Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:16 PM EDT

PDB ID	:	4L6V / pdb_00004l6v
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	:	2013-06-13
Resolution	:	3.80 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:

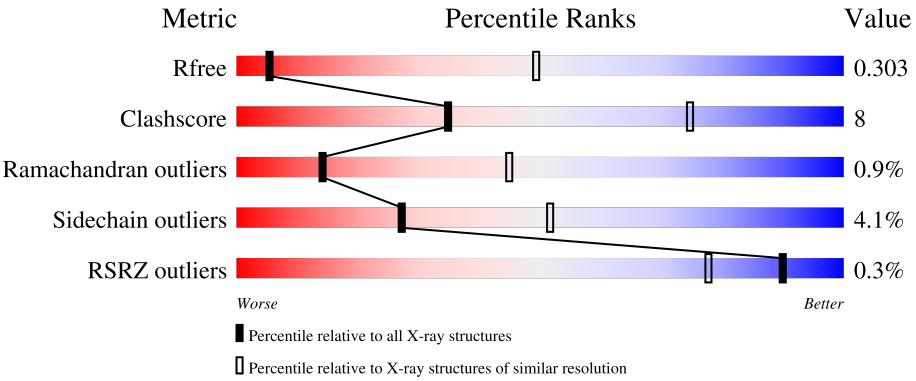
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1	751	89% 9% •
1	A	751	88% 10% •
1	a	751	89% 9% •
2	2	731	88% 11% •
2	B	731	87% 12% •

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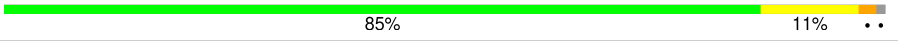
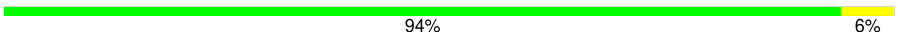
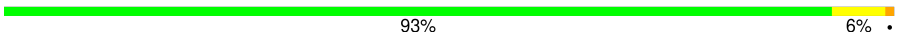
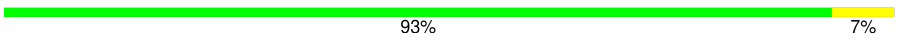
Mol	Chain	Length	Quality of chain
2	b	731	
3	3	81	
3	C	81	
3	c	81	
4	4	141	
4	D	141	
4	d	141	
5	5	74	
5	E	74	
5	e	74	
6	6	125	
6	F	125	
6	f	125	
7	8	157	
7	L	157	
7	l	157	
8	7	31	
8	M	31	
8	m	31	
9	9	40	
9	I	40	
9	i	40	
10	0	128	
10	K	128	
10	k	128	

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	SF4	3	3002	-	-	X	-
13	SF4	3	3003	-	-	X	-
13	SF4	A	3001	-	-	X	-
13	SF4	C	3002	-	-	X	-
13	SF4	C	3003	-	-	X	-
13	SF4	a	3001	-	-	X	-
13	SF4	c	3002	-	-	X	-
13	SF4	c	3003	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 68370 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
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	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			
2	b	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	2	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			
3	c	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	3	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
			1079	683	187	206	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			
4	4	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	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
			529	332	93	104			
5	e	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	5	68	Total	C	N	O	0	0	0
			529	332	93	104			

- Molecule 6 is a protein called Fusion protein of Photosystem I subunit III and subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O	0	0	0
			676	420	126	130			
6	f	125	Total	C	N	O	0	0	0
			685	429	126	130			
6	6	125	Total	C	N	O	0	0	0
			685	429	126	130			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	CYS	-	linker	UNP L8AII8
F	42	SER	-	linker	UNP L8AII8
F	43	CYS	-	linker	UNP L8AII8
F	53	ILE	LEU	engineered mutation	UNP L8AII8
f	41	CYS	-	linker	UNP L8AII8
f	42	SER	-	linker	UNP L8AII8
f	43	CYS	-	linker	UNP L8AII8
f	53	ILE	LEU	engineered mutation	UNP L8AII8
6	41	CYS	-	linker	UNP L8AII8
6	42	SER	-	linker	UNP L8AII8
6	43	CYS	-	linker	UNP L8AII8
6	53	ILE	LEU	engineered mutation	UNP L8AII8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	l	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	8	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	m	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	7	31	Total	C	N	O	0	0	0
			235	157	36	42			

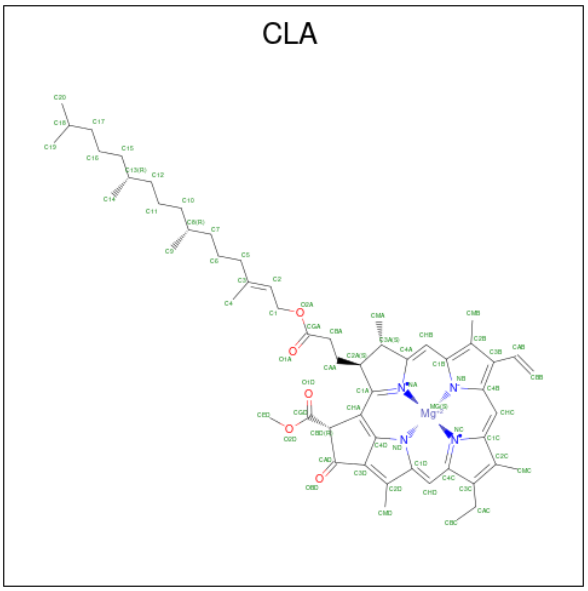
- Molecule 9 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	i	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	9	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	I	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	k	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	0	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
11	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
11	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
11	2	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
11	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	2	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
11	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
11	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	2	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
11	2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	2	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
11	2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	8	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	8	1	Total 46	C 36	Mg 1	N 4	O 5	0	0

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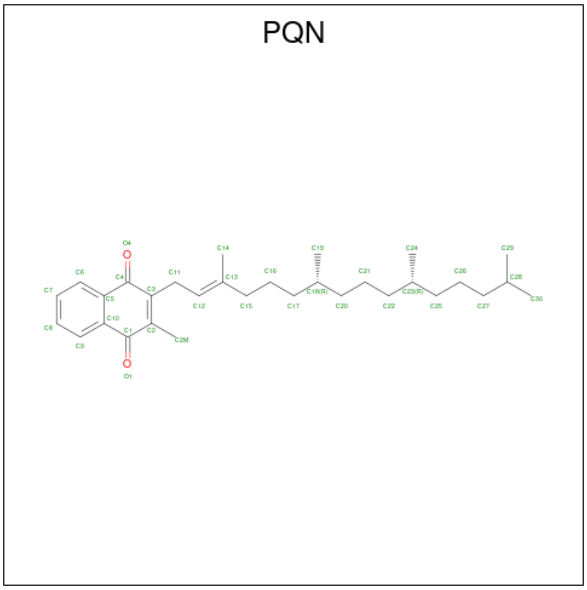
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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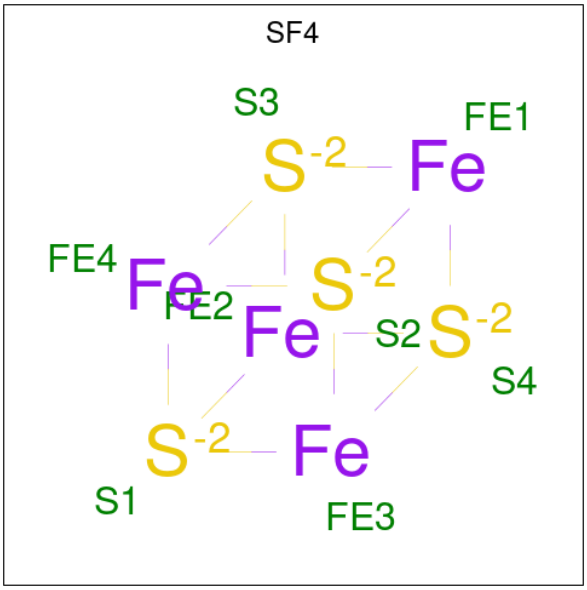
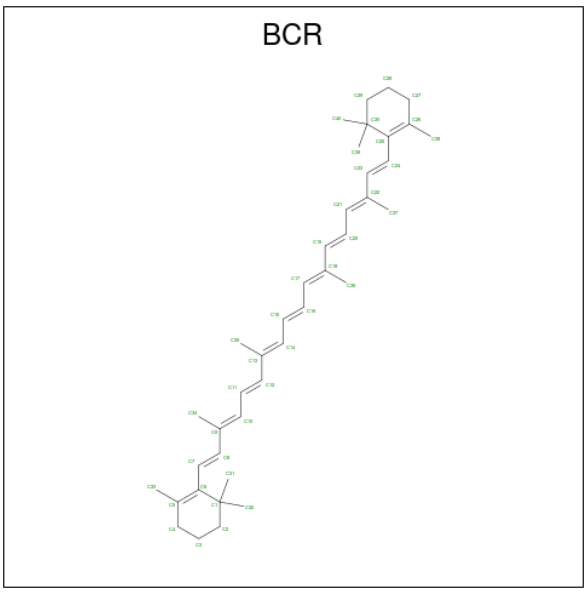
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	1	1	Total C O 33 31 2	0	0
12	2	1	Total C O 33 31 2	0	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Fe S 8 4 4	0	0
13	C	1	Total Fe S 8 4 4	0	0
13	C	1	Total Fe S 8 4 4	0	0
13	a	1	Total Fe S 8 4 4	0	0
13	c	1	Total Fe S 8 4 4	0	0
13	c	1	Total Fe S 8 4 4	0	0
13	1	1	Total Fe S 8 4 4	0	0
13	3	1	Total Fe S 8 4 4	0	0
13	3	1	Total Fe S 8 4 4	0	0

- 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	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	F	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	M	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
14	f	1	Total C 40 40	0	0
14	f	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	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	8	1	Total C 40 40	0	0

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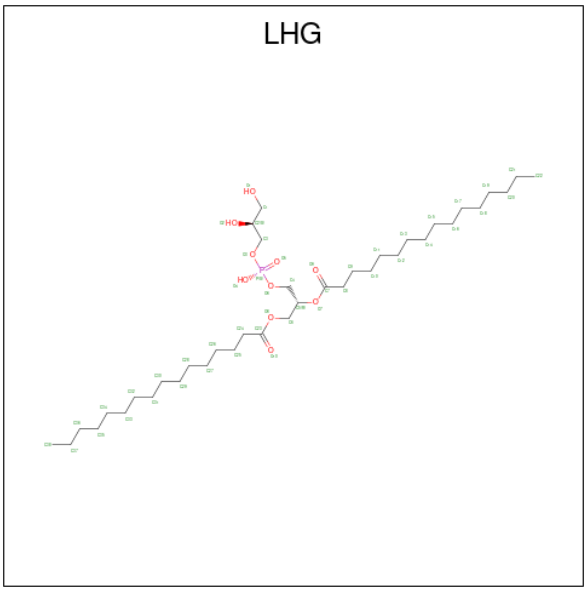
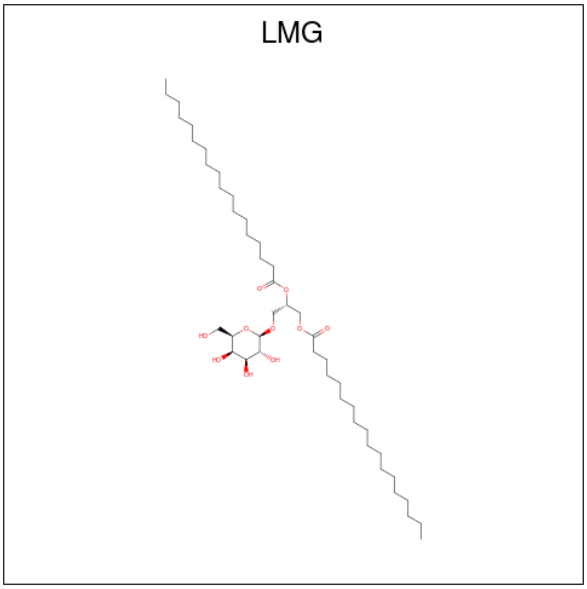
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O P 49 38 10 1	0	0
15	A	1	Total C O P 49 38 10 1	0	0
15	B	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	b	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	2	1	Total C O P 49 38 10 1	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



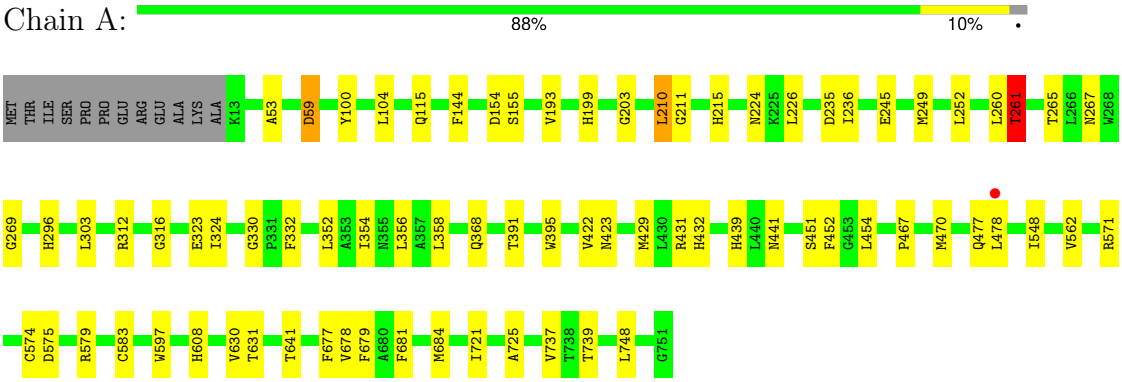
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C O 55 45 10	0	0
16	b	1	Total C O 55 45 10	0	0
16	2	1	Total C O 55 45 10	0	0

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.

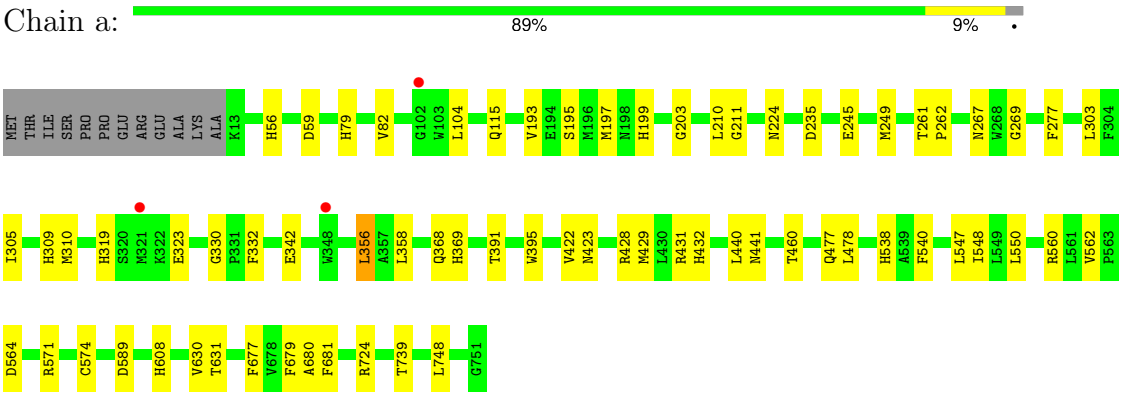
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



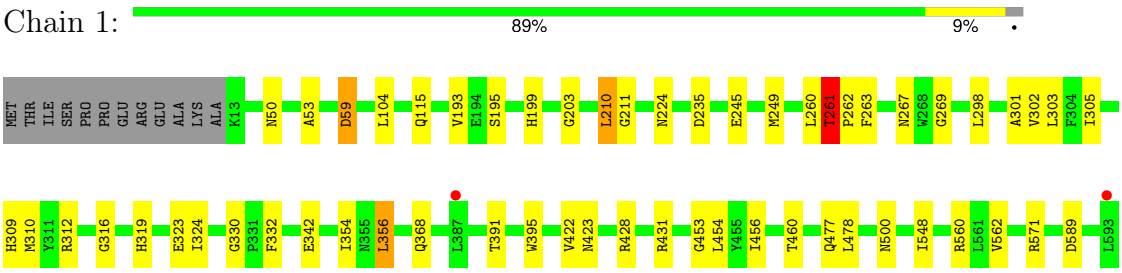
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

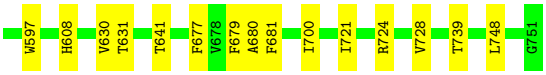
Chain a:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

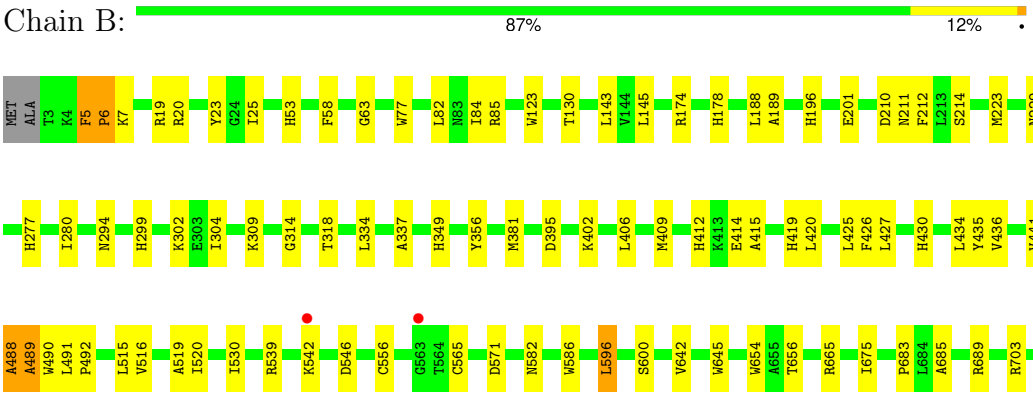
Chain 1:





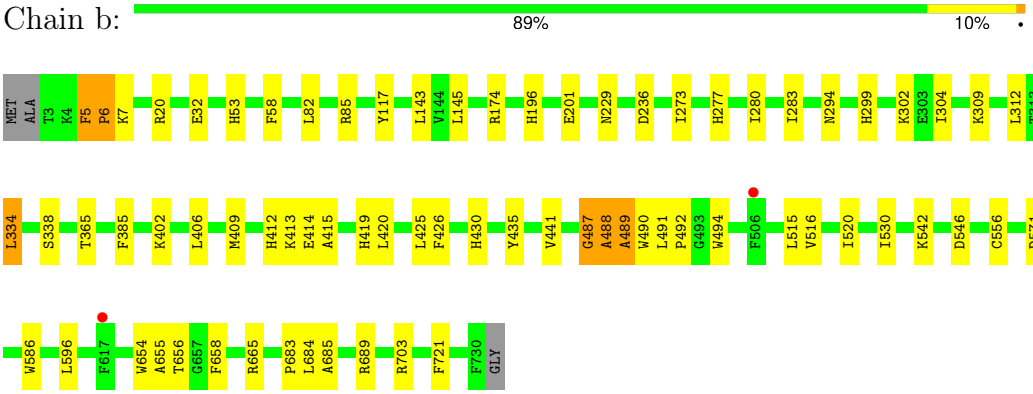
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



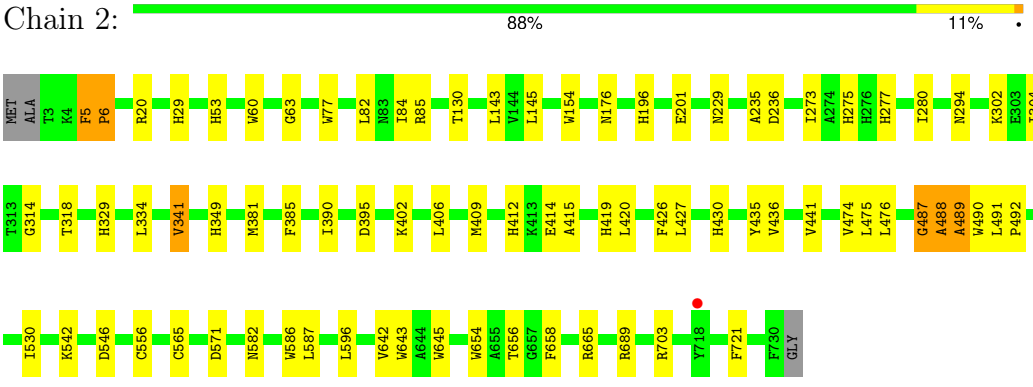
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



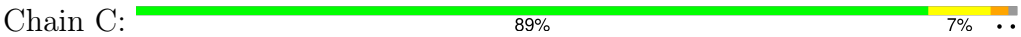
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

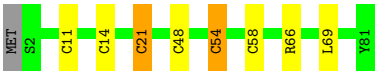
Chain 2:



• Molecule 3: Photosystem I iron-sulfur center

Chain C:



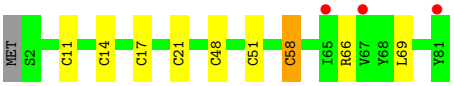


• Molecule 3: Photosystem I iron-sulfur center

Chain c:

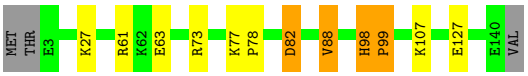
• Molecule 3: Photosystem I iron-sulfur center

Chain 3:



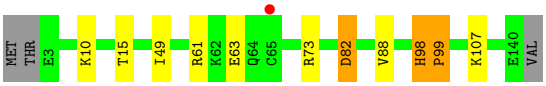
• Molecule 4: Photosystem I subunit II

Chain D:



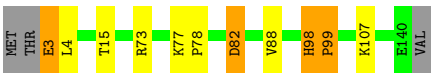
• Molecule 4: Photosystem I subunit II

Chain d:



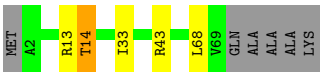
• Molecule 4: Photosystem I subunit II

Chain 4:



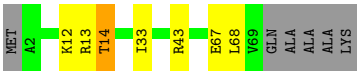
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



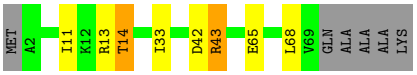
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



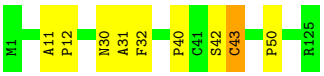
• Molecule 5: Photosystem I reaction center subunit IV

Chain 5:



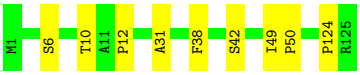
• Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain F:



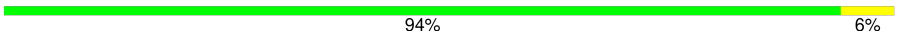
• Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

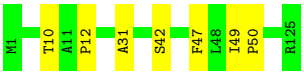
Chain f:



• Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

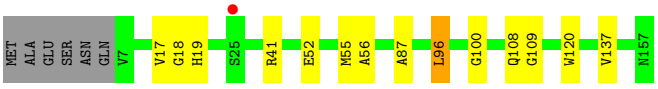
Chain 6:





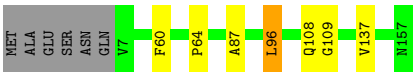
• Molecule 7: Photosystem I reaction center subunit XI

Chain L:



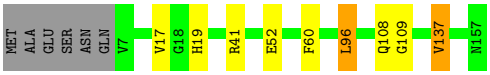
• Molecule 7: Photosystem I reaction center subunit XI

Chain l:



• Molecule 7: Photosystem I reaction center subunit XI

Chain 8:

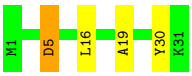


• Molecule 8: Photosystem I reaction center subunit XII

Chain M:

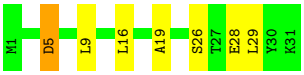
• Molecule 8: Photosystem I reaction center subunit XII

Chain m:



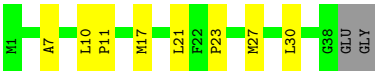
• Molecule 8: Photosystem I reaction center subunit XII

Chain 7:



• Molecule 9: Photosystem I subunit III

Chain i:

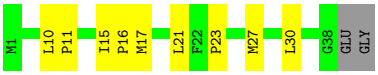


• Molecule 9: Photosystem I subunit III

Chain 9:

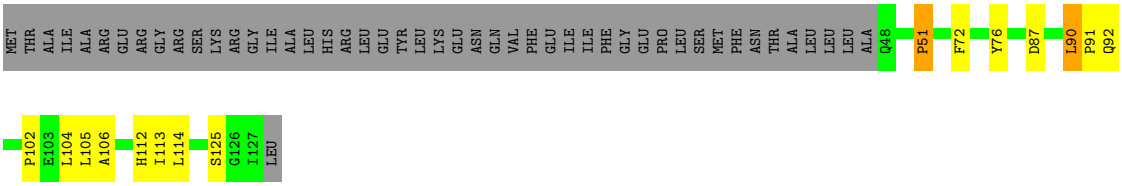
• Molecule 9: Photosystem I subunit III

Chain I:



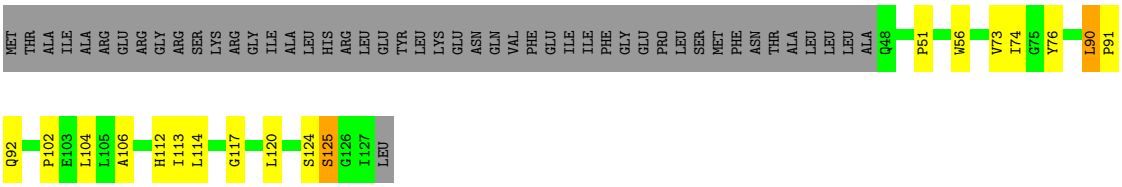
• Molecule 10: Photosystem I reaction center subunit VIII

Chain K:



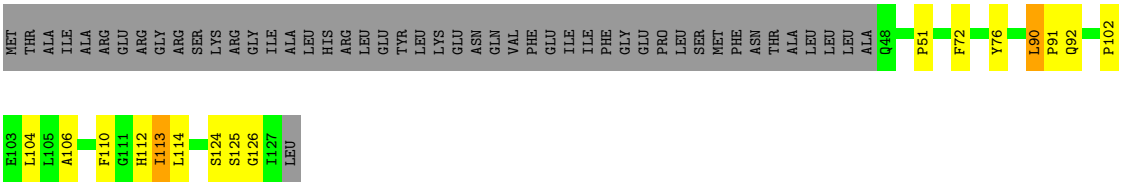
• Molecule 10: Photosystem I reaction center subunit VIII

Chain k:



• Molecule 10: Photosystem I reaction center subunit VIII

Chain 0:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	214.62Å 133.68Å 219.85Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-3.80) 77.5 (30.00-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.02 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2-1309, REFMAC 5.7.0032	Depositor
R, R_{free}	0.253 , 0.297 0.265 , 0.303	Depositor DCC
R_{free} test set	7809 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	93.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 105.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å^2)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 (i)

5.1 Standard geometry (i)

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

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	1	0.30	0/5970	0.66	2/8138 (0.0%)
1	A	0.31	0/5970	0.65	2/8138 (0.0%)
1	a	0.30	0/5970	0.66	0/8138
2	2	0.30	0/5976	0.64	1/8173 (0.0%)
2	B	0.31	0/5976	0.64	1/8173 (0.0%)
2	b	0.30	0/5976	0.64	1/8173 (0.0%)
3	3	0.34	0/610	0.67	0/826
3	C	0.33	0/610	0.66	0/826
3	c	0.34	0/610	0.64	0/826
4	4	0.31	0/1103	0.61	0/1487
4	D	0.30	0/1103	0.61	0/1487
4	d	0.30	0/1103	0.61	0/1487
5	5	0.30	0/538	0.67	0/729
5	E	0.29	0/538	0.63	0/729
5	e	0.29	0/538	0.64	0/729
6	6	0.36	0/700	0.92	1/976 (0.1%)
6	F	0.41	0/690	0.97	0/963
6	f	0.36	0/700	0.90	0/976
7	8	0.31	0/1163	0.67	0/1580
7	L	0.31	0/1163	0.67	0/1580
7	l	0.30	0/1163	0.67	0/1580
8	7	0.38	0/238	0.66	0/323
8	M	0.37	0/238	0.67	0/323
8	m	0.34	0/238	0.68	0/323
9	9	0.37	0/308	0.71	0/421
9	I	0.36	0/308	0.69	0/421
9	i	0.34	0/308	0.64	0/421
10	0	0.35	0/504	0.84	0/688
10	K	0.36	0/504	0.81	0/688
10	k	0.34	0/504	0.83	1/688 (0.1%)
All	All	0.31	0/51320	0.67	9/70010 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	47	PHE	N-CA-C	-5.47	106.38	113.16
1	1	261	THR	CA-C-N	-5.18	113.58	119.28
1	1	261	THR	C-N-CA	-5.18	113.58	119.28
2	B	665	ARG	N-CA-C	5.15	116.58	110.97
2	2	665	ARG	N-CA-C	5.12	116.55	110.97
1	A	261	THR	CA-C-N	-5.07	113.71	119.28
1	A	261	THR	C-N-CA	-5.07	113.71	119.28
2	b	665	ARG	N-CA-C	5.04	116.47	110.97
10	k	56	TRP	CB-CA-C	-5.03	110.38	117.23

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	5	PHE	Peptide
4	4	98	HIS	Peptide
2	B	5	PHE	Peptide
4	D	98	HIS	Peptide
6	F	40	PRO	Mainchain
2	b	5	PHE	Peptide
4	d	98	HIS	Peptide
10	k	125	SER	Peptide

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	1	5772	0	5621	58	0
1	A	5772	0	5621	61	0
1	a	5772	0	5621	66	0
2	2	5765	0	5546	54	0
2	B	5765	0	5546	60	0
2	b	5765	0	5545	44	0
3	3	600	0	588	21	0
3	C	600	0	586	14	0
3	c	600	0	587	23	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	6	0
4	d	1079	0	1073	6	0
5	5	529	0	506	4	0
5	E	529	0	506	1	0
5	e	529	0	506	2	0
6	6	685	0	411	3	0
6	F	676	0	395	5	0
6	f	685	0	411	6	0
7	8	1133	0	1108	6	0
7	L	1133	0	1108	7	0
7	l	1133	0	1108	5	0
8	7	235	0	253	9	0
8	M	235	0	253	7	0
8	m	235	0	253	5	0
9	9	297	0	295	10	0
9	I	297	0	295	6	0
9	i	297	0	295	4	0
10	0	496	0	439	5	0
10	K	496	0	439	5	0
10	k	496	0	439	8	0
11	0	115	0	111	4	0
11	1	2546	0	2430	95	0
11	2	2313	0	2213	97	0
11	8	176	0	177	7	0
11	A	2546	0	2435	96	0
11	B	2313	0	2213	85	0
11	K	115	0	111	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	176	0	177	4	0
11	a	2546	0	2434	94	0
11	b	2313	0	2213	97	0
11	k	115	0	111	5	0
11	l	176	0	177	7	0
12	1	33	0	45	0	0
12	2	33	0	45	1	0
12	A	33	0	45	2	0
12	B	33	0	45	1	0
12	a	33	0	46	3	0
12	b	33	0	45	1	0
13	1	8	0	0	1	0
13	3	16	0	0	20	0
13	A	8	0	0	3	0
13	C	16	0	0	13	0
13	a	8	0	0	2	0
13	c	16	0	0	20	0
14	1	200	0	242	23	0
14	2	320	0	391	43	0
14	6	120	0	147	20	0
14	7	40	0	49	5	0
14	8	80	0	97	15	0
14	A	200	0	244	26	0
14	B	320	0	390	44	0
14	F	120	0	146	15	0
14	L	80	0	97	14	0
14	M	40	0	49	5	0
14	a	200	0	243	16	0
14	b	320	0	389	38	0
14	f	120	0	147	15	0
14	l	80	0	97	11	0
14	m	40	0	49	4	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	9	0
15	B	49	0	74	4	0
15	a	98	0	148	11	0
15	b	49	0	74	5	0
16	2	55	0	86	2	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	1010	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 8.

All (1010) 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)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:a:56:HIS:CG	11:a:1103:CLA:HBB2	1.23	1.62
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:c:58:CYS:SG	13:c:3003:SF4:FE1	0.94	1.57
3:c:11:CYS:SG	13:c:3003:SF4:FE3	0.96	1.54
3:c:48:CYS:SG	13:c:3002:SF4:FE4	1.05	1.48
3:c:14:CYS:SG	13:c:3003:SF4:FE2	1.10	1.44
1:a:56:HIS:CD2	11:a:1103:CLA:HBB2	1.55	1.40
1:a:56:HIS:CG	11:a:1103:CLA:CBB	2.07	1.36
3:C:54:CYS:SG	13:C:3002:SF4:FE3	1.22	1.29
3:3:58:CYS:SG	13:3:3003:SF4:FE1	1.23	1.29
3:3:14:CYS:SG	13:3:3003:SF4:FE2	1.29	1.23
3:C:14:CYS:SG	13:C:3003:SF4:FE2	1.31	1.22
3:C:48:CYS:SG	13:C:3002:SF4:S3	2.39	1.20
3:c:21:CYS:SG	13:c:3002:SF4:S1	2.51	1.06
3:3:51:CYS:SG	13:3:3002:SF4:FE1	1.45	1.06
3:3:58:CYS:SG	13:3:3003:SF4:S3	2.58	1.02
3:c:14:CYS:HG	13:c:3003:SF4:FE2	0.75	1.02
3:C:21:CYS:SG	13:C:3002:SF4:S1	2.57	0.97
1:A:583:CYS:HG	13:A:3001:SF4:FE2	0.73	0.97
3:c:14:CYS:SG	13:c:3003:SF4:S4	2.64	0.96
3:c:51:CYS:HG	13:c:3002:SF4:FE1	0.65	0.93
2:2:586:TRP:CZ2	11:2:1021:CLA:H201	2.05	0.92
1:a:56:HIS:CD2	11:a:1103:CLA:CBB	2.42	0.92
3:3:48:CYS:HG	13:3:3002:SF4:FE4	0.83	0.91
3:C:54:CYS:HG	13:C:3002:SF4:FE3	0.65	0.91
3:c:51:CYS:SG	13:c:3002:SF4:FE1	1.63	0.90
3:3:17:CYS:HG	13:3:3003:SF4:FE4	0.61	0.90
11:b:1222:CLA:HBA1	11:b:1223:CLA:OBD	1.71	0.90
3:c:48:CYS:HG	13:c:3002:SF4:FE4	0.87	0.88
1:a:56:HIS:CB	11:a:1103:CLA:HBB2	2.02	0.88
14:B:4004:BCR:H403	14:B:4004:BCR:H23C	1.58	0.85
3:3:11:CYS:HG	13:3:3003:SF4:FE3	0.88	0.85
14:b:4004:BCR:H403	14:b:4004:BCR:H23C	1.58	0.85
3:c:11:CYS:HG	13:c:3003:SF4:FE3	0.54	0.84
3:3:48:CYS:SG	13:3:3002:SF4:S1	2.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:4018:BCR:H14C	9:I:23:PRO:CG	2.08	0.83
3:3:17:CYS:SG	13:3:3003:SF4:FE4	1.71	0.82
3:c:58:CYS:HG	13:c:3003:SF4:FE1	0.85	0.82
11:a:1127:CLA:HHC	11:a:1127:CLA:HBB1	1.62	0.81
11:A:1123:CLA:HHC	11:A:1123:CLA:HBB1	1.63	0.81
3:C:48:CYS:SG	13:C:3002:SF4:S1	2.79	0.80
14:L:4019:BCR:H321	14:L:4019:BCR:HC8	1.62	0.80
11:A:1134:CLA:HHC	11:A:1134:CLA:HBB1	1.63	0.80
3:3:58:CYS:SG	13:3:3003:SF4:S2	2.80	0.80
1:1:395:TRP:CD1	11:1:1126:CLA:HAB	2.17	0.80
1:a:56:HIS:ND1	11:a:1103:CLA:CBB	2.45	0.79
1:a:574:CYS:SG	13:a:3001:SF4:S3	2.80	0.79
11:a:1103:CLA:H51	11:a:1111:CLA:H12	1.64	0.79
11:a:1801:CLA:C1C	15:a:5003:LHG:HC31	2.13	0.79
11:A:1801:CLA:HHC	11:A:1801:CLA:HBB1	1.65	0.79
11:B:1227:CLA:HBC3	11:B:1227:CLA:HHD	1.65	0.78
14:2:4004:BCR:H403	14:2:4004:BCR:H23C	1.65	0.78
1:A:583:CYS:SG	13:A:3001:SF4:FE2	1.75	0.78
11:A:1140:CLA:HHC	11:A:1140:CLA:HBB1	1.67	0.77
3:c:58:CYS:SG	13:c:3003:SF4:S2	2.82	0.77
11:1:1107:CLA:HHC	11:1:1107:CLA:HBB1	1.67	0.77
3:3:11:CYS:SG	13:3:3003:SF4:S2	2.81	0.77
6:f:10:THR:CB	14:f:4013:BCR:H401	2.14	0.77
1:A:395:TRP:CD1	11:A:1126:CLA:HAB	2.20	0.77
11:1:1131:CLA:HAB	11:1:1132:CLA:HHB	1.66	0.76
7:8:96:LEU:HG	14:8:4019:BCR:H24C	1.67	0.76
11:2:1231:CLA:HHC	11:2:1231:CLA:HBB1	1.65	0.76
1:A:354:ILE:HD11	14:A:4007:BCR:HC7	1.66	0.76
14:A:4001:BCR:H331	14:A:4002:BCR:H24C	1.66	0.76
14:B:4014:BCR:HC21	11:B:1229:CLA:HBB2	1.68	0.76
3:3:21:CYS:SG	13:3:3002:SF4:S1	2.78	0.75
11:a:1237:CLA:HHC	11:a:1237:CLA:HBB1	1.69	0.75
11:a:1128:CLA:HHC	11:a:1128:CLA:HBB1	1.68	0.75
14:B:4014:BCR:HC21	11:B:1229:CLA:CBB	2.17	0.74
1:A:193:VAL:CG1	11:A:1123:CLA:HHD	2.17	0.74
14:8:4019:BCR:H321	14:8:4019:BCR:HC8	1.69	0.74
11:a:1116:CLA:HHC	11:a:1116:CLA:HBB1	1.69	0.74
11:A:1129:CLA:HHC	11:A:1129:CLA:HBB1	1.70	0.74
11:B:1229:CLA:HHC	11:B:1229:CLA:HBB1	1.69	0.74
11:a:1125:CLA:HHC	11:a:1125:CLA:HBB1	1.68	0.74
6:F:12:PRO:HG2	14:F:4013:BCR:H401	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:4001:BCR:C33	14:a:4002:BCR:H24C	2.16	0.74
11:b:1214:CLA:HHC	11:b:1214:CLA:HBB1	1.68	0.74
11:a:1110:CLA:HHC	11:a:1110:CLA:HBB1	1.69	0.73
1:a:56:HIS:CB	11:a:1103:CLA:CBB	2.63	0.73
14:l:4019:BCR:H321	14:l:4019:BCR:HC8	1.69	0.73
11:1:1125:CLA:HBC2	11:1:1125:CLA:HHD	1.70	0.73
11:a:1111:CLA:HHC	11:a:1111:CLA:HBB1	1.71	0.73
14:f:4018:BCR:H402	14:f:4020:BCR:H353	1.68	0.73
11:b:1021:CLA:HHC	11:b:1021:CLA:HBB1	1.69	0.73
3:3:21:CYS:SG	13:3:3002:SF4:S3	2.80	0.73
11:k:1402:CLA:HHC	11:k:1402:CLA:HBB1	1.70	0.72
2:2:426:PHE:O	2:2:430:HIS:ND1	2.23	0.72
2:B:656:THR:HA	11:B:1023:CLA:HAB	1.72	0.72
11:B:1229:CLA:H201	11:B:1235:CLA:C15	2.20	0.72
2:b:426:PHE:CE2	11:b:1235:CLA:HAB	2.24	0.72
11:A:1110:CLA:HHC	11:A:1110:CLA:HBB1	1.70	0.72
6:f:12:PRO:HB3	14:f:4013:BCR:H19C	1.71	0.71
1:1:571:ARG:NH1	15:1:5001:LHG:O10	2.23	0.71
11:1:1128:CLA:HHC	11:1:1128:CLA:HBB1	1.72	0.71
14:F:4013:BCR:H392	14:F:4013:BCR:H23C	1.72	0.71
14:6:4018:BCR:H14C	9:9:23:PRO:CG	2.21	0.71
14:6:4013:BCR:H23C	14:6:4013:BCR:H392	1.72	0.71
11:A:1126:CLA:H42	14:B:4011:BCR:HC7	1.73	0.71
11:a:1134:CLA:HHC	11:a:1134:CLA:HBB1	1.72	0.71
1:a:571:ARG:NH1	15:a:5001:LHG:O10	2.24	0.71
14:2:4009:BCR:H353	15:2:5004:LHG:H202	1.72	0.70
11:1:1106:CLA:H191	11:1:1109:CLA:H91	1.73	0.70
11:A:1101:CLA:H202	11:A:1126:CLA:H203	1.73	0.70
1:A:330:GLY:HA3	15:A:5003:LHG:HC32	1.73	0.70
1:1:330:GLY:HA3	15:1:5003:LHG:HC32	1.72	0.70
11:A:1136:CLA:HBB1	11:A:1136:CLA:HHC	1.74	0.70
11:2:1220:CLA:HBC2	11:2:1220:CLA:HHD	1.73	0.70
3:c:58:CYS:SG	13:c:3003:SF4:S3	2.85	0.70
11:b:1227:CLA:HBC3	11:b:1227:CLA:HHD	1.73	0.69
2:b:656:THR:HA	11:b:1023:CLA:HAB	1.75	0.69
2:2:309:LYS:O	15:2:5004:LHG:HC31	1.93	0.69
14:1:4008:BCR:C8	11:1:1124:CLA:HAB	2.21	0.69
2:b:415:ALA:O	2:b:419:HIS:ND1	2.26	0.69
15:1:5001:LHG:H202	11:1:1128:CLA:H202	1.75	0.69
14:b:4006:BCR:H392	14:b:4006:BCR:H23C	1.74	0.69
2:b:309:LYS:O	15:b:5004:LHG:HC31	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1238:CLA:H142	14:F:4020:BCR:HC8	1.75	0.68
11:L:1501:CLA:H43	14:L:4022:BCR:H14C	1.73	0.68
11:B:1222:CLA:HMB3	11:B:1223:CLA:H202	1.74	0.68
11:1:1104:CLA:HHC	11:1:1104:CLA:HBB1	1.74	0.68
3:c:48:CYS:SG	13:c:3002:SF4:S1	2.92	0.68
11:1:1115:CLA:CHD	11:0:1401:CLA:HBA1	2.24	0.68
11:1:1012:CLA:C1B	11:2:1021:CLA:H203	2.24	0.68
14:A:4008:BCR:C8	11:A:1124:CLA:HAB	2.24	0.67
11:1:1110:CLA:HHC	11:1:1110:CLA:HBB1	1.76	0.67
11:1:1131:CLA:HAB	11:1:1132:CLA:CHB	2.25	0.67
4:D:82:ASP:OD1	4:D:82:ASP:N	2.28	0.67
7:l:96:LEU:HG	14:l:4019:BCR:H24C	1.76	0.67
11:1:1012:CLA:C2B	11:2:1021:CLA:H203	2.25	0.67
2:2:426:PHE:CE2	11:2:1235:CLA:HAB	2.29	0.67
2:B:654:TRP:CD2	11:B:1021:CLA:HMA2	2.29	0.67
11:B:1238:CLA:C14	14:F:4020:BCR:HC8	2.25	0.67
1:A:681:PHE:HA	11:B:1013:CLA:HAB	1.75	0.67
14:a:4008:BCR:HC8	11:a:1124:CLA:HAB	1.75	0.67
2:B:23:TYR:CE2	16:B:5002:LMG:HC71	2.31	0.66
2:2:426:PHE:CD2	11:2:1235:CLA:HAB	2.31	0.66
14:A:4003:BCR:H403	14:A:4003:BCR:H23C	1.78	0.66
11:b:1223:CLA:HBC3	11:b:1223:CLA:HHD	1.78	0.66
14:B:4005:BCR:H343	11:B:1209:CLA:HMC1	1.76	0.66
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC2	1.77	0.66
14:F:4018:BCR:H14C	9:I:23:PRO:HG3	1.77	0.66
1:a:560:ARG:O	4:d:61:ARG:NH1	2.29	0.66
14:B:4009:BCR:H23C	11:B:1227:CLA:CBC	2.26	0.65
14:b:4004:BCR:H14C	11:b:1217:CLA:HBB1	1.78	0.65
14:A:4007:BCR:H19C	11:A:1122:CLA:H43	1.76	0.65
2:b:426:PHE:O	2:b:430:HIS:ND1	2.30	0.65
6:F:12:PRO:CG	14:F:4013:BCR:H401	2.27	0.65
2:B:546:ASP:OD2	3:C:66:ARG:NH1	2.29	0.65
3:C:48:CYS:SG	13:C:3002:SF4:S2	2.95	0.65
11:8:1501:CLA:HBA2	14:8:4022:BCR:H363	1.77	0.65
11:A:1124:CLA:H12	11:A:1135:CLA:HMA2	1.78	0.65
15:1:5003:LHG:H302	11:1:1137:CLA:H102	1.79	0.65
8:M:16:LEU:CD2	14:M:4021:BCR:H19C	2.27	0.65
13:A:3001:SF4:S2	2:B:565:CYS:SG	2.95	0.64
14:b:4017:BCR:HC7	11:b:1205:CLA:C10	2.27	0.64
1:a:395:TRP:CD1	11:a:1126:CLA:HAB	2.33	0.64
14:1:4001:BCR:C33	14:1:4002:BCR:H24C	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:56:HIS:HB3	11:a:1103:CLA:CBB	2.26	0.64
1:1:312:ARG:NH2	1:1:316:GLY:O	2.29	0.64
1:a:574:CYS:HG	13:a:3001:SF4:FE4	1.15	0.64
11:b:1222:CLA:CBA	11:b:1223:CLA:OBD	2.45	0.64
14:a:4001:BCR:H333	14:a:4002:BCR:H24C	1.78	0.64
11:B:1222:CLA:CMB	11:B:1223:CLA:H202	2.28	0.64
16:2:5002:LMG:H202	11:2:1201:CLA:HBC1	1.80	0.64
3:3:14:CYS:SG	13:3:3003:SF4:S4	2.95	0.64
11:b:1206:CLA:H43	14:f:4018:BCR:H342	1.80	0.63
10:K:102:PRO:O	10:K:106:ALA:N	2.30	0.63
1:a:330:GLY:HA3	15:a:5003:LHG:HC32	1.79	0.63
14:2:4009:BCR:H23C	11:2:1227:CLA:HBC1	1.79	0.63
2:B:530:ILE:HG12	11:B:1013:CLA:HMD3	1.79	0.63
2:B:656:THR:CA	11:B:1023:CLA:HAB	2.28	0.63
11:A:1137:CLA:HAB	11:A:1129:CLA:CBB	2.29	0.63
1:a:79:HIS:CE1	11:a:1103:CLA:HMA2	2.34	0.63
1:A:597:TRP:HH2	11:A:1022:CLA:HAB	1.64	0.62
11:a:1132:CLA:H201	14:l:4022:BCR:H343	1.81	0.62
1:A:597:TRP:CH2	11:A:1022:CLA:HAB	2.34	0.62
11:2:1212:CLA:HHC	11:2:1212:CLA:HBB1	1.81	0.62
7:L:96:LEU:HG	14:L:4019:BCR:H24C	1.80	0.62
11:b:1221:CLA:HMB3	11:b:1223:CLA:H8	1.82	0.62
1:1:597:TRP:CH2	11:1:1022:CLA:HAB	2.34	0.62
11:A:1138:CLA:HHD	14:B:4014:BCR:C38	2.30	0.62
2:B:415:ALA:O	2:B:419:HIS:ND1	2.33	0.62
11:1:1022:CLA:H172	14:2:4017:BCR:H343	1.82	0.62
13:1:3001:SF4:S2	2:2:565:CYS:SG	2.97	0.62
11:1:1112:CLA:CMC	11:1:1113:CLA:HAB	2.30	0.61
11:a:1012:CLA:CHB	11:b:1021:CLA:H202	2.30	0.61
11:2:1206:CLA:H43	14:6:4018:BCR:H342	1.81	0.61
14:6:4018:BCR:H14C	9:9:23:PRO:HG3	1.82	0.61
11:b:1220:CLA:HMB3	11:b:1240:CLA:HAB	1.81	0.61
11:K:1402:CLA:HHC	11:K:1402:CLA:HBB1	1.81	0.61
11:A:1125:CLA:CBC	11:A:1125:CLA:HHD	2.31	0.61
8:m:16:LEU:HD23	14:m:4021:BCR:H19C	1.82	0.61
11:A:1115:CLA:HBC3	11:A:1115:CLA:HHD	1.83	0.61
14:a:4007:BCR:H352	11:a:1119:CLA:H71	1.82	0.61
11:2:1206:CLA:H201	9:9:23:PRO:HA	1.83	0.61
11:1:1106:CLA:HHC	11:1:1106:CLA:HBB1	1.82	0.61
1:A:677:PHE:CD1	14:B:4011:BCR:H363	2.35	0.61
14:A:4008:BCR:HC8	11:A:1124:CLA:HAB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:677:PHE:CG	14:2:4011:BCR:H363	2.35	0.61
11:1:1801:CLA:C1C	15:1:5003:LHG:HC31	2.31	0.60
11:1:1137:CLA:HAB	11:1:1129:CLA:CBB	2.32	0.60
2:2:520:ILE:HD13	11:2:1234:CLA:HAB	1.83	0.60
14:2:4017:BCR:H342	11:2:1205:CLA:C10	2.32	0.60
11:a:1131:CLA:H192	11:b:1023:CLA:H201	1.83	0.60
11:b:1225:CLA:C16	11:b:1211:CLA:HAB	2.31	0.60
6:6:10:THR:CB	14:6:4013:BCR:H401	2.31	0.60
11:L:1501:CLA:C4	14:L:4022:BCR:H14C	2.32	0.60
11:A:1119:CLA:HHD	11:A:1119:CLA:HBC2	1.82	0.60
11:a:1126:CLA:C4	14:b:4011:BCR:HC7	2.31	0.59
1:1:597:TRP:HH2	11:1:1022:CLA:HAB	1.67	0.59
2:2:312:LEU:HD23	15:2:5004:LHG:HC61	1.85	0.59
2:B:488:ALA:O	2:B:490:TRP:N	2.35	0.59
11:B:1210:CLA:HHD	11:B:1210:CLA:HBC2	1.85	0.59
7:L:41:ARG:NH2	7:L:52:GLU:OE2	2.35	0.59
1:a:681:PHE:HA	11:b:1013:CLA:HAB	1.85	0.59
14:1:4008:BCR:HC8	11:1:1124:CLA:HAB	1.84	0.59
11:2:1214:CLA:H92	11:2:1231:CLA:O1A	2.03	0.59
2:B:188:LEU:HD21	14:B:4004:BCR:H331	1.85	0.59
14:a:4002:BCR:H14C	11:a:1112:CLA:HBB1	1.84	0.59
14:b:4010:BCR:HC41	11:b:1223:CLA:HMA3	1.85	0.58
2:B:381:MET:HE1	14:B:4010:BCR:H361	1.85	0.58
3:C:14:CYS:HG	13:C:3003:SF4:FE2	1.15	0.58
14:1:4007:BCR:H341	11:1:1123:CLA:HAB	1.86	0.58
2:2:312:LEU:HD22	15:2:5004:LHG:HC42	1.85	0.58
3:C:21:CYS:SG	13:C:3002:SF4:S3	2.84	0.58
14:F:4018:BCR:H402	14:F:4020:BCR:H353	1.86	0.58
11:b:1205:CLA:C1A	11:b:1205:CLA:CGA	2.82	0.58
1:1:302:VAL:HG22	14:1:4001:BCR:H352	1.83	0.58
11:2:1231:CLA:C4C	11:2:1232:CLA:HAB	2.34	0.58
2:B:63:GLY:HA3	11:B:1204:CLA:HAB	1.85	0.58
11:2:1205:CLA:HAB	11:2:1206:CLA:HAA2	1.85	0.58
4:D:61:ARG:NH2	4:D:63:GLU:OE1	2.36	0.58
2:b:656:THR:CA	11:b:1023:CLA:HAB	2.33	0.58
14:2:4014:BCR:HC21	11:2:1229:CLA:CBB	2.34	0.58
3:c:14:CYS:SG	13:c:3003:SF4:S3	3.02	0.58
11:A:1022:CLA:H172	14:B:4017:BCR:H343	1.85	0.58
11:2:1205:CLA:C1A	11:2:1205:CLA:CGA	2.81	0.58
2:b:299:HIS:NE2	11:b:1219:CLA:OBD	2.35	0.58
2:b:426:PHE:HE2	11:b:1235:CLA:HAB	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:16:LEU:HD23	14:7:4021:BCR:H19C	1.84	0.58
10:k:102:PRO:O	10:k:106:ALA:N	2.36	0.58
14:B:4005:BCR:HC8	14:B:4005:BCR:H321	1.86	0.57
11:B:1205:CLA:C1A	11:B:1205:CLA:CGA	2.82	0.57
11:1:1133:CLA:HHC	11:1:1133:CLA:HBB1	1.86	0.57
14:2:4014:BCR:HC21	11:2:1229:CLA:HBB1	1.86	0.57
11:B:1202:CLA:H161	11:B:1210:CLA:HMD2	1.86	0.57
2:2:530:ILE:HG12	11:2:1013:CLA:HMD3	1.85	0.57
11:2:1204:CLA:H2	14:6:4018:BCR:HC32	1.86	0.57
14:A:4007:BCR:HC41	11:A:1119:CLA:H191	1.86	0.57
2:2:488:ALA:O	2:2:490:TRP:N	2.37	0.57
4:d:82:ASP:OD1	4:d:82:ASP:N	2.38	0.57
11:A:1125:CLA:C4B	11:A:1133:CLA:HMA3	2.35	0.57
11:A:1126:CLA:C4C	14:B:4011:BCR:HC42	2.34	0.57
14:f:4020:BCR:H333	7:l:87:ALA:HB3	1.85	0.57
14:2:4009:BCR:H23C	11:2:1227:CLA:CBC	2.34	0.57
14:f:4018:BCR:H14C	9:i:23:PRO:CG	2.34	0.57
14:f:4013:BCR:H392	14:f:4013:BCR:H23C	1.87	0.57
14:1:4003:BCR:H321	14:1:4003:BCR:HC8	1.86	0.57
8:7:16:LEU:CD2	14:7:4021:BCR:H19C	2.35	0.57
11:A:1138:CLA:HBB1	11:A:1138:CLA:HHC	1.87	0.57
14:2:4005:BCR:H321	14:2:4005:BCR:HC8	1.86	0.57
11:B:1201:CLA:HMA2	8:M:29:LEU:HD23	1.86	0.57
11:2:1240:CLA:HHC	11:2:1240:CLA:HBB1	1.87	0.57
11:a:1801:CLA:HMA2	15:a:5003:LHG:HC62	1.87	0.57
11:1:1106:CLA:H191	11:1:1109:CLA:C9	2.33	0.57
11:A:1131:CLA:H203	11:B:1023:CLA:H201	1.85	0.56
11:1:1115:CLA:C1D	11:0:1401:CLA:HBA1	2.35	0.56
14:6:4020:BCR:HC22	9:9:20:TRP:CD1	2.40	0.56
8:M:16:LEU:HD23	14:M:4021:BCR:H19C	1.87	0.56
8:m:16:LEU:CD2	14:m:4021:BCR:H19C	2.36	0.56
1:1:50:ASN:ND2	15:1:5001:LHG:HC12	2.21	0.56
14:1:4008:BCR:C8	14:1:4008:BCR:H331	2.35	0.56
1:A:193:VAL:HG13	11:A:1123:CLA:HMD3	1.88	0.56
1:A:548:ILE:HG12	11:B:1023:CLA:HMD3	1.88	0.56
14:b:4010:BCR:C19	11:b:1223:CLA:H111	2.35	0.56
5:5:13:ARG:NH1	5:5:65:GLU:OE2	2.39	0.56
1:A:684:MET:HE2	12:A:2001:PQN:H2M3	1.87	0.56
11:B:1224:CLA:HBC2	11:B:1224:CLA:HHD	1.86	0.56
14:b:4010:BCR:H392	14:b:4010:BCR:H23C	1.88	0.56
14:2:4014:BCR:H333	11:2:1230:CLA:H51	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:8:1501:CLA:C4	14:8:4022:BCR:H14C	2.35	0.56
11:A:1012:CLA:CHB	11:B:1021:CLA:H202	2.36	0.56
2:B:273:ILE:O	2:B:277:HIS:ND1	2.39	0.56
5:5:42:ASP:OD2	5:5:43:ARG:NH1	2.39	0.56
12:2:2002:PQN:H302	11:2:1239:CLA:C1	2.36	0.55
1:A:395:TRP:NE1	11:A:1126:CLA:HAB	2.22	0.55
14:A:4003:BCR:H23C	14:A:4003:BCR:C40	2.36	0.55
11:A:1114:CLA:HHC	11:A:1114:CLA:HBB1	1.89	0.55
11:l:1501:CLA:H41	14:l:4022:BCR:H14C	1.88	0.55
11:1:1801:CLA:HMA1	15:1:5003:LHG:HC62	1.88	0.55
3:3:11:CYS:SG	13:3:3003:SF4:S4	3.04	0.55
1:1:199:HIS:O	1:1:203:GLY:N	2.40	0.55
11:2:1227:CLA:HBC3	11:2:1227:CLA:HHD	1.88	0.55
1:a:211:GLY:CA	14:a:4002:BCR:H363	2.36	0.55
1:a:677:PHE:CG	14:b:4011:BCR:H363	2.41	0.55
14:b:4014:BCR:HC21	11:b:1229:CLA:HBB2	1.89	0.55
11:b:1220:CLA:HHD	11:b:1220:CLA:HBC2	1.88	0.55
14:1:4001:BCR:HC42	11:1:1113:CLA:HBB1	1.87	0.55
10:k:120:LEU:HD13	11:k:1401:CLA:H11	1.87	0.55
15:B:5004:LHG:H262	15:B:5004:LHG:HC82	1.88	0.55
1:a:560:ARG:NH2	4:d:15:THR:O	2.40	0.55
11:a:1119:CLA:HMB2	11:a:1123:CLA:CED	2.37	0.55
2:2:645:TRP:CZ3	14:2:4017:BCR:HC21	2.41	0.55
11:A:1104:CLA:CMD	11:A:1106:CLA:H202	2.37	0.55
1:a:679:PHE:CD2	11:a:1011:CLA:HMA3	2.42	0.55
11:b:1208:CLA:HHC	11:b:1208:CLA:HBB1	1.88	0.55
2:b:530:ILE:HG12	11:b:1013:CLA:HMD3	1.87	0.55
2:2:176:ASN:HB3	11:2:1217:CLA:HMD2	1.89	0.55
2:B:5:PHE:CG	2:B:6:PRO:CD	2.90	0.55
3:C:54:CYS:SG	13:C:3002:SF4:S4	2.99	0.55
14:A:4008:BCR:H342	11:A:1124:CLA:CHC	2.37	0.54
11:a:1801:CLA:HAB	11:a:1122:CLA:HMB1	1.89	0.54
1:A:193:VAL:HG11	11:A:1123:CLA:HHD	1.89	0.54
11:1:1801:CLA:HBB1	11:1:1121:CLA:HAB	1.89	0.54
11:1:1106:CLA:C9	11:1:1128:CLA:H203	2.38	0.54
1:A:391:THR:OG1	11:A:1126:CLA:HMB2	2.08	0.54
14:2:4017:BCR:C8	14:2:4017:BCR:H331	2.38	0.54
11:0:1402:CLA:HHC	11:0:1402:CLA:HBB1	1.90	0.54
11:a:1801:CLA:HAB	11:a:1122:CLA:HHB	1.89	0.54
1:A:211:GLY:CA	14:A:4002:BCR:H363	2.38	0.54
1:a:677:PHE:CD1	14:b:4011:BCR:H363	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:4009:BCR:H321	14:b:4009:BCR:HC8	1.89	0.54
14:b:4010:BCR:H14C	11:b:1222:CLA:HMA3	1.90	0.54
11:b:1228:CLA:HHC	11:b:1228:CLA:HBB1	1.88	0.54
11:1:1101:CLA:H203	11:1:1140:CLA:H152	1.90	0.54
2:2:63:GLY:HA3	11:2:1204:CLA:HAB	1.90	0.54
11:2:1201:CLA:HMA2	8:7:29:LEU:HD23	1.89	0.54
1:A:571:ARG:HD2	15:A:5001:LHG:HC42	1.89	0.54
2:B:130:THR:OG1	2:B:201:GLU:OE1	2.26	0.54
8:M:12:LEU:HD13	14:M:4021:BCR:H372	1.89	0.54
11:b:1221:CLA:CMB	11:b:1223:CLA:H8	2.38	0.54
11:B:1238:CLA:O1A	14:L:4019:BCR:H363	2.08	0.54
2:b:5:PHE:CG	2:b:6:PRO:CD	2.90	0.54
2:B:349:HIS:ND1	11:B:1214:CLA:OBD	2.37	0.53
2:b:58:PHE:CE1	14:b:4005:BCR:H373	2.43	0.53
14:b:4017:BCR:H342	11:b:1205:CLA:C10	2.38	0.53
11:A:1101:CLA:C20	11:A:1126:CLA:H203	2.38	0.53
14:b:4010:BCR:C19	11:b:1223:CLA:H93	2.38	0.53
11:A:1801:CLA:C1C	15:A:5003:LHG:HC31	2.38	0.53
14:A:4008:BCR:H353	11:A:1119:CLA:H62	1.90	0.53
2:b:656:THR:N	11:b:1023:CLA:HAB	2.23	0.53
14:1:4002:BCR:HC41	11:1:1103:CLA:H142	1.91	0.53
11:1:1137:CLA:HAB	11:1:1129:CLA:HBB2	1.91	0.53
1:A:574:CYS:HB3	1:A:583:CYS:HA	1.90	0.53
11:b:1225:CLA:H162	11:b:1211:CLA:HAB	1.91	0.53
14:b:4014:BCR:HC21	11:b:1229:CLA:CBB	2.39	0.53
2:2:5:PHE:CG	2:2:6:PRO:CD	2.92	0.53
2:B:210:ASP:OD1	2:B:211:ASN:ND2	2.38	0.53
12:a:2001:PQN:H243	11:b:1013:CLA:H202	1.90	0.53
1:1:263:PHE:CE2	14:1:4001:BCR:H343	2.43	0.53
2:2:546:ASP:OD2	3:3:66:ARG:NH1	2.41	0.53
11:a:1112:CLA:CMC	11:a:1113:CLA:HAB	2.38	0.53
11:l:1501:CLA:H202	11:l:1503:CLA:C1	2.40	0.53
1:A:332:PHE:HB2	15:A:5003:LHG:HC41	1.91	0.52
1:A:681:PHE:CA	11:B:1013:CLA:HAB	2.39	0.52
8:M:16:LEU:HD21	14:M:4021:BCR:H19C	1.90	0.52
4:d:61:ARG:NH2	4:d:63:GLU:OE1	2.41	0.52
3:3:11:CYS:SG	13:3:3003:SF4:S1	3.07	0.52
14:B:4006:BCR:H372	11:B:1225:CLA:H142	1.92	0.52
3:C:54:CYS:SG	13:C:3002:SF4:S2	3.08	0.52
7:L:55:MET:HB3	14:L:4022:BCR:H19C	1.92	0.52
11:a:1106:CLA:HHC	11:a:1106:CLA:HBB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:1204:CLA:H93	14:f:4018:BCR:HC31	1.90	0.52
11:a:1110:CLA:HAB	11:a:1118:CLA:H61	1.91	0.52
1:1:680:ALA:C	11:2:1013:CLA:HAB	2.34	0.52
14:b:4010:BCR:H19C	11:b:1223:CLA:H111	1.92	0.52
14:b:4017:BCR:H362	11:b:1023:CLA:H143	1.91	0.52
2:2:349:HIS:ND1	11:2:1214:CLA:OBD	2.42	0.52
14:B:4009:BCR:C13	15:B:5004:LHG:H202	2.39	0.52
2:b:283:ILE:HD13	11:b:1214:CLA:HMC1	1.92	0.52
1:A:678:VAL:HG11	11:A:1140:CLA:HMB2	1.92	0.52
1:1:548:ILE:HG12	11:2:1023:CLA:HMD3	1.90	0.52
10:0:102:PRO:O	10:0:106:ALA:N	2.41	0.52
11:b:1238:CLA:C2	14:l:4019:BCR:H363	2.39	0.51
1:1:560:ARG:NH2	4:4:15:THR:O	2.44	0.51
9:9:7:ALA:N	8:7:5:ASP:OD1	2.41	0.51
11:8:1503:CLA:HBC1	14:8:4022:BCR:H341	1.91	0.51
2:B:520:ILE:HD13	11:B:1234:CLA:HAB	1.92	0.51
6:F:30:ASN:O	6:F:32:PHE:N	2.43	0.51
11:A:1237:CLA:HHC	11:A:1237:CLA:HBB1	1.92	0.51
2:b:273:ILE:O	2:b:277:HIS:ND1	2.41	0.51
15:b:5004:LHG:HC62	11:b:1220:CLA:HBB1	1.93	0.51
14:B:4011:BCR:H23C	14:B:4011:BCR:H392	1.92	0.51
1:a:441:ASN:ND2	11:a:1237:CLA:OBD	2.43	0.51
2:B:337:ALA:HB2	14:B:4010:BCR:H372	1.93	0.51
2:B:656:THR:N	11:B:1023:CLA:HAB	2.26	0.51
2:b:488:ALA:O	2:b:490:TRP:N	2.42	0.51
3:3:48:CYS:SG	13:3:3002:SF4:S3	2.99	0.51
11:a:1125:CLA:HED1	11:a:1133:CLA:HAB	1.92	0.51
3:c:11:CYS:SG	13:c:3003:SF4:S4	3.06	0.51
1:1:193:VAL:CG1	11:1:1123:CLA:HHD	2.41	0.51
2:b:546:ASP:OD2	3:c:66:ARG:NH1	2.43	0.51
1:1:298:LEU:HD21	11:1:1115:CLA:HMB1	1.92	0.51
14:2:4014:BCR:H382	14:2:4014:BCR:H23C	1.91	0.51
14:A:4008:BCR:C8	14:A:4008:BCR:H331	2.41	0.51
2:B:426:PHE:O	2:B:430:HIS:ND1	2.37	0.51
2:B:571:ASP:OD1	2:B:703:ARG:NH2	2.44	0.51
14:B:4010:BCR:H392	14:B:4010:BCR:H23C	1.93	0.51
11:B:1013:CLA:HMA2	11:B:1013:CLA:H2	1.91	0.51
1:1:395:TRP:HD1	11:1:1126:CLA:HAB	1.71	0.51
14:6:4020:BCR:HC22	9:9:20:TRP:NE1	2.26	0.51
1:A:725:ALA:HB2	15:A:5001:LHG:HC62	1.91	0.51
11:B:1228:CLA:HMC2	11:B:1236:CLA:HAC2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:56:HIS:CE1	11:a:1103:CLA:CBB	2.94	0.51
5:e:12:LYS:NZ	5:e:67:GLU:OE1	2.28	0.51
14:2:4017:BCR:H362	11:2:1023:CLA:H111	1.93	0.51
7:8:41:ARG:NH2	7:8:52:GLU:OE2	2.41	0.51
11:a:1119:CLA:HBB1	11:a:1119:CLA:HHC	1.93	0.51
11:a:1012:CLA:H42	14:b:4011:BCR:H362	1.93	0.50
1:1:456:ILE:HG21	11:1:1132:CLA:HMC1	1.93	0.50
2:2:654:TRP:CD2	11:2:1021:CLA:HMA2	2.47	0.50
2:B:487:GLY:O	2:B:489:ALA:N	2.44	0.50
14:2:4009:BCR:H353	15:2:5004:LHG:C20	2.40	0.50
11:8:1501:CLA:H41	14:8:4022:BCR:H14C	1.93	0.50
11:L:1501:CLA:HBA2	14:L:4022:BCR:H363	1.94	0.50
3:3:48:CYS:SG	13:3:3002:SF4:S2	3.08	0.50
14:b:4009:BCR:H23C	11:b:1227:CLA:CBC	2.40	0.50
11:l:1501:CLA:H202	11:l:1503:CLA:C2	2.42	0.50
11:B:1013:CLA:CGA	11:B:1013:CLA:H3A	2.42	0.50
1:a:267:ASN:O	1:a:269:GLY:N	2.43	0.50
2:2:436:VAL:HB	11:2:1230:CLA:HMC2	1.94	0.50
11:2:1238:CLA:O1A	14:8:4019:BCR:H363	2.12	0.50
14:A:4003:BCR:H353	11:A:1111:CLA:C15	2.42	0.50
1:a:538:HIS:ND1	11:a:1135:CLA:HAB	2.27	0.50
3:c:11:CYS:SG	13:c:3003:SF4:S2	3.08	0.50
6:f:12:PRO:CB	14:f:4013:BCR:H19C	2.42	0.50
11:B:1212:CLA:HAB	11:B:1211:CLA:HMC1	1.92	0.50
11:b:1212:CLA:HHC	11:b:1212:CLA:HBB1	1.93	0.50
11:B:1226:CLA:HHC	11:B:1226:CLA:HBB1	1.94	0.50
3:c:11:CYS:SG	13:c:3003:SF4:S1	3.10	0.50
3:C:14:CYS:SG	13:C:3003:SF4:S4	3.10	0.49
11:a:1133:CLA:HMB1	11:a:1135:CLA:HED1	1.93	0.49
1:1:332:PHE:O	1:1:428:ARG:NH2	2.45	0.49
1:1:354:ILE:HD11	14:1:4007:BCR:HC7	1.94	0.49
1:1:681:PHE:HA	11:2:1013:CLA:HAB	1.93	0.49
11:1:1130:CLA:HHC	11:1:1130:CLA:HBB1	1.94	0.49
11:1:1133:CLA:HHC	11:1:1133:CLA:CBB	2.42	0.49
1:1:589:ASP:OD1	1:1:724:ARG:NH1	2.44	0.49
2:2:415:ALA:O	2:2:419:HIS:ND1	2.43	0.49
11:A:1138:CLA:HHD	14:B:4014:BCR:H381	1.94	0.49
1:1:677:PHE:CD1	14:2:4011:BCR:H363	2.47	0.49
1:a:199:HIS:O	1:a:203:GLY:N	2.44	0.49
11:1:1237:CLA:H3A	14:6:4020:BCR:H401	1.94	0.49
11:1:1022:CLA:H203	11:2:1206:CLA:H51	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LYS:O	15:B:5004:LHG:HC31	2.12	0.49
11:B:1212:CLA:HAB	11:B:1211:CLA:CMC	2.43	0.49
1:A:199:HIS:O	1:A:203:GLY:N	2.44	0.49
1:1:460:THR:HG23	11:2:1206:CLA:HMC1	1.93	0.49
7:8:137:VAL:HG23	14:8:4022:BCR:H403	1.93	0.49
1:a:391:THR:OG1	11:a:1126:CLA:HMB1	2.12	0.49
11:a:1119:CLA:HMB2	11:a:1123:CLA:HED2	1.95	0.49
11:2:1212:CLA:HHC	11:2:1212:CLA:CBB	2.43	0.49
6:6:12:PRO:CG	14:6:4013:BCR:H403	2.43	0.49
1:A:454:LEU:HD23	11:A:1132:CLA:HAB	1.95	0.49
11:A:1125:CLA:HHD	11:A:1125:CLA:HBC3	1.94	0.49
1:a:680:ALA:C	11:b:1013:CLA:HAB	2.38	0.49
11:b:1229:CLA:HHC	11:b:1229:CLA:HBB1	1.94	0.49
14:1:4007:BCR:H352	11:1:1119:CLA:H71	1.94	0.49
14:8:4019:BCR:H392	14:8:4019:BCR:H23C	1.94	0.49
10:K:90:LEU:CB	10:K:91:PRO:CD	2.91	0.49
11:a:1138:CLA:HHD	14:b:4014:BCR:C38	2.43	0.49
2:2:312:LEU:CD2	15:2:5004:LHG:HC42	2.43	0.49
10:k:117:GLY:HA3	11:k:1401:CLA:C3B	2.43	0.49
11:A:1022:CLA:C17	14:B:4017:BCR:H343	2.43	0.48
2:b:334:LEU:HB3	14:b:4010:BCR:H401	1.94	0.48
1:1:267:ASN:O	1:1:269:GLY:N	2.45	0.48
14:2:4014:BCR:HC41	11:2:1229:CLA:CBB	2.43	0.48
14:2:4011:BCR:H321	14:2:4011:BCR:HC8	1.95	0.48
11:8:1501:CLA:H202	11:8:1503:CLA:H2	1.95	0.48
1:a:540:PHE:HE2	11:a:1022:CLA:HAB	1.79	0.48
11:1:1106:CLA:H91	11:1:1106:CLA:H111	1.72	0.48
2:2:587:LEU:CD1	11:2:1234:CLA:HBB2	2.44	0.48
1:A:352:LEU:HD11	11:A:1128:CLA:HBB1	1.94	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:C8	2.44	0.48
11:B:1223:CLA:HED1	11:B:1231:CLA:HAB	1.94	0.48
3:c:21:CYS:SG	13:c:3002:SF4:S3	2.93	0.48
11:2:1238:CLA:HHC	11:2:1238:CLA:HBB1	1.96	0.48
1:A:215:HIS:HB2	11:A:1112:CLA:CHC	2.44	0.48
14:A:4007:BCR:H24C	11:A:1137:CLA:C9	2.43	0.48
1:a:540:PHE:CE2	11:a:1022:CLA:HAB	2.48	0.48
1:1:195:SER:O	1:1:199:HIS:ND1	2.36	0.48
2:2:587:LEU:HD12	11:2:1234:CLA:HBB2	1.94	0.48
11:1:1125:CLA:HHD	11:1:1125:CLA:CBC	2.42	0.48
11:2:1220:CLA:HMD3	11:2:1221:CLA:HHC	1.96	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:HC8	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:1128:CLA:H172	14:2:4011:BCR:H342	1.96	0.48
11:A:1104:CLA:HMD2	11:A:1106:CLA:H202	1.96	0.48
11:A:1121:CLA:HHC	11:A:1121:CLA:HBB1	1.95	0.48
2:B:586:TRP:CE2	11:B:1021:CLA:H191	2.49	0.48
11:1:1106:CLA:H93	11:1:1128:CLA:H203	1.96	0.48
14:2:4010:BCR:H23C	14:2:4010:BCR:H392	1.95	0.48
11:A:1102:CLA:HAB	11:A:1104:CLA:CAD	2.44	0.48
11:A:1119:CLA:HMB2	11:A:1123:CLA:HED2	1.95	0.48
1:1:193:VAL:HG13	11:1:1123:CLA:HMD1	1.95	0.48
11:1:1107:CLA:H12	14:6:4013:BCR:H14C	1.96	0.48
1:A:267:ASN:O	1:A:269:GLY:N	2.46	0.47
14:B:4017:BCR:H15C	14:B:4017:BCR:H351	1.61	0.47
11:B:1221:CLA:CMB	11:B:1223:CLA:H8	2.43	0.47
1:a:197:MET:HE2	11:a:1119:CLA:HMA2	1.96	0.47
14:b:4004:BCR:H15C	14:b:4004:BCR:H351	1.61	0.47
1:1:681:PHE:N	11:2:1013:CLA:HAB	2.29	0.47
14:2:4005:BCR:H343	11:2:1209:CLA:HMC2	1.95	0.47
14:A:4007:BCR:H15C	14:A:4007:BCR:H351	1.64	0.47
11:2:1013:CLA:H2	11:2:1013:CLA:HMA3	1.96	0.47
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.47	0.47
11:B:1225:CLA:C16	11:B:1211:CLA:HAB	2.44	0.47
14:b:4009:BCR:H353	15:b:5004:LHG:H223	1.96	0.47
14:1:4001:BCR:H332	14:1:4002:BCR:H24C	1.96	0.47
14:1:4007:BCR:H372	15:1:5003:LHG:H262	1.95	0.47
1:A:429:MET:HA	1:A:432:HIS:CE1	2.50	0.47
11:A:1138:CLA:HHD	14:B:4014:BCR:H383	1.96	0.47
2:B:539:ARG:NH2	4:D:127:GLU:OE1	2.41	0.47
14:B:4014:BCR:H351	14:B:4014:BCR:H15C	1.56	0.47
14:a:4003:BCR:H402	11:a:1103:CLA:H72	1.95	0.47
7:l:64:PRO:HA	11:l:1503:CLA:HMB1	1.96	0.47
1:1:423:ASN:OD1	1:1:431:ARG:NH2	2.48	0.47
2:2:586:TRP:CE2	11:2:1021:CLA:H201	2.48	0.47
6:F:42:SER:O	6:F:43:CYS:CB	2.63	0.47
14:a:4007:BCR:H15C	14:a:4007:BCR:H351	1.66	0.47
11:b:1238:CLA:H2	14:l:4019:BCR:H363	1.96	0.47
14:2:4010:BCR:H363	11:2:1222:CLA:C2B	2.44	0.47
11:b:1207:CLA:HHC	11:b:1207:CLA:HBB1	1.95	0.47
11:b:1208:CLA:HHC	11:b:1208:CLA:CBB	2.45	0.47
11:1:1117:CLA:HAB	11:1:1117:CLA:C11	2.45	0.47
7:8:96:LEU:CG	14:8:4019:BCR:H24C	2.43	0.47
14:A:4002:BCR:H351	14:A:4002:BCR:H15C	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1104:CLA:HMD2	11:A:1106:CLA:C20	2.44	0.47
2:B:586:TRP:CD2	11:B:1021:CLA:H191	2.50	0.47
14:B:4009:BCR:C14	15:B:5004:LHG:H202	2.45	0.47
2:b:520:ILE:HD13	11:b:1234:CLA:HAB	1.96	0.47
14:b:4011:BCR:H351	14:b:4011:BCR:H15C	1.70	0.47
14:f:4018:BCR:H14C	9:i:23:PRO:HG3	1.96	0.47
1:1:679:PHE:CD2	11:1:1011:CLA:HMA3	2.50	0.47
14:1:4001:BCR:H331	14:1:4002:BCR:H24C	1.96	0.47
14:2:4010:BCR:H351	14:2:4010:BCR:H15C	1.54	0.47
14:6:4018:BCR:H382	14:6:4018:BCR:H23C	1.96	0.47
11:B:1205:CLA:HAB	11:B:1206:CLA:HAA2	1.97	0.47
1:a:195:SER:O	1:a:199:HIS:ND1	2.41	0.47
11:b:1219:CLA:HMB3	11:b:1240:CLA:HBC3	1.96	0.47
14:2:4006:BCR:H351	14:2:4006:BCR:H15C	1.72	0.47
14:2:4017:BCR:H351	14:2:4017:BCR:H15C	1.65	0.47
11:2:1238:CLA:H193	14:6:4018:BCR:H362	1.95	0.47
12:a:2001:PQN:C24	11:b:1013:CLA:H202	2.45	0.47
2:b:312:LEU:HD22	15:b:5004:LHG:HC42	1.96	0.47
11:2:1013:CLA:CGA	11:2:1013:CLA:H3A	2.44	0.47
1:A:324:ILE:HD13	11:A:1121:CLA:HMD2	1.97	0.47
14:A:4007:BCR:HC41	11:A:1119:CLA:C19	2.45	0.47
11:A:1136:CLA:HHC	11:A:1136:CLA:CBB	2.44	0.47
11:a:1112:CLA:HBB1	11:a:1112:CLA:HHC	1.97	0.47
11:b:1201:CLA:HAB	11:b:1203:CLA:CAD	2.44	0.47
8:7:26:SER:HB3	14:7:4021:BCR:HC41	1.97	0.47
11:A:1114:CLA:HHC	11:A:1114:CLA:CBB	2.45	0.46
11:a:1133:CLA:HHC	11:a:1133:CLA:HBB1	1.97	0.46
11:2:1231:CLA:NC	11:2:1232:CLA:HAB	2.30	0.46
1:a:589:ASP:OD1	1:a:724:ARG:NH1	2.45	0.46
11:b:1217:CLA:HBB1	11:b:1217:CLA:HHC	1.95	0.46
11:1:1115:CLA:CBB	11:1:1115:CLA:HHC	2.45	0.46
11:2:1212:CLA:HAB	11:2:1211:CLA:CMC	2.45	0.46
14:A:4001:BCR:H15C	14:A:4001:BCR:H351	1.54	0.46
2:B:642:VAL:HG22	11:B:1206:CLA:HHD	1.97	0.46
11:1:1112:CLA:HHC	11:1:1112:CLA:HBB1	1.97	0.46
14:F:4018:BCR:H14C	9:I:23:PRO:HG2	1.96	0.46
1:a:571:ARG:HD2	15:a:5001:LHG:HC42	1.97	0.46
1:1:210:LEU:HB2	1:1:301:ALA:HB1	1.98	0.46
10:k:124:SER:O	10:k:125:SER:C	2.57	0.46
10:0:90:LEU:CB	10:0:91:PRO:CD	2.93	0.46
11:A:1138:CLA:HHC	11:A:1138:CLA:CBB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:193:VAL:CG1	11:a:1123:CLA:HHD	2.45	0.46
1:1:342:GLU:OE1	1:1:342:GLU:N	2.45	0.46
14:1:4001:BCR:H24C	10:0:110:PHE:HB2	1.97	0.46
2:2:721:PHE:CD1	11:2:1021:CLA:HMD2	2.50	0.46
14:2:4014:BCR:H15C	14:2:4014:BCR:H351	1.65	0.46
10:k:90:LEU:CB	10:k:91:PRO:CD	2.94	0.46
1:a:330:GLY:N	15:a:5003:LHG:HC2	2.30	0.46
1:a:681:PHE:CA	11:b:1013:CLA:HAB	2.45	0.46
11:b:1220:CLA:CMD	11:b:1221:CLA:HMC1	2.46	0.46
11:1:1105:CLA:C2	14:6:4013:BCR:H342	2.46	0.46
2:2:5:PHE:HB2	9:9:34:ILE:HA	1.98	0.46
2:B:582:ASN:ND2	2:B:586:TRP:CZ2	2.83	0.46
14:B:4005:BCR:H343	11:B:1209:CLA:CMC	2.44	0.46
14:B:4010:BCR:H332	11:B:1223:CLA:HED2	1.97	0.46
11:B:1023:CLA:H193	14:F:4018:BCR:H19C	1.97	0.46
14:F:4020:BCR:HC42	7:L:87:ALA:HB1	1.96	0.46
11:a:1125:CLA:HHD	11:a:1125:CLA:HBC2	1.97	0.46
2:b:53:HIS:CE1	11:b:1202:CLA:HMA2	2.51	0.46
14:A:4003:BCR:H403	14:A:4003:BCR:C23	2.43	0.46
1:a:277:PHE:CD2	11:a:1116:CLA:HMB3	2.51	0.46
1:a:369:HIS:ND1	11:a:1116:CLA:OBD	2.49	0.46
11:a:1101:CLA:H52	11:a:1101:CLA:H8	1.76	0.46
11:b:1235:CLA:HMA3	11:b:1236:CLA:HED1	1.98	0.46
1:1:356:LEU:HD11	11:1:1128:CLA:CBB	2.46	0.46
14:F:4018:BCR:H24C	14:F:4018:BCR:H371	1.65	0.46
14:a:4008:BCR:C8	11:a:1124:CLA:HAB	2.45	0.46
11:a:1126:CLA:C4C	14:b:4011:BCR:HC42	2.46	0.46
2:b:117:TYR:HA	2:b:365:THR:HG22	1.98	0.46
14:b:4009:BCR:H23C	11:b:1227:CLA:HBC1	1.98	0.46
1:1:453:GLY:C	11:1:1132:CLA:HAB	2.41	0.46
11:1:1117:CLA:HAB	11:1:1117:CLA:H111	1.97	0.46
9:9:31:PHE:HB2	14:8:4019:BCR:H14C	1.97	0.46
11:A:1012:CLA:H43	14:B:4011:BCR:H362	1.97	0.45
11:b:1210:CLA:HHC	11:b:1210:CLA:HBB1	1.97	0.45
11:1:1101:CLA:HAB	11:1:1102:CLA:C2C	2.46	0.45
14:6:4013:BCR:H351	14:6:4013:BCR:H15C	1.62	0.45
1:A:53:ALA:HB2	15:A:5001:LHG:HC82	1.98	0.45
2:B:58:PHE:CE1	14:B:4005:BCR:H373	2.51	0.45
2:B:434:LEU:HD23	11:B:1230:CLA:HBB1	1.97	0.45
1:1:721:ILE:HG21	15:1:5001:LHG:HC42	1.97	0.45
11:1:1134:CLA:HHC	11:1:1134:CLA:HBB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:TYR:CE2	2:B:515:LEU:HB3	2.52	0.45
1:a:460:THR:HG23	11:b:1206:CLA:HMC3	1.98	0.45
11:a:1103:CLA:H51	11:a:1111:CLA:C1	2.42	0.45
2:b:571:ASP:OD1	2:b:703:ARG:NH2	2.48	0.45
11:1:1237:CLA:CHA	11:1:1237:CLA:HBA1	2.45	0.45
14:2:4005:BCR:HC7	11:2:1209:CLA:HMC3	1.99	0.45
11:A:1131:CLA:HAB	11:A:1132:CLA:HHB	1.98	0.45
2:B:519:ALA:HB1	11:B:1021:CLA:C19	2.46	0.45
11:a:1117:CLA:H111	11:a:1117:CLA:HAB	1.99	0.45
1:1:199:HIS:CE1	11:1:1118:CLA:HMD3	2.52	0.45
1:1:700:ILE:HD13	11:1:1138:CLA:HMD1	1.97	0.45
14:a:4003:BCR:H402	14:a:4003:BCR:H23C	1.96	0.45
14:2:4017:BCR:H331	14:2:4017:BCR:HC8	1.99	0.45
1:A:193:VAL:HG13	11:A:1123:CLA:HHD	1.98	0.45
11:A:1104:CLA:H3A	11:A:1128:CLA:HAB	1.99	0.45
11:B:1204:CLA:HHB	11:B:1205:CLA:HMB3	1.98	0.45
11:B:1231:CLA:HHC	11:B:1231:CLA:HBB1	1.99	0.45
9:i:7:ALA:N	8:m:5:ASP:OD1	2.49	0.45
11:1:1138:CLA:HAA2	11:2:1228:CLA:HMB2	1.98	0.45
2:b:7:LYS:NZ	8:m:30:TYR:O	2.50	0.45
14:b:4017:BCR:H351	14:b:4017:BCR:H15C	1.60	0.45
1:1:203:GLY:HA2	11:1:1118:CLA:HBC1	1.97	0.45
1:1:395:TRP:NE1	11:1:1126:CLA:HAB	2.32	0.45
1:A:721:ILE:HG21	15:A:5001:LHG:HC42	1.99	0.45
1:A:737:VAL:HG22	14:B:4011:BCR:H321	1.99	0.45
12:A:2001:PQN:H251	11:B:1013:CLA:H202	1.99	0.45
11:B:1215:CLA:CGA	11:B:1215:CLA:H3A	2.46	0.45
7:L:17:VAL:O	7:L:19:HIS:N	2.49	0.45
1:a:79:HIS:ND1	11:a:1103:CLA:HMA2	2.31	0.45
15:a:5003:LHG:H171	15:a:5003:LHG:H301	1.98	0.45
11:b:1228:CLA:HHC	11:b:1228:CLA:CBB	2.47	0.45
14:1:4008:BCR:HC8	14:1:4008:BCR:H331	1.98	0.45
11:1:1101:CLA:H201	11:1:1012:CLA:H203	1.99	0.45
2:2:5:PHE:HB3	2:2:20:ARG:NH1	2.32	0.45
2:2:130:THR:OG1	2:2:201:GLU:OE1	2.34	0.45
2:2:487:GLY:O	2:2:489:ALA:N	2.50	0.45
14:2:4017:BCR:H24C	14:2:4017:BCR:H371	1.78	0.45
2:B:53:HIS:CE1	11:B:1202:CLA:HMA2	2.52	0.45
1:a:358:LEU:HG	11:a:1123:CLA:HMB1	1.98	0.45
1:a:681:PHE:N	11:b:1013:CLA:HAB	2.31	0.45
14:a:4003:BCR:H351	14:a:4003:BCR:H15C	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:4007:BCR:C34	11:1:1123:CLA:HAB	2.45	0.45
14:6:4018:BCR:H351	14:6:4018:BCR:H15C	1.62	0.45
14:A:4003:BCR:H15C	14:A:4003:BCR:H351	1.64	0.45
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB2	1.97	0.45
2:B:212:PHE:CG	11:B:1211:CLA:HMD1	2.52	0.45
14:B:4006:BCR:H392	14:B:4006:BCR:H23C	1.97	0.45
11:b:1013:CLA:H2	11:b:1013:CLA:HMA3	1.98	0.45
11:b:1228:CLA:HMC2	11:b:1236:CLA:HAC2	1.99	0.45
14:2:4009:BCR:H321	14:2:4009:BCR:HC8	1.99	0.45
14:2:4011:BCR:H15C	14:2:4011:BCR:H351	1.77	0.45
11:8:1501:CLA:HHC	11:8:1501:CLA:HBB1	1.98	0.45
2:b:413:LYS:NZ	6:f:124:PRO:O	2.40	0.44
2:b:655:ALA:C	11:b:1023:CLA:HAB	2.42	0.44
11:l:1501:CLA:H202	11:l:1503:CLA:H2	1.99	0.44
11:L:1501:CLA:CBA	14:L:4022:BCR:H363	2.46	0.44
14:L:4019:BCR:HC7	14:L:4019:BCR:H331	1.58	0.44
11:a:1105:CLA:CBB	11:a:1105:CLA:HHC	2.48	0.44
1:1:59:ASP:OD1	1:1:59:ASP:N	2.50	0.44
11:1:1130:CLA:HBC2	11:1:1137:CLA:HMC3	1.99	0.44
1:A:59:ASP:N	1:A:59:ASP:OD1	2.49	0.44
2:B:25:ILE:HG12	14:L:4019:BCR:HC41	1.99	0.44
11:B:1207:CLA:C2	11:B:1207:CLA:HMA1	2.48	0.44
11:B:1223:CLA:HBC3	11:B:1223:CLA:HHD	1.98	0.44
4:4:3:GLU:HB3	4:4:4:LEU:H	1.61	0.44
1:A:100:TYR:HA	1:A:144:PHE:CE2	2.53	0.44
11:A:1102:CLA:H203	11:A:1106:CLA:C14	2.48	0.44
14:B:4005:BCR:H351	14:B:4005:BCR:H15C	1.64	0.44
11:b:1212:CLA:HHC	11:b:1212:CLA:CBB	2.48	0.44
14:2:4005:BCR:H351	14:2:4005:BCR:H15C	1.77	0.44
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.61	0.44
9:i:10:LEU:HB2	9:i:11:PRO:HD3	2.00	0.44
14:1:4007:BCR:H351	14:1:4007:BCR:H15C	1.56	0.44
2:2:381:MET:HE1	14:2:4010:BCR:H361	1.98	0.44
11:2:1240:CLA:HHC	11:2:1240:CLA:CBB	2.47	0.44
5:5:13:ARG:O	5:5:14:THR:HB	2.18	0.44
6:6:49:ILE:CB	6:6:50:PRO:HD3	2.47	0.44
1:A:203:GLY:HA2	11:A:1118:CLA:HBC1	1.98	0.44
11:A:1104:CLA:HHB	11:A:1128:CLA:HAB	1.99	0.44
11:b:1238:CLA:C1	14:l:4019:BCR:H363	2.47	0.44
1:1:454:LEU:CD2	11:1:1132:CLA:HMB2	2.48	0.44
2:2:275:HIS:HB3	11:2:1214:CLA:HMB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:1023:CLA:CGA	11:2:1023:CLA:H3A	2.47	0.44
11:B:1207:CLA:HMA1	11:B:1207:CLA:H2	1.99	0.44
11:a:1137:CLA:HAB	11:a:1129:CLA:CBB	2.47	0.44
2:b:338:SER:HB3	11:b:1221:CLA:H42	2.00	0.44
2:2:312:LEU:HB2	15:2:5004:LHG:HC42	1.99	0.44
11:8:1501:CLA:H43	14:8:4022:BCR:H14C	1.99	0.44
8:7:9:LEU:HD12	14:7:4021:BCR:H401	1.99	0.44
11:A:1102:CLA:H142	11:A:1107:CLA:H202	2.00	0.44
14:B:4005:BCR:HC7	11:B:1209:CLA:CMC	2.47	0.44
6:F:11:ALA:N	6:F:12:PRO:HD2	2.33	0.44
1:a:356:LEU:HD11	11:a:1128:CLA:CBB	2.47	0.44
11:b:1013:CLA:H3A	11:b:1013:CLA:CGA	2.48	0.44
11:b:1220:CLA:HMD3	11:b:1221:CLA:HMC1	2.00	0.44
2:2:582:ASN:ND2	2:2:586:TRP:CZ2	2.86	0.44
1:A:226:LEU:HD21	1:A:252:LEU:HD11	2.00	0.44
11:A:1104:CLA:HBC3	11:A:1104:CLA:HHD	2.00	0.44
14:F:4018:BCR:H351	14:F:4018:BCR:H15C	1.63	0.44
11:a:1108:CLA:HHC	11:a:1108:CLA:HBB1	2.00	0.44
11:b:1210:CLA:HBC2	11:b:1210:CLA:HHD	2.00	0.44
3:c:17:CYS:HB2	3:c:54:CYS:HB3	2.00	0.44
6:f:49:ILE:CB	6:f:50:PRO:HD3	2.48	0.44
14:A:4003:BCR:H23C	11:A:1103:CLA:H72	2.00	0.43
14:F:4018:BCR:H14C	9:I:23:PRO:CB	2.48	0.43
1:a:59:ASP:OD1	1:a:59:ASP:N	2.51	0.43
1:a:440:LEU:HD23	1:a:547:LEU:HA	1.99	0.43
14:a:4001:BCR:H14C	11:a:1118:CLA:HBB1	1.99	0.43
12:b:2002:PQN:H291	14:l:4019:BCR:HC8	2.00	0.43
1:1:728:VAL:CG1	15:1:5001:LHG:H301	2.47	0.43
11:1:1119:CLA:HMB2	11:1:1123:CLA:CED	2.48	0.43
11:2:1205:CLA:CGA	11:2:1205:CLA:CHA	2.96	0.43
11:2:1210:CLA:H203	11:2:1225:CLA:C3D	2.48	0.43
11:A:1115:CLA:HBB1	11:A:1115:CLA:HHC	2.00	0.43
2:B:77:TRP:HA	2:B:84:ILE:HG21	2.00	0.43
11:a:1133:CLA:HHC	11:a:1133:CLA:CBB	2.48	0.43
1:1:500:ASN:ND2	11:1:1115:CLA:OBD	2.51	0.43
14:6:4020:BCR:H351	14:6:4020:BCR:H15C	1.66	0.43
7:8:17:VAL:O	7:8:19:HIS:N	2.48	0.43
1:A:354:ILE:CD1	14:A:4007:BCR:HC7	2.42	0.43
1:A:608:HIS:C	1:A:608:HIS:CD2	2.96	0.43
11:A:1136:CLA:C1A	11:A:1136:CLA:CGA	2.96	0.43
2:B:299:HIS:NE2	11:B:1219:CLA:OBD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:LEU:O	2:B:600:SER:OG	2.31	0.43
2:B:721:PHE:CD1	11:B:1021:CLA:HMD2	2.53	0.43
11:B:1238:CLA:H193	14:F:4018:BCR:H362	2.00	0.43
11:a:1107:CLA:CBA	11:a:1107:CLA:HBD	2.48	0.43
2:b:385:PHE:CZ	14:b:4010:BCR:H373	2.52	0.43
14:f:4018:BCR:H24C	14:f:4018:BCR:H371	1.61	0.43
14:f:4018:BCR:H351	14:f:4018:BCR:H15C	1.62	0.43
8:m:19:ALA:HB2	14:m:4021:BCR:H15C	1.99	0.43
11:1:1128:CLA:H201	11:1:1140:CLA:H2	2.00	0.43
14:A:4002:BCR:C14	11:A:1112:CLA:HBB1	2.48	0.43
11:A:1022:CLA:CAD	11:B:1021:CLA:HMB2	2.48	0.43
11:A:1118:CLA:H3A	10:K:105:LEU:HD12	2.01	0.43
1:a:342:GLU:OE1	1:a:342:GLU:N	2.48	0.43
2:b:412:HIS:O	2:b:412:HIS:ND1	2.52	0.43
11:b:1201:CLA:HHC	11:b:1203:CLA:OBD	2.19	0.43
14:1:4003:BCR:H371	11:1:1127:CLA:H62	2.01	0.43
11:1:1126:CLA:C4C	14:2:4011:BCR:HC42	2.48	0.43
2:2:53:HIS:CE1	11:2:1202:CLA:HMA2	2.53	0.43
1:A:296:HIS:HE1	11:A:1117:CLA:C2B	2.31	0.43
14:B:4004:BCR:H15C	14:B:4004:BCR:H351	1.60	0.43
11:B:1204:CLA:H92	14:M:4021:BCR:C14	2.48	0.43
4:D:98:HIS:CG	4:D:99:PRO:CD	3.01	0.43
11:b:1207:CLA:HHC	11:b:1207:CLA:CBB	2.48	0.43
11:1:1125:CLA:CAB	11:1:1133:CLA:HMA2	2.47	0.43
2:2:273:ILE:O	2:2:277:HIS:ND1	2.50	0.43
2:2:427:LEU:HD11	11:2:1235:CLA:HMB1	2.01	0.43
9:9:10:LEU:HB2	9:9:11:PRO:HD3	2.01	0.43
1:A:358:LEU:HG	11:A:1123:CLA:HMB3	2.00	0.43
11:a:1125:CLA:HHC	11:a:1125:CLA:CBB	2.43	0.43
2:b:5:PHE:HB3	2:b:20:ARG:NH1	2.34	0.43
14:f:4020:BCR:H333	7:l:87:ALA:CB	2.47	0.43
11:2:1207:CLA:HHC	11:2:1207:CLA:CBB	2.48	0.43
11:a:1801:CLA:CHC	15:a:5003:LHG:HC31	2.49	0.43
11:a:1119:CLA:OBD	11:a:1121:CLA:HHD	2.18	0.43
14:b:4005:BCR:H321	14:b:4005:BCR:HC8	2.00	0.43
11:b:1223:CLA:HBD	11:b:1223:CLA:HAA2	2.00	0.43
11:l:1501:CLA:C4	14:l:4022:BCR:H14C	2.49	0.43
14:2:4011:BCR:H23C	11:2:1230:CLA:HMC1	2.01	0.43
1:A:210:LEU:HD11	14:A:4001:BCR:HC8	2.01	0.43
11:A:1237:CLA:HHD	14:B:4017:BCR:H383	2.00	0.43
2:B:211:ASN:O	2:B:214:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:721:PHE:CD1	11:b:1021:CLA:HMD2	2.54	0.43
14:b:4006:BCR:H282	11:b:1211:CLA:HMA3	2.01	0.43
11:A:1237:CLA:HHC	11:A:1237:CLA:CBB	2.48	0.43
1:a:330:GLY:HA3	15:a:5003:LHG:HC2	2.00	0.43
1:a:550:LEU:HD11	11:a:1119:CLA:H202	2.00	0.43
2:b:582:ASN:ND2	2:b:586:TRP:CZ2	2.87	0.43
11:2:1239:CLA:HHC	11:2:1239:CLA:HBB1	2.00	0.43
1:a:564:ASP:OD1	1:a:564:ASP:N	2.51	0.43
2:b:491:LEU:N	2:b:492:PRO:CD	2.82	0.43
14:b:4005:BCR:H351	14:b:4005:BCR:H15C	1.73	0.43
1:1:571:ARG:NE	15:1:5001:LHG:O5	2.51	0.43
1:A:261:THR:O	1:A:265:THR:N	2.48	0.42
1:A:269:GLY:HA3	10:K:51:PRO:HG3	2.01	0.42
14:A:4002:BCR:HC41	11:A:1103:CLA:H142	2.01	0.42
2:B:642:VAL:CG2	11:B:1206:CLA:HHD	2.49	0.42
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC1	1.99	0.42
7:l:60:PHE:CD1	7:l:60:PHE:C	2.97	0.42
15:1:5001:LHG:C20	11:1:1128:CLA:H202	2.47	0.42
10:0:124:SER:O	10:0:125:SER:C	2.62	0.42
1:A:312:ARG:NH2	1:A:316:GLY:O	2.52	0.42
12:B:2002:PQN:H291	14:L:4019:BCR:H342	2.00	0.42
11:B:1021:CLA:HBA2	11:B:1021:CLA:H3A	1.91	0.42
11:B:1220:CLA:HBC2	11:B:1220:CLA:HHD	2.01	0.42
2:b:174:ARG:NH2	11:b:1221:CLA:HMD2	2.34	0.42
11:2:1013:CLA:HMA3	11:2:1013:CLA:C2	2.49	0.42
11:2:1021:CLA:HBA1	11:2:1021:CLA:H3A	1.78	0.42
14:8:4022:BCR:H351	14:8:4022:BCR:H15C	1.66	0.42
1:A:608:HIS:CD2	11:A:1135:CLA:HMC3	2.55	0.42
1:a:310:MET:HE1	11:a:1119:CLA:C1D	2.49	0.42
1:a:608:HIS:C	1:a:608:HIS:CD2	2.97	0.42
14:a:4001:BCR:H351	14:a:4001:BCR:H15C	1.60	0.42
1:1:263:PHE:CZ	14:1:4001:BCR:H343	2.54	0.42
11:1:1103:CLA:CGA	11:1:1103:CLA:H3A	2.49	0.42
2:2:656:THR:HA	11:2:1023:CLA:HAB	2.01	0.42
11:2:1206:CLA:CMB	11:2:1207:CLA:C1C	2.97	0.42
2:B:427:LEU:HD11	11:B:1235:CLA:HMB1	2.01	0.42
5:E:13:ARG:O	5:E:14:THR:HB	2.18	0.42
1:a:193:VAL:HG13	11:a:1123:CLA:HMD3	2.02	0.42
1:a:423:ASN:OD1	1:a:431:ARG:NH2	2.52	0.42
11:a:1801:CLA:NC	15:a:5003:LHG:HC31	2.34	0.42
11:a:1119:CLA:H93	11:a:1123:CLA:HMB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:4011:BCR:H23C	11:b:1230:CLA:HMC3	2.02	0.42
11:1:1134:CLA:O1A	11:0:1401:CLA:O1D	2.36	0.42
11:2:1207:CLA:H2A	11:2:1207:CLA:O2A	2.20	0.42
10:k:120:LEU:HD13	11:k:1401:CLA:C1	2.49	0.42
10:0:110:PHE:HA	10:0:113:ILE:HG22	2.00	0.42
11:B:1201:CLA:HMA2	8:M:29:LEU:CD2	2.48	0.42
11:a:1124:CLA:H12	11:a:1135:CLA:HMA2	2.00	0.42
6:f:6:SER:O	6:f:10:THR:N	2.52	0.42
2:2:77:TRP:HA	2:2:84:ILE:HG21	2.01	0.42
2:2:412:HIS:O	2:2:412:HIS:ND1	2.53	0.42
11:2:1208:CLA:CBB	11:2:1208:CLA:HHC	2.50	0.42
14:8:4022:BCR:H24C	14:8:4022:BCR:H371	1.78	0.42
11:A:1125:CLA:HHD	11:A:1125:CLA:HBC2	1.99	0.42
14:B:4017:BCR:HC32	11:B:1205:CLA:HMC2	2.01	0.42
14:b:4010:BCR:C20	11:b:1223:CLA:H91	2.50	0.42
11:b:1201:CLA:HMC3	11:b:1203:CLA:OBD	2.19	0.42
11:b:1209:CLA:CBB	11:b:1209:CLA:HHC	2.50	0.42
1:1:260:LEU:O	1:1:261:THR:OG1	2.31	0.42
2:2:385:PHE:CE2	14:2:4010:BCR:H373	2.55	0.42
2:2:435:TYR:CE2	2:2:515:LEU:HB3	2.55	0.42
11:2:1201:CLA:HMA2	8:7:29:LEU:CD2	2.49	0.42
11:2:1202:CLA:H141	11:2:1202:CLA:C17	2.49	0.42
4:4:77:LYS:HB2	4:4:78:PRO:HD3	2.00	0.42
2:B:178:HIS:ND1	11:B:1221:CLA:O1D	2.53	0.42
2:B:425:LEU:HB3	11:B:1229:CLA:CED	2.48	0.42
14:B:4010:BCR:H15C	14:B:4010:BCR:H351	1.62	0.42
4:D:27:LYS:HG3	4:D:88:VAL:HG13	2.02	0.42
1:a:211:GLY:HA2	14:a:4002:BCR:H363	2.02	0.42
1:1:262:PRO:O	1:1:267:ASN:N	2.49	0.42
1:1:305:ILE:O	1:1:309:HIS:ND1	2.53	0.42
11:1:1237:CLA:HMD3	14:2:4017:BCR:H383	2.00	0.42
2:2:294:ASN:OD1	2:2:294:ASN:N	2.52	0.42
2:2:642:VAL:HG12	2:2:643:TRP:N	2.35	0.42
1:A:395:TRP:HE1	11:A:1126:CLA:HAB	1.85	0.42
1:A:467:PRO:HA	1:A:470:MET:HG2	2.02	0.42
11:A:1119:CLA:HMB2	11:A:1123:CLA:CED	2.49	0.42
2:B:294:ASN:N	2:B:294:ASN:OD1	2.52	0.42
2:B:412:HIS:ND1	2:B:412:HIS:O	2.52	0.42
14:B:4010:BCR:HC21	11:B:1223:CLA:CMA	2.49	0.42
7:L:100:GLY:HA3	7:L:120:TRP:CD1	2.55	0.42
11:b:1204:CLA:HHB	11:b:1205:CLA:HMB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:13:ARG:O	5:e:14:THR:HB	2.19	0.42
11:2:1207:CLA:HHC	11:2:1207:CLA:HBB1	2.01	0.42
1:A:226:LEU:HD12	1:A:236:ILE:HG23	2.01	0.42
11:A:1011:CLA:HBA2	11:A:1011:CLA:H3A	1.89	0.42
2:B:683:PRO:C	2:B:685:ALA:H	2.28	0.42
14:B:4010:BCR:H332	11:B:1223:CLA:CED	2.50	0.42
11:B:1201:CLA:HAC1	14:L:4019:BCR:HC32	2.01	0.42
1:a:429:MET:HA	1:a:432:HIS:CE1	2.55	0.42
14:a:4003:BCR:C23	14:a:4003:BCR:C40	2.98	0.42
11:a:1112:CLA:HMC3	11:a:1113:CLA:HAB	2.01	0.42
14:l:4019:BCR:HC8	14:l:4019:BCR:C32	2.44	0.42
1:1:211:GLY:CA	14:1:4002:BCR:H363	2.50	0.42
1:1:681:PHE:CA	11:2:1013:CLA:HAB	2.49	0.42
11:1:1237:CLA:C10	14:8:4019:BCR:H361	2.50	0.42
2:2:341:VAL:HG13	11:2:1222:CLA:HED1	2.01	0.42
11:2:1202:CLA:H142	11:2:1202:CLA:CAD	2.49	0.42
4:4:98:HIS:CG	4:4:99:PRO:CD	3.03	0.42
2:B:189:ALA:HA	11:B:1212:CLA:HAB	2.02	0.42
11:a:1108:CLA:HHC	11:a:1108:CLA:CBB	2.50	0.42
11:b:1205:CLA:HAB	11:b:1206:CLA:O1A	2.19	0.42
4:d:98:HIS:CG	4:d:99:PRO:CD	3.03	0.42
11:1:1130:CLA:HHC	11:1:1130:CLA:CBB	2.50	0.42
11:2:1238:CLA:HHC	11:2:1238:CLA:CBB	2.49	0.42
1:A:679:PHE:CD2	11:A:1011:CLA:HMA3	2.55	0.41
2:b:435:TYR:CE2	2:b:515:LEU:HB3	2.55	0.41
14:b:4014:BCR:H351	14:b:4014:BCR:H15C	1.66	0.41
11:b:1209:CLA:HHC	11:b:1209:CLA:HBB1	2.00	0.41
14:l:4022:BCR:H351	14:l:4022:BCR:H15C	1.76	0.41
11:1:1112:CLA:HMC3	11:1:1113:CLA:HAB	2.02	0.41
1:A:571:ARG:NH1	15:A:5001:LHG:O10	2.51	0.41
2:B:491:LEU:N	2:B:492:PRO:CD	2.83	0.41
11:a:1138:CLA:HMD2	2:b:425:LEU:HD21	2.01	0.41
14:f:4020:BCR:H15C	14:f:4020:BCR:H351	1.74	0.41
11:A:1801:CLA:C2C	15:A:5003:LHG:HC31	2.51	0.41
11:A:1118:CLA:H3A	10:K:105:LEU:CD1	2.50	0.41
1:a:262:PRO:O	1:a:267:ASN:N	2.52	0.41
1:a:608:HIS:CD2	11:a:1135:CLA:HMC3	2.55	0.41
1:1:319:HIS:HB3	1:1:324:ILE:HD11	2.02	0.41
2:B:123:TRP:HA	2:B:356:TYR:CD1	2.56	0.41
2:B:436:VAL:HB	11:B:1230:CLA:HMC2	2.02	0.41
11:B:1222:CLA:CAD	11:B:1234:CLA:HBB1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:4019:BCR:H321	14:L:4019:BCR:C8	2.43	0.41
1:a:305:ILE:O	1:a:309:HIS:ND1	2.53	0.41
1:a:681:PHE:HA	11:b:1013:CLA:CAB	2.49	0.41
12:a:2001:PQN:H201	11:a:1101:CLA:H12	2.03	0.41
11:a:1103:CLA:HBB1	11:a:1104:CLA:HBA1	2.03	0.41
11:a:1131:CLA:HAB	11:a:1132:CLA:HHB	2.02	0.41
2:b:654:TRP:CD2	11:b:1021:CLA:HMA2	2.55	0.41
1:1:391:THR:OG1	11:1:1126:CLA:HMB1	2.20	0.41
14:1:4007:BCR:H363	11:1:1122:CLA:H143	2.01	0.41
11:1:1106:CLA:H91	11:1:1128:CLA:H203	2.01	0.41
11:1:1110:CLA:HAB	11:1:1118:CLA:H61	2.02	0.41
9:I:15:ILE:HB	9:I:16:PRO:HD3	2.03	0.41
1:a:332:PHE:O	1:a:428:ARG:NH2	2.54	0.41
11:a:1138:CLA:C1A	11:a:1138:CLA:CGA	2.98	0.41
2:b:312:LEU:HB2	15:b:5004:LHG:HC42	2.01	0.41
2:b:658:PHE:HB3	11:b:1023:CLA:HMC2	2.02	0.41
2:2:571:ASP:OD1	2:2:703:ARG:NH2	2.52	0.41
4:4:82:ASP:OD1	4:4:82:ASP:N	2.52	0.41
7:8:60:PHE:CD1	7:8:60:PHE:C	2.99	0.41
1:A:679:PHE:CG	11:A:1011:CLA:HMA3	2.56	0.41
2:B:174:ARG:HB3	11:B:1221:CLA:HMD1	2.03	0.41
2:b:294:ASN:OD1	2:b:294:ASN:N	2.52	0.41
1:1:608:HIS:CD2	1:1:608:HIS:C	2.98	0.41
1:1:721:ILE:CG2	15:1:5001:LHG:HC42	2.50	0.41
2:2:491:LEU:N	2:2:492:PRO:CD	2.84	0.41
14:2:4004:BCR:H15C	14:2:4004:BCR:H351	1.67	0.41
8:7:19:ALA:HB2	14:7:4021:BCR:C15	2.50	0.41
9:I:10:LEU:HB2	9:I:11:PRO:HD3	2.02	0.41
2:B:5:PHE:HB3	2:B:20:ARG:NH1	2.36	0.41
2:B:7:LYS:NZ	8:M:30:TYR:O	2.48	0.41
4:D:77:LYS:HB2	4:D:78:PRO:HD3	2.02	0.41
11:a:1119:CLA:OBD	11:a:1121:CLA:HMD3	2.21	0.41
2:b:494:TRP:CE2	11:b:1231:CLA:HED2	2.56	0.41
14:b:4010:BCR:C20	11:b:1223:CLA:C9	2.98	0.41
10:k:73:VAL:HG13	10:k:74:ILE:N	2.36	0.41
14:A:4003:BCR:C40	14:A:4003:BCR:C23	2.98	0.41
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB1	2.01	0.41
2:b:586:TRP:CD2	11:b:1021:CLA:H191	2.55	0.41
11:b:1220:CLA:HHB	11:b:1240:CLA:HAB	2.02	0.41
2:2:60:TRP:HA	11:2:1204:CLA:HBB2	2.02	0.41
14:2:4014:BCR:HC41	11:2:1229:CLA:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4017:BCR:H352	11:2:1239:CLA:HBA2	2.03	0.41
10:k:120:LEU:CD1	11:k:1401:CLA:H11	2.49	0.41
1:A:575:ASP:OD2	1:A:579:ARG:NH1	2.53	0.41
2:B:645:TRP:CZ3	14:B:4017:BCR:HC21	2.56	0.41
11:B:1227:CLA:HMA3	11:B:1228:CLA:HED2	2.03	0.41
1:a:310:MET:O	1:a:319:HIS:N	2.54	0.41
14:a:4007:BCR:H341	11:a:1123:CLA:HAB	2.02	0.41
11:a:1103:CLA:H111	11:a:1103:CLA:H71	1.64	0.41
11:a:1119:CLA:HHC	11:a:1119:CLA:CBB	2.50	0.41
11:a:1121:CLA:CBB	11:a:1121:CLA:HHC	2.51	0.41
14:f:4013:BCR:H15C	14:f:4013:BCR:H351	1.72	0.41
1:1:53:ALA:HB2	15:1:5001:LHG:HC91	2.03	0.41
1:1:310:MET:O	1:1:319:HIS:N	2.54	0.41
2:2:154:TRP:CD1	8:7:28:GLU:HG3	2.56	0.41
2:2:329:HIS:CE1	2:2:390:ILE:HG21	2.56	0.41
2:2:520:ILE:HG21	11:2:1234:CLA:HAB	2.03	0.41
11:2:1202:CLA:H141	11:2:1202:CLA:H171	2.03	0.41
11:2:1238:CLA:C19	14:6:4018:BCR:H362	2.51	0.41
1:A:260:LEU:O	1:A:261:THR:OG1	2.32	0.41
11:A:1107:CLA:HBD	11:A:1107:CLA:HBA1	2.04	0.41
2:b:684:LEU:HD12	11:l:1502:CLA:HMD3	2.03	0.41
11:1:1801:CLA:CMA	15:1:5003:LHG:HC62	2.51	0.41
11:2:1239:CLA:HHC	11:2:1239:CLA:CBB	2.51	0.41
1:A:154:ASP:OD1	1:A:155:SER:N	2.55	0.40
11:B:1207:CLA:H2A	11:B:1207:CLA:O2A	2.20	0.40
1:a:203:GLY:HA2	11:a:1118:CLA:HBC1	2.03	0.40
1:a:332:PHE:HB2	15:a:5003:LHG:HC41	2.02	0.40
11:1:1022:CLA:H203	11:2:1206:CLA:H62	2.03	0.40
11:1:1106:CLA:HHC	11:1:1106:CLA:CBB	2.49	0.40
11:1:1107:CLA:C1	14:6:4013:BCR:H14C	2.51	0.40
11:1:1012:CLA:CHB	11:2:1021:CLA:H203	2.51	0.40
14:6:4018:BCR:H14C	9:9:23:PRO:HG2	2.00	0.40
1:A:439:HIS:CE1	11:A:1129:CLA:HMB2	2.57	0.40
11:A:1112:CLA:HBC2	11:A:1112:CLA:HHD	2.03	0.40
2:B:19:ARG:HG2	2:B:23:TYR:CD1	2.56	0.40
2:B:656:THR:HA	11:B:1023:CLA:CAB	2.46	0.40
7:L:56:ALA:HA	14:L:4022:BCR:H15C	2.03	0.40
2:b:683:PRO:C	2:b:685:ALA:H	2.28	0.40
11:b:1204:CLA:H92	14:m:4021:BCR:C14	2.52	0.40
4:d:10:LYS:HG3	4:d:49:ILE:HD11	2.03	0.40
1:1:456:ILE:CG2	11:1:1132:CLA:HMC1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:476:LEU:HD12	11:2:1231:CLA:HED3	2.03	0.40
14:2:4010:BCR:HC21	11:2:1223:CLA:CMA	2.51	0.40
5:5:11:ILE:N	5:5:11:ILE:HD12	2.36	0.40
1:A:451:SER:OG	1:A:452:PHE:N	2.55	0.40
11:A:1122:CLA:HMD2	11:A:1123:CLA:CBB	2.52	0.40
11:B:1226:CLA:C19	11:B:1239:CLA:HMA3	2.52	0.40
14:b:4017:BCR:C8	14:b:4017:BCR:H331	2.51	0.40
11:b:1222:CLA:CMB	11:b:1223:CLA:H202	2.51	0.40
11:b:1223:CLA:H111	11:b:1223:CLA:H93	1.85	0.40
11:1:1801:CLA:H3A	11:1:1801:CLA:HBA2	1.93	0.40
11:1:1111:CLA:CGA	11:1:1111:CLA:H3A	2.51	0.40
16:2:5002:LMG:H442	11:2:1224:CLA:HMC2	2.03	0.40
11:2:1231:CLA:C4C	11:2:1232:CLA:CAB	2.99	0.40
11:K:1402:CLA:HHC	11:K:1402:CLA:CBB	2.49	0.40
11:K:1402:CLA:CGA	11:K:1402:CLA:C1A	3.00	0.40
1:A:441:ASN:ND2	2:B:675:ILE:HG12	2.36	0.40
2:B:223:MET:N	2:B:223:MET:SD	2.94	0.40
1:a:548:ILE:HG12	11:b:1023:CLA:HMD3	2.02	0.40
11:b:1219:CLA:C1A	11:b:1219:CLA:CGA	2.98	0.40
3:c:17:CYS:SG	3:c:18:VAL:N	2.95	0.40
1:1:728:VAL:HG13	15:1:5001:LHG:H301	2.04	0.40
11:1:1134:CLA:HHC	11:1:1134:CLA:CBB	2.50	0.40
2:2:29:HIS:ND1	11:2:1203:CLA:O1A	2.54	0.40
2:2:654:TRP:CH2	2:2:658:PHE:CZ	3.10	0.40
1:A:395:TRP:HD1	11:A:1126:CLA:HAB	1.79	0.40
1:a:199:HIS:CE1	11:a:1118:CLA:HMD3	2.57	0.40
11:a:1801:CLA:HBB1	11:a:1121:CLA:CAB	2.52	0.40
2:b:487:GLY:O	2:b:489:ALA:N	2.54	0.40
2:2:475:LEU:HD13	11:2:1231:CLA:HHD	2.03	0.40
14:2:4011:BCR:H23C	11:2:1230:CLA:CMC	2.52	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	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	36	67
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	36	67
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	36	67
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	12	43
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	16	48
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	16	48
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	18	51
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	18	51
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	18	51
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	8	36
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	8	36
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	8	36
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	7	35
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	4	29
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	7	35
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	9	38
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	6	32
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	9	38
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	1	17
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	14
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	14 45

