1D-ND	-2.47	1.34	1.37
15	A	1110	CLA	C1B-NB	-2.47	1.34	1.37
15	B	1227	CLA	C1D-C2D	2.47	1.50	1.45
15	A	1133	CLA	C1B-NB	-2.47	1.34	1.37
15	A	1022	CLA	C1B-NB	-2.47	1.34	1.37
15	A	1126	CLA	C1B-C2B	2.47	1.48	1.43
15	B	1219	CLA	C1D-ND	-2.47	1.34	1.37
15	B	1239	CLA	C4C-C3C	2.46	1.49	1.45
15	A	1138	CLA	C3B-C4B	2.46	1.49	1.42
15	A	1110	CLA	C1C-NC	-2.46	1.34	1.37
15	A	1106	CLA	C1B-NB	-2.46	1.34	1.37
15	B	1207	CLA	C1D-ND	-2.46	1.34	1.37
15	B	1206	CLA	C4C-C3C	2.46	1.49	1.45
15	A	1114	CLA	C1D-ND	-2.46	1.34	1.37
15	A	1112	CLA	C1D-C2D	2.46	1.50	1.45
15	A	1136	CLA	C1D-ND	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	1303	CLA	C1D-C2D	2.46	1.50	1.45
15	A	1101	CLA	C1B-C2B	2.46	1.48	1.43
15	B	1202	CLA	C1D-ND	-2.45	1.34	1.37
15	B	1204	CLA	C1D-ND	-2.45	1.34	1.37
15	A	1116	CLA	C4B-NB	-2.45	1.34	1.37
15	K	1401	CLA	C1D-C2D	2.45	1.50	1.45
15	J	1302	CLA	C1D-C2D	2.45	1.50	1.45
15	A	1115	CLA	C1B-NB	-2.45	1.34	1.37
15	A	1113	CLA	C1D-C2D	2.45	1.50	1.45
15	A	1114	CLA	C1B-NB	-2.44	1.34	1.37
15	B	1236	CLA	C1B-NB	-2.44	1.34	1.37
15	A	1134	CLA	C1D-ND	-2.44	1.34	1.37
15	A	1116	CLA	C1B-NB	-2.44	1.34	1.37
15	A	1126	CLA	C1D-ND	-2.44	1.34	1.37
15	A	1116	CLA	C1D-ND	-2.44	1.34	1.37
15	B	1239	CLA	C1D-ND	-2.44	1.34	1.37
15	B	1216	CLA	C4C-C3C	2.43	1.49	1.45
15	A	1135	CLA	C1D-C2D	2.43	1.50	1.45
15	A	1107	CLA	C1B-NB	-2.43	1.34	1.37
15	A	1122	CLA	C3B-C4B	2.43	1.49	1.42
15	B	1210	CLA	C1D-C2D	2.43	1.50	1.45
15	A	1111	CLA	C1D-ND	-2.43	1.34	1.37
15	A	1129	CLA	C1D-ND	-2.43	1.34	1.37
15	K	1402	CLA	C1D-ND	-2.43	1.34	1.37
15	J	1303	CLA	C1B-NB	-2.43	1.34	1.37
15	A	1110	CLA	C4B-NB	-2.43	1.34	1.37
15	F	1139	CLA	C1C-NC	-2.42	1.34	1.37
15	B	1224	CLA	C4B-NB	-2.42	1.34	1.37
15	B	1234	CLA	C1C-NC	-2.42	1.34	1.37
15	A	1111	CLA	C4B-NB	-2.42	1.34	1.37
15	B	1232	CLA	C1B-NB	-2.42	1.34	1.37
15	B	1232	CLA	C1D-C2D	2.42	1.50	1.45
15	A	1104	CLA	C1B-NB	-2.42	1.34	1.37
15	A	1138	CLA	C1B-NB	-2.42	1.34	1.37
15	B	1209	CLA	C1D-ND	-2.42	1.34	1.37
15	F	1139	CLA	C1B-NB	-2.42	1.34	1.37
15	A	1801	CLA	C1B-NB	-2.41	1.34	1.37
15	B	1236	CLA	C1C-C2C	2.41	1.49	1.44
15	A	1133	CLA	C4C-C3C	2.41	1.49	1.45
15	B	1212	CLA	C1B-NB	-2.41	1.34	1.37
15	B	1234	CLA	C1D-C2D	2.41	1.50	1.45
15	B	1201	CLA	C1D-C2D	2.41	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	1401	CLA	C4B-NB	-2.41	1.34	1.37
15	J	1303	CLA	C1D-ND	-2.41	1.34	1.37
15	A	1105	CLA	C4C-C3C	2.41	1.49	1.45
15	A	1115	CLA	C1C-NC	-2.41	1.34	1.37
15	A	1118	CLA	C1D-C2D	2.41	1.50	1.45
15	K	1401	CLA	C1B-NB	-2.40	1.34	1.37
13	A	1108	CL0	CHB-C4A	-2.40	1.35	1.38
15	B	1023	CLA	C1C-NC	-2.40	1.34	1.37
15	A	1138	CLA	C1B-C2B	2.40	1.48	1.43
15	B	1225	CLA	C4B-NB	-2.40	1.34	1.37
15	A	1136	CLA	C4B-NB	-2.40	1.34	1.37
15	B	1217	CLA	C1B-NB	-2.40	1.34	1.37
15	A	1801	CLA	C1D-C2D	2.40	1.50	1.45
15	A	1116	CLA	C4C-C3C	2.40	1.49	1.45
15	A	1131	CLA	C1C-NC	-2.40	1.34	1.37
15	A	1107	CLA	C3B-C4B	2.40	1.49	1.42
15	K	1401	CLA	C1D-ND	-2.40	1.34	1.37
15	K	1402	CLA	C1B-NB	-2.40	1.34	1.37
15	A	1132	CLA	C1D-C2D	2.39	1.50	1.45
15	A	1137	CLA	C4B-NB	-2.39	1.34	1.37
15	B	1013	CLA	C1C-NC	-2.39	1.34	1.37
15	A	1130	CLA	C1B-C2B	2.39	1.48	1.43
15	A	1120	CLA	C1B-NB	-2.39	1.34	1.37
15	A	1801	CLA	C1C-NC	-2.39	1.34	1.37
15	B	1217	CLA	C1D-C2D	2.39	1.50	1.45
15	B	1239	CLA	C1C-NC	-2.39	1.34	1.37
15	A	1106	CLA	C1C-NC	-2.38	1.34	1.37
15	B	1218	CLA	C1D-C2D	2.38	1.50	1.45
15	B	1220	CLA	C1B-NB	-2.38	1.34	1.37
15	B	1215	CLA	C1C-NC	-2.38	1.34	1.37
15	A	1134	CLA	C1B-NB	-2.38	1.34	1.37
15	B	1234	CLA	C1B-NB	-2.37	1.34	1.37
15	B	1222	CLA	C1C-NC	-2.37	1.34	1.37
15	B	1228	CLA	C1D-ND	-2.37	1.34	1.37
15	B	1231	CLA	C1B-NB	-2.37	1.34	1.37
15	B	1240	CLA	C1B-NB	-2.37	1.34	1.37
15	A	1110	CLA	C1D-C2D	2.37	1.50	1.45
15	A	1113	CLA	C4C-C3C	2.37	1.49	1.45
15	B	1204	CLA	C4C-C3C	2.37	1.49	1.45
15	A	1138	CLA	C1C-C2C	2.37	1.49	1.44
15	B	1212	CLA	C1D-C2D	2.36	1.50	1.45
15	A	1119	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1208	CLA	C1C-NC	-2.36	1.34	1.37
15	A	1126	CLA	C1B-NB	-2.36	1.34	1.37
15	B	1201	CLA	C1B-NB	-2.36	1.34	1.37
15	A	1103	CLA	C1D-ND	-2.36	1.34	1.37
15	F	1410	CLA	C1B-NB	-2.36	1.34	1.37
15	A	1137	CLA	C4C-C3C	2.36	1.49	1.45
15	A	1120	CLA	C4C-C3C	2.35	1.49	1.45
15	J	1303	CLA	C4C-C3C	2.35	1.49	1.45
15	B	1211	CLA	C1B-NB	-2.35	1.34	1.37
15	A	1140	CLA	C1C-NC	-2.35	1.34	1.37
15	A	1126	CLA	C3B-C4B	2.35	1.49	1.42
15	B	1215	CLA	C4C-C3C	2.35	1.49	1.45
15	B	1203	CLA	C1C-NC	-2.35	1.34	1.37
15	B	1211	CLA	C1C-NC	-2.35	1.34	1.37
15	A	1137	CLA	C1D-C2D	2.35	1.50	1.45
15	A	1113	CLA	C1C-NC	-2.35	1.34	1.37
15	B	1236	CLA	C3B-C4B	2.35	1.49	1.42
15	B	1225	CLA	C1D-C2D	2.35	1.50	1.45
15	A	1113	CLA	C3B-C4B	2.34	1.49	1.42
15	A	1102	CLA	C1C-NC	-2.34	1.34	1.37
15	B	1221	CLA	C4B-NB	-2.34	1.34	1.37
15	A	1103	CLA	C1C-NC	-2.34	1.34	1.37
15	K	1401	CLA	C1C-NC	-2.34	1.34	1.37
15	A	1131	CLA	C4C-C3C	2.34	1.49	1.45
15	B	1235	CLA	C1D-C2D	2.34	1.50	1.45
15	A	1121	CLA	C4C-C3C	2.34	1.49	1.45
15	B	1238	CLA	C1B-NB	-2.34	1.34	1.37
14	A	4008	BCR	C30-C25	-2.34	1.50	1.53
15	A	1105	CLA	C1C-NC	-2.34	1.34	1.37
15	B	1210	CLA	C1C-NC	-2.34	1.34	1.37
15	B	1240	CLA	C4C-C3C	2.34	1.49	1.45
15	B	1229	CLA	C1C-NC	-2.34	1.34	1.37
15	A	1022	CLA	C1D-C2D	2.34	1.50	1.45
15	A	1121	CLA	C1C-NC	-2.34	1.34	1.37
15	B	1219	CLA	C4B-NB	-2.34	1.34	1.37
15	B	1204	CLA	C4B-NB	-2.34	1.34	1.37
15	A	1107	CLA	C1B-C2B	2.34	1.48	1.43
15	B	1224	CLA	C1D-ND	-2.33	1.34	1.37
15	A	1140	CLA	C1D-C2D	2.33	1.50	1.45
15	A	1102	CLA	C4B-NB	-2.33	1.34	1.37
15	F	1139	CLA	C1D-C2D	2.33	1.50	1.45
15	K	1401	CLA	C4C-C3C	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1227	CLA	C4C-C3C	2.33	1.49	1.45
15	B	1218	CLA	C1C-NC	-2.33	1.34	1.37
15	B	1222	CLA	C1D-C2D	2.33	1.49	1.45
15	B	1208	CLA	C4B-NB	-2.33	1.34	1.37
15	F	1301	CLA	C1D-C2D	2.33	1.49	1.45
15	A	1135	CLA	C4C-C3C	2.33	1.49	1.45
15	B	1222	CLA	C4B-NB	-2.33	1.34	1.37
15	B	1226	CLA	C1D-C2D	2.33	1.49	1.45
15	B	1214	CLA	C4C-C3C	2.33	1.49	1.45
15	B	1205	CLA	C1C-NC	-2.32	1.34	1.37
15	J	1302	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1111	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1135	CLA	C1B-NB	-2.32	1.34	1.37
15	B	1238	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1109	CLA	C1C-NC	-2.32	1.34	1.37
15	B	1209	CLA	C4B-NB	-2.32	1.34	1.37
15	B	1237	CLA	C1D-ND	-2.32	1.34	1.37
15	B	1207	CLA	C4C-C3C	2.32	1.49	1.45
15	B	1228	CLA	C4B-NB	-2.32	1.34	1.37
15	B	1212	CLA	C1C-NC	-2.32	1.34	1.37
15	A	1132	CLA	C1B-NB	-2.31	1.34	1.37
15	K	1402	CLA	C4B-NB	-2.31	1.34	1.37
15	A	1128	CLA	C3B-C4B	2.31	1.49	1.42
15	A	1101	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1135	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1127	CLA	C4B-NB	-2.31	1.34	1.37
15	B	1227	CLA	C1B-NB	-2.31	1.34	1.37
15	B	1237	CLA	C4C-C3C	2.31	1.49	1.45
15	B	1227	CLA	C1C-NC	-2.31	1.34	1.37
15	A	1116	CLA	C1C-NC	-2.30	1.34	1.37
15	B	1202	CLA	C1C-NC	-2.30	1.34	1.37
15	B	1207	CLA	C4B-NB	-2.30	1.34	1.37
15	A	1135	CLA	C4B-NB	-2.30	1.34	1.37
15	B	1208	CLA	C4C-C3C	2.30	1.48	1.45
15	F	1139	CLA	C3B-C4B	2.30	1.49	1.42
15	A	1122	CLA	C1C-NC	-2.30	1.34	1.37
15	A	1136	CLA	C1B-NB	-2.30	1.34	1.37
15	A	1109	CLA	C1B-NB	-2.30	1.34	1.37
15	A	1136	CLA	C1C-NC	-2.30	1.34	1.37
15	A	1114	CLA	C4B-NB	-2.29	1.34	1.37
15	A	1132	CLA	C4B-NB	-2.29	1.34	1.37
15	A	1119	CLA	C4C-C3C	2.29	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1140	CLA	C1B-NB	-2.29	1.34	1.37
15	B	1211	CLA	C1D-C2D	2.29	1.49	1.45
15	J	1303	CLA	C1C-NC	-2.29	1.34	1.37
15	B	1203	CLA	C4C-C3C	2.29	1.48	1.45
15	A	1120	CLA	C1C-NC	-2.29	1.34	1.37
14	F	4015	BCR	C30-C25	-2.29	1.50	1.53
15	A	1115	CLA	C1D-C2D	2.29	1.49	1.45
15	A	1111	CLA	C4C-C3C	2.29	1.48	1.45
15	A	1134	CLA	C4C-C3C	2.29	1.48	1.45
15	B	1206	CLA	C1C-NC	-2.29	1.34	1.37
15	B	1216	CLA	C1C-NC	-2.28	1.34	1.37
15	A	1124	CLA	C4C-C3C	2.28	1.48	1.45
15	A	1121	CLA	C1B-NB	-2.28	1.34	1.37
15	K	1402	CLA	C1C-NC	-2.28	1.34	1.37
15	B	1220	CLA	C4C-C3C	2.28	1.48	1.45
15	A	1133	CLA	C4B-NB	-2.28	1.34	1.37
15	A	1123	CLA	C1D-ND	-2.28	1.34	1.37
15	A	1012	CLA	C4C-C3C	2.28	1.48	1.45
15	A	1101	CLA	C1D-C2D	2.28	1.49	1.45
15	A	1129	CLA	C4C-C3C	2.28	1.48	1.45
15	B	1202	CLA	C4B-NB	-2.28	1.34	1.37
15	B	1021	CLA	C1D-C2D	2.28	1.49	1.45
15	A	1106	CLA	C4B-NB	-2.28	1.34	1.37
15	A	1133	CLA	C1C-NC	-2.28	1.34	1.37
15	B	1210	CLA	C4C-C3C	2.28	1.48	1.45
15	B	1210	CLA	C4B-NB	-2.28	1.34	1.37
15	B	1013	CLA	C1D-C2D	2.28	1.49	1.45
15	B	1232	CLA	C4C-C3C	2.28	1.48	1.45
15	B	1219	CLA	C4C-C3C	2.27	1.48	1.45
15	B	1232	CLA	C1C-NC	-2.27	1.34	1.37
15	A	1123	CLA	C4B-NB	-2.27	1.34	1.37
15	B	1229	CLA	C1D-C2D	2.27	1.49	1.45
15	A	1136	CLA	C4C-C3C	2.27	1.48	1.45
15	A	1103	CLA	C4B-NB	-2.27	1.34	1.37
15	B	1235	CLA	C1C-C2C	2.27	1.49	1.44
15	A	1127	CLA	C1C-NC	-2.27	1.34	1.37
15	B	1215	CLA	C4B-NB	-2.27	1.34	1.37
15	B	1211	CLA	C4B-NB	-2.27	1.34	1.37
15	B	1237	CLA	C1B-NB	-2.27	1.34	1.37
15	B	1223	CLA	C1C-C2C	2.27	1.49	1.44
15	A	1137	CLA	C1C-NC	-2.27	1.34	1.37
15	B	1207	CLA	C1C-NC	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1104	CLA	C1C-NC	-2.26	1.34	1.37
15	B	1230	CLA	C1C-NC	-2.26	1.34	1.37
15	A	1134	CLA	C4B-NB	-2.26	1.34	1.37
15	A	1125	CLA	C1C-NC	-2.26	1.34	1.37
15	B	1201	CLA	C1C-NC	-2.26	1.34	1.37
15	B	1023	CLA	C4C-C3C	2.26	1.48	1.45
15	J	1302	CLA	C3B-C4B	2.26	1.49	1.42
15	A	1134	CLA	C1C-NC	-2.26	1.34	1.37
15	A	1125	CLA	C3B-C4B	2.26	1.49	1.42
15	A	1125	CLA	C1C-C2C	2.26	1.49	1.44
15	B	1205	CLA	C1B-NB	-2.26	1.34	1.37
15	A	1129	CLA	C4B-NB	-2.26	1.34	1.37
15	A	1114	CLA	C1C-NC	-2.26	1.34	1.37
15	B	1221	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1123	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1112	CLA	C3B-C4B	2.25	1.49	1.42
15	A	1124	CLA	C1C-NC	-2.25	1.34	1.37
15	B	1204	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1132	CLA	C1C-NC	-2.25	1.34	1.37
15	B	1237	CLA	C1C-NC	-2.25	1.34	1.37
15	K	1402	CLA	C4C-C3C	2.25	1.48	1.45
14	B	4009	BCR	C30-C25	-2.25	1.50	1.53
15	A	1118	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1119	CLA	C1C-NC	-2.25	1.34	1.37
15	A	1131	CLA	C3B-C4B	2.25	1.49	1.42
15	B	1220	CLA	C4B-NB	-2.25	1.34	1.37
15	B	1234	CLA	C4B-NB	-2.25	1.34	1.37
15	B	1235	CLA	C4B-NB	-2.25	1.34	1.37
15	A	1117	CLA	C1C-NC	-2.24	1.34	1.37
15	B	1224	CLA	C1C-NC	-2.24	1.34	1.37
15	A	1118	CLA	C4B-NB	-2.24	1.34	1.37
15	B	1239	CLA	C1B-NB	-2.24	1.34	1.37
15	A	1130	CLA	C3B-C4B	2.24	1.49	1.42
15	B	1213	CLA	C4C-C3C	2.24	1.48	1.45
15	J	1302	CLA	C4C-C3C	2.24	1.48	1.45
15	B	1230	CLA	C4B-NB	-2.24	1.34	1.37
15	B	1217	CLA	C4C-C3C	2.23	1.48	1.45
15	A	1107	CLA	C4B-NB	-2.23	1.34	1.37
15	B	1209	CLA	C1C-NC	-2.23	1.34	1.37
15	A	1104	CLA	C3B-C4B	2.23	1.49	1.42
15	A	1130	CLA	C4B-NB	-2.23	1.34	1.37
15	B	1226	CLA	C4B-NB	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1223	CLA	C1D-C2D	2.23	1.49	1.45
15	B	1021	CLA	C1C-NC	-2.23	1.34	1.37
15	B	1217	CLA	C1C-NC	-2.23	1.34	1.37
15	B	1203	CLA	C4B-NB	-2.23	1.34	1.37
15	B	1215	CLA	C1B-NB	-2.23	1.34	1.37
15	J	1303	CLA	C4B-NB	-2.22	1.34	1.37
15	B	1239	CLA	C4B-NB	-2.22	1.34	1.37
15	B	1238	CLA	C4C-C3C	2.22	1.48	1.45
15	A	1107	CLA	C4C-C3C	2.22	1.48	1.45
15	B	1218	CLA	C4C-C3C	2.22	1.48	1.45
15	B	1235	CLA	C3B-C4B	2.22	1.49	1.42
15	B	1202	CLA	C4C-C3C	2.22	1.48	1.45
15	F	1301	CLA	C1C-NC	-2.21	1.34	1.37
15	B	1213	CLA	C1C-NC	-2.21	1.34	1.37
15	F	1410	CLA	C1C-NC	-2.21	1.34	1.37
15	B	1201	CLA	C4B-NB	-2.21	1.35	1.37
15	B	1235	CLA	C1C-NC	-2.21	1.34	1.37
15	B	1228	CLA	C3B-C4B	2.21	1.49	1.42
15	B	1217	CLA	C4B-NB	-2.21	1.35	1.37
15	B	1201	CLA	C4C-C3C	2.21	1.48	1.45
15	F	1139	CLA	C1C-C2C	2.21	1.49	1.44
15	A	1110	CLA	C4C-C3C	2.20	1.48	1.45
15	A	1130	CLA	C4C-C3C	2.20	1.48	1.45
15	A	1126	CLA	C4C-C3C	2.20	1.48	1.45
15	A	1022	CLA	C1C-NC	-2.20	1.34	1.37
15	B	1227	CLA	C4B-NB	-2.20	1.35	1.37
15	B	1231	CLA	C3B-C4B	2.20	1.49	1.42
15	A	1130	CLA	C1C-NC	-2.20	1.34	1.37
15	B	1228	CLA	C1C-NC	-2.20	1.34	1.37
15	A	1102	CLA	C4C-C3C	2.20	1.48	1.45
15	A	1104	CLA	C1C-C2C	2.20	1.49	1.44
15	A	1126	CLA	C1C-NC	-2.20	1.34	1.37
15	A	1801	CLA	C4C-C3C	2.20	1.48	1.45
15	B	1221	CLA	C4C-C3C	2.20	1.48	1.45
15	B	1220	CLA	C1C-NC	-2.20	1.34	1.37
15	A	1117	CLA	C3B-C4B	2.19	1.49	1.42
15	A	1115	CLA	C4B-NB	-2.19	1.35	1.37
15	A	1117	CLA	C4C-C3C	2.19	1.48	1.45
15	B	1214	CLA	C3B-C4B	2.19	1.49	1.42
15	B	1021	CLA	C4C-C3C	2.19	1.48	1.45
15	A	1102	CLA	C3B-C4B	2.19	1.49	1.42
15	A	1127	CLA	C1D-C2D	2.18	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1240	CLA	C1C-NC	-2.18	1.34	1.37
15	A	1112	CLA	C4C-C3C	2.18	1.48	1.45
15	F	1410	CLA	C4B-NB	-2.18	1.35	1.37
15	A	1119	CLA	C3B-C4B	2.18	1.49	1.42
15	B	1214	CLA	C4B-NB	-2.18	1.35	1.37
15	B	1021	CLA	C3B-C4B	2.18	1.49	1.42
15	B	1206	CLA	C4B-NB	-2.18	1.35	1.37
15	A	1140	CLA	C3B-C4B	2.17	1.49	1.42
15	A	1120	CLA	C4B-NB	-2.17	1.35	1.37
15	A	1138	CLA	C1C-NC	-2.17	1.34	1.37
15	B	1213	CLA	C1B-NB	-2.17	1.35	1.37
15	A	1134	CLA	C3B-C4B	2.17	1.49	1.42
15	B	1219	CLA	C1C-NC	-2.17	1.34	1.37
15	B	1223	CLA	C3B-C4B	2.17	1.49	1.42
15	A	1109	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1221	CLA	C1D-C2D	2.16	1.49	1.45
15	B	1225	CLA	C1C-NC	-2.16	1.34	1.37
15	A	1126	CLA	C4B-NB	-2.16	1.35	1.37
15	A	1115	CLA	C3B-C4B	2.16	1.49	1.42
15	A	1130	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1218	CLA	C3B-C4B	2.16	1.49	1.42
15	B	1228	CLA	C4C-C3C	2.16	1.48	1.45
15	A	1109	CLA	C3B-C4B	2.16	1.49	1.42
15	B	1013	CLA	C3B-C4B	2.16	1.49	1.42
15	B	1220	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1212	CLA	C4B-NB	-2.15	1.35	1.37
15	B	1240	CLA	C3B-C4B	2.15	1.49	1.42
15	A	1125	CLA	C1D-C2D	2.15	1.49	1.45
15	A	1106	CLA	C4C-C3C	2.15	1.48	1.45
15	B	1205	CLA	C1D-C2D	2.15	1.49	1.45
15	B	1223	CLA	C1C-NC	-2.15	1.34	1.37
15	B	1214	CLA	C1C-NC	-2.15	1.34	1.37
15	F	1301	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1213	CLA	C3B-C4B	2.15	1.49	1.42
15	A	1103	CLA	C4C-C3C	2.15	1.48	1.45
15	B	1216	CLA	C4B-NB	-2.15	1.35	1.37
15	B	1220	CLA	C3B-C4B	2.14	1.49	1.42
15	A	1129	CLA	C1C-NC	-2.14	1.34	1.37
15	F	1410	CLA	C4C-C3C	2.14	1.48	1.45
15	B	1225	CLA	C4C-C3C	2.14	1.48	1.45
15	B	1229	CLA	C1B-NB	-2.14	1.35	1.37
15	A	1103	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1236	CLA	C4B-NB	-2.14	1.35	1.37
15	B	1212	CLA	C4C-C3C	2.14	1.48	1.45
15	A	1012	CLA	C3B-C4B	2.14	1.49	1.42
14	B	4017	BCR	C30-C25	-2.14	1.51	1.53
15	A	1127	CLA	C4C-C3C	2.14	1.48	1.45
15	F	1301	CLA	C4B-NB	-2.14	1.35	1.37
15	A	1122	CLA	C1C-C2C	2.13	1.48	1.44
15	F	1139	CLA	C4C-C3C	2.13	1.48	1.45
15	B	1234	CLA	C4C-C3C	2.13	1.48	1.45
15	A	1124	CLA	C4B-NB	-2.13	1.35	1.37
15	A	1105	CLA	C1B-NB	-2.13	1.35	1.37
15	A	1012	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1122	CLA	C4C-C3C	2.13	1.48	1.45
15	B	1218	CLA	C4B-NB	-2.13	1.35	1.37
15	A	1140	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1121	CLA	C4B-NB	-2.13	1.35	1.37
15	B	1205	CLA	C4B-NB	-2.12	1.35	1.37
15	F	1301	CLA	C3B-C4B	2.12	1.48	1.42
15	J	1303	CLA	C3B-C4B	2.12	1.48	1.42
15	A	1117	CLA	C4B-NB	-2.12	1.35	1.37
15	A	1022	CLA	C1C-C2C	2.12	1.48	1.44
15	A	1106	CLA	C3B-C4B	2.12	1.48	1.42
15	B	1237	CLA	C3B-C4B	2.11	1.48	1.42
15	A	1132	CLA	C4C-C3C	2.11	1.48	1.45
15	B	1013	CLA	C4B-NB	-2.11	1.35	1.37
15	B	1222	CLA	C4C-C3C	2.11	1.48	1.45
15	B	1231	CLA	C4C-C3C	2.11	1.48	1.45
14	A	4002	BCR	C30-C25	-2.11	1.51	1.53
15	A	1111	CLA	C3B-C4B	2.11	1.48	1.42
15	A	1022	CLA	C4C-C3C	2.11	1.48	1.45
15	J	1302	CLA	C4B-NB	-2.11	1.35	1.37
15	B	1217	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1201	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1230	CLA	C1C-C2C	2.10	1.48	1.44
15	B	1229	CLA	C4B-NB	-2.10	1.35	1.37
15	B	1238	CLA	C3B-C4B	2.10	1.48	1.42
15	A	1125	CLA	C4B-NB	-2.10	1.35	1.37
15	B	1202	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1210	CLA	C3B-C4B	2.10	1.48	1.42
15	A	1124	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1230	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1206	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1119	CLA	C4B-NB	-2.10	1.35	1.37
15	A	1128	CLA	C1D-C2D	2.10	1.49	1.45
15	A	1114	CLA	C3B-C4B	2.10	1.48	1.42
15	F	1410	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1231	CLA	C4B-NB	-2.09	1.35	1.37
15	A	1112	CLA	C1C-NC	-2.09	1.34	1.37
15	A	1131	CLA	C4B-NB	-2.09	1.35	1.37
15	K	1401	CLA	C3B-C4B	2.09	1.48	1.42
15	A	1022	CLA	C3B-C4B	2.09	1.48	1.42
15	A	1121	CLA	C3B-C4B	2.09	1.48	1.42
15	B	1207	CLA	C3B-C4B	2.09	1.48	1.42
15	B	1240	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1021	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1237	CLA	C4B-NB	-2.09	1.35	1.37
15	A	1022	CLA	C4B-NB	-2.09	1.35	1.37
15	B	1236	CLA	C1C-NC	-2.09	1.34	1.37
15	A	1012	CLA	C1C-NC	-2.08	1.34	1.37
15	A	1012	CLA	C1D-C2D	2.08	1.49	1.45
15	B	1212	CLA	C3B-C4B	2.08	1.48	1.42
15	B	1228	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1109	CLA	C4B-NB	-2.08	1.35	1.37
15	B	1213	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1101	CLA	C1C-C2C	2.07	1.48	1.44
15	F	1410	CLA	C1C-C2C	2.07	1.48	1.44
15	A	1113	CLA	C4B-NB	-2.07	1.35	1.37
15	A	1133	CLA	C3B-C4B	2.07	1.48	1.42
15	B	1219	CLA	C3B-C4B	2.07	1.48	1.42
15	A	1112	CLA	C1C-C2C	2.07	1.48	1.44
15	B	1217	CLA	C1C-C2C	2.07	1.48	1.44
15	A	1128	CLA	C4C-C3C	2.06	1.48	1.45
15	B	1226	CLA	C1C-NC	-2.06	1.34	1.37
15	B	1227	CLA	C1C-C2C	2.06	1.48	1.44
15	B	1232	CLA	C4B-NB	-2.06	1.35	1.37
15	A	1126	CLA	C1C-C2C	2.06	1.48	1.44
15	B	1226	CLA	C4C-C3C	2.06	1.48	1.45
15	B	1238	CLA	C4B-NB	-2.06	1.35	1.37
15	B	1211	CLA	C4C-C3C	2.06	1.48	1.45
15	B	1225	CLA	C3B-C4B	2.06	1.48	1.42
15	B	1229	CLA	C1C-C2C	2.06	1.48	1.44
15	A	1112	CLA	C4B-NB	-2.06	1.35	1.37
15	B	1021	CLA	C4B-NB	-2.06	1.35	1.37
15	B	1208	CLA	C3B-C4B	2.05	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1225	CLA	C1C-C2C	2.05	1.48	1.44
15	F	1301	CLA	C4C-C3C	2.04	1.48	1.45
15	A	1119	CLA	C1C-C2C	2.04	1.48	1.44
15	B	1219	CLA	C1C-C2C	2.04	1.48	1.44
15	B	1215	CLA	C3B-C4B	2.04	1.48	1.42
15	B	1212	CLA	C1C-C2C	2.04	1.48	1.44
15	A	1801	CLA	C3B-C4B	2.04	1.48	1.42
15	B	1205	CLA	C4C-C3C	2.04	1.48	1.45
15	B	1224	CLA	C4C-C3C	2.04	1.48	1.45
15	B	1221	CLA	C1C-C2C	2.03	1.48	1.44
15	B	1211	CLA	C1C-C2C	2.03	1.48	1.44
15	A	1115	CLA	C4C-C3C	2.03	1.48	1.45
15	A	1801	CLA	C1C-C2C	2.03	1.48	1.44
15	A	1129	CLA	C3B-C4B	2.03	1.48	1.42
15	A	1101	CLA	C4B-NB	-2.03	1.35	1.37
15	A	1120	CLA	C3B-C4B	2.03	1.48	1.42
15	B	1216	CLA	C3B-C4B	2.02	1.48	1.42
15	B	1209	CLA	C3B-C4B	2.02	1.48	1.42
15	A	1138	CLA	C4B-NB	-2.02	1.35	1.37
15	B	1229	CLA	C3B-C4B	2.02	1.48	1.42
15	A	1101	CLA	C4C-C3C	2.02	1.48	1.45
15	J	1303	CLA	C1C-C2C	2.02	1.48	1.44
15	A	1140	CLA	C4B-NB	-2.02	1.35	1.37
15	A	1801	CLA	C4B-NB	-2.02	1.35	1.37
15	B	1221	CLA	C3B-C4B	2.02	1.48	1.42
15	B	1226	CLA	C3B-C4B	2.01	1.48	1.42
15	B	1237	CLA	C1C-C2C	2.01	1.48	1.44
15	B	1223	CLA	C4B-NB	-2.01	1.35	1.37
15	A	1127	CLA	C3B-C4B	2.01	1.48	1.42
15	B	1204	CLA	C3B-C4B	2.01	1.48	1.42
15	A	1127	CLA	C1C-C2C	2.01	1.48	1.44
14	J	4013	BCR	C30-C25	-2.01	1.51	1.53
15	A	1107	CLA	C1C-C2C	2.01	1.48	1.44
15	B	1240	CLA	C4B-NB	-2.00	1.35	1.37
15	B	1023	CLA	C3B-C4B	2.00	1.48	1.42
15	A	1105	CLA	C1C-C2C	2.00	1.48	1.44