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR
2	b	6	PRO
4	d	99	PRO
1	1	261	THR
2	2	6	PRO
4	4	99	PRO
6	6	42	SER
10	K	92	GLN
10	K	125	SER
10	k	92	GLN
10	0	92	GLN
2	B	488	ALA
2	B	489	ALA
5	E	14	THR
7	L	108	GLN
2	b	488	ALA
5	e	14	THR
6	f	42	SER
2	2	488	ALA
2	2	489	ALA
5	5	14	THR
7	8	108	GLN
10	K	90	LEU
10	k	90	LEU
10	0	90	LEU
10	0	126	GLY
2	B	556	CYS
6	F	31	ALA
2	b	489	ALA
2	b	556	CYS
7	l	108	GLN
2	2	314	GLY
2	2	487	GLY

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Mol	Chain	Res	Type
2	2	556	CYS
1	A	115	GLN
2	B	314	GLY
2	B	487	GLY
7	L	109	GLY
1	a	115	GLN
2	b	487	GLY
6	f	31	ALA
1	1	115	GLN
6	6	31	ALA
10	k	51	PRO
6	F	50	PRO
2	2	235	ALA
2	b	314	GLY
7	l	109	GLY
7	8	109	GLY
10	K	51	PRO
10	K	87	ASP
10	0	51	PRO
7	L	18	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	588/603 (98%)	568 (97%)	20 (3%)	32	55
1	A	588/603 (98%)	568 (97%)	20 (3%)	32	55
1	a	588/603 (98%)	569 (97%)	19 (3%)	34	56
2	2	582/583 (100%)	557 (96%)	25 (4%)	26	50
2	B	582/583 (100%)	559 (96%)	23 (4%)	28	52
2	b	582/583 (100%)	557 (96%)	25 (4%)	26	50
3	3	68/69 (99%)	66 (97%)	2 (3%)	37	58
3	C	68/69 (99%)	63 (93%)	5 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	68/69 (99%)	65 (96%)	3 (4%)	25	49
4	4	113/116 (97%)	108 (96%)	5 (4%)	25	49
4	D	113/116 (97%)	109 (96%)	4 (4%)	32	54
4	d	113/116 (97%)	109 (96%)	4 (4%)	32	54
5	5	56/60 (93%)	53 (95%)	3 (5%)	20	45
5	E	56/60 (93%)	53 (95%)	3 (5%)	20	45
5	e	56/60 (93%)	53 (95%)	3 (5%)	20	45
6	6	21/106 (20%)	21 (100%)	0	100	100
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	23	47
7	8	113/118 (96%)	111 (98%)	2 (2%)	51	67
7	L	113/118 (96%)	111 (98%)	2 (2%)	51	67
7	l	113/118 (96%)	111 (98%)	2 (2%)	51	67
8	7	24/25 (96%)	23 (96%)	1 (4%)	26	50
8	M	24/25 (96%)	23 (96%)	1 (4%)	26	50
8	m	24/25 (96%)	23 (96%)	1 (4%)	26	50
9	9	31/32 (97%)	27 (87%)	4 (13%)	4	20
9	I	31/32 (97%)	27 (87%)	4 (13%)	4	20
9	i	31/32 (97%)	27 (87%)	4 (13%)	4	20
10	0	37/100 (37%)	31 (84%)	6 (16%)	2	14
10	K	37/100 (37%)	31 (84%)	6 (16%)	2	14
10	k	37/100 (37%)	32 (86%)	5 (14%)	4	19
All	All	4897/5436 (90%)	4694 (96%)	203 (4%)	27	51

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	104	LEU
1	A	210	LEU
1	A	224	ASN
1	A	235	ASP
1	A	245	GLU
1	A	249	MET

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	323	GLU
1	A	356	LEU
1	A	368	GLN
1	A	422	VAL
1	A	477	GLN
1	A	478	LEU
1	A	562	VAL
1	A	630	VAL
1	A	631	THR
1	A	641	THR
1	A	739	THR
1	A	748	LEU
2	B	82	LEU
2	B	85	ARG
2	B	143	LEU
2	B	145	LEU
2	B	196	HIS
2	B	229	ASN
2	B	236	ASP
2	B	280	ILE
2	B	302	LYS
2	B	304	ILE
2	B	318	THR
2	B	334	LEU
2	B	395	ASP
2	B	402	LYS
2	B	406	LEU
2	B	409	MET
2	B	414	GLU
2	B	420	LEU
2	B	441	VAL
2	B	516	VAL
2	B	542	LYS
2	B	596	LEU
2	B	689	ARG
3	C	11	CYS
3	C	21	CYS
3	C	54	CYS
3	C	58	CYS
3	C	69	LEU
4	D	73	ARG

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Mol	Chain	Res	Type
4	D	82	ASP
4	D	88	VAL
4	D	107	LYS
5	E	33	ILE
5	E	43	ARG
5	E	68	LEU
7	L	96	LEU
7	L	137	VAL
8	M	5	ASP
1	a	82	VAL
1	a	104	LEU
1	a	210	LEU
1	a	224	ASN
1	a	235	ASP
1	a	245	GLU
1	a	249	MET
1	a	303	LEU
1	a	323	GLU
1	a	356	LEU
1	a	368	GLN
1	a	422	VAL
1	a	477	GLN
1	a	478	LEU
1	a	562	VAL
1	a	630	VAL
1	a	631	THR
1	a	739	THR
1	a	748	LEU
2	b	32	GLU
2	b	82	LEU
2	b	85	ARG
2	b	143	LEU
2	b	145	LEU
2	b	196	HIS
2	b	201	GLU
2	b	229	ASN
2	b	236	ASP
2	b	280	ILE
2	b	302	LYS
2	b	304	ILE
2	b	318	THR
2	b	334	LEU

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Mol	Chain	Res	Type
2	b	402	LYS
2	b	406	LEU
2	b	409	MET
2	b	414	GLU
2	b	420	LEU
2	b	441	VAL
2	b	516	VAL
2	b	542	LYS
2	b	573	PHE
2	b	596	LEU
2	b	689	ARG
3	c	21	CYS
3	c	58	CYS
3	c	69	LEU
4	d	73	ARG
4	d	82	ASP
4	d	88	VAL
4	d	107	LYS
5	e	33	ILE
5	e	43	ARG
5	e	68	LEU
6	f	38	PHE
9	i	17	MET
9	i	21	LEU
9	i	27	MET
9	i	30	LEU
7	l	96	LEU
7	l	137	VAL
8	m	5	ASP
1	1	59	ASP
1	1	104	LEU
1	1	210	LEU
1	1	224	ASN
1	1	235	ASP
1	1	245	GLU
1	1	249	MET
1	1	303	LEU
1	1	323	GLU
1	1	356	LEU
1	1	368	GLN
1	1	422	VAL
1	1	477	GLN

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Mol	Chain	Res	Type
1	1	478	LEU
1	1	562	VAL
1	1	630	VAL
1	1	631	THR
1	1	641	THR
1	1	739	THR
1	1	748	LEU
2	2	82	LEU
2	2	85	ARG
2	2	143	LEU
2	2	145	LEU
2	2	196	HIS
2	2	229	ASN
2	2	236	ASP
2	2	280	ILE
2	2	302	LYS
2	2	304	ILE
2	2	318	THR
2	2	334	LEU
2	2	341	VAL
2	2	395	ASP
2	2	402	LYS
2	2	406	LEU
2	2	409	MET
2	2	414	GLU
2	2	420	LEU
2	2	441	VAL
2	2	474	VAL
2	2	516	VAL
2	2	542	LYS
2	2	596	LEU
2	2	689	ARG
3	3	58	CYS
3	3	69	LEU
4	4	3	GLU
4	4	73	ARG
4	4	82	ASP
4	4	88	VAL
4	4	107	LYS
5	5	33	ILE
5	5	43	ARG
5	5	68	LEU

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Mol	Chain	Res	Type
9	9	17	MET
9	9	21	LEU
9	9	27	MET
9	9	30	LEU
7	8	96	LEU
7	8	137	VAL
8	7	5	ASP
10	K	72	PHE
10	K	76	TYR
10	K	104	LEU
10	K	112	HIS
10	K	113	ILE
10	K	114	LEU
9	I	17	MET
9	I	21	LEU
9	I	27	MET
9	I	30	LEU
10	k	76	TYR
10	k	104	LEU
10	k	112	HIS
10	k	113	ILE
10	k	114	LEU
10	0	72	PHE
10	0	76	TYR
10	0	104	LEU
10	0	112	HIS
10	0	113	ILE
10	0	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	135	HIS
1	A	192	ASN
1	A	224	ASN
1	A	296	HIS
1	A	368	GLN
1	A	393	HIS
1	A	432	HIS
1	A	536	HIS
1	A	608	HIS

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Mol	Chain	Res	Type
1	A	714	GLN
2	B	29	HIS
2	B	34	HIS
2	B	53	HIS
2	B	89	HIS
2	B	114	ASN
2	B	317	HIS
2	B	373	HIS
2	B	437	HIS
2	B	582	ASN
2	B	602	ASN
2	B	627	GLN
4	D	51	ASN
4	D	64	GLN
7	L	105	GLN
1	a	93	HIS
1	a	135	HIS
1	a	192	ASN
1	a	224	ASN
1	a	296	HIS
1	a	368	GLN
1	a	393	HIS
1	a	432	HIS
1	a	538	HIS
1	a	608	HIS
1	a	676	HIS
2	b	34	HIS
2	b	53	HIS
2	b	114	ASN
2	b	437	HIS
2	b	582	ASN
4	d	64	GLN
1	1	50	ASN
1	1	56	HIS
1	1	76	HIS
1	1	79	HIS
1	1	192	ASN
1	1	224	ASN
1	1	296	HIS
1	1	393	HIS
1	1	432	HIS
1	1	488	HIS

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Mol	Chain	Res	Type
1	1	608	HIS
1	1	653	GLN
2	2	34	HIS
2	2	53	HIS
2	2	89	HIS
2	2	317	HIS
2	2	329	HIS
2	2	373	HIS
2	2	437	HIS
2	2	450	GLN
2	2	582	ASN
4	4	64	GLN
7	8	19	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

357 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CLA	1	1135	-	55,59,73	2.65	23 (41%)	64,96,113	2.80	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	2	1214	2	63,67,73	2.48	21 (33%)	74,105,113	2.53	26 (35%)
11	CLA	K	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.55	29 (35%)
14	BCR	B	4009	-	41,41,41	2.58	6 (14%)	56,56,56	6.86	21 (37%)
11	CLA	b	1214	2	63,67,73	2.47	22 (34%)	74,105,113	2.59	30 (40%)
14	BCR	A	4008	-	41,41,41	2.55	7 (17%)	56,56,56	6.83	29 (51%)
11	CLA	a	1801	15	56,60,73	2.65	22 (39%)	65,97,113	2.74	24 (36%)
11	CLA	B	1023	-	69,73,73	2.32	22 (31%)	82,113,113	2.51	30 (36%)
16	LMG	b	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.04	4 (6%)
11	CLA	2	1211	-	50,54,73	2.81	21 (42%)	59,90,113	2.76	21 (35%)
11	CLA	B	1223	-	69,73,73	2.38	22 (31%)	82,113,113	2.48	28 (34%)
11	CLA	8	1501	-	69,73,73	2.35	22 (31%)	82,113,113	2.53	27 (32%)
14	BCR	b	4006	-	41,41,41	2.59	6 (14%)	56,56,56	7.09	26 (46%)
11	CLA	2	1239	2	50,54,73	2.86	22 (44%)	59,90,113	2.73	22 (37%)
11	CLA	1	1132	1	69,73,73	2.35	22 (31%)	82,113,113	2.40	24 (29%)
11	CLA	b	1239	-	50,54,73	2.84	22 (44%)	59,90,113	2.76	23 (38%)
11	CLA	a	1135	-	55,59,73	2.65	21 (38%)	64,96,113	2.74	25 (39%)
14	BCR	A	4007	-	41,41,41	2.59	7 (17%)	56,56,56	6.97	21 (37%)
11	CLA	2	1023	-	69,73,73	2.35	22 (31%)	82,113,113	2.59	30 (36%)
11	CLA	2	1232	-	49,53,73	2.71	22 (44%)	58,89,113	2.72	22 (37%)
11	CLA	B	1226	2	69,73,73	2.34	22 (31%)	82,113,113	2.52	27 (32%)
11	CLA	b	1232	-	49,53,73	2.71	21 (42%)	58,89,113	2.71	21 (36%)
11	CLA	2	1223	2	69,73,73	2.38	22 (31%)	82,113,113	2.47	29 (35%)
11	CLA	2	1212	-	49,53,73	2.69	21 (42%)	58,89,113	2.71	22 (37%)
15	LHG	2	5004	11	48,48,48	0.96	2 (4%)	51,54,54	1.07	3 (5%)
11	CLA	A	1123	-	69,73,73	2.35	22 (31%)	82,113,113	2.52	28 (34%)
11	CLA	B	1221	-	58,62,73	2.56	21 (36%)	68,99,113	2.73	25 (36%)
11	CLA	b	1219	-	59,63,73	2.58	22 (37%)	70,101,113	2.58	25 (35%)
15	LHG	b	5004	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	4 (7%)
11	CLA	A	1103	1	69,73,73	2.36	22 (31%)	82,113,113	2.51	26 (31%)
11	CLA	2	1226	2	69,73,73	2.35	21 (30%)	82,113,113	2.51	24 (29%)
11	CLA	2	1224	-	59,63,73	2.53	21 (35%)	70,101,113	2.81	27 (38%)
13	SF4	A	3001	1,2	0,12,12	-	-	-		
11	CLA	2	1203	-	69,73,73	2.34	21 (30%)	82,113,113	2.50	28 (34%)
11	CLA	A	1129	-	50,54,73	2.82	22 (44%)	59,90,113	2.67	23 (38%)
11	CLA	B	1208	-	49,53,73	2.70	22 (44%)	58,89,113	2.76	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	A	1112	1	49,53,73	2.71	21 (42%)	58,89,113	2.84	24 (41%)
11	CLA	A	1122	-	63,67,73	2.46	21 (33%)	74,105,113	2.70	26 (35%)
11	CLA	1	1118	1	65,69,73	2.41	21 (32%)	77,108,113	2.49	27 (35%)
11	CLA	1	1121	1	50,54,73	2.84	22 (44%)	59,90,113	2.76	22 (37%)
12	PQN	a	2001	-	34,34,34	1.66	2 (5%)	43,45,45	1.06	4 (9%)
14	BCR	f	4018	-	41,41,41	2.66	7 (17%)	56,56,56	6.50	25 (44%)
11	CLA	b	1212	-	49,53,73	2.68	22 (44%)	58,89,113	2.81	20 (34%)
11	CLA	2	1235	-	64,68,73	2.46	23 (35%)	76,107,113	2.58	29 (38%)
11	CLA	b	1235	-	64,68,73	2.47	23 (35%)	76,107,113	2.60	29 (38%)
11	CLA	A	1109	1,11	69,73,73	2.38	22 (31%)	82,113,113	2.52	24 (29%)
14	BCR	b	4010	-	41,41,41	2.61	6 (14%)	56,56,56	6.86	21 (37%)
11	CLA	A	1131	1	69,73,73	2.38	21 (30%)	82,113,113	2.43	27 (32%)
11	CLA	8	1502	7	50,54,73	2.81	22 (44%)	59,90,113	2.80	22 (37%)
11	CLA	b	1201	2	58,62,73	2.57	22 (37%)	68,99,113	2.70	26 (38%)
11	CLA	A	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.38	28 (34%)
14	BCR	B	4017	-	41,41,41	2.60	7 (17%)	56,56,56	6.76	29 (51%)
11	CLA	2	1021	-	69,73,73	2.36	22 (31%)	82,113,113	2.53	30 (36%)
14	BCR	a	4003	-	41,41,41	2.60	6 (14%)	56,56,56	6.33	27 (48%)
14	BCR	2	4004	-	41,41,41	2.55	6 (14%)	56,56,56	6.62	29 (51%)
11	CLA	A	1130	1	50,54,73	2.83	21 (42%)	59,90,113	2.70	20 (33%)
11	CLA	1	1104	1	69,73,73	2.34	21 (30%)	82,113,113	2.52	27 (32%)
13	SF4	c	3003	3	0,12,12	-	-	-		
14	BCR	A	4001	-	41,41,41	2.60	7 (17%)	56,56,56	6.54	25 (44%)
14	BCR	A	4002	-	41,41,41	2.57	7 (17%)	56,56,56	6.45	23 (41%)
14	BCR	2	4009	-	41,41,41	2.55	6 (14%)	56,56,56	6.91	23 (41%)
11	CLA	2	1238	-	69,73,73	2.36	22 (31%)	82,113,113	2.40	25 (30%)
11	CLA	A	1117	1	69,73,73	2.41	22 (31%)	82,113,113	2.39	25 (30%)
11	CLA	a	1112	-	49,53,73	2.70	20 (40%)	58,89,113	2.75	23 (39%)
11	CLA	2	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.53	27 (32%)
11	CLA	a	1120	1	50,54,73	2.84	23 (46%)	59,90,113	2.81	22 (37%)
14	BCR	8	4022	-	41,41,41	2.59	6 (14%)	56,56,56	6.65	30 (53%)
15	LHG	A	5001	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	4 (7%)
11	CLA	B	1222	-	60,64,73	2.56	22 (36%)	71,102,113	2.74	28 (39%)
11	CLA	a	1126	1	69,73,73	2.38	23 (33%)	82,113,113	2.49	25 (30%)
11	CLA	b	1240	-	49,53,73	2.72	22 (44%)	58,89,113	2.75	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	1	1112	-	49,53,73	2.70	21 (42%)	58,89,113	2.80	24 (41%)
11	CLA	a	1110	1	58,62,73	2.59	22 (37%)	68,99,113	2.64	27 (39%)
11	CLA	A	1126	1	69,73,73	2.38	21 (30%)	82,113,113	2.56	26 (31%)
11	CLA	b	1202	2	69,73,73	2.36	22 (31%)	82,113,113	2.49	24 (29%)
11	CLA	b	1225	-	69,73,73	2.39	22 (31%)	82,113,113	2.38	24 (29%)
11	CLA	1	1134	-	50,54,73	2.84	22 (44%)	59,90,113	2.76	22 (37%)
11	CLA	A	1108	1	49,53,73	2.68	21 (42%)	58,89,113	2.76	23 (39%)
14	BCR	B	4006	-	41,41,41	2.57	6 (14%)	56,56,56	6.97	26 (46%)
11	CLA	B	1230	2	62,66,73	2.49	20 (32%)	73,104,113	2.60	27 (36%)
11	CLA	A	1135	-	55,59,73	2.64	22 (40%)	64,96,113	2.78	27 (42%)
11	CLA	B	1220	2	50,54,73	2.82	21 (42%)	59,90,113	2.65	21 (35%)
11	CLA	1	1122	-	63,67,73	2.49	22 (34%)	74,105,113	2.58	25 (33%)
11	CLA	B	1231	-	49,53,73	2.70	21 (42%)	58,89,113	2.79	24 (41%)
11	CLA	1	1127	-	69,73,73	2.38	22 (31%)	82,113,113	2.39	25 (30%)
11	CLA	b	1210	2	69,73,73	2.38	22 (31%)	82,113,113	2.48	31 (37%)
11	CLA	a	1138	1	50,54,73	2.84	22 (44%)	59,90,113	2.81	23 (38%)
11	CLA	b	1234	-	64,68,73	2.46	21 (32%)	76,107,113	2.53	25 (32%)
14	BCR	7	4021	-	41,41,41	2.60	6 (14%)	56,56,56	6.77	21 (37%)
11	CLA	b	1216	-	69,73,73	2.39	22 (31%)	82,113,113	2.43	29 (35%)
11	CLA	1	1133	-	50,54,73	2.84	21 (42%)	59,90,113	2.70	22 (37%)
14	BCR	B	4005	-	41,41,41	2.61	7 (17%)	56,56,56	6.69	25 (44%)
11	CLA	B	1216	-	69,73,73	2.37	22 (31%)	82,113,113	2.41	27 (32%)
11	CLA	1	1140	1	69,73,73	2.38	22 (31%)	82,113,113	2.55	27 (32%)
11	CLA	1	1139	-	54,58,73	2.69	23 (42%)	64,95,113	2.71	24 (37%)
11	CLA	1	1120	1	50,54,73	2.85	23 (46%)	59,90,113	2.76	22 (37%)
11	CLA	a	1132	1	69,73,73	2.38	22 (31%)	82,113,113	2.45	26 (31%)
11	CLA	A	1136	1	50,54,73	2.81	22 (44%)	59,90,113	2.76	23 (38%)
11	CLA	A	1105	1	52,56,73	2.71	22 (42%)	61,92,113	2.75	23 (37%)
11	CLA	B	1234	-	64,68,73	2.43	21 (32%)	76,107,113	2.60	29 (38%)
11	CLA	B	1217	-	51,55,73	2.71	22 (43%)	60,91,113	2.79	23 (38%)
11	CLA	1	1116	-	58,62,73	2.59	22 (37%)	68,99,113	2.68	26 (38%)
11	CLA	1	1137	-	69,73,73	2.36	22 (31%)	82,113,113	2.60	25 (30%)
11	CLA	L	1502	7	50,54,73	2.81	20 (40%)	59,90,113	2.80	21 (35%)
11	CLA	1	1128	1	69,73,73	2.36	21 (30%)	82,113,113	2.37	25 (30%)
11	CLA	b	1211	-	50,54,73	2.84	22 (44%)	59,90,113	2.72	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	A	1125	1	56,60,73	2.65	21 (37%)	65,97,113	2.81	29 (44%)
11	CLA	1	1131	1	69,73,73	2.36	22 (31%)	82,113,113	2.46	25 (30%)
11	CLA	1	1101	-	69,73,73	2.36	21 (30%)	82,113,113	2.47	28 (34%)
11	CLA	B	1215	2	69,73,73	2.36	22 (31%)	82,113,113	2.57	27 (32%)
11	CLA	a	1103	1	69,73,73	2.39	22 (31%)	82,113,113	2.43	25 (30%)
11	CLA	B	1206	2	69,73,73	2.34	21 (30%)	82,113,113	2.42	26 (31%)
11	CLA	a	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.45	26 (31%)
11	CLA	b	1227	-	49,53,73	2.70	20 (40%)	58,89,113	2.83	22 (37%)
14	BCR	f	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.76	22 (39%)
11	CLA	1	1136	-	50,54,73	2.82	21 (42%)	59,90,113	2.76	22 (37%)
11	CLA	2	1229	2	69,73,73	2.37	23 (33%)	82,113,113	2.46	27 (32%)
11	CLA	a	1117	1	69,73,73	2.37	22 (31%)	82,113,113	2.47	26 (31%)
11	CLA	a	1121	-	50,54,73	2.85	22 (44%)	59,90,113	2.77	23 (38%)
11	CLA	A	1114	-	50,54,73	2.84	22 (44%)	59,90,113	2.66	21 (35%)
11	CLA	B	1214	2	63,67,73	2.46	22 (34%)	74,105,113	2.72	28 (37%)
15	LHG	B	5004	11	48,48,48	0.96	2 (4%)	51,54,54	1.14	4 (7%)
11	CLA	2	1205	2	59,63,73	2.50	20 (33%)	70,101,113	2.69	24 (34%)
11	CLA	a	1102	1,11	69,73,73	2.37	22 (31%)	82,113,113	2.46	25 (30%)
14	BCR	a	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.90	23 (41%)
11	CLA	B	1202	2	69,73,73	2.39	22 (31%)	82,113,113	2.47	25 (30%)
14	BCR	L	4022	-	41,41,41	2.56	6 (14%)	56,56,56	6.25	25 (44%)
13	SF4	3	3002	3	0,12,12	-	-	-		
11	CLA	a	1123	-	69,73,73	2.37	21 (30%)	82,113,113	2.43	25 (30%)
14	BCR	b	4011	-	41,41,41	2.58	7 (17%)	56,56,56	6.94	25 (44%)
11	CLA	a	1108	-	49,53,73	2.70	21 (42%)	58,89,113	2.76	22 (37%)
11	CLA	A	1022	-	69,73,73	2.36	21 (30%)	82,113,113	2.40	28 (34%)
14	BCR	8	4019	-	41,41,41	2.58	6 (14%)	56,56,56	6.80	22 (39%)
11	CLA	A	1012	-	69,73,73	2.35	22 (31%)	82,113,113	2.56	27 (32%)
11	CLA	1	1801	15	56,60,73	2.65	22 (39%)	65,97,113	2.78	26 (40%)
11	CLA	a	1115	1	50,54,73	2.84	23 (46%)	59,90,113	2.71	23 (38%)
11	CLA	B	1239	2	50,54,73	2.82	22 (44%)	59,90,113	2.76	20 (33%)
11	CLA	2	1202	2	69,73,73	2.38	22 (31%)	82,113,113	2.48	24 (29%)
14	BCR	f	4020	-	41,41,41	2.61	6 (14%)	56,56,56	6.73	22 (39%)
11	CLA	A	1110	1	58,62,73	2.58	22 (37%)	68,99,113	2.71	26 (38%)
11	CLA	a	1107	1	69,73,73	2.35	21 (30%)	82,113,113	2.61	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	B	1235	-	64,68,73	2.47	23 (35%)	76,107,113	2.55	23 (30%)
11	CLA	B	1232	-	49,53,73	2.70	20 (40%)	58,89,113	2.74	21 (36%)
11	CLA	A	1106	1	69,73,73	2.38	21 (30%)	82,113,113	2.46	23 (28%)
11	CLA	a	1104	1	69,73,73	2.34	22 (31%)	82,113,113	2.51	28 (34%)
11	CLA	2	1209	-	49,53,73	2.71	21 (42%)	58,89,113	2.75	23 (39%)
11	CLA	a	1011	1	69,73,73	2.38	23 (33%)	82,113,113	2.47	26 (31%)
11	CLA	1	1012	-	69,73,73	2.37	21 (30%)	82,113,113	2.52	26 (31%)
11	CLA	a	1109	1,11	69,73,73	2.39	22 (31%)	82,113,113	2.51	25 (30%)
14	BCR	L	4019	-	41,41,41	2.53	6 (14%)	56,56,56	6.74	24 (42%)
14	BCR	F	4013	-	41,41,41	2.60	6 (14%)	56,56,56	6.93	21 (37%)
13	SF4	a	3001	1,2	0,12,12	-	-	-		
11	CLA	a	1122	-	63,67,73	2.49	22 (34%)	74,105,113	2.63	26 (35%)
11	CLA	b	1204	2	69,73,73	2.35	22 (31%)	82,113,113	2.42	23 (28%)
11	CLA	b	1209	-	49,53,73	2.71	21 (42%)	58,89,113	2.76	22 (37%)
11	CLA	2	1201	2	58,62,73	2.59	21 (36%)	68,99,113	2.63	24 (35%)
15	LHG	1	5003	11	48,48,48	0.96	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	1	1105	-	52,56,73	2.72	22 (42%)	61,92,113	2.78	23 (37%)
14	BCR	A	4003	-	41,41,41	2.66	6 (14%)	56,56,56	6.43	24 (42%)
11	CLA	A	1118	1	65,69,73	2.40	20 (30%)	77,108,113	2.56	25 (32%)
11	CLA	B	1203	2	69,73,73	2.35	21 (30%)	82,113,113	2.47	23 (28%)
11	CLA	b	1215	2	69,73,73	2.39	22 (31%)	82,113,113	2.53	29 (35%)
14	BCR	a	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.67	25 (44%)
11	CLA	1	1111	1	64,68,73	2.41	21 (32%)	76,107,113	2.68	30 (39%)
11	CLA	B	1204	2	69,73,73	2.33	21 (30%)	82,113,113	2.49	27 (32%)
11	CLA	1	1109	-	69,73,73	2.36	21 (30%)	82,113,113	2.49	25 (30%)
11	CLA	L	1503	-	69,73,73	2.33	20 (28%)	82,113,113	2.50	23 (28%)
11	CLA	a	1131	1	69,73,73	2.37	21 (30%)	82,113,113	2.44	29 (35%)
11	CLA	1	1022	-	69,73,73	2.38	22 (31%)	82,113,113	2.38	28 (34%)
13	SF4	C	3002	3	0,12,12	-	-	-		
11	CLA	b	1218	-	49,53,73	2.71	21 (42%)	58,89,113	2.75	22 (37%)
11	CLA	b	1021	-	69,73,73	2.38	22 (31%)	82,113,113	2.54	32 (39%)
14	BCR	m	4021	-	41,41,41	2.64	6 (14%)	56,56,56	6.66	24 (42%)
15	LHG	a	5003	11	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
11	CLA	1	1119	-	69,73,73	2.36	21 (30%)	82,113,113	2.48	27 (32%)
11	CLA	B	1238	-	69,73,73	2.34	20 (28%)	82,113,113	2.43	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	a	1105	1	52,56,73	2.74	21 (40%)	61,92,113	2.81	23 (37%)
11	CLA	B	1210	2	69,73,73	2.37	22 (31%)	82,113,113	2.49	27 (32%)
14	BCR	B	4011	-	41,41,41	2.63	7 (17%)	56,56,56	6.86	27 (48%)
11	CLA	1	1106	1	69,73,73	2.37	22 (31%)	82,113,113	2.41	26 (31%)
11	CLA	A	1140	1	69,73,73	2.36	22 (31%)	82,113,113	2.49	26 (31%)
14	BCR	1	4003	-	41,41,41	2.60	6 (14%)	56,56,56	6.53	27 (48%)
11	CLA	A	1121	1	50,54,73	2.85	22 (44%)	59,90,113	2.71	20 (33%)
11	CLA	1	1115	1	50,54,73	2.83	21 (42%)	59,90,113	2.75	22 (37%)
11	CLA	0	1402	-	54,58,73	2.70	22 (40%)	64,95,113	2.72	22 (34%)
11	CLA	A	1139	-	54,58,73	2.68	23 (42%)	64,95,113	2.71	24 (37%)
11	CLA	b	1222	-	60,64,73	2.54	22 (36%)	71,102,113	2.76	26 (36%)
11	CLA	b	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.53	26 (31%)
11	CLA	B	1213	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	25 (30%)
11	CLA	A	1113	-	49,53,73	2.68	21 (42%)	58,89,113	2.77	22 (37%)
11	CLA	a	1129	-	50,54,73	2.82	22 (44%)	59,90,113	2.78	21 (35%)
11	CLA	A	1127	1	69,73,73	2.35	21 (30%)	82,113,113	2.47	26 (31%)
11	CLA	B	1207	-	69,73,73	2.34	21 (30%)	82,113,113	2.57	24 (29%)
12	PQN	b	2002	-	34,34,34	1.67	2 (5%)	43,45,45	1.14	5 (11%)
11	CLA	B	1240	15	49,53,73	2.72	22 (44%)	58,89,113	2.74	23 (39%)
11	CLA	A	1124	-	59,63,73	2.56	22 (37%)	70,101,113	2.66	29 (41%)
11	CLA	2	1231	-	49,53,73	2.71	21 (42%)	58,89,113	2.83	26 (44%)
11	CLA	2	1210	-	69,73,73	2.34	22 (31%)	82,113,113	2.54	29 (35%)
11	CLA	B	1228	2	54,58,73	2.69	22 (40%)	64,95,113	2.71	23 (35%)
11	CLA	2	1234	-	64,68,73	2.43	21 (32%)	76,107,113	2.56	27 (35%)
14	BCR	1	4001	-	41,41,41	2.57	6 (14%)	56,56,56	6.70	27 (48%)
14	BCR	B	4014	-	41,41,41	2.59	7 (17%)	56,56,56	6.44	24 (42%)
11	CLA	a	1136	1	50,54,73	2.82	21 (42%)	59,90,113	2.77	21 (35%)
11	CLA	A	1107	1	69,73,73	2.33	21 (30%)	82,113,113	2.52	26 (31%)
11	CLA	B	1013	-	69,73,73	2.36	22 (31%)	82,113,113	2.47	27 (32%)
11	CLA	1	1129	-	50,54,73	2.84	22 (44%)	59,90,113	2.77	21 (35%)
14	BCR	2	4005	-	41,41,41	2.58	7 (17%)	56,56,56	6.53	20 (35%)
11	CLA	2	1240	15	49,53,73	2.71	21 (42%)	58,89,113	2.70	21 (36%)
14	BCR	b	4005	-	41,41,41	2.58	6 (14%)	56,56,56	6.74	25 (44%)
14	BCR	l	4022	-	41,41,41	2.57	6 (14%)	56,56,56	6.56	26 (46%)
14	BCR	a	4002	-	41,41,41	2.59	7 (17%)	56,56,56	6.74	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	k	1402	10	54,58,73	2.68	22 (40%)	64,95,113	2.71	24 (37%)
11	CLA	a	1012	-	69,73,73	2.38	23 (33%)	82,113,113	2.45	23 (28%)
11	CLA	a	1137	-	69,73,73	2.37	21 (30%)	82,113,113	2.57	27 (32%)
11	CLA	A	1137	1	69,73,73	2.37	23 (33%)	82,113,113	2.61	28 (34%)
11	CLA	A	1128	1	69,73,73	2.34	20 (28%)	82,113,113	2.40	25 (30%)
11	CLA	a	1101	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	26 (31%)
14	BCR	1	4002	-	41,41,41	2.56	7 (17%)	56,56,56	7.09	22 (39%)
11	CLA	A	1101	1	69,73,73	2.34	22 (31%)	82,113,113	2.44	26 (31%)
11	CLA	2	1206	2	69,73,73	2.35	21 (30%)	82,113,113	2.39	24 (29%)
11	CLA	A	1237	-	59,63,73	2.54	22 (37%)	70,101,113	2.63	25 (35%)
11	CLA	a	1118	1	65,69,73	2.41	22 (33%)	77,108,113	2.54	26 (33%)
11	CLA	a	1237	-	59,63,73	2.53	22 (37%)	70,101,113	2.61	25 (35%)
11	CLA	a	1111	1	64,68,73	2.41	23 (35%)	76,107,113	2.62	29 (38%)
11	CLA	1	1110	1	58,62,73	2.59	22 (37%)	68,99,113	2.70	26 (38%)
15	LHG	1	5001	-	48,48,48	0.95	2 (4%)	51,54,54	1.10	4 (7%)
11	CLA	a	1124	-	59,63,73	2.56	22 (37%)	70,101,113	2.71	27 (38%)
11	CLA	b	1230	-	62,66,73	2.53	21 (33%)	73,104,113	2.64	27 (36%)
11	CLA	a	1125	-	56,60,73	2.60	22 (39%)	65,97,113	2.70	24 (36%)
11	CLA	b	1206	2	69,73,73	2.36	21 (30%)	82,113,113	2.42	25 (30%)
11	CLA	1	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.75	22 (37%)
14	BCR	B	4004	-	41,41,41	2.61	6 (14%)	56,56,56	6.71	27 (48%)
11	CLA	2	1213	-	69,73,73	2.41	23 (33%)	82,113,113	2.56	27 (32%)
11	CLA	2	1225	2	69,73,73	2.38	22 (31%)	82,113,113	2.44	25 (30%)
14	BCR	2	4017	-	41,41,41	2.61	7 (17%)	56,56,56	6.69	27 (48%)
11	CLA	2	1230	2	62,66,73	2.51	22 (35%)	73,104,113	2.62	27 (36%)
11	CLA	b	1213	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	25 (30%)
11	CLA	b	1023	-	69,73,73	2.34	21 (30%)	82,113,113	2.51	29 (35%)
14	BCR	a	4008	-	41,41,41	2.60	7 (17%)	56,56,56	6.71	28 (50%)
11	CLA	B	1227	-	49,53,73	2.68	20 (40%)	58,89,113	2.86	22 (37%)
11	CLA	b	1223	-	69,73,73	2.38	21 (30%)	82,113,113	2.40	26 (31%)
11	CLA	a	1114	-	50,54,73	2.84	21 (42%)	59,90,113	2.69	21 (35%)
14	BCR	b	4017	-	41,41,41	2.63	7 (17%)	56,56,56	6.81	27 (48%)
11	CLA	B	1211	-	50,54,73	2.82	21 (42%)	59,90,113	2.71	21 (35%)
15	LHG	a	5001	-	48,48,48	0.96	2 (4%)	51,54,54	1.08	4 (7%)
11	CLA	b	1205	2	59,63,73	2.53	21 (35%)	70,101,113	2.65	25 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	2	1227	-	49,53,73	2.68	20 (40%)	58,89,113	2.82	22 (37%)
11	CLA	b	1226	2	69,73,73	2.35	22 (31%)	82,113,113	2.44	27 (32%)
11	CLA	A	1115	1	50,54,73	2.86	23 (46%)	59,90,113	2.75	23 (38%)
11	CLA	b	1224	-	59,63,73	2.56	23 (38%)	70,101,113	2.71	26 (37%)
11	CLA	a	1113	-	49,53,73	2.70	21 (42%)	58,89,113	2.73	22 (37%)
11	CLA	A	1111	1	64,68,73	2.43	22 (34%)	76,107,113	2.56	25 (32%)
11	CLA	B	1205	2	59,63,73	2.51	19 (32%)	70,101,113	2.77	24 (34%)
11	CLA	1	1114	-	50,54,73	2.85	22 (44%)	59,90,113	2.70	21 (35%)
16	LMG	B	5002	-	55,55,55	0.90	2 (3%)	63,63,63	1.08	4 (6%)
11	CLA	1	1103	1	69,73,73	2.36	21 (30%)	82,113,113	2.55	27 (32%)
11	CLA	2	1236	2	51,55,73	2.72	23 (45%)	60,91,113	2.84	22 (36%)
13	SF4	3	3003	-	0,12,12	-	-	-		
11	CLA	1	1125	-	56,60,73	2.62	22 (39%)	65,97,113	2.77	27 (41%)
14	BCR	l	4019	-	41,41,41	2.59	6 (14%)	56,56,56	6.87	20 (35%)
11	CLA	0	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.56	29 (35%)
11	CLA	B	1224	-	59,63,73	2.53	22 (37%)	70,101,113	2.82	25 (35%)
11	CLA	1	1237	-	59,63,73	2.52	22 (37%)	70,101,113	2.67	27 (38%)
11	CLA	b	1221	-	58,62,73	2.58	23 (39%)	68,99,113	2.80	27 (39%)
11	CLA	2	1208	-	49,53,73	2.69	21 (42%)	58,89,113	2.72	19 (32%)
11	CLA	A	1011	1	69,73,73	2.34	22 (31%)	82,113,113	2.49	25 (30%)
11	CLA	2	1013	-	69,73,73	2.37	22 (31%)	82,113,113	2.51	28 (34%)
11	CLA	a	1022	-	69,73,73	2.37	21 (30%)	82,113,113	2.35	24 (29%)
11	CLA	b	1208	-	49,53,73	2.71	21 (42%)	58,89,113	2.76	21 (36%)
16	LMG	2	5002	-	55,55,55	0.91	2 (3%)	63,63,63	1.07	4 (6%)
11	CLA	1	1107	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	25 (30%)
11	CLA	b	1013	-	69,73,73	2.38	22 (31%)	82,113,113	2.45	28 (34%)
11	CLA	8	1503	-	69,73,73	2.39	22 (31%)	82,113,113	2.41	24 (29%)
11	CLA	1	1138	1	50,54,73	2.81	22 (44%)	59,90,113	2.72	20 (33%)
14	BCR	2	4006	-	41,41,41	2.56	6 (14%)	56,56,56	6.98	28 (50%)
11	CLA	1	1117	-	69,73,73	2.38	22 (31%)	82,113,113	2.43	26 (31%)
14	BCR	1	4008	-	41,41,41	2.58	7 (17%)	56,56,56	6.94	26 (46%)
11	CLA	B	1212	-	49,53,73	2.70	22 (44%)	58,89,113	2.74	21 (36%)
11	CLA	a	1106	1	69,73,73	2.37	22 (31%)	82,113,113	2.45	27 (32%)
13	SF4	1	3001	1,2	0,12,12	-	-	-		
11	CLA	1	1102	1	69,73,73	2.38	23 (33%)	82,113,113	2.40	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	2	1221	-	58,62,73	2.57	23 (39%)	68,99,113	2.72	26 (38%)
14	BCR	b	4014	-	41,41,41	2.58	7 (17%)	56,56,56	6.64	23 (41%)
11	CLA	b	1203	2	69,73,73	2.36	23 (33%)	82,113,113	2.47	24 (29%)
14	BCR	b	4004	-	41,41,41	2.56	6 (14%)	56,56,56	6.72	25 (44%)
11	CLA	2	1219	2	59,63,73	2.58	23 (38%)	70,101,113	2.67	25 (35%)
11	CLA	B	1209	-	49,53,73	2.70	21 (42%)	58,89,113	2.74	22 (37%)
11	CLA	A	1102	1,11	69,73,73	2.38	22 (31%)	82,113,113	2.48	27 (32%)
11	CLA	1	1108	-	49,53,73	2.70	21 (42%)	58,89,113	2.76	20 (34%)
11	CLA	l	1503	-	69,73,73	2.36	22 (31%)	82,113,113	2.44	24 (29%)
12	PQN	A	2001	-	34,34,34	1.68	2 (5%)	43,45,45	1.16	5 (11%)
11	CLA	A	1104	1	69,73,73	2.31	21 (30%)	82,113,113	2.62	28 (34%)
11	CLA	A	1116	-	58,62,73	2.60	23 (39%)	68,99,113	2.67	27 (39%)
11	CLA	2	1215	2	69,73,73	2.38	21 (30%)	82,113,113	2.56	28 (34%)
11	CLA	b	1236	-	51,55,73	2.71	23 (45%)	60,91,113	2.87	21 (35%)
11	CLA	2	1204	2	69,73,73	2.37	22 (31%)	82,113,113	2.42	26 (31%)
11	CLA	B	1219	2	59,63,73	2.56	22 (37%)	70,101,113	2.57	25 (35%)
11	CLA	B	1236	2	51,55,73	2.67	22 (43%)	60,91,113	2.88	23 (38%)
11	CLA	B	1201	2	58,62,73	2.56	22 (37%)	68,99,113	2.72	28 (41%)
11	CLA	2	1228	2	54,58,73	2.68	22 (40%)	64,95,113	2.72	25 (39%)
11	CLA	A	1133	-	50,54,73	2.82	21 (42%)	59,90,113	2.76	24 (40%)
12	PQN	B	2002	-	34,34,34	1.68	2 (5%)	43,45,45	1.17	4 (9%)
11	CLA	B	1218	-	49,53,73	2.69	21 (42%)	58,89,113	2.77	21 (36%)
11	CLA	b	1231	-	49,53,73	2.69	21 (42%)	58,89,113	2.78	23 (39%)
11	CLA	2	1222	-	60,64,73	2.54	22 (36%)	71,102,113	2.67	27 (38%)
13	SF4	C	3003	3	0,12,12	-	-	-		
11	CLA	a	1133	-	50,54,73	2.83	21 (42%)	59,90,113	2.75	23 (38%)
14	BCR	6	4013	-	41,41,41	2.56	6 (14%)	56,56,56	6.77	23 (41%)
11	CLA	A	1120	1	50,54,73	2.86	22 (44%)	59,90,113	2.75	22 (37%)
11	CLA	1	1130	1	50,54,73	2.85	22 (44%)	59,90,113	2.66	21 (35%)
11	CLA	a	1134	-	50,54,73	2.83	22 (44%)	59,90,113	2.75	24 (40%)
12	PQN	2	2002	-	34,34,34	1.67	2 (5%)	43,45,45	1.12	7 (16%)
14	BCR	M	4021	-	41,41,41	2.60	6 (14%)	56,56,56	6.73	19 (33%)
11	CLA	A	1134	1	50,54,73	2.83	22 (44%)	59,90,113	2.72	23 (38%)
11	CLA	b	1229	-	69,73,73	2.37	22 (31%)	82,113,113	2.44	26 (31%)
11	CLA	b	1228	2	54,58,73	2.68	22 (40%)	64,95,113	2.71	24 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	BCR	B	4010	-	41,41,41	2.57	6 (14%)	56,56,56	6.56	26 (46%)
13	SF4	c	3002	3	0,12,12	-	-	-		
14	BCR	6	4020	-	41,41,41	2.67	7 (17%)	56,56,56	6.68	24 (42%)
14	BCR	2	4011	-	41,41,41	2.62	7 (17%)	56,56,56	6.92	25 (44%)
14	BCR	b	4009	-	41,41,41	2.50	6 (14%)	56,56,56	7.08	24 (42%)
11	CLA	b	1238	-	69,73,73	2.36	22 (31%)	82,113,113	2.41	25 (30%)
11	CLA	a	1116	-	58,62,73	2.60	22 (37%)	68,99,113	2.66	27 (39%)
11	CLA	l	1501	7	69,73,73	2.37	23 (33%)	82,113,113	2.50	25 (30%)
14	BCR	F	4020	-	41,41,41	2.61	6 (14%)	56,56,56	6.57	23 (41%)
11	CLA	B	1225	2	69,73,73	2.37	22 (31%)	82,113,113	2.37	25 (30%)
12	PQN	1	2001	-	34,34,34	1.70	2 (5%)	43,45,45	1.12	4 (9%)
14	BCR	2	4010	-	41,41,41	2.65	7 (17%)	56,56,56	6.55	27 (48%)
11	CLA	1	1123	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	24 (29%)
11	CLA	1	1011	1	69,73,73	2.35	22 (31%)	82,113,113	2.67	26 (31%)
11	CLA	L	1501	7	69,73,73	2.37	22 (31%)	82,113,113	2.47	25 (30%)
11	CLA	a	1128	1	69,73,73	2.37	21 (30%)	82,113,113	2.43	26 (31%)
11	CLA	2	1216	-	69,73,73	2.38	23 (33%)	82,113,113	2.44	25 (30%)
11	CLA	a	1127	-	69,73,73	2.37	22 (31%)	82,113,113	2.45	31 (37%)
11	CLA	A	1132	1	69,73,73	2.37	21 (30%)	82,113,113	2.53	25 (30%)
11	CLA	1	1124	-	59,63,73	2.55	22 (37%)	70,101,113	2.67	25 (35%)
14	BCR	F	4018	-	41,41,41	2.70	7 (17%)	56,56,56	6.72	24 (42%)
11	CLA	2	1217	2	51,55,73	2.73	21 (41%)	60,91,113	2.80	25 (41%)
14	BCR	2	4014	-	41,41,41	2.61	6 (14%)	56,56,56	6.58	23 (41%)
11	CLA	a	1140	-	69,73,73	2.36	21 (30%)	82,113,113	2.46	26 (31%)
11	CLA	2	1218	-	49,53,73	2.68	21 (42%)	58,89,113	2.79	22 (37%)
11	CLA	b	1217	-	51,55,73	2.72	23 (45%)	60,91,113	2.79	21 (35%)
11	CLA	a	1139	-	54,58,73	2.70	21 (38%)	64,95,113	2.69	23 (35%)
11	CLA	K	1402	10	54,58,73	2.66	22 (40%)	64,95,113	2.68	23 (35%)
11	CLA	l	1502	7	50,54,73	2.81	22 (44%)	59,90,113	2.77	21 (35%)
11	CLA	2	1220	2	50,54,73	2.83	21 (42%)	59,90,113	2.73	21 (35%)
11	CLA	b	1220	2	50,54,73	2.87	21 (42%)	59,90,113	2.68	22 (37%)
11	CLA	A	1138	1	50,54,73	2.80	22 (44%)	59,90,113	2.83	22 (37%)
11	CLA	k	1401	-	69,73,73	2.37	21 (30%)	82,113,113	2.56	29 (35%)
14	BCR	6	4018	-	41,41,41	2.68	7 (17%)	56,56,56	6.44	26 (46%)
11	CLA	A	1801	15	56,60,73	2.68	22 (39%)	65,97,113	2.75	28 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	LHG	A	5003	11	48,48,48	0.95	2 (4%)	51,54,54	1.15	4 (7%)
11	CLA	1	1126	1	69,73,73	2.38	23 (33%)	82,113,113	2.50	29 (35%)
11	CLA	B	1229	2	69,73,73	2.37	22 (31%)	82,113,113	2.45	28 (34%)
14	BCR	1	4007	-	41,41,41	2.55	6 (14%)	56,56,56	6.82	25 (44%)
11	CLA	a	1130	1	50,54,73	2.86	22 (44%)	59,90,113	2.69	21 (35%)
11	CLA	B	1021	-	69,73,73	2.33	21 (30%)	82,113,113	2.61	30 (36%)