All (2623) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4009	BCR	C16-C17-C18	27.25	165.49	127.28
14	F	4016	BCR	C20-C21-C22	25.81	163.47	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4006	BCR	C20-C21-C22	24.39	161.49	127.28
14	A	4008	BCR	C20-C21-C22	23.67	160.48	127.28
14	A	4007	BCR	C20-C21-C22	23.67	160.48	127.28
14	B	4014	BCR	C16-C17-C18	23.51	160.24	127.28
14	B	4010	BCR	C20-C21-C22	23.48	160.21	127.28
14	F	4015	BCR	C20-C21-C22	22.60	158.97	127.28
14	A	4008	BCR	C16-C17-C18	22.59	158.97	127.28
14	A	4007	BCR	C16-C17-C18	22.30	158.55	127.28
14	J	4013	BCR	C20-C21-C22	22.27	158.50	127.28
14	F	4015	BCR	C16-C17-C18	22.22	158.44	127.28
14	B	4011	BCR	C16-C17-C18	22.22	158.44	127.28
14	A	4003	BCR	C16-C17-C18	21.67	157.67	127.28
14	B	4010	BCR	C16-C17-C18	21.58	157.54	127.28
14	A	4002	BCR	C20-C21-C22	21.45	157.36	127.28
14	B	4017	BCR	C20-C21-C22	21.35	157.23	127.28
14	F	4016	BCR	C16-C17-C18	21.05	156.80	127.28
14	J	4013	BCR	C16-C17-C18	20.90	156.59	127.28
14	B	4006	BCR	C16-C17-C18	20.82	156.48	127.28
14	A	4002	BCR	C15-C16-C17	20.77	166.01	123.52
14	B	4005	BCR	C20-C21-C22	20.68	156.28	127.28
14	F	4016	BCR	C15-C16-C17	20.66	165.79	123.52
14	A	4001	BCR	C20-C21-C22	20.58	156.15	127.28
14	B	4005	BCR	C15-C16-C17	20.53	165.52	123.52
14	B	4009	BCR	C20-C21-C22	20.52	156.06	127.28
14	B	4017	BCR	C16-C17-C18	20.32	155.78	127.28
14	B	4017	BCR	C15-C16-C17	20.25	164.95	123.52
14	A	4012	BCR	C15-C16-C17	20.18	164.81	123.52
14	A	4003	BCR	C20-C21-C22	20.14	155.53	127.28
14	B	4014	BCR	C20-C21-C22	20.11	155.48	127.28
14	A	4003	BCR	C15-C16-C17	20.05	164.55	123.52
14	B	4004	BCR	C20-C21-C22	20.05	155.40	127.28
14	B	4004	BCR	C15-C16-C17	20.03	164.51	123.52
14	A	4012	BCR	C16-C17-C18	19.79	155.03	127.28
14	A	4001	BCR	C15-C16-C17	19.77	163.98	123.52
14	A	4001	BCR	C16-C17-C18	19.74	154.96	127.28
14	B	4006	BCR	C15-C16-C17	19.72	163.88	123.52
14	B	4011	BCR	C20-C21-C22	19.70	154.90	127.28
14	B	4005	BCR	C16-C17-C18	19.45	154.56	127.28
14	J	4013	BCR	C15-C16-C17	19.42	163.25	123.52
14	B	4011	BCR	C15-C16-C17	19.34	163.09	123.52
14	A	4002	BCR	C16-C17-C18	19.33	154.39	127.28
14	A	4007	BCR	C15-C16-C17	19.28	162.96	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4012	BCR	C20-C21-C22	19.24	154.26	127.28
14	B	4010	BCR	C15-C16-C17	19.05	162.50	123.52
14	F	4015	BCR	C10-C11-C12	18.81	177.72	123.20
14	A	4008	BCR	C15-C16-C17	18.81	162.01	123.52
14	B	4004	BCR	C16-C17-C18	18.74	153.56	127.28
14	B	4005	BCR	C10-C11-C12	18.63	177.17	123.20
14	B	4014	BCR	C10-C11-C12	18.60	177.11	123.20
14	J	4013	BCR	C10-C11-C12	18.60	177.10	123.20
14	B	4014	BCR	C15-C16-C17	18.60	161.57	123.52
14	A	4008	BCR	C10-C11-C12	18.53	176.90	123.20
14	B	4017	BCR	C10-C11-C12	18.53	176.89	123.20
14	B	4006	BCR	C10-C11-C12	18.51	176.83	123.20
14	A	4002	BCR	C10-C11-C12	18.44	176.64	123.20
14	A	4007	BCR	C10-C11-C12	18.26	176.12	123.20
14	B	4010	BCR	C10-C11-C12	18.23	176.01	123.20
14	B	4004	BCR	C10-C11-C12	18.07	175.56	123.20
14	F	4016	BCR	C10-C11-C12	17.98	175.29	123.20
14	A	4003	BCR	C10-C11-C12	17.86	174.95	123.20
14	F	4015	BCR	C15-C16-C17	17.75	159.85	123.52
14	B	4011	BCR	C11-C10-C9	17.44	151.74	127.28
14	B	4011	BCR	C10-C11-C12	16.80	171.87	123.20
14	A	4012	BCR	C10-C11-C12	16.51	171.03	123.20
14	B	4009	BCR	C16-C15-C14	16.50	157.29	123.52
14	B	4009	BCR	C10-C11-C12	16.37	170.63	123.20
14	A	4001	BCR	C10-C11-C12	16.09	169.83	123.20
14	B	4009	BCR	C15-C16-C17	15.92	156.10	123.52
14	F	4015	BCR	C16-C15-C14	15.02	154.25	123.52
14	B	4014	BCR	C16-C15-C14	15.02	154.24	123.52
14	B	4004	BCR	C21-C20-C19	14.83	166.17	123.20
14	A	4001	BCR	C21-C20-C19	14.65	165.64	123.20
14	A	4012	BCR	C21-C20-C19	14.49	165.18	123.20
14	B	4014	BCR	C21-C20-C19	14.40	164.92	123.20
14	A	4003	BCR	C21-C20-C19	14.35	164.79	123.20
14	B	4005	BCR	C21-C20-C19	14.32	164.70	123.20
14	B	4017	BCR	C11-C10-C9	14.19	147.18	127.28
14	B	4009	BCR	C21-C20-C19	14.19	164.32	123.20
14	B	4017	BCR	C21-C20-C19	14.15	164.19	123.20
14	A	4002	BCR	C21-C20-C19	13.99	163.73	123.20
14	A	4008	BCR	C16-C15-C14	13.90	151.97	123.52
14	B	4014	BCR	C11-C10-C9	13.89	146.75	127.28
14	B	4011	BCR	C21-C20-C19	13.63	162.71	123.20
14	J	4013	BCR	C16-C15-C14	13.61	151.38	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4010	BCR	C16-C15-C14	13.60	151.35	123.52
14	B	4006	BCR	C11-C10-C9	13.58	146.32	127.28
14	B	4010	BCR	C11-C10-C9	13.58	146.32	127.28
14	A	4003	BCR	C16-C15-C14	13.54	151.22	123.52
14	A	4008	BCR	C11-C10-C9	13.49	146.20	127.28
14	F	4016	BCR	C21-C20-C19	13.49	162.28	123.20
14	B	4004	BCR	C16-C15-C14	13.48	151.10	123.52
14	F	4015	BCR	C21-C20-C19	13.36	161.92	123.20
14	J	4013	BCR	C11-C10-C9	13.32	145.96	127.28
14	A	4007	BCR	C16-C15-C14	13.32	150.78	123.52
14	A	4007	BCR	C11-C10-C9	13.31	145.94	127.28
14	A	4008	BCR	C21-C20-C19	13.22	161.50	123.20
14	A	4001	BCR	C16-C15-C14	13.12	150.36	123.52
14	B	4011	BCR	C16-C15-C14	13.09	150.29	123.52
14	A	4007	BCR	C21-C20-C19	13.08	161.09	123.20
14	B	4005	BCR	C11-C10-C9	13.04	145.57	127.28
14	B	4010	BCR	C21-C20-C19	13.03	160.97	123.20
14	B	4017	BCR	C16-C15-C14	12.91	149.93	123.52
14	B	4006	BCR	C21-C20-C19	12.86	160.47	123.20
14	A	4002	BCR	C11-C10-C9	12.80	145.23	127.28
14	B	4004	BCR	C11-C10-C9	12.76	145.18	127.28
14	B	4011	BCR	C11-C12-C13	12.65	161.04	126.36
14	J	4013	BCR	C21-C20-C19	12.63	159.80	123.20
14	B	4006	BCR	C16-C15-C14	12.52	149.13	123.52
14	B	4005	BCR	C16-C15-C14	12.40	148.90	123.52
14	F	4015	BCR	C11-C10-C9	12.27	144.48	127.28
14	F	4016	BCR	C16-C15-C14	12.18	148.45	123.52
14	A	4012	BCR	C16-C15-C14	11.99	148.06	123.52
14	A	4002	BCR	C16-C15-C14	11.89	147.85	123.52
13	A	1108	CL0	C1B-CHB-C4A	11.87	128.96	121.32
14	F	4016	BCR	C11-C10-C9	11.81	143.84	127.28
14	B	4009	BCR	C11-C10-C9	11.80	143.82	127.28
14	A	4002	BCR	C11-C12-C13	11.78	158.66	126.36
14	A	4003	BCR	C11-C10-C9	11.73	143.73	127.28
14	A	4007	BCR	C11-C12-C13	11.62	158.23	126.36
14	B	4005	BCR	C11-C12-C13	11.39	157.59	126.36
14	J	4013	BCR	C11-C12-C13	11.26	157.25	126.36
14	A	4008	BCR	C11-C12-C13	11.25	157.22	126.36
13	A	1011	CL0	C1B-CHB-C4A	11.19	128.52	121.32
14	F	4015	BCR	C11-C12-C13	11.19	157.06	126.36
14	A	4012	BCR	C11-C12-C13	11.18	157.01	126.36
14	B	4010	BCR	C11-C12-C13	11.12	156.85	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4006	BCR	C11-C12-C13	11.12	156.85	126.36
14	B	4004	BCR	C11-C12-C13	11.01	156.54	126.36
14	A	4012	BCR	C11-C10-C9	10.81	142.44	127.28
14	B	4017	BCR	C11-C12-C13	10.80	155.99	126.36
14	A	4003	BCR	C11-C12-C13	10.78	155.91	126.36
14	B	4014	BCR	C11-C12-C13	10.66	155.58	126.36
14	A	4001	BCR	C11-C10-C9	10.63	142.18	127.28
14	A	4001	BCR	C11-C12-C13	9.89	153.49	126.36
14	B	4009	BCR	C11-C12-C13	9.76	153.13	126.36
15	A	1126	CLA	CMD-C2D-C1D	9.58	141.59	124.73
13	A	1011	CL0	O2D-CGD-CBD	9.49	121.38	110.95
14	F	4016	BCR	C11-C12-C13	9.08	151.27	126.36
15	A	1129	CLA	CMD-C2D-C1D	8.87	140.35	124.73
14	F	4016	BCR	C20-C19-C18	8.83	150.57	126.36
15	A	1122	CLA	CMD-C2D-C1D	8.83	140.27	124.73
14	A	4007	BCR	C20-C19-C18	8.83	150.57	126.36
14	A	4008	BCR	C20-C19-C18	8.73	150.30	126.36
14	B	4010	BCR	C20-C19-C18	8.72	150.28	126.36
15	A	1107	CLA	CMD-C2D-C1D	8.58	139.84	124.73
15	B	1237	CLA	CMD-C2D-C1D	8.56	139.81	124.73
15	B	1231	CLA	CMD-C2D-C1D	8.53	139.76	124.73
15	B	1230	CLA	CMD-C2D-C1D	8.41	139.54	124.73
15	A	1120	CLA	CMD-C2D-C1D	8.41	139.54	124.73
15	B	1224	CLA	CMD-C2D-C1D	8.40	139.52	124.73
15	B	1204	CLA	CMD-C2D-C1D	8.37	139.47	124.73
15	B	1239	CLA	CMD-C2D-C1D	8.36	139.46	124.73
15	B	1206	CLA	CMD-C2D-C1D	8.36	139.45	124.73
15	A	1134	CLA	CMD-C2D-C1D	8.33	139.40	124.73
15	A	1125	CLA	CMD-C2D-C1D	8.32	139.39	124.73
15	B	1203	CLA	CMD-C2D-C1D	8.30	139.34	124.73
15	K	1401	CLA	CMD-C2D-C1D	8.28	139.32	124.73
15	B	1228	CLA	CMD-C2D-C1D	8.26	139.28	124.73
15	B	1209	CLA	CMD-C2D-C1D	8.25	139.26	124.73
14	B	4006	BCR	C20-C19-C18	8.24	148.96	126.36
15	A	1103	CLA	CMD-C2D-C1D	8.23	139.22	124.73
15	A	1109	CLA	CMD-C2D-C1D	8.22	139.21	124.73
15	A	1123	CLA	CMD-C2D-C1D	8.22	139.21	124.73
15	F	1139	CLA	CMD-C2D-C1D	8.22	139.20	124.73
15	A	1130	CLA	CMD-C2D-C1D	8.21	139.19	124.73
14	J	4013	BCR	C20-C19-C18	8.20	148.86	126.36
15	B	1227	CLA	CMD-C2D-C1D	8.18	139.14	124.73
15	A	1114	CLA	CMD-C2D-C1D	8.18	139.13	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	1303	CLA	CMD-C2D-C1D	8.17	139.11	124.73
15	B	1236	CLA	CMD-C2D-C1D	8.15	139.08	124.73
15	A	1113	CLA	CMD-C2D-C1D	8.15	139.07	124.73
14	B	4011	BCR	C20-C19-C18	8.14	148.69	126.36
15	B	1219	CLA	CMD-C2D-C1D	8.13	139.05	124.73
15	K	1402	CLA	CMD-C2D-C1D	8.13	139.05	124.73
15	B	1213	CLA	CMD-C2D-C1D	8.11	139.02	124.73
15	A	1136	CLA	CMD-C2D-C1D	8.11	139.01	124.73
15	A	1106	CLA	CMD-C2D-C1D	8.10	139.00	124.73
15	B	1207	CLA	CMD-C2D-C1D	8.10	139.00	124.73
15	B	1208	CLA	CMD-C2D-C1D	8.09	138.97	124.73
15	A	1104	CLA	CMD-C2D-C1D	8.08	138.96	124.73
15	J	1302	CLA	CMD-C2D-C1D	8.08	138.96	124.73
15	A	1801	CLA	CMD-C2D-C1D	8.07	138.94	124.73
15	A	1116	CLA	CMD-C2D-C1D	8.07	138.93	124.73
15	A	1105	CLA	CMD-C2D-C1D	8.07	138.93	124.73
15	A	1110	CLA	CMD-C2D-C1D	8.05	138.91	124.73
15	B	1202	CLA	CMD-C2D-C1D	8.05	138.90	124.73
15	B	1234	CLA	CMD-C2D-C1D	8.05	138.90	124.73
15	B	1216	CLA	CMD-C2D-C1D	8.04	138.88	124.73
15	F	1410	CLA	CMD-C2D-C1D	8.04	138.88	124.73
15	A	1131	CLA	CMD-C2D-C1D	8.02	138.85	124.73
15	B	1214	CLA	CMD-C2D-C1D	8.01	138.84	124.73
15	B	1226	CLA	CMD-C2D-C1D	8.01	138.84	124.73
15	A	1124	CLA	CMD-C2D-C1D	8.01	138.83	124.73
15	A	1121	CLA	CMD-C2D-C1D	8.00	138.82	124.73
15	B	1240	CLA	CMD-C2D-C1D	7.98	138.79	124.73
15	A	1140	CLA	CMD-C2D-C1D	7.97	138.75	124.73
15	A	1111	CLA	CMD-C2D-C1D	7.96	138.74	124.73
15	A	1118	CLA	CMD-C2D-C1D	7.96	138.74	124.73
15	A	1112	CLA	CMD-C2D-C1D	7.94	138.71	124.73
15	A	1133	CLA	CMD-C2D-C1D	7.94	138.71	124.73
15	B	1223	CLA	CMD-C2D-C1D	7.94	138.70	124.73
15	A	1135	CLA	CMD-C2D-C1D	7.92	138.68	124.73
15	B	1210	CLA	CMD-C2D-C1D	7.91	138.66	124.73
15	A	1137	CLA	CMD-C2D-C1D	7.90	138.65	124.73
15	B	1021	CLA	CMD-C2D-C1D	7.86	138.57	124.73
15	B	1229	CLA	CMD-C2D-C1D	7.86	138.57	124.73
15	B	1225	CLA	CMD-C2D-C1D	7.85	138.55	124.73
15	B	1218	CLA	CMD-C2D-C1D	7.85	138.55	124.73
15	A	1132	CLA	CMD-C2D-C1D	7.83	138.51	124.73
15	B	1201	CLA	CMD-C2D-C1D	7.82	138.50	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1238	CLA	CMD-C2D-C1D	7.82	138.50	124.73
15	A	1119	CLA	CMD-C2D-C1D	7.79	138.45	124.73
15	B	1215	CLA	CMD-C2D-C1D	7.78	138.43	124.73
14	F	4015	BCR	C20-C19-C18	7.77	147.67	126.36
15	B	1023	CLA	CMD-C2D-C1D	7.76	138.40	124.73
15	B	1211	CLA	CMD-C2D-C1D	7.75	138.38	124.73
15	A	1127	CLA	CMD-C2D-C1D	7.75	138.37	124.73
15	B	1212	CLA	CMD-C2D-C1D	7.74	138.36	124.73
15	B	1217	CLA	CMD-C2D-C1D	7.72	138.33	124.73
15	B	1232	CLA	CMD-C2D-C1D	7.72	138.32	124.73
15	A	1115	CLA	CMD-C2D-C1D	7.71	138.30	124.73
15	A	1117	CLA	CMD-C2D-C1D	7.70	138.29	124.73
15	B	1235	CLA	CMD-C2D-C1D	7.70	138.29	124.73
15	A	1101	CLA	CMD-C2D-C1D	7.64	138.19	124.73
15	A	1138	CLA	CMD-C2D-C1D	7.61	138.13	124.73
15	B	1220	CLA	CMD-C2D-C1D	7.59	138.10	124.73
15	A	1102	CLA	CMD-C2D-C1D	7.59	138.09	124.73
15	F	1301	CLA	CMD-C2D-C1D	7.52	137.98	124.73
14	B	4014	BCR	C20-C19-C18	7.52	146.97	126.36
15	B	1222	CLA	CMD-C2D-C1D	7.46	137.87	124.73
15	A	1128	CLA	CMD-C2D-C1D	7.42	137.80	124.73
15	B	1221	CLA	CMD-C2D-C1D	7.41	137.77	124.73
15	B	1013	CLA	CMD-C2D-C1D	7.40	137.76	124.73
15	B	1205	CLA	CMD-C2D-C1D	7.14	137.31	124.73
15	A	1022	CLA	CMD-C2D-C1D	7.11	137.25	124.73
14	A	4003	BCR	C20-C19-C18	7.08	145.77	126.36
15	B	1222	CLA	O2D-CGD-CBD	6.93	123.35	111.23
14	B	4009	BCR	C20-C19-C18	6.87	145.19	126.36
14	B	4017	BCR	C20-C19-C18	6.86	145.18	126.36
14	A	4002	BCR	C20-C19-C18	6.85	145.15	126.36
15	B	1205	CLA	O2D-CGD-CBD	6.84	123.18	111.23
14	A	4012	BCR	C20-C19-C18	6.83	145.10	126.36
14	B	4005	BCR	C20-C19-C18	6.83	145.09	126.36
15	B	1221	CLA	C4A-NA-C1A	6.83	109.79	106.68
15	B	1226	CLA	O2D-CGD-CBD	6.78	123.08	111.23
15	A	1136	CLA	C4A-NA-C1A	6.78	109.77	106.68
14	A	4001	BCR	C20-C19-C18	6.67	144.66	126.36
15	B	1222	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	B	1021	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	B	1205	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	1229	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	A	1106	CLA	O2D-CGD-CBD	6.57	122.71	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1118	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	B	4004	BCR	C20-C19-C18	6.47	144.12	126.36
13	A	1108	CL0	O2D-CGD-CBD	6.47	118.06	110.95
15	B	1203	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	A	1128	CLA	O2D-CGD-CBD	6.42	122.46	111.23
15	A	1801	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	B	1239	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	A	1012	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	A	1123	CLA	O2D-CGD-CBD	6.31	122.25	111.23
15	B	1201	CLA	O2D-CGD-CBD	6.26	122.17	111.23
14	B	4009	BCR	C15-C14-C13	-6.24	118.53	127.28
15	A	1101	CLA	O2D-CGD-CBD	6.22	122.10	111.23
15	A	1132	CLA	C4A-NA-C1A	6.19	109.50	106.68
15	B	1234	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	K	1402	CLA	C4A-NA-C1A	6.16	109.49	106.68
15	B	1215	CLA	C2C-C1C-NC	6.16	116.45	109.98
15	B	1239	CLA	C2C-C1C-NC	6.16	116.45	109.98
15	A	1012	CLA	CMD-C2D-C1D	6.14	135.54	124.73
15	A	1115	CLA	C4A-NA-C1A	6.14	109.48	106.68
15	B	1226	CLA	C4A-NA-C1A	6.14	109.48	106.68
15	A	1125	CLA	O2D-CGD-CBD	6.13	121.94	111.23
15	B	1235	CLA	C4A-NA-C1A	6.11	109.47	106.68
15	B	1013	CLA	C4A-NA-C1A	6.10	109.46	106.68
15	F	1139	CLA	C4A-NA-C1A	6.09	109.46	106.68
15	A	1123	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	A	1135	CLA	C2C-C1C-NC	6.06	116.35	109.98
15	B	1231	CLA	C4A-NA-C1A	6.05	109.44	106.68
15	A	1128	CLA	C4A-NA-C1A	6.05	109.44	106.68
15	B	1207	CLA	C2C-C1C-NC	6.05	116.33	109.98
15	B	1203	CLA	C2C-C1C-NC	6.04	116.33	109.98
15	A	1131	CLA	C2C-C1C-NC	6.04	116.32	109.98
15	B	1201	CLA	C4A-NA-C1A	6.03	109.43	106.68
15	B	1235	CLA	C1D-ND-C4D	-6.02	102.09	106.31
15	A	1128	CLA	C2C-C1C-NC	6.01	116.30	109.98
15	A	1109	CLA	C1D-ND-C4D	-6.00	102.10	106.31
15	A	1120	CLA	C4A-NA-C1A	5.99	109.41	106.68
15	A	1131	CLA	O2D-CGD-CBD	5.99	121.70	111.23
15	B	1228	CLA	C1D-ND-C4D	-5.99	102.11	106.31
15	A	1123	CLA	C2C-C1C-NC	5.99	116.27	109.98
15	A	1136	CLA	C2C-C1C-NC	5.98	116.26	109.98
15	B	1209	CLA	C4A-NA-C1A	5.97	109.40	106.68
15	A	1118	CLA	C1D-ND-C4D	-5.97	102.12	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1227	CLA	O2D-CGD-CBD	5.97	121.66	111.23
15	A	1140	CLA	C4A-NA-C1A	5.96	109.40	106.68
15	A	1136	CLA	C1D-ND-C4D	-5.96	102.13	106.31
15	A	1137	CLA	C2C-C1C-NC	5.96	116.24	109.98
15	A	1137	CLA	C4A-NA-C1A	5.96	109.40	106.68
15	B	1231	CLA	C2C-C1C-NC	5.95	116.23	109.98
15	B	1212	CLA	C4A-NA-C1A	5.94	109.39	106.68
15	J	1303	CLA	C4A-NA-C1A	5.94	109.39	106.68
15	A	1801	CLA	C2C-C1C-NC	5.93	116.21	109.98
15	A	1133	CLA	C2C-C1C-NC	5.93	116.21	109.98
15	B	1232	CLA	C2C-C1C-NC	5.93	116.21	109.98
15	B	1023	CLA	C4A-NA-C1A	5.92	109.38	106.68
15	J	1302	CLA	C2C-C1C-NC	5.92	116.20	109.98
15	B	1207	CLA	C4A-NA-C1A	5.92	109.38	106.68
15	B	1237	CLA	C4A-NA-C1A	5.91	109.38	106.68
15	B	1211	CLA	O2D-CGD-CBD	5.91	121.55	111.23
15	B	1227	CLA	C4A-NA-C1A	5.90	109.37	106.68
15	B	1221	CLA	O2D-CGD-CBD	5.90	121.54	111.23
15	B	1209	CLA	C2C-C1C-NC	5.89	116.17	109.98
15	A	1133	CLA	C4A-NA-C1A	5.88	109.36	106.68
15	K	1402	CLA	C1D-ND-C4D	-5.88	102.19	106.31
15	A	1132	CLA	C1D-ND-C4D	-5.88	102.19	106.31
15	B	1230	CLA	C4A-NA-C1A	5.87	109.36	106.68
15	A	1120	CLA	C2C-C1C-NC	5.87	116.15	109.98
15	B	1221	CLA	C2C-C1C-NC	5.87	116.14	109.98
15	B	1232	CLA	C4A-NA-C1A	5.86	109.35	106.68
15	A	1113	CLA	C2C-C1C-NC	5.86	116.14	109.98
15	A	1132	CLA	O2D-CGD-CBD	5.85	121.46	111.23
15	A	1105	CLA	C2C-C1C-NC	5.85	116.13	109.98
15	B	1227	CLA	C2C-C1C-NC	5.85	116.13	109.98
15	A	1127	CLA	C4A-NA-C1A	5.85	109.35	106.68
15	A	1106	CLA	C4A-NA-C1A	5.85	109.35	106.68
15	B	1205	CLA	C2C-C1C-NC	5.85	116.12	109.98
15	B	1212	CLA	O2D-CGD-CBD	5.85	121.45	111.23
15	B	1229	CLA	C2D-C1D-ND	5.84	115.91	110.13
15	A	1012	CLA	C2C-C1C-NC	5.83	116.10	109.98
15	B	1204	CLA	C4A-NA-C1A	5.83	109.34	106.68
15	B	1202	CLA	C4A-NA-C1A	5.82	109.33	106.68
15	B	1204	CLA	C2C-C1C-NC	5.81	116.09	109.98
15	J	1303	CLA	C2C-C1C-NC	5.81	116.08	109.98
15	B	1235	CLA	C2D-C1D-ND	5.80	115.87	110.13
15	A	1126	CLA	O2D-CGD-CBD	5.80	121.36	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1229	CLA	C1D-ND-C4D	-5.79	102.25	106.31
15	A	1131	CLA	C1D-ND-C4D	-5.79	102.25	106.31
15	B	1222	CLA	C2C-C1C-NC	5.78	116.05	109.98
15	J	1302	CLA	C4A-NA-C1A	5.78	109.32	106.68
15	A	1110	CLA	C2C-C1C-NC	5.77	116.05	109.98
15	A	1102	CLA	C4A-NA-C1A	5.77	109.31	106.68
15	A	1102	CLA	O2D-CGD-CBD	5.77	121.32	111.23
15	B	1225	CLA	C2C-C1C-NC	5.77	116.04	109.98
15	A	1114	CLA	C2C-C1C-NC	5.76	116.04	109.98
15	B	1226	CLA	C2C-C1C-NC	5.76	116.04	109.98
15	A	1137	CLA	O2D-CGD-CBD	5.76	121.29	111.23
15	A	1116	CLA	C2C-C1C-NC	5.76	116.03	109.98
15	A	1127	CLA	C2C-C1C-NC	5.76	116.03	109.98
15	A	1107	CLA	C1D-ND-C4D	-5.75	102.28	106.31
15	K	1402	CLA	C2C-C1C-NC	5.75	116.02	109.98
15	B	1238	CLA	C2C-C1C-NC	5.75	116.02	109.98
15	A	1125	CLA	C2D-C1D-ND	5.75	115.81	110.13
15	K	1401	CLA	C4A-NA-C1A	5.74	109.30	106.68
15	A	1115	CLA	C1D-ND-C4D	-5.74	102.28	106.31
15	A	1103	CLA	C1D-ND-C4D	-5.74	102.28	106.31
15	A	1112	CLA	C4A-NA-C1A	5.74	109.30	106.68
15	A	1129	CLA	C4A-NA-C1A	5.74	109.30	106.68
15	A	1121	CLA	C2C-C1C-NC	5.73	116.00	109.98
15	B	1224	CLA	O2D-CGD-CBD	5.73	121.24	111.23
15	A	1131	CLA	C4A-NA-C1A	5.72	109.29	106.68
15	A	1129	CLA	C2C-C1C-NC	5.72	115.99	109.98
15	A	1122	CLA	C1D-ND-C4D	-5.72	102.30	106.31
15	B	1234	CLA	C2C-C1C-NC	5.71	115.98	109.98
15	A	1101	CLA	CAA-C2A-C3A	-5.71	97.58	113.00
15	A	1103	CLA	C4A-NA-C1A	5.70	109.28	106.68
15	A	1126	CLA	C4A-NA-C1A	5.69	109.28	106.68
15	A	1104	CLA	C1C-C2C-C3C	-5.69	100.99	106.98
15	K	1401	CLA	C2C-C1C-NC	5.69	115.96	109.98
15	A	1118	CLA	C2C-C1C-NC	5.68	115.95	109.98
15	B	1217	CLA	O2D-CGD-CBD	5.68	121.16	111.23
15	A	1124	CLA	C2C-C1C-NC	5.68	115.94	109.98
15	B	1206	CLA	C2C-C1C-NC	5.68	115.94	109.98
14	J	4013	BCR	C7-C8-C9	-5.67	117.84	126.23
15	A	1125	CLA	C3D-C2D-C1D	-5.67	98.10	105.83
15	B	1202	CLA	C1D-ND-C4D	-5.66	102.34	106.31
15	A	1140	CLA	C1D-ND-C4D	-5.66	102.34	106.31
15	A	1130	CLA	O2D-CGD-CBD	5.65	121.11	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1022	CLA	C2C-C1C-NC	5.65	115.92	109.98
15	J	1303	CLA	C1D-ND-C4D	-5.64	102.35	106.31
15	B	1229	CLA	C2C-C1C-NC	5.63	115.90	109.98
15	A	1118	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
15	B	1212	CLA	C2C-C1C-NC	5.63	115.89	109.98
15	B	1217	CLA	C2C-C1C-NC	5.63	115.89	109.98
15	A	1138	CLA	C1D-ND-C4D	-5.63	102.36	106.31
15	B	1216	CLA	C2C-C1C-NC	5.61	115.88	109.98
15	B	1201	CLA	C2C-C1C-NC	5.61	115.88	109.98
15	B	1224	CLA	C2C-C1C-NC	5.61	115.88	109.98
15	B	1219	CLA	C4A-NA-C1A	5.61	109.24	106.68
15	B	1219	CLA	C2C-C1C-NC	5.61	115.87	109.98
15	A	1116	CLA	O2D-CGD-CBD	5.60	121.03	111.23
15	B	1218	CLA	C2C-C1C-NC	5.60	115.87	109.98
15	F	1139	CLA	C2C-C1C-NC	5.60	115.86	109.98
15	B	1225	CLA	C4A-NA-C1A	5.60	109.23	106.68
15	B	1237	CLA	C2C-C1C-NC	5.60	115.86	109.98
15	A	1111	CLA	C4A-NA-C1A	5.59	109.23	106.68
15	B	1231	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
15	F	1139	CLA	C1D-ND-C4D	-5.59	102.39	106.31
15	B	1023	CLA	C2C-C1C-NC	5.59	115.85	109.98
15	A	1118	CLA	C2D-C1D-ND	5.58	115.65	110.13
15	B	1210	CLA	C4A-NA-C1A	5.58	109.23	106.68
15	A	1114	CLA	C1D-ND-C4D	-5.58	102.39	106.31
15	A	1134	CLA	C2C-C1C-NC	5.58	115.84	109.98
15	B	1223	CLA	C4A-NA-C1A	5.58	109.22	106.68
15	F	1410	CLA	C2C-C1C-NC	5.58	115.84	109.98
15	B	1013	CLA	C1D-ND-C4D	-5.58	102.40	106.31
15	B	1209	CLA	O2D-CGD-CBD	5.58	120.98	111.23
15	A	1105	CLA	O2D-CGD-CBD	5.57	120.97	111.23
15	B	1235	CLA	O2D-CGD-CBD	5.57	120.97	111.23
15	B	1211	CLA	C4A-NA-C1A	5.57	109.22	106.68
15	A	1134	CLA	C4A-NA-C1A	5.57	109.22	106.68
15	B	1208	CLA	C2C-C1C-NC	5.56	115.83	109.98
15	J	1302	CLA	C1D-ND-C4D	-5.56	102.41	106.31
15	A	1134	CLA	C1D-ND-C4D	-5.56	102.41	106.31
15	B	1234	CLA	O2D-CGD-CBD	5.56	120.94	111.23
15	B	1240	CLA	C4A-NA-C1A	5.55	109.21	106.68
15	B	1240	CLA	C2C-C1C-NC	5.55	115.81	109.98
15	A	1135	CLA	C4A-NA-C1A	5.55	109.21	106.68
15	F	1410	CLA	O2D-CGD-CBD	5.55	120.93	111.23
15	A	1121	CLA	C4A-NA-C1A	5.55	109.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1021	CLA	C2C-C1C-NC	5.55	115.81	109.98
15	A	1132	CLA	C2D-C1D-ND	5.55	115.62	110.13
15	B	1202	CLA	O2D-CGD-CBD	5.55	120.93	111.23
15	B	1203	CLA	C1C-C2C-C3C	-5.55	101.15	106.98
15	B	1217	CLA	C4A-NA-C1A	5.55	109.21	106.68
15	B	1207	CLA	C1D-ND-C4D	-5.54	102.42	106.31
15	A	1125	CLA	C4A-NA-C1A	5.54	109.21	106.68
15	A	1116	CLA	C4A-NA-C1A	5.54	109.20	106.68
15	B	1215	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
15	B	1202	CLA	C2C-C1C-NC	5.53	115.79	109.98
15	A	1125	CLA	C1D-ND-C4D	-5.53	102.43	106.31
15	B	1232	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
15	B	1208	CLA	C4A-NA-C1A	5.51	109.19	106.68
15	B	1222	CLA	C2D-C1D-ND	5.51	115.58	110.13
15	A	1119	CLA	C2C-C1C-NC	5.51	115.77	109.98
15	B	1013	CLA	O2A-CGA-O1A	-5.51	109.84	123.63
15	A	1112	CLA	C2C-C1C-NC	5.50	115.76	109.98
15	A	1111	CLA	C1D-ND-C4D	-5.50	102.45	106.31
15	A	1135	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
15	K	1401	CLA	C1D-ND-C4D	-5.50	102.45	106.31
15	B	1229	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
15	B	1230	CLA	C2C-C1C-NC	5.50	115.76	109.98
15	A	1132	CLA	C2C-C1C-NC	5.50	115.76	109.98
15	B	1236	CLA	O2D-CGD-CBD	5.50	120.84	111.23
15	A	1012	CLA	C2D-C1D-ND	5.50	115.57	110.13
15	B	1214	CLA	O2D-CGD-CBD	5.50	120.84	111.23
15	B	1218	CLA	C4-C3-C5	5.50	122.60	116.13
15	B	1218	CLA	C4A-NA-C1A	5.49	109.18	106.68
15	A	1137	CLA	C1D-ND-C4D	-5.49	102.46	106.31
15	B	1215	CLA	O2D-CGD-CBD	5.49	120.82	111.23
15	B	1239	CLA	C1C-C2C-C3C	-5.48	101.21	106.98
15	A	1118	CLA	O2D-CGD-CBD	5.48	120.81	111.23
15	A	1109	CLA	C4A-NA-C1A	5.48	109.18	106.68
15	A	1104	CLA	C4A-NA-C1A	5.47	109.18	106.68
15	A	1112	CLA	O2D-CGD-CBD	5.47	120.80	111.23
15	B	1236	CLA	C1D-ND-C4D	-5.47	102.47	106.31
15	A	1114	CLA	O2D-CGD-CBD	5.47	120.79	111.23
15	A	1101	CLA	C4A-NA-C1A	5.47	109.17	106.68
15	A	1109	CLA	C2D-C1D-ND	5.47	115.54	110.13
15	A	1138	CLA	C2D-C1D-ND	5.47	115.54	110.13
15	A	1105	CLA	C3B-C2B-C1B	-5.47	100.73	107.17
15	B	1204	CLA	C1D-ND-C4D	-5.47	102.48	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1230	CLA	O2D-CGD-CBD	5.46	120.78	111.23
15	A	1131	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
15	A	1102	CLA	C2C-C1C-NC	5.46	115.72	109.98
15	B	1226	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
15	B	1219	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
15	A	1801	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
15	B	1219	CLA	C1D-ND-C4D	-5.46	102.48	106.31
15	A	1119	CLA	O2A-CGA-O1A	-5.46	109.98	123.63
15	B	1213	CLA	C2C-C1C-NC	5.45	115.70	109.98
15	A	1106	CLA	C2C-C1C-NC	5.45	115.70	109.98
15	B	1221	CLA	O2A-CGA-O1A	-5.45	110.00	123.63
15	B	1207	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
15	B	1023	CLA	C1D-ND-C4D	-5.44	102.49	106.31
15	B	1221	CLA	C1D-ND-C4D	-5.44	102.49	106.31
15	B	1227	CLA	C1C-C2C-C3C	-5.44	101.25	106.98
15	A	1113	CLA	C1D-ND-C4D	-5.44	102.49	106.31
15	B	1205	CLA	O2A-CGA-O1A	-5.44	110.02	123.63
15	B	1224	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
15	J	1302	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
15	B	1221	CLA	C2D-C1D-ND	5.43	115.50	110.13
15	A	1104	CLA	C1D-ND-C4D	-5.43	102.50	106.31
15	A	1136	CLA	O2D-CGD-CBD	5.43	120.72	111.23
15	B	1223	CLA	O2D-CGD-CBD	5.43	120.72	111.23
15	A	1133	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
15	A	1128	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
15	F	1301	CLA	C4A-NA-C1A	5.42	109.15	106.68
15	A	1115	CLA	C2D-C1D-ND	5.42	115.49	110.13
15	B	1204	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
15	B	1213	CLA	C1D-ND-C4D	-5.42	102.51	106.31
15	A	1112	CLA	C1D-ND-C4D	-5.42	102.51	106.31
15	B	1235	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
15	B	1222	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
15	F	1301	CLA	C2C-C1C-NC	5.41	115.66	109.98
15	B	1229	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
15	B	1239	CLA	O2D-CGD-CBD	5.41	120.68	111.23
15	A	1022	CLA	C1C-C2C-C3C	-5.41	101.30	106.98
15	B	1235	CLA	O2A-CGA-O1A	-5.40	110.11	123.63
15	B	1230	CLA	C1D-ND-C4D	-5.40	102.52	106.31
15	A	1105	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
15	A	1120	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
15	B	1238	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
15	A	1124	CLA	C4A-NA-C1A	5.40	109.14	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1212	CLA	C1D-ND-C4D	-5.40	102.52	106.31
15	B	1205	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
15	B	1208	CLA	C1D-ND-C4D	-5.40	102.52	106.31
15	B	1213	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
15	A	1114	CLA	C4A-NA-C1A	5.40	109.14	106.68
15	A	1127	CLA	C1D-ND-C4D	-5.40	102.53	106.31
15	A	1124	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
15	A	1116	CLA	C1D-ND-C4D	-5.39	102.53	106.31
15	A	1115	CLA	C2C-C1C-NC	5.39	115.64	109.98
15	B	1215	CLA	C4A-NA-C1A	5.39	109.14	106.68
15	A	1106	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
15	A	1113	CLA	C4A-NA-C1A	5.39	109.14	106.68
15	B	1223	CLA	C2C-C1C-NC	5.39	115.64	109.98
15	B	1013	CLA	C3B-C2B-C1B	-5.38	100.82	107.17
15	B	1228	CLA	C2D-C1D-ND	5.38	115.45	110.13
15	A	1136	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
15	A	1137	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
15	K	1402	CLA	C2D-C1D-ND	5.38	115.45	110.13
15	B	1206	CLA	C4A-NA-C1A	5.37	109.13	106.68
15	B	1212	CLA	C2D-C1D-ND	5.37	115.44	110.13
15	A	1129	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
15	B	1221	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
15	A	1140	CLA	C2D-C1D-ND	5.36	115.44	110.13
15	B	1223	CLA	C2D-C1D-ND	5.36	115.43	110.13
15	B	1218	CLA	O2D-CGD-CBD	5.36	120.60	111.23
15	B	1013	CLA	C2D-C1D-ND	5.36	115.43	110.13
15	A	1110	CLA	C1D-ND-C4D	-5.36	102.55	106.31
15	F	1139	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
15	B	1234	CLA	C1D-ND-C4D	-5.36	102.55	106.31
15	A	1131	CLA	C2D-C1D-ND	5.36	115.43	110.13
15	B	1214	CLA	C2C-C1C-NC	5.35	115.60	109.98
15	A	1105	CLA	C4A-NA-C1A	5.35	109.12	106.68
15	B	1238	CLA	C4A-NA-C1A	5.35	109.12	106.68
15	B	1208	CLA	C1C-C2C-C3C	-5.35	101.36	106.98
15	A	1127	CLA	C1C-C2C-C3C	-5.35	101.36	106.98
15	A	1126	CLA	C1D-ND-C4D	-5.34	102.56	106.31
15	A	1124	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
15	B	1218	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
15	B	1212	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
15	B	1225	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
15	A	1136	CLA	O2A-CGA-O1A	-5.34	110.28	123.63
15	B	1219	CLA	O2D-CGD-CBD	5.34	120.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1207	CLA	O2D-CGD-CBD	5.33	120.55	111.23
15	B	1202	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
15	A	1136	CLA	C2D-C1D-ND	5.33	115.40	110.13
15	B	1236	CLA	C2D-C1D-ND	5.33	115.40	110.13
15	A	1117	CLA	C2C-C1C-NC	5.33	115.58	109.98
15	B	1211	CLA	C2C-C1C-NC	5.33	115.58	109.98
15	A	1140	CLA	O2D-CGD-CBD	5.33	120.55	111.23
15	B	1226	CLA	C1D-ND-C4D	-5.33	102.57	106.31
15	A	1104	CLA	C2C-C1C-NC	5.33	115.58	109.98
15	J	1303	CLA	C2D-C1D-ND	5.33	115.40	110.13
15	B	1223	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
15	A	1132	CLA	O2A-CGA-O1A	-5.33	110.31	123.63
15	A	1129	CLA	O2D-CGD-CBD	5.32	120.54	111.23
15	K	1402	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
15	J	1302	CLA	C2D-C1D-ND	5.32	115.39	110.13
15	B	1202	CLA	C2D-C1D-ND	5.32	115.39	110.13
15	A	1126	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
15	B	1222	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
15	B	1213	CLA	O2D-CGD-CBD	5.31	120.51	111.23
15	A	1134	CLA	C2D-C1D-ND	5.31	115.38	110.13
15	B	1224	CLA	C1D-ND-C4D	-5.31	102.59	106.31
15	B	1222	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
15	A	1107	CLA	O2D-CGD-CBD	5.30	120.50	111.23
15	B	1224	CLA	C4A-NA-C1A	5.30	109.10	106.68
15	F	1410	CLA	C4A-NA-C1A	5.30	109.10	106.68
15	A	1110	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	B	4017	BCR	C24-C23-C22	-5.30	118.39	126.23
15	B	1236	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
15	B	1231	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	F	4016	BCR	C38-C26-C25	-5.30	118.70	124.48
15	B	1201	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
15	A	1012	CLA	O2D-CGD-CBD	5.29	120.48	111.23
15	B	1237	CLA	C1D-ND-C4D	-5.29	102.60	106.31
15	F	1410	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
15	A	1109	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
15	B	1206	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
15	A	1113	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
15	A	1801	CLA	O2A-CGA-O1A	-5.28	110.41	123.63
15	B	1213	CLA	C4A-NA-C1A	5.28	109.09	106.68
15	B	1217	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
15	A	1121	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
15	B	1209	CLA	C1C-C2C-C3C	-5.28	101.43	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1138	CLA	C4A-NA-C1A	5.28	109.09	106.68
15	B	1021	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
15	A	1106	CLA	C1D-ND-C4D	-5.27	102.61	106.31
15	A	1114	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
15	B	1216	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
15	B	1230	CLA	C4-C3-C5	5.26	124.37	115.23
15	F	1301	CLA	C2D-C1D-ND	5.26	115.34	110.13
15	A	1104	CLA	C2D-C1D-ND	5.26	115.33	110.13
15	B	1202	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
15	B	1013	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
15	A	1132	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
15	B	1013	CLA	C2C-C1C-NC	5.25	115.50	109.98
15	B	1210	CLA	O2A-CGA-O1A	-5.25	110.49	123.63
15	A	1134	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
15	A	1106	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
15	A	1118	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
15	B	1235	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
15	B	1237	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
15	A	1129	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
15	B	1216	CLA	C1D-ND-C4D	-5.24	102.63	106.31
15	A	1138	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
15	A	1116	CLA	C1C-C2C-C3C	-5.24	101.46	106.98
15	A	1111	CLA	C2C-C1C-NC	5.24	115.49	109.98
15	B	1210	CLA	C2C-C1C-NC	5.24	115.49	109.98
15	B	1222	CLA	C1D-ND-C4D	-5.24	102.64	106.31
15	B	1220	CLA	C2C-C1C-NC	5.24	115.48	109.98
15	F	1301	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
15	B	1234	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
15	B	1231	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
15	B	1231	CLA	C1D-ND-C4D	-5.23	102.64	106.31
15	B	1230	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
15	A	1121	CLA	C1D-ND-C4D	-5.22	102.65	106.31
15	A	1109	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
15	B	1236	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
15	A	1102	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
15	A	1119	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
15	B	1214	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
15	A	1116	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
15	B	1238	CLA	C1D-ND-C4D	-5.21	102.65	106.31
15	B	1228	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
15	B	1207	CLA	C2D-C1D-ND	5.21	115.28	110.13
15	A	1102	CLA	C1C-C2C-C3C	-5.21	101.50	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1234	CLA	C2D-C1D-ND	5.21	115.28	110.13
15	B	1223	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
15	B	1023	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
15	A	1111	CLA	C2D-C1D-ND	5.20	115.27	110.13
15	A	1111	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
15	A	1112	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
15	A	1110	CLA	C2D-C1D-ND	5.20	115.27	110.13
15	A	1012	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
15	B	1212	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
15	A	1103	CLA	O2D-CGD-CBD	5.19	120.31	111.23
15	A	1130	CLA	C2C-C1C-NC	5.19	115.43	109.98
15	K	1401	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
15	A	1102	CLA	C2D-C1D-ND	5.19	115.26	110.13
15	A	1140	CLA	C2C-C1C-NC	5.19	115.43	109.98
15	A	1801	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
15	A	1131	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
15	A	1101	CLA	C2C-C1C-NC	5.19	115.43	109.98
15	B	1227	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
15	B	1238	CLA	C2D-C1D-ND	5.18	115.25	110.13
15	A	1102	CLA	O2A-CGA-O1A	-5.18	110.67	123.63
15	F	1410	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
15	B	1224	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
15	A	1134	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
15	A	1129	CLA	C1D-ND-C4D	-5.18	102.68	106.31
15	F	1139	CLA	C2D-C1D-ND	5.18	115.25	110.13
15	J	1303	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
15	B	1236	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
15	A	1123	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
15	A	1130	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
15	F	1410	CLA	C2D-C1D-ND	5.18	115.25	110.13
15	F	1410	CLA	C1D-ND-C4D	-5.18	102.68	106.31
15	A	1801	CLA	C2D-C1D-ND	5.17	115.25	110.13
15	A	1113	CLA	C2D-C1D-ND	5.17	115.25	110.13
15	A	1104	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
15	A	1115	CLA	O2D-CGD-CBD	5.17	120.27	111.23
15	A	1105	CLA	C1D-ND-C4D	-5.17	102.68	106.31
15	K	1402	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
15	A	1135	CLA	C1D-ND-C4D	-5.17	102.69	106.31
15	A	1102	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
15	B	1240	CLA	C1D-ND-C4D	-5.17	102.69	106.31
15	B	1226	CLA	C2D-C1D-ND	5.17	115.24	110.13
15	A	1133	CLA	O2D-CGD-CBD	5.16	120.26	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1110	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
15	J	1303	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
15	B	1204	CLA	O2D-CGD-CBD	5.16	120.25	111.23
15	A	1012	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	A	4012	BCR	C38-C26-C25	-5.15	118.86	124.48
15	B	1231	CLA	C2D-C1D-ND	5.15	115.22	110.13
15	A	1103	CLA	C2C-C1C-NC	5.15	115.39	109.98
15	B	1211	CLA	C1D-ND-C4D	-5.15	102.70	106.31
15	F	1301	CLA	O2D-CGD-CBD	5.15	120.23	111.23
15	B	1238	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
15	A	1131	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
15	J	1302	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
15	A	1114	CLA	C2D-C1D-ND	5.15	115.22	110.13
15	A	1111	CLA	O2A-CGA-O1A	-5.15	110.76	123.63
15	A	1110	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
15	B	1234	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
15	A	1106	CLA	C2D-C1D-ND	5.14	115.22	110.13
15	B	1230	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
14	A	4001	BCR	C7-C8-C9	-5.14	118.63	126.23
15	K	1401	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
15	A	1022	CLA	O2D-CGD-CBD	5.14	120.22	111.23
15	A	1123	CLA	C1D-ND-C4D	-5.14	102.71	106.31
15	B	1240	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
15	B	1210	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
15	A	1130	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
15	A	1117	CLA	C4A-NA-C1A	5.14	109.02	106.68
15	A	1138	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
15	B	1240	CLA	C2D-C1D-ND	5.13	115.21	110.13
15	K	1401	CLA	C2D-C1D-ND	5.13	115.21	110.13
15	B	1202	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
15	A	1137	CLA	C2D-C1D-ND	5.13	115.21	110.13
15	A	1111	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	B	1229	CLA	O2D-CGD-CBD	5.13	120.20	111.23
15	A	1106	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	B	1235	CLA	C2C-C1C-NC	5.13	115.37	109.98
15	A	1104	CLA	O2D-CGD-CBD	5.13	120.20	111.23
15	B	1219	CLA	C2D-C1D-ND	5.13	115.20	110.13
15	B	1220	CLA	C1D-ND-C4D	-5.13	102.71	106.31
15	B	1240	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	B	1023	CLA	C2D-C1D-ND	5.13	115.20	110.13
15	A	1135	CLA	O2A-CGA-O1A	-5.13	110.81	123.63
15	B	1232	CLA	C2D-C1D-ND	5.13	115.20	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1210	CLA	C1D-ND-C4D	-5.13	102.72	106.31
15	B	1232	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
15	B	1209	CLA	C1D-ND-C4D	-5.12	102.72	106.31
15	A	1112	CLA	C2D-C1D-ND	5.12	115.19	110.13
15	B	1217	CLA	C2D-C1D-ND	5.12	115.19	110.13
15	B	1021	CLA	O2A-CGA-O1A	-5.12	110.83	123.63
15	F	1301	CLA	C1D-ND-C4D	-5.12	102.72	106.31
15	F	1301	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
15	A	1120	CLA	C1D-ND-C4D	-5.12	102.72	106.31
15	B	1203	CLA	C1D-ND-C4D	-5.12	102.72	106.31
15	B	1023	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
15	B	1227	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
15	B	1221	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
15	B	1211	CLA	C1C-C2C-C3C	-5.11	101.60	106.98
15	A	1136	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
15	B	1203	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	B	1224	CLA	C2D-C1D-ND	5.11	115.18	110.13
15	B	1210	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	A	1103	CLA	C2D-C1D-ND	5.10	115.18	110.13
15	B	1219	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
15	B	1207	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
15	A	1122	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
15	A	1140	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
15	A	1115	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
15	B	1223	CLA	C1D-ND-C4D	-5.10	102.73	106.31
15	A	1109	CLA	C2C-C1C-NC	5.10	115.33	109.98
14	B	4006	BCR	C38-C26-C25	-5.10	118.92	124.48
15	A	1113	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
15	B	1210	CLA	C2D-C1D-ND	5.09	115.17	110.13
15	A	1105	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
15	B	1220	CLA	C1C-C2C-C3C	-5.09	101.62	106.98
15	B	1227	CLA	C1D-ND-C4D	-5.09	102.74	106.31
15	A	1126	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
15	B	1224	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
15	A	1104	CLA	O2A-CGA-O1A	-5.09	110.91	123.63
15	A	1125	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
15	A	1107	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
15	A	1121	CLA	O2D-CGD-CBD	5.08	120.11	111.23
15	A	1105	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
15	A	1119	CLA	C1D-ND-C4D	-5.08	102.75	106.31
15	B	1226	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
15	A	1132	CLA	C1C-C2C-C3C	-5.08	101.64	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1219	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
15	B	1228	CLA	C2C-C1C-NC	5.07	115.31	109.98
15	A	1140	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
15	B	1217	CLA	C1D-ND-C4D	-5.07	102.75	106.31
15	A	1124	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
15	A	1114	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
15	B	1214	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
15	A	1109	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
15	A	1111	CLA	O2D-CGD-CBD	5.07	120.09	111.23
15	B	1220	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
15	A	1122	CLA	C2C-C1C-NC	5.07	115.30	109.98
15	B	1232	CLA	C1D-ND-C4D	-5.07	102.76	106.31
15	A	1103	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
15	B	1202	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
15	A	1101	CLA	C1D-ND-C4D	-5.07	102.76	106.31
15	B	1218	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
15	A	1117	CLA	C1C-C2C-C3C	-5.06	101.65	106.98
15	B	1215	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
15	B	1208	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
15	K	1401	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
15	A	1022	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
15	F	1410	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
15	J	1303	CLA	O2D-CGD-CBD	5.05	120.06	111.23
15	B	1226	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
15	B	1217	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
15	B	1208	CLA	C2D-C1D-ND	5.05	115.12	110.13
15	B	1237	CLA	O2D-CGD-CBD	5.04	120.05	111.23
15	B	1214	CLA	O2A-CGA-O1A	-5.04	111.01	123.63
15	B	1217	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
15	A	1104	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
15	F	1301	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
15	A	1133	CLA	C1D-ND-C4D	-5.04	102.78	106.31
15	F	1139	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
15	A	1123	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
15	B	1225	CLA	O2D-CGD-CBD	5.02	120.01	111.23
15	A	1135	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
15	A	1117	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
15	B	1225	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
15	A	1101	CLA	C2D-C1D-ND	5.02	115.09	110.13
15	A	1117	CLA	C2D-C1D-ND	5.02	115.09	110.13
15	B	1013	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
15	A	1121	CLA	C2D-C1D-ND	5.02	115.09	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1023	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
15	A	1112	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
15	A	1135	CLA	C2D-C1D-ND	5.02	115.09	110.13
15	A	1120	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
15	K	1401	CLA	O2D-CGD-CBD	5.01	119.99	111.23
15	A	1123	CLA	O2A-CGA-O1A	-5.01	111.09	123.63
15	B	1213	CLA	C2D-C1D-ND	5.01	115.08	110.13
15	B	1205	CLA	C1D-ND-C4D	-5.01	102.80	106.31
15	B	1218	CLA	C1D-ND-C4D	-5.01	102.80	106.31
15	B	1227	CLA	C2D-C1D-ND	5.01	115.08	110.13
14	A	4003	BCR	C7-C8-C9	-5.01	118.83	126.23
15	A	1122	CLA	O2D-CGD-CBD	5.01	119.98	111.23
15	B	1206	CLA	C1D-ND-C4D	-5.00	102.80	106.31
15	B	1206	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
15	B	1237	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
15	B	1234	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
15	B	1206	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
15	A	1119	CLA	O2D-CGD-CBD	5.00	119.97	111.23
15	A	1121	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
15	A	1107	CLA	C2C-C1C-NC	5.00	115.23	109.98
15	B	1239	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
15	A	1022	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
15	F	1410	CLA	C4-C3-C5	5.00	123.90	115.23
15	B	1220	CLA	C2D-C1D-ND	5.00	115.07	110.13
15	B	1230	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	B	1228	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
15	B	1213	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	B	1209	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	A	1117	CLA	C1D-ND-C4D	-4.99	102.81	106.31
15	A	1122	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	B	1204	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
15	B	1230	CLA	C2D-C1D-ND	4.99	115.06	110.13
15	B	1210	CLA	O2D-CGD-CBD	4.99	119.94	111.23
15	B	1201	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
15	A	1130	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
15	A	1022	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
15	A	1128	CLA	C2D-C1D-ND	4.98	115.05	110.13
15	B	1203	CLA	C2D-C1D-ND	4.98	115.05	110.13
15	A	1116	CLA	C2D-C1D-ND	4.98	115.05	110.13
15	A	1109	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
15	A	1137	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
15	B	1240	CLA	C3B-C2B-C1B	-4.98	101.30	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1216	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
15	A	1801	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
15	B	1229	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
15	A	1110	CLA	C4A-NA-C1A	4.97	108.95	106.68
15	B	1204	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
15	A	1132	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
13	A	1108	CL0	O2A-CGA-O1A	-4.97	110.54	123.33
15	A	1105	CLA	C2D-C1D-ND	4.97	115.05	110.13
15	B	1201	CLA	C1D-ND-C4D	-4.97	102.83	106.31
15	A	1112	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
15	A	1130	CLA	O2A-CGA-O1A	-4.97	111.20	123.63
15	A	1137	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
15	A	1119	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
15	A	1101	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
15	B	1220	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
15	A	1107	CLA	C2D-C1D-ND	4.96	115.03	110.13
15	B	1238	CLA	O2D-CGD-CBD	4.96	119.90	111.23
15	B	1021	CLA	C1D-ND-C4D	-4.96	102.83	106.31
15	J	1302	CLA	O2D-CGD-CBD	4.96	119.89	111.23
15	A	1133	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
15	A	1122	CLA	C2D-C1D-ND	4.96	115.03	110.13
15	A	1116	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
15	B	1216	CLA	O2D-CGD-CBD	4.95	119.89	111.23
15	A	1801	CLA	C1D-ND-C4D	-4.95	102.84	106.31
15	B	1228	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
15	A	1022	CLA	C4A-NA-C1A	4.94	108.94	106.68
15	B	1219	CLA	O2A-CGA-O1A	-4.94	111.26	123.63
15	B	1204	CLA	C2D-C1D-ND	4.94	115.02	110.13
13	A	1011	CL0	O2A-CGA-O1A	-4.94	111.27	123.63
15	A	1117	CLA	O2D-CGD-CBD	4.94	119.87	111.23
15	A	1022	CLA	C2D-C1D-ND	4.94	115.02	110.13
15	A	1103	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
15	A	1107	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
15	B	1220	CLA	O2D-CGD-CBD	4.94	119.86	111.23
15	B	1201	CLA	C2D-C1D-ND	4.94	115.01	110.13
15	B	1217	CLA	O2A-CGA-O1A	-4.94	111.28	123.63
15	B	1205	CLA	C2D-C1D-ND	4.93	115.01	110.13
15	B	1214	CLA	C1D-ND-C4D	-4.93	102.85	106.31
15	B	1211	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
15	A	1127	CLA	C2D-C1D-ND	4.93	115.01	110.13
15	B	1201	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
15	A	1127	CLA	O2D-CGD-CBD	4.93	119.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1134	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
15	A	1119	CLA	C2D-C1D-ND	4.93	115.01	110.13
15	B	1215	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
15	A	1129	CLA	C2D-C1D-ND	4.93	115.00	110.13
15	B	1208	CLA	O2D-CGD-CBD	4.93	119.84	111.23
15	A	1117	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
15	B	1214	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
15	B	1239	CLA	C1D-ND-C4D	-4.92	102.86	106.31
15	A	1107	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
15	B	1208	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
15	A	1124	CLA	C2D-C1D-ND	4.92	115.00	110.13
15	A	1110	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
15	A	1120	CLA	C2D-C1D-ND	4.92	115.00	110.13
15	A	1140	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
15	B	1211	CLA	C2D-C1D-ND	4.92	114.99	110.13
15	B	1216	CLA	C2D-C1D-ND	4.91	114.99	110.13
15	B	1235	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
15	B	1209	CLA	C2D-C1D-ND	4.91	114.99	110.13
15	B	1236	CLA	O2A-CGA-O1A	-4.91	111.34	123.63
15	A	1137	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
15	B	1236	CLA	C2C-C1C-NC	4.91	115.14	109.98
15	A	1124	CLA	C1D-ND-C4D	-4.91	102.87	106.31
15	B	1021	CLA	C2D-C1D-ND	4.90	114.98	110.13
15	A	1102	CLA	C1D-ND-C4D	-4.90	102.87	106.31
15	A	1119	CLA	C4A-NA-C1A	4.90	108.92	106.68
15	B	1228	CLA	C4A-NA-C1A	4.89	108.91	106.68
15	B	1218	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
15	A	1126	CLA	C1C-C2C-C3C	-4.89	101.83	106.98
15	A	1123	CLA	C2D-C1D-ND	4.89	114.97	110.13
15	B	1213	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
15	B	1203	CLA	O2D-CGD-CBD	4.89	119.77	111.23
15	K	1402	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
15	A	1128	CLA	C1D-ND-C4D	-4.88	102.89	106.31
15	B	1225	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	A	4003	BCR	C38-C26-C25	-4.88	119.16	124.48
15	A	1120	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
14	A	4008	BCR	C33-C5-C6	-4.88	119.16	124.48
15	B	1220	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
15	B	1228	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
15	B	1212	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
15	A	1111	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
15	B	1203	CLA	C3B-C2B-C1B	-4.87	101.43	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	1303	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
15	B	1237	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
15	B	1223	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
15	B	1209	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
15	A	1115	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
15	A	1136	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
15	F	1301	CLA	O2A-CGA-O1A	-4.85	110.87	123.33
15	A	1128	CLA	O2A-CGA-O1A	-4.84	111.51	123.63
15	A	1109	CLA	C4-C3-C5	4.84	123.63	115.23
15	A	1133	CLA	C2D-C1D-ND	4.84	114.92	110.13
15	A	1101	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
15	B	1206	CLA	C2D-C1D-ND	4.84	114.92	110.13
15	F	1139	CLA	O2D-CGD-CBD	4.84	119.69	111.23
15	B	1218	CLA	C2D-C1D-ND	4.84	114.92	110.13
15	B	1211	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
15	B	1215	CLA	C2D-C1D-ND	4.84	114.92	110.13
15	A	1128	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
15	B	1230	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
15	B	1237	CLA	C2D-C1D-ND	4.84	114.91	110.13
14	B	4011	BCR	C34-C9-C10	-4.84	114.98	122.82
15	A	1138	CLA	O2D-CGD-CBD	4.83	119.68	111.23
14	A	4002	BCR	C24-C23-C22	-4.83	119.08	126.23
15	B	1238	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
15	B	1221	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
15	A	1125	CLA	C2C-C1C-NC	4.83	115.05	109.98
15	A	1120	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
15	A	1126	CLA	C2C-C1C-NC	4.82	115.05	109.98
15	A	1107	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
15	A	1012	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
15	B	1207	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
15	B	1221	CLA	O2A-CGA-CBA	4.82	126.52	111.83
15	A	1121	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
15	B	1021	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
15	A	1120	CLA	O2D-CGD-CBD	4.81	119.64	111.23
15	B	1225	CLA	C1D-ND-C4D	-4.81	102.94	106.31
15	B	1228	CLA	O2D-CGD-CBD	4.81	119.64	111.23
15	B	1240	CLA	O2D-CGD-CBD	4.81	119.64	111.23
15	A	1103	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
15	A	1113	CLA	O2D-CGD-CBD	4.81	119.63	111.23
15	A	1114	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
15	A	1122	CLA	C4A-NA-C1A	4.80	108.87	106.68
15	A	1124	CLA	O2D-CGD-CBD	4.80	119.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1122	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
15	A	1130	CLA	C1D-ND-C4D	-4.80	102.95	106.31
15	A	1135	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
15	A	1114	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
15	B	1234	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
15	F	1410	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
15	B	1227	CLA	O2A-CGA-O1A	-4.79	111.02	123.33
15	B	1231	CLA	O2D-CGD-CBD	4.79	119.60	111.23
15	B	1214	CLA	C2D-C1D-ND	4.79	114.86	110.13
15	A	1126	CLA	C2D-C1D-ND	4.78	114.86	110.13
15	A	1118	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
15	A	1101	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
15	B	1023	CLA	O2A-CGA-O1A	-4.78	111.68	123.63
15	A	1012	CLA	C1D-ND-C4D	-4.77	102.96	106.31
15	A	1140	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
15	B	1216	CLA	C4A-NA-C1A	4.77	108.86	106.68
15	B	1206	CLA	O2D-CGD-CBD	4.77	119.57	111.23
15	A	1135	CLA	O2D-CGD-CBD	4.77	119.57	111.23
15	A	1116	CLA	O2A-CGA-O1A	-4.77	111.71	123.63
15	B	1239	CLA	C2D-C1D-ND	4.76	114.84	110.13
15	A	1127	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
14	B	4014	BCR	C7-C8-C9	-4.76	119.19	126.23
15	A	1110	CLA	O2D-CGD-CBD	4.76	119.55	111.23
15	B	1225	CLA	C4-C3-C5	4.76	123.49	115.23
15	B	1225	CLA	C2D-C1D-ND	4.76	114.83	110.13
15	B	1210	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
15	B	1215	CLA	C1D-ND-C4D	-4.75	102.98	106.31
15	A	1801	CLA	O2D-CGD-CBD	4.75	119.53	111.23
15	A	1120	CLA	O2A-C1-C2	4.75	120.29	108.99
15	B	1205	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
15	B	1023	CLA	O2D-CGD-CBD	4.75	119.53	111.23
15	B	1215	CLA	O2A-CGA-O1A	-4.74	111.77	123.63
15	B	1231	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
15	A	1112	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
15	B	1205	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
15	B	1216	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
15	A	1012	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
15	A	1022	CLA	C1D-ND-C4D	-4.72	103.00	106.31
15	A	1122	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
15	B	1239	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
15	J	1302	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
15	A	1113	CLA	O2A-CGA-O1A	-4.71	111.21	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1119	CLA	O2A-C1-C2	4.71	120.21	108.99
14	J	4013	BCR	C3-C4-C5	-4.71	105.66	114.06
15	B	1021	CLA	O2D-CGD-CBD	4.71	119.46	111.23
15	B	1215	CLA	C4-C3-C5	4.71	123.40	115.23
15	A	1130	CLA	C2D-C1D-ND	4.70	114.78	110.13
15	A	1136	CLA	O2A-CGA-CBA	4.70	126.17	111.83
15	A	1119	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
15	A	1115	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
15	B	1240	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
15	B	1209	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
15	A	1127	CLA	O2A-CGA-O1A	-4.69	111.88	123.63
15	B	1218	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
15	A	1133	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
15	B	1224	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
15	B	1237	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
15	A	1107	CLA	C4A-NA-C1A	4.69	108.82	106.68
15	A	1123	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
15	B	1212	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	B	4009	BCR	C24-C23-C22	-4.69	119.30	126.23
14	B	4009	BCR	C7-C8-C9	-4.69	119.30	126.23
15	B	1208	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
15	A	1117	CLA	O2A-CGA-O1A	-4.68	111.92	123.63
15	A	1125	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
15	B	1214	CLA	C4A-NA-C1A	4.66	108.81	106.68
14	B	4009	BCR	C33-C5-C6	-4.66	119.40	124.48
15	B	1223	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
15	A	1129	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
15	B	1232	CLA	O2A-CGA-O1A	-4.66	111.36	123.33
15	A	1125	CLA	O2A-CGA-O1A	-4.65	111.99	123.63
15	A	1113	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
14	B	4004	BCR	C33-C5-C6	-4.64	119.43	124.48
14	B	4014	BCR	C33-C5-C6	-4.62	119.44	124.48
15	K	1402	CLA	O2D-CGD-CBD	4.62	119.31	111.23
15	A	1109	CLA	O2D-CGD-CBD	4.61	119.30	111.23
15	A	1131	CLA	O2A-CGA-CBA	4.61	125.89	111.83
14	F	4015	BCR	C24-C23-C22	-4.61	119.42	126.23
14	A	4008	BCR	C24-C23-C22	-4.60	119.43	126.23
15	A	1132	CLA	O2A-CGA-CBA	4.60	125.86	111.83
15	A	1127	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
15	B	1225	CLA	O2A-CGA-O1A	-4.59	112.16	123.63
15	A	1138	CLA	C1C-C2C-C3C	-4.58	102.16	106.98
14	B	4014	BCR	C24-C23-C22	-4.58	119.46	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1114	CLA	O2A-C1-C2	4.58	119.89	108.99
12	B	5004	LHG	O7-C7-C8	4.58	121.38	111.48
14	B	4014	BCR	C38-C26-C25	-4.57	119.49	124.48
15	B	1232	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
15	A	1126	CLA	O2A-CGA-O1A	-4.56	112.22	123.63
14	B	4011	BCR	C24-C23-C22	-4.56	119.49	126.23
15	B	1224	CLA	O2A-CGA-CBA	4.55	125.72	111.83
14	F	4015	BCR	C33-C5-C6	-4.55	119.52	124.48
15	B	1229	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
15	B	1232	CLA	O2D-CGD-CBD	4.55	119.18	111.23
15	A	1106	CLA	O2A-CGA-O1A	-4.54	112.27	123.63
14	A	4012	BCR	C24-C23-C22	-4.54	119.53	126.23
15	B	1226	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
15	B	1203	CLA	O2A-CGA-O1A	-4.52	112.33	123.63
15	J	1302	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
15	B	1021	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
12	A	5003	LHG	O7-C7-C8	4.50	121.21	111.48
15	B	1213	CLA	O2A-CGA-O1A	-4.49	112.39	123.63
15	B	1013	CLA	O2D-CGD-CBD	4.49	119.08	111.23
14	B	4017	BCR	C33-C5-C6	-4.48	119.59	124.48
15	B	1236	CLA	C4A-NA-C1A	4.47	108.72	106.68
15	B	1222	CLA	O2A-CGA-O1A	-4.47	112.44	123.63
15	B	1216	CLA	O2A-CGA-O1A	-4.46	112.48	123.63
15	B	1218	CLA	O2A-CGA-CBA	4.45	125.39	111.83
15	A	1801	CLA	O2A-CGA-CBA	4.44	125.38	111.83
15	A	1138	CLA	O2A-CGA-O1A	-4.44	112.52	123.63
15	A	1104	CLA	O2A-CGA-CBA	4.44	125.38	111.83
15	B	1220	CLA	C4A-NA-C1A	4.43	108.70	106.68
15	A	1111	CLA	O2A-CGA-CBA	4.39	125.23	111.83
15	F	1139	CLA	O2A-CGA-O1A	-4.39	112.64	123.63
15	A	1131	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
15	B	1013	CLA	O2A-CGA-CBA	4.39	125.22	111.83
15	B	1230	CLA	O2A-CGA-CBA	4.38	125.19	111.83
15	A	1122	CLA	C4-C3-C5	4.38	122.83	115.23
15	F	1139	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
15	A	1101	CLA	O2A-CGA-O1A	-4.36	112.72	123.63
15	A	1119	CLA	O2A-CGA-CBA	4.35	125.11	111.83
15	B	1239	CLA	O2A-CGA-O1A	-4.35	110.21	123.20
15	A	1138	CLA	C2C-C1C-NC	4.33	114.53	109.98
15	B	1013	CLA	C1-O2A-CGA	4.32	127.10	116.65
15	B	1021	CLA	O2A-CGA-CBA	4.32	125.00	111.83
15	B	1231	CLA	O2A-CGA-CBA	4.31	124.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1210	CLA	O2A-CGA-CBA	4.31	124.96	111.83
15	A	1121	CLA	O2A-CGA-O1A	-4.30	110.35	123.20
15	B	1235	CLA	O2A-CGA-CBA	4.30	124.95	111.83
15	B	1214	CLA	O2A-CGA-CBA	4.29	124.92	111.83
14	B	4010	BCR	C33-C5-C6	-4.28	119.81	124.48
14	A	4001	BCR	C33-C5-C6	-4.28	119.81	124.48
14	A	4003	BCR	C24-C23-C22	-4.27	119.92	126.23
15	A	1103	CLA	O2A-CGA-O1A	-4.26	112.98	123.63
14	B	4004	BCR	C38-C26-C25	-4.26	119.84	124.48
15	A	1102	CLA	O2A-CGA-CBA	4.26	124.81	111.83
14	B	4011	BCR	C33-C5-C6	-4.25	119.84	124.48
15	A	1116	CLA	O2A-CGA-CBA	4.25	124.79	111.83
14	F	4015	BCR	C7-C8-C9	-4.23	119.97	126.23
15	A	1120	CLA	O2A-CGA-CBA	4.22	124.71	111.83
14	B	4017	BCR	C7-C8-C9	-4.22	119.99	126.23
13	A	1011	CL0	CMA-C3A-C4A	-4.22	105.52	114.61
15	A	1109	CLA	O2A-CGA-CBA	4.21	124.67	111.83
15	B	1217	CLA	O2A-CGA-CBA	4.20	124.65	111.83
15	B	1236	CLA	CMC-C2C-C1C	4.20	131.60	125.03
14	A	4012	BCR	C33-C5-C6	-4.20	119.90	124.48
15	A	1130	CLA	O2A-CGA-CBA	4.20	124.63	111.83
15	A	1130	CLA	C4A-NA-C1A	4.18	108.59	106.68
15	A	1126	CLA	CHD-C1D-ND	-4.17	118.93	124.80
15	A	1134	CLA	O2D-CGD-CBD	4.17	118.52	111.23
13	A	1108	CL0	CHA-C1A-C2A	-4.16	123.53	133.31
14	B	4011	BCR	C38-C26-C25	-4.16	119.94	124.48
15	B	1204	CLA	O2A-CGA-O1A	-4.16	110.77	123.20
14	F	4015	BCR	C15-C14-C13	-4.15	121.45	127.28
15	A	1124	CLA	O2A-CGA-O1A	-4.14	113.26	123.63
13	A	1108	CL0	C1C-CHC-C4B	4.14	130.89	116.07
14	A	4003	BCR	C33-C5-C6	-4.14	119.97	124.48
15	B	1214	CLA	C4-C3-C5	4.13	122.39	115.23
15	A	1107	CLA	O2A-CGA-CBA	4.13	124.42	111.83
15	A	1135	CLA	O2A-CGA-CBA	4.13	124.41	111.83
15	B	1205	CLA	O2A-CGA-CBA	4.12	124.39	111.83
15	J	1303	CLA	O2A-CGA-O1A	-4.12	110.91	123.20
14	A	4002	BCR	C33-C5-C6	-4.12	119.99	124.48
14	B	4011	BCR	C7-C8-C9	-4.11	120.15	126.23
15	A	1115	CLA	O2A-CGA-O1A	-4.11	110.93	123.20
15	B	1202	CLA	O2A-CGA-CBA	4.11	124.35	111.83
15	A	1137	CLA	O2A-CGA-CBA	4.09	124.32	111.83
15	B	1201	CLA	O2A-CGA-O1A	-4.09	110.99	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1133	CLA	O2A-CGA-O1A	-4.09	110.99	123.20
14	F	4016	BCR	C33-C5-C6	-4.09	120.02	124.48
15	K	1401	CLA	O2A-CGA-O1A	-4.08	111.03	123.20
15	B	1211	CLA	O2A-CGA-O1A	-4.07	111.04	123.20
15	B	1207	CLA	O2A-CGA-O1A	-4.07	111.06	123.20
15	B	1013	CLA	O2A-C1-C2	4.07	123.76	108.11
15	A	1118	CLA	O2A-CGA-O1A	-4.06	111.07	123.20
15	B	1223	CLA	O2A-CGA-CBA	4.06	124.22	111.83
14	B	4010	BCR	C38-C26-C25	-4.06	120.06	124.48
15	B	1219	CLA	O2A-CGA-CBA	4.06	124.20	111.83
15	A	1128	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
13	A	1011	CL0	CHA-C1A-C2A	-4.05	123.80	133.31
12	A	5001	LHG	O7-C7-C8	4.05	120.23	111.48
15	A	1110	CLA	O2A-CGA-CBA	4.04	124.17	111.83
15	B	1226	CLA	O2A-CGA-CBA	4.04	124.15	111.83
14	B	4005	BCR	C33-C5-C6	-4.04	120.08	124.48
15	A	1129	CLA	O2A-CGA-O1A	-4.04	111.15	123.20
15	B	1215	CLA	O2A-CGA-CBA	4.04	124.14	111.83
15	A	1117	CLA	O2A-CGA-CBA	4.02	124.10	111.83
15	K	1402	CLA	O2A-CGA-O1A	-4.02	111.19	123.20
15	B	1236	CLA	O2A-CGA-CBA	4.02	124.09	111.83
15	A	1127	CLA	O2A-CGA-CBA	4.02	124.08	111.83
15	B	1234	CLA	O2A-CGA-CBA	4.02	124.08	111.83
15	A	1140	CLA	O2A-CGA-CBA	4.01	124.07	111.83
17	B	5002	LMG	O7-C10-C11	3.99	120.11	111.48
13	A	1011	CL0	O2A-CGA-CBA	3.99	124.00	111.83
15	B	1236	CLA	CHD-C1D-ND	-3.97	119.21	124.80
13	A	1108	CL0	CBC-CAC-C3C	-3.95	107.22	112.87
15	A	1109	CLA	CHD-C1D-ND	-3.94	119.26	124.80
10	B	2002	PQN	C14-C13-C15	3.94	122.06	115.23
14	A	4001	BCR	C24-C23-C22	-3.93	120.42	126.23
15	A	1124	CLA	C1-O2A-CGA	3.93	126.16	116.65
15	A	1114	CLA	O2A-CGA-CBA	3.93	123.80	111.83
15	A	1125	CLA	O2A-CGA-CBA	3.92	123.80	111.83
15	A	1012	CLA	O2A-C1-C2	3.91	123.15	108.11
15	A	1104	CLA	CHD-C1D-ND	-3.91	119.31	124.80
15	B	1215	CLA	O2A-C1-C2	3.91	123.14	108.11
15	B	1231	CLA	CHD-C1D-ND	-3.91	119.31	124.80
15	B	1220	CLA	O2A-CGA-CBA	3.90	123.72	111.83
12	A	5005	LHG	O7-C7-C8	3.90	119.91	111.48
14	A	4001	BCR	C38-C26-C25	-3.89	120.24	124.48
15	B	1228	CLA	O2A-CGA-CBA	3.89	123.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1023	CLA	O2A-CGA-CBA	3.89	123.69	111.83
15	B	1206	CLA	O2A-CGA-O1A	-3.87	111.66	123.20
15	A	1022	CLA	O2A-CGA-CBA	3.86	123.61	111.83
15	A	1134	CLA	O2A-CGA-O1A	-3.86	111.68	123.20
14	A	4007	BCR	C38-C26-C25	-3.86	120.28	124.48
15	B	1229	CLA	O2A-CGA-CBA	3.85	123.59	111.83
15	A	1130	CLA	CHD-C1D-ND	-3.84	119.40	124.80
15	A	1122	CLA	CHD-C1D-ND	-3.83	119.42	124.80
15	B	1214	CLA	CHD-C1D-ND	-3.83	119.42	124.80
14	A	4008	BCR	C7-C8-C9	-3.82	120.58	126.23
14	B	4006	BCR	C33-C5-C6	-3.82	120.32	124.48
15	B	1213	CLA	O2A-CGA-CBA	3.82	123.47	111.83
15	B	1227	CLA	CMB-C2B-C1B	3.81	131.22	125.42
13	A	1011	CL0	C1C-CHC-C4B	3.80	129.68	116.07
15	B	1208	CLA	CHD-C1D-ND	-3.80	119.46	124.80
15	A	1012	CLA	O2A-CGA-CBA	3.79	123.39	111.83
14	B	4005	BCR	C7-C8-C9	-3.78	120.64	126.23
15	B	1203	CLA	O2A-C1-C2	3.78	122.65	108.11
15	A	1123	CLA	O2A-CGA-CBA	3.77	123.34	111.83
15	A	1128	CLA	O2A-CGA-CBA	3.77	123.33	111.83
14	B	4004	BCR	C19-C18-C17	3.76	124.92	119.01
15	A	1106	CLA	O2A-CGA-CBA	3.76	123.30	111.83
15	A	1105	CLA	O2A-CGA-CBA	3.75	123.28	111.83
14	B	4005	BCR	C24-C23-C22	-3.74	120.70	126.23
15	F	1410	CLA	O2A-CGA-CBA	3.73	123.22	111.83
15	A	1126	CLA	C2B-C1B-NB	3.72	114.19	110.33
15	A	1138	CLA	O2A-CGA-CBA	3.72	123.18	111.83
15	F	1410	CLA	CHD-C1D-ND	-3.72	119.57	124.80
15	A	1107	CLA	CHD-C1D-ND	-3.72	119.57	124.80
15	B	1237	CLA	O2A-CGA-CBA	3.71	123.15	111.83
15	B	1213	CLA	CHD-C1D-ND	-3.70	119.59	124.80
15	B	1228	CLA	CHD-C1D-ND	-3.70	119.60	124.80
15	A	1106	CLA	C1-O2A-CGA	3.70	125.60	116.65
15	A	1117	CLA	CHD-C1D-ND	-3.69	119.61	124.80
15	A	1127	CLA	C4-C3-C5	3.68	121.62	115.23
15	B	1219	CLA	CHD-C1D-ND	-3.68	119.62	124.80
15	B	1216	CLA	CHD-C1D-ND	-3.68	119.63	124.80
15	A	1105	CLA	CHD-C1D-ND	-3.67	119.64	124.80
15	A	1124	CLA	C2B-C1B-NB	3.67	114.13	110.33
15	B	1238	CLA	CHD-C1D-ND	-3.67	119.64	124.80
15	B	1220	CLA	CHD-C1D-ND	-3.67	119.64	124.80
15	A	1126	CLA	O2A-CGA-CBA	3.66	123.01	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1108	CL0	C4D-ND-C1D	-3.66	102.44	105.22
15	A	1106	CLA	CHD-C1D-ND	-3.65	119.67	124.80
15	A	1104	CLA	C1-C2-C3	-3.65	120.22	126.20
15	A	1135	CLA	CHD-C1D-ND	-3.65	119.67	124.80
15	A	1138	CLA	C2B-C1B-NB	3.65	114.11	110.33
15	A	1129	CLA	CHD-C1D-ND	-3.64	119.68	124.80
15	A	1123	CLA	CAC-C3C-C4C	3.64	129.52	124.79
15	A	1110	CLA	CHD-C1D-ND	-3.63	119.69	124.80
15	B	1220	CLA	C1-O2A-CGA	3.63	125.44	116.65
15	B	1239	CLA	CHD-C1D-ND	-3.61	119.72	124.80
15	B	1220	CLA	O2A-C1-C2	3.61	121.99	108.11
15	B	1223	CLA	C1-C2-C3	-3.60	120.30	126.20
15	B	1237	CLA	CHD-C1D-ND	-3.60	119.74	124.80
13	A	1108	CL0	CMC-C2C-C1C	3.60	131.21	124.73
15	B	1206	CLA	CHD-C1D-ND	-3.60	119.74	124.80
15	F	1139	CLA	O2A-CGA-CBA	3.59	122.79	111.83
15	A	1135	CLA	O2A-C1-C2	3.59	121.93	108.11
15	A	1124	CLA	O2A-C1-C2	3.59	121.92	108.11
15	B	1212	CLA	CHD-C1D-ND	-3.59	119.76	124.80
15	B	1204	CLA	CHD-C1D-ND	-3.58	119.76	124.80
15	B	1232	CLA	CHD-C1D-ND	-3.58	119.77	124.80
15	A	1136	CLA	CHD-C1D-ND	-3.58	119.77	124.80
15	B	1218	CLA	O2A-C1-C2	3.57	121.86	108.11
15	A	1126	CLA	CMD-C2D-C3D	-3.57	119.51	127.69
15	A	1127	CLA	O2A-C1-C2	3.56	121.82	108.11
14	A	4008	BCR	C27-C26-C25	-3.56	117.89	122.70
15	A	1102	CLA	C2B-C1B-NB	3.56	114.02	110.33
15	B	1229	CLA	C1-C2-C3	-3.56	120.36	126.20
15	B	1214	CLA	C4-C3-C2	-3.56	114.48	123.63
15	B	1023	CLA	CHD-C1D-ND	-3.56	119.79	124.80
15	B	1229	CLA	CHD-C1D-ND	-3.56	119.79	124.80
15	B	1224	CLA	CHD-C1D-ND	-3.56	119.80	124.80
15	B	1230	CLA	CHD-C1D-ND	-3.56	119.80	124.80
15	B	1234	CLA	CHD-C1D-ND	-3.55	119.80	124.80
15	A	1121	CLA	O2A-CGA-CBA	3.55	125.56	112.14
15	B	1215	CLA	CHD-C1D-ND	-3.55	119.81	124.80
15	A	1140	CLA	CHD-C1D-ND	-3.55	119.81	124.80
15	A	1119	CLA	CHD-C1D-ND	-3.55	119.81	124.80
15	A	1105	CLA	O2A-C1-C2	3.55	121.75	108.11
15	A	1124	CLA	CHD-C1D-ND	-3.54	119.83	124.80
15	A	1125	CLA	OBD-CAD-C3D	-3.53	120.16	128.42
15	B	1214	CLA	C2B-C1B-NB	3.53	113.99	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1203	CLA	CHD-C1D-ND	-3.53	119.83	124.80
15	A	1102	CLA	CHD-C1D-ND	-3.53	119.84	124.80
15	A	1120	CLA	CHD-C1D-ND	-3.53	119.84	124.80
15	A	1114	CLA	CHD-C1D-ND	-3.53	119.84	124.80
15	A	1121	CLA	CHD-C1D-ND	-3.53	119.84	124.80
15	A	1130	CLA	C2B-C1B-NB	3.53	113.98	110.33
14	B	4017	BCR	C3-C4-C5	-3.52	107.77	114.06
15	K	1401	CLA	O2A-CGA-CBA	3.52	125.44	112.14
15	A	1022	CLA	CHD-C1D-ND	-3.52	119.85	124.80
15	A	1138	CLA	CMC-C2C-C1C	3.51	130.52	125.03
15	A	1118	CLA	CHD-C1D-ND	-3.51	119.86	124.80
15	F	1301	CLA	CHD-C1D-ND	-3.51	119.86	124.80
15	A	1134	CLA	CHD-C1D-ND	-3.50	119.88	124.80
15	B	1235	CLA	CHD-C1D-ND	-3.50	119.88	124.80
15	A	1106	CLA	C2B-C1B-NB	3.50	113.95	110.33
15	B	1210	CLA	C2B-C1B-NB	3.49	113.94	110.33
15	B	1227	CLA	CHD-C1D-ND	-3.48	119.90	124.80
15	B	1225	CLA	O2A-CGA-CBA	3.48	122.46	111.83
15	A	1113	CLA	CHD-C1D-ND	-3.48	119.90	124.80
15	B	1240	CLA	CHD-C1D-ND	-3.48	119.91	124.80
15	A	1110	CLA	O2A-C1-C2	3.48	121.49	108.11
15	B	1210	CLA	CHD-C1D-ND	-3.47	119.91	124.80
15	B	1237	CLA	C4-C3-C5	3.47	121.25	115.23
15	B	1202	CLA	CHD-C1D-ND	-3.47	119.92	124.80
15	A	1116	CLA	CHD-C1D-ND	-3.47	119.92	124.80
15	B	1217	CLA	CHD-C1D-ND	-3.47	119.92	124.80
15	K	1402	CLA	CHD-C1D-ND	-3.47	119.92	124.80
15	B	1216	CLA	O2A-CGA-CBA	3.47	122.40	111.83
15	B	1013	CLA	CHD-C1D-ND	-3.46	119.93	124.80
15	A	1110	CLA	C1-C2-C3	-3.46	120.53	126.20
15	B	1218	CLA	CHD-C1D-ND	-3.46	119.93	124.80
15	A	1101	CLA	O2A-CGA-CBA	3.46	122.37	111.83
15	B	1231	CLA	O2A-C1-C2	3.46	121.41	108.11
15	A	1138	CLA	CHD-C1D-ND	-3.46	119.94	124.80
15	B	1234	CLA	O2A-C1-C2	3.45	121.40	108.11
15	B	1203	CLA	O2A-CGA-CBA	3.45	122.35	111.83
15	B	1239	CLA	O2A-CGA-CBA	3.45	125.16	112.14
15	A	1109	CLA	O2A-C1-C2	3.45	121.37	108.11
15	B	1207	CLA	CHD-C1D-ND	-3.45	119.95	124.80
15	B	1223	CLA	CHD-C1D-ND	-3.44	119.95	124.80
13	A	1108	CL0	O2A-CGA-CBA	3.44	124.86	114.00
15	B	1013	CLA	C2B-C1B-NB	3.43	113.89	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	1139	CLA	CHD-C1D-ND	-3.43	119.98	124.80
14	A	4001	BCR	C19-C18-C17	3.42	124.39	119.01
15	A	1104	CLA	CMC-C2C-C1C	3.42	130.38	125.03
15	A	1111	CLA	CHD-C1D-ND	-3.42	119.99	124.80
15	A	1117	CLA	O2A-C1-C2	3.41	121.24	108.11
15	A	1012	CLA	C1-O2A-CGA	3.41	124.91	116.65
15	B	1209	CLA	O2A-CGA-CBA	3.41	124.77	114.00
15	A	1112	CLA	CHD-C1D-ND	-3.41	120.01	124.80
15	B	1222	CLA	C2B-C1B-NB	3.41	113.86	110.33
14	B	4006	BCR	C34-C9-C10	-3.41	117.30	122.82
15	A	1133	CLA	CHD-C1D-ND	-3.40	120.01	124.80
12	B	5004	LHG	C5-O7-C7	-3.40	109.66	117.80
14	A	4012	BCR	C37-C22-C21	-3.40	117.31	122.82
15	A	1125	CLA	CHD-C1D-ND	-3.39	120.03	124.80
15	B	1222	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	A	4003	BCR	C34-C9-C10	-3.39	117.32	122.82
15	B	1213	CLA	O2A-C1-C2	3.39	121.16	108.11
15	B	1226	CLA	O2A-C1-C2	3.38	121.13	108.11
14	F	4015	BCR	C38-C26-C25	-3.38	120.80	124.48
14	B	4005	BCR	C38-C26-C25	-3.38	120.80	124.48
15	A	1131	CLA	CHD-C1D-ND	-3.38	120.05	124.80
15	B	1219	CLA	O2A-C1-C2	3.38	121.10	108.11
15	A	1103	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	J	4013	BCR	C30-C25-C26	-3.37	118.03	122.64
14	B	4009	BCR	C19-C18-C17	3.37	124.31	119.01
14	A	4002	BCR	C38-C26-C25	-3.37	120.81	124.48
15	B	1219	CLA	C2B-C1B-NB	3.37	113.82	110.33
15	A	1132	CLA	CHD-C1D-ND	-3.36	120.08	124.80
15	B	1201	CLA	CHD-C1D-ND	-3.36	120.08	124.80
15	A	1138	CLA	CED-O2D-CGD	3.35	123.53	115.92
14	B	4005	BCR	C19-C18-C17	3.35	124.28	119.01
15	B	1222	CLA	C1-O2A-CGA	3.35	124.76	116.65
14	A	4008	BCR	C38-C26-C27	3.35	120.73	113.60
15	A	1106	CLA	O2A-C1-C2	3.34	120.97	108.11
15	A	1104	CLA	C2B-C1B-NB	3.34	113.79	110.33
15	J	1302	CLA	CHD-C1D-ND	-3.34	120.11	124.80
14	F	4016	BCR	C12-C13-C14	3.34	124.26	119.01
14	B	4009	BCR	C38-C26-C25	-3.33	120.85	124.48
15	B	1236	CLA	C2B-C1B-NB	3.33	113.78	110.33
15	A	1801	CLA	CHD-C1D-ND	-3.33	120.11	124.80
15	B	1209	CLA	CHD-C1D-ND	-3.33	120.11	124.80
15	B	1226	CLA	CHD-C1D-ND	-3.33	120.12	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1122	CLA	O2A-CGA-CBA	3.32	121.97	111.83
14	F	4016	BCR	C3-C4-C5	-3.32	108.14	114.06
15	A	1125	CLA	CMC-C2C-C1C	3.31	130.21	125.03
15	B	1211	CLA	CMC-C2C-C1C	3.31	130.21	125.03
15	B	1206	CLA	C2B-C1B-NB	3.31	113.76	110.33
15	A	1135	CLA	C4-C3-C5	3.31	120.97	115.23
15	A	1132	CLA	C1-C2-C3	-3.31	120.78	126.20
15	B	1211	CLA	CHD-C1D-ND	-3.31	120.15	124.80
15	K	1401	CLA	CHD-C1D-ND	-3.31	120.15	124.80
14	B	4010	BCR	C24-C23-C22	-3.31	121.34	126.23
15	A	1107	CLA	C3D-C4D-ND	3.30	115.36	109.99
13	A	1011	CL0	O2A-C1-C2	3.30	120.82	108.11
15	A	1122	CLA	C4-C3-C2	-3.30	115.15	123.63
15	A	1137	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	B	4017	BCR	C19-C18-C17	3.30	124.20	119.01
15	J	1303	CLA	CHD-C1D-ND	-3.30	120.16	124.80
15	B	1232	CLA	O2A-CGA-CBA	3.30	124.42	114.00
14	A	4007	BCR	C33-C5-C6	-3.30	120.89	124.48
14	A	4012	BCR	C7-C8-C9	-3.29	121.36	126.23
15	J	1303	CLA	O2A-CGA-CBA	3.29	124.58	112.14
15	A	1122	CLA	C3D-C4D-ND	3.29	115.33	109.99
15	A	1115	CLA	O2A-CGA-CBA	3.29	124.56	112.14
15	A	1109	CLA	C3D-C4D-ND	3.29	115.33	109.99
15	B	1239	CLA	CMB-C2B-C1B	3.28	130.42	125.42
15	A	1131	CLA	O2A-C1-C2	3.28	120.74	108.11
15	A	1115	CLA	CHD-C1D-ND	-3.28	120.19	124.80
14	B	4014	BCR	C37-C22-C21	-3.28	117.51	122.82
15	B	1223	CLA	O2A-C1-C2	3.26	120.67	108.11
14	B	4011	BCR	C37-C22-C21	-3.26	117.53	122.82
15	B	1235	CLA	CMC-C2C-C1C	3.26	130.13	125.03
15	F	1301	CLA	C2B-C1B-NB	3.26	113.70	110.33
15	A	1123	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
15	A	1022	CLA	OBD-CAD-C3D	-3.25	120.81	128.42
15	B	1204	CLA	O2A-CGA-CBA	3.25	124.42	112.14
15	A	1105	CLA	CMB-C2B-C1B	3.25	130.37	125.42
14	A	4002	BCR	C19-C18-C17	3.25	124.12	119.01
15	A	1117	CLA	C2B-C1B-NB	3.25	113.69	110.33
14	A	4001	BCR	C36-C18-C17	-3.24	117.56	122.82
14	B	4006	BCR	C7-C8-C9	-3.24	121.44	126.23
15	A	1116	CLA	CMB-C2B-C1B	3.24	130.36	125.42
15	A	1136	CLA	C3D-C4D-ND	3.24	115.25	109.99
15	B	1013	CLA	C3D-C4D-ND	3.24	115.25	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1203	CLA	CMB-C2B-C1B	3.24	130.35	125.42
15	A	1107	CLA	C2B-C1B-NB	3.23	113.68	110.33
15	A	1111	CLA	O2A-C1-C2	3.23	120.54	108.11
15	A	1113	CLA	O2A-CGA-CBA	3.23	124.20	114.00
15	B	1240	CLA	O2A-CGA-CBA	3.22	124.18	114.00
12	A	5003	LHG	C5-O7-C7	-3.22	110.09	117.80
15	B	1213	CLA	C3D-C4D-ND	3.22	115.22	109.99
15	A	1134	CLA	O2A-CGA-CBA	3.22	124.30	112.14
14	A	4007	BCR	C24-C23-C22	-3.22	121.47	126.23
15	B	1021	CLA	CMA-C3A-C4A	-3.21	103.13	111.77
15	B	1226	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
15	B	1222	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
14	B	4004	BCR	C36-C18-C17	-3.21	117.62	122.82
15	B	1228	CLA	C3D-C4D-ND	3.21	115.20	109.99
15	K	1402	CLA	O2A-CGA-CBA	3.21	124.26	112.14
15	A	1132	CLA	CMB-C2B-C1B	3.21	130.30	125.42
15	B	1220	CLA	C2B-C1B-NB	3.20	113.65	110.33
15	B	1215	CLA	C1-O2A-CGA	3.19	124.38	116.65
15	A	1126	CLA	C4D-C3D-CAD	3.19	111.57	108.11
15	B	1023	CLA	C3D-C4D-ND	3.19	115.17	109.99
15	A	1123	CLA	CHD-C1D-ND	-3.19	120.32	124.80
14	A	4002	BCR	C38-C26-C27	3.18	120.38	113.60
15	A	1127	CLA	C3D-C4D-ND	3.18	115.16	109.99
15	A	1110	CLA	C2B-C1B-NB	3.18	113.62	110.33
15	A	1103	CLA	C4D-C3D-CAD	3.18	111.56	108.11
15	B	1212	CLA	O2A-CGA-CBA	3.18	124.04	114.00
15	B	1204	CLA	C3D-C4D-ND	3.18	115.15	109.99
15	A	1119	CLA	C2B-C1B-NB	3.17	113.62	110.33
15	J	1302	CLA	O2A-CGA-CBA	3.17	124.02	114.00
15	A	1122	CLA	C2B-C1B-NB	3.17	113.62	110.33
15	F	1139	CLA	C4D-C3D-CAD	3.17	111.55	108.11
14	B	4011	BCR	C8-C9-C10	3.17	124.00	119.01
15	A	1125	CLA	C4D-C3D-CAD	3.17	111.55	108.11
15	B	1229	CLA	CMB-C2B-C1B	3.17	130.24	125.42
15	A	1112	CLA	C2B-C1B-NB	3.16	113.61	110.33
15	A	1115	CLA	C3D-C4D-ND	3.16	115.13	109.99
15	B	1220	CLA	C3D-C4D-ND	3.16	115.13	109.99
15	B	1216	CLA	C3D-C4D-ND	3.16	115.13	109.99
14	B	4009	BCR	C34-C9-C10	-3.16	117.69	122.82
15	A	1101	CLA	C2B-C1B-NB	3.16	113.60	110.33
15	A	1103	CLA	O2A-C1-C2	3.16	120.26	108.11
15	F	1301	CLA	O2A-CGA-CBA	3.16	123.97	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1208	CLA	C3D-C4D-ND	3.15	115.11	109.99
15	B	1217	CLA	O2A-C1-C2	3.15	119.70	108.40
15	A	1125	CLA	O2A-C1-C2	3.15	120.22	108.11
14	A	4002	BCR	C7-C8-C9	-3.15	121.58	126.23
14	B	4011	BCR	C23-C22-C21	3.15	123.96	119.01
15	B	1208	CLA	O2A-CGA-CBA	3.14	123.93	114.00
14	A	4008	BCR	C30-C25-C26	-3.14	118.34	122.64
15	A	1111	CLA	C2B-C1B-NB	3.14	113.58	110.33
15	B	1205	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	B	1021	CLA	CHD-C1D-ND	-3.14	120.39	124.80
15	B	1211	CLA	O2A-CGA-CBA	3.14	123.99	112.14
15	F	1410	CLA	CMC-C2C-C1C	3.14	129.94	125.03
15	A	1128	CLA	CHD-C1D-ND	-3.14	120.39	124.80
15	A	1127	CLA	CHD-C1D-ND	-3.13	120.39	124.80
15	A	1109	CLA	C2B-C1B-NB	3.13	113.57	110.33
15	A	1114	CLA	C3D-C4D-ND	3.13	115.08	109.99
15	J	1303	CLA	CMB-C2B-C1B	3.13	130.19	125.42
15	A	1129	CLA	O2A-CGA-CBA	3.13	123.96	112.14
15	A	1116	CLA	C3D-C4D-ND	3.13	115.07	109.99
15	A	1109	CLA	C1-O2A-CGA	3.13	124.22	116.65
14	A	4007	BCR	C38-C26-C27	3.13	120.26	113.60
15	A	1103	CLA	O2A-CGA-CBA	3.13	121.36	111.83
15	B	1230	CLA	O2A-C1-C2	3.13	120.14	108.11
15	A	1118	CLA	O2A-CGA-CBA	3.12	123.94	112.14
15	B	1240	CLA	C2B-C1B-NB	3.12	113.56	110.33
15	A	1128	CLA	O2A-C1-C2	3.12	120.12	108.11
15	A	1118	CLA	C3D-C4D-ND	3.12	115.06	109.99
14	B	4009	BCR	C3-C4-C5	-3.12	108.50	114.06
14	A	4001	BCR	C37-C22-C21	-3.12	117.77	122.82
15	B	1201	CLA	C2B-C1B-NB	3.11	113.55	110.33
15	K	1402	CLA	C3D-C4D-ND	3.11	115.04	109.99
15	B	1201	CLA	O2A-CGA-CBA	3.11	123.89	112.14
15	A	1107	CLA	CAA-C2A-C1A	-3.11	101.78	111.97
15	B	1225	CLA	CMC-C2C-C1C	3.11	129.89	125.03
15	A	1801	CLA	C4D-C3D-CAD	3.11	111.48	108.11
15	B	1236	CLA	O2A-C1-C2	3.10	120.06	108.11
15	B	1230	CLA	C3D-C4D-ND	3.10	115.03	109.99
15	B	1023	CLA	O2A-C1-C2	3.10	120.04	108.11
15	B	1230	CLA	CMC-C2C-C1C	3.10	129.88	125.03
15	A	1140	CLA	C3D-C4D-ND	3.10	115.03	109.99
15	B	1216	CLA	C1-O2A-CGA	3.10	124.15	116.65
15	A	1131	CLA	C3D-C4D-ND	3.10	115.02	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1202	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	A	1104	CLA	C3D-C4D-ND	3.09	115.02	109.99
15	A	1101	CLA	CHD-C1D-ND	-3.09	120.45	124.80
15	B	1237	CLA	CMC-C2C-C1C	3.09	129.87	125.03
15	B	1225	CLA	CHD-C1D-ND	-3.09	120.45	124.80
15	A	1126	CLA	C3D-C4D-ND	3.09	115.01	109.99
15	B	1208	CLA	C2B-C1B-NB	3.09	113.53	110.33
15	A	1125	CLA	C2B-C1B-NB	3.09	113.53	110.33
15	A	1132	CLA	C3D-C4D-ND	3.09	115.00	109.99
15	A	1112	CLA	O2A-CGA-CBA	3.09	123.75	114.00
15	A	1120	CLA	C4D-C3D-CAD	3.08	111.45	108.11
15	F	1410	CLA	C4-C3-C2	-3.08	115.71	123.63
15	A	1130	CLA	O2A-C1-C2	3.08	119.97	108.11
15	A	1138	CLA	C1-C2-C3	-3.08	121.15	126.20
14	B	4011	BCR	C33-C5-C4	3.08	120.16	113.60
15	B	1221	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	J	4013	BCR	C38-C26-C25	-3.08	121.13	124.48
14	B	4014	BCR	C23-C22-C21	3.07	123.84	119.01
15	A	1103	CLA	C3D-C4D-ND	3.07	114.98	109.99
15	F	1410	CLA	C2B-C1B-NB	3.07	113.51	110.33
15	A	1128	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
15	A	1105	CLA	C3D-C4D-ND	3.07	114.98	109.99
14	A	4001	BCR	C3-C4-C5	-3.07	108.58	114.06
15	B	1227	CLA	O2A-CGA-CBA	3.07	123.69	114.00
15	B	1206	CLA	C4D-C3D-CAD	3.07	111.44	108.11
15	B	1228	CLA	C2B-C1B-NB	3.07	113.51	110.33
15	B	1021	CLA	C4D-C3D-CAD	3.07	111.44	108.11
14	A	4003	BCR	C37-C22-C21	-3.07	117.85	122.82
15	A	1110	CLA	C3D-C4D-ND	3.06	114.97	109.99
15	A	1022	CLA	O2A-C1-C2	3.06	119.90	108.11
15	B	1235	CLA	C3D-C4D-ND	3.06	114.96	109.99
15	A	1133	CLA	O2A-CGA-CBA	3.06	123.69	112.14
15	B	1236	CLA	C3D-C4D-ND	3.05	114.95	109.99
15	B	1213	CLA	CMC-C2C-C1C	3.05	129.80	125.03
15	A	1022	CLA	C2B-C1B-NB	3.05	113.49	110.33
15	B	1219	CLA	C3D-C4D-ND	3.05	114.94	109.99
15	A	1122	CLA	CMD-C2D-C3D	-3.05	120.70	127.69
15	A	1122	CLA	CMC-C2C-C1C	3.05	129.79	125.03
14	A	4007	BCR	C3-C4-C5	-3.05	108.62	114.06
15	B	1023	CLA	CMB-C2B-C1B	3.05	130.06	125.42
15	A	1111	CLA	C3D-C4D-ND	3.05	114.94	109.99
15	A	1121	CLA	C3D-C4D-ND	3.04	114.94	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1126	CLA	O2A-C1-C2	3.04	119.82	108.11
15	A	1012	CLA	CHD-C1D-ND	-3.04	120.52	124.80
15	B	1021	CLA	O2A-C1-C2	3.04	119.82	108.11
15	A	1101	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	B	1211	CLA	C3D-C4D-ND	3.04	114.93	109.99
15	A	1127	CLA	C4D-C3D-CAD	3.04	111.41	108.11
15	B	1207	CLA	O2A-CGA-CBA	3.04	123.62	112.14
15	A	1112	CLA	C3D-C4D-ND	3.04	114.93	109.99
15	A	1135	CLA	C3D-C4D-ND	3.04	114.93	109.99
15	A	1125	CLA	C3C-C4C-NC	3.04	114.32	110.43
15	B	1224	CLA	C2B-C1B-NB	3.04	113.47	110.33
15	A	1106	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	A	1123	CLA	C4D-C3D-CAD	3.04	111.40	108.11
15	A	1104	CLA	O2A-C1-C2	3.03	119.79	108.11
15	A	1022	CLA	C3D-C4D-ND	3.03	114.92	109.99
15	B	1210	CLA	O2A-C1-C2	3.03	119.78	108.11
15	A	1117	CLA	C1-O2A-CGA	3.03	123.99	116.65
15	F	1139	CLA	CMC-C2C-C1C	3.03	129.77	125.03
15	A	1105	CLA	C2B-C1B-NB	3.03	113.47	110.33
15	A	1137	CLA	O2A-C1-C2	3.03	119.76	108.11
15	A	1101	CLA	C4D-C3D-CAD	3.03	111.39	108.11
15	B	1227	CLA	C2B-C1B-NB	3.03	113.47	110.33
15	A	1102	CLA	O2A-C1-C2	3.03	119.75	108.11
15	A	1109	CLA	CMC-C2C-C1C	3.03	129.76	125.03
15	A	1119	CLA	C3D-C4D-ND	3.03	114.90	109.99
15	A	1125	CLA	C1-O2A-CGA	3.02	123.97	116.65
14	A	4001	BCR	C30-C25-C26	-3.02	118.50	122.64
15	A	1125	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	A	4012	BCR	C36-C18-C17	-3.02	117.92	122.82
15	A	1132	CLA	O2A-C1-C2	3.02	119.74	108.11
14	B	4004	BCR	C7-C8-C9	-3.02	121.77	126.23
15	F	1410	CLA	O2A-C1-C2	3.02	119.73	108.11
15	B	1237	CLA	C3D-C4D-ND	3.02	114.90	109.99
14	B	4005	BCR	C36-C18-C17	-3.02	117.92	122.82
15	B	1234	CLA	C3D-C4D-ND	3.02	114.89	109.99
15	B	1202	CLA	C3D-C4D-ND	3.02	114.89	109.99
15	B	1214	CLA	C3D-C4D-ND	3.01	114.89	109.99
15	B	1218	CLA	C4D-C3D-CAD	3.01	111.38	108.11
15	B	1238	CLA	C3D-C4D-ND	3.01	114.88	109.99
15	J	1303	CLA	C4D-C3D-CAD	3.01	111.37	108.11
15	A	1138	CLA	C3D-C4D-ND	3.00	114.87	109.99
15	F	1301	CLA	CMC-C2C-C1C	3.00	129.73	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1801	CLA	C2B-C1B-NB	3.00	113.44	110.33
15	A	1117	CLA	C3D-C4D-ND	3.00	114.87	109.99
15	K	1402	CLA	CMB-C2B-C1B	3.00	129.99	125.42
15	B	1218	CLA	C3D-C4D-ND	3.00	114.86	109.99
15	A	1121	CLA	CMB-C2B-C1B	3.00	129.99	125.42
15	A	1137	CLA	C3D-C4D-ND	3.00	114.86	109.99
15	B	1239	CLA	C4D-C3D-CAD	3.00	111.36	108.11
15	A	1113	CLA	C3D-C4D-ND	3.00	114.86	109.99
15	K	1401	CLA	C2B-C1B-NB	3.00	113.44	110.33
15	B	1217	CLA	C2B-C1B-NB	3.00	113.43	110.33
15	B	1231	CLA	C2B-C1B-NB	3.00	113.43	110.33
15	B	1207	CLA	C3D-C4D-ND	3.00	114.86	109.99
14	J	4013	BCR	C15-C14-C13	-2.99	123.08	127.28
15	A	1129	CLA	C4D-C3D-CAD	2.99	111.36	108.11
15	A	1130	CLA	C3D-C4D-ND	2.99	114.85	109.99
15	F	1139	CLA	C3D-C4D-ND	2.99	114.85	109.99
15	A	1106	CLA	CMC-C2C-C1C	2.99	129.71	125.03
15	B	1206	CLA	O2A-CGA-CBA	2.99	123.42	112.14
14	B	4010	BCR	C3-C4-C5	-2.99	108.73	114.06
15	A	1106	CLA	C3D-C4D-ND	2.99	114.84	109.99
15	A	1133	CLA	C3D-C4D-ND	2.99	114.84	109.99
15	B	1216	CLA	C2B-C1B-NB	2.99	113.42	110.33
14	F	4016	BCR	C35-C13-C14	-2.98	117.98	122.82
15	B	1237	CLA	C4D-C3D-CAD	2.98	111.35	108.11
15	B	1223	CLA	CMC-C2C-C1C	2.98	129.70	125.03
15	B	1237	CLA	C4-C3-C2	-2.98	115.98	123.63
15	B	1201	CLA	CMC-C2C-C1C	2.97	129.68	125.03
15	K	1401	CLA	C3D-C4D-ND	2.97	114.81	109.99
15	A	1121	CLA	C4D-C3D-CAD	2.97	111.33	108.11
14	A	4002	BCR	C34-C9-C8	2.96	122.61	118.09
15	B	1223	CLA	C2B-C1B-NB	2.96	113.40	110.33
14	B	4009	BCR	C36-C18-C17	-2.96	118.02	122.82
15	B	1230	CLA	C4-C3-C2	-2.96	116.03	123.63
15	A	1116	CLA	C4D-C3D-CAD	2.96	111.32	108.11
15	A	1107	CLA	C4D-C3D-CAD	2.95	111.31	108.11
15	A	1134	CLA	C3D-C4D-ND	2.95	114.79	109.99
15	J	1303	CLA	C3D-C4D-ND	2.95	114.78	109.99
13	A	1011	CL0	O2D-CGD-O1D	-2.95	118.10	123.85
15	B	1213	CLA	C2B-C1B-NB	2.95	113.39	110.33
15	A	1012	CLA	C2B-C1B-NB	2.95	113.39	110.33
15	B	1222	CLA	O2A-CGA-CBA	2.95	120.83	111.83
15	A	1105	CLA	CMC-C2C-C1C	2.95	129.64	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	1302	CLA	C3D-C4D-ND	2.95	114.78	109.99
15	A	1136	CLA	C1-O2A-CGA	2.95	123.79	116.65
15	A	1122	CLA	C4D-C3D-CAD	2.95	111.31	108.11
15	B	1217	CLA	CMC-C2C-C1C	2.95	129.64	125.03
14	B	4009	BCR	C38-C26-C27	2.95	119.88	113.60
15	A	1022	CLA	CMC-C2C-C1C	2.94	129.63	125.03
15	B	1202	CLA	C2B-C1B-NB	2.94	113.38	110.33
15	A	1112	CLA	CMC-C2C-C1C	2.94	129.63	125.03
15	A	1136	CLA	CMB-C2B-C1B	2.94	129.90	125.42
15	F	1410	CLA	C3D-C4D-ND	2.94	114.76	109.99
15	A	1124	CLA	O2A-CGA-CBA	2.94	120.79	111.83
15	J	1302	CLA	C4D-C3D-CAD	2.94	111.29	108.11
15	B	1206	CLA	C3D-C4D-ND	2.93	114.75	109.99
15	B	1209	CLA	C4D-C3D-CAD	2.93	111.29	108.11
15	B	1212	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	A	4012	BCR	C19-C18-C17	2.93	123.62	119.01
10	A	2001	PQN	C14-C13-C15	2.93	120.31	115.23
15	A	1129	CLA	CMD-C2D-C3D	-2.93	120.98	127.69
15	A	1126	CLA	CMC-C2C-C1C	2.93	129.61	125.03
15	B	1237	CLA	C2B-C1B-NB	2.92	113.36	110.33
15	B	1229	CLA	C3D-C4D-ND	2.92	114.74	109.99
15	A	1120	CLA	C2B-C1B-NB	2.92	113.36	110.33
14	B	4004	BCR	C37-C22-C21	-2.92	118.08	122.82
15	B	1231	CLA	C3D-C4D-ND	2.92	114.73	109.99
15	B	1210	CLA	CAC-C3C-C4C	2.92	128.59	124.79
15	B	1202	CLA	C1-C2-C3	-2.92	121.42	126.20
15	B	1227	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	1205	CLA	C4D-C3D-CAD	2.92	111.27	108.11
15	B	1225	CLA	C2B-C1B-NB	2.92	113.35	110.33
15	B	1224	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
15	B	1229	CLA	O2A-C1-C2	2.91	119.32	108.11
15	A	1128	CLA	C4D-C3D-CAD	2.91	111.27	108.11
15	B	1224	CLA	O2A-C1-C2	2.91	119.31	108.11
15	B	1205	CLA	C3D-C4D-ND	2.91	114.72	109.99
15	B	1222	CLA	CMB-C2B-C1B	2.91	129.85	125.42
15	K	1401	CLA	C4D-C3D-CAD	2.91	111.26	108.11
14	B	4006	BCR	C34-C9-C8	2.91	122.53	118.09
15	B	1232	CLA	C3D-C4D-ND	2.90	114.71	109.99
15	B	1238	CLA	C2B-C1B-NB	2.90	113.34	110.33
15	A	1012	CLA	C3C-C4C-NC	2.90	114.15	110.43
15	B	1203	CLA	C3D-C4D-ND	2.90	114.71	109.99
15	A	1109	CLA	C4D-C3D-CAD	2.90	111.26	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1107	CLA	CMD-C2D-C3D	-2.90	121.04	127.69
15	B	1239	CLA	C3D-C4D-ND	2.90	114.70	109.99
14	A	4001	BCR	C34-C9-C10	-2.90	118.12	122.82
15	B	1209	CLA	C3D-C4D-ND	2.90	114.69	109.99
15	B	1201	CLA	C3D-C4D-ND	2.90	114.69	109.99
15	B	1215	CLA	C1-C2-C3	-2.90	121.45	126.20
15	B	1212	CLA	C2B-C1B-NB	2.90	113.33	110.33
15	A	1129	CLA	C3D-C4D-ND	2.89	114.69	109.99
15	A	1116	CLA	O2A-C1-C2	2.89	119.25	108.11
15	A	1012	CLA	C4-C3-C5	2.89	120.25	115.23
15	K	1401	CLA	CMB-C2B-C1B	2.89	129.82	125.42
15	B	1231	CLA	C4-C3-C5	2.89	120.25	115.23
15	B	1214	CLA	CMC-C2C-C1C	2.89	129.55	125.03
15	B	1023	CLA	C2B-C1B-NB	2.89	113.32	110.33
15	B	1215	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	B	4017	BCR	C34-C9-C10	-2.89	118.14	122.82
13	A	1011	CL0	C4D-ND-C1D	-2.89	103.03	105.22
15	B	1240	CLA	C3D-C4D-ND	2.89	114.68	109.99
15	A	1130	CLA	CMC-C2C-C1C	2.89	129.54	125.03
14	F	4016	BCR	C8-C7-C6	-2.88	119.29	127.00
14	A	4002	BCR	C27-C26-C25	-2.88	118.81	122.70
15	B	1209	CLA	C2B-C1B-NB	2.88	113.32	110.33
15	A	1101	CLA	O2A-C1-C2	2.88	119.20	108.11
15	A	1105	CLA	CBB-CAB-C3B	-2.88	113.12	127.53
15	B	1219	CLA	CMC-C2C-C1C	2.88	129.53	125.03
15	B	1227	CLA	C3D-C4D-ND	2.88	114.67	109.99
15	B	1217	CLA	C3D-C4D-ND	2.88	114.67	109.99
15	B	1021	CLA	C3D-C4D-ND	2.88	114.67	109.99
15	A	1101	CLA	C3D-C4D-ND	2.88	114.66	109.99
15	B	1205	CLA	C1-C2-C3	-2.88	121.49	126.20
15	B	1219	CLA	C4-C3-C5	2.87	120.22	115.23
15	B	1220	CLA	CMC-C2C-C1C	2.87	129.53	125.03
15	A	1134	CLA	C4D-C3D-CAD	2.87	111.23	108.11
15	B	1224	CLA	C3D-C4D-ND	2.87	114.66	109.99
15	B	1210	CLA	C3D-C4D-ND	2.87	114.66	109.99
15	B	1229	CLA	CMC-C2C-C1C	2.87	129.52	125.03
15	B	1215	CLA	C2B-C1B-NB	2.87	113.30	110.33
15	B	1211	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	B	4011	BCR	C28-C27-C26	-2.87	108.94	114.06
14	J	4013	BCR	C4-C5-C6	-2.87	118.83	122.70
15	A	1107	CLA	C1-C2-C3	-2.87	122.13	126.76
15	B	1221	CLA	CHD-C1D-ND	-2.86	120.77	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4005	BCR	C37-C22-C21	-2.86	118.18	122.82
15	A	1128	CLA	C3D-C4D-ND	2.86	114.64	109.99
15	A	1102	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	B	1204	CLA	C4D-C3D-CAD	2.86	111.21	108.11
15	B	1210	CLA	CMC-C2C-C1C	2.86	129.50	125.03
15	A	1801	CLA	O2A-C1-C2	2.86	119.10	108.11
15	A	1134	CLA	C2B-C1B-NB	2.86	113.29	110.33
14	B	4006	BCR	C3-C4-C5	-2.86	108.96	114.06
15	F	1301	CLA	C3D-C4D-ND	2.86	114.63	109.99
15	A	1123	CLA	C3D-C4D-ND	2.85	114.62	109.99
15	B	1203	CLA	C2B-C1B-NB	2.85	113.28	110.33
15	B	1205	CLA	CHD-C1D-ND	-2.85	120.79	124.80
15	A	1118	CLA	CMB-C2B-C1B	2.85	129.76	125.42
15	A	1106	CLA	CMB-C2B-C1B	2.85	129.76	125.42
14	J	4013	BCR	C33-C5-C4	2.85	119.67	113.60
14	J	4013	BCR	C38-C26-C27	2.85	119.66	113.60
15	A	1137	CLA	C4D-C3D-CAD	2.85	111.20	108.11
15	A	1101	CLA	CMC-C2C-C1C	2.85	129.48	125.03
15	B	1238	CLA	CMC-C2C-C1C	2.84	129.48	125.03
15	A	1124	CLA	C3D-C4D-ND	2.84	114.61	109.99
14	A	4008	BCR	C38-C26-C25	-2.84	121.38	124.48
14	B	4017	BCR	C36-C18-C17	-2.84	118.21	122.82
15	A	1138	CLA	O2A-C1-C2	2.84	119.04	108.11
15	B	1225	CLA	O2A-C1-C2	2.84	119.04	108.11
15	B	1226	CLA	C3D-C4D-ND	2.84	114.60	109.99
15	A	1120	CLA	C3D-C4D-ND	2.83	114.59	109.99
15	B	1237	CLA	CMD-C2D-C3D	-2.83	121.19	127.69
14	F	4016	BCR	C23-C24-C25	-2.83	119.43	127.00
15	A	1121	CLA	CMC-C2C-C1C	2.83	129.46	125.03
15	A	1131	CLA	CMC-C2C-C1C	2.83	129.46	125.03
15	B	1225	CLA	C3D-C4D-ND	2.83	114.59	109.99
15	A	1140	CLA	C2B-C1B-NB	2.83	113.26	110.33
15	A	1132	CLA	C4-C3-C5	2.83	120.14	115.23
15	B	1206	CLA	CMC-C2C-C1C	2.83	129.45	125.03
15	A	1111	CLA	CAC-C3C-C4C	2.83	128.47	124.79
15	B	1201	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
15	J	1302	CLA	CMC-C2C-C1C	2.83	129.45	125.03
15	A	1113	CLA	C2B-C1B-NB	2.82	113.25	110.33
15	B	1218	CLA	C2B-C1B-NB	2.82	113.25	110.33
14	A	4003	BCR	C33-C5-C4	2.82	119.61	113.60
15	A	1124	CLA	C4D-C3D-CAD	2.82	111.17	108.11
15	B	1224	CLA	C4D-C3D-CAD	2.82	111.17	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1205	CLA	O2A-C1-C2	2.82	118.94	108.11
14	B	4010	BCR	C34-C9-C8	2.81	122.39	118.09
15	B	1203	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	K	1402	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	A	1102	CLA	C3D-C4D-ND	2.81	114.55	109.99
15	A	1136	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	B	1202	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	B	1230	CLA	C4D-C3D-CAD	2.81	111.16	108.11
15	B	1021	CLA	CMC-C2C-C1C	2.81	129.42	125.03
15	A	1112	CLA	C4D-C3D-CAD	2.81	111.15	108.11
15	A	1140	CLA	C4D-C3D-CAD	2.81	111.15	108.11
15	B	1205	CLA	CMB-C2B-C1B	2.81	129.69	125.42
15	B	1223	CLA	C3C-C4C-NC	2.80	114.02	110.43
15	B	1204	CLA	C2B-C1B-NB	2.80	113.23	110.33
15	A	1116	CLA	C2B-C1B-NB	2.80	113.23	110.33
14	A	4002	BCR	C36-C18-C17	-2.80	118.28	122.82
15	F	1139	CLA	CMB-C2B-C1B	2.80	129.68	125.42
14	F	4015	BCR	C38-C26-C27	2.80	119.56	113.60
14	A	4002	BCR	C34-C9-C10	-2.80	118.28	122.82
14	B	4006	BCR	C33-C5-C4	2.80	119.56	113.60
15	A	1135	CLA	C1-O2A-CGA	2.79	123.41	116.65
15	B	1219	CLA	C4D-C3D-CAD	2.79	111.14	108.11
14	B	4006	BCR	C36-C18-C17	-2.79	118.29	122.82
15	B	1227	CLA	C4D-C3D-CAD	2.79	111.14	108.11
14	A	4012	BCR	C23-C22-C21	2.79	123.39	119.01
15	F	1410	CLA	CMB-C2B-C1B	2.79	129.66	125.42
15	B	1207	CLA	C4D-C3D-CAD	2.79	111.13	108.11
15	B	1234	CLA	C2B-C1B-NB	2.78	113.21	110.33
15	B	1230	CLA	C3C-C4C-NC	2.78	114.00	110.43
15	A	1124	CLA	CMB-C2B-C1B	2.78	129.66	125.42
15	A	1140	CLA	CMC-C2C-C1C	2.78	129.38	125.03
15	B	1212	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	B	4017	BCR	C27-C26-C25	-2.78	118.95	122.70
15	B	1222	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
13	A	1011	CL0	O1D-CGD-CBD	-2.78	120.51	124.72
15	B	1202	CLA	O2A-C1-C2	2.78	118.79	108.11
15	A	1012	CLA	CMC-C2C-C1C	2.78	129.37	125.03
15	A	1138	CLA	C1-O2A-CGA	2.78	123.37	116.65
15	A	1127	CLA	CMC-C2C-C1C	2.78	129.37	125.03
15	A	1134	CLA	CMC-C2C-C1C	2.77	129.37	125.03
15	A	1128	CLA	C2B-C1B-NB	2.77	113.20	110.33
15	B	1203	CLA	C1-O2A-CGA	2.77	123.36	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1221	CLA	C3D-C4D-ND	2.77	114.49	109.99
15	B	1234	CLA	C1-O2A-CGA	2.77	123.35	116.65
15	B	1211	CLA	C2B-C1B-NB	2.77	113.19	110.33
15	A	1123	CLA	CMC-C2C-C1C	2.77	129.35	125.03
10	B	2002	PQN	C2M-C2-C3	-2.76	119.91	124.45
15	A	1115	CLA	C4D-C3D-CAD	2.76	111.11	108.11
14	A	4002	BCR	C3-C4-C5	-2.76	109.13	114.06
15	B	1209	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
15	B	1013	CLA	C1-C2-C3	-2.76	121.67	126.20
14	B	4014	BCR	C15-C14-C13	-2.76	123.40	127.28
15	B	1217	CLA	C4D-C3D-CAD	2.76	111.11	108.11
15	B	1229	CLA	C4D-C3D-CAD	2.76	111.11	108.11
12	A	5005	LHG	O8-C23-C24	2.76	120.25	111.83
15	A	1121	CLA	C2B-C1B-NB	2.76	113.19	110.33
15	B	1236	CLA	C4D-C3D-CAD	2.76	111.10	108.11
15	B	1205	CLA	O1D-CGD-CBD	-2.76	119.08	124.52
15	A	1118	CLA	CMC-C2C-C1C	2.76	129.34	125.03
14	B	4011	BCR	C38-C26-C27	2.75	119.47	113.60
15	B	1235	CLA	C2B-C1B-NB	2.75	113.18	110.33
15	B	1223	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
15	B	1021	CLA	C2B-C1B-NB	2.75	113.18	110.33
15	A	1140	CLA	O2A-C1-C2	2.75	118.69	108.11
15	A	1801	CLA	C3C-C4C-NC	2.75	113.95	110.43
15	B	1223	CLA	C4D-C3D-CAD	2.75	111.09	108.11
14	A	4003	BCR	C23-C22-C21	2.75	123.33	119.01
15	B	1232	CLA	C2B-C1B-NB	2.75	113.18	110.33
15	A	1103	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
15	B	1215	CLA	CMB-C2B-C1B	2.75	129.60	125.42
12	A	5001	LHG	C5-O7-C7	-2.74	111.23	117.80
15	B	1217	CLA	CMB-C2B-C1B	2.74	129.60	125.42
15	B	1206	CLA	CAC-C3C-C4C	2.74	128.36	124.79
15	A	1129	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	J	4013	BCR	C33-C5-C6	-2.74	121.50	124.48
15	B	1207	CLA	CMB-C2B-C1B	2.74	129.59	125.42
15	B	1214	CLA	C4D-C3D-CAD	2.74	111.08	108.11
15	B	1235	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	B	1213	CLA	C1-O2A-CGA	2.74	123.28	116.65
15	B	1204	CLA	CMB-C2B-C1B	2.74	129.59	125.42
15	F	1139	CLA	O2A-C1-C2	2.74	118.64	108.11
15	A	1102	CLA	CMC-C2C-C1C	2.74	129.31	125.03
15	B	1202	CLA	CMB-C2B-C1B	2.74	129.58	125.42
15	B	1228	CLA	O2A-C1-C2	2.74	118.63	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1215	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	A	1137	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	A	4001	BCR	C38-C26-C27	2.73	119.42	113.60
15	B	1225	CLA	C4D-C3D-CAD	2.73	111.07	108.11
15	B	1221	CLA	C3C-C4C-NC	2.73	113.93	110.43
15	K	1402	CLA	CMC-C2C-C1C	2.73	129.30	125.03
15	A	1131	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	B	5004	LHG	O8-C23-C24	2.73	120.16	111.83
15	A	1103	CLA	C1-O2A-CGA	2.73	123.26	116.65
15	B	1230	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
15	B	1212	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
15	A	1103	CLA	C2B-C1B-NB	2.72	113.15	110.33
14	F	4016	BCR	C34-C9-C8	2.72	122.25	118.09
15	B	1236	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
15	A	1114	CLA	C4D-C3D-CAD	2.72	111.06	108.11
15	B	1223	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	B	4005	BCR	C3-C4-C5	-2.72	109.20	114.06
15	A	1138	CLA	C4-C3-C5	2.72	119.95	115.23
15	A	1104	CLA	CMB-C2B-C1B	2.72	129.56	125.42
15	A	1124	CLA	CMC-C2C-C1C	2.72	129.28	125.03
15	A	1133	CLA	C4D-C3D-CAD	2.72	111.06	108.11
15	B	1217	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
15	A	1111	CLA	CMC-C2C-C1C	2.71	129.28	125.03
15	A	1113	CLA	CMC-C2C-C1C	2.71	129.27	125.03
15	B	1221	CLA	CMC-C2C-C1C	2.71	129.27	125.03
15	B	1226	CLA	C4D-C3D-CAD	2.71	111.05	108.11
15	B	1209	CLA	CAC-C3C-C4C	2.71	128.32	124.79
14	A	4007	BCR	C23-C24-C25	-2.71	119.75	127.00
15	A	1117	CLA	CMC-C2C-C1C	2.71	129.27	125.03
15	A	1120	CLA	CMD-C2D-C3D	-2.71	121.47	127.69
15	B	1205	CLA	CMC-C2C-C1C	2.71	129.26	125.03
15	A	1135	CLA	C4-C3-C2	-2.71	116.68	123.63
15	B	1222	CLA	C3D-C4D-ND	2.71	114.39	109.99
15	B	1212	CLA	C4D-C3D-CAD	2.71	111.05	108.11
15	A	1110	CLA	CMC-C2C-C1C	2.71	129.26	125.03
15	B	1218	CLA	CMC-C2C-C1C	2.70	129.26	125.03
15	B	1204	CLA	CMC-C2C-C1C	2.70	129.26	125.03
15	A	1135	CLA	C2B-C1B-NB	2.70	113.13	110.33
15	A	1133	CLA	CMC-C2C-C1C	2.70	129.25	125.03
15	F	1139	CLA	C2B-C1B-NB	2.70	113.13	110.33
14	J	4013	BCR	C2-C1-C6	2.70	114.36	110.44
15	B	1229	CLA	C2B-C1B-NB	2.70	113.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1234	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
15	B	1220	CLA	CED-O2D-CGD	2.70	122.03	115.92
14	A	4007	BCR	C7-C8-C9	-2.70	122.25	126.23
15	B	1204	CLA	CMD-C2D-C3D	-2.70	121.51	127.69
15	B	1215	CLA	C4-C3-C2	-2.70	116.70	123.63
15	F	1301	CLA	C4D-C3D-CAD	2.70	111.03	108.11
15	A	1110	CLA	CMB-C2B-C1B	2.69	129.52	125.42
15	A	1118	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
15	A	1012	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	A	4008	BCR	C15-C14-C13	-2.69	123.50	127.28
15	A	1116	CLA	C1-O2A-CGA	2.69	123.17	116.65
15	A	1104	CLA	C4-C3-C5	2.69	119.90	115.23
14	J	4013	BCR	C23-C24-C25	-2.69	119.81	127.00
15	A	1123	CLA	O2A-C1-C2	2.69	118.45	108.11
15	B	1239	CLA	CMD-C2D-C3D	-2.68	121.53	127.69
17	B	5002	LMG	O8-C28-C29	2.68	120.02	111.83
15	B	1240	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	B	4006	BCR	C24-C23-C22	-2.68	122.27	126.23
15	B	1206	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
15	B	1232	CLA	C4D-C3D-CAD	2.68	111.02	108.11
14	A	4008	BCR	C3-C4-C5	-2.68	109.28	114.06
15	B	1235	CLA	O2A-C1-C2	2.68	118.41	108.11
15	B	1224	CLA	C1-O2A-CGA	2.68	123.13	116.65
15	B	1207	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
13	A	1011	CL0	CMC-C2C-C1C	2.67	129.54	124.73
15	B	1215	CLA	CMC-C2C-C1C	2.67	129.21	125.03
15	A	1801	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
14	A	4003	BCR	C3-C4-C5	-2.67	109.29	114.06
15	B	1234	CLA	CMB-C2B-C1B	2.67	129.49	125.42
15	A	1127	CLA	C3C-C4C-NC	2.67	113.85	110.43
15	A	1138	CLA	C4D-C3D-CAD	2.67	111.00	108.11
15	B	1237	CLA	O2A-C1-C2	2.67	118.37	108.11
15	A	1114	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
15	A	1113	CLA	C4D-C3D-CAD	2.66	111.00	108.11
15	A	1115	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	A	4012	BCR	C3-C4-C5	-2.66	109.31	114.06
15	A	1110	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	A	4002	BCR	C30-C25-C26	-2.66	119.00	122.64
15	B	1224	CLA	CMC-C2C-C1C	2.66	129.19	125.03
15	A	1105	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
15	B	1232	CLA	CMB-C2B-C1B	2.66	129.47	125.42
15	A	1126	CLA	O2D-CGD-O1D	-2.66	118.68	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1115	CLA	C3C-C4C-NC	2.65	113.83	110.43
15	A	1119	CLA	CMC-C2C-C1C	2.65	129.18	125.03
15	A	1118	CLA	C4D-C3D-CAD	2.65	110.99	108.11
15	A	1130	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	A	1135	CLA	CMC-C2C-C1C	2.65	129.18	125.03
15	A	1132	CLA	C4D-C3D-CAD	2.65	110.98	108.11
15	A	1120	CLA	CMB-C2B-C1B	2.65	129.45	125.42
14	B	4011	BCR	C1-C6-C5	-2.65	119.02	122.64
15	B	1211	CLA	C4D-C3D-CAD	2.64	110.98	108.11
15	B	1207	CLA	C2B-C1B-NB	2.64	113.06	110.33
15	A	1128	CLA	C1-O2A-CGA	2.64	123.04	116.65
15	A	1125	CLA	C3D-C4D-ND	2.64	114.28	109.99
15	A	1103	CLA	CMB-C2B-C1B	2.64	129.44	125.42
15	B	1231	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
14	A	4003	BCR	C15-C14-C13	-2.64	123.58	127.28
15	B	1218	CLA	C1-O2A-CGA	2.63	123.03	116.65
14	B	4017	BCR	C38-C26-C27	2.63	119.21	113.60
15	B	1226	CLA	O1D-CGD-CBD	-2.63	119.32	124.52
15	B	1213	CLA	C4D-C3D-CAD	2.63	110.97	108.11
15	B	1223	CLA	C4-C3-C5	2.63	119.80	115.23
15	A	1801	CLA	C3D-C4D-ND	2.63	114.26	109.99
15	B	1240	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	B	4010	BCR	C36-C18-C17	-2.63	118.56	122.82
14	B	4004	BCR	C33-C5-C4	2.63	119.20	113.60
15	A	1114	CLA	C2B-C1B-NB	2.63	113.05	110.33
15	A	1107	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	B	4010	BCR	C30-C25-C26	-2.63	119.05	122.64
15	B	1201	CLA	C4D-C3D-CAD	2.62	110.96	108.11
15	A	1118	CLA	C2B-C1B-NB	2.62	113.05	110.33
15	A	1122	CLA	O2A-C1-C2	2.62	118.21	108.11
15	J	1303	CLA	C2B-C1B-NB	2.62	113.05	110.33
15	A	1129	CLA	CMC-C2C-C1C	2.62	129.13	125.03
15	A	1106	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
15	A	1103	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
15	A	1012	CLA	OBD-CAD-C3D	-2.62	122.29	128.42
15	A	1127	CLA	C1-O2A-CGA	2.62	122.99	116.65
15	A	1132	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
15	A	1116	CLA	CMC-C2C-C1C	2.62	129.12	125.03
14	A	4008	BCR	C23-C24-C25	-2.61	120.02	127.00
15	J	1303	CLA	CMC-C2C-C1C	2.61	129.12	125.03
15	A	1022	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
15	B	1023	CLA	O2D-CGD-O1D	-2.61	118.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	1303	CLA	C3C-C4C-NC	2.61	113.78	110.43
15	A	1111	CLA	C4D-C3D-CAD	2.61	110.94	108.11
15	A	1131	CLA	C4D-C3D-CAD	2.61	110.94	108.11
15	J	1302	CLA	CMB-C2B-C1B	2.61	129.39	125.42
15	B	1222	CLA	C4-C3-C5	2.61	119.76	115.23
15	B	1228	CLA	C4D-C3D-CAD	2.61	110.94	108.11
15	A	1137	CLA	C2B-C1B-NB	2.61	113.03	110.33
15	A	1131	CLA	CAC-C3C-C4C	2.61	128.18	124.79
15	B	1013	CLA	CMB-C2B-C1B	2.61	129.39	125.42
15	A	1022	CLA	CMB-C2B-C1B	2.61	129.39	125.42
15	A	1022	CLA	C4-C3-C5	2.61	119.75	115.23
15	B	1231	CLA	C4D-C3D-CAD	2.61	110.94	108.11
15	A	1123	CLA	C2B-C1B-NB	2.60	113.03	110.33
15	A	1129	CLA	CMB-C2B-C1B	2.60	129.38	125.42
15	B	1209	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
15	B	1224	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
15	B	1213	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
15	B	1211	CLA	CMB-C2B-C1B	2.60	129.38	125.42
15	B	1221	CLA	C2B-C1B-NB	2.60	113.02	110.33
15	A	1131	CLA	CMB-C2B-C1B	2.60	129.38	125.42
14	B	4004	BCR	C23-C22-C21	2.60	123.10	119.01
15	B	1205	CLA	C2B-C1B-NB	2.60	113.02	110.33
15	B	1228	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	J	4013	BCR	C36-C18-C17	-2.60	118.61	122.82
15	B	1236	CLA	C1-C2-C3	-2.59	122.56	126.76
15	A	1120	CLA	CMC-C2C-C1C	2.59	129.09	125.03
15	B	1021	CLA	CMB-C2B-C1B	2.59	129.37	125.42
15	A	1101	CLA	C3C-C4C-NC	2.59	113.75	110.43
15	K	1401	CLA	CMC-C2C-C1C	2.59	129.08	125.03
15	A	1012	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
15	K	1401	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
15	B	1239	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
15	B	1210	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	J	4013	BCR	C27-C26-C25	-2.59	119.21	122.70
15	A	1119	CLA	C4D-C3D-CAD	2.59	110.92	108.11
15	B	1235	CLA	C3C-C4C-NC	2.59	113.74	110.43
15	A	1106	CLA	C4D-C3D-CAD	2.58	110.91	108.11
15	A	1105	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	B	4017	BCR	C33-C5-C4	2.58	119.10	113.60
15	B	1205	CLA	C3C-C4C-NC	2.58	113.73	110.43
15	F	1410	CLA	C4D-C3D-CAD	2.58	110.91	108.11
15	A	1130	CLA	CMD-C2D-C3D	-2.58	121.78	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4003	BCR	C36-C18-C17	-2.58	118.64	122.82
14	B	4009	BCR	C37-C22-C21	-2.58	118.64	122.82
15	A	1133	CLA	C2B-C1B-NB	2.58	113.00	110.33
15	B	1225	CLA	C3C-C4C-NC	2.58	113.73	110.43
14	A	4002	BCR	C35-C13-C12	2.57	122.02	118.09
15	A	1107	CLA	O2A-C1-C2	2.57	118.01	108.11
15	A	1140	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1111	CLA	CMB-C2B-C1B	2.57	129.34	125.42
15	A	1116	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	B	1013	CLA	CBB-CAB-C3B	-2.57	114.67	127.53
15	B	1219	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1136	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1114	CLA	CMC-C2C-C1C	2.57	129.05	125.03
15	A	1132	CLA	C3C-C4C-NC	2.57	113.72	110.43
15	B	1203	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
15	A	1136	CLA	CMC-C2C-C1C	2.57	129.05	125.03
15	B	1216	CLA	CMC-C2C-C1C	2.57	129.05	125.03
15	B	1218	CLA	CMB-C2B-C1B	2.57	129.33	125.42
15	J	1302	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	A	1114	CLA	CMB-C2B-C1B	2.57	129.33	125.42
15	B	1229	CLA	C3C-C4C-NC	2.57	113.72	110.43
15	A	1103	CLA	CMC-C2C-C1C	2.56	129.04	125.03
14	B	4011	BCR	C3-C4-C5	-2.56	109.49	114.06
10	A	2001	PQN	C2M-C2-C3	-2.56	120.24	124.45
12	A	5003	LHG	O8-C23-C24	2.56	119.65	111.83
15	A	1123	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
15	B	1214	CLA	O2A-C1-C2	2.56	117.95	108.11
15	B	1206	CLA	CMB-C2B-C1B	2.56	129.31	125.42
15	A	1101	CLA	CHB-C4A-NA	2.56	128.09	124.40
15	A	1135	CLA	C4D-C3D-CAD	2.56	110.88	108.11
15	A	1112	CLA	CMB-C2B-C1B	2.56	129.31	125.42
15	B	1201	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
15	F	1139	CLA	CMD-C2D-C3D	-2.55	121.83	127.69
13	A	1011	CL0	C1-O2A-CGA	2.55	122.83	116.65
15	B	1222	CLA	C4D-C3D-CAD	2.55	110.87	108.11
14	B	4005	BCR	C23-C22-C21	2.55	123.02	119.01
14	B	4009	BCR	C30-C25-C26	-2.55	119.16	122.64
15	B	1227	CLA	CMC-C2C-C1C	2.55	129.01	125.03
14	B	4004	BCR	C38-C26-C27	2.55	119.02	113.60
15	A	1801	CLA	CMB-C2B-C1B	2.54	129.29	125.42
14	B	4004	BCR	C1-C6-C5	-2.54	119.16	122.64
15	B	1023	CLA	C4D-C3D-CAD	2.54	110.86	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1207	CLA	CMC-C2C-C1C	2.54	129.00	125.03
15	B	1218	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
15	B	1230	CLA	C2B-C1B-NB	2.54	112.96	110.33
15	B	1226	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	B	4009	BCR	C27-C26-C25	-2.54	119.28	122.70
15	B	1215	CLA	C4D-C3D-CAD	2.53	110.86	108.11
15	J	1302	CLA	C2B-C1B-NB	2.53	112.95	110.33
15	B	1208	CLA	C4D-C3D-CAD	2.53	110.86	108.11
15	A	1130	CLA	C4D-C3D-CAD	2.53	110.85	108.11
15	A	1115	CLA	C2B-C1B-NB	2.53	112.95	110.33
15	F	1410	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
15	B	1232	CLA	CMC-C2C-C1C	2.53	128.98	125.03
15	B	1238	CLA	CMB-C2B-C1B	2.52	129.26	125.42
14	B	4017	BCR	C30-C25-C26	-2.52	119.19	122.64
15	B	1222	CLA	C3C-C4C-NC	2.52	113.66	110.43
15	A	1012	CLA	C4D-C3D-CAD	2.52	110.84	108.11
15	B	1221	CLA	C4D-C3D-CAD	2.52	110.84	108.11
15	B	1213	CLA	CMB-C2B-C1B	2.52	129.26	125.42
15	B	1218	CLA	C1-C2-C3	-2.52	122.07	126.20
15	B	1234	CLA	C4D-C3D-CAD	2.52	110.84	108.11
15	B	1013	CLA	CED-O2D-CGD	2.52	121.63	115.92
15	A	1109	CLA	CMB-C2B-C1B	2.52	129.25	125.42
15	B	1235	CLA	CMB-C2B-C1B	2.52	129.25	125.42
15	A	1102	CLA	C4-C3-C5	2.52	119.59	115.23
15	B	1230	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
14	A	4008	BCR	C33-C5-C4	2.51	118.95	113.60
15	B	1239	CLA	C2B-C1B-NB	2.51	112.93	110.33
15	A	1134	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
15	A	1105	CLA	C1-O2A-CGA	2.51	122.72	116.65
15	B	1219	CLA	CMB-C2B-C3B	2.51	132.45	126.55
15	B	1236	CLA	CMB-C2B-C1B	2.51	129.24	125.42
15	B	1203	CLA	CMC-C2C-C1C	2.51	128.95	125.03
15	B	1216	CLA	C4D-C3D-CAD	2.51	110.83	108.11
15	A	1133	CLA	CAC-C3C-C4C	2.51	128.05	124.79
15	B	1237	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
12	A	5005	LHG	C5-O7-C7	-2.51	111.80	117.80
15	B	1021	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
15	B	1013	CLA	C4D-C3D-CAD	2.50	110.83	108.11
15	B	1214	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
15	A	1115	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
15	A	1114	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
15	B	1221	CLA	O2A-C1-C2	2.50	117.72	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1022	CLA	C3C-C4C-NC	2.50	113.63	110.43
15	B	1222	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	B	1213	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
15	F	1301	CLA	C3C-C4C-NC	2.49	113.62	110.43
15	A	1109	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
15	B	1021	CLA	CMA-C3A-C2A	-2.49	104.34	113.98
15	B	1209	CLA	CMC-C2C-C1C	2.49	128.93	125.03
15	A	1107	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
15	A	1133	CLA	CMB-C2B-C1B	2.49	129.21	125.42
15	A	1133	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
15	A	1137	CLA	C3C-C4C-NC	2.49	113.62	110.43
15	A	1122	CLA	CMB-C2B-C1B	2.49	129.21	125.42
14	A	4001	BCR	C15-C14-C13	-2.49	123.79	127.28
14	B	4011	BCR	C35-C13-C12	2.48	121.88	118.09
15	B	1229	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
15	B	1225	CLA	C5-C3-C2	-2.48	115.59	121.17
15	A	1116	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
15	B	1231	CLA	CED-O2D-CGD	2.48	121.54	115.92
15	A	1112	CLA	C3C-C4C-NC	2.48	113.61	110.43
15	A	1129	CLA	C2B-C1B-NB	2.48	112.89	110.33
15	B	1228	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
15	A	1132	CLA	C2B-C1B-NB	2.48	112.89	110.33
15	B	1237	CLA	CMB-C2B-C1B	2.47	129.19	125.42
15	A	1122	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
15	B	1240	CLA	C3C-C4C-NC	2.47	113.60	110.43
14	J	4013	BCR	C37-C22-C21	-2.47	118.81	122.82
15	A	1140	CLA	C3C-C4C-NC	2.47	113.59	110.43
15	A	1123	CLA	CMB-C2B-C1B	2.47	129.18	125.42
15	B	1208	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
15	A	1101	CLA	CBA-CAA-C2A	2.47	121.13	113.79
15	A	1117	CLA	C4D-C3D-CAD	2.46	110.78	108.11
15	A	1112	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	B	1013	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	B	1225	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	B	1221	CLA	C4-C3-C2	-2.46	117.31	123.63
15	B	1218	CLA	C4-C3-C2	-2.46	117.31	123.63
16	J	1304	LMU	C1B-O1B-C4'	-2.46	112.15	117.98
15	A	1113	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
15	B	1214	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
15	B	1219	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
15	A	1130	CLA	CHB-C1B-C2B	-2.46	120.29	127.43
15	A	1128	CLA	O1D-CGD-CBD	-2.46	119.67	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1104	CLA	C4D-C3D-CAD	2.46	110.78	108.11
15	A	1128	CLA	C3C-C4C-NC	2.46	113.58	110.43
15	F	1301	CLA	CMB-C2B-C1B	2.45	129.16	125.42
15	B	1220	CLA	C4D-C3D-CAD	2.45	110.77	108.11
15	A	1126	CLA	C1-C2-C3	-2.45	122.18	126.20
15	B	1238	CLA	C4D-C3D-CAD	2.45	110.77	108.11
15	B	1227	CLA	C3C-C4C-NC	2.45	113.57	110.43
15	F	1139	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	F	4016	BCR	C36-C18-C17	-2.45	118.84	122.82
14	F	4016	BCR	C7-C6-C5	-2.45	115.91	121.56
15	A	1138	CLA	CHB-C1B-C2B	-2.45	120.31	127.43
15	B	1210	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	B	1231	CLA	CMB-C2B-C1B	2.45	129.15	125.42
15	B	1220	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	B	1235	CLA	C4D-C3D-CAD	2.45	110.77	108.11
15	A	1131	CLA	C2B-C1B-NB	2.45	112.86	110.33
15	K	1402	CLA	C2B-C1B-NB	2.45	112.86	110.33
15	F	1301	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
15	B	1216	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
15	A	1109	CLA	CMD-C2D-C3D	-2.44	122.08	127.69
15	A	1121	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
15	B	1204	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
15	A	1137	CLA	CMC-C2C-C1C	2.44	128.85	125.03
15	A	1101	CLA	C1-O2A-CGA	2.44	122.56	116.65
15	A	1114	CLA	CAC-C3C-C4C	2.44	127.96	124.79
15	A	1109	CLA	C1-C2-C3	-2.44	122.20	126.20
15	B	1208	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
14	A	4007	BCR	C28-C27-C26	-2.44	109.71	114.06
15	B	1212	CLA	CMB-C2B-C1B	2.44	129.13	125.42
15	J	1303	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
15	A	1110	CLA	C4-C3-C5	2.44	119.45	115.23
15	B	1227	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	B	4017	BCR	C38-C26-C25	-2.43	121.83	124.48
15	B	1219	CLA	C4-C3-C2	-2.43	117.38	123.63
15	B	1216	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
15	B	1203	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
14	B	4017	BCR	C34-C9-C8	2.43	121.80	118.09
16	B	1301	LMU	C1B-O1B-C4'	-2.43	112.22	117.98
14	A	4007	BCR	C30-C25-C26	-2.43	119.32	122.64
15	J	1302	CLA	C3C-C4C-NC	2.43	113.54	110.43
15	B	1207	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	A	4012	BCR	C34-C9-C10	-2.43	118.89	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1119	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
15	A	1127	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
14	A	4012	BCR	C8-C7-C6	-2.42	120.52	127.00
15	A	1120	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
15	B	1021	CLA	C3C-C4C-NC	2.42	113.53	110.43
15	A	1104	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
15	A	1136	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
15	B	1207	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
15	B	1216	CLA	O2A-C1-C2	2.42	117.42	108.11
15	A	1801	CLA	C1-C2-C3	-2.42	122.23	126.20
15	A	1125	CLA	CMB-C2B-C1B	2.42	129.10	125.42
15	A	1117	CLA	CMB-C2B-C1B	2.41	129.09	125.42
15	A	1131	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
15	B	1021	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
15	B	1223	CLA	OBD-CAD-C3D	-2.41	122.78	128.42
15	B	1013	CLA	C3C-C4C-NC	2.41	113.52	110.43
15	A	1131	CLA	C1-C2-C3	-2.41	122.25	126.20
10	A	2001	PQN	C11-C3-C2	-2.41	120.76	124.89
15	A	1105	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	J	4013	BCR	C34-C9-C10	-2.41	118.92	122.82
15	A	1121	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	F	4016	BCR	C38-C26-C27	2.41	118.72	113.60
15	A	1134	CLA	C3C-C4C-NC	2.40	113.51	110.43
15	B	1226	CLA	C3C-C4C-NC	2.40	113.51	110.43
15	A	1106	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
15	A	1125	CLA	CHD-C4C-C3C	-2.40	121.27	124.77
15	K	1402	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
14	A	4002	BCR	C23-C24-C25	-2.40	120.58	127.00
14	F	4015	BCR	C8-C7-C6	-2.40	120.58	127.00
15	A	1132	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
14	A	4007	BCR	C27-C26-C25	-2.40	119.46	122.70
15	K	1402	CLA	C3C-C4C-NC	2.40	113.50	110.43
15	B	1234	CLA	CMC-C2C-C1C	2.40	128.78	125.03
15	B	1216	CLA	C4-C3-C5	2.40	119.39	115.23
15	B	1225	CLA	CBA-CAA-C2A	2.40	120.93	113.79
15	A	1110	CLA	C4D-C3D-CAD	2.40	110.71	108.11
15	B	1212	CLA	C3C-C4C-NC	2.40	113.50	110.43
15	B	1236	CLA	C3C-C4C-NC	2.40	113.50	110.43
13	A	1108	CL0	CED-O2D-CGD	2.40	121.35	115.92
15	A	1105	CLA	CAC-C3C-C4C	2.39	127.91	124.79
15	B	1021	CLA	C1-O2A-CGA	2.39	122.44	116.65
15	A	1117	CLA	O2D-CGD-O1D	-2.39	119.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	4015	BCR	C30-C25-C26	-2.39	119.37	122.64
15	A	1128	CLA	C1-C2-C3	-2.39	122.28	126.20
15	J	1303	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	B	1230	CLA	CMB-C2B-C1B	2.39	129.05	125.42
15	B	1236	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
15	B	1237	CLA	CAC-C3C-C4C	2.39	127.89	124.79
15	B	1232	CLA	C3C-C4C-NC	2.38	113.48	110.43
15	B	1234	CLA	C4-C3-C2	-2.38	117.50	123.63
15	A	1110	CLA	CAC-C3C-C4C	2.38	127.89	124.79
15	A	1119	CLA	C1-O2A-CGA	2.38	122.42	116.65
15	B	1239	CLA	CAC-C3C-C4C	2.38	127.89	124.79
15	A	1133	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
15	A	1113	CLA	C3C-C4C-NC	2.38	113.48	110.43
15	B	1226	CLA	C2B-C1B-NB	2.38	112.79	110.33
15	F	1139	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
15	A	1119	CLA	CHB-C1B-C2B	-2.38	120.53	127.43
15	J	1302	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
15	A	1112	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
15	A	1132	CLA	CMC-C2C-C1C	2.37	128.75	125.03
15	B	1231	CLA	C4-C3-C2	-2.37	117.53	123.63
15	B	1228	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
15	B	1226	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
10	A	2001	PQN	C11-C12-C13	-2.37	122.75	126.83
15	A	1124	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
15	A	1126	CLA	CHB-C1B-C2B	-2.37	120.56	127.43
15	A	1135	CLA	C3C-C4C-NC	2.36	113.46	110.43
15	B	1217	CLA	C3C-C4C-NC	2.36	113.46	110.43
15	A	1104	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
15	B	1202	CLA	CMC-C2C-C1C	2.36	128.73	125.03
15	A	1113	CLA	CMB-C2B-C1B	2.36	129.02	125.42
15	A	1107	CLA	CAA-CBA-CGA	-2.36	106.50	113.21
15	B	1202	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
15	B	1225	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
15	K	1401	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
15	A	1113	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	A	4001	BCR	C30-C25-C24	2.36	122.05	115.65
15	B	1234	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
10	B	2002	PQN	C11-C3-C2	-2.36	120.85	124.89
13	A	1011	CL0	CBC-CAC-C3C	-2.36	109.50	112.87
15	F	1410	CLA	C3C-C4C-NC	2.35	113.45	110.43
15	B	1021	CLA	CBA-CAA-C2A	2.35	120.80	113.79
15	A	1127	CLA	CMD-C2D-C3D	-2.35	122.29	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1137	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
15	B	1218	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
15	B	1222	CLA	CMC-C2C-C1C	2.35	128.71	125.03
14	B	4010	BCR	C34-C9-C10	-2.35	119.01	122.82
15	A	1801	CLA	C1-O2A-CGA	2.35	122.34	116.65
15	B	1234	CLA	C3C-C4C-NC	2.35	113.44	110.43
15	A	1110	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
15	A	1801	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
15	B	1013	CLA	CMC-C2C-C1C	2.34	128.69	125.03
14	B	4004	BCR	C30-C25-C26	-2.34	119.44	122.64
15	A	1111	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
15	A	1130	CLA	C1-O2A-CGA	2.34	122.31	116.65
15	A	1107	CLA	CHB-C1B-C2B	-2.34	120.64	127.43
14	B	4006	BCR	C23-C24-C25	-2.34	120.76	127.00
14	A	4003	BCR	C28-C27-C26	-2.34	109.89	114.06
14	B	4017	BCR	C37-C22-C21	-2.34	119.03	122.82
15	A	1116	CLA	C3C-C4C-NC	2.34	113.42	110.43
15	A	1136	CLA	C2B-C1B-NB	2.33	112.75	110.33
15	A	1136	CLA	O2A-C1-C2	2.33	117.09	108.11
15	A	1136	CLA	C3C-C4C-NC	2.33	113.42	110.43
15	A	1121	CLA	C3C-C4C-NC	2.33	113.42	110.43
15	B	1203	CLA	C1-C2-C3	-2.33	122.38	126.20
15	A	1126	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
15	B	1228	CLA	C3C-C4C-NC	2.33	113.42	110.43
14	A	4003	BCR	C19-C18-C17	2.33	122.67	119.01
15	A	1135	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	B	4004	BCR	C15-C14-C13	-2.33	124.02	127.28
15	F	1410	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
15	B	1215	CLA	C3C-C4C-NC	2.32	113.40	110.43
15	A	1104	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
15	B	1206	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
15	A	1140	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
14	F	4016	BCR	C34-C9-C10	-2.32	119.06	122.82
15	B	1240	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
15	K	1401	CLA	CAC-C3C-C4C	2.31	127.80	124.79
15	A	1103	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	A	1113	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
15	B	1240	CLA	CMB-C2B-C1B	2.31	128.94	125.42
15	B	1211	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
14	A	4007	BCR	C33-C5-C4	2.31	118.52	113.60
15	A	1131	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
15	B	1201	CLA	CMD-C2D-C3D	-2.31	122.39	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4007	BCR	C34-C9-C8	2.31	121.61	118.09
15	A	1119	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	F	4015	BCR	C3-C4-C5	-2.31	109.94	114.06
14	B	4004	BCR	C34-C9-C10	-2.31	119.08	122.82
14	B	4009	BCR	C33-C5-C4	2.31	118.51	113.60
15	A	1012	CLA	CMB-C2B-C1B	2.31	128.93	125.42
15	A	1101	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
15	A	1111	CLA	C1-O2A-CGA	2.30	122.23	116.65
12	A	5001	LHG	O8-C23-C24	2.30	118.86	111.83
15	A	1127	CLA	C2B-C1B-NB	2.30	112.71	110.33
15	A	1110	CLA	C3C-C4C-NC	2.30	113.38	110.43
15	A	1136	CLA	CAC-C3C-C4C	2.30	127.78	124.79
15	A	1124	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
14	A	4003	BCR	C38-C26-C27	2.30	118.49	113.60
15	K	1402	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
12	B	5004	LHG	O7-C7-O9	-2.29	118.34	123.70
15	A	1131	CLA	C3C-C4C-NC	2.29	113.37	110.43
15	B	1211	CLA	C3C-C4C-NC	2.29	113.37	110.43
15	A	1111	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
14	B	4009	BCR	C8-C9-C10	2.29	122.61	119.01
15	B	1212	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
15	A	1012	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	B	1240	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
15	B	1232	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
15	B	1201	CLA	C3C-C4C-NC	2.29	113.36	110.43
15	A	1133	CLA	C3C-C4C-NC	2.28	113.36	110.43
15	A	1105	CLA	C3C-C4C-NC	2.28	113.35	110.43
15	A	1138	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
15	A	1129	CLA	C3C-C4C-NC	2.28	113.35	110.43
15	A	1112	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	K	1401	CLA	C3C-C4C-NC	2.28	113.35	110.43
15	A	1140	CLA	CMB-C2B-C1B	2.28	128.89	125.42
14	F	4015	BCR	C23-C24-C25	-2.28	120.92	127.00
15	B	1239	CLA	CMC-C2C-C1C	2.28	128.59	125.03
15	B	1235	CLA	C4-C3-C5	2.28	119.18	115.23
15	A	1129	CLA	OBD-CAD-C3D	-2.27	123.10	128.42
15	B	1219	CLA	C1-O2A-CGA	2.27	122.16	116.65
15	A	1121	CLA	CAC-C3C-C4C	2.27	127.75	124.79
15	B	1210	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
15	B	1235	CLA	C1-O2A-CGA	2.27	122.15	116.65
15	B	1023	CLA	CMC-C2C-C1C	2.27	128.58	125.03
15	B	1225	CLA	CMB-C2B-C1B	2.27	128.87	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	4015	BCR	C27-C26-C25	-2.27	119.64	122.70
15	A	1119	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
15	B	1238	CLA	C3C-C4C-NC	2.27	113.33	110.43
15	A	1102	CLA	C4D-C3D-CAD	2.26	110.56	108.11
14	B	4010	BCR	C33-C5-C4	2.26	118.42	113.60
15	B	1228	CLA	CMB-C2B-C3B	2.26	131.87	126.55
15	A	1124	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	B	1236	CLA	C1-O2A-CGA	2.26	122.12	116.65
15	A	1125	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
14	A	4008	BCR	C28-C27-C26	-2.25	110.04	114.06
13	A	1108	CL0	CGD-CBD-CAD	-2.25	103.55	110.85
15	B	1204	CLA	CAC-C3C-C4C	2.25	127.72	124.79
15	A	1101	CLA	C4-C3-C2	-2.25	117.84	123.63
15	B	1231	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
15	A	1124	CLA	C1-C2-C3	-2.25	122.51	126.20
15	A	1102	CLA	C1-O2A-CGA	2.25	122.09	116.65
15	B	1202	CLA	C3C-C4C-NC	2.25	113.31	110.43
15	A	1107	CLA	C4B-CHC-C1C	2.25	131.53	126.25
15	B	1215	CLA	CAC-C3C-C4C	2.25	127.72	124.79
15	A	1119	CLA	CED-O2D-CGD	2.25	121.01	115.92
15	A	1125	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
15	A	1103	CLA	CED-O2D-CGD	2.25	121.01	115.92
15	A	1117	CLA	C1-C2-C3	-2.25	122.52	126.20
15	A	1115	CLA	CMB-C2B-C1B	2.25	128.84	125.42
15	A	1111	CLA	CHB-C4A-NA	2.24	127.64	124.40
15	A	1126	CLA	CAC-C3C-C4C	2.24	127.71	124.79
15	A	1130	CLA	C3C-C4C-NC	2.24	113.30	110.43
15	F	1301	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	A	1140	CLA	C1-C2-C3	-2.24	122.53	126.20
15	B	1021	CLA	CED-O2D-CGD	2.24	120.99	115.92
15	A	1116	CLA	CAC-C3C-C4C	2.24	127.70	124.79
15	A	1117	CLA	C4-C3-C5	2.24	119.11	115.23
15	A	1124	CLA	C3C-C4C-NC	2.24	113.30	110.43
15	A	1135	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
14	F	4015	BCR	C32-C1-C6	-2.23	106.74	110.24
15	B	1231	CLA	C3C-C4C-NC	2.23	113.29	110.43
15	B	1208	CLA	CMC-C2C-C1C	2.23	128.52	125.03
15	A	1135	CLA	CMB-C2B-C1B	2.23	128.81	125.42
15	B	1238	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
15	B	1236	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
15	B	1202	CLA	CHB-C4A-NA	2.23	127.61	124.40
14	A	4012	BCR	C38-C26-C27	2.23	118.34	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1116	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
15	A	1107	CLA	C5-C3-C4	2.22	119.71	114.59
15	A	1101	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
15	F	1410	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
15	A	1117	CLA	C3C-C4C-NC	2.22	113.28	110.43
14	B	4010	BCR	C38-C26-C27	2.22	118.34	113.60
15	B	1013	CLA	CHB-C4A-NA	2.22	127.61	124.40
15	A	1118	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
15	B	1023	CLA	C4-C3-C5	2.22	119.08	115.23
15	A	1127	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
15	B	1214	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
15	A	1137	CLA	CMB-C2B-C1B	2.22	128.80	125.42
12	A	5003	LHG	O7-C7-O9	-2.22	118.52	123.70
15	A	1101	CLA	CHB-C1B-C2B	-2.22	121.00	127.43
15	A	1117	CLA	CHB-C1B-C2B	-2.21	121.00	127.43
15	A	1112	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
15	A	1103	CLA	CAC-C3C-C4C	2.21	127.67	124.79
14	A	4001	BCR	C31-C1-C6	-2.21	106.77	110.24
15	B	1021	CLA	CHB-C4A-NA	2.21	127.59	124.40
15	B	1209	CLA	C3C-C4C-NC	2.21	113.27	110.43
15	B	1220	CLA	C3C-C4C-NC	2.21	113.27	110.43
15	B	1023	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
15	B	1227	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
13	A	1108	CL0	OBD-CAD-C3D	-2.21	124.44	127.89
15	A	1102	CLA	C3C-C4C-NC	2.21	113.26	110.43
15	A	1140	CLA	C4-C3-C5	2.21	119.06	115.23
14	B	4006	BCR	C15-C14-C13	-2.21	124.18	127.28
15	A	1127	CLA	CED-O2D-CGD	2.21	120.92	115.92
14	B	4005	BCR	C23-C24-C25	-2.21	121.10	127.00
14	A	4001	BCR	C23-C22-C21	2.21	122.48	119.01
15	B	1226	CLA	CMB-C2B-C1B	2.21	128.78	125.42
15	B	1234	CLA	C5-C3-C2	2.21	126.12	121.17
15	B	1228	CLA	CED-O2D-CGD	2.21	120.92	115.92
13	A	1011	CL0	C4C-C3C-C2C	-2.20	104.67	113.37
15	B	1220	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
15	B	1230	CLA	C1-C2-C3	-2.20	122.59	126.20
15	A	1123	CLA	C3C-C4C-NC	2.20	113.25	110.43
15	B	1215	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
14	F	4015	BCR	C19-C18-C17	2.20	122.47	119.01
15	A	1126	CLA	C6-C5-C3	-2.20	108.11	113.47
15	A	1137	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
15	B	1214	CLA	O1D-CGD-CBD	-2.20	120.18	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1211	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
10	B	2002	PQN	C11-C12-C13	-2.20	123.05	126.83
14	F	4016	BCR	C7-C8-C9	-2.20	122.99	126.23
15	B	1211	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	A	4007	BCR	C34-C9-C10	-2.19	119.27	122.82
15	A	1114	CLA	C3C-C4C-NC	2.19	113.24	110.43
15	A	1120	CLA	C3C-C4C-NC	2.19	113.24	110.43
15	B	1227	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	A	1122	CLA	C4B-CHC-C1C	2.19	131.39	126.25
15	A	1130	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
15	B	1201	CLA	CAC-C3C-C4C	2.19	127.63	124.79
15	B	1210	CLA	C3C-C4C-NC	2.18	113.23	110.43
15	B	1237	CLA	C3C-C4C-NC	2.18	113.23	110.43
14	J	4013	BCR	C19-C18-C17	2.18	122.44	119.01
15	B	1216	CLA	CHB-C1B-C2B	-2.18	121.10	127.43
15	A	1123	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
15	A	1118	CLA	C3C-C4C-NC	2.18	113.22	110.43
15	B	1023	CLA	CAC-C3C-C4C	2.18	127.62	124.79
15	B	1238	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	B	4014	BCR	C34-C9-C10	-2.18	119.29	122.82
13	A	1108	CL0	C4C-C3C-C2C	-2.17	104.79	113.37
15	A	1122	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
15	A	1104	CLA	C3C-C4C-NC	2.17	113.21	110.43
15	A	1131	CLA	C4B-CHC-C1C	2.17	131.34	126.25
15	A	1138	CLA	C3C-C4C-NC	2.17	113.20	110.43
15	B	1217	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
15	A	1116	CLA	C4-C3-C5	2.17	118.99	115.23
15	B	1230	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
15	A	1113	CLA	C4B-CHC-C1C	2.16	131.33	126.25
15	A	1109	CLA	C4-C3-C2	-2.16	118.07	123.63
15	A	1117	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
15	B	1223	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
15	A	1022	CLA	C4D-C3D-CAD	2.16	110.45	108.11
15	A	1128	CLA	CMB-C2B-C1B	2.16	128.71	125.42
16	B	1301	LMU	O5'-C5'-C4'	2.16	114.19	109.72
15	A	1107	CLA	C3C-C4C-NC	2.16	113.19	110.43
15	B	1218	CLA	C3C-C4C-NC	2.16	113.19	110.43
15	K	1401	CLA	CED-O2D-CGD	2.16	120.81	115.92
14	B	4010	BCR	C7-C8-C9	-2.15	123.05	126.23
15	B	1217	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
14	B	4004	BCR	C23-C24-C25	-2.15	121.25	127.00
15	B	1023	CLA	CBB-CAB-C3B	-2.15	116.79	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1135	CLA	CED-O2D-CGD	2.15	120.79	115.92
15	B	1203	CLA	C3C-C4C-NC	2.15	113.18	110.43
15	A	1126	CLA	C4-C3-C5	2.14	118.95	115.23
14	B	4005	BCR	C35-C13-C12	2.14	121.36	118.09
15	B	1225	CLA	C1-O2A-CGA	2.14	121.84	116.65
15	K	1401	CLA	CHB-C4A-NA	2.14	127.49	124.40
15	B	1221	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	A	4003	BCR	C23-C24-C25	-2.14	121.28	127.00
15	B	1220	CLA	CMB-C2B-C3B	2.14	131.59	126.55
15	A	1102	CLA	CHB-C4A-NA	2.14	127.49	124.40
15	A	1106	CLA	C6-C5-C3	-2.14	108.26	113.47
15	A	1101	CLA	CMB-C2B-C1B	2.14	128.67	125.42
15	B	1228	CLA	CHB-C1B-C2B	-2.14	121.23	127.43
15	B	1231	CLA	CMC-C2C-C1C	2.13	128.37	125.03
14	F	4015	BCR	C36-C18-C17	-2.13	119.36	122.82
15	B	1224	CLA	CMB-C2B-C1B	2.13	128.67	125.42
15	A	1131	CLA	CED-O2D-CGD	2.13	120.75	115.92
15	B	1210	CLA	C6-C5-C3	-2.13	108.28	113.47
15	B	1209	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	A	4001	BCR	C33-C5-C4	2.13	118.14	113.60
15	F	1139	CLA	C4-C3-C2	-2.13	118.16	123.63
15	A	1126	CLA	CMB-C2B-C1B	2.13	128.66	125.42
15	A	1134	CLA	CMB-C2B-C1B	2.13	128.66	125.42
15	A	1107	CLA	CAC-C3C-C4C	2.13	127.56	124.79
15	B	1207	CLA	CHB-C4A-NA	2.13	127.47	124.40
14	B	4004	BCR	C30-C25-C24	2.13	121.42	115.65
14	F	4016	BCR	C1-C6-C7	2.12	121.41	115.65
15	A	1104	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
14	J	4013	BCR	C35-C13-C12	2.12	121.33	118.09
15	J	1302	CLA	CAC-C3C-C4C	2.12	127.55	124.79
15	B	1023	CLA	C1-O2A-CGA	2.12	121.78	116.65
15	A	1115	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
14	B	4006	BCR	C29-C28-C27	2.12	115.94	111.28
15	A	1124	CLA	CHB-C1B-C2B	-2.12	121.27	127.43
15	A	1132	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
13	A	1108	CL0	O2D-CGD-O1D	-2.12	119.72	123.85
15	B	1013	CLA	C4-C3-C5	2.12	118.90	115.23
15	B	1021	CLA	C4-C3-C5	2.12	118.90	115.23
15	B	1232	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
15	B	1220	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
15	B	1223	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
15	B	1201	CLA	CMB-C2B-C1B	2.12	128.64	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1230	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
15	B	1206	CLA	CHB-C4A-NA	2.11	127.45	124.40
16	B	1301	LMU	O1'-C1'-C2'	-2.11	105.06	108.27
15	A	1105	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
15	A	1107	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
15	A	1118	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	A	4012	BCR	C35-C13-C12	2.11	121.31	118.09
15	A	1124	CLA	CED-O2D-CGD	2.11	120.70	115.92
15	A	1126	CLA	CHB-C4A-NA	2.11	127.44	124.40
14	B	4004	BCR	C24-C23-C22	-2.11	123.11	126.23
15	B	1013	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
15	B	1216	CLA	C3C-C4C-NC	2.11	113.13	110.43
15	A	1109	CLA	C3C-C4C-NC	2.10	113.13	110.43
15	A	1114	CLA	C1-O2A-CGA	2.10	121.74	116.65
15	A	1117	CLA	C6-C5-C3	-2.10	108.34	113.47
15	B	1239	CLA	C3C-C4C-NC	2.10	113.12	110.43
13	A	1011	CL0	C4C-CHD-C1D	2.10	123.59	116.07
15	A	1119	CLA	CAC-C3C-C4C	2.10	127.52	124.79
13	A	1108	CL0	CMA-C3A-C4A	-2.10	110.09	114.61
14	A	4007	BCR	C35-C13-C12	2.10	121.29	118.09
15	A	1115	CLA	CAC-C3C-C4C	2.10	127.52	124.79
15	A	1123	CLA	C4-C3-C5	2.10	118.87	115.23
13	A	1011	CL0	C2C-C1C-NC	2.09	116.38	110.46
14	B	4017	BCR	C31-C1-C6	-2.09	106.96	110.24
14	A	4007	BCR	C36-C18-C17	-2.09	119.43	122.82
15	B	1205	CLA	C4-C3-C5	2.09	118.86	115.23
14	A	4003	BCR	C8-C9-C10	2.09	122.30	119.01
15	B	1023	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	B	4006	BCR	C37-C22-C21	-2.09	119.43	122.82
15	B	1212	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
15	A	1102	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
15	B	1216	CLA	CAC-C3C-C4C	2.09	127.51	124.79
15	B	1235	CLA	CHB-C4A-NA	2.09	127.42	124.40
15	A	1125	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
15	B	1013	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
12	A	5005	LHG	O7-C7-O9	-2.09	118.83	123.70
15	B	1023	CLA	C3C-C4C-NC	2.09	113.10	110.43
14	B	4004	BCR	C3-C4-C5	-2.08	110.34	114.06
14	B	4011	BCR	C1-C6-C7	2.08	121.30	115.65
15	B	1219	CLA	C1-C2-C3	-2.08	122.79	126.20
15	J	1302	CLA	C4B-CHC-C1C	2.08	131.14	126.25
15	A	1111	CLA	C3C-C4C-NC	2.08	113.09	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1239	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
16	B	1301	LMU	C1'-O5'-C5'	2.08	117.78	113.72
14	B	4014	BCR	C3-C4-C5	-2.08	110.35	114.06
14	B	4010	BCR	C8-C7-C6	-2.08	121.45	127.00
15	B	1209	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	F	4016	BCR	C33-C5-C4	2.08	118.03	113.60
14	B	4004	BCR	C1-C6-C7	2.08	121.28	115.65
15	B	1232	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
15	A	1126	CLA	C1-O2A-CGA	2.08	121.67	116.65
15	A	1128	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
14	B	4010	BCR	C30-C25-C24	2.07	121.27	115.65
15	A	1128	CLA	CMC-C2C-C1C	2.07	128.27	125.03
15	A	1136	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
15	A	1123	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	A	4002	BCR	C37-C22-C21	-2.07	119.46	122.82
15	B	1214	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	A	4012	BCR	C34-C9-C8	2.07	121.25	118.09
15	A	1122	CLA	C3C-C4C-NC	2.06	113.08	110.43
15	B	1229	CLA	C1-O2A-CGA	2.06	121.64	116.65
15	B	1213	CLA	C3C-C4C-NC	2.06	113.07	110.43
15	A	1122	CLA	CED-O2D-CGD	2.06	120.59	115.92
15	A	1129	CLA	CAC-C3C-C4C	2.06	127.47	124.79
15	B	1234	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
14	B	4005	BCR	C38-C26-C27	2.06	117.98	113.60
14	F	4015	BCR	C35-C13-C14	-2.06	119.48	122.82
15	B	1208	CLA	CMB-C2B-C3B	2.06	131.39	126.55
15	A	1128	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
15	B	1229	CLA	CMD-C2D-C3D	-2.06	122.98	127.69
14	B	4005	BCR	C1-C6-C7	2.05	121.22	115.65
14	B	4009	BCR	C23-C24-C25	-2.05	121.52	127.00
15	A	1106	CLA	C3C-C4C-NC	2.05	113.06	110.43
14	B	4005	BCR	C34-C9-C10	-2.05	119.49	122.82
15	B	1209	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
14	B	4017	BCR	C15-C14-C13	-2.05	124.40	127.28
15	F	1139	CLA	C4B-CHC-C1C	2.05	131.06	126.25
15	A	1125	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
14	B	4014	BCR	C38-C26-C27	2.05	117.96	113.60
15	B	1218	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
15	B	1210	CLA	C16-C15-C13	-2.04	109.17	115.97
15	A	1128	CLA	CHB-C4A-NA	2.04	127.35	124.40
15	B	1021	CLA	C11-C12-C13	-2.04	109.17	115.97
15	A	1801	CLA	CAC-C3C-C2C	2.04	131.31	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4005	BCR	C33-C5-C4	2.04	117.95	113.60
15	A	1801	CLA	CHB-C4A-NA	2.04	127.35	124.40
15	B	1239	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
15	A	1113	CLA	CHB-C4A-NA	2.04	127.34	124.40
15	A	1116	CLA	CHB-C4A-NA	2.04	127.34	124.40
15	A	1102	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
15	B	1205	CLA	C1-O2A-CGA	2.04	121.58	116.65
15	B	1206	CLA	C3C-C4C-NC	2.04	113.04	110.43
15	A	1107	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
15	B	1204	CLA	CHB-C4A-NA	2.04	127.34	124.40
15	A	1120	CLA	CED-O2D-CGD	2.04	120.53	115.92
15	B	1238	CLA	CAC-C3C-C4C	2.04	127.44	124.79
15	B	1214	CLA	CMB-C2B-C1B	2.03	128.51	125.42
14	A	4008	BCR	C35-C13-C12	2.03	121.19	118.09
15	B	1235	CLA	C1-C2-C3	-2.03	122.87	126.20
15	B	1235	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
15	B	1240	CLA	CAC-C3C-C4C	2.03	127.43	124.79
15	A	1136	CLA	CED-O2D-CGD	2.03	120.52	115.92
15	B	1236	CLA	CHD-C4C-C3C	-2.03	121.82	124.77
14	A	4008	BCR	C34-C9-C10	-2.03	119.53	122.82
15	B	1219	CLA	C3C-C4C-NC	2.03	113.03	110.43
15	B	1220	CLA	CAC-C3C-C4C	2.03	127.43	124.79
15	A	1801	CLA	C4-C3-C2	-2.03	118.42	123.63
14	A	4008	BCR	C30-C25-C24	2.03	121.15	115.65
15	A	1109	CLA	CED-O2D-CGD	2.03	120.51	115.92
15	B	1210	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
15	J	1303	CLA	CHB-C4A-NA	2.02	127.32	124.40
15	A	1138	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
15	B	1224	CLA	C3C-C4C-NC	2.02	113.02	110.43
14	A	4002	BCR	C33-C5-C4	2.02	117.91	113.60
15	B	1231	CLA	C1-O2A-CGA	2.02	121.55	116.65
15	A	1120	CLA	CHB-C4A-NA	2.02	127.32	124.40
15	A	1134	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
15	A	1128	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
14	B	4006	BCR	C19-C18-C17	2.02	122.19	119.01
14	B	4006	BCR	C30-C25-C24	2.02	121.13	115.65
15	A	1138	CLA	CHB-C4A-NA	2.02	127.32	124.40
15	J	1303	CLA	CAC-C3C-C4C	2.02	127.42	124.79
15	B	1207	CLA	CAC-C3C-C4C	2.02	127.42	124.79
15	B	1224	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
15	A	1120	CLA	CAC-C3C-C4C	2.02	127.41	124.79
15	F	1139	CLA	C1-C2-C3	-2.02	122.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1119	CLA	CMB-C2B-C3B	2.02	131.29	126.55
15	A	1129	CLA	CHB-C4A-NA	2.02	127.31	124.40
15	B	1206	CLA	CED-O2D-CGD	2.01	120.49	115.92
15	A	1114	CLA	O1D-CGD-CBD	-2.01	120.54	124.52
15	B	1223	CLA	C1-O2A-CGA	2.01	121.53	116.65
15	K	1402	CLA	CAC-C3C-C4C	2.01	127.41	124.79
15	B	1231	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
15	B	1209	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
15	A	1101	CLA	C4B-CHC-C1C	2.01	130.97	126.25
14	B	4010	BCR	C37-C22-C21	-2.01	119.56	122.82
14	B	4011	BCR	C4-C5-C6	-2.00	120.00	122.70
15	B	1240	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
15	A	1136	CLA	CHB-C4A-NA	2.00	127.29	124.40
15	B	1226	CLA	CHB-C4A-NA	2.00	127.29	124.40
15	B	1210	CLA	CMB-C2B-C3B	2.00	131.26	126.55
15	K	1402	CLA	CED-O2D-CGD	2.00	120.46	115.92
15	B	1218	CLA	OBD-CAD-C3D	-2.00	123.74	128.42