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
11	CLA	1	1135	-	-	9/23/99/115	-
11	CLA	2	1214	2	-	13/32/108/115	-
11	CLA	K	1401	-	-	22/39/115/115	-
14	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1214	2	-	10/32/108/115	-
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	a	1801	15	-	13/24/100/115	-
11	CLA	B	1023	-	-	14/39/115/115	-
16	LMG	b	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	2	1211	-	-	9/17/93/115	-
11	CLA	B	1223	-	-	10/39/115/115	-
11	CLA	8	1501	-	-	14/39/115/115	-
14	BCR	b	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	2	1239	2	-	10/17/93/115	-
11	CLA	1	1132	1	-	9/39/115/115	-
11	CLA	b	1239	-	-	7/17/93/115	-
11	CLA	a	1135	-	-	9/23/99/115	-
14	BCR	A	4007	-	-	13/29/63/63	0/2/2/2
11	CLA	2	1023	-	-	14/39/115/115	-
11	CLA	2	1232	-	-	7/15/91/115	-
11	CLA	B	1226	2	-	13/39/115/115	-
11	CLA	b	1232	-	-	6/15/91/115	-
11	CLA	2	1223	2	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1212	-	-	2/15/91/115	-
15	LHG	2	5004	11	-	28/53/53/53	-
11	CLA	A	1123	-	-	15/39/115/115	-
11	CLA	B	1221	-	-	10/26/102/115	-
11	CLA	b	1219	-	-	9/27/103/115	-
15	LHG	b	5004	-	-	24/53/53/53	-
11	CLA	A	1103	1	-	14/39/115/115	-
11	CLA	2	1226	2	-	13/39/115/115	-
11	CLA	2	1224	-	-	10/27/103/115	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
11	CLA	2	1203	-	-	16/39/115/115	-
11	CLA	A	1129	-	-	5/17/93/115	-
11	CLA	B	1208	-	-	5/15/91/115	-
11	CLA	A	1112	1	-	9/15/91/115	-
11	CLA	A	1122	-	-	10/32/108/115	-
11	CLA	1	1118	1	-	21/35/111/115	-
11	CLA	1	1121	1	-	8/17/93/115	-
12	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
14	BCR	f	4018	-	-	6/29/63/63	0/2/2/2
11	CLA	b	1212	-	-	5/15/91/115	-
11	CLA	2	1235	-	-	14/33/109/115	-
11	CLA	b	1235	-	-	13/33/109/115	-
11	CLA	A	1109	1,11	-	15/39/115/115	-
14	BCR	b	4010	-	-	11/29/63/63	0/2/2/2
11	CLA	A	1131	1	-	14/39/115/115	-
11	CLA	8	1502	7	-	5/17/93/115	-
11	CLA	b	1201	2	-	10/26/102/115	-
11	CLA	A	1119	-	-	16/39/115/115	-
14	BCR	B	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	2	1021	-	-	19/39/115/115	-
14	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	BCR	2	4004	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1130	1	-	7/17/93/115	-
11	CLA	1	1104	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	c	3003	3	-	-	0/6/5/5
14	BCR	A	4001	-	-	9/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
14	BCR	2	4009	-	-	15/29/63/63	0/2/2/2
11	CLA	2	1238	-	-	12/39/115/115	-
11	CLA	A	1117	1	-	12/39/115/115	-
11	CLA	a	1112	-	-	2/15/91/115	-
11	CLA	2	1207	-	-	14/39/115/115	-
11	CLA	a	1120	1	-	9/17/93/115	-
14	BCR	8	4022	-	-	6/29/63/63	0/2/2/2
15	LHG	A	5001	-	-	29/53/53/53	-
11	CLA	B	1222	-	-	15/29/105/115	-
11	CLA	a	1126	1	-	18/39/115/115	-
11	CLA	b	1240	-	-	9/15/91/115	-
11	CLA	1	1112	-	-	2/15/91/115	-
11	CLA	a	1110	1	-	10/26/102/115	-
11	CLA	A	1126	1	-	14/39/115/115	-
11	CLA	b	1202	2	-	17/39/115/115	-
11	CLA	b	1225	-	-	14/39/115/115	-
11	CLA	1	1134	-	-	5/17/93/115	-
11	CLA	A	1108	1	-	3/15/91/115	-
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
11	CLA	B	1230	2	-	9/31/107/115	-
11	CLA	A	1135	-	-	8/23/99/115	-
11	CLA	B	1220	2	-	6/17/93/115	-
11	CLA	1	1122	-	-	18/32/108/115	-
11	CLA	B	1231	-	-	9/15/91/115	-
11	CLA	1	1127	-	-	17/39/115/115	-
11	CLA	b	1210	2	-	18/39/115/115	-
11	CLA	a	1138	1	-	7/17/93/115	-
11	CLA	b	1234	-	-	14/33/109/115	-
14	BCR	7	4021	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1216	-	-	15/39/115/115	-
11	CLA	1	1133	-	-	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
11	CLA	B	1216	-	-	10/39/115/115	-
11	CLA	1	1140	1	-	16/39/115/115	-
11	CLA	1	1139	-	-	10/21/97/115	-
11	CLA	1	1120	1	-	9/17/93/115	-
11	CLA	a	1132	1	-	17/39/115/115	-
11	CLA	A	1136	1	-	4/17/93/115	-
11	CLA	A	1105	1	-	7/19/95/115	-
11	CLA	B	1234	-	-	15/33/109/115	-
11	CLA	B	1217	-	-	12/18/94/115	-
11	CLA	1	1116	-	-	11/26/102/115	-
11	CLA	1	1137	-	-	18/39/115/115	-
11	CLA	L	1502	7	-	7/17/93/115	-
11	CLA	1	1128	1	-	12/39/115/115	-
11	CLA	b	1211	-	-	6/17/93/115	-
11	CLA	A	1125	1	-	11/24/100/115	-
11	CLA	1	1131	1	-	22/39/115/115	-
11	CLA	1	1101	-	-	21/39/115/115	-
11	CLA	B	1215	2	-	14/39/115/115	-
11	CLA	a	1103	1	-	19/39/115/115	-
11	CLA	B	1206	2	-	13/39/115/115	-
11	CLA	a	1119	-	-	14/39/115/115	-
11	CLA	b	1227	-	-	10/15/91/115	-
14	BCR	f	4013	-	-	17/29/63/63	0/2/2/2
11	CLA	1	1136	-	-	8/17/93/115	-
11	CLA	2	1229	2	-	16/39/115/115	-
11	CLA	a	1117	1	-	18/39/115/115	-
11	CLA	a	1121	-	-	5/17/93/115	-
11	CLA	A	1114	-	-	7/17/93/115	-
11	CLA	B	1214	2	-	13/32/108/115	-
15	LHG	B	5004	11	-	24/53/53/53	-
11	CLA	2	1205	2	-	8/27/103/115	-
11	CLA	a	1102	1,11	-	13/39/115/115	-
14	BCR	a	4007	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1202	2	-	17/39/115/115	-
14	BCR	L	4022	-	-	10/29/63/63	0/2/2/2
13	SF4	3	3002	3	-	-	0/6/5/5
11	CLA	a	1123	-	-	16/39/115/115	-
14	BCR	b	4011	-	-	15/29/63/63	0/2/2/2
11	CLA	a	1108	-	-	4/15/91/115	-
11	CLA	A	1022	-	-	15/39/115/115	-
14	BCR	8	4019	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1012	-	-	17/39/115/115	-
11	CLA	1	1801	15	-	15/24/100/115	-
11	CLA	a	1115	1	-	4/17/93/115	-
11	CLA	B	1239	2	-	10/17/93/115	-
11	CLA	2	1202	2	-	14/39/115/115	-
14	BCR	f	4020	-	-	15/29/63/63	0/2/2/2
11	CLA	A	1110	1	-	11/26/102/115	-
11	CLA	a	1107	1	-	11/39/115/115	-
11	CLA	B	1235	-	-	14/33/109/115	-
11	CLA	B	1232	-	-	7/15/91/115	-
11	CLA	A	1106	1	-	17/39/115/115	-
11	CLA	a	1104	1	-	14/39/115/115	-
11	CLA	2	1209	-	-	6/15/91/115	-
11	CLA	a	1011	1	-	11/39/115/115	-
11	CLA	1	1012	-	-	19/39/115/115	-
11	CLA	a	1109	1,11	-	19/39/115/115	-
14	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
14	BCR	F	4013	-	-	15/29/63/63	0/2/2/2
13	SF4	a	3001	1,2	-	-	0/6/5/5
11	CLA	a	1122	-	-	13/32/108/115	-
11	CLA	b	1204	2	-	15/39/115/115	-
11	CLA	b	1209	-	-	7/15/91/115	-
11	CLA	2	1201	2	-	8/26/102/115	-
15	LHG	1	5003	11	-	31/53/53/53	-
11	CLA	1	1105	-	-	5/19/95/115	-
14	BCR	A	4003	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1118	1	-	17/35/111/115	-
11	CLA	B	1203	2	-	16/39/115/115	-
11	CLA	b	1215	2	-	12/39/115/115	-
14	BCR	a	4001	-	-	10/29/63/63	0/2/2/2
11	CLA	1	1111	1	-	17/33/109/115	-
11	CLA	B	1204	2	-	14/39/115/115	-
11	CLA	1	1109	-	-	16/39/115/115	-
11	CLA	L	1503	-	-	15/39/115/115	-
11	CLA	a	1131	1	-	18/39/115/115	-
11	CLA	1	1022	-	-	16/39/115/115	-
13	SF4	C	3002	3	-	-	0/6/5/5
11	CLA	b	1218	-	-	4/15/91/115	-
11	CLA	b	1021	-	-	23/39/115/115	-
14	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
15	LHG	a	5003	11	-	24/53/53/53	-
11	CLA	1	1119	-	-	17/39/115/115	-
11	CLA	B	1238	-	-	11/39/115/115	-
11	CLA	a	1105	1	-	6/19/95/115	-
11	CLA	B	1210	2	-	25/39/115/115	-
14	BCR	B	4011	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1106	1	-	23/39/115/115	-
11	CLA	A	1140	1	-	16/39/115/115	-
14	BCR	1	4003	-	-	12/29/63/63	0/2/2/2
11	CLA	A	1121	1	-	5/17/93/115	-
11	CLA	1	1115	1	-	4/17/93/115	-
11	CLA	0	1402	-	-	5/21/97/115	-
11	CLA	A	1139	-	-	9/21/97/115	-
11	CLA	b	1222	-	-	14/29/105/115	-
11	CLA	b	1207	-	-	14/39/115/115	-
11	CLA	B	1213	-	-	18/39/115/115	-
11	CLA	A	1113	-	-	7/15/91/115	-
11	CLA	a	1129	-	-	8/17/93/115	-
11	CLA	A	1127	1	-	12/39/115/115	-
11	CLA	B	1207	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	B	1240	15	-	8/15/91/115	-
11	CLA	A	1124	-	-	14/27/103/115	-
11	CLA	2	1231	-	-	4/15/91/115	-
11	CLA	2	1210	-	-	15/39/115/115	-
11	CLA	B	1228	2	-	8/21/97/115	-
11	CLA	2	1234	-	-	17/33/109/115	-
14	BCR	1	4001	-	-	11/29/63/63	0/2/2/2
14	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
11	CLA	a	1136	1	-	5/17/93/115	-
11	CLA	A	1107	1	-	13/39/115/115	-
11	CLA	B	1013	-	-	18/39/115/115	-
11	CLA	1	1129	-	-	7/17/93/115	-
14	BCR	2	4005	-	-	9/29/63/63	0/2/2/2
11	CLA	2	1240	15	-	5/15/91/115	-
14	BCR	b	4005	-	-	13/29/63/63	0/2/2/2
14	BCR	l	4022	-	-	11/29/63/63	0/2/2/2
14	BCR	a	4002	-	-	15/29/63/63	0/2/2/2
11	CLA	k	1402	10	-	5/21/97/115	-
11	CLA	a	1012	-	-	21/39/115/115	-
11	CLA	a	1137	-	-	13/39/115/115	-
11	CLA	A	1137	1	-	11/39/115/115	-
11	CLA	A	1128	1	-	13/39/115/115	-
11	CLA	a	1101	-	-	19/39/115/115	-
14	BCR	1	4002	-	-	13/29/63/63	0/2/2/2
11	CLA	A	1101	1	-	17/39/115/115	-
11	CLA	2	1206	2	-	16/39/115/115	-
11	CLA	A	1237	-	-	11/27/103/115	-
11	CLA	a	1118	1	-	10/35/111/115	-
11	CLA	a	1237	-	-	10/27/103/115	-
11	CLA	a	1111	1	-	17/33/109/115	-
11	CLA	1	1110	1	-	14/26/102/115	-
15	LHG	1	5001	-	-	25/53/53/53	-
11	CLA	a	1124	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1230	-	-	12/31/107/115	-
11	CLA	a	1125	-	-	7/24/100/115	-
11	CLA	b	1206	2	-	14/39/115/115	-
11	CLA	1	1113	-	-	7/15/91/115	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
11	CLA	2	1213	-	-	17/39/115/115	-
11	CLA	2	1225	2	-	12/39/115/115	-
14	BCR	2	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	2	1230	2	-	9/31/107/115	-
11	CLA	b	1213	-	-	14/39/115/115	-
11	CLA	b	1023	-	-	17/39/115/115	-
14	BCR	a	4008	-	-	11/29/63/63	0/2/2/2
11	CLA	B	1227	-	-	6/15/91/115	-
11	CLA	b	1223	-	-	19/39/115/115	-
11	CLA	a	1114	-	-	6/17/93/115	-
14	BCR	b	4017	-	-	6/29/63/63	0/2/2/2
11	CLA	B	1211	-	-	7/17/93/115	-
15	LHG	a	5001	-	-	29/53/53/53	-
11	CLA	b	1205	2	-	10/27/103/115	-
11	CLA	2	1227	-	-	9/15/91/115	-
11	CLA	b	1226	2	-	13/39/115/115	-
11	CLA	A	1115	1	-	7/17/93/115	-
11	CLA	b	1224	-	-	12/27/103/115	-
11	CLA	a	1113	-	-	4/15/91/115	-
11	CLA	A	1111	1	-	16/33/109/115	-
11	CLA	B	1205	2	-	11/27/103/115	-
11	CLA	1	1114	-	-	10/17/93/115	-
16	LMG	B	5002	-	-	27/50/70/70	0/1/1/1
11	CLA	1	1103	1	-	19/39/115/115	-
11	CLA	2	1236	2	-	8/18/94/115	-
13	SF4	3	3003	-	-	-	0/6/5/5
11	CLA	1	1125	-	-	10/24/100/115	-
14	BCR	l	4019	-	-	17/29/63/63	0/2/2/2
11	CLA	0	1401	-	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1224	-	-	11/27/103/115	-
11	CLA	1	1237	-	-	9/27/103/115	-
11	CLA	b	1221	-	-	9/26/102/115	-
11	CLA	2	1208	-	-	3/15/91/115	-
11	CLA	A	1011	1	-	16/39/115/115	-
11	CLA	2	1013	-	-	15/39/115/115	-
11	CLA	a	1022	-	-	12/39/115/115	-
11	CLA	b	1208	-	-	4/15/91/115	-
16	LMG	2	5002	-	-	30/50/70/70	0/1/1/1
11	CLA	1	1107	-	-	14/39/115/115	-
11	CLA	b	1013	-	-	12/39/115/115	-
11	CLA	8	1503	-	-	12/39/115/115	-
11	CLA	1	1138	1	-	6/17/93/115	-
14	BCR	2	4006	-	-	13/29/63/63	0/2/2/2
11	CLA	1	1117	-	-	13/39/115/115	-
14	BCR	1	4008	-	-	10/29/63/63	0/2/2/2
11	CLA	B	1212	-	-	9/15/91/115	-
11	CLA	a	1106	1	-	19/39/115/115	-
13	SF4	1	3001	1,2	-	-	0/6/5/5
11	CLA	1	1102	1	-	14/39/115/115	-
11	CLA	2	1221	-	-	8/26/102/115	-
14	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
11	CLA	b	1203	2	-	14/39/115/115	-
14	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
11	CLA	2	1219	2	-	10/27/103/115	-
11	CLA	B	1209	-	-	6/15/91/115	-
11	CLA	A	1102	1,11	-	19/39/115/115	-
11	CLA	1	1108	-	-	7/15/91/115	-
11	CLA	l	1503	-	-	18/39/115/115	-
12	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
11	CLA	A	1104	1	-	22/39/115/115	-
11	CLA	A	1116	-	-	10/26/102/115	-
11	CLA	2	1215	2	-	17/39/115/115	-
11	CLA	b	1236	-	-	10/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1204	2	-	10/39/115/115	-
11	CLA	B	1219	2	-	10/27/103/115	-
11	CLA	B	1236	2	-	8/18/94/115	-
11	CLA	B	1201	2	-	10/26/102/115	-
11	CLA	2	1228	2	-	5/21/97/115	-
11	CLA	A	1133	-	-	4/17/93/115	-
12	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
11	CLA	B	1218	-	-	4/15/91/115	-
11	CLA	b	1231	-	-	7/15/91/115	-
11	CLA	2	1222	-	-	13/29/105/115	-
13	SF4	C	3003	3	-	-	0/6/5/5
11	CLA	a	1133	-	-	4/17/93/115	-
14	BCR	6	4013	-	-	16/29/63/63	0/2/2/2
11	CLA	A	1120	1	-	6/17/93/115	-
11	CLA	1	1130	1	-	5/17/93/115	-
11	CLA	a	1134	-	-	5/17/93/115	-
12	PQN	2	2002	-	-	8/23/43/43	0/2/2/2
14	BCR	M	4021	-	-	8/29/63/63	0/2/2/2
11	CLA	A	1134	1	-	5/17/93/115	-
11	CLA	b	1229	-	-	20/39/115/115	-
11	CLA	b	1228	2	-	5/21/97/115	-
14	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
13	SF4	c	3002	3	-	-	0/6/5/5
14	BCR	6	4020	-	-	15/29/63/63	0/2/2/2
14	BCR	2	4011	-	-	13/29/63/63	0/2/2/2
14	BCR	b	4009	-	-	14/29/63/63	0/2/2/2
11	CLA	b	1238	-	-	13/39/115/115	-
11	CLA	a	1116	-	-	9/26/102/115	-
11	CLA	l	1501	7	-	16/39/115/115	-
14	BCR	F	4020	-	-	12/29/63/63	0/2/2/2
11	CLA	B	1225	2	-	14/39/115/115	-
12	PQN	1	2001	-	-	7/23/43/43	0/2/2/2
14	BCR	2	4010	-	-	10/29/63/63	0/2/2/2
11	CLA	1	1123	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1011	1	-	12/39/115/115	-
11	CLA	L	1501	7	-	14/39/115/115	-
11	CLA	a	1128	1	-	10/39/115/115	-
11	CLA	2	1216	-	-	17/39/115/115	-
11	CLA	a	1127	-	-	12/39/115/115	-
11	CLA	A	1132	1	-	18/39/115/115	-
11	CLA	1	1124	-	-	13/27/103/115	-
14	BCR	F	4018	-	-	5/29/63/63	0/2/2/2
11	CLA	2	1217	2	-	14/18/94/115	-
14	BCR	2	4014	-	-	14/29/63/63	0/2/2/2
11	CLA	a	1140	-	-	14/39/115/115	-
11	CLA	2	1218	-	-	5/15/91/115	-
11	CLA	b	1217	-	-	6/18/94/115	-
11	CLA	a	1139	-	-	9/21/97/115	-
11	CLA	K	1402	10	-	6/21/97/115	-
11	CLA	l	1502	7	-	4/17/93/115	-
11	CLA	2	1220	2	-	6/17/93/115	-
11	CLA	b	1220	2	-	6/17/93/115	-
11	CLA	A	1138	1	-	0/17/93/115	-
11	CLA	k	1401	-	-	22/39/115/115	-
14	BCR	6	4018	-	-	10/29/63/63	0/2/2/2
11	CLA	A	1801	15	-	13/24/100/115	-
15	LHG	A	5003	11	-	30/53/53/53	-
11	CLA	1	1126	1	-	20/39/115/115	-
11	CLA	B	1229	2	-	20/39/115/115	-
14	BCR	1	4007	-	-	12/29/63/63	0/2/2/2
11	CLA	a	1130	1	-	7/17/93/115	-
11	CLA	B	1021	-	-	22/39/115/115	-