All (86) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CL0	ND
13	A	1011	CL0	NC
13	A	1011	CL0	NA
13	A	1108	CL0	ND
13	A	1108	CL0	NC
13	A	1108	CL0	NA
15	A	1801	CLA	ND
15	A	1022	CLA	ND
15	A	1101	CLA	ND
15	A	1102	CLA	ND
15	A	1103	CLA	ND
15	A	1104	CLA	ND
15	A	1105	CLA	ND
15	A	1106	CLA	ND
15	A	1110	CLA	ND
15	A	1111	CLA	ND
15	A	1112	CLA	ND
15	A	1113	CLA	ND
15	A	1116	CLA	ND
15	A	1117	CLA	ND
15	A	1118	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1122	CLA	ND
15	A	1123	CLA	ND
15	A	1124	CLA	ND
15	A	1125	CLA	ND
15	A	1127	CLA	ND
15	A	1128	CLA	ND
15	A	1136	CLA	ND
15	A	1137	CLA	ND
15	A	1138	CLA	ND
15	A	1140	CLA	ND
15	A	1012	CLA	ND
15	A	1114	CLA	ND
15	A	1115	CLA	ND
15	A	1120	CLA	ND
15	A	1121	CLA	ND
15	A	1129	CLA	ND
15	A	1130	CLA	ND
15	A	1131	CLA	ND
15	A	1132	CLA	ND
15	A	1133	CLA	ND
15	A	1134	CLA	ND
15	A	1135	CLA	ND
15	B	1240	CLA	ND
15	B	1021	CLA	ND
15	B	1023	CLA	ND
15	B	1202	CLA	ND
15	B	1203	CLA	ND
15	B	1205	CLA	ND
15	B	1207	CLA	ND
15	B	1208	CLA	ND
15	B	1209	CLA	ND
15	B	1210	CLA	ND
15	B	1212	CLA	ND
15	B	1215	CLA	ND
15	B	1217	CLA	ND
15	B	1218	CLA	ND
15	B	1219	CLA	ND
15	B	1220	CLA	ND
15	B	1221	CLA	ND
15	B	1223	CLA	ND
15	B	1224	CLA	ND
15	B	1225	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1226	CLA	ND
15	B	1228	CLA	ND
15	B	1229	CLA	ND
15	B	1230	CLA	ND
15	B	1231	CLA	ND
15	B	1232	CLA	ND
15	B	1234	CLA	ND
15	B	1235	CLA	ND
15	B	1236	CLA	ND
15	B	1201	CLA	ND
15	B	1204	CLA	ND
15	B	1206	CLA	ND
15	B	1211	CLA	ND
15	B	1237	CLA	ND
15	B	1238	CLA	ND
15	B	1239	CLA	ND
15	F	1410	CLA	ND
15	F	1139	CLA	ND
15	F	1301	CLA	ND
15	J	1303	CLA	ND
15	J	1302	CLA	ND
15	K	1401	CLA	ND
15	K	1402	CLA	ND

All (1356) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	5001	LHG	C1-C2-C3-O3
12	A	5003	LHG	C1-C2-C3-O3
12	A	5003	LHG	C3-O3-P-O6
12	A	5003	LHG	C4-O6-P-O3
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
12	A	5005	LHG	C3-O3-P-O6
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
13	A	1108	CL0	CBD-CGD-O2D-CED
14	A	4001	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
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
14	A	4002	BCR	C7-C8-C9-C10
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C11-C10-C9-C34
14	A	4003	BCR	C7-C8-C9-C10
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	A	4007	BCR	C7-C8-C9-C10
14	A	4007	BCR	C7-C8-C9-C34
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
14	A	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
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
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
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C23-C24-C25-C26
14	B	4006	BCR	C23-C24-C25-C30
14	B	4009	BCR	C11-C10-C9-C8
14	B	4009	BCR	C11-C10-C9-C34
14	B	4009	BCR	C10-C11-C12-C13
14	B	4010	BCR	C17-C18-C19-C20
14	B	4010	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	B	4010	BCR	C23-C24-C25-C30
14	B	4011	BCR	C7-C8-C9-C10
14	B	4011	BCR	C7-C8-C9-C34
14	B	4011	BCR	C23-C24-C25-C26
14	B	4011	BCR	C23-C24-C25-C30
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	4017	BCR	C7-C8-C9-C10
14	B	4017	BCR	C11-C10-C9-C8
14	B	4017	BCR	C11-C10-C9-C34
14	B	4017	BCR	C10-C11-C12-C13
14	F	4015	BCR	C17-C18-C19-C20
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	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	1801	CLA	CBA-CGA-O2A-C1
15	A	1801	CLA	O1A-CGA-O2A-C1
15	A	1801	CLA	C2B-C3B-CAB-CBB
15	A	1801	CLA	C4B-C3B-CAB-CBB
15	A	1801	CLA	CAD-CBD-CGD-O1D
15	A	1801	CLA	CAD-CBD-CGD-O2D
15	A	1022	CLA	C2-C1-O2A-CGA
15	A	1022	CLA	C2B-C3B-CAB-CBB
15	A	1022	CLA	C4B-C3B-CAB-CBB
15	A	1022	CLA	CBD-CGD-O2D-CED
15	A	1102	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	A	1104	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1104	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
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	A	1109	CLA	CBD-CGD-O2D-CED
15	A	1110	CLA	C1A-C2A-CAA-CBA
15	A	1111	CLA	C2B-C3B-CAB-CBB
15	A	1111	CLA	C4B-C3B-CAB-CBB
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C3A-C2A-CAA-CBA
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1113	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1118	CLA	CAD-CBD-CGD-O2D
15	A	1123	CLA	C1A-C2A-CAA-CBA
15	A	1123	CLA	C3A-C2A-CAA-CBA
15	A	1123	CLA	C2-C1-O2A-CGA
15	A	1124	CLA	C1A-C2A-CAA-CBA
15	A	1124	CLA	C3A-C2A-CAA-CBA
15	A	1126	CLA	C4B-C3B-CAB-CBB
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1127	CLA	C4-C3-C5-C6
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1137	CLA	C2-C1-O2A-CGA
15	A	1012	CLA	C2B-C3B-CAB-CBB
15	A	1012	CLA	C4B-C3B-CAB-CBB
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	CAD-CBD-CGD-O2D
15	A	1115	CLA	CBA-CGA-O2A-C1
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	A	1120	CLA	C3A-C2A-CAA-CBA
15	A	1120	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	C3A-C2A-CAA-CBA
15	A	1129	CLA	CBA-CGA-O2A-C1
15	A	1129	CLA	C2B-C3B-CAB-CBB
15	A	1129	CLA	C4B-C3B-CAB-CBB
15	A	1132	CLA	C2B-C3B-CAB-CBB
15	A	1132	CLA	C4B-C3B-CAB-CBB
15	A	1132	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	1132	CLA	CHA-CBD-CGD-O2D
15	A	1132	CLA	C11-C10-C8-C7
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	1134	CLA	CBA-CGA-O2A-C1
15	A	1134	CLA	CBD-CGD-O2D-CED
15	A	1135	CLA	CBD-CGD-O2D-CED
15	B	1013	CLA	C2-C1-O2A-CGA
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
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	B	1202	CLA	CAD-CBD-CGD-O1D
15	B	1202	CLA	CAD-CBD-CGD-O2D
15	B	1205	CLA	CHA-CBD-CGD-O1D
15	B	1205	CLA	CHA-CBD-CGD-O2D
15	B	1207	CLA	CBD-CGD-O2D-CED
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	B	1212	CLA	C2B-C3B-CAB-CBB
15	B	1212	CLA	C4B-C3B-CAB-CBB
15	B	1213	CLA	C2B-C3B-CAB-CBB
15	B	1213	CLA	C4B-C3B-CAB-CBB
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1215	CLA	CBD-CGD-O2D-CED
15	B	1215	CLA	C11-C12-C13-C14
15	B	1216	CLA	C2B-C3B-CAB-CBB
15	B	1216	CLA	C4B-C3B-CAB-CBB
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
15	B	1219	CLA	C2-C1-O2A-CGA
15	B	1220	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
15	B	1222	CLA	C1A-C2A-CAA-CBA
15	B	1222	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1224	CLA	CBD-CGD-O2D-CED
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1225	CLA	C3A-C2A-CAA-CBA
15	B	1225	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	C2B-C3B-CAB-CBB
15	B	1226	CLA	C4B-C3B-CAB-CBB
15	B	1226	CLA	CHA-CBD-CGD-O1D
15	B	1226	CLA	CHA-CBD-CGD-O2D
15	B	1227	CLA	C2B-C3B-CAB-CBB
15	B	1227	CLA	C4B-C3B-CAB-CBB
15	B	1228	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	C1A-C2A-CAA-CBA
15	B	1229	CLA	C4B-C3B-CAB-CBB
15	B	1230	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	B	1231	CLA	CBD-CGD-O2D-CED
15	B	1236	CLA	CBD-CGD-O2D-CED
15	B	1204	CLA	C2B-C3B-CAB-CBB
15	B	1204	CLA	C4B-C3B-CAB-CBB
15	B	1206	CLA	CBA-CGA-O2A-C1
15	B	1206	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C3A-C2A-CAA-CBA
15	B	1237	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	B	1239	CLA	C3A-C2A-CAA-CBA
15	B	1239	CLA	CBD-CGD-O2D-CED
15	F	1410	CLA	C4-C3-C5-C6
15	F	1139	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	C1A-C2A-CAA-CBA
15	J	1302	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	CAD-CBD-CGD-O1D
15	K	1401	CLA	CAD-CBD-CGD-O2D
15	A	1109	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	A	1124	CLA	O1D-CGD-O2D-CED
15	A	1134	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1203	CLA	O1D-CGD-O2D-CED
15	B	1208	CLA	O1D-CGD-O2D-CED
15	B	1238	CLA	O1D-CGD-O2D-CED
15	J	1303	CLA	O1D-CGD-O2D-CED
15	A	1117	CLA	O1D-CGD-O2D-CED
15	B	1240	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	B	1231	CLA	O1D-CGD-O2D-CED
15	B	1232	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	K	1402	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1111	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	A	1118	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	B	1240	CLA	CBD-CGD-O2D-CED
15	B	1203	CLA	CBD-CGD-O2D-CED
15	B	1208	CLA	CBD-CGD-O2D-CED
15	B	1210	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED
15	B	1219	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	F	1410	CLA	CBD-CGD-O2D-CED
15	J	1303	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	CBD-CGD-O2D-CED
15	K	1401	CLA	CBD-CGD-O2D-CED
15	K	1402	CLA	CBD-CGD-O2D-CED
15	A	1110	CLA	O1A-CGA-O2A-C1
15	B	1013	CLA	O1A-CGA-O2A-C1
15	F	1410	CLA	O1A-CGA-O2A-C1
15	A	1115	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	O1A-CGA-O2A-C1
15	A	1133	CLA	O1A-CGA-O2A-C1
15	A	1134	CLA	O1A-CGA-O2A-C1
15	B	1206	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1A-CGA-O2A-C1
15	K	1401	CLA	O1A-CGA-O2A-C1
15	A	1801	CLA	C4C-C3C-CAC-CBC
15	A	1104	CLA	O1D-CGD-O2D-CED
15	B	1211	CLA	CBA-CGA-O2A-C1
12	A	5005	LHG	C5-C6-O8-C23
15	A	1131	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	CBA-CGA-O2A-C1
15	A	1102	CLA	O1A-CGA-O2A-C1
15	A	1109	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	O1A-CGA-O2A-C1
15	A	1132	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	O1A-CGA-O2A-C1
15	B	1237	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	O1A-CGA-O2A-C1
15	A	1022	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	A	1111	CLA	O1D-CGD-O2D-CED
15	A	1120	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	B	1218	CLA	O1D-CGD-O2D-CED
15	F	1410	CLA	O1D-CGD-O2D-CED
13	A	1108	CL0	O1D-CGD-O2D-CED
15	A	1105	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	O1D-CGD-O2D-CED
15	B	1215	CLA	O1D-CGD-O2D-CED
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	A	1130	CLA	CBD-CGD-O2D-CED
15	B	1205	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	CBD-CGD-O2D-CED
15	B	1223	CLA	CBD-CGD-O2D-CED
15	A	1123	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1239	CLA	O1D-CGD-O2D-CED
15	A	1118	CLA	CBA-CGA-O2A-C1
15	A	1126	CLA	C3-C5-C6-C7
15	A	1136	CLA	C3-C5-C6-C7
15	A	1012	CLA	C3-C5-C6-C7
15	A	1131	CLA	C3-C5-C6-C7
15	A	1132	CLA	C3-C5-C6-C7
15	B	1205	CLA	C3-C5-C6-C7
15	A	1801	CLA	C2C-C3C-CAC-CBC
15	A	1104	CLA	CBA-CGA-O2A-C1
15	A	1109	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	A	1119	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
15	B	1013	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	CBA-CGA-O2A-C1
15	B	1210	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	B	1237	CLA	CBA-CGA-O2A-C1
15	F	1410	CLA	CBA-CGA-O2A-C1
15	A	1801	CLA	CBD-CGD-O2D-CED
15	A	1106	CLA	CBD-CGD-O2D-CED
15	A	1122	CLA	CBD-CGD-O2D-CED
15	A	1125	CLA	CBD-CGD-O2D-CED
15	A	1136	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CBD-CGD-O2D-CED
15	B	1212	CLA	CBD-CGD-O2D-CED
15	B	1213	CLA	CBD-CGD-O2D-CED
15	B	1220	CLA	CBD-CGD-O2D-CED
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	CBD-CGD-O2D-CED
15	B	1201	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	C2-C1-O2A-CGA
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	O1D-CGD-O2D-CED
15	B	1207	CLA	O1D-CGD-O2D-CED
15	B	1210	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	F	1301	CLA	O1D-CGD-O2D-CED
15	F	1139	CLA	O1D-CGD-O2D-CED
15	B	1215	CLA	C4-C3-C5-C6
15	A	1127	CLA	C2-C3-C5-C6
15	F	1410	CLA	C2-C3-C5-C6
15	K	1402	CLA	CBA-CGA-O2A-C1
15	B	1013	CLA	CBD-CGD-O2D-CED
15	B	1214	CLA	CBD-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
16	B	1301	LMU	O5B-C5B-C6B-O6B
17	B	5002	LMG	O6-C5-C6-O5
15	A	1128	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	C3-C5-C6-C7
15	A	1102	CLA	CBA-CGA-O2A-C1
15	A	1130	CLA	CBA-CGA-O2A-C1
15	A	1132	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	CBA-CGA-O2A-C1
15	B	1226	CLA	CBA-CGA-O2A-C1
15	K	1402	CLA	O1A-CGA-O2A-C1
16	J	1304	LMU	C4B-C5B-C6B-O6B
14	A	4007	BCR	C19-C20-C21-C22
14	A	4008	BCR	C19-C20-C21-C22
14	B	4009	BCR	C9-C10-C11-C12
14	B	4014	BCR	C15-C16-C17-C18
15	A	1104	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	B	1221	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1D-CGD-O2D-CED
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	B	1228	CLA	O1D-CGD-O2D-CED
15	K	1401	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	C3-C5-C6-C7
15	B	1216	CLA	C3-C5-C6-C7
15	A	1102	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CBD-CGD-O2D-CED
12	A	5001	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
12	A	5003	LHG	O2-C2-C3-O3
15	A	1116	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1
17	B	5002	LMG	C29-C28-O8-C9
15	B	1202	CLA	O1A-CGA-O2A-C1
15	B	1210	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBA-CGA-O2A-C1
15	B	1239	CLA	CBA-CGA-O2A-C1
15	A	1138	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1A-CGA-O2A-C1
17	B	5002	LMG	C4-C5-C6-O5
15	A	1123	CLA	C3-C5-C6-C7
15	A	1127	CLA	C3-C5-C6-C7
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	CBA-CGA-O2A-C1
15	A	1109	CLA	C4-C3-C5-C6
15	B	1214	CLA	C4-C3-C5-C6
15	B	1225	CLA	C4-C3-C5-C6
15	B	1230	CLA	C4-C3-C5-C6
15	A	1109	CLA	C2-C3-C5-C6
15	B	1225	CLA	C2-C3-C5-C6
15	B	1230	CLA	C2-C3-C5-C6
16	B	1301	LMU	C4B-C5B-C6B-O6B
15	B	1232	CLA	C2A-CAA-CBA-CGA
15	B	1217	CLA	O1D-CGD-O2D-CED
15	B	1226	CLA	O1D-CGD-O2D-CED
17	B	5002	LMG	O10-C28-O8-C9
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	CBD-CGD-O2D-CED
15	B	1235	CLA	CBD-CGD-O2D-CED
15	B	1204	CLA	CBD-CGD-O2D-CED
16	J	1304	LMU	O5B-C5B-C6B-O6B
16	B	1301	LMU	O5'-C5'-C6'-O6'
15	A	1801	CLA	O1D-CGD-O2D-CED
15	B	1230	CLA	O1D-CGD-O2D-CED
14	B	4017	BCR	C9-C10-C11-C12
15	B	1218	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1130	CLA	O1D-CGD-O2D-CED
15	B	1220	CLA	O1D-CGD-O2D-CED
15	B	1223	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	CBA-CGA-O2A-C1
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	B	1205	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	B	1212	CLA	O1D-CGD-O2D-CED
15	B	1213	CLA	O1D-CGD-O2D-CED
15	B	1201	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	C2-C3-C5-C6
15	B	1215	CLA	C2-C3-C5-C6
15	A	1105	CLA	C11-C10-C8-C9
15	A	1105	CLA	C11-C12-C13-C14
15	A	1106	CLA	C14-C13-C15-C16
15	A	1128	CLA	C6-C7-C8-C9
15	B	1013	CLA	C14-C13-C15-C16
15	B	1203	CLA	C14-C13-C15-C16
15	B	1234	CLA	C14-C13-C15-C16
15	A	1106	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	A	1137	CLA	CBD-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	A	1136	CLA	O1D-CGD-O2D-CED
14	A	4008	BCR	C7-C8-C9-C34
14	B	4004	BCR	C7-C8-C9-C34
14	B	4005	BCR	C7-C8-C9-C34
14	B	4005	BCR	C37-C22-C23-C24
14	B	4006	BCR	C37-C22-C23-C24
14	B	4009	BCR	C7-C8-C9-C34
14	B	4010	BCR	C36-C18-C19-C20
14	B	4011	BCR	C36-C18-C19-C20
14	B	4011	BCR	C37-C22-C23-C24
14	B	4014	BCR	C37-C22-C23-C24
14	B	4017	BCR	C7-C8-C9-C34
14	F	4015	BCR	C36-C18-C19-C20
14	F	4016	BCR	C37-C22-C23-C24
14	J	4013	BCR	C7-C8-C9-C34
14	A	4003	BCR	C17-C18-C19-C20
14	A	4007	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C7-C8-C9-C10
14	A	4012	BCR	C21-C22-C23-C24
14	B	4005	BCR	C7-C8-C9-C10
14	B	4006	BCR	C21-C22-C23-C24
14	B	4009	BCR	C7-C8-C9-C10
14	B	4011	BCR	C21-C22-C23-C24
14	J	4013	BCR	C7-C8-C9-C10
15	A	1140	CLA	O1A-CGA-O2A-C1
15	B	1235	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	C2-C1-O2A-CGA
15	A	1104	CLA	C2-C1-O2A-CGA
15	A	1117	CLA	C2-C1-O2A-CGA
15	B	1203	CLA	C2-C1-O2A-CGA
15	B	1213	CLA	C2-C1-O2A-CGA
15	B	1214	CLA	C2-C1-O2A-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1218	CLA	C2-C1-O2A-CGA
15	A	1129	CLA	O1D-CGD-O2D-CED
16	B	1301	LMU	C4'-C5'-C6'-O6'
10	A	2001	PQN	C18-C20-C21-C22
15	A	1012	CLA	C5-C6-C7-C8
15	B	1216	CLA	C15-C16-C17-C18
15	A	1122	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	CBA-CGA-O2A-C1
10	B	2002	PQN	C15-C16-C17-C18
15	B	1210	CLA	C8-C10-C11-C12
15	B	1228	CLA	C10-C11-C12-C13
14	B	4004	BCR	C19-C20-C21-C22
15	B	1239	CLA	O1A-CGA-O2A-C1
15	B	1220	CLA	C3-C5-C6-C7
15	B	1225	CLA	C5-C6-C7-C8
15	B	1230	CLA	O1A-CGA-O2A-C1
12	A	5005	LHG	C8-C7-O7-C5
15	B	1211	CLA	O1D-CGD-O2D-CED
15	B	1222	CLA	CBA-CGA-O2A-C1
15	A	1122	CLA	C10-C11-C12-C13
15	A	1126	CLA	C10-C11-C12-C13
15	B	1203	CLA	C10-C11-C12-C13
15	A	1119	CLA	C2A-CAA-CBA-CGA
15	A	1134	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	C2A-CAA-CBA-CGA
15	B	1219	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	B	2002	PQN	C18-C20-C21-C22
15	A	1104	CLA	C15-C16-C17-C18
15	A	1127	CLA	C8-C10-C11-C12
15	B	1023	CLA	C15-C16-C17-C18
15	B	1216	CLA	C13-C15-C16-C17
15	B	1221	CLA	C5-C6-C7-C8
15	B	1225	CLA	C13-C15-C16-C17
15	B	1234	CLA	C8-C10-C11-C12
15	F	1410	CLA	C10-C11-C12-C13
12	B	5004	LHG	C23-C24-C25-C26
15	B	1202	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	C13-C15-C16-C17
15	A	1126	CLA	C13-C15-C16-C17
15	A	1127	CLA	C15-C16-C17-C18
15	B	1023	CLA	C8-C10-C11-C12
15	B	1210	CLA	C5-C6-C7-C8
15	B	1220	CLA	C5-C6-C7-C8
15	B	1224	CLA	C8-C10-C11-C12
15	B	1224	CLA	C15-C16-C17-C18
15	B	1226	CLA	C8-C10-C11-C12
15	B	1226	CLA	C13-C15-C16-C17
15	B	1229	CLA	C8-C10-C11-C12
15	A	1105	CLA	C13-C15-C16-C17
15	B	1021	CLA	C13-C15-C16-C17
15	B	1215	CLA	C5-C6-C7-C8
16	B	1301	LMU	O1'-C1-C2-C3
15	B	1207	CLA	CBA-CGA-O2A-C1
16	J	1304	LMU	O1'-C1-C2-C3
15	A	1102	CLA	O1D-CGD-O2D-CED
15	B	1013	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	O1D-CGD-O2D-CED
15	A	1102	CLA	C13-C15-C16-C17
15	B	1202	CLA	C15-C16-C17-C18
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1135	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	O1D-CGD-O2D-CED
15	A	1128	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	C8-C10-C11-C12
15	B	1013	CLA	C10-C11-C12-C13
15	B	1231	CLA	C3-C5-C6-C7
15	A	1132	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	4001	BCR	C19-C20-C21-C22
14	A	4003	BCR	C13-C14-C15-C16
15	A	1101	CLA	C10-C11-C12-C13
12	A	5005	LHG	O9-C7-O7-C5
15	A	1801	CLA	C2A-CAA-CBA-CGA
15	A	1111	CLA	C2A-CAA-CBA-CGA
15	F	1139	CLA	CBA-CGA-O2A-C1
15	A	1105	CLA	C5-C6-C7-C8
15	A	1122	CLA	C8-C10-C11-C12
15	B	1021	CLA	C8-C10-C11-C12
15	B	1202	CLA	C13-C15-C16-C17
15	B	1223	CLA	C5-C6-C7-C8
15	B	1230	CLA	C13-C15-C16-C17
15	B	1234	CLA	C10-C11-C12-C13
15	B	1234	CLA	C15-C16-C17-C18
15	A	1117	CLA	C3-C5-C6-C7
15	A	1012	CLA	C15-C16-C17-C18
15	B	1235	CLA	C15-C16-C17-C18
15	A	1103	CLA	C8-C10-C11-C12
15	B	1231	CLA	C5-C6-C7-C8
15	A	1132	CLA	O1D-CGD-O2D-CED
15	A	1122	CLA	CBA-CGA-O2A-C1
15	A	1131	CLA	CBA-CGA-O2A-C1
15	A	1117	CLA	C13-C15-C16-C17
14	A	4012	BCR	C11-C10-C9-C34
14	B	4004	BCR	C11-C10-C9-C34
14	A	4003	BCR	C37-C22-C23-C24
14	A	4007	BCR	C37-C22-C23-C24
14	F	4015	BCR	C7-C8-C9-C34
14	F	4015	BCR	C37-C22-C23-C24
14	B	4011	BCR	C17-C18-C19-C20
14	B	4014	BCR	C21-C22-C23-C24
14	F	4015	BCR	C7-C8-C9-C10
15	B	1222	CLA	O1A-CGA-O2A-C1
15	A	1126	CLA	C2A-CAA-CBA-CGA
15	A	1140	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C5-C6-C7-C8
15	B	1224	CLA	C13-C15-C16-C17
15	A	1012	CLA	O2A-C1-C2-C3
14	F	4015	BCR	C15-C16-C17-C18
15	A	1126	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	B	1203	CLA	C16-C17-C18-C19
15	B	1229	CLA	C16-C17-C18-C20
15	B	1222	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	C3-C5-C6-C7
15	B	1221	CLA	C15-C16-C17-C18
14	A	4002	BCR	C11-C10-C9-C8
14	A	4012	BCR	C11-C10-C9-C8
14	B	4004	BCR	C11-C10-C9-C8
14	F	4016	BCR	C11-C10-C9-C8
17	B	5002	LMG	C11-C10-O7-C8
15	A	1109	CLA	C15-C16-C17-C18
15	A	1127	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	C8-C10-C11-C12
15	A	1105	CLA	C15-C16-C17-C18
15	A	1132	CLA	C5-C6-C7-C8
15	F	1139	CLA	C8-C10-C11-C12
15	A	1101	CLA	C2-C1-O2A-CGA
15	A	1126	CLA	C2-C1-O2A-CGA
15	A	1114	CLA	C2-C1-O2A-CGA
15	A	1130	CLA	C2-C1-O2A-CGA
15	A	1135	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	C2-C1-O2A-CGA
13	A	1011	CL0	C16-C17-C18-C19
15	A	1103	CLA	C16-C17-C18-C19
15	A	1128	CLA	C16-C17-C18-C19
15	B	1210	CLA	C15-C16-C17-C18
12	B	5004	LHG	C13-C14-C15-C16
17	B	5002	LMG	C32-C33-C34-C35
17	B	5002	LMG	C23-C24-C25-C26
12	A	5003	LHG	C30-C31-C32-C33
17	B	5002	LMG	C14-C15-C16-C17
17	B	5002	LMG	O9-C10-O7-C8
12	A	5005	LHG	O1-C1-C2-O2
12	B	5004	LHG	O1-C1-C2-O2
12	A	5003	LHG	C11-C12-C13-C14
12	A	5005	LHG	C10-C11-C12-C13
16	B	1301	LMU	C6-C7-C8-C9
15	B	1235	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	C4B-C3B-CAB-CBB
15	A	1109	CLA	C4B-C3B-CAB-CBB
15	A	1127	CLA	C4B-C3B-CAB-CBB
15	A	1140	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	B	1023	CLA	C4B-C3B-CAB-CBB
15	B	1221	CLA	C4B-C3B-CAB-CBB
15	B	1224	CLA	C4B-C3B-CAB-CBB
15	B	1225	CLA	C4B-C3B-CAB-CBB
15	B	1206	CLA	C4B-C3B-CAB-CBB
16	B	1301	LMU	C3-C4-C5-C6
17	B	5002	LMG	C33-C34-C35-C36
15	A	1103	CLA	C16-C17-C18-C20
15	A	1111	CLA	C11-C12-C13-C14
15	A	1126	CLA	C16-C17-C18-C19
15	B	1223	CLA	C16-C17-C18-C19
15	B	1223	CLA	C16-C17-C18-C20
15	B	1229	CLA	C16-C17-C18-C19
15	B	1229	CLA	O1D-CGD-O2D-CED
12	A	5005	LHG	C9-C10-C11-C12
15	A	1122	CLA	C11-C12-C13-C15
15	A	1122	CLA	C5-C6-C7-C8
15	A	1123	CLA	C10-C11-C12-C13
15	F	1139	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	A	1107	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C3A-C2A-CAA-CBA
15	A	1131	CLA	C3A-C2A-CAA-CBA
15	B	1234	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
15	B	1216	CLA	C8-C10-C11-C12
15	B	1204	CLA	O1D-CGD-O2D-CED
14	B	4014	BCR	C9-C10-C11-C12
13	A	1011	CL0	C16-C17-C18-C20
15	A	1111	CLA	C11-C12-C13-C15
15	B	1234	CLA	CBA-CGA-O2A-C1
12	A	5001	LHG	C28-C29-C30-C31
15	A	1103	CLA	C10-C11-C12-C13
16	B	1301	LMU	C2-C3-C4-C5
15	A	1127	CLA	O1A-CGA-O2A-C1
15	A	1131	CLA	O1A-CGA-O2A-C1
12	A	5003	LHG	C33-C34-C35-C36
15	B	1203	CLA	C16-C17-C18-C20
12	A	5003	LHG	C7-C8-C9-C10
14	A	4001	BCR	C23-C24-C25-C30
14	A	4008	BCR	C1-C6-C7-C8
14	A	4012	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	A	4012	BCR	C23-C24-C25-C30
14	B	4005	BCR	C1-C6-C7-C8
14	B	4009	BCR	C1-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
15	A	1109	CLA	C2B-C3B-CAB-CBB
15	A	1126	CLA	C2B-C3B-CAB-CBB
15	A	1127	CLA	C2B-C3B-CAB-CBB
15	A	1140	CLA	C2B-C3B-CAB-CBB
15	B	1214	CLA	C2B-C3B-CAB-CBB
15	B	1229	CLA	C2B-C3B-CAB-CBB
15	A	1107	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	C3-C5-C6-C7
15	B	1228	CLA	C3-C5-C6-C7
12	A	5003	LHG	C14-C15-C16-C17
12	B	5004	LHG	C11-C12-C13-C14
15	A	1136	CLA	C2A-CAA-CBA-CGA
15	A	1122	CLA	O1A-CGA-O2A-C1
16	J	1304	LMU	C6-C7-C8-C9
15	A	1110	CLA	C4-C3-C5-C6
15	B	1231	CLA	C4-C3-C5-C6
12	A	5001	LHG	C31-C32-C33-C34
14	B	4005	BCR	C10-C11-C12-C13
14	J	4013	BCR	C10-C11-C12-C13
15	A	1119	CLA	C8-C10-C11-C12
15	B	1223	CLA	C15-C16-C17-C18
15	A	1122	CLA	C2-C3-C5-C6
15	A	1137	CLA	CBA-CGA-O2A-C1
16	J	1304	LMU	C7-C8-C9-C10
15	A	1124	CLA	C5-C6-C7-C8
15	B	1231	CLA	C8-C10-C11-C12
12	A	5001	LHG	C11-C12-C13-C14
12	A	5001	LHG	C25-C26-C27-C28
12	A	5003	LHG	C28-C29-C30-C31
17	B	5002	LMG	C2-C1-O1-C7
15	B	1224	CLA	C5-C6-C7-C8
15	B	1228	CLA	C13-C15-C16-C17
10	B	2002	PQN	C20-C21-C22-C23
15	A	1128	CLA	CBA-CGA-O2A-C1
14	A	4001	BCR	C13-C14-C15-C16
14	A	4001	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	B	4011	BCR	C19-C20-C21-C22
15	A	1101	CLA	C16-C17-C18-C19
15	A	1128	CLA	C16-C17-C18-C20
10	B	2002	PQN	C25-C26-C27-C28
15	A	1101	CLA	C8-C10-C11-C12
15	A	1117	CLA	C10-C11-C12-C13
15	B	1230	CLA	C8-C10-C11-C12
14	B	4010	BCR	C37-C22-C23-C24
14	B	4010	BCR	C21-C22-C23-C24
12	A	5005	LHG	C25-C26-C27-C28
15	B	1225	CLA	C2A-CAA-CBA-CGA
15	A	1110	CLA	CBD-CGD-O2D-CED
17	B	5002	LMG	C11-C12-C13-C14
15	A	1122	CLA	C13-C15-C16-C17
15	A	1136	CLA	C15-C16-C17-C18
15	B	1214	CLA	C8-C10-C11-C12
15	B	1021	CLA	C15-C16-C17-C18
15	B	1234	CLA	O1A-CGA-O2A-C1
16	J	1304	LMU	C2-C3-C4-C5
15	A	1122	CLA	C3-C5-C6-C7
15	B	1228	CLA	C15-C16-C17-C18
15	B	1237	CLA	C5-C6-C7-C8
12	A	5001	LHG	C24-C25-C26-C27
17	B	5002	LMG	C21-C22-C23-C24
15	F	1139	CLA	C2-C1-O2A-CGA
15	A	1103	CLA	C5-C6-C7-C8
15	A	1117	CLA	C8-C10-C11-C12
12	B	5004	LHG	C11-C10-C9-C8
12	B	5004	LHG	C9-C10-C11-C12
15	A	1135	CLA	C4-C3-C5-C6
15	B	1228	CLA	C4-C3-C5-C6
15	A	1110	CLA	C2-C3-C5-C6
12	A	5001	LHG	C26-C27-C28-C29
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	A	1127	CLA	C2A-CAA-CBA-CGA
15	A	1115	CLA	C2A-CAA-CBA-CGA
16	B	1301	LMU	C5-C6-C7-C8
15	B	1225	CLA	C10-C11-C12-C13
15	A	1107	CLA	O1A-CGA-O2A-C1
15	A	1128	CLA	O1A-CGA-O2A-C1
15	A	1137	CLA	O1A-CGA-O2A-C1
15	A	1102	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1107	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1117	CLA	C1A-C2A-CAA-CBA
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	A	1122	CLA	C1A-C2A-CAA-CBA
15	A	1129	CLA	C1A-C2A-CAA-CBA
15	A	1131	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	B	1208	CLA	C1A-C2A-CAA-CBA
15	B	1209	CLA	C1A-C2A-CAA-CBA
15	B	1212	CLA	C1A-C2A-CAA-CBA
15	B	1215	CLA	C1A-C2A-CAA-CBA
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	B	1217	CLA	C1A-C2A-CAA-CBA
15	B	1218	CLA	C1A-C2A-CAA-CBA
15	B	1226	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	B	1239	CLA	C1A-C2A-CAA-CBA
15	K	1401	CLA	C1A-C2A-CAA-CBA
12	A	5001	LHG	O6-C4-C5-C6
15	A	1104	CLA	C11-C12-C13-C15
15	A	1105	CLA	C11-C12-C13-C15
15	A	1136	CLA	C12-C13-C15-C16
15	B	1021	CLA	C6-C7-C8-C10
15	B	1215	CLA	C11-C10-C8-C7
15	B	1224	CLA	C11-C12-C13-C15
15	B	1226	CLA	C6-C7-C8-C10
15	A	1101	CLA	C16-C17-C18-C20
15	A	1127	CLA	C16-C17-C18-C19
12	A	5003	LHG	C11-C10-C9-C8
15	A	1128	CLA	C10-C11-C12-C13
15	B	1215	CLA	C15-C16-C17-C18
15	A	1137	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C11-C10-C8-C9
15	A	1117	CLA	C6-C7-C8-C9
15	A	1136	CLA	C14-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C9
15	B	1202	CLA	C11-C12-C13-C14
15	B	1214	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	B	1215	CLA	C11-C10-C8-C9
15	B	1223	CLA	C6-C7-C8-C9
15	B	1226	CLA	C6-C7-C8-C9
14	A	4012	BCR	C19-C20-C21-C22
15	B	1213	CLA	CBA-CGA-O2A-C1
15	B	1231	CLA	C2C-C3C-CAC-CBC
16	B	1301	LMU	C2'-C1'-O1'-C1
12	A	5003	LHG	C23-C24-C25-C26
17	B	5002	LMG	O1-C7-C8-C9
15	A	1117	CLA	C15-C16-C17-C18
12	A	5001	LHG	C17-C18-C19-C20
15	B	1207	CLA	C2C-C3C-CAC-CBC
15	A	1106	CLA	C5-C6-C7-C8
15	A	1131	CLA	C5-C6-C7-C8
13	A	1011	CL0	CHA-CBD-CGD-O1D
13	A	1011	CL0	CHA-CBD-CGD-O2D
15	A	1012	CLA	C10-C11-C12-C13
15	B	1207	CLA	O1A-CGA-O2A-C1
14	B	4014	BCR	C17-C18-C19-C20
15	A	1130	CLA	C2A-CAA-CBA-CGA
12	A	5001	LHG	C29-C30-C31-C32
14	A	4008	BCR	C18-C19-C20-C21
14	A	4008	BCR	C9-C10-C11-C12
15	A	1127	CLA	C16-C17-C18-C20
12	A	5005	LHG	O6-C4-C5-O7
15	B	1213	CLA	O1A-CGA-O2A-C1
15	A	1122	CLA	C4-C3-C5-C6
15	B	1228	CLA	C2-C3-C5-C6
12	A	5005	LHG	C11-C12-C13-C14
12	A	5005	LHG	O7-C5-C6-O8
12	B	5004	LHG	C26-C27-C28-C29
15	A	1127	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	CAA-CBA-CGA-O2A
15	B	1215	CLA	CAA-CBA-CGA-O2A
15	B	1217	CLA	CAA-CBA-CGA-O2A
15	B	1228	CLA	CAA-CBA-CGA-O2A
15	A	1105	CLA	C3-C5-C6-C7
15	B	1203	CLA	C13-C15-C16-C17
15	A	1137	CLA	C2C-C3C-CAC-CBC
15	B	1220	CLA	CBA-CGA-O2A-C1
15	B	1223	CLA	C3-C5-C6-C7
14	J	4013	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	B	1205	CLA	C4-C3-C5-C6
12	A	5001	LHG	C35-C36-C37-C38
15	A	1110	CLA	C5-C6-C7-C8
16	J	1304	LMU	C4-C5-C6-C7
16	B	1301	LMU	C2-C1-O1'-C1'
15	A	1104	CLA	C11-C12-C13-C14
15	B	1021	CLA	C14-C13-C15-C16
15	B	1210	CLA	C11-C12-C13-C14
15	B	1216	CLA	C6-C7-C8-C9
12	B	5004	LHG	C28-C29-C30-C31
15	A	1104	CLA	C13-C15-C16-C17
15	A	1124	CLA	C4B-C3B-CAB-CBB
15	A	1120	CLA	C4B-C3B-CAB-CBB
15	B	1013	CLA	C4B-C3B-CAB-CBB
15	B	1202	CLA	C4B-C3B-CAB-CBB
15	B	1214	CLA	C4B-C3B-CAB-CBB
15	B	1222	CLA	C4B-C3B-CAB-CBB
15	B	1232	CLA	C4B-C3B-CAB-CBB
15	B	1235	CLA	C4B-C3B-CAB-CBB
17	B	5002	LMG	C41-C42-C43-C44
15	A	1118	CLA	C2A-CAA-CBA-CGA
12	A	5005	LHG	O6-C4-C5-C6
15	A	1106	CLA	C11-C10-C8-C7
15	A	1117	CLA	C12-C13-C15-C16
15	B	1021	CLA	C12-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C7
15	B	1202	CLA	C11-C12-C13-C15
15	B	1210	CLA	C11-C12-C13-C15
15	B	1216	CLA	C6-C7-C8-C10
15	B	1230	CLA	C12-C13-C15-C16
15	F	1139	CLA	C12-C13-C15-C16
10	A	2001	PQN	C25-C26-C27-C28
15	A	1103	CLA	C3A-C2A-CAA-CBA
15	B	1209	CLA	C3A-C2A-CAA-CBA
15	B	1229	CLA	C3A-C2A-CAA-CBA
15	F	1410	CLA	C3A-C2A-CAA-CBA
15	A	1135	CLA	C2-C3-C5-C6
17	B	5002	LMG	O6-C1-O1-C7
14	B	4006	BCR	C19-C20-C21-C22
14	B	4009	BCR	C19-C20-C21-C22
14	B	4010	BCR	C19-C20-C21-C22
14	B	4009	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	B	5004	LHG	C25-C26-C27-C28
12	A	5005	LHG	C4-C5-C6-O8
15	B	1202	CLA	C10-C11-C12-C13
12	B	5004	LHG	C35-C36-C37-C38
17	B	5002	LMG	C31-C32-C33-C34
15	B	1220	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	C3-C5-C6-C7
15	B	1239	CLA	C2C-C3C-CAC-CBC
14	B	4009	BCR	C5-C6-C7-C8
14	F	4015	BCR	C1-C6-C7-C8
15	A	1105	CLA	C2B-C3B-CAB-CBB
15	B	1232	CLA	C2B-C3B-CAB-CBB
15	B	1235	CLA	C2B-C3B-CAB-CBB
15	A	1111	CLA	C8-C10-C11-C12
12	A	5003	LHG	C2-C3-O3-P
15	A	1022	CLA	C15-C16-C17-C18
15	B	1235	CLA	C8-C10-C11-C12
12	B	5004	LHG	O7-C5-C6-O8
15	B	1205	CLA	C2-C3-C5-C6
12	A	5003	LHG	C31-C32-C33-C34
15	A	1101	CLA	C14-C13-C15-C16
15	B	1230	CLA	C14-C13-C15-C16
17	B	5002	LMG	C24-C25-C26-C27
15	B	1229	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C8-C10-C11-C12
15	A	1109	CLA	C5-C6-C7-C8
12	A	5001	LHG	O1-C1-C2-O2
15	A	1022	CLA	CBA-CGA-O2A-C1
15	A	1110	CLA	O1D-CGD-O2D-CED
17	B	5002	LMG	C17-C18-C19-C20
17	B	5002	LMG	C40-C41-C42-C43
15	A	1119	CLA	C3-C5-C6-C7
15	B	1236	CLA	CBA-CGA-O2A-C1
15	B	1229	CLA	C13-C15-C16-C17
15	A	1101	CLA	C12-C13-C15-C16
15	A	1119	CLA	C11-C12-C13-C15
15	B	1222	CLA	C6-C7-C8-C10
15	B	1235	CLA	C6-C7-C8-C10
17	B	5002	LMG	C13-C14-C15-C16
15	A	1138	CLA	C5-C6-C7-C8
14	A	4003	BCR	C21-C22-C23-C24
14	B	4009	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	F	4015	BCR	C21-C22-C23-C24
15	B	1236	CLA	O1A-CGA-O2A-C1
15	B	1231	CLA	C4C-C3C-CAC-CBC
15	A	1127	CLA	C10-C11-C12-C13
15	B	1202	CLA	C8-C10-C11-C12
15	B	1237	CLA	C2A-CAA-CBA-CGA
15	B	1231	CLA	C2-C3-C5-C6
17	B	5002	LMG	C42-C43-C44-C45
17	B	5002	LMG	C9-C8-O7-C10
15	J	1303	CLA	C2C-C3C-CAC-CBC
16	B	1301	LMU	C1-C2-C3-C4
14	B	4011	BCR	C11-C10-C9-C8
12	A	5003	LHG	O6-C4-C5-O7
15	A	1119	CLA	O2A-C1-C2-C3
17	B	5002	LMG	C7-C8-C9-O8
15	A	1103	CLA	C4-C3-C5-C6
15	A	1123	CLA	C4-C3-C5-C6
15	A	1123	CLA	C8-C10-C11-C12
15	B	1235	CLA	C3-C5-C6-C7
17	B	5002	LMG	O1-C7-C8-O7
15	A	1119	CLA	C11-C12-C13-C14
15	A	1122	CLA	C14-C13-C15-C16
15	B	1222	CLA	C6-C7-C8-C9
15	B	1235	CLA	C6-C7-C8-C9
12	B	5004	LHG	C34-C35-C36-C37
15	B	1229	CLA	C15-C16-C17-C18
15	B	1236	CLA	C2-C1-O2A-CGA
15	A	1122	CLA	C16-C17-C18-C19
15	A	1127	CLA	C13-C15-C16-C17
15	A	1106	CLA	C10-C11-C12-C13
15	B	1013	CLA	C3-C5-C6-C7
15	B	1237	CLA	C3-C5-C6-C7
13	A	1108	CL0	C4C-C3C-CAC-CBC
14	A	4007	BCR	C18-C19-C20-C21
14	F	4016	BCR	C18-C19-C20-C21
14	J	4013	BCR	C18-C19-C20-C21
15	A	1140	CLA	C16-C17-C18-C19
15	B	1205	CLA	C6-C7-C8-C10
14	B	4014	BCR	C36-C18-C19-C20
15	A	1105	CLA	C4B-C3B-CAB-CBB
15	A	1117	CLA	C4B-C3B-CAB-CBB
15	B	1240	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	B	1021	CLA	C4B-C3B-CAB-CBB
15	B	1205	CLA	C4B-C3B-CAB-CBB
15	B	1209	CLA	C4B-C3B-CAB-CBB
15	B	1217	CLA	C4B-C3B-CAB-CBB
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	F	1410	CLA	C4B-C3B-CAB-CBB
15	F	1301	CLA	C4B-C3B-CAB-CBB
15	B	1224	CLA	C4-C3-C5-C6
12	A	5003	LHG	C16-C17-C18-C19
15	A	1136	CLA	C16-C17-C18-C20
15	B	1226	CLA	C15-C16-C17-C18
15	A	1022	CLA	O1A-CGA-O2A-C1
15	A	1012	CLA	C2A-CAA-CBA-CGA
15	B	1207	CLA	C4C-C3C-CAC-CBC
15	A	1102	CLA	C12-C13-C15-C16
15	A	1117	CLA	C11-C12-C13-C15
15	A	1138	CLA	C11-C10-C8-C7
15	B	1013	CLA	C12-C13-C15-C16
15	B	1203	CLA	C12-C13-C15-C16
15	B	1228	CLA	C11-C12-C13-C15
15	B	1229	CLA	C11-C10-C8-C7
15	B	1231	CLA	C6-C7-C8-C10
15	F	1410	CLA	C6-C7-C8-C10
15	F	1410	CLA	C12-C13-C15-C16
12	A	5001	LHG	C11-C10-C9-C8
17	B	5002	LMG	C36-C37-C38-C39
12	A	5001	LHG	O6-C4-C5-O7
12	A	5001	LHG	C8-C7-O7-C5
15	A	1117	CLA	C14-C13-C15-C16
15	A	1122	CLA	C11-C12-C13-C14
12	A	5005	LHG	C11-C10-C9-C8
15	A	1120	CLA	C1-C2-C3-C4
17	B	5002	LMG	C38-C39-C40-C41
17	B	5002	LMG	O7-C8-C9-O8
15	B	1216	CLA	C10-C11-C12-C13
15	B	1230	CLA	C5-C6-C7-C8
12	B	5004	LHG	C33-C34-C35-C36
15	A	1123	CLA	C2-C3-C5-C6
15	A	1102	CLA	CAD-CBD-CGD-O2D
15	A	1111	CLA	CAD-CBD-CGD-O2D
15	A	1129	CLA	CAD-CBD-CGD-O2D
15	B	1223	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	B	1301	LMU	O5'-C1'-O1'-C1
12	A	5001	LHG	C19-C20-C21-C22
12	A	5003	LHG	C3-O3-P-O5
12	A	5003	LHG	C4-O6-P-O5
14	A	4002	BCR	C19-C20-C21-C22
14	B	4011	BCR	C11-C10-C9-C34
15	A	1102	CLA	CAD-CBD-CGD-O1D
15	A	1111	CLA	CAD-CBD-CGD-O1D
15	A	1118	CLA	CAD-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	A	1124	CLA	CHA-CBD-CGD-O1D
15	A	1124	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CAD-CBD-CGD-O1D
15	B	1212	CLA	CHA-CBD-CGD-O1D
15	B	1212	CLA	CHA-CBD-CGD-O2D
15	B	1223	CLA	CAD-CBD-CGD-O1D
15	B	1211	CLA	CAD-CBD-CGD-O1D
12	A	5003	LHG	C13-C14-C15-C16
14	B	4004	BCR	C23-C24-C25-C26
15	A	1103	CLA	C2B-C3B-CAB-CBB
15	B	1240	CLA	C2B-C3B-CAB-CBB
15	B	1023	CLA	C2B-C3B-CAB-CBB
15	B	1205	CLA	C2B-C3B-CAB-CBB
15	B	1217	CLA	C2B-C3B-CAB-CBB
15	B	1221	CLA	C2B-C3B-CAB-CBB
15	B	1222	CLA	C2B-C3B-CAB-CBB
15	B	1224	CLA	C2B-C3B-CAB-CBB
15	B	1225	CLA	C2B-C3B-CAB-CBB
15	B	1206	CLA	C2B-C3B-CAB-CBB
15	A	1103	CLA	C2-C3-C5-C6
17	B	5002	LMG	C15-C16-C17-C18
12	A	5003	LHG	C24-C23-O8-C6
12	A	5005	LHG	C12-C13-C14-C15
15	B	1202	CLA	C3-C5-C6-C7
14	B	4010	BCR	C18-C19-C20-C21
15	K	1402	CLA	CAA-CBA-CGA-O2A
15	A	1117	CLA	C5-C6-C7-C8
12	A	5003	LHG	O6-C4-C5-C6
15	B	1204	CLA	CBA-CGA-O2A-C1
15	F	1410	CLA	C6-C7-C8-C9
15	F	1139	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	A	1137	CLA	C4C-C3C-CAC-CBC
15	B	1202	CLA	C4-C3-C5-C6
12	A	5001	LHG	O9-C7-O7-C5
15	B	1210	CLA	C10-C11-C12-C13
14	B	4004	BCR	C9-C10-C11-C12
15	B	1237	CLA	C2-C1-O2A-CGA
12	B	5004	LHG	C4-C5-C6-O8
15	B	1226	CLA	C5-C6-C7-C8
14	B	4014	BCR	C14-C15-C16-C17
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	B	1219	CLA	CAA-CBA-CGA-O2A
15	J	1303	CLA	C2A-CAA-CBA-CGA
15	A	1116	CLA	O1A-CGA-O2A-C1
15	B	1224	CLA	C2-C3-C5-C6
15	B	1239	CLA	C4C-C3C-CAC-CBC
15	J	1303	CLA	C4C-C3C-CAC-CBC
15	A	1101	CLA	C15-C16-C17-C18
15	B	1228	CLA	CAA-CBA-CGA-O1A
10	A	2001	PQN	C21-C22-C23-C24
15	B	1231	CLA	C6-C7-C8-C9
15	B	1211	CLA	C4B-C3B-CAB-CBB
15	A	1112	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	C16-C17-C18-C20
15	B	1217	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	C5-C6-C7-C8
15	A	1136	CLA	C16-C17-C18-C19
12	A	5003	LHG	C9-C10-C11-C12
12	A	5003	LHG	O10-C23-O8-C6
13	A	1011	CL0	O1A-CGA-O2A-C1
12	A	5005	LHG	O2-C2-C3-O3
12	A	5003	LHG	C10-C11-C12-C13
15	B	1229	CLA	C5-C6-C7-C8
15	A	1022	CLA	C4-C3-C5-C6
15	A	1140	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	CAA-CBA-CGA-O2A
14	B	4006	BCR	C20-C21-C22-C37
14	B	4009	BCR	C16-C17-C18-C36
14	B	4011	BCR	C16-C17-C18-C36
14	F	4015	BCR	C11-C10-C9-C34
14	F	4016	BCR	C35-C13-C14-C15
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	B	1225	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	A	5001	LHG	C14-C15-C16-C17
14	B	4006	BCR	C13-C14-C15-C16
15	A	1105	CLA	C2-C1-O2A-CGA
15	A	1109	CLA	C2-C1-O2A-CGA
15	B	1013	CLA	C13-C15-C16-C17
15	B	1232	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	C5-C6-C7-C8
15	A	1112	CLA	CAA-CBA-CGA-O1A
12	B	5004	LHG	C15-C16-C17-C18
15	B	1232	CLA	CAA-CBA-CGA-O1A
15	A	1102	CLA	C14-C13-C15-C16
15	A	1103	CLA	C6-C7-C8-C9
15	A	1123	CLA	C11-C10-C8-C9
15	A	1136	CLA	C6-C7-C8-C9
15	B	1013	CLA	C6-C7-C8-C9
15	B	1021	CLA	C11-C10-C8-C9
12	A	5001	LHG	O1-C1-C2-C3
15	A	1114	CLA	C2C-C3C-CAC-CBC
15	A	1113	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	CAA-CBA-CGA-O1A
15	B	1225	CLA	C15-C16-C17-C18
14	B	4006	BCR	C20-C21-C22-C23
14	B	4009	BCR	C16-C17-C18-C19
14	B	4011	BCR	C16-C17-C18-C19
14	F	4016	BCR	C12-C13-C14-C15
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	B	1223	CLA	C1A-C2A-CAA-CBA
15	B	1228	CLA	C1A-C2A-CAA-CBA
15	B	1232	CLA	C1A-C2A-CAA-CBA
15	F	1410	CLA	C1A-C2A-CAA-CBA
15	A	1101	CLA	C5-C6-C7-C8
14	A	4001	BCR	C1-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C30
14	A	4008	BCR	C5-C6-C7-C8
14	A	4012	BCR	C1-C6-C7-C8
14	B	4004	BCR	C23-C24-C25-C30
14	B	4011	BCR	C1-C6-C7-C8
14	B	4017	BCR	C1-C6-C7-C8
14	B	4017	BCR	C5-C6-C7-C8
14	F	4015	BCR	C5-C6-C7-C8
14	J	4013	BCR	C1-C6-C7-C8
15	A	1117	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	A	1124	CLA	C2B-C3B-CAB-CBB
15	A	1135	CLA	C2B-C3B-CAB-CBB
15	B	1013	CLA	C2B-C3B-CAB-CBB
15	B	1021	CLA	C2B-C3B-CAB-CBB
15	B	1202	CLA	C2B-C3B-CAB-CBB
15	B	1209	CLA	C2B-C3B-CAB-CBB
15	F	1410	CLA	C2B-C3B-CAB-CBB
15	F	1301	CLA	C2B-C3B-CAB-CBB
15	B	1240	CLA	CAA-CBA-CGA-O2A
15	B	1230	CLA	C16-C17-C18-C20
10	A	2001	PQN	C21-C22-C23-C25
15	A	1106	CLA	C12-C13-C15-C16
15	A	1012	CLA	C11-C12-C13-C15
15	B	1023	CLA	C12-C13-C15-C16
15	B	1221	CLA	C12-C13-C15-C16
15	F	1139	CLA	C6-C7-C8-C10
15	B	1013	CLA	C2A-CAA-CBA-CGA
15	A	1113	CLA	CAA-CBA-CGA-O2A
14	B	4006	BCR	C7-C8-C9-C34
15	B	1223	CLA	C4-C3-C5-C6
15	A	1022	CLA	C2-C3-C5-C6
15	B	1202	CLA	C2-C3-C5-C6
15	A	1111	CLA	C10-C11-C12-C13
15	F	1410	CLA	C2A-CAA-CBA-CGA
15	B	1209	CLA	CAA-CBA-CGA-O2A
15	A	1119	CLA	C14-C13-C15-C16
15	A	1128	CLA	C11-C10-C8-C9
12	A	5005	LHG	C24-C25-C26-C27
15	B	1215	CLA	CAA-CBA-CGA-O1A
16	J	1304	LMU	C9-C10-C11-C12
12	A	5001	LHG	C15-C16-C17-C18
15	A	1136	CLA	C4-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	A	1132	CLA	C4-C3-C5-C6
15	B	1013	CLA	C4-C3-C5-C6
12	B	5004	LHG	C31-C32-C33-C34
15	A	1123	CLA	C5-C6-C7-C8
15	F	1410	CLA	C8-C10-C11-C12
15	A	1116	CLA	CBA-CGA-O2A-C1
15	A	1140	CLA	C10-C11-C12-C13
15	B	1234	CLA	C13-C15-C16-C17
15	F	1301	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1125	CLA	C4-C3-C5-C6
10	A	2001	PQN	C23-C25-C26-C27
15	A	1135	CLA	C4B-C3B-CAB-CBB
15	B	1023	CLA	C10-C11-C12-C13
15	B	1229	CLA	C10-C11-C12-C13
15	A	1106	CLA	C16-C17-C18-C20
15	B	1209	CLA	CAA-CBA-CGA-O1A
15	B	1223	CLA	C8-C10-C11-C12
15	B	1223	CLA	C13-C15-C16-C17
12	A	5001	LHG	C12-C13-C14-C15
15	A	1117	CLA	C11-C12-C13-C14
15	A	1132	CLA	C11-C10-C8-C9
15	B	1229	CLA	C11-C10-C8-C9
15	F	1410	CLA	C15-C16-C17-C18
15	F	1139	CLA	C15-C16-C17-C18
15	A	1114	CLA	C2A-CAA-CBA-CGA
15	B	1218	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C2-C1-O2A-CGA
15	B	1219	CLA	C3A-C2A-CAA-CBA
15	B	1223	CLA	C3A-C2A-CAA-CBA
15	A	1012	CLA	C13-C15-C16-C17
13	A	1011	CL0	CBA-CGA-O2A-C1
15	F	1301	CLA	CAA-CBA-CGA-O1A
16	B	1301	LMU	C4-C5-C6-C7
14	B	4014	BCR	C19-C20-C21-C22
15	F	1139	CLA	C16-C17-C18-C20
10	A	2001	PQN	C20-C21-C22-C23
12	A	5001	LHG	O8-C23-C24-C25
15	B	1021	CLA	CAA-CBA-CGA-O2A
10	A	2001	PQN	C19-C18-C20-C21
15	A	1138	CLA	C11-C10-C8-C9
15	B	1214	CLA	C6-C7-C8-C9
15	F	1410	CLA	C14-C13-C15-C16
15	A	1131	CLA	C2C-C3C-CAC-CBC
12	A	5001	LHG	C13-C14-C15-C16
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	A	1105	CLA	C11-C10-C8-C7
15	A	1119	CLA	C12-C13-C15-C16
15	A	1123	CLA	C11-C10-C8-C7
15	A	1128	CLA	C6-C7-C8-C10
15	A	1128	CLA	C11-C10-C8-C7
15	B	1013	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	B	1023	CLA	C11-C12-C13-C15
15	B	1223	CLA	C6-C7-C8-C10
15	B	1234	CLA	C12-C13-C15-C16
15	B	1234	CLA	C3-C5-C6-C7
14	A	4001	BCR	C5-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C26
14	B	4011	BCR	C5-C6-C7-C8
14	J	4013	BCR	C5-C6-C7-C8
15	A	1123	CLA	C2B-C3B-CAB-CBB
15	A	1120	CLA	C2B-C3B-CAB-CBB
15	B	1211	CLA	C2B-C3B-CAB-CBB
15	K	1402	CLA	C2B-C3B-CAB-CBB
15	B	1202	CLA	CAA-CBA-CGA-O2A
15	B	1210	CLA	CAA-CBA-CGA-O2A
15	A	1102	CLA	C2-C1-O2A-CGA
15	B	1210	CLA	C2-C1-O2A-CGA
15	B	1216	CLA	C2-C1-O2A-CGA
15	B	1231	CLA	CAA-CBA-CGA-O2A
15	B	1206	CLA	CAA-CBA-CGA-O2A
16	J	1304	LMU	C2B-C1B-O1B-C4'
15	B	1205	CLA	C5-C6-C7-C8
15	A	1022	CLA	C13-C15-C16-C17
12	A	5001	LHG	O7-C7-C8-C9
14	B	4005	BCR	C19-C20-C21-C22
12	A	5001	LHG	C27-C28-C29-C30
16	J	1304	LMU	O5B-C1B-O1B-C4'
15	K	1401	CLA	CAA-CBA-CGA-O2A
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	A	1128	CLA	C15-C16-C17-C18
15	B	1023	CLA	C14-C13-C15-C16
15	B	1221	CLA	C14-C13-C15-C16
15	A	1136	CLA	CAA-CBA-CGA-O2A
15	A	1116	CLA	C4B-C3B-CAB-CBB
15	A	1118	CLA	C4B-C3B-CAB-CBB
15	A	1123	CLA	C4B-C3B-CAB-CBB
15	A	1125	CLA	C4B-C3B-CAB-CBB
15	A	1114	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	C4B-C3B-CAB-CBB
15	B	1213	CLA	C1A-C2A-CAA-CBA
15	B	1219	CLA	C1A-C2A-CAA-CBA
15	B	1223	CLA	C4B-C3B-CAB-CBB
15	K	1402	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	B	5004	LHG	C19-C20-C21-C22
15	B	1222	CLA	C2C-C3C-CAC-CBC
15	A	1120	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	A	1134	CLA	CAA-CBA-CGA-O2A
15	A	1135	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	O1A-CGA-O2A-C1
15	A	1114	CLA	C4C-C3C-CAC-CBC
15	A	1129	CLA	CAA-CBA-CGA-O2A
15	B	1207	CLA	CAA-CBA-CGA-O2A
13	A	1108	CL0	C2A-CAA-CBA-CGA
15	A	1123	CLA	C15-C16-C17-C18
15	A	1116	CLA	C2-C1-O2A-CGA
12	A	5005	LHG	O8-C23-C24-C25
15	B	1021	CLA	C11-C10-C8-C7
15	B	1215	CLA	C11-C12-C13-C15
15	B	1225	CLA	C6-C7-C8-C10
15	B	1229	CLA	C11-C12-C13-C15
15	B	1223	CLA	C2-C3-C5-C6
15	B	1228	CLA	C2C-C3C-CAC-CBC
15	B	1234	CLA	C5-C6-C7-C8
15	A	1120	CLA	O2A-C1-C2-C3
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	K	1401	CLA	CAA-CBA-CGA-O1A
15	B	1210	CLA	CAA-CBA-CGA-O1A
15	B	1231	CLA	CAA-CBA-CGA-O1A
15	A	1101	CLA	C11-C10-C8-C9
15	A	1012	CLA	C11-C12-C13-C14
15	B	1228	CLA	C11-C12-C13-C14
15	B	1229	CLA	C11-C12-C13-C14
15	F	1139	CLA	C6-C7-C8-C9
15	A	1115	CLA	CAA-CBA-CGA-O2A
13	A	1108	CL0	C2C-C3C-CAC-CBC
15	A	1134	CLA	CAA-CBA-CGA-O1A
15	B	1021	CLA	CAA-CBA-CGA-O1A
15	B	1206	CLA	CAA-CBA-CGA-O1A
15	B	1201	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	C5-C6-C7-C8
12	A	5005	LHG	C26-C27-C28-C29
15	B	1203	CLA	O1A-CGA-O2A-C1
15	F	1410	CLA	C13-C15-C16-C17
15	A	1102	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	B	1205	CLA	C6-C7-C8-C9
14	A	4002	BCR	C11-C12-C13-C14
12	A	5001	LHG	O9-C7-C8-C9
15	A	1136	CLA	CAA-CBA-CGA-O1A
15	B	1202	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	B	1013	CLA	C16-C17-C18-C20
15	B	1230	CLA	C16-C17-C18-C19
12	A	5001	LHG	O10-C23-C24-C25
15	A	1012	CLA	C8-C10-C11-C12
15	B	1228	CLA	C8-C10-C11-C12
15	A	1127	CLA	CAA-CBA-CGA-O2A
12	A	5005	LHG	O10-C23-C24-C25
15	B	1207	CLA	CAA-CBA-CGA-O1A
15	A	1140	CLA	CAD-CBD-CGD-O2D
15	A	1121	CLA	CAD-CBD-CGD-O2D
15	B	1210	CLA	CAD-CBD-CGD-O2D
15	B	1201	CLA	CAD-CBD-CGD-O2D
15	B	1211	CLA	CAD-CBD-CGD-O2D
15	B	1211	CLA	CAA-CBA-CGA-O2A
16	B	1301	LMU	C7-C8-C9-C10
15	A	1110	CLA	C2-C1-O2A-CGA
15	A	1131	CLA	C2-C1-O2A-CGA
15	B	1225	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	CAA-CBA-CGA-O2A
15	B	1224	CLA	O1A-CGA-O2A-C1
15	A	1106	CLA	C16-C17-C18-C19
15	A	1122	CLA	C16-C17-C18-C20
17	B	5002	LMG	C34-C35-C36-C37
15	B	1205	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	B	1212	CLA	C2C-C3C-CAC-CBC
15	A	1116	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	CAA-CBA-CGA-O2A
15	B	1213	CLA	CAA-CBA-CGA-O2A
15	A	1120	CLA	CAA-CBA-CGA-O1A
15	A	1129	CLA	CAA-CBA-CGA-O1A
15	B	1229	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

98 monomers are involved in 218 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1102	CLA	2	0
15	A	1113	CLA	1	0
15	B	1021	CLA	1	0
15	B	1216	CLA	2	0
15	J	1302	CLA	2	0
12	B	5004	LHG	2	0
15	B	1239	CLA	1	0
15	A	1126	CLA	7	0
15	A	1135	CLA	1	0
14	A	4001	BCR	3	0
15	A	1109	CLA	2	0
15	A	1122	CLA	6	0
15	B	1222	CLA	3	0
14	B	4014	BCR	2	0
15	B	1240	CLA	1	0
15	A	1112	CLA	2	0
15	B	1205	CLA	1	0
15	A	1105	CLA	2	0
15	A	1127	CLA	4	0
15	A	1128	CLA	3	0
15	B	1202	CLA	1	0
15	B	1217	CLA	1	0
15	B	1214	CLA	1	0
14	A	4003	BCR	3	0
15	B	1228	CLA	1	0
14	B	4011	BCR	7	0
15	A	1131	CLA	2	0
15	A	1124	CLA	3	0
14	B	4010	BCR	5	0
15	B	1231	CLA	4	0
15	B	1215	CLA	4	0
15	B	1206	CLA	2	0
14	B	4004	BCR	3	0
10	B	2002	PQN	2	0
15	B	1210	CLA	2	0
15	B	1224	CLA	3	0
15	B	1218	CLA	2	0
15	A	1012	CLA	1	0
15	A	1132	CLA	1	0
15	B	1213	CLA	1	0
12	A	5001	LHG	1	0
14	B	4006	BCR	1	0
14	B	4017	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1211	CLA	2	0
15	B	1220	CLA	2	0
15	A	1138	CLA	2	0
15	A	1101	CLA	3	0
15	B	1226	CLA	2	0
15	A	1110	CLA	11	0
15	B	1230	CLA	2	0
15	A	1111	CLA	1	0
14	A	4002	BCR	3	0
16	J	1304	LMU	2	0
15	A	1125	CLA	1	0
15	B	1235	CLA	5	0
12	A	5005	LHG	10	0
15	B	1229	CLA	4	0
15	B	1201	CLA	1	0
14	F	4016	BCR	2	0
15	A	1107	CLA	4	0
15	A	1022	CLA	2	0
15	A	1133	CLA	3	0
15	B	1227	CLA	2	0
14	A	4007	BCR	2	0
14	B	4005	BCR	1	0
14	B	4009	BCR	1	0
14	F	4015	BCR	6	0
15	B	1236	CLA	5	0
15	B	1212	CLA	2	0
15	F	1139	CLA	3	0
13	A	1011	CL0	8	0
14	A	4012	BCR	5	0
15	B	1221	CLA	5	0
15	A	1129	CLA	1	0
15	B	1237	CLA	1	0
14	A	4008	BCR	5	0
15	K	1402	CLA	1	0
15	A	1120	CLA	1	0
15	K	1401	CLA	1	0
15	A	1123	CLA	4	0
15	A	1801	CLA	2	0
15	A	1137	CLA	1	0
15	B	1023	CLA	6	0
15	A	1118	CLA	2	0
17	B	5002	LMG	2	0

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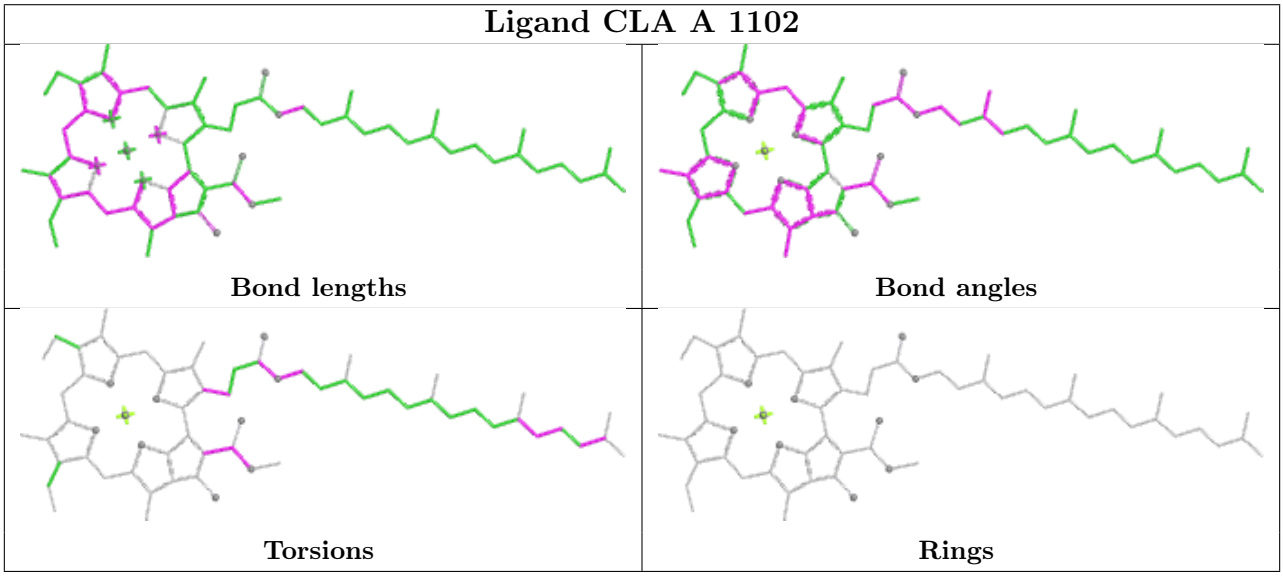
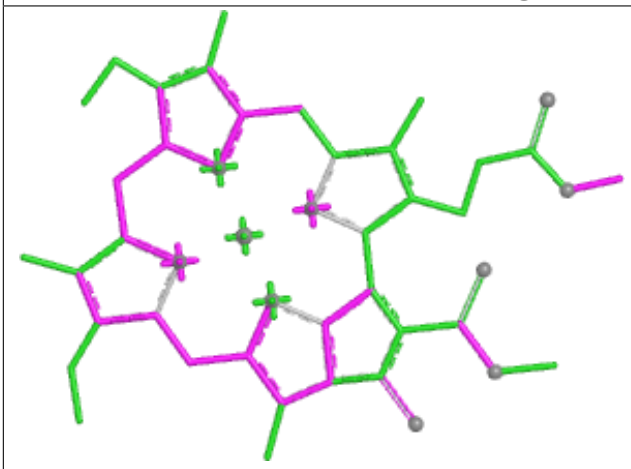
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1106	CLA	1	0
15	A	1104	CLA	2	0
15	B	1232	CLA	2	0
15	B	1203	CLA	2	0
15	F	1301	CLA	1	0
13	A	1108	CL0	2	0
15	A	1114	CLA	2	0
15	B	1013	CLA	10	0
15	A	1103	CLA	6	0
15	A	1119	CLA	2	0
12	A	5003	LHG	7	0
14	J	4013	BCR	3	0
15	A	1121	CLA	2	0

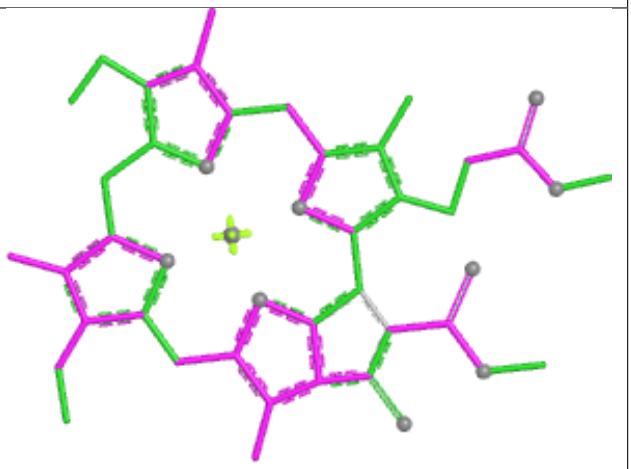
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



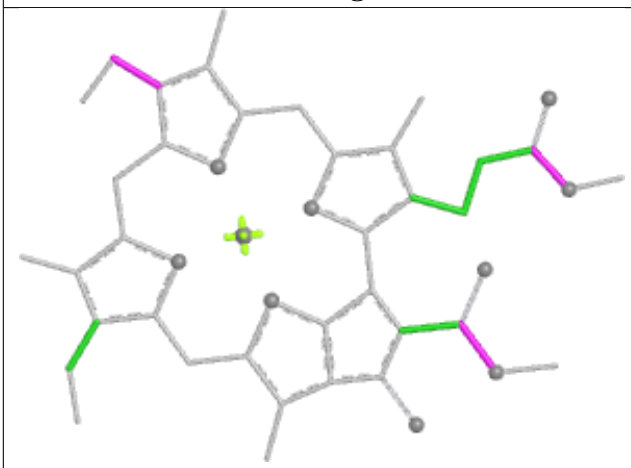
Ligand CLA B 1204



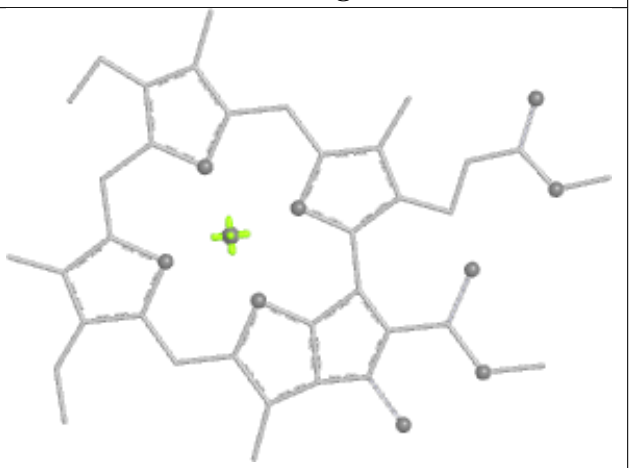
Bond lengths



Bond angles

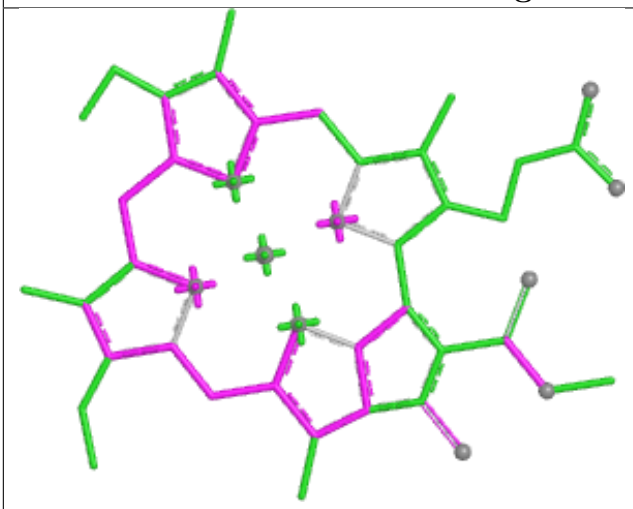


Torsions

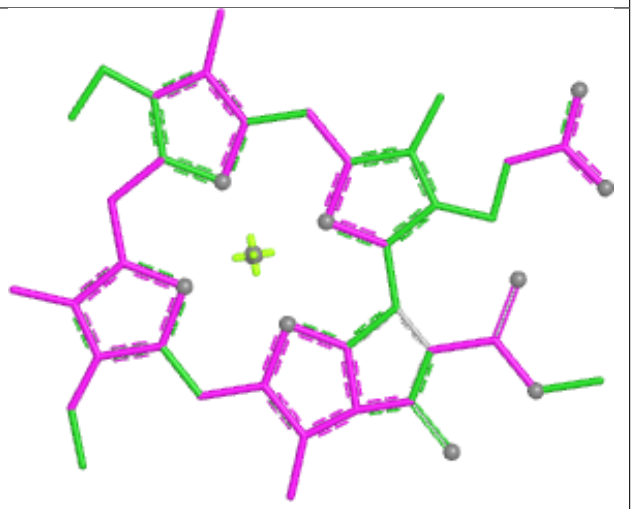


Rings

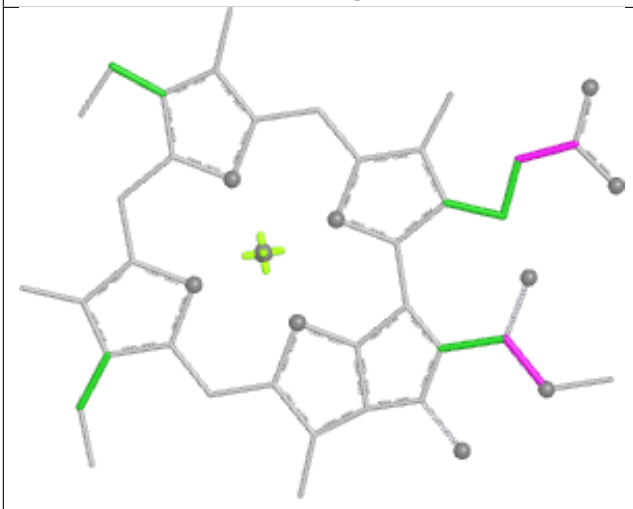
Ligand CLA A 1113



Bond lengths



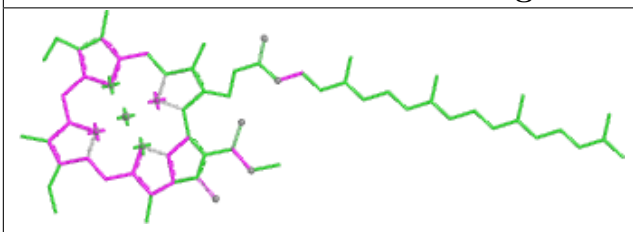
Bond angles



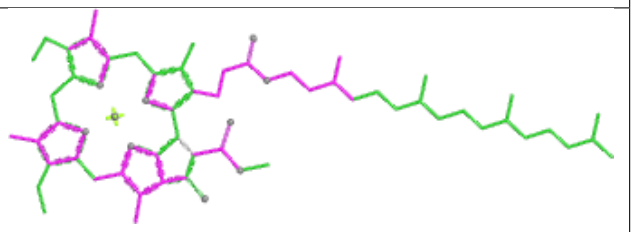
Torsions

Rings

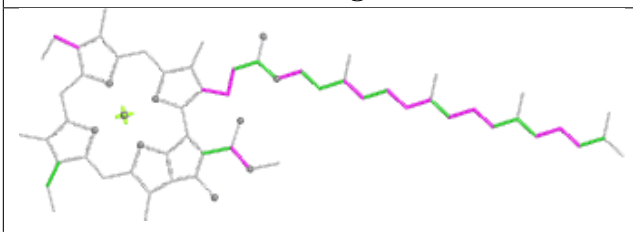
Ligand CLA B 1225



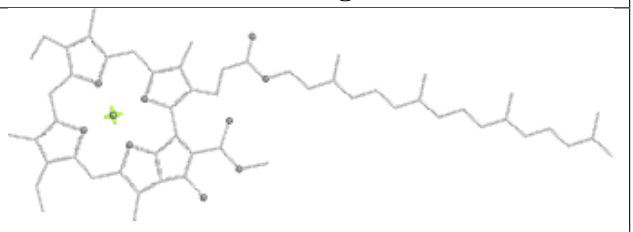
Bond lengths



Bond angles

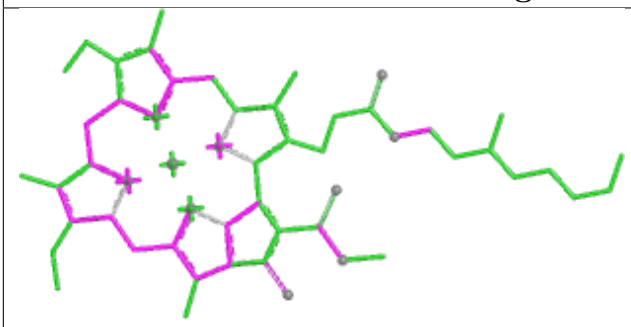


Torsions



Rings

Ligand CLA A 1116



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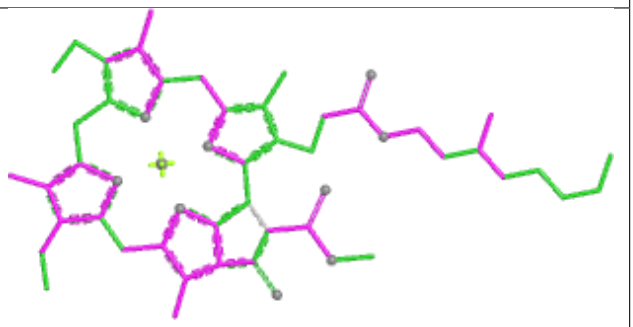
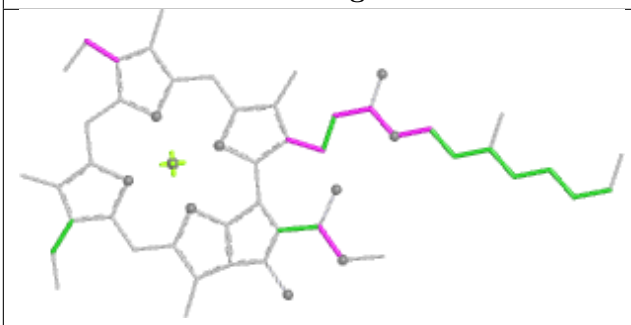
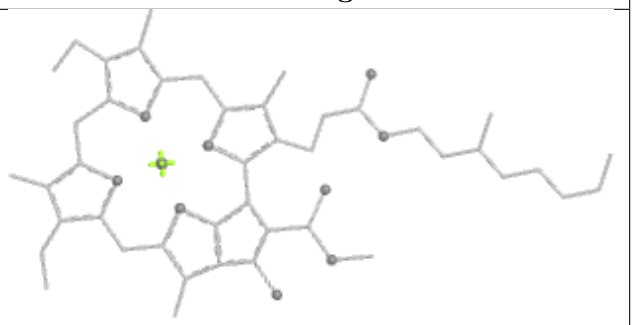


Bond angles

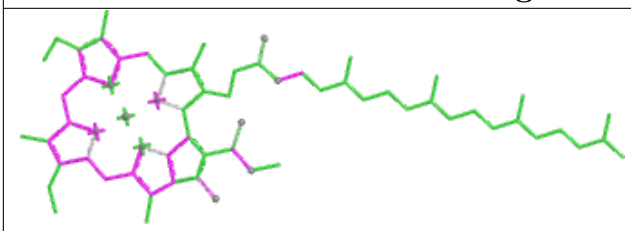


Torsions

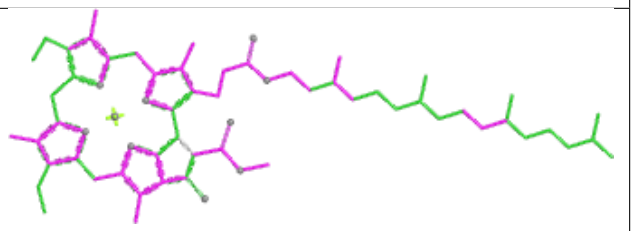


Rings

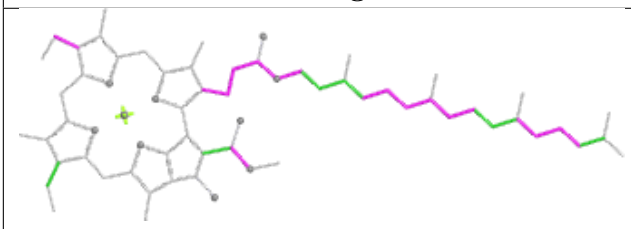
Ligand CLA B 1021



Bond lengths



Bond angles



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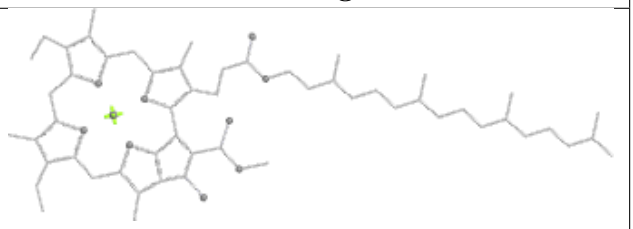

Rings

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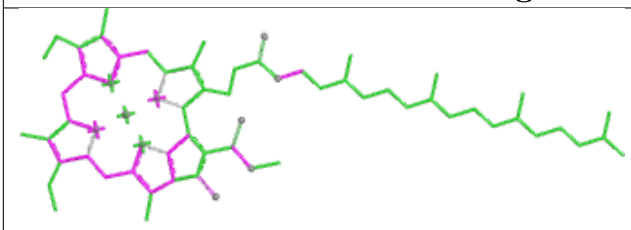

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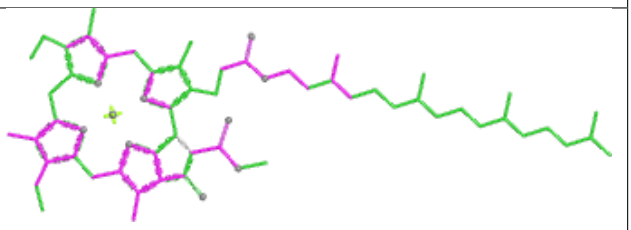

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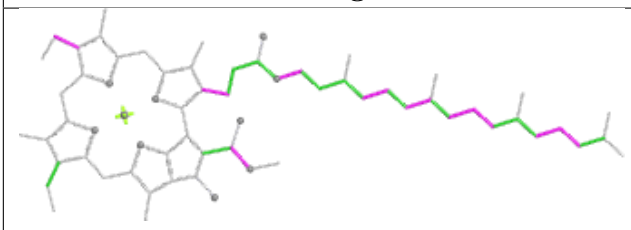