All (6320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1125	CLA	MG-NA	9.70	2.29	2.06
11	a	1103	CLA	MG-NA	9.70	2.29	2.06
11	B	1223	CLA	MG-NA	9.65	2.29	2.06
11	b	1223	CLA	MG-NA	9.64	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1139	CLA	MG-NA	9.64	2.29	2.06
11	1	1123	CLA	MG-NA	9.63	2.29	2.06
11	A	1120	CLA	MG-NA	9.63	2.29	2.06
11	b	1221	CLA	MG-NA	9.63	2.29	2.06
11	b	1220	CLA	MG-NA	9.61	2.29	2.06
11	1	1012	CLA	MG-NA	9.61	2.29	2.06
11	2	1216	CLA	MG-NA	9.61	2.29	2.06
11	1	1011	CLA	MG-NA	9.60	2.29	2.06
11	1	1120	CLA	MG-NA	9.59	2.29	2.06
11	2	1219	CLA	MG-NA	9.59	2.29	2.06
11	a	1012	CLA	MG-NA	9.59	2.29	2.06
11	b	1225	CLA	MG-NA	9.59	2.29	2.06
11	2	1214	CLA	MG-NA	9.59	2.29	2.06
11	1	1110	CLA	MG-NA	9.59	2.29	2.06
11	A	1110	CLA	MG-NA	9.58	2.29	2.06
11	b	1230	CLA	MG-NA	9.58	2.29	2.06
11	a	1121	CLA	MG-NA	9.57	2.29	2.06
11	A	1112	CLA	MG-NA	9.57	2.29	2.06
11	1	1102	CLA	MG-NA	9.57	2.29	2.06
11	b	1234	CLA	MG-NA	9.57	2.29	2.06
11	1	1135	CLA	MG-NA	9.57	2.29	2.06
11	2	1232	CLA	MG-NA	9.56	2.29	2.06
11	A	1123	CLA	MG-NA	9.56	2.29	2.06
11	B	1240	CLA	MG-NA	9.55	2.29	2.06
11	a	1123	CLA	MG-NA	9.55	2.29	2.06
11	2	1212	CLA	MG-NA	9.55	2.29	2.06
11	2	1209	CLA	MG-NA	9.55	2.28	2.06
11	A	1114	CLA	MG-NA	9.54	2.28	2.06
11	2	1240	CLA	MG-NA	9.54	2.28	2.06
11	2	1221	CLA	MG-NA	9.54	2.28	2.06
11	b	1219	CLA	MG-NA	9.54	2.28	2.06
11	b	1021	CLA	MG-NA	9.54	2.28	2.06
11	b	1208	CLA	MG-NA	9.54	2.28	2.06
11	a	1022	CLA	MG-NA	9.54	2.28	2.06
11	2	1206	CLA	MG-NA	9.54	2.28	2.06
11	B	1209	CLA	MG-NA	9.53	2.28	2.06
11	1	1022	CLA	MG-NA	9.53	2.28	2.06
11	1	1140	CLA	MG-NA	9.53	2.28	2.06
11	1	1139	CLA	MG-NA	9.53	2.28	2.06
11	b	1240	CLA	MG-NA	9.52	2.28	2.06
11	a	1113	CLA	MG-NA	9.52	2.28	2.06
11	a	1011	CLA	MG-NA	9.52	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1223	CLA	MG-NA	9.52	2.28	2.06
11	A	1134	CLA	MG-NA	9.52	2.28	2.06
11	b	1215	CLA	MG-NA	9.52	2.28	2.06
11	B	1220	CLA	MG-NA	9.51	2.28	2.06
11	1	1115	CLA	MG-NA	9.51	2.28	2.06
11	1	1126	CLA	MG-NA	9.51	2.28	2.06
11	b	1203	CLA	MG-NA	9.51	2.28	2.06
11	B	1221	CLA	MG-NA	9.50	2.28	2.06
11	a	1107	CLA	MG-NA	9.50	2.28	2.06
11	2	1239	CLA	MG-NA	9.50	2.28	2.06
11	A	1116	CLA	MG-NA	9.50	2.28	2.06
11	1	1121	CLA	MG-NA	9.50	2.28	2.06
11	B	1225	CLA	MG-NA	9.50	2.28	2.06
11	8	1503	CLA	MG-NA	9.50	2.28	2.06
11	2	1220	CLA	MG-NA	9.50	2.28	2.06
11	a	1126	CLA	MG-NA	9.50	2.28	2.06
11	A	1801	CLA	MG-NA	9.50	2.28	2.06
11	1	1113	CLA	MG-NA	9.50	2.28	2.06
11	b	1224	CLA	MG-NA	9.50	2.28	2.06
11	k	1401	CLA	MG-NA	9.50	2.28	2.06
11	a	1125	CLA	MG-NA	9.50	2.28	2.06
11	L	1501	CLA	MG-NA	9.49	2.28	2.06
11	a	1120	CLA	MG-NA	9.49	2.28	2.06
11	2	1235	CLA	MG-NA	9.49	2.28	2.06
11	2	1222	CLA	MG-NA	9.49	2.28	2.06
11	a	1101	CLA	MG-NA	9.49	2.28	2.06
11	a	1801	CLA	MG-NA	9.49	2.28	2.06
11	b	1217	CLA	MG-NA	9.49	2.28	2.06
11	a	1105	CLA	MG-NA	9.49	2.28	2.06
11	b	1216	CLA	MG-NA	9.49	2.28	2.06
11	l	1501	CLA	MG-NA	9.48	2.28	2.06
11	a	1114	CLA	MG-NA	9.48	2.28	2.06
11	A	1139	CLA	MG-NA	9.48	2.28	2.06
11	2	1225	CLA	MG-NA	9.48	2.28	2.06
11	B	1231	CLA	MG-NA	9.48	2.28	2.06
11	b	1227	CLA	MG-NA	9.48	2.28	2.06
11	a	1115	CLA	MG-NA	9.48	2.28	2.06
11	b	1211	CLA	MG-NA	9.48	2.28	2.06
11	K	1401	CLA	MG-NA	9.48	2.28	2.06
11	2	1230	CLA	MG-NA	9.48	2.28	2.06
11	2	1231	CLA	MG-NA	9.47	2.28	2.06
11	B	1232	CLA	MG-NA	9.47	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1127	CLA	MG-NA	9.47	2.28	2.06
11	B	1229	CLA	MG-NA	9.47	2.28	2.06
11	b	1235	CLA	MG-NA	9.47	2.28	2.06
11	A	1121	CLA	MG-NA	9.47	2.28	2.06
11	b	1239	CLA	MG-NA	9.47	2.28	2.06
11	a	1108	CLA	MG-NA	9.47	2.28	2.06
11	0	1401	CLA	MG-NA	9.47	2.28	2.06
11	b	1228	CLA	MG-NA	9.47	2.28	2.06
11	a	1130	CLA	MG-NA	9.47	2.28	2.06
11	1	1127	CLA	MG-NA	9.47	2.28	2.06
11	B	1215	CLA	MG-NA	9.46	2.28	2.06
11	1	1801	CLA	MG-NA	9.46	2.28	2.06
11	b	1210	CLA	MG-NA	9.46	2.28	2.06
11	1	1134	CLA	MG-NA	9.46	2.28	2.06
11	2	1229	CLA	MG-NA	9.46	2.28	2.06
11	a	1112	CLA	MG-NA	9.46	2.28	2.06
11	1	1112	CLA	MG-NA	9.46	2.28	2.06
11	a	1140	CLA	MG-NA	9.46	2.28	2.06
11	b	1232	CLA	MG-NA	9.46	2.28	2.06
11	1	1114	CLA	MG-NA	9.46	2.28	2.06
11	B	1218	CLA	MG-NA	9.46	2.28	2.06
11	1	1103	CLA	MG-NA	9.46	2.28	2.06
11	1	1116	CLA	MG-NA	9.46	2.28	2.06
11	2	1213	CLA	MG-NA	9.45	2.28	2.06
11	b	1218	CLA	MG-NA	9.45	2.28	2.06
11	2	1202	CLA	MG-NA	9.45	2.28	2.06
11	b	1212	CLA	MG-NA	9.45	2.28	2.06
11	A	1140	CLA	MG-NA	9.45	2.28	2.06
11	1	1117	CLA	MG-NA	9.45	2.28	2.06
11	A	1124	CLA	MG-NA	9.45	2.28	2.06
11	1	1125	CLA	MG-NA	9.45	2.28	2.06
11	b	1204	CLA	MG-NA	9.45	2.28	2.06
11	A	1105	CLA	MG-NA	9.44	2.28	2.06
11	a	1109	CLA	MG-NA	9.44	2.28	2.06
11	a	1124	CLA	MG-NA	9.44	2.28	2.06
11	2	1234	CLA	MG-NA	9.44	2.28	2.06
11	8	1502	CLA	MG-NA	9.44	2.28	2.06
11	a	1133	CLA	MG-NA	9.44	2.28	2.06
11	B	1239	CLA	MG-NA	9.44	2.28	2.06
11	1	1108	CLA	MG-NA	9.44	2.28	2.06
11	A	1101	CLA	MG-NA	9.44	2.28	2.06
11	B	1222	CLA	MG-NA	9.44	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1135	CLA	MG-NA	9.44	2.28	2.06
11	1	1133	CLA	MG-NA	9.44	2.28	2.06
11	a	1128	CLA	MG-NA	9.43	2.28	2.06
11	A	1131	CLA	MG-NA	9.43	2.28	2.06
11	B	1219	CLA	MG-NA	9.43	2.28	2.06
11	b	1229	CLA	MG-NA	9.43	2.28	2.06
11	2	1204	CLA	MG-NA	9.43	2.28	2.06
11	A	1012	CLA	MG-NA	9.43	2.28	2.06
11	2	1236	CLA	MG-NA	9.42	2.28	2.06
11	b	1231	CLA	MG-NA	9.42	2.28	2.06
11	A	1113	CLA	MG-NA	9.42	2.28	2.06
11	2	1228	CLA	MG-NA	9.42	2.28	2.06
11	a	1116	CLA	MG-NA	9.42	2.28	2.06
11	1	1107	CLA	MG-NA	9.42	2.28	2.06
11	B	1234	CLA	MG-NA	9.42	2.28	2.06
11	1	1130	CLA	MG-NA	9.42	2.28	2.06
11	1	1137	CLA	MG-NA	9.42	2.28	2.06
11	2	1217	CLA	MG-NA	9.42	2.28	2.06
11	a	1102	CLA	MG-NA	9.41	2.28	2.06
11	b	1213	CLA	MG-NA	9.41	2.28	2.06
11	B	1210	CLA	MG-NA	9.41	2.28	2.06
11	b	1214	CLA	MG-NA	9.41	2.28	2.06
11	a	1117	CLA	MG-NA	9.41	2.28	2.06
11	A	1130	CLA	MG-NA	9.41	2.28	2.06
11	a	1131	CLA	MG-NA	9.41	2.28	2.06
11	1	1122	CLA	MG-NA	9.41	2.28	2.06
11	a	1110	CLA	MG-NA	9.41	2.28	2.06
11	2	1201	CLA	MG-NA	9.41	2.28	2.06
11	1	1124	CLA	MG-NA	9.41	2.28	2.06
11	l	1502	CLA	MG-NA	9.41	2.28	2.06
11	B	1228	CLA	MG-NA	9.41	2.28	2.06
11	b	1202	CLA	MG-NA	9.41	2.28	2.06
11	B	1212	CLA	MG-NA	9.40	2.28	2.06
11	B	1213	CLA	MG-NA	9.40	2.28	2.06
11	a	1132	CLA	MG-NA	9.40	2.28	2.06
11	a	1106	CLA	MG-NA	9.40	2.28	2.06
11	a	1134	CLA	MG-NA	9.40	2.28	2.06
11	l	1503	CLA	MG-NA	9.40	2.28	2.06
11	1	1129	CLA	MG-NA	9.40	2.28	2.06
11	2	1215	CLA	MG-NA	9.40	2.28	2.06
11	A	1129	CLA	MG-NA	9.40	2.28	2.06
11	a	1137	CLA	MG-NA	9.40	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1206	CLA	MG-NA	9.39	2.28	2.06
11	2	1238	CLA	MG-NA	9.39	2.28	2.06
11	8	1501	CLA	MG-NA	9.39	2.28	2.06
11	1	1101	CLA	MG-NA	9.39	2.28	2.06
11	b	1222	CLA	MG-NA	9.39	2.28	2.06
11	a	1122	CLA	MG-NA	9.39	2.28	2.06
11	A	1107	CLA	MG-NA	9.39	2.28	2.06
11	2	1227	CLA	MG-NA	9.39	2.28	2.06
11	b	1236	CLA	MG-NA	9.39	2.28	2.06
11	A	1115	CLA	MG-NA	9.39	2.28	2.06
11	a	1138	CLA	MG-NA	9.39	2.28	2.06
11	2	1218	CLA	MG-NA	9.39	2.28	2.06
11	a	1136	CLA	MG-NA	9.39	2.28	2.06
11	b	1209	CLA	MG-NA	9.38	2.28	2.06
11	2	1224	CLA	MG-NA	9.38	2.28	2.06
11	A	1102	CLA	MG-NA	9.38	2.28	2.06
11	B	1235	CLA	MG-NA	9.38	2.28	2.06
11	B	1206	CLA	MG-NA	9.38	2.28	2.06
11	L	1503	CLA	MG-NA	9.38	2.28	2.06
11	1	1131	CLA	MG-NA	9.38	2.28	2.06
11	1	1119	CLA	MG-NA	9.38	2.28	2.06
11	0	1402	CLA	MG-NA	9.38	2.28	2.06
11	1	1105	CLA	MG-NA	9.38	2.28	2.06
11	A	1011	CLA	MG-NA	9.38	2.28	2.06
11	A	1117	CLA	MG-NA	9.38	2.28	2.06
11	B	1230	CLA	MG-NA	9.37	2.28	2.06
11	b	1207	CLA	MG-NA	9.37	2.28	2.06
11	A	1127	CLA	MG-NA	9.37	2.28	2.06
11	B	1203	CLA	MG-NA	9.37	2.28	2.06
11	A	1022	CLA	MG-NA	9.37	2.28	2.06
11	B	1227	CLA	MG-NA	9.36	2.28	2.06
11	B	1214	CLA	MG-NA	9.36	2.28	2.06
11	1	1128	CLA	MG-NA	9.36	2.28	2.06
11	B	1208	CLA	MG-NA	9.36	2.28	2.06
11	B	1217	CLA	MG-NA	9.36	2.28	2.06
11	B	1202	CLA	MG-NA	9.36	2.28	2.06
11	b	1226	CLA	MG-NA	9.36	2.28	2.06
11	1	1132	CLA	MG-NA	9.36	2.28	2.06
11	b	1238	CLA	MG-NA	9.35	2.28	2.06
11	a	1119	CLA	MG-NA	9.35	2.28	2.06
11	A	1132	CLA	MG-NA	9.35	2.28	2.06
11	A	1126	CLA	MG-NA	9.34	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	1502	CLA	MG-NA	9.34	2.28	2.06
11	A	1135	CLA	MG-NA	9.34	2.28	2.06
11	2	1021	CLA	MG-NA	9.34	2.28	2.06
11	A	1108	CLA	MG-NA	9.33	2.28	2.06
11	B	1207	CLA	MG-NA	9.33	2.28	2.06
11	A	1137	CLA	MG-NA	9.33	2.28	2.06
11	a	1237	CLA	MG-NA	9.33	2.28	2.06
11	A	1136	CLA	MG-NA	9.33	2.28	2.06
11	2	1203	CLA	MG-NA	9.33	2.28	2.06
11	a	1111	CLA	MG-NA	9.33	2.28	2.06
11	A	1106	CLA	MG-NA	9.33	2.28	2.06
11	B	1224	CLA	MG-NA	9.32	2.28	2.06
11	b	1013	CLA	MG-NA	9.32	2.28	2.06
11	A	1111	CLA	MG-NA	9.32	2.28	2.06
11	B	1205	CLA	MG-NA	9.31	2.28	2.06
11	1	1109	CLA	MG-NA	9.31	2.28	2.06
11	1	1106	CLA	MG-NA	9.31	2.28	2.06
11	2	1210	CLA	MG-NA	9.31	2.28	2.06
11	A	1103	CLA	MG-NA	9.31	2.28	2.06
11	a	1129	CLA	MG-NA	9.31	2.28	2.06
11	a	1104	CLA	MG-NA	9.30	2.28	2.06
11	B	1236	CLA	MG-NA	9.30	2.28	2.06
11	B	1216	CLA	MG-NA	9.30	2.28	2.06
11	1	1136	CLA	MG-NA	9.30	2.28	2.06
11	B	1226	CLA	MG-NA	9.29	2.28	2.06
11	b	1023	CLA	MG-NA	9.29	2.28	2.06
11	1	1104	CLA	MG-NA	9.29	2.28	2.06
11	1	1237	CLA	MG-NA	9.29	2.28	2.06
11	2	1226	CLA	MG-NA	9.29	2.28	2.06
11	B	1204	CLA	MG-NA	9.29	2.28	2.06
11	A	1109	CLA	MG-NA	9.29	2.28	2.06
11	2	1208	CLA	MG-NA	9.29	2.28	2.06
11	2	1013	CLA	MG-NA	9.28	2.28	2.06
11	A	1122	CLA	MG-NA	9.28	2.28	2.06
11	A	1138	CLA	MG-NA	9.28	2.28	2.06
11	K	1402	CLA	MG-NA	9.28	2.28	2.06
11	b	1205	CLA	MG-NA	9.28	2.28	2.06
11	B	1201	CLA	MG-NA	9.28	2.28	2.06
11	A	1133	CLA	MG-NA	9.27	2.28	2.06
11	k	1402	CLA	MG-NA	9.27	2.28	2.06
11	1	1118	CLA	MG-NA	9.27	2.28	2.06
11	A	1119	CLA	MG-NA	9.27	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1207	CLA	MG-NA	9.26	2.28	2.06
11	B	1238	CLA	MG-NA	9.26	2.28	2.06
11	B	1023	CLA	MG-NA	9.26	2.28	2.06
11	1	1138	CLA	MG-NA	9.25	2.28	2.06
11	A	1237	CLA	MG-NA	9.24	2.28	2.06
11	B	1211	CLA	MG-NA	9.24	2.28	2.06
11	2	1205	CLA	MG-NA	9.24	2.28	2.06
11	B	1021	CLA	MG-NA	9.22	2.28	2.06
11	b	1201	CLA	MG-NA	9.22	2.28	2.06
11	A	1128	CLA	MG-NA	9.22	2.28	2.06
11	1	1111	CLA	MG-NA	9.20	2.28	2.06
11	2	1023	CLA	MG-NA	9.19	2.28	2.06
11	B	1013	CLA	MG-NA	9.19	2.28	2.06
11	a	1118	CLA	MG-NA	9.19	2.28	2.06
11	2	1211	CLA	MG-NA	9.14	2.28	2.06
11	A	1118	CLA	MG-NA	9.10	2.27	2.06
11	A	1104	CLA	MG-NA	9.07	2.27	2.06
14	m	4021	BCR	C8-C9	-8.47	1.27	1.46
14	f	4013	BCR	C8-C9	-8.42	1.27	1.46
14	A	4003	BCR	C8-C9	-8.41	1.27	1.46
14	F	4013	BCR	C8-C9	-8.38	1.28	1.46
14	2	4011	BCR	C8-C9	-8.35	1.28	1.46
14	F	4018	BCR	C8-C9	-8.34	1.28	1.46
14	l	4019	BCR	C8-C9	-8.34	1.28	1.46
14	6	4018	BCR	C8-C9	-8.33	1.28	1.46
14	f	4018	BCR	C8-C9	-8.31	1.28	1.46
14	B	4011	BCR	C8-C9	-8.31	1.28	1.46
14	7	4021	BCR	C8-C9	-8.30	1.28	1.46
14	B	4004	BCR	C8-C9	-8.29	1.28	1.46
14	b	4006	BCR	C8-C9	-8.29	1.28	1.46
14	M	4021	BCR	C8-C9	-8.29	1.28	1.46
14	2	4014	BCR	C8-C9	-8.29	1.28	1.46
14	2	4010	BCR	C8-C9	-8.28	1.28	1.46
14	a	4008	BCR	C8-C9	-8.27	1.28	1.46
14	B	4006	BCR	C8-C9	-8.27	1.28	1.46
14	a	4003	BCR	C8-C9	-8.27	1.28	1.46
14	b	4010	BCR	C8-C9	-8.26	1.28	1.46
14	6	4013	BCR	C8-C9	-8.26	1.28	1.46
14	6	4020	BCR	C8-C9	-8.25	1.28	1.46
14	B	4010	BCR	C8-C9	-8.25	1.28	1.46
14	8	4019	BCR	C8-C9	-8.25	1.28	1.46
14	2	4005	BCR	C8-C9	-8.23	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	4014	BCR	C8-C9	-8.23	1.28	1.46
14	1	4003	BCR	C8-C9	-8.23	1.28	1.46
14	f	4020	BCR	C8-C9	-8.21	1.28	1.46
14	b	4005	BCR	C8-C9	-8.21	1.28	1.46
14	B	4005	BCR	C8-C9	-8.20	1.28	1.46
14	A	4001	BCR	C8-C9	-8.19	1.28	1.46
14	1	4008	BCR	C8-C9	-8.19	1.28	1.46
14	F	4020	BCR	C8-C9	-8.17	1.28	1.46
14	A	4003	BCR	C11-C10	-8.17	1.17	1.43
14	L	4022	BCR	C8-C9	-8.16	1.28	1.46
14	a	4002	BCR	C8-C9	-8.15	1.28	1.46
14	F	4018	BCR	C11-C10	-8.13	1.18	1.43
14	2	4009	BCR	C8-C9	-8.11	1.28	1.46
14	2	4010	BCR	C11-C10	-8.09	1.18	1.43
12	1	2001	PQN	C3-C2	8.08	1.49	1.35
14	a	4007	BCR	C8-C9	-8.08	1.28	1.46
14	A	4002	BCR	C8-C9	-8.07	1.28	1.46
14	m	4021	BCR	C11-C10	-8.07	1.18	1.43
14	l	4022	BCR	C8-C9	-8.07	1.28	1.46
14	a	4001	BCR	C8-C9	-8.07	1.28	1.46
14	8	4022	BCR	C8-C9	-8.06	1.28	1.46
14	2	4006	BCR	C8-C9	-8.06	1.28	1.46
14	6	4020	BCR	C11-C10	-8.06	1.18	1.43
14	M	4021	BCR	C11-C10	-8.04	1.18	1.43
14	1	4001	BCR	C8-C9	-8.04	1.28	1.46
14	b	4011	BCR	C8-C9	-8.04	1.28	1.46
14	A	4007	BCR	C8-C9	-8.03	1.28	1.46
14	B	4014	BCR	C8-C9	-8.03	1.28	1.46
14	B	4009	BCR	C8-C9	-8.01	1.28	1.46
12	B	2002	PQN	C3-C2	8.00	1.49	1.35
14	B	4017	BCR	C8-C9	-8.00	1.28	1.46
14	2	4004	BCR	C8-C9	-8.00	1.28	1.46
14	2	4017	BCR	C8-C9	-7.99	1.28	1.46
14	b	4004	BCR	C8-C9	-7.99	1.28	1.46
14	1	4007	BCR	C8-C9	-7.99	1.28	1.46
14	1	4002	BCR	C8-C9	-7.99	1.28	1.46
14	L	4019	BCR	C8-C9	-7.96	1.28	1.46
14	b	4017	BCR	C11-C10	-7.96	1.18	1.43
12	2	2002	PQN	C3-C2	7.94	1.49	1.35
14	b	4010	BCR	C11-C10	-7.94	1.18	1.43
12	A	2001	PQN	C3-C2	7.93	1.49	1.35
14	B	4009	BCR	C11-C10	-7.93	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	4018	BCR	C11-C10	-7.93	1.18	1.43
14	l	4019	BCR	C11-C10	-7.92	1.18	1.43
14	B	4004	BCR	C11-C10	-7.92	1.18	1.43
14	B	4011	BCR	C11-C10	-7.91	1.18	1.43
14	F	4013	BCR	C11-C10	-7.91	1.18	1.43
14	F	4020	BCR	C11-C10	-7.91	1.18	1.43
14	f	4020	BCR	C11-C10	-7.91	1.18	1.43
14	2	4011	BCR	C11-C10	-7.90	1.18	1.43
14	a	4008	BCR	C11-C10	-7.90	1.18	1.43
14	f	4013	BCR	C11-C10	-7.90	1.18	1.43
12	b	2002	PQN	C3-C2	7.90	1.49	1.35
14	7	4021	BCR	C11-C10	-7.88	1.18	1.43
14	b	4009	BCR	C8-C9	-7.88	1.29	1.46
14	A	4008	BCR	C8-C9	-7.88	1.29	1.46
14	1	4003	BCR	C11-C10	-7.87	1.18	1.43
14	8	4022	BCR	C11-C10	-7.87	1.18	1.43
12	a	2001	PQN	C3-C2	7.87	1.49	1.35
14	a	4002	BCR	C11-C10	-7.87	1.18	1.43
14	B	4005	BCR	C11-C10	-7.86	1.18	1.43
14	2	4017	BCR	C11-C10	-7.85	1.18	1.43
14	2	4014	BCR	C11-C10	-7.85	1.18	1.43
14	b	4017	BCR	C8-C9	-7.84	1.29	1.46
14	b	4004	BCR	C11-C10	-7.84	1.18	1.43
14	f	4018	BCR	C11-C10	-7.83	1.18	1.43
14	A	4007	BCR	C11-C10	-7.83	1.18	1.43
14	1	4008	BCR	C11-C10	-7.82	1.18	1.43
14	b	4006	BCR	C11-C10	-7.82	1.18	1.43
14	b	4011	BCR	C11-C10	-7.82	1.18	1.43
14	b	4005	BCR	C11-C10	-7.81	1.19	1.43
14	B	4017	BCR	C11-C10	-7.79	1.19	1.43
14	2	4005	BCR	C11-C10	-7.79	1.19	1.43
14	l	4022	BCR	C11-C10	-7.78	1.19	1.43
14	a	4007	BCR	C11-C10	-7.78	1.19	1.43
14	a	4003	BCR	C11-C10	-7.76	1.19	1.43
14	1	4001	BCR	C11-C10	-7.75	1.19	1.43
14	1	4007	BCR	C11-C10	-7.74	1.19	1.43
14	b	4014	BCR	C11-C10	-7.74	1.19	1.43
14	8	4019	BCR	C11-C10	-7.74	1.19	1.43
14	a	4001	BCR	C11-C10	-7.74	1.19	1.43
14	B	4006	BCR	C11-C10	-7.74	1.19	1.43
14	2	4009	BCR	C11-C10	-7.73	1.19	1.43
14	2	4004	BCR	C11-C10	-7.73	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	4006	BCR	C11-C10	-7.73	1.19	1.43
14	A	4001	BCR	C11-C10	-7.72	1.19	1.43
14	6	4013	BCR	C11-C10	-7.72	1.19	1.43
14	B	4010	BCR	C11-C10	-7.72	1.19	1.43
14	1	4002	BCR	C11-C10	-7.71	1.19	1.43
14	A	4008	BCR	C11-C10	-7.70	1.19	1.43
14	L	4019	BCR	C11-C10	-7.68	1.19	1.43
14	B	4014	BCR	C11-C10	-7.67	1.19	1.43
14	6	4018	BCR	C20-C21	-7.61	1.19	1.43
14	A	4002	BCR	C11-C10	-7.61	1.19	1.43
14	b	4009	BCR	C11-C10	-7.56	1.19	1.43
14	L	4022	BCR	C11-C10	-7.55	1.19	1.43
14	6	4018	BCR	C16-C17	-7.51	1.19	1.43
14	F	4018	BCR	C20-C21	-7.50	1.19	1.43
14	f	4018	BCR	C20-C21	-7.48	1.20	1.43
14	f	4018	BCR	C16-C17	-7.47	1.20	1.43
14	f	4013	BCR	C20-C21	-7.45	1.20	1.43
14	2	4017	BCR	C20-C21	-7.44	1.20	1.43
14	B	4017	BCR	C20-C21	-7.43	1.20	1.43
14	6	4020	BCR	C20-C21	-7.42	1.20	1.43
14	b	4017	BCR	C20-C21	-7.40	1.20	1.43
14	F	4018	BCR	C16-C17	-7.39	1.20	1.43
14	a	4003	BCR	C16-C17	-7.35	1.20	1.43
14	A	4003	BCR	C20-C21	-7.35	1.20	1.43
14	b	4017	BCR	C16-C17	-7.35	1.20	1.43
14	6	4020	BCR	C16-C17	-7.34	1.20	1.43
14	A	4003	BCR	C16-C17	-7.33	1.20	1.43
14	a	4003	BCR	C20-C21	-7.32	1.20	1.43
14	f	4013	BCR	C16-C17	-7.31	1.20	1.43
14	L	4022	BCR	C20-C21	-7.31	1.20	1.43
14	B	4014	BCR	C16-C17	-7.30	1.20	1.43
14	8	4022	BCR	C20-C21	-7.30	1.20	1.43
14	B	4014	BCR	C20-C21	-7.29	1.20	1.43
14	F	4020	BCR	C20-C21	-7.28	1.20	1.43
14	b	4006	BCR	C20-C21	-7.28	1.20	1.43
14	B	4005	BCR	C20-C21	-7.28	1.20	1.43
14	B	4011	BCR	C16-C17	-7.28	1.20	1.43
14	8	4019	BCR	C20-C21	-7.27	1.20	1.43
14	2	4010	BCR	C20-C21	-7.27	1.20	1.43
14	B	4004	BCR	C20-C21	-7.27	1.20	1.43
14	B	4011	BCR	C20-C21	-7.26	1.20	1.43
14	f	4020	BCR	C16-C17	-7.26	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	m	4021	BCR	C16-C17	-7.26	1.20	1.43
14	f	4020	BCR	C20-C21	-7.25	1.20	1.43
14	2	4005	BCR	C20-C21	-7.24	1.20	1.43
14	B	4009	BCR	C20-C21	-7.24	1.20	1.43
14	l	4019	BCR	C20-C21	-7.23	1.20	1.43
14	6	4013	BCR	C20-C21	-7.23	1.20	1.43
14	2	4011	BCR	C20-C21	-7.22	1.20	1.43
14	B	4005	BCR	C16-C17	-7.22	1.20	1.43
14	b	4004	BCR	C20-C21	-7.22	1.20	1.43
14	1	4003	BCR	C20-C21	-7.22	1.20	1.43
14	l	4022	BCR	C20-C21	-7.21	1.20	1.43
14	a	4002	BCR	C20-C21	-7.21	1.20	1.43
14	b	4011	BCR	C20-C21	-7.21	1.20	1.43
14	2	4010	BCR	C16-C17	-7.21	1.20	1.43
14	2	4017	BCR	C16-C17	-7.20	1.20	1.43
14	a	4008	BCR	C20-C21	-7.20	1.20	1.43
14	b	4010	BCR	C20-C21	-7.20	1.20	1.43
14	B	4017	BCR	C16-C17	-7.20	1.20	1.43
14	a	4001	BCR	C20-C21	-7.19	1.20	1.43
14	7	4021	BCR	C20-C21	-7.18	1.20	1.43
14	F	4013	BCR	C20-C21	-7.18	1.20	1.43
14	2	4011	BCR	C16-C17	-7.18	1.20	1.43
14	A	4008	BCR	C20-C21	-7.17	1.20	1.43
14	2	4014	BCR	C16-C17	-7.17	1.20	1.43
14	b	4011	BCR	C16-C17	-7.17	1.21	1.43
14	6	4013	BCR	C16-C17	-7.17	1.21	1.43
14	1	4007	BCR	C20-C21	-7.17	1.21	1.43
14	A	4007	BCR	C16-C17	-7.17	1.21	1.43
14	L	4022	BCR	C16-C17	-7.17	1.21	1.43
14	1	4008	BCR	C20-C21	-7.17	1.21	1.43
14	1	4003	BCR	C16-C17	-7.16	1.21	1.43
14	F	4020	BCR	C16-C17	-7.16	1.21	1.43
14	2	4004	BCR	C20-C21	-7.16	1.21	1.43
14	a	4008	BCR	C16-C17	-7.16	1.21	1.43
14	b	4005	BCR	C20-C21	-7.16	1.21	1.43
14	b	4010	BCR	C16-C17	-7.15	1.21	1.43
14	8	4022	BCR	C16-C17	-7.15	1.21	1.43
14	A	4007	BCR	C20-C21	-7.15	1.21	1.43
14	A	4002	BCR	C20-C21	-7.15	1.21	1.43
14	B	4006	BCR	C20-C21	-7.15	1.21	1.43
14	7	4021	BCR	C16-C17	-7.14	1.21	1.43
14	1	4001	BCR	C20-C21	-7.14	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	m	4021	BCR	C20-C21	-7.14	1.21	1.43
14	B	4010	BCR	C20-C21	-7.13	1.21	1.43
14	A	4008	BCR	C16-C17	-7.13	1.21	1.43
14	2	4006	BCR	C20-C21	-7.12	1.21	1.43
14	B	4004	BCR	C16-C17	-7.12	1.21	1.43
14	a	4007	BCR	C20-C21	-7.12	1.21	1.43
14	b	4006	BCR	C16-C17	-7.11	1.21	1.43
14	1	4008	BCR	C16-C17	-7.11	1.21	1.43
14	A	4001	BCR	C20-C21	-7.10	1.21	1.43
14	b	4005	BCR	C16-C17	-7.10	1.21	1.43
14	A	4001	BCR	C16-C17	-7.10	1.21	1.43
14	b	4014	BCR	C16-C17	-7.09	1.21	1.43
14	1	4002	BCR	C20-C21	-7.09	1.21	1.43
14	2	4005	BCR	C16-C17	-7.08	1.21	1.43
14	a	4002	BCR	C16-C17	-7.08	1.21	1.43
14	2	4009	BCR	C20-C21	-7.08	1.21	1.43
14	2	4004	BCR	C16-C17	-7.08	1.21	1.43
14	a	4007	BCR	C16-C17	-7.08	1.21	1.43
14	1	4007	BCR	C16-C17	-7.08	1.21	1.43
14	l	4019	BCR	C16-C17	-7.07	1.21	1.43
14	1	4001	BCR	C16-C17	-7.07	1.21	1.43
14	F	4013	BCR	C16-C17	-7.06	1.21	1.43
14	l	4022	BCR	C16-C17	-7.06	1.21	1.43
14	B	4010	BCR	C16-C17	-7.06	1.21	1.43
14	M	4021	BCR	C20-C21	-7.05	1.21	1.43
14	8	4019	BCR	C16-C17	-7.05	1.21	1.43
14	1	4002	BCR	C16-C17	-7.05	1.21	1.43
14	L	4019	BCR	C20-C21	-7.05	1.21	1.43
14	A	4002	BCR	C16-C17	-7.04	1.21	1.43
14	M	4021	BCR	C16-C17	-7.04	1.21	1.43
14	B	4009	BCR	C16-C17	-7.03	1.21	1.43
14	2	4009	BCR	C16-C17	-7.03	1.21	1.43
14	B	4006	BCR	C16-C17	-7.03	1.21	1.43
14	b	4004	BCR	C16-C17	-7.02	1.21	1.43
14	b	4009	BCR	C20-C21	-7.02	1.21	1.43
14	2	4006	BCR	C16-C17	-7.01	1.21	1.43
14	b	4014	BCR	C20-C21	-7.01	1.21	1.43
14	a	4001	BCR	C16-C17	-7.01	1.21	1.43
14	L	4019	BCR	C16-C17	-7.00	1.21	1.43
14	2	4014	BCR	C20-C21	-7.00	1.21	1.43
11	a	1121	CLA	O2A-C1	6.96	1.60	1.45
11	a	1120	CLA	O2A-C1	6.89	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1211	CLA	O2A-C1	6.89	1.60	1.45
14	b	4009	BCR	C16-C17	-6.89	1.21	1.43
11	A	1121	CLA	O2A-C1	6.87	1.60	1.45
11	1	1130	CLA	O2A-C1	6.86	1.60	1.45
11	A	1134	CLA	O2A-C1	6.86	1.60	1.45
11	A	1129	CLA	O2A-C1	6.86	1.60	1.45
11	L	1502	CLA	O2A-C1	6.86	1.60	1.45
11	1	1134	CLA	O2A-C1	6.85	1.60	1.45
11	a	1130	CLA	O2A-C1	6.85	1.60	1.45
11	a	1133	CLA	O2A-C1	6.84	1.60	1.45
11	1	1133	CLA	O2A-C1	6.84	1.60	1.45
11	2	1239	CLA	O2A-C1	6.84	1.60	1.45
11	1	1121	CLA	O2A-C1	6.84	1.60	1.45
11	a	1138	CLA	O2A-C1	6.83	1.60	1.45
11	a	1115	CLA	O2A-C1	6.83	1.60	1.45
11	1	1136	CLA	O2A-C1	6.83	1.60	1.45
11	1	1138	CLA	O2A-C1	6.83	1.60	1.45
11	A	1120	CLA	O2A-C1	6.82	1.60	1.45
11	1	1120	CLA	O2A-C1	6.82	1.60	1.45
11	b	1220	CLA	O2A-C1	6.82	1.60	1.45
11	a	1114	CLA	O2A-C1	6.82	1.60	1.45
11	2	1220	CLA	O2A-C1	6.82	1.60	1.45
11	A	1138	CLA	O2A-C1	6.82	1.60	1.45
11	A	1114	CLA	O2A-C1	6.81	1.60	1.45
11	l	1502	CLA	O2A-C1	6.81	1.60	1.45
11	1	1114	CLA	O2A-C1	6.81	1.60	1.45
11	A	1130	CLA	O2A-C1	6.81	1.60	1.45
11	1	1115	CLA	O2A-C1	6.81	1.60	1.45
11	b	1211	CLA	O2A-C1	6.81	1.60	1.45
11	a	1129	CLA	O2A-C1	6.80	1.60	1.45
11	B	1211	CLA	O2A-C1	6.80	1.60	1.45
11	A	1136	CLA	O2A-C1	6.80	1.60	1.45
11	A	1115	CLA	O2A-C1	6.79	1.60	1.45
11	a	1136	CLA	O2A-C1	6.79	1.60	1.45
11	8	1502	CLA	O2A-C1	6.79	1.60	1.45
11	b	1239	CLA	O2A-C1	6.78	1.60	1.45
11	1	1129	CLA	O2A-C1	6.78	1.60	1.45
11	A	1133	CLA	O2A-C1	6.78	1.60	1.45
11	B	1239	CLA	O2A-C1	6.75	1.60	1.45
11	a	1134	CLA	O2A-C1	6.74	1.60	1.45
11	B	1220	CLA	O2A-C1	6.72	1.60	1.45
11	B	1230	CLA	O2A-C1	5.75	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1106	CLA	O2A-C1	5.74	1.61	1.46
11	1	1106	CLA	O2A-C1	5.74	1.61	1.46
11	A	1117	CLA	O2A-C1	5.72	1.61	1.46
11	b	1230	CLA	O2A-C1	5.72	1.61	1.46
11	2	1207	CLA	O2A-C1	5.68	1.61	1.46
11	1	1107	CLA	O2A-C1	5.67	1.61	1.46
11	a	1122	CLA	O2A-C1	5.67	1.61	1.46
11	a	1132	CLA	O2A-C1	5.64	1.61	1.46
11	A	1116	CLA	O2A-C1	5.64	1.61	1.46
11	a	1105	CLA	O2A-C1	5.63	1.61	1.46
11	A	1132	CLA	O2A-C1	5.62	1.61	1.46
11	2	1201	CLA	O2A-C1	5.61	1.61	1.46
11	k	1402	CLA	O2A-C1	5.61	1.61	1.46
11	2	1230	CLA	O2A-C1	5.60	1.61	1.46
11	A	1119	CLA	O2A-C1	5.60	1.61	1.46
11	a	1116	CLA	O2A-C1	5.60	1.61	1.46
11	2	1238	CLA	O2A-C1	5.60	1.61	1.46
11	b	1207	CLA	O2A-C1	5.58	1.61	1.46
11	1	1801	CLA	O2A-C1	5.57	1.61	1.46
11	a	1137	CLA	O2A-C1	5.57	1.61	1.46
11	A	1801	CLA	O2A-C1	5.56	1.61	1.46
11	a	1117	CLA	O2A-C1	5.56	1.61	1.46
11	a	1801	CLA	O2A-C1	5.56	1.61	1.46
11	B	1207	CLA	O2A-C1	5.54	1.61	1.46
11	1	1119	CLA	O2A-C1	5.54	1.61	1.46
11	b	1210	CLA	O2A-C1	5.54	1.61	1.46
11	2	1215	CLA	O2A-C1	5.54	1.61	1.46
11	1	1117	CLA	O2A-C1	5.53	1.61	1.46
11	a	1109	CLA	O2A-C1	5.53	1.61	1.46
11	b	1013	CLA	O2A-C1	5.53	1.61	1.46
11	a	1140	CLA	O2A-C1	5.53	1.61	1.46
11	B	1221	CLA	O2A-C1	5.53	1.61	1.46
11	a	1118	CLA	O2A-C1	5.53	1.61	1.46
11	A	1131	CLA	O2A-C1	5.53	1.61	1.46
11	a	1237	CLA	O2A-C1	5.52	1.61	1.46
11	A	1102	CLA	O2A-C1	5.52	1.61	1.46
11	B	1013	CLA	O2A-C1	5.52	1.61	1.46
11	1	1102	CLA	O2A-C1	5.51	1.61	1.46
11	A	1126	CLA	CHC-C1C	5.51	1.49	1.38
11	K	1402	CLA	O2A-C1	5.51	1.60	1.46
11	a	1102	CLA	O2A-C1	5.51	1.60	1.46
11	1	1012	CLA	O2A-C1	5.51	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1128	CLA	O2A-C1	5.50	1.60	1.46
11	b	1214	CLA	O2A-C1	5.50	1.60	1.46
11	A	1118	CLA	O2A-C1	5.50	1.60	1.46
11	1	1109	CLA	O2A-C1	5.49	1.60	1.46
11	2	1221	CLA	O2A-C1	5.49	1.60	1.46
11	A	1107	CLA	O2A-C1	5.49	1.60	1.46
11	1	1135	CLA	O2A-C1	5.49	1.60	1.46
11	1	1140	CLA	O2A-C1	5.49	1.60	1.46
11	1	1122	CLA	O2A-C1	5.49	1.60	1.46
11	B	1235	CLA	O2A-C1	5.49	1.60	1.46
11	1	1116	CLA	O2A-C1	5.49	1.60	1.46
11	0	1402	CLA	O2A-C1	5.48	1.60	1.46
11	A	1109	CLA	O2A-C1	5.48	1.60	1.46
11	b	1215	CLA	O2A-C1	5.48	1.60	1.46
11	b	1223	CLA	O2A-C1	5.48	1.60	1.46
11	b	1228	CLA	O2A-C1	5.48	1.60	1.46
11	a	1131	CLA	O2A-C1	5.48	1.60	1.46
11	B	1222	CLA	O2A-C1	5.48	1.60	1.46
11	A	1135	CLA	O2A-C1	5.47	1.60	1.46
11	a	1012	CLA	O2A-C1	5.47	1.60	1.46
11	a	1106	CLA	O2A-C1	5.47	1.60	1.46
11	2	1222	CLA	O2A-C1	5.47	1.60	1.46
11	2	1013	CLA	O2A-C1	5.47	1.60	1.46
11	2	1223	CLA	O2A-C1	5.47	1.60	1.46
11	1	1237	CLA	O2A-C1	5.46	1.60	1.46
11	L	1501	CLA	O2A-C1	5.46	1.60	1.46
11	A	1122	CLA	O2A-C1	5.46	1.60	1.46
11	B	1226	CLA	O2A-C1	5.46	1.60	1.46
11	b	1224	CLA	O2A-C1	5.46	1.60	1.46
11	A	1237	CLA	O2A-C1	5.45	1.60	1.46
11	2	1023	CLA	O2A-C1	5.45	1.60	1.46
11	B	1219	CLA	O2A-C1	5.45	1.60	1.46
11	a	1139	CLA	O2A-C1	5.44	1.60	1.46
11	A	1125	CLA	O2A-C1	5.44	1.60	1.46
11	B	1223	CLA	O2A-C1	5.43	1.60	1.46
11	2	1216	CLA	O2A-C1	5.43	1.60	1.46
11	b	1225	CLA	O2A-C1	5.43	1.60	1.46
11	2	1214	CLA	O2A-C1	5.43	1.60	1.46
11	b	1229	CLA	O2A-C1	5.43	1.60	1.46
11	A	1140	CLA	O2A-C1	5.43	1.60	1.46
11	b	1205	CLA	O2A-C1	5.43	1.60	1.46
11	1	1137	CLA	O2A-C1	5.43	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1111	CLA	O2A-C1	5.43	1.60	1.46
11	B	1238	CLA	O2A-C1	5.43	1.60	1.46
11	B	1228	CLA	O2A-C1	5.43	1.60	1.46
11	1	1118	CLA	O2A-C1	5.43	1.60	1.46
11	2	1206	CLA	O2A-C1	5.42	1.60	1.46
11	B	1225	CLA	O2A-C1	5.42	1.60	1.46
11	1	1105	CLA	O2A-C1	5.42	1.60	1.46
11	2	1210	CLA	O2A-C1	5.42	1.60	1.46
11	a	1022	CLA	O2A-C1	5.42	1.60	1.46
11	B	1216	CLA	O2A-C1	5.42	1.60	1.46
11	1	1022	CLA	O2A-C1	5.42	1.60	1.46
11	a	1110	CLA	O2A-C1	5.42	1.60	1.46
11	2	1228	CLA	O2A-C1	5.41	1.60	1.46
11	8	1503	CLA	O2A-C1	5.41	1.60	1.46
11	b	1206	CLA	O2A-C1	5.41	1.60	1.46
11	B	1234	CLA	O2A-C1	5.41	1.60	1.46
11	2	1203	CLA	O2A-C1	5.41	1.60	1.46
11	a	1135	CLA	O2A-C1	5.40	1.60	1.46
11	b	1021	CLA	O2A-C1	5.40	1.60	1.46
11	2	1235	CLA	O2A-C1	5.40	1.60	1.46
11	B	1201	CLA	O2A-C1	5.40	1.60	1.46
11	B	1229	CLA	O2A-C1	5.40	1.60	1.46
11	l	1501	CLA	O2A-C1	5.40	1.60	1.46
11	A	1128	CLA	O2A-C1	5.40	1.60	1.46
11	k	1401	CLA	O2A-C1	5.40	1.60	1.46
11	a	1119	CLA	O2A-C1	5.40	1.60	1.46
11	B	1210	CLA	O2A-C1	5.39	1.60	1.46
11	a	1107	CLA	O2A-C1	5.39	1.60	1.46
11	2	1202	CLA	O2A-C1	5.39	1.60	1.46
11	1	1132	CLA	O2A-C1	5.39	1.60	1.46
11	A	1105	CLA	O2A-C1	5.39	1.60	1.46
11	B	1205	CLA	O2A-C1	5.39	1.60	1.46
11	A	1124	CLA	O2A-C1	5.39	1.60	1.46
11	B	1224	CLA	O2A-C1	5.39	1.60	1.46
11	b	1216	CLA	O2A-C1	5.39	1.60	1.46
11	2	1213	CLA	O2A-C1	5.39	1.60	1.46
11	b	1234	CLA	O2A-C1	5.39	1.60	1.46
11	a	1011	CLA	O2D-CGD	5.38	1.46	1.33
11	a	1101	CLA	O2A-C1	5.38	1.60	1.46
11	b	1226	CLA	O2A-C1	5.38	1.60	1.46
11	1	1128	CLA	O2A-C1	5.38	1.60	1.46
11	B	1206	CLA	O2A-C1	5.38	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1126	CLA	O2A-C1	5.38	1.60	1.46
11	l	1503	CLA	O2A-C1	5.37	1.60	1.46
11	b	1219	CLA	O2A-C1	5.37	1.60	1.46
11	K	1401	CLA	O2A-C1	5.37	1.60	1.46
11	b	1238	CLA	O2A-C1	5.37	1.60	1.46
11	B	1214	CLA	O2A-C1	5.37	1.60	1.46
11	A	1112	CLA	CHC-C1C	5.37	1.49	1.38
11	L	1503	CLA	O2A-C1	5.37	1.60	1.46
11	B	1213	CLA	O2A-C1	5.37	1.60	1.46
11	b	1222	CLA	O2A-C1	5.36	1.60	1.46
11	a	1123	CLA	O2A-C1	5.36	1.60	1.46
11	b	1202	CLA	O2A-C1	5.36	1.60	1.46
11	b	1023	CLA	O2A-C1	5.36	1.60	1.46
11	B	1202	CLA	O2A-C1	5.35	1.60	1.46
11	2	1226	CLA	O2A-C1	5.35	1.60	1.46
11	A	1137	CLA	O2A-C1	5.35	1.60	1.46
11	2	1234	CLA	O2A-C1	5.35	1.60	1.46
11	0	1401	CLA	O2A-C1	5.34	1.60	1.46
11	A	1123	CLA	O2A-C1	5.34	1.60	1.46
11	2	1204	CLA	O2A-C1	5.34	1.60	1.46
11	B	1203	CLA	O2A-C1	5.34	1.60	1.46
11	a	1124	CLA	O2A-C1	5.34	1.60	1.46
11	2	1229	CLA	O2A-C1	5.34	1.60	1.46
11	1	1104	CLA	O2A-C1	5.33	1.60	1.46
11	b	1213	CLA	O2A-C1	5.33	1.60	1.46
11	a	1011	CLA	O2A-C1	5.33	1.60	1.46
11	a	1104	CLA	O2A-C1	5.32	1.60	1.46
11	1	1125	CLA	O2A-C1	5.32	1.60	1.46
11	8	1501	CLA	O2A-C1	5.32	1.60	1.46
11	B	1023	CLA	O2A-C1	5.32	1.60	1.46
11	b	1203	CLA	O2A-C1	5.31	1.60	1.46
11	B	1204	CLA	O2A-C1	5.31	1.60	1.46
11	a	1126	CLA	CHC-C1C	5.31	1.49	1.38
11	A	1103	CLA	CHC-C1C	5.31	1.49	1.38
11	b	1221	CLA	O2A-C1	5.31	1.60	1.46
11	a	1125	CLA	O2A-C1	5.31	1.60	1.46
11	1	1110	CLA	O2A-C1	5.30	1.60	1.46
11	1	1011	CLA	O2A-C1	5.30	1.60	1.46
11	A	1103	CLA	O2A-C1	5.30	1.60	1.46
11	1	1103	CLA	O2A-C1	5.30	1.60	1.46
11	a	1127	CLA	O2A-C1	5.30	1.60	1.46
11	A	1109	CLA	O2D-CGD	5.30	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1021	CLA	O2A-C1	5.29	1.60	1.46
11	1	1139	CLA	O2A-C1	5.29	1.60	1.46
11	2	1224	CLA	O2A-C1	5.29	1.60	1.46
11	1	1123	CLA	O2A-C1	5.29	1.60	1.46
11	A	1139	CLA	O2A-C1	5.29	1.60	1.46
11	a	1127	CLA	O2D-CGD	5.29	1.46	1.33
11	1	1124	CLA	O2A-C1	5.28	1.60	1.46
11	a	1101	CLA	O2D-CGD	5.28	1.46	1.33
11	B	1202	CLA	CHC-C1C	5.28	1.49	1.38
11	2	1021	CLA	O2A-C1	5.28	1.60	1.46
11	a	1103	CLA	O2A-C1	5.28	1.60	1.46
11	1	1138	CLA	O2D-CGD	5.28	1.46	1.33
11	2	1225	CLA	O2A-C1	5.28	1.60	1.46
11	A	1127	CLA	O2A-C1	5.28	1.60	1.46
11	A	1101	CLA	O2A-C1	5.27	1.60	1.46
11	2	1205	CLA	O2A-C1	5.27	1.60	1.46
11	b	1201	CLA	O2A-C1	5.27	1.60	1.46
11	A	1133	CLA	O2D-CGD	5.26	1.46	1.33
11	a	1112	CLA	CHC-C1C	5.26	1.49	1.38
11	A	1022	CLA	O2A-C1	5.26	1.60	1.46
11	1	1131	CLA	O2A-C1	5.26	1.60	1.46
11	A	1110	CLA	O2A-C1	5.26	1.60	1.46
11	A	1117	CLA	CHC-C1C	5.25	1.49	1.38
11	2	1223	CLA	CHC-C1C	5.25	1.49	1.38
11	a	1126	CLA	O2A-C1	5.25	1.60	1.46
11	A	1104	CLA	O2A-C1	5.25	1.60	1.46
11	A	1012	CLA	O2A-C1	5.25	1.60	1.46
11	2	1219	CLA	O2A-C1	5.24	1.60	1.46
11	b	1235	CLA	O2A-C1	5.24	1.60	1.46
11	A	1116	CLA	CHC-C1C	5.24	1.49	1.38
11	A	1111	CLA	CHC-C1C	5.24	1.49	1.38
11	1	1126	CLA	CHC-C1C	5.23	1.49	1.38
11	B	1215	CLA	O2A-C1	5.23	1.60	1.46
11	A	1115	CLA	O2D-CGD	5.23	1.46	1.33
11	1	1121	CLA	O2D-CGD	5.23	1.46	1.33
11	2	1230	CLA	O2D-CGD	5.23	1.46	1.33
11	A	1011	CLA	O2A-C1	5.22	1.60	1.46
11	2	1228	CLA	O2D-CGD	5.22	1.46	1.33
11	2	1216	CLA	O2D-CGD	5.22	1.46	1.33
11	b	1210	CLA	CHC-C1C	5.22	1.48	1.38
11	b	1221	CLA	CHC-C1C	5.22	1.48	1.38
11	a	1108	CLA	O2D-CGD	5.22	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1213	CLA	O2D-CGD	5.21	1.46	1.33
11	b	1218	CLA	O2D-CGD	5.21	1.46	1.33
11	2	1023	CLA	O2D-CGD	5.21	1.46	1.33
11	b	1224	CLA	O2D-CGD	5.21	1.46	1.33
11	b	1213	CLA	O2D-CGD	5.21	1.46	1.33
11	1	1112	CLA	O2D-CGD	5.21	1.46	1.33
11	b	1021	CLA	O2D-CGD	5.20	1.46	1.33
11	2	1213	CLA	CHC-C1C	5.20	1.48	1.38
11	B	1214	CLA	CHC-C1C	5.20	1.48	1.38
11	a	1119	CLA	O2D-CGD	5.20	1.46	1.33
11	2	1235	CLA	CHC-C1C	5.20	1.48	1.38
11	2	1239	CLA	O2D-CGD	5.20	1.46	1.33
11	b	1207	CLA	O2D-CGD	5.20	1.46	1.33
11	A	1011	CLA	O2D-CGD	5.20	1.46	1.33
11	1	1109	CLA	O2D-CGD	5.20	1.46	1.33
11	a	1115	CLA	CHC-C1C	5.20	1.48	1.38
11	2	1208	CLA	O2D-CGD	5.19	1.46	1.33
11	b	1213	CLA	CHC-C1C	5.19	1.48	1.38
11	1	1127	CLA	O2A-C1	5.19	1.60	1.46
11	a	1105	CLA	O2D-CGD	5.19	1.46	1.33
11	A	1119	CLA	O2D-CGD	5.19	1.46	1.33
11	b	1219	CLA	O2D-CGD	5.19	1.46	1.33
11	1	1125	CLA	O2D-CGD	5.19	1.46	1.33
11	2	1204	CLA	O2D-CGD	5.19	1.46	1.33
11	1	1126	CLA	O2A-C1	5.19	1.60	1.46
11	b	1202	CLA	CHC-C1C	5.19	1.48	1.38
11	a	1115	CLA	O2D-CGD	5.19	1.46	1.33
11	a	1139	CLA	O2D-CGD	5.18	1.46	1.33
11	a	1114	CLA	O2D-CGD	5.18	1.46	1.33
11	A	1237	CLA	O2D-CGD	5.18	1.46	1.33
11	A	1801	CLA	C3C-C2C	5.18	1.47	1.36
11	2	1211	CLA	O2D-CGD	5.18	1.46	1.33
11	a	1109	CLA	O2D-CGD	5.18	1.46	1.33
11	a	1120	CLA	O2D-CGD	5.18	1.46	1.33
11	A	1137	CLA	CHC-C1C	5.18	1.48	1.38
11	1	1101	CLA	O2A-C1	5.18	1.60	1.46
11	B	1218	CLA	O2D-CGD	5.18	1.46	1.33
11	B	1230	CLA	O2D-CGD	5.18	1.46	1.33
11	a	1131	CLA	O2D-CGD	5.18	1.46	1.33
11	1	1108	CLA	O2D-CGD	5.18	1.46	1.33
11	1	1122	CLA	CHC-C1C	5.18	1.48	1.38
11	a	1103	CLA	O2D-CGD	5.17	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1503	CLA	O2D-CGD	5.17	1.46	1.33
11	b	1228	CLA	O2D-CGD	5.17	1.45	1.33
11	A	1116	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1111	CLA	CHC-C1C	5.17	1.48	1.38
11	B	1232	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1136	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1130	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1235	CLA	O2D-CGD	5.17	1.45	1.33
11	B	1219	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1114	CLA	O2D-CGD	5.17	1.45	1.33
11	a	1126	CLA	O2D-CGD	5.17	1.45	1.33
11	A	1139	CLA	O2D-CGD	5.17	1.45	1.33
11	2	1013	CLA	O2D-CGD	5.17	1.45	1.33
11	1	1122	CLA	O2D-CGD	5.17	1.45	1.33
11	2	1021	CLA	O2D-CGD	5.16	1.45	1.33
11	b	1216	CLA	O2D-CGD	5.16	1.45	1.33
11	b	1215	CLA	O2D-CGD	5.16	1.45	1.33
11	B	1217	CLA	O2D-CGD	5.16	1.45	1.33
11	B	1212	CLA	CHC-C1C	5.16	1.48	1.38
11	a	1136	CLA	O2D-CGD	5.16	1.45	1.33
11	a	1102	CLA	O2D-CGD	5.16	1.45	1.33
11	a	1138	CLA	O2D-CGD	5.16	1.45	1.33
11	A	1106	CLA	O2D-CGD	5.16	1.45	1.33
11	A	1125	CLA	O2D-CGD	5.16	1.45	1.33
11	2	1219	CLA	CHC-C1C	5.16	1.48	1.38
11	b	1236	CLA	CHC-C1C	5.16	1.48	1.38
11	A	1140	CLA	O2D-CGD	5.16	1.45	1.33
11	1	1133	CLA	O2D-CGD	5.16	1.45	1.33
11	a	1122	CLA	CHC-C1C	5.16	1.48	1.38
11	b	1204	CLA	O2A-C1	5.16	1.60	1.46
11	b	1206	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1128	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1136	CLA	O2D-CGD	5.15	1.45	1.33
11	B	1208	CLA	O2D-CGD	5.15	1.45	1.33
11	2	1227	CLA	O2D-CGD	5.15	1.45	1.33
11	2	1236	CLA	O2D-CGD	5.15	1.45	1.33
11	1	1115	CLA	O2D-CGD	5.15	1.45	1.33
11	1	1128	CLA	O2D-CGD	5.15	1.45	1.33
11	B	1228	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1801	CLA	O2D-CGD	5.15	1.45	1.33
11	a	1130	CLA	O2D-CGD	5.15	1.45	1.33
11	1	1101	CLA	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1203	CLA	O2D-CGD	5.15	1.45	1.33
11	2	1220	CLA	O2D-CGD	5.15	1.45	1.33
11	A	1111	CLA	O2A-C1	5.14	1.60	1.46
11	1	1113	CLA	O2D-CGD	5.14	1.45	1.33
11	k	1402	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1235	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1204	CLA	CHC-C1C	5.14	1.48	1.38
11	B	1214	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1235	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1202	CLA	O2D-CGD	5.14	1.45	1.33
11	A	1138	CLA	O2D-CGD	5.14	1.45	1.33
11	1	1119	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1013	CLA	O2D-CGD	5.14	1.45	1.33
11	1	1105	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1209	CLA	O2D-CGD	5.14	1.45	1.33
11	2	1236	CLA	CHC-C1C	5.14	1.48	1.38
11	1	1139	CLA	O2D-CGD	5.14	1.45	1.33
11	A	1115	CLA	CHC-C1C	5.14	1.48	1.38
11	A	1104	CLA	O2D-CGD	5.14	1.45	1.33
11	0	1401	CLA	O2D-CGD	5.14	1.45	1.33
11	b	1214	CLA	CHC-C1C	5.13	1.48	1.38
11	A	1102	CLA	O2D-CGD	5.13	1.45	1.33
11	B	1240	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1201	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1230	CLA	O2D-CGD	5.13	1.45	1.33
11	a	1128	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1202	CLA	O2D-CGD	5.13	1.45	1.33
11	2	1213	CLA	O2D-CGD	5.13	1.45	1.33
11	A	1112	CLA	O2D-CGD	5.13	1.45	1.33
11	2	1202	CLA	CHC-C1C	5.13	1.48	1.38
11	2	1215	CLA	O2D-CGD	5.13	1.45	1.33
11	a	1123	CLA	O2D-CGD	5.13	1.45	1.33
11	l	1501	CLA	O2D-CGD	5.13	1.45	1.33
11	1	1117	CLA	O2D-CGD	5.13	1.45	1.33
11	K	1401	CLA	O2D-CGD	5.13	1.45	1.33
11	a	1801	CLA	CHC-C1C	5.13	1.48	1.38
11	A	1126	CLA	O2D-CGD	5.13	1.45	1.33
11	b	1234	CLA	O2D-CGD	5.13	1.45	1.33
11	B	1240	CLA	CHC-C1C	5.13	1.48	1.38
11	B	1208	CLA	CHC-C1C	5.13	1.48	1.38
11	0	1402	CLA	CHC-C1C	5.13	1.48	1.38
11	a	1129	CLA	O2D-CGD	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1108	CLA	O2D-CGD	5.12	1.45	1.33
11	1	1118	CLA	O2D-CGD	5.12	1.45	1.33
11	k	1401	CLA	O2D-CGD	5.12	1.45	1.33
11	1	1134	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1216	CLA	O2D-CGD	5.12	1.45	1.33
11	2	1213	CLA	C3C-C2C	5.12	1.47	1.36
11	1	1120	CLA	O2D-CGD	5.12	1.45	1.33
11	2	1210	CLA	CHC-C1C	5.12	1.48	1.38
11	A	1123	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1204	CLA	O2D-CGD	5.12	1.45	1.33
11	1	1112	CLA	CHC-C1C	5.12	1.48	1.38
11	A	1124	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1208	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1212	CLA	O2D-CGD	5.12	1.45	1.33
11	1	1140	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1240	CLA	O2D-CGD	5.12	1.45	1.33
11	A	1022	CLA	CHC-C1C	5.12	1.48	1.38
11	b	1217	CLA	O2D-CGD	5.12	1.45	1.33
11	2	1229	CLA	CHC-C1C	5.12	1.48	1.38
11	b	1232	CLA	O2D-CGD	5.12	1.45	1.33
11	1	1106	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1023	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1111	CLA	O2A-C1	5.12	1.59	1.46
11	a	1012	CLA	O2D-CGD	5.12	1.45	1.33
11	b	1227	CLA	O2D-CGD	5.12	1.45	1.33
11	B	1210	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1110	CLA	O2D-CGD	5.12	1.45	1.33
11	a	1116	CLA	CHC-C1C	5.12	1.48	1.38
11	b	1205	CLA	O2D-CGD	5.11	1.45	1.33
11	8	1503	CLA	CHC-C1C	5.11	1.48	1.38
11	b	1204	CLA	O2D-CGD	5.11	1.45	1.33
11	b	1225	CLA	O2D-CGD	5.11	1.45	1.33
11	1	1801	CLA	O2D-CGD	5.11	1.45	1.33
11	2	1219	CLA	O2D-CGD	5.11	1.45	1.33
11	B	1235	CLA	CHC-C1C	5.11	1.48	1.38
11	1	1129	CLA	CHC-C1C	5.11	1.48	1.38
11	a	1116	CLA	O2D-CGD	5.11	1.45	1.33
11	a	1121	CLA	O2D-CGD	5.11	1.45	1.33
11	A	1113	CLA	CHC-C1C	5.11	1.48	1.38
11	1	1129	CLA	O2D-CGD	5.11	1.45	1.33
11	B	1236	CLA	CHC-C1C	5.11	1.48	1.38
11	a	1133	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1126	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1013	CLA	CHC-C1C	5.10	1.48	1.38
11	a	1118	CLA	O2D-CGD	5.10	1.45	1.33
11	l	1503	CLA	O2D-CGD	5.10	1.45	1.33
11	B	1213	CLA	CHC-C1C	5.10	1.48	1.38
11	1	1104	CLA	O2D-CGD	5.10	1.45	1.33
11	0	1402	CLA	O2D-CGD	5.10	1.45	1.33
11	a	1104	CLA	CHC-C1C	5.10	1.48	1.38
11	1	1022	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1234	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1225	CLA	O2D-CGD	5.10	1.45	1.33
11	1	1127	CLA	O2D-CGD	5.10	1.45	1.33
11	A	1139	CLA	CHC-C1C	5.10	1.48	1.38
11	8	1501	CLA	O2D-CGD	5.10	1.45	1.33
11	B	1223	CLA	CHC-C1C	5.10	1.48	1.38
11	A	1114	CLA	O2D-CGD	5.10	1.45	1.33
11	2	1217	CLA	O2D-CGD	5.10	1.45	1.33
11	L	1501	CLA	O2D-CGD	5.10	1.45	1.33
11	1	1123	CLA	O2D-CGD	5.09	1.45	1.33
11	B	1223	CLA	O2D-CGD	5.09	1.45	1.33
11	a	1134	CLA	O2D-CGD	5.09	1.45	1.33
11	1	1116	CLA	O2D-CGD	5.09	1.45	1.33
11	A	1113	CLA	O2D-CGD	5.09	1.45	1.33
11	A	1120	CLA	CHC-C1C	5.09	1.48	1.38
11	B	1224	CLA	CHC-C1C	5.09	1.48	1.38
11	1	1125	CLA	CHC-C1C	5.09	1.48	1.38
11	A	1137	CLA	O2D-CGD	5.09	1.45	1.33
11	b	1235	CLA	CHC-C1C	5.09	1.48	1.38
11	a	1132	CLA	O2D-CGD	5.09	1.45	1.33
11	A	1012	CLA	O2D-CGD	5.09	1.45	1.33
11	1	1135	CLA	O2D-CGD	5.09	1.45	1.33
11	A	1131	CLA	O2D-CGD	5.09	1.45	1.33
11	1	1124	CLA	O2D-CGD	5.09	1.45	1.33
11	2	1209	CLA	O2D-CGD	5.09	1.45	1.33
11	B	1225	CLA	O2D-CGD	5.08	1.45	1.33
11	2	1232	CLA	O2D-CGD	5.08	1.45	1.33
11	A	1127	CLA	O2D-CGD	5.08	1.45	1.33
11	A	1130	CLA	O2D-CGD	5.08	1.45	1.33
11	a	1012	CLA	CHC-C1C	5.08	1.48	1.38
11	b	1226	CLA	CHC-C1C	5.08	1.48	1.38
11	B	1013	CLA	CHC-C1C	5.08	1.48	1.38
11	b	1216	CLA	CHC-C1C	5.08	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1222	CLA	CHC-C1C	5.08	1.48	1.38
11	a	1113	CLA	O2D-CGD	5.08	1.45	1.33
11	2	1212	CLA	O2D-CGD	5.08	1.45	1.33
11	a	1122	CLA	O2D-CGD	5.08	1.45	1.33
11	2	1218	CLA	O2D-CGD	5.08	1.45	1.33
11	A	1118	CLA	O2D-CGD	5.08	1.45	1.33
11	1	1022	CLA	CHC-C1C	5.07	1.48	1.38
11	a	1022	CLA	O2D-CGD	5.07	1.45	1.33
11	a	1104	CLA	O2D-CGD	5.07	1.45	1.33
11	B	1227	CLA	O2D-CGD	5.07	1.45	1.33
11	b	1013	CLA	CHC-C1C	5.07	1.48	1.38
11	b	1240	CLA	CHC-C1C	5.07	1.48	1.38
11	2	1232	CLA	CHC-C1C	5.07	1.48	1.38
11	B	1222	CLA	O2D-CGD	5.07	1.45	1.33
11	a	1135	CLA	O2D-CGD	5.07	1.45	1.33
11	A	1121	CLA	O2D-CGD	5.07	1.45	1.33
11	a	1112	CLA	O2D-CGD	5.07	1.45	1.33
11	b	1239	CLA	O2D-CGD	5.07	1.45	1.33
11	2	1240	CLA	O2D-CGD	5.07	1.45	1.33
11	k	1402	CLA	CHC-C1C	5.07	1.48	1.38
11	B	1206	CLA	O2D-CGD	5.07	1.45	1.33
11	b	1220	CLA	O2D-CGD	5.07	1.45	1.33
11	1	1116	CLA	CHC-C1C	5.07	1.48	1.38
11	A	1132	CLA	O2D-CGD	5.07	1.45	1.33
11	L	1502	CLA	O2D-CGD	5.07	1.45	1.33
11	a	1117	CLA	O2D-CGD	5.07	1.45	1.33
11	2	1206	CLA	O2D-CGD	5.07	1.45	1.33
11	B	1224	CLA	O2D-CGD	5.06	1.45	1.33
11	1	1131	CLA	O2D-CGD	5.06	1.45	1.33
11	A	1108	CLA	CHC-C1C	5.06	1.48	1.38
11	B	1209	CLA	O2D-CGD	5.06	1.45	1.33
12	A	2001	PQN	C10-C5	5.06	1.48	1.40
11	B	1202	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1229	CLA	O2D-CGD	5.06	1.45	1.33
11	1	1103	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1225	CLA	CHC-C1C	5.06	1.48	1.38
11	b	1222	CLA	O2D-CGD	5.06	1.45	1.33
11	2	1222	CLA	O2D-CGD	5.06	1.45	1.33
11	A	1107	CLA	CHC-C1C	5.06	1.48	1.38
11	B	1210	CLA	CHC-C1C	5.06	1.48	1.38
11	B	1215	CLA	O2D-CGD	5.06	1.45	1.33
11	b	1210	CLA	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1231	CLA	CHC-C1C	5.06	1.48	1.38
11	b	1214	CLA	O2D-CGD	5.06	1.45	1.33
11	L	1501	CLA	CHC-C1C	5.05	1.48	1.38
11	a	1140	CLA	O2D-CGD	5.05	1.45	1.33
11	K	1402	CLA	O2D-CGD	5.05	1.45	1.33
11	2	1214	CLA	O2D-CGD	5.05	1.45	1.33
11	2	1224	CLA	O2D-CGD	5.05	1.45	1.33
11	1	1108	CLA	CHC-C1C	5.05	1.48	1.38
11	a	1237	CLA	O2D-CGD	5.05	1.45	1.33
11	B	1221	CLA	CHC-C1C	5.05	1.48	1.38
11	1	1107	CLA	O2D-CGD	5.05	1.45	1.33
11	a	1125	CLA	O2D-CGD	5.05	1.45	1.33
11	B	1239	CLA	O2D-CGD	5.05	1.45	1.33
11	1	1102	CLA	CHC-C1C	5.05	1.48	1.38
11	2	1218	CLA	CHC-C1C	5.05	1.48	1.38
11	a	1134	CLA	CHC-C1C	5.05	1.48	1.38
11	B	1212	CLA	O2D-CGD	5.04	1.45	1.33
11	2	1201	CLA	O2D-CGD	5.04	1.45	1.33
11	2	1226	CLA	O2D-CGD	5.04	1.45	1.33
11	l	1502	CLA	CHC-C1C	5.04	1.48	1.38
11	8	1502	CLA	CHC-C1C	5.04	1.48	1.38
11	B	1211	CLA	O2D-CGD	5.04	1.45	1.33
11	A	1022	CLA	O2D-CGD	5.04	1.45	1.33
11	B	1226	CLA	O2D-CGD	5.04	1.45	1.33
11	1	1237	CLA	O2D-CGD	5.04	1.45	1.33
11	B	1013	CLA	O2D-CGD	5.04	1.45	1.33
11	2	1229	CLA	O2D-CGD	5.04	1.45	1.33
11	b	1201	CLA	CHC-C1C	5.04	1.48	1.38
11	B	1221	CLA	O2D-CGD	5.04	1.45	1.33
11	A	1120	CLA	O2D-CGD	5.04	1.45	1.33
11	A	1134	CLA	O2D-CGD	5.04	1.45	1.33
11	l	1502	CLA	O2D-CGD	5.04	1.45	1.33
11	b	1224	CLA	CHC-C1C	5.03	1.48	1.38
12	b	2002	PQN	C10-C5	5.03	1.48	1.40
11	B	1203	CLA	O2D-CGD	5.03	1.45	1.33
11	b	1221	CLA	O2D-CGD	5.03	1.45	1.33
11	B	1021	CLA	O2D-CGD	5.03	1.45	1.33
11	b	1218	CLA	CHC-C1C	5.03	1.48	1.38
11	B	1234	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1012	CLA	CHC-C1C	5.03	1.48	1.38
11	a	1106	CLA	O2D-CGD	5.03	1.45	1.33
11	B	1236	CLA	O2D-CGD	5.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1217	CLA	CHC-C1C	5.03	1.48	1.38
11	l	1501	CLA	CHC-C1C	5.03	1.48	1.38
11	B	1207	CLA	O2D-CGD	5.03	1.45	1.33
11	1	1012	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1129	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1117	CLA	O2D-CGD	5.03	1.45	1.33
11	b	1211	CLA	CHC-C1C	5.02	1.48	1.38
11	0	1401	CLA	CHC-C1C	5.02	1.48	1.38
11	a	1132	CLA	CHC-C1C	5.02	1.48	1.38
11	2	1223	CLA	O2D-CGD	5.02	1.45	1.33
11	A	1122	CLA	CHC-C1C	5.02	1.48	1.38
11	a	1109	CLA	CHC-C1C	5.02	1.48	1.38
11	2	1207	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1113	CLA	CHC-C1C	5.02	1.48	1.38
11	1	1130	CLA	CHC-C1C	5.02	1.48	1.38
11	B	1216	CLA	CHC-C1C	5.02	1.48	1.38
11	1	1137	CLA	O2D-CGD	5.02	1.45	1.33
11	a	1117	CLA	CHC-C1C	5.02	1.48	1.38
11	1	1134	CLA	CHC-C1C	5.02	1.48	1.38
11	B	1201	CLA	O2D-CGD	5.02	1.45	1.33
11	A	1135	CLA	O2D-CGD	5.02	1.45	1.33
11	A	1130	CLA	CHC-C1C	5.02	1.48	1.38
11	1	1137	CLA	CHC-C1C	5.02	1.48	1.38
11	1	1111	CLA	O2D-CGD	5.01	1.45	1.33
11	b	1238	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1124	CLA	CHC-C1C	5.01	1.48	1.38
11	2	1210	CLA	O2D-CGD	5.01	1.45	1.33
11	1	1011	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1111	CLA	CHC-C1C	5.01	1.48	1.38
11	2	1211	CLA	CHC-C1C	5.01	1.48	1.38
11	1	1110	CLA	O2D-CGD	5.01	1.45	1.33
11	b	1236	CLA	O2D-CGD	5.01	1.45	1.33
11	b	1211	CLA	O2D-CGD	5.01	1.45	1.33
11	2	1238	CLA	O2D-CGD	5.00	1.45	1.33
11	a	1130	CLA	CHC-C1C	5.00	1.48	1.38
11	2	1216	CLA	CHC-C1C	5.00	1.48	1.38
11	a	1113	CLA	CHC-C1C	5.00	1.48	1.38
11	b	1203	CLA	CHC-C1C	5.00	1.48	1.38
11	a	1129	CLA	CHC-C1C	5.00	1.48	1.38
11	a	1801	CLA	O2D-CGD	5.00	1.45	1.33
11	2	1225	CLA	CHC-C1C	5.00	1.48	1.38
11	2	1221	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1128	CLA	CHC-C1C	5.00	1.48	1.38
11	1	1119	CLA	CHC-C1C	4.99	1.48	1.38
12	a	2001	PQN	C10-C5	4.99	1.48	1.40
11	2	1221	CLA	CHC-C1C	4.99	1.48	1.38
11	A	1109	CLA	CHC-C1C	4.99	1.48	1.38
11	B	1225	CLA	CHC-C1C	4.99	1.48	1.38
11	1	1136	CLA	CHC-C1C	4.99	1.48	1.38
11	2	1222	CLA	CHC-C1C	4.99	1.48	1.38
11	B	1238	CLA	O2D-CGD	4.99	1.45	1.33
11	a	1137	CLA	O2D-CGD	4.99	1.45	1.33
11	1	1106	CLA	CHC-C1C	4.99	1.48	1.38
11	A	1101	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1215	CLA	CHC-C1C	4.99	1.48	1.38
11	A	1121	CLA	CHC-C1C	4.99	1.48	1.38
11	A	1124	CLA	CHC-C1C	4.99	1.48	1.38
11	a	1124	CLA	O2D-CGD	4.99	1.45	1.33
11	1	1120	CLA	CHC-C1C	4.98	1.48	1.38
12	2	2002	PQN	C10-C5	4.98	1.48	1.40
11	1	1801	CLA	C3C-C2C	4.98	1.47	1.36
11	k	1401	CLA	CHC-C1C	4.98	1.48	1.38
11	B	1205	CLA	O2D-CGD	4.98	1.45	1.33
11	L	1503	CLA	O2D-CGD	4.98	1.45	1.33
11	K	1401	CLA	CHC-C1C	4.98	1.48	1.38
11	1	1121	CLA	CHC-C1C	4.98	1.48	1.38
11	a	1106	CLA	CHC-C1C	4.97	1.48	1.38
11	2	1205	CLA	O2D-CGD	4.97	1.45	1.33
11	A	1102	CLA	CHC-C1C	4.97	1.48	1.38
11	A	1127	CLA	CHC-C1C	4.97	1.48	1.38
11	A	1105	CLA	CHC-C1C	4.97	1.48	1.38
11	A	1103	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1220	CLA	CHC-C1C	4.97	1.48	1.38
11	1	1801	CLA	CHC-C1C	4.97	1.48	1.38
11	1	1102	CLA	O2D-CGD	4.97	1.45	1.33
11	B	1023	CLA	O2D-CGD	4.97	1.45	1.33
11	B	1219	CLA	CHC-C1C	4.97	1.48	1.38
11	2	1209	CLA	CHC-C1C	4.97	1.48	1.38
11	B	1239	CLA	CHC-C1C	4.97	1.48	1.38
11	A	1101	CLA	CHC-C1C	4.97	1.48	1.38
12	1	2001	PQN	C10-C5	4.96	1.48	1.40
11	b	1226	CLA	O2D-CGD	4.96	1.45	1.33
11	2	1226	CLA	CHC-C1C	4.96	1.48	1.38
11	A	1111	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1220	CLA	O2D-CGD	4.96	1.45	1.33
11	B	1229	CLA	O2D-CGD	4.96	1.45	1.33
11	L	1502	CLA	CHC-C1C	4.96	1.48	1.38
11	a	1137	CLA	CHC-C1C	4.96	1.48	1.38
11	b	1229	CLA	CHC-C1C	4.96	1.48	1.38
11	2	1230	CLA	CHC-C1C	4.96	1.48	1.38
11	1	1118	CLA	CHC-C1C	4.96	1.48	1.38
11	a	1111	CLA	O2D-CGD	4.96	1.45	1.33
11	b	1203	CLA	O2D-CGD	4.96	1.45	1.33
11	1	1127	CLA	CHC-C1C	4.96	1.48	1.38
11	1	1135	CLA	CHC-C1C	4.96	1.48	1.38
11	l	1503	CLA	CHC-C1C	4.95	1.48	1.38
11	2	1228	CLA	CHC-C1C	4.95	1.48	1.38
11	a	1107	CLA	O2D-CGD	4.95	1.45	1.33
12	B	2002	PQN	C10-C5	4.95	1.48	1.40
11	b	1204	CLA	CHC-C1C	4.95	1.48	1.38
11	b	1209	CLA	CHC-C1C	4.95	1.48	1.38
11	A	1129	CLA	CHC-C1C	4.95	1.48	1.38
11	A	1131	CLA	CHC-C1C	4.95	1.48	1.38
11	B	1228	CLA	CHC-C1C	4.95	1.48	1.38
11	a	1108	CLA	CHC-C1C	4.95	1.48	1.38
11	a	1101	CLA	CHC-C1C	4.95	1.48	1.38
11	A	1104	CLA	CHC-C1C	4.95	1.48	1.38
11	1	1139	CLA	CHC-C1C	4.95	1.48	1.38
11	b	1232	CLA	CHC-C1C	4.94	1.48	1.38
11	B	1211	CLA	CHC-C1C	4.94	1.48	1.38
11	b	1238	CLA	CHC-C1C	4.94	1.48	1.38
11	1	1124	CLA	CHC-C1C	4.94	1.48	1.38
11	1	1012	CLA	CHC-C1C	4.94	1.48	1.38
11	b	1223	CLA	O2D-CGD	4.94	1.45	1.33
11	2	1231	CLA	CHC-C1C	4.94	1.48	1.38
11	B	1226	CLA	CHC-C1C	4.94	1.48	1.38
11	a	1107	CLA	CHC-C1C	4.94	1.48	1.38
11	1	1110	CLA	CHC-C1C	4.94	1.48	1.38
11	b	1217	CLA	CHC-C1C	4.94	1.48	1.38
11	a	1123	CLA	CHC-C1C	4.94	1.48	1.38
11	a	1103	CLA	CHC-C1C	4.94	1.48	1.38
11	a	1140	CLA	CHC-C1C	4.94	1.48	1.38
11	A	1135	CLA	CHC-C1C	4.93	1.48	1.38
11	A	1119	CLA	CHC-C1C	4.93	1.48	1.38
11	b	1227	CLA	CHC-C1C	4.93	1.48	1.38
11	1	1138	CLA	CHC-C1C	4.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1132	CLA	CHC-C1C	4.93	1.48	1.38
11	2	1023	CLA	CHC-C1C	4.93	1.48	1.38
11	A	1105	CLA	O2D-CGD	4.93	1.45	1.33
11	1	1105	CLA	CHC-C1C	4.93	1.48	1.38
11	B	1238	CLA	CHC-C1C	4.92	1.48	1.38
11	a	1121	CLA	CHC-C1C	4.92	1.48	1.38
11	B	1023	CLA	CHC-C1C	4.92	1.48	1.38
11	B	1207	CLA	CHC-C1C	4.92	1.48	1.38
11	B	1209	CLA	CHC-C1C	4.92	1.48	1.38
11	1	1140	CLA	CHC-C1C	4.92	1.48	1.38
11	2	1224	CLA	CHC-C1C	4.92	1.48	1.38
11	b	1023	CLA	CHC-C1C	4.92	1.48	1.38
11	b	1230	CLA	CHC-C1C	4.92	1.48	1.38
11	1	1132	CLA	O2D-CGD	4.92	1.45	1.33
11	1	1107	CLA	CHC-C1C	4.92	1.48	1.38
11	1	1131	CLA	CHC-C1C	4.92	1.48	1.38
11	2	1021	CLA	CHC-C1C	4.92	1.48	1.38
11	2	1217	CLA	CHC-C1C	4.92	1.48	1.38
11	a	1102	CLA	CHC-C1C	4.91	1.48	1.38
11	1	1101	CLA	CHC-C1C	4.91	1.48	1.38
11	B	1231	CLA	CHD-C1D	4.91	1.48	1.38
11	2	1205	CLA	CHC-C1C	4.91	1.48	1.38
11	2	1240	CLA	CHC-C1C	4.91	1.48	1.38
11	1	1123	CLA	CHC-C1C	4.91	1.48	1.38
11	1	1103	CLA	CHC-C1C	4.91	1.48	1.38
11	2	1208	CLA	CHC-C1C	4.91	1.48	1.38
11	B	1218	CLA	CHC-C1C	4.91	1.48	1.38
11	a	1125	CLA	CHC-C1C	4.91	1.48	1.38
11	b	1021	CLA	CHC-C1C	4.90	1.48	1.38
11	a	1237	CLA	CHC-C1C	4.90	1.48	1.38
11	8	1502	CLA	O2D-CGD	4.90	1.45	1.33
11	A	1132	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1138	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1128	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1120	CLA	CHC-C1C	4.89	1.48	1.38
11	A	1110	CLA	CHC-C1C	4.89	1.48	1.38
11	b	1228	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1022	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1114	CLA	CHC-C1C	4.89	1.48	1.38
11	a	1131	CLA	CHC-C1C	4.89	1.48	1.38
11	b	1219	CLA	CHC-C1C	4.89	1.48	1.38
11	A	1237	CLA	CHC-C1C	4.88	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1222	CLA	CHC-C1C	4.88	1.48	1.38
11	1	1237	CLA	CHC-C1C	4.88	1.48	1.38
11	B	1203	CLA	CHC-C1C	4.88	1.48	1.38
11	2	1214	CLA	CHC-C1C	4.88	1.48	1.38
11	1	1104	CLA	CHC-C1C	4.88	1.48	1.38
11	2	1220	CLA	CHC-C1C	4.88	1.48	1.38
11	A	1011	CLA	CHC-C1C	4.87	1.48	1.38
11	1	1114	CLA	CHC-C1C	4.87	1.48	1.38
11	1	1117	CLA	CHC-C1C	4.87	1.48	1.38
11	K	1402	CLA	CHC-C1C	4.87	1.48	1.38
11	a	1136	CLA	CHC-C1C	4.87	1.48	1.38
11	a	1110	CLA	CHC-C1C	4.87	1.48	1.38
11	A	1106	CLA	CHC-C1C	4.87	1.48	1.38
11	A	1801	CLA	CHC-C1C	4.87	1.48	1.38
11	A	1110	CLA	O2D-CGD	4.87	1.45	1.33
11	B	1231	CLA	O2D-CGD	4.87	1.45	1.33
11	a	1139	CLA	CHD-C1D	4.86	1.47	1.38
11	B	1220	CLA	CHC-C1C	4.86	1.48	1.38
11	B	1215	CLA	CHC-C1C	4.85	1.48	1.38
11	A	1122	CLA	O2D-CGD	4.85	1.45	1.33
11	2	1239	CLA	CHC-C1C	4.85	1.48	1.38
11	2	1238	CLA	CHC-C1C	4.85	1.48	1.38
11	b	1208	CLA	CHC-C1C	4.84	1.48	1.38
11	2	1231	CLA	CHD-C1D	4.83	1.47	1.38
11	a	1138	CLA	CHD-C1D	4.83	1.47	1.38
11	8	1501	CLA	CHC-C1C	4.83	1.48	1.38
11	2	1203	CLA	CHC-C1C	4.83	1.48	1.38
11	A	1136	CLA	CHC-C1C	4.82	1.48	1.38
11	B	1204	CLA	CHC-C1C	4.82	1.48	1.38
11	b	1212	CLA	CHC-C1C	4.82	1.48	1.38
11	2	1201	CLA	CHC-C1C	4.82	1.48	1.38
11	B	1201	CLA	CHC-C1C	4.82	1.48	1.38
11	b	1240	CLA	C3C-C2C	4.82	1.47	1.36
11	1	1128	CLA	CHC-C1C	4.81	1.48	1.38
11	b	1205	CLA	CHC-C1C	4.81	1.48	1.38
11	b	1223	CLA	CHC-C1C	4.81	1.48	1.38
11	2	1215	CLA	CHC-C1C	4.81	1.48	1.38
11	a	1105	CLA	CHC-C1C	4.81	1.48	1.38
11	B	1229	CLA	CHC-C1C	4.80	1.48	1.38
11	a	1801	CLA	C3C-C2C	4.80	1.47	1.36
11	B	1232	CLA	CHD-C1D	4.80	1.47	1.38
11	b	1231	CLA	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1118	CLA	CHC-C1C	4.79	1.48	1.38
11	A	1118	CLA	CHC-C1C	4.79	1.48	1.38
11	A	1114	CLA	CHC-C1C	4.78	1.48	1.38
11	B	1217	CLA	O2A-C1	4.78	1.61	1.46
11	b	1239	CLA	CHC-C1C	4.78	1.48	1.38
11	2	1225	CLA	CHD-C1D	4.77	1.47	1.38
11	a	1127	CLA	CHC-C1C	4.77	1.48	1.38
11	A	1102	CLA	CHD-C1D	4.77	1.47	1.38
11	1	1109	CLA	CHC-C1C	4.77	1.48	1.38
11	A	1119	CLA	C3C-C2C	4.77	1.47	1.36
11	B	1231	CLA	CHC-C1C	4.77	1.48	1.38
11	a	1139	CLA	CHC-C1C	4.77	1.48	1.38
11	A	1106	CLA	CHD-C1D	4.77	1.47	1.38
11	2	1227	CLA	CHC-C1C	4.76	1.48	1.38
11	A	1109	CLA	CHD-C1D	4.76	1.47	1.38
11	b	1208	CLA	CHD-C1D	4.76	1.47	1.38
11	B	1021	CLA	CHC-C1C	4.76	1.48	1.38
11	a	1135	CLA	CHC-C1C	4.76	1.48	1.38
11	1	1114	CLA	CHD-C1D	4.76	1.47	1.38
11	B	1216	CLA	CHD-C1D	4.76	1.47	1.38
11	L	1503	CLA	CHC-C1C	4.75	1.48	1.38
11	a	1011	CLA	CHC-C1C	4.75	1.48	1.38
11	2	1212	CLA	CHC-C1C	4.75	1.48	1.38
11	a	1133	CLA	CHC-C1C	4.75	1.48	1.38
11	B	1205	CLA	CHC-C1C	4.74	1.48	1.38
11	A	1120	CLA	CHD-C1D	4.74	1.47	1.38
11	A	1117	CLA	CHD-C1D	4.74	1.47	1.38
11	b	1206	CLA	CHD-C1D	4.74	1.47	1.38
11	2	1207	CLA	CHC-C1C	4.74	1.48	1.38
11	a	1127	CLA	CHD-C1D	4.73	1.47	1.38
11	1	1133	CLA	CHD-C1D	4.73	1.47	1.38
11	B	1232	CLA	CHC-C1C	4.73	1.48	1.38
11	b	1215	CLA	CHD-C1D	4.73	1.47	1.38
11	2	1231	CLA	O2D-CGD	4.73	1.44	1.33
11	a	1119	CLA	CHD-C1D	4.73	1.47	1.38
11	2	1013	CLA	CHD-C1D	4.73	1.47	1.38
11	2	1209	CLA	CHD-C1D	4.73	1.47	1.38
11	b	1231	CLA	CHD-C1D	4.73	1.47	1.38
11	1	1139	CLA	CHD-C1D	4.73	1.47	1.38
11	2	1234	CLA	CHC-C1C	4.72	1.47	1.38
11	A	1138	CLA	CHD-C1D	4.72	1.47	1.38
11	b	1225	CLA	CHD-C1D	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1217	CLA	CHD-C1D	4.72	1.47	1.38
11	B	1228	CLA	CHD-C1D	4.72	1.47	1.38
11	A	1140	CLA	CHC-C1C	4.72	1.47	1.38
11	b	1239	CLA	CHD-C1D	4.72	1.47	1.38
11	A	1134	CLA	CHD-C1D	4.72	1.47	1.38
11	1	1110	CLA	CHD-C1D	4.72	1.47	1.38
11	1	1123	CLA	CHD-C1D	4.72	1.47	1.38
11	a	1121	CLA	CHD-C1D	4.72	1.47	1.38
11	B	1220	CLA	CHD-C1D	4.72	1.47	1.38
11	a	1109	CLA	CHD-C1D	4.72	1.47	1.38
11	1	1115	CLA	CHC-C1C	4.71	1.47	1.38
11	b	1209	CLA	CHD-C1D	4.71	1.47	1.38
11	A	1801	CLA	CHD-C1D	4.71	1.47	1.38
11	2	1217	CLA	O2A-C1	4.71	1.61	1.46
11	2	1206	CLA	CHC-C1C	4.71	1.47	1.38
11	b	1013	CLA	CHD-C1D	4.71	1.47	1.38
11	2	1215	CLA	CHD-C1D	4.71	1.47	1.38
11	A	1114	CLA	CHD-C1D	4.71	1.47	1.38
11	B	1236	CLA	O2A-C1	4.71	1.61	1.46
11	2	1232	CLA	CHD-C1D	4.71	1.47	1.38
11	b	1232	CLA	CHD-C1D	4.71	1.47	1.38
11	A	1121	CLA	CHD-C1D	4.70	1.47	1.38
11	1	1133	CLA	CHC-C1C	4.70	1.47	1.38
11	K	1402	CLA	C3C-C2C	4.70	1.46	1.36
11	1	1103	CLA	CHD-C1D	4.70	1.47	1.38
11	a	1801	CLA	CHD-C1D	4.70	1.47	1.38
11	a	1103	CLA	CHD-C1D	4.70	1.47	1.38
11	a	1123	CLA	CHD-C1D	4.70	1.47	1.38
11	a	1131	CLA	CHD-C1D	4.70	1.47	1.38
11	A	1138	CLA	CHC-C1C	4.70	1.47	1.38
11	b	1234	CLA	CHC-C1C	4.69	1.47	1.38
11	b	1228	CLA	CHD-C1D	4.69	1.47	1.38
11	B	1209	CLA	CHD-C1D	4.69	1.47	1.38
11	a	1105	CLA	CHD-C1D	4.69	1.47	1.38
11	A	1115	CLA	C3C-C2C	4.69	1.46	1.36
11	a	1130	CLA	CHD-C1D	4.69	1.47	1.38
11	b	1206	CLA	CHC-C1C	4.68	1.47	1.38
11	B	1215	CLA	CHD-C1D	4.68	1.47	1.38
11	a	1133	CLA	CHD-C1D	4.68	1.47	1.38
11	2	1239	CLA	CHD-C1D	4.68	1.47	1.38
11	1	1130	CLA	CHD-C1D	4.68	1.47	1.38
11	b	1236	CLA	O2A-C1	4.68	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1135	CLA	CHD-C1D	4.68	1.47	1.38
11	A	1107	CLA	O2D-CGD	4.68	1.44	1.33
11	A	1134	CLA	CHC-C1C	4.68	1.47	1.38
11	A	1131	CLA	CHD-C1D	4.68	1.47	1.38
11	2	1223	CLA	C3C-C2C	4.68	1.46	1.36
11	A	1117	CLA	C3C-C2C	4.68	1.46	1.36
11	1	1121	CLA	CHD-C1D	4.68	1.47	1.38
11	1	1117	CLA	CHD-C1D	4.67	1.47	1.38
11	b	1229	CLA	C3C-C2C	4.67	1.46	1.36
11	1	1109	CLA	CHD-C1D	4.67	1.47	1.38
11	b	1216	CLA	CHD-C1D	4.67	1.47	1.38
11	0	1402	CLA	C3C-C2C	4.67	1.46	1.36
11	B	1228	CLA	C3C-C2C	4.67	1.46	1.36
11	1	1130	CLA	C3C-C2C	4.67	1.46	1.36
11	B	1230	CLA	CHC-C1C	4.67	1.47	1.38
11	a	1119	CLA	CHC-C1C	4.67	1.47	1.38
11	B	1202	CLA	CHD-C1D	4.67	1.47	1.38
11	2	1201	CLA	CHD-C1D	4.67	1.47	1.38
11	1	1128	CLA	CHD-C1D	4.67	1.47	1.38
11	A	1104	CLA	C3C-C2C	4.66	1.46	1.36
11	2	1021	CLA	CHD-C1D	4.66	1.47	1.38
11	1	1127	CLA	CHD-C1D	4.66	1.47	1.38
11	1	1131	CLA	CHD-C1D	4.66	1.47	1.38
11	1	1120	CLA	CHD-C1D	4.66	1.47	1.38
11	8	1503	CLA	CHD-C1D	4.66	1.47	1.38
11	B	1217	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1220	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1124	CLA	CHD-C1D	4.66	1.47	1.38
11	b	1217	CLA	C3C-C2C	4.65	1.46	1.36
11	A	1123	CLA	CHD-C1D	4.65	1.47	1.38
11	1	1105	CLA	CHD-C1D	4.65	1.47	1.38
11	a	1128	CLA	C3C-C2C	4.65	1.46	1.36
11	1	1011	CLA	CHC-C1C	4.65	1.47	1.38
11	B	1223	CLA	C3C-C2C	4.65	1.46	1.36
11	a	1011	CLA	CHD-C1D	4.65	1.47	1.38
11	b	1218	CLA	CHD-C1D	4.65	1.47	1.38
11	A	1012	CLA	C3C-C2C	4.65	1.46	1.36
11	a	1114	CLA	CHD-C1D	4.65	1.47	1.38
11	a	1120	CLA	C3C-C2C	4.65	1.46	1.36
11	a	1102	CLA	CHD-C1D	4.64	1.47	1.38
11	B	1211	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1103	CLA	C3C-C2C	4.64	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1116	CLA	CHD-C1D	4.64	1.47	1.38
11	A	1133	CLA	CHD-C1D	4.64	1.47	1.38
11	B	1013	CLA	CHD-C1D	4.64	1.47	1.38
11	K	1401	CLA	CHD-C1D	4.64	1.47	1.38
11	2	1202	CLA	CHD-C1D	4.64	1.47	1.38
11	B	1227	CLA	CHC-C1C	4.64	1.47	1.38
11	1	1120	CLA	C3C-C2C	4.63	1.46	1.36
11	2	1229	CLA	CHD-C1D	4.63	1.47	1.38
11	a	1132	CLA	CHD-C1D	4.63	1.47	1.38
11	a	1134	CLA	CHD-C1D	4.63	1.47	1.38
11	1	1135	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1102	CLA	CHD-C1D	4.63	1.47	1.38
11	1	1134	CLA	CHD-C1D	4.63	1.47	1.38
11	1	1124	CLA	CHD-C1D	4.63	1.47	1.38
11	b	1222	CLA	CHD-C1D	4.63	1.47	1.38
11	B	1225	CLA	CHD-C1D	4.63	1.47	1.38
11	0	1401	CLA	CHD-C1D	4.63	1.47	1.38
11	2	1239	CLA	C3C-C2C	4.63	1.46	1.36
11	2	1236	CLA	O2A-C1	4.63	1.60	1.46
11	a	1108	CLA	CHD-C1D	4.63	1.47	1.38
11	2	1228	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1128	CLA	C3C-C2C	4.62	1.46	1.36
11	b	1227	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1204	CLA	CHD-C1D	4.62	1.47	1.38
11	b	1021	CLA	CHD-C1D	4.62	1.47	1.38
11	a	1135	CLA	C3C-C2C	4.62	1.46	1.36
11	2	1206	CLA	CHD-C1D	4.62	1.47	1.38
11	b	1235	CLA	CHD-C1D	4.62	1.47	1.38
11	k	1401	CLA	CHD-C1D	4.62	1.47	1.38
11	B	1222	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1201	CLA	CHD-C1D	4.62	1.47	1.38
11	a	1110	CLA	CHD-C1D	4.62	1.47	1.38
11	2	1227	CLA	CHD-C1D	4.62	1.47	1.38
11	b	1216	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1201	CLA	C3C-C2C	4.62	1.46	1.36
11	b	1228	CLA	C3C-C2C	4.62	1.46	1.36
11	A	1132	CLA	CHD-C1D	4.62	1.47	1.38
11	1	1101	CLA	CHD-C1D	4.62	1.47	1.38
11	2	1228	CLA	CHD-C1D	4.62	1.47	1.38
11	A	1111	CLA	CHD-C1D	4.61	1.47	1.38
11	a	1128	CLA	CHD-C1D	4.61	1.47	1.38
11	B	1224	CLA	C3C-C2C	4.61	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1236	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1124	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1118	CLA	CHD-C1D	4.61	1.47	1.38
11	2	1204	CLA	CHD-C1D	4.61	1.47	1.38
11	A	1112	CLA	C3C-C2C	4.61	1.46	1.36
11	B	1234	CLA	CHD-C1D	4.61	1.47	1.38
11	0	1402	CLA	CHD-C1D	4.61	1.47	1.38
11	A	1121	CLA	C3C-C2C	4.61	1.46	1.36
11	b	1226	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1022	CLA	C3C-C2C	4.61	1.46	1.36
11	2	1219	CLA	C3C-C2C	4.61	1.46	1.36
11	b	1234	CLA	CHD-C1D	4.61	1.47	1.38
11	2	1240	CLA	CHD-C1D	4.61	1.47	1.38
11	8	1501	CLA	CHD-C1D	4.61	1.47	1.38
11	1	1108	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1140	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1135	CLA	CHD-C1D	4.61	1.47	1.38
11	b	1211	CLA	CHD-C1D	4.61	1.47	1.38
11	1	1116	CLA	CHD-C1D	4.61	1.47	1.38
11	b	1219	CLA	CHD-C1D	4.61	1.47	1.38
11	L	1501	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1012	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1132	CLA	CHD-C1D	4.61	1.47	1.38
11	b	1218	CLA	C3C-C2C	4.60	1.46	1.36
11	1	1106	CLA	CHD-C1D	4.60	1.47	1.38
11	k	1402	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1109	CLA	C3C-C2C	4.60	1.46	1.36
11	B	1234	CLA	CHC-C1C	4.60	1.47	1.38
11	a	1112	CLA	CHD-C1D	4.60	1.47	1.38
11	b	1238	CLA	CHD-C1D	4.60	1.47	1.38
11	2	1214	CLA	CHD-C1D	4.60	1.47	1.38
11	b	1021	CLA	C3C-C2C	4.60	1.46	1.36
11	a	1109	CLA	C3C-C2C	4.60	1.46	1.36
11	a	1106	CLA	CHD-C1D	4.60	1.47	1.38
11	a	1132	CLA	C3C-C2C	4.60	1.46	1.36
11	b	1203	CLA	C3C-C2C	4.60	1.46	1.36
11	b	1201	CLA	CHD-C1D	4.60	1.47	1.38
11	a	1110	CLA	C3C-C2C	4.60	1.46	1.36
11	1	1129	CLA	C3C-C2C	4.60	1.46	1.36
11	a	1113	CLA	CHD-C1D	4.60	1.47	1.38
11	b	1207	CLA	CHC-C1C	4.60	1.47	1.38
11	1	1139	CLA	C3C-C2C	4.60	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1114	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1110	CLA	CHD-C1D	4.60	1.47	1.38
11	a	1137	CLA	CHD-C1D	4.59	1.47	1.38
11	2	1216	CLA	CHD-C1D	4.59	1.47	1.38
11	b	1229	CLA	CHD-C1D	4.59	1.47	1.38
11	b	1230	CLA	CHD-C1D	4.59	1.47	1.38
11	b	1239	CLA	C3C-C2C	4.59	1.46	1.36
11	b	1234	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1133	CLA	CHC-C1C	4.59	1.47	1.38
11	B	1206	CLA	CHC-C1C	4.59	1.47	1.38
11	B	1229	CLA	CHD-C1D	4.59	1.47	1.38
11	b	1213	CLA	CHD-C1D	4.59	1.47	1.38
11	2	1208	CLA	CHD-C1D	4.59	1.47	1.38
11	a	1130	CLA	C3C-C2C	4.59	1.46	1.36
11	b	1235	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1208	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1102	CLA	C3C-C2C	4.59	1.46	1.36
11	l	1501	CLA	C3C-C2C	4.59	1.46	1.36
11	2	1226	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1218	CLA	CHD-C1D	4.59	1.47	1.38
11	b	1204	CLA	CHD-C1D	4.59	1.47	1.38
11	2	1218	CLA	CHD-C1D	4.59	1.47	1.38
11	A	1126	CLA	C3C-C2C	4.59	1.46	1.36
11	a	1101	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1011	CLA	CHD-C1D	4.59	1.47	1.38
11	a	1124	CLA	CHD-C1D	4.59	1.47	1.38
11	B	1219	CLA	CHD-C1D	4.58	1.47	1.38
11	A	1130	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1022	CLA	CHD-C1D	4.58	1.47	1.38
11	b	1224	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1238	CLA	CHD-C1D	4.58	1.47	1.38
11	b	1222	CLA	C3C-C2C	4.58	1.46	1.36
11	b	1201	CLA	C3C-C2C	4.58	1.46	1.36
11	8	1502	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1202	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1238	CLA	C3C-C2C	4.58	1.46	1.36
11	k	1402	CLA	CHD-C1D	4.58	1.47	1.38
11	A	1115	CLA	CHD-C1D	4.58	1.47	1.38
11	b	1220	CLA	CHD-C1D	4.58	1.47	1.38
11	B	1216	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1217	CLA	C3C-C2C	4.58	1.46	1.36
11	A	1237	CLA	CHD-C1D	4.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1136	CLA	CHD-C1D	4.58	1.47	1.38
11	1	1109	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1240	CLA	CHD-C1D	4.58	1.47	1.38
11	b	1217	CLA	CHD-C1D	4.58	1.47	1.38
11	2	1222	CLA	CHD-C1D	4.58	1.47	1.38
11	A	1139	CLA	CHD-C1D	4.58	1.47	1.38
11	B	1208	CLA	CHD-C1D	4.58	1.47	1.38
11	A	1132	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1229	CLA	C3C-C2C	4.58	1.46	1.36
11	A	1123	CLA	CHC-C1C	4.58	1.47	1.38
11	1	1138	CLA	CHD-C1D	4.58	1.47	1.38
11	1	1126	CLA	CHD-C1D	4.58	1.47	1.38
11	B	1212	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1106	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1235	CLA	CHD-C1D	4.58	1.47	1.38
11	B	1229	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1104	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1119	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1232	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1206	CLA	CHD-C1D	4.58	1.47	1.38
11	1	1113	CLA	C3C-C2C	4.57	1.46	1.36
11	B	1240	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1129	CLA	C3C-C2C	4.57	1.46	1.36
11	A	1101	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1133	CLA	C3C-C2C	4.57	1.46	1.36
11	B	1227	CLA	CHD-C1D	4.57	1.47	1.38
11	B	1203	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1213	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1137	CLA	C3C-C2C	4.57	1.46	1.36
11	A	1125	CLA	CHD-C1D	4.57	1.47	1.38
11	1	1136	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1240	CLA	CHD-C1D	4.57	1.47	1.38
11	B	1203	CLA	CHD-C1D	4.57	1.47	1.38
11	1	1124	CLA	C3C-C2C	4.57	1.46	1.36
11	B	1021	CLA	CHD-C1D	4.57	1.47	1.38
11	B	1213	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1115	CLA	C3C-C2C	4.57	1.46	1.36
11	A	1108	CLA	CHD-C1D	4.57	1.47	1.38
11	B	1239	CLA	CHD-C1D	4.57	1.47	1.38
11	1	1022	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1107	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1125	CLA	C3C-C2C	4.57	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1108	CLA	CHD-C1D	4.56	1.47	1.38
11	B	1235	CLA	C3C-C2C	4.56	1.46	1.36
11	2	1234	CLA	CHD-C1D	4.56	1.47	1.38
11	1	1112	CLA	CHD-C1D	4.56	1.47	1.38
11	A	1103	CLA	CHD-C1D	4.56	1.47	1.38
11	b	1238	CLA	C3C-C2C	4.56	1.46	1.36
11	A	1105	CLA	CHD-C1D	4.56	1.47	1.38
11	2	1023	CLA	CHD-C1D	4.56	1.47	1.38
11	B	1213	CLA	CHD-C1D	4.56	1.47	1.38
11	a	1022	CLA	C3C-C2C	4.56	1.46	1.36
11	b	1209	CLA	C3C-C2C	4.56	1.46	1.36
11	a	1022	CLA	CHD-C1D	4.56	1.47	1.38
11	a	1101	CLA	CHD-C1D	4.56	1.47	1.38
11	2	1201	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1237	CLA	CHD-C1D	4.55	1.47	1.38
11	a	1102	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1227	CLA	C3C-C2C	4.55	1.46	1.36
11	L	1502	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1204	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1128	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1240	CLA	C3C-C2C	4.55	1.46	1.36
11	b	1236	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1124	CLA	C3C-C2C	4.55	1.46	1.36
11	b	1013	CLA	C3C-C2C	4.55	1.46	1.36
11	2	1203	CLA	CHD-C1D	4.55	1.47	1.38
11	2	1213	CLA	CHD-C1D	4.55	1.47	1.38
11	2	1236	CLA	C3C-C2C	4.55	1.46	1.36
11	B	1212	CLA	CHD-C1D	4.55	1.47	1.38
11	B	1218	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1119	CLA	CHD-C1D	4.55	1.47	1.38
11	a	1116	CLA	C3C-C2C	4.55	1.46	1.36
14	F	4018	BCR	C10-C9	-4.55	1.25	1.35
11	a	1140	CLA	CHD-C1D	4.55	1.47	1.38
11	2	1208	CLA	C3C-C2C	4.55	1.46	1.36
11	B	1227	CLA	C3C-C2C	4.54	1.46	1.36
11	1	1125	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1139	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1117	CLA	CHD-C1D	4.54	1.47	1.38
11	b	1205	CLA	CHD-C1D	4.54	1.47	1.38
11	2	1224	CLA	C3C-C2C	4.54	1.46	1.36
11	1	1801	CLA	CHD-C1D	4.54	1.47	1.38
11	b	1203	CLA	CHD-C1D	4.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1231	CLA	C3C-C2C	4.54	1.46	1.36
11	8	1503	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1022	CLA	CHD-C1D	4.54	1.47	1.38
11	1	1116	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1012	CLA	C3C-C2C	4.54	1.46	1.36
11	b	1215	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1140	CLA	CHD-C1D	4.54	1.47	1.38
11	B	1230	CLA	CHD-C1D	4.54	1.47	1.38
11	a	1115	CLA	C3C-C2C	4.54	1.46	1.36
11	1	1113	CLA	CHD-C1D	4.54	1.47	1.38
11	B	1221	CLA	C3C-C2C	4.54	1.46	1.36
11	1	1121	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1126	CLA	CHD-C1D	4.54	1.47	1.38
11	B	1215	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1122	CLA	CHD-C1D	4.53	1.47	1.38
11	a	1134	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1115	CLA	CHD-C1D	4.53	1.47	1.38
11	B	1238	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1112	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1133	CLA	C3C-C2C	4.53	1.46	1.36
11	A	1131	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1112	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1140	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1137	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1105	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1117	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1113	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1132	CLA	C3C-C2C	4.53	1.46	1.36
11	b	1223	CLA	CHD-C1D	4.53	1.47	1.38
11	1	1134	CLA	C3C-C2C	4.53	1.46	1.36
11	a	1119	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1136	CLA	CHD-C1D	4.53	1.47	1.38
11	1	1119	CLA	CHD-C1D	4.53	1.47	1.38
11	b	1211	CLA	C3C-C2C	4.53	1.46	1.36
11	1	1140	CLA	CHD-C1D	4.52	1.47	1.38
11	2	1223	CLA	CHD-C1D	4.52	1.47	1.38
11	b	1231	CLA	C3C-C2C	4.52	1.46	1.36
11	k	1401	CLA	C3C-C2C	4.52	1.46	1.36
11	a	1118	CLA	C3C-C2C	4.52	1.46	1.36
11	B	1210	CLA	CHD-C1D	4.52	1.47	1.38
11	A	1110	CLA	C3C-C2C	4.52	1.46	1.36
11	A	1133	CLA	C3C-C2C	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1013	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1215	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1021	CLA	C3C-C2C	4.52	1.46	1.36
11	A	1125	CLA	CHC-C1C	4.52	1.47	1.38
11	b	1212	CLA	CHD-C1D	4.52	1.47	1.38
11	A	1114	CLA	C3C-C2C	4.52	1.46	1.36
11	1	1122	CLA	C3C-C2C	4.52	1.46	1.36
11	l	1503	CLA	CHD-C1D	4.52	1.47	1.38
11	2	1220	CLA	CHD-C1D	4.52	1.47	1.38
11	a	1136	CLA	C3C-C2C	4.52	1.46	1.36
11	A	1102	CLA	C3C-C2C	4.52	1.46	1.36
11	A	1120	CLA	C3C-C2C	4.52	1.46	1.36
11	1	1117	CLA	C3C-C2C	4.52	1.46	1.36
11	1	1127	CLA	C3C-C2C	4.52	1.46	1.36
11	b	1023	CLA	CHD-C1D	4.52	1.47	1.38
11	a	1131	CLA	C3C-C2C	4.51	1.46	1.36
11	b	1236	CLA	CHD-C1D	4.51	1.47	1.38
11	b	1225	CLA	C3C-C2C	4.51	1.46	1.36
11	a	1120	CLA	CHD-C1D	4.51	1.47	1.38
11	B	1211	CLA	C3D-C4D	-4.51	1.34	1.44
11	B	1209	CLA	C3C-C2C	4.51	1.46	1.36
11	B	1220	CLA	C3C-C2C	4.51	1.46	1.36
11	2	1212	CLA	CHD-C1D	4.51	1.47	1.38
11	8	1501	CLA	C3C-C2C	4.51	1.46	1.36
11	A	1106	CLA	C3C-C2C	4.51	1.46	1.36
11	A	1135	CLA	C3C-C2C	4.51	1.46	1.36
11	b	1232	CLA	C3C-C2C	4.51	1.46	1.36
11	A	1129	CLA	C3C-C2C	4.51	1.46	1.36
11	A	1119	CLA	C3D-C4D	-4.50	1.34	1.44
11	B	1021	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1217	CLA	O2A-C1	4.50	1.60	1.46
11	a	1122	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1206	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1125	CLA	C3C-C2C	4.50	1.46	1.36
11	1	1138	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1113	CLA	CHD-C1D	4.50	1.47	1.38
11	L	1501	CLA	CHD-C1D	4.50	1.47	1.38
11	A	1116	CLA	CHD-C1D	4.50	1.47	1.38
11	2	1212	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1127	CLA	CHD-C1D	4.50	1.47	1.38
11	a	1105	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1136	CLA	C3C-C2C	4.50	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1239	CLA	C3C-C2C	4.50	1.46	1.36
11	a	1121	CLA	C3C-C2C	4.50	1.46	1.36
11	a	1011	CLA	C3C-C2C	4.50	1.46	1.36
11	B	1211	CLA	CHD-C1D	4.50	1.47	1.38
11	b	1226	CLA	CHD-C1D	4.50	1.47	1.38
11	A	1113	CLA	C3C-C2C	4.50	1.46	1.36
11	2	1209	CLA	C3C-C2C	4.50	1.46	1.36
11	A	1130	CLA	CHD-C1D	4.50	1.47	1.38
11	a	1104	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1208	CLA	C3C-C2C	4.50	1.46	1.36
11	2	1222	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1227	CLA	CHD-C1D	4.50	1.47	1.38
11	K	1401	CLA	C3C-C2C	4.50	1.46	1.36
11	b	1230	CLA	C3C-C2C	4.49	1.46	1.36
11	B	1225	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1112	CLA	CHD-C1D	4.49	1.47	1.38
11	A	1137	CLA	C3C-C2C	4.49	1.46	1.36
11	B	1226	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1128	CLA	CHD-C1D	4.49	1.47	1.38
11	0	1401	CLA	C3C-C2C	4.49	1.46	1.36
11	l	1503	CLA	C3C-C2C	4.49	1.46	1.36
11	2	1210	CLA	CHD-C1D	4.49	1.47	1.38
11	2	1235	CLA	CHD-C1D	4.49	1.47	1.38
11	1	1131	CLA	C3C-C2C	4.49	1.46	1.36
11	a	1012	CLA	CHD-C1D	4.49	1.47	1.38
11	2	1218	CLA	C3C-C2C	4.48	1.46	1.36
11	1	1129	CLA	CHD-C1D	4.48	1.47	1.38
11	b	1223	CLA	C3C-C2C	4.48	1.46	1.36
11	a	1129	CLA	CHD-C1D	4.48	1.47	1.38
11	1	1110	CLA	C3C-C2C	4.48	1.46	1.36
11	1	1104	CLA	CHD-C1D	4.48	1.47	1.38
11	b	1204	CLA	C3C-C2C	4.48	1.46	1.36
11	b	1210	CLA	CHD-C1D	4.48	1.47	1.38
11	1	1107	CLA	CHD-C1D	4.48	1.47	1.38
11	a	1127	CLA	C3C-C2C	4.48	1.46	1.36
11	a	1118	CLA	CHD-C1D	4.48	1.47	1.38
11	2	1230	CLA	C3C-C2C	4.48	1.46	1.36
11	A	1127	CLA	C3C-C2C	4.48	1.46	1.36
11	B	1226	CLA	CHD-C1D	4.48	1.47	1.38
11	a	1114	CLA	C3C-C2C	4.47	1.46	1.36
11	A	1136	CLA	CHD-C1D	4.47	1.47	1.38
11	1	1011	CLA	CHD-C1D	4.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1135	CLA	CHD-C1D	4.47	1.47	1.38
11	2	1211	CLA	C3C-C2C	4.47	1.46	1.36
11	a	1104	CLA	CHD-C1D	4.47	1.47	1.38
11	2	1216	CLA	C3C-C2C	4.47	1.46	1.36
14	m	4021	BCR	C10-C9	-4.47	1.25	1.35
11	2	1225	CLA	C3C-C2C	4.47	1.46	1.36
11	K	1402	CLA	CHD-C1D	4.47	1.47	1.38
11	a	1108	CLA	C3C-C2C	4.47	1.46	1.36
11	b	1219	CLA	C3C-C2C	4.47	1.46	1.36
11	l	1502	CLA	C3C-C2C	4.46	1.46	1.36
11	B	1219	CLA	C3C-C2C	4.46	1.46	1.36
11	B	1013	CLA	C3C-C2C	4.46	1.46	1.36
11	2	1207	CLA	CHD-C1D	4.46	1.47	1.38
11	2	1211	CLA	CHD-C1D	4.46	1.47	1.38
11	B	1231	CLA	C3C-C2C	4.46	1.46	1.36
11	2	1214	CLA	C3C-C2C	4.46	1.46	1.36
11	1	1126	CLA	C3C-C2C	4.46	1.46	1.36
11	2	1230	CLA	CHD-C1D	4.46	1.47	1.38
11	1	1011	CLA	C3C-C2C	4.46	1.46	1.36
11	2	1221	CLA	C3C-C2C	4.46	1.46	1.36
11	1	1137	CLA	CHD-C1D	4.45	1.47	1.38
11	2	1236	CLA	CHD-C1D	4.45	1.47	1.38
11	A	1011	CLA	C3C-C2C	4.45	1.46	1.36
11	a	1237	CLA	CHD-C1D	4.45	1.47	1.38
11	A	1122	CLA	C3C-C2C	4.45	1.46	1.36
11	2	1219	CLA	CHD-C1D	4.45	1.47	1.38
11	b	1212	CLA	C3C-C2C	4.45	1.46	1.36
11	a	1138	CLA	C3C-C2C	4.45	1.46	1.36
11	1	1106	CLA	C3C-C2C	4.45	1.46	1.36
11	A	1105	CLA	C3C-C2C	4.45	1.46	1.36
11	1	1101	CLA	C3C-C2C	4.45	1.46	1.36
11	b	1202	CLA	C3C-C2C	4.44	1.46	1.36
11	a	1107	CLA	C3C-C2C	4.44	1.46	1.36
11	a	1139	CLA	C3C-C2C	4.44	1.46	1.36
11	A	1108	CLA	C3C-C2C	4.44	1.46	1.36
11	A	1237	CLA	C3C-C2C	4.44	1.46	1.36
11	B	1207	CLA	C3C-C2C	4.44	1.46	1.36
11	a	1126	CLA	CHD-C1D	4.44	1.47	1.38
11	l	1501	CLA	CHD-C1D	4.44	1.47	1.38
11	A	1107	CLA	C3C-C2C	4.44	1.46	1.36
11	B	1238	CLA	CHD-C1D	4.44	1.47	1.38
11	L	1502	CLA	CHD-C1D	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1214	CLA	CHD-C1D	4.44	1.47	1.38
11	b	1214	CLA	CHD-C1D	4.44	1.47	1.38
11	1	1122	CLA	CHD-C1D	4.43	1.47	1.38
11	b	1224	CLA	CHD-C1D	4.43	1.47	1.38
11	b	1207	CLA	CHD-C1D	4.43	1.47	1.38
11	a	1126	CLA	C3C-C2C	4.43	1.46	1.36
11	2	1220	CLA	C3C-C2C	4.43	1.46	1.36
11	A	1137	CLA	CHD-C1D	4.43	1.47	1.38
11	B	1207	CLA	CHD-C1D	4.43	1.47	1.38
11	a	1111	CLA	CHD-C1D	4.42	1.47	1.38
11	b	1023	CLA	C3C-C2C	4.42	1.46	1.36
11	B	1217	CLA	CHD-C1D	4.42	1.47	1.38
11	1	1118	CLA	CHD-C1D	4.42	1.47	1.38
11	2	1226	CLA	CHD-C1D	4.42	1.47	1.38
11	A	1134	CLA	C3C-C2C	4.42	1.46	1.36
11	A	1126	CLA	CHC-C4B	4.42	1.49	1.39
11	2	1203	CLA	C3C-C2C	4.42	1.46	1.36
11	b	1221	CLA	C3C-C2C	4.42	1.46	1.36
11	B	1223	CLA	CHD-C1D	4.42	1.47	1.38
11	2	1202	CLA	C3C-C2C	4.42	1.46	1.36
11	A	1125	CLA	C3D-C4D	-4.42	1.34	1.44
11	B	1204	CLA	C3C-C2C	4.42	1.46	1.36
11	b	1202	CLA	CHD-C1D	4.41	1.47	1.38
11	l	1502	CLA	CHD-C1D	4.41	1.47	1.38
11	2	1221	CLA	CHD-C1D	4.41	1.47	1.38
11	1	1118	CLA	C3C-C2C	4.41	1.46	1.36
11	B	1232	CLA	C3C-C2C	4.41	1.46	1.36
11	L	1503	CLA	CHD-C1D	4.40	1.47	1.38
11	L	1503	CLA	C3C-C2C	4.40	1.46	1.36
11	b	1205	CLA	C3C-C2C	4.40	1.46	1.36
11	a	1125	CLA	C3D-C4D	-4.40	1.34	1.44
11	2	1214	CLA	C3D-C4D	-4.40	1.34	1.44
15	A	5003	LHG	O8-C23	4.40	1.46	1.33
11	a	1103	CLA	C3D-C4D	-4.40	1.34	1.44
11	b	1221	CLA	CHD-C1D	4.39	1.47	1.38
11	A	1012	CLA	CHD-C1D	4.39	1.47	1.38
11	1	1125	CLA	CHD-C1D	4.39	1.47	1.38
11	1	1022	CLA	C3D-C4D	-4.39	1.34	1.44
11	a	1107	CLA	CHD-C1D	4.39	1.47	1.38
11	B	1234	CLA	C3C-C2C	4.38	1.46	1.36
14	2	4014	BCR	C10-C9	-4.38	1.25	1.35
11	2	1224	CLA	CHD-C1D	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1023	CLA	C3C-C2C	4.38	1.46	1.36
11	b	1214	CLA	C3C-C2C	4.38	1.46	1.36
11	B	1206	CLA	C3C-C2C	4.37	1.46	1.36
11	B	1023	CLA	CHD-C1D	4.37	1.47	1.38
15	a	5001	LHG	O8-C23	4.37	1.46	1.33
11	B	1216	CLA	C3D-C4D	-4.37	1.34	1.44
11	A	1121	CLA	C3D-C4D	-4.37	1.34	1.44
14	2	4010	BCR	C10-C9	-4.37	1.25	1.35
15	1	5003	LHG	O8-C23	4.37	1.46	1.33
11	2	1206	CLA	C3C-C2C	4.37	1.46	1.36
11	2	1234	CLA	C3C-C2C	4.37	1.46	1.36
11	2	1202	CLA	C3D-C4D	-4.37	1.34	1.44
11	A	1129	CLA	CHD-C1D	4.37	1.46	1.38
11	1	1237	CLA	C3C-C2C	4.36	1.46	1.36
11	2	1205	CLA	C3C-C2C	4.36	1.46	1.36
11	8	1502	CLA	CHD-C1D	4.36	1.46	1.38
11	A	1116	CLA	C3C-C2C	4.35	1.46	1.36
11	A	1103	CLA	C3C-C2C	4.35	1.46	1.36
11	A	1140	CLA	C3C-C2C	4.35	1.46	1.36
11	b	1207	CLA	C3C-C2C	4.35	1.46	1.36
11	B	1205	CLA	CHD-C1D	4.35	1.46	1.38
11	B	1236	CLA	C3D-C4D	-4.34	1.34	1.44
11	b	1210	CLA	C3C-C2C	4.34	1.46	1.36
11	A	1122	CLA	CHD-C1D	4.34	1.46	1.38
11	B	1205	CLA	C3C-C2C	4.34	1.46	1.36
11	A	1122	CLA	C3D-C4D	-4.34	1.34	1.44
14	M	4021	BCR	C10-C9	-4.34	1.25	1.35
11	B	1214	CLA	C3C-C2C	4.34	1.46	1.36
11	1	1115	CLA	C3D-C4D	-4.34	1.34	1.44
11	a	1119	CLA	C3D-C4D	-4.34	1.34	1.44
14	8	4022	BCR	C10-C9	-4.33	1.25	1.35
11	a	1130	CLA	C3D-C4D	-4.33	1.34	1.44
11	B	1223	CLA	C3D-C4D	-4.33	1.34	1.44
11	a	1022	CLA	C3D-C4D	-4.33	1.34	1.44
11	1	1103	CLA	C3C-C2C	4.33	1.46	1.36
11	a	1127	CLA	C3D-C4D	-4.33	1.34	1.44
11	a	1125	CLA	CHD-C1D	4.33	1.46	1.38
11	2	1225	CLA	C3D-C4D	-4.33	1.34	1.44
11	1	1237	CLA	C3D-C4D	-4.33	1.34	1.44
11	1	1106	CLA	C3D-C4D	-4.32	1.34	1.44
11	1	1111	CLA	CHD-C1D	4.32	1.46	1.38
11	2	1223	CLA	C3D-C4D	-4.32	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1222	CLA	CHD-C1D	4.32	1.46	1.38
11	1	1012	CLA	CHD-C1D	4.32	1.46	1.38
11	1	1123	CLA	C3C-C2C	4.32	1.46	1.36
11	A	1104	CLA	C3D-C4D	-4.32	1.34	1.44
15	B	5004	LHG	O8-C23	4.32	1.45	1.33
11	A	1112	CLA	CHC-C4B	4.32	1.49	1.39
11	a	1126	CLA	CHC-C4B	4.32	1.49	1.39
11	B	1210	CLA	C3C-C2C	4.32	1.46	1.36
11	A	1132	CLA	C3D-C4D	-4.32	1.34	1.44
11	2	1235	CLA	C3C-C2C	4.32	1.46	1.36
11	a	1138	CLA	C3D-C4D	-4.31	1.34	1.44
11	a	1115	CLA	CHD-C1D	4.31	1.46	1.38
11	1	1125	CLA	C3D-C4D	-4.31	1.34	1.44
11	A	1106	CLA	C3D-C4D	-4.31	1.34	1.44
11	2	1226	CLA	C3D-C4D	-4.31	1.34	1.44
11	A	1101	CLA	CHD-C1D	4.31	1.46	1.38
11	B	1221	CLA	CHD-C1D	4.30	1.46	1.38
11	B	1023	CLA	C3C-C2C	4.30	1.46	1.36
15	1	5001	LHG	O8-C23	4.30	1.45	1.33
11	b	1216	CLA	C3D-C4D	-4.30	1.34	1.44
14	6	4020	BCR	C10-C9	-4.30	1.25	1.35
11	b	1236	CLA	C3D-C4D	-4.30	1.34	1.44
11	A	1118	CLA	C3D-C4D	-4.30	1.34	1.44
11	2	1205	CLA	C3D-C4D	-4.30	1.34	1.44
11	a	1115	CLA	CHC-C4B	4.30	1.49	1.39
11	A	1022	CLA	C3D-C4D	-4.30	1.34	1.44
11	A	1127	CLA	C3D-C4D	-4.30	1.34	1.44
11	K	1402	CLA	C3D-C4D	-4.30	1.34	1.44
11	a	1123	CLA	C3C-C2C	4.30	1.46	1.36
15	a	5003	LHG	O8-C23	4.30	1.45	1.33
11	a	1139	CLA	C3D-C4D	-4.30	1.34	1.44
11	A	1137	CLA	C3D-C4D	-4.29	1.34	1.44
11	B	1217	CLA	C3D-C4D	-4.29	1.34	1.44
11	1	1126	CLA	CHC-C4B	4.29	1.49	1.39
11	A	1118	CLA	C3C-C2C	4.29	1.46	1.36
16	2	5002	LMG	O8-C28	4.29	1.45	1.33
11	1	1105	CLA	C3D-C4D	-4.29	1.34	1.44
11	b	1226	CLA	C3D-C4D	-4.29	1.34	1.44
11	A	1123	CLA	C3C-C2C	4.29	1.46	1.36
11	1	1131	CLA	C3D-C4D	-4.29	1.34	1.44
11	a	1124	CLA	C3D-C4D	-4.29	1.34	1.44
11	a	1237	CLA	C3C-C2C	4.29	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1115	CLA	CHC-C4B	4.29	1.49	1.39
11	a	1110	CLA	C3D-C4D	-4.28	1.34	1.44
11	a	1237	CLA	CHB-C1B	4.28	1.49	1.39
11	B	1208	CLA	C3D-C4D	-4.28	1.34	1.44
11	a	1118	CLA	C3D-C4D	-4.28	1.34	1.44
11	A	1136	CLA	C3D-C4D	-4.28	1.34	1.44
11	B	1207	CLA	C3D-C4D	-4.28	1.34	1.44
11	b	1223	CLA	C3D-C4D	-4.28	1.34	1.44
11	1	1133	CLA	C3D-C4D	-4.28	1.34	1.44
11	1	1136	CLA	C3D-C4D	-4.28	1.34	1.44
11	b	1220	CLA	C3D-C4D	-4.28	1.34	1.44
14	B	4004	BCR	C10-C9	-4.28	1.25	1.35
11	B	1203	CLA	C3D-C4D	-4.28	1.34	1.44
11	1	1101	CLA	C3D-C4D	-4.28	1.34	1.44
11	L	1502	CLA	C3D-C4D	-4.27	1.34	1.44
11	a	1115	CLA	C3D-C4D	-4.27	1.34	1.44
11	A	1115	CLA	C3D-C4D	-4.27	1.34	1.44
11	B	1202	CLA	CHC-C4B	4.27	1.49	1.39
11	A	1237	CLA	C3D-C4D	-4.27	1.34	1.44
11	a	1112	CLA	CHC-C4B	4.27	1.49	1.39
11	2	1205	CLA	CHD-C1D	4.27	1.46	1.38
11	1	1129	CLA	C3D-C4D	-4.27	1.34	1.44
15	2	5004	LHG	O8-C23	4.27	1.45	1.33
11	2	1201	CLA	C3D-C4D	-4.27	1.34	1.44
11	2	1236	CLA	C3D-C4D	-4.27	1.34	1.44
11	A	1104	CLA	CHD-C1D	4.27	1.46	1.38
11	1	1109	CLA	C3D-C4D	-4.27	1.34	1.44
11	1	1119	CLA	C3D-C4D	-4.27	1.34	1.44
11	1	1128	CLA	C3D-C4D	-4.27	1.34	1.44
11	A	1103	CLA	C3D-C4D	-4.26	1.34	1.44
11	A	1130	CLA	C3D-C4D	-4.26	1.34	1.44
11	A	1108	CLA	C3D-C4D	-4.26	1.34	1.44
15	b	5004	LHG	O8-C23	4.26	1.45	1.33
11	1	1118	CLA	C3D-C4D	-4.26	1.34	1.44
11	b	1206	CLA	C3D-C4D	-4.26	1.34	1.44
11	A	1117	CLA	CHC-C4B	4.26	1.49	1.39
11	1	1130	CLA	C3D-C4D	-4.26	1.34	1.44
11	2	1238	CLA	C3D-C4D	-4.26	1.34	1.44
11	2	1218	CLA	C3D-C4D	-4.26	1.34	1.44
11	B	1202	CLA	C3D-C4D	-4.26	1.34	1.44
11	A	1133	CLA	C3D-C4D	-4.26	1.34	1.44
11	b	1201	CLA	C3D-C4D	-4.26	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1217	CLA	C3D-C4D	-4.26	1.34	1.44
11	B	1201	CLA	C3D-C4D	-4.26	1.34	1.44
11	b	1204	CLA	C3D-C4D	-4.26	1.34	1.44
11	a	1135	CLA	C3D-C4D	-4.26	1.34	1.44
11	2	1220	CLA	C3D-C4D	-4.25	1.34	1.44
16	b	5002	LMG	O8-C28	4.25	1.45	1.33
11	2	1213	CLA	C3D-C4D	-4.25	1.34	1.44
11	B	1218	CLA	C3D-C4D	-4.25	1.34	1.44
11	2	1206	CLA	C3D-C4D	-4.25	1.34	1.44
11	2	1216	CLA	C3D-C4D	-4.25	1.34	1.44
11	B	1230	CLA	C3C-C2C	4.25	1.45	1.36
11	b	1210	CLA	CHC-C4B	4.25	1.49	1.39
11	2	1207	CLA	C3D-C4D	-4.25	1.34	1.44
11	a	1129	CLA	C3D-C4D	-4.25	1.34	1.44
11	k	1402	CLA	C3D-C4D	-4.25	1.34	1.44
11	A	1117	CLA	C3D-C4D	-4.25	1.34	1.44
11	B	1230	CLA	C3D-C4D	-4.25	1.34	1.44
11	B	1224	CLA	C3D-C4D	-4.25	1.34	1.44
11	b	1225	CLA	C3D-C4D	-4.25	1.34	1.44
11	2	1023	CLA	C3D-C4D	-4.25	1.34	1.44
11	b	1202	CLA	CHC-C4B	4.25	1.48	1.39
11	A	1105	CLA	C3D-C4D	-4.25	1.34	1.44
11	A	1139	CLA	C3D-C4D	-4.25	1.34	1.44
11	A	1135	CLA	C3D-C4D	-4.25	1.34	1.44
11	a	1123	CLA	C3D-C4D	-4.25	1.34	1.44
11	2	1203	CLA	C3D-C4D	-4.25	1.34	1.44
11	B	1219	CLA	C3D-C4D	-4.25	1.34	1.44
11	0	1402	CLA	C3D-C4D	-4.25	1.34	1.44
11	b	1214	CLA	CHC-C4B	4.24	1.48	1.39
11	B	1214	CLA	C3D-C4D	-4.24	1.34	1.44
11	B	1206	CLA	C3D-C4D	-4.24	1.34	1.44
11	A	1111	CLA	C3C-C2C	4.24	1.45	1.36
15	2	5004	LHG	O7-C7	4.24	1.46	1.34
11	A	1126	CLA	C3D-C4D	-4.24	1.34	1.44
11	A	1801	CLA	C3D-C4D	-4.24	1.34	1.44
11	B	1235	CLA	C3D-C4D	-4.24	1.34	1.44
11	B	1023	CLA	C3D-C4D	-4.24	1.34	1.44
11	1	1139	CLA	C3D-C4D	-4.24	1.34	1.44
14	b	4017	BCR	C10-C9	-4.24	1.26	1.35
11	A	1123	CLA	C3D-C4D	-4.24	1.34	1.44
11	A	1129	CLA	C3D-C4D	-4.24	1.34	1.44
11	1	1114	CLA	C3D-C4D	-4.24	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1223	CLA	CHC-C4B	4.24	1.48	1.39
11	2	1013	CLA	C3D-C4D	-4.24	1.34	1.44
11	A	1120	CLA	C3D-C4D	-4.24	1.34	1.44
11	2	1213	CLA	CHC-C4B	4.24	1.48	1.39
11	A	1116	CLA	CHC-C4B	4.24	1.48	1.39
11	B	1225	CLA	C3D-C4D	-4.24	1.34	1.44
14	b	4010	BCR	C10-C9	-4.23	1.26	1.35
11	B	1021	CLA	C3D-C4D	-4.23	1.34	1.44
11	B	1234	CLA	C3D-C4D	-4.23	1.34	1.44
11	b	1215	CLA	C3D-C4D	-4.23	1.34	1.44
11	A	1103	CLA	CHC-C4B	4.23	1.48	1.39
11	0	1402	CLA	CHC-C4B	4.23	1.48	1.39
11	A	1131	CLA	C3D-C4D	-4.23	1.34	1.44
11	1	1117	CLA	C3D-C4D	-4.23	1.34	1.44
11	2	1204	CLA	C3D-C4D	-4.23	1.34	1.44
11	A	1107	CLA	CHD-C1D	4.23	1.46	1.38
11	b	1240	CLA	C3D-C4D	-4.23	1.34	1.44
14	F	4013	BCR	C10-C9	-4.23	1.26	1.35
11	1	1122	CLA	C3D-C4D	-4.23	1.34	1.44
14	A	4001	BCR	C10-C9	-4.23	1.26	1.35
11	B	1222	CLA	C3D-C4D	-4.23	1.34	1.44
11	a	1132	CLA	C3D-C4D	-4.23	1.34	1.44
11	A	1114	CLA	C3D-C4D	-4.23	1.34	1.44
11	B	1204	CLA	C3D-C4D	-4.23	1.34	1.44
11	2	1210	CLA	C3D-C4D	-4.23	1.34	1.44
14	2	4011	BCR	C10-C9	-4.23	1.26	1.35
11	B	1212	CLA	C3D-C4D	-4.23	1.34	1.44
11	a	1122	CLA	C3D-C4D	-4.23	1.34	1.44
11	B	1236	CLA	CHD-C1D	4.23	1.46	1.38
11	B	1226	CLA	C3D-C4D	-4.23	1.34	1.44
11	b	1213	CLA	C3D-C4D	-4.23	1.34	1.44
11	2	1222	CLA	C3D-C4D	-4.23	1.34	1.44
14	f	4018	BCR	C10-C9	-4.23	1.26	1.35
11	A	1137	CLA	CHC-C4B	4.23	1.48	1.39
11	a	1136	CLA	C3D-C4D	-4.23	1.34	1.44
11	b	1211	CLA	C3D-C4D	-4.23	1.34	1.44
11	a	1128	CLA	C3D-C4D	-4.22	1.34	1.44
11	b	1232	CLA	C3D-C4D	-4.22	1.34	1.44
11	2	1232	CLA	C3D-C4D	-4.22	1.34	1.44
11	a	1105	CLA	C3D-C4D	-4.22	1.34	1.44
11	1	1124	CLA	C3D-C4D	-4.22	1.34	1.44
11	B	1013	CLA	C3D-C4D	-4.22	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1217	CLA	C3D-C4D	-4.22	1.34	1.44
11	B	1220	CLA	C3D-C4D	-4.22	1.34	1.44
11	b	1227	CLA	C3D-C4D	-4.22	1.34	1.44
11	8	1503	CLA	C3D-C4D	-4.22	1.34	1.44
11	B	1232	CLA	C3D-C4D	-4.22	1.34	1.44
11	b	1238	CLA	C3D-C4D	-4.22	1.34	1.44
11	2	1234	CLA	C3D-C4D	-4.22	1.34	1.44
11	2	1207	CLA	C3C-C2C	4.22	1.45	1.36
11	a	1140	CLA	C3D-C4D	-4.22	1.34	1.44
11	2	1212	CLA	C3D-C4D	-4.22	1.34	1.44
11	b	1214	CLA	C3D-C4D	-4.22	1.34	1.44
11	b	1221	CLA	CHC-C4B	4.22	1.48	1.39
11	B	1227	CLA	C3D-C4D	-4.22	1.34	1.44
11	a	1104	CLA	C3D-C4D	-4.22	1.34	1.44
11	B	1229	CLA	C3D-C4D	-4.22	1.34	1.44
11	2	1236	CLA	CHC-C4B	4.22	1.48	1.39
11	A	1138	CLA	C3D-C4D	-4.21	1.34	1.44
11	a	1137	CLA	C3D-C4D	-4.21	1.34	1.44
11	2	1228	CLA	C3D-C4D	-4.21	1.34	1.44
11	A	1140	CLA	C3D-C4D	-4.21	1.34	1.44
11	1	1112	CLA	C3D-C4D	-4.21	1.34	1.44
11	A	1101	CLA	C3D-C4D	-4.21	1.34	1.44
11	b	1218	CLA	C3D-C4D	-4.21	1.34	1.44
11	a	1131	CLA	C3D-C4D	-4.21	1.34	1.44
11	b	1209	CLA	C3D-C4D	-4.21	1.34	1.44
11	2	1219	CLA	CHC-C4B	4.21	1.48	1.39
11	b	1228	CLA	C3D-C4D	-4.21	1.34	1.44
11	a	1133	CLA	C3D-C4D	-4.21	1.34	1.44
11	A	1134	CLA	C3D-C4D	-4.21	1.34	1.44
11	1	1127	CLA	C3D-C4D	-4.21	1.34	1.44
11	b	1023	CLA	C3D-C4D	-4.21	1.34	1.44
11	1	1123	CLA	C3D-C4D	-4.21	1.34	1.44
11	1	1126	CLA	C3D-C4D	-4.21	1.34	1.44
14	F	4020	BCR	C10-C9	-4.21	1.26	1.35
11	1	1107	CLA	C3D-C4D	-4.20	1.34	1.44
11	1	1104	CLA	C3D-C4D	-4.20	1.34	1.44
14	A	4007	BCR	C10-C9	-4.20	1.26	1.35
11	a	1116	CLA	CHC-C4B	4.20	1.48	1.39
11	b	1208	CLA	C3D-C4D	-4.20	1.34	1.44
11	1	1138	CLA	C3D-C4D	-4.20	1.34	1.44
11	2	1224	CLA	C3D-C4D	-4.20	1.34	1.44
11	8	1502	CLA	C3D-C4D	-4.20	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4005	BCR	C10-C9	-4.20	1.26	1.35
11	l	1503	CLA	C3D-C4D	-4.20	1.34	1.44
11	2	1235	CLA	CHC-C4B	4.20	1.48	1.39
11	A	1109	CLA	C3D-C4D	-4.20	1.34	1.44
11	a	1121	CLA	C3D-C4D	-4.20	1.34	1.44
11	b	1230	CLA	C3D-C4D	-4.20	1.34	1.44
11	A	1110	CLA	C3D-C4D	-4.20	1.34	1.44
11	1	1121	CLA	C3D-C4D	-4.20	1.34	1.44
14	6	4018	BCR	C10-C9	-4.20	1.26	1.35
11	a	1116	CLA	C3D-C4D	-4.20	1.34	1.44
11	b	1235	CLA	C3D-C4D	-4.20	1.34	1.44
11	2	1211	CLA	C3D-C4D	-4.20	1.34	1.44
11	2	1231	CLA	CHD-C4C	4.20	1.48	1.39
11	1	1111	CLA	CHC-C4B	4.20	1.48	1.39
11	a	1801	CLA	C3D-C4D	-4.20	1.34	1.44
14	1	4003	BCR	C10-C9	-4.19	1.26	1.35
11	a	1108	CLA	C3D-C4D	-4.19	1.34	1.44
14	A	4003	BCR	C10-C9	-4.19	1.26	1.35
11	A	1128	CLA	C3D-C4D	-4.19	1.34	1.44
11	B	1215	CLA	C3D-C4D	-4.19	1.34	1.44
11	b	1224	CLA	C3D-C4D	-4.19	1.34	1.44
11	b	1231	CLA	C3D-C4D	-4.19	1.34	1.44
11	2	1227	CLA	C3D-C4D	-4.19	1.34	1.44
14	f	4020	BCR	C10-C9	-4.19	1.26	1.35
11	A	1111	CLA	C3D-C4D	-4.19	1.34	1.44
11	2	1230	CLA	C3D-C4D	-4.19	1.34	1.44
11	b	1222	CLA	C3D-C4D	-4.19	1.34	1.44
11	A	1102	CLA	C3D-C4D	-4.19	1.34	1.44
11	2	1239	CLA	C3D-C4D	-4.19	1.34	1.44
11	B	1214	CLA	CHC-C4B	4.19	1.48	1.39
11	B	1222	CLA	CHC-C4B	4.19	1.48	1.39
11	A	1124	CLA	C3D-C4D	-4.19	1.34	1.44
11	1	1103	CLA	C3D-C4D	-4.19	1.34	1.44
11	2	1235	CLA	C3D-C4D	-4.19	1.34	1.44
11	2	1202	CLA	CHC-C4B	4.19	1.48	1.39
14	A	4002	BCR	C10-C9	-4.19	1.26	1.35
11	1	1116	CLA	C3D-C4D	-4.19	1.34	1.44
11	1	1140	CLA	C3D-C4D	-4.19	1.34	1.44
11	1	1135	CLA	C3D-C4D	-4.19	1.34	1.44
15	B	5004	LHG	O7-C7	4.18	1.46	1.34
11	2	1219	CLA	C3D-C4D	-4.18	1.34	1.44
14	B	4011	BCR	C10-C9	-4.18	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	5002	LMG	O8-C28	4.18	1.45	1.33
11	a	1126	CLA	C3D-C4D	-4.18	1.34	1.44
11	1	1132	CLA	C3D-C4D	-4.18	1.34	1.44
11	a	1104	CLA	CHC-C4B	4.18	1.48	1.39
11	B	1238	CLA	C3D-C4D	-4.18	1.34	1.44
11	a	1101	CLA	C3D-C4D	-4.18	1.34	1.44
11	A	1118	CLA	CHB-C1B	4.18	1.48	1.39
11	1	1110	CLA	C3D-C4D	-4.18	1.34	1.44
11	2	1231	CLA	C3D-C4D	-4.18	1.34	1.44
11	A	1101	CLA	CHC-C4B	4.18	1.48	1.39
11	B	1224	CLA	CHC-C4B	4.18	1.48	1.39
11	b	1223	CLA	CHB-C1B	4.18	1.48	1.39
11	L	1503	CLA	C3D-C4D	-4.18	1.34	1.44
11	a	1134	CLA	C3D-C4D	-4.18	1.34	1.44
11	2	1209	CLA	C3D-C4D	-4.18	1.34	1.44
11	B	1213	CLA	C3D-C4D	-4.18	1.34	1.44
11	1	1134	CLA	C3D-C4D	-4.18	1.34	1.44
11	b	1229	CLA	C3D-C4D	-4.18	1.34	1.44
11	b	1219	CLA	C3D-C4D	-4.18	1.34	1.44
11	b	1213	CLA	CHC-C4B	4.18	1.48	1.39
11	B	1240	CLA	CHC-C4B	4.18	1.48	1.39
11	B	1235	CLA	CHC-C4B	4.18	1.48	1.39
11	1	1122	CLA	CHC-C4B	4.18	1.48	1.39
11	A	1121	CLA	CHD-C4C	4.18	1.48	1.39
11	b	1202	CLA	C3D-C4D	-4.18	1.34	1.44
11	a	1112	CLA	C3D-C4D	-4.18	1.34	1.44
11	2	1225	CLA	CHD-C4C	4.17	1.48	1.39
11	A	1111	CLA	CHC-C4B	4.17	1.48	1.39
11	a	1237	CLA	C3D-C4D	-4.17	1.34	1.44
11	B	1208	CLA	CHC-C4B	4.17	1.48	1.39
11	B	1221	CLA	C3D-C4D	-4.17	1.34	1.44
11	b	1013	CLA	C3D-C4D	-4.17	1.34	1.44
11	a	1109	CLA	C3D-C4D	-4.17	1.34	1.44
15	A	5001	LHG	O8-C23	4.17	1.45	1.33
11	A	1112	CLA	C3D-C4D	-4.17	1.34	1.44
11	a	1111	CLA	CHC-C4B	4.17	1.48	1.39
14	8	4019	BCR	C10-C9	-4.17	1.26	1.35
11	B	1228	CLA	C3D-C4D	-4.17	1.34	1.44
11	b	1207	CLA	C3D-C4D	-4.17	1.34	1.44
11	a	1122	CLA	CHC-C4B	4.17	1.48	1.39
11	b	1212	CLA	C3D-C4D	-4.17	1.34	1.44
11	2	1202	CLA	CHB-C1B	4.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1021	CLA	C3D-C4D	-4.17	1.34	1.44
11	a	1111	CLA	C3C-C2C	4.17	1.45	1.36
11	b	1205	CLA	C3D-C4D	-4.16	1.34	1.44
11	1	1113	CLA	C3D-C4D	-4.16	1.34	1.44
15	a	5001	LHG	O7-C7	4.16	1.46	1.34
11	a	1106	CLA	C3D-C4D	-4.16	1.34	1.44
11	2	1215	CLA	C3D-C4D	-4.16	1.34	1.44
15	1	5001	LHG	O7-C7	4.16	1.46	1.34
11	b	1208	CLA	CHB-C1B	4.16	1.48	1.39
11	B	1236	CLA	CHC-C4B	4.16	1.48	1.39
11	1	1108	CLA	C3D-C4D	-4.16	1.34	1.44
11	B	1239	CLA	C3D-C4D	-4.16	1.34	1.44
11	2	1236	CLA	CHB-C1B	4.16	1.48	1.39
11	a	1139	CLA	CHD-C4C	4.16	1.48	1.39
11	B	1210	CLA	C3D-C4D	-4.16	1.34	1.44
11	b	1235	CLA	CHC-C4B	4.16	1.48	1.39
11	2	1240	CLA	C3D-C4D	-4.16	1.34	1.44
11	2	1208	CLA	C3D-C4D	-4.16	1.34	1.44
11	a	1011	CLA	C3D-C4D	-4.16	1.34	1.44
11	a	1114	CLA	C3D-C4D	-4.16	1.34	1.44
11	k	1401	CLA	C3D-C4D	-4.16	1.34	1.44
11	B	1240	CLA	C3D-C4D	-4.15	1.34	1.44
11	l	1502	CLA	C3D-C4D	-4.15	1.34	1.44
11	B	1205	CLA	C3D-C4D	-4.15	1.34	1.44
11	B	1231	CLA	C3D-C4D	-4.15	1.34	1.44
11	a	1102	CLA	C3D-C4D	-4.15	1.34	1.44
11	1	1125	CLA	CHC-C4B	4.15	1.48	1.39
11	2	1021	CLA	C3D-C4D	-4.15	1.34	1.44
11	A	1139	CLA	CHC-C4B	4.15	1.48	1.39
11	2	1205	CLA	CHB-C1B	4.15	1.48	1.39
11	b	1239	CLA	C3D-C4D	-4.15	1.34	1.44
11	A	1136	CLA	CHB-C1B	4.15	1.48	1.39
11	K	1401	CLA	C3D-C4D	-4.15	1.34	1.44
11	a	1120	CLA	C3D-C4D	-4.15	1.34	1.44
11	A	1011	CLA	C3D-C4D	-4.15	1.34	1.44
14	7	4021	BCR	C10-C9	-4.15	1.26	1.35
11	L	1501	CLA	C3D-C4D	-4.14	1.34	1.44
11	b	1234	CLA	C3D-C4D	-4.14	1.34	1.44
11	A	1113	CLA	C3D-C4D	-4.14	1.34	1.44
11	1	1111	CLA	C3D-C4D	-4.14	1.34	1.44
11	8	1501	CLA	C3D-C4D	-4.14	1.34	1.44
11	a	1113	CLA	C3D-C4D	-4.14	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1801	CLA	C3D-C4D	-4.14	1.34	1.44
11	0	1401	CLA	C3D-C4D	-4.14	1.34	1.44
11	B	1209	CLA	C3D-C4D	-4.14	1.34	1.44
11	b	1210	CLA	C3D-C4D	-4.14	1.34	1.44
11	8	1503	CLA	CHC-C4B	4.14	1.48	1.39
11	A	1110	CLA	CHB-C1B	4.14	1.48	1.39
11	2	1229	CLA	CHC-C4B	4.14	1.48	1.39
15	1	5003	LHG	O7-C7	4.14	1.46	1.34
11	2	1229	CLA	C3D-C4D	-4.14	1.34	1.44
11	b	1236	CLA	CHC-C4B	4.14	1.48	1.39
11	1	1136	CLA	CHB-C1B	4.14	1.48	1.39
11	l	1501	CLA	C3D-C4D	-4.14	1.34	1.44
11	a	1133	CLA	CHB-C1B	4.13	1.48	1.39
11	2	1210	CLA	CHC-C4B	4.13	1.48	1.39
11	a	1117	CLA	C3D-C4D	-4.13	1.34	1.44
11	b	1013	CLA	CHC-C4B	4.13	1.48	1.39
11	2	1226	CLA	CHB-C1B	4.13	1.48	1.39
11	B	1234	CLA	CHB-C1B	4.13	1.48	1.39
14	a	4002	BCR	C10-C9	-4.13	1.26	1.35
11	A	1132	CLA	CHB-C1B	4.13	1.48	1.39
11	B	1212	CLA	CHC-C4B	4.13	1.48	1.39
11	B	1216	CLA	CHD-C4C	4.13	1.48	1.39
11	A	1107	CLA	C3D-C4D	-4.13	1.34	1.44
11	a	1109	CLA	CHD-C4C	4.13	1.48	1.39
11	b	1212	CLA	CHB-C1B	4.13	1.48	1.39
14	b	4005	BCR	C10-C9	-4.13	1.26	1.35
11	A	1105	CLA	CHB-C1B	4.13	1.48	1.39
11	b	1234	CLA	CHB-C1B	4.12	1.48	1.39
14	B	4014	BCR	C10-C9	-4.12	1.26	1.35
11	b	1226	CLA	CHC-C4B	4.12	1.48	1.39
11	b	1203	CLA	C3D-C4D	-4.12	1.34	1.44
11	1	1102	CLA	C3D-C4D	-4.12	1.34	1.44
11	2	1221	CLA	C3D-C4D	-4.12	1.34	1.44
11	B	1232	CLA	CHD-C4C	4.12	1.48	1.39
11	A	1109	CLA	CHD-C4C	4.12	1.48	1.39
11	1	1111	CLA	C3C-C2C	4.12	1.45	1.36
15	A	5001	LHG	O7-C7	4.12	1.45	1.34
11	2	1210	CLA	C3C-C2C	4.12	1.45	1.36
11	b	1208	CLA	CHD-C4C	4.12	1.48	1.39
16	B	5002	LMG	O7-C10	4.12	1.45	1.34
11	A	1120	CLA	CHC-C4B	4.12	1.48	1.39
11	a	1138	CLA	CHD-C4C	4.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1132	CLA	CHC-C4B	4.12	1.48	1.39
11	2	1231	CLA	CHC-C4B	4.11	1.48	1.39
11	B	1227	CLA	CHB-C1B	4.11	1.48	1.39
11	8	1502	CLA	CHC-C4B	4.11	1.48	1.39
11	b	1221	CLA	C3D-C4D	-4.11	1.34	1.44
11	a	1111	CLA	C3D-C4D	-4.11	1.34	1.44
11	b	1218	CLA	CHC-C4B	4.11	1.48	1.39
11	A	1120	CLA	CHD-C4C	4.11	1.48	1.39
11	A	1138	CLA	C3C-C2C	4.11	1.45	1.36
11	1	1112	CLA	CHC-C4B	4.11	1.48	1.39
11	2	1208	CLA	CHB-C1B	4.11	1.48	1.39
11	1	1127	CLA	CHD-C4C	4.11	1.48	1.39
11	l	1502	CLA	CHC-C4B	4.11	1.48	1.39
11	b	1240	CLA	CHC-C4B	4.11	1.48	1.39
11	A	1117	CLA	CHD-C4C	4.11	1.48	1.39
11	1	1137	CLA	C3D-C4D	-4.11	1.34	1.44
11	B	1231	CLA	CHD-C4C	4.11	1.48	1.39
11	B	1223	CLA	CHC-C4B	4.11	1.48	1.39
11	b	1221	CLA	CHB-C1B	4.10	1.48	1.39
11	l	1501	CLA	CHC-C4B	4.10	1.48	1.39
11	b	1201	CLA	CHC-C4B	4.10	1.48	1.39
11	b	1216	CLA	CHC-C4B	4.10	1.48	1.39
11	A	1121	CLA	CHC-C4B	4.10	1.48	1.39
11	A	1801	CLA	CHD-C4C	4.10	1.48	1.39
11	a	1111	CLA	CHB-C1B	4.10	1.48	1.39
11	B	1227	CLA	CHD-C4C	4.10	1.48	1.39
11	A	1113	CLA	CHC-C4B	4.10	1.48	1.39
11	B	1224	CLA	CHD-C1D	4.10	1.46	1.38
11	a	1125	CLA	CHC-C4B	4.10	1.48	1.39
11	A	1116	CLA	C3D-C4D	-4.10	1.35	1.44
11	B	1228	CLA	CHD-C4C	4.10	1.48	1.39
11	A	1130	CLA	CHC-C4B	4.10	1.48	1.39
11	B	1213	CLA	CHB-C1B	4.10	1.48	1.39
11	b	1211	CLA	CHB-C1B	4.10	1.48	1.39
11	1	1129	CLA	CHC-C4B	4.10	1.48	1.39
11	2	1232	CLA	CHC-C4B	4.10	1.48	1.39
11	1	1108	CLA	CHC-C4B	4.09	1.48	1.39
11	A	1125	CLA	CHB-C1B	4.09	1.48	1.39
11	1	1130	CLA	CHC-C4B	4.09	1.48	1.39
11	a	1136	CLA	CHB-C1B	4.09	1.48	1.39
11	1	1129	CLA	CHB-C1B	4.09	1.48	1.39
11	a	1105	CLA	CHB-C1B	4.09	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1115	CLA	CHB-C1B	4.09	1.48	1.39
11	1	1107	CLA	CHB-C1B	4.09	1.48	1.39
11	b	1229	CLA	CHC-C4B	4.09	1.48	1.39
11	b	1231	CLA	CHD-C4C	4.09	1.48	1.39
11	a	1130	CLA	CHD-C4C	4.08	1.48	1.39
11	2	1216	CLA	CHC-C4B	4.08	1.48	1.39
11	a	1801	CLA	CHD-C4C	4.08	1.48	1.39
16	2	5002	LMG	O7-C10	4.08	1.45	1.34
11	L	1501	CLA	CHC-C4B	4.08	1.48	1.39
11	1	1134	CLA	CHC-C4B	4.08	1.48	1.39
11	2	1232	CLA	CHD-C4C	4.08	1.48	1.39
11	A	1022	CLA	CHC-C4B	4.08	1.48	1.39
11	B	1232	CLA	CHB-C1B	4.08	1.48	1.39
11	1	1127	CLA	OBD-CAD	4.08	1.29	1.22
11	1	1102	CLA	CHC-C4B	4.08	1.48	1.39
11	1	1116	CLA	CHC-C4B	4.08	1.48	1.39
11	1	1122	CLA	CHB-C1B	4.08	1.48	1.39
11	a	1118	CLA	CHB-C1B	4.08	1.48	1.39
11	a	1114	CLA	CHB-C1B	4.08	1.48	1.39
11	B	1013	CLA	CHC-C4B	4.08	1.48	1.39
11	1	1119	CLA	CHC-C4B	4.08	1.48	1.39
11	2	1204	CLA	CHC-C4B	4.08	1.48	1.39
11	b	1013	CLA	CHD-C4C	4.08	1.48	1.39
11	1	1114	CLA	CHD-C4C	4.08	1.48	1.39
11	1	1120	CLA	CHC-C4B	4.08	1.48	1.39
11	B	1220	CLA	CHD-C4C	4.07	1.48	1.39
11	1	1114	CLA	CHB-C1B	4.07	1.48	1.39
11	B	1213	CLA	CHC-C4B	4.07	1.48	1.39
11	b	1203	CLA	CHC-C4B	4.07	1.48	1.39
11	2	1213	CLA	CHB-C1B	4.07	1.48	1.39
11	1	1113	CLA	CHB-C1B	4.07	1.48	1.39
11	b	1224	CLA	CHC-C4B	4.07	1.48	1.39
11	A	1102	CLA	CHD-C4C	4.07	1.48	1.39
14	B	4006	BCR	C10-C9	-4.07	1.26	1.35
11	A	1140	CLA	CHB-C1B	4.07	1.48	1.39
11	b	1232	CLA	CHD-C4C	4.07	1.48	1.39
11	1	1139	CLA	CHD-C4C	4.07	1.48	1.39
11	B	1226	CLA	CHC-C4B	4.07	1.48	1.39
11	1	1101	CLA	CHD-C4C	4.07	1.48	1.39
11	B	1208	CLA	CHB-C1B	4.07	1.48	1.39
11	b	1231	CLA	CHC-C4B	4.07	1.48	1.39
11	2	1205	CLA	CHC-C4B	4.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1113	CLA	CHB-C1B	4.07	1.48	1.39
11	b	1239	CLA	CHD-C4C	4.07	1.48	1.39
11	1	1139	CLA	CHC-C4B	4.07	1.48	1.39
11	a	1121	CLA	CHC-C4B	4.07	1.48	1.39
11	b	1219	CLA	CHB-C1B	4.07	1.48	1.39
11	A	1114	CLA	CHB-C1B	4.07	1.48	1.39
11	a	1108	CLA	CHB-C1B	4.07	1.48	1.39
11	a	1012	CLA	CHC-C4B	4.07	1.48	1.39
11	1	1109	CLA	CHD-C4C	4.07	1.48	1.39
14	l	4022	BCR	C10-C9	-4.06	1.26	1.35
11	1	1120	CLA	C3D-C4D	-4.06	1.35	1.44
11	k	1402	CLA	CHC-C4B	4.06	1.48	1.39
15	b	5004	LHG	O7-C7	4.06	1.45	1.34
11	a	1106	CLA	CHC-C4B	4.06	1.48	1.39
11	1	1133	CLA	CHB-C1B	4.06	1.48	1.39
11	b	1206	CLA	CHD-C4C	4.06	1.48	1.39
11	a	1117	CLA	CHC-C4B	4.06	1.48	1.39
11	b	1238	CLA	CHC-C4B	4.06	1.48	1.39
14	b	4004	BCR	C10-C9	-4.06	1.26	1.35
11	a	1113	CLA	CHC-C4B	4.06	1.48	1.39
11	b	1213	CLA	CHB-C1B	4.06	1.48	1.39
11	B	1224	CLA	CHB-C1B	4.06	1.48	1.39
11	A	1107	CLA	CHC-C4B	4.06	1.48	1.39
11	1	1124	CLA	CHC-C4B	4.06	1.48	1.39
11	a	1130	CLA	CHC-C4B	4.06	1.48	1.39
11	b	1216	CLA	CHB-C1B	4.06	1.48	1.39
11	2	1013	CLA	CHC-C4B	4.06	1.48	1.39
11	A	1108	CLA	CHC-C4B	4.06	1.48	1.39