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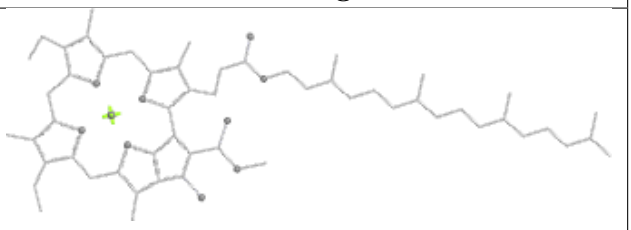
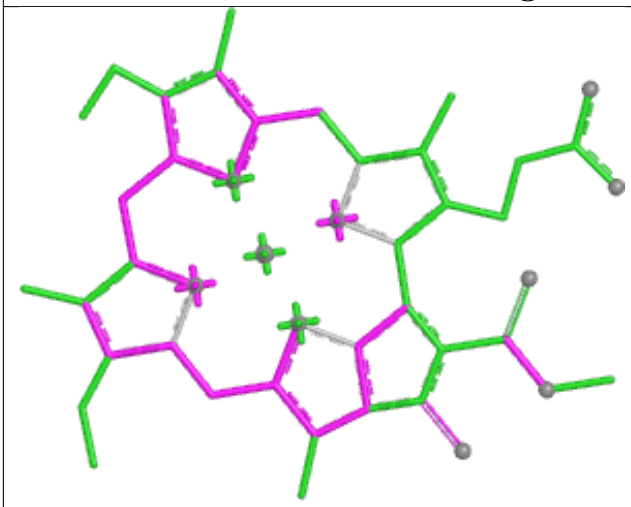


Rings

Ligand CLA J 1302



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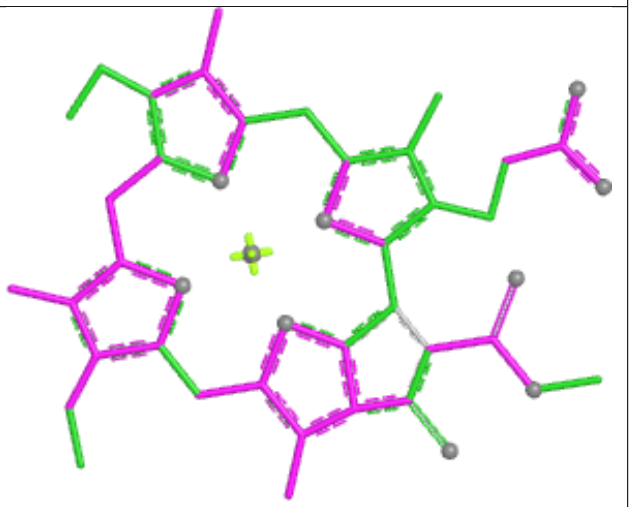
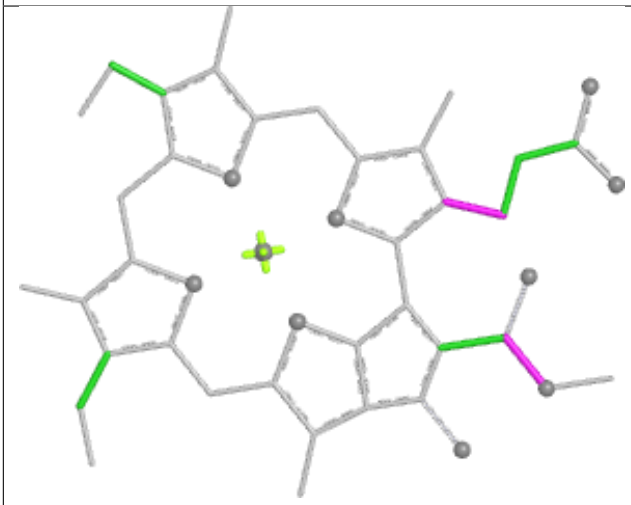


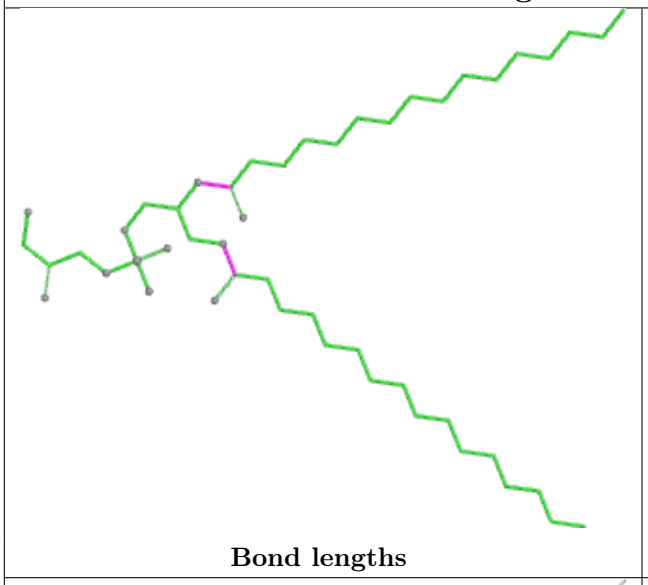
Bond angles



Torsions

Rings

Ligand LHG B 5004



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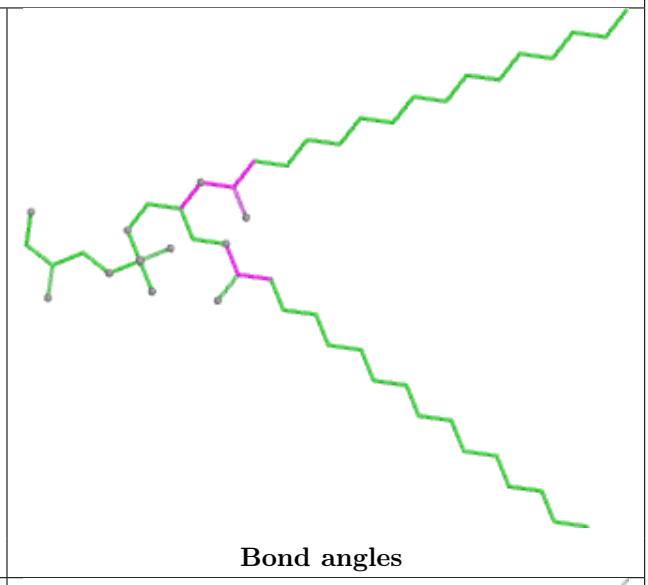
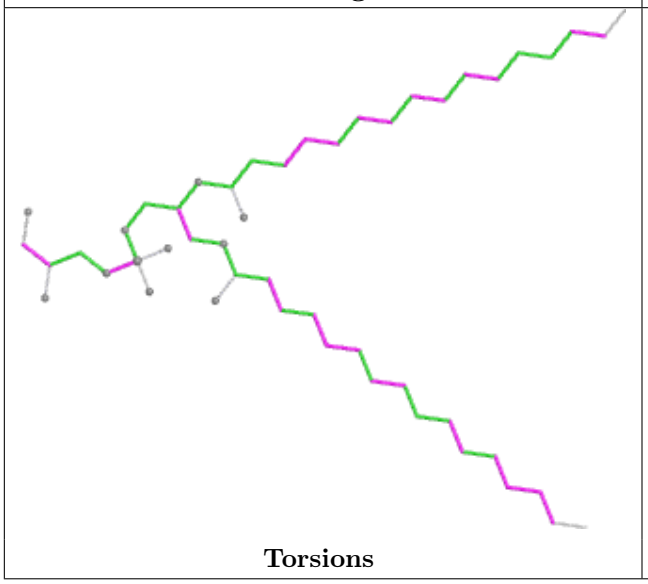
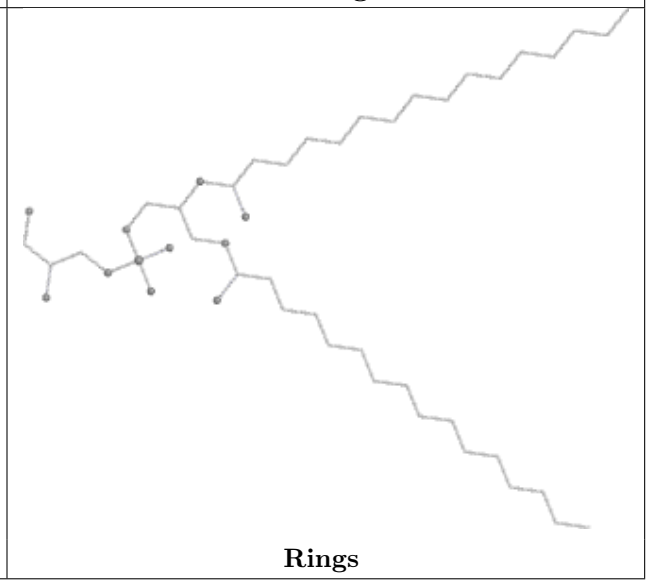


Bond angles

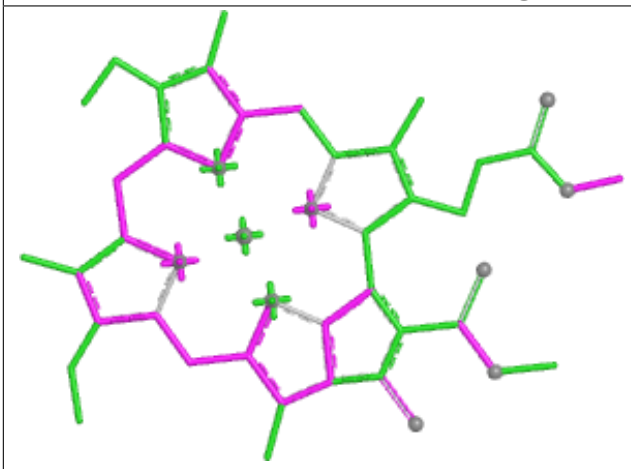


Torsions



Rings

Ligand CLA B 1239



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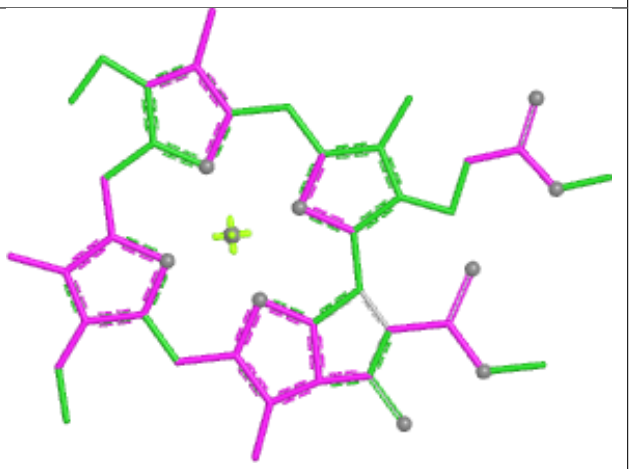
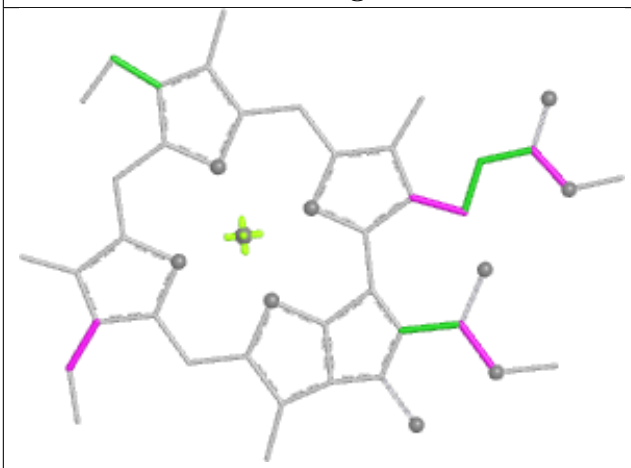
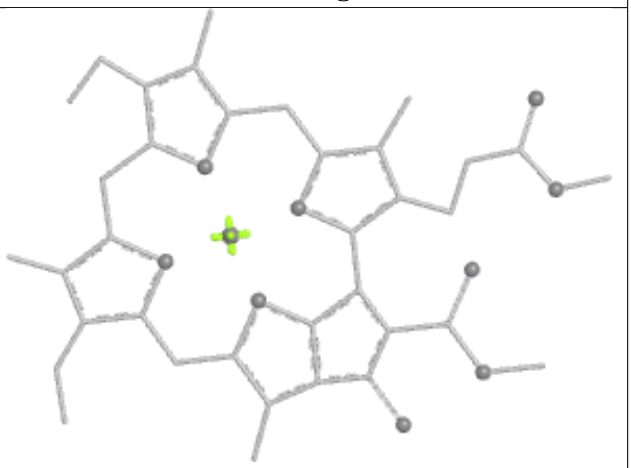


Bond angles

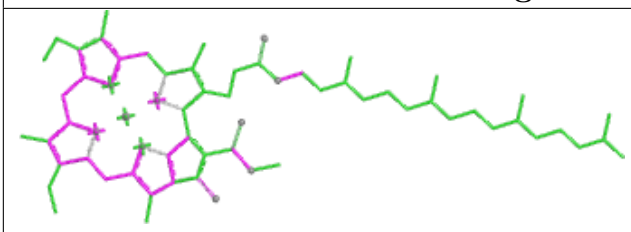


Torsions



Rings

Ligand CLA A 1126



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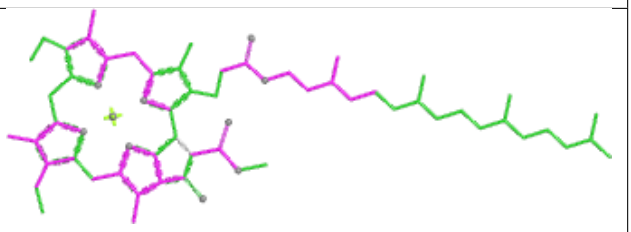
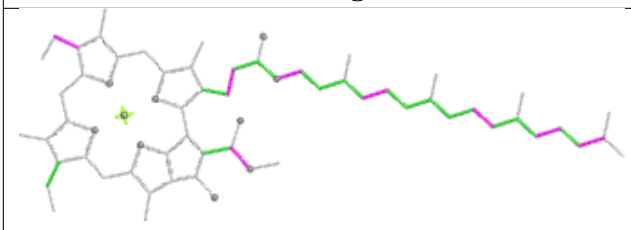
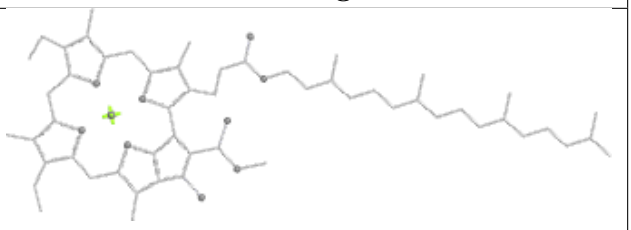


Bond angles

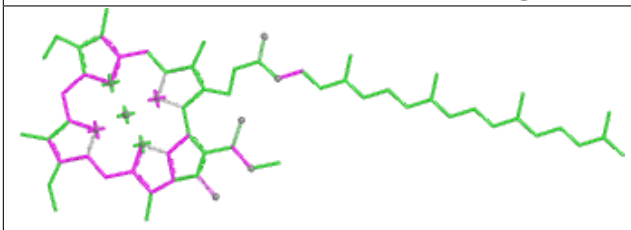


Torsions

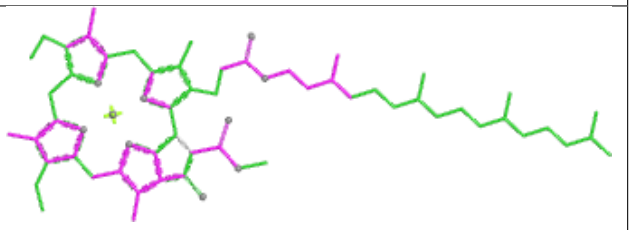


Rings

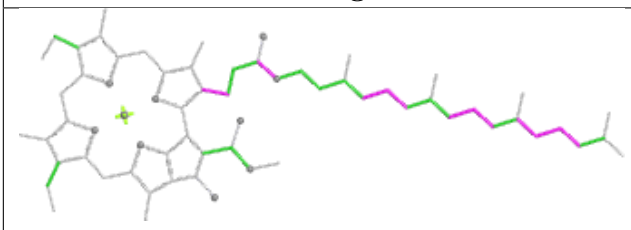
Ligand CLA B 1234



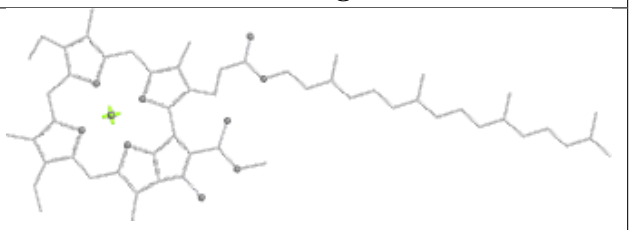
Bond lengths



Bond angles

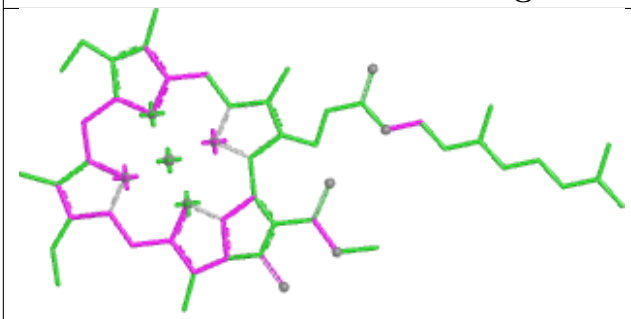


Torsions

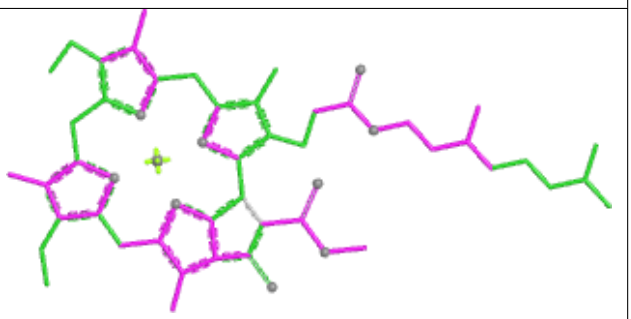


Rings

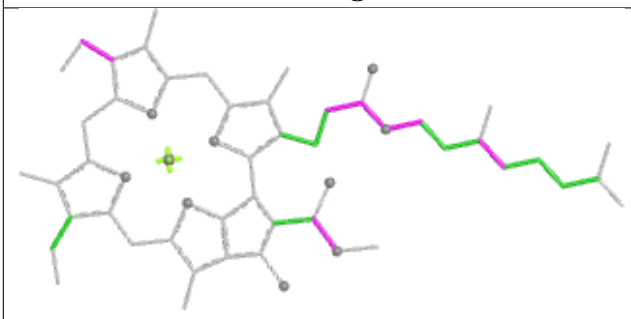
Ligand CLA A 1135



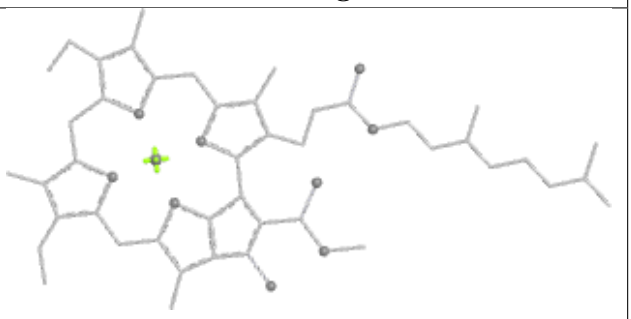
Bond lengths



Bond angles

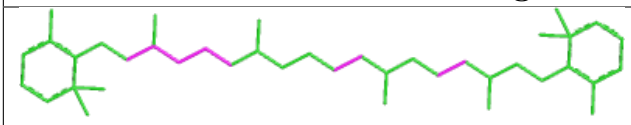


Torsions

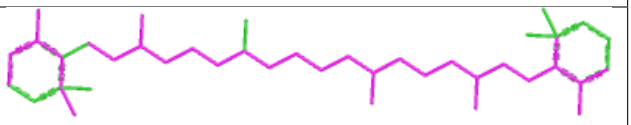


Rings

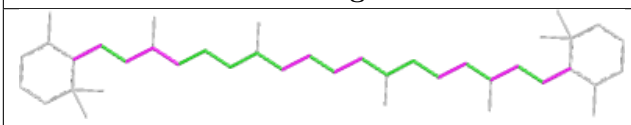
Ligand BCR A 4001



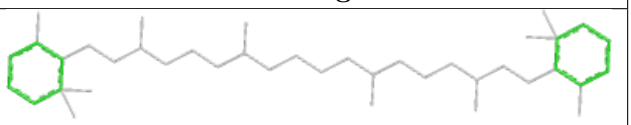
Bond lengths



Bond angles

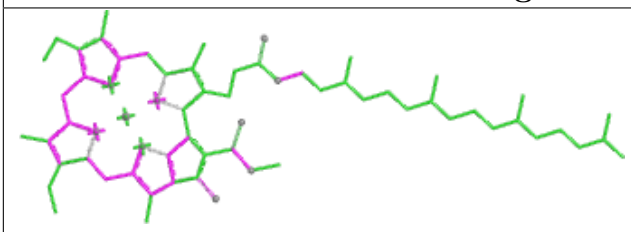


Torsions



Rings

Ligand CLA A 1109



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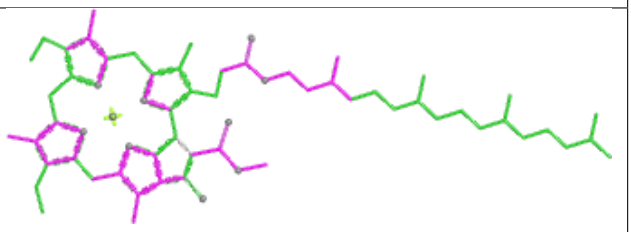
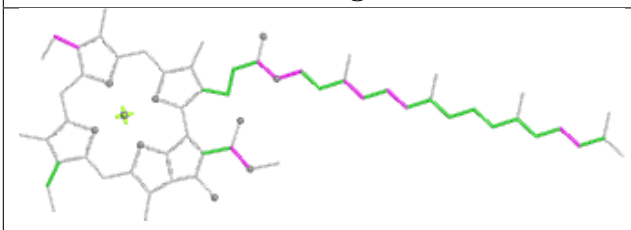
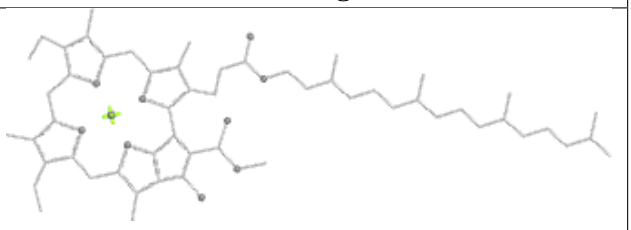


Bond angles

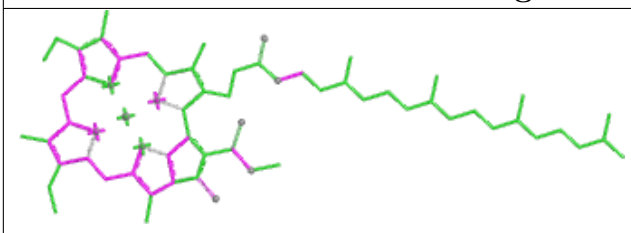


Torsions



Rings

Ligand CLA A 1122



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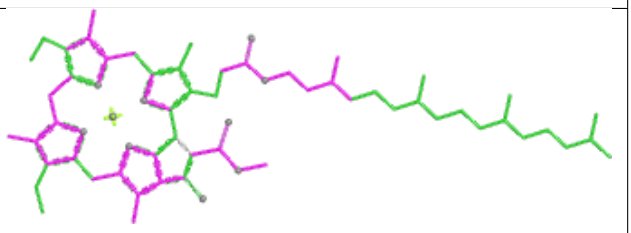
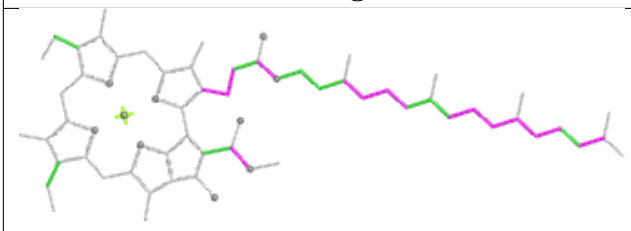
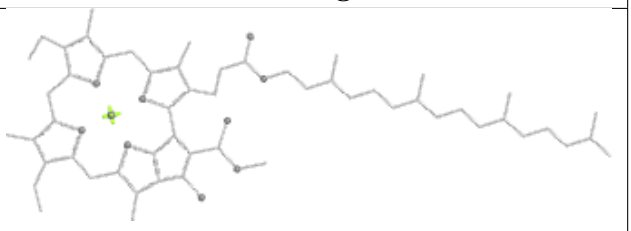


Bond angles

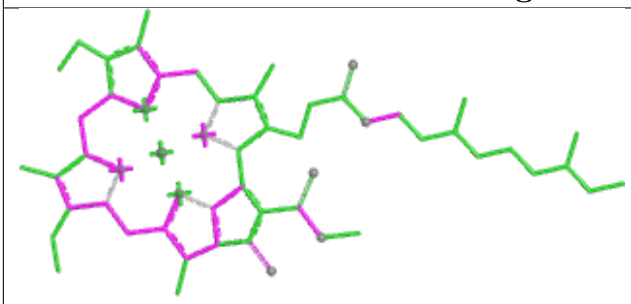


Torsions

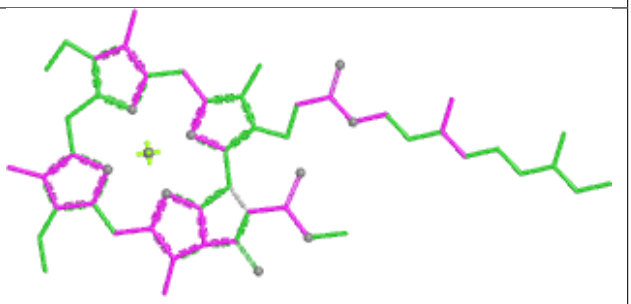


Rings

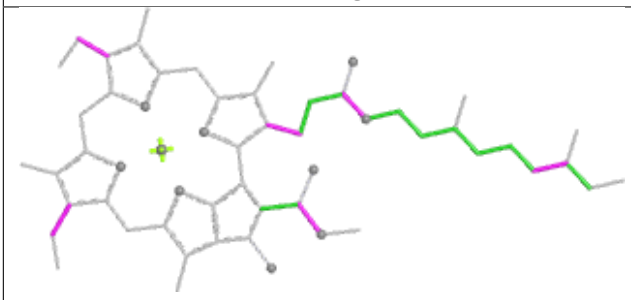
Ligand CLA B 1222



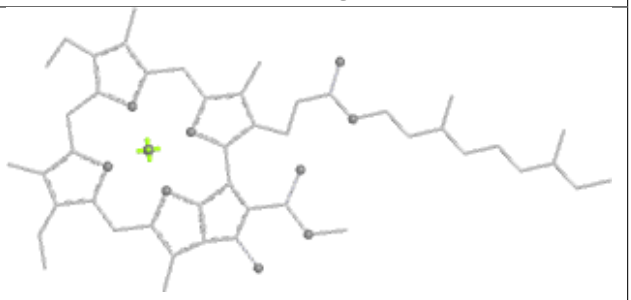
Bond lengths



Bond angles

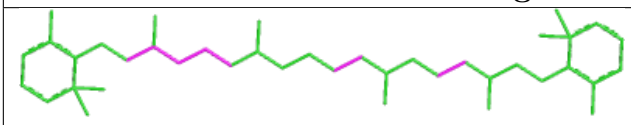


Torsions



Rings

Ligand BCR B 4014



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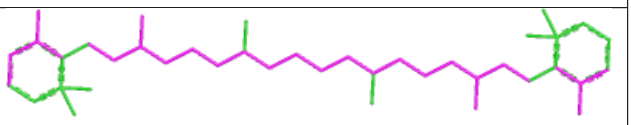
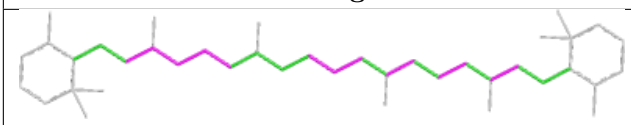


Bond angles



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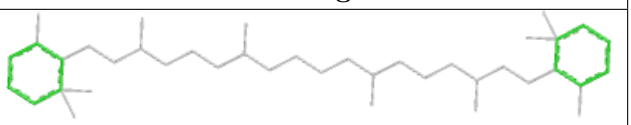
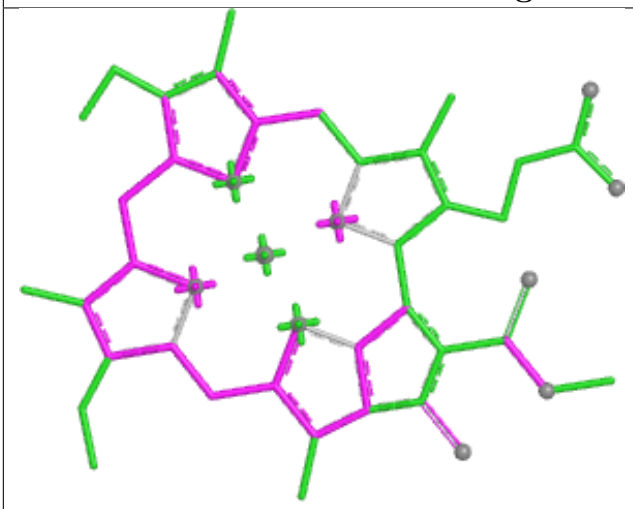
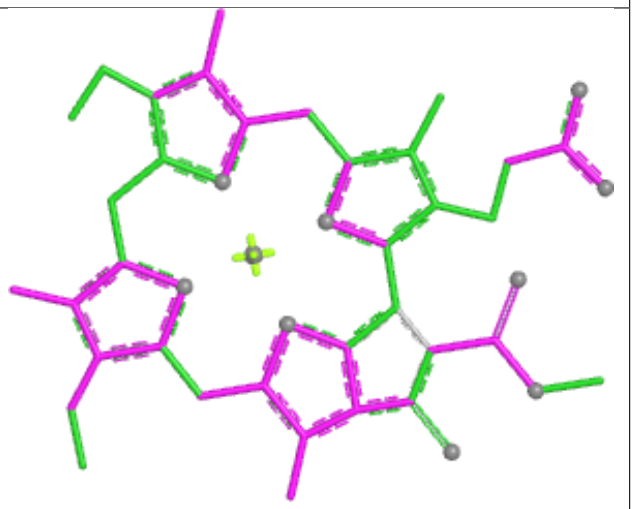


Rings

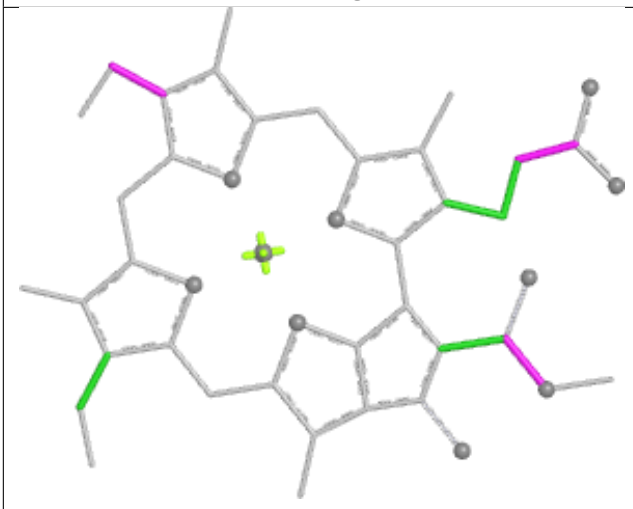
Ligand CLA B 1240



Bond lengths



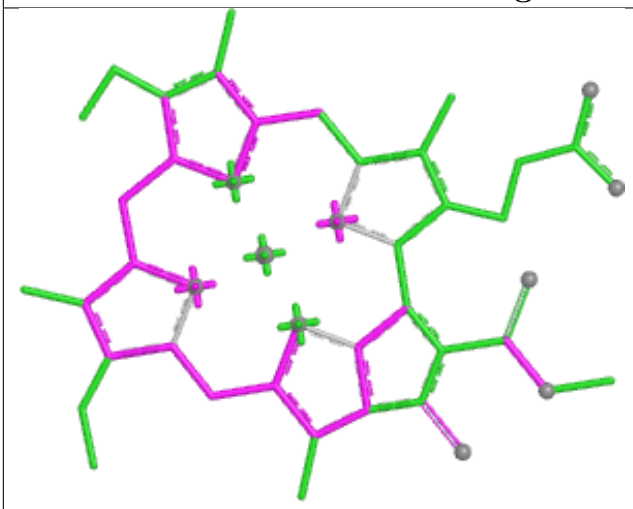
Bond angles



Torsions

Rings

Ligand CLA A 1112



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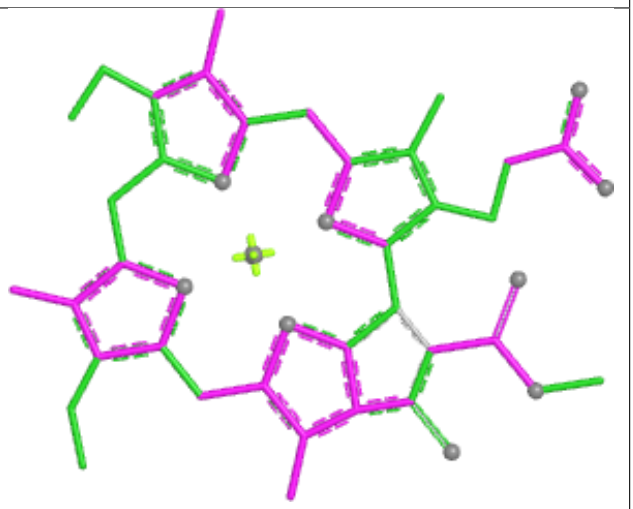
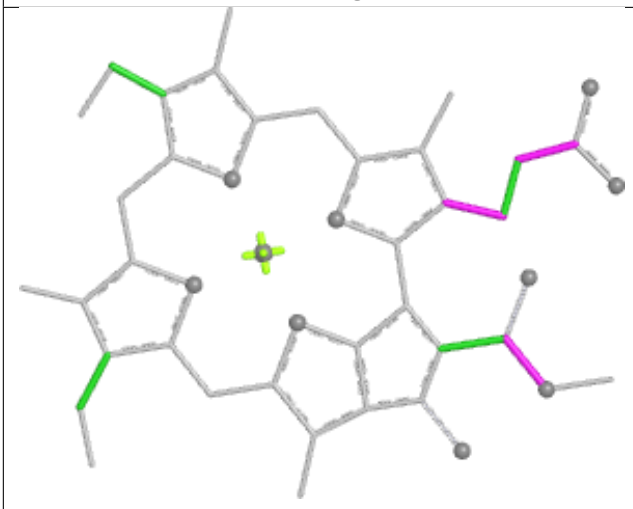


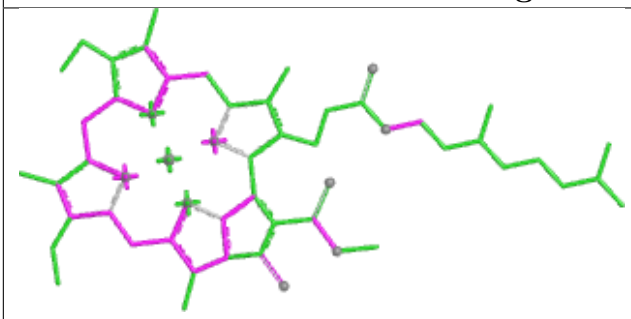
Bond angles



Torsions

Rings

Ligand CLA B 1205



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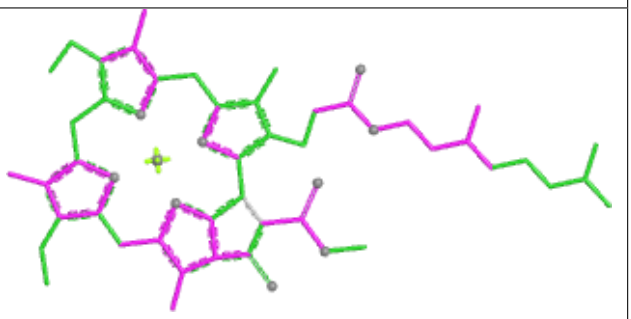
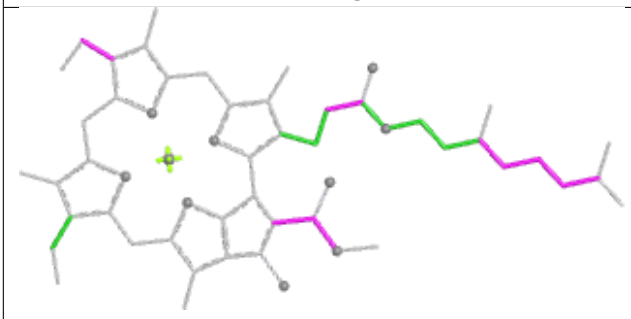
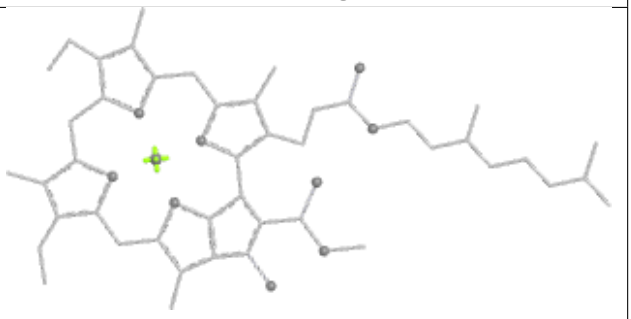


Bond angles

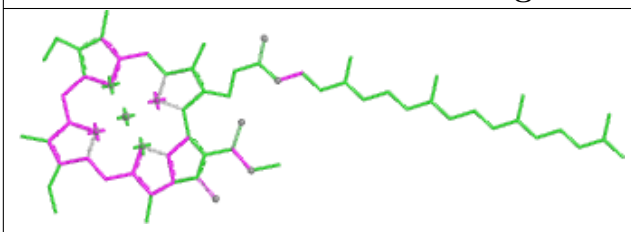


Torsions

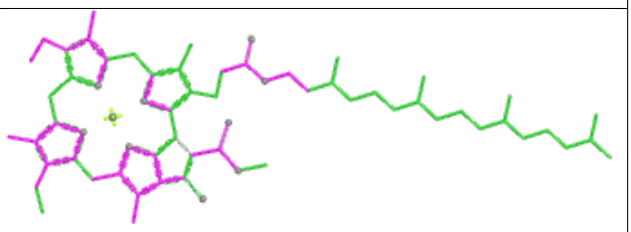


Rings

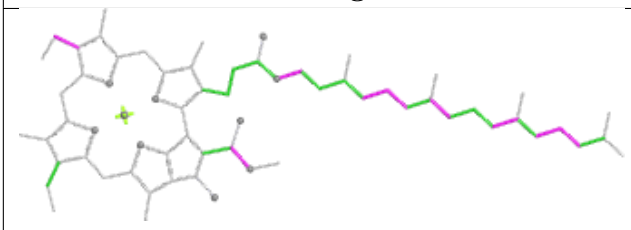
Ligand CLA A 1105



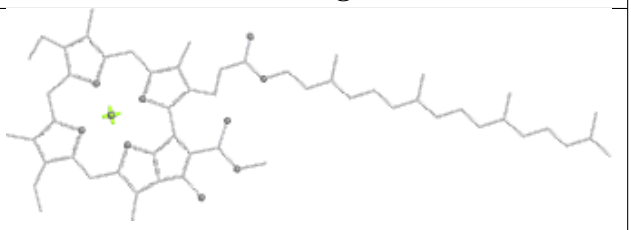
Bond lengths



Bond angles

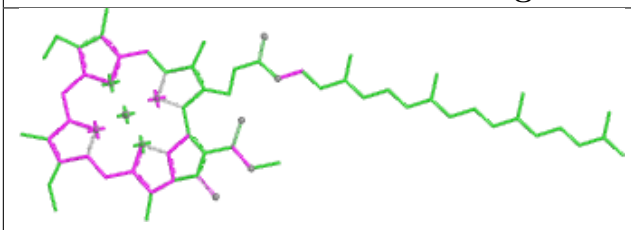


Torsions



Rings

Ligand CLA A 1127



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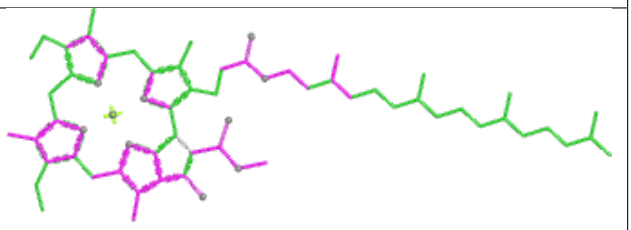
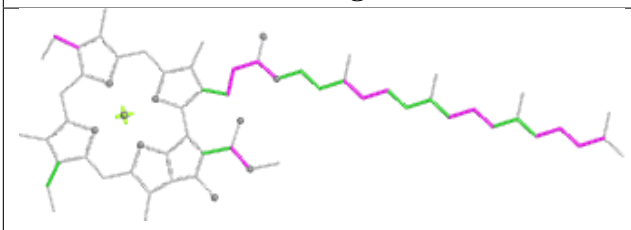


Bond angles



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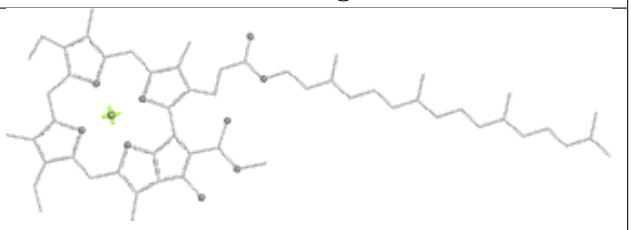
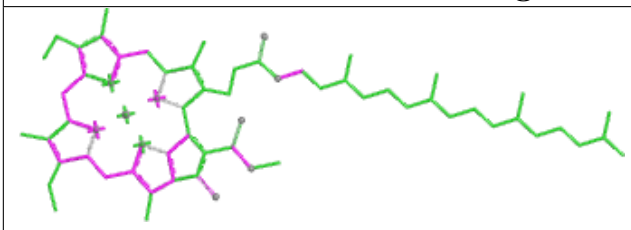


Rings

Ligand CLA A 1128



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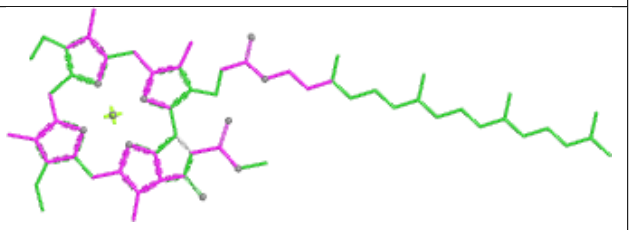
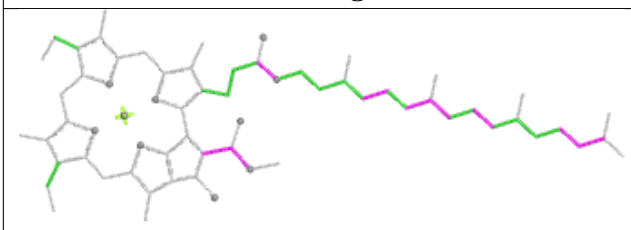
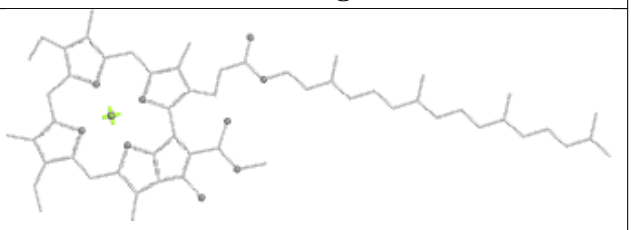


Bond angles

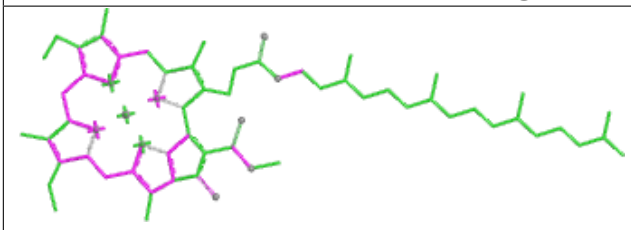


Torsions

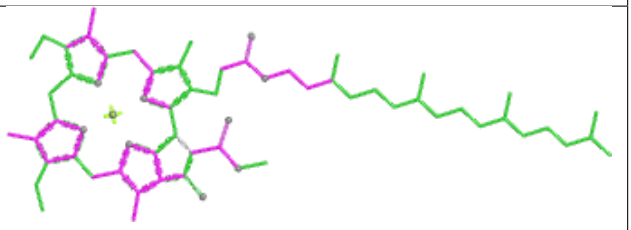


Rings

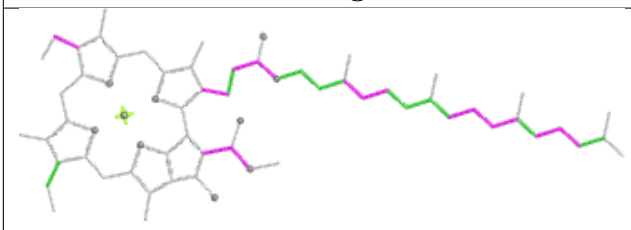
Ligand CLA B 1202



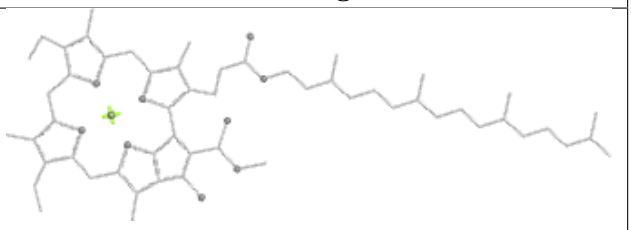
Bond lengths



Bond angles

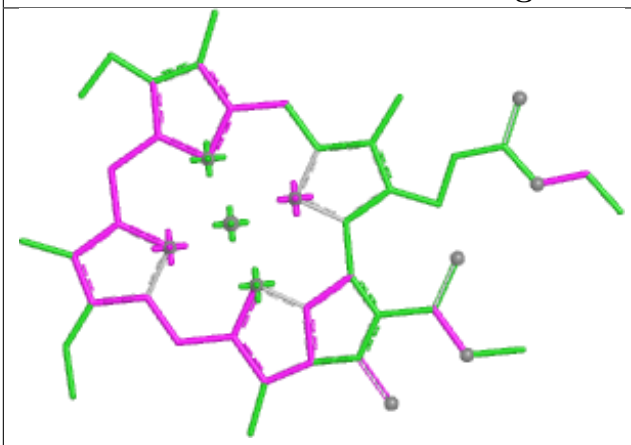


Torsions

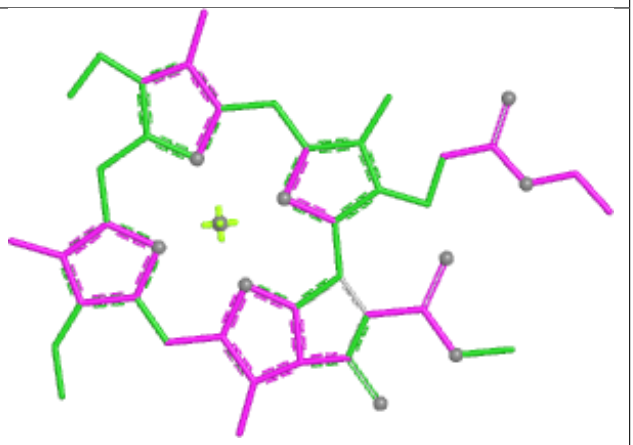


Rings

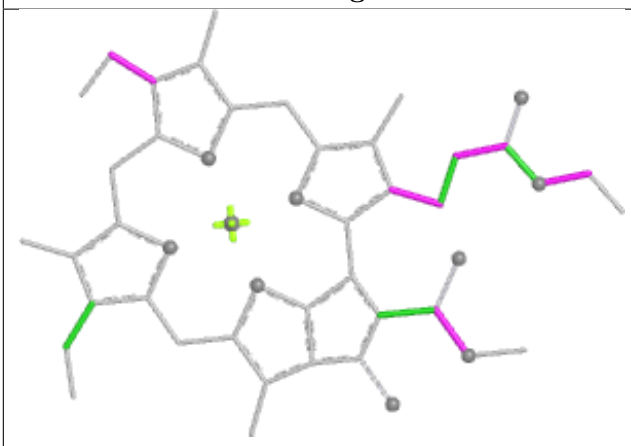
Ligand CLA B 1217



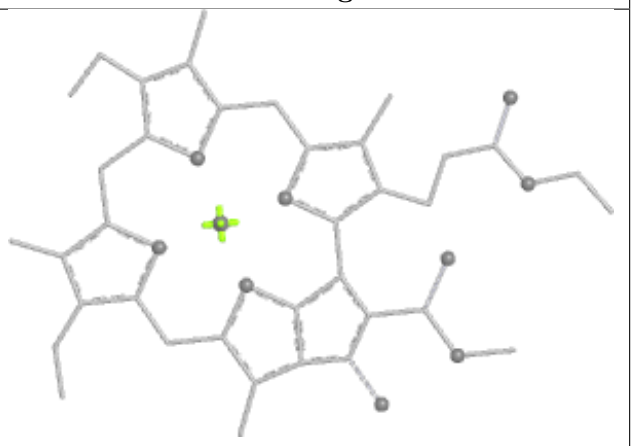
Bond lengths



Bond angles

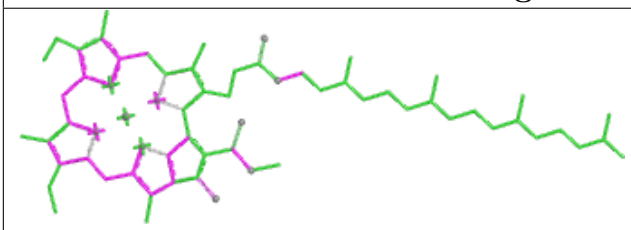


Torsions

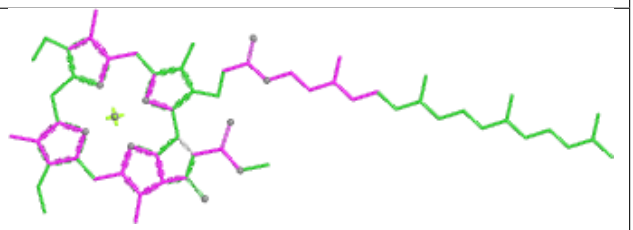


Rings

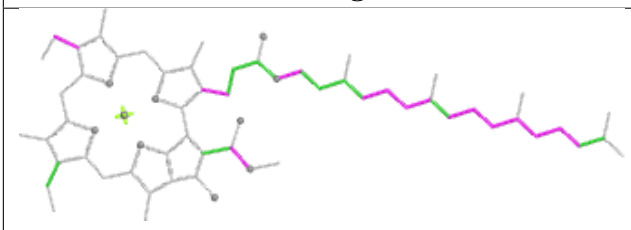
Ligand CLA A 1117



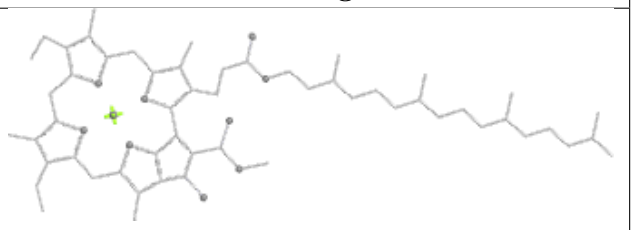
Bond lengths



Bond angles

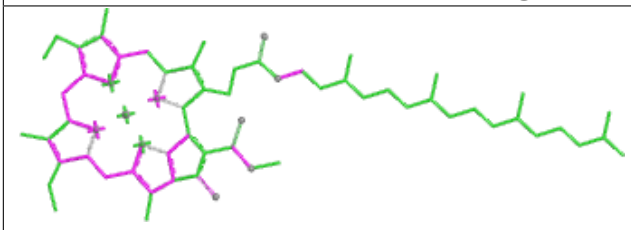


Torsions

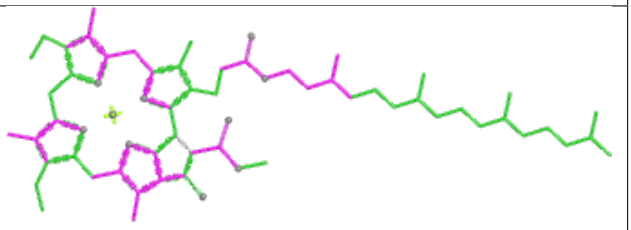


Rings

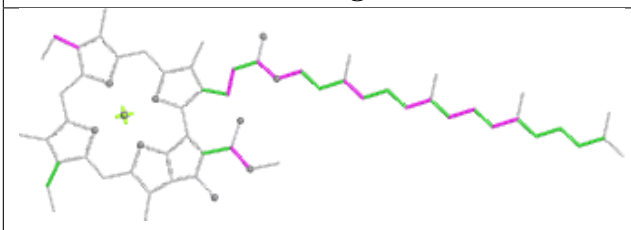
Ligand CLA B 1214



Bond lengths



Bond angles



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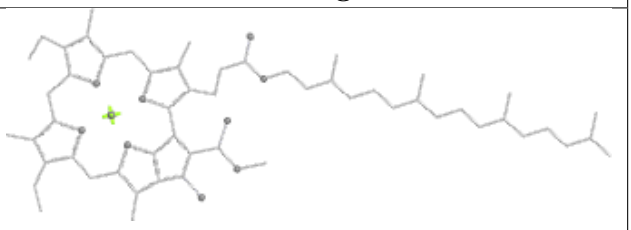
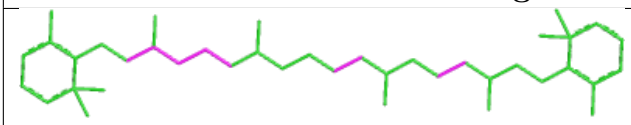


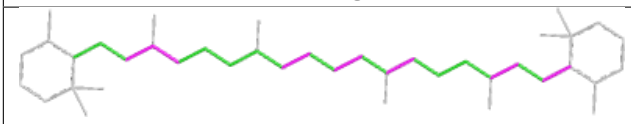
Rings

Ligand BCR A 4003

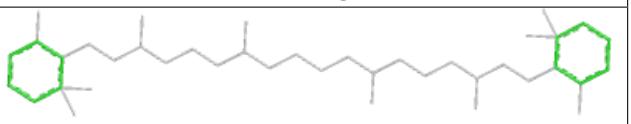


Bond lengths

Bond angles

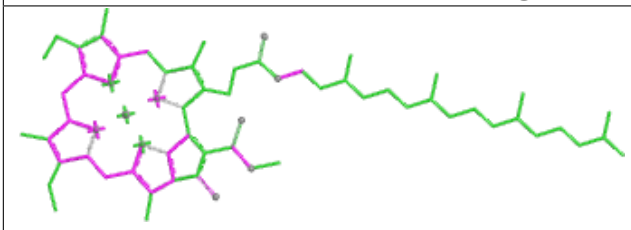


Torsions

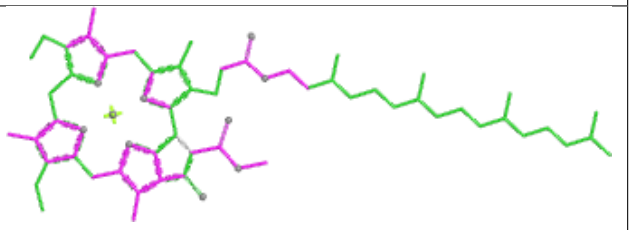


Rings

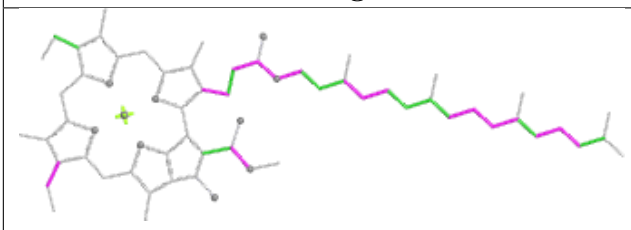
Ligand CLA B 1228



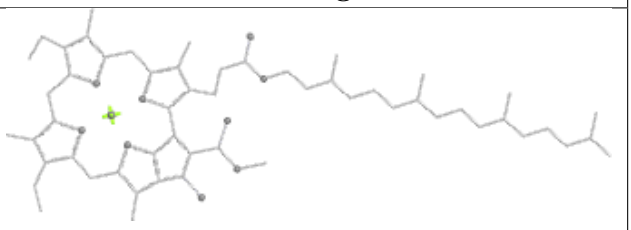
Bond lengths



Bond angles

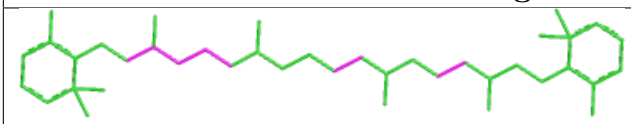


Torsions

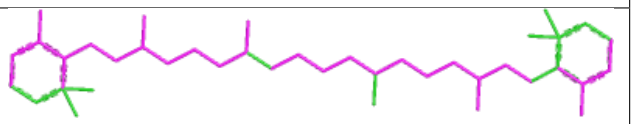


Rings

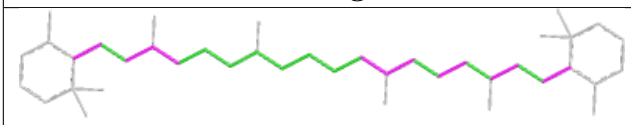
Ligand BCR B 4011



Bond lengths



Bond angles



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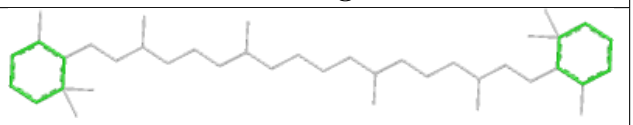
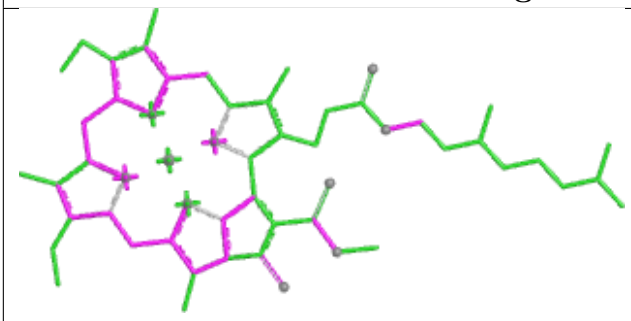
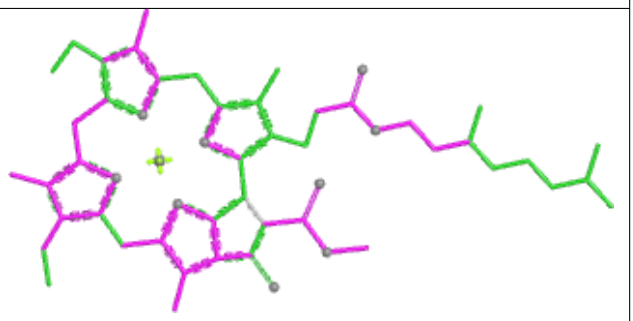


Rings

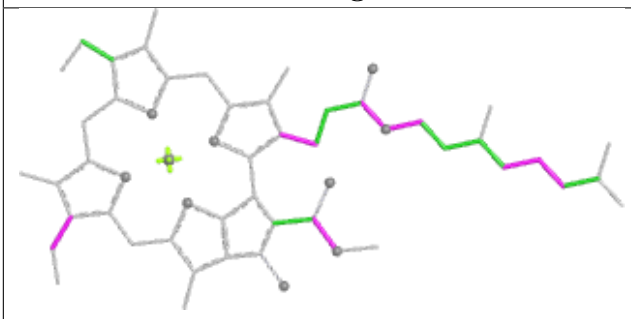
Ligand CLA A 1131



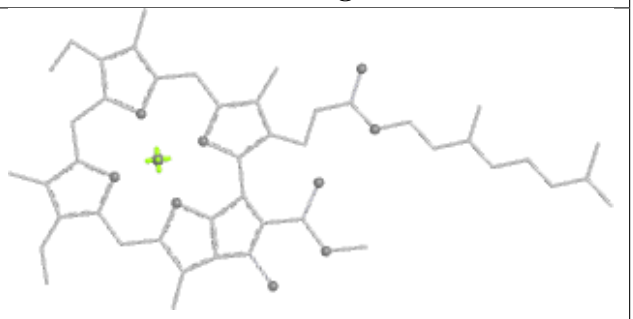
Bond lengths



Bond angles

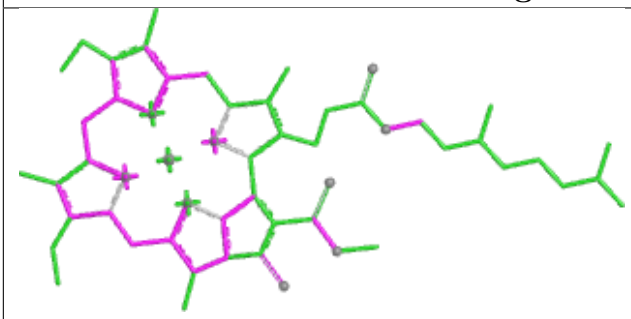


Torsions

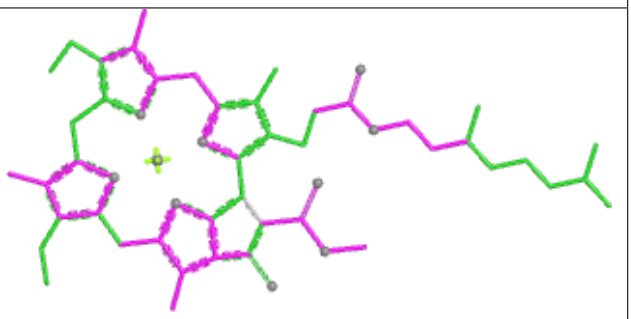


Rings

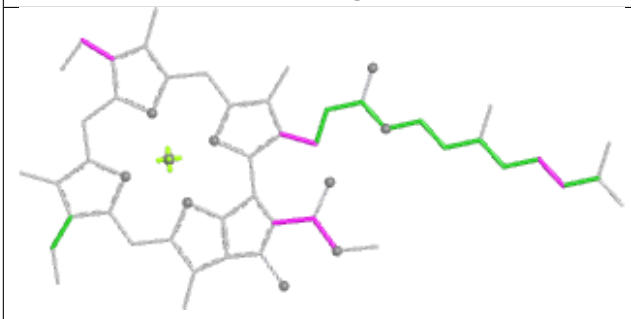
Ligand CLA A 1124



Bond lengths



Bond angles



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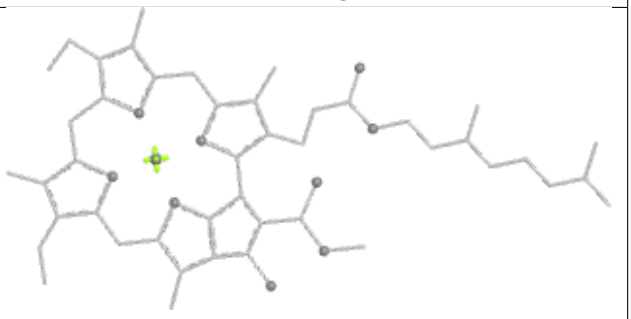
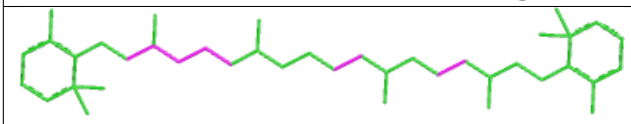
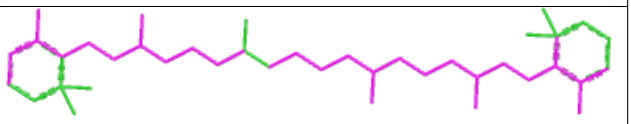


Rings

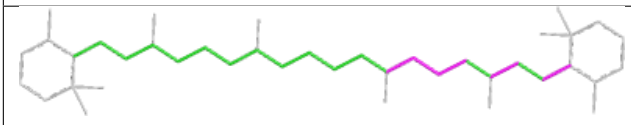
Ligand BCR B 4010



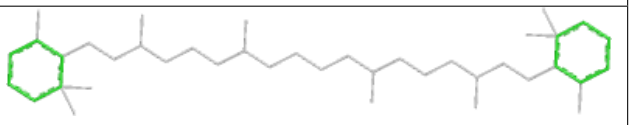
Bond lengths



Bond angles

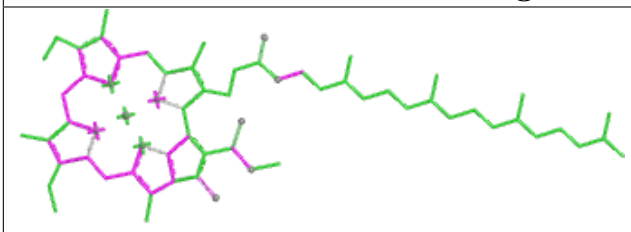


Torsions

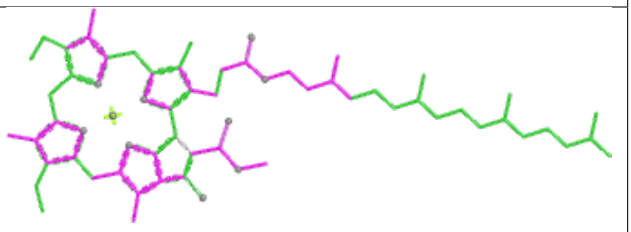


Rings

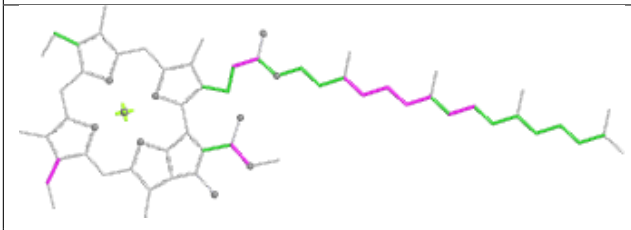
Ligand CLA B 1231



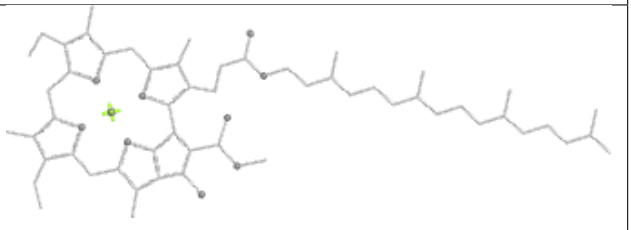
Bond lengths



Bond angles

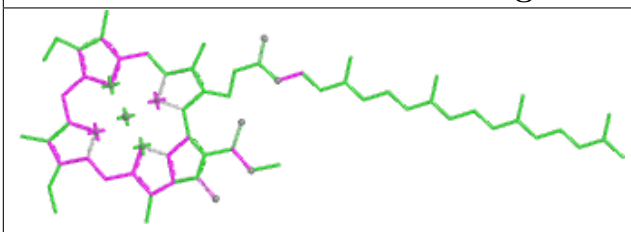


Torsions



Rings

Ligand CLA B 1215



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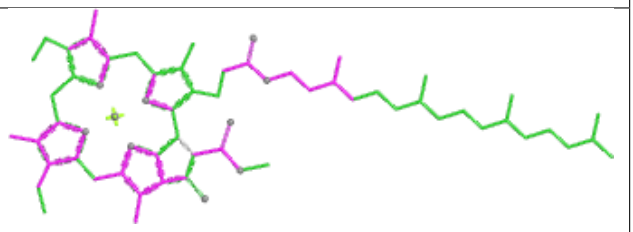
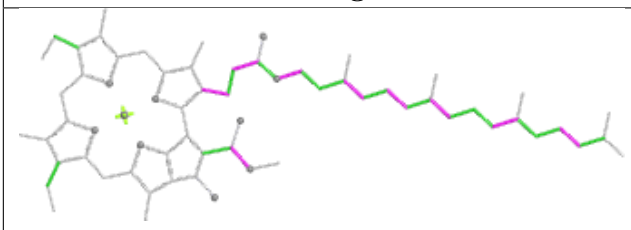
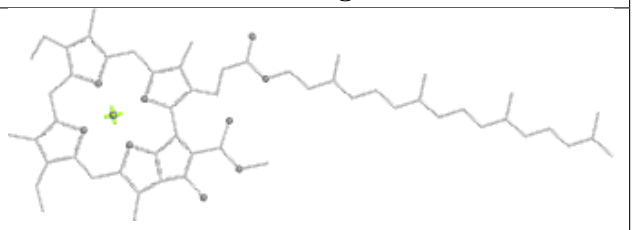


Bond angles

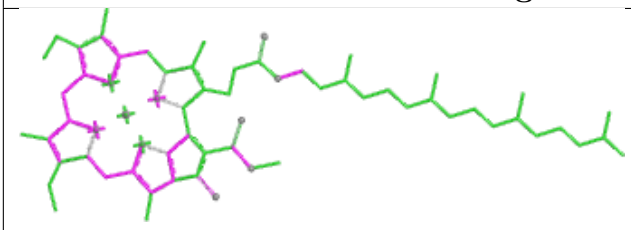


Torsions

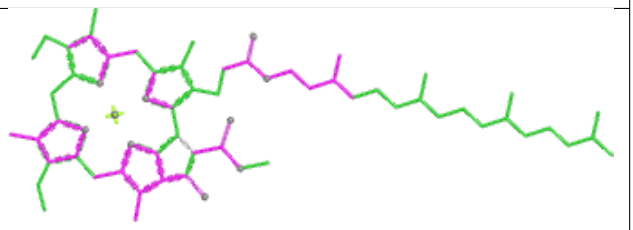


Rings

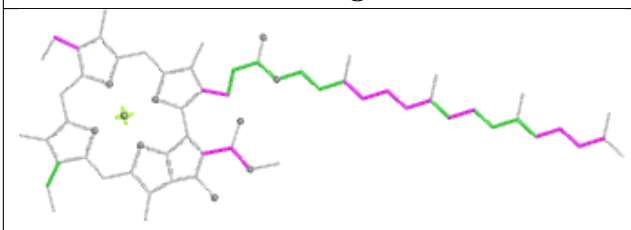
Ligand CLA B 1223



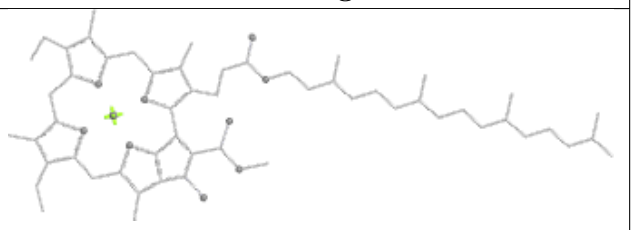
Bond lengths



Bond angles

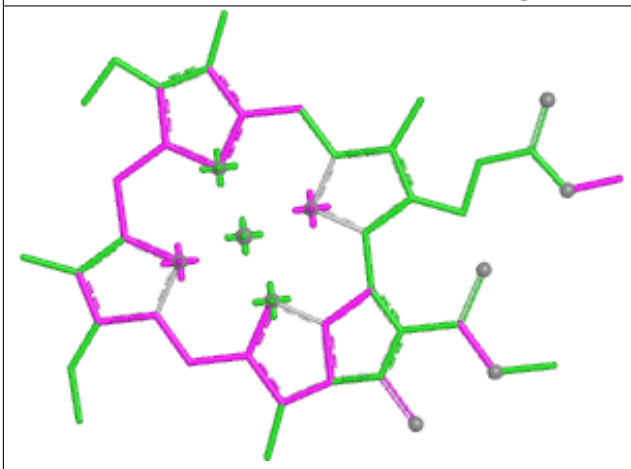


Torsions

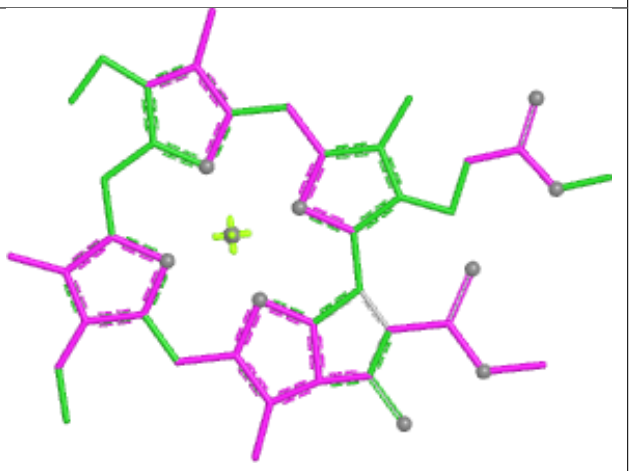


Rings

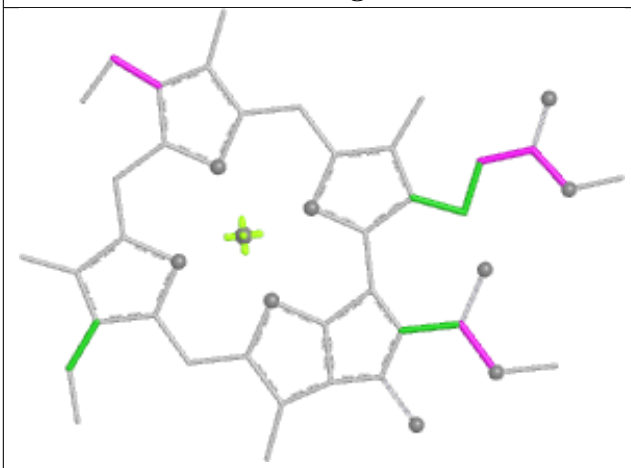
Ligand CLA B 1206



Bond lengths



Bond angles



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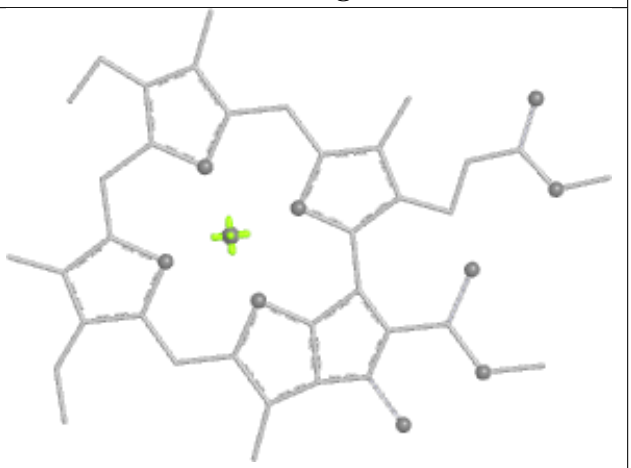
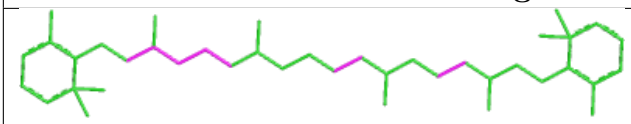


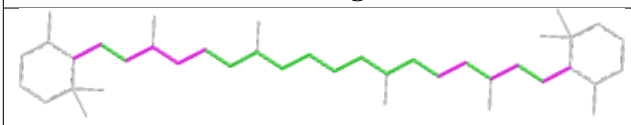
Rings

Ligand BCR B 4004

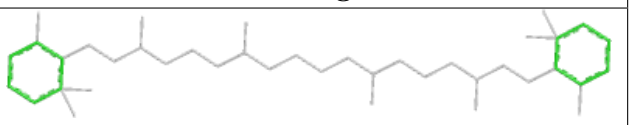


Bond lengths

Bond angles

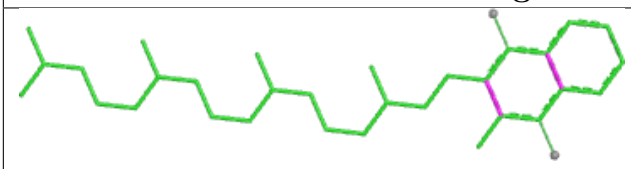


Torsions

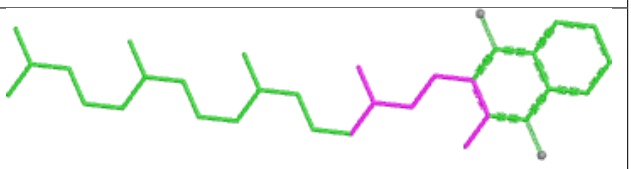


Rings

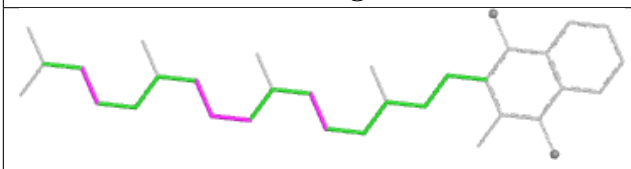
Ligand PQN B 2002



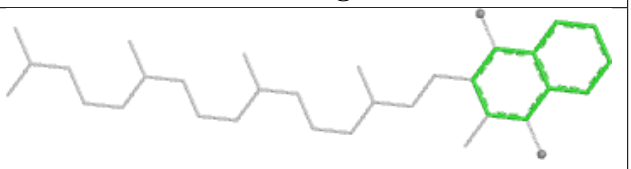
Bond lengths



Bond angles

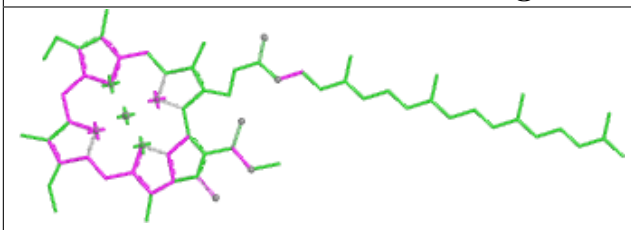


Torsions

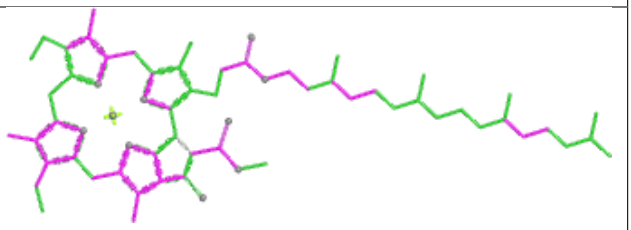


Rings

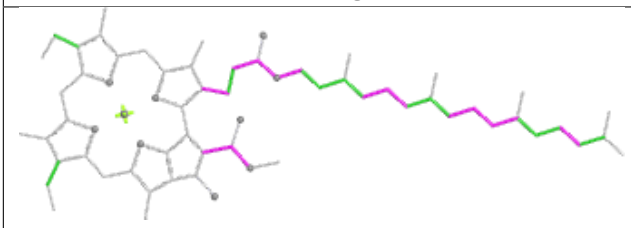
Ligand CLA B 1210



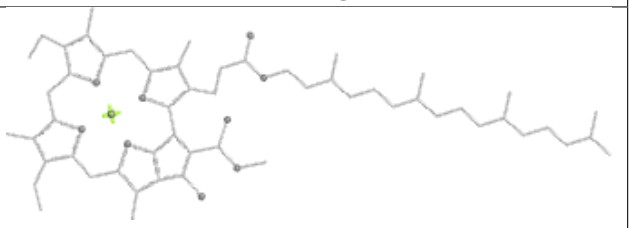
Bond lengths



Bond angles

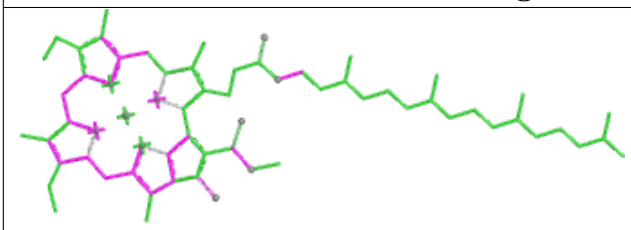


Torsions

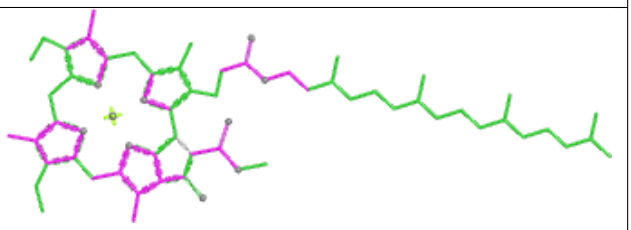


Rings

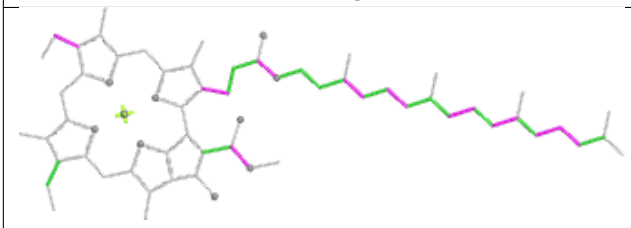
Ligand CLA B 1224



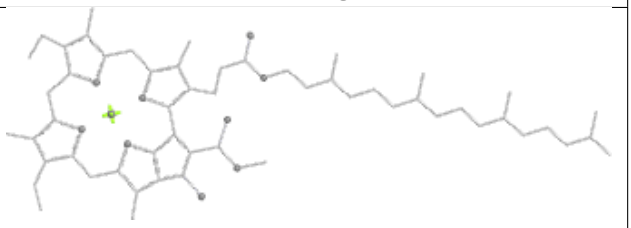
Bond lengths



Bond angles

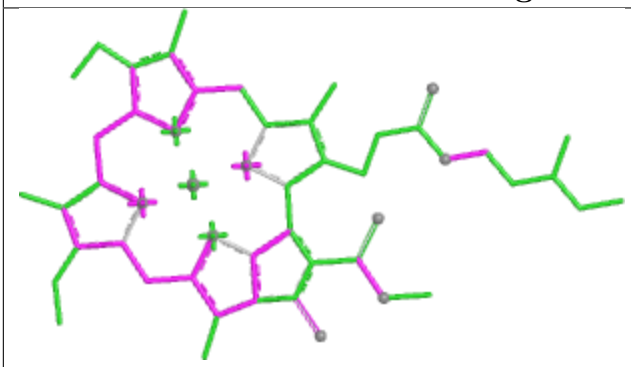


Torsions



Rings

Ligand CLA B 1218



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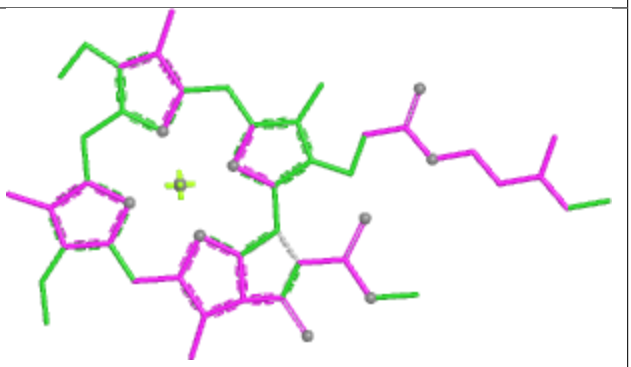
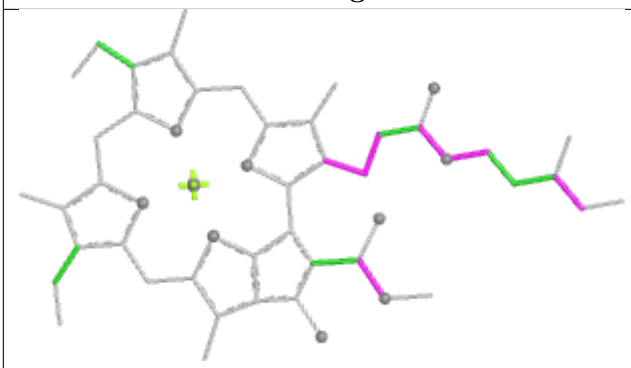
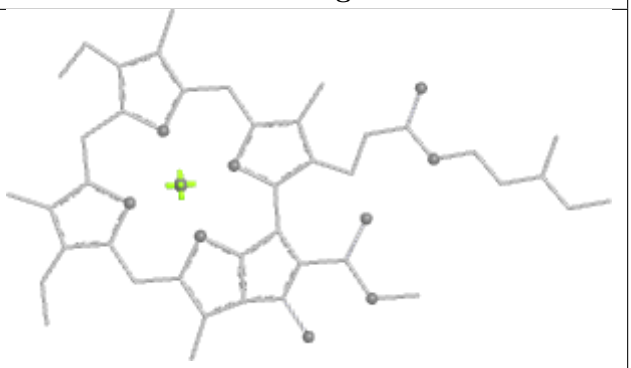


Bond angles

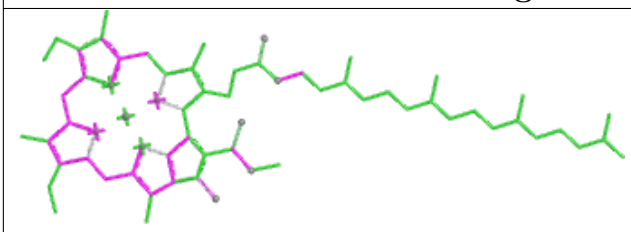


Torsions



Rings

Ligand CLA A 1012



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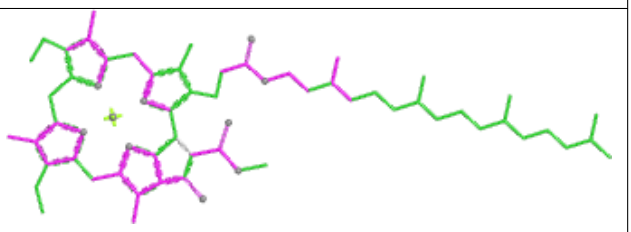
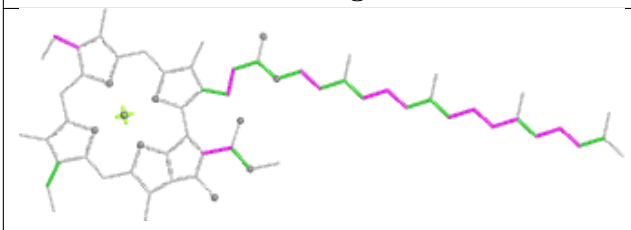


Bond angles



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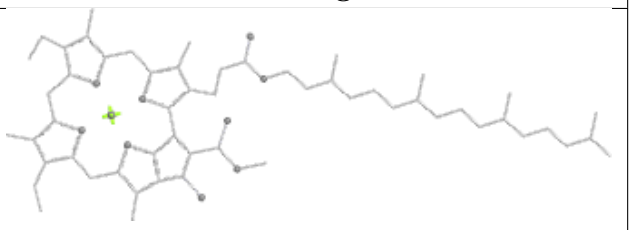
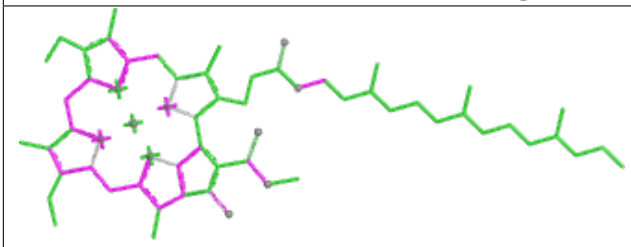
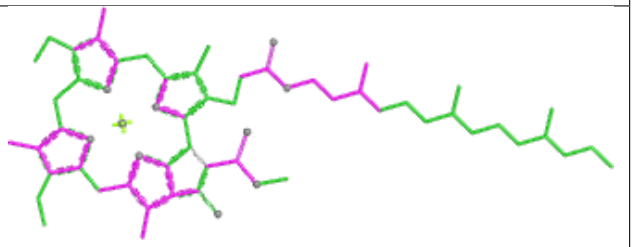


Rings

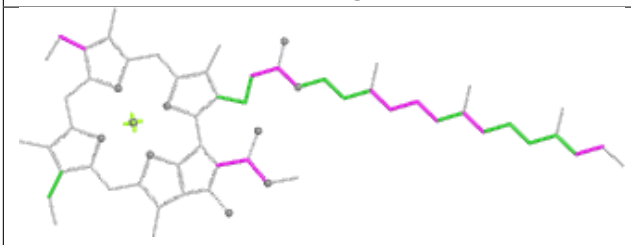
Ligand CLA A 1132



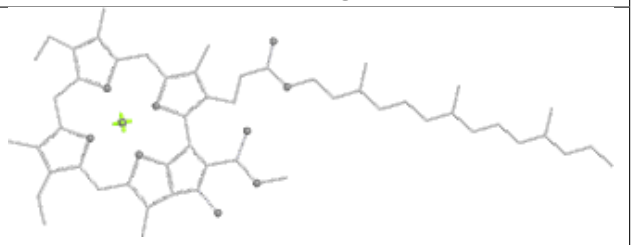
Bond lengths



Bond angles

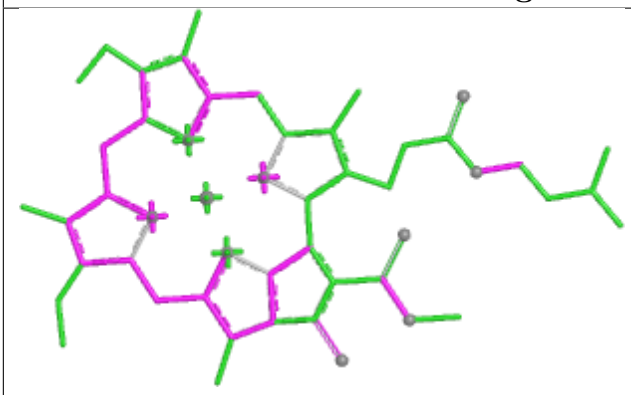


Torsions

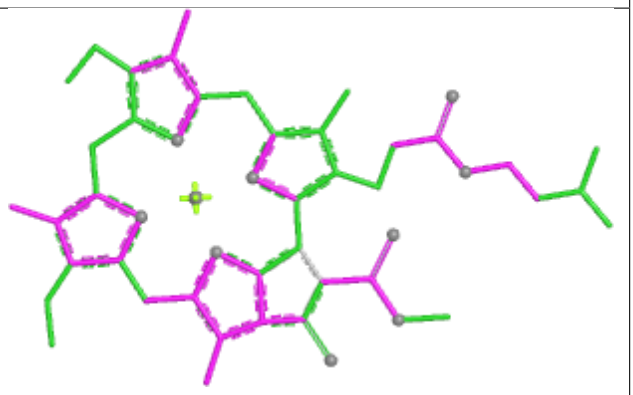


Rings

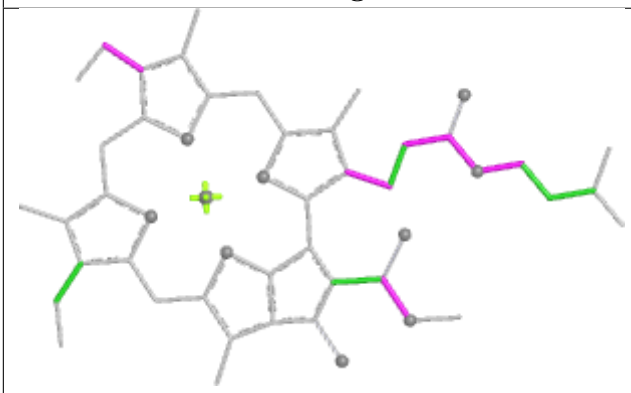
Ligand CLA B 1213



Bond lengths



Bond angles



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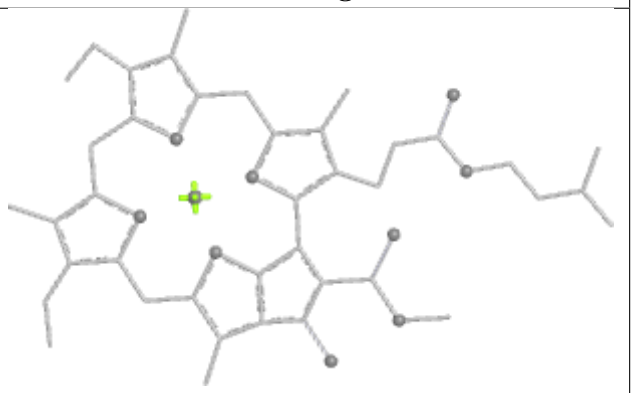
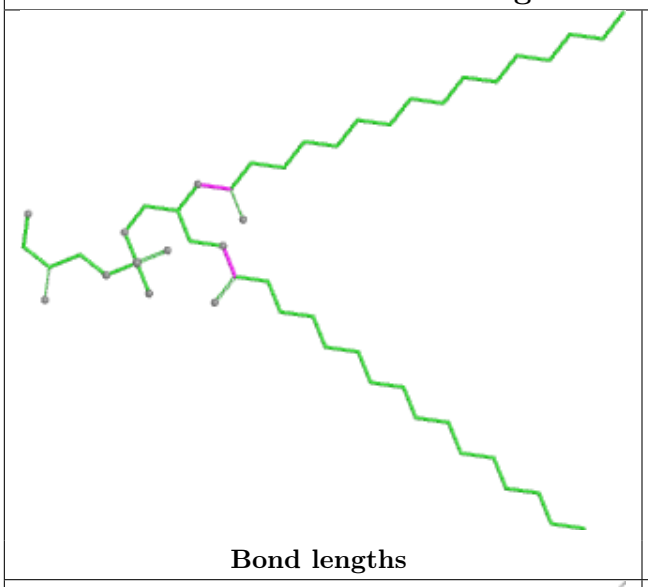
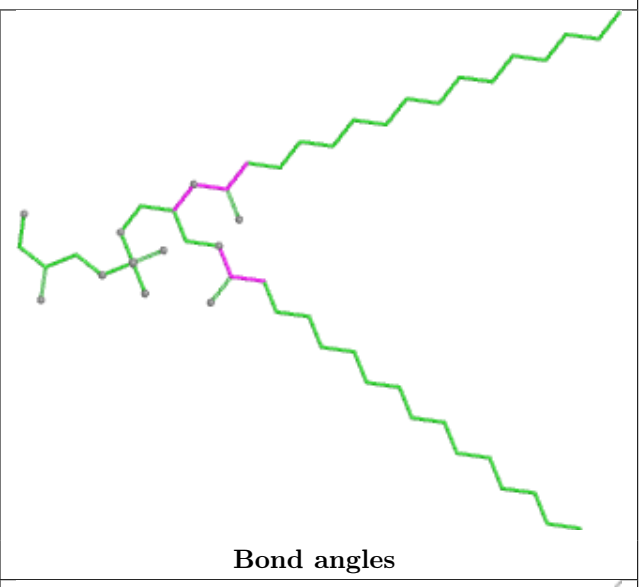


Rings

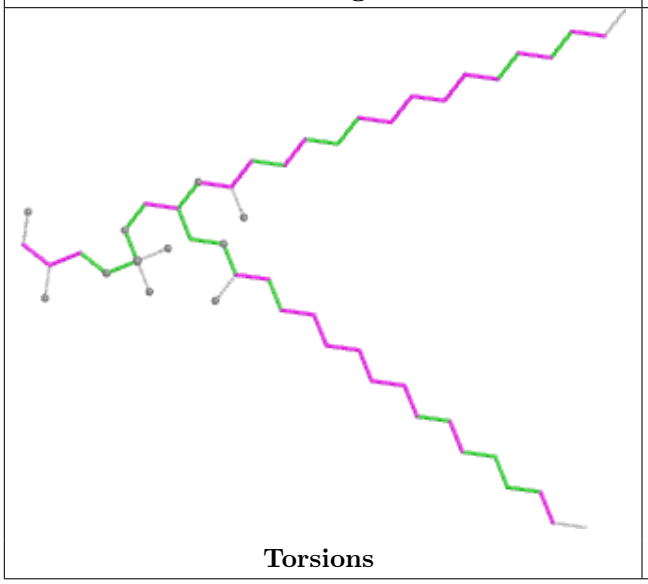
Ligand LHG A 5001



Bond lengths



Bond angles



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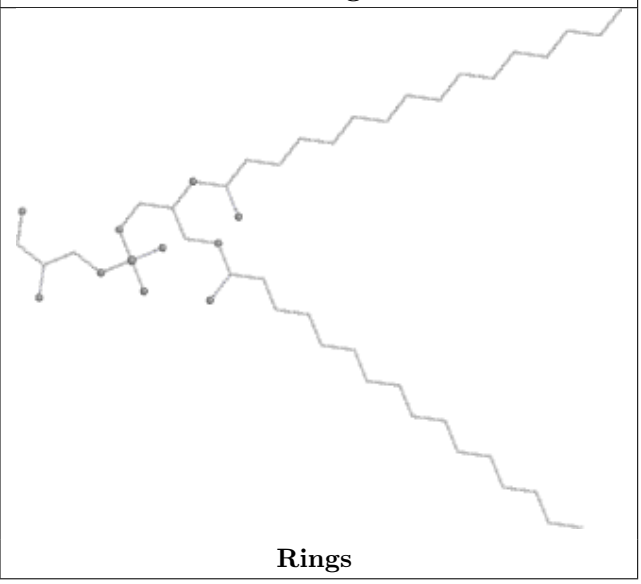
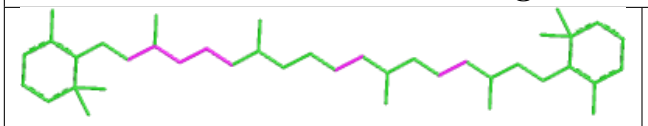


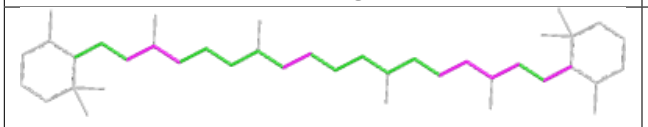
Rings

Ligand BCR B 4006

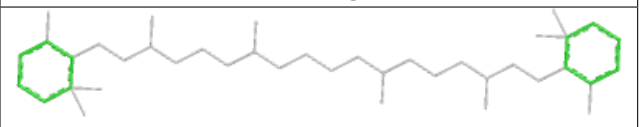


Bond lengths

Bond angles

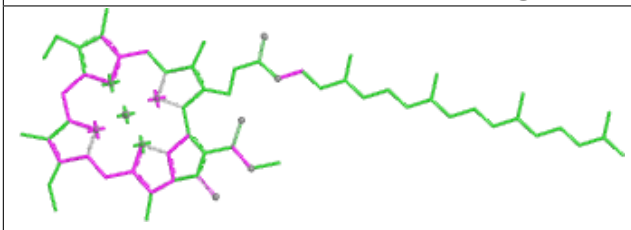


Torsions

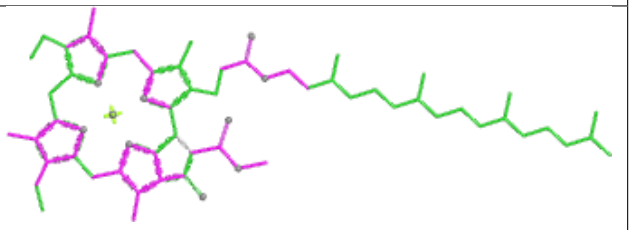


Rings

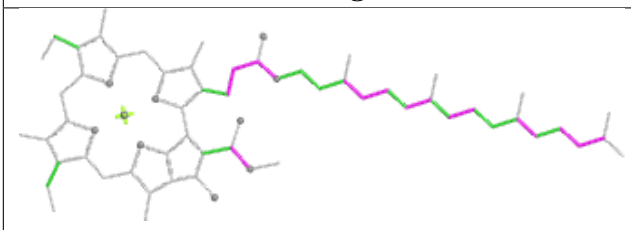
Ligand CLA A 1136



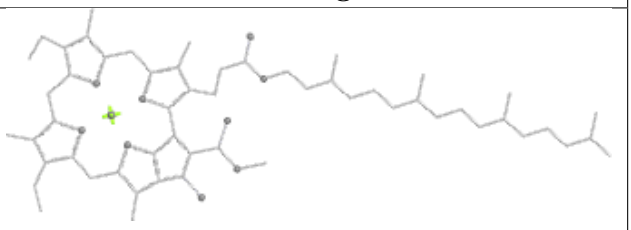
Bond lengths



Bond angles

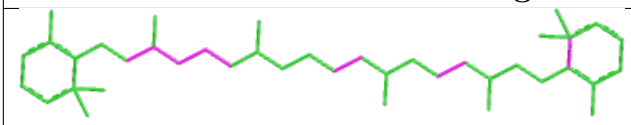


Torsions



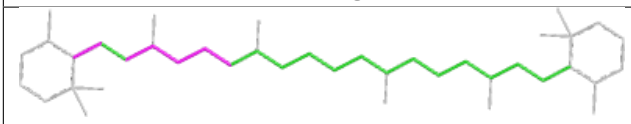
Rings

Ligand BCR B 4017

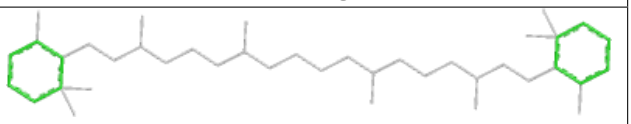


Bond lengths

Bond angles

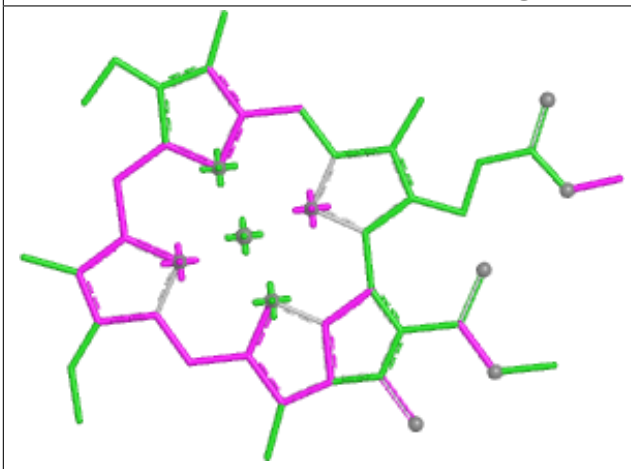


Torsions

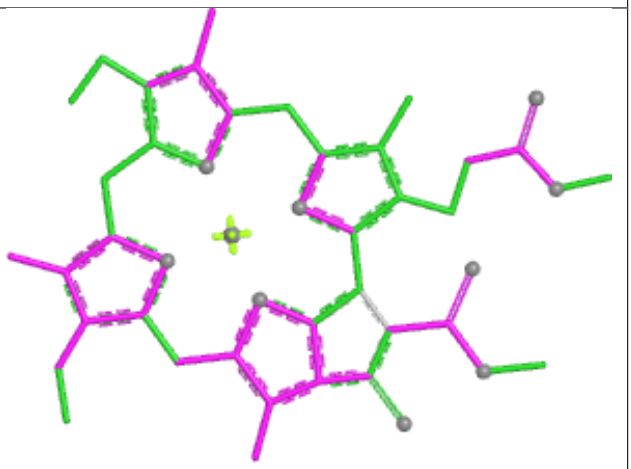


Rings

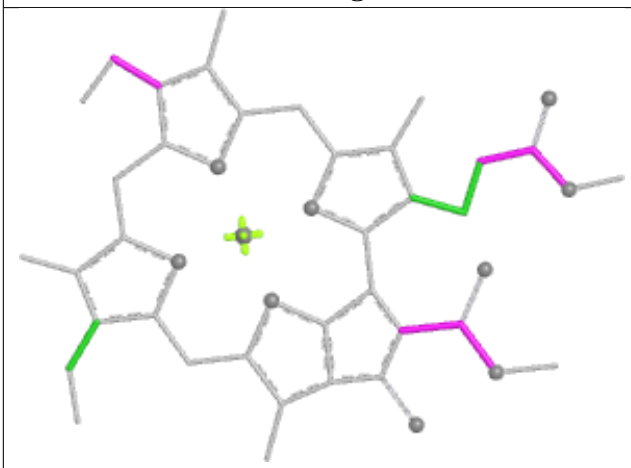
Ligand CLA B 1211



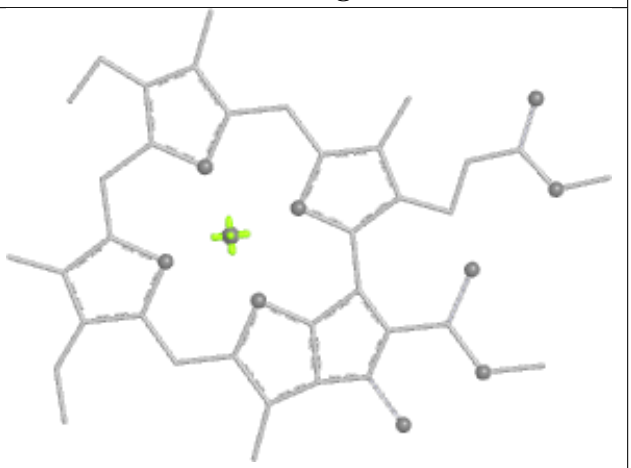
Bond lengths



Bond angles

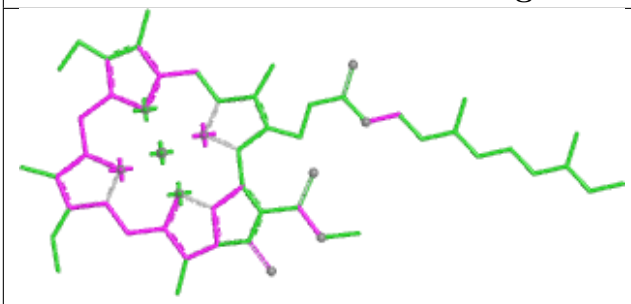


Torsions

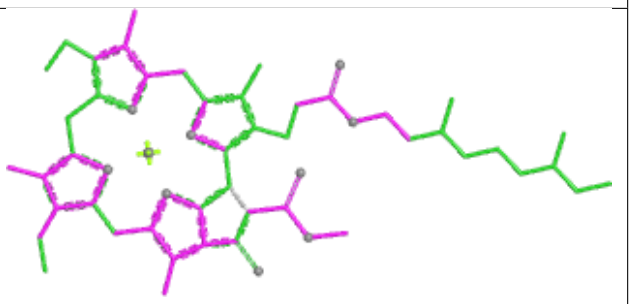


Rings

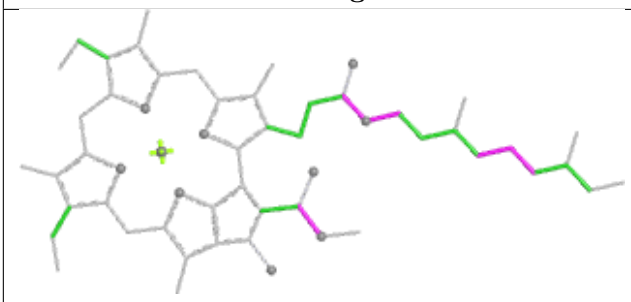
Ligand CLA B 1220



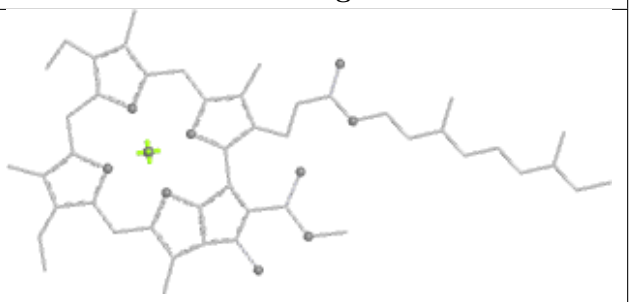
Bond lengths



Bond angles

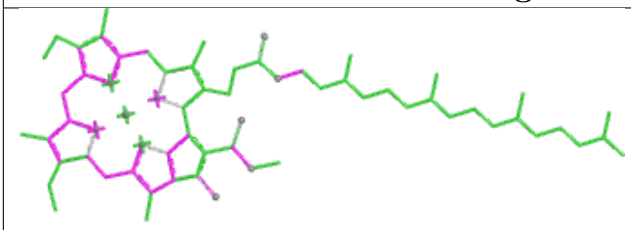


Torsions



Rings

Ligand CLA A 1138



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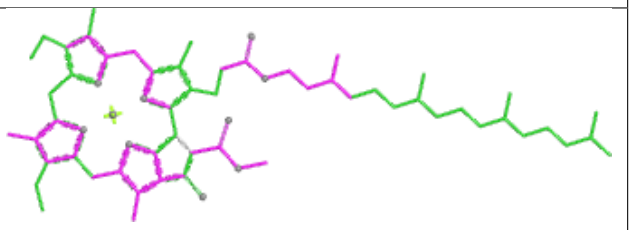
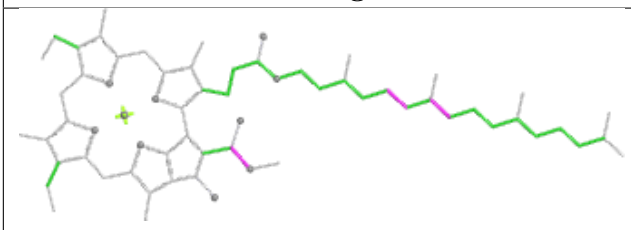


Bond angles



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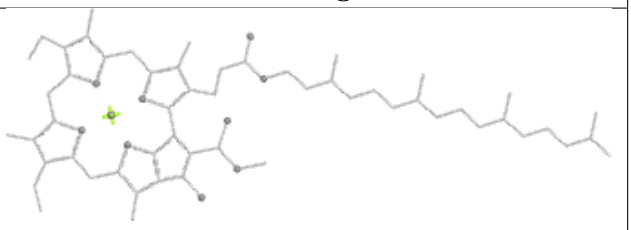
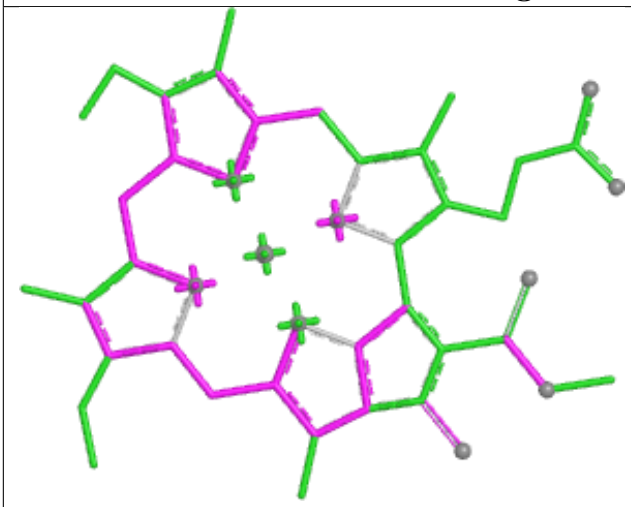
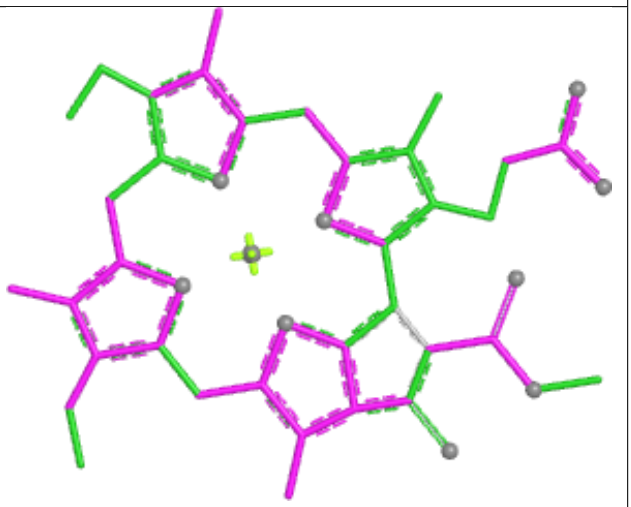


Rings

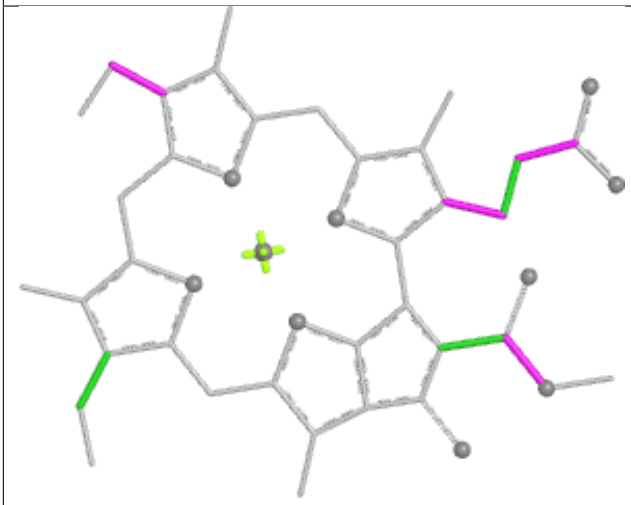
Ligand CLA B 1209



Bond lengths



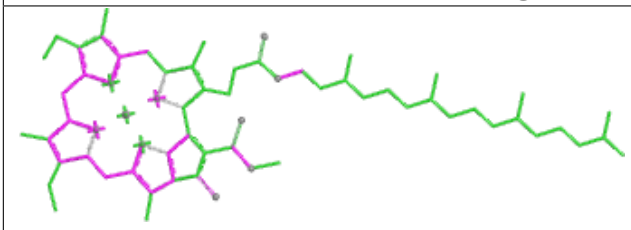
Bond angles



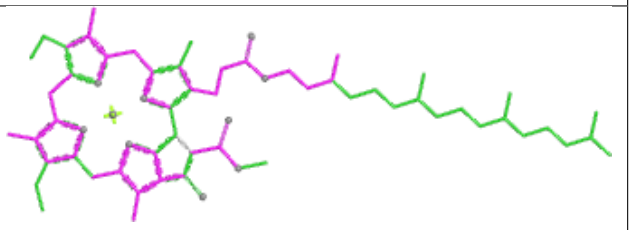
Torsions

Rings

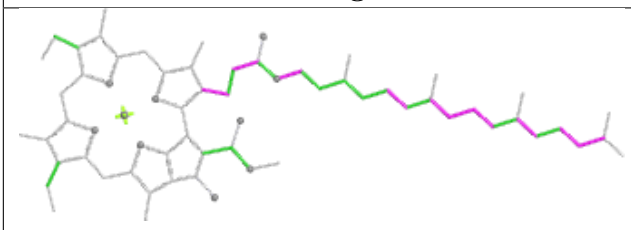
Ligand CLA A 1101



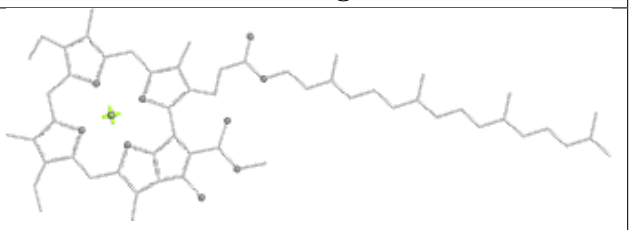
Bond lengths



Bond angles

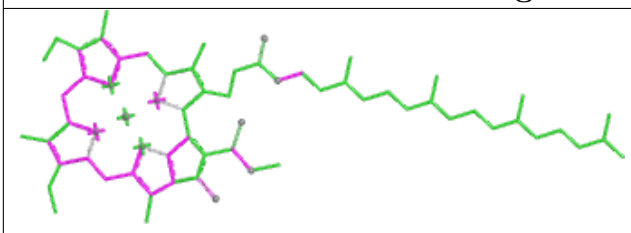


Torsions

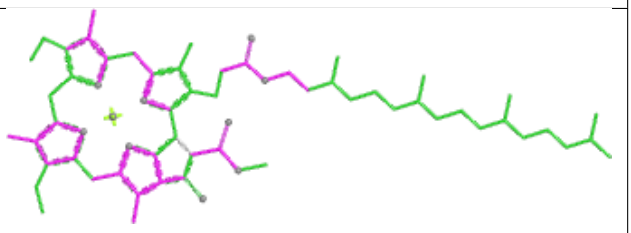


Rings

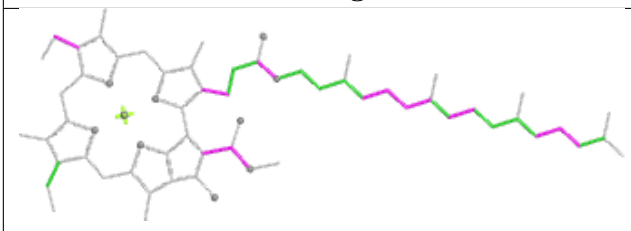
Ligand CLA B 1226



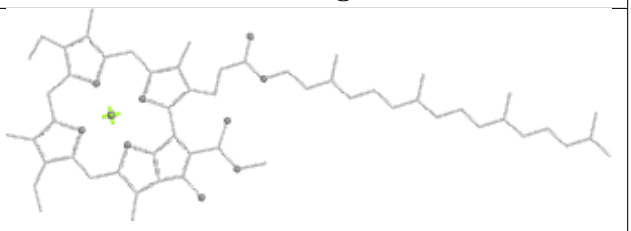
Bond lengths



Bond angles

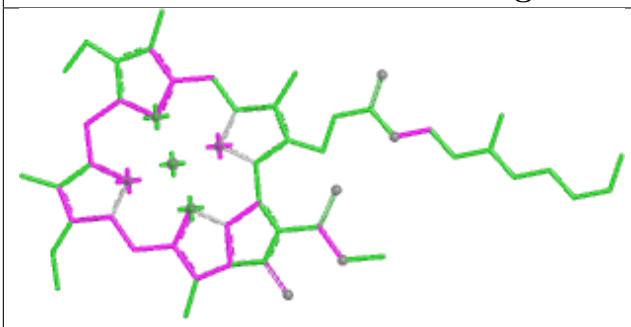


Torsions

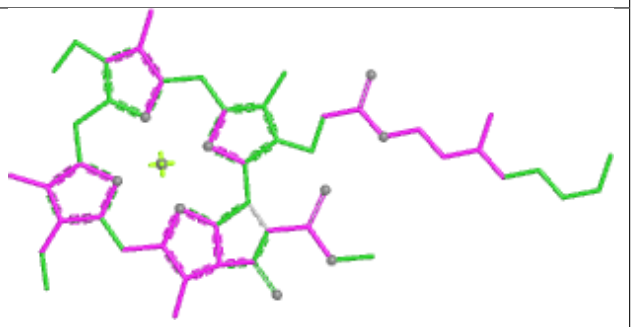


Rings

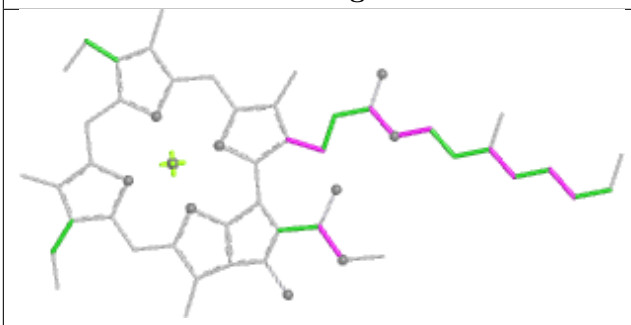
Ligand CLA A 1110



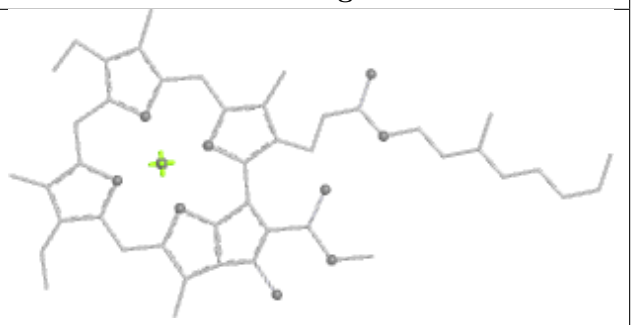
Bond lengths



Bond angles

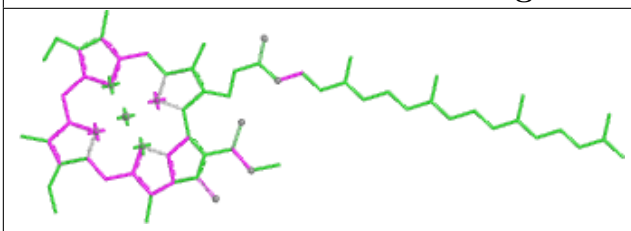


Torsions

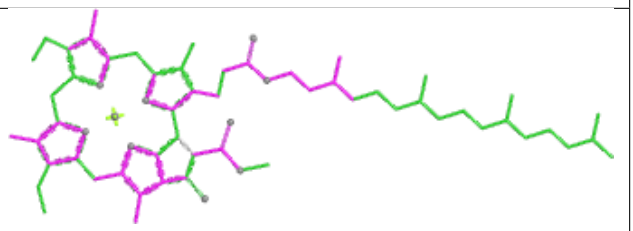


Rings

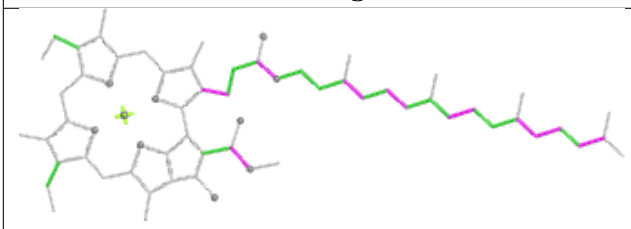
Ligand CLA B 1230



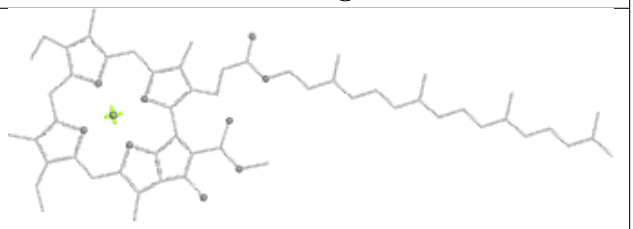
Bond lengths



Bond angles

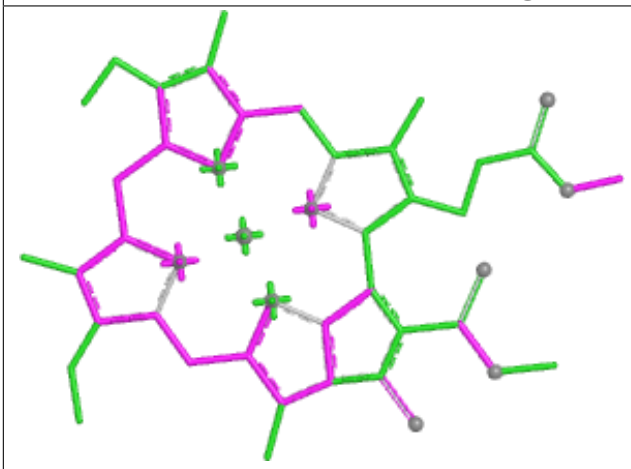


Torsions



Rings

Ligand CLA J 1303



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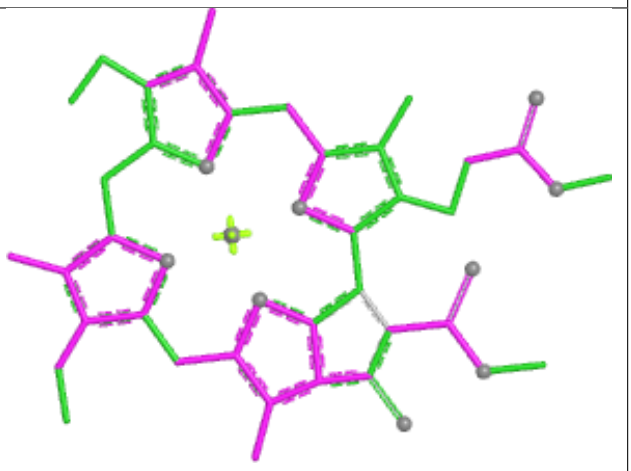
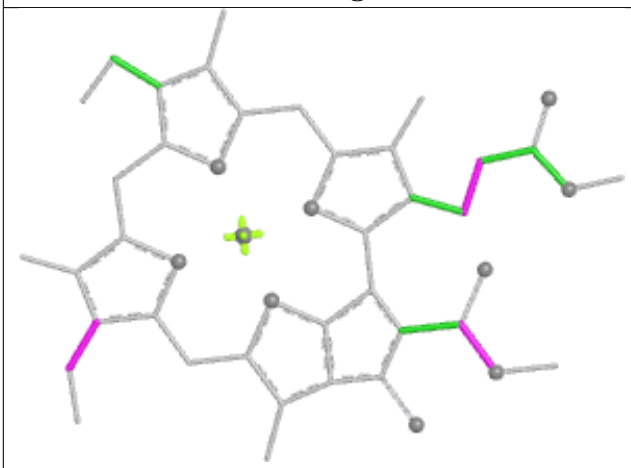
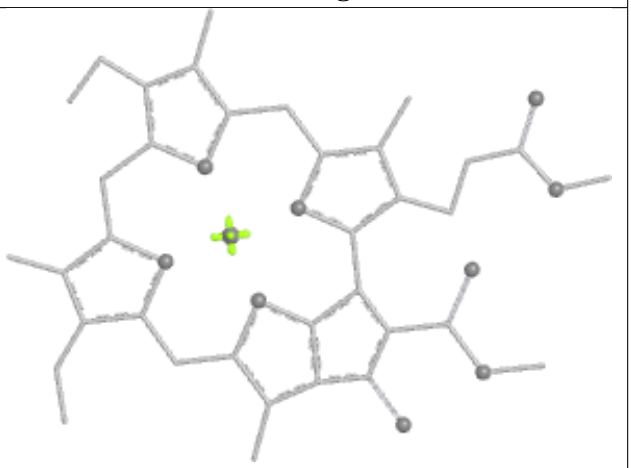


Bond angles

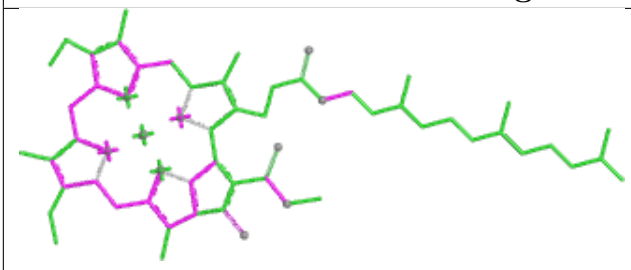


Torsions

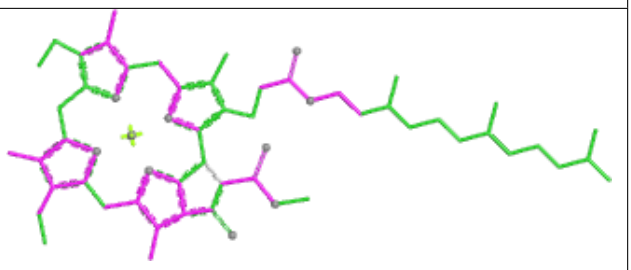


Rings

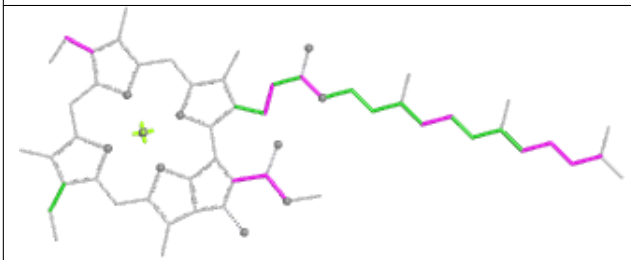
Ligand CLA A 1111



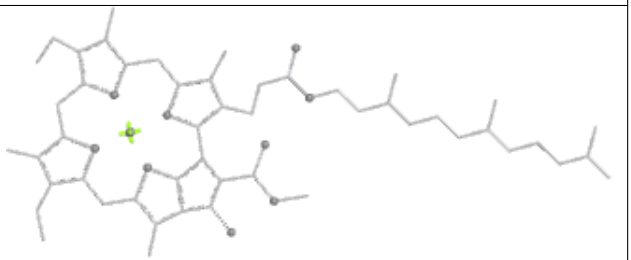
Bond lengths



Bond angles

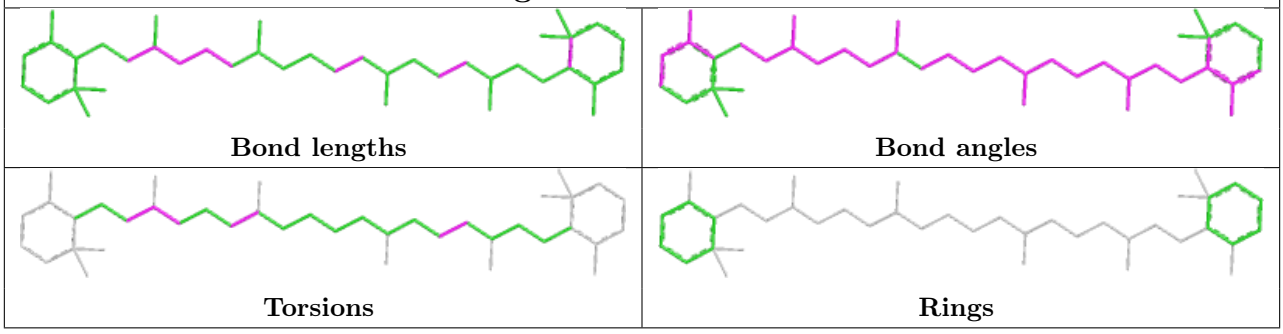


Torsions

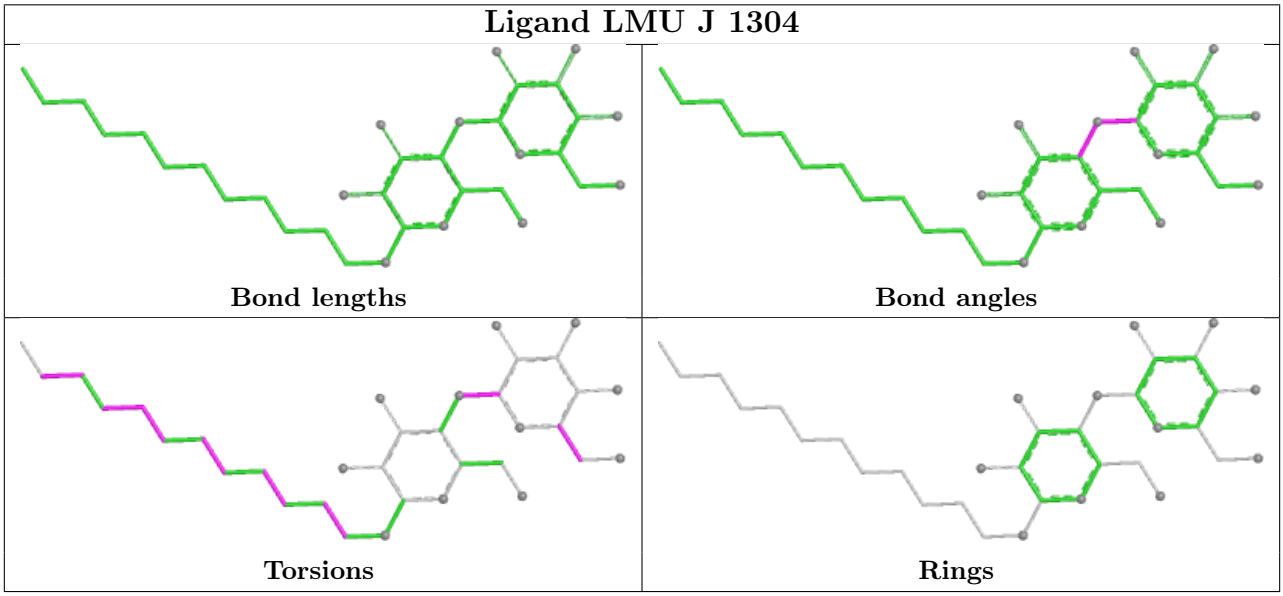


Rings

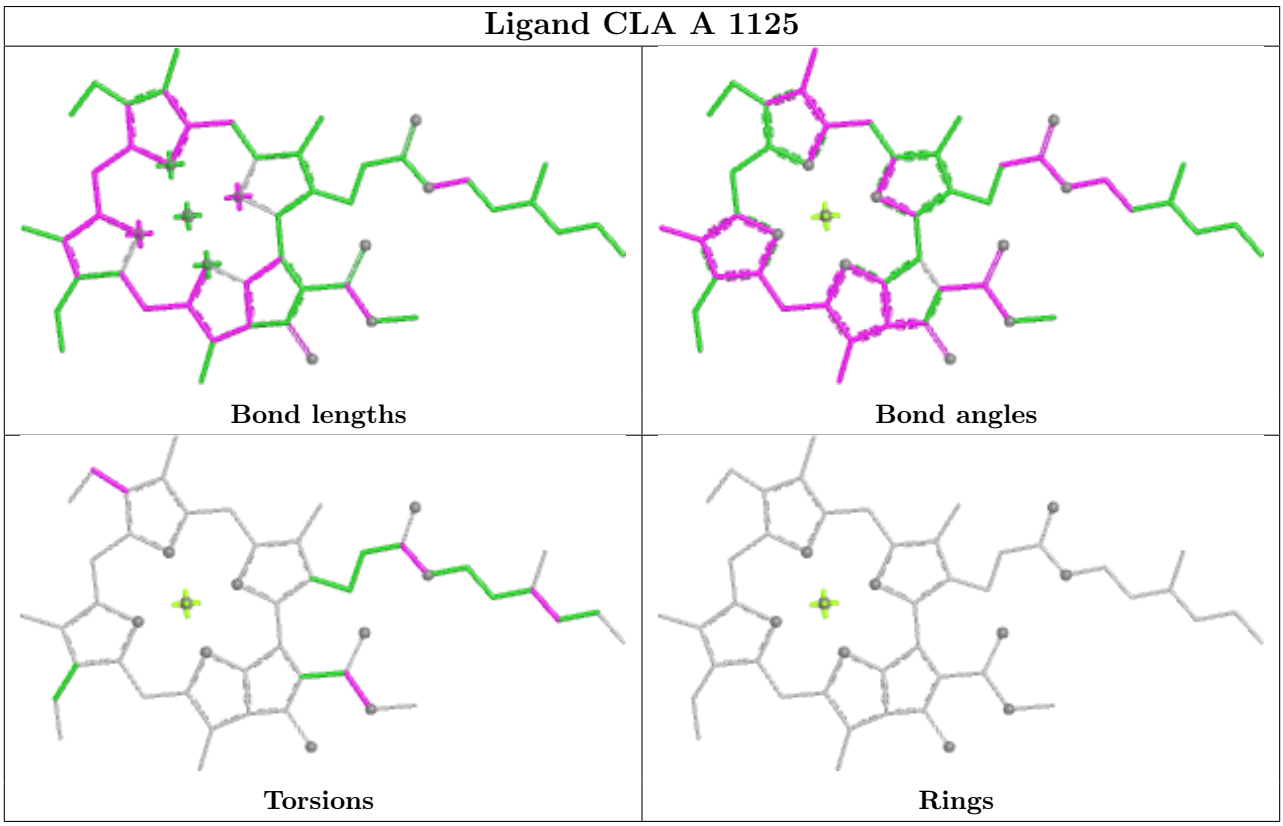
Ligand BCR A 4002



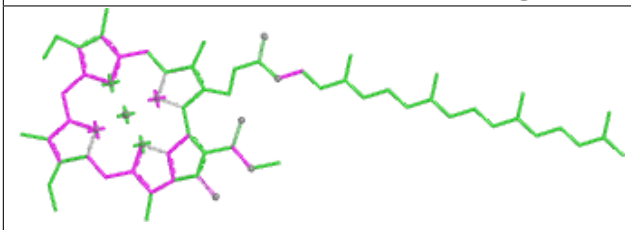
Ligand LMU J 1304



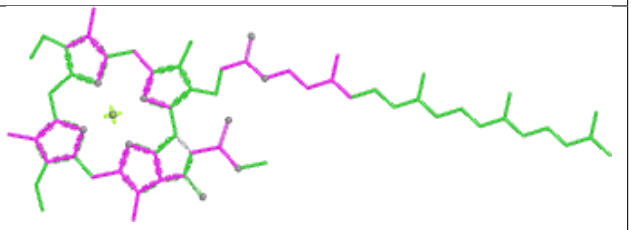
Ligand CLA A 1125



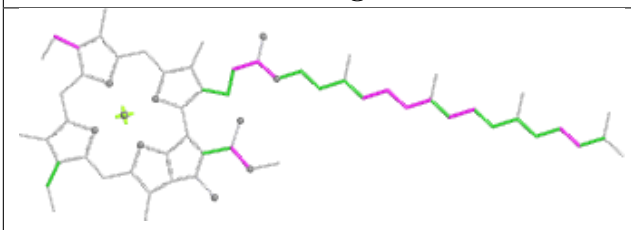
Ligand CLA B 1235



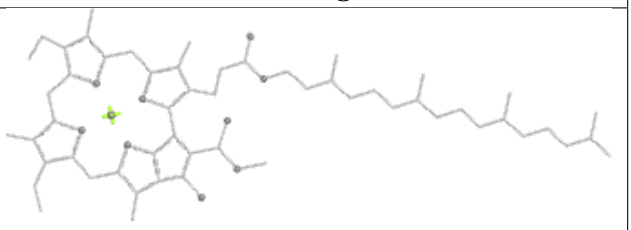
Bond lengths



Bond angles

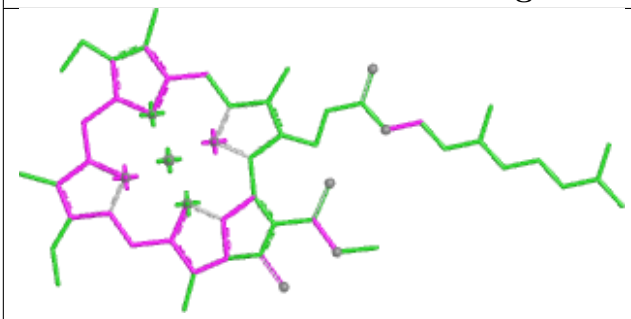


Torsions

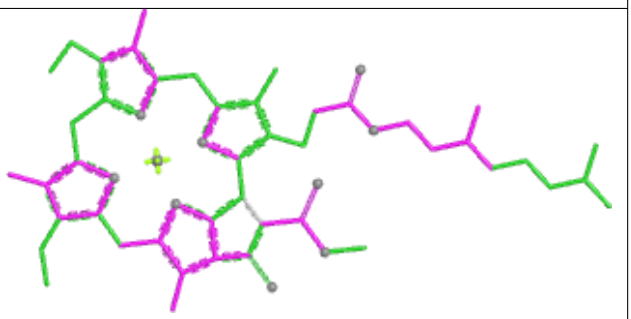


Rings

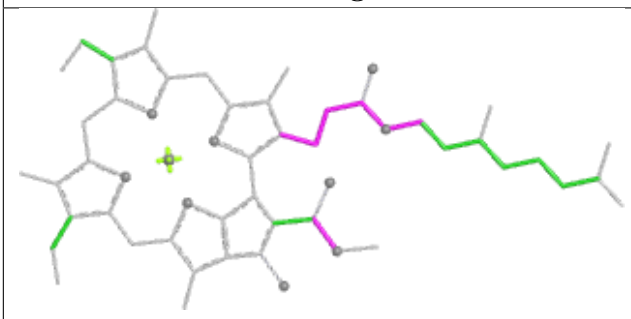
Ligand CLA B 1219



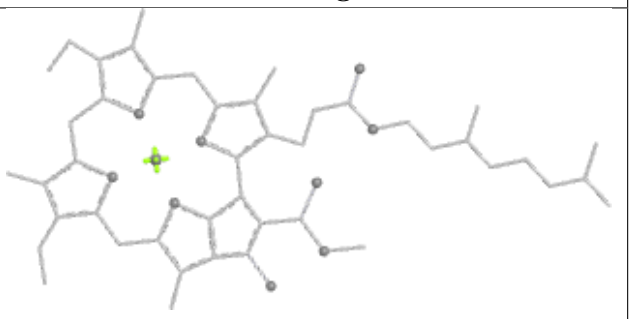
Bond lengths



Bond angles

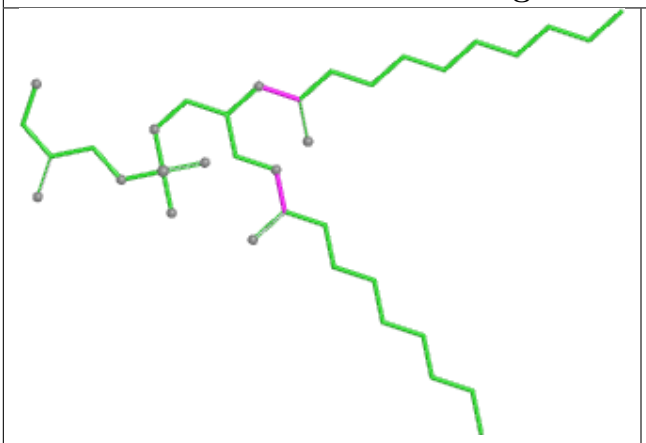


Torsions

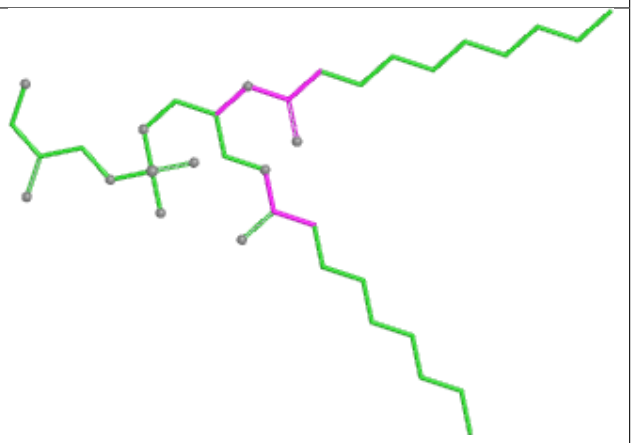


Rings

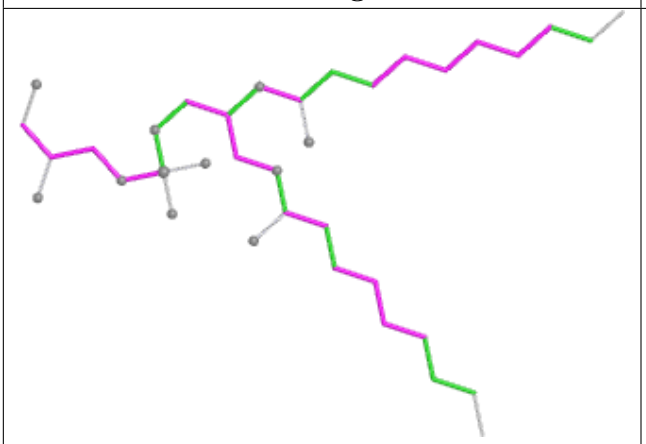
Ligand LHG A 5005



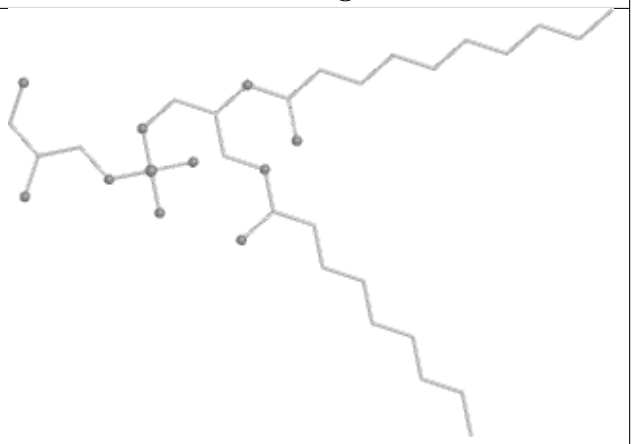
Bond lengths



Bond angles

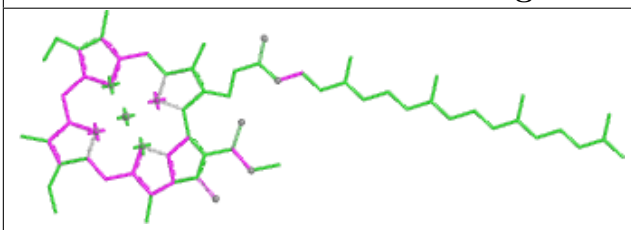


Torsions



Rings

Ligand CLA B 1229



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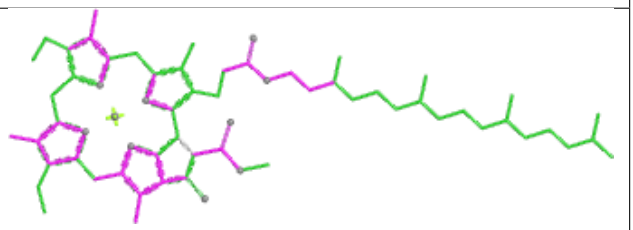
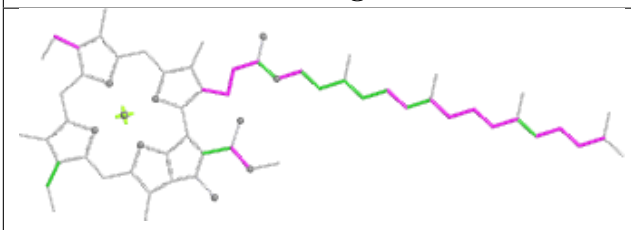
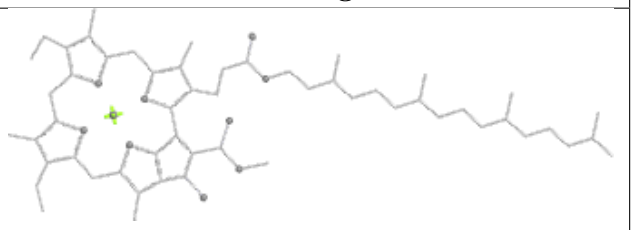


Bond angles

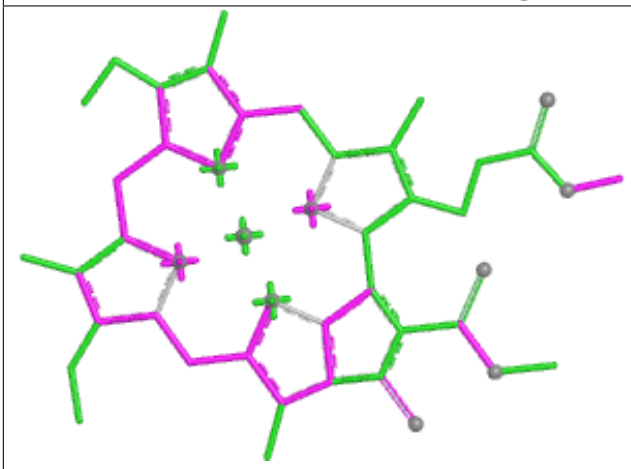


Torsions



Rings

Ligand CLA B 1201



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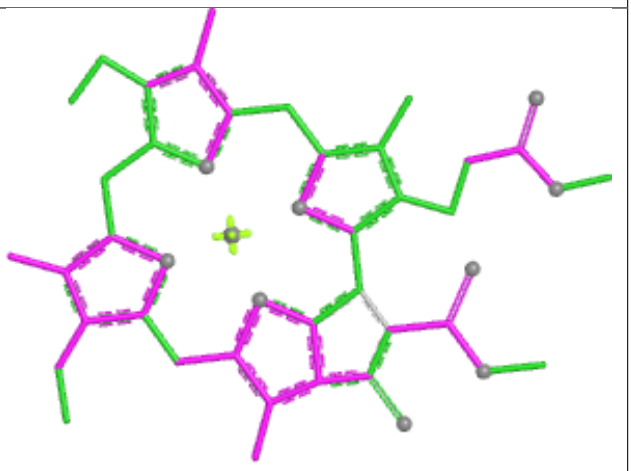
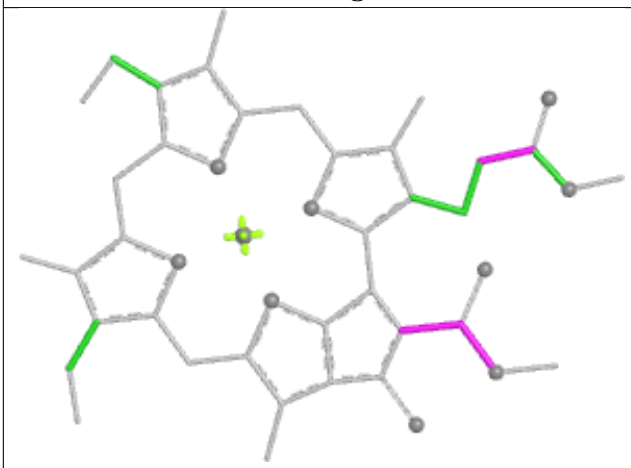


Bond angles



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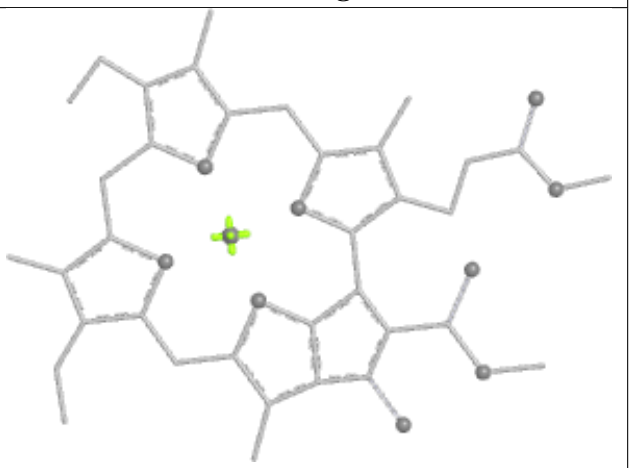
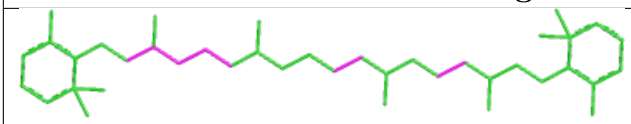


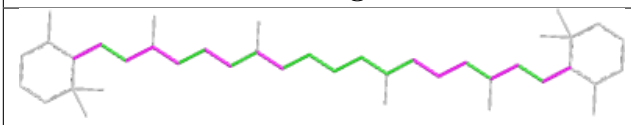
Rings

Ligand BCR F 4016



Bond lengths

Bond angles



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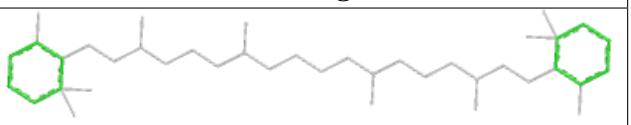
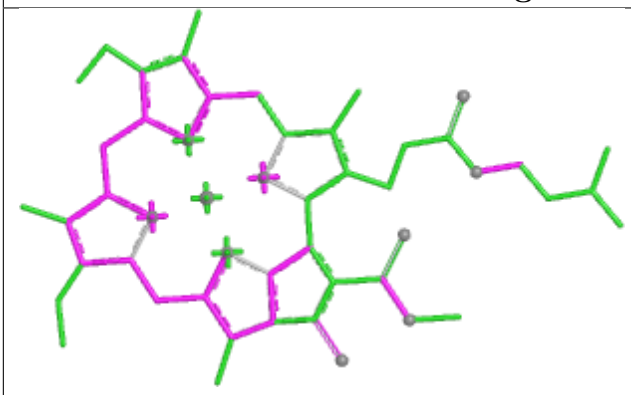
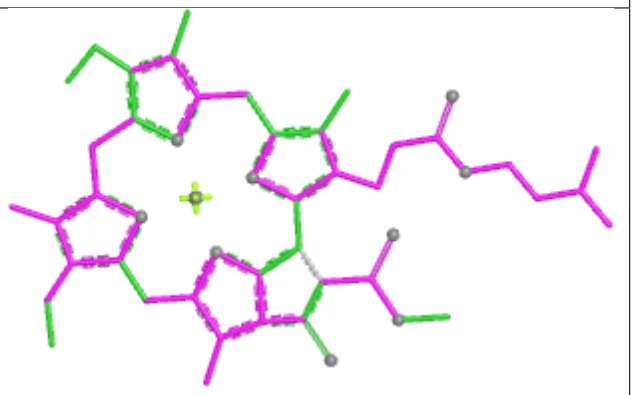


Rings

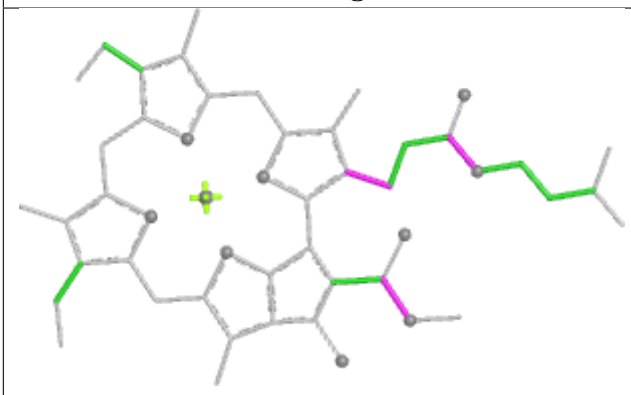
Ligand CLA A 1107



Bond lengths



Bond angles



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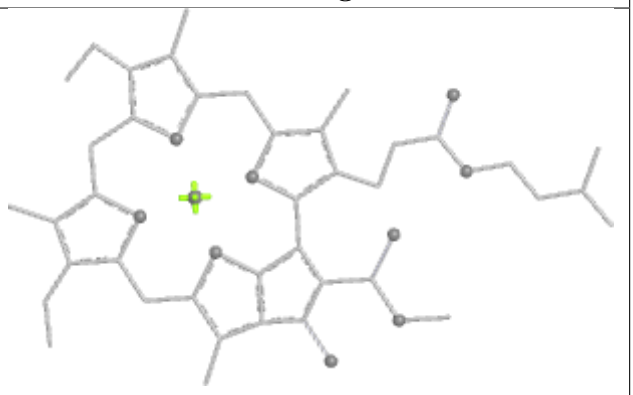
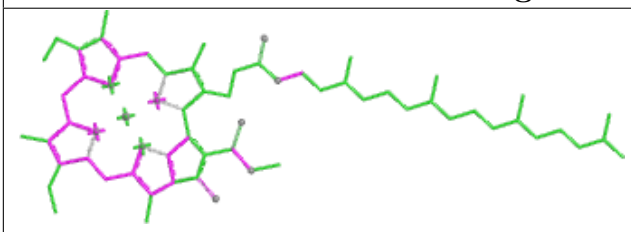
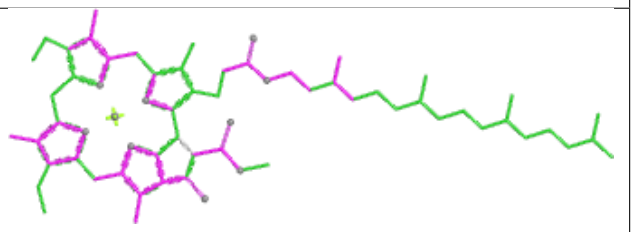


Rings

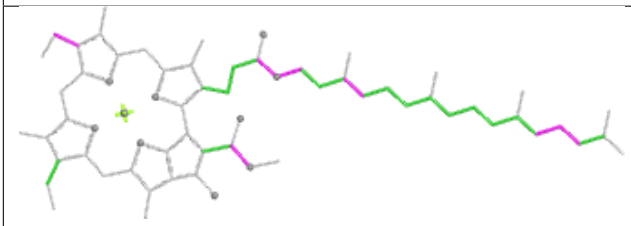
Ligand CLA A 1022



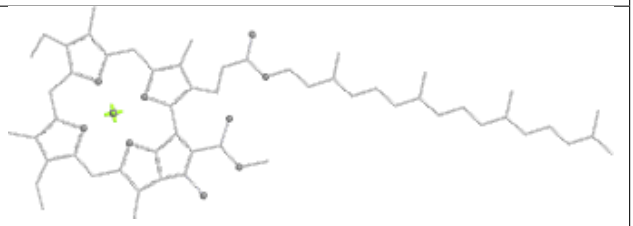
Bond lengths



Bond angles

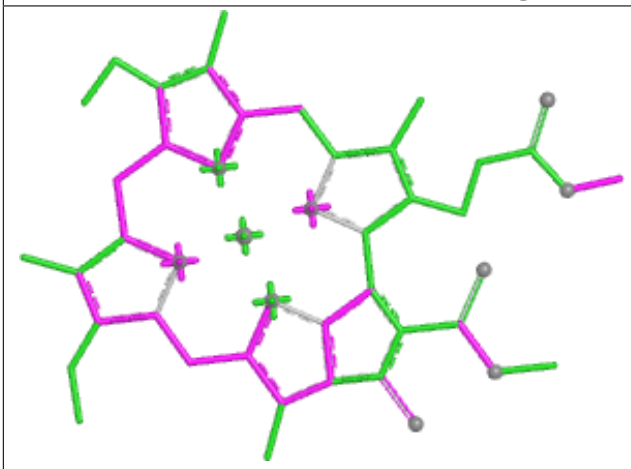


Torsions

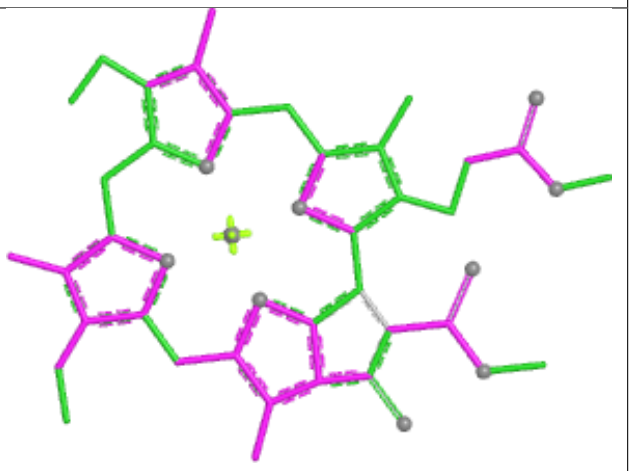


Rings

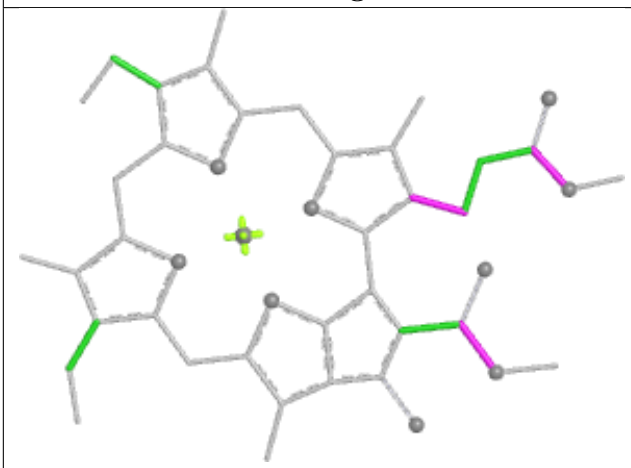
Ligand CLA A 1133



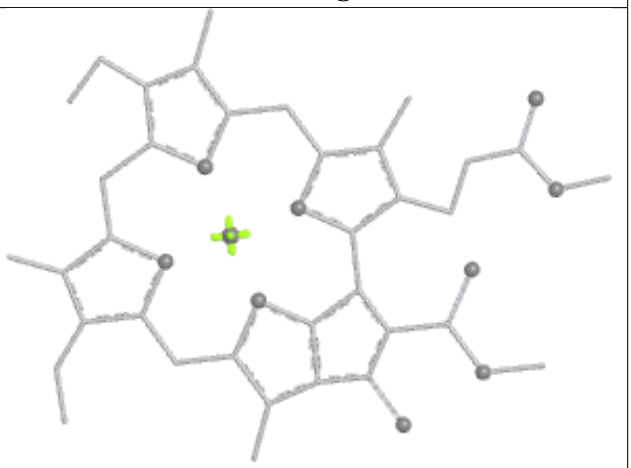
Bond lengths



Bond angles

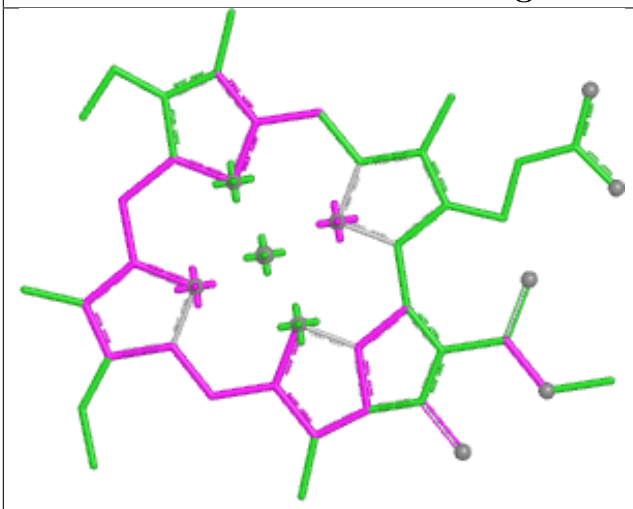


Torsions



Rings

Ligand CLA B 1227



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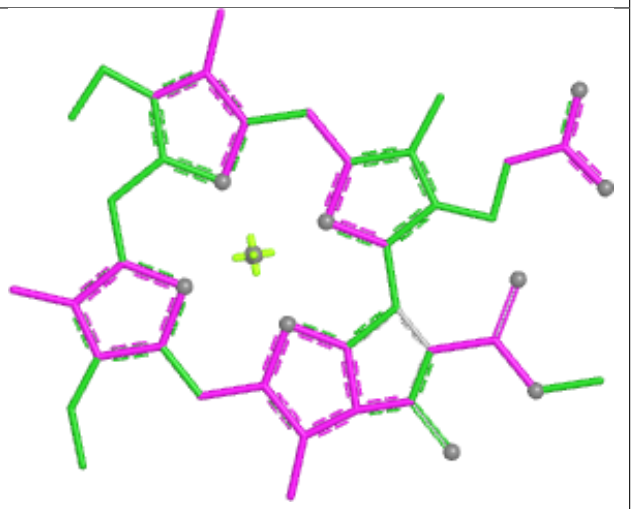
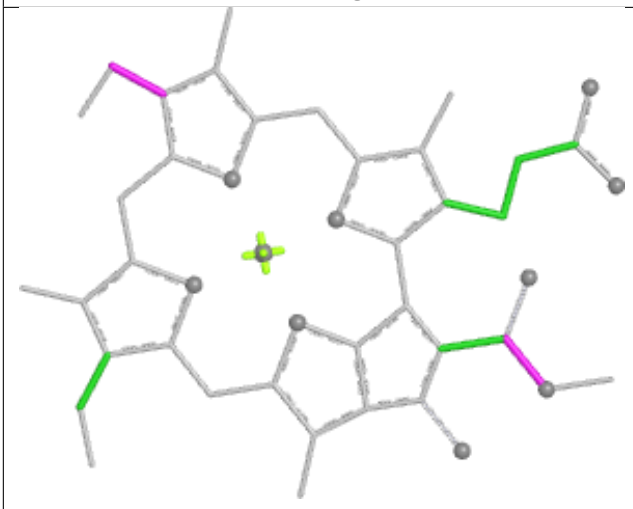


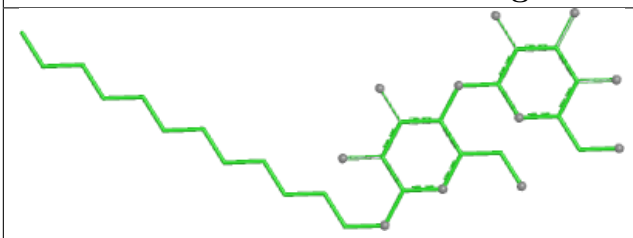
Bond angles



Torsions

Rings

Ligand LMU B 1301



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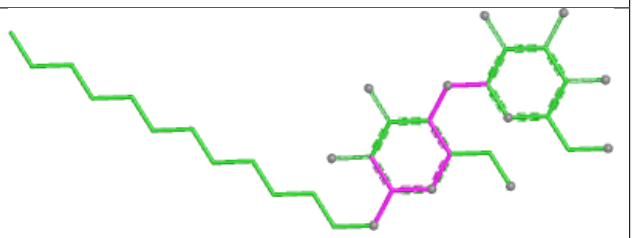
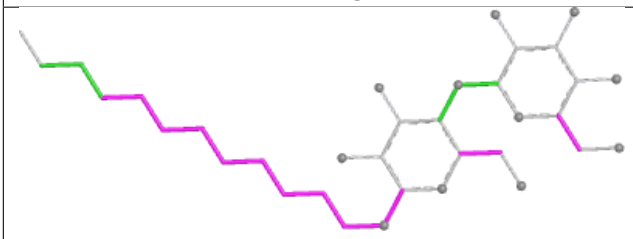
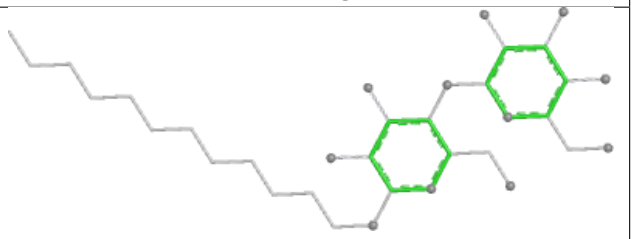


Bond angles

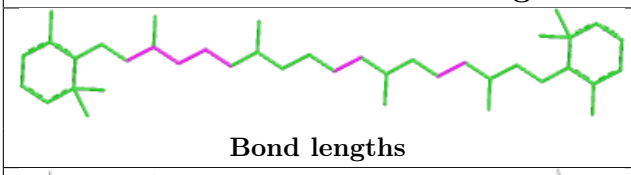


Torsions



Rings

Ligand BCR A 4007



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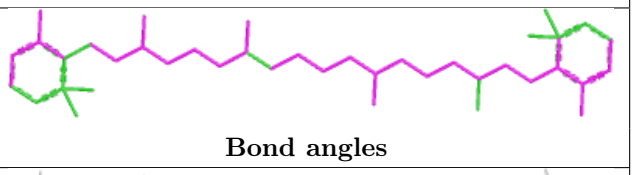
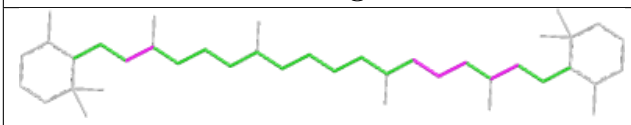


Bond angles



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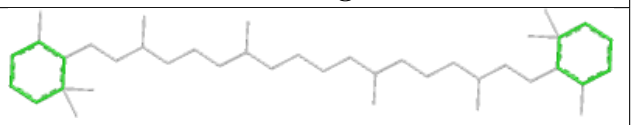
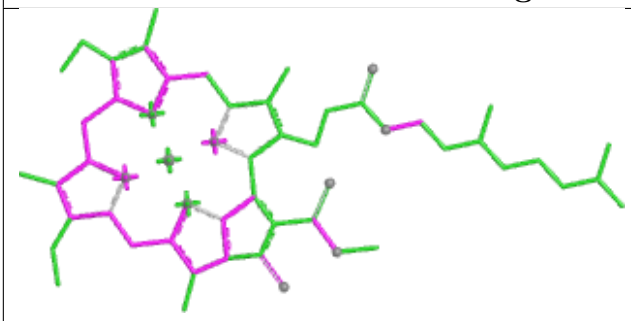
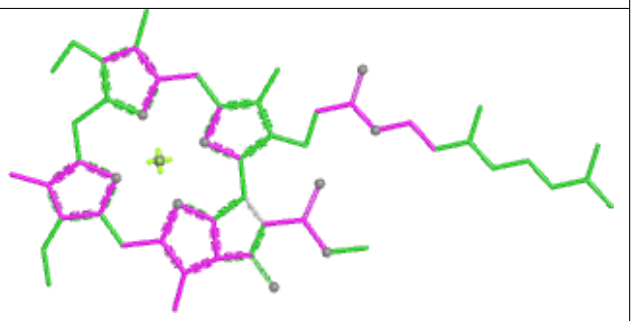


Rings

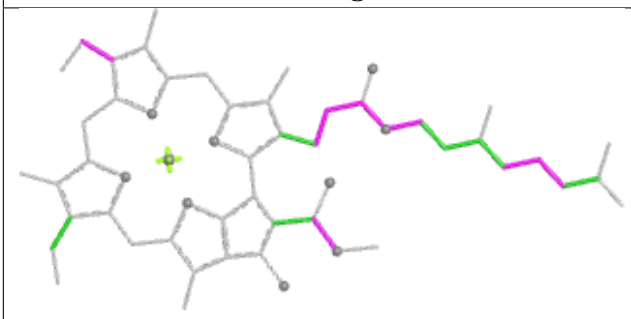
Ligand CLA A 1130



Bond lengths



Bond angles



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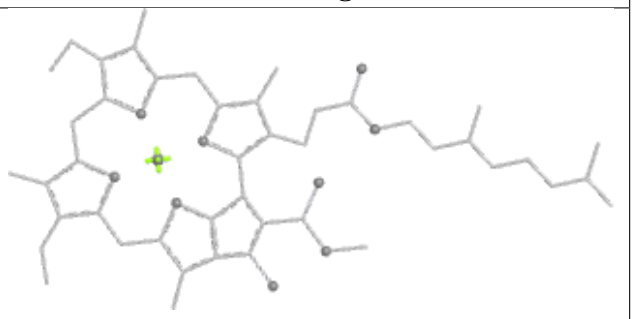
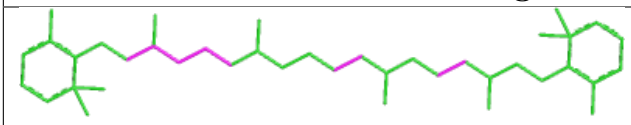
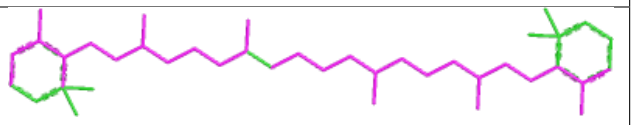


Rings

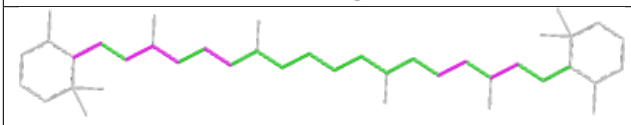
Ligand BCR B 4005



Bond lengths



Bond angles



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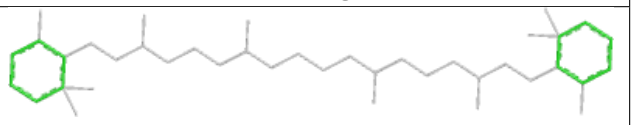
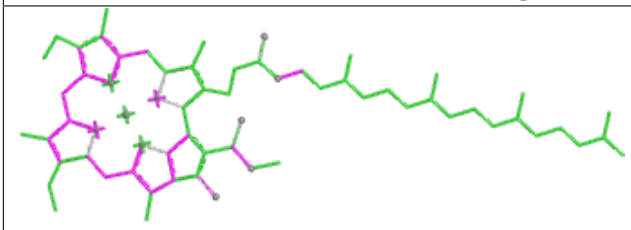


Rings

Ligand CLA A 1140



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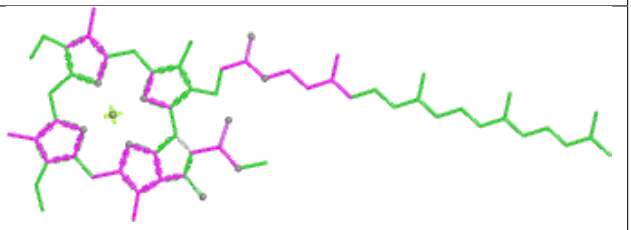
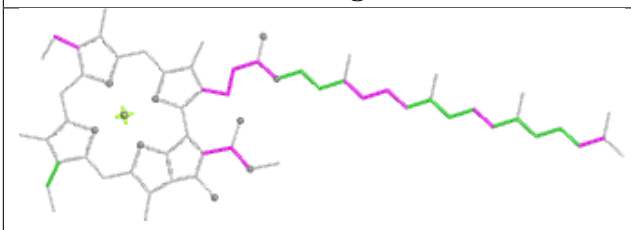


Bond angles



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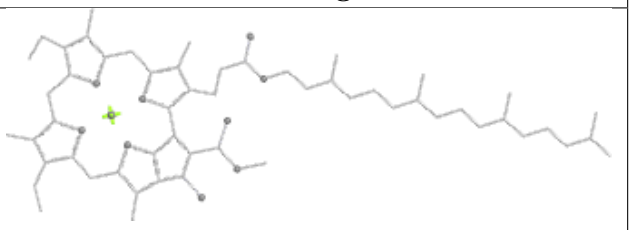
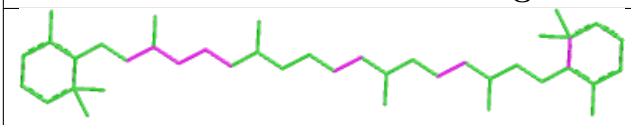


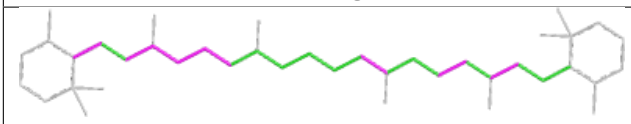
Rings

Ligand BCR B 4009



Bond lengths

Bond angles



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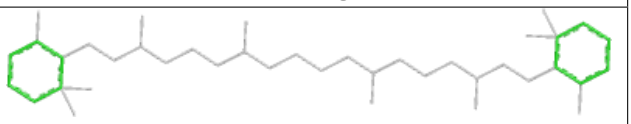
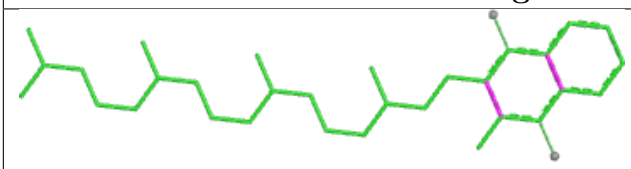
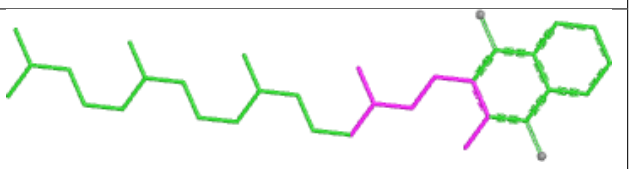


Rings

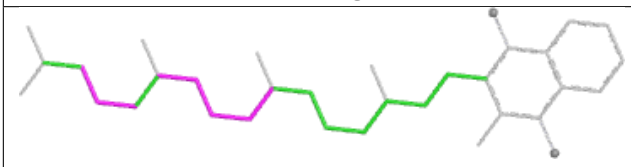
Ligand PQN A 2001



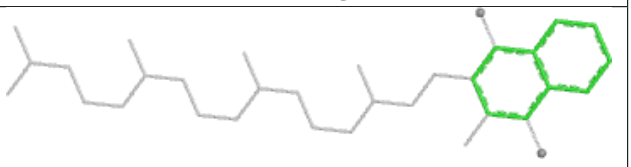
Bond lengths



Bond angles

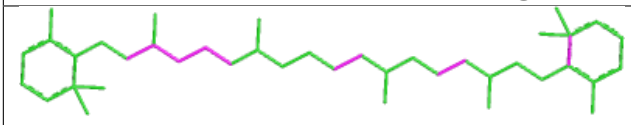


Torsions



Rings

Ligand BCR F 4015



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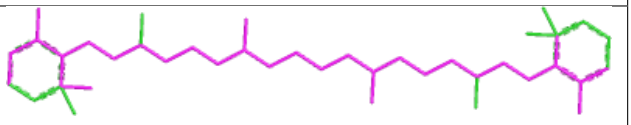
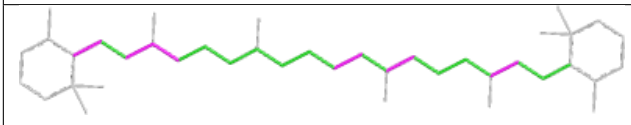
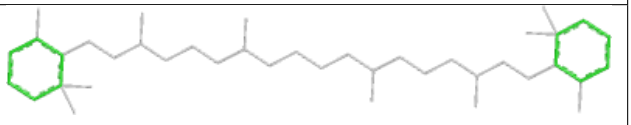


Bond angles

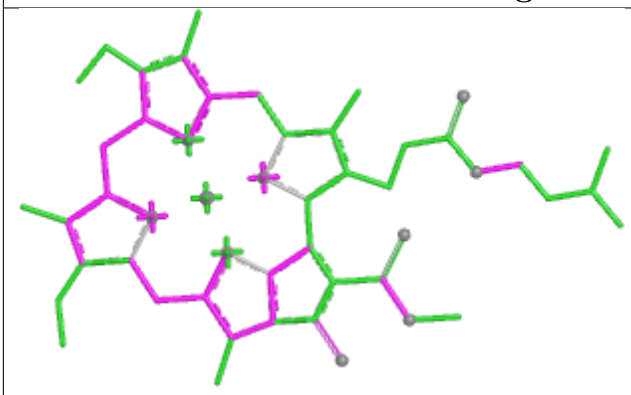


Torsions



Rings

Ligand CLA B 1236



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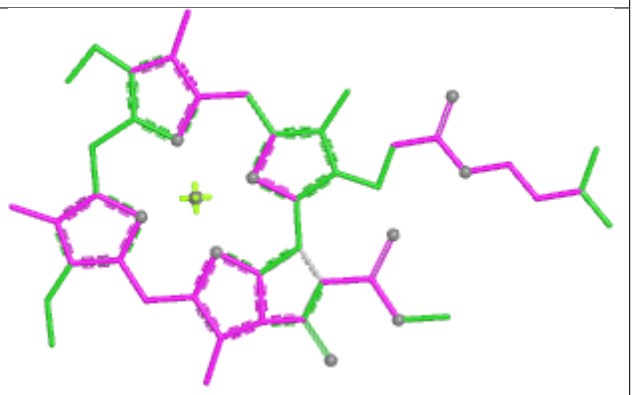
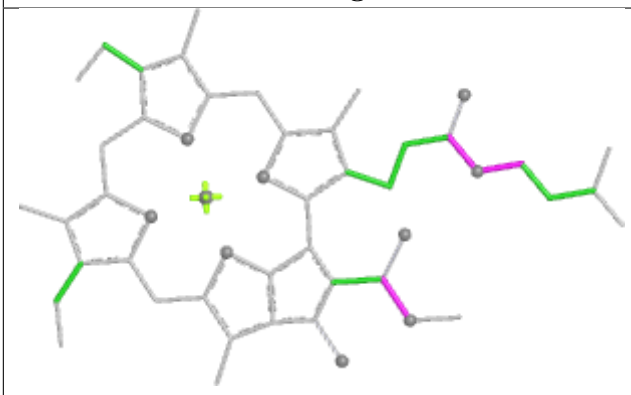
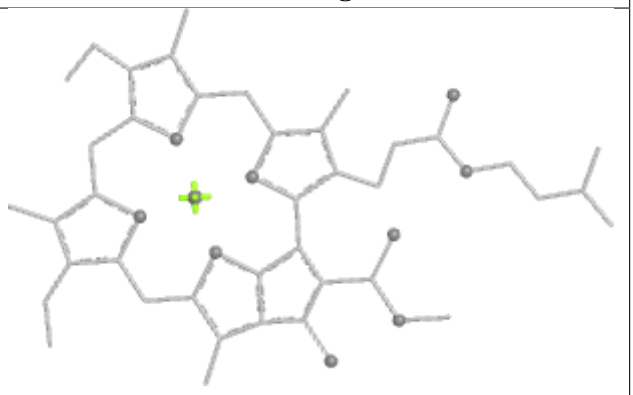


Bond angles

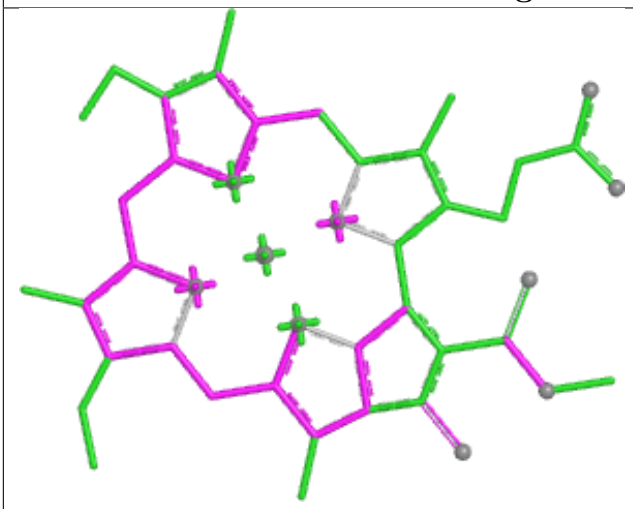


Torsions

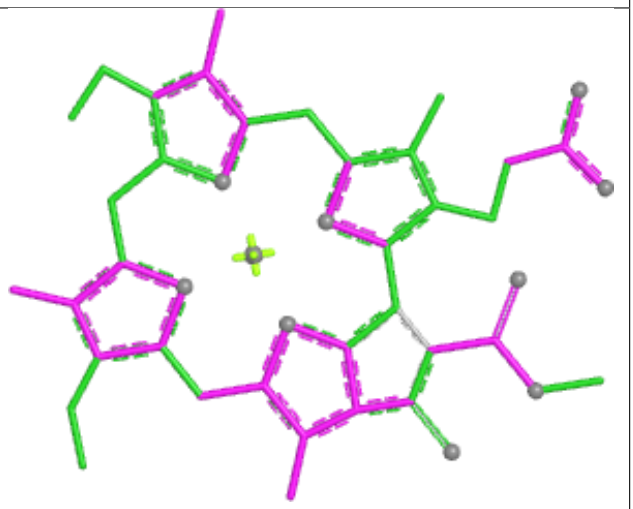


Rings

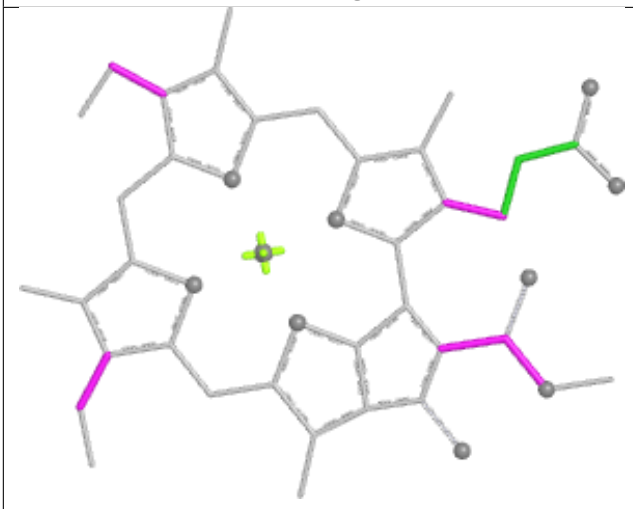
Ligand CLA B 1212



Bond lengths



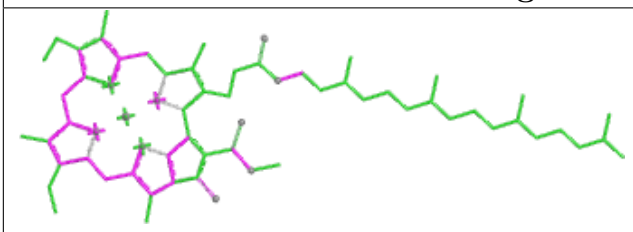
Bond angles



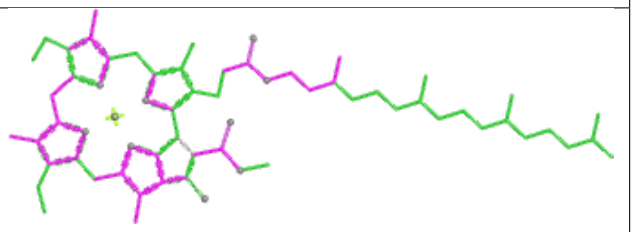
Torsions

Rings

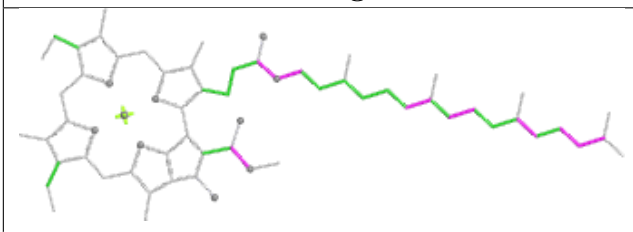
Ligand CLA F 1139



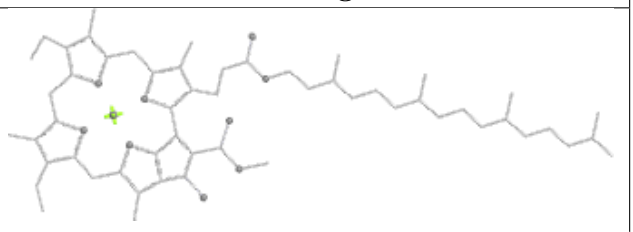
Bond lengths



Bond angles

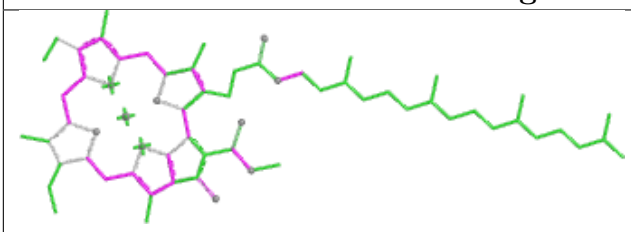


Torsions



Rings

Ligand CL0 A 1011



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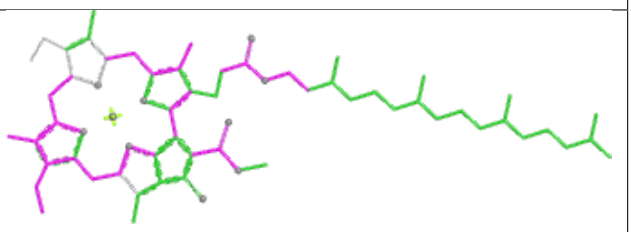
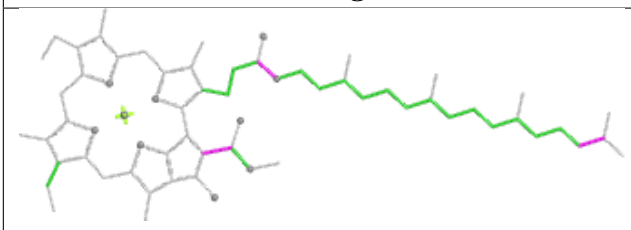
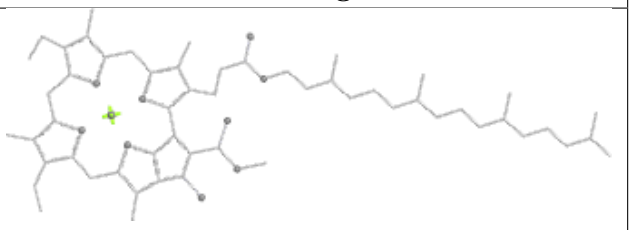


Bond angles

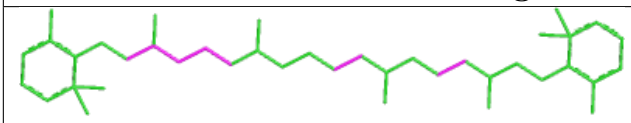


Torsions

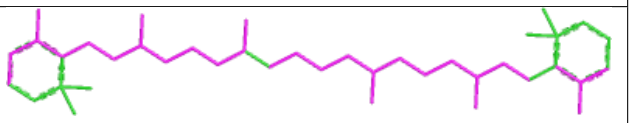


Rings

Ligand BCR A 4012

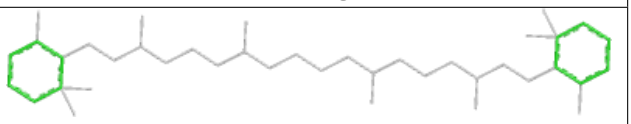


Bond lengths



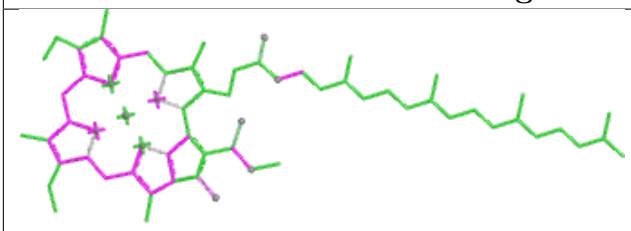
Bond angles

Torsions

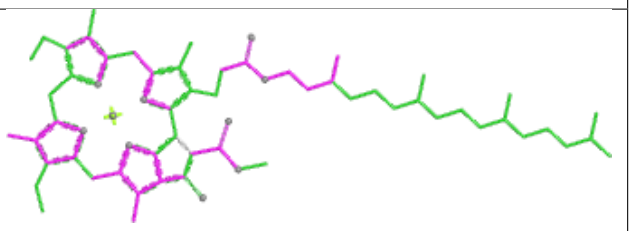


Rings

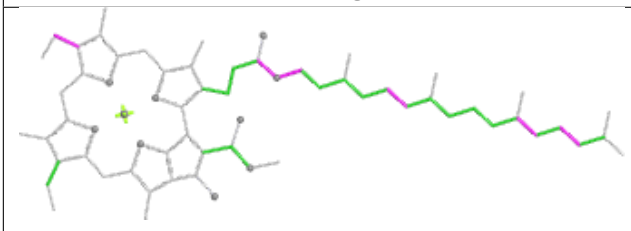
Ligand CLA B 1221



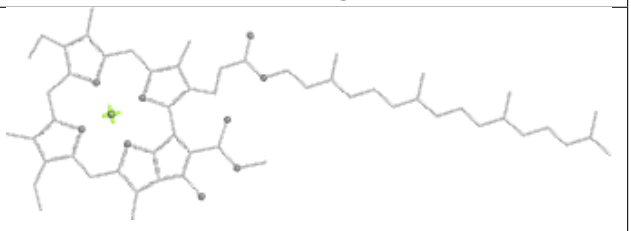
Bond lengths



Bond angles

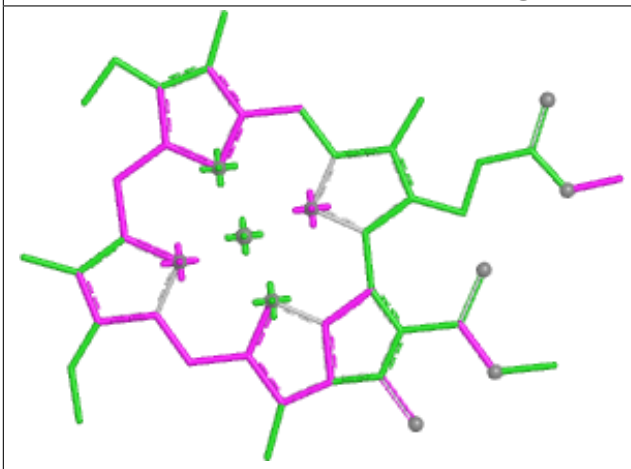


Torsions



Rings

Ligand CLA A 1115



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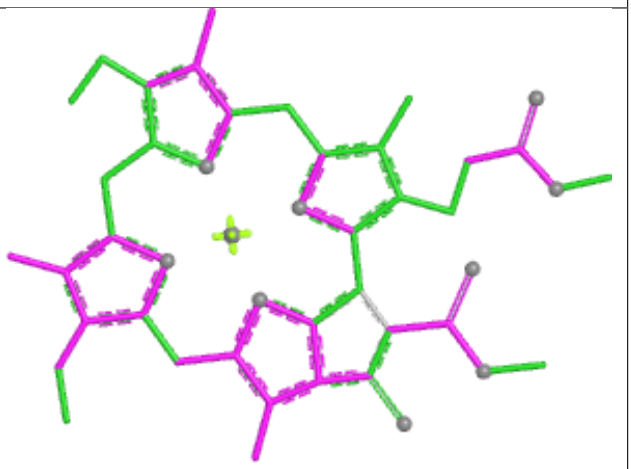
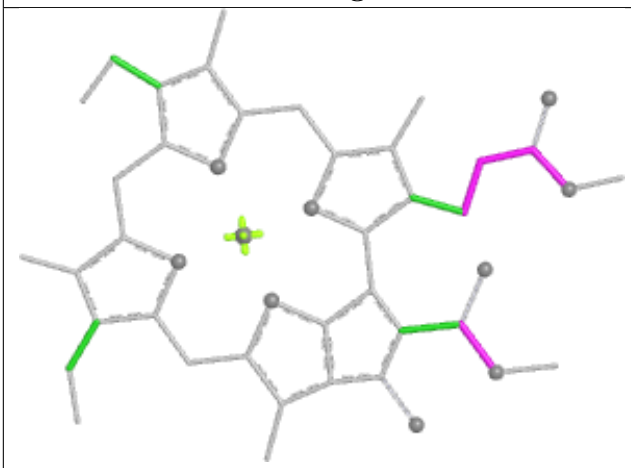


Bond angles



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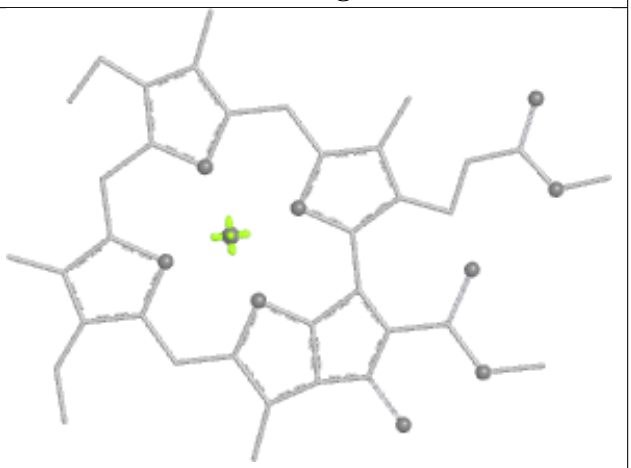
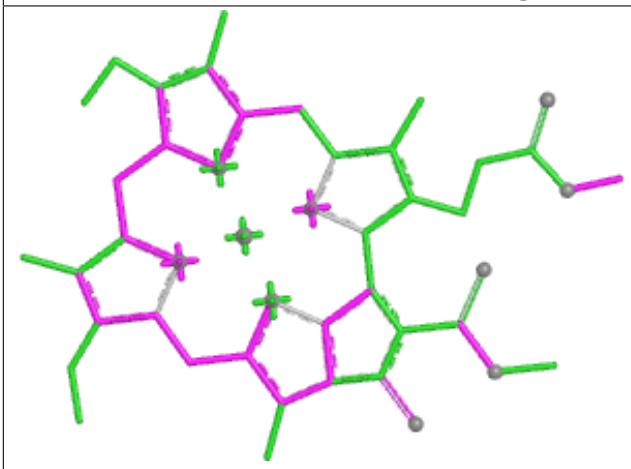


Rings

Ligand CLA A 1129



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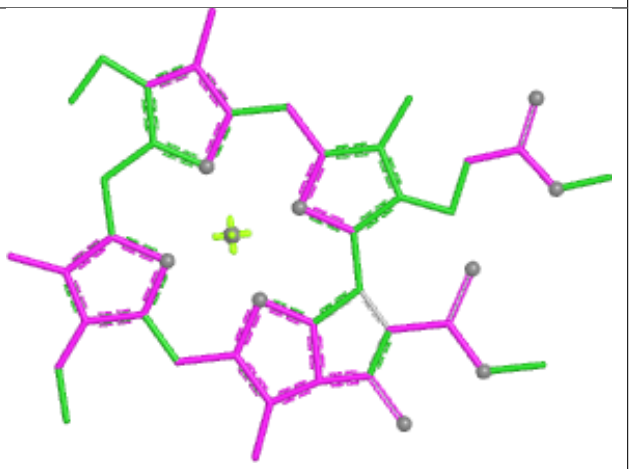
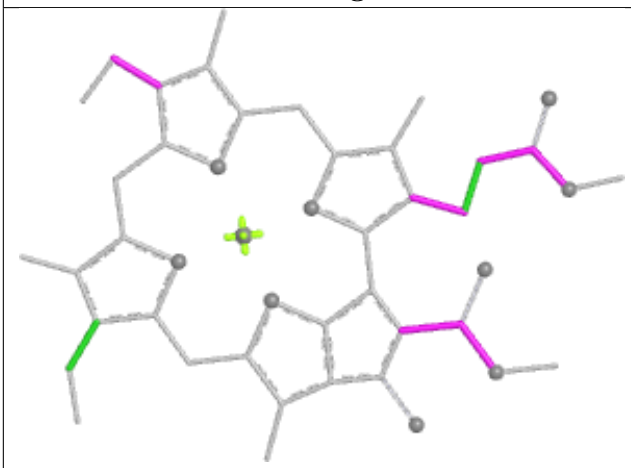


Bond angles



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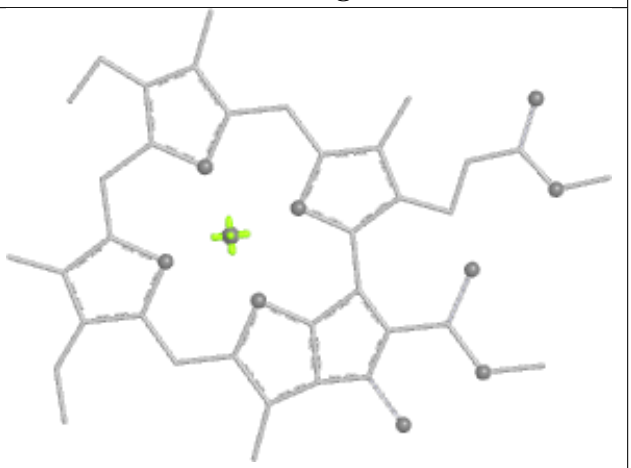
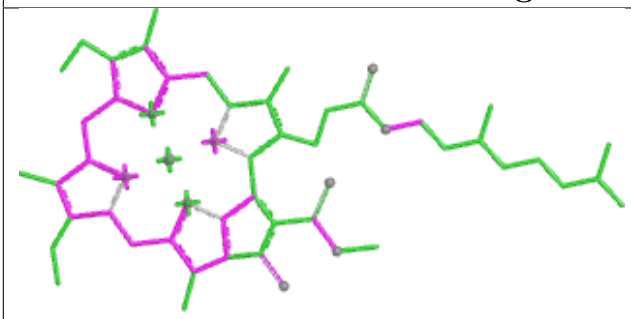
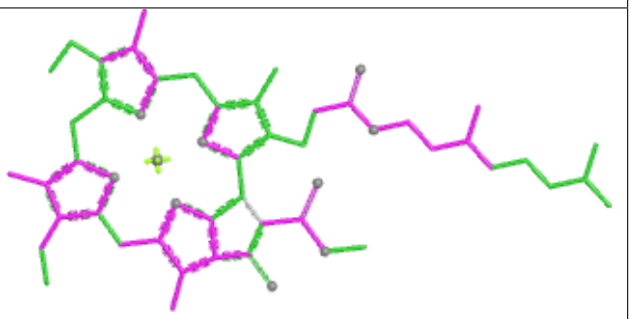