11	2	1224	CLA	CHB-C1B	4.06	1.48	1.39
11	B	1218	CLA	CHB-C1B	4.06	1.48	1.39
11	a	1801	CLA	CHC-C4B	4.06	1.48	1.39
11	A	1124	CLA	CHD-C4C	4.06	1.48	1.39
14	B	4017	BCR	C10-C9	-4.06	1.26	1.35
11	1	1107	CLA	CHC-C4B	4.05	1.48	1.39
11	2	1201	CLA	CHB-C1B	4.05	1.48	1.39
11	2	1013	CLA	CHD-C4C	4.05	1.48	1.39
11	a	1139	CLA	CHB-C1B	4.05	1.48	1.39
14	b	4006	BCR	C10-C9	-4.05	1.26	1.35
14	2	4017	BCR	C10-C9	-4.05	1.26	1.35
11	1	1130	CLA	CHD-C4C	4.05	1.48	1.39
11	A	1127	CLA	CHC-C4B	4.05	1.48	1.39
11	1	1121	CLA	CHD-C4C	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1230	CLA	CHB-C1B	4.05	1.48	1.39
11	a	1134	CLA	CHC-C4B	4.05	1.48	1.39
11	b	1215	CLA	CHD-C4C	4.05	1.48	1.39
11	1	1105	CLA	CHD-C4C	4.05	1.48	1.39
11	A	1129	CLA	CHC-C4B	4.05	1.48	1.39
11	b	1021	CLA	CHC-C4B	4.05	1.48	1.39
11	b	1232	CLA	CHC-C4B	4.05	1.48	1.39
11	2	1217	CLA	CHD-C4C	4.05	1.48	1.39
11	b	1220	CLA	CHC-C4B	4.05	1.48	1.39
11	a	1123	CLA	CHD-C4C	4.05	1.48	1.39
11	b	1217	CLA	CHC-C4B	4.05	1.48	1.39
11	2	1216	CLA	CHB-C1B	4.05	1.48	1.39
11	1	1135	CLA	CHC-C4B	4.05	1.48	1.39
11	2	1215	CLA	CHD-C4C	4.05	1.48	1.39
11	1	1110	CLA	CHD-C4C	4.05	1.48	1.39
11	l	1502	CLA	CHB-C1B	4.05	1.48	1.39
11	2	1238	CLA	CHC-C4B	4.05	1.48	1.39
11	a	1105	CLA	CHD-C4C	4.05	1.48	1.39
11	2	1230	CLA	CHC-C4B	4.05	1.48	1.39
11	b	1211	CLA	CHC-C4B	4.05	1.48	1.39
11	A	1109	CLA	CHC-C4B	4.05	1.48	1.39
11	A	1138	CLA	CHD-C4C	4.05	1.48	1.39
11	B	1023	CLA	CHC-C4B	4.04	1.48	1.39
11	A	1131	CLA	CHD-C4C	4.04	1.48	1.39
11	a	1110	CLA	CHD-C4C	4.04	1.48	1.39
11	B	1210	CLA	CHC-C4B	4.04	1.48	1.39
11	a	1124	CLA	CHC-C4B	4.04	1.48	1.39
11	1	1131	CLA	CHB-C1B	4.04	1.48	1.39
11	2	1226	CLA	CHC-C4B	4.04	1.48	1.39
11	L	1502	CLA	CHC-C4B	4.04	1.48	1.39
14	a	4007	BCR	C10-C9	-4.04	1.26	1.35
11	1	1012	CLA	CHB-C1B	4.04	1.48	1.39
11	0	1402	CLA	CHB-C1B	4.04	1.48	1.39
11	a	1107	CLA	C3D-C4D	-4.04	1.35	1.44
11	1	1137	CLA	CHC-C4B	4.04	1.48	1.39
11	a	1129	CLA	CHB-C1B	4.04	1.48	1.39
11	b	1236	CLA	CHB-C1B	4.04	1.48	1.39
11	a	1135	CLA	CHD-C4C	4.04	1.48	1.39
15	a	5003	LHG	O7-C7	4.04	1.45	1.34
11	B	1236	CLA	CHB-C1B	4.04	1.48	1.39
11	a	1137	CLA	CHB-C1B	4.04	1.48	1.39
11	2	1239	CLA	CHB-C1B	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1136	CLA	CHC-C4B	4.04	1.48	1.39
11	1	1105	CLA	CHC-C4B	4.04	1.48	1.39
11	b	1227	CLA	CHD-C4C	4.04	1.48	1.39
11	b	1224	CLA	CHB-C1B	4.04	1.48	1.39
11	b	1209	CLA	CHB-C1B	4.04	1.48	1.39
11	1	1132	CLA	CHD-C4C	4.04	1.48	1.39
11	b	1218	CLA	CHD-C4C	4.04	1.48	1.39
11	a	1110	CLA	CHC-C4B	4.04	1.48	1.39
11	1	1123	CLA	CHD-C4C	4.04	1.48	1.39
11	1	1108	CLA	CHB-C1B	4.03	1.48	1.39
11	1	1113	CLA	CHC-C4B	4.03	1.48	1.39
11	A	1103	CLA	CHB-C1B	4.03	1.48	1.39
11	A	1131	CLA	CHB-C1B	4.03	1.48	1.39
11	b	1209	CLA	CHD-C4C	4.03	1.48	1.39
11	b	1228	CLA	CHD-C4C	4.03	1.48	1.39
11	A	1012	CLA	C3D-C4D	-4.03	1.35	1.44
11	B	1216	CLA	CHC-C4B	4.03	1.48	1.39
11	2	1227	CLA	CHB-C1B	4.03	1.48	1.39
11	2	1211	CLA	CHB-C1B	4.03	1.48	1.39
11	A	1128	CLA	CHB-C1B	4.03	1.48	1.39
11	A	1102	CLA	CHC-C4B	4.03	1.48	1.39
11	A	1105	CLA	CHC-C4B	4.03	1.48	1.39
11	1	1138	CLA	CHB-C1B	4.03	1.48	1.39
11	B	1229	CLA	CHD-C4C	4.03	1.48	1.39
11	2	1202	CLA	CHD-C4C	4.03	1.48	1.39
14	a	4001	BCR	C10-C9	-4.03	1.26	1.35
11	A	1012	CLA	CHC-C4B	4.03	1.48	1.39
11	a	1129	CLA	CHC-C4B	4.03	1.48	1.39
11	1	1106	CLA	CHB-C1B	4.03	1.48	1.39
11	2	1023	CLA	CHC-C4B	4.03	1.48	1.39
11	a	1108	CLA	CHC-C4B	4.03	1.48	1.39
11	1	1012	CLA	C3D-C4D	-4.03	1.35	1.44
14	b	4011	BCR	C10-C9	-4.03	1.26	1.35
11	1	1237	CLA	CHB-C1B	4.03	1.48	1.39
11	A	1125	CLA	CHD-C4C	4.03	1.48	1.39
11	2	1209	CLA	CHD-C4C	4.03	1.48	1.39
11	1	1022	CLA	CHC-C4B	4.03	1.48	1.39
11	a	1134	CLA	CHD-C4C	4.03	1.48	1.39
11	B	1210	CLA	CHB-C1B	4.03	1.48	1.39
11	1	1127	CLA	CHB-C1B	4.03	1.48	1.39
11	B	1211	CLA	CHB-C1B	4.02	1.48	1.39
11	1	1117	CLA	CHD-C4C	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1229	CLA	CHD-C4C	4.02	1.48	1.39
11	A	1131	CLA	CHC-C4B	4.02	1.48	1.39
11	B	1205	CLA	CHB-C1B	4.02	1.48	1.39
11	a	1109	CLA	CHC-C4B	4.02	1.48	1.39
11	2	1212	CLA	CHB-C1B	4.02	1.48	1.39
11	A	1106	CLA	CHD-C4C	4.02	1.48	1.39
11	b	1220	CLA	CHB-C1B	4.02	1.48	1.39
11	2	1222	CLA	CHC-C4B	4.02	1.48	1.39
11	a	1103	CLA	CHD-C4C	4.02	1.48	1.39
11	2	1220	CLA	CHB-C1B	4.02	1.48	1.39
11	a	1101	CLA	CHD-C4C	4.02	1.48	1.39
11	b	1217	CLA	CHD-C4C	4.02	1.48	1.39
11	B	1211	CLA	CHC-C4B	4.02	1.48	1.39
11	B	1217	CLA	CHC-C4B	4.02	1.48	1.39
11	a	1137	CLA	CHC-C4B	4.02	1.48	1.39
11	A	1134	CLA	CHB-C1B	4.02	1.48	1.39
11	B	1239	CLA	CHB-C1B	4.02	1.48	1.39
14	B	4009	BCR	C10-C9	-4.02	1.26	1.35
11	1	1012	CLA	CHC-C4B	4.02	1.48	1.39
11	2	1240	CLA	CHB-C1B	4.02	1.48	1.39
11	a	1119	CLA	CHB-C1B	4.02	1.48	1.39
11	B	1219	CLA	CHC-C4B	4.02	1.48	1.39
11	A	1129	CLA	CHB-C1B	4.02	1.48	1.39
11	2	1201	CLA	CHD-C4C	4.02	1.48	1.39
11	B	1203	CLA	CHC-C4B	4.02	1.48	1.39
11	b	1227	CLA	CHB-C1B	4.02	1.48	1.39
11	1	1104	CLA	CHC-C4B	4.02	1.48	1.39
11	1	1110	CLA	CHC-C4B	4.02	1.48	1.39
11	1	1131	CLA	CHD-C4C	4.02	1.48	1.39
11	A	1122	CLA	CHB-C1B	4.02	1.48	1.39
11	b	1239	CLA	CHB-C1B	4.02	1.48	1.39
11	a	1114	CLA	CHD-C4C	4.02	1.48	1.39
11	b	1226	CLA	CHB-C1B	4.02	1.48	1.39
11	B	1229	CLA	CHB-C1B	4.02	1.48	1.39
11	b	1222	CLA	CHC-C4B	4.02	1.48	1.39
11	2	1228	CLA	CHC-C4B	4.02	1.48	1.39
11	A	1139	CLA	CHD-C4C	4.01	1.48	1.39
11	a	1112	CLA	CHD-C4C	4.01	1.48	1.39
11	1	1126	CLA	CHD-C4C	4.01	1.48	1.39
11	A	1104	CLA	CHC-C4B	4.01	1.48	1.39
11	2	1239	CLA	CHD-C4C	4.01	1.48	1.39
11	2	1227	CLA	CHD-C4C	4.01	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1503	CLA	CHD-C4C	4.01	1.48	1.39
11	A	1110	CLA	CHC-C4B	4.01	1.48	1.39
11	A	1115	CLA	CHD-C4C	4.01	1.48	1.39
11	1	1011	CLA	C3D-C4D	-4.01	1.35	1.44
11	A	1124	CLA	CHC-C4B	4.01	1.48	1.39
11	B	1218	CLA	CHD-C4C	4.01	1.48	1.39
11	a	1131	CLA	CHD-C4C	4.01	1.48	1.39
11	A	1121	CLA	CHB-C1B	4.01	1.48	1.39
11	b	1212	CLA	CHC-C4B	4.01	1.48	1.39
11	a	1012	CLA	C3D-C4D	-4.01	1.35	1.44
11	B	1239	CLA	CHC-C4B	4.01	1.48	1.39
11	a	1131	CLA	CHC-C4B	4.01	1.48	1.39
11	1	1115	CLA	CHC-C4B	4.01	1.48	1.39
11	1	1118	CLA	CHC-C4B	4.01	1.48	1.39
11	b	1206	CLA	CHB-C1B	4.01	1.48	1.39
11	2	1239	CLA	CHC-C4B	4.01	1.48	1.39
11	a	1119	CLA	CHD-C4C	4.01	1.48	1.39
11	a	1140	CLA	CHD-C4C	4.01	1.48	1.39
11	B	1206	CLA	CHB-C1B	4.01	1.48	1.39
11	2	1221	CLA	CHC-C4B	4.01	1.48	1.39
11	1	1106	CLA	CHD-C4C	4.00	1.48	1.39
11	A	1122	CLA	CHC-C4B	4.00	1.48	1.39
11	1	1127	CLA	CHC-C4B	4.00	1.48	1.39
11	b	1232	CLA	CHB-C1B	4.00	1.48	1.39
11	2	1240	CLA	CHC-C4B	4.00	1.48	1.39
11	b	1225	CLA	CHC-C4B	4.00	1.48	1.39
11	A	1125	CLA	MG-NC	4.00	2.15	2.06
11	a	1132	CLA	CHD-C4C	4.00	1.48	1.39
11	a	1121	CLA	CHD-C4C	4.00	1.48	1.39
11	a	1117	CLA	CHB-C1B	4.00	1.48	1.39
11	1	1140	CLA	CHC-C4B	4.00	1.48	1.39
11	2	1204	CLA	CHD-C4C	4.00	1.48	1.39
11	A	1237	CLA	CHB-C1B	4.00	1.48	1.39
11	1	1134	CLA	CHB-C1B	4.00	1.48	1.39
11	b	1240	CLA	CHD-C4C	4.00	1.48	1.39
11	b	1227	CLA	CHC-C4B	4.00	1.48	1.39
11	1	1105	CLA	CHB-C1B	4.00	1.48	1.39
11	1	1106	CLA	CHC-C4B	4.00	1.48	1.39
11	2	1206	CLA	CHB-C1B	4.00	1.48	1.39
11	a	1135	CLA	CHB-C1B	4.00	1.48	1.39
11	b	1218	CLA	CHB-C1B	4.00	1.48	1.39
11	A	1132	CLA	CHD-C4C	4.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1208	CLA	CHD-C4C	4.00	1.48	1.39
11	1	1120	CLA	CHD-C4C	4.00	1.48	1.39
11	1	1101	CLA	CHC-C4B	4.00	1.48	1.39
11	1	1131	CLA	CHC-C4B	4.00	1.48	1.39
11	B	1215	CLA	CHD-C4C	4.00	1.48	1.39
11	A	1126	CLA	CHD-C4C	4.00	1.48	1.39
11	B	1223	CLA	CHB-C1B	4.00	1.48	1.39
11	B	1238	CLA	CHB-C1B	4.00	1.48	1.39
11	1	1116	CLA	CHB-C1B	4.00	1.48	1.39
11	2	1213	CLA	CHD-C4C	4.00	1.48	1.39
14	2	4009	BCR	C10-C9	-4.00	1.26	1.35
11	1	1115	CLA	CHD-C4C	4.00	1.48	1.39
11	l	1503	CLA	CHC-C4B	4.00	1.48	1.39
11	1	1121	CLA	CHC-C4B	4.00	1.48	1.39
11	a	1128	CLA	CHD-C4C	4.00	1.48	1.39
11	b	1238	CLA	CHD-C4C	4.00	1.48	1.39
11	1	1118	CLA	CHB-C1B	4.00	1.48	1.39
11	1	1128	CLA	CHD-C4C	4.00	1.48	1.39
11	b	1209	CLA	CHC-C4B	4.00	1.48	1.39
11	A	1118	CLA	CHD-C4C	3.99	1.48	1.39
11	2	1208	CLA	CHD-C4C	3.99	1.48	1.39
11	A	1134	CLA	CHD-C4C	3.99	1.48	1.39
11	2	1214	CLA	CHD-C4C	3.99	1.48	1.39
11	1	1133	CLA	CHD-C4C	3.99	1.48	1.39
15	A	5003	LHG	O7-C7	3.99	1.45	1.34
11	2	1222	CLA	CHD-C4C	3.99	1.48	1.39
11	2	1229	CLA	CHD-C4C	3.99	1.48	1.39
11	a	1131	CLA	CHB-C1B	3.99	1.48	1.39
11	1	1801	CLA	CHD-C4C	3.99	1.48	1.39
11	A	1135	CLA	CHC-C4B	3.99	1.48	1.39
11	a	1102	CLA	CHC-C4B	3.99	1.48	1.39
11	a	1140	CLA	CHB-C1B	3.99	1.48	1.39
11	1	1121	CLA	CHB-C1B	3.99	1.48	1.39
11	B	1239	CLA	CHD-C4C	3.99	1.48	1.39
11	A	1108	CLA	CHB-C1B	3.99	1.48	1.39
11	A	1119	CLA	CHD-C4C	3.99	1.48	1.39
11	2	1234	CLA	CHB-C1B	3.99	1.48	1.39
14	L	4019	BCR	C10-C9	-3.99	1.26	1.35
11	B	1217	CLA	CHB-C1B	3.99	1.48	1.39
11	2	1211	CLA	CHC-C4B	3.99	1.48	1.39
11	1	1112	CLA	CHB-C1B	3.99	1.48	1.39
11	1	1116	CLA	CHD-C4C	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1130	CLA	CHB-C1B	3.99	1.48	1.39
11	a	1103	CLA	CHC-C4B	3.99	1.48	1.39
11	a	1140	CLA	CHC-C4B	3.99	1.48	1.39
11	b	1230	CLA	CHB-C1B	3.99	1.48	1.39
11	a	1237	CLA	CHC-C4B	3.99	1.48	1.39
11	1	1801	CLA	CHC-C4B	3.99	1.48	1.39
11	A	1123	CLA	CHD-C4C	3.99	1.48	1.39
14	1	4001	BCR	C10-C9	-3.99	1.26	1.35
11	1	1128	CLA	CHB-C1B	3.99	1.48	1.39
11	B	1228	CLA	CHC-C4B	3.98	1.48	1.39
11	2	1240	CLA	CHD-C4C	3.98	1.48	1.39
14	2	4006	BCR	C10-C9	-3.98	1.26	1.35
11	2	1218	CLA	CHC-C4B	3.98	1.48	1.39
11	a	1102	CLA	CHD-C4C	3.98	1.48	1.39
11	B	1207	CLA	CHC-C4B	3.98	1.48	1.39
14	1	4002	BCR	C10-C9	-3.98	1.26	1.35
11	A	1130	CLA	CHD-C4C	3.98	1.48	1.39
11	1	1124	CLA	CHD-C4C	3.98	1.48	1.39
11	1	1134	CLA	CHD-C4C	3.98	1.48	1.39
11	a	1126	CLA	CHB-C1B	3.98	1.48	1.39
11	2	1224	CLA	CHC-C4B	3.98	1.48	1.39
11	B	1204	CLA	CHD-C4C	3.98	1.48	1.39
11	A	1113	CLA	CHB-C1B	3.98	1.48	1.39
11	b	1228	CLA	CHC-C4B	3.98	1.48	1.39
11	b	1204	CLA	CHD-C4C	3.98	1.48	1.39
11	A	1135	CLA	CHD-C4C	3.98	1.48	1.39
11	1	1102	CLA	CHD-C4C	3.98	1.48	1.39
11	1	1140	CLA	CHB-C1B	3.98	1.48	1.39
11	2	1208	CLA	CHC-C4B	3.98	1.48	1.39
11	2	1228	CLA	CHD-C4C	3.98	1.48	1.39
11	2	1234	CLA	CHD-C4C	3.98	1.48	1.39
11	B	1221	CLA	CHC-C4B	3.98	1.48	1.39
11	b	1208	CLA	CHC-C4B	3.98	1.48	1.39
11	A	1801	CLA	CHC-C4B	3.98	1.48	1.39
11	A	1132	CLA	CHC-C4B	3.98	1.48	1.39
11	b	1201	CLA	CHB-C1B	3.98	1.48	1.39
11	A	1104	CLA	CHB-C1B	3.98	1.48	1.39
11	b	1216	CLA	CHD-C4C	3.98	1.48	1.39
11	A	1133	CLA	CHB-C1B	3.98	1.48	1.39
16	b	5002	LMG	O7-C10	3.97	1.45	1.34
11	2	1217	CLA	CHC-C4B	3.97	1.48	1.39
11	2	1223	CLA	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1139	CLA	MG-NC	3.97	2.15	2.06
11	l	1503	CLA	CHD-C4C	3.97	1.48	1.39
11	1	1112	CLA	CHD-C4C	3.97	1.48	1.39
11	L	1503	CLA	CHB-C1B	3.97	1.48	1.39
11	a	1120	CLA	CHB-C1B	3.97	1.48	1.39
11	A	1022	CLA	CHD-C4C	3.97	1.48	1.39
11	b	1225	CLA	CHD-C4C	3.97	1.48	1.39
11	A	1137	CLA	CHB-C1B	3.97	1.48	1.39
11	1	1109	CLA	CHB-C1B	3.97	1.48	1.39
11	b	1236	CLA	CHD-C4C	3.97	1.48	1.39
11	b	1240	CLA	CHB-C1B	3.97	1.48	1.39
11	B	1203	CLA	CHD-C4C	3.97	1.48	1.39
11	B	1235	CLA	CHB-C1B	3.97	1.48	1.39
11	b	1204	CLA	CHC-C4B	3.97	1.48	1.39
11	A	1115	CLA	CHB-C1B	3.97	1.48	1.39
11	A	1128	CLA	CHC-C4B	3.97	1.48	1.39
11	a	1128	CLA	CHB-C1B	3.97	1.48	1.39
11	B	1219	CLA	CHB-C1B	3.97	1.48	1.39
11	B	1225	CLA	CHC-C4B	3.97	1.48	1.39
11	a	1125	CLA	CHB-C1B	3.97	1.48	1.39
11	a	1123	CLA	CHB-C1B	3.97	1.48	1.39
11	2	1218	CLA	CHB-C1B	3.96	1.48	1.39
11	1	1119	CLA	CHD-C4C	3.96	1.48	1.39
11	A	1114	CLA	CHC-C4B	3.96	1.48	1.39
11	1	1137	CLA	CHB-C1B	3.96	1.48	1.39
11	b	1235	CLA	CHD-C4C	3.96	1.48	1.39
11	A	1101	CLA	CHB-C1B	3.96	1.48	1.39
11	B	1202	CLA	CHD-C4C	3.96	1.48	1.39
11	B	1209	CLA	CHD-C4C	3.96	1.48	1.39
11	A	1114	CLA	CHD-C4C	3.96	1.48	1.39
11	a	1117	CLA	CHD-C4C	3.96	1.48	1.39
11	b	1222	CLA	CHD-C4C	3.96	1.48	1.39
11	b	1235	CLA	CHB-C1B	3.96	1.48	1.39
11	b	1201	CLA	CHD-C4C	3.96	1.48	1.39
11	1	1022	CLA	CHD-C4C	3.96	1.48	1.39
14	b	4014	BCR	C10-C9	-3.96	1.26	1.35
11	2	1214	CLA	CHB-C1B	3.96	1.48	1.39
11	a	1110	CLA	CHB-C1B	3.96	1.48	1.39
11	2	1238	CLA	CHD-C4C	3.96	1.48	1.39
11	0	1402	CLA	CHD-C4C	3.96	1.48	1.39
11	B	1201	CLA	CHD-C4C	3.96	1.48	1.39
11	a	1107	CLA	CHC-C4B	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1127	CLA	CHB-C1B	3.96	1.48	1.39
11	1	1103	CLA	CHD-C4C	3.96	1.48	1.39
11	1	1123	CLA	CHC-C4B	3.96	1.48	1.39
11	1	1125	CLA	CHD-C4C	3.96	1.48	1.39
11	A	1138	CLA	CHB-C1B	3.96	1.48	1.39
11	2	1218	CLA	CHD-C4C	3.96	1.48	1.39
11	b	1204	CLA	CHB-C1B	3.96	1.48	1.39
11	b	1207	CLA	CHB-C1B	3.96	1.48	1.39
11	k	1402	CLA	CHB-C1B	3.96	1.48	1.39
11	a	1123	CLA	CHC-C4B	3.95	1.48	1.39
11	b	1023	CLA	CHC-C4B	3.95	1.48	1.39
11	K	1402	CLA	CHB-C1B	3.95	1.48	1.39
11	b	1230	CLA	MG-NC	3.95	2.15	2.06
11	A	1136	CLA	CHC-C4B	3.95	1.48	1.39
11	2	1217	CLA	CHB-C1B	3.95	1.48	1.39
11	a	1122	CLA	CHB-C1B	3.95	1.48	1.39
11	b	1211	CLA	CHD-C4C	3.95	1.48	1.39
11	1	1123	CLA	MG-NC	3.95	2.15	2.06
11	B	1229	CLA	CHC-C4B	3.95	1.48	1.39
11	a	1120	CLA	CHC-C4B	3.95	1.48	1.39
11	2	1204	CLA	CHB-C1B	3.95	1.48	1.39
11	a	1133	CLA	CHD-C4C	3.95	1.48	1.39
11	8	1503	CLA	CHB-C1B	3.95	1.48	1.39
11	2	1212	CLA	CHC-C4B	3.95	1.48	1.39
11	a	1105	CLA	CHC-C4B	3.95	1.48	1.39
11	b	1229	CLA	CHB-C1B	3.95	1.48	1.39
11	A	1108	CLA	CHD-C4C	3.95	1.48	1.39
11	a	1137	CLA	CHD-C4C	3.95	1.48	1.39
11	b	1230	CLA	CHC-C4B	3.95	1.48	1.39
11	k	1401	CLA	CHB-C1B	3.95	1.48	1.39
14	1	4007	BCR	C10-C9	-3.95	1.26	1.35
11	a	1022	CLA	CHC-C4B	3.95	1.48	1.39
11	2	1220	CLA	CHD-C4C	3.95	1.48	1.39
11	B	1203	CLA	CHB-C1B	3.95	1.48	1.39
11	B	1228	CLA	CHB-C1B	3.95	1.48	1.39
11	1	1132	CLA	CHC-C4B	3.95	1.48	1.39
11	a	1124	CLA	CHD-C4C	3.95	1.48	1.39
11	b	1219	CLA	CHC-C4B	3.94	1.48	1.39
11	A	1110	CLA	CHD-C4C	3.94	1.48	1.39
11	1	1138	CLA	CHD-C4C	3.94	1.48	1.39
11	a	1136	CLA	CHC-C4B	3.94	1.48	1.39
11	A	1140	CLA	CHC-C4B	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1209	CLA	CHB-C1B	3.94	1.48	1.39
11	A	1140	CLA	CHD-C4C	3.94	1.48	1.39
11	2	1206	CLA	CHD-C4C	3.94	1.48	1.39
11	2	1214	CLA	CHC-C4B	3.94	1.48	1.39
11	2	1210	CLA	CHB-C1B	3.94	1.48	1.39
11	2	1225	CLA	CHC-C4B	3.94	1.48	1.39
11	k	1401	CLA	CHC-C4B	3.94	1.48	1.39
11	b	1213	CLA	CHD-C4C	3.94	1.48	1.39
11	B	1240	CLA	CHD-C4C	3.94	1.48	1.39
11	2	1215	CLA	CHB-C1B	3.94	1.48	1.39
11	a	1114	CLA	CHC-C4B	3.94	1.48	1.39
11	a	1128	CLA	CHC-C4B	3.94	1.48	1.39
11	b	1215	CLA	CHC-C4B	3.94	1.48	1.39
11	1	1101	CLA	CHB-C1B	3.94	1.48	1.39
11	8	1501	CLA	CHD-C4C	3.94	1.48	1.39
11	2	1220	CLA	CHC-C4B	3.94	1.48	1.39
11	1	1139	CLA	CHB-C1B	3.94	1.48	1.39
11	b	1234	CLA	CHD-C4C	3.94	1.48	1.39
11	A	1119	CLA	CHC-C4B	3.94	1.48	1.39
11	1	1103	CLA	CHC-C4B	3.94	1.48	1.39
11	2	1219	CLA	CHB-C1B	3.94	1.48	1.39
11	b	1220	CLA	MG-NC	3.94	2.15	2.06
11	a	1116	CLA	CHD-C4C	3.94	1.48	1.39
11	1	1119	CLA	CHB-C1B	3.94	1.48	1.39
11	a	1101	CLA	CHB-C1B	3.94	1.48	1.39
11	1	1117	CLA	CHB-C1B	3.94	1.48	1.39
11	B	1238	CLA	CHC-C4B	3.93	1.48	1.39
11	2	1216	CLA	MG-NC	3.93	2.15	2.06
11	a	1108	CLA	CHD-C4C	3.93	1.48	1.39
11	B	1240	CLA	CHB-C1B	3.93	1.48	1.39
11	2	1232	CLA	CHB-C1B	3.93	1.48	1.39
11	B	1235	CLA	CHD-C4C	3.93	1.48	1.39
11	1	1123	CLA	CHB-C1B	3.93	1.48	1.39
11	b	1220	CLA	CHD-C4C	3.93	1.48	1.39
11	b	1219	CLA	CHD-C4C	3.93	1.48	1.39
11	k	1402	CLA	CHD-C4C	3.93	1.48	1.39
11	K	1402	CLA	CHC-C4B	3.93	1.48	1.39
11	B	1212	CLA	CHD-C4C	3.93	1.48	1.39
11	2	1203	CLA	CHD-C4C	3.93	1.48	1.39
11	A	1105	CLA	CHD-C4C	3.93	1.48	1.39
11	B	1206	CLA	CHD-C4C	3.93	1.48	1.39
11	a	1118	CLA	CHC-C4B	3.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1401	CLA	CHC-C4B	3.93	1.48	1.39
11	L	1503	CLA	CHD-C4C	3.93	1.48	1.39
11	a	1012	CLA	CHB-C1B	3.93	1.48	1.39
11	b	1217	CLA	CHB-C1B	3.93	1.48	1.39
11	b	1222	CLA	CHB-C1B	3.93	1.48	1.39
11	b	1203	CLA	CHD-C4C	3.93	1.48	1.39
11	b	1210	CLA	CHB-C1B	3.93	1.48	1.39
11	1	1114	CLA	CHC-C4B	3.93	1.48	1.39
11	1	1135	CLA	CHB-C1B	3.93	1.48	1.39
11	B	1219	CLA	CHD-C4C	3.92	1.48	1.39
11	L	1502	CLA	CHB-C1B	3.92	1.48	1.39
11	a	1136	CLA	CHD-C4C	3.92	1.48	1.39
11	b	1202	CLA	CHB-C1B	3.92	1.48	1.39
11	1	1237	CLA	CHC-C4B	3.92	1.48	1.39
11	0	1401	CLA	CHC-C4B	3.92	1.48	1.39
11	b	1221	CLA	MG-NC	3.92	2.15	2.06
11	B	1211	CLA	CHD-C4C	3.92	1.48	1.39
11	a	1127	CLA	CHD-C4C	3.92	1.48	1.39
11	2	1209	CLA	CHC-C4B	3.92	1.48	1.39
11	2	1215	CLA	CHC-C4B	3.92	1.48	1.39
11	B	1218	CLA	CHC-C4B	3.92	1.48	1.39
11	a	1011	CLA	CHD-C4C	3.92	1.48	1.39
14	A	4008	BCR	C10-C9	-3.92	1.26	1.35
14	l	4019	BCR	C10-C9	-3.92	1.26	1.35
11	a	1130	CLA	CHB-C1B	3.92	1.48	1.39
11	a	1121	CLA	CHB-C1B	3.92	1.48	1.39
11	a	1106	CLA	CHD-C4C	3.92	1.48	1.39
11	a	1109	CLA	CHB-C1B	3.92	1.48	1.39
11	B	1215	CLA	CHC-C4B	3.92	1.48	1.39
11	0	1401	CLA	CHB-C1B	3.92	1.48	1.39
11	2	1223	CLA	CHD-C4C	3.92	1.48	1.39
11	b	1238	CLA	CHB-C1B	3.92	1.48	1.39
11	b	1205	CLA	CHB-C1B	3.92	1.48	1.39
11	8	1502	CLA	CHB-C1B	3.92	1.48	1.39
11	1	1115	CLA	CHB-C1B	3.91	1.48	1.39
11	1	1117	CLA	CHC-C4B	3.91	1.48	1.39
11	K	1401	CLA	CHB-C1B	3.91	1.48	1.39
11	1	1133	CLA	CHC-C4B	3.91	1.48	1.39
11	B	1234	CLA	CHD-C4C	3.91	1.48	1.39
14	2	4004	BCR	C10-C9	-3.91	1.26	1.35
11	A	1109	CLA	CHB-C1B	3.91	1.48	1.39
11	b	1021	CLA	CHB-C1B	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1237	CLA	CHD-C4C	3.91	1.48	1.39
11	a	1103	CLA	CHB-C1B	3.91	1.48	1.39
11	A	1011	CLA	CHD-C4C	3.91	1.48	1.39
11	B	1223	CLA	CHD-C4C	3.91	1.48	1.39
11	1	1129	CLA	CHD-C4C	3.91	1.48	1.39
11	a	1101	CLA	CHC-C4B	3.91	1.48	1.39
11	a	1022	CLA	CHD-C4C	3.91	1.48	1.39
11	2	1230	CLA	CHB-C1B	3.91	1.48	1.39
11	2	1219	CLA	CHD-C4C	3.91	1.48	1.39
11	A	1111	CLA	CHD-C4C	3.91	1.48	1.39
11	1	1126	CLA	CHB-C1B	3.91	1.48	1.39
11	b	1226	CLA	CHD-C4C	3.91	1.48	1.39
11	B	1013	CLA	CHD-C4C	3.90	1.48	1.39
11	2	1235	CLA	CHB-C1B	3.90	1.48	1.39
11	B	1225	CLA	CHD-C4C	3.90	1.48	1.39
11	A	1123	CLA	CHB-C1B	3.90	1.48	1.39
11	A	1133	CLA	CHD-C4C	3.90	1.48	1.39
11	A	1237	CLA	CHC-C4B	3.90	1.48	1.39
11	1	1120	CLA	CHB-C1B	3.90	1.48	1.39
11	b	1021	CLA	CHD-C4C	3.90	1.48	1.39
11	b	1205	CLA	CHC-C4B	3.90	1.48	1.39
11	2	1021	CLA	CHC-C4B	3.90	1.48	1.39
11	a	1012	CLA	MG-NC	3.90	2.15	2.06
11	B	1209	CLA	CHC-C4B	3.90	1.48	1.39
11	1	1130	CLA	CHB-C1B	3.90	1.48	1.39
11	2	1221	CLA	CHB-C1B	3.90	1.48	1.39
11	a	1121	CLA	MG-NC	3.90	2.15	2.06
11	2	1238	CLA	CHB-C1B	3.90	1.48	1.39
11	b	1212	CLA	CHD-C4C	3.90	1.48	1.39
11	B	1226	CLA	CHB-C1B	3.90	1.48	1.39
11	l	1501	CLA	CHB-C1B	3.90	1.48	1.39
11	b	1223	CLA	CHD-C4C	3.90	1.48	1.39
11	A	1139	CLA	CHB-C1B	3.90	1.48	1.39
11	A	1011	CLA	CHC-C4B	3.90	1.48	1.39
11	A	1237	CLA	CHD-C4C	3.89	1.48	1.39
11	B	1212	CLA	CHB-C1B	3.89	1.48	1.39
11	2	1021	CLA	CHD-C4C	3.89	1.48	1.39
11	B	1205	CLA	CHC-C4B	3.89	1.48	1.39
11	a	1138	CLA	CHC-C4B	3.89	1.48	1.39
11	1	1128	CLA	CHC-C4B	3.89	1.48	1.39
11	1	1011	CLA	CHB-C1B	3.89	1.48	1.39
11	B	1238	CLA	CHD-C4C	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1113	CLA	CHD-C4C	3.89	1.48	1.39
11	1	1140	CLA	CHD-C4C	3.89	1.48	1.39
11	B	1202	CLA	CHB-C1B	3.89	1.48	1.39
11	b	1214	CLA	CHB-C1B	3.89	1.48	1.39
11	A	1112	CLA	CHD-C4C	3.89	1.48	1.39
11	a	1104	CLA	CHD-C4C	3.89	1.48	1.39
11	1	1108	CLA	CHD-C4C	3.89	1.48	1.39
11	B	1217	CLA	CHD-C4C	3.89	1.48	1.39
11	2	1222	CLA	CHB-C1B	3.89	1.48	1.39
11	1	1104	CLA	CHD-C4C	3.89	1.48	1.39
11	a	1113	CLA	CHD-C4C	3.89	1.48	1.39
11	a	1022	CLA	CHB-C1B	3.89	1.48	1.39
11	a	1107	CLA	CHB-C1B	3.89	1.48	1.39
14	2	4005	BCR	C10-C9	-3.89	1.26	1.35
11	A	1136	CLA	CHD-C4C	3.89	1.48	1.39
11	B	1221	CLA	CHB-C1B	3.88	1.48	1.39
11	1	1109	CLA	CHC-C4B	3.88	1.48	1.39
11	B	1213	CLA	CHD-C4C	3.88	1.48	1.39
11	2	1023	CLA	CHD-C4C	3.88	1.48	1.39
11	A	1118	CLA	CHC-C4B	3.88	1.48	1.39
11	B	1201	CLA	CHC-C4B	3.88	1.48	1.39
11	2	1228	CLA	CHB-C1B	3.88	1.48	1.39
11	1	1103	CLA	CHB-C1B	3.88	1.48	1.39
11	b	1223	CLA	CHC-C4B	3.88	1.48	1.39
11	A	1107	CLA	CHB-C1B	3.88	1.48	1.39
11	1	1138	CLA	CHC-C4B	3.88	1.48	1.39
11	K	1401	CLA	CHD-C4C	3.88	1.48	1.39
11	1	1110	CLA	MG-NC	3.88	2.15	2.06
11	1	1124	CLA	CHB-C1B	3.88	1.48	1.39
11	A	1111	CLA	CHB-C1B	3.88	1.48	1.39
11	2	1217	CLA	MG-NC	3.88	2.15	2.06
11	8	1501	CLA	CHC-C4B	3.88	1.48	1.39
11	a	1120	CLA	CHD-C4C	3.88	1.48	1.39
11	a	1123	CLA	MG-NC	3.88	2.15	2.06
11	B	1201	CLA	CHB-C1B	3.87	1.48	1.39
11	1	1022	CLA	CHB-C1B	3.87	1.48	1.39
11	2	1207	CLA	CHC-C4B	3.87	1.48	1.39
11	B	1220	CLA	CHC-C4B	3.87	1.48	1.39
11	k	1401	CLA	CHD-C4C	3.87	1.48	1.39
11	a	1133	CLA	CHC-C4B	3.87	1.48	1.39
11	A	1120	CLA	OBD-CAD	3.87	1.29	1.22
11	2	1209	CLA	CHB-C1B	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1106	CLA	CHC-C4B	3.87	1.48	1.39
11	a	1123	CLA	OBD-CAD	3.87	1.29	1.22
11	A	1103	CLA	CHD-C4C	3.87	1.48	1.39
11	1	1136	CLA	CHD-C4C	3.87	1.48	1.39
11	2	1203	CLA	CHC-C4B	3.87	1.48	1.39
11	2	1227	CLA	CHC-C4B	3.87	1.48	1.39
11	A	1127	CLA	CHB-C1B	3.87	1.48	1.39
11	2	1232	CLA	MG-NC	3.87	2.15	2.06
11	2	1212	CLA	CHD-C4C	3.86	1.48	1.39
11	0	1401	CLA	CHD-C4C	3.86	1.48	1.39
11	b	1228	CLA	CHB-C1B	3.86	1.48	1.39
11	B	1215	CLA	CHB-C1B	3.86	1.48	1.39
11	a	1129	CLA	CHD-C4C	3.86	1.48	1.39
11	l	1501	CLA	CHD-C4C	3.86	1.48	1.39
11	A	1120	CLA	CHB-C1B	3.86	1.48	1.39
11	1	1012	CLA	MG-NC	3.86	2.15	2.06
11	1	1118	CLA	CHD-C4C	3.86	1.48	1.39
11	2	1203	CLA	CHB-C1B	3.86	1.48	1.39
11	a	1118	CLA	CHD-C4C	3.86	1.48	1.39
11	1	1801	CLA	CHB-C1B	3.86	1.48	1.39
11	b	1219	CLA	MG-NC	3.86	2.15	2.06
11	2	1239	CLA	MG-NC	3.86	2.15	2.06
11	a	1114	CLA	MG-NC	3.86	2.15	2.06
11	a	1134	CLA	CHB-C1B	3.86	1.48	1.39
11	B	1204	CLA	CHB-C1B	3.86	1.48	1.39
11	L	1502	CLA	CHD-C4C	3.86	1.48	1.39
11	1	1104	CLA	CHB-C1B	3.85	1.48	1.39
11	A	1127	CLA	CHD-C4C	3.85	1.48	1.39
11	1	1102	CLA	MG-NC	3.85	2.15	2.06
11	l	1503	CLA	CHB-C1B	3.85	1.48	1.39
11	2	1225	CLA	CHB-C1B	3.85	1.48	1.39
11	b	1224	CLA	CHD-C4C	3.85	1.48	1.39
11	2	1229	CLA	CHB-C1B	3.85	1.48	1.39
11	b	1230	CLA	CHD-C4C	3.85	1.48	1.39
11	A	1112	CLA	CHB-C1B	3.85	1.48	1.39
11	b	1214	CLA	CHD-C4C	3.85	1.48	1.39
11	b	1215	CLA	CHB-C1B	3.85	1.48	1.39
11	a	1139	CLA	CHC-C4B	3.85	1.48	1.39
11	b	1203	CLA	CHB-C1B	3.85	1.48	1.39
11	b	1223	CLA	MG-NC	3.85	2.15	2.06
11	b	1239	CLA	CHC-C4B	3.85	1.48	1.39
11	B	1214	CLA	CHB-C1B	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1216	CLA	CHB-C1B	3.84	1.48	1.39
11	2	1240	CLA	MG-NC	3.84	2.15	2.06
11	B	1207	CLA	CHD-C4C	3.84	1.47	1.39
11	L	1501	CLA	CHD-C4C	3.84	1.47	1.39
11	b	1225	CLA	CHB-C1B	3.84	1.48	1.39
11	a	1125	CLA	CHD-C4C	3.84	1.47	1.39
11	A	1123	CLA	CHC-C4B	3.84	1.48	1.39
11	A	1137	CLA	CHD-C4C	3.84	1.47	1.39
11	b	1023	CLA	CHD-C4C	3.84	1.47	1.39
11	A	1124	CLA	MG-NC	3.84	2.15	2.06
11	1	1122	CLA	CHD-C4C	3.84	1.47	1.39
11	A	1138	CLA	CHC-C4B	3.84	1.48	1.39
11	B	1220	CLA	CHB-C1B	3.84	1.48	1.39
11	2	1234	CLA	CHC-C4B	3.84	1.48	1.39
11	A	1114	CLA	MG-NC	3.83	2.15	2.06
11	b	1232	CLA	MG-NC	3.83	2.15	2.06
11	a	1116	CLA	CHB-C1B	3.83	1.48	1.39
11	1	1139	CLA	MG-NC	3.83	2.15	2.06
11	L	1503	CLA	CHC-C4B	3.83	1.48	1.39
11	1	1125	CLA	CHB-C1B	3.83	1.48	1.39
11	B	1231	CLA	CHC-C4B	3.83	1.48	1.39
11	2	1207	CLA	CHD-C4C	3.83	1.47	1.39
11	B	1232	CLA	MG-NC	3.83	2.15	2.06
11	1	1135	CLA	CHD-C4C	3.83	1.47	1.39
11	a	1011	CLA	CHC-C4B	3.83	1.48	1.39
11	K	1402	CLA	CHD-C4C	3.83	1.47	1.39
11	1	1011	CLA	CHD-C4C	3.83	1.47	1.39
11	B	1207	CLA	CHB-C1B	3.83	1.48	1.39
11	1	1132	CLA	CHB-C1B	3.83	1.48	1.39
11	A	1801	CLA	MG-NC	3.83	2.15	2.06
11	B	1225	CLA	CHB-C1B	3.83	1.48	1.39
11	a	1022	CLA	MG-NC	3.83	2.15	2.06
11	B	1210	CLA	CHD-C4C	3.83	1.47	1.39
11	b	1224	CLA	MG-NC	3.83	2.15	2.06
11	B	1240	CLA	MG-NC	3.83	2.15	2.06
11	a	1012	CLA	CHD-C4C	3.82	1.47	1.39
14	B	4010	BCR	C10-C9	-3.82	1.27	1.35
11	b	1240	CLA	MG-NC	3.82	2.15	2.06
11	B	1204	CLA	CHC-C4B	3.82	1.48	1.39
11	a	1122	CLA	CHD-C4C	3.82	1.47	1.39
11	B	1230	CLA	CHC-C4B	3.82	1.48	1.39
11	a	1106	CLA	CHB-C1B	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1223	CLA	MG-NC	3.82	2.15	2.06
11	A	1101	CLA	CHD-C4C	3.82	1.47	1.39
11	2	1216	CLA	CHD-C4C	3.82	1.47	1.39
11	2	1209	CLA	OBD-CAD	3.82	1.29	1.22
11	a	1138	CLA	CHB-C1B	3.82	1.48	1.39
11	a	1117	CLA	OBD-CAD	3.82	1.29	1.22
11	2	1215	CLA	MG-NC	3.82	2.15	2.06
11	B	1021	CLA	CHD-C4C	3.82	1.47	1.39
11	b	1210	CLA	CHD-C4C	3.82	1.47	1.39
11	2	1202	CLA	OBD-CAD	3.82	1.29	1.22
11	1	1137	CLA	CHD-C4C	3.82	1.47	1.39
11	b	1225	CLA	MG-NC	3.82	2.15	2.06
11	A	1128	CLA	CHD-C4C	3.82	1.47	1.39
11	2	1236	CLA	CHD-C4C	3.82	1.47	1.39
11	A	1104	CLA	CHD-C4C	3.82	1.47	1.39
11	a	1126	CLA	CHD-C4C	3.82	1.47	1.39
11	1	1120	CLA	MG-NC	3.82	2.15	2.06
11	2	1201	CLA	CHC-C4B	3.82	1.48	1.39
11	A	1109	CLA	OBD-CAD	3.82	1.29	1.22
11	2	1231	CLA	MG-NC	3.82	2.15	2.06
11	A	1131	CLA	MG-NC	3.81	2.15	2.06
11	b	1234	CLA	MG-NC	3.81	2.15	2.06
11	a	1111	CLA	CHD-C4C	3.81	1.47	1.39
11	a	1119	CLA	CHC-C4B	3.81	1.48	1.39
11	b	1023	CLA	CHB-C1B	3.81	1.48	1.39
11	A	1123	CLA	MG-NC	3.81	2.15	2.06
11	1	1022	CLA	MG-NC	3.81	2.15	2.06
11	2	1210	CLA	CHD-C4C	3.81	1.47	1.39
14	b	4009	BCR	C10-C9	-3.81	1.27	1.35
11	1	1135	CLA	MG-NC	3.81	2.15	2.06
11	a	1127	CLA	CHC-C4B	3.81	1.48	1.39
11	B	1222	CLA	OBD-CAD	3.81	1.29	1.22
11	b	1210	CLA	MG-NC	3.81	2.15	2.06
11	b	1205	CLA	CHD-C4C	3.81	1.47	1.39
11	b	1215	CLA	OBD-CAD	3.81	1.29	1.22
11	2	1222	CLA	OBD-CAD	3.81	1.29	1.22
11	2	1212	CLA	MG-NC	3.81	2.15	2.06
11	A	1134	CLA	CHC-C4B	3.81	1.48	1.39
11	b	1013	CLA	OBD-CAD	3.81	1.29	1.22
11	2	1230	CLA	MG-NC	3.80	2.15	2.06
11	B	1205	CLA	OBD-CAD	3.80	1.29	1.22
11	2	1227	CLA	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1102	CLA	CHB-C1B	3.80	1.47	1.39
11	B	1210	CLA	OBD-CAD	3.80	1.29	1.22
11	1	1102	CLA	CHB-C1B	3.80	1.47	1.39
11	b	1202	CLA	CHD-C4C	3.80	1.47	1.39
11	B	1230	CLA	OBD-CAD	3.80	1.29	1.22
11	2	1235	CLA	CHD-C4C	3.80	1.47	1.39
11	2	1201	CLA	OBD-CAD	3.80	1.29	1.22
11	L	1501	CLA	CHB-C1B	3.80	1.47	1.39
11	2	1219	CLA	MG-NC	3.80	2.15	2.06
11	2	1211	CLA	CHD-C4C	3.80	1.47	1.39
11	A	1106	CLA	CHB-C1B	3.80	1.47	1.39
11	1	1110	CLA	CHB-C1B	3.80	1.47	1.39
11	b	1208	CLA	MG-NC	3.80	2.15	2.06
11	B	1021	CLA	OBD-CAD	3.80	1.29	1.22
11	B	1231	CLA	MG-NC	3.80	2.15	2.06
11	B	1232	CLA	CHC-C4B	3.80	1.47	1.39
11	a	1113	CLA	MG-NC	3.80	2.15	2.06
11	A	1139	CLA	MG-NC	3.80	2.15	2.06
11	B	1213	CLA	OBD-CAD	3.80	1.29	1.22
11	2	1206	CLA	MG-NC	3.80	2.15	2.06
11	a	1801	CLA	CHB-C1B	3.80	1.47	1.39
11	A	1022	CLA	OBD-CAD	3.80	1.29	1.22
11	1	1108	CLA	OBD-CAD	3.80	1.29	1.22
11	A	1116	CLA	CHD-C4C	3.80	1.47	1.39
11	b	1231	CLA	OBD-CAD	3.80	1.29	1.22
11	B	1212	CLA	OBD-CAD	3.80	1.29	1.22
11	2	1212	CLA	OBD-CAD	3.80	1.29	1.22
11	A	1129	CLA	CHD-C4C	3.80	1.47	1.39
11	B	1222	CLA	CHB-C1B	3.80	1.47	1.39
11	A	1139	CLA	OBD-CAD	3.80	1.29	1.22
11	b	1227	CLA	MG-NC	3.79	2.15	2.06
11	B	1214	CLA	CHD-C4C	3.79	1.47	1.39
11	2	1220	CLA	MG-NC	3.79	2.15	2.06
11	2	1213	CLA	OBD-CAD	3.79	1.29	1.22
11	2	1231	CLA	OBD-CAD	3.79	1.29	1.22
11	2	1201	CLA	MG-NC	3.79	2.15	2.06
11	a	1135	CLA	CHC-C4B	3.79	1.47	1.39
11	a	1101	CLA	MG-NC	3.79	2.15	2.06
11	b	1225	CLA	OBD-CAD	3.79	1.29	1.22
11	1	1111	CLA	OBD-CAD	3.79	1.29	1.22
11	A	1012	CLA	CHB-C1B	3.79	1.47	1.39
11	B	1202	CLA	OBD-CAD	3.79	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1211	CLA	OBD-CAD	3.79	1.29	1.22
11	a	1101	CLA	OBD-CAD	3.79	1.29	1.22
11	a	1801	CLA	MG-NC	3.79	2.15	2.06
11	a	1132	CLA	CHB-C1B	3.79	1.47	1.39
11	B	1226	CLA	CHD-C4C	3.79	1.47	1.39
11	a	1237	CLA	OBD-CAD	3.79	1.29	1.22
11	a	1124	CLA	CHB-C1B	3.79	1.47	1.39
11	b	1023	CLA	OBD-CAD	3.79	1.29	1.22
11	a	1107	CLA	MG-NC	3.79	2.15	2.06
11	1	1133	CLA	MG-NC	3.79	2.15	2.06
11	b	1220	CLA	OBD-CAD	3.79	1.29	1.22
11	1	1114	CLA	OBD-CAD	3.79	1.29	1.22
11	0	1402	CLA	OBD-CAD	3.79	1.29	1.22
11	1	1140	CLA	MG-NC	3.79	2.15	2.06
11	1	1117	CLA	OBD-CAD	3.79	1.29	1.22
11	2	1232	CLA	OBD-CAD	3.79	1.29	1.22
11	1	1115	CLA	MG-NC	3.79	2.15	2.06
11	l	1502	CLA	OBD-CAD	3.78	1.29	1.22
11	b	1239	CLA	MG-NC	3.78	2.15	2.06
11	A	1122	CLA	OBD-CAD	3.78	1.29	1.22
11	b	1203	CLA	MG-NC	3.78	2.15	2.06
11	2	1224	CLA	CHD-C4C	3.78	1.47	1.39
11	B	1222	CLA	MG-NC	3.78	2.15	2.06
11	1	1113	CLA	MG-NC	3.78	2.15	2.06
11	a	1114	CLA	OBD-CAD	3.78	1.29	1.22
11	A	1113	CLA	CHD-C4C	3.78	1.47	1.39
11	a	1011	CLA	CHB-C1B	3.78	1.47	1.39
11	b	1021	CLA	MG-NC	3.78	2.15	2.06
11	a	1011	CLA	OBD-CAD	3.78	1.29	1.22
11	b	1230	CLA	OBD-CAD	3.78	1.29	1.22
11	2	1021	CLA	OBD-CAD	3.78	1.29	1.22
11	1	1133	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1220	CLA	MG-NC	3.78	2.15	2.06
11	a	1126	CLA	MG-NC	3.78	2.15	2.06
11	a	1104	CLA	OBD-CAD	3.78	1.29	1.22
11	a	1137	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1209	CLA	MG-NC	3.78	2.15	2.06
11	A	1102	CLA	CHB-C1B	3.78	1.47	1.39
11	B	1231	CLA	OBD-CAD	3.78	1.29	1.22
11	2	1013	CLA	OBD-CAD	3.78	1.29	1.22
11	A	1131	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1225	CLA	OBD-CAD	3.78	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1240	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1021	CLA	CHC-C4B	3.78	1.47	1.39
11	A	1117	CLA	OBD-CAD	3.78	1.29	1.22
11	1	1011	CLA	OBD-CAD	3.78	1.29	1.22
11	2	1023	CLA	OBD-CAD	3.78	1.29	1.22
11	a	1108	CLA	MG-NC	3.78	2.15	2.06
11	A	1116	CLA	OBD-CAD	3.78	1.29	1.22
11	b	1216	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1201	CLA	OBD-CAD	3.78	1.29	1.22
11	B	1240	CLA	OBD-CAD	3.78	1.29	1.22
11	a	1135	CLA	MG-NC	3.78	2.15	2.06
11	2	1226	CLA	OBD-CAD	3.78	1.29	1.22
11	0	1401	CLA	MG-NC	3.78	2.15	2.06
11	b	1232	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1126	CLA	OBD-CAD	3.77	1.29	1.22
11	B	1222	CLA	CHD-C4C	3.77	1.47	1.39
11	a	1126	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1104	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1129	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1114	CLA	MG-NC	3.77	2.15	2.06
11	A	1138	CLA	OBD-CAD	3.77	1.29	1.22
11	b	1212	CLA	MG-NC	3.77	2.15	2.06
11	2	1223	CLA	MG-NC	3.77	2.15	2.06
11	A	1101	CLA	OBD-CAD	3.77	1.29	1.22
11	A	1011	CLA	OBD-CAD	3.77	1.29	1.22
11	A	1135	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1130	CLA	OBD-CAD	3.77	1.29	1.22
11	A	1110	CLA	OBD-CAD	3.77	1.29	1.22
11	2	1239	CLA	OBD-CAD	3.77	1.29	1.22
11	b	1207	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1022	CLA	OBD-CAD	3.77	1.29	1.22
11	A	1110	CLA	MG-NC	3.77	2.15	2.06
11	A	1134	CLA	MG-NC	3.77	2.15	2.06
11	b	1205	CLA	OBD-CAD	3.77	1.29	1.22
11	B	1013	CLA	OBD-CAD	3.77	1.29	1.22
11	8	1503	CLA	MG-NC	3.77	2.15	2.06
11	a	1115	CLA	OBD-CAD	3.77	1.29	1.22
11	2	1215	CLA	OBD-CAD	3.77	1.29	1.22
11	a	1112	CLA	CHB-C1B	3.77	1.47	1.39
11	B	1230	CLA	MG-NC	3.77	2.15	2.06
11	1	1101	CLA	MG-NC	3.77	2.15	2.06
11	A	1012	CLA	CHD-C4C	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1103	CLA	OBD-CAD	3.77	1.29	1.22
11	a	1129	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1011	CLA	MG-NC	3.77	2.15	2.06
11	a	1110	CLA	OBD-CAD	3.77	1.29	1.22
11	a	1139	CLA	OBD-CAD	3.77	1.29	1.22
11	1	1107	CLA	CHD-C4C	3.77	1.47	1.39
11	b	1216	CLA	MG-NC	3.77	2.15	2.06
11	A	1116	CLA	CHB-C1B	3.77	1.47	1.39
11	2	1221	CLA	CHD-C4C	3.77	1.47	1.39
11	B	1013	CLA	CHB-C1B	3.76	1.47	1.39
11	A	1111	CLA	OBD-CAD	3.76	1.29	1.22
11	b	1213	CLA	OBD-CAD	3.76	1.29	1.22
11	b	1211	CLA	MG-NC	3.76	2.15	2.06
11	1	1129	CLA	MG-NC	3.76	2.15	2.06
11	B	1239	CLA	OBD-CAD	3.76	1.29	1.22
11	B	1023	CLA	CHB-C1B	3.76	1.47	1.39
11	2	1207	CLA	CHB-C1B	3.76	1.47	1.39
11	B	1229	CLA	OBD-CAD	3.76	1.29	1.22
11	B	1238	CLA	OBD-CAD	3.76	1.29	1.22
11	1	1128	CLA	OBD-CAD	3.76	1.29	1.22
11	2	1208	CLA	OBD-CAD	3.76	1.29	1.22
11	1	1108	CLA	MG-NC	3.76	2.15	2.06
11	a	1140	CLA	MG-NC	3.76	2.15	2.06
11	a	1012	CLA	OBD-CAD	3.76	1.29	1.22
11	A	1125	CLA	CHC-C4B	3.76	1.47	1.39
11	A	1108	CLA	OBD-CAD	3.76	1.29	1.22
11	1	1103	CLA	OBD-CAD	3.76	1.29	1.22
11	2	1230	CLA	CHD-C4C	3.76	1.47	1.39
11	B	1206	CLA	OBD-CAD	3.76	1.29	1.22
11	1	1140	CLA	OBD-CAD	3.76	1.29	1.22
11	A	1132	CLA	MG-NC	3.76	2.15	2.06
11	a	1102	CLA	MG-NC	3.76	2.15	2.06
11	b	1240	CLA	OBD-CAD	3.76	1.29	1.22
11	2	1229	CLA	MG-NC	3.76	2.15	2.06
11	1	1107	CLA	OBD-CAD	3.76	1.29	1.22
11	B	1225	CLA	MG-NC	3.76	2.15	2.06
11	L	1501	CLA	MG-NC	3.76	2.15	2.06
11	b	1207	CLA	CHC-C4B	3.76	1.47	1.39
11	A	1117	CLA	CHB-C1B	3.76	1.47	1.39
11	b	1206	CLA	CHC-C4B	3.76	1.47	1.39
11	2	1234	CLA	MG-NC	3.76	2.15	2.06
11	b	1021	CLA	OBD-CAD	3.76	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1801	CLA	OBD-CAD	3.76	1.29	1.22
11	a	1128	CLA	OBD-CAD	3.76	1.29	1.22
11	a	1134	CLA	OBD-CAD	3.76	1.29	1.22
11	k	1402	CLA	OBD-CAD	3.76	1.29	1.22
11	A	1102	CLA	MG-NC	3.76	2.15	2.06
11	2	1226	CLA	CHD-C4C	3.76	1.47	1.39
11	B	1227	CLA	CHC-C4B	3.76	1.47	1.39
11	1	1112	CLA	MG-NC	3.76	2.15	2.06
11	1	1113	CLA	OBD-CAD	3.76	1.29	1.22
11	1	1116	CLA	OBD-CAD	3.76	1.29	1.22
11	b	1235	CLA	MG-NC	3.76	2.15	2.06
11	a	1113	CLA	OBD-CAD	3.76	1.28	1.22
11	b	1210	CLA	OBD-CAD	3.76	1.28	1.22
11	B	1221	CLA	MG-NC	3.76	2.15	2.06
11	2	1230	CLA	OBD-CAD	3.76	1.28	1.22
11	1	1134	CLA	MG-NC	3.75	2.15	2.06
11	b	1207	CLA	CHD-C4C	3.75	1.47	1.39
11	K	1401	CLA	MG-NC	3.75	2.15	2.06
11	B	1021	CLA	CHB-C1B	3.75	1.47	1.39
11	B	1226	CLA	OBD-CAD	3.75	1.28	1.22
11	b	1227	CLA	OBD-CAD	3.75	1.28	1.22
11	A	1133	CLA	CHC-C4B	3.75	1.47	1.39
11	2	1206	CLA	CHC-C4B	3.75	1.47	1.39
11	a	1109	CLA	MG-NC	3.75	2.15	2.06
11	a	1120	CLA	MG-NC	3.75	2.15	2.06
11	A	1107	CLA	OBD-CAD	3.75	1.28	1.22
11	2	1219	CLA	OBD-CAD	3.75	1.28	1.22
11	1	1132	CLA	OBD-CAD	3.75	1.28	1.22
11	2	1229	CLA	OBD-CAD	3.75	1.28	1.22
11	1	1123	CLA	OBD-CAD	3.75	1.28	1.22
11	a	1115	CLA	CHD-C4C	3.75	1.47	1.39
11	8	1501	CLA	MG-NC	3.75	2.15	2.06
11	a	1107	CLA	CHD-C4C	3.75	1.47	1.39
11	a	1105	CLA	MG-NC	3.75	2.15	2.06
11	1	1125	CLA	MG-NC	3.75	2.15	2.06
11	a	1105	CLA	OBD-CAD	3.75	1.28	1.22
11	a	1138	CLA	OBD-CAD	3.75	1.28	1.22
11	1	1139	CLA	OBD-CAD	3.75	1.28	1.22
11	8	1501	CLA	CHB-C1B	3.75	1.47	1.39
11	A	1132	CLA	OBD-CAD	3.75	1.28	1.22
11	b	1218	CLA	OBD-CAD	3.75	1.28	1.22
11	1	1101	CLA	OBD-CAD	3.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1129	CLA	MG-NC	3.75	2.15	2.06
11	a	1116	CLA	OBD-CAD	3.75	1.28	1.22
11	b	1234	CLA	OBD-CAD	3.75	1.28	1.22
11	2	1221	CLA	OBD-CAD	3.75	1.28	1.22
11	A	1127	CLA	MG-NC	3.75	2.15	2.06
11	A	1101	CLA	MG-NC	3.75	2.15	2.06
11	b	1239	CLA	OBD-CAD	3.75	1.28	1.22
11	a	1112	CLA	OBD-CAD	3.75	1.28	1.22
11	a	1135	CLA	OBD-CAD	3.75	1.28	1.22
11	1	1120	CLA	OBD-CAD	3.75	1.28	1.22
11	2	1213	CLA	MG-NC	3.75	2.15	2.06
11	B	1203	CLA	OBD-CAD	3.75	1.28	1.22
11	a	1133	CLA	OBD-CAD	3.74	1.28	1.22
11	B	1229	CLA	MG-NC	3.74	2.15	2.06
11	1	1118	CLA	OBD-CAD	3.74	1.28	1.22
11	b	1222	CLA	MG-NC	3.74	2.15	2.06
11	A	1119	CLA	CHB-C1B	3.74	1.47	1.39
11	A	1114	CLA	OBD-CAD	3.74	1.28	1.22
11	0	1401	CLA	OBD-CAD	3.74	1.28	1.22
11	2	1222	CLA	MG-NC	3.74	2.15	2.06
11	a	1140	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1124	CLA	MG-NC	3.74	2.15	2.06
11	a	1111	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1132	CLA	OBD-CAD	3.74	1.28	1.22
11	b	1208	CLA	OBD-CAD	3.74	1.28	1.22
11	B	1204	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1120	CLA	OBD-CAD	3.74	1.28	1.22
11	1	1801	CLA	OBD-CAD	3.74	1.28	1.22
11	A	1133	CLA	OBD-CAD	3.74	1.28	1.22
11	B	1227	CLA	MG-NC	3.74	2.15	2.06
11	1	1102	CLA	OBD-CAD	3.74	1.28	1.22
11	1	1112	CLA	OBD-CAD	3.74	1.28	1.22
11	B	1219	CLA	MG-NC	3.74	2.15	2.06
11	b	1217	CLA	MG-NC	3.74	2.15	2.06
11	1	1131	CLA	MG-NC	3.74	2.15	2.06
11	b	1212	CLA	OBD-CAD	3.74	1.28	1.22
11	A	1112	CLA	MG-NC	3.74	2.15	2.06
11	b	1222	CLA	OBD-CAD	3.74	1.28	1.22
11	k	1401	CLA	OBD-CAD	3.74	1.28	1.22
11	1	1801	CLA	MG-NC	3.74	2.15	2.06
11	B	1215	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1127	CLA	MG-NC	3.74	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1011	CLA	CHC-C4B	3.74	1.47	1.39
11	b	1229	CLA	OBD-CAD	3.74	1.28	1.22
11	b	1206	CLA	OBD-CAD	3.74	1.28	1.22
11	l	1501	CLA	OBD-CAD	3.74	1.28	1.22
11	K	1401	CLA	OBD-CAD	3.74	1.28	1.22
11	2	1225	CLA	MG-NC	3.74	2.15	2.06
11	l	1503	CLA	OBD-CAD	3.74	1.28	1.22
11	2	1228	CLA	OBD-CAD	3.74	1.28	1.22
11	1	1111	CLA	CHB-C1B	3.74	1.47	1.39
11	1	1121	CLA	MG-NC	3.74	2.15	2.06
11	B	1218	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1122	CLA	OBD-CAD	3.74	1.28	1.22
11	a	1110	CLA	MG-NC	3.74	2.15	2.06
11	b	1203	CLA	OBD-CAD	3.73	1.28	1.22
11	a	1108	CLA	OBD-CAD	3.73	1.28	1.22
11	B	1234	CLA	MG-NC	3.73	2.15	2.06
11	A	1128	CLA	OBD-CAD	3.73	1.28	1.22
11	b	1201	CLA	OBD-CAD	3.73	1.28	1.22
11	2	1205	CLA	OBD-CAD	3.73	1.28	1.22
11	a	1131	CLA	OBD-CAD	3.73	1.28	1.22
11	8	1501	CLA	OBD-CAD	3.73	1.28	1.22
11	B	1235	CLA	MG-NC	3.73	2.15	2.06
11	B	1232	CLA	OBD-CAD	3.73	1.28	1.22
11	1	1110	CLA	OBD-CAD	3.73	1.28	1.22
11	l	1501	CLA	MG-NC	3.73	2.15	2.06
11	B	1234	CLA	CHC-C4B	3.73	1.47	1.39
11	2	1227	CLA	MG-NC	3.73	2.15	2.06
11	k	1401	CLA	MG-NC	3.73	2.15	2.06
11	A	1112	CLA	OBD-CAD	3.73	1.28	1.22
11	B	1224	CLA	OBD-CAD	3.73	1.28	1.22
11	a	1106	CLA	OBD-CAD	3.73	1.28	1.22
11	B	1212	CLA	MG-NC	3.73	2.15	2.06
11	b	1213	CLA	MG-NC	3.73	2.15	2.06
11	a	1136	CLA	OBD-CAD	3.73	1.28	1.22
11	a	1112	CLA	MG-NC	3.73	2.15	2.06
11	A	1116	CLA	MG-NC	3.73	2.15	2.06
11	a	1102	CLA	OBD-CAD	3.73	1.28	1.22
11	1	1105	CLA	OBD-CAD	3.73	1.28	1.22
11	2	1218	CLA	OBD-CAD	3.73	1.28	1.22
11	A	1126	CLA	OBD-CAD	3.73	1.28	1.22
11	A	1123	CLA	OBD-CAD	3.73	1.28	1.22
11	b	1202	CLA	OBD-CAD	3.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1225	CLA	OBD-CAD	3.72	1.28	1.22
11	a	1133	CLA	MG-NC	3.72	2.15	2.06
11	K	1402	CLA	OBD-CAD	3.72	1.28	1.22
11	b	1013	CLA	CHB-C1B	3.72	1.47	1.39
11	b	1209	CLA	MG-NC	3.72	2.15	2.06
11	B	1208	CLA	OBD-CAD	3.72	1.28	1.22
11	l	1502	CLA	MG-NC	3.72	2.15	2.06
11	B	1206	CLA	CHC-C4B	3.72	1.47	1.39
11	A	1130	CLA	OBD-CAD	3.72	1.28	1.22
11	B	1228	CLA	OBD-CAD	3.72	1.28	1.22
11	2	1206	CLA	OBD-CAD	3.72	1.28	1.22
11	2	1207	CLA	OBD-CAD	3.72	1.28	1.22
11	2	1209	CLA	MG-NC	3.72	2.15	2.06
11	1	1116	CLA	MG-NC	3.72	2.15	2.06
11	l	1502	CLA	CHD-C4C	3.72	1.47	1.39
11	1	1132	CLA	MG-NC	3.72	2.15	2.06
11	1	1122	CLA	OBD-CAD	3.72	1.28	1.22
11	a	1106	CLA	MG-NC	3.72	2.15	2.06
11	1	1122	CLA	MG-NC	3.72	2.15	2.06
11	2	1221	CLA	MG-NC	3.72	2.15	2.06
11	B	1227	CLA	OBD-CAD	3.72	1.28	1.22
11	a	1109	CLA	OBD-CAD	3.72	1.28	1.22
11	1	1134	CLA	OBD-CAD	3.72	1.28	1.22
11	1	1126	CLA	MG-NC	3.72	2.15	2.06
11	B	1205	CLA	CHD-C4C	3.71	1.47	1.39
11	1	1136	CLA	OBD-CAD	3.71	1.28	1.22
11	A	1134	CLA	OBD-CAD	3.71	1.28	1.22
11	A	1121	CLA	MG-NC	3.71	2.15	2.06
11	A	1102	CLA	OBD-CAD	3.71	1.28	1.22
11	B	1209	CLA	OBD-CAD	3.71	1.28	1.22
11	a	1115	CLA	MG-NC	3.71	2.15	2.06
11	b	1218	CLA	MG-NC	3.71	2.15	2.06
11	a	1801	CLA	OBD-CAD	3.71	1.28	1.22
11	2	1204	CLA	OBD-CAD	3.71	1.28	1.22
11	B	1230	CLA	CHD-C4C	3.71	1.47	1.39
11	2	1235	CLA	MG-NC	3.71	2.15	2.06
11	8	1502	CLA	MG-NC	3.71	2.15	2.06
11	b	1209	CLA	OBD-CAD	3.71	1.28	1.22
11	1	1138	CLA	OBD-CAD	3.71	1.28	1.22
11	a	1104	CLA	CHB-C1B	3.71	1.47	1.39
11	a	1130	CLA	OBD-CAD	3.71	1.28	1.22
11	2	1238	CLA	MG-NC	3.71	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1137	CLA	MG-NC	3.71	2.15	2.06
11	2	1214	CLA	OBD-CAD	3.71	1.28	1.22
11	A	1012	CLA	OBD-CAD	3.70	1.28	1.22
11	2	1210	CLA	OBD-CAD	3.70	1.28	1.22
11	1	1106	CLA	OBD-CAD	3.70	1.28	1.22
11	B	1234	CLA	OBD-CAD	3.70	1.28	1.22
11	b	1223	CLA	OBD-CAD	3.70	1.28	1.22
11	1	1111	CLA	CHD-C4C	3.70	1.47	1.39
11	a	1237	CLA	CHD-C4C	3.70	1.47	1.39
11	8	1502	CLA	CHD-C4C	3.70	1.47	1.39
11	b	1221	CLA	OBD-CAD	3.70	1.28	1.22
11	a	1103	CLA	MG-NC	3.70	2.15	2.06
11	1	1124	CLA	MG-NC	3.70	2.15	2.06
11	a	1118	CLA	OBD-CAD	3.70	1.28	1.22
11	1	1131	CLA	OBD-CAD	3.70	1.28	1.22
11	a	1011	CLA	MG-NC	3.70	2.15	2.06
11	b	1234	CLA	CHC-C4B	3.70	1.47	1.39
11	A	1105	CLA	OBD-CAD	3.70	1.28	1.22
11	L	1502	CLA	OBD-CAD	3.70	1.28	1.22
11	2	1238	CLA	OBD-CAD	3.70	1.28	1.22
11	1	1105	CLA	MG-NC	3.70	2.15	2.06
11	B	1235	CLA	OBD-CAD	3.70	1.28	1.22
11	2	1235	CLA	OBD-CAD	3.69	1.28	1.22
11	B	1236	CLA	CHD-C4C	3.69	1.47	1.39
11	a	1121	CLA	OBD-CAD	3.69	1.28	1.22
11	1	1117	CLA	MG-NC	3.69	2.15	2.06
11	A	1124	CLA	OBD-CAD	3.69	1.28	1.22
11	B	1220	CLA	OBD-CAD	3.69	1.28	1.22
11	B	1207	CLA	OBD-CAD	3.69	1.28	1.22
11	b	1226	CLA	MG-NC	3.69	2.15	2.06
11	B	1210	CLA	MG-NC	3.69	2.15	2.06
11	A	1118	CLA	OBD-CAD	3.69	1.28	1.22
11	1	1109	CLA	OBD-CAD	3.69	1.28	1.22
11	b	1205	CLA	MG-NC	3.69	2.15	2.06
11	2	1228	CLA	MG-NC	3.69	2.15	2.06
11	8	1502	CLA	OBD-CAD	3.69	1.28	1.22
11	2	1021	CLA	MG-NC	3.69	2.15	2.06
11	A	1022	CLA	CHB-C1B	3.69	1.47	1.39
11	L	1503	CLA	OBD-CAD	3.69	1.28	1.22
14	1	4008	BCR	C10-C9	-3.69	1.27	1.35
11	A	1140	CLA	OBD-CAD	3.69	1.28	1.22
11	8	1503	CLA	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1022	CLA	OBD-CAD	3.69	1.28	1.22
11	1	1124	CLA	OBD-CAD	3.69	1.28	1.22
11	2	1236	CLA	MG-NC	3.69	2.15	2.06
11	b	1201	CLA	MG-NC	3.69	2.15	2.06
11	B	1023	CLA	CHD-C4C	3.69	1.47	1.39
11	A	1104	CLA	OBD-CAD	3.69	1.28	1.22
11	b	1235	CLA	OBD-CAD	3.69	1.28	1.22
11	L	1501	CLA	OBD-CAD	3.69	1.28	1.22
11	b	1217	CLA	OBD-CAD	3.69	1.28	1.22
11	b	1221	CLA	CHD-C4C	3.69	1.47	1.39
11	1	1119	CLA	OBD-CAD	3.68	1.28	1.22
11	A	1113	CLA	MG-NC	3.68	2.15	2.06
11	1	1103	CLA	MG-NC	3.68	2.15	2.06
11	A	1012	CLA	MG-NC	3.68	2.15	2.06
11	a	1111	CLA	MG-NC	3.68	2.15	2.06
11	b	1204	CLA	OBD-CAD	3.68	1.28	1.22
11	b	1224	CLA	OBD-CAD	3.68	1.28	1.22
11	B	1215	CLA	MG-NC	3.68	2.15	2.06
11	A	1136	CLA	OBD-CAD	3.68	1.28	1.22
11	B	1211	CLA	OBD-CAD	3.68	1.28	1.22
11	B	1239	CLA	MG-NC	3.68	2.15	2.06
11	2	1220	CLA	OBD-CAD	3.68	1.28	1.22
11	2	1224	CLA	OBD-CAD	3.68	1.28	1.22
11	1	1107	CLA	MG-NC	3.68	2.15	2.06
11	B	1216	CLA	OBD-CAD	3.68	1.28	1.22
11	a	1131	CLA	MG-NC	3.68	2.15	2.06
11	A	1126	CLA	MG-NC	3.68	2.15	2.06
11	b	1214	CLA	MG-NC	3.68	2.15	2.06
11	b	1228	CLA	OBD-CAD	3.67	1.28	1.22
11	a	1117	CLA	MG-NC	3.67	2.15	2.06
14	a	4003	BCR	C10-C9	-3.67	1.27	1.35
11	B	1217	CLA	MG-NC	3.67	2.15	2.06
11	a	1122	CLA	MG-NC	3.67	2.15	2.06
11	A	1113	CLA	OBD-CAD	3.67	1.28	1.22
11	A	1115	CLA	MG-NC	3.67	2.15	2.06
11	A	1107	CLA	CHD-C4C	3.67	1.47	1.39
11	1	1012	CLA	CHD-C4C	3.67	1.47	1.39
11	A	1122	CLA	CHD-C4C	3.67	1.47	1.39
11	2	1231	CLA	CHB-C1B	3.67	1.47	1.39
11	B	1202	CLA	MG-NC	3.67	2.15	2.06
11	B	1224	CLA	CHD-C4C	3.67	1.47	1.39
11	a	1138	CLA	MG-NC	3.67	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1204	CLA	MG-NC	3.67	2.15	2.06
11	B	1214	CLA	OBD-CAD	3.67	1.28	1.22
11	a	1124	CLA	OBD-CAD	3.67	1.28	1.22
11	B	1023	CLA	OBD-CAD	3.67	1.28	1.22
11	2	1224	CLA	MG-NC	3.67	2.15	2.06
11	B	1206	CLA	MG-NC	3.67	2.15	2.06
11	A	1237	CLA	OBD-CAD	3.67	1.28	1.22
11	l	1503	CLA	MG-NC	3.67	2.15	2.06
11	b	1207	CLA	MG-NC	3.67	2.15	2.06
11	A	1126	CLA	CHB-C1B	3.67	1.47	1.39
11	2	1216	CLA	OBD-CAD	3.67	1.28	1.22
11	A	1130	CLA	MG-NC	3.66	2.15	2.06
11	B	1224	CLA	MG-NC	3.66	2.15	2.06
11	A	1801	CLA	CHB-C1B	3.66	1.47	1.39
11	A	1133	CLA	MG-NC	3.66	2.15	2.06
11	b	1229	CLA	MG-NC	3.66	2.15	2.06
11	b	1202	CLA	MG-NC	3.66	2.15	2.06
11	a	1107	CLA	OBD-CAD	3.66	1.28	1.22
11	a	1134	CLA	MG-NC	3.66	2.15	2.06
11	b	1231	CLA	MG-NC	3.66	2.15	2.06
11	A	1129	CLA	OBD-CAD	3.66	1.28	1.22
11	B	1214	CLA	MG-NC	3.66	2.15	2.06
11	a	1132	CLA	MG-NC	3.66	2.15	2.06
11	1	1137	CLA	MG-NC	3.66	2.15	2.06
11	b	1219	CLA	OBD-CAD	3.66	1.28	1.22
11	A	1105	CLA	MG-NC	3.66	2.15	2.06
11	a	1125	CLA	MG-NC	3.66	2.15	2.06
11	A	1137	CLA	OBD-CAD	3.66	1.28	1.22
11	A	1137	CLA	MG-NC	3.66	2.15	2.06
11	B	1213	CLA	MG-NC	3.65	2.15	2.06
11	A	1106	CLA	OBD-CAD	3.65	1.28	1.22
11	b	1211	CLA	OBD-CAD	3.65	1.28	1.22
11	b	1238	CLA	MG-NC	3.65	2.14	2.06
11	b	1231	CLA	CHB-C1B	3.65	1.47	1.39
11	A	1140	CLA	MG-NC	3.65	2.14	2.06
11	1	1137	CLA	OBD-CAD	3.65	1.28	1.22
11	2	1210	CLA	MG-NC	3.65	2.14	2.06
11	A	1124	CLA	CHB-C1B	3.65	1.47	1.39
11	B	1219	CLA	OBD-CAD	3.65	1.28	1.22
11	a	1128	CLA	MG-NC	3.65	2.14	2.06
11	b	1228	CLA	MG-NC	3.65	2.14	2.06
11	A	1106	CLA	MG-NC	3.64	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1121	CLA	OBD-CAD	3.64	1.28	1.22
11	1	1109	CLA	MG-NC	3.64	2.14	2.06
11	1	1130	CLA	MG-NC	3.64	2.14	2.06
11	B	1211	CLA	MG-NC	3.64	2.14	2.06
11	2	1203	CLA	OBD-CAD	3.64	1.28	1.22
11	0	1402	CLA	MG-NC	3.64	2.14	2.06
11	b	1214	CLA	OBD-CAD	3.64	1.28	1.22
11	2	1203	CLA	MG-NC	3.64	2.14	2.06
11	a	1129	CLA	MG-NC	3.64	2.14	2.06
11	B	1208	CLA	MG-NC	3.63	2.14	2.06
11	B	1231	CLA	CHB-C1B	3.63	1.47	1.39
11	a	1127	CLA	OBD-CAD	3.63	1.28	1.22
11	2	1205	CLA	CHD-C4C	3.63	1.47	1.39
11	b	1215	CLA	MG-NC	3.63	2.14	2.06
11	a	1116	CLA	MG-NC	3.63	2.14	2.06
11	A	1115	CLA	OBD-CAD	3.63	1.28	1.22
11	1	1136	CLA	MG-NC	3.63	2.14	2.06
11	B	1207	CLA	MG-NC	3.63	2.14	2.06
11	B	1221	CLA	CHD-C4C	3.63	1.47	1.39
11	a	1130	CLA	MG-NC	3.63	2.14	2.06
11	2	1013	CLA	CHB-C1B	3.63	1.47	1.39
11	L	1503	CLA	MG-NC	3.63	2.14	2.06
11	1	1135	CLA	OBD-CAD	3.63	1.28	1.22
11	2	1234	CLA	OBD-CAD	3.63	1.28	1.22
14	F	4018	BCR	C11-C12	-3.63	1.25	1.34
11	a	1237	CLA	MG-NC	3.63	2.14	2.06
11	A	1111	CLA	MG-NC	3.62	2.14	2.06
11	2	1204	CLA	MG-NC	3.62	2.14	2.06
14	a	4008	BCR	C10-C9	-3.62	1.27	1.35
11	a	1103	CLA	OBD-CAD	3.62	1.28	1.22
11	B	1226	CLA	MG-NC	3.62	2.14	2.06
11	A	1011	CLA	CHB-C1B	3.62	1.47	1.39
11	B	1201	CLA	MG-NC	3.62	2.14	2.06
11	b	1238	CLA	OBD-CAD	3.62	1.28	1.22
11	B	1203	CLA	MG-NC	3.62	2.14	2.06
11	b	1206	CLA	MG-NC	3.62	2.14	2.06
11	B	1221	CLA	OBD-CAD	3.62	1.28	1.22
11	2	1208	CLA	MG-NC	3.62	2.14	2.06
11	2	1023	CLA	MG-NC	3.61	2.14	2.06
11	B	1216	CLA	MG-NC	3.61	2.14	2.06
11	b	1023	CLA	MG-NC	3.61	2.14	2.06
11	b	1236	CLA	MG-NC	3.61	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1136	CLA	MG-NC	3.61	2.14	2.06
11	B	1218	CLA	MG-NC	3.61	2.14	2.06
11	B	1205	CLA	MG-NC	3.61	2.14	2.06
11	1	1118	CLA	MG-NC	3.61	2.14	2.06
11	A	1120	CLA	MG-NC	3.61	2.14	2.06
11	1	1128	CLA	MG-NC	3.61	2.14	2.06
11	B	1023	CLA	MG-NC	3.61	2.14	2.06
11	1	1119	CLA	MG-NC	3.60	2.14	2.06
11	A	1135	CLA	CHB-C1B	3.60	1.47	1.39
11	a	1136	CLA	MG-NC	3.60	2.14	2.06
11	2	1021	CLA	CHB-C1B	3.60	1.47	1.39
11	B	1238	CLA	MG-NC	3.60	2.14	2.06
11	A	1237	CLA	MG-NC	3.60	2.14	2.06
11	b	1013	CLA	MG-NC	3.59	2.14	2.06
11	B	1228	CLA	MG-NC	3.59	2.14	2.06
11	a	1118	CLA	MG-NC	3.59	2.14	2.06
11	2	1202	CLA	MG-NC	3.59	2.14	2.06
11	b	1236	CLA	OBD-CAD	3.59	1.28	1.22
11	A	1117	CLA	MG-NC	3.59	2.14	2.06
11	a	1119	CLA	MG-NC	3.59	2.14	2.06
11	a	1104	CLA	MG-NC	3.58	2.14	2.06
11	1	1127	CLA	MG-NC	3.58	2.14	2.06
11	1	1012	CLA	OBD-CAD	3.58	1.28	1.22
11	A	1135	CLA	MG-NC	3.58	2.14	2.06
11	A	1107	CLA	MG-NC	3.57	2.14	2.06
11	A	1022	CLA	MG-NC	3.57	2.14	2.06
11	2	1217	CLA	OBD-CAD	3.57	1.28	1.22
11	k	1402	CLA	MG-NC	3.56	2.14	2.06
11	1	1125	CLA	OBD-CAD	3.56	1.28	1.22
11	A	1138	CLA	MG-NC	3.56	2.14	2.06
11	2	1226	CLA	MG-NC	3.56	2.14	2.06
11	L	1502	CLA	MG-NC	3.55	2.14	2.06
11	B	1021	CLA	MG-NC	3.55	2.14	2.06
11	A	1108	CLA	MG-NC	3.55	2.14	2.06
11	2	1214	CLA	MG-NC	3.55	2.14	2.06
11	2	1205	CLA	MG-NC	3.55	2.14	2.06
11	A	1121	CLA	OBD-CAD	3.55	1.28	1.22
11	2	1223	CLA	OBD-CAD	3.55	1.28	1.22
11	1	1237	CLA	MG-NC	3.54	2.14	2.06
11	A	1109	CLA	MG-NC	3.54	2.14	2.06
11	b	1226	CLA	OBD-CAD	3.54	1.28	1.22
11	B	1217	CLA	OBD-CAD	3.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1119	CLA	MG-NC	3.54	2.14	2.06
11	2	1207	CLA	MG-NC	3.53	2.14	2.06
11	A	1011	CLA	MG-NC	3.53	2.14	2.06
11	2	1211	CLA	MG-NC	3.53	2.14	2.06
11	A	1128	CLA	MG-NC	3.52	2.14	2.06
11	1	1138	CLA	MG-NC	3.52	2.14	2.06
11	1	1104	CLA	MG-NC	3.52	2.14	2.06
11	1	1106	CLA	MG-NC	3.52	2.14	2.06
11	A	1103	CLA	MG-NC	3.52	2.14	2.06
14	L	4022	BCR	C10-C9	-3.52	1.27	1.35
11	B	1236	CLA	MG-NC	3.52	2.14	2.06
11	B	1013	CLA	MG-NC	3.51	2.14	2.06
11	2	1023	CLA	CHB-C1B	3.51	1.47	1.39
11	B	1204	CLA	MG-NC	3.50	2.14	2.06
11	2	1013	CLA	MG-NC	3.50	2.14	2.06
11	2	1236	CLA	OBD-CAD	3.50	1.28	1.22
14	A	4003	BCR	C11-C12	-3.49	1.25	1.34
14	6	4013	BCR	C10-C9	-3.49	1.27	1.35
14	m	4021	BCR	C11-C12	-3.49	1.25	1.34
11	K	1402	CLA	MG-NC	3.48	2.14	2.06
11	A	1127	CLA	OBD-CAD	3.47	1.28	1.22
11	1	1237	CLA	OBD-CAD	3.47	1.28	1.22
11	A	1118	CLA	MG-NC	3.46	2.14	2.06
11	a	1119	CLA	OBD-CAD	3.46	1.28	1.22
11	A	1104	CLA	MG-NC	3.44	2.14	2.06
11	2	1218	CLA	MG-NC	3.44	2.14	2.06
14	f	4013	BCR	C10-C9	-3.44	1.27	1.35
14	2	4014	BCR	C11-C12	-3.44	1.25	1.34
11	B	1223	CLA	OBD-CAD	3.43	1.28	1.22
11	1	1115	CLA	OBD-CAD	3.42	1.28	1.22
14	6	4020	BCR	C11-C12	-3.41	1.25	1.34
11	A	1122	CLA	MG-NC	3.40	2.14	2.06
11	A	1012	CLA	C3D-C2D	3.40	1.48	1.39
11	1	1111	CLA	MG-NC	3.39	2.14	2.06
11	a	1125	CLA	OBD-CAD	3.37	1.28	1.22
14	6	4018	BCR	C11-C12	-3.35	1.25	1.34
14	M	4021	BCR	C11-C12	-3.35	1.25	1.34
11	a	1012	CLA	C3D-C2D	3.35	1.48	1.39
14	2	4010	BCR	C11-C12	-3.33	1.26	1.34
11	1	1012	CLA	C3D-C2D	3.31	1.48	1.39
14	b	4017	BCR	C11-C12	-3.29	1.26	1.34
14	2	4011	BCR	C11-C12	-3.28	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	4003	BCR	C11-C12	-3.28	1.26	1.34
11	a	1011	CLA	C4D-CHA	3.28	1.49	1.38
14	B	4011	BCR	C11-C12	-3.27	1.26	1.34
14	7	4021	BCR	C11-C12	-3.27	1.26	1.34
14	f	4020	BCR	C11-C12	-3.27	1.26	1.34
11	A	1119	CLA	OBD-CAD	3.26	1.28	1.22
14	B	4004	BCR	C11-C12	-3.25	1.26	1.34
11	a	1022	CLA	C3D-C2D	3.25	1.47	1.39
14	B	4009	BCR	C11-C12	-3.24	1.26	1.34
14	b	4004	BCR	C11-C12	-3.24	1.26	1.34
11	B	1236	CLA	OBD-CAD	3.23	1.28	1.22
14	b	4010	BCR	C11-C12	-3.23	1.26	1.34
14	B	4005	BCR	C11-C12	-3.23	1.26	1.34
14	A	4001	BCR	C11-C12	-3.22	1.26	1.34
14	b	4014	BCR	C11-C12	-3.22	1.26	1.34
14	F	4020	BCR	C11-C12	-3.21	1.26	1.34
11	A	1125	CLA	OBD-CAD	3.20	1.28	1.22
14	b	4005	BCR	C11-C12	-3.19	1.26	1.34
14	a	4008	BCR	C11-C12	-3.18	1.26	1.34
11	A	1132	CLA	C1B-C2B	3.18	1.50	1.43
14	f	4018	BCR	C11-C12	-3.18	1.26	1.34
11	B	1013	CLA	C3D-C2D	3.18	1.47	1.39
14	b	4011	BCR	C11-C12	-3.17	1.26	1.34
11	A	1022	CLA	C3D-C2D	3.17	1.47	1.39
14	A	4007	BCR	C11-C12	-3.17	1.26	1.34
14	8	4022	BCR	C11-C12	-3.16	1.26	1.34
14	2	4017	BCR	C11-C12	-3.15	1.26	1.34
11	1	1022	CLA	C3D-C2D	3.15	1.47	1.39
14	1	4008	BCR	C11-C12	-3.15	1.26	1.34
14	b	4006	BCR	C11-C12	-3.14	1.26	1.34
11	A	1011	CLA	C4D-CHA	3.14	1.49	1.38
14	l	4019	BCR	C11-C12	-3.14	1.26	1.34
11	b	1232	CLA	C3D-C2D	3.14	1.47	1.39
14	F	4013	BCR	C11-C12	-3.14	1.26	1.34
14	f	4013	BCR	C11-C12	-3.13	1.26	1.34
11	b	1215	CLA	C3D-C2D	3.13	1.47	1.39
11	2	1208	CLA	C3D-C2D	3.13	1.47	1.39
11	A	1127	CLA	C3D-C2D	3.13	1.47	1.39
11	A	1128	CLA	C3D-C2D	3.13	1.47	1.39
14	B	4017	BCR	C11-C12	-3.12	1.26	1.34
11	B	1205	CLA	C1B-C2B	3.12	1.50	1.43
11	2	1212	CLA	C3D-C2D	3.12	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1117	CLA	C3D-C2D	3.11	1.47	1.39
11	A	1011	CLA	C1B-NB	-3.11	1.33	1.37
11	B	1234	CLA	C1B-C2B	3.11	1.50	1.43
11	2	1230	CLA	C3D-C2D	3.11	1.47	1.39
11	1	1114	CLA	C3D-C2D	3.10	1.47	1.39
11	B	1231	CLA	C3D-C2D	3.10	1.47	1.39
11	b	1219	CLA	C3D-C2D	3.10	1.47	1.39
11	b	1013	CLA	C3D-C2D	3.10	1.47	1.39
11	a	1130	CLA	C3D-C2D	3.10	1.47	1.39
11	1	1012	CLA	C1D-ND	-3.10	1.33	1.37
11	b	1208	CLA	C3D-C2D	3.09	1.47	1.39
14	2	4006	BCR	C11-C12	-3.09	1.26	1.34
11	B	1230	CLA	C3D-C2D	3.09	1.47	1.39
14	l	4022	BCR	C11-C12	-3.09	1.26	1.34
11	a	1119	CLA	C3D-C2D	3.09	1.47	1.39
11	A	1102	CLA	C3D-C2D	3.09	1.47	1.39
11	2	1013	CLA	C3D-C2D	3.09	1.47	1.39
11	a	1128	CLA	C3D-C2D	3.09	1.47	1.39
11	1	1110	CLA	C3D-C2D	3.09	1.47	1.39
11	2	1205	CLA	C1D-ND	-3.09	1.33	1.37
11	a	1109	CLA	C3D-C2D	3.09	1.47	1.39
14	a	4007	BCR	C11-C12	-3.09	1.26	1.34
11	A	1131	CLA	C3D-C2D	3.09	1.47	1.39
11	A	1109	CLA	C3D-C2D	3.09	1.47	1.39
11	1	1117	CLA	C3D-C2D	3.09	1.47	1.39
11	l	1503	CLA	C3D-C2D	3.08	1.47	1.39
14	B	4006	BCR	C11-C12	-3.08	1.26	1.34
11	2	1023	CLA	C3D-C2D	3.08	1.47	1.39
11	a	1114	CLA	C3D-C2D	3.08	1.47	1.39
11	1	1120	CLA	C3D-C2D	3.08	1.47	1.39
11	A	1133	CLA	C3D-C2D	3.08	1.47	1.39
14	L	4019	BCR	C11-C12	-3.08	1.26	1.34
11	A	1012	CLA	C1D-ND	-3.08	1.33	1.37
11	k	1402	CLA	C3D-C2D	3.08	1.47	1.39
11	2	1217	CLA	C3D-C2D	3.07	1.47	1.39
11	a	1110	CLA	C3D-C2D	3.07	1.47	1.39
11	b	1228	CLA	C3D-C2D	3.07	1.47	1.39
14	a	4001	BCR	C11-C12	-3.07	1.26	1.34
11	b	1229	CLA	C3D-C2D	3.07	1.47	1.39
11	b	1211	CLA	C3D-C2D	3.07	1.47	1.39
11	a	1117	CLA	C3D-C2D	3.07	1.47	1.39
11	B	1209	CLA	C3D-C2D	3.07	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1137	CLA	C3D-C2D	3.06	1.47	1.39
11	2	1215	CLA	C3D-C2D	3.06	1.47	1.39
11	B	1228	CLA	C3D-C2D	3.06	1.47	1.39
11	B	1232	CLA	C3D-C2D	3.06	1.47	1.39
11	K	1401	CLA	C1B-C2B	3.06	1.50	1.43
11	a	1132	CLA	C3D-C2D	3.06	1.47	1.39
11	1	1128	CLA	C3D-C2D	3.06	1.47	1.39
11	1	1133	CLA	C3D-C2D	3.06	1.47	1.39
11	b	1230	CLA	C3D-C2D	3.06	1.47	1.39
11	2	1236	CLA	C3D-C2D	3.06	1.47	1.39
14	2	4009	BCR	C11-C12	-3.06	1.26	1.34
14	a	4002	BCR	C11-C12	-3.06	1.26	1.34
11	k	1401	CLA	C1B-C2B	3.06	1.50	1.43
11	a	1107	CLA	C4D-CHA	3.06	1.48	1.38
11	b	1212	CLA	C1B-C2B	3.06	1.50	1.43
11	0	1401	CLA	C1B-C2B	3.06	1.50	1.43
11	a	1011	CLA	C1B-NB	-3.06	1.33	1.37
11	B	1212	CLA	C3D-C2D	3.06	1.47	1.39
11	a	1131	CLA	C3D-C2D	3.06	1.47	1.39
11	b	1238	CLA	C3D-C2D	3.06	1.47	1.39
11	1	1105	CLA	C3D-C2D	3.05	1.47	1.39
14	2	4005	BCR	C11-C12	-3.05	1.26	1.34
11	1	1132	CLA	C3D-C2D	3.05	1.47	1.39
11	B	1229	CLA	C3D-C2D	3.05	1.47	1.39
11	2	1021	CLA	C4D-CHA	3.05	1.48	1.38
14	1	4001	BCR	C11-C12	-3.05	1.26	1.34
11	2	1227	CLA	C3D-C2D	3.05	1.47	1.39
14	a	4003	BCR	C11-C12	-3.05	1.26	1.34
11	2	1204	CLA	C3D-C2D	3.05	1.47	1.39
11	A	1106	CLA	C3D-C2D	3.05	1.47	1.39
11	A	1130	CLA	C3D-C2D	3.05	1.47	1.39
11	B	1206	CLA	C3D-C2D	3.05	1.47	1.39
11	A	1114	CLA	C3D-C2D	3.05	1.47	1.39
11	b	1223	CLA	C1B-C2B	3.05	1.50	1.43
11	b	1203	CLA	C3D-C2D	3.05	1.47	1.39
11	a	1133	CLA	C3D-C2D	3.05	1.47	1.39
11	a	1120	CLA	C4D-CHA	3.05	1.48	1.38
11	A	1135	CLA	C3D-C2D	3.04	1.47	1.39
11	l	1501	CLA	C3D-C2D	3.04	1.47	1.39
11	1	1126	CLA	C3D-C2D	3.04	1.47	1.39
11	2	1239	CLA	C3D-C2D	3.04	1.47	1.39
11	a	1126	CLA	C3D-C2D	3.04	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1101	CLA	C3D-C2D	3.04	1.47	1.39
11	1	1103	CLA	C4D-CHA	3.04	1.48	1.38
11	1	1801	CLA	C3D-C2D	3.04	1.47	1.39
11	1	1130	CLA	C3D-C2D	3.04	1.47	1.39
11	2	1228	CLA	C3D-C2D	3.04	1.47	1.39
11	2	1021	CLA	C3D-C2D	3.04	1.47	1.39
11	2	1213	CLA	C3D-C2D	3.03	1.47	1.39
11	a	1102	CLA	C3D-C2D	3.03	1.47	1.39
14	2	4004	BCR	C11-C12	-3.03	1.26	1.34
11	b	1218	CLA	C3D-C2D	3.03	1.47	1.39
11	B	1221	CLA	C4D-CHA	3.03	1.48	1.38
11	B	1231	CLA	C4D-CHA	3.03	1.48	1.38
11	B	1213	CLA	C3D-C2D	3.03	1.47	1.39
11	1	1109	CLA	C3D-C2D	3.03	1.47	1.39
14	1	4002	BCR	C11-C12	-3.03	1.26	1.34
11	K	1402	CLA	C3D-C2D	3.03	1.47	1.39
11	b	1206	CLA	C3D-C2D	3.03	1.47	1.39
11	a	1123	CLA	C3D-C2D	3.03	1.47	1.39
11	A	1111	CLA	C3D-C2D	3.03	1.47	1.39
11	l	1502	CLA	C3D-C2D	3.03	1.47	1.39
11	2	1206	CLA	C3D-C2D	3.03	1.47	1.39
11	B	1235	CLA	C3D-C2D	3.03	1.47	1.39
11	a	1122	CLA	C3D-C2D	3.02	1.47	1.39
11	B	1210	CLA	C3D-C2D	3.02	1.47	1.39
11	1	1119	CLA	C3D-C2D	3.02	1.47	1.39
11	A	1124	CLA	C3D-C2D	3.02	1.47	1.39
11	b	1204	CLA	C3D-C2D	3.02	1.47	1.39
14	L	4022	BCR	C11-C12	-3.02	1.26	1.34
11	B	1227	CLA	C1B-C2B	3.02	1.50	1.43
11	a	1011	CLA	C3D-C2D	3.02	1.47	1.39
11	2	1021	CLA	C1B-NB	-3.02	1.33	1.37
11	b	1239	CLA	C3D-C2D	3.02	1.47	1.39
11	b	1234	CLA	C3D-C2D	3.02	1.47	1.39
11	1	1123	CLA	C3D-C2D	3.02	1.47	1.39
11	A	1011	CLA	C3D-C2D	3.02	1.47	1.39
11	1	1122	CLA	C3D-C2D	3.02	1.47	1.39
11	1	1135	CLA	C3D-C2D	3.02	1.47	1.39
11	a	1105	CLA	C3D-C2D	3.02	1.47	1.39
11	2	1221	CLA	C4D-CHA	3.02	1.48	1.38
11	B	1215	CLA	C3D-C2D	3.02	1.47	1.39
11	a	1101	CLA	C3D-C2D	3.01	1.47	1.39
11	8	1503	CLA	C3D-C2D	3.01	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1240	CLA	C3D-C2D	3.01	1.47	1.39
11	A	1116	CLA	C3D-C2D	3.01	1.47	1.39
11	A	1108	CLA	C3D-C2D	3.01	1.47	1.39
11	1	1138	CLA	C3D-C2D	3.01	1.47	1.39
11	a	1801	CLA	C3D-C2D	3.01	1.47	1.39
11	A	1237	CLA	C3D-C2D	3.01	1.47	1.39
11	a	1105	CLA	C1B-C2B	3.01	1.50	1.43
11	2	1234	CLA	C3D-C2D	3.01	1.47	1.39
11	b	1217	CLA	C3D-C2D	3.01	1.47	1.39
11	b	1240	CLA	C3D-C2D	3.01	1.47	1.39
11	1	1102	CLA	C3D-C2D	3.01	1.47	1.39
11	2	1238	CLA	C3D-C2D	3.01	1.47	1.39
14	A	4008	BCR	C11-C12	-3.01	1.26	1.34
11	b	1214	CLA	C3D-C2D	3.01	1.47	1.39
11	2	1229	CLA	C3D-C2D	3.01	1.47	1.39
11	a	1137	CLA	C3D-C2D	3.01	1.47	1.39
11	B	1204	CLA	C3D-C2D	3.01	1.47	1.39
11	B	1227	CLA	C3D-C2D	3.01	1.47	1.39
11	B	1234	CLA	C3D-C2D	3.00	1.47	1.39
11	a	1106	CLA	C3D-C2D	3.00	1.47	1.39
11	2	1231	CLA	C4D-CHA	3.00	1.48	1.38
11	b	1023	CLA	C3D-C2D	3.00	1.47	1.39
11	2	1209	CLA	C3D-C2D	3.00	1.47	1.39
11	B	1208	CLA	C3D-C2D	3.00	1.47	1.39
11	B	1239	CLA	C3D-C2D	3.00	1.47	1.39
11	1	1121	CLA	C3D-C2D	3.00	1.47	1.39
11	A	1125	CLA	C1B-C2B	3.00	1.50	1.43
11	a	1127	CLA	C3D-C2D	3.00	1.47	1.39
11	0	1402	CLA	C3D-C2D	3.00	1.47	1.39
11	8	1501	CLA	C4D-CHA	3.00	1.48	1.38
14	B	4010	BCR	C11-C12	-3.00	1.26	1.34
11	a	1134	CLA	C3D-C2D	3.00	1.47	1.39
11	B	1220	CLA	C3D-C2D	3.00	1.47	1.39
11	a	1129	CLA	C3D-C2D	3.00	1.47	1.39
11	b	1212	CLA	C3D-C2D	3.00	1.47	1.39
11	8	1502	CLA	C3D-C2D	3.00	1.47	1.39
11	b	1209	CLA	C3D-C2D	3.00	1.47	1.39
11	1	1118	CLA	C3D-C2D	3.00	1.47	1.39
11	2	1201	CLA	C1B-C2B	3.00	1.50	1.43
11	b	1227	CLA	C3D-C2D	3.00	1.47	1.39
11	B	1013	CLA	C1D-ND	-3.00	1.33	1.37
11	8	1501	CLA	C3D-C2D	3.00	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1139	CLA	C3D-C2D	3.00	1.47	1.39
11	a	1117	CLA	C1B-C2B	3.00	1.50	1.43
11	A	1110	CLA	C3D-C2D	2.99	1.47	1.39
11	1	1102	CLA	C4D-CHA	2.99	1.48	1.38
14	1	4007	BCR	C11-C12	-2.99	1.26	1.34
11	a	1124	CLA	C3D-C2D	2.99	1.47	1.39
11	1	1127	CLA	C3D-C2D	2.99	1.47	1.39
11	1	1112	CLA	C3D-C2D	2.99	1.47	1.39
11	L	1503	CLA	C1B-C2B	2.99	1.50	1.43
11	B	1240	CLA	C3D-C2D	2.99	1.47	1.39
11	L	1503	CLA	C3D-C2D	2.99	1.47	1.39
11	2	1207	CLA	C3D-C2D	2.99	1.47	1.39
11	a	1108	CLA	C3D-C2D	2.99	1.47	1.39
14	B	4014	BCR	C11-C12	-2.99	1.26	1.34
11	1	1131	CLA	C3D-C2D	2.99	1.47	1.39
11	a	1103	CLA	C3D-C2D	2.99	1.47	1.39
11	2	1218	CLA	C3D-C2D	2.99	1.47	1.39
11	k	1401	CLA	C4D-CHA	2.99	1.48	1.38
11	2	1210	CLA	C3D-C2D	2.99	1.47	1.39
11	2	1232	CLA	C3D-C2D	2.99	1.47	1.39
11	B	1219	CLA	C3D-C2D	2.99	1.47	1.39
11	a	1108	CLA	C1B-C2B	2.98	1.50	1.43
11	1	1134	CLA	C3D-C2D	2.98	1.47	1.39
11	b	1216	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1104	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1140	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1011	CLA	C4D-CHA	2.98	1.48	1.38
11	b	1210	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1113	CLA	C3D-C2D	2.98	1.47	1.39
11	b	1021	CLA	C3D-C2D	2.98	1.47	1.39
11	2	1211	CLA	C3D-C2D	2.98	1.47	1.39
11	A	1801	CLA	C3D-C2D	2.98	1.47	1.39
11	b	1220	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1115	CLA	C3D-C2D	2.98	1.47	1.39
11	A	1118	CLA	C1B-C2B	2.98	1.50	1.43
11	2	1208	CLA	C1B-C2B	2.98	1.50	1.43
11	A	1139	CLA	C3D-C2D	2.98	1.47	1.39
11	B	1216	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1136	CLA	C1B-C2B	2.98	1.50	1.43
11	L	1501	CLA	C3D-C2D	2.98	1.47	1.39
11	A	1113	CLA	C3D-C2D	2.98	1.47	1.39
11	B	1021	CLA	C1B-C2B	2.98	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1011	CLA	C1B-NB	-2.98	1.33	1.37
11	0	1401	CLA	C4D-CHA	2.98	1.48	1.38
11	a	1112	CLA	C3D-C2D	2.98	1.47	1.39
11	a	1106	CLA	C4D-CHA	2.98	1.48	1.38
11	a	1140	CLA	C3D-C2D	2.98	1.47	1.39
11	1	1108	CLA	C3D-C2D	2.98	1.47	1.39
11	B	1222	CLA	C3D-C2D	2.97	1.47	1.39
11	A	1125	CLA	C3D-C2D	2.97	1.47	1.39
11	A	1140	CLA	C3D-C2D	2.97	1.47	1.39
11	a	1136	CLA	C3D-C2D	2.97	1.47	1.39
11	1	1110	CLA	C4D-CHA	2.97	1.48	1.38
11	L	1502	CLA	C3D-C2D	2.97	1.47	1.39
11	b	1201	CLA	C3D-C2D	2.97	1.47	1.39
11	a	1104	CLA	C3D-C2D	2.97	1.47	1.39
11	K	1401	CLA	C4D-CHA	2.97	1.48	1.38
14	6	4013	BCR	C11-C12	-2.97	1.26	1.34
11	b	1221	CLA	C4D-CHA	2.97	1.48	1.38
11	B	1218	CLA	C1B-C2B	2.97	1.50	1.43
14	8	4019	BCR	C11-C12	-2.97	1.26	1.34
11	2	1235	CLA	C3D-C2D	2.97	1.47	1.39
11	b	1205	CLA	C3D-C2D	2.97	1.47	1.39
11	0	1401	CLA	C3D-C2D	2.96	1.47	1.39
11	2	1205	CLA	C1B-C2B	2.96	1.50	1.43
11	B	1205	CLA	C4D-CHA	2.96	1.48	1.38
11	a	1113	CLA	C3D-C2D	2.96	1.47	1.39
11	2	1220	CLA	C3D-C2D	2.96	1.47	1.39
11	B	1021	CLA	C4D-CHA	2.96	1.48	1.38
11	2	1219	CLA	C4D-CHA	2.96	1.48	1.38
11	a	1138	CLA	C4D-CHA	2.96	1.48	1.38
11	b	1226	CLA	C3D-C2D	2.96	1.47	1.39
11	1	1123	CLA	C4D-CHA	2.96	1.48	1.38
11	b	1222	CLA	C3D-C2D	2.96	1.47	1.39
11	B	1021	CLA	C3D-C2D	2.96	1.47	1.39
11	a	1120	CLA	C3D-C2D	2.96	1.47	1.39
11	A	1125	CLA	C4C-C3C	2.96	1.50	1.45
11	A	1102	CLA	C4D-CHA	2.96	1.48	1.38
11	a	1102	CLA	C4D-CHA	2.96	1.48	1.38
11	2	1224	CLA	C1B-C2B	2.96	1.50	1.43
11	B	1202	CLA	C3D-C2D	2.96	1.47	1.39
11	B	1240	CLA	C4D-CHA	2.95	1.48	1.38
11	B	1222	CLA	C1D-ND	-2.95	1.34	1.37
11	b	1230	CLA	C4D-CHA	2.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1222	CLA	C4D-CHA	2.95	1.48	1.38
11	A	1119	CLA	C3D-C2D	2.95	1.47	1.39
11	2	1223	CLA	C3D-C2D	2.95	1.47	1.39
11	b	1219	CLA	C4D-CHA	2.95	1.48	1.38
11	A	1121	CLA	C3D-C2D	2.95	1.47	1.39
11	b	1213	CLA	C3D-C2D	2.95	1.47	1.39
11	A	1132	CLA	C3D-C2D	2.95	1.47	1.39
11	B	1214	CLA	C3D-C2D	2.95	1.47	1.39
11	a	1138	CLA	C3D-C2D	2.95	1.47	1.39
11	2	1221	CLA	C3D-C2D	2.95	1.47	1.39
11	1	1113	CLA	C1B-C2B	2.95	1.50	1.43
11	1	1135	CLA	C4D-CHA	2.95	1.48	1.38
14	A	4002	BCR	C11-C12	-2.95	1.27	1.34
11	B	1232	CLA	C1B-C2B	2.95	1.50	1.43
11	a	1114	CLA	C1B-C2B	2.95	1.50	1.43
11	a	1118	CLA	C1B-C2B	2.94	1.50	1.43
11	1	1116	CLA	C3D-C2D	2.94	1.47	1.39
11	1	1124	CLA	C3D-C2D	2.94	1.47	1.39
11	K	1401	CLA	C3D-C2D	2.94	1.47	1.39
11	b	1224	CLA	C1B-C2B	2.94	1.50	1.43
11	A	1116	CLA	C4D-CHA	2.94	1.48	1.38
11	1	1103	CLA	C1B-C2B	2.94	1.50	1.43
11	b	1222	CLA	C4D-CHA	2.94	1.48	1.38
11	A	1134	CLA	C3D-C2D	2.94	1.47	1.39
11	b	1230	CLA	C1B-C2B	2.94	1.50	1.43
11	b	1207	CLA	C1B-C2B	2.94	1.50	1.43
11	A	1115	CLA	C3D-C2D	2.94	1.47	1.39
11	B	1023	CLA	C3D-C2D	2.94	1.47	1.39
11	A	1114	CLA	C1B-C2B	2.94	1.50	1.43
11	b	1021	CLA	C4D-CHA	2.94	1.48	1.38
11	a	1121	CLA	C4D-CHA	2.94	1.48	1.38
11	b	1205	CLA	C1B-C2B	2.94	1.50	1.43
11	b	1239	CLA	C1B-C2B	2.94	1.50	1.43
11	A	1106	CLA	C1B-C2B	2.94	1.50	1.43
11	1	1120	CLA	C4D-CHA	2.94	1.48	1.38
11	a	1139	CLA	C1B-C2B	2.94	1.50	1.43
11	k	1401	CLA	C3D-C2D	2.94	1.47	1.39
11	b	1234	CLA	C4D-CHA	2.94	1.48	1.38
11	a	1113	CLA	C1B-C2B	2.93	1.50	1.43
11	A	1138	CLA	C3D-C2D	2.93	1.47	1.39
11	a	1127	CLA	C1B-NB	-2.93	1.34	1.37
11	1	1125	CLA	C3D-C2D	2.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1214	CLA	C3D-C2D	2.93	1.47	1.39
11	a	1121	CLA	C3D-C2D	2.93	1.47	1.39
11	A	1103	CLA	C1B-C2B	2.93	1.50	1.43
11	B	1238	CLA	C3D-C2D	2.93	1.47	1.39
11	1	1140	CLA	C4D-CHA	2.93	1.48	1.38
11	b	1209	CLA	C1B-C2B	2.93	1.50	1.43
11	b	1235	CLA	C3D-C2D	2.93	1.47	1.39
11	a	1237	CLA	C3D-C2D	2.93	1.47	1.39
11	B	1209	CLA	C4D-CHA	2.93	1.48	1.38
11	B	1206	CLA	C1B-C2B	2.93	1.50	1.43
11	a	1135	CLA	C3D-C2D	2.93	1.47	1.39
11	b	1234	CLA	C1B-C2B	2.93	1.50	1.43
11	b	1202	CLA	C4D-CHA	2.93	1.48	1.38
11	a	1118	CLA	C3D-C2D	2.93	1.47	1.39
11	1	1118	CLA	C1D-ND	-2.93	1.34	1.37
11	a	1129	CLA	C1B-C2B	2.93	1.50	1.43
11	2	1227	CLA	C1B-C2B	2.93	1.50	1.43
11	1	1106	CLA	C3D-C2D	2.93	1.47	1.39
11	b	1231	CLA	C3D-C2D	2.93	1.47	1.39
11	A	1801	CLA	C4D-CHA	2.93	1.48	1.38
11	B	1218	CLA	C3D-C2D	2.93	1.47	1.39
11	1	1136	CLA	C3D-C2D	2.93	1.47	1.39
11	2	1216	CLA	C4D-CHA	2.93	1.48	1.38
11	1	1121	CLA	C1B-C2B	2.93	1.50	1.43
11	2	1222	CLA	C3D-C2D	2.92	1.47	1.39
11	b	1204	CLA	C1B-C2B	2.92	1.50	1.43
11	A	1129	CLA	C3D-C2D	2.92	1.47	1.39
11	a	1139	CLA	C3D-C2D	2.92	1.47	1.39
11	A	1122	CLA	C1B-C2B	2.92	1.50	1.43
11	2	1203	CLA	C3D-C2D	2.92	1.47	1.39
11	2	1217	CLA	C4D-CHA	2.92	1.48	1.38
11	a	1111	CLA	C3D-C2D	2.92	1.47	1.39
11	b	1221	CLA	C3D-C2D	2.92	1.47	1.39
11	B	1201	CLA	C4D-CHA	2.92	1.48	1.38
11	a	1111	CLA	C1B-C2B	2.92	1.50	1.43
11	2	1234	CLA	C1B-C2B	2.92	1.50	1.43
11	a	1116	CLA	C3D-C2D	2.92	1.47	1.39
11	A	1138	CLA	C1B-C2B	2.92	1.50	1.43
11	B	1221	CLA	C3D-C2D	2.92	1.47	1.39
11	A	1120	CLA	C3D-C2D	2.92	1.47	1.39
11	b	1211	CLA	C1B-C2B	2.92	1.50	1.43
11	A	1125	CLA	C4D-CHA	2.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1105	CLA	C1B-C2B	2.92	1.50	1.43
11	B	1223	CLA	C3D-C2D	2.91	1.46	1.39
11	A	1112	CLA	C4D-CHA	2.91	1.48	1.38
11	L	1501	CLA	C4D-CHA	2.91	1.48	1.38
11	b	1222	CLA	C1B-C2B	2.91	1.50	1.43
11	1	1138	CLA	C1B-C2B	2.91	1.50	1.43
11	b	1223	CLA	C3D-C2D	2.91	1.46	1.39
11	1	1137	CLA	C4D-CHA	2.91	1.48	1.38
11	B	1229	CLA	C1B-C2B	2.91	1.50	1.43
11	A	1104	CLA	C1D-ND	-2.91	1.34	1.37
11	b	1207	CLA	C3D-C2D	2.91	1.46	1.39
11	a	1237	CLA	C1B-C2B	2.91	1.50	1.43
11	B	1230	CLA	C1B-C2B	2.91	1.50	1.43
11	A	1117	CLA	C1B-NB	-2.91	1.34	1.37
11	A	1136	CLA	C3D-C2D	2.91	1.46	1.39
11	b	1239	CLA	C4D-CHA	2.91	1.48	1.38
11	2	1203	CLA	C4D-CHA	2.91	1.48	1.38
11	2	1201	CLA	C3D-C2D	2.91	1.46	1.39
11	a	1113	CLA	C4D-CHA	2.91	1.48	1.38
11	B	1219	CLA	C4D-CHA	2.91	1.48	1.38
11	l	1501	CLA	C4D-CHA	2.91	1.48	1.38
11	A	1140	CLA	C4D-CHA	2.91	1.48	1.38
11	a	1126	CLA	C4D-CHA	2.91	1.48	1.38
11	B	1213	CLA	C1B-C2B	2.91	1.49	1.43
11	1	1237	CLA	C3D-C2D	2.91	1.46	1.39
11	a	1120	CLA	C1B-C2B	2.91	1.49	1.43
11	2	1230	CLA	C4D-CHA	2.91	1.48	1.38
11	b	1202	CLA	C3D-C2D	2.91	1.46	1.39
11	A	1122	CLA	C1D-ND	-2.91	1.34	1.37
11	2	1239	CLA	C1B-C2B	2.90	1.49	1.43
11	1	1801	CLA	C4D-CHA	2.90	1.48	1.38
11	A	1124	CLA	C4D-CHA	2.90	1.48	1.38
11	2	1201	CLA	C4D-CHA	2.90	1.48	1.38
11	A	1105	CLA	C3D-C2D	2.90	1.46	1.39
11	b	1224	CLA	C3D-C2D	2.90	1.46	1.39
11	b	1203	CLA	C4D-CHA	2.90	1.48	1.38
11	2	1215	CLA	C4D-CHA	2.90	1.48	1.38
11	2	1216	CLA	C3D-C2D	2.90	1.46	1.39
11	A	1110	CLA	C1B-C2B	2.90	1.49	1.43
11	A	1133	CLA	C4D-CHA	2.90	1.48	1.38
11	1	1121	CLA	C4D-CHA	2.90	1.48	1.38
11	A	1122	CLA	C3D-C2D	2.90	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1113	CLA	C4D-CHA	2.90	1.48	1.38
11	b	1208	CLA	C1B-C2B	2.90	1.49	1.43
11	1	1108	CLA	C1B-C2B	2.90	1.49	1.43
11	2	1239	CLA	C4D-CHA	2.90	1.48	1.38
11	B	1217	CLA	C3D-C2D	2.90	1.46	1.39
11	b	1235	CLA	C4D-CHA	2.90	1.48	1.38
11	A	1110	CLA	C4D-CHA	2.90	1.48	1.38
11	2	1222	CLA	C4D-CHA	2.90	1.48	1.38
11	2	1209	CLA	C4D-CHA	2.90	1.48	1.38
11	A	1137	CLA	C3D-C2D	2.90	1.46	1.39
11	1	1105	CLA	C1B-C2B	2.90	1.49	1.43
11	a	1139	CLA	C4D-CHA	2.90	1.48	1.38
11	B	1203	CLA	C3D-C2D	2.89	1.46	1.39
11	2	1217	CLA	C1B-C2B	2.89	1.49	1.43
11	B	1205	CLA	C3D-C2D	2.89	1.46	1.39
11	B	1230	CLA	C4D-CHA	2.89	1.48	1.38
11	1	1011	CLA	C3D-C2D	2.89	1.46	1.39
11	2	1213	CLA	C1B-C2B	2.89	1.49	1.43
11	b	1231	CLA	C4D-CHA	2.89	1.48	1.38
11	1	1237	CLA	C1B-C2B	2.89	1.49	1.43
11	1	1129	CLA	C3D-C2D	2.89	1.46	1.39
11	b	1228	CLA	C4D-CHA	2.89	1.48	1.38
11	b	1220	CLA	C1B-C2B	2.89	1.49	1.43
11	1	1131	CLA	C1B-C2B	2.89	1.49	1.43
11	B	1225	CLA	C3D-C2D	2.89	1.46	1.39
11	2	1231	CLA	C3D-C2D	2.89	1.46	1.39
11	a	1125	CLA	C3D-C2D	2.89	1.46	1.39
11	B	1236	CLA	C1B-C2B	2.89	1.49	1.43
11	a	1112	CLA	C4D-CHA	2.89	1.48	1.38
11	2	1206	CLA	C4D-CHA	2.89	1.48	1.38
11	B	1236	CLA	C3D-C2D	2.89	1.46	1.39
11	a	1115	CLA	C3D-C2D	2.88	1.46	1.39
11	b	1224	CLA	C4D-CHA	2.88	1.48	1.38
11	2	1226	CLA	C1B-C2B	2.88	1.49	1.43
11	a	1135	CLA	C4D-CHA	2.88	1.48	1.38
11	b	1207	CLA	C4D-CHA	2.88	1.48	1.38
11	1	1103	CLA	C3D-C2D	2.88	1.46	1.39
11	2	1234	CLA	C4D-CHA	2.88	1.48	1.38
11	b	1201	CLA	C1B-C2B	2.88	1.49	1.43
11	A	1131	CLA	C4D-CHA	2.88	1.48	1.38
11	a	1136	CLA	C1B-C2B	2.88	1.49	1.43
11	2	1240	CLA	C4D-CHA	2.88	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1107	CLA	C3D-C2D	2.88	1.46	1.39
11	A	1104	CLA	C1B-C2B	2.88	1.49	1.43
11	B	1207	CLA	C3D-C2D	2.88	1.46	1.39
11	a	1012	CLA	C4D-CHA	2.88	1.48	1.38
11	2	1235	CLA	C4D-CHA	2.88	1.48	1.38
11	B	1232	CLA	C4D-CHA	2.88	1.48	1.38
11	1	1108	CLA	C4D-CHA	2.88	1.48	1.38
11	A	1134	CLA	C4D-CHA	2.87	1.48	1.38
11	B	1210	CLA	C4D-CHA	2.87	1.48	1.38
11	1	1115	CLA	C1B-C2B	2.87	1.49	1.43
11	2	1013	CLA	C4D-CHA	2.87	1.48	1.38
11	a	1131	CLA	C4D-CHA	2.87	1.48	1.38
11	a	1133	CLA	C1B-C2B	2.87	1.49	1.43
11	1	1101	CLA	C1B-C2B	2.87	1.49	1.43
11	B	1204	CLA	C1B-C2B	2.87	1.49	1.43
11	a	1012	CLA	C1D-ND	-2.87	1.34	1.37
11	A	1123	CLA	C3D-C2D	2.87	1.46	1.39
11	A	1022	CLA	C1D-ND	-2.87	1.34	1.37
11	A	1126	CLA	C3D-C2D	2.87	1.46	1.39
11	B	1239	CLA	C1B-C2B	2.87	1.49	1.43
11	a	1138	CLA	C1B-C2B	2.87	1.49	1.43
11	1	1109	CLA	C1B-C2B	2.87	1.49	1.43
11	B	1226	CLA	C3D-C2D	2.87	1.46	1.39
11	b	1219	CLA	C1B-C2B	2.87	1.49	1.43
11	a	1130	CLA	C4D-CHA	2.87	1.48	1.38
11	B	1207	CLA	C1B-C2B	2.87	1.49	1.43
11	B	1227	CLA	C4D-CHA	2.87	1.48	1.38
11	A	1123	CLA	C4D-CHA	2.87	1.48	1.38
11	1	1111	CLA	C3D-C2D	2.87	1.46	1.39
11	A	1108	CLA	C1B-C2B	2.87	1.49	1.43
11	A	1129	CLA	C4D-CHA	2.87	1.48	1.38
11	a	1114	CLA	C4D-CHA	2.87	1.48	1.38
11	B	1202	CLA	C4D-CHA	2.87	1.48	1.38
11	A	1111	CLA	C4D-CHA	2.87	1.48	1.38
11	b	1220	CLA	C4D-CHA	2.87	1.48	1.38
11	2	1206	CLA	C1D-ND	-2.87	1.34	1.37
14	b	4009	BCR	C11-C12	-2.87	1.27	1.34
11	b	1213	CLA	C1B-C2B	2.87	1.49	1.43
11	A	1131	CLA	C1B-C2B	2.86	1.49	1.43
11	2	1228	CLA	C4D-CHA	2.86	1.48	1.38
11	B	1217	CLA	C4D-CHA	2.86	1.48	1.38
11	2	1214	CLA	C1D-ND	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1137	CLA	C1B-C2B	2.86	1.49	1.43
11	a	1132	CLA	C4D-CHA	2.86	1.48	1.38
11	1	1140	CLA	C1B-C2B	2.86	1.49	1.43
11	2	1218	CLA	C1B-C2B	2.86	1.49	1.43
11	a	1123	CLA	C4D-CHA	2.86	1.48	1.38
11	b	1210	CLA	C4D-CHA	2.86	1.48	1.38
11	1	1118	CLA	C1B-C2B	2.86	1.49	1.43
11	A	1118	CLA	C3D-C2D	2.86	1.46	1.39
11	B	1201	CLA	C1B-C2B	2.86	1.49	1.43
11	2	1229	CLA	C4D-CHA	2.86	1.48	1.38
11	2	1212	CLA	C4D-CHA	2.86	1.48	1.38
11	B	1234	CLA	C4D-CHA	2.86	1.48	1.38
11	2	1222	CLA	C1B-C2B	2.86	1.49	1.43
11	A	1131	CLA	C1D-ND	-2.86	1.34	1.37
11	A	1135	CLA	C1D-ND	-2.86	1.34	1.37
11	1	1127	CLA	C1B-C2B	2.86	1.49	1.43
11	B	1201	CLA	C3D-C2D	2.86	1.46	1.39
11	2	1212	CLA	C1B-C2B	2.86	1.49	1.43
11	2	1236	CLA	C1B-C2B	2.86	1.49	1.43
11	8	1503	CLA	C4D-CHA	2.86	1.48	1.38
11	A	1140	CLA	C1B-C2B	2.86	1.49	1.43
11	1	1137	CLA	C1B-C2B	2.86	1.49	1.43
11	A	1132	CLA	C4D-CHA	2.85	1.48	1.38
11	A	1112	CLA	C3D-C2D	2.85	1.46	1.39
11	1	1133	CLA	C4D-CHA	2.85	1.48	1.38
11	b	1225	CLA	C3D-C2D	2.85	1.46	1.39
11	1	1107	CLA	C1B-C2B	2.85	1.49	1.43
11	b	1212	CLA	C4D-CHA	2.85	1.48	1.38
11	2	1211	CLA	C1B-C2B	2.85	1.49	1.43
11	2	1218	CLA	C4D-CHA	2.85	1.48	1.38
11	2	1207	CLA	C1B-C2B	2.85	1.49	1.43
11	a	1108	CLA	C4D-CHA	2.85	1.48	1.38
11	A	1103	CLA	C4D-CHA	2.85	1.48	1.38
11	b	1205	CLA	C4D-CHA	2.85	1.48	1.38
11	B	1215	CLA	C4D-CHA	2.85	1.48	1.38
11	a	1801	CLA	C4D-CHA	2.85	1.48	1.38
11	a	1103	CLA	C4D-CHA	2.85	1.48	1.38
11	B	1225	CLA	C4D-CHA	2.85	1.48	1.38
11	A	1109	CLA	C1B-C2B	2.85	1.49	1.43
11	8	1502	CLA	C4D-CHA	2.85	1.48	1.38
11	b	1217	CLA	C4D-CHA	2.85	1.48	1.38
11	B	1203	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1215	CLA	C4D-CHA	2.85	1.48	1.38
11	A	1133	CLA	C4B-NB	-2.85	1.34	1.37
11	A	1134	CLA	C1B-NB	-2.85	1.34	1.37
11	1	1114	CLA	C1B-C2B	2.85	1.49	1.43
11	1	1112	CLA	C4D-CHA	2.85	1.48	1.38
11	a	1107	CLA	C1B-C2B	2.85	1.49	1.43
11	a	1129	CLA	C4D-CHA	2.85	1.48	1.38
11	A	1138	CLA	C4D-CHA	2.84	1.48	1.38
11	B	1239	CLA	C4D-CHA	2.84	1.48	1.38
11	B	1211	CLA	C1D-ND	-2.84	1.34	1.37
11	2	1220	CLA	C1B-C2B	2.84	1.49	1.43
11	2	1203	CLA	C1B-C2B	2.84	1.49	1.43
11	B	1223	CLA	C4D-CHA	2.84	1.48	1.38
11	B	1220	CLA	C4D-CHA	2.84	1.48	1.38
11	B	1224	CLA	C1B-C2B	2.84	1.49	1.43
11	a	1125	CLA	C4D-CHA	2.84	1.48	1.38
11	B	1205	CLA	C1D-ND	-2.84	1.34	1.37
11	b	1232	CLA	C1B-C2B	2.84	1.49	1.43
11	1	1012	CLA	C4D-CHA	2.84	1.48	1.38
11	1	1111	CLA	C4D-CHA	2.84	1.48	1.38
11	2	1219	CLA	C3D-C2D	2.84	1.46	1.39
11	a	1107	CLA	C3D-C2D	2.84	1.46	1.39
11	1	1124	CLA	C4D-CHA	2.84	1.48	1.38
11	a	1131	CLA	C1B-C2B	2.84	1.49	1.43
11	a	1101	CLA	C4D-CHA	2.84	1.48	1.38
11	l	1502	CLA	C1B-C2B	2.84	1.49	1.43
11	1	1133	CLA	C1B-C2B	2.84	1.49	1.43
11	A	1121	CLA	C1D-C2D	2.84	1.51	1.45
11	2	1225	CLA	C3D-C2D	2.84	1.46	1.39
11	1	1135	CLA	C1B-C2B	2.84	1.49	1.43
11	b	1236	CLA	C3D-C2D	2.84	1.46	1.39
11	B	1210	CLA	C1B-C2B	2.84	1.49	1.43
11	A	1109	CLA	C1D-C2D	2.84	1.51	1.45
11	B	1222	CLA	C1B-NB	-2.84	1.34	1.37
11	1	1022	CLA	C1D-ND	-2.84	1.34	1.37
11	b	1225	CLA	C4D-CHA	2.84	1.48	1.38
11	A	1106	CLA	C4D-CHA	2.84	1.48	1.38
11	a	1109	CLA	C1B-C2B	2.84	1.49	1.43
11	b	1221	CLA	C1B-C2B	2.84	1.49	1.43
11	A	1114	CLA	C4D-CHA	2.84	1.48	1.38
11	b	1220	CLA	C1D-ND	-2.84	1.34	1.37
11	1	1126	CLA	C4D-CHA	2.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1101	CLA	C1B-C2B	2.83	1.49	1.43
11	2	1202	CLA	C3D-C2D	2.83	1.46	1.39
11	A	1133	CLA	C1B-C2B	2.83	1.49	1.43
11	A	1136	CLA	C1B-C2B	2.83	1.49	1.43
11	b	1013	CLA	C1D-ND	-2.83	1.34	1.37
11	1	1132	CLA	C4D-CHA	2.83	1.48	1.38
11	1	1134	CLA	C4D-CHA	2.83	1.48	1.38
11	b	1235	CLA	C1B-C2B	2.83	1.49	1.43
11	b	1209	CLA	C4D-CHA	2.83	1.48	1.38
11	2	1211	CLA	C1D-ND	-2.83	1.34	1.37
11	2	1205	CLA	C3D-C2D	2.83	1.46	1.39
11	1	1125	CLA	C4D-CHA	2.83	1.48	1.38
11	A	1103	CLA	C3D-C2D	2.83	1.46	1.39
11	B	1203	CLA	C4D-CHA	2.83	1.48	1.38
11	b	1240	CLA	C1B-C2B	2.83	1.49	1.43
11	A	1128	CLA	C1D-ND	-2.83	1.34	1.37
11	b	1205	CLA	C1D-ND	-2.83	1.34	1.37
11	A	1126	CLA	C4D-CHA	2.83	1.48	1.38
11	2	1214	CLA	C1B-C2B	2.83	1.49	1.43
11	a	1135	CLA	C1B-C2B	2.83	1.49	1.43
11	b	1218	CLA	C1B-C2B	2.83	1.49	1.43
11	B	1226	CLA	C4D-CHA	2.83	1.48	1.38
11	1	1117	CLA	C4D-CHA	2.83	1.48	1.38
11	A	1118	CLA	C1D-ND	-2.83	1.34	1.37
11	b	1013	CLA	C4D-CHA	2.82	1.48	1.38
11	b	1021	CLA	C1B-NB	-2.82	1.34	1.37
11	a	1116	CLA	C4D-CHA	2.82	1.48	1.38
11	a	1134	CLA	C4D-CHA	2.82	1.48	1.38
11	2	1240	CLA	C1B-C2B	2.82	1.49	1.43
11	1	1116	CLA	C4D-CHA	2.82	1.48	1.38
11	1	1130	CLA	C4D-CHA	2.82	1.48	1.38
11	2	1204	CLA	C1D-ND	-2.82	1.34	1.37
11	b	1023	CLA	C4D-CHA	2.82	1.48	1.38
11	1	1129	CLA	C1B-C2B	2.82	1.49	1.43
11	B	1207	CLA	C4D-CHA	2.82	1.48	1.38
11	A	1120	CLA	C4D-CHA	2.82	1.48	1.38
11	A	1137	CLA	C1B-C2B	2.82	1.49	1.43
11	B	1013	CLA	C4D-CHA	2.82	1.48	1.38
11	a	1118	CLA	C1D-ND	-2.82	1.34	1.37
11	1	1116	CLA	C1B-C2B	2.82	1.49	1.43
11	A	1012	CLA	C4D-CHA	2.82	1.48	1.38
11	B	1214	CLA	C4D-CHA	2.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1227	CLA	C4D-CHA	2.82	1.48	1.38
11	A	1113	CLA	C4D-CHA	2.82	1.48	1.38
11	2	1224	CLA	C4D-CHA	2.82	1.48	1.38
11	a	1022	CLA	C1D-ND	-2.82	1.34	1.37
11	1	1107	CLA	C4D-CHA	2.82	1.48	1.38
11	a	1102	CLA	C1B-C2B	2.82	1.49	1.43
11	a	1105	CLA	C4D-CHA	2.82	1.48	1.38
11	a	1133	CLA	C4D-CHA	2.82	1.48	1.38
11	1	1138	CLA	C4D-CHA	2.82	1.48	1.38
11	1	1120	CLA	C1B-C2B	2.81	1.49	1.43
11	B	1206	CLA	C4D-CHA	2.81	1.48	1.38
11	2	1220	CLA	C4D-CHA	2.81	1.48	1.38
11	A	1801	CLA	C4C-C3C	2.81	1.49	1.45
11	A	1107	CLA	C4D-CHA	2.81	1.48	1.38
11	A	1130	CLA	C1B-C2B	2.81	1.49	1.43
11	1	1115	CLA	C4D-CHA	2.81	1.48	1.38
11	1	1106	CLA	C1B-C2B	2.81	1.49	1.43
11	L	1502	CLA	C1B-C2B	2.81	1.49	1.43
11	1	1132	CLA	C1B-C2B	2.81	1.49	1.43
11	K	1402	CLA	C1B-C2B	2.81	1.49	1.43
11	2	1207	CLA	C4D-CHA	2.81	1.48	1.38
11	1	1109	CLA	C4D-CHA	2.81	1.48	1.38
11	b	1202	CLA	C1B-C2B	2.81	1.49	1.43
11	1	1012	CLA	C1B-C2B	2.81	1.49	1.43
11	8	1503	CLA	C1B-C2B	2.81	1.49	1.43
11	2	1236	CLA	C4D-CHA	2.81	1.48	1.38
11	A	1130	CLA	C4D-CHA	2.81	1.48	1.38
11	a	1117	CLA	C4D-CHA	2.81	1.48	1.38
11	a	1106	CLA	C1B-C2B	2.81	1.49	1.43
11	B	1225	CLA	C1B-C2B	2.81	1.49	1.43
11	A	1237	CLA	C1B-C2B	2.81	1.49	1.43
11	B	1240	CLA	C1B-C2B	2.81	1.49	1.43
11	a	1130	CLA	C1B-C2B	2.81	1.49	1.43
11	b	1232	CLA	C4D-CHA	2.81	1.48	1.38
11	2	1232	CLA	C4D-CHA	2.81	1.48	1.38
11	B	1228	CLA	C4D-CHA	2.81	1.48	1.38
11	A	1125	CLA	C4B-NB	-2.81	1.34	1.37
11	B	1202	CLA	C1B-NB	-2.81	1.34	1.37
11	B	1230	CLA	C1D-ND	-2.81	1.34	1.37
11	a	1127	CLA	C1D-ND	-2.80	1.34	1.37
11	b	1223	CLA	C4D-CHA	2.80	1.48	1.38
11	1	1117	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1225	CLA	C4D-CHA	2.80	1.48	1.38
11	B	1235	CLA	C4D-CHA	2.80	1.48	1.38
11	a	1109	CLA	C4D-CHA	2.80	1.48	1.38
11	B	1235	CLA	C1B-C2B	2.80	1.49	1.43
11	2	1023	CLA	C4D-CHA	2.80	1.48	1.38
11	A	1101	CLA	C3D-C2D	2.80	1.46	1.39
11	b	1216	CLA	C4D-CHA	2.80	1.48	1.38
11	A	1104	CLA	C3D-C2D	2.80	1.46	1.39
11	a	1140	CLA	C4D-CHA	2.80	1.48	1.38
11	8	1502	CLA	C1B-C2B	2.80	1.49	1.43
11	1	1129	CLA	C4D-CHA	2.80	1.48	1.38
11	1	1112	CLA	C1B-C2B	2.80	1.49	1.43
11	2	1230	CLA	C1D-ND	-2.80	1.34	1.37
11	l	1501	CLA	C1B-C2B	2.80	1.49	1.43
11	A	1117	CLA	C4D-CHA	2.80	1.48	1.38
11	B	1225	CLA	C1D-ND	-2.80	1.34	1.37
11	b	1238	CLA	C1B-C2B	2.80	1.49	1.43
11	a	1128	CLA	C4D-CHA	2.80	1.48	1.38
11	2	1223	CLA	C4D-CHA	2.80	1.48	1.38
11	B	1217	CLA	C1B-C2B	2.80	1.49	1.43
11	b	1201	CLA	C4D-CHA	2.80	1.48	1.38
11	A	1139	CLA	C4D-CHA	2.79	1.48	1.38
11	B	1212	CLA	C4D-CHA	2.79	1.48	1.38
11	1	1114	CLA	C4D-CHA	2.79	1.48	1.38
11	2	1204	CLA	C4D-CHA	2.79	1.48	1.38
11	a	1111	CLA	C4D-CHA	2.79	1.48	1.38
11	A	1113	CLA	C1B-C2B	2.79	1.49	1.43
11	1	1124	CLA	C1B-C2B	2.79	1.49	1.43
11	1	1122	CLA	C1B-C2B	2.79	1.49	1.43
11	1	1022	CLA	C4D-CHA	2.79	1.48	1.38
11	b	1227	CLA	C4D-CHA	2.79	1.48	1.38
11	1	1118	CLA	C4D-CHA	2.79	1.48	1.38
11	B	1218	CLA	C4D-CHA	2.79	1.48	1.38
11	a	1124	CLA	C4D-CHA	2.79	1.48	1.38
11	l	1502	CLA	C4D-CHA	2.79	1.48	1.38
11	A	1237	CLA	C4D-CHA	2.79	1.48	1.38
11	B	1204	CLA	C4D-CHA	2.79	1.48	1.38
11	a	1104	CLA	C4D-CHA	2.79	1.48	1.38
11	2	1208	CLA	C4D-CHA	2.79	1.48	1.38
11	A	1115	CLA	C1D-ND	-2.79	1.34	1.37
11	2	1221	CLA	C1B-NB	-2.79	1.34	1.37
11	2	1220	CLA	C1D-ND	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1211	CLA	C4D-CHA	2.79	1.48	1.38
11	A	1102	CLA	C1B-C2B	2.79	1.49	1.43
11	1	1128	CLA	C4D-CHA	2.79	1.48	1.38
11	2	1230	CLA	C1B-C2B	2.79	1.49	1.43
11	b	1227	CLA	C1D-ND	-2.79	1.34	1.37
11	2	1226	CLA	C3D-C2D	2.79	1.46	1.39
11	b	1217	CLA	C1B-C2B	2.79	1.49	1.43
11	B	1207	CLA	C1D-ND	-2.79	1.34	1.37
11	B	1225	CLA	C1B-NB	-2.79	1.34	1.37
11	A	1128	CLA	C4D-CHA	2.79	1.47	1.38
11	2	1215	CLA	C1B-C2B	2.79	1.49	1.43
11	b	1230	CLA	C1D-ND	-2.79	1.34	1.37
11	B	1023	CLA	C1B-C2B	2.79	1.49	1.43
11	a	1115	CLA	C1D-ND	-2.78	1.34	1.37
11	1	1139	CLA	C1B-C2B	2.78	1.49	1.43
11	2	1204	CLA	C1B-C2B	2.78	1.49	1.43
11	2	1225	CLA	C1B-NB	-2.78	1.34	1.37
11	a	1103	CLA	C1B-C2B	2.78	1.49	1.43
11	B	1229	CLA	C4D-CHA	2.78	1.47	1.38
11	2	1238	CLA	C4D-CHA	2.78	1.47	1.38
11	a	1122	CLA	C4D-CHA	2.78	1.47	1.38
11	b	1204	CLA	C4D-CHA	2.78	1.47	1.38
11	a	1011	CLA	C1B-C2B	2.78	1.49	1.43
11	a	1136	CLA	C4D-CHA	2.78	1.47	1.38
11	B	1214	CLA	C1B-C2B	2.78	1.49	1.43
11	a	1119	CLA	C4D-CHA	2.78	1.47	1.38
11	b	1206	CLA	C4D-CHA	2.78	1.47	1.38
11	1	1104	CLA	C4D-CHA	2.78	1.47	1.38
11	a	1124	CLA	C1B-C2B	2.78	1.49	1.43
11	a	1115	CLA	C1B-C2B	2.78	1.49	1.43
11	B	1023	CLA	C1D-ND	-2.78	1.34	1.37
11	A	1121	CLA	C1B-C2B	2.78	1.49	1.43
11	2	1225	CLA	C1D-C2D	2.78	1.50	1.45
11	b	1225	CLA	C1B-NB	-2.78	1.34	1.37
11	2	1208	CLA	C1D-ND	-2.78	1.34	1.37
11	b	1227	CLA	C1B-C2B	2.77	1.49	1.43
11	2	1021	CLA	C1D-ND	-2.77	1.34	1.37
11	1	1134	CLA	C1B-C2B	2.77	1.49	1.43
11	b	1214	CLA	C4D-CHA	2.77	1.47	1.38
11	2	1219	CLA	C1B-C2B	2.77	1.49	1.43
11	L	1501	CLA	C1B-C2B	2.77	1.49	1.43
11	1	1106	CLA	C1D-ND	-2.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1119	CLA	C1B-NB	-2.77	1.34	1.37
11	l	1503	CLA	C1D-ND	-2.77	1.34	1.37
11	B	1219	CLA	C1B-C2B	2.77	1.49	1.43
11	B	1021	CLA	C1D-ND	-2.77	1.34	1.37
11	1	1011	CLA	C1D-ND	-2.77	1.34	1.37
11	a	1012	CLA	C1B-C2B	2.77	1.49	1.43
11	b	1208	CLA	C4D-CHA	2.77	1.47	1.38
11	2	1235	CLA	C1B-C2B	2.77	1.49	1.43
11	A	1107	CLA	C3D-C2D	2.77	1.46	1.39
11	2	1207	CLA	C1C-NC	-2.77	1.33	1.37
11	B	1228	CLA	C1B-C2B	2.77	1.49	1.43
11	B	1213	CLA	C4D-CHA	2.77	1.47	1.38
11	B	1221	CLA	C1B-NB	-2.77	1.34	1.37
11	1	1104	CLA	C1B-C2B	2.77	1.49	1.43
11	A	1117	CLA	C1D-ND	-2.77	1.34	1.37
11	A	1139	CLA	C1B-C2B	2.77	1.49	1.43
11	a	1022	CLA	C4D-CHA	2.77	1.47	1.38
11	b	1211	CLA	C4D-CHA	2.77	1.47	1.38
11	l	1503	CLA	C1B-C2B	2.77	1.49	1.43
11	b	1218	CLA	C4D-CHA	2.76	1.47	1.38
11	l	1503	CLA	C4D-CHA	2.76	1.47	1.38
11	B	1208	CLA	C1B-C2B	2.76	1.49	1.43
11	b	1229	CLA	C1B-C2B	2.76	1.49	1.43
11	B	1021	CLA	C1B-NB	-2.76	1.34	1.37
11	B	1211	CLA	C1B-C2B	2.76	1.49	1.43
11	1	1101	CLA	C4D-CHA	2.76	1.47	1.38
11	A	1012	CLA	C1B-C2B	2.76	1.49	1.43
11	B	1238	CLA	C1B-C2B	2.76	1.49	1.43
11	A	1135	CLA	C4D-CHA	2.76	1.47	1.38
11	1	1122	CLA	C4D-CHA	2.76	1.47	1.38
11	A	1107	CLA	C1B-C2B	2.76	1.49	1.43
11	B	1215	CLA	C1B-C2B	2.76	1.49	1.43
11	1	1131	CLA	C4D-CHA	2.76	1.47	1.38
11	a	1110	CLA	C1B-C2B	2.76	1.49	1.43
11	a	1110	CLA	C4D-CHA	2.76	1.47	1.38
11	a	1103	CLA	C1D-ND	-2.76	1.34	1.37
11	a	1127	CLA	C4D-CHA	2.76	1.47	1.38
11	b	1236	CLA	C1B-C2B	2.75	1.49	1.43
11	b	1226	CLA	C4D-CHA	2.75	1.47	1.38
11	L	1503	CLA	C4D-CHA	2.75	1.47	1.38
11	A	1115	CLA	C1B-C2B	2.75	1.49	1.43
11	2	1223	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1023	CLA	C1B-C2B	2.75	1.49	1.43
11	2	1202	CLA	C4D-CHA	2.75	1.47	1.38
11	a	1125	CLA	C1B-C2B	2.75	1.49	1.43
11	2	1219	CLA	C1B-NB	-2.75	1.34	1.37
11	B	1212	CLA	C1B-C2B	2.75	1.49	1.43
11	B	1208	CLA	C4D-CHA	2.75	1.47	1.38
11	a	1119	CLA	C1B-C2B	2.75	1.49	1.43
11	B	1216	CLA	C1D-C2D	2.75	1.50	1.45
11	A	1115	CLA	C4D-CHA	2.75	1.47	1.38
11	b	1213	CLA	C4D-CHA	2.75	1.47	1.38
11	a	1130	CLA	C1D-ND	-2.75	1.34	1.37
11	2	1209	CLA	C1B-C2B	2.75	1.49	1.43
11	A	1801	CLA	C1D-ND	-2.75	1.34	1.37
11	B	1212	CLA	C1D-ND	-2.75	1.34	1.37
11	B	1023	CLA	C4D-CHA	2.75	1.47	1.38
11	2	1226	CLA	C4D-CHA	2.75	1.47	1.38
11	1	1128	CLA	C1D-ND	-2.75	1.34	1.37
11	1	1801	CLA	C1B-C2B	2.75	1.49	1.43
11	2	1226	CLA	C1D-ND	-2.74	1.34	1.37
11	2	1224	CLA	C3D-C2D	2.74	1.46	1.39
11	a	1137	CLA	C4D-CHA	2.74	1.47	1.38
11	2	1023	CLA	C4B-NB	-2.74	1.34	1.37
11	2	1206	CLA	C1B-NB	-2.74	1.34	1.37
11	1	1139	CLA	C4D-CHA	2.74	1.47	1.38
11	a	1118	CLA	C4D-CHA	2.74	1.47	1.38
11	A	1119	CLA	C1D-ND	-2.74	1.34	1.37
11	2	1210	CLA	C4D-CHA	2.74	1.47	1.38
11	A	1022	CLA	C4D-CHA	2.74	1.47	1.38
11	A	1102	CLA	C1D-ND	-2.74	1.34	1.37
11	2	1229	CLA	C1B-C2B	2.74	1.49	1.43
11	2	1232	CLA	C1B-C2B	2.74	1.49	1.43
11	0	1402	CLA	C1B-C2B	2.74	1.49	1.43
11	b	1210	CLA	C1B-C2B	2.74	1.49	1.43
11	b	1229	CLA	C4D-CHA	2.74	1.47	1.38
11	a	1140	CLA	C1D-ND	-2.74	1.34	1.37
11	b	1240	CLA	C4D-CHA	2.74	1.47	1.38
11	A	1138	CLA	C1D-C2D	2.74	1.50	1.45
11	A	1101	CLA	C1B-C2B	2.74	1.49	1.43
11	B	1202	CLA	C1B-C2B	2.73	1.49	1.43
11	a	1121	CLA	C1B-C2B	2.73	1.49	1.43
11	A	1101	CLA	C1D-ND	-2.73	1.34	1.37
11	A	1124	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1223	CLA	C1B-C2B	2.73	1.49	1.43
11	B	1217	CLA	C1D-ND	-2.73	1.34	1.37
11	1	1101	CLA	C1D-ND	-2.73	1.34	1.37
11	2	1202	CLA	C1B-C2B	2.73	1.49	1.43
11	2	1221	CLA	C1B-C2B	2.73	1.49	1.43
11	A	1105	CLA	C4D-CHA	2.73	1.47	1.38
11	b	1236	CLA	C4D-CHA	2.73	1.47	1.38
11	A	1101	CLA	C4D-CHA	2.73	1.47	1.38
11	b	1206	CLA	C1B-C2B	2.73	1.49	1.43
11	1	1119	CLA	C4D-CHA	2.73	1.47	1.38
11	b	1219	CLA	C1D-ND	-2.73	1.34	1.37
11	b	1206	CLA	C1B-NB	-2.73	1.34	1.37
11	A	1801	CLA	C1C-NC	-2.73	1.33	1.37
11	l	1501	CLA	C1D-ND	-2.73	1.34	1.37
11	2	1210	CLA	C1B-C2B	2.73	1.49	1.43
11	A	1109	CLA	C4D-CHA	2.73	1.47	1.38
11	A	1108	CLA	C4D-CHA	2.73	1.47	1.38
11	1	1136	CLA	C4D-CHA	2.73	1.47	1.38
11	2	1023	CLA	C1D-ND	-2.73	1.34	1.37
11	2	1214	CLA	C4D-CHA	2.73	1.47	1.38
11	B	1224	CLA	C1D-ND	-2.73	1.34	1.37
11	b	1216	CLA	C1B-NB	-2.73	1.34	1.37
11	1	1125	CLA	C1D-ND	-2.73	1.34	1.37
11	A	1128	CLA	C1B-C2B	2.73	1.49	1.43
11	a	1109	CLA	C1D-C2D	2.73	1.50	1.45
11	A	1123	CLA	C1B-C2B	2.72	1.49	1.43
11	B	1209	CLA	C1B-C2B	2.72	1.49	1.43
11	2	1013	CLA	C1D-ND	-2.72	1.34	1.37
11	A	1133	CLA	C1D-ND	-2.72	1.34	1.37
11	a	1120	CLA	C1D-ND	-2.72	1.34	1.37
11	a	1126	CLA	C1D-ND	-2.72	1.34	1.37
11	a	1122	CLA	C1B-C2B	2.72	1.49	1.43
11	A	1121	CLA	C4D-CHA	2.72	1.47	1.38
11	1	1125	CLA	C1B-C2B	2.72	1.49	1.43
11	b	1238	CLA	C4D-CHA	2.72	1.47	1.38
11	2	1205	CLA	C4D-CHA	2.72	1.47	1.38
11	2	1021	CLA	C1B-C2B	2.72	1.49	1.43
11	A	1136	CLA	C4D-CHA	2.72	1.47	1.38
11	1	1130	CLA	C1D-ND	-2.72	1.34	1.37
11	L	1503	CLA	C1D-ND	-2.72	1.34	1.37
11	2	1212	CLA	C1D-ND	-2.72	1.34	1.37
11	1	1105	CLA	C4D-CHA	2.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1206	CLA	C1D-ND	-2.72	1.34	1.37
11	A	1127	CLA	C4D-CHA	2.72	1.47	1.38
11	1	1011	CLA	C1B-C2B	2.72	1.49	1.43
11	L	1502	CLA	C4D-CHA	2.72	1.47	1.38
11	A	1118	CLA	C4D-CHA	2.72	1.47	1.38
11	b	1216	CLA	C1D-ND	-2.72	1.34	1.37
11	B	1226	CLA	C1B-NB	-2.71	1.34	1.37
11	a	1116	CLA	C1B-NB	-2.71	1.34	1.37
11	A	1127	CLA	C1D-ND	-2.71	1.34	1.37
11	A	1140	CLA	C1C-NC	-2.71	1.33	1.37
11	a	1140	CLA	C1B-C2B	2.71	1.49	1.43
11	b	1231	CLA	C1B-C2B	2.71	1.49	1.43
11	B	1227	CLA	C1D-ND	-2.71	1.34	1.37
11	b	1219	CLA	C1B-NB	-2.71	1.34	1.37
11	1	1106	CLA	C4D-CHA	2.71	1.47	1.38
11	b	1229	CLA	C1D-ND	-2.71	1.34	1.37
11	1	1123	CLA	C1B-C2B	2.71	1.49	1.43
11	B	1238	CLA	C4D-CHA	2.71	1.47	1.38
11	B	1210	CLA	C4C-C3C	2.71	1.49	1.45
11	1	1237	CLA	C4D-CHA	2.71	1.47	1.38
11	b	1021	CLA	C1B-C2B	2.71	1.49	1.43
11	b	1203	CLA	C1B-C2B	2.71	1.49	1.43
11	a	1127	CLA	C1B-C2B	2.71	1.49	1.43
11	b	1215	CLA	C1D-ND	-2.71	1.34	1.37
11	A	1130	CLA	C1D-ND	-2.71	1.34	1.37
11	B	1208	CLA	C1D-ND	-2.71	1.34	1.37
11	2	1202	CLA	C1B-NB	-2.71	1.34	1.37
11	1	1111	CLA	C1B-C2B	2.71	1.49	1.43
11	a	1106	CLA	C1D-ND	-2.70	1.34	1.37
11	a	1801	CLA	C1B-C2B	2.70	1.49	1.43
11	1	1119	CLA	C1B-C2B	2.70	1.49	1.43
11	B	1236	CLA	C4D-CHA	2.70	1.47	1.38
11	a	1110	CLA	C1D-ND	-2.70	1.34	1.37
11	1	1127	CLA	C1D-ND	-2.70	1.34	1.37
11	1	1135	CLA	C1D-ND	-2.70	1.34	1.37
11	a	1115	CLA	C4D-CHA	2.70	1.47	1.38
11	2	1225	CLA	C1B-C2B	2.70	1.49	1.43
11	A	1119	CLA	C4D-CHA	2.70	1.47	1.38
11	2	1209	CLA	C1B-NB	-2.70	1.34	1.37
11	2	1216	CLA	C1D-ND	-2.70	1.34	1.37
11	0	1402	CLA	C4D-CHA	2.70	1.47	1.38
11	a	1022	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	1402	CLA	C1B-C2B	2.70	1.49	1.43
11	a	1128	CLA	C1B-C2B	2.70	1.49	1.43
11	a	1123	CLA	C1B-C2B	2.70	1.49	1.43
11	a	1112	CLA	C1B-C2B	2.70	1.49	1.43
11	b	1235	CLA	C1B-NB	-2.69	1.34	1.37
11	A	1127	CLA	C1B-C2B	2.69	1.49	1.43
11	8	1501	CLA	C1B-C2B	2.69	1.49	1.43
11	a	1104	CLA	C1B-C2B	2.69	1.49	1.43
11	A	1127	CLA	C1B-NB	-2.69	1.34	1.37
11	2	1226	CLA	C1B-NB	-2.69	1.34	1.37
11	A	1122	CLA	C1B-NB	-2.69	1.34	1.37
11	2	1023	CLA	C1B-C2B	2.69	1.49	1.43
11	2	1238	CLA	C1B-C2B	2.69	1.49	1.43
11	B	1224	CLA	C3D-C2D	2.69	1.46	1.39
11	2	1228	CLA	C1B-C2B	2.69	1.49	1.43
11	b	1222	CLA	C1D-ND	-2.68	1.34	1.37
11	B	1228	CLA	C1D-C2D	2.68	1.50	1.45
11	A	1129	CLA	C1B-C2B	2.68	1.49	1.43
11	1	1127	CLA	C4D-CHA	2.68	1.47	1.38
11	a	1132	CLA	C1D-ND	-2.68	1.34	1.37
11	8	1503	CLA	C1B-NB	-2.68	1.34	1.37
11	2	1228	CLA	C1D-ND	-2.68	1.34	1.37
11	b	1225	CLA	C1B-C2B	2.68	1.49	1.43
11	1	1801	CLA	C1D-ND	-2.68	1.34	1.37
11	b	1226	CLA	C1B-C2B	2.68	1.49	1.43
11	B	1209	CLA	C1B-NB	-2.68	1.34	1.37
11	L	1501	CLA	C1D-ND	-2.68	1.34	1.37
11	a	1101	CLA	C1D-ND	-2.68	1.34	1.37
11	A	1116	CLA	C1B-NB	-2.68	1.34	1.37
11	a	1128	CLA	C1D-ND	-2.68	1.34	1.37
11	a	1237	CLA	C4D-CHA	2.68	1.47	1.38
11	B	1222	CLA	C1B-C2B	2.68	1.49	1.43
11	B	1208	CLA	C1D-C2D	2.68	1.50	1.45
11	a	1138	CLA	C1D-C2D	2.68	1.50	1.45
11	B	1238	CLA	C1D-ND	-2.68	1.34	1.37
11	2	1222	CLA	C1D-ND	-2.68	1.34	1.37
11	A	1120	CLA	C1B-C2B	2.68	1.49	1.43
11	A	1139	CLA	C1D-ND	-2.68	1.34	1.37
11	B	1216	CLA	C4D-CHA	2.68	1.47	1.38
11	A	1126	CLA	C1D-ND	-2.68	1.34	1.37
11	a	1117	CLA	C1D-ND	-2.68	1.34	1.37
11	a	1123	CLA	C1B-NB	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1227	CLA	C1D-ND	-2.68	1.34	1.37
11	A	1112	CLA	C1B-NB	-2.68	1.34	1.37
11	a	1134	CLA	C1B-NB	-2.67	1.34	1.37
11	b	1232	CLA	C1D-ND	-2.67	1.34	1.37
11	b	1206	CLA	C1D-ND	-2.67	1.34	1.37
11	B	1231	CLA	C4C-C3C	2.67	1.49	1.45
11	A	1105	CLA	C1D-ND	-2.67	1.34	1.37
11	1	1102	CLA	C1B-C2B	2.67	1.49	1.43
11	k	1402	CLA	C4D-CHA	2.67	1.47	1.38
11	B	1211	CLA	C4B-NB	-2.67	1.34	1.37
11	a	1104	CLA	C1D-ND	-2.67	1.34	1.37
11	8	1502	CLA	C1D-ND	-2.67	1.34	1.37
11	K	1402	CLA	C4D-CHA	2.67	1.47	1.38
11	A	1111	CLA	C1B-C2B	2.67	1.49	1.43
11	a	1135	CLA	C1D-ND	-2.67	1.34	1.37
11	A	1104	CLA	C4D-CHA	2.67	1.47	1.38
11	b	1215	CLA	C1B-C2B	2.67	1.49	1.43
11	B	1231	CLA	C1B-C2B	2.67	1.49	1.43
11	a	1121	CLA	C1D-C2D	2.67	1.50	1.45
11	B	1219	CLA	C1D-ND	-2.67	1.34	1.37
11	a	1122	CLA	C1D-ND	-2.67	1.34	1.37
11	1	1126	CLA	C1D-ND	-2.67	1.34	1.37
11	1	1110	CLA	C1B-C2B	2.66	1.49	1.43
11	B	1231	CLA	C1B-NB	-2.66	1.34	1.37
11	B	1240	CLA	C1D-ND	-2.66	1.34	1.37
11	A	1116	CLA	C1D-ND	-2.66	1.34	1.37
11	B	1229	CLA	C1D-ND	-2.66	1.34	1.37
11	1	1131	CLA	C1D-ND	-2.66	1.34	1.37
11	a	1107	CLA	C1B-NB	-2.66	1.34	1.37
11	a	1119	CLA	C1C-NC	-2.66	1.33	1.37
11	2	1207	CLA	C1D-ND	-2.66	1.34	1.37
11	2	1216	CLA	C1B-NB	-2.66	1.34	1.37
11	2	1231	CLA	C1B-NB	-2.66	1.34	1.37
11	B	1221	CLA	C1B-C2B	2.66	1.49	1.43
11	2	1213	CLA	C4D-CHA	2.66	1.47	1.38
11	a	1131	CLA	C1D-ND	-2.66	1.34	1.37
11	a	1011	CLA	C1D-ND	-2.66	1.34	1.37
11	B	1224	CLA	C4D-CHA	2.65	1.47	1.38
11	b	1211	CLA	C1D-ND	-2.65	1.34	1.37
11	2	1202	CLA	C1D-C2D	2.65	1.50	1.45
11	b	1225	CLA	C1D-ND	-2.65	1.34	1.37
11	b	1220	CLA	C4C-C3C	2.65	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1111	CLA	C1B-NB	-2.65	1.34	1.37
11	2	1217	CLA	C1D-ND	-2.65	1.34	1.37
11	8	1503	CLA	C1D-ND	-2.65	1.34	1.37
11	A	1137	CLA	C4D-CHA	2.65	1.47	1.38
11	A	1112	CLA	C1B-C2B	2.65	1.49	1.43
11	1	1117	CLA	C1B-NB	-2.65	1.34	1.37
11	b	1209	CLA	C4C-C3C	2.65	1.49	1.45
11	A	1108	CLA	C1D-C2D	2.64	1.50	1.45
11	A	1137	CLA	C1D-ND	-2.64	1.34	1.37
11	1	1139	CLA	C1D-ND	-2.64	1.34	1.37
11	B	1204	CLA	C1D-ND	-2.64	1.34	1.37
11	b	1201	CLA	C1D-ND	-2.64	1.34	1.37
11	1	1104	CLA	C1D-ND	-2.64	1.34	1.37
11	1	1105	CLA	C1D-ND	-2.64	1.34	1.37
11	1	1115	CLA	C1D-ND	-2.64	1.34	1.37
11	2	1232	CLA	C1D-C2D	2.64	1.50	1.45
11	8	1501	CLA	C1B-NB	-2.64	1.34	1.37
11	1	1119	CLA	C1D-ND	-2.64	1.34	1.37
11	2	1213	CLA	C1D-C2D	2.64	1.50	1.45
11	b	1232	CLA	C1D-C2D	2.64	1.50	1.45
11	A	1129	CLA	C1D-ND	-2.64	1.34	1.37
11	b	1023	CLA	C1D-ND	-2.64	1.34	1.37
11	l	1502	CLA	C1D-ND	-2.64	1.34	1.37
11	b	1231	CLA	C1D-C2D	2.64	1.50	1.45
11	b	1013	CLA	C1B-NB	-2.64	1.34	1.37
11	2	1215	CLA	C1B-NB	-2.64	1.34	1.37
11	a	1139	CLA	C4C-C3C	2.64	1.49	1.45
11	b	1215	CLA	C1B-NB	-2.64	1.34	1.37
11	1	1114	CLA	C1D-C2D	2.64	1.50	1.45
11	A	1107	CLA	C1B-NB	-2.63	1.34	1.37
11	B	1223	CLA	C1D-ND	-2.63	1.34	1.37
11	B	1201	CLA	C1D-ND	-2.63	1.34	1.37
11	1	1133	CLA	C4C-C3C	2.63	1.49	1.45
11	b	1208	CLA	C1D-C2D	2.63	1.50	1.45
11	b	1238	CLA	C1D-C2D	2.63	1.50	1.45
11	b	1207	CLA	C1C-NC	-2.63	1.33	1.37
11	A	1124	CLA	C1D-ND	-2.63	1.34	1.37
11	b	1204	CLA	C1D-ND	-2.63	1.34	1.37
11	1	1115	CLA	C4B-NB	-2.63	1.34	1.37
11	a	1122	CLA	C1B-NB	-2.63	1.34	1.37
11	1	1117	CLA	C1D-ND	-2.63	1.34	1.37
11	A	1011	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1105	CLA	C1D-C2D	2.63	1.50	1.45
11	1	1107	CLA	C1B-NB	-2.62	1.34	1.37
11	A	1122	CLA	C4D-CHA	2.62	1.47	1.38
11	B	1226	CLA	C1D-ND	-2.62	1.34	1.37
11	a	1126	CLA	C1B-C2B	2.62	1.49	1.43
11	0	1402	CLA	C1D-C2D	2.62	1.50	1.45
11	B	1013	CLA	C1B-NB	-2.62	1.34	1.37
11	B	1220	CLA	C1B-NB	-2.62	1.34	1.37
11	B	1218	CLA	C1D-C2D	2.62	1.50	1.45
11	b	1236	CLA	C1D-C2D	2.62	1.50	1.45
11	a	1124	CLA	C1D-ND	-2.62	1.34	1.37
11	2	1221	CLA	C1D-ND	-2.62	1.34	1.37
11	B	1215	CLA	C1D-C2D	2.62	1.50	1.45
11	1	1122	CLA	C1D-ND	-2.62	1.34	1.37
11	A	1135	CLA	C1B-C2B	2.62	1.49	1.43
11	1	1120	CLA	C1D-ND	-2.62	1.34	1.37
11	1	1130	CLA	C1D-C2D	2.62	1.50	1.45
11	B	1227	CLA	C4C-C3C	2.62	1.49	1.45
11	b	1228	CLA	C1B-C2B	2.62	1.49	1.43
11	A	1022	CLA	C1B-NB	-2.62	1.34	1.37
11	b	1228	CLA	C1D-ND	-2.62	1.34	1.37
11	A	1134	CLA	C1B-C2B	2.62	1.49	1.43
11	A	1125	CLA	C1D-ND	-2.62	1.34	1.37
11	b	1240	CLA	C1D-ND	-2.62	1.34	1.37
11	1	1109	CLA	C1D-C2D	2.61	1.50	1.45
11	B	1211	CLA	C3D-C2D	2.61	1.46	1.39
11	A	1011	CLA	C1D-ND	-2.61	1.34	1.37
11	1	1132	CLA	C1D-ND	-2.61	1.34	1.37
11	A	1136	CLA	C1D-ND	-2.61	1.34	1.37
11	b	1203	CLA	C1D-ND	-2.61	1.34	1.37
11	A	1135	CLA	C4B-NB	-2.61	1.34	1.37
11	2	1023	CLA	C1B-NB	-2.61	1.34	1.37
11	A	1120	CLA	C1D-ND	-2.61	1.34	1.37
11	2	1209	CLA	C1D-C2D	2.61	1.50	1.45
11	b	1228	CLA	C1B-NB	-2.61	1.34	1.37
11	a	1132	CLA	C1B-C2B	2.61	1.49	1.43
11	1	1139	CLA	C1D-C2D	2.61	1.50	1.45
11	a	1134	CLA	C1D-C2D	2.61	1.50	1.45
11	a	1127	CLA	C4C-C3C	2.61	1.49	1.45
11	b	1207	CLA	C1D-ND	-2.61	1.34	1.37
11	1	1128	CLA	C1B-NB	-2.61	1.34	1.37
11	B	1230	CLA	C1C-NC	-2.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1213	CLA	C1B-NB	-2.61	1.34	1.37
11	B	1239	CLA	C1D-ND	-2.61	1.34	1.37
11	a	1123	CLA	C1D-C2D	2.61	1.50	1.45
11	A	1123	CLA	C4C-C3C	2.61	1.49	1.45
11	A	1106	CLA	C1D-ND	-2.60	1.34	1.37
11	b	1226	CLA	C1D-ND	-2.60	1.34	1.37
11	b	1208	CLA	C1D-ND	-2.60	1.34	1.37
11	2	1207	CLA	C4B-NB	-2.60	1.34	1.37
11	K	1402	CLA	C1C-NC	-2.60	1.33	1.37
11	B	1204	CLA	C1D-C2D	2.60	1.50	1.45
11	a	1105	CLA	C1D-C2D	2.60	1.50	1.45
11	b	1218	CLA	C1D-C2D	2.60	1.50	1.45
11	1	1126	CLA	C1B-C2B	2.60	1.49	1.43
11	a	1237	CLA	C1D-ND	-2.60	1.34	1.37
11	2	1215	CLA	C1D-ND	-2.60	1.34	1.37
11	1	1127	CLA	C1D-C2D	2.60	1.50	1.45
11	2	1216	CLA	C1B-C2B	2.60	1.49	1.43
11	B	1204	CLA	C1B-NB	-2.60	1.34	1.37
11	1	1140	CLA	C1D-ND	-2.60	1.34	1.37
11	1	1121	CLA	C1D-C2D	2.60	1.50	1.45
11	1	1103	CLA	C1D-C2D	2.60	1.50	1.45
11	B	1210	CLA	C1B-NB	-2.60	1.34	1.37
11	b	1023	CLA	C1B-NB	-2.60	1.34	1.37
11	A	1801	CLA	C1B-C2B	2.60	1.49	1.43
11	B	1220	CLA	C1D-ND	-2.59	1.34	1.37
11	1	1134	CLA	C1D-C2D	2.59	1.50	1.45
11	A	1133	CLA	C1B-NB	-2.59	1.34	1.37
11	b	1221	CLA	C1B-NB	-2.59	1.34	1.37
11	1	1129	CLA	C1D-ND	-2.59	1.34	1.37
11	a	1130	CLA	C1D-C2D	2.59	1.50	1.45
11	1	1124	CLA	C1D-C2D	2.59	1.50	1.45
11	B	1013	CLA	C1B-C2B	2.59	1.49	1.43
11	2	1013	CLA	C1B-C2B	2.59	1.49	1.43
11	b	1218	CLA	C1D-ND	-2.59	1.34	1.37
11	a	1801	CLA	C1D-ND	-2.59	1.34	1.37
11	b	1021	CLA	C1D-ND	-2.59	1.34	1.37
11	b	1215	CLA	C1D-C2D	2.59	1.50	1.45
11	B	1221	CLA	C1D-ND	-2.59	1.34	1.37
11	b	1214	CLA	C1B-C2B	2.59	1.49	1.43
11	1	1237	CLA	C1D-C2D	2.59	1.50	1.45
11	A	1107	CLA	C1D-ND	-2.59	1.34	1.37
11	A	1129	CLA	C1B-NB	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1106	CLA	C4B-NB	-2.59	1.34	1.37
11	B	1238	CLA	C1D-C2D	2.59	1.50	1.45
11	a	1134	CLA	C1B-C2B	2.59	1.49	1.43
11	A	1103	CLA	C1D-C2D	2.59	1.50	1.45
11	B	1211	CLA	C4D-CHA	2.59	1.47	1.38
11	1	1119	CLA	C1D-C2D	2.59	1.50	1.45
11	B	1232	CLA	C1D-C2D	2.58	1.50	1.45
11	B	1216	CLA	C1B-NB	-2.58	1.34	1.37
11	1	1124	CLA	C1D-ND	-2.58	1.34	1.37
11	2	1023	CLA	C1C-NC	-2.58	1.33	1.37
11	b	1209	CLA	C1D-C2D	2.58	1.50	1.45
11	1	1103	CLA	C1B-NB	-2.58	1.34	1.37
11	b	1240	CLA	C1D-C2D	2.58	1.50	1.45
11	k	1402	CLA	C1D-C2D	2.58	1.50	1.45
11	1	1128	CLA	C1B-C2B	2.58	1.49	1.43
11	A	1132	CLA	C1D-ND	-2.58	1.34	1.37
11	a	1105	CLA	C1D-ND	-2.58	1.34	1.37
11	2	1204	CLA	C1D-C2D	2.58	1.50	1.45
11	B	1232	CLA	C1D-ND	-2.58	1.34	1.37
11	B	1023	CLA	C4B-NB	-2.58	1.34	1.37
11	1	1114	CLA	C1D-ND	-2.58	1.34	1.37
11	2	1223	CLA	C1D-ND	-2.58	1.34	1.37
11	2	1235	CLA	C1D-ND	-2.58	1.34	1.37
11	L	1503	CLA	C1B-NB	-2.58	1.34	1.37
11	b	1223	CLA	C1B-NB	-2.58	1.34	1.37
11	b	1229	CLA	C1D-C2D	2.58	1.50	1.45
11	A	1110	CLA	C1D-ND	-2.58	1.34	1.37
11	a	1119	CLA	C1D-ND	-2.58	1.34	1.37
11	1	1102	CLA	C1D-ND	-2.58	1.34	1.37
11	A	1126	CLA	C1B-NB	-2.58	1.34	1.37
11	b	1212	CLA	C1D-ND	-2.58	1.34	1.37
11	B	1203	CLA	C1D-C2D	2.58	1.50	1.45
11	B	1211	CLA	C1B-NB	-2.58	1.34	1.37
11	1	1130	CLA	C1B-NB	-2.58	1.34	1.37
11	2	1214	CLA	C1B-NB	-2.58	1.34	1.37
11	2	1217	CLA	C4C-C3C	2.58	1.49	1.45
11	l	1503	CLA	C1D-C2D	2.58	1.50	1.45
11	1	1012	CLA	C1B-NB	-2.57	1.34	1.37