Rings

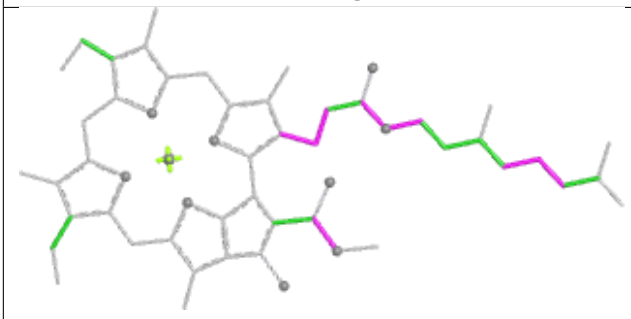
Ligand CLA B 1237



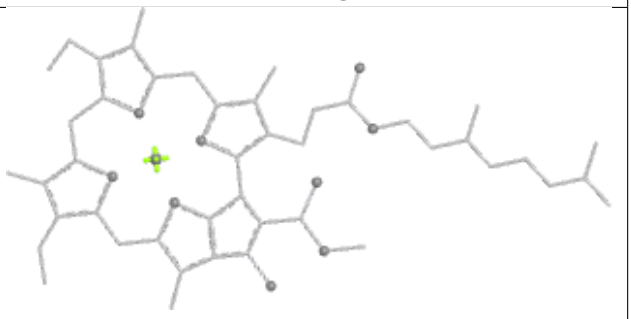
Bond lengths



Bond angles

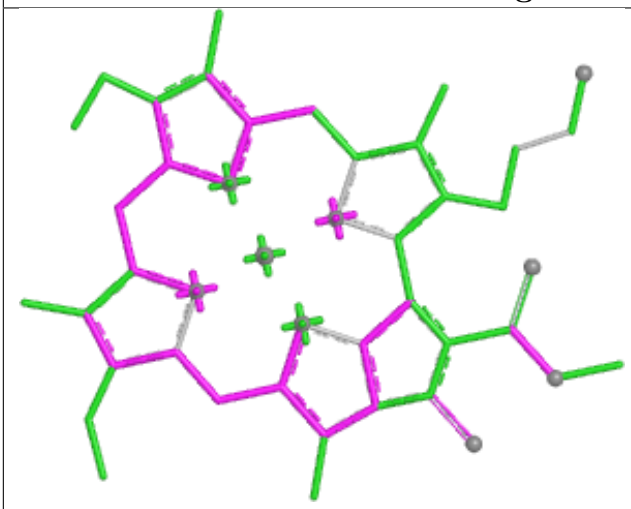


Torsions



Rings

Ligand CLA B 1238



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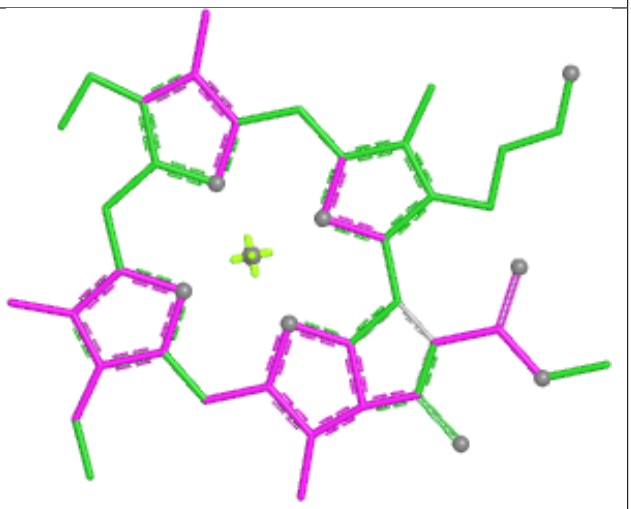
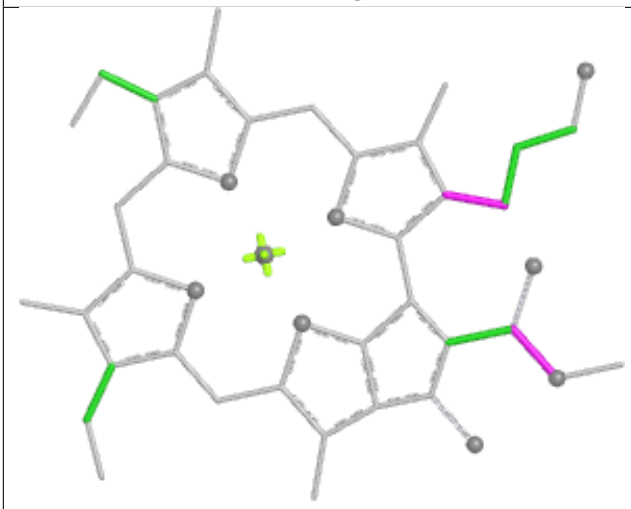


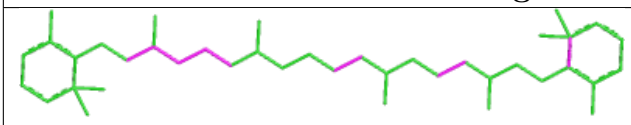
Bond angles



Torsions

Rings

Ligand BCR A 4008



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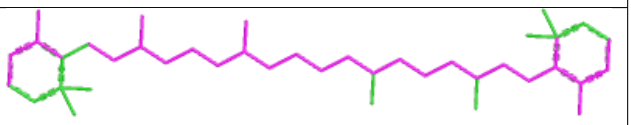
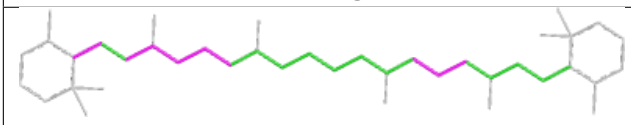
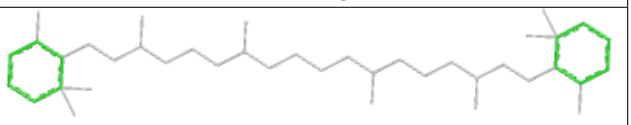


Bond angles

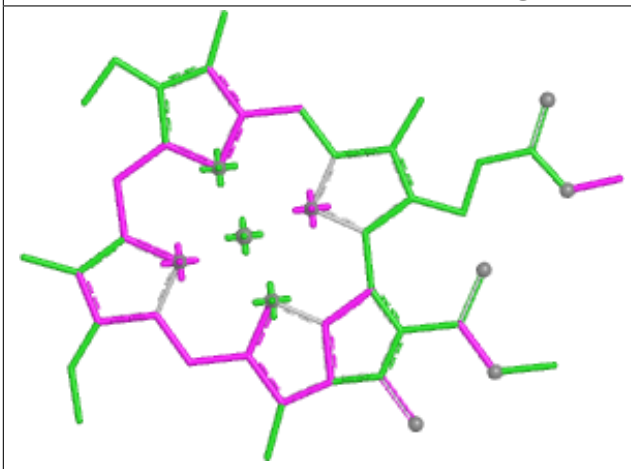


Torsions

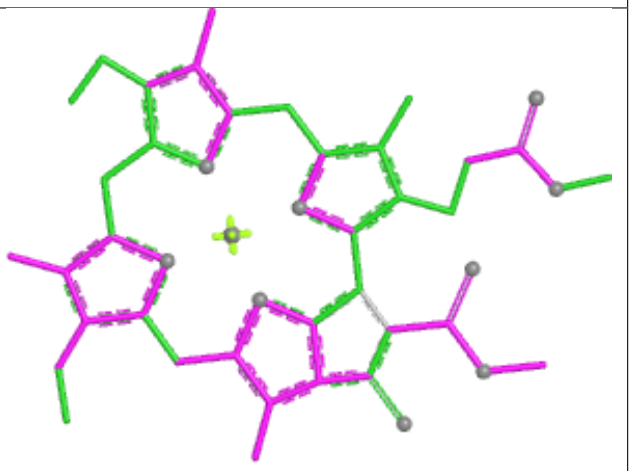


Rings

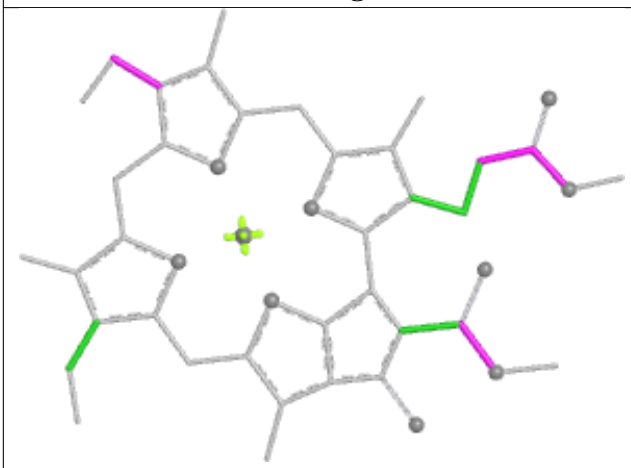
Ligand CLA K 1402



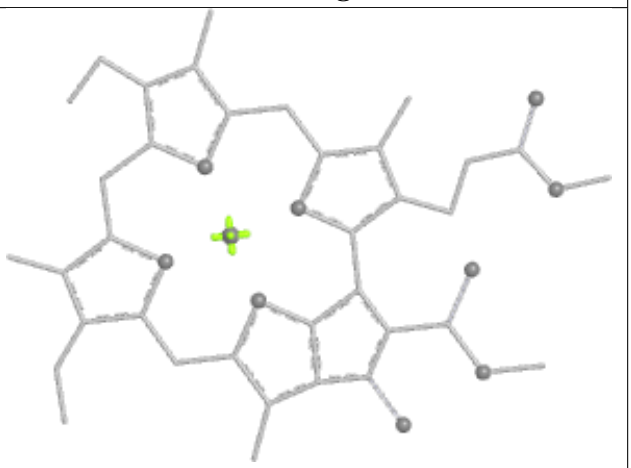
Bond lengths



Bond angles

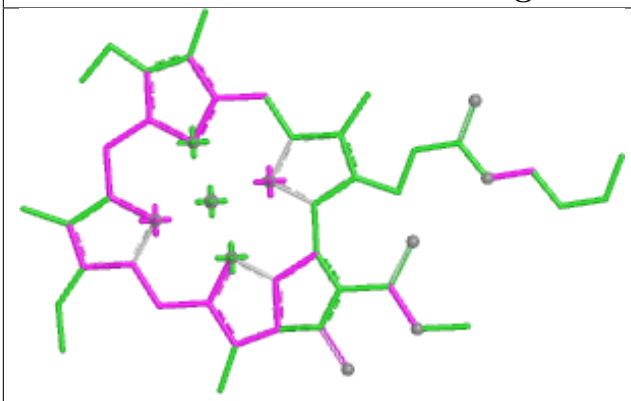


Torsions



Rings

Ligand CLA A 1120



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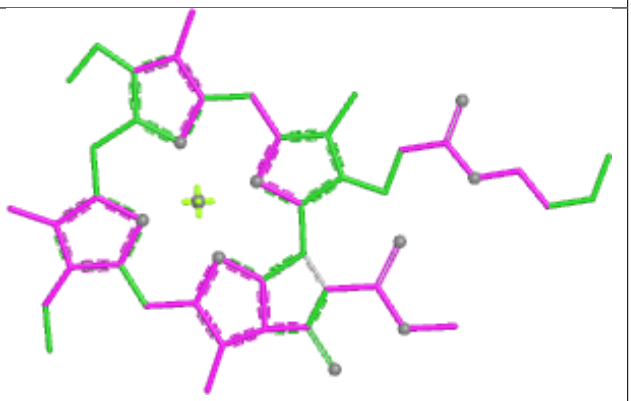
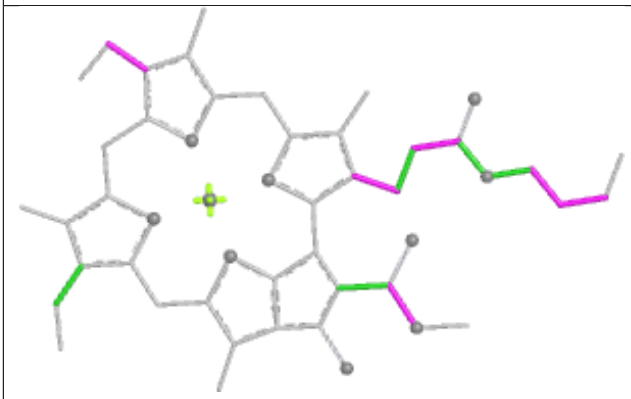
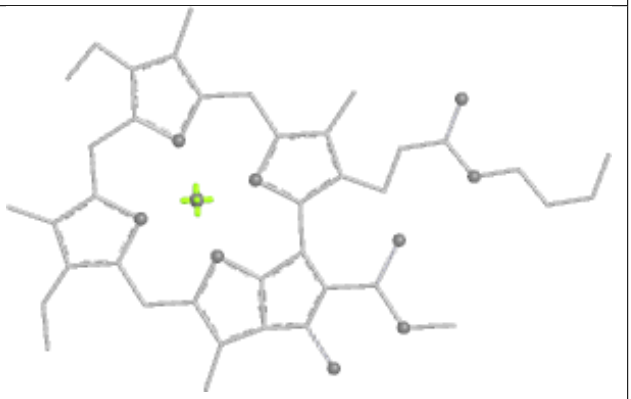


Bond angles

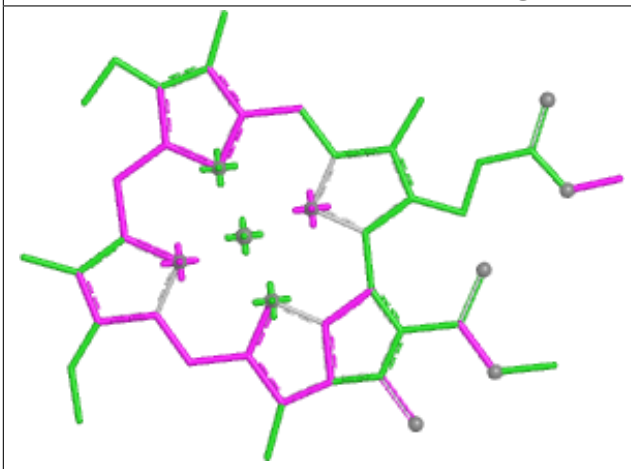


Torsions



Rings

Ligand CLA K 1401



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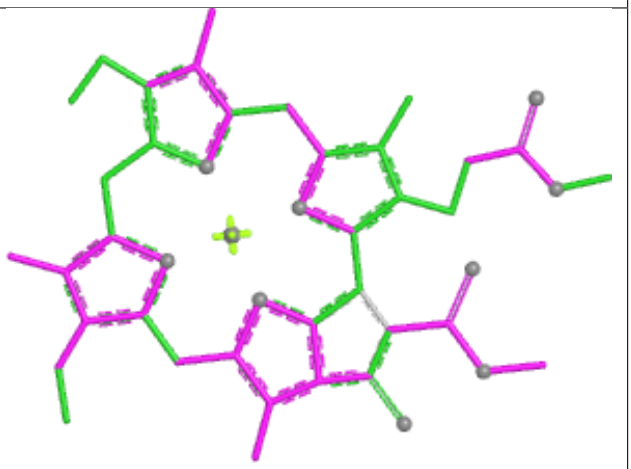
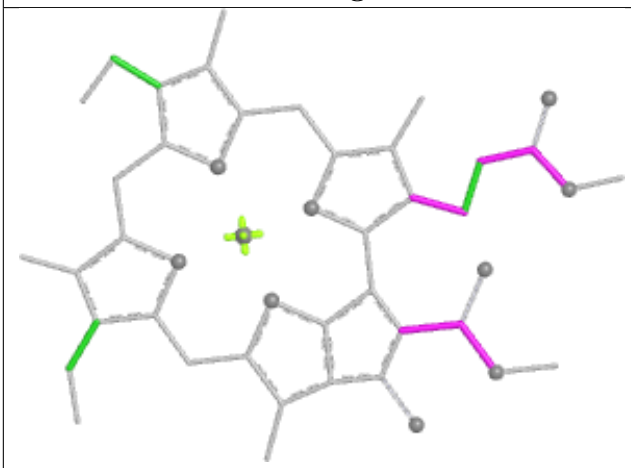
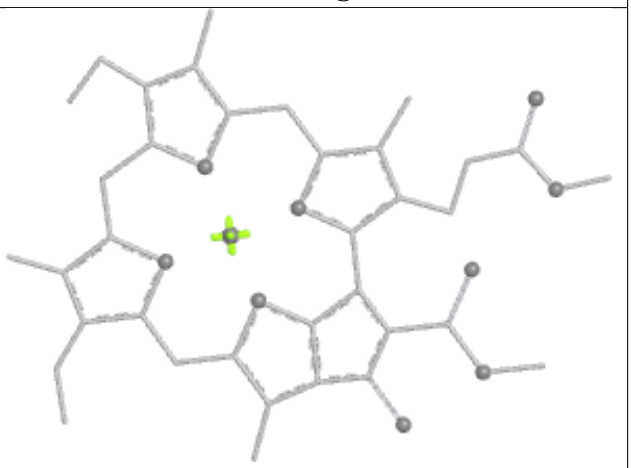


Bond angles

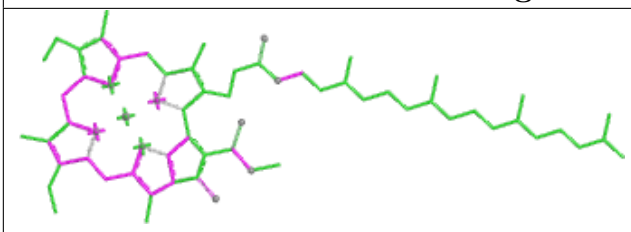


Torsions



Rings

Ligand CLA A 1123



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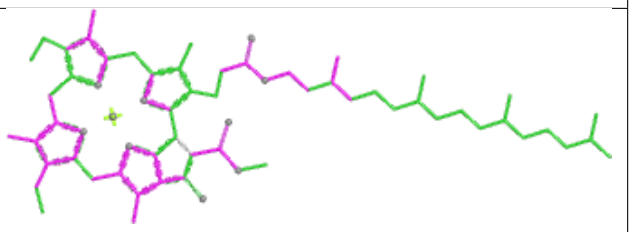
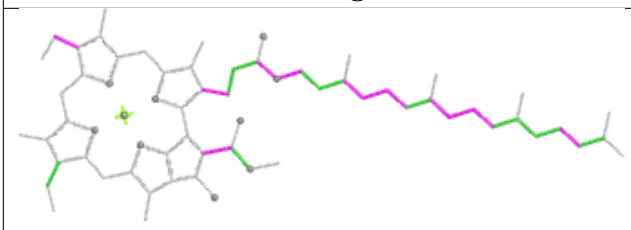
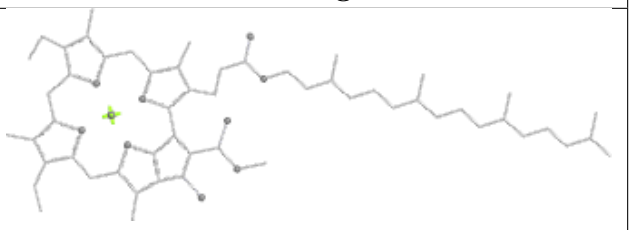


Bond angles

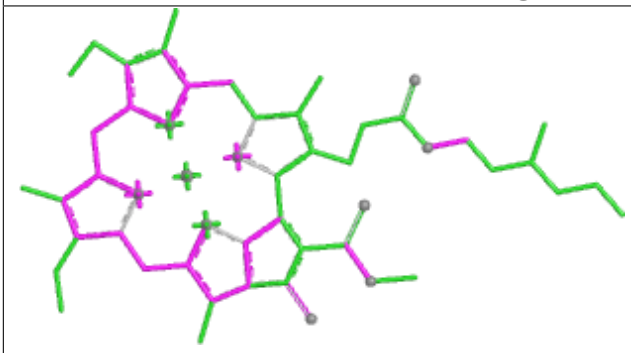


Torsions

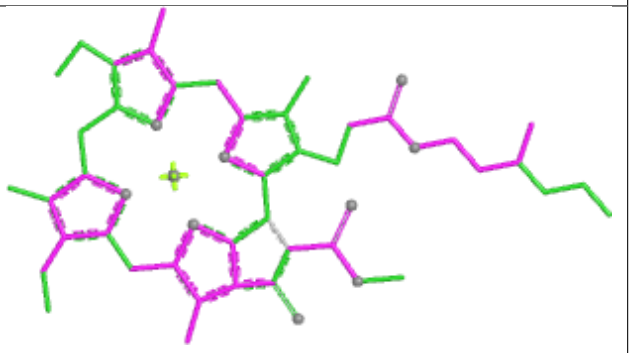


Rings

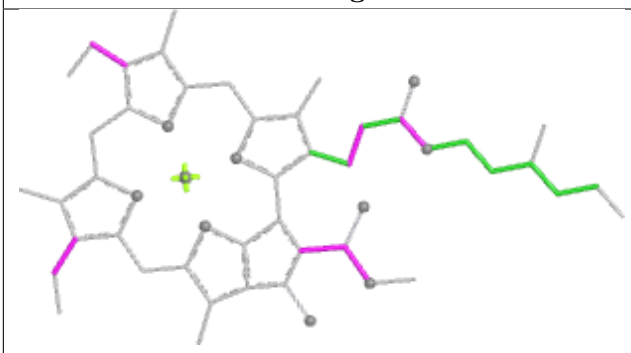
Ligand CLA A 1801



Bond lengths



Bond angles



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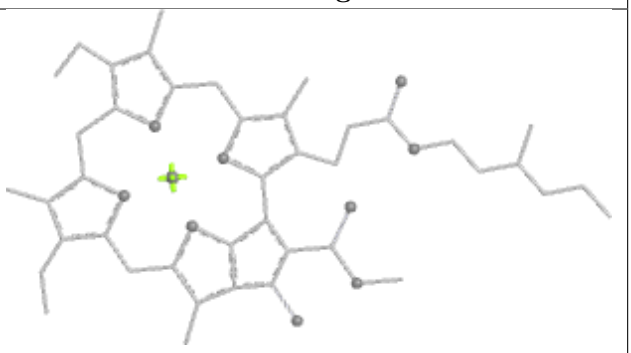
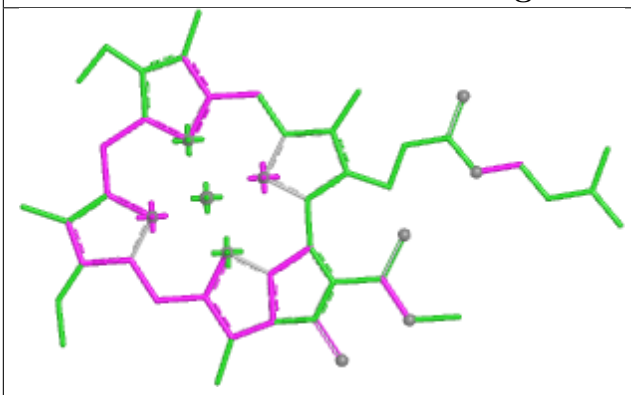
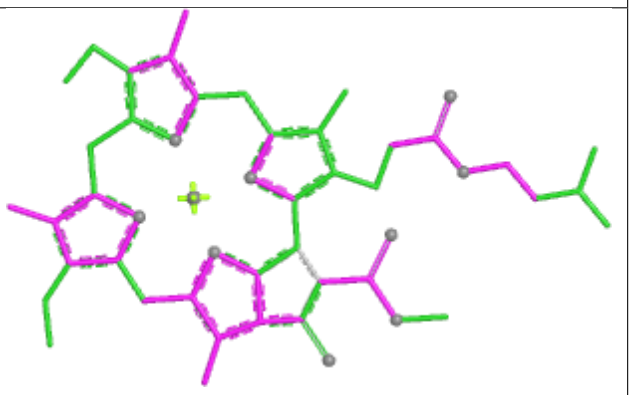


Rings

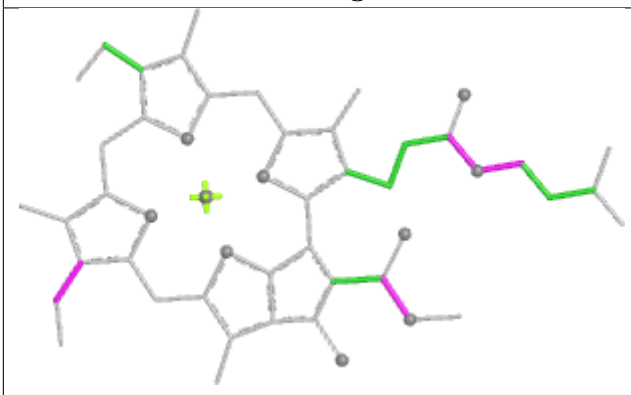
Ligand CLA A 1137



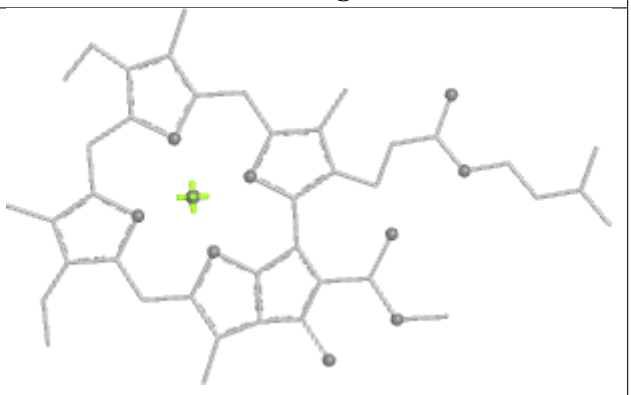
Bond lengths



Bond angles

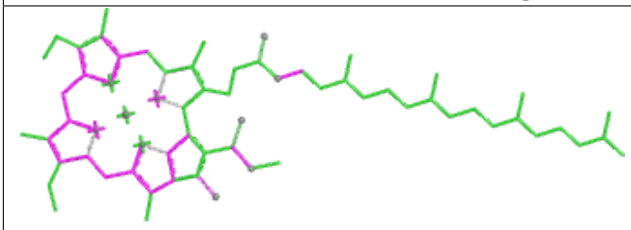


Torsions

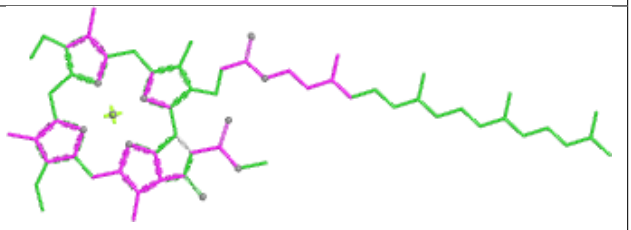


Rings

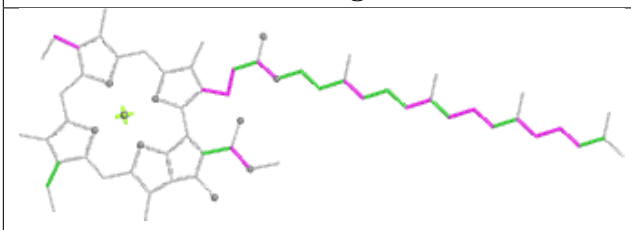
Ligand CLA F 1410



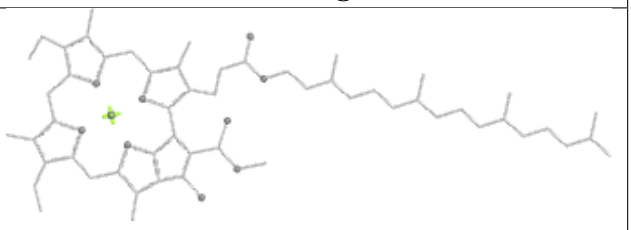
Bond lengths



Bond angles

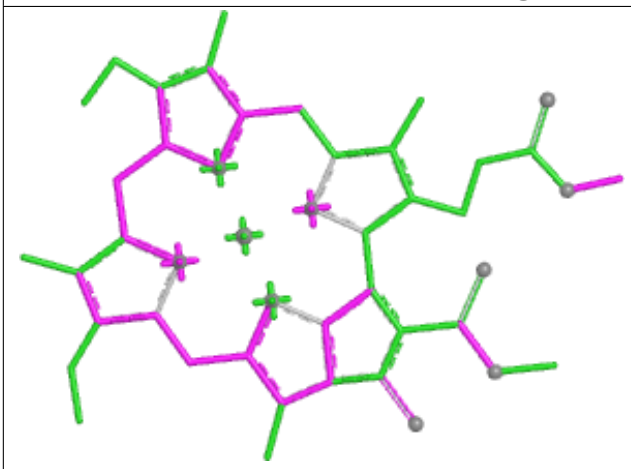


Torsions

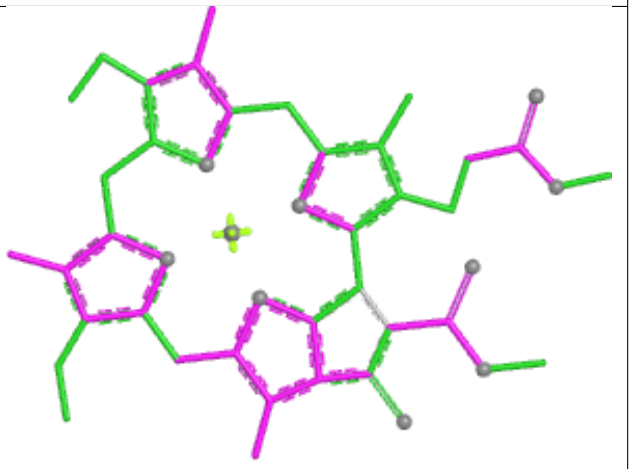


Rings

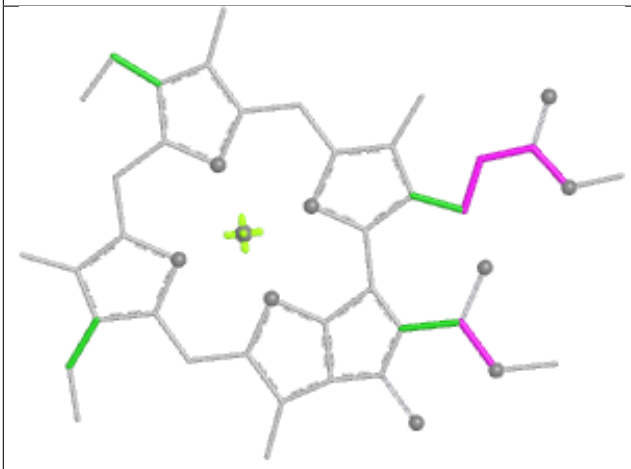
Ligand CLA A 1134



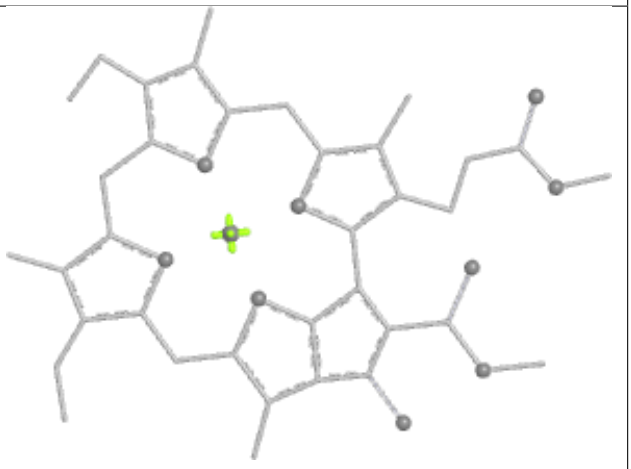
Bond lengths



Bond angles

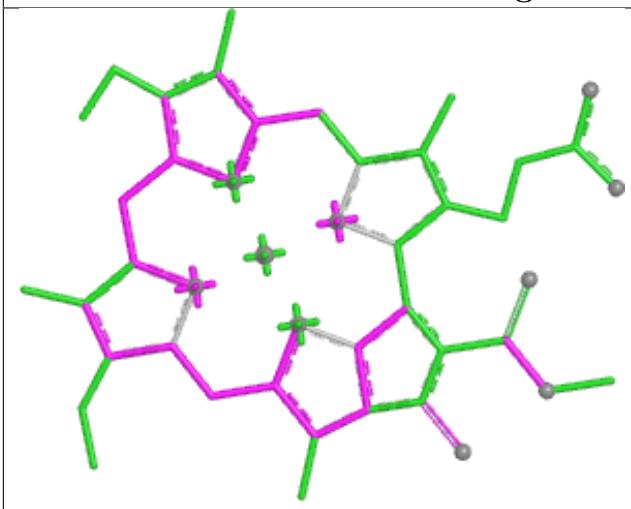


Torsions



Rings

Ligand CLA B 1208



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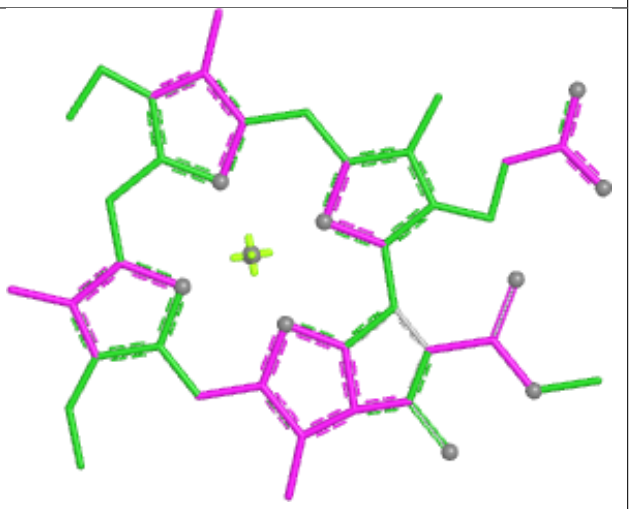
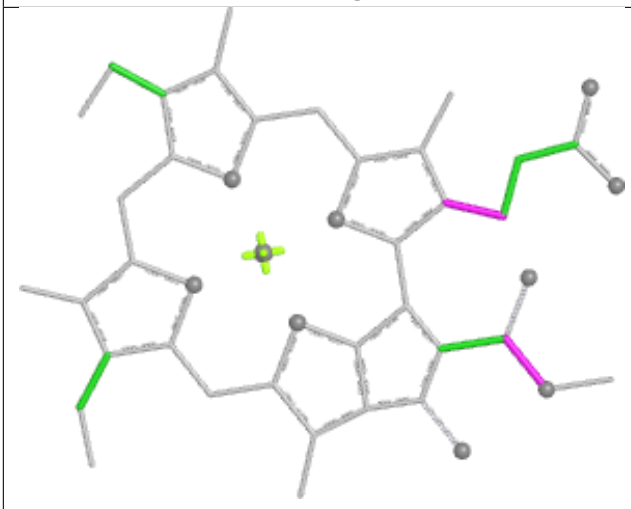


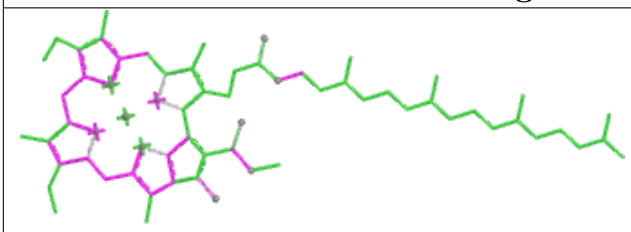
Bond angles



Torsions

Rings

Ligand CLA B 1023



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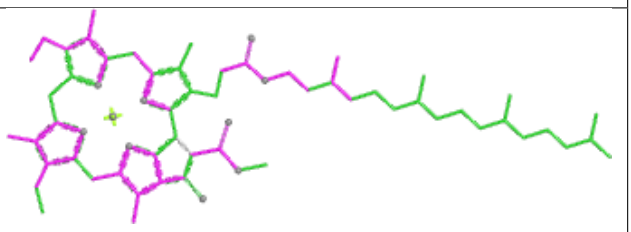
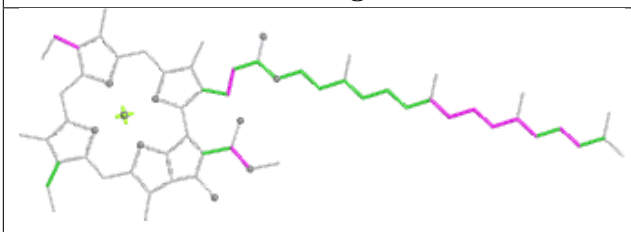
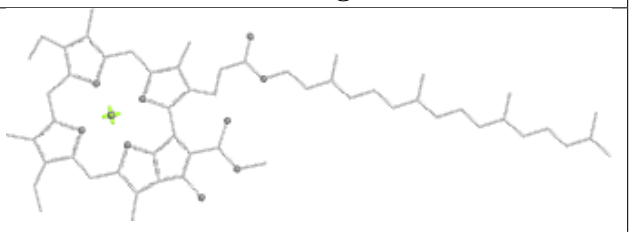


Bond angles

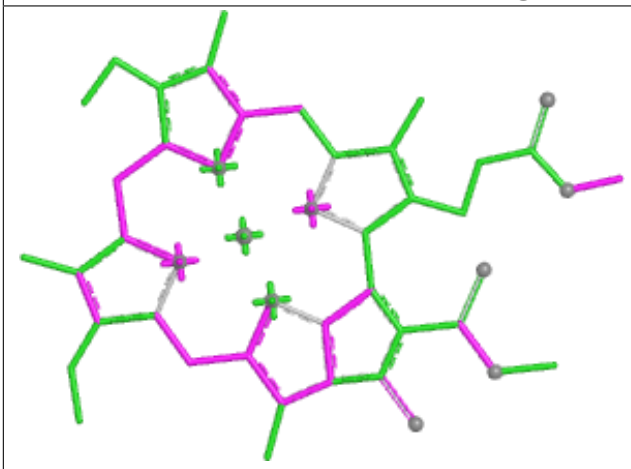


Torsions



Rings

Ligand CLA A 1118



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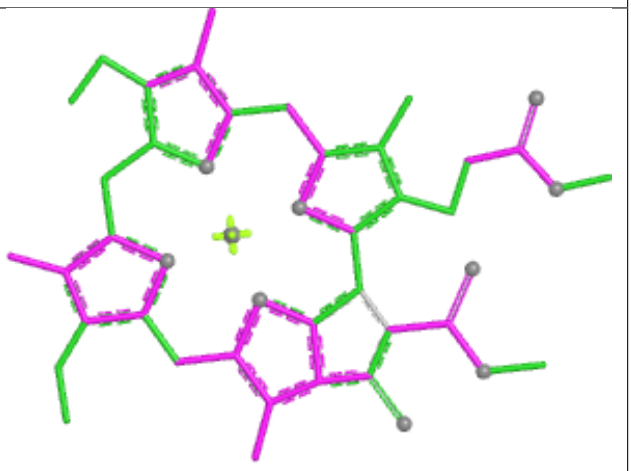
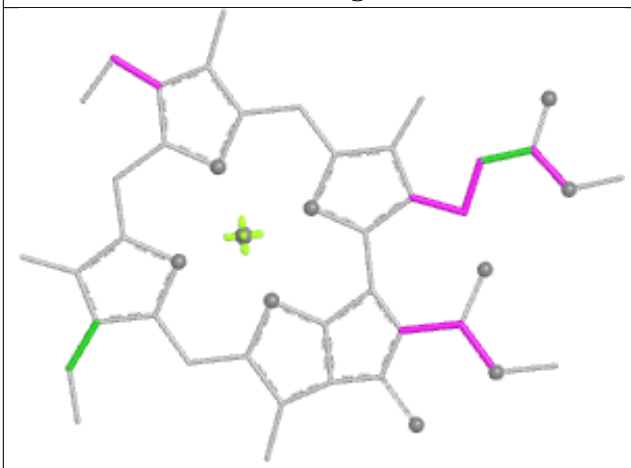


Bond angles



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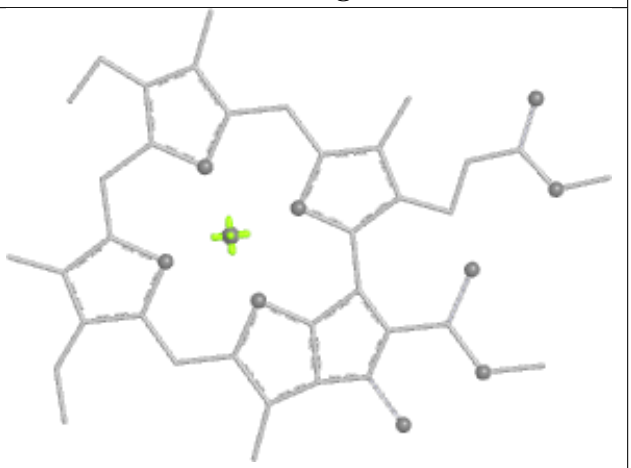
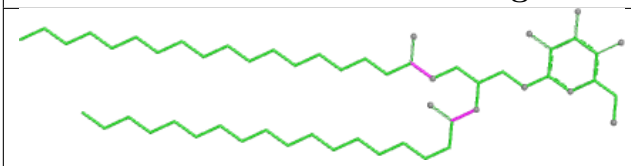
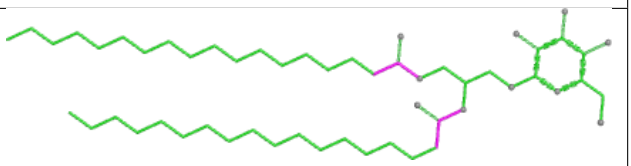


Rings

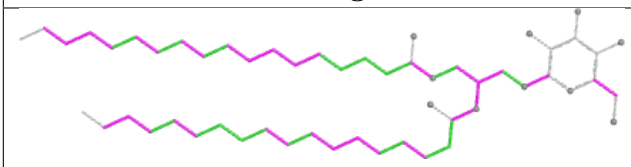
Ligand LMG B 5002



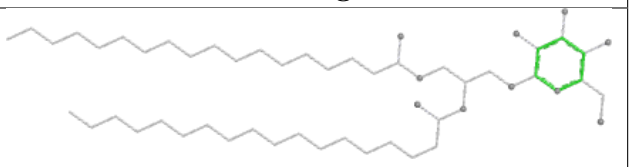
Bond lengths



Bond angles

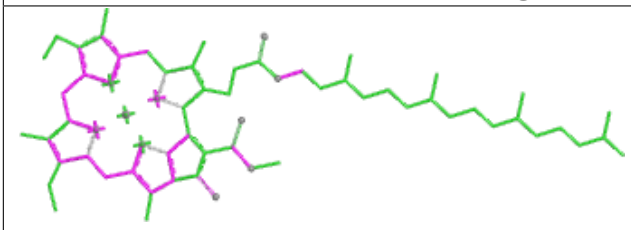


Torsions



Rings

Ligand CLA A 1106



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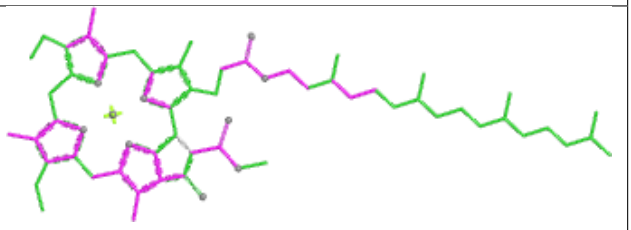
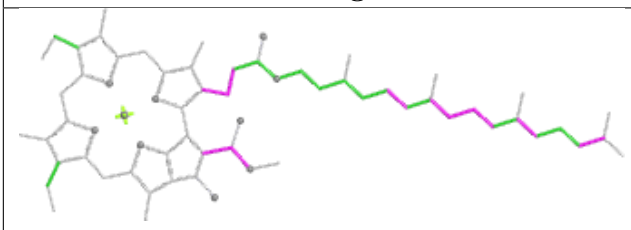


Bond angles



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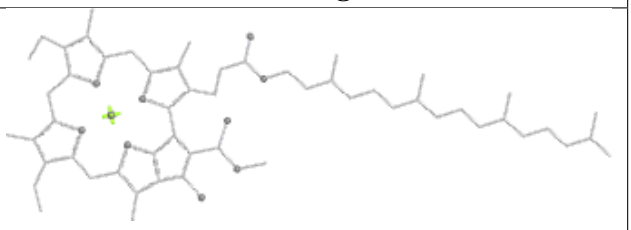
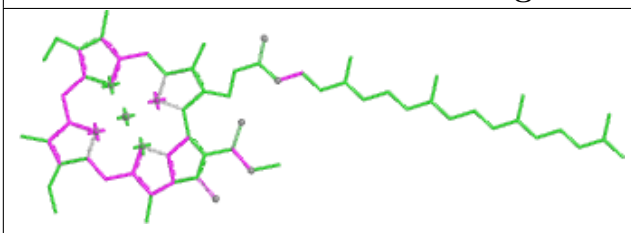


Rings

Ligand CLA A 1104



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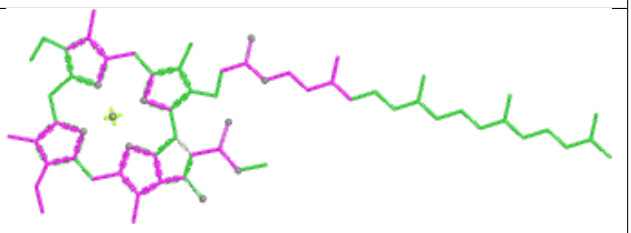
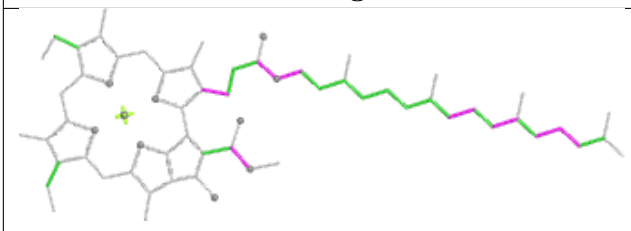
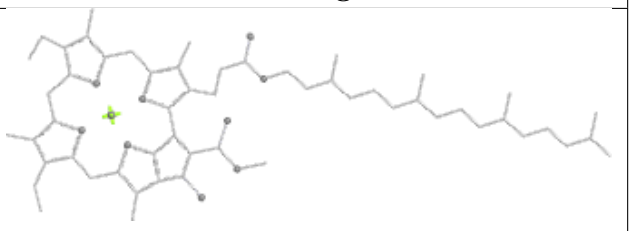


Bond angles

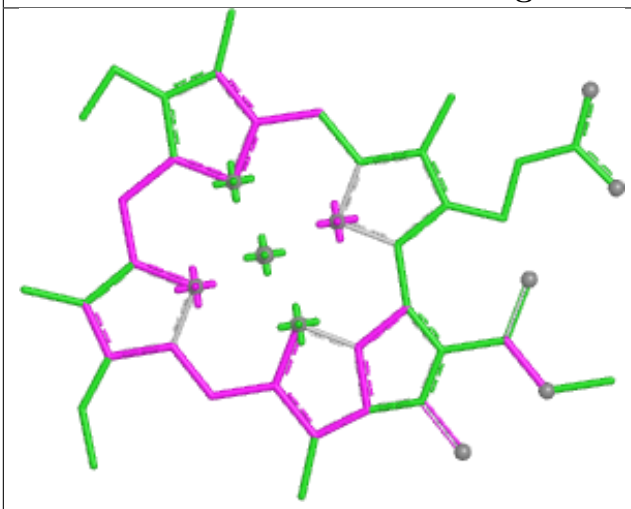


Torsions



Rings

Ligand CLA B 1232



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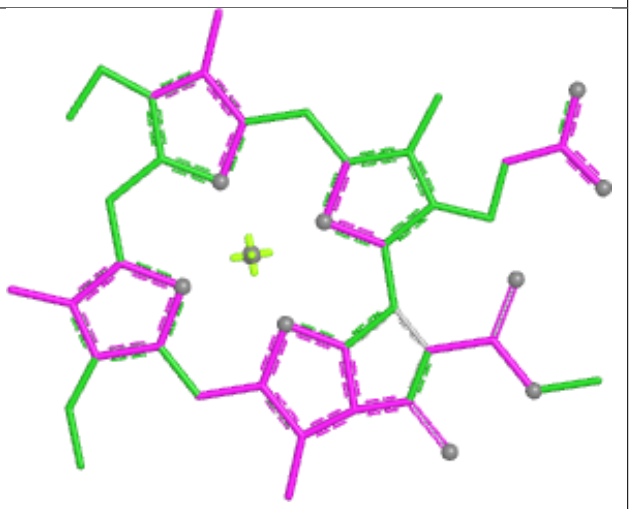
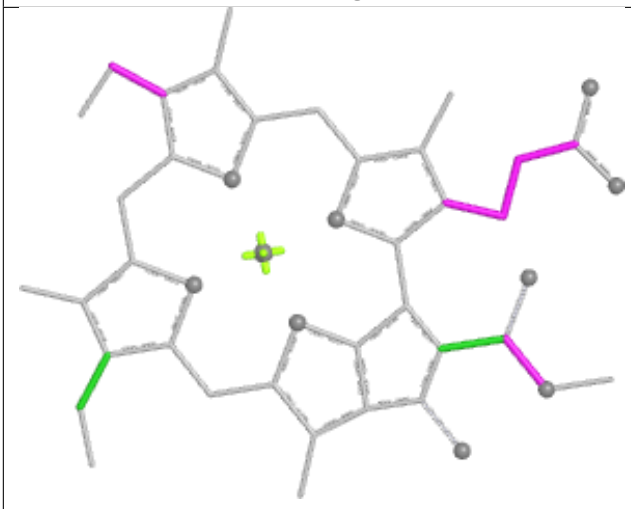


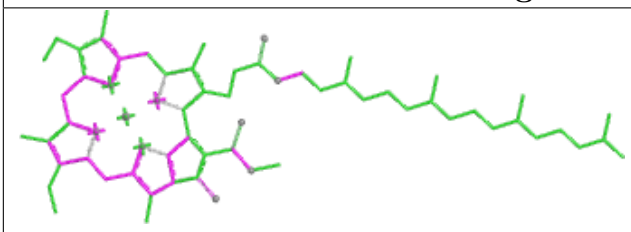
Bond angles



Torsions

Rings

Ligand CLA B 1203



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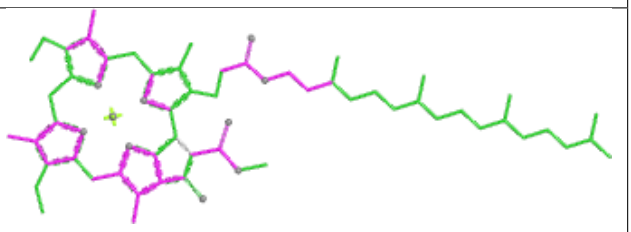
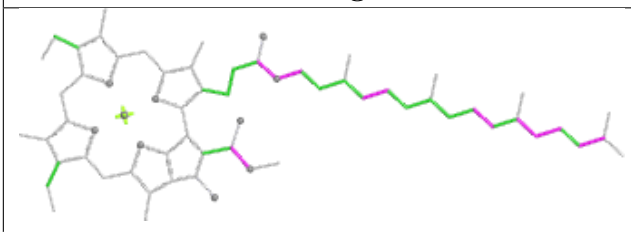
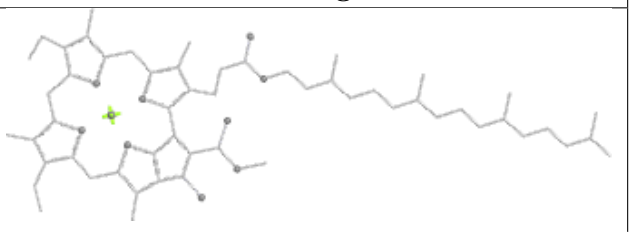


Bond angles

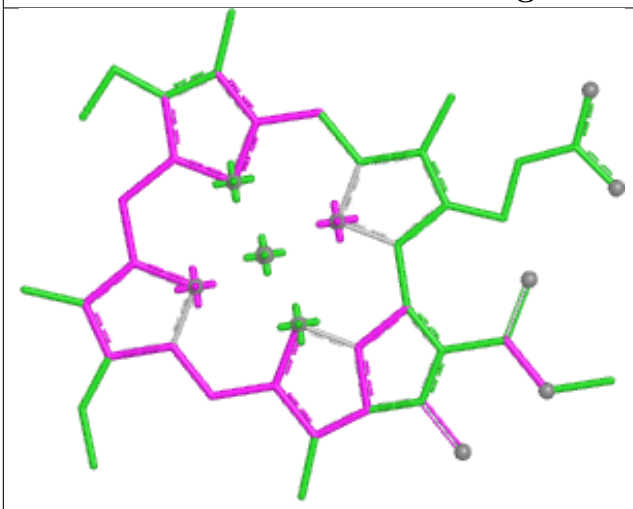


Torsions



Rings

Ligand CLA F 1301



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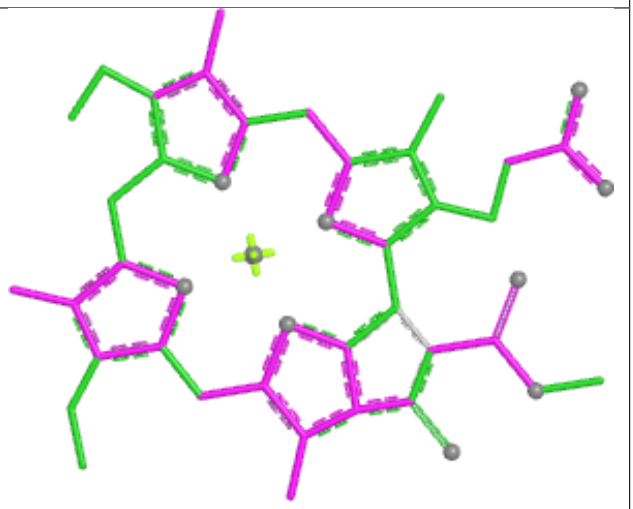
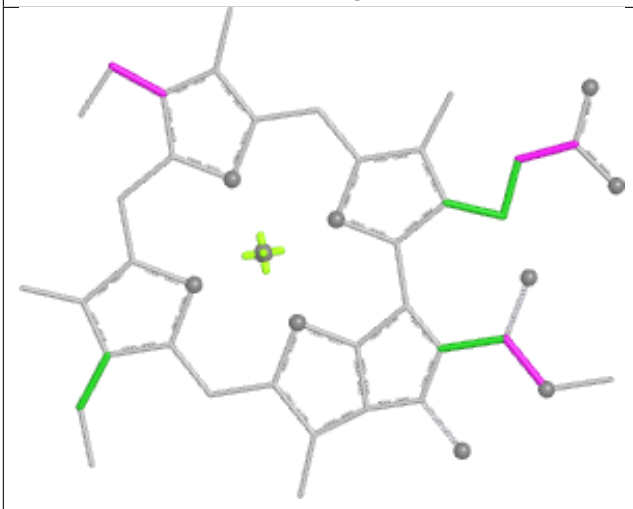


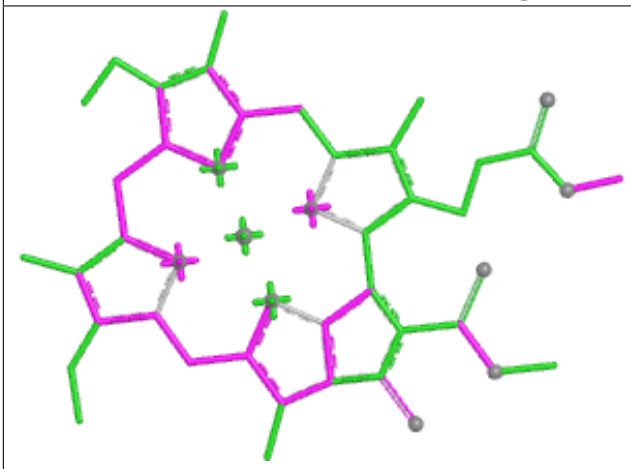
Bond angles



Torsions

Rings

Ligand CLA B 1207



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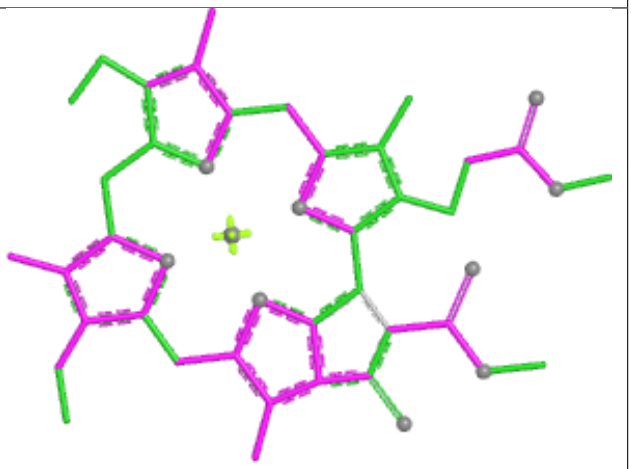
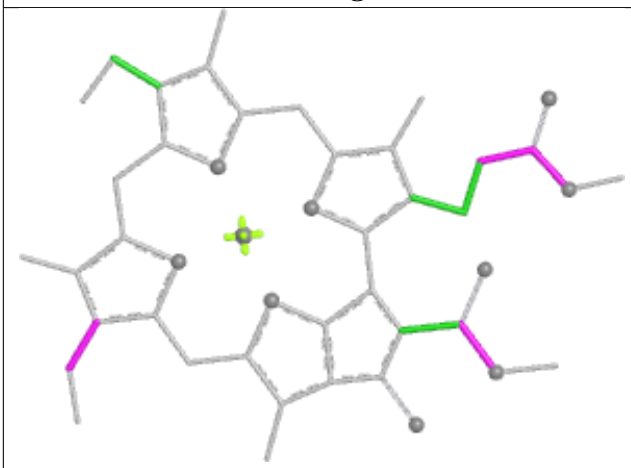
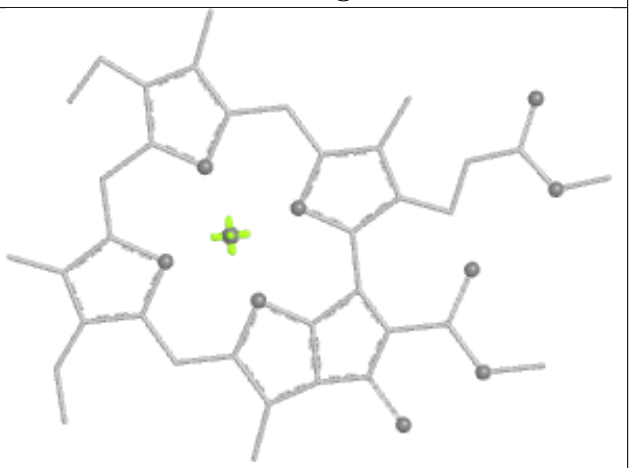


Bond angles

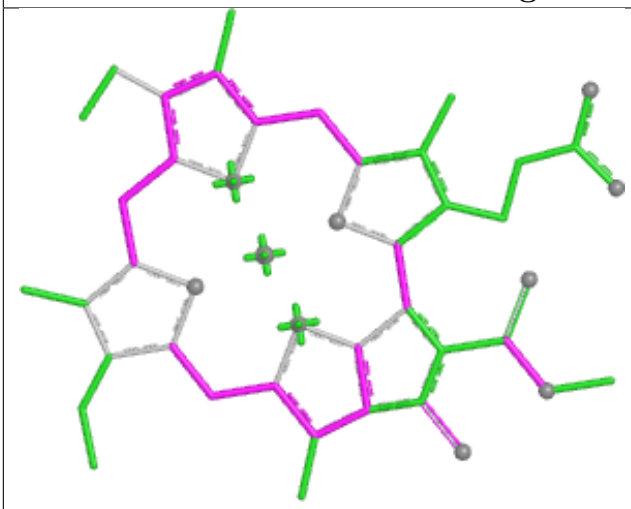


Torsions



Rings

Ligand CL0 A 1108



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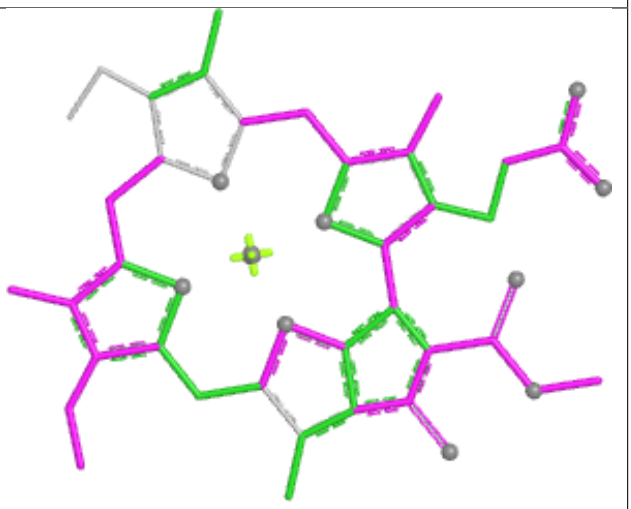
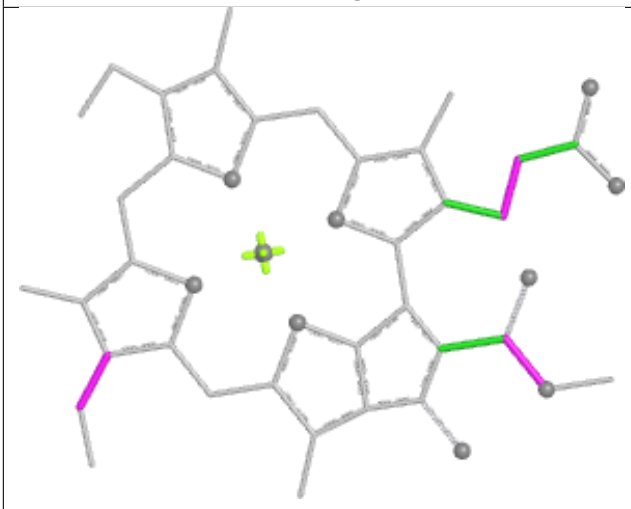


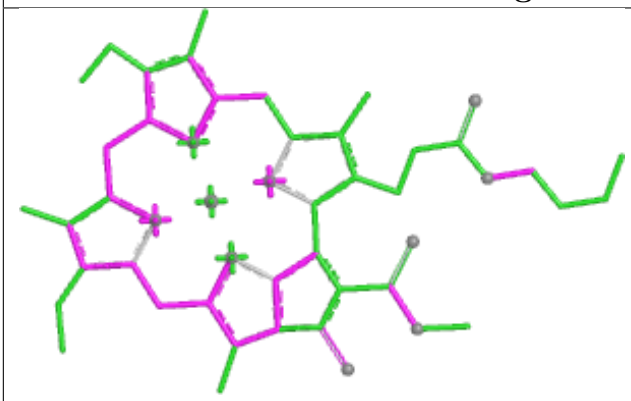
Bond angles



Torsions

Rings

Ligand CLA A 1114



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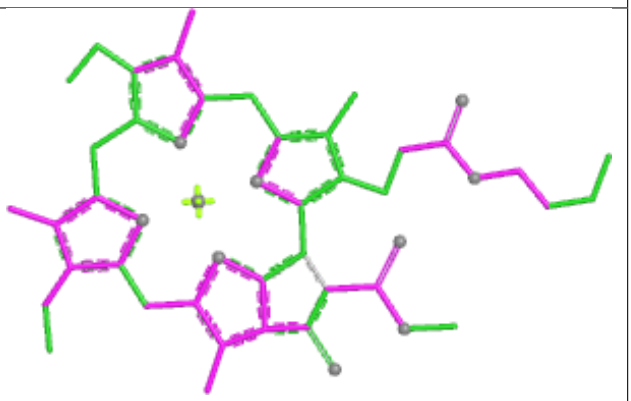
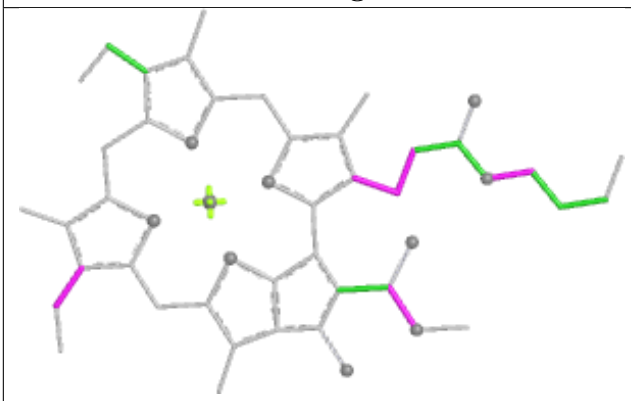
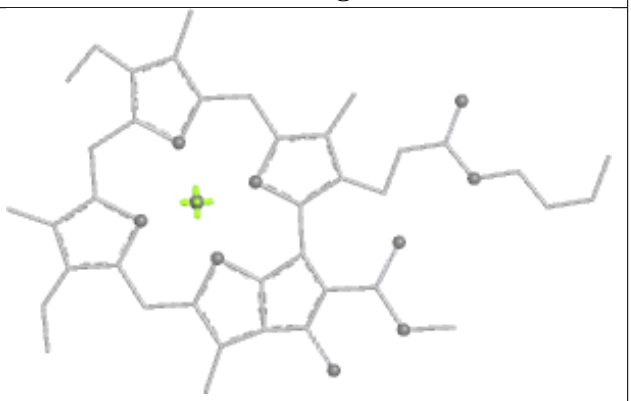


Bond angles

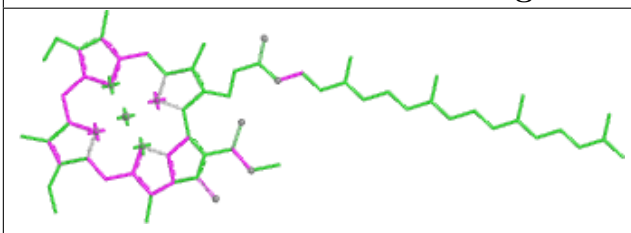


Torsions



Rings

Ligand CLA B 1013



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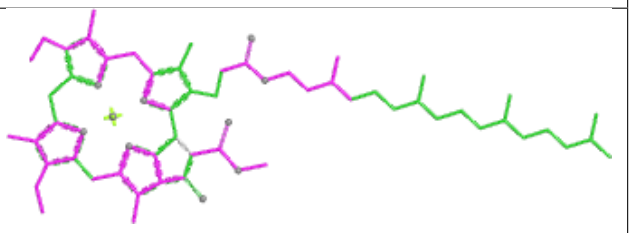
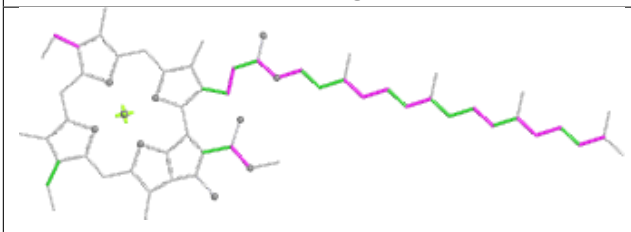
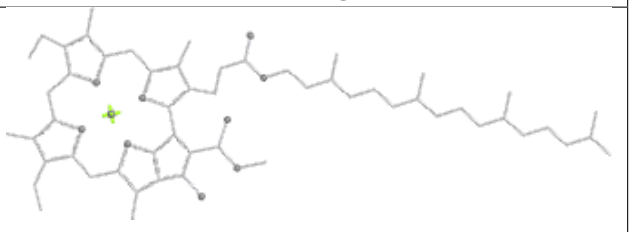


Bond angles

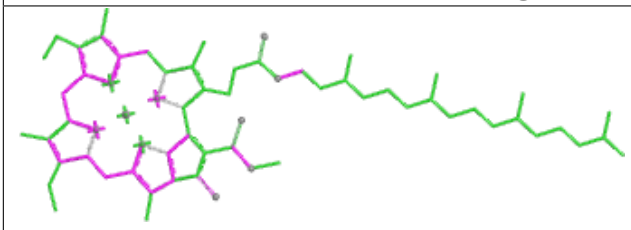


Torsions

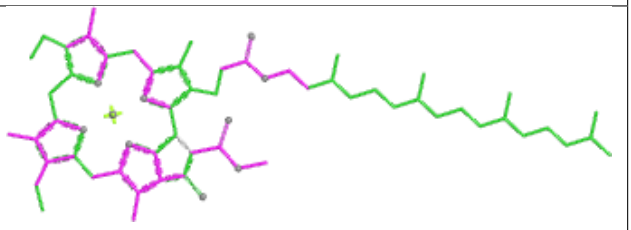


Rings

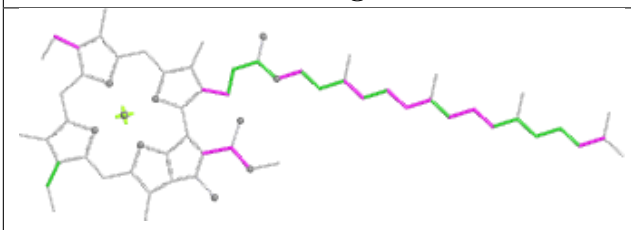
Ligand CLA A 1103



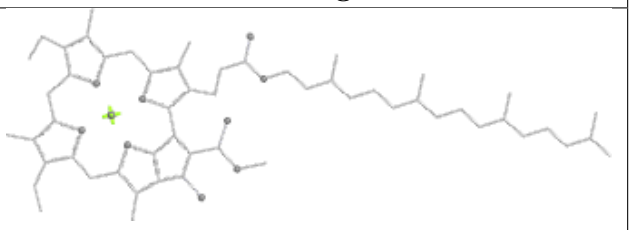
Bond lengths



Bond angles

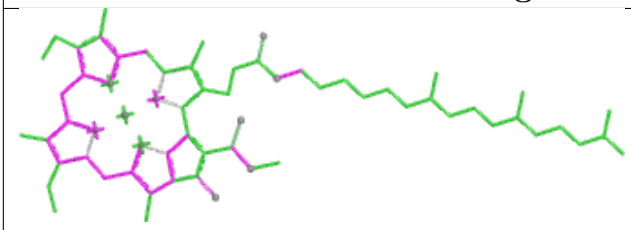


Torsions

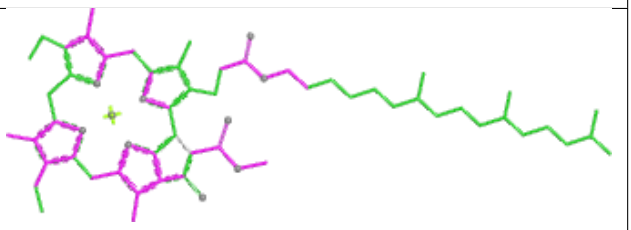


Rings

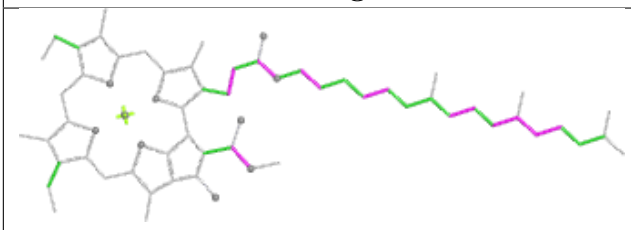
Ligand CLA A 1119



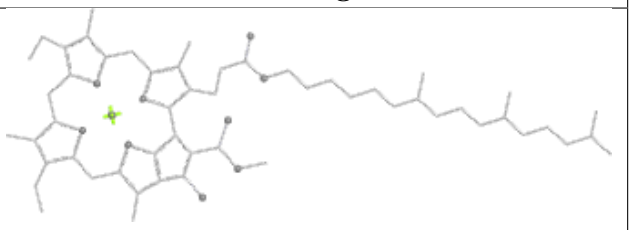
Bond lengths



Bond angles

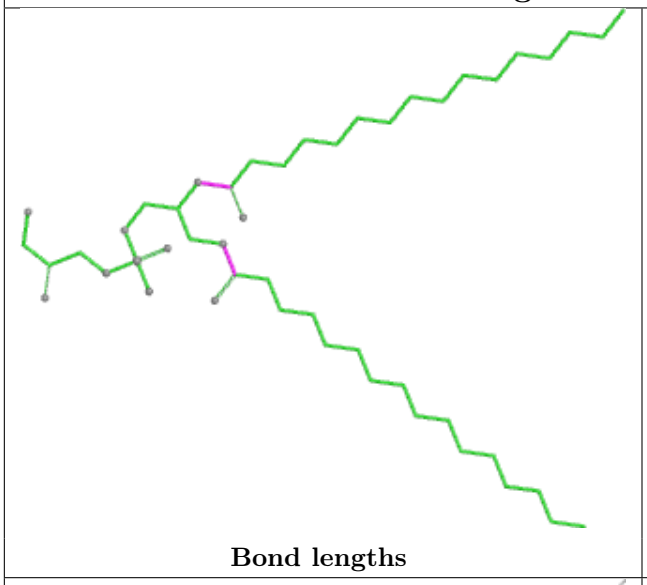


Torsions

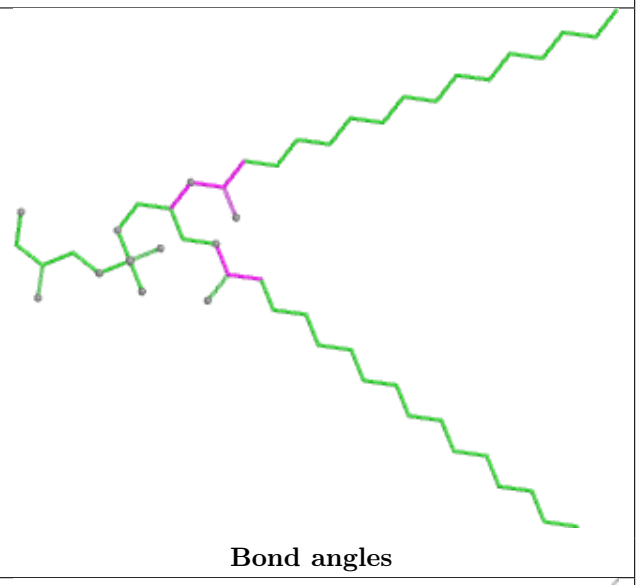


Rings

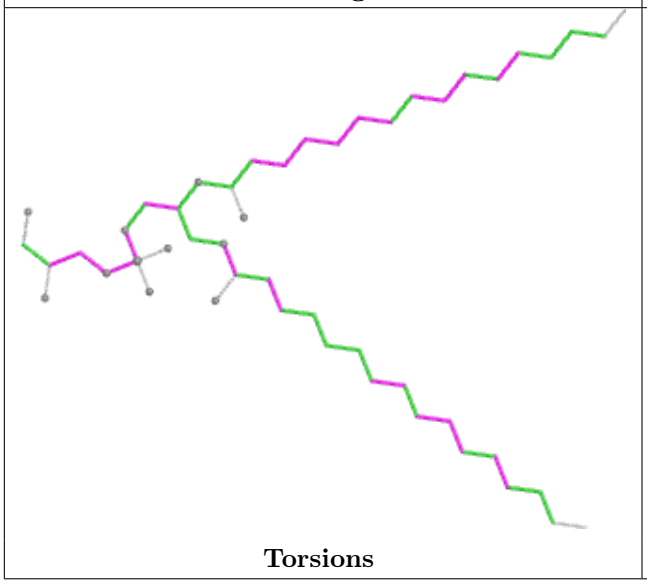
Ligand LHG A 5003



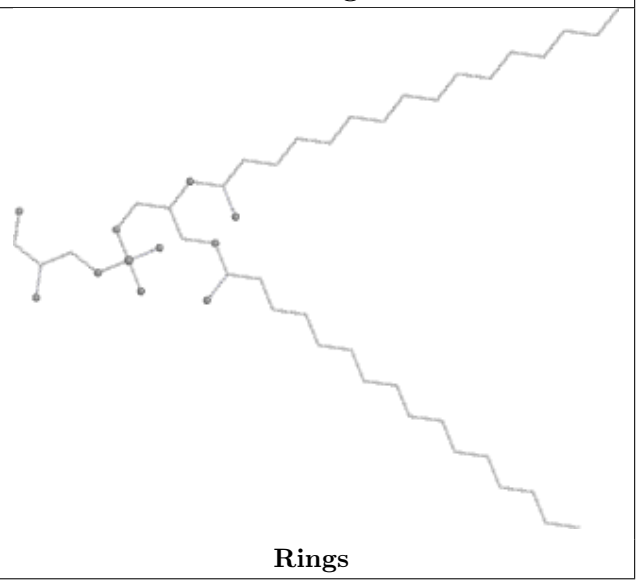
Bond lengths



Bond angles

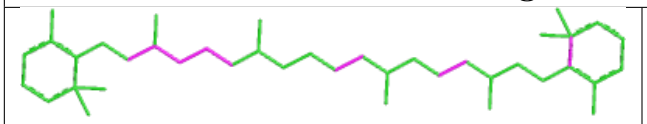


Torsions



Rings

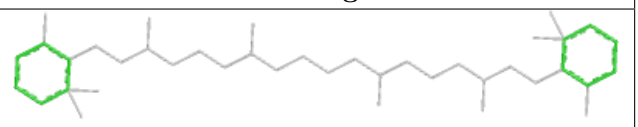
Ligand BCR J 4013



Bond lengths

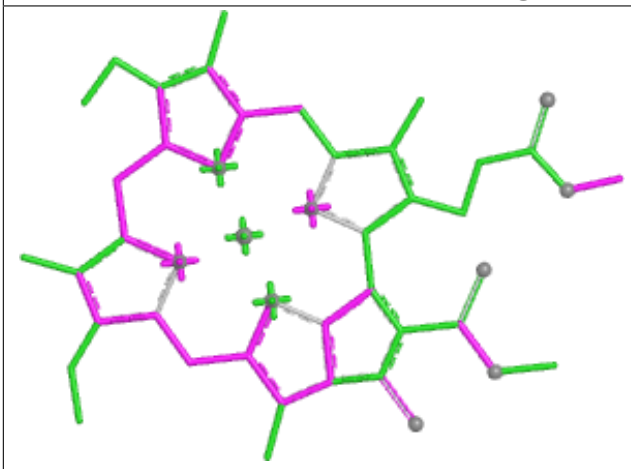
Bond angles

Torsions

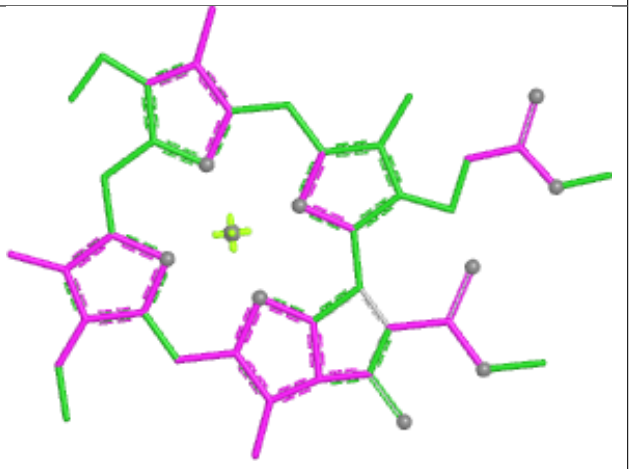


Rings

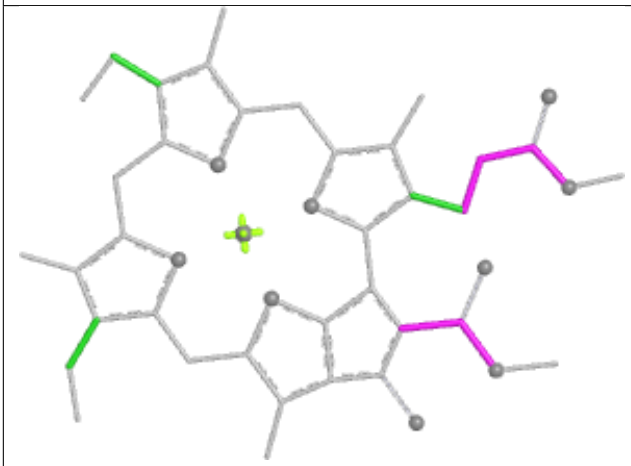
Ligand CLA A 1121



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.01	10 (1%) 73 64	43, 90, 141, 226	0
2	B	728/731 (99%)	-0.06	8 (1%) 78 70	53, 83, 126, 179	0
3	C	80/81 (98%)	0.09	3 (3%) 44 35	60, 72, 95, 105	0
4	D	138/141 (97%)	0.24	4 (2%) 53 43	72, 90, 125, 161	0
5	E	68/74 (91%)	0.13	1 (1%) 72 63	59, 75, 109, 138	0
6	F	141/165 (85%)	-0.10	2 (1%) 73 64	64, 82, 111, 169	0
7	J	40/40 (100%)	-0.28	0 100 100	66, 76, 124, 148	0
8	K	53/128 (41%)	1.14	9 (16%) 4 3	134, 160, 207, 253	0
9	M	30/31 (96%)	0.55	3 (10%) 12 9	109, 132, 158, 172	0
All	All	2017/2142 (94%)	0.02	40 (1%) 65 56	43, 86, 145, 253	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	PRO	5.5
5	E	14	THR	4.5
9	M	2	ALA	4.2
8	K	127	ILE	4.1
1	A	751	GLY	3.6
8	K	56	TRP	3.6
8	K	60	VAL	3.5
2	B	687	LEU	3.3
1	A	114	ALA	3.2
2	B	294	ASN	3.1
1	A	280	GLY	3.1
2	B	215	THR	2.9
4	D	36	SER	2.8
1	A	259	GLY	2.8
3	C	48	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
8	K	54	ALA	2.6
8	K	78	ALA	2.6
9	M	3	LEU	2.6
3	C	61	ASP	2.6
8	K	64	MET	2.5
1	A	285	THR	2.5
1	A	260	LEU	2.4
8	K	101	LEU	2.4
4	D	4	LEU	2.4
4	D	113	GLU	2.4
1	A	290	LEU	2.4
1	A	511	GLY	2.4
6	F	95	ASN	2.3
6	F	3	ASP	2.3
8	K	122	LEU	2.3
9	M	4	SER	2.3
2	B	730	PHE	2.3
2	B	480	ASP	2.3
2	B	214	SER	2.3
4	D	102	GLY	2.1
2	B	673	GLU	2.1
1	A	488	HIS	2.1
1	A	381	ILE	2.1
3	C	40	ALA	2.0
8	K	116	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
16	LMU	J	1304	35/35	0.55	0.15	91,159,172,173	0
16	LMU	B	1301	35/35	0.59	0.17	120,136,148,154	0
15	CLA	B	1207	46/65	0.69	0.16	118,164,185,189	0
12	LHG	A	5005	36/49	0.78	0.16	103,143,182,188	0
15	CLA	B	1213	50/65	0.78	0.16	89,104,128,136	0
15	CLA	K	1402	46/65	0.80	0.18	163,187,214,221	0
15	CLA	K	1401	46/65	0.81	0.17	120,155,169,173	0
15	CLA	A	1110	54/65	0.81	0.15	96,121,150,154	0
14	BCR	A	4001	40/40	0.83	0.17	111,127,138,140	0
15	CLA	A	1132	62/65	0.83	0.16	74,105,153,156	0
12	LHG	A	5003	49/49	0.84	0.15	91,121,142,143	0
15	CLA	A	1801	52/65	0.84	0.14	100,122,154,158	0
14	BCR	A	4007	40/40	0.86	0.14	69,86,137,139	0
15	CLA	J	1303	46/65	0.86	0.11	94,114,141,159	0
14	BCR	A	4008	40/40	0.86	0.13	67,93,105,115	0
14	BCR	B	4009	40/40	0.87	0.14	72,103,147,151	0
15	CLA	J	1302	45/65	0.87	0.10	82,93,138,150	0
15	CLA	A	1114	49/65	0.88	0.13	98,124,137,150	0
13	CL0	A	1108	45/65	0.88	0.15	86,113,154,170	0
14	BCR	A	4003	40/40	0.88	0.15	69,111,146,146	0
15	CLA	B	1208	45/65	0.88	0.11	88,114,130,140	0
14	BCR	B	4004	40/40	0.88	0.14	101,115,147,151	0
15	CLA	F	1410	65/65	0.88	0.13	69,96,135,147	0
15	CLA	A	1120	49/65	0.89	0.12	101,116,140,156	0
15	CLA	B	1230	65/65	0.89	0.15	53,68,118,125	0
15	CLA	B	1231	65/65	0.89	0.12	66,89,115,138	0
12	LHG	B	5004	49/49	0.89	0.12	59,88,99,106	0
15	CLA	B	1212	45/65	0.89	0.12	101,117,128,143	0
17	LMG	B	5002	55/55	0.89	0.14	71,101,130,137	0
15	CLA	B	1218	51/65	0.90	0.11	86,98,125,159	0
15	CLA	B	1228	65/65	0.90	0.12	54,74,105,114	0
15	CLA	A	1105	65/65	0.90	0.13	70,96,111,120	0
14	BCR	J	4013	40/40	0.90	0.15	78,97,112,121	0
15	CLA	A	1134	46/65	0.90	0.10	109,127,151,186	0
15	CLA	A	1135	55/65	0.90	0.14	70,98,132,135	0
15	CLA	B	1240	45/65	0.90	0.10	71,83,124,151	0
15	CLA	A	1111	60/65	0.90	0.13	78,96,107,112	0
15	CLA	A	1113	45/65	0.90	0.10	112,129,158,162	0
15	CLA	A	1124	55/65	0.90	0.12	61,92,120,129	0
14	BCR	B	4005	40/40	0.90	0.13	73,93,125,128	0
15	CLA	B	1217	47/65	0.90	0.11	96,114,132,157	0
15	CLA	B	1224	65/65	0.91	0.12	60,78,98,108	0
14	BCR	B	4006	40/40	0.91	0.13	86,109,141,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CLA	A	1118	46/65	0.91	0.12	99,113,135,154	0
15	CLA	A	1102	65/65	0.91	0.12	55,81,107,112	0
15	CLA	B	1203	65/65	0.91	0.10	62,83,99,104	0
15	CLA	F	1301	45/65	0.91	0.10	54,75,97,131	0
15	CLA	A	1125	52/65	0.91	0.12	76,98,124,133	0
14	BCR	A	4002	40/40	0.91	0.12	88,109,128,130	0
14	BCR	F	4015	40/40	0.91	0.13	52,73,107,111	0
15	CLA	A	1121	46/65	0.91	0.11	91,114,141,163	0
15	CLA	B	1214	65/65	0.91	0.14	72,89,119,133	0
15	CLA	A	1131	55/65	0.91	0.10	78,107,126,140	0
10	PQN	B	2002	33/33	0.91	0.10	59,79,99,105	0
15	CLA	B	1232	45/65	0.92	0.10	72,89,109,115	0
15	CLA	B	1234	65/65	0.92	0.12	56,73,108,120	0
15	CLA	B	1236	50/65	0.92	0.11	52,72,106,114	0
15	CLA	B	1201	46/65	0.92	0.10	72,83,107,123	0
15	CLA	A	1133	46/65	0.92	0.09	86,103,118,128	0
15	CLA	A	1122	65/65	0.92	0.11	74,91,119,129	0
15	CLA	B	1219	55/65	0.92	0.10	74,86,119,142	0
15	CLA	B	1221	65/65	0.92	0.12	68,79,105,125	0
15	CLA	B	1222	56/65	0.92	0.10	52,66,101,108	0
14	BCR	B	4010	40/40	0.92	0.12	55,74,102,113	0
12	LHG	A	5001	49/49	0.92	0.12	49,70,91,100	0
15	CLA	A	1119	64/65	0.92	0.13	78,97,115,137	0
15	CLA	B	1216	65/65	0.92	0.10	67,91,106,118	0
15	CLA	B	1225	65/65	0.93	0.11	66,80,100,104	0
15	CLA	B	1226	65/65	0.93	0.12	54,79,133,144	0
15	CLA	B	1227	45/65	0.93	0.10	54,72,94,98	0
15	CLA	A	1109	65/65	0.93	0.12	66,81,105,112	0
15	CLA	B	1023	65/65	0.93	0.11	55,79,111,119	0
15	CLA	A	1126	65/65	0.93	0.11	63,80,101,116	0
15	CLA	A	1136	65/65	0.93	0.12	78,105,139,142	0
14	BCR	F	4016	40/40	0.93	0.10	59,72,89,94	0
15	CLA	B	1210	65/65	0.93	0.12	75,95,108,120	0
15	CLA	A	1115	46/65	0.93	0.11	109,129,140,151	0
15	CLA	B	1204	46/65	0.93	0.09	79,96,115,137	0
14	BCR	B	4011	40/40	0.93	0.10	49,67,84,91	0
14	BCR	B	4014	40/40	0.93	0.11	46,62,88,89	0
15	CLA	A	1129	46/65	0.93	0.11	76,92,115,151	0
15	CLA	A	1130	55/65	0.93	0.10	82,106,133,139	0
15	CLA	A	1116	54/65	0.93	0.13	84,113,130,141	0
15	CLA	A	1101	65/65	0.93	0.10	55,73,89,96	0
14	BCR	B	4017	40/40	0.93	0.10	70,87,101,104	0

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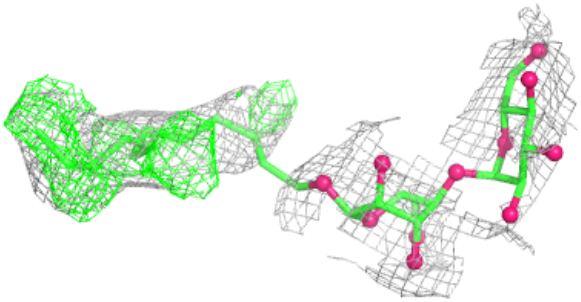
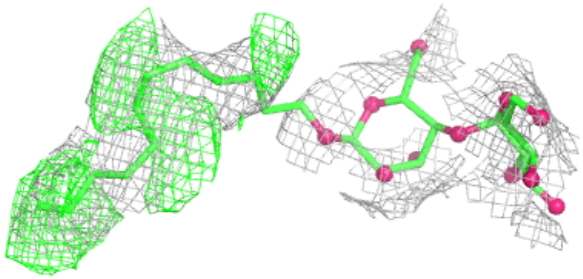
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CLA	A	1103	65/65	0.93	0.13	61,80,108,118	0
10	PQN	A	2001	33/33	0.93	0.10	45,57,68,74	0
15	CLA	A	1127	65/65	0.94	0.12	67,79,100,106	0
15	CLA	A	1106	65/65	0.94	0.11	59,79,98,109	0
15	CLA	B	1215	65/65	0.94	0.11	72,85,104,106	0
15	CLA	A	1137	50/65	0.94	0.09	72,94,128,134	0
15	CLA	B	1235	65/65	0.94	0.09	55,66,85,92	0
15	CLA	A	1012	65/65	0.94	0.12	47,60,86,93	0
15	CLA	A	1117	65/65	0.94	0.10	80,100,111,113	0
15	CLA	B	1013	65/65	0.94	0.10	46,53,77,89	0
15	CLA	B	1211	46/65	0.94	0.09	90,106,116,133	0
15	CLA	B	1237	55/65	0.94	0.09	71,82,117,132	0
15	CLA	B	1238	44/65	0.94	0.09	68,80,92,111	0
15	CLA	B	1239	46/65	0.94	0.09	62,78,107,141	0
15	CLA	B	1220	56/65	0.94	0.10	61,77,111,119	0
15	CLA	A	1107	50/65	0.94	0.09	56,64,98,112	0
14	BCR	A	4012	40/40	0.94	0.09	55,77,87,91	0
15	CLA	B	1223	65/65	0.94	0.11	59,77,94,98	0
15	CLA	A	1022	65/65	0.94	0.11	53,78,96,103	0
15	CLA	A	1104	65/65	0.94	0.10	58,72,83,96	0
15	CLA	B	1209	45/65	0.94	0.10	102,113,134,148	0
15	CLA	A	1112	45/65	0.94	0.11	89,115,127,130	0
11	SF4	C	3002	8/8	0.94	0.11	60,88,151,152	0
15	CLA	F	1139	65/65	0.95	0.11	47,58,90,98	0
15	CLA	B	1229	65/65	0.95	0.09	50,62,86,107	0
15	CLA	A	1140	65/65	0.95	0.09	52,73,103,116	0
15	CLA	B	1206	46/65	0.95	0.10	78,100,119,149	0
13	CL0	A	1011	65/65	0.95	0.11	51,69,81,99	0
15	CLA	B	1205	55/65	0.95	0.10	68,87,100,112	0
15	CLA	A	1128	65/65	0.95	0.10	54,74,90,101	0
11	SF4	A	3001	8/8	0.95	0.16	50,62,210,290	0
15	CLA	A	1123	65/65	0.95	0.11	75,88,98,104	0
15	CLA	B	1202	65/65	0.96	0.11	67,82,99,106	0
15	CLA	B	1021	65/65	0.96	0.10	49,69,80,84	0
15	CLA	A	1138	65/65	0.96	0.09	47,55,69,77	0
11	SF4	C	3003	8/8	0.98	0.12	60,67,100,115	0
18	CL	B	6000	1/1	0.98	0.08	82,82,82,82	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 LMU J 1304:

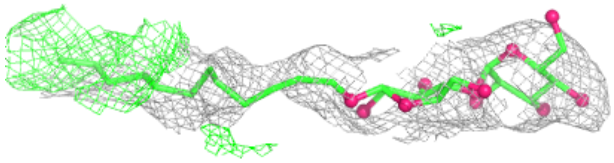
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

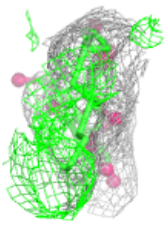




Electron density around LMU B 1301:

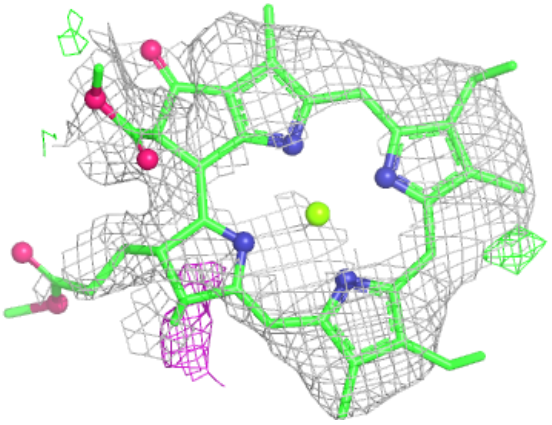
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

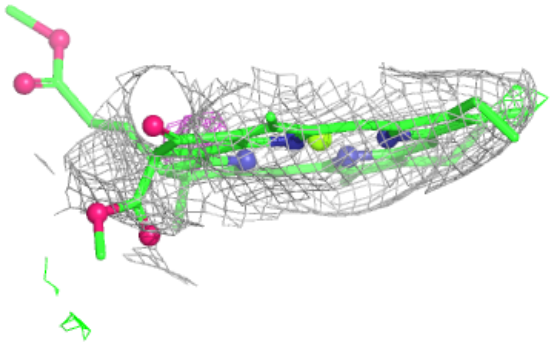


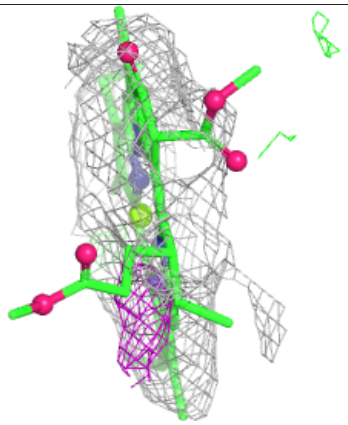


Electron density around CLA B 1207:

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

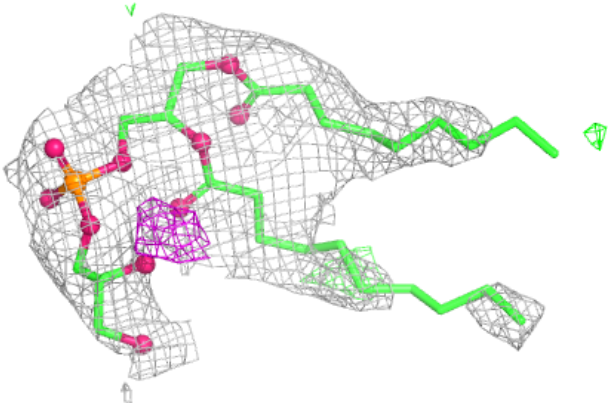


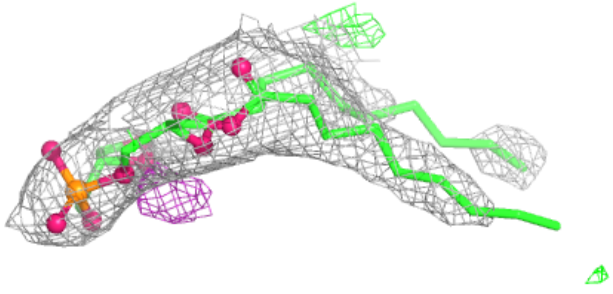


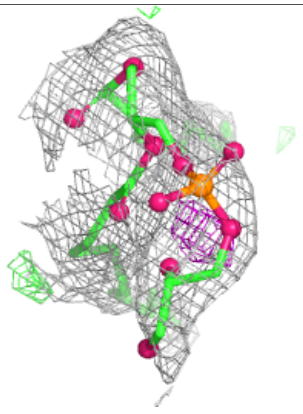


Electron density around LHG A 5005:

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

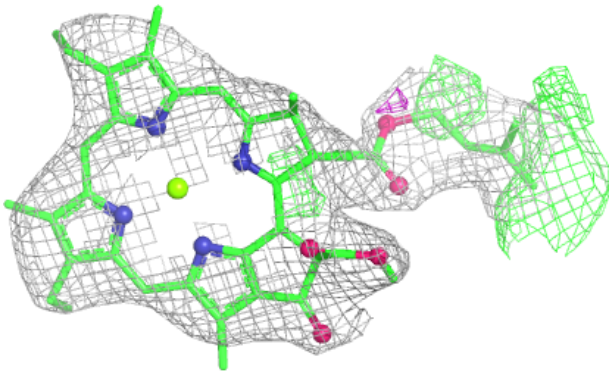


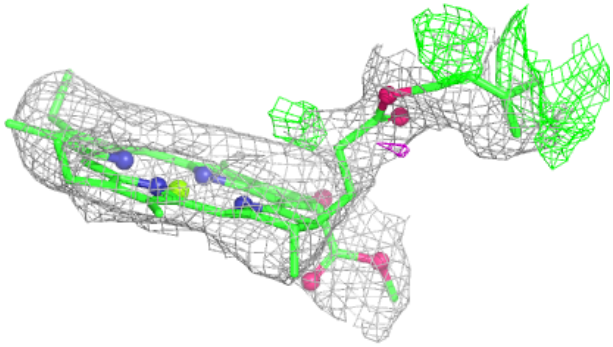


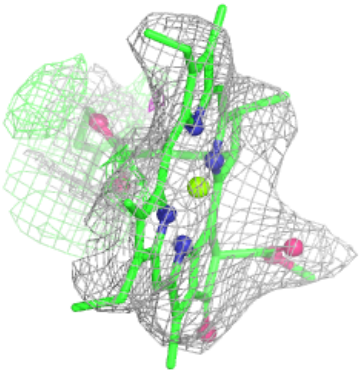


Electron density around CLA B 1213:

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

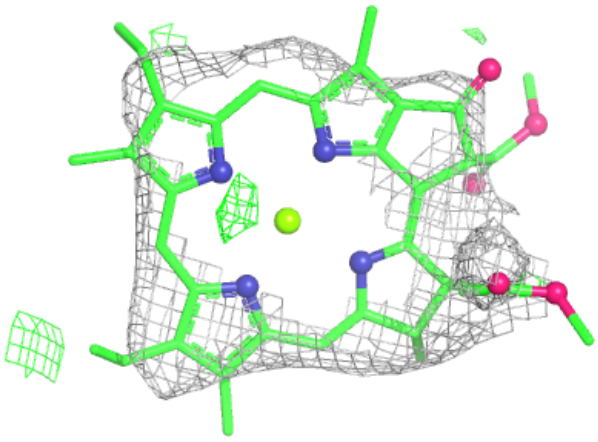


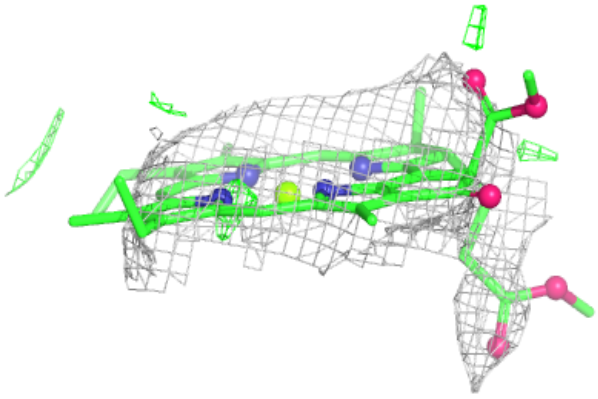


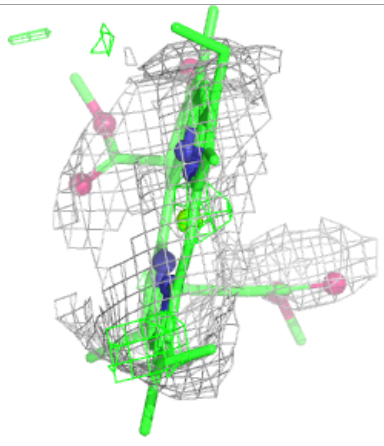


Electron density around CLA K 1402:

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

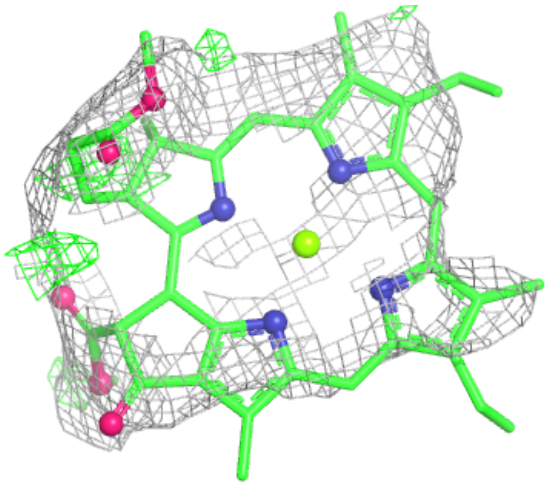


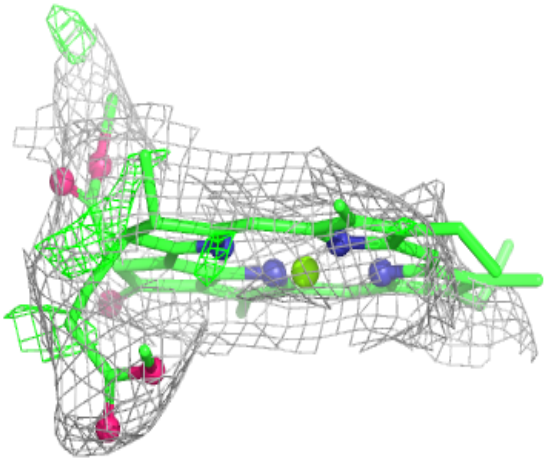




Electron density around CLA K 1401:

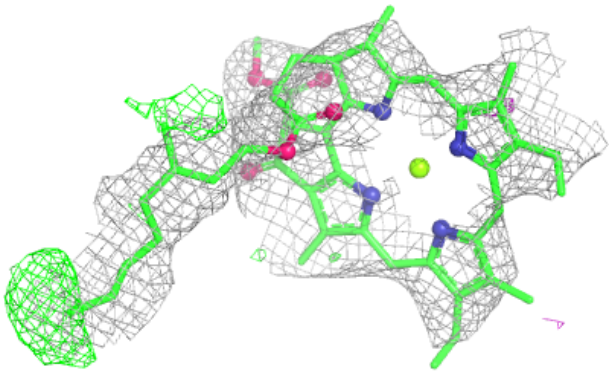
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

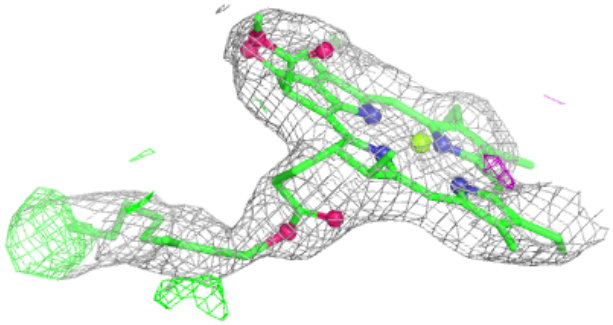


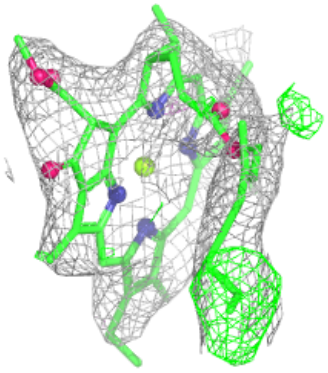


Electron density around CLA A 1110:

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

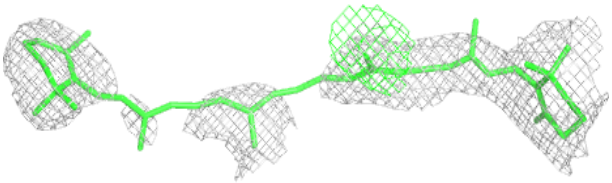


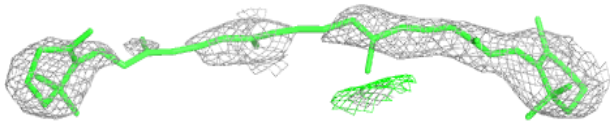


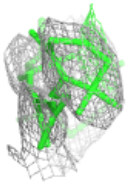


Electron density around BCR A 4001:

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

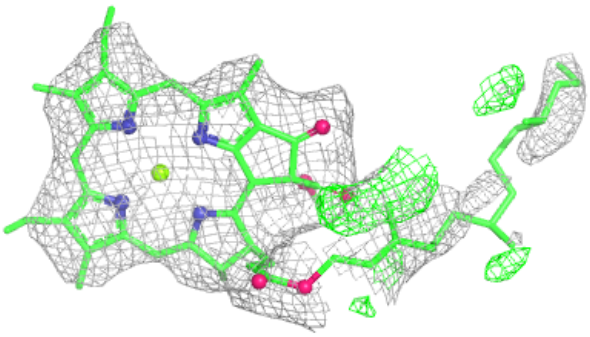


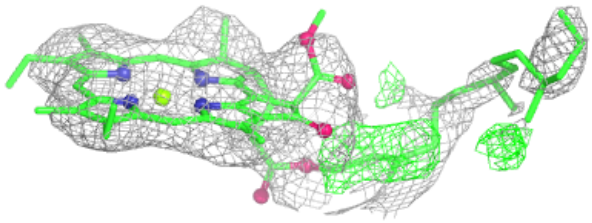


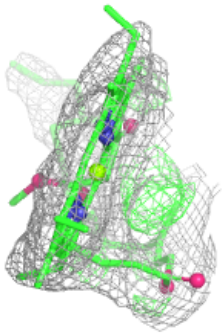


Electron density around CLA A 1132:

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

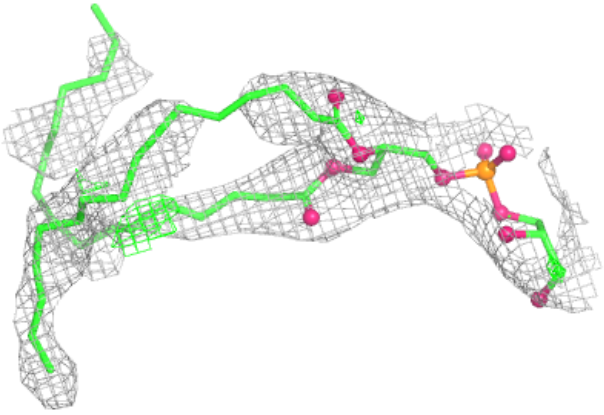


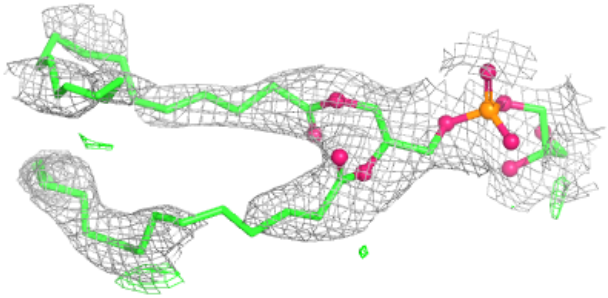


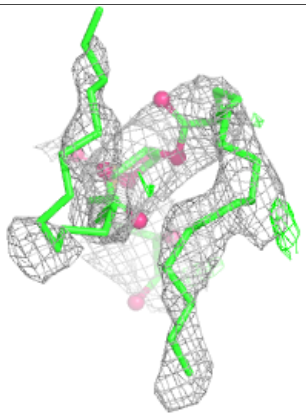


Electron density around LHG A 5003:

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

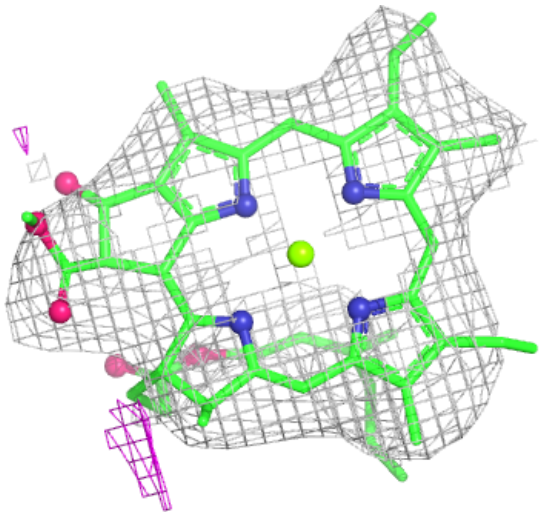


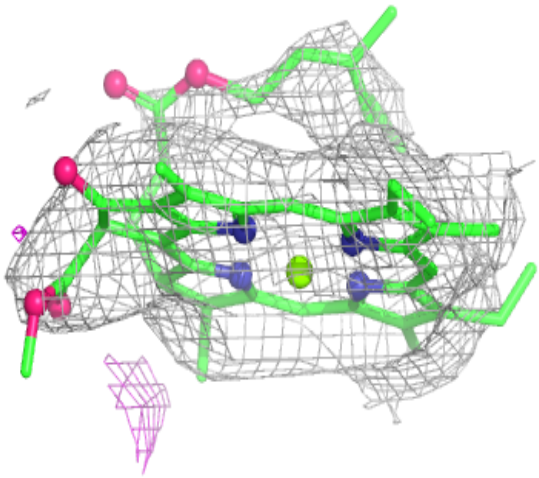


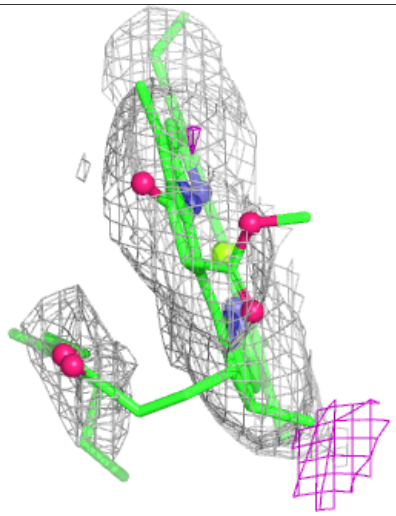


Electron density around CLA A 1801:

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

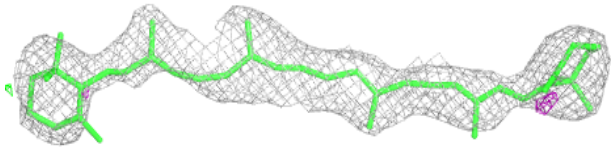


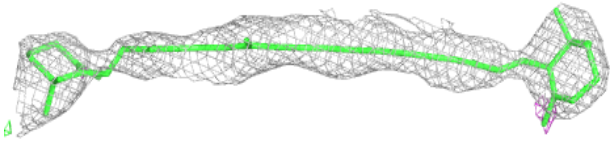


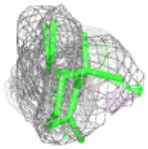


Electron density around BCR A 4007:

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

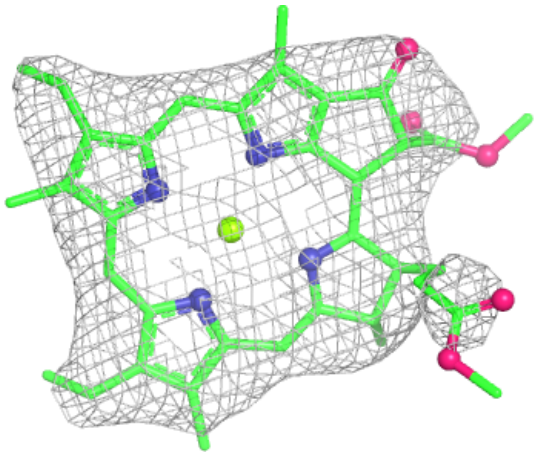


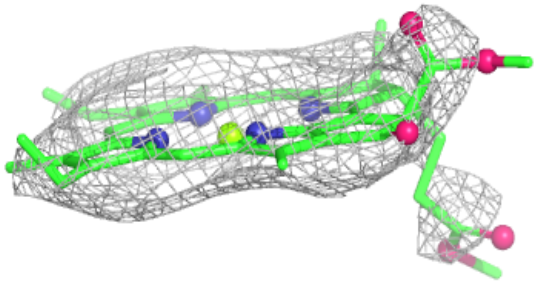


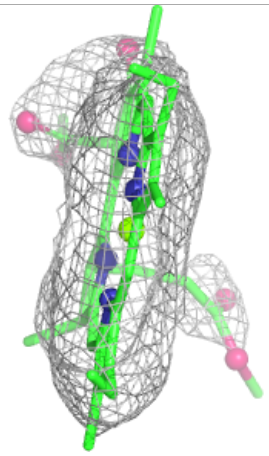


Electron density around CLA J 1303:

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

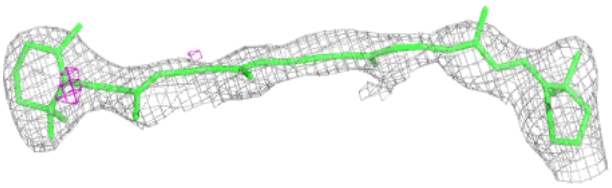


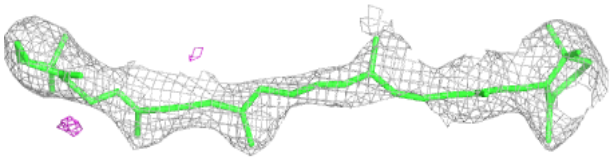


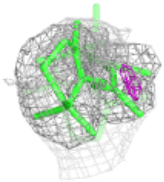


Electron density around BCR A 4008:

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

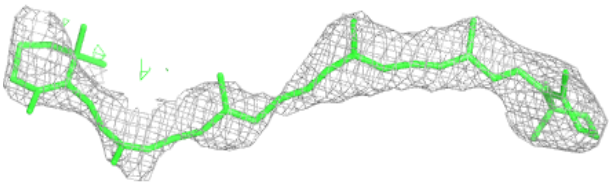


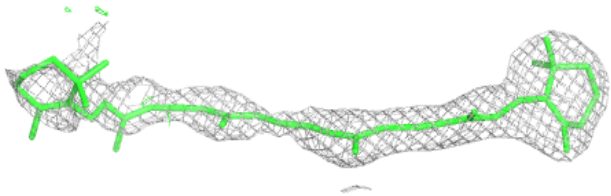


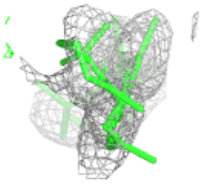


Electron density around BCR B 4009:

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

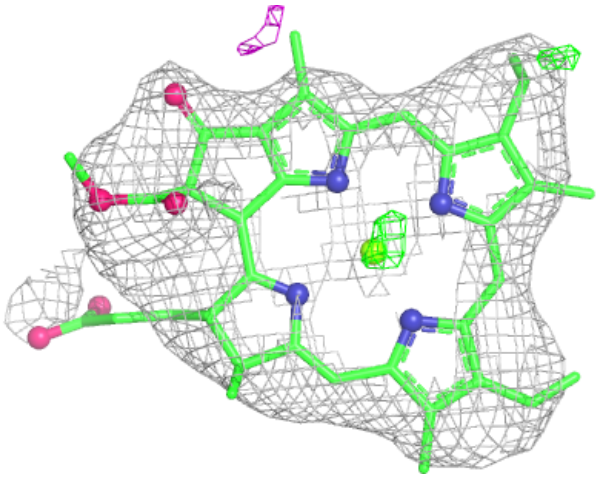


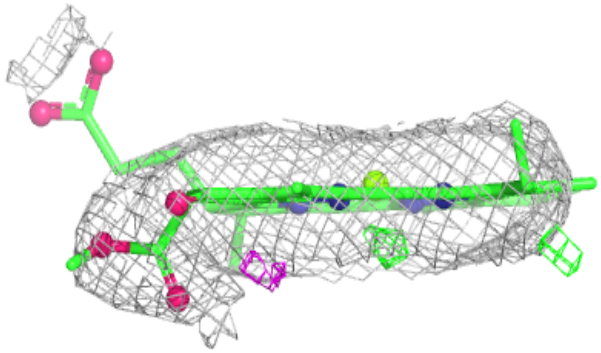


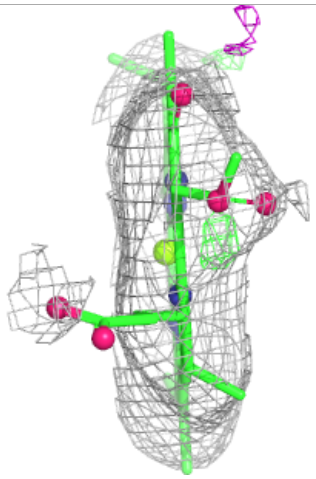


Electron density around CLA J 1302:

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

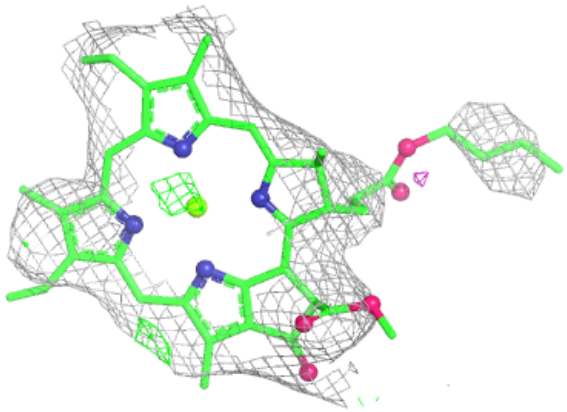


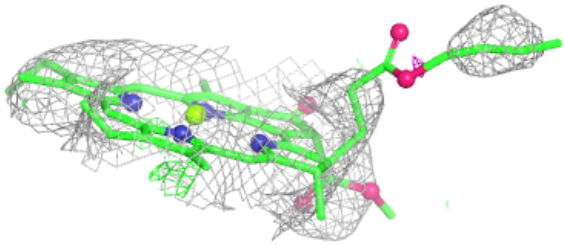


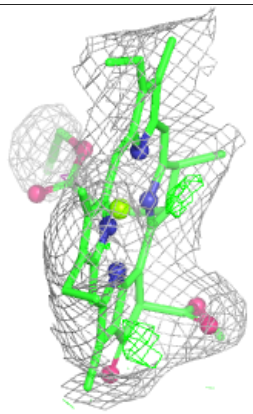


Electron density around CLA A 1114:

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

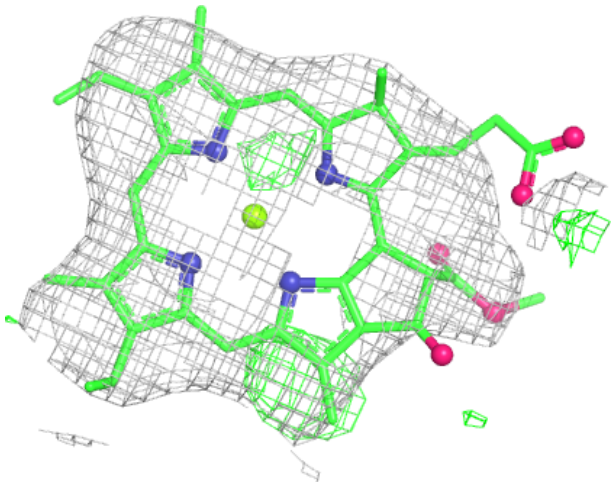


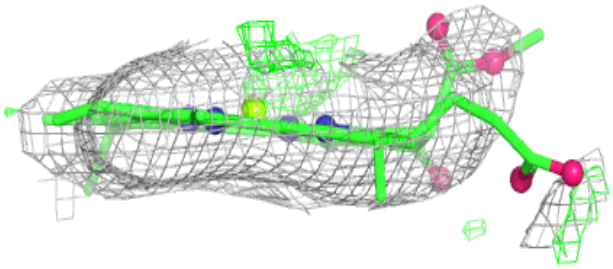


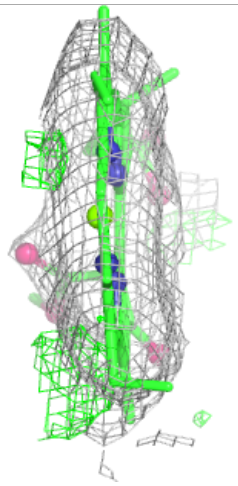


Electron density around CL0 A 1108:

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

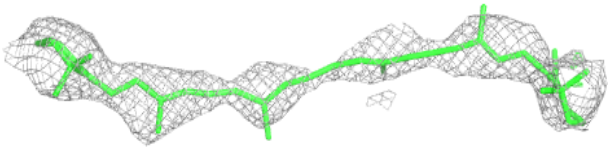


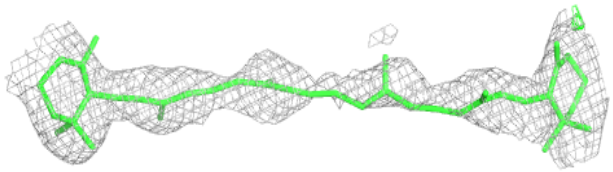


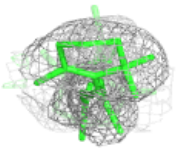


Electron density around BCR A 4003:

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

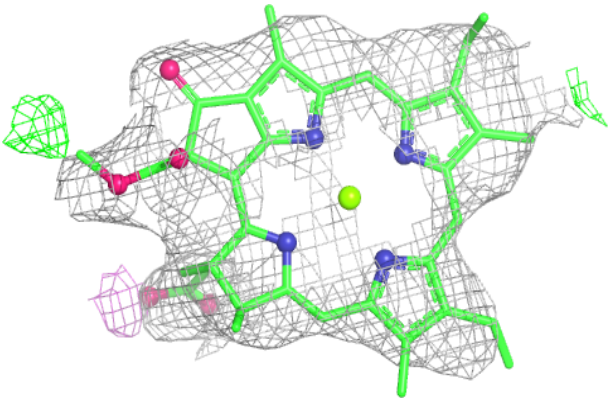


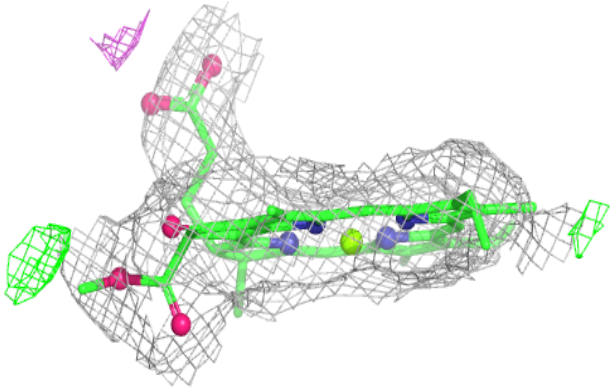


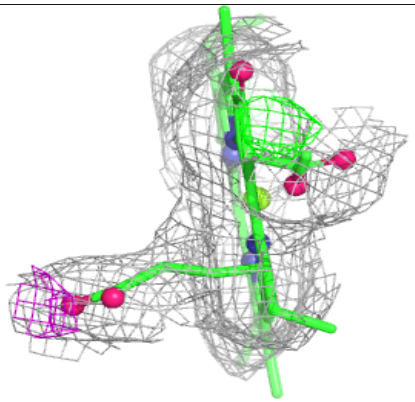


Electron density around CLA B 1208:

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

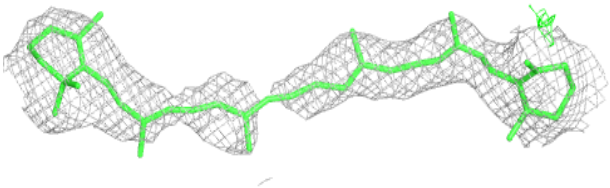


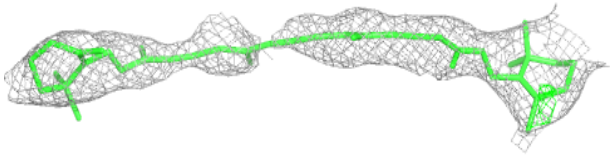


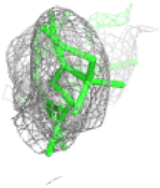


Electron density around BCR B 4004:

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

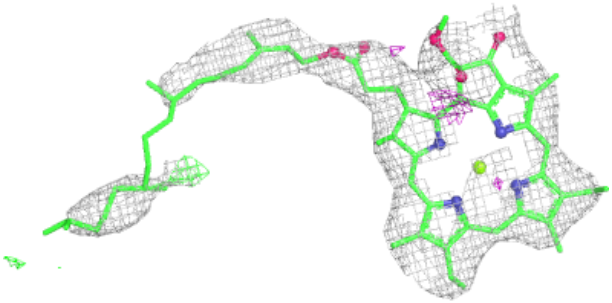


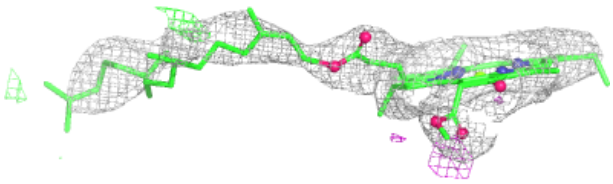




Electron density around CLA F 1410:

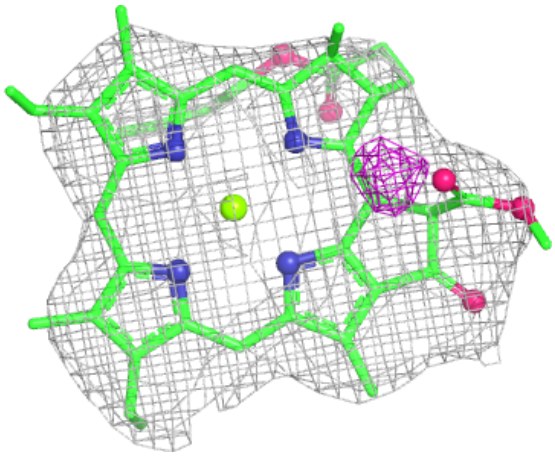
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

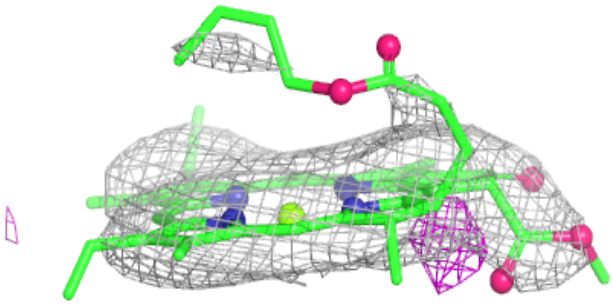


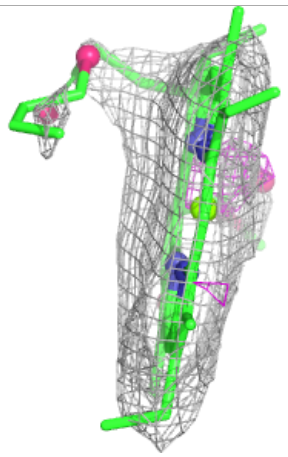


Electron density around CLA A 1120:

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

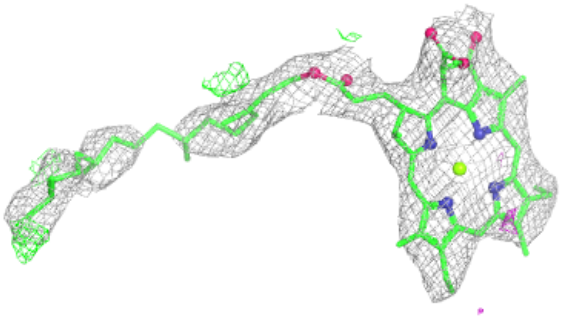


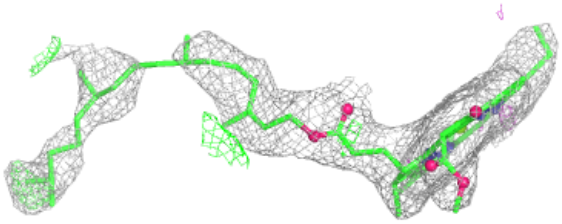


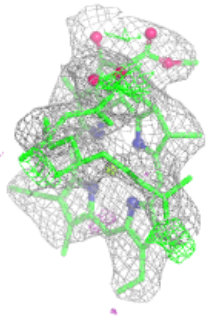


Electron density around CLA B 1230:

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

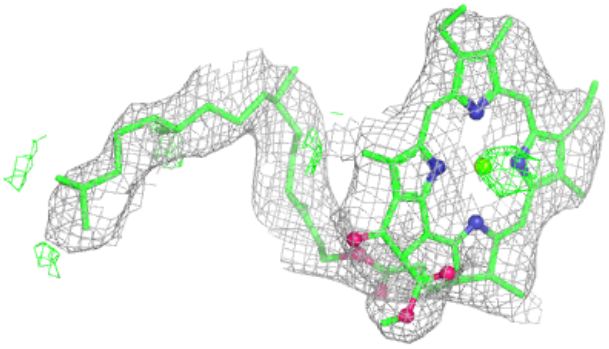


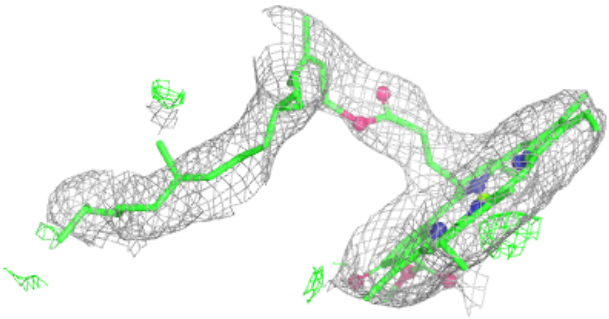




Electron density around CLA B 1231:

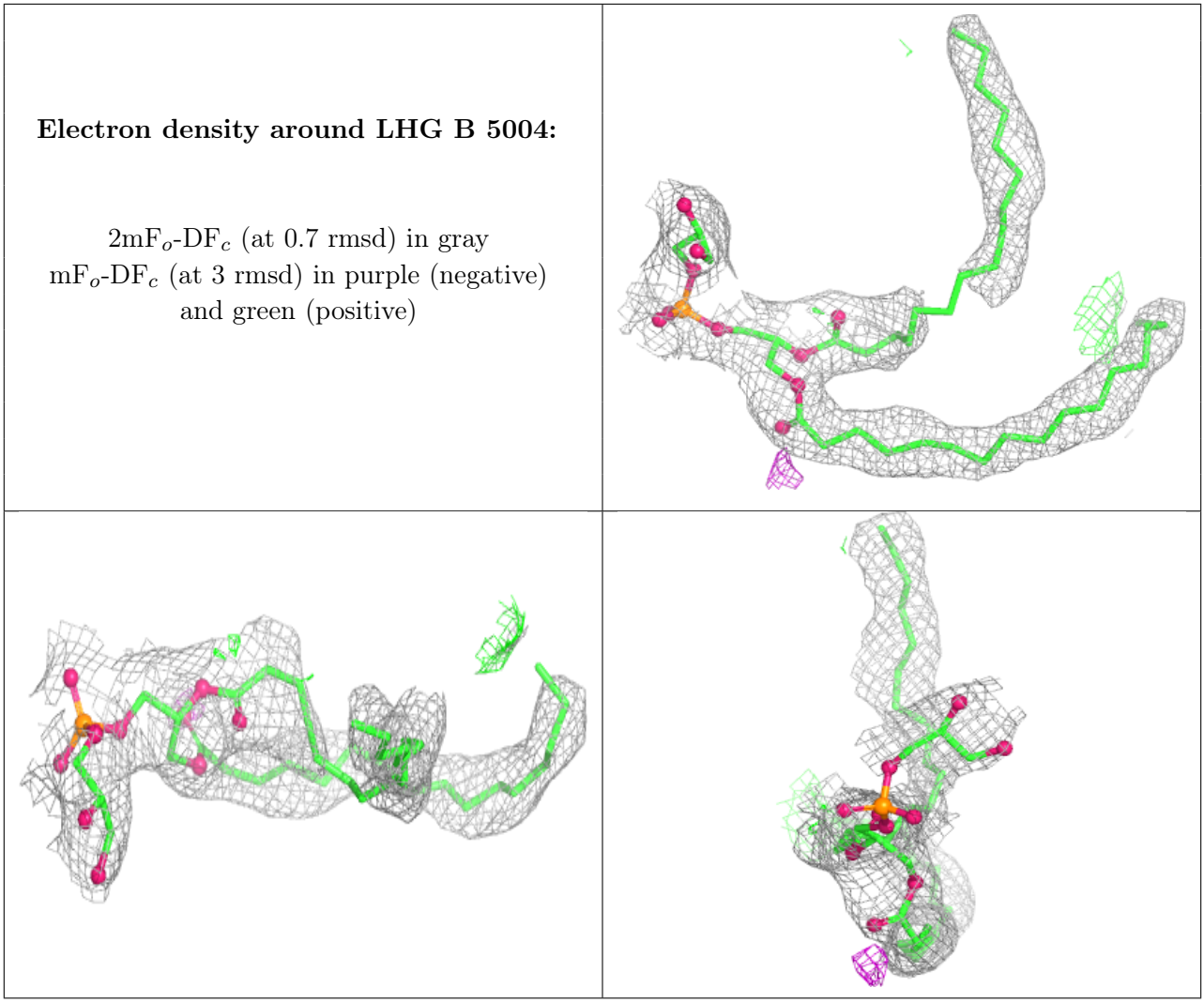
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





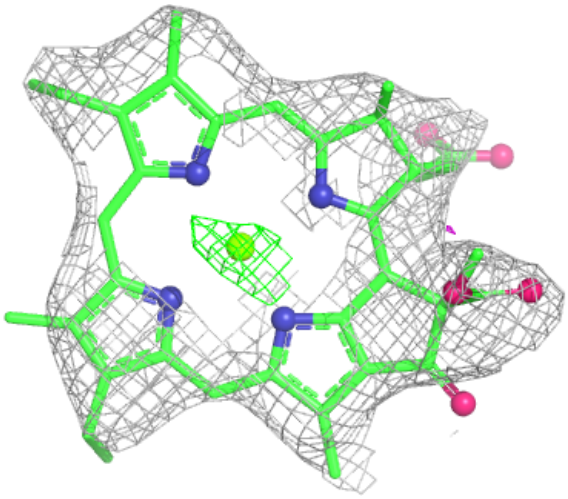
Electron density around LHG B 5004:

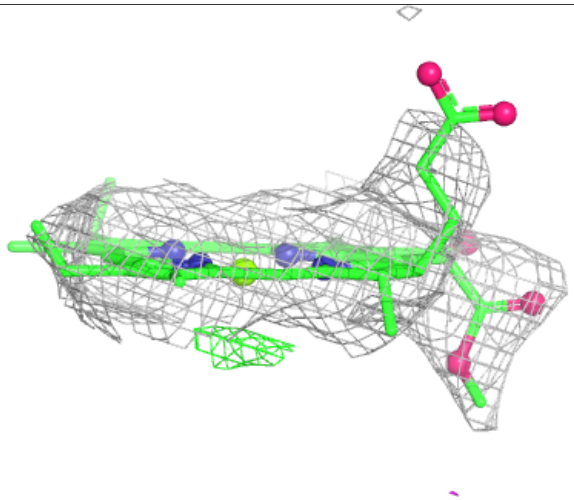
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

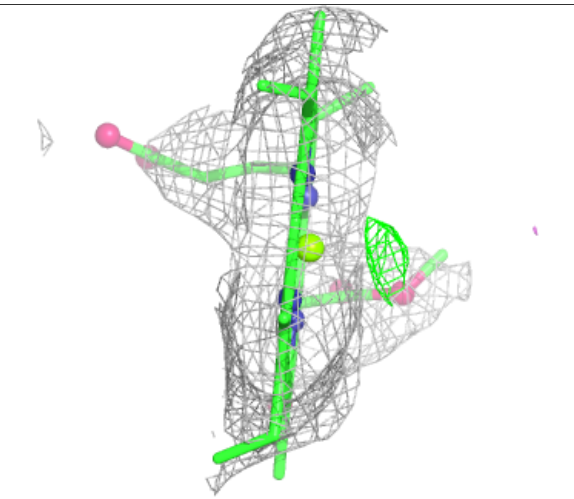


Electron density around CLA B 1212:

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

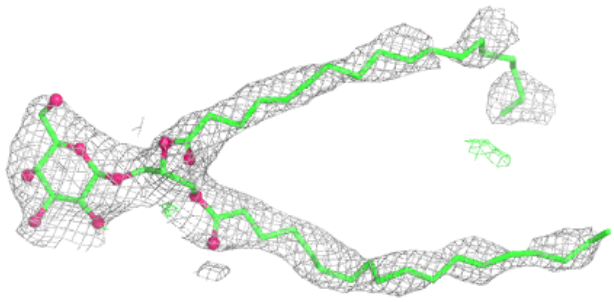


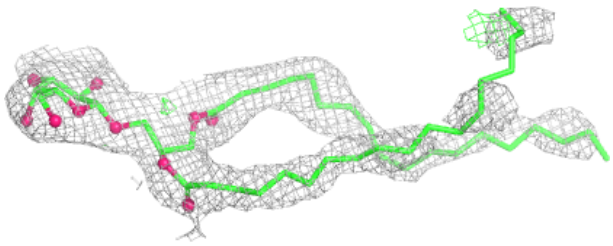


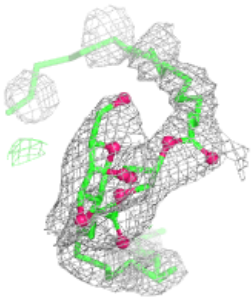


Electron density around LMG B 5002:

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

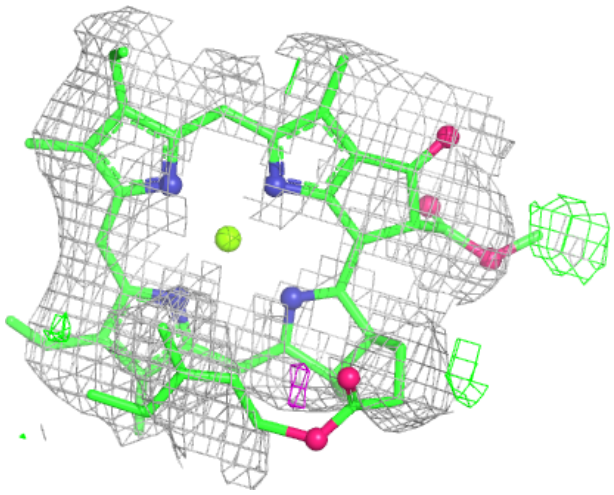


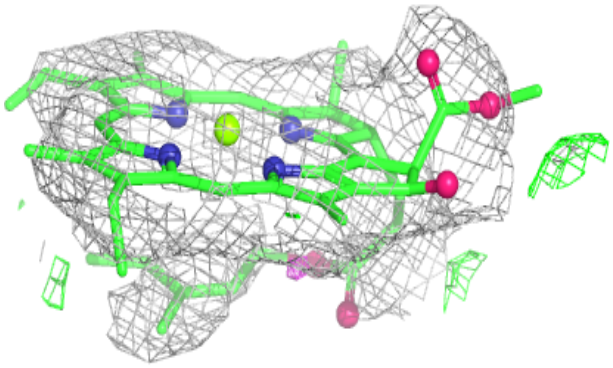


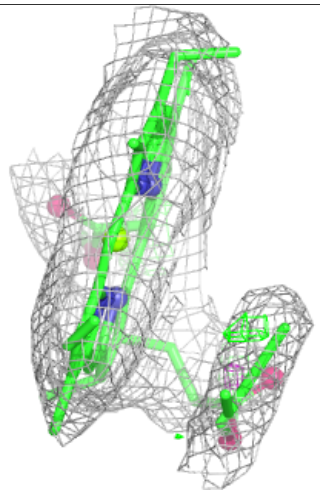


Electron density around CLA B 1218:

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

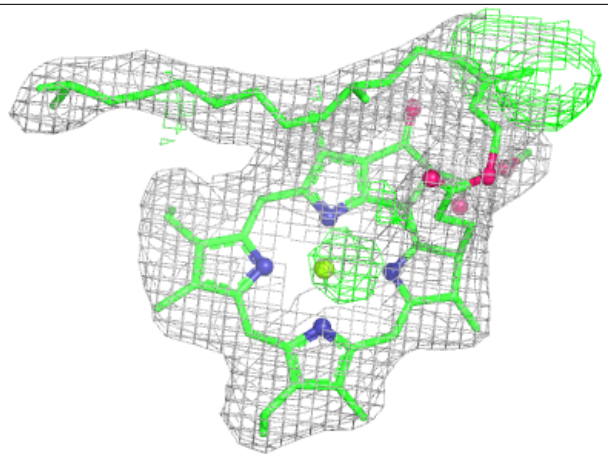


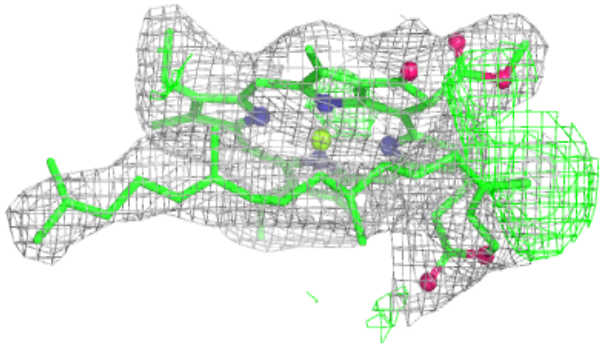


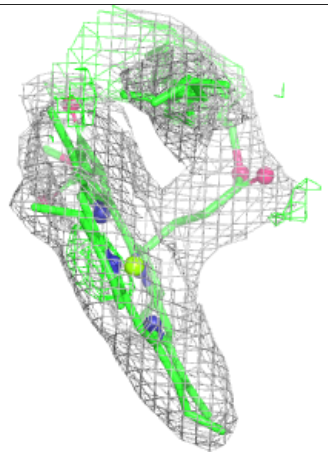


Electron density around CLA B 1228:

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

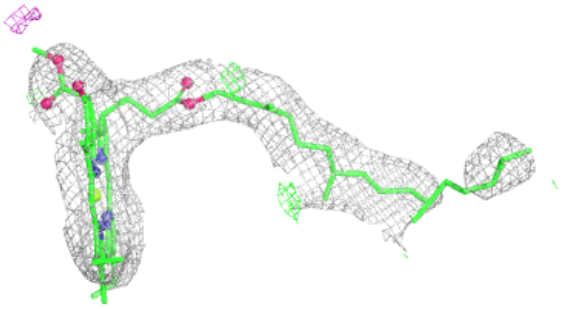


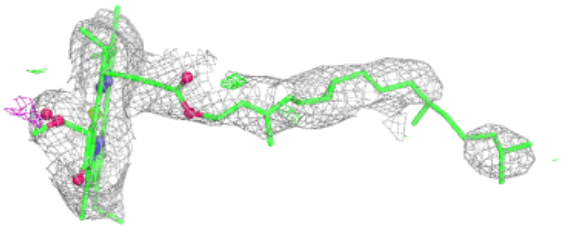


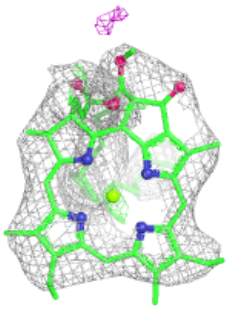


Electron density around CLA A 1105:

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

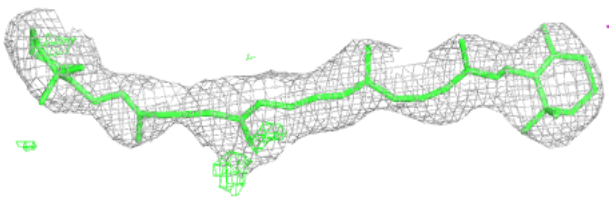


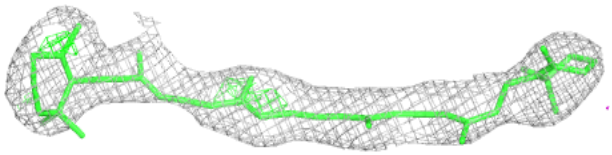


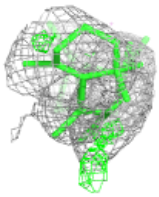


Electron density around BCR J 4013:

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

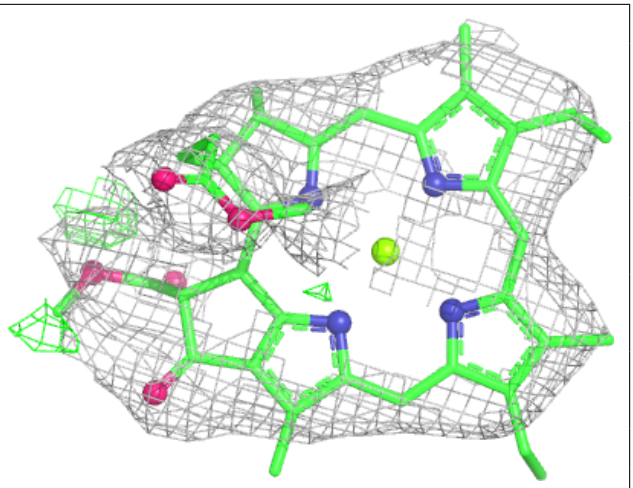


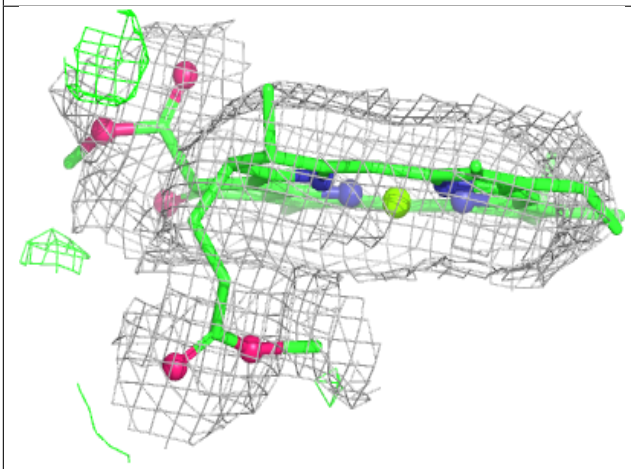


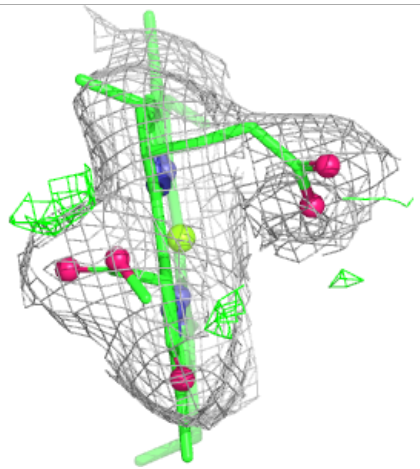


Electron density around CLA A 1134:

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

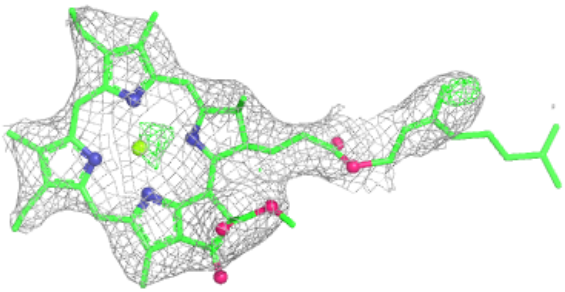


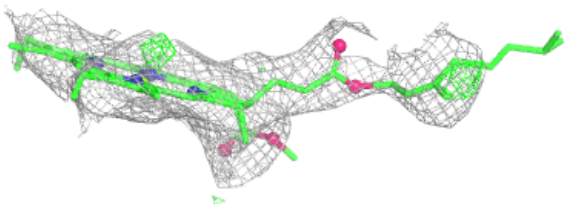


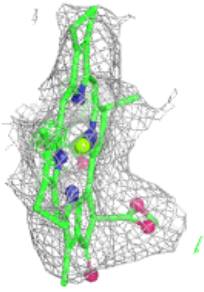


Electron density around CLA A 1135:

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

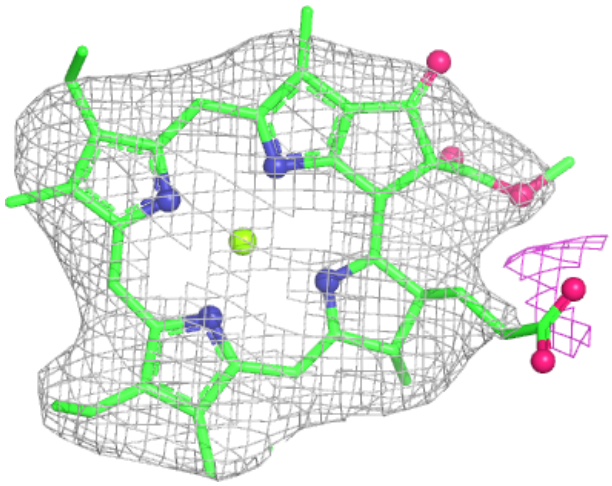


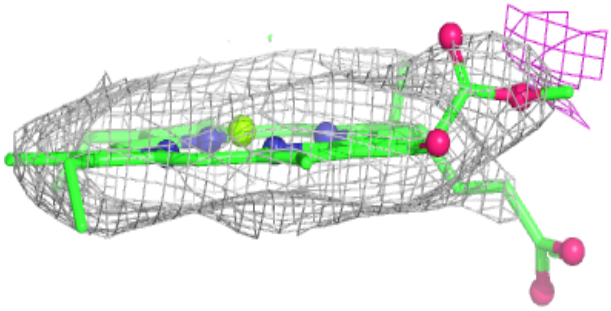


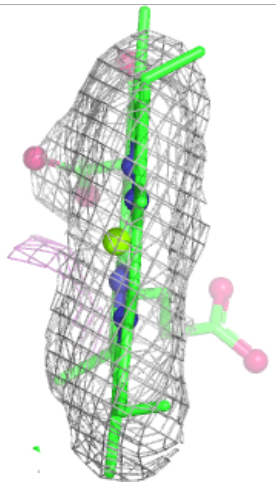


Electron density around CLA B 1240:

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

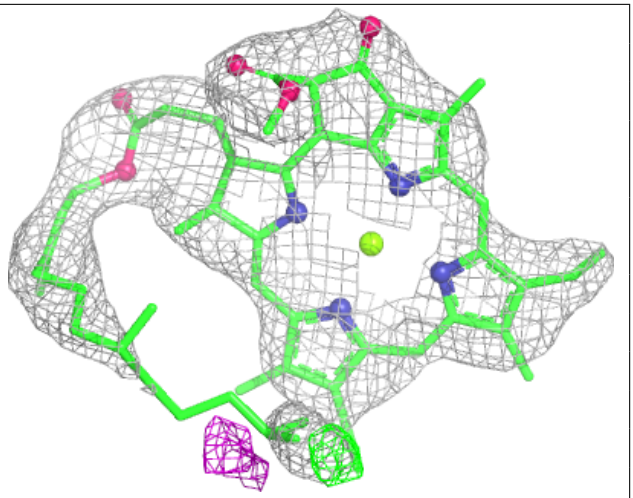


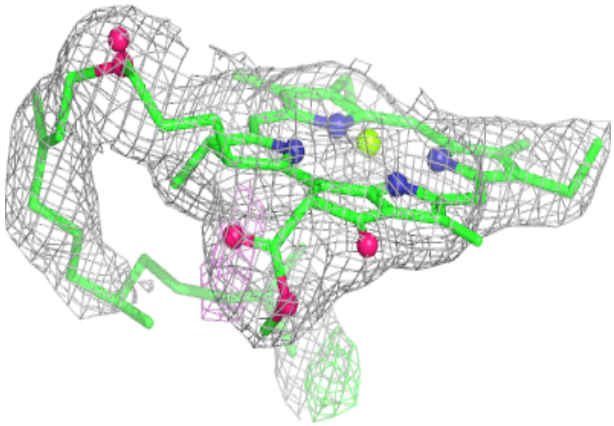


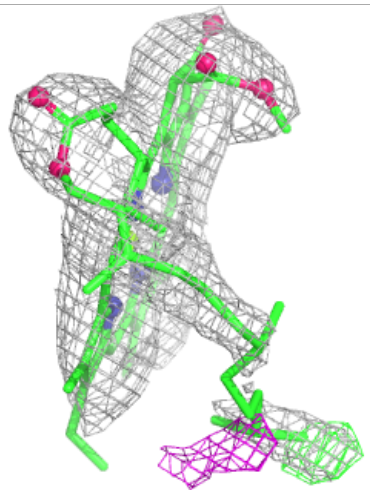


Electron density around CLA A 1111:

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

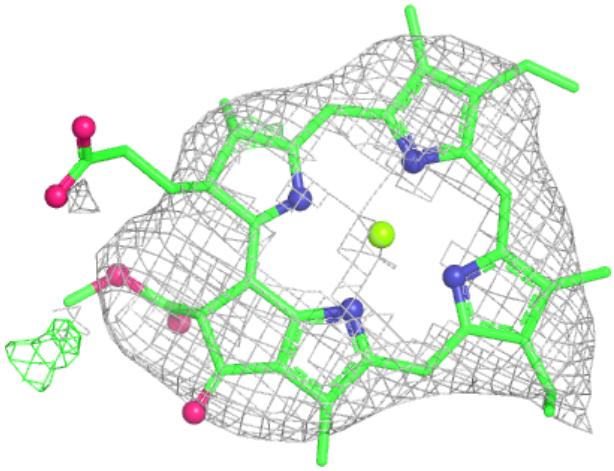


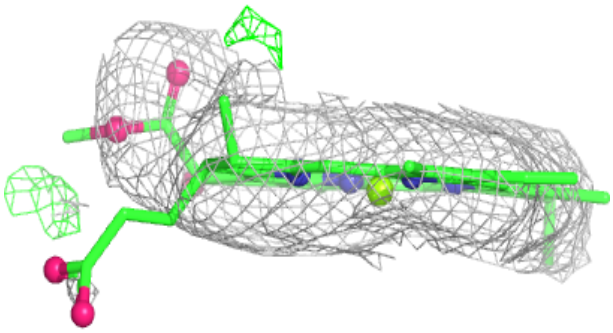


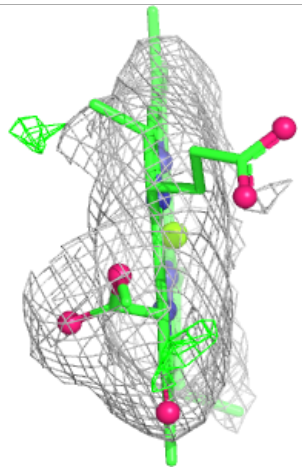


Electron density around CLA A 1113:

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

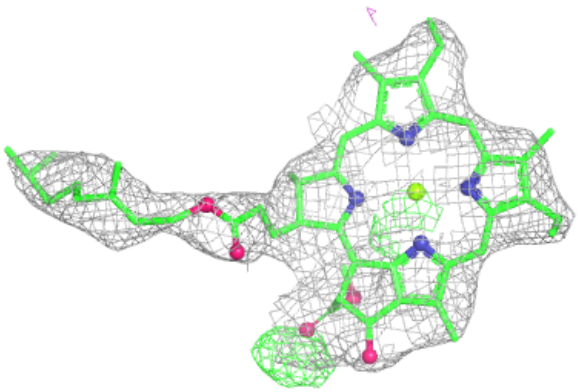


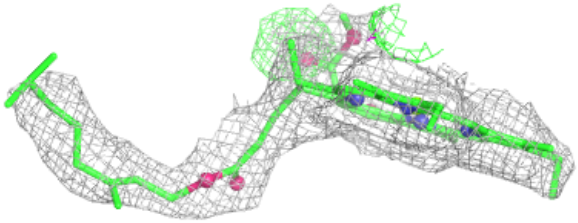


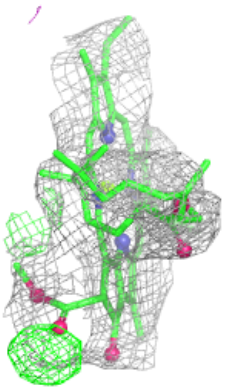


Electron density around CLA A 1124:

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

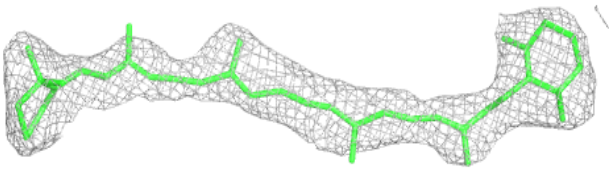


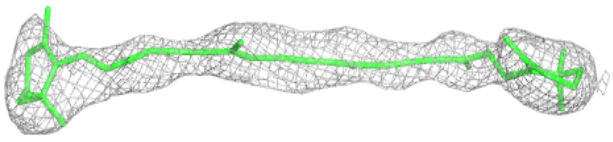


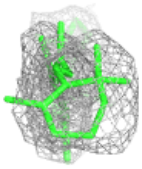


Electron density around BCR B 4005:

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

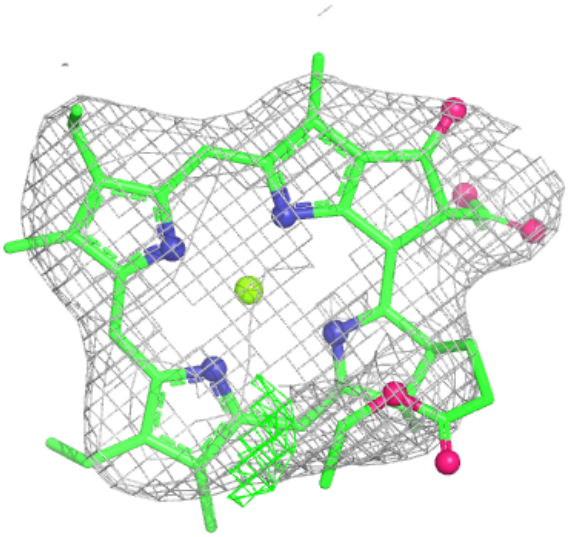


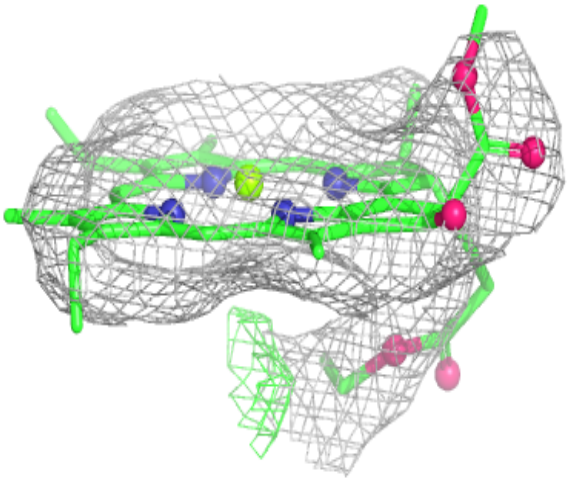


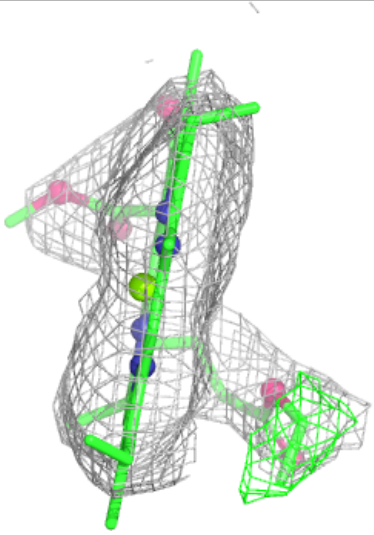


Electron density around CLA B 1217:

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

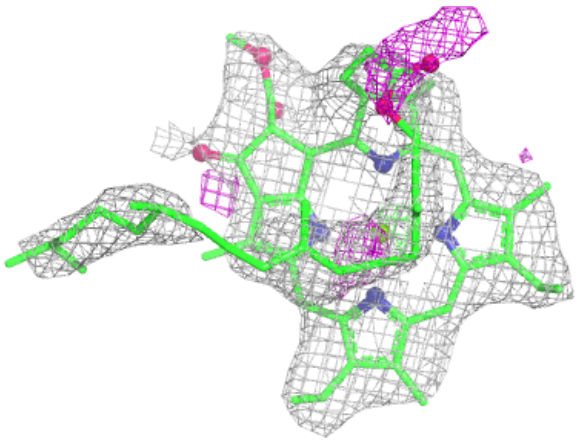


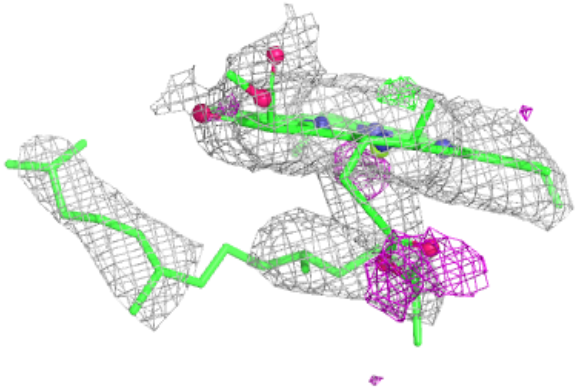


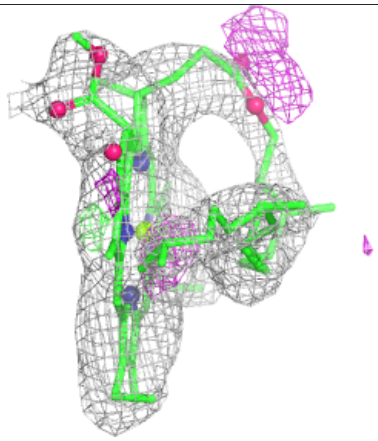


Electron density around CLA B 1224:

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

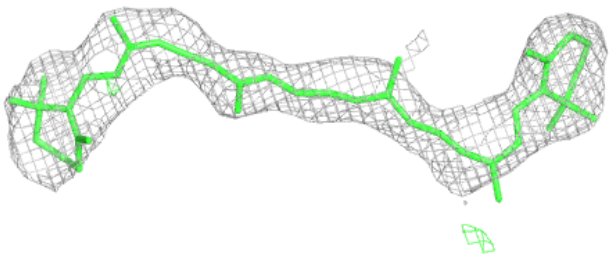


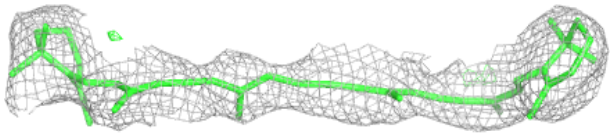


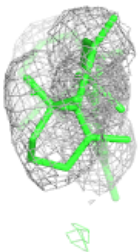


Electron density around BCR B 4006:

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

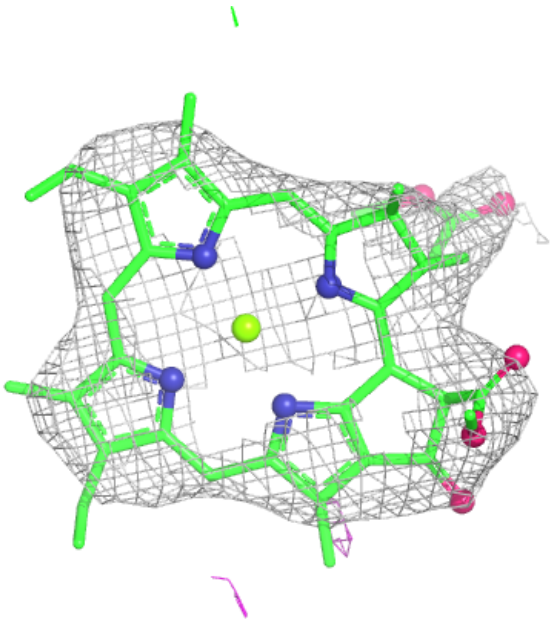


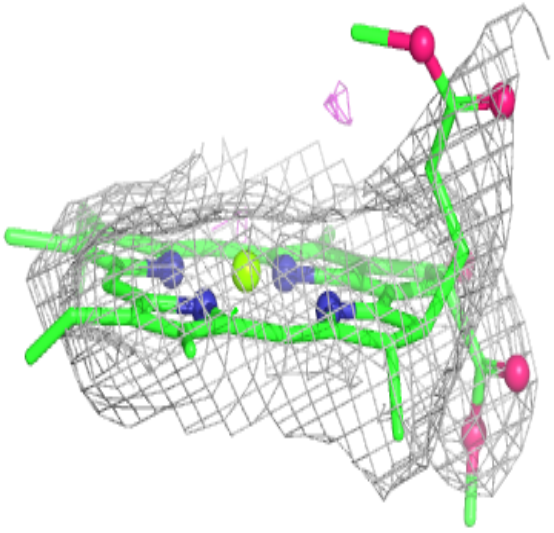


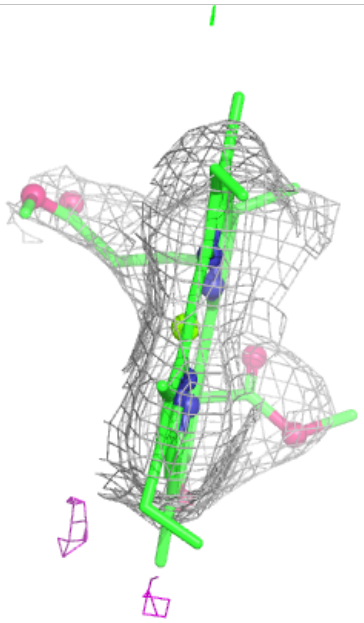


Electron density around CLA A 1118:

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

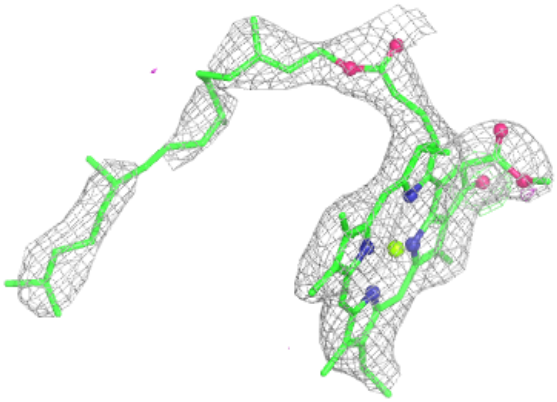


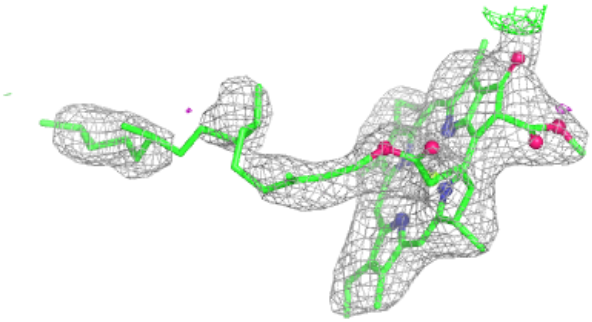


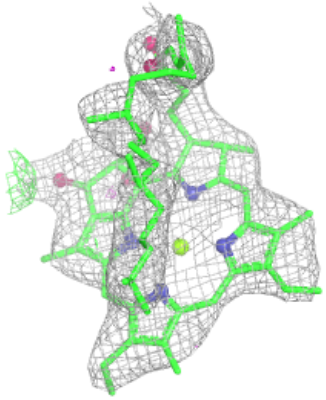


Electron density around CLA A 1102:

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

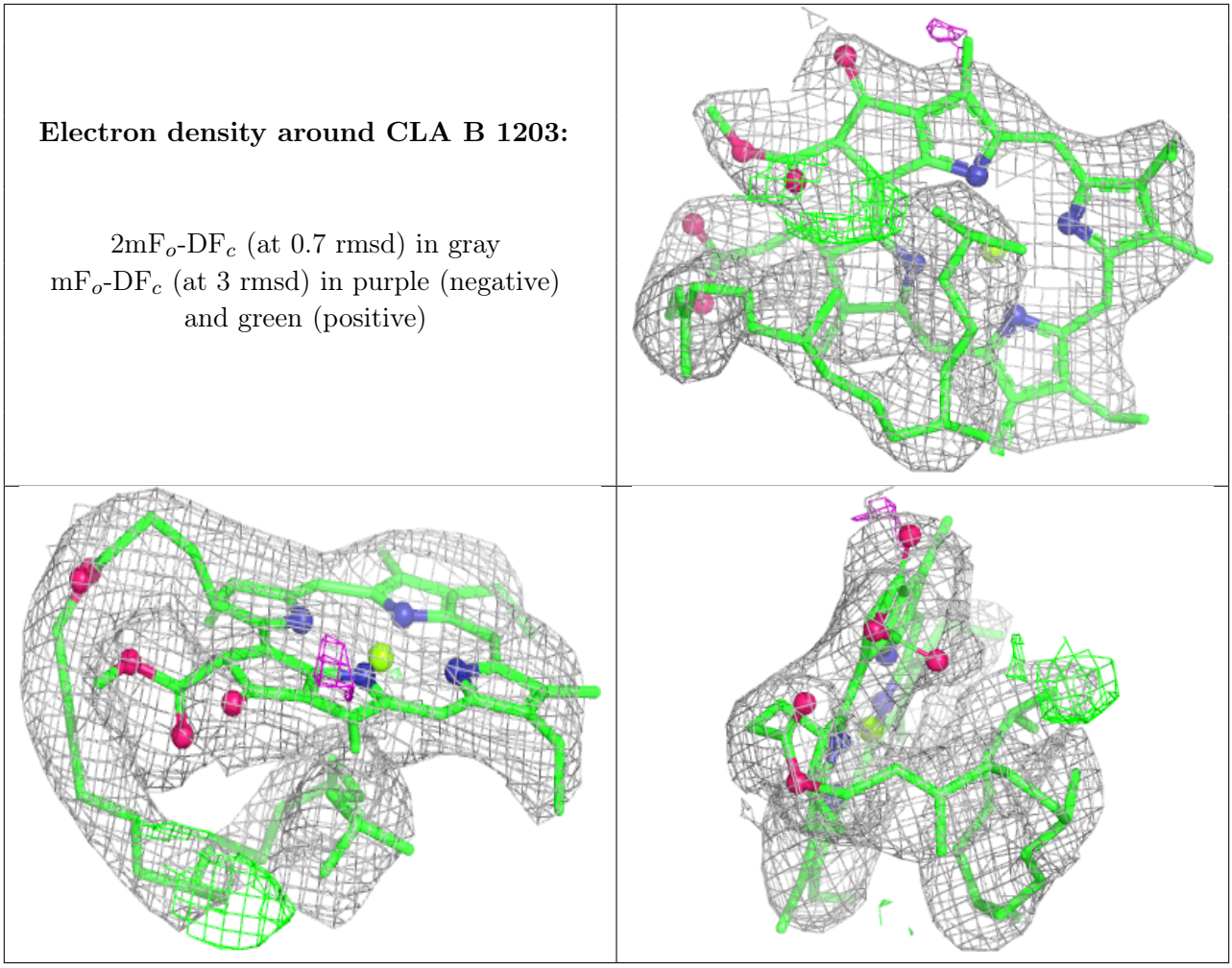






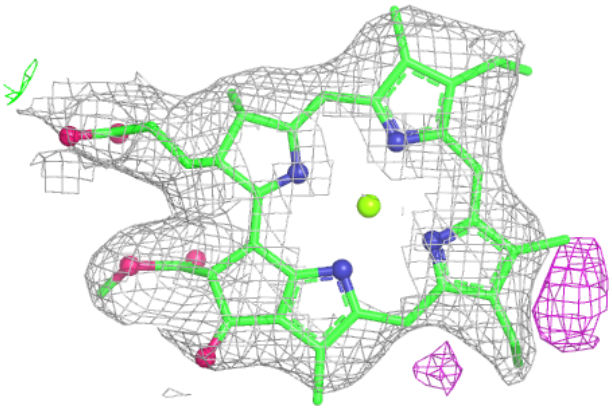
Electron density around CLA B 1203:

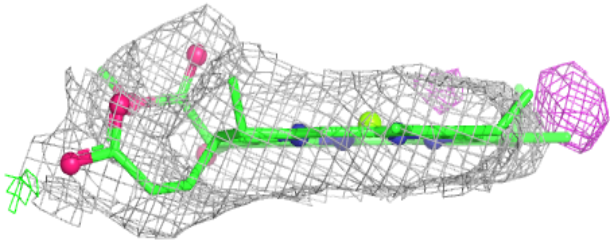
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

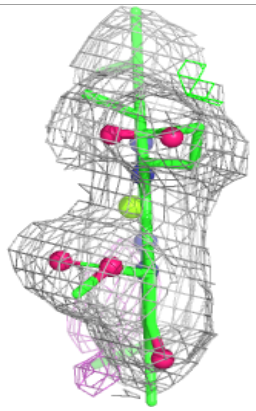


Electron density around CLA F 1301:

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

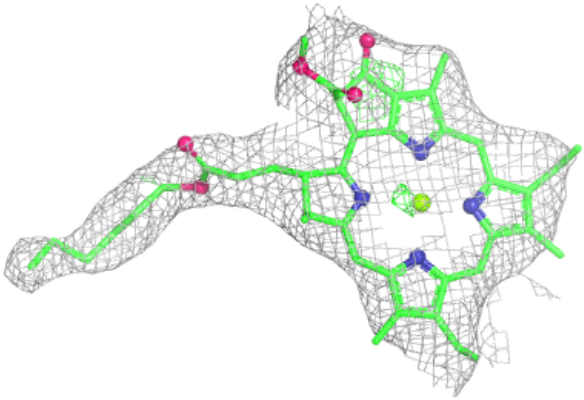


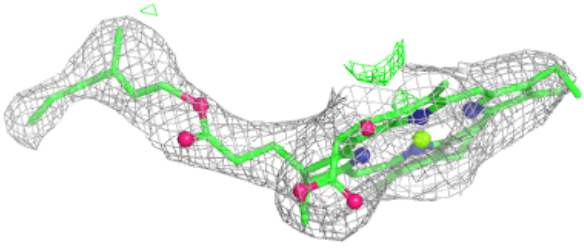




Electron density around CLA A 1125:

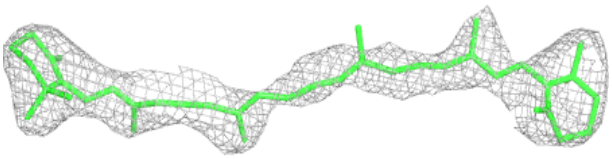
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

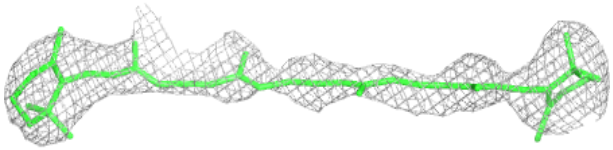


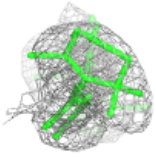


Electron density around BCR A 4002:

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

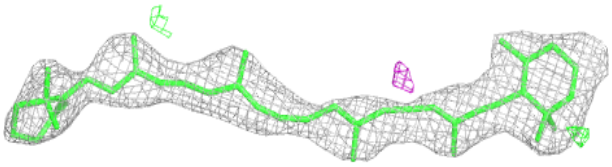


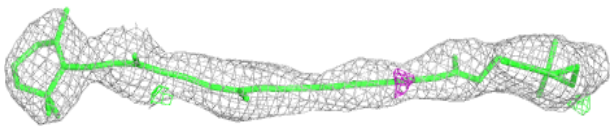


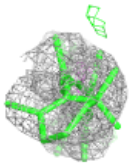


Electron density around BCR F 4015:

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

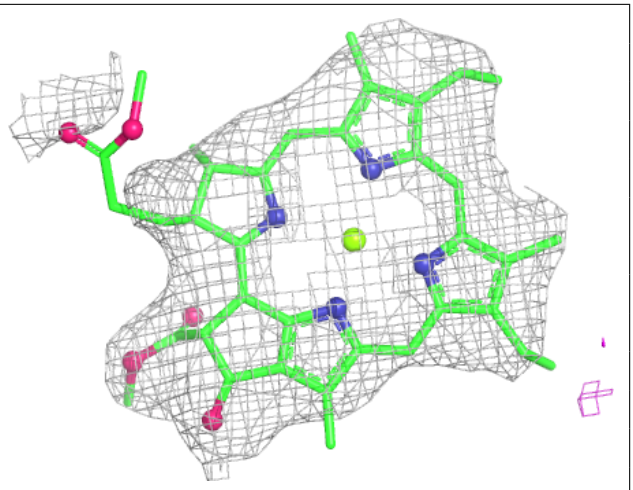


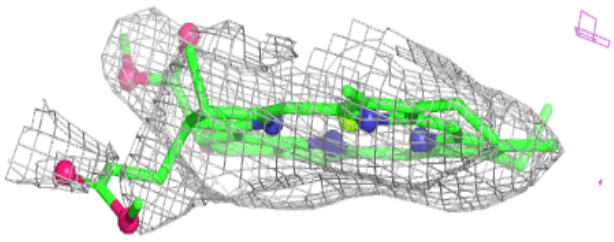


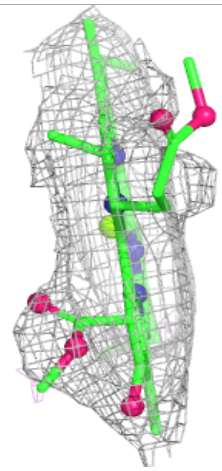


Electron density around CLA A 1121:

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

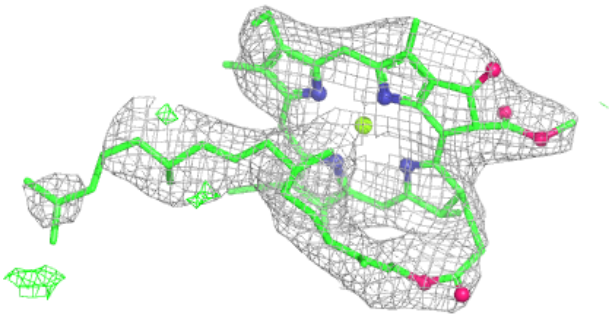


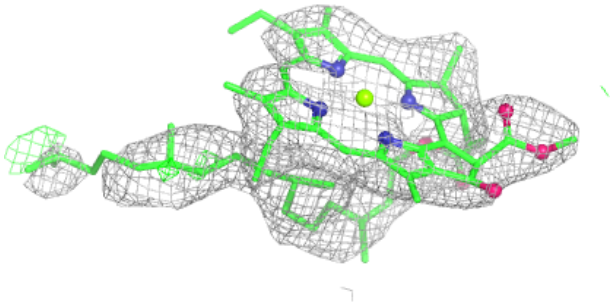


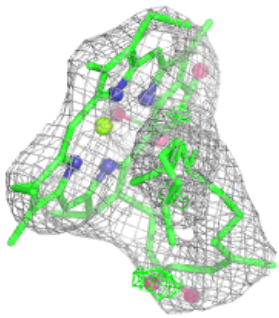


Electron density around CLA B 1214:

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

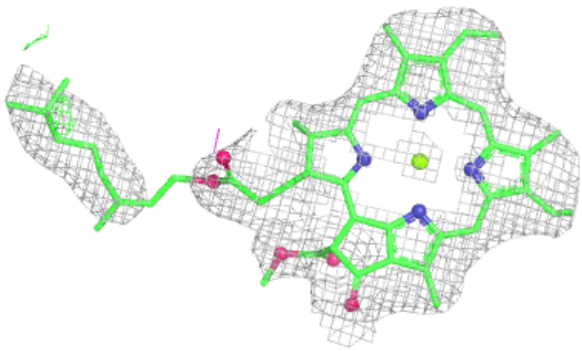


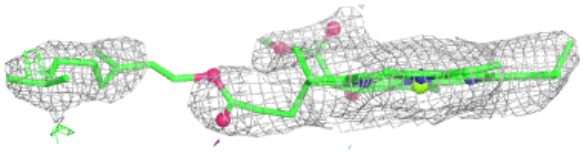


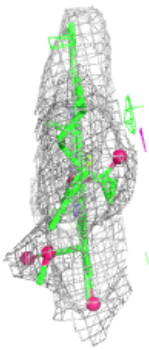


Electron density around CLA A 1131:

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

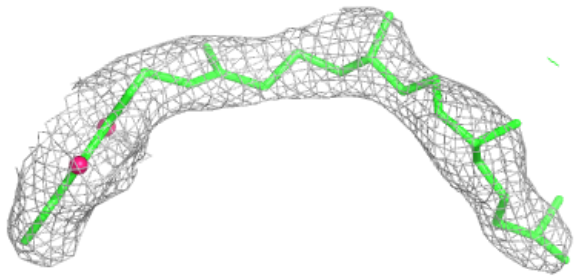


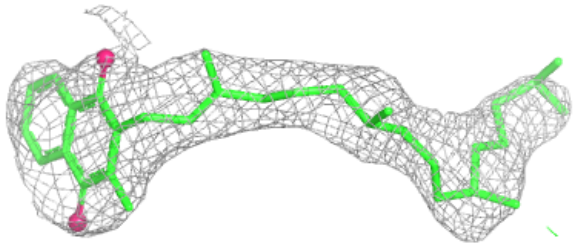


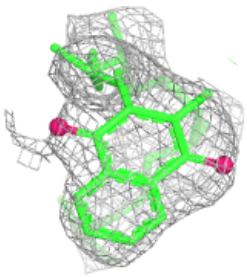


Electron density around PQN B 2002:

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

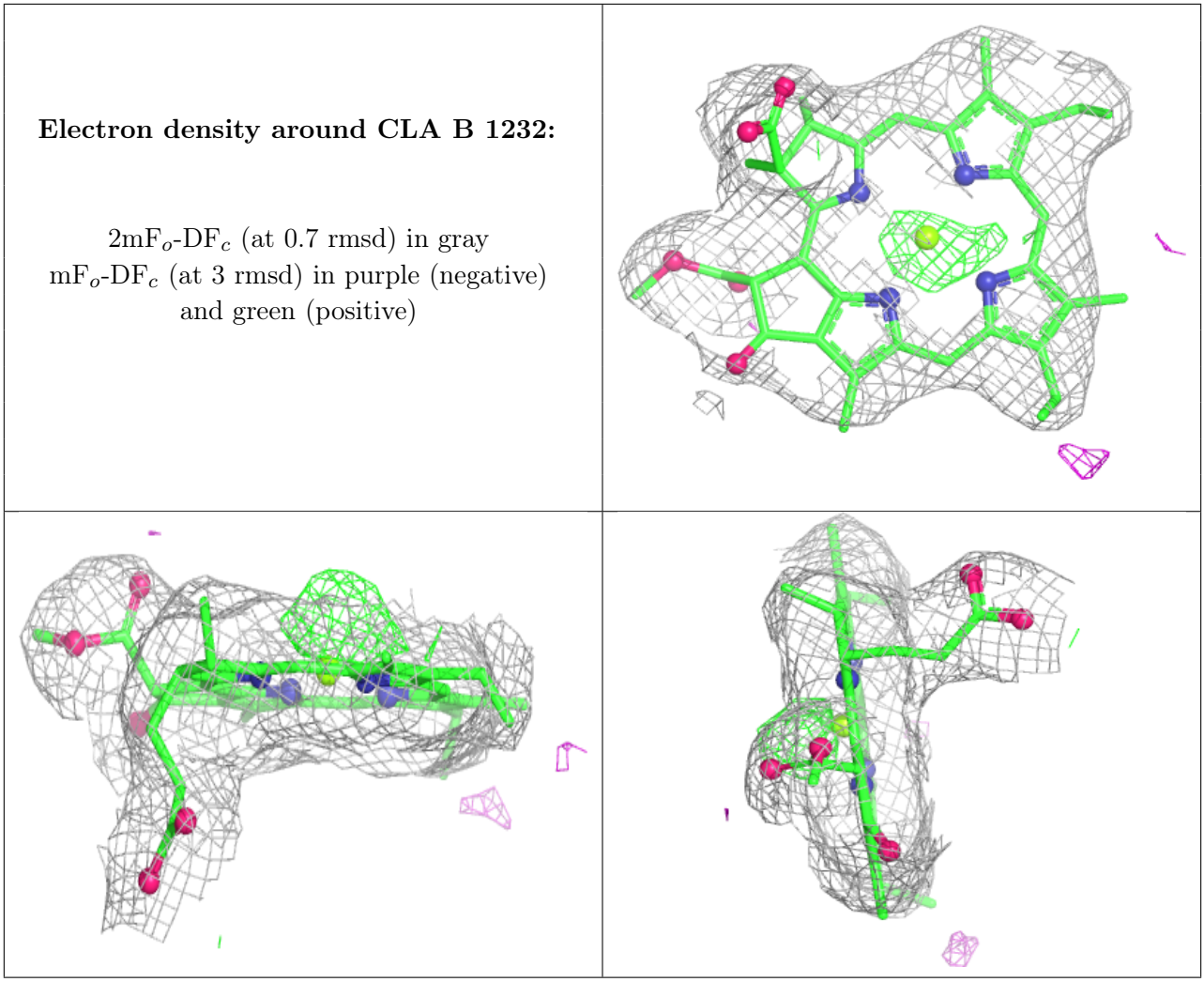






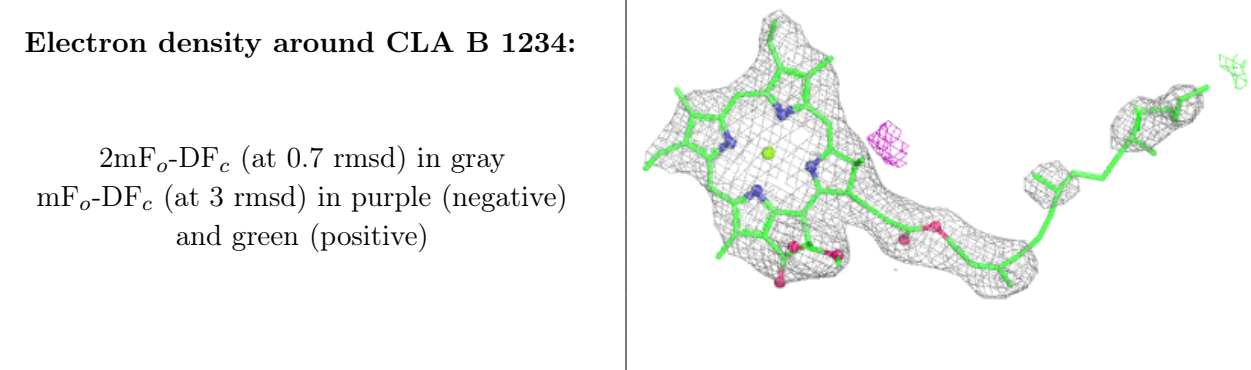
Electron density around CLA B 1232:

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



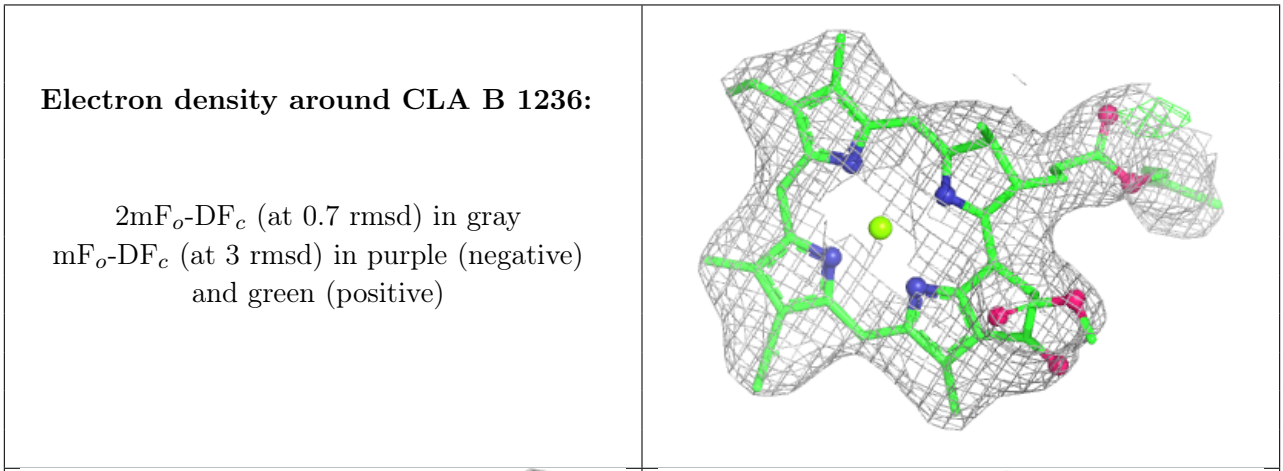
Electron density around CLA B 1234:

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



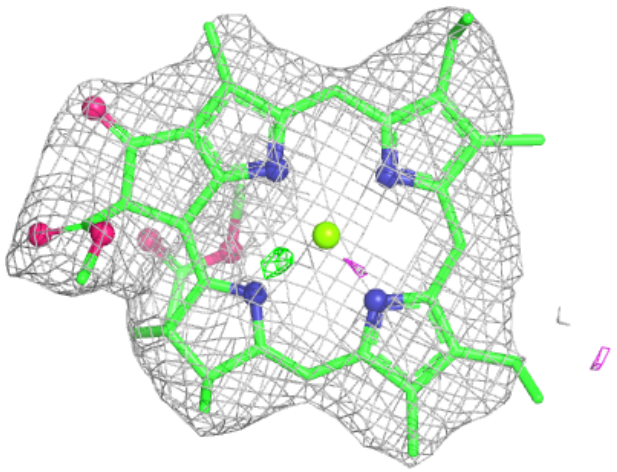
Electron density around CLA B 1236:

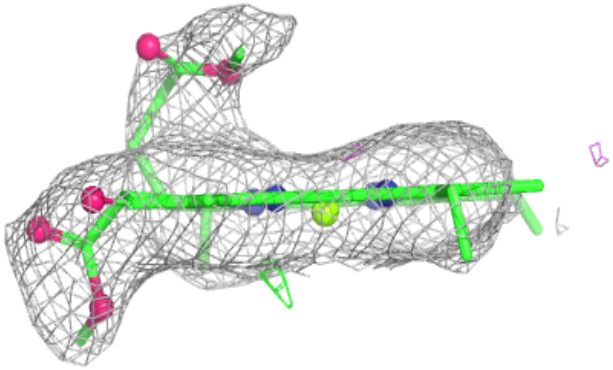
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

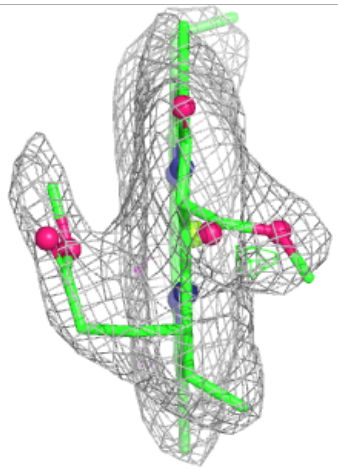


Electron density around CLA B 1201:

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

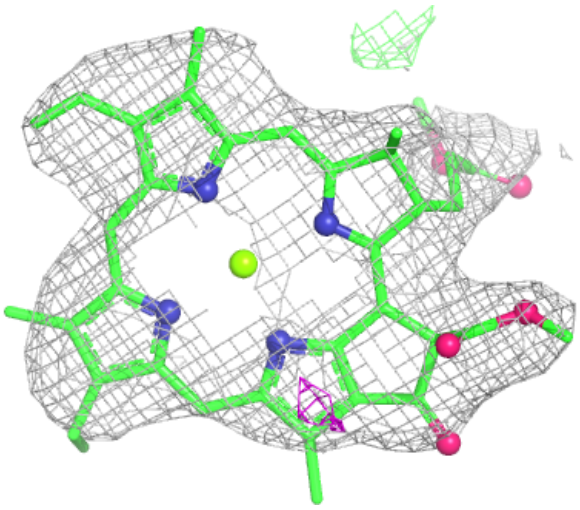


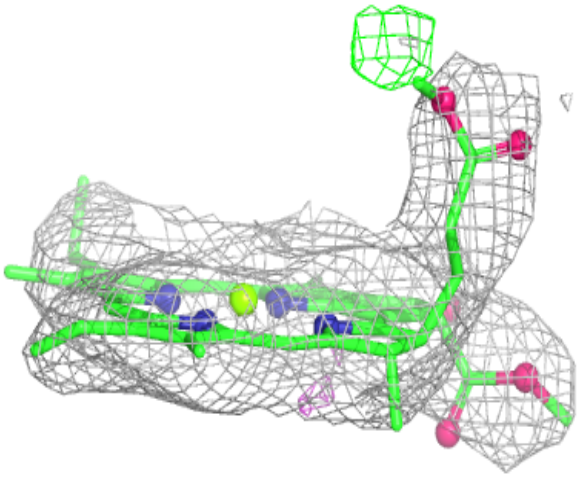


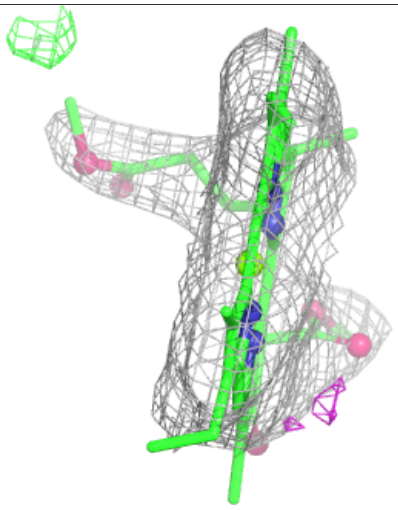


Electron density around CLA A 1133:

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

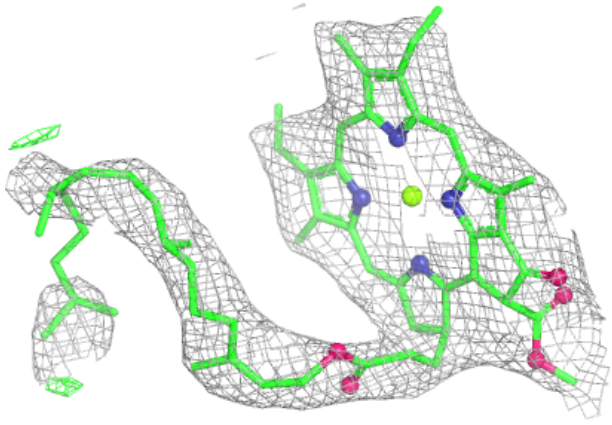


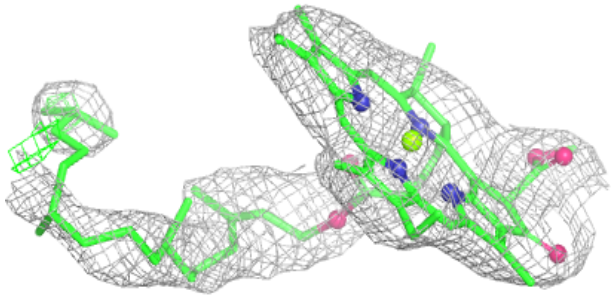


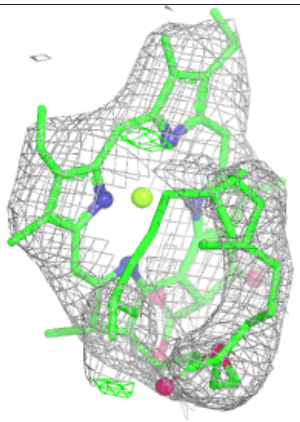


Electron density around CLA A 1122:

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

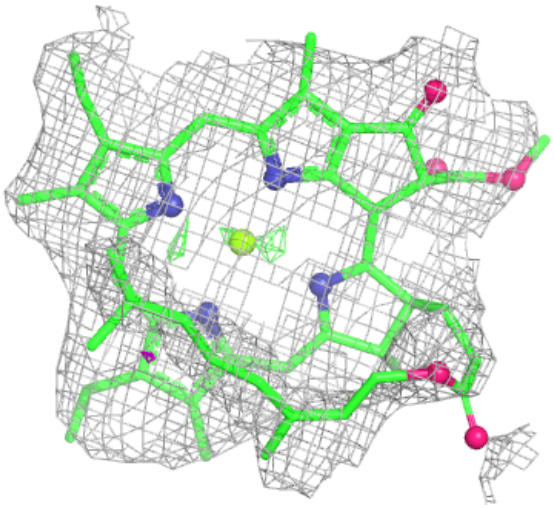


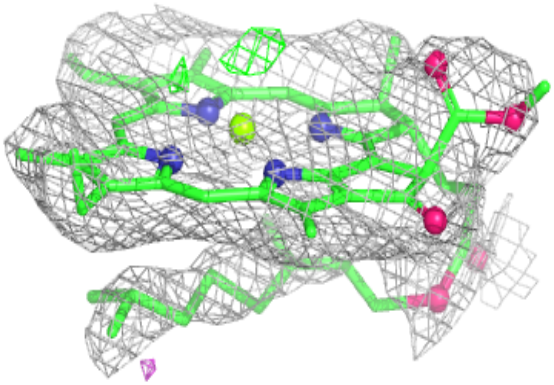


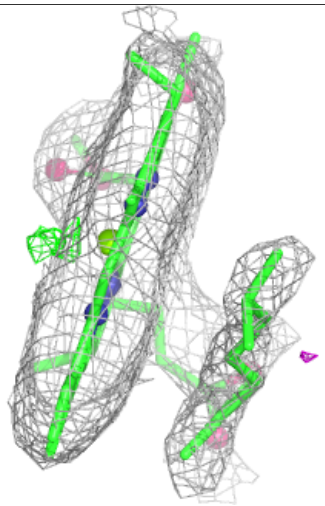


Electron density around CLA B 1219:

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

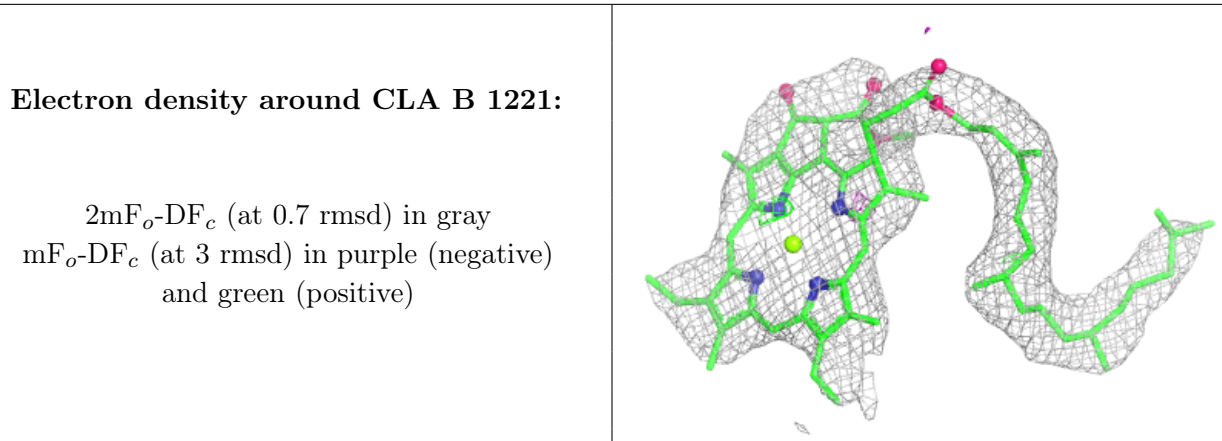






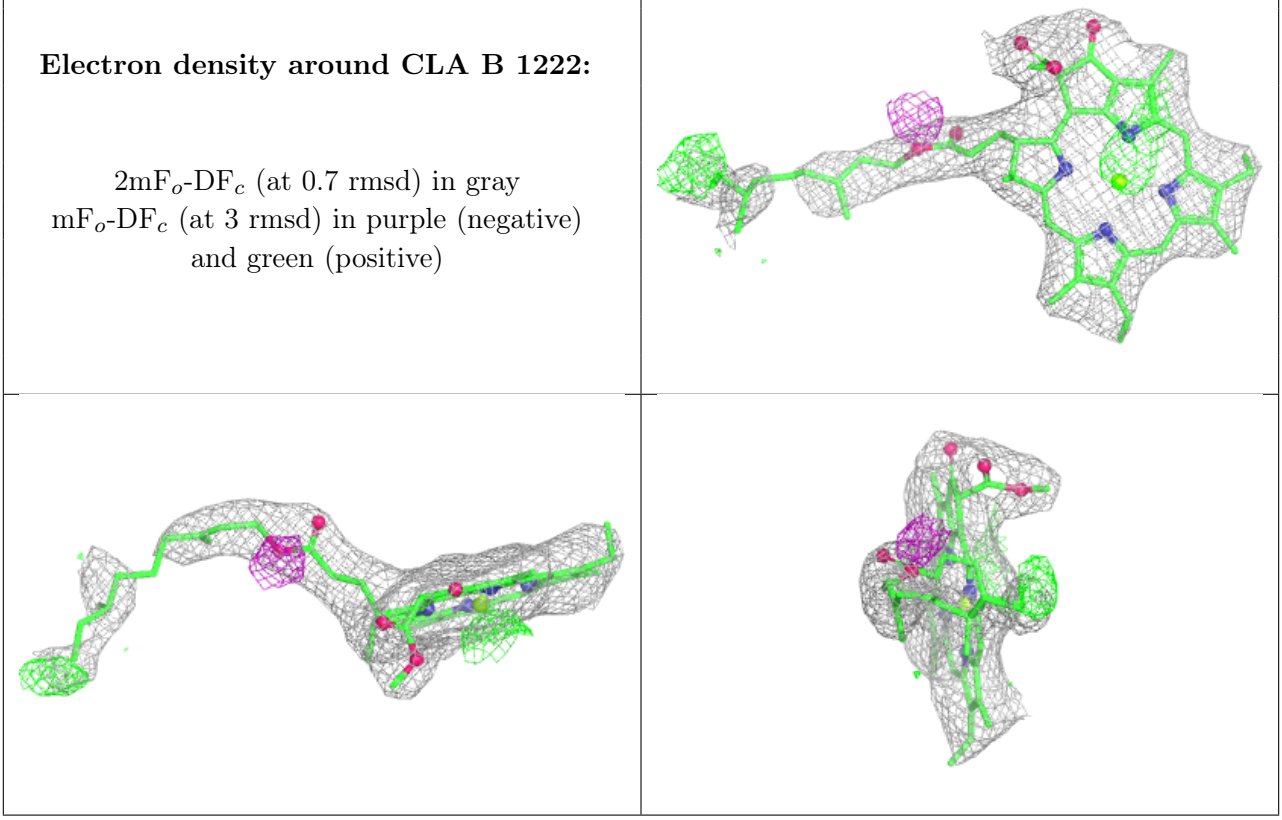
Electron density around CLA B 1221:

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



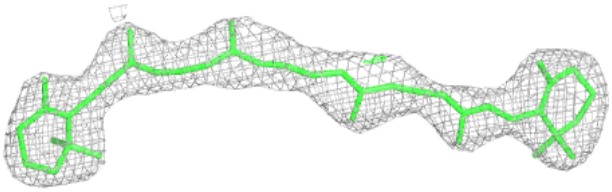
Electron density around CLA B 1222:

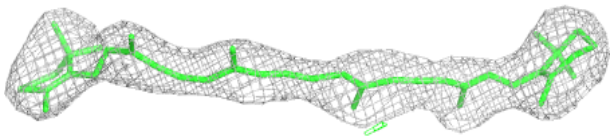
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

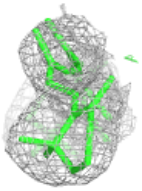


Electron density around BCR B 4010:

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

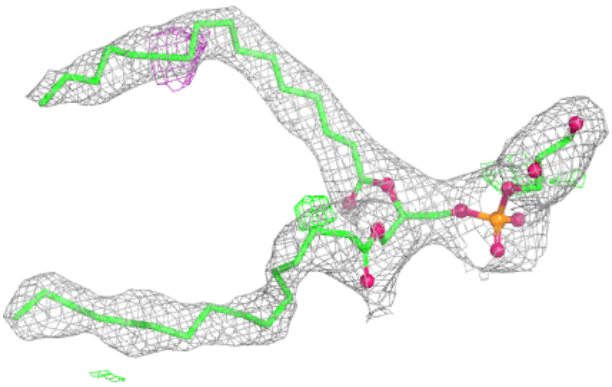


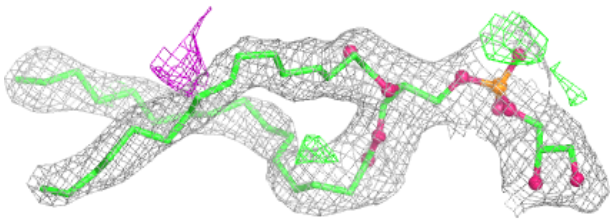


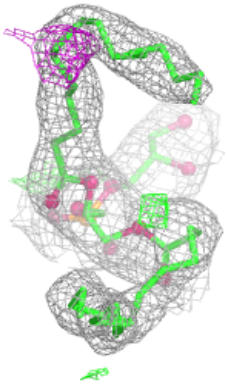


Electron density around LHG A 5001:

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

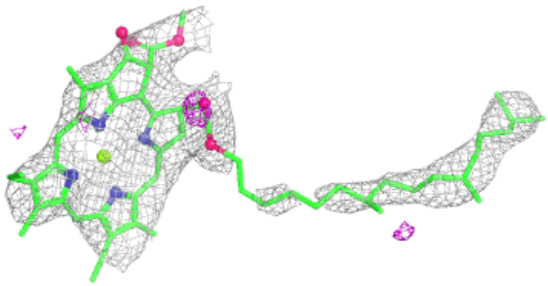


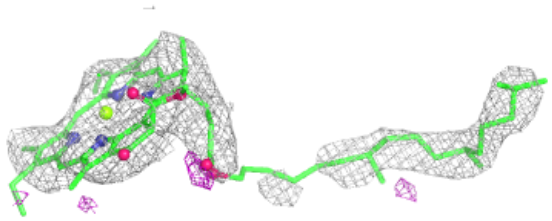


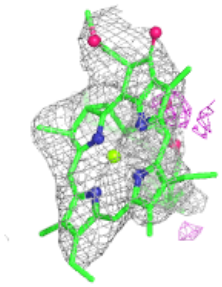


Electron density around CLA A 1119:

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

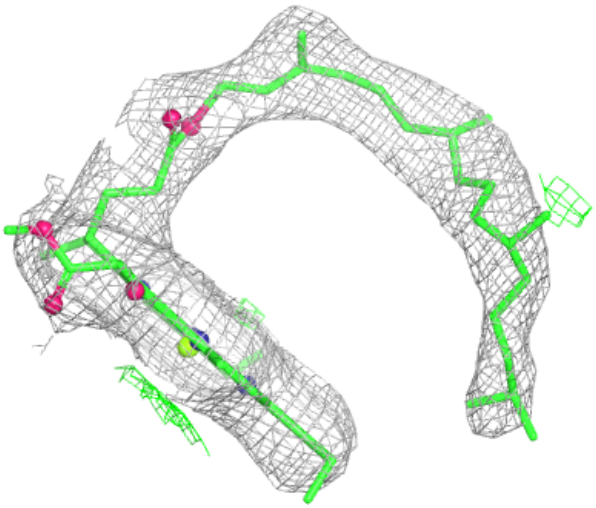


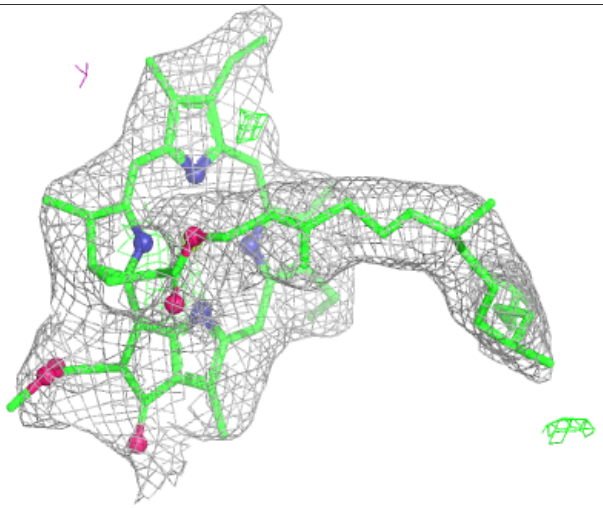


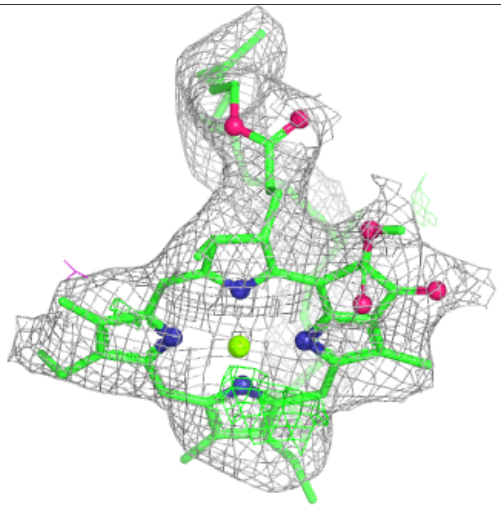


Electron density around CLA B 1216:

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

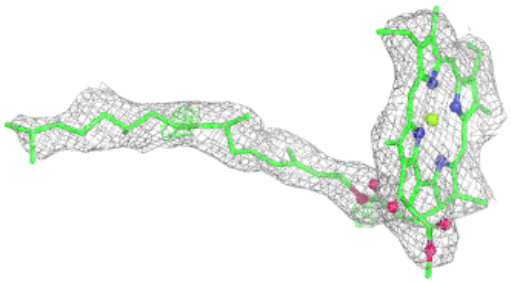


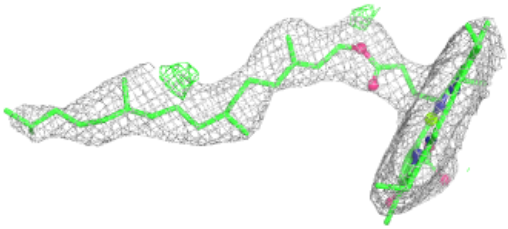


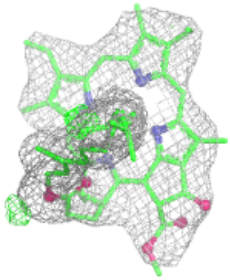


Electron density around CLA B 1225:

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

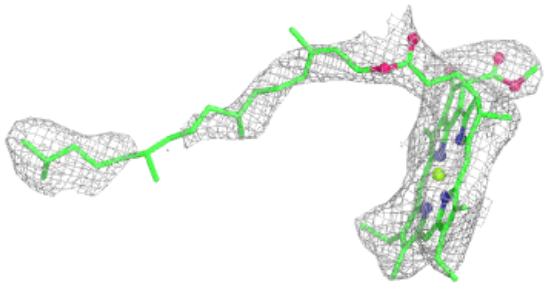


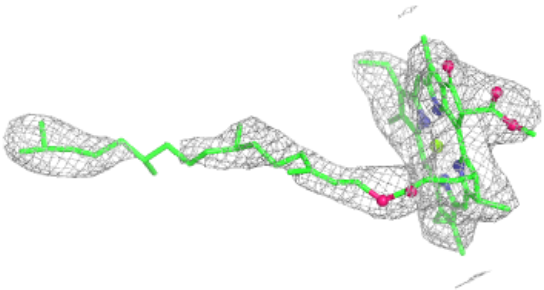


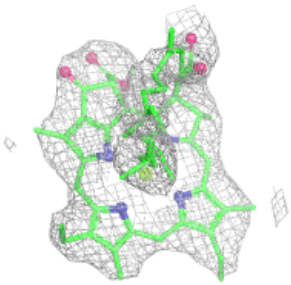


Electron density around CLA B 1226:

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

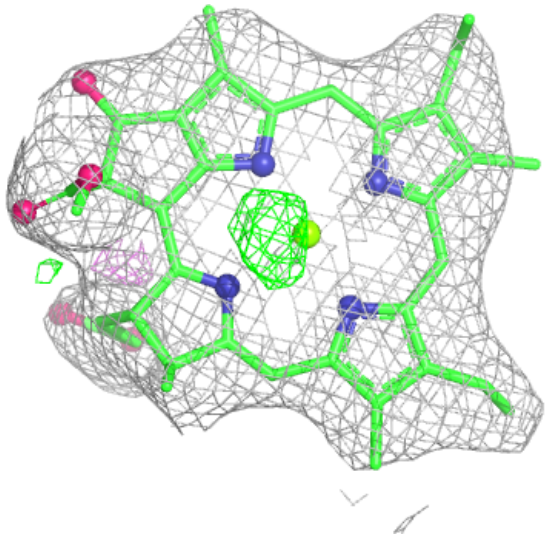


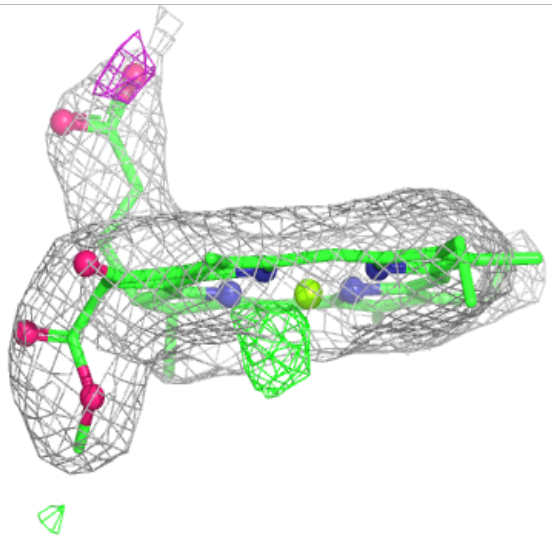


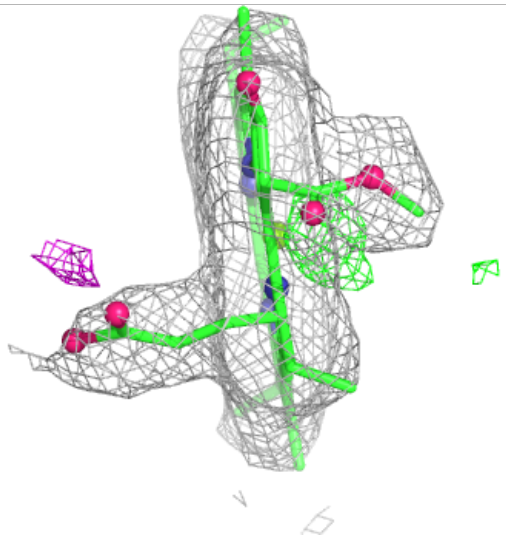


Electron density around CLA B 1227:

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

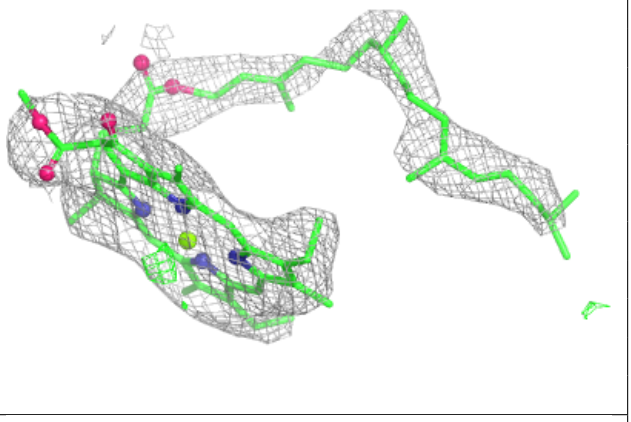


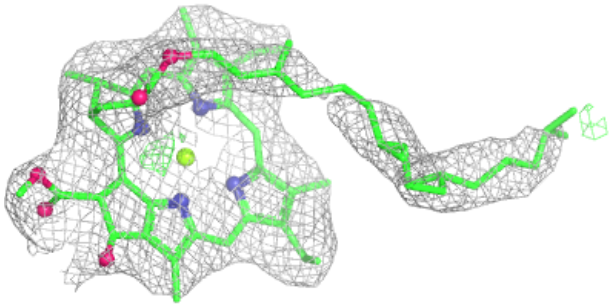


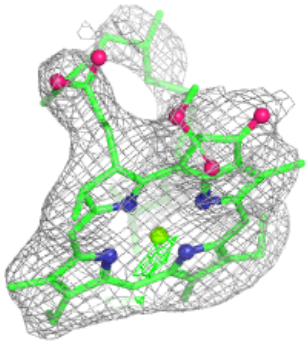


Electron density around CLA A 1109:

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

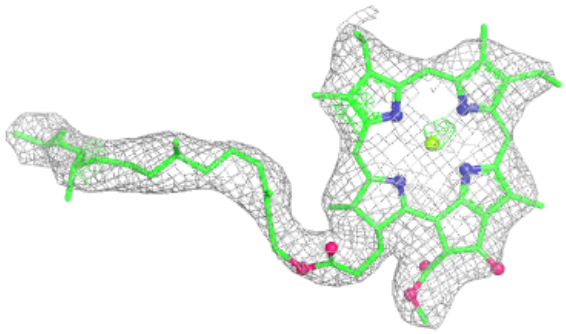


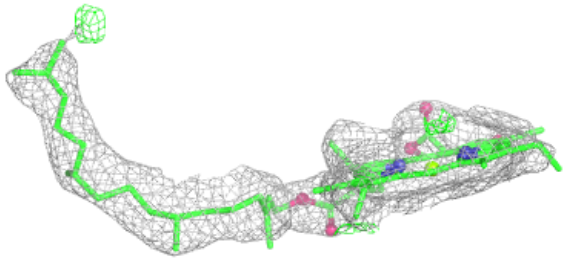


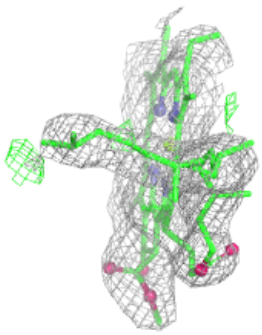


Electron density around CLA B 1023:

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

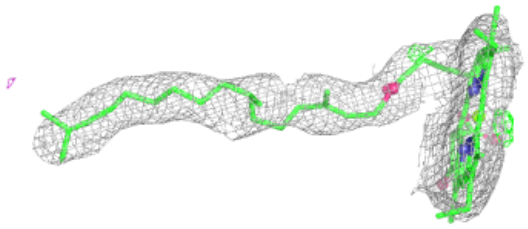


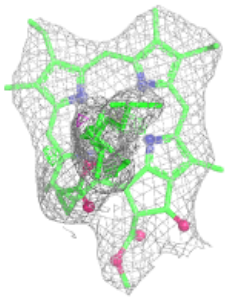




Electron density around CLA A 1126:

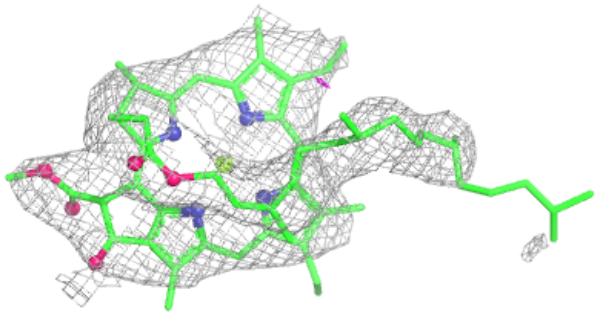
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

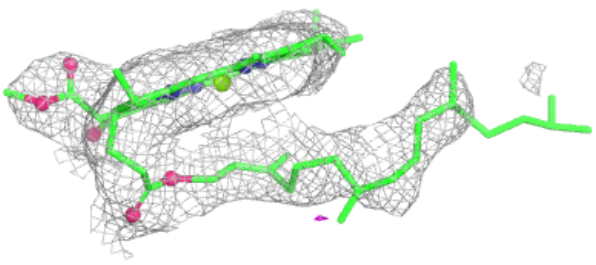


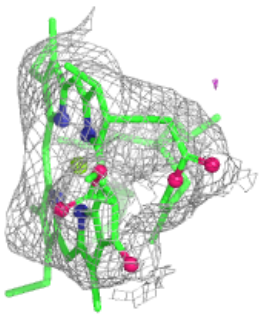


Electron density around CLA A 1136:

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

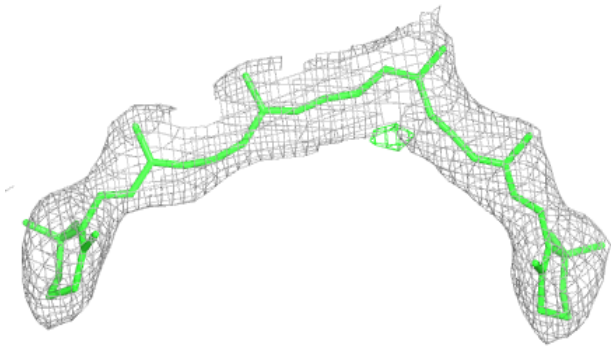


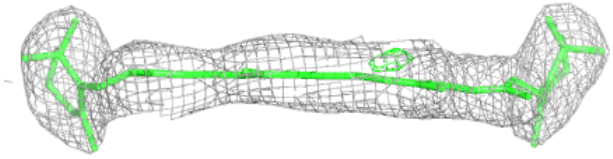


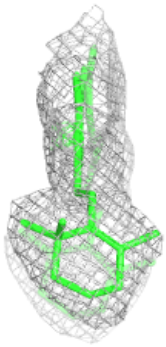


Electron density around BCR F 4016:

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

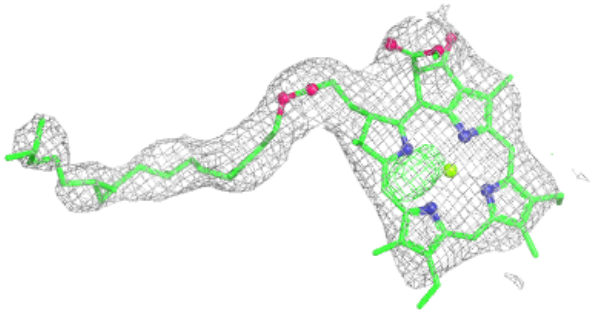


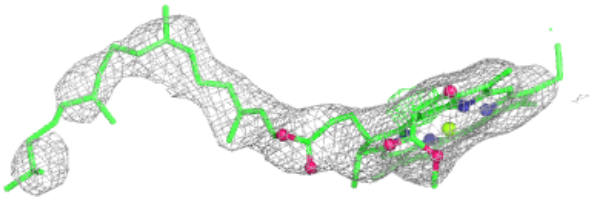




Electron density around CLA B 1210:

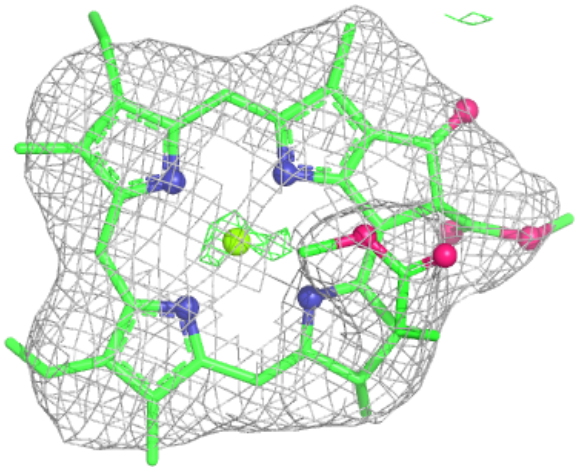
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

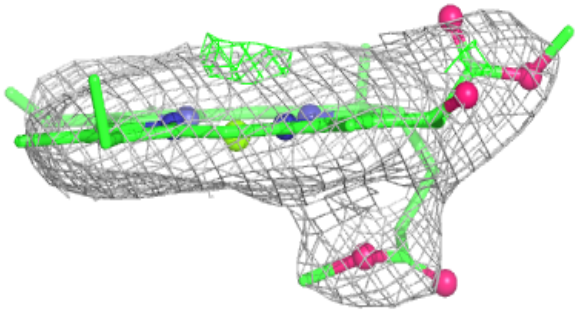


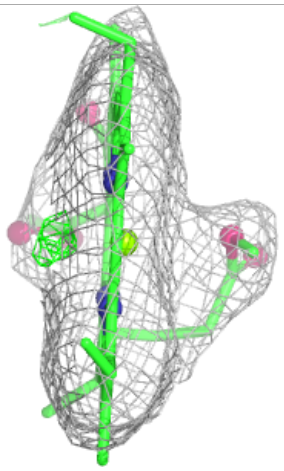


Electron density around CLA A 1115:

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

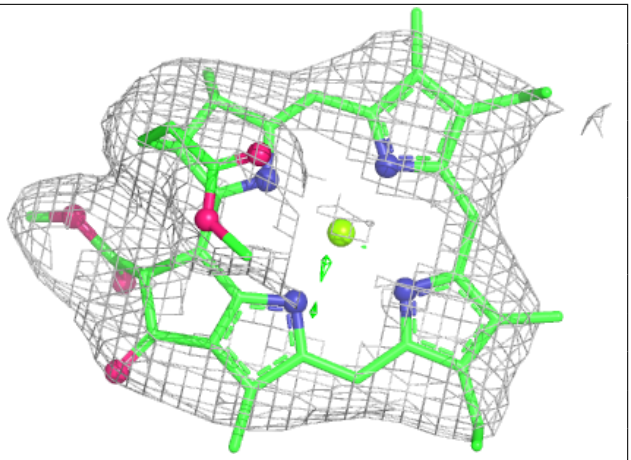


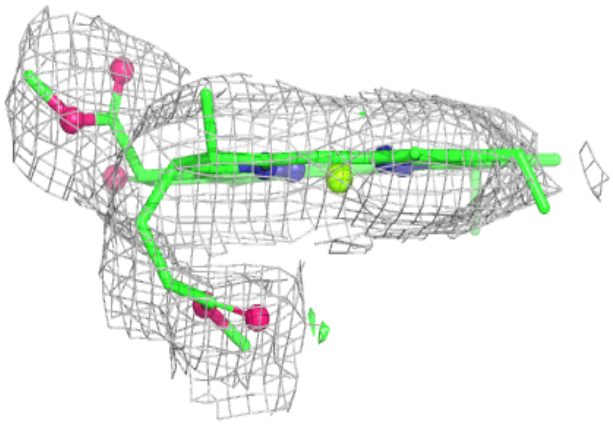


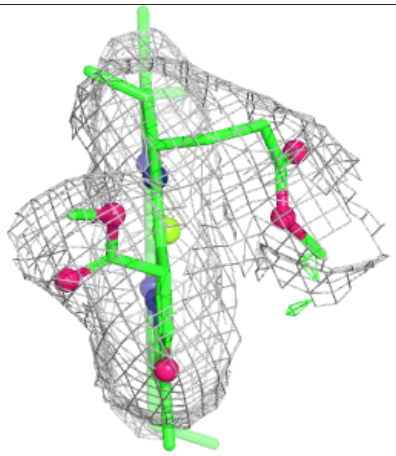


Electron density around CLA B 1204:

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

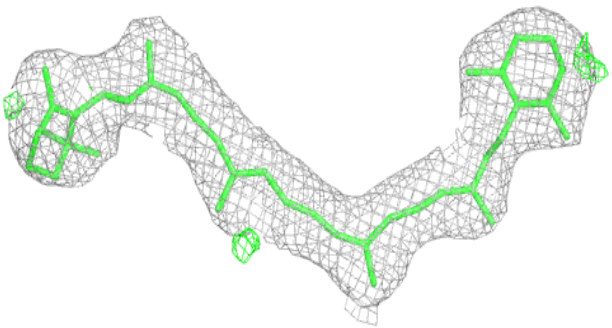


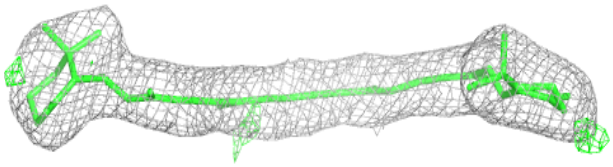


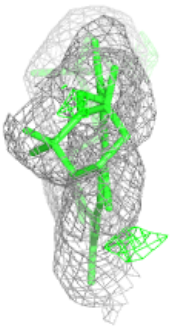


Electron density around BCR B 4011:

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

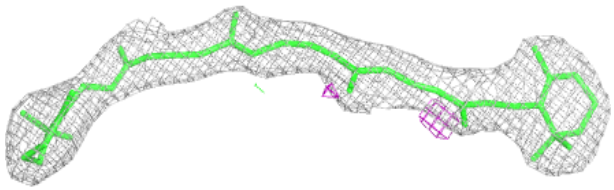


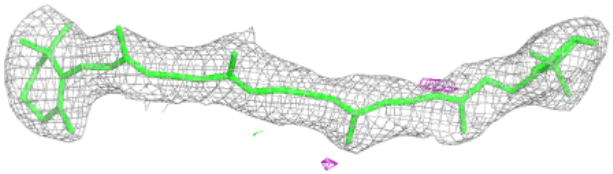


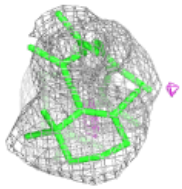


Electron density around BCR B 4014:

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

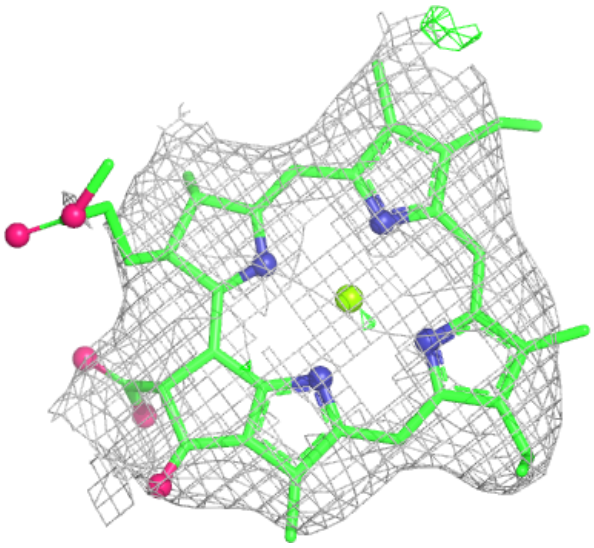


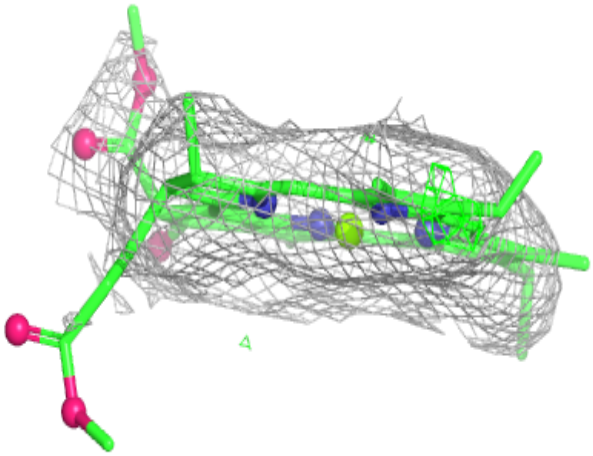


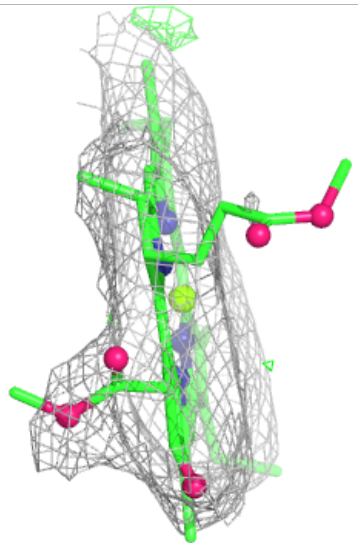


Electron density around CLA A 1129:

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

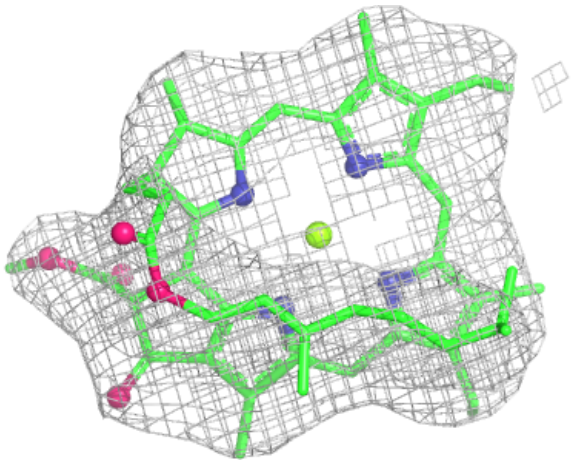


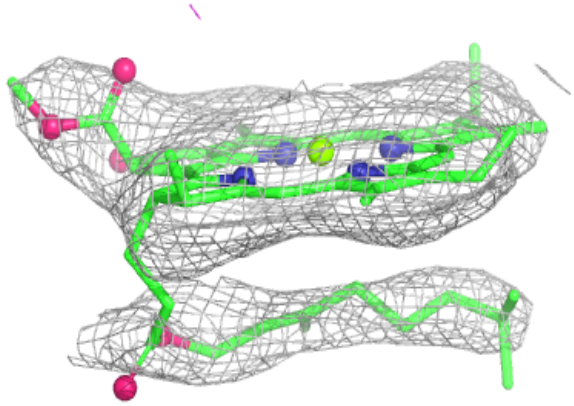


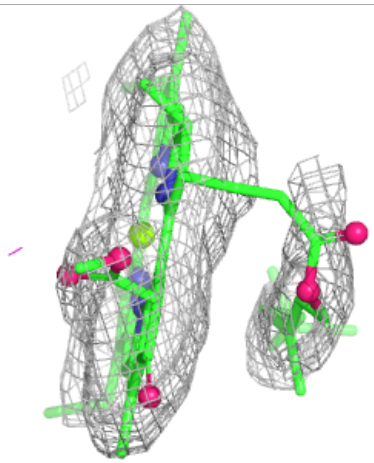


Electron density around CLA A 1130:

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

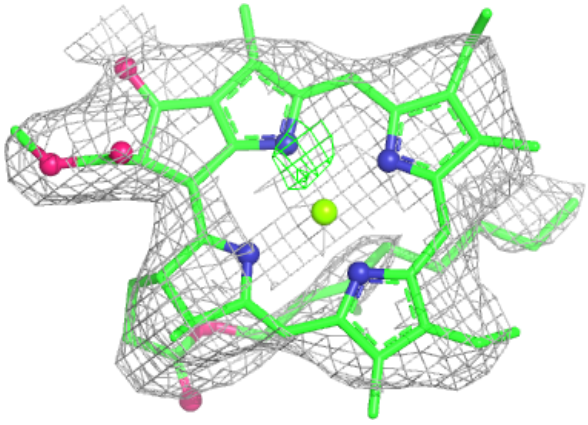


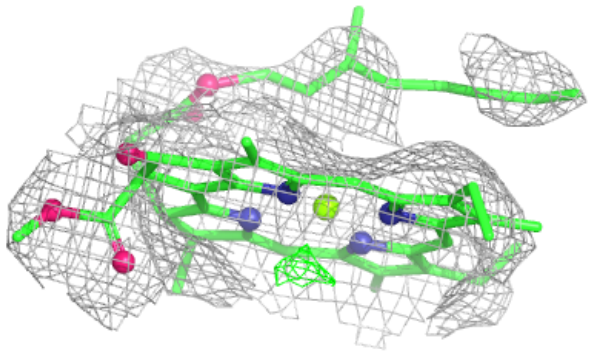


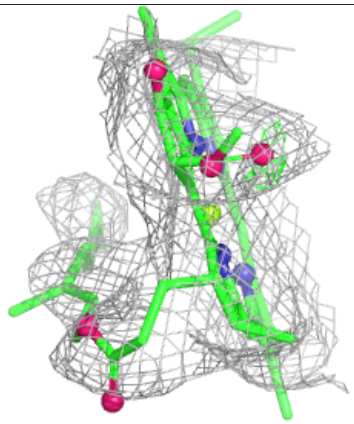


Electron density around CLA A 1116:

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

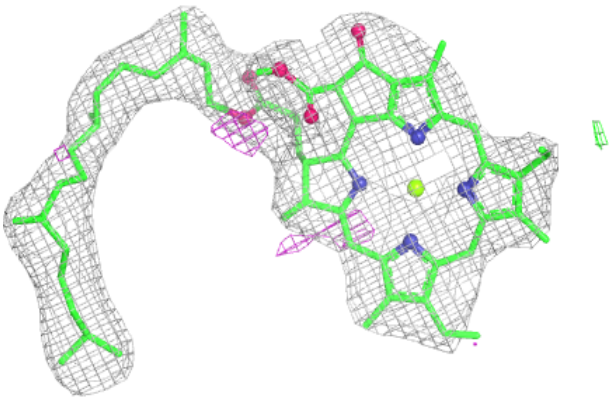


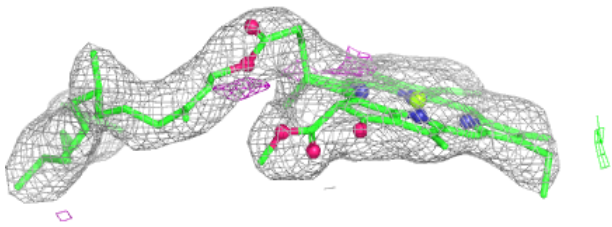




Electron density around CLA A 1101:

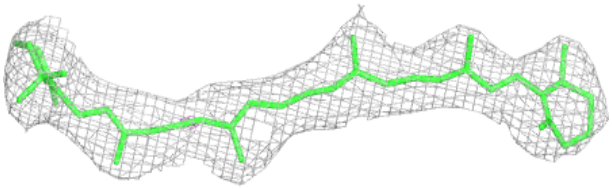
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

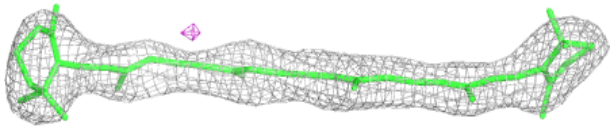


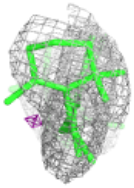


Electron density around BCR B 4017:

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

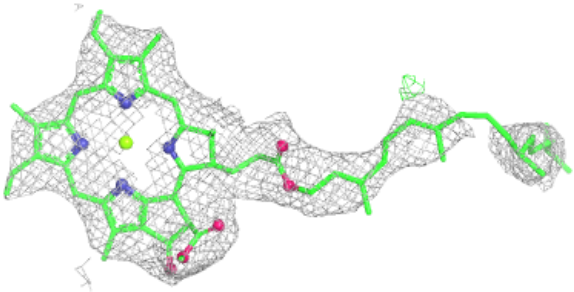


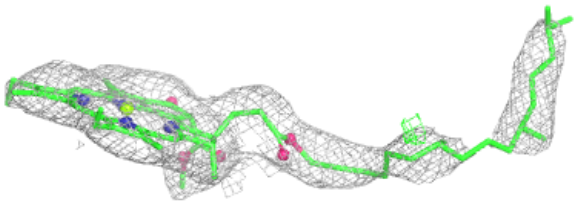


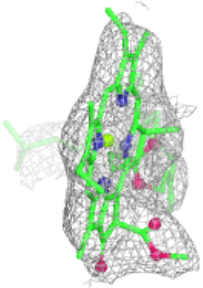


Electron density around CLA A 1103:

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

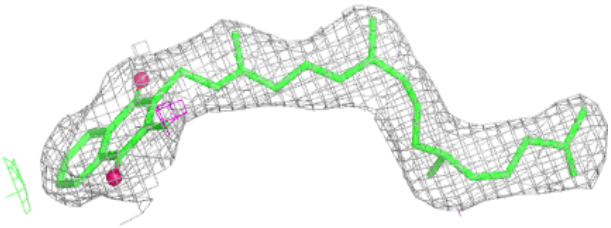


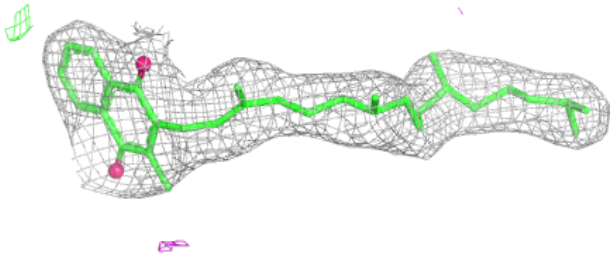


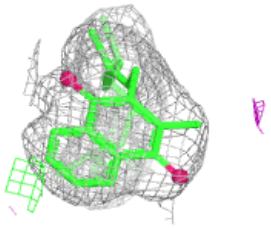


Electron density around PQN A 2001:

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

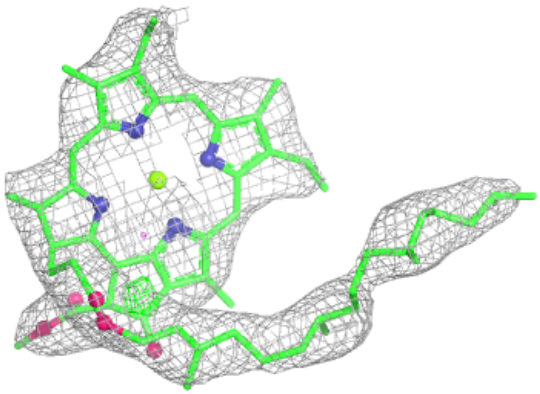


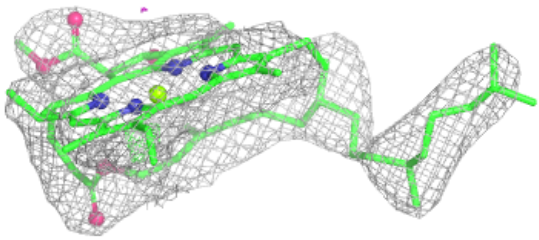


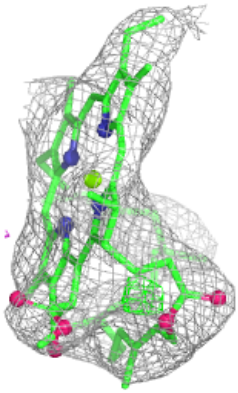


Electron density around CLA A 1127:

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

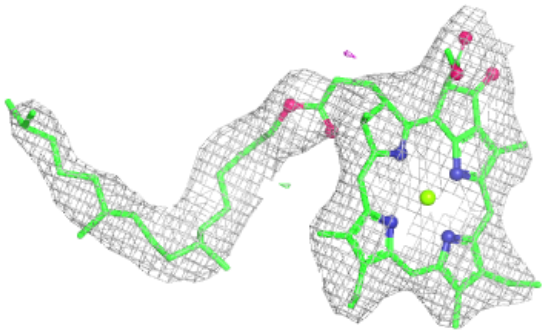


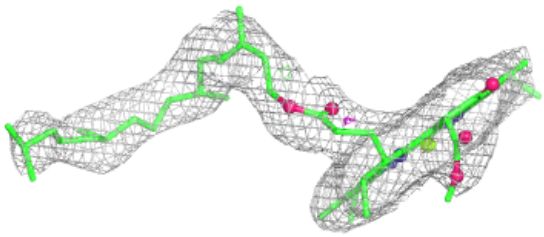


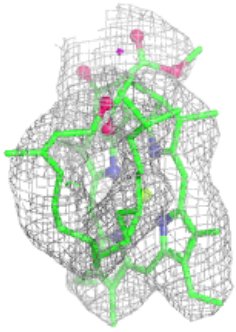


Electron density around CLA A 1106:

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

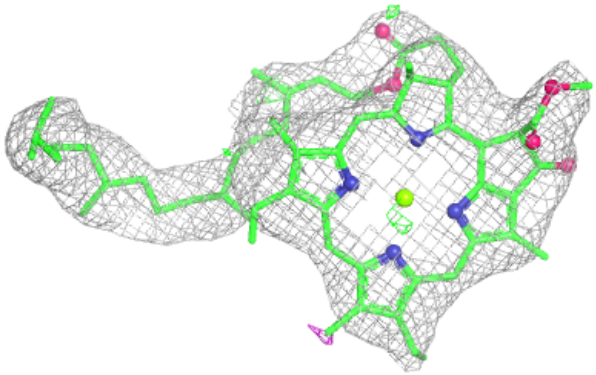


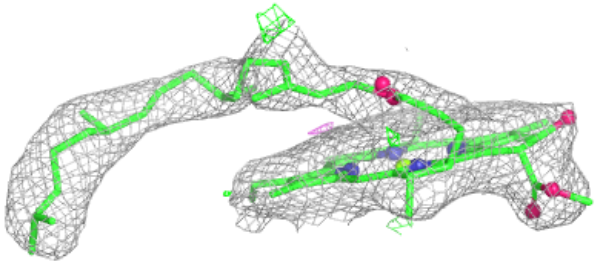


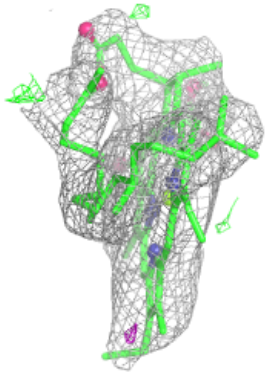


Electron density around CLA B 1215:

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

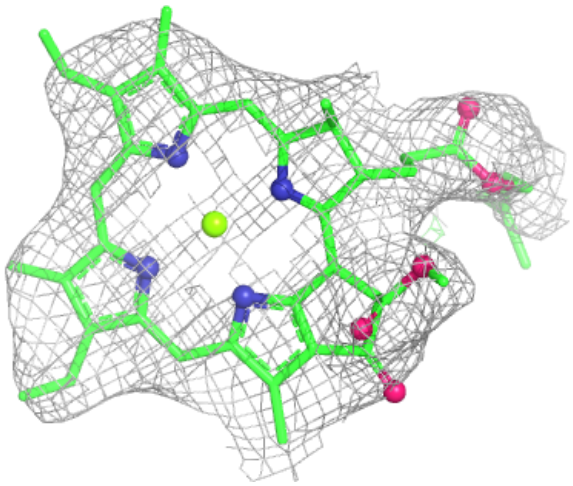


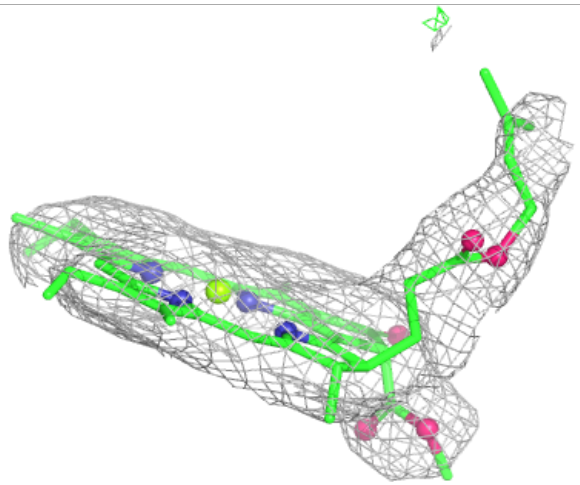


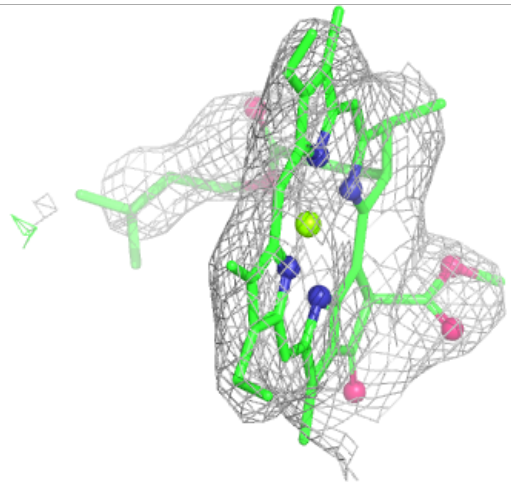


Electron density around CLA A 1137:

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

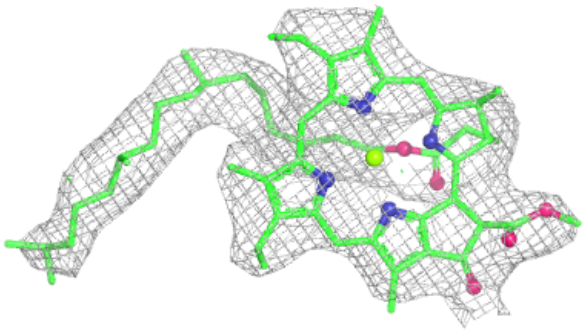


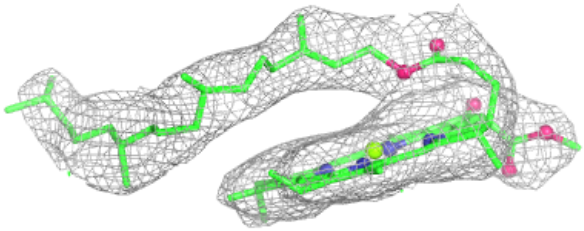


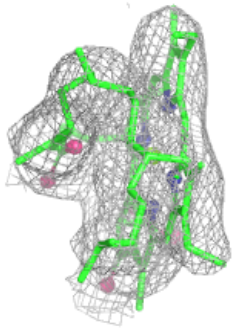


Electron density around CLA B 1235:

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

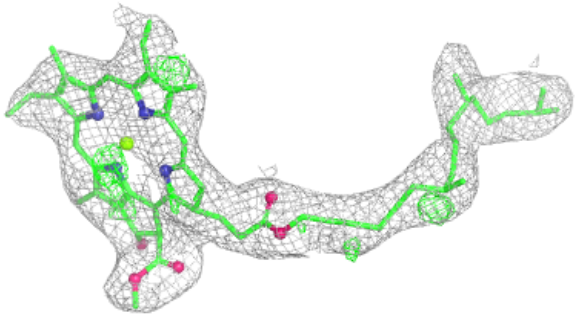


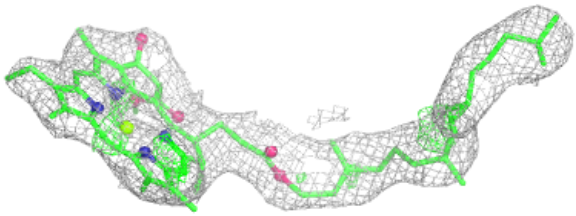


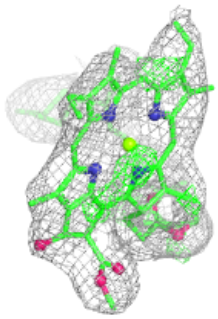


Electron density around CLA A 1012:

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

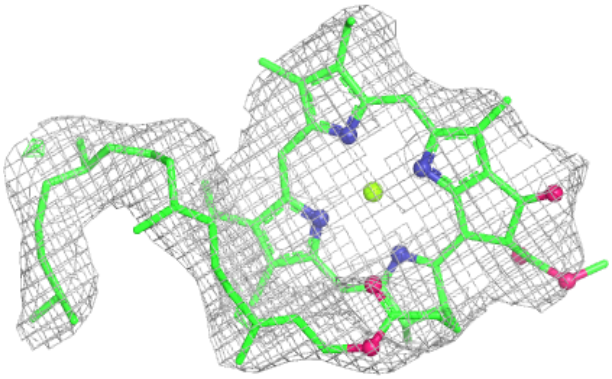


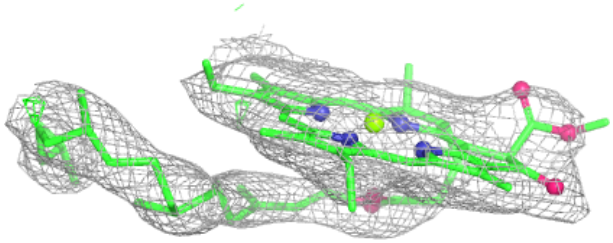


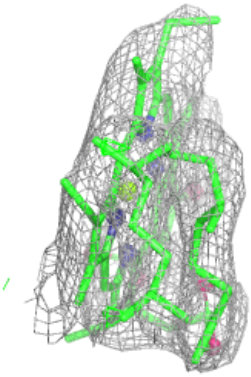


Electron density around CLA A 1117:

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

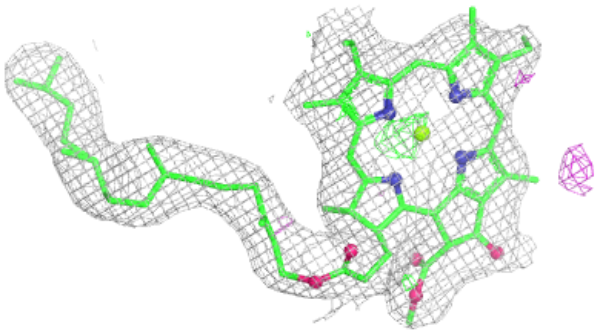


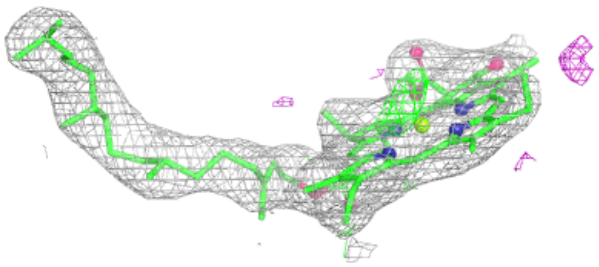




Electron density around CLA B 1013:

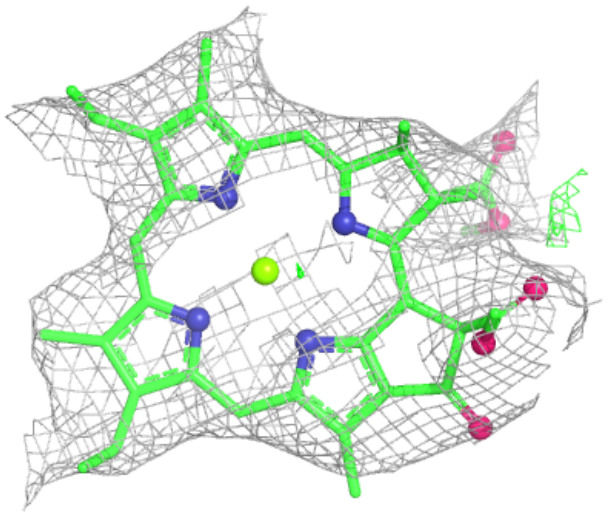
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

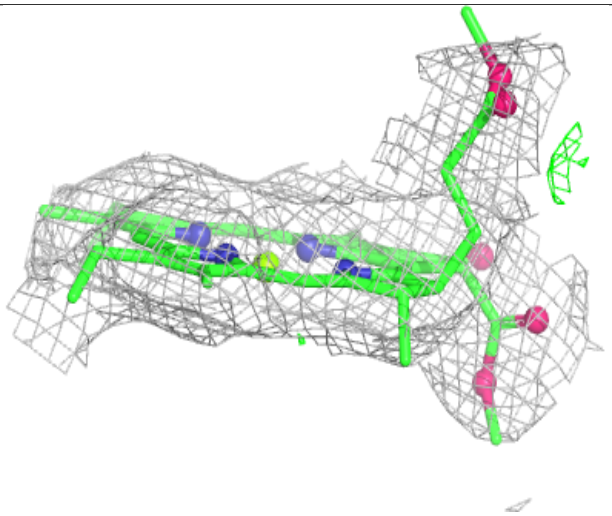


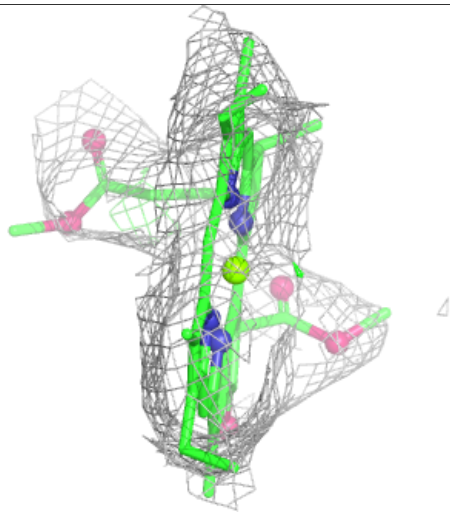


Electron density around CLA B 1211:

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

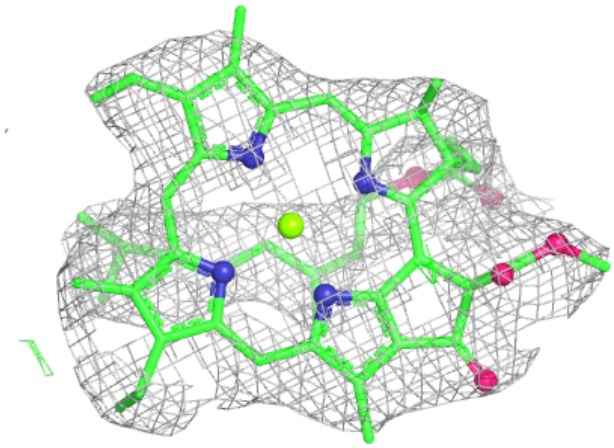


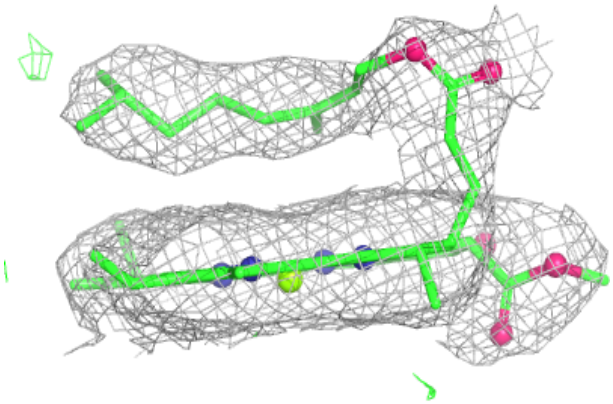


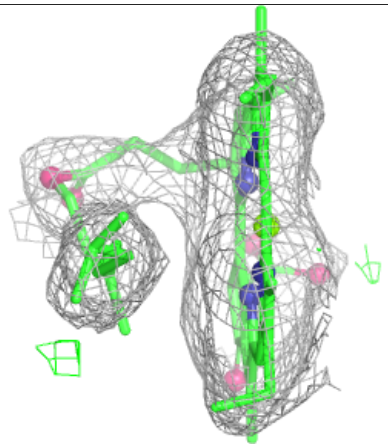


Electron density around CLA B 1237:

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

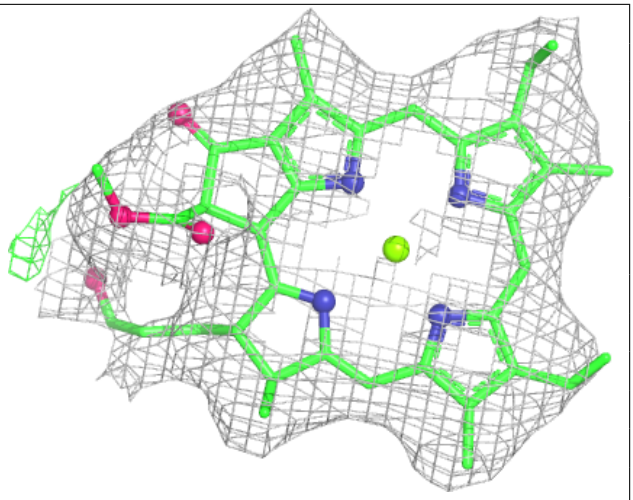


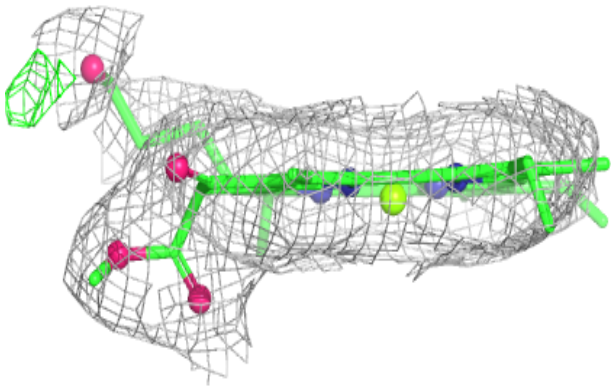


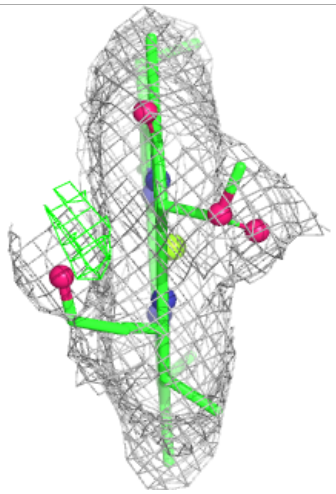


Electron density around CLA B 1238:

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

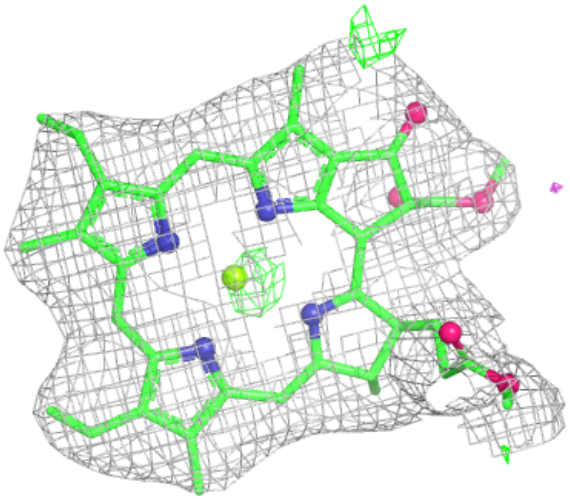


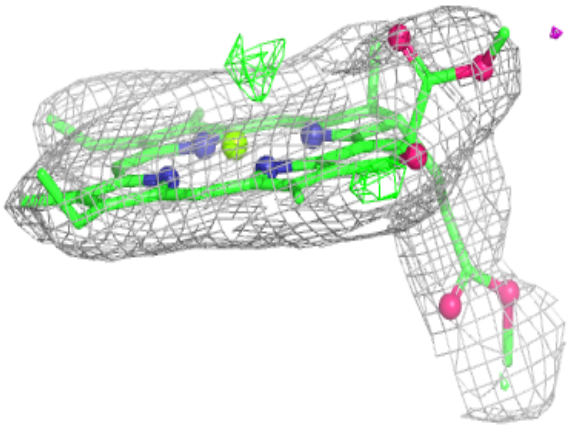


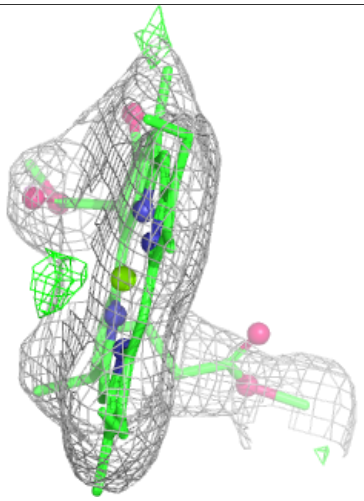


Electron density around CLA B 1239:

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

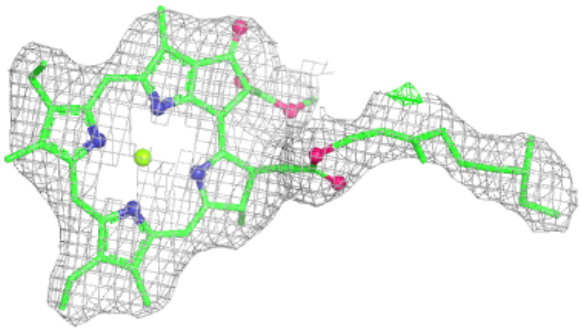


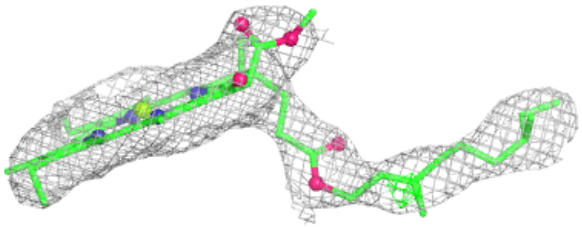


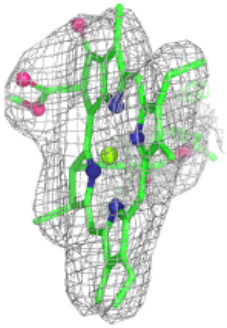


Electron density around CLA B 1220:

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

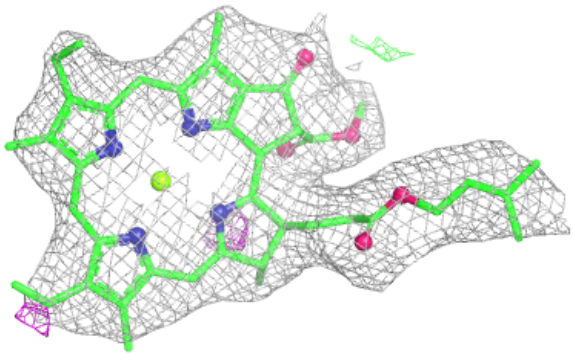


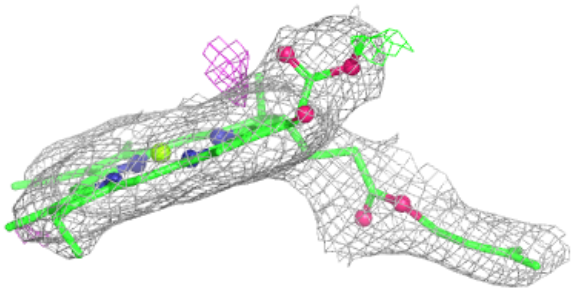


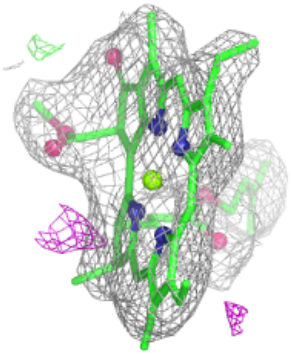


Electron density around CLA A 1107:

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

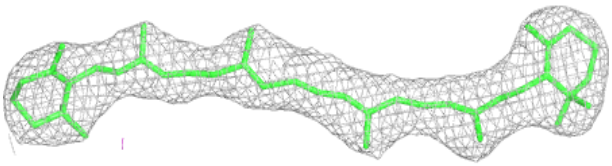


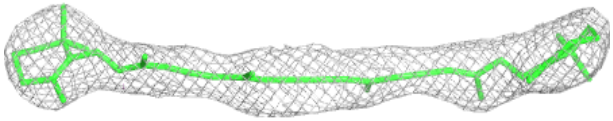


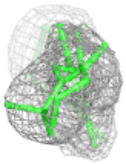


Electron density around BCR A 4012:

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

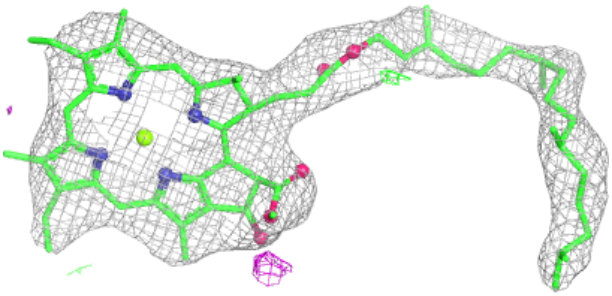


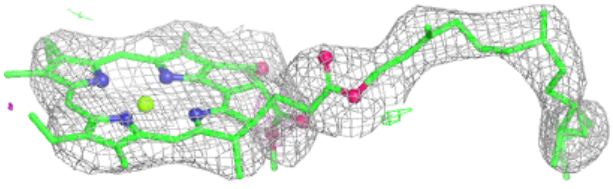


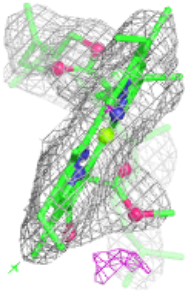


Electron density around CLA B 1223:

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

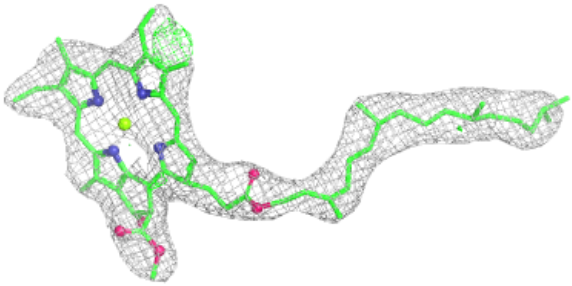


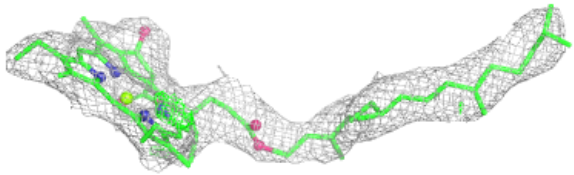


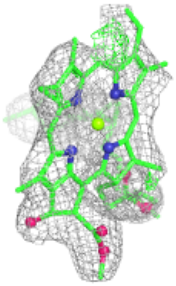


Electron density around CLA A 1022:

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

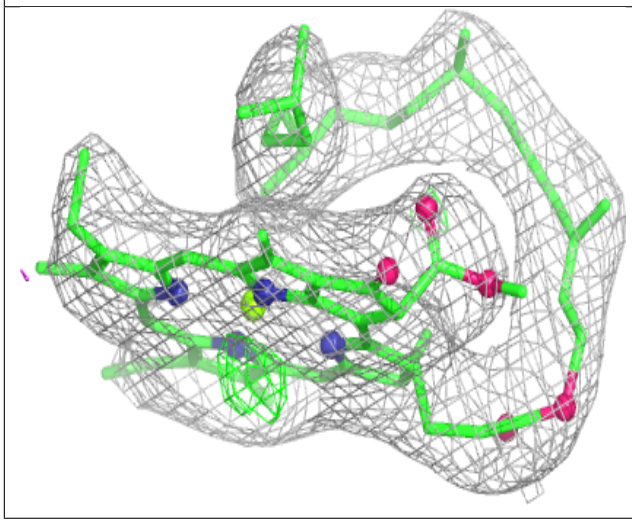


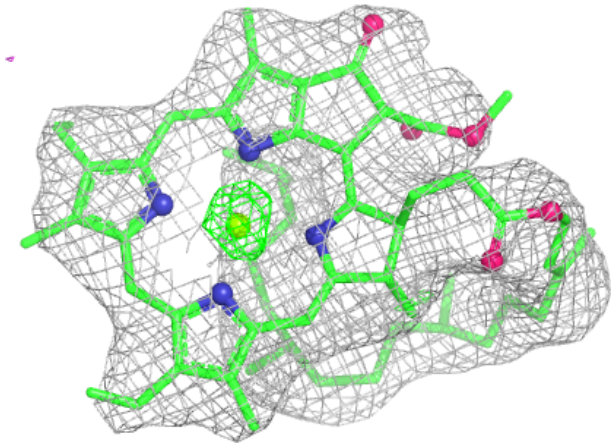


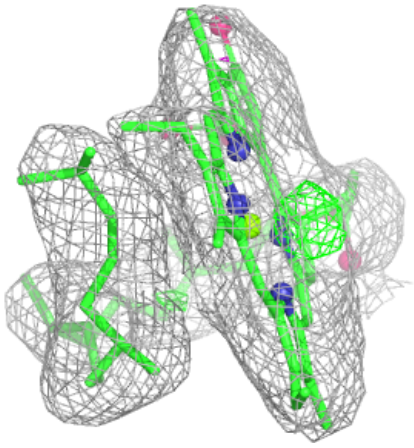


Electron density around CLA A 1104:

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

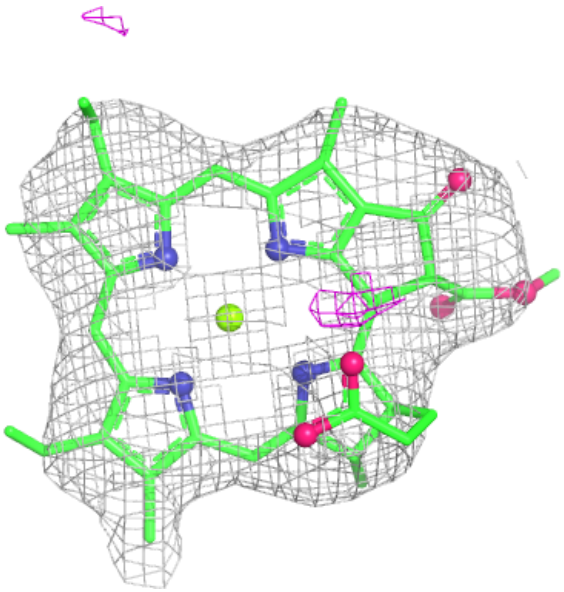


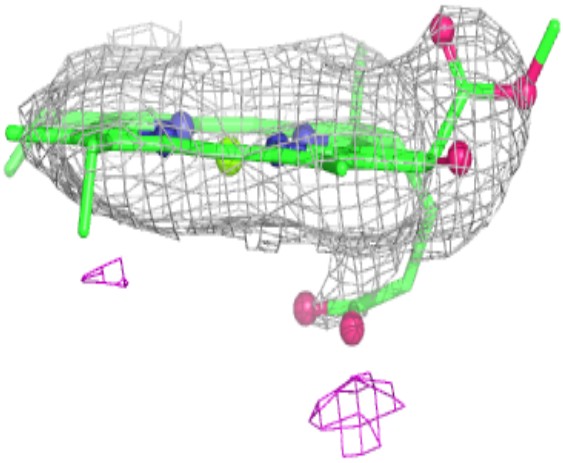


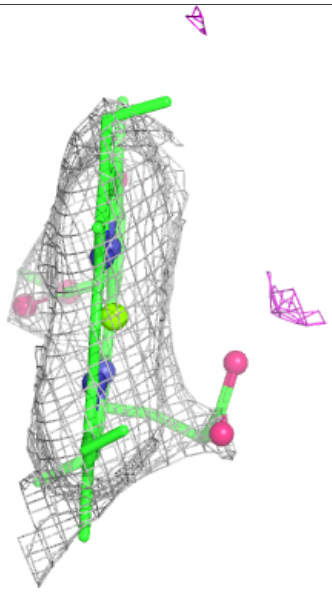


Electron density around CLA B 1209:

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

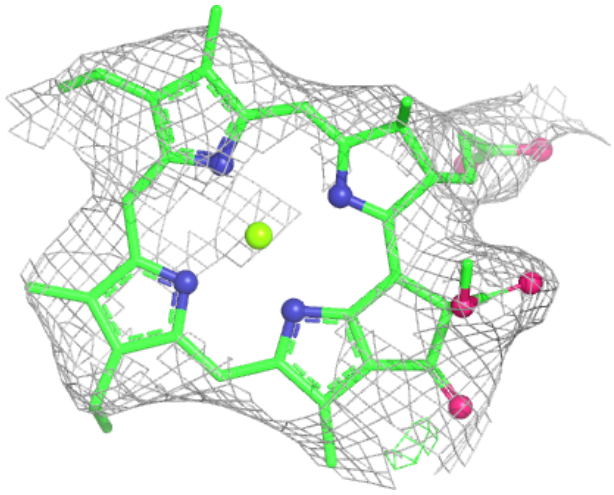


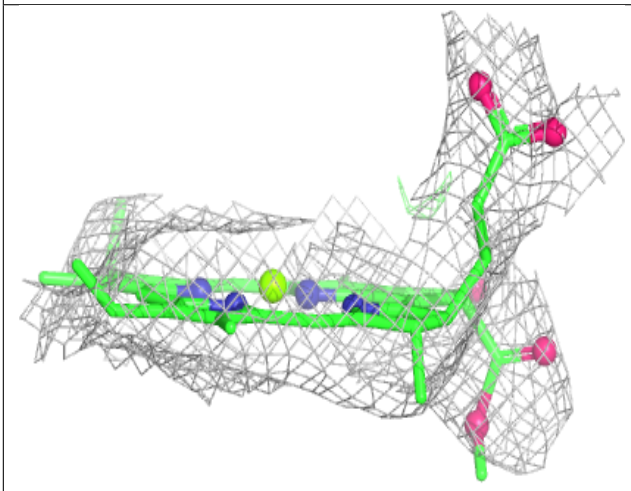


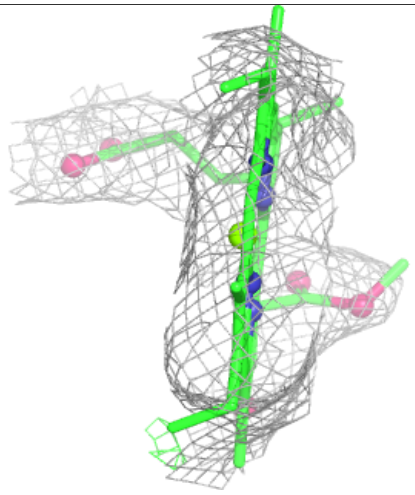


Electron density around CLA A 1112:

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

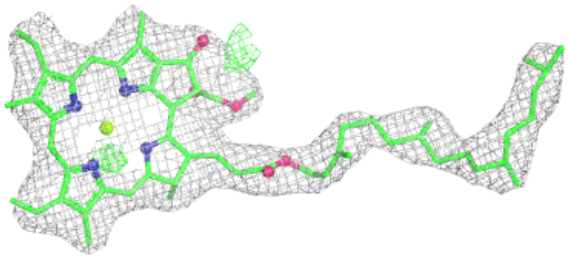


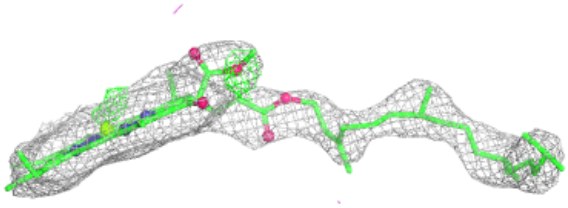


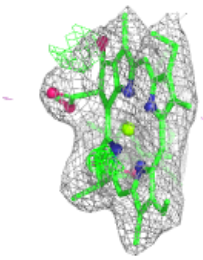


Electron density around CLA F 1139:

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

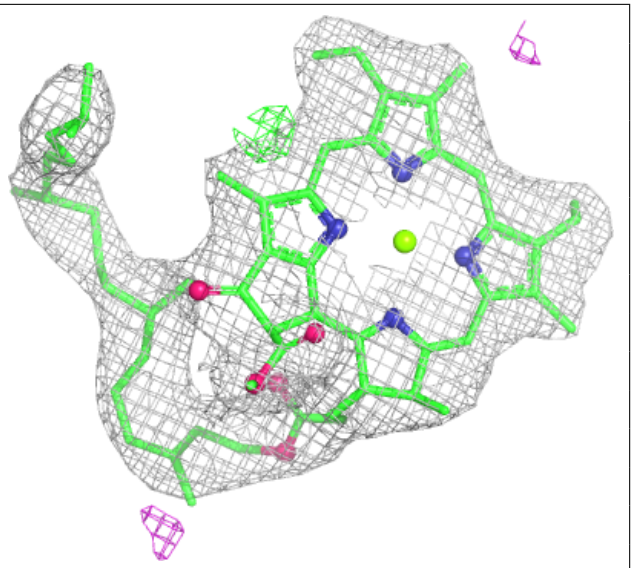


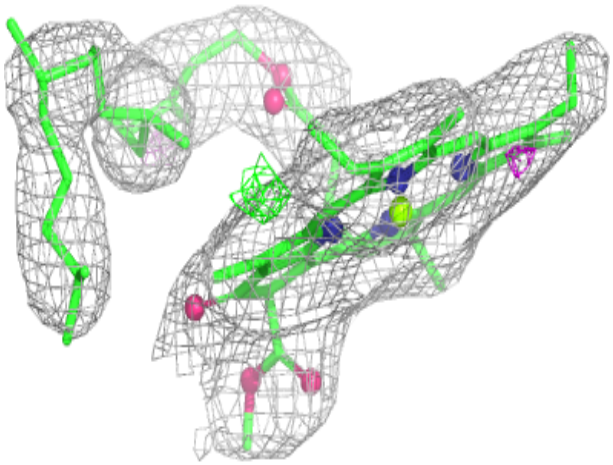


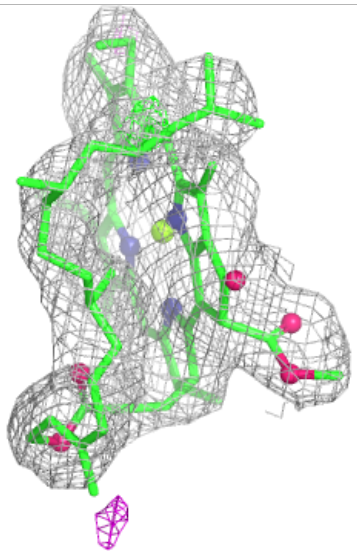


Electron density around CLA B 1229:

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

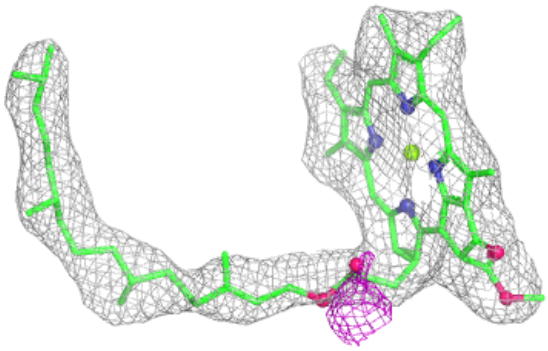


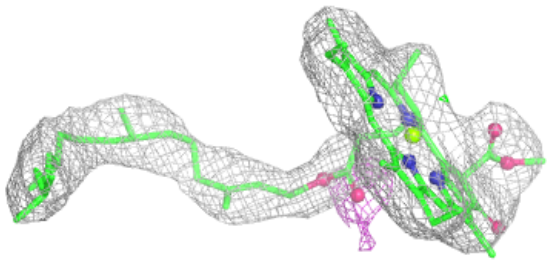


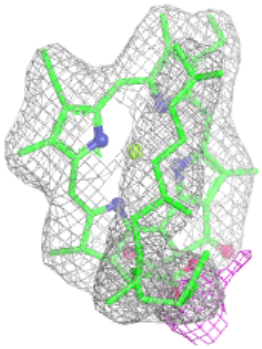


Electron density around CLA A 1140:

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

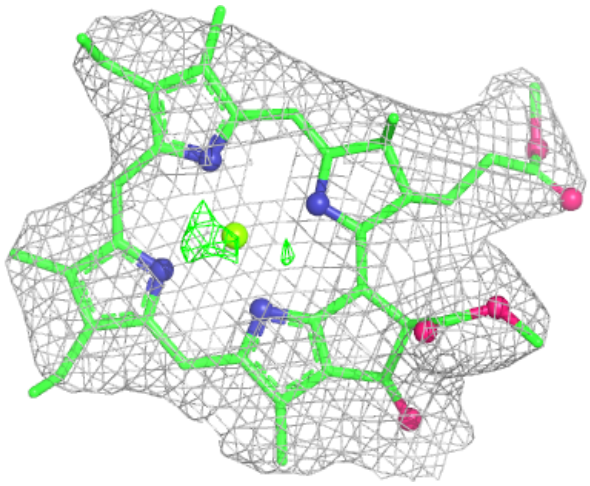


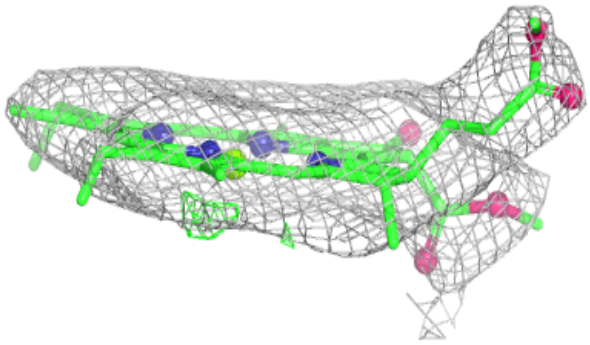


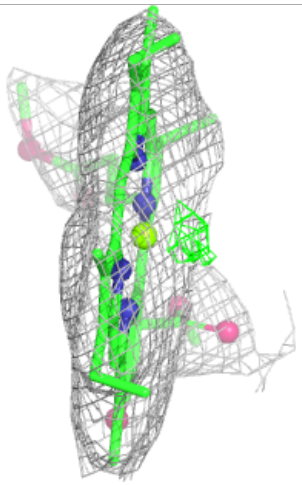


Electron density around CLA B 1206:

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

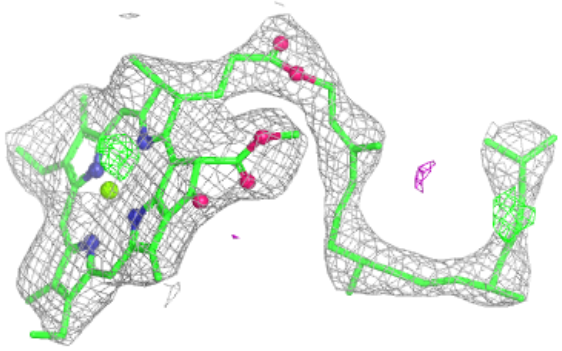


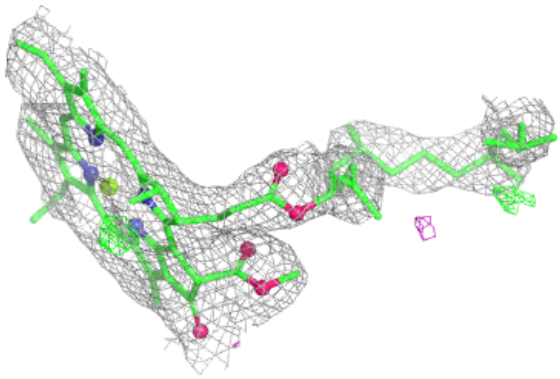


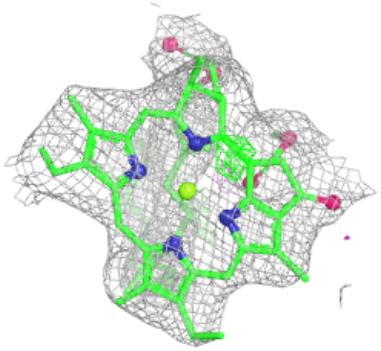


Electron density around CL0 A 1011:

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

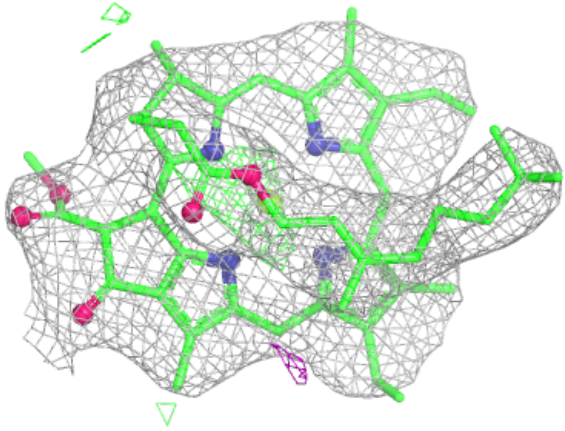


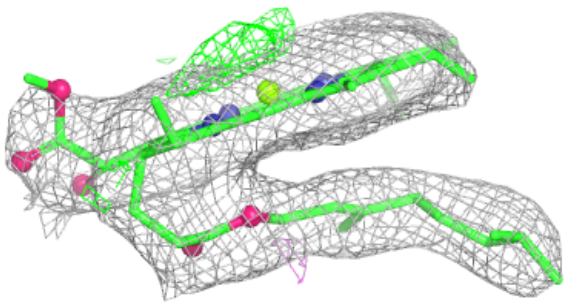


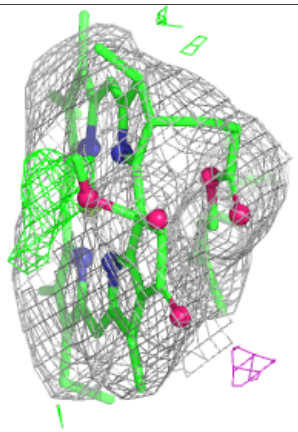


Electron density around CLA B 1205:

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

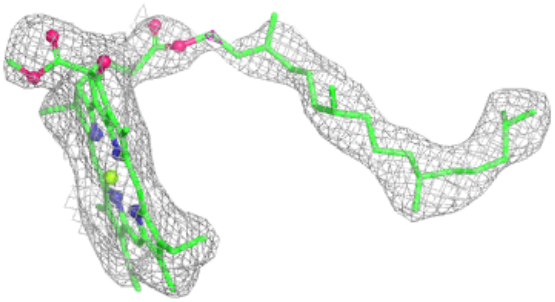


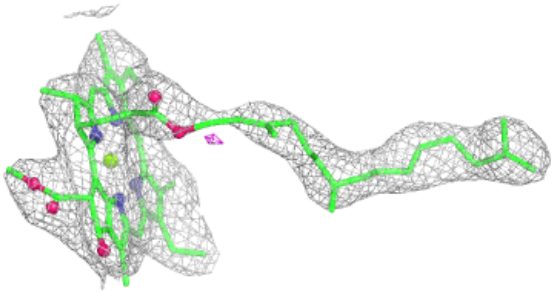


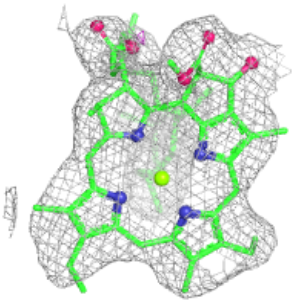


Electron density around CLA A 1128:

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

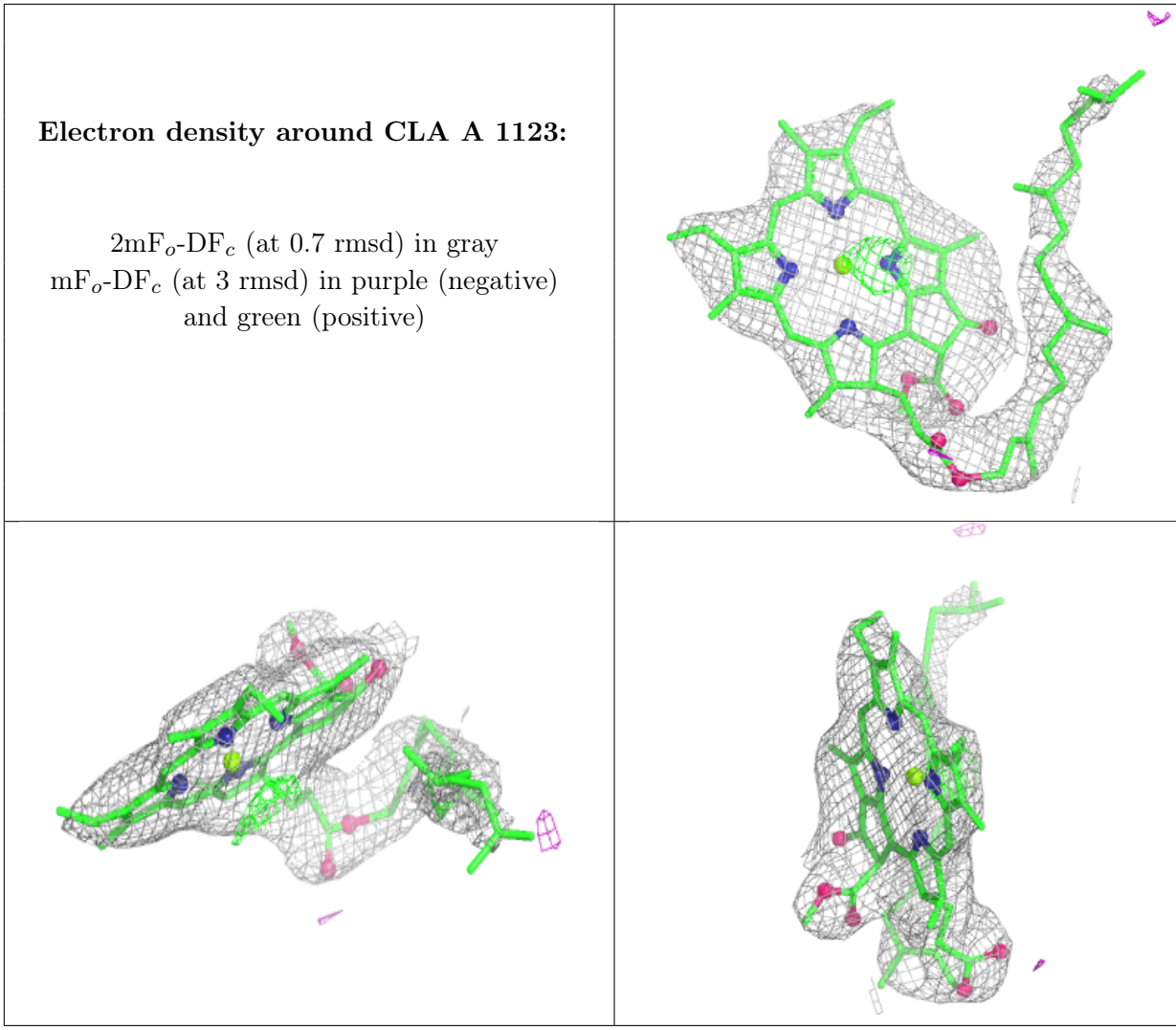






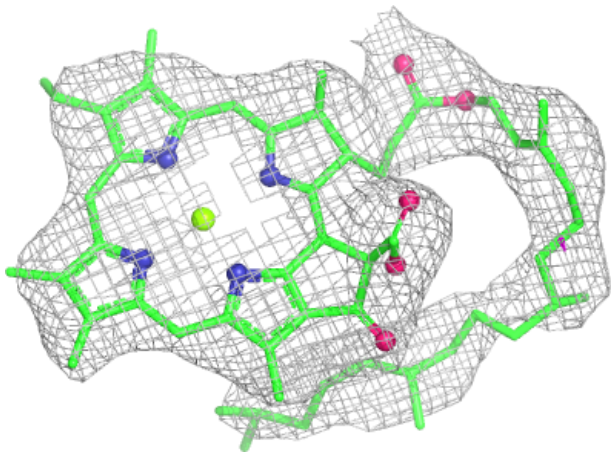
Electron density around CLA A 1123:

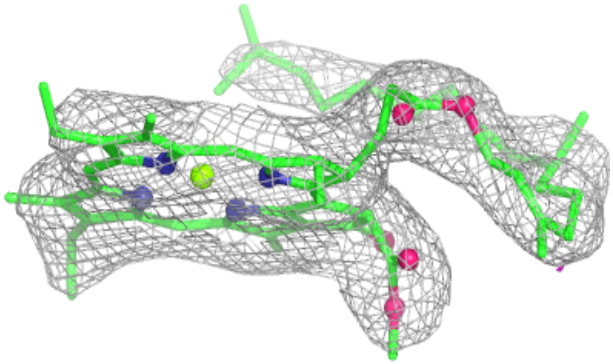
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

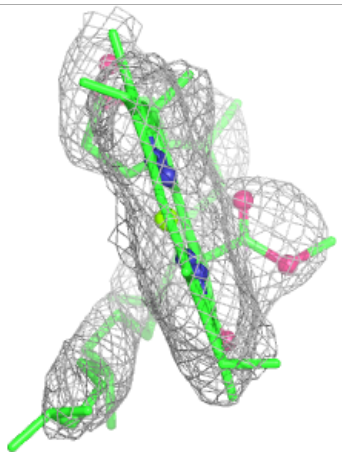


Electron density around CLA B 1202:

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

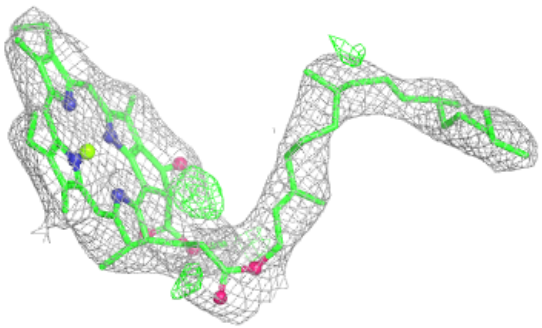


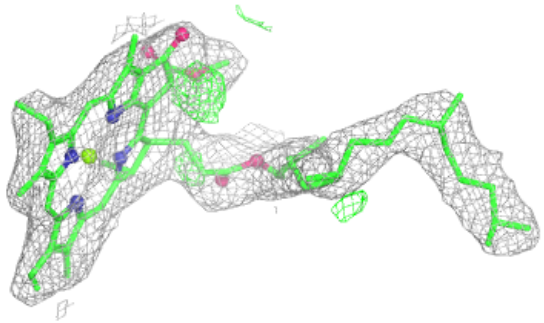


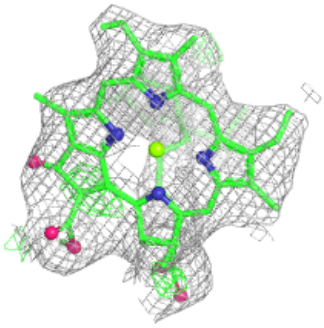


Electron density around CLA B 1021:

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

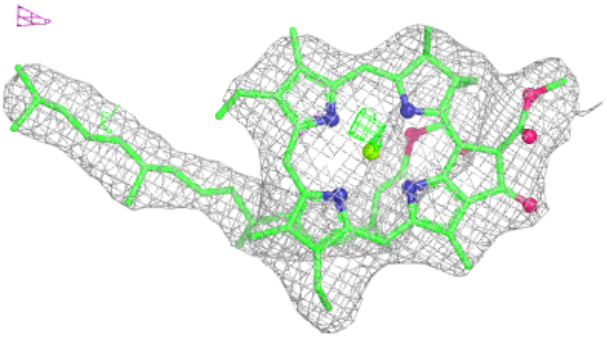


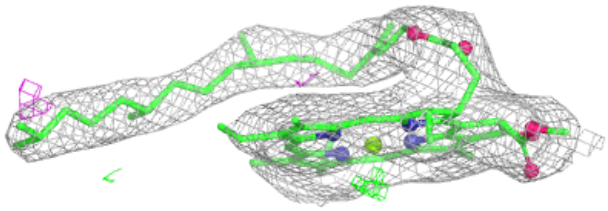


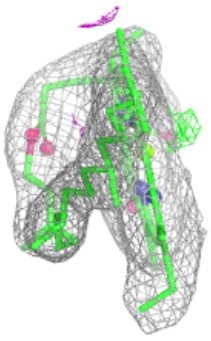


Electron density around CLA A 1138:

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







6.5 Other polymers (i)

There are no such residues in this entry.