11	A	1120	CLA	C1D-C2D	2.57	1.50	1.45
11	1	1112	CLA	C1B-NB	-2.57	1.34	1.37
11	1	1134	CLA	C1B-NB	-2.57	1.34	1.37
11	a	1119	CLA	C1D-C2D	2.57	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1206	CLA	C1B-C2B	2.57	1.49	1.43
11	1	1022	CLA	C1B-C2B	2.57	1.49	1.43
11	a	1116	CLA	C1D-C2D	2.57	1.50	1.45
11	A	1137	CLA	C4B-NB	-2.57	1.34	1.37
11	L	1502	CLA	C1D-ND	-2.57	1.34	1.37
11	2	1203	CLA	C1D-ND	-2.57	1.34	1.37
11	A	1134	CLA	C1D-C2D	2.57	1.50	1.45
11	b	1239	CLA	C1D-C2D	2.57	1.50	1.45
11	B	1236	CLA	C1D-ND	-2.57	1.34	1.37
11	a	1801	CLA	C1D-C2D	2.57	1.50	1.45
11	a	1103	CLA	C1B-NB	-2.57	1.34	1.37
11	1	1137	CLA	C1B-NB	-2.57	1.34	1.37
11	B	1232	CLA	C4C-C3C	2.57	1.49	1.45
11	A	1109	CLA	C1D-ND	-2.57	1.34	1.37
11	2	1013	CLA	C1B-NB	-2.57	1.34	1.37
11	2	1211	CLA	C1B-NB	-2.57	1.34	1.37
11	k	1401	CLA	C1B-NB	-2.57	1.34	1.37
11	8	1503	CLA	C1D-C2D	2.57	1.50	1.45
11	A	1114	CLA	C1D-ND	-2.57	1.34	1.37
11	A	1123	CLA	C1D-C2D	2.57	1.50	1.45
11	2	1231	CLA	C1B-C2B	2.57	1.49	1.43
11	b	1223	CLA	C1D-ND	-2.57	1.34	1.37
11	b	1234	CLA	C1D-ND	-2.57	1.34	1.37
11	2	1219	CLA	C1D-ND	-2.57	1.34	1.37
11	A	1012	CLA	C1B-NB	-2.57	1.34	1.37
11	a	1114	CLA	C1D-ND	-2.57	1.34	1.37
11	2	1224	CLA	C1D-ND	-2.57	1.34	1.37
11	2	1209	CLA	C4C-C3C	2.57	1.49	1.45
11	b	1235	CLA	C1D-C2D	2.56	1.50	1.45
11	1	1116	CLA	C1D-C2D	2.56	1.50	1.45
11	1	1107	CLA	C1D-ND	-2.56	1.34	1.37
11	1	1138	CLA	C1D-C2D	2.56	1.50	1.45
11	a	1129	CLA	C1D-ND	-2.56	1.34	1.37
11	K	1401	CLA	C1B-NB	-2.56	1.34	1.37
11	B	1226	CLA	C1B-C2B	2.56	1.49	1.43
11	1	1117	CLA	C1D-C2D	2.56	1.50	1.45
11	A	1237	CLA	C1B-NB	-2.56	1.34	1.37
11	2	1203	CLA	C1B-NB	-2.56	1.34	1.37
11	a	1114	CLA	C1D-C2D	2.56	1.50	1.45
11	A	1116	CLA	C1B-C2B	2.56	1.49	1.43
11	2	1229	CLA	C1D-ND	-2.56	1.34	1.37
11	B	1202	CLA	C1D-C2D	2.56	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1102	CLA	C1D-ND	-2.56	1.34	1.37
11	a	1125	CLA	C1D-ND	-2.56	1.34	1.37
11	A	1130	CLA	C1D-C2D	2.56	1.50	1.45
11	A	1111	CLA	C1B-NB	-2.56	1.34	1.37
11	A	1117	CLA	C1D-C2D	2.56	1.50	1.45
11	1	1112	CLA	C1D-C2D	2.56	1.50	1.45
11	B	1220	CLA	C1D-C2D	2.56	1.50	1.45
11	1	1123	CLA	C1D-ND	-2.56	1.34	1.37
11	1	1129	CLA	C1B-NB	-2.56	1.34	1.37
11	a	1125	CLA	C1C-NC	-2.56	1.33	1.37
11	a	1139	CLA	C1D-C2D	2.55	1.50	1.45
11	2	1223	CLA	C1D-C2D	2.55	1.50	1.45
11	a	1108	CLA	C1D-C2D	2.55	1.50	1.45
11	1	1101	CLA	C1D-C2D	2.55	1.50	1.45
11	A	1119	CLA	C1C-NC	-2.55	1.33	1.37
11	B	1215	CLA	C1B-NB	-2.55	1.34	1.37
11	2	1213	CLA	C1D-ND	-2.55	1.34	1.37
11	8	1501	CLA	C1D-ND	-2.55	1.34	1.37
11	B	1216	CLA	C1D-ND	-2.55	1.34	1.37
11	b	1238	CLA	C1D-ND	-2.55	1.34	1.37
11	1	1110	CLA	C1D-ND	-2.55	1.34	1.37
11	1	1121	CLA	C1D-ND	-2.55	1.34	1.37
11	1	1106	CLA	C1B-NB	-2.55	1.34	1.37
11	A	1801	CLA	C1B-NB	-2.55	1.34	1.37
11	b	1209	CLA	C1B-NB	-2.55	1.34	1.37
11	1	1118	CLA	C1B-NB	-2.55	1.34	1.37
11	B	1231	CLA	C1D-ND	-2.55	1.34	1.37
11	B	1235	CLA	C1D-ND	-2.55	1.34	1.37
11	a	1123	CLA	C1D-ND	-2.55	1.34	1.37
11	B	1229	CLA	C1D-C2D	2.55	1.50	1.45
14	f	4018	BCR	C30-C25	-2.55	1.50	1.53
11	b	1204	CLA	C1D-C2D	2.55	1.50	1.45
11	b	1023	CLA	C4B-NB	-2.55	1.34	1.37
11	B	1234	CLA	C1D-ND	-2.55	1.34	1.37
11	a	1139	CLA	C1D-ND	-2.55	1.34	1.37
11	B	1216	CLA	C4B-NB	-2.55	1.34	1.37
11	A	1115	CLA	C1D-C2D	2.54	1.50	1.45
11	b	1234	CLA	C4C-C3C	2.54	1.49	1.45
11	a	1101	CLA	C1D-C2D	2.54	1.50	1.45
11	A	1237	CLA	C1D-ND	-2.54	1.34	1.37
11	B	1230	CLA	C1B-NB	-2.54	1.34	1.37
11	2	1238	CLA	C1D-ND	-2.54	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1133	CLA	C1C-NC	-2.54	1.33	1.37
11	B	1220	CLA	C1B-C2B	2.54	1.49	1.43
11	B	1215	CLA	C1D-ND	-2.54	1.34	1.37
11	a	1237	CLA	C1B-NB	-2.54	1.34	1.37
11	b	1206	CLA	C1D-C2D	2.54	1.50	1.45
11	a	1117	CLA	C1D-C2D	2.54	1.50	1.45
11	1	1106	CLA	C1D-C2D	2.54	1.50	1.45
11	2	1013	CLA	C1D-C2D	2.54	1.50	1.45
11	A	1134	CLA	C4C-C3C	2.54	1.49	1.45
11	2	1230	CLA	C1C-NC	-2.54	1.33	1.37
11	2	1227	CLA	C1D-C2D	2.54	1.50	1.45
11	a	1118	CLA	C1B-NB	-2.54	1.34	1.37
11	1	1128	CLA	C1C-NC	-2.54	1.33	1.37
11	B	1228	CLA	C1D-ND	-2.54	1.34	1.37
11	b	1226	CLA	C1B-NB	-2.54	1.34	1.37
11	8	1502	CLA	C1B-NB	-2.54	1.34	1.37
11	a	1124	CLA	C1D-C2D	2.54	1.50	1.45
11	B	1213	CLA	C1D-ND	-2.54	1.34	1.37
11	b	1217	CLA	C1D-ND	-2.54	1.34	1.37
11	2	1218	CLA	C1D-C2D	2.54	1.50	1.45
11	A	1137	CLA	C1B-NB	-2.54	1.34	1.37
11	b	1202	CLA	C1B-NB	-2.54	1.34	1.37
11	2	1231	CLA	C1D-C2D	2.54	1.50	1.45
11	a	1138	CLA	C4C-C3C	2.54	1.49	1.45
11	a	1112	CLA	C1B-NB	-2.53	1.34	1.37
11	a	1137	CLA	C4B-NB	-2.53	1.34	1.37
11	b	1231	CLA	C1D-ND	-2.53	1.34	1.37
11	1	1123	CLA	C1B-NB	-2.53	1.34	1.37
11	1	1108	CLA	C1D-C2D	2.53	1.50	1.45
11	b	1216	CLA	C1B-C2B	2.53	1.49	1.43
11	B	1023	CLA	C1C-NC	-2.53	1.33	1.37
11	A	1135	CLA	C1D-C2D	2.53	1.50	1.45
11	1	1237	CLA	C1B-NB	-2.53	1.34	1.37
11	B	1214	CLA	C1D-ND	-2.53	1.34	1.37
11	B	1209	CLA	C4C-C3C	2.53	1.49	1.45
11	a	1128	CLA	C1C-NC	-2.53	1.33	1.37
11	b	1231	CLA	C1B-NB	-2.53	1.34	1.37
11	a	1112	CLA	C1D-C2D	2.53	1.50	1.45
11	b	1207	CLA	C1B-NB	-2.53	1.34	1.37
11	2	1236	CLA	C1D-ND	-2.53	1.34	1.37
11	b	1228	CLA	C1D-C2D	2.53	1.50	1.45
11	1	1123	CLA	C1D-C2D	2.53	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1013	CLA	C1B-C2B	2.53	1.49	1.43
11	A	1113	CLA	C1B-NB	-2.53	1.34	1.37
11	1	1112	CLA	C1D-ND	-2.53	1.34	1.37
11	A	1114	CLA	C1D-C2D	2.53	1.50	1.45
11	L	1503	CLA	C1D-C2D	2.53	1.50	1.45
11	1	1126	CLA	C1D-C2D	2.53	1.50	1.45
11	A	1105	CLA	C1D-C2D	2.52	1.50	1.45
11	2	1239	CLA	C1D-C2D	2.52	1.50	1.45
11	B	1206	CLA	C1C-NC	-2.52	1.33	1.37
11	2	1228	CLA	C1B-NB	-2.52	1.34	1.37
11	2	1234	CLA	C1D-ND	-2.52	1.34	1.37
11	a	1135	CLA	C4C-C3C	2.52	1.49	1.45
11	A	1103	CLA	C1B-NB	-2.52	1.34	1.37
11	0	1401	CLA	C1B-NB	-2.52	1.34	1.37
11	A	1106	CLA	C1D-C2D	2.52	1.50	1.45
11	a	1102	CLA	C1B-NB	-2.52	1.34	1.37
11	K	1402	CLA	C1D-ND	-2.52	1.34	1.37
11	2	1212	CLA	C1C-NC	-2.52	1.33	1.37
11	A	1108	CLA	C1D-ND	-2.52	1.34	1.37
11	2	1232	CLA	C1D-ND	-2.52	1.34	1.37
11	A	1135	CLA	C1C-NC	-2.52	1.33	1.37
11	b	1217	CLA	C1D-C2D	2.52	1.50	1.45
11	a	1103	CLA	C1D-C2D	2.52	1.50	1.45
11	1	1130	CLA	C1B-C2B	2.52	1.49	1.43
11	a	1011	CLA	C4B-NB	-2.52	1.34	1.37
11	1	1122	CLA	C1B-NB	-2.52	1.34	1.37
11	1	1127	CLA	C1B-NB	-2.52	1.34	1.37
11	a	1131	CLA	C1D-C2D	2.52	1.50	1.45
11	b	1227	CLA	C1D-C2D	2.52	1.50	1.45
11	B	1201	CLA	C1B-NB	-2.52	1.34	1.37
11	A	1128	CLA	C1B-NB	-2.52	1.34	1.37
11	B	1231	CLA	C1D-C2D	2.52	1.50	1.45
11	2	1218	CLA	C1D-ND	-2.52	1.34	1.37
11	2	1220	CLA	C4C-C3C	2.52	1.49	1.45
11	B	1214	CLA	C1B-NB	-2.51	1.34	1.37
11	2	1201	CLA	C1D-ND	-2.51	1.34	1.37
11	2	1209	CLA	C1D-ND	-2.51	1.34	1.37
11	a	1133	CLA	C4C-C3C	2.51	1.49	1.45
11	B	1235	CLA	C1D-C2D	2.51	1.50	1.45
11	A	1140	CLA	C1D-ND	-2.51	1.34	1.37
11	B	1240	CLA	C1D-C2D	2.51	1.50	1.45
11	1	1114	CLA	C4C-C3C	2.51	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1123	CLA	C1D-ND	-2.51	1.34	1.37
11	1	1116	CLA	C1B-NB	-2.51	1.34	1.37
11	1	1133	CLA	C1D-C2D	2.51	1.50	1.45
11	B	1240	CLA	C1B-NB	-2.51	1.34	1.37
11	b	1208	CLA	C4C-C3C	2.51	1.49	1.45
11	A	1125	CLA	C1B-NB	-2.51	1.34	1.37
11	a	1106	CLA	C1B-NB	-2.51	1.34	1.37
11	1	1137	CLA	C4B-NB	-2.51	1.34	1.37
11	a	1132	CLA	C1D-C2D	2.51	1.50	1.45
11	A	1113	CLA	C1D-ND	-2.51	1.34	1.37
11	a	1133	CLA	C1D-C2D	2.51	1.50	1.45
11	B	1219	CLA	C1B-NB	-2.51	1.34	1.37
11	a	1120	CLA	C1B-NB	-2.51	1.34	1.37
11	2	1240	CLA	C1D-ND	-2.51	1.34	1.37
11	2	1238	CLA	C1D-C2D	2.51	1.50	1.45
11	a	1135	CLA	C1B-NB	-2.51	1.34	1.37
11	b	1214	CLA	C1B-NB	-2.51	1.34	1.37
11	1	1110	CLA	C1D-C2D	2.51	1.50	1.45
11	1	1109	CLA	C1D-ND	-2.51	1.34	1.37
11	b	1213	CLA	C1D-C2D	2.51	1.50	1.45
11	1	1115	CLA	C1C-NC	-2.51	1.34	1.37
11	a	1128	CLA	C1B-NB	-2.51	1.34	1.37
11	1	1110	CLA	C4C-C3C	2.50	1.49	1.45
11	a	1136	CLA	C1D-C2D	2.50	1.50	1.45
11	B	1234	CLA	C1C-NC	-2.50	1.34	1.37
11	k	1402	CLA	C1C-NC	-2.50	1.34	1.37
11	b	1013	CLA	C1D-C2D	2.50	1.50	1.45
11	b	1202	CLA	C1D-C2D	2.50	1.50	1.45
11	a	1110	CLA	C1D-C2D	2.50	1.50	1.45
11	a	1137	CLA	C1D-C2D	2.50	1.50	1.45
11	1	1801	CLA	C1D-C2D	2.50	1.50	1.45
11	a	1116	CLA	C1B-C2B	2.50	1.49	1.43
11	2	1215	CLA	C1D-C2D	2.50	1.50	1.45
11	2	1235	CLA	C1B-NB	-2.50	1.34	1.37
11	k	1402	CLA	C1D-ND	-2.50	1.34	1.37
11	A	1801	CLA	C1D-C2D	2.50	1.50	1.45
11	2	1222	CLA	C1D-C2D	2.50	1.50	1.45
11	k	1401	CLA	C1D-C2D	2.50	1.50	1.45
11	B	1201	CLA	C1C-NC	-2.50	1.34	1.37
11	B	1213	CLA	C1D-C2D	2.50	1.50	1.45
11	1	1104	CLA	C1D-C2D	2.50	1.50	1.45
11	2	1234	CLA	C1D-C2D	2.50	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1022	CLA	C1B-NB	-2.50	1.34	1.37
11	b	1230	CLA	C4C-C3C	2.50	1.49	1.45
11	2	1203	CLA	C1D-C2D	2.50	1.50	1.45
11	b	1210	CLA	C4C-C3C	2.50	1.49	1.45
11	B	1210	CLA	C1D-ND	-2.50	1.34	1.37
11	B	1223	CLA	C1B-NB	-2.50	1.34	1.37
11	2	1229	CLA	C1D-C2D	2.50	1.50	1.45
11	1	1132	CLA	C1D-C2D	2.49	1.50	1.45
11	B	1216	CLA	C1B-C2B	2.49	1.49	1.43
11	1	1138	CLA	C1D-ND	-2.49	1.34	1.37
11	2	1212	CLA	C1B-NB	-2.49	1.34	1.37
11	1	1125	CLA	C4C-C3C	2.49	1.49	1.45
11	B	1212	CLA	C1D-C2D	2.49	1.50	1.45
11	B	1227	CLA	C1D-C2D	2.49	1.50	1.45
11	2	1210	CLA	C1D-C2D	2.49	1.50	1.45
11	A	1112	CLA	C1D-ND	-2.49	1.34	1.37
11	B	1021	CLA	C4B-NB	-2.49	1.34	1.37
11	B	1203	CLA	C1B-NB	-2.49	1.34	1.37
11	b	1214	CLA	C1D-ND	-2.49	1.34	1.37
11	1	1131	CLA	C1D-C2D	2.49	1.50	1.45
11	A	1114	CLA	C4C-C3C	2.49	1.49	1.45
11	B	1207	CLA	C1C-NC	-2.49	1.34	1.37
11	1	1133	CLA	C4B-NB	-2.49	1.34	1.37
11	2	1228	CLA	C1D-C2D	2.49	1.50	1.45
11	A	1123	CLA	C1C-NC	-2.49	1.34	1.37
11	1	1123	CLA	C4C-C3C	2.49	1.49	1.45
11	B	1239	CLA	C1D-C2D	2.49	1.50	1.45
11	b	1234	CLA	C1B-NB	-2.49	1.34	1.37
11	A	1124	CLA	C1D-C2D	2.49	1.50	1.45
11	a	1104	CLA	C1D-C2D	2.49	1.50	1.45
11	B	1209	CLA	C1D-C2D	2.49	1.50	1.45
11	1	1801	CLA	C1C-NC	-2.49	1.34	1.37
11	b	1209	CLA	C1D-ND	-2.49	1.34	1.37
11	1	1113	CLA	C1B-NB	-2.49	1.34	1.37
11	A	1136	CLA	C1D-C2D	2.49	1.50	1.45
11	A	1119	CLA	C1D-C2D	2.49	1.50	1.45
11	1	1137	CLA	C1D-ND	-2.49	1.34	1.37
11	2	1239	CLA	C1D-ND	-2.49	1.34	1.37
11	A	1119	CLA	C4C-C3C	2.48	1.49	1.45
11	A	1123	CLA	C1B-NB	-2.48	1.34	1.37
11	B	1202	CLA	C1D-ND	-2.48	1.34	1.37
11	2	1210	CLA	C4B-NB	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1223	CLA	C1D-C2D	2.48	1.50	1.45
11	B	1228	CLA	C4C-C3C	2.48	1.49	1.45
11	B	1229	CLA	C1C-NC	-2.48	1.34	1.37
11	b	1211	CLA	C1D-C2D	2.48	1.50	1.45
11	b	1210	CLA	C1D-ND	-2.48	1.34	1.37
11	B	1216	CLA	C4C-C3C	2.48	1.49	1.45
11	1	1136	CLA	C1D-C2D	2.48	1.50	1.45
11	A	1133	CLA	C4C-C3C	2.48	1.49	1.45
11	a	1121	CLA	C1D-ND	-2.48	1.34	1.37
11	b	1213	CLA	C1D-ND	-2.48	1.34	1.37
11	b	1221	CLA	C1D-ND	-2.48	1.34	1.37
11	1	1108	CLA	C1D-ND	-2.48	1.34	1.37
11	b	1210	CLA	C1D-C2D	2.48	1.50	1.45
11	a	1108	CLA	C1B-NB	-2.48	1.34	1.37
11	A	1126	CLA	C1D-C2D	2.48	1.50	1.45
11	a	1109	CLA	C1D-ND	-2.48	1.34	1.37
11	a	1137	CLA	C1B-NB	-2.48	1.34	1.37
11	b	1224	CLA	C1D-ND	-2.48	1.34	1.37
11	2	1214	CLA	C1D-C2D	2.48	1.50	1.45
11	k	1402	CLA	C1B-NB	-2.48	1.34	1.37
11	2	1240	CLA	C4C-C3C	2.47	1.49	1.45
11	A	1138	CLA	C1B-NB	-2.47	1.34	1.37
11	A	1135	CLA	C1B-NB	-2.47	1.34	1.37
11	b	1236	CLA	C1B-NB	-2.47	1.34	1.37
11	1	1103	CLA	C4B-NB	-2.47	1.34	1.37
11	b	1203	CLA	C1D-C2D	2.47	1.50	1.45
11	K	1401	CLA	C1D-C2D	2.47	1.50	1.45
11	b	1234	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1102	CLA	C1D-C2D	2.47	1.50	1.45
11	b	1239	CLA	C4C-C3C	2.47	1.49	1.45
11	2	1214	CLA	C1C-NC	-2.47	1.34	1.37
11	A	1022	CLA	C1B-C2B	2.47	1.48	1.43
11	B	1224	CLA	C1B-NB	-2.47	1.34	1.37
11	a	1101	CLA	C1B-NB	-2.47	1.34	1.37
11	1	1120	CLA	C1B-NB	-2.47	1.34	1.37
11	a	1129	CLA	C1D-C2D	2.47	1.50	1.45
11	b	1210	CLA	C1B-NB	-2.47	1.34	1.37
11	b	1214	CLA	C1D-C2D	2.47	1.50	1.45
11	2	1210	CLA	C1B-NB	-2.47	1.34	1.37
11	A	1112	CLA	C3B-C4B	2.47	1.49	1.42
11	a	1135	CLA	C1D-C2D	2.47	1.50	1.45
11	B	1203	CLA	C1D-ND	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1124	CLA	C1B-NB	-2.47	1.34	1.37
11	a	1137	CLA	C1D-ND	-2.47	1.34	1.37
11	l	1501	CLA	C1B-NB	-2.47	1.34	1.37
11	1	1113	CLA	C1D-ND	-2.47	1.34	1.37
11	b	1239	CLA	C1D-ND	-2.47	1.34	1.37
11	1	1136	CLA	C1D-ND	-2.47	1.34	1.37
11	a	1113	CLA	C1D-ND	-2.47	1.34	1.37
11	B	1234	CLA	C1D-C2D	2.46	1.50	1.45
11	2	1235	CLA	C1D-C2D	2.46	1.50	1.45
11	B	1209	CLA	C1D-ND	-2.46	1.34	1.37
11	0	1401	CLA	C1D-ND	-2.46	1.34	1.37
11	a	1102	CLA	C1D-C2D	2.46	1.50	1.45
11	2	1239	CLA	C4C-C3C	2.46	1.49	1.45
11	A	1237	CLA	C1C-NC	-2.46	1.34	1.37
11	A	1125	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1133	CLA	C1B-NB	-2.46	1.34	1.37
11	a	1113	CLA	C1B-NB	-2.46	1.34	1.37
11	2	1210	CLA	C1D-ND	-2.46	1.34	1.37
11	b	1216	CLA	C4C-C3C	2.46	1.49	1.45
11	B	1218	CLA	C1C-NC	-2.46	1.34	1.37
11	B	1206	CLA	C1B-NB	-2.46	1.34	1.37
11	a	1119	CLA	C1B-NB	-2.46	1.34	1.37
11	B	1227	CLA	C1C-NC	-2.46	1.34	1.37
11	B	1207	CLA	C1B-NB	-2.46	1.34	1.37
11	A	1112	CLA	C1D-C2D	2.46	1.50	1.45
11	2	1236	CLA	C1B-NB	-2.46	1.34	1.37
11	0	1401	CLA	C1D-C2D	2.46	1.50	1.45
11	b	1225	CLA	C4C-C3C	2.46	1.49	1.45
11	a	1108	CLA	C1D-ND	-2.46	1.34	1.37
11	b	1201	CLA	C1B-NB	-2.46	1.34	1.37
11	1	1133	CLA	C1B-NB	-2.46	1.34	1.37
11	A	1122	CLA	C1C-NC	-2.46	1.34	1.37
11	B	1205	CLA	C1B-NB	-2.46	1.34	1.37
11	0	1402	CLA	C1D-ND	-2.46	1.34	1.37
11	a	1801	CLA	C4C-C3C	2.46	1.49	1.45
11	A	1111	CLA	C1D-C2D	2.46	1.50	1.45
11	1	1133	CLA	C1D-ND	-2.46	1.34	1.37
11	1	1111	CLA	C1D-ND	-2.46	1.34	1.37
11	B	1228	CLA	C1C-NC	-2.46	1.34	1.37
11	a	1125	CLA	C1B-NB	-2.46	1.34	1.37
11	2	1208	CLA	C1D-C2D	2.45	1.50	1.45
11	2	1217	CLA	C1B-NB	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1237	CLA	C1D-C2D	2.45	1.50	1.45
11	A	1102	CLA	C1B-NB	-2.45	1.34	1.37
11	1	1110	CLA	C1B-NB	-2.45	1.34	1.37
11	2	1240	CLA	C1D-C2D	2.45	1.50	1.45
11	A	1012	CLA	C1C-NC	-2.45	1.34	1.37
11	a	1128	CLA	C1D-C2D	2.45	1.50	1.45
11	A	1106	CLA	C1C-NC	-2.45	1.34	1.37
11	2	1232	CLA	C4C-C3C	2.45	1.49	1.45
11	A	1131	CLA	C1D-C2D	2.45	1.50	1.45
11	a	1012	CLA	C1B-NB	-2.45	1.34	1.37
11	b	1239	CLA	C1C-NC	-2.45	1.34	1.37
11	L	1502	CLA	C1D-C2D	2.45	1.50	1.45
11	2	1218	CLA	C1C-NC	-2.45	1.34	1.37
11	B	1225	CLA	C4B-NB	-2.45	1.34	1.37
11	L	1502	CLA	C1B-NB	-2.45	1.34	1.37
11	1	1022	CLA	C1B-NB	-2.45	1.34	1.37
11	2	1214	CLA	C4B-NB	-2.45	1.34	1.37
11	1	1102	CLA	C1D-C2D	2.45	1.50	1.45
11	B	1238	CLA	C1B-NB	-2.45	1.34	1.37
11	1	1237	CLA	C1D-ND	-2.45	1.34	1.37
11	1	1125	CLA	C1D-C2D	2.45	1.50	1.45
11	k	1401	CLA	C1D-ND	-2.45	1.34	1.37
11	1	1115	CLA	C1D-C2D	2.45	1.50	1.45
11	B	1230	CLA	C4B-NB	-2.45	1.34	1.37
11	B	1220	CLA	C4C-C3C	2.44	1.49	1.45
11	2	1219	CLA	C1D-C2D	2.44	1.50	1.45
11	1	1129	CLA	C1D-C2D	2.44	1.50	1.45
11	B	1023	CLA	C1B-NB	-2.44	1.34	1.37
11	a	1129	CLA	C1B-NB	-2.44	1.34	1.37
11	2	1208	CLA	C1C-NC	-2.44	1.34	1.37
14	6	4018	BCR	C30-C25	-2.44	1.50	1.53
11	1	1109	CLA	C1B-NB	-2.44	1.34	1.37
11	l	1503	CLA	C1B-NB	-2.44	1.34	1.37
11	A	1110	CLA	C1C-NC	-2.44	1.34	1.37
11	A	1139	CLA	C1D-C2D	2.44	1.50	1.45
11	a	1801	CLA	C1B-NB	-2.44	1.34	1.37
11	A	1128	CLA	C1C-NC	-2.44	1.34	1.37
11	A	1111	CLA	C1D-ND	-2.44	1.34	1.37
11	1	1102	CLA	C1B-NB	-2.44	1.34	1.37
11	1	1116	CLA	C1D-ND	-2.44	1.34	1.37
11	2	1211	CLA	C4B-NB	-2.44	1.34	1.37
11	a	1112	CLA	C3B-C4B	2.44	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1124	CLA	C4C-C3C	2.44	1.49	1.45
11	b	1227	CLA	C1B-NB	-2.44	1.34	1.37
11	a	1124	CLA	C1C-NC	-2.44	1.34	1.37
11	A	1111	CLA	C4B-NB	-2.44	1.34	1.37
11	a	1126	CLA	C1B-NB	-2.44	1.34	1.37
11	B	1203	CLA	C1C-NC	-2.44	1.34	1.37
11	1	1139	CLA	C4C-C3C	2.44	1.49	1.45
11	2	1201	CLA	C4C-C3C	2.44	1.49	1.45
11	B	1218	CLA	C1D-ND	-2.44	1.34	1.37
11	a	1139	CLA	C1B-NB	-2.44	1.34	1.37
11	1	1104	CLA	C1B-NB	-2.44	1.34	1.37
11	K	1402	CLA	C1B-NB	-2.44	1.34	1.37
11	b	1223	CLA	C1D-C2D	2.44	1.50	1.45
11	A	1137	CLA	C1D-C2D	2.44	1.50	1.45
11	a	1116	CLA	C1D-ND	-2.44	1.34	1.37
11	b	1235	CLA	C4B-NB	-2.44	1.34	1.37
11	1	1108	CLA	C1B-NB	-2.44	1.34	1.37
11	K	1401	CLA	C1D-ND	-2.44	1.34	1.37
11	a	1131	CLA	C1B-NB	-2.44	1.34	1.37
11	b	1206	CLA	C4C-C3C	2.44	1.49	1.45
11	B	1227	CLA	C1B-NB	-2.44	1.34	1.37
11	a	1115	CLA	C1C-NC	-2.43	1.34	1.37
11	1	1107	CLA	C1C-NC	-2.43	1.34	1.37
11	2	1216	CLA	C4C-C3C	2.43	1.49	1.45
11	a	1118	CLA	C1C-NC	-2.43	1.34	1.37
11	1	1801	CLA	C1B-NB	-2.43	1.34	1.37
11	1	1132	CLA	C1B-NB	-2.43	1.34	1.37
11	K	1402	CLA	C1D-C2D	2.43	1.50	1.45
11	B	1228	CLA	C1B-NB	-2.43	1.34	1.37
11	a	1110	CLA	C1B-NB	-2.43	1.34	1.37
11	b	1239	CLA	C1B-NB	-2.43	1.34	1.37
11	1	1125	CLA	C1B-NB	-2.43	1.34	1.37
11	2	1227	CLA	C4C-C3C	2.43	1.49	1.45
11	a	1133	CLA	C1D-ND	-2.43	1.34	1.37
11	L	1502	CLA	C4B-NB	-2.43	1.34	1.37
11	l	1502	CLA	C1B-NB	-2.43	1.34	1.37
11	A	1109	CLA	C1B-NB	-2.43	1.34	1.37
11	A	1127	CLA	C4B-NB	-2.43	1.34	1.37
11	b	1216	CLA	C1D-C2D	2.43	1.50	1.45
11	b	1238	CLA	C1C-NC	-2.43	1.34	1.37
11	A	1113	CLA	C1D-C2D	2.43	1.50	1.45
11	A	1117	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1106	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1122	CLA	C4B-NB	-2.42	1.34	1.37
11	B	1235	CLA	C1B-NB	-2.42	1.34	1.37
11	b	1234	CLA	C1D-C2D	2.42	1.50	1.45
11	2	1224	CLA	C1D-C2D	2.42	1.50	1.45
11	A	1125	CLA	C1D-C2D	2.42	1.50	1.45
11	B	1210	CLA	C4B-NB	-2.42	1.34	1.37
11	1	1139	CLA	C1B-NB	-2.42	1.34	1.37
11	A	1129	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1205	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1236	CLA	C1D-C2D	2.42	1.50	1.45
11	1	1138	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1121	CLA	C1D-ND	-2.42	1.34	1.37
11	b	1219	CLA	C4B-NB	-2.42	1.34	1.37
11	b	1212	CLA	C1D-C2D	2.42	1.50	1.45
11	a	1111	CLA	C1B-NB	-2.42	1.34	1.37
11	b	1235	CLA	C1D-ND	-2.42	1.34	1.37
11	a	1110	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1114	CLA	C1C-NC	-2.42	1.34	1.37
11	2	1235	CLA	C4B-NB	-2.42	1.34	1.37
11	1	1109	CLA	C1C-NC	-2.42	1.34	1.37
11	B	1210	CLA	C1C-NC	-2.42	1.34	1.37
11	A	1110	CLA	C1B-NB	-2.42	1.34	1.37
11	2	1217	CLA	C1D-C2D	2.42	1.50	1.45
11	1	1111	CLA	C1C-NC	-2.42	1.34	1.37
11	L	1501	CLA	C1D-C2D	2.42	1.50	1.45
11	1	1113	CLA	C1D-C2D	2.42	1.50	1.45
11	a	1112	CLA	C1D-ND	-2.42	1.34	1.37
11	A	1237	CLA	C4B-NB	-2.42	1.34	1.37
11	B	1206	CLA	C4B-NB	-2.42	1.34	1.37
11	a	1136	CLA	C1D-ND	-2.42	1.34	1.37
11	b	1222	CLA	C1D-C2D	2.42	1.50	1.45
11	A	1022	CLA	C1D-C2D	2.41	1.50	1.45
11	b	1209	CLA	C1C-NC	-2.41	1.34	1.37
11	8	1501	CLA	C1D-C2D	2.41	1.50	1.45
11	2	1201	CLA	C1D-C2D	2.41	1.50	1.45
11	a	1103	CLA	C4B-NB	-2.41	1.34	1.37
11	a	1113	CLA	C1D-C2D	2.41	1.50	1.45
11	A	1108	CLA	C1B-NB	-2.41	1.34	1.37
11	B	1217	CLA	C1D-C2D	2.41	1.50	1.45
11	1	1133	CLA	C1C-NC	-2.41	1.34	1.37
11	a	1134	CLA	C4C-C3C	2.41	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1230	CLA	C1B-NB	-2.41	1.34	1.37
11	B	1219	CLA	C1D-C2D	2.41	1.50	1.45
11	A	1120	CLA	C1B-NB	-2.41	1.34	1.37
11	1	1126	CLA	C1B-NB	-2.41	1.34	1.37
11	2	1224	CLA	C1B-NB	-2.41	1.34	1.37
11	b	1223	CLA	C4C-C3C	2.41	1.49	1.45
11	b	1205	CLA	C1C-NC	-2.41	1.34	1.37
11	b	1206	CLA	C1C-NC	-2.41	1.34	1.37
11	1	1120	CLA	C1D-C2D	2.41	1.50	1.45
11	a	1119	CLA	C4C-C3C	2.41	1.49	1.45
11	2	1231	CLA	C1D-ND	-2.41	1.34	1.37
11	2	1236	CLA	C1D-C2D	2.41	1.50	1.45
11	A	1108	CLA	C4B-NB	-2.41	1.34	1.37
11	2	1218	CLA	C1B-NB	-2.41	1.34	1.37
11	B	1229	CLA	C4C-C3C	2.41	1.49	1.45
11	B	1013	CLA	C1C-NC	-2.41	1.34	1.37
11	2	1207	CLA	C1B-NB	-2.41	1.34	1.37
11	1	1125	CLA	C1C-NC	-2.41	1.34	1.37
11	A	1118	CLA	C1B-NB	-2.40	1.34	1.37
11	B	1202	CLA	C4B-NB	-2.40	1.34	1.37
11	A	1126	CLA	C1B-C2B	2.40	1.48	1.43
11	1	1127	CLA	C4B-NB	-2.40	1.34	1.37
11	2	1213	CLA	C1B-NB	-2.40	1.34	1.37
11	A	1136	CLA	C1C-NC	-2.40	1.34	1.37
11	b	1023	CLA	C1C-NC	-2.40	1.34	1.37
11	a	1140	CLA	C1D-C2D	2.40	1.50	1.45
11	a	1135	CLA	C1C-NC	-2.40	1.34	1.37
11	a	1138	CLA	C1B-NB	-2.40	1.34	1.37
11	2	1021	CLA	C4B-NB	-2.40	1.34	1.37
11	b	1203	CLA	C1B-NB	-2.40	1.34	1.37
11	b	1204	CLA	C1B-NB	-2.40	1.34	1.37
11	2	1238	CLA	C1C-NC	-2.40	1.34	1.37
11	2	1240	CLA	C1C-NC	-2.40	1.34	1.37
11	1	1128	CLA	C1D-C2D	2.40	1.50	1.45
11	A	1138	CLA	C1C-NC	-2.40	1.34	1.37
11	b	1230	CLA	C1C-NC	-2.40	1.34	1.37
11	b	1209	CLA	C4B-NB	-2.40	1.34	1.37
11	2	1224	CLA	C1C-NC	-2.40	1.34	1.37
11	A	1118	CLA	C1D-C2D	2.40	1.50	1.45
11	a	1111	CLA	C1D-C2D	2.40	1.50	1.45
11	a	1123	CLA	C4C-C3C	2.40	1.49	1.45
11	b	1232	CLA	C4C-C3C	2.40	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1136	CLA	C1C-NC	-2.40	1.34	1.37
11	A	1104	CLA	C1B-NB	-2.40	1.34	1.37
11	2	1240	CLA	C1B-NB	-2.40	1.34	1.37
11	1	1022	CLA	C1D-C2D	2.40	1.50	1.45
11	b	1222	CLA	C1B-NB	-2.40	1.34	1.37
11	B	1021	CLA	C1C-NC	-2.40	1.34	1.37
11	b	1224	CLA	C1D-C2D	2.40	1.50	1.45
11	A	1140	CLA	C1B-NB	-2.40	1.34	1.37
11	A	1133	CLA	C1D-C2D	2.39	1.50	1.45
11	b	1023	CLA	C1D-C2D	2.39	1.50	1.45
11	2	1227	CLA	C1C-NC	-2.39	1.34	1.37
11	8	1501	CLA	C1C-NC	-2.39	1.34	1.37
11	A	1134	CLA	C1D-ND	-2.39	1.34	1.37
11	B	1212	CLA	C1B-NB	-2.39	1.34	1.37
11	2	1213	CLA	C4B-NB	-2.39	1.34	1.37
11	2	1223	CLA	C1B-NB	-2.39	1.34	1.37
11	B	1208	CLA	C1B-NB	-2.39	1.34	1.37
11	2	1203	CLA	C4B-NB	-2.39	1.34	1.37
11	2	1225	CLA	C1D-ND	-2.39	1.34	1.37
11	A	1110	CLA	C4C-C3C	2.39	1.49	1.45
11	1	1117	CLA	C1C-NC	-2.39	1.34	1.37
11	2	1226	CLA	C1C-NC	-2.39	1.34	1.37
11	B	1235	CLA	C4B-NB	-2.39	1.34	1.37
11	A	1022	CLA	C1C-NC	-2.39	1.34	1.37
11	b	1213	CLA	C1B-NB	-2.39	1.34	1.37
11	a	1237	CLA	C1C-NC	-2.39	1.34	1.37
11	b	1212	CLA	C1C-NC	-2.39	1.34	1.37
11	b	1227	CLA	C4C-C3C	2.39	1.49	1.45
11	A	1108	CLA	C1C-NC	-2.39	1.34	1.37
11	B	1224	CLA	C1C-NC	-2.39	1.34	1.37
11	a	1106	CLA	C1C-NC	-2.39	1.34	1.37
11	a	1127	CLA	C1C-NC	-2.39	1.34	1.37
11	b	1225	CLA	C1D-C2D	2.39	1.50	1.45
11	a	1133	CLA	C1C-NC	-2.39	1.34	1.37
11	2	1238	CLA	C1B-NB	-2.39	1.34	1.37
11	K	1402	CLA	C4B-NB	-2.39	1.34	1.37
11	a	1120	CLA	C1D-C2D	2.39	1.50	1.45
11	A	1118	CLA	C1C-NC	-2.39	1.34	1.37
11	A	1124	CLA	C1C-NC	-2.39	1.34	1.37
11	2	1206	CLA	C1C-NC	-2.39	1.34	1.37
11	A	1107	CLA	C4B-NB	-2.39	1.34	1.37
11	a	1116	CLA	C1C-NC	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1201	CLA	C1D-C2D	2.38	1.50	1.45
11	a	1121	CLA	C4C-C3C	2.38	1.49	1.45
11	A	1101	CLA	C1D-C2D	2.38	1.50	1.45
11	1	1140	CLA	C1D-C2D	2.38	1.50	1.45
11	a	1104	CLA	C1B-NB	-2.38	1.34	1.37
11	a	1136	CLA	C1B-NB	-2.38	1.34	1.37
11	b	1207	CLA	C4B-NB	-2.38	1.34	1.37
11	2	1222	CLA	C1B-NB	-2.38	1.34	1.37
11	a	1134	CLA	C1D-ND	-2.38	1.34	1.37
11	0	1402	CLA	C1B-NB	-2.38	1.34	1.37
11	A	1126	CLA	C3B-C4B	2.38	1.49	1.42
11	L	1502	CLA	C1C-NC	-2.38	1.34	1.37
11	A	1116	CLA	C1D-C2D	2.38	1.50	1.45
11	A	1131	CLA	C1B-NB	-2.38	1.34	1.37
11	b	1236	CLA	C1D-ND	-2.38	1.34	1.37
11	a	1138	CLA	C1C-NC	-2.38	1.34	1.37
11	L	1501	CLA	C1B-NB	-2.38	1.34	1.37
11	a	1109	CLA	C1B-NB	-2.38	1.34	1.37
11	b	1211	CLA	C1B-NB	-2.38	1.34	1.37
11	1	1012	CLA	C1C-NC	-2.38	1.34	1.37
11	A	1117	CLA	C4B-NB	-2.38	1.34	1.37
11	b	1228	CLA	C4C-C3C	2.38	1.49	1.45
11	B	1226	CLA	C1C-NC	-2.38	1.34	1.37
11	2	1239	CLA	C1B-NB	-2.38	1.34	1.37
11	A	1132	CLA	C1D-C2D	2.38	1.50	1.45
11	a	1113	CLA	C4C-C3C	2.38	1.49	1.45
11	B	1210	CLA	C1D-C2D	2.38	1.50	1.45
11	2	1224	CLA	C4B-NB	-2.38	1.34	1.37
11	1	1134	CLA	C4C-C3C	2.38	1.49	1.45
11	B	1232	CLA	C1C-NC	-2.38	1.34	1.37
11	A	1131	CLA	C4C-C3C	2.38	1.49	1.45
11	A	1139	CLA	C1B-NB	-2.38	1.34	1.37
11	a	1130	CLA	C1B-NB	-2.38	1.34	1.37
11	2	1202	CLA	C1D-ND	-2.38	1.34	1.37
11	0	1402	CLA	C1C-NC	-2.38	1.34	1.37
11	B	1207	CLA	C1D-C2D	2.37	1.50	1.45
11	A	1107	CLA	C1C-NC	-2.37	1.34	1.37
11	2	1205	CLA	C1C-NC	-2.37	1.34	1.37
11	a	1107	CLA	C4B-NB	-2.37	1.34	1.37
11	1	1131	CLA	C4B-NB	-2.37	1.34	1.37
11	B	1215	CLA	C1C-NC	-2.37	1.34	1.37
11	A	1132	CLA	C4B-NB	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1201	CLA	C1C-NC	-2.37	1.34	1.37
11	A	1134	CLA	C1C-NC	-2.37	1.34	1.37
11	b	1217	CLA	C1C-NC	-2.37	1.34	1.37
11	A	1122	CLA	C1D-C2D	2.37	1.50	1.45
11	2	1219	CLA	C3B-C4B	2.37	1.49	1.42
11	2	1231	CLA	C3B-C4B	2.37	1.49	1.42
11	1	1104	CLA	C1C-NC	-2.37	1.34	1.37
11	B	1214	CLA	C1D-C2D	2.37	1.50	1.45
11	2	1023	CLA	C4C-C3C	2.37	1.49	1.45
11	B	1201	CLA	C1D-C2D	2.37	1.50	1.45
11	2	1223	CLA	C3B-C4B	2.37	1.49	1.42
11	A	1116	CLA	C4B-NB	-2.37	1.34	1.37
11	b	1220	CLA	C1B-NB	-2.37	1.34	1.37
11	1	1131	CLA	C1C-NC	-2.37	1.34	1.37
11	a	1111	CLA	C1D-ND	-2.37	1.34	1.37
11	a	1140	CLA	C1B-NB	-2.37	1.34	1.37
11	1	1124	CLA	C1B-NB	-2.37	1.34	1.37
11	a	1103	CLA	C4C-C3C	2.37	1.49	1.45
11	a	1105	CLA	C4C-C3C	2.37	1.49	1.45
11	a	1022	CLA	C4B-NB	-2.37	1.34	1.37
11	2	1230	CLA	C4B-NB	-2.37	1.34	1.37
11	B	1221	CLA	C4B-NB	-2.37	1.34	1.37
11	1	1134	CLA	C1D-ND	-2.37	1.34	1.37
11	2	1220	CLA	C1B-NB	-2.37	1.34	1.37
11	1	1136	CLA	C1C-NC	-2.37	1.34	1.37
11	2	1220	CLA	C1D-C2D	2.36	1.50	1.45
11	a	1116	CLA	C3B-C4B	2.36	1.49	1.42
11	b	1205	CLA	C4B-NB	-2.36	1.34	1.37
11	2	1201	CLA	C1C-NC	-2.36	1.34	1.37
11	2	1203	CLA	C1C-NC	-2.36	1.34	1.37
11	1	1103	CLA	C4C-C3C	2.36	1.49	1.45
11	2	1225	CLA	C4C-C3C	2.36	1.49	1.45
11	A	1103	CLA	C1D-ND	-2.36	1.34	1.37
11	B	1217	CLA	C1B-NB	-2.36	1.34	1.37
11	A	1012	CLA	C4B-NB	-2.36	1.34	1.37
11	a	1130	CLA	C4B-NB	-2.36	1.34	1.37
11	1	1122	CLA	C4B-NB	-2.36	1.34	1.37
11	a	1116	CLA	C4C-C3C	2.36	1.49	1.45
11	a	1130	CLA	C4C-C3C	2.36	1.49	1.45
11	1	1237	CLA	C1C-NC	-2.36	1.34	1.37
11	0	1401	CLA	C4B-NB	-2.36	1.34	1.37
11	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)
11	1	1120	CLA	C4C-C3C	2.36	1.49	1.45
11	a	1134	CLA	C1C-NC	-2.36	1.34	1.37
11	b	1228	CLA	C1C-NC	-2.36	1.34	1.37
11	1	1118	CLA	C1C-NC	-2.36	1.34	1.37
11	B	1224	CLA	C1D-C2D	2.36	1.50	1.45
11	a	1114	CLA	C4C-C3C	2.36	1.49	1.45
11	2	1231	CLA	C4C-C3C	2.36	1.49	1.45
11	b	1214	CLA	C1C-NC	-2.36	1.34	1.37
11	1	1105	CLA	C1C-NC	-2.36	1.34	1.37
11	A	1136	CLA	C1B-NB	-2.36	1.34	1.37
11	a	1124	CLA	C4B-NB	-2.36	1.34	1.37
14	6	4020	BCR	C30-C25	-2.36	1.50	1.53
11	a	1132	CLA	C1B-NB	-2.36	1.34	1.37
11	b	1217	CLA	C1B-NB	-2.36	1.34	1.37
11	A	1131	CLA	C4B-NB	-2.36	1.34	1.37
11	A	1117	CLA	C3B-C4B	2.36	1.49	1.42
11	a	1135	CLA	C4B-NB	-2.36	1.34	1.37
11	1	1116	CLA	C4C-C3C	2.35	1.49	1.45
11	B	1211	CLA	C1C-NC	-2.35	1.34	1.37
11	b	1220	CLA	C1C-NC	-2.35	1.34	1.37
11	b	1224	CLA	C1B-NB	-2.35	1.34	1.37
11	8	1502	CLA	C4B-NB	-2.35	1.34	1.37
11	1	1130	CLA	C1C-NC	-2.35	1.34	1.37
11	b	1226	CLA	C1D-C2D	2.35	1.50	1.45
11	b	1211	CLA	C4B-NB	-2.35	1.34	1.37
11	2	1239	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1222	CLA	C4B-NB	-2.35	1.34	1.37
11	1	1111	CLA	C4B-NB	-2.35	1.34	1.37
11	2	1215	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1214	CLA	C4B-NB	-2.35	1.34	1.37
11	a	1133	CLA	C4B-NB	-2.35	1.34	1.37
11	B	1216	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1219	CLA	C1C-NC	-2.35	1.34	1.37
11	1	1140	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1236	CLA	C4B-NB	-2.35	1.34	1.37
11	b	1230	CLA	C1B-NB	-2.35	1.34	1.37
11	1	1119	CLA	C1C-NC	-2.35	1.34	1.37
11	b	1021	CLA	C4C-C3C	2.35	1.49	1.45
11	a	1136	CLA	C4B-NB	-2.35	1.34	1.37
11	2	1211	CLA	C1D-C2D	2.35	1.50	1.45
11	A	1106	CLA	C4C-C3C	2.35	1.49	1.45
11	A	1109	CLA	C1C-NC	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1105	CLA	C1C-NC	-2.35	1.34	1.37
11	B	1206	CLA	C1D-C2D	2.35	1.50	1.45
11	2	1209	CLA	C4B-NB	-2.35	1.34	1.37
11	2	1229	CLA	C1B-NB	-2.35	1.34	1.37
11	A	1101	CLA	C1B-NB	-2.35	1.34	1.37
11	a	1109	CLA	C4C-C3C	2.35	1.49	1.45
11	a	1124	CLA	C1B-NB	-2.35	1.34	1.37
11	a	1022	CLA	C1D-C2D	2.35	1.50	1.45
11	a	1124	CLA	C4C-C3C	2.34	1.49	1.45
11	1	1137	CLA	C1D-C2D	2.34	1.50	1.45
11	1	1135	CLA	C1D-C2D	2.34	1.50	1.45
11	K	1401	CLA	C4B-NB	-2.34	1.34	1.37
11	a	1130	CLA	C1C-NC	-2.34	1.34	1.37
11	b	1211	CLA	C4C-C3C	2.34	1.49	1.45
11	B	1238	CLA	C1C-NC	-2.34	1.34	1.37
11	2	1210	CLA	C1C-NC	-2.34	1.34	1.37
11	B	1206	CLA	C4C-C3C	2.34	1.49	1.45
11	b	1240	CLA	C1C-NC	-2.34	1.34	1.37
11	B	1219	CLA	C4B-NB	-2.34	1.34	1.37
11	a	1117	CLA	C1B-NB	-2.34	1.34	1.37
11	2	1236	CLA	C4B-NB	-2.34	1.34	1.37
11	k	1401	CLA	C4B-NB	-2.34	1.34	1.37
11	8	1502	CLA	C1C-NC	-2.34	1.34	1.37
11	2	1021	CLA	C4C-C3C	2.34	1.49	1.45
11	A	1140	CLA	C4C-C3C	2.34	1.49	1.45
11	B	1201	CLA	C4C-C3C	2.34	1.49	1.45
11	1	1011	CLA	C1C-NC	-2.34	1.34	1.37
11	2	1217	CLA	C1C-NC	-2.34	1.34	1.37
11	1	1122	CLA	C1D-C2D	2.34	1.50	1.45
11	B	1013	CLA	C4B-NB	-2.34	1.34	1.37
11	1	1108	CLA	C4B-NB	-2.34	1.34	1.37
11	1	1135	CLA	C1B-NB	-2.34	1.34	1.37
11	k	1401	CLA	C1C-NC	-2.34	1.34	1.37
11	A	1130	CLA	C4B-NB	-2.34	1.34	1.37
11	B	1209	CLA	C1C-NC	-2.34	1.34	1.37
11	1	1132	CLA	C1C-NC	-2.34	1.34	1.37
11	2	1220	CLA	C1C-NC	-2.34	1.34	1.37
11	A	1137	CLA	C1C-NC	-2.34	1.34	1.37
11	B	1209	CLA	C4B-NB	-2.33	1.34	1.37
11	A	1132	CLA	C1C-NC	-2.33	1.34	1.37
11	1	1127	CLA	C1C-NC	-2.33	1.34	1.37
11	a	1122	CLA	C4B-NB	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	1503	CLA	C4B-NB	-2.33	1.34	1.37
11	2	1013	CLA	C1C-NC	-2.33	1.34	1.37
11	2	1234	CLA	C1B-NB	-2.33	1.34	1.37
11	a	1107	CLA	C1D-C2D	2.33	1.49	1.45
11	a	1125	CLA	C1D-C2D	2.33	1.49	1.45
11	B	1201	CLA	C4B-NB	-2.33	1.34	1.37
11	1	1128	CLA	C4C-C3C	2.33	1.49	1.45
11	2	1213	CLA	C1C-NC	-2.33	1.34	1.37
11	B	1236	CLA	C1B-NB	-2.33	1.34	1.37
11	a	1110	CLA	C4C-C3C	2.33	1.49	1.45
11	a	1120	CLA	C1C-NC	-2.33	1.34	1.37
11	b	1202	CLA	C1D-ND	-2.33	1.34	1.37
11	k	1402	CLA	C4C-C3C	2.33	1.49	1.45
11	B	1239	CLA	C1C-NC	-2.33	1.34	1.37
11	B	1228	CLA	C4B-NB	-2.33	1.34	1.37
11	b	1204	CLA	C1C-NC	-2.33	1.34	1.37
11	a	1131	CLA	C4C-C3C	2.33	1.49	1.45
11	A	1129	CLA	C1D-C2D	2.33	1.49	1.45
11	2	1230	CLA	C4C-C3C	2.33	1.49	1.45
11	2	1205	CLA	C1B-NB	-2.33	1.34	1.37
11	a	1122	CLA	C1D-C2D	2.33	1.49	1.45
11	k	1402	CLA	C3B-C4B	2.33	1.49	1.42
11	b	1222	CLA	C1C-NC	-2.33	1.34	1.37
11	a	1108	CLA	C4C-C3C	2.33	1.49	1.45
11	B	1234	CLA	C4B-NB	-2.33	1.34	1.37
11	a	1131	CLA	C4B-NB	-2.33	1.34	1.37
11	a	1128	CLA	C4C-C3C	2.33	1.49	1.45
11	b	1236	CLA	C4B-NB	-2.32	1.34	1.37
11	B	1232	CLA	C1B-NB	-2.32	1.34	1.37
11	b	1222	CLA	C4B-NB	-2.32	1.34	1.37
11	b	1214	CLA	C3B-C4B	2.32	1.49	1.42
11	a	1131	CLA	C1C-NC	-2.32	1.34	1.37
11	a	1129	CLA	C4B-NB	-2.32	1.34	1.37
11	b	1230	CLA	C4B-NB	-2.32	1.34	1.37
11	B	1207	CLA	C4B-NB	-2.32	1.34	1.37
11	2	1225	CLA	C4B-NB	-2.32	1.34	1.37
11	a	1126	CLA	C1D-C2D	2.32	1.49	1.45
11	b	1223	CLA	C1C-NC	-2.32	1.34	1.37
14	2	4017	BCR	C30-C25	-2.32	1.50	1.53
11	a	1114	CLA	C1B-NB	-2.32	1.34	1.37
11	1	1104	CLA	C3B-C4B	2.32	1.49	1.42
11	1	1111	CLA	C1D-C2D	2.32	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1204	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1217	CLA	C1C-NC	-2.32	1.34	1.37
11	a	1022	CLA	C1C-NC	-2.32	1.34	1.37
11	b	1208	CLA	C1B-NB	-2.32	1.34	1.37
11	1	1138	CLA	C1B-NB	-2.32	1.34	1.37
11	1	1136	CLA	C4B-NB	-2.32	1.34	1.37
11	2	1202	CLA	C4B-NB	-2.32	1.34	1.37
11	b	1225	CLA	C4B-NB	-2.32	1.34	1.37
11	A	1102	CLA	C4C-C3C	2.32	1.49	1.45
11	1	1140	CLA	C1B-NB	-2.32	1.34	1.37
14	B	4011	BCR	C1-C6	-2.32	1.50	1.53
11	A	1110	CLA	C1D-C2D	2.32	1.49	1.45
11	a	1101	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1239	CLA	C1B-NB	-2.32	1.34	1.37
11	2	1234	CLA	C4B-NB	-2.32	1.34	1.37
11	1	1101	CLA	C1C-NC	-2.32	1.34	1.37
11	1	1114	CLA	C1C-NC	-2.32	1.34	1.37
11	1	1135	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1202	CLA	C3B-C4B	2.32	1.49	1.42
11	a	1132	CLA	C1C-NC	-2.32	1.34	1.37
11	a	1132	CLA	C4B-NB	-2.32	1.34	1.37
11	A	1138	CLA	C1D-ND	-2.32	1.34	1.37
11	a	1105	CLA	C4B-NB	-2.32	1.34	1.37
11	1	1107	CLA	C4B-NB	-2.32	1.34	1.37
11	K	1401	CLA	C1C-NC	-2.32	1.34	1.37
11	0	1401	CLA	C1C-NC	-2.32	1.34	1.37
11	A	1117	CLA	C1C-NC	-2.31	1.34	1.37
11	b	1208	CLA	C1C-NC	-2.31	1.34	1.37
11	1	1103	CLA	C1C-NC	-2.31	1.34	1.37
11	A	1140	CLA	C1D-C2D	2.31	1.49	1.45
11	L	1501	CLA	C1C-NC	-2.31	1.34	1.37
11	b	1220	CLA	C4B-NB	-2.31	1.34	1.37
11	2	1227	CLA	C1B-NB	-2.31	1.34	1.37
11	2	1206	CLA	C4C-C3C	2.31	1.49	1.45
11	a	1128	CLA	C3B-C4B	2.31	1.49	1.42
11	a	1134	CLA	C3B-C4B	2.31	1.49	1.42
11	A	1113	CLA	C4B-NB	-2.31	1.34	1.37
11	a	1111	CLA	C1C-NC	-2.31	1.34	1.37
11	b	1210	CLA	C4B-NB	-2.31	1.34	1.37
11	1	1101	CLA	C4B-NB	-2.31	1.34	1.37
11	1	1121	CLA	C1B-NB	-2.31	1.34	1.37
11	B	1226	CLA	C1D-C2D	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1121	CLA	C1B-NB	-2.31	1.34	1.37
11	b	1219	CLA	C1D-C2D	2.31	1.49	1.45
11	b	1231	CLA	C4C-C3C	2.31	1.49	1.45
11	A	1136	CLA	C4C-C3C	2.31	1.49	1.45
11	A	1011	CLA	C4B-NB	-2.31	1.34	1.37
11	A	1120	CLA	C1C-NC	-2.31	1.34	1.37
11	B	1231	CLA	C1C-NC	-2.31	1.34	1.37
11	1	1022	CLA	C1C-NC	-2.31	1.34	1.37
11	A	1129	CLA	C4C-C3C	2.31	1.49	1.45
11	b	1215	CLA	C4C-C3C	2.31	1.49	1.45
11	0	1401	CLA	C4C-C3C	2.31	1.49	1.45
11	B	1221	CLA	C1C-NC	-2.31	1.34	1.37
11	a	1115	CLA	C1B-NB	-2.31	1.34	1.37
11	b	1229	CLA	C1B-NB	-2.31	1.34	1.37
11	1	1105	CLA	C4B-NB	-2.31	1.34	1.37
11	a	1105	CLA	C1B-NB	-2.31	1.34	1.37
11	b	1205	CLA	C1B-NB	-2.31	1.34	1.37
11	1	1124	CLA	C1C-NC	-2.31	1.34	1.37
11	A	1132	CLA	C4C-C3C	2.31	1.49	1.45
11	a	1112	CLA	C4C-C3C	2.31	1.49	1.45
11	B	1215	CLA	C4B-NB	-2.31	1.34	1.37
11	a	1140	CLA	C1C-NC	-2.30	1.34	1.37
11	2	1229	CLA	C4C-C3C	2.30	1.48	1.45
11	a	1117	CLA	C1C-NC	-2.30	1.34	1.37
11	b	1219	CLA	C1C-NC	-2.30	1.34	1.37
11	2	1216	CLA	C4B-NB	-2.30	1.34	1.37
11	2	1221	CLA	C4B-NB	-2.30	1.34	1.37
11	2	1226	CLA	C1D-C2D	2.30	1.49	1.45
11	2	1215	CLA	C4B-NB	-2.30	1.34	1.37
11	1	1107	CLA	C1D-C2D	2.30	1.49	1.45
11	A	1115	CLA	C1B-NB	-2.30	1.34	1.37
11	2	1234	CLA	C1C-NC	-2.30	1.34	1.37
11	a	1103	CLA	C1C-NC	-2.30	1.34	1.37
11	a	1122	CLA	C1C-NC	-2.30	1.34	1.37
11	b	1204	CLA	C4B-NB	-2.30	1.34	1.37
11	2	1208	CLA	C1B-NB	-2.30	1.34	1.37
11	1	1801	CLA	C4C-C3C	2.30	1.48	1.45
11	A	1127	CLA	C1D-C2D	2.30	1.49	1.45
11	B	1234	CLA	C4C-C3C	2.30	1.48	1.45
11	a	1101	CLA	C4B-NB	-2.30	1.34	1.37
11	A	1111	CLA	C4C-C3C	2.30	1.48	1.45
11	A	1135	CLA	C4C-C3C	2.30	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1218	CLA	C1B-NB	-2.30	1.34	1.37
11	A	1127	CLA	C1C-NC	-2.30	1.34	1.37
11	a	1118	CLA	C1D-C2D	2.30	1.49	1.45
11	B	1220	CLA	C1C-NC	-2.30	1.34	1.37
11	A	1114	CLA	C1B-NB	-2.30	1.34	1.37
11	1	1116	CLA	C4B-NB	-2.30	1.34	1.37
11	A	1105	CLA	C1C-NC	-2.30	1.34	1.37
11	a	1129	CLA	C1C-NC	-2.30	1.34	1.37
11	A	1104	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1114	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1214	CLA	C4C-C3C	2.29	1.48	1.45
11	a	1113	CLA	C4B-NB	-2.29	1.34	1.37
11	b	1224	CLA	C4B-NB	-2.29	1.34	1.37
11	b	1238	CLA	C1B-NB	-2.29	1.34	1.37
11	A	1101	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1137	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1127	CLA	C1D-C2D	2.29	1.49	1.45
11	B	1240	CLA	C4C-C3C	2.29	1.48	1.45
11	2	1207	CLA	C1D-C2D	2.29	1.49	1.45
11	b	1216	CLA	C4B-NB	-2.29	1.34	1.37
11	K	1401	CLA	C4C-C3C	2.29	1.48	1.45
11	A	1129	CLA	C3B-C4B	2.29	1.49	1.42
11	a	1237	CLA	C1D-C2D	2.29	1.49	1.45
11	l	1502	CLA	C1D-C2D	2.29	1.49	1.45
11	b	1218	CLA	C1B-NB	-2.29	1.34	1.37
11	b	1229	CLA	C1C-NC	-2.29	1.34	1.37
11	1	1237	CLA	C4B-NB	-2.29	1.34	1.37
11	2	1217	CLA	C4B-NB	-2.29	1.34	1.37
11	2	1228	CLA	C1C-NC	-2.29	1.34	1.37
11	1	1114	CLA	C1B-NB	-2.29	1.34	1.37
11	2	1204	CLA	C1B-NB	-2.29	1.34	1.37
11	2	1206	CLA	C1D-C2D	2.29	1.49	1.45
11	A	1115	CLA	C1C-NC	-2.29	1.34	1.37
11	B	1222	CLA	C1C-NC	-2.29	1.34	1.37
11	a	1801	CLA	C1C-NC	-2.29	1.34	1.37
11	l	1501	CLA	C1C-NC	-2.29	1.34	1.37
11	8	1503	CLA	C3B-C4B	2.29	1.49	1.42
11	B	1204	CLA	C4B-NB	-2.29	1.34	1.37
11	A	1120	CLA	C4C-C3C	2.29	1.48	1.45
11	b	1210	CLA	C1C-NC	-2.29	1.34	1.37
11	1	1127	CLA	C4C-C3C	2.29	1.48	1.45
11	B	1224	CLA	C4B-NB	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1229	CLA	C1B-NB	-2.29	1.34	1.37
11	b	1238	CLA	C4B-NB	-2.29	1.34	1.37
11	b	1013	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1202	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1204	CLA	C1C-NC	-2.29	1.34	1.37
11	2	1212	CLA	C4C-C3C	2.29	1.48	1.45
11	b	1224	CLA	C4C-C3C	2.29	1.48	1.45
11	b	1218	CLA	C1C-NC	-2.28	1.34	1.37
11	L	1503	CLA	C1C-NC	-2.28	1.34	1.37
11	1	1136	CLA	C4C-C3C	2.28	1.48	1.45
11	a	1121	CLA	C1B-NB	-2.28	1.34	1.37
11	2	1220	CLA	C4B-NB	-2.28	1.34	1.37
11	1	1106	CLA	C4C-C3C	2.28	1.48	1.45
11	B	1214	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1236	CLA	C1C-NC	-2.28	1.34	1.37
11	l	1503	CLA	C1C-NC	-2.28	1.34	1.37
11	a	1126	CLA	C3B-C4B	2.28	1.49	1.42
11	A	1801	CLA	C3B-C4B	2.28	1.49	1.42
11	A	1103	CLA	C3B-C4B	2.28	1.49	1.42
11	1	1115	CLA	C1B-NB	-2.28	1.34	1.37
11	1	1132	CLA	C4C-C3C	2.28	1.48	1.45
11	a	1106	CLA	C3B-C4B	2.28	1.49	1.42
11	l	1501	CLA	C1D-C2D	2.28	1.49	1.45
11	1	1101	CLA	C4C-C3C	2.28	1.48	1.45
11	1	1121	CLA	C4C-C3C	2.28	1.48	1.45
11	0	1402	CLA	C4C-C3C	2.28	1.48	1.45
11	B	1226	CLA	C4B-NB	-2.28	1.34	1.37
11	a	1119	CLA	C4B-NB	-2.28	1.34	1.37
11	a	1125	CLA	C4B-NB	-2.28	1.34	1.37
11	b	1221	CLA	C4B-NB	-2.28	1.34	1.37
11	a	1012	CLA	C1C-NC	-2.28	1.34	1.37
11	b	1219	CLA	C4C-C3C	2.28	1.48	1.45
11	2	1212	CLA	C1D-C2D	2.28	1.49	1.45
11	1	1115	CLA	C4C-C3C	2.28	1.48	1.45
11	B	1231	CLA	C4B-NB	-2.28	1.34	1.37
11	1	1131	CLA	C1B-NB	-2.28	1.34	1.37
11	1	1113	CLA	C4C-C3C	2.28	1.48	1.45
11	a	1107	CLA	C1C-NC	-2.28	1.34	1.37
11	1	1137	CLA	C1C-NC	-2.28	1.34	1.37
11	1	1112	CLA	C4C-C3C	2.28	1.48	1.45
11	b	1206	CLA	C4B-NB	-2.28	1.34	1.37
11	b	1224	CLA	C1C-NC	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	4018	BCR	C30-C25	-2.27	1.50	1.53
11	1	1136	CLA	C1B-NB	-2.27	1.34	1.37
11	1	1110	CLA	C3B-C4B	2.27	1.49	1.42
11	b	1203	CLA	C1C-NC	-2.27	1.34	1.37
11	b	1240	CLA	C4C-C3C	2.27	1.48	1.45
11	8	1503	CLA	C4B-NB	-2.27	1.34	1.37
11	k	1401	CLA	C4C-C3C	2.27	1.48	1.45
11	1	1134	CLA	C1C-NC	-2.27	1.34	1.37
11	a	1138	CLA	C1D-ND	-2.27	1.34	1.37
11	b	1202	CLA	C4B-NB	-2.27	1.34	1.37
11	1	1101	CLA	C1B-NB	-2.27	1.34	1.37
11	A	1104	CLA	C1D-C2D	2.27	1.49	1.45
11	A	1022	CLA	C4B-NB	-2.27	1.34	1.37
11	1	1109	CLA	C4B-NB	-2.27	1.34	1.37
11	1	1110	CLA	C1C-NC	-2.27	1.34	1.37
11	1	1109	CLA	C4C-C3C	2.27	1.48	1.45
11	B	1222	CLA	C3B-C4B	2.27	1.49	1.42
11	A	1130	CLA	C1C-NC	-2.27	1.34	1.37
11	l	1502	CLA	C1C-NC	-2.27	1.34	1.37
11	a	1102	CLA	C4B-NB	-2.27	1.34	1.37
11	b	1220	CLA	C1D-C2D	2.27	1.49	1.45
11	2	1023	CLA	C1D-C2D	2.27	1.49	1.45
11	a	1106	CLA	C1D-C2D	2.27	1.49	1.45
11	1	1111	CLA	C3B-C4B	2.27	1.49	1.42
11	B	1234	CLA	C1B-NB	-2.27	1.34	1.37
11	2	1226	CLA	C4B-NB	-2.27	1.34	1.37
11	B	1218	CLA	C4C-C3C	2.27	1.48	1.45
11	B	1213	CLA	C4B-NB	-2.27	1.34	1.37
11	b	1232	CLA	C1B-NB	-2.27	1.34	1.37
11	b	1240	CLA	C1B-NB	-2.27	1.34	1.37
11	A	1103	CLA	C1C-NC	-2.27	1.34	1.37
11	2	1209	CLA	C1C-NC	-2.27	1.34	1.37
11	b	1013	CLA	C4C-C3C	2.27	1.48	1.45
11	a	1126	CLA	C1C-C2C	2.27	1.49	1.44
11	A	1120	CLA	C4B-NB	-2.26	1.34	1.37
11	a	1108	CLA	C4B-NB	-2.26	1.34	1.37
11	1	1120	CLA	C1C-NC	-2.26	1.34	1.37
11	1	1105	CLA	C4C-C3C	2.26	1.48	1.45
11	2	1227	CLA	C4B-NB	-2.26	1.34	1.37
11	A	1107	CLA	C1D-C2D	2.26	1.49	1.45
11	A	1115	CLA	C3B-C4B	2.26	1.49	1.42
11	a	1102	CLA	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1121	CLA	C1C-NC	-2.26	1.34	1.37
11	A	1011	CLA	C1C-NC	-2.26	1.34	1.37
11	2	1223	CLA	C1C-NC	-2.26	1.34	1.37
11	b	1210	CLA	C3B-C4B	2.26	1.49	1.42
11	b	1238	CLA	C4C-C3C	2.26	1.48	1.45
11	A	1128	CLA	C1D-C2D	2.26	1.49	1.45
11	0	1402	CLA	C4B-NB	-2.26	1.34	1.37
11	A	1111	CLA	C1C-NC	-2.26	1.34	1.37
14	b	4017	BCR	C30-C25	-2.26	1.50	1.53
11	1	1119	CLA	C1B-NB	-2.26	1.34	1.37
11	1	1108	CLA	C1C-NC	-2.26	1.34	1.37
11	2	1238	CLA	C4B-NB	-2.26	1.34	1.37
11	2	1215	CLA	C4C-C3C	2.26	1.48	1.45
11	a	1115	CLA	C1D-C2D	2.26	1.49	1.45
11	a	1110	CLA	C3B-C4B	2.26	1.49	1.42
11	a	1108	CLA	C1C-NC	-2.26	1.34	1.37
11	1	1128	CLA	C3B-C4B	2.26	1.49	1.42
11	2	1201	CLA	C1B-NB	-2.26	1.34	1.37
11	a	1104	CLA	C1C-NC	-2.26	1.34	1.37
11	b	1218	CLA	C4C-C3C	2.26	1.48	1.45
11	1	1122	CLA	C1C-NC	-2.26	1.34	1.37
11	A	1114	CLA	C4B-NB	-2.26	1.34	1.37
11	a	1121	CLA	C4B-NB	-2.26	1.34	1.37
11	b	1215	CLA	C1C-NC	-2.26	1.34	1.37
11	a	1117	CLA	C4B-NB	-2.26	1.34	1.37
11	b	1201	CLA	C4B-NB	-2.26	1.34	1.37
11	8	1501	CLA	C4C-C3C	2.26	1.48	1.45
11	A	1103	CLA	C4B-NB	-2.26	1.34	1.37
11	2	1211	CLA	C1C-NC	-2.26	1.34	1.37
11	B	1203	CLA	C4B-NB	-2.25	1.34	1.37
11	B	1202	CLA	C1C-NC	-2.25	1.34	1.37
11	b	1213	CLA	C4B-NB	-2.25	1.34	1.37
11	1	1103	CLA	C1D-ND	-2.25	1.34	1.37
11	1	1134	CLA	C4B-NB	-2.25	1.34	1.37
11	B	1240	CLA	C3B-C4B	2.25	1.49	1.42
11	1	1011	CLA	C4B-NB	-2.25	1.34	1.37
11	a	1104	CLA	C4B-NB	-2.25	1.34	1.37
11	1	1121	CLA	C1C-NC	-2.25	1.34	1.37
11	2	1231	CLA	C1C-NC	-2.25	1.34	1.37
11	A	1138	CLA	C4B-NB	-2.25	1.34	1.37
11	2	1238	CLA	C4C-C3C	2.25	1.48	1.45
11	B	1219	CLA	C4C-C3C	2.25	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1112	CLA	C3B-C4B	2.25	1.49	1.42
14	a	4008	BCR	C30-C25	-2.25	1.50	1.53
11	a	1102	CLA	C1C-NC	-2.25	1.34	1.37
11	1	1129	CLA	C4B-NB	-2.25	1.34	1.37
11	2	1201	CLA	C4B-NB	-2.25	1.34	1.37
11	b	1211	CLA	C1C-NC	-2.25	1.34	1.37
11	a	1111	CLA	C3B-C4B	2.25	1.49	1.42
11	1	1117	CLA	C4B-NB	-2.25	1.34	1.37
11	a	1106	CLA	C4C-C3C	2.25	1.48	1.45
11	b	1239	CLA	C4B-NB	-2.25	1.34	1.37
11	b	1218	CLA	C3B-C4B	2.25	1.49	1.42
11	1	1125	CLA	C4B-NB	-2.25	1.34	1.37
11	A	1117	CLA	C4C-C3C	2.24	1.48	1.45
11	B	1225	CLA	C1D-C2D	2.24	1.49	1.45
11	B	1211	CLA	C1D-C2D	2.24	1.49	1.45
11	A	1136	CLA	C4B-NB	-2.24	1.34	1.37
11	b	1021	CLA	C1D-C2D	2.24	1.49	1.45
11	1	1129	CLA	C4C-C3C	2.24	1.48	1.45
11	1	1129	CLA	C1C-NC	-2.24	1.34	1.37
11	8	1503	CLA	C1C-NC	-2.24	1.34	1.37
11	a	1022	CLA	C4C-C3C	2.24	1.48	1.45
11	a	1011	CLA	C1C-NC	-2.24	1.34	1.37
11	B	1223	CLA	C3B-C4B	2.24	1.49	1.42
11	8	1502	CLA	C1D-C2D	2.24	1.49	1.45
11	a	1107	CLA	C1D-ND	-2.24	1.34	1.37
11	b	1226	CLA	C1C-NC	-2.24	1.34	1.37
11	A	1131	CLA	C1C-NC	-2.24	1.34	1.37
11	2	1213	CLA	C4C-C3C	2.24	1.48	1.45
11	b	1021	CLA	C3B-C4B	2.24	1.49	1.42
11	b	1231	CLA	C3B-C4B	2.24	1.49	1.42
11	B	1223	CLA	C4C-C3C	2.24	1.48	1.45
11	b	1235	CLA	C4C-C3C	2.24	1.48	1.45
11	2	1232	CLA	C1B-NB	-2.24	1.34	1.37
11	2	1208	CLA	C4B-NB	-2.24	1.34	1.37
11	2	1212	CLA	C4B-NB	-2.24	1.34	1.37
11	0	1402	CLA	C3B-C4B	2.23	1.49	1.42
11	a	1121	CLA	C1C-NC	-2.23	1.34	1.37
11	B	1215	CLA	C4C-C3C	2.23	1.48	1.45
11	2	1235	CLA	C1C-NC	-2.23	1.34	1.37
11	L	1503	CLA	C4B-NB	-2.23	1.34	1.37
11	l	1502	CLA	C4B-NB	-2.23	1.34	1.37
11	a	1137	CLA	C4C-C3C	2.23	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1011	CLA	C4C-C3C	2.23	1.48	1.45
11	1	1022	CLA	C4C-C3C	2.23	1.48	1.45
11	B	1232	CLA	C4B-NB	-2.23	1.34	1.37
11	2	1222	CLA	C1C-NC	-2.23	1.34	1.37
11	B	1212	CLA	C4B-NB	-2.23	1.34	1.37
11	B	1238	CLA	C4B-NB	-2.23	1.34	1.37
11	1	1117	CLA	C4C-C3C	2.23	1.48	1.45
11	A	1138	CLA	C4C-C3C	2.23	1.48	1.45
11	2	1229	CLA	C1C-NC	-2.23	1.34	1.37
11	B	1218	CLA	C4B-NB	-2.23	1.34	1.37
11	2	1219	CLA	C1C-NC	-2.23	1.34	1.37
11	2	1221	CLA	C1D-C2D	2.23	1.49	1.45
11	A	1011	CLA	C3B-C4B	2.23	1.49	1.42
11	B	1223	CLA	C1C-NC	-2.23	1.34	1.37
11	1	1108	CLA	C4C-C3C	2.23	1.48	1.45
11	1	1126	CLA	C1C-NC	-2.23	1.34	1.37
11	b	1217	CLA	C4C-C3C	2.23	1.48	1.45
11	8	1503	CLA	C4C-C3C	2.23	1.48	1.45
11	A	1123	CLA	C4B-NB	-2.23	1.34	1.37
11	A	1139	CLA	C1C-C2C	2.22	1.49	1.44
11	A	1112	CLA	C4C-C3C	2.22	1.48	1.45
11	B	1220	CLA	C4B-NB	-2.22	1.34	1.37
11	a	1127	CLA	C4B-NB	-2.22	1.34	1.37
11	b	1207	CLA	C1D-C2D	2.22	1.49	1.45
11	1	1114	CLA	C4B-NB	-2.22	1.34	1.37
11	a	1140	CLA	C4C-C3C	2.22	1.48	1.45
11	B	1208	CLA	C1C-NC	-2.22	1.34	1.37
11	b	1021	CLA	C1C-NC	-2.22	1.34	1.37
11	b	1213	CLA	C4C-C3C	2.22	1.48	1.45
11	A	1102	CLA	C1C-NC	-2.22	1.34	1.37
11	B	1212	CLA	C1C-NC	-2.22	1.34	1.37
11	b	1231	CLA	C1C-NC	-2.22	1.34	1.37
11	a	1138	CLA	C4B-NB	-2.22	1.34	1.37
11	B	1225	CLA	C1C-NC	-2.22	1.34	1.37
11	1	1130	CLA	C4C-C3C	2.22	1.48	1.45
11	b	1229	CLA	C3B-C4B	2.22	1.49	1.42
11	1	1123	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1219	CLA	C4B-NB	-2.22	1.34	1.37
11	2	1228	CLA	C4B-NB	-2.22	1.34	1.37
11	1	1126	CLA	C3B-C4B	2.22	1.49	1.42
11	B	1213	CLA	C1C-NC	-2.22	1.34	1.37
11	1	1139	CLA	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1102	CLA	C4C-C3C	2.22	1.48	1.45
11	b	1227	CLA	C1C-NC	-2.22	1.34	1.37
11	1	1102	CLA	C4B-NB	-2.22	1.34	1.37
11	A	1121	CLA	C3B-C4B	2.22	1.49	1.42
11	a	1125	CLA	C3B-C4B	2.22	1.49	1.42
11	a	1109	CLA	C1C-NC	-2.21	1.34	1.37
11	A	1140	CLA	C3B-C4B	2.21	1.49	1.42
14	A	4008	BCR	C30-C25	-2.21	1.50	1.53
11	A	1124	CLA	C4B-NB	-2.21	1.35	1.37
11	b	1202	CLA	C1C-NC	-2.21	1.34	1.37
11	2	1021	CLA	C1C-NC	-2.21	1.34	1.37
11	2	1013	CLA	C4B-NB	-2.21	1.35	1.37
11	1	1237	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1113	CLA	C1C-NC	-2.21	1.34	1.37
11	B	1217	CLA	C4B-NB	-2.21	1.35	1.37
11	a	1115	CLA	C3B-C4B	2.21	1.49	1.42
11	b	1214	CLA	C4B-NB	-2.21	1.35	1.37
11	a	1109	CLA	C3B-C4B	2.21	1.49	1.42
14	B	4014	BCR	C30-C25	-2.21	1.51	1.53
11	A	1115	CLA	C4B-NB	-2.21	1.35	1.37
11	A	1130	CLA	C1B-NB	-2.21	1.35	1.37
11	a	1116	CLA	C4B-NB	-2.21	1.35	1.37
11	1	1140	CLA	C4C-C3C	2.21	1.48	1.45
11	b	1212	CLA	C1B-NB	-2.21	1.35	1.37
11	b	1214	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1134	CLA	C3B-C4B	2.21	1.49	1.42
11	b	1232	CLA	C4B-NB	-2.21	1.35	1.37
11	1	1113	CLA	C4B-NB	-2.20	1.35	1.37
11	k	1402	CLA	C4B-NB	-2.20	1.35	1.37
11	1	1130	CLA	C3B-C4B	2.20	1.49	1.42
11	b	1221	CLA	C1D-C2D	2.20	1.49	1.45
11	b	1222	CLA	C4C-C3C	2.20	1.48	1.45
11	1	1131	CLA	C4C-C3C	2.20	1.48	1.45
11	B	1226	CLA	C3B-C4B	2.20	1.49	1.42
11	B	1227	CLA	C4B-NB	-2.20	1.35	1.37
11	B	1229	CLA	C4B-NB	-2.20	1.35	1.37
11	b	1223	CLA	C3B-C4B	2.20	1.49	1.42
11	2	1221	CLA	C1C-NC	-2.20	1.34	1.37
11	2	1218	CLA	C3B-C4B	2.20	1.49	1.42
11	b	1230	CLA	C1D-C2D	2.20	1.49	1.45
11	B	1205	CLA	C4B-NB	-2.20	1.35	1.37
11	b	1013	CLA	C4B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1116	CLA	C4C-C3C	2.20	1.48	1.45
11	A	1121	CLA	C4C-C3C	2.20	1.48	1.45
11	2	1222	CLA	C4B-NB	-2.20	1.35	1.37
11	B	1230	CLA	C4C-C3C	2.20	1.48	1.45
11	b	1228	CLA	C4B-NB	-2.20	1.35	1.37
11	1	1120	CLA	C4B-NB	-2.20	1.35	1.37
14	B	4005	BCR	C30-C25	-2.20	1.51	1.53
11	2	1013	CLA	C3B-C4B	2.20	1.49	1.42
11	A	1110	CLA	C3B-C4B	2.20	1.49	1.42
11	2	1219	CLA	C1C-C2C	2.20	1.49	1.44
11	1	1118	CLA	C4B-NB	-2.20	1.35	1.37
11	2	1232	CLA	C1C-NC	-2.20	1.34	1.37
11	1	1132	CLA	C4B-NB	-2.20	1.35	1.37
11	1	1135	CLA	C4B-NB	-2.20	1.35	1.37
11	b	1207	CLA	C4C-C3C	2.20	1.48	1.45
11	b	1240	CLA	C4B-NB	-2.20	1.35	1.37
11	A	1128	CLA	C3B-C4B	2.20	1.49	1.42
11	a	1101	CLA	C4C-C3C	2.20	1.48	1.45
11	B	1240	CLA	C1C-C2C	2.20	1.49	1.44
11	a	1106	CLA	C4B-NB	-2.20	1.35	1.37
11	B	1213	CLA	C4C-C3C	2.19	1.48	1.45
11	2	1234	CLA	C4C-C3C	2.19	1.48	1.45
11	A	1115	CLA	C4C-C3C	2.19	1.48	1.45
11	B	1214	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1011	CLA	C1D-C2D	2.19	1.49	1.45
11	A	1137	CLA	C3B-C4B	2.19	1.49	1.42
11	1	1138	CLA	C4B-NB	-2.19	1.35	1.37
11	A	1115	CLA	C1C-C2C	2.19	1.49	1.44
11	B	1235	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1212	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1217	CLA	C3B-C4B	2.19	1.49	1.42
11	b	1201	CLA	C3B-C4B	2.19	1.49	1.42
11	2	1236	CLA	C1C-NC	-2.19	1.34	1.37
11	A	1105	CLA	C1B-NB	-2.19	1.35	1.37
11	B	1013	CLA	C1D-C2D	2.19	1.49	1.45
11	a	1136	CLA	C4C-C3C	2.19	1.48	1.45
11	A	1801	CLA	C4B-NB	-2.19	1.35	1.37
11	B	1202	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1102	CLA	C1C-C2C	2.19	1.49	1.44
11	B	1231	CLA	C3B-C4B	2.19	1.49	1.42
11	B	1225	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1124	CLA	C4B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1012	CLA	C4B-NB	-2.19	1.35	1.37
11	1	1106	CLA	C3B-C4B	2.19	1.49	1.42
11	a	1139	CLA	C1C-NC	-2.18	1.34	1.37
11	b	1235	CLA	C1C-NC	-2.18	1.34	1.37
11	a	1011	CLA	C1D-C2D	2.18	1.49	1.45
11	a	1012	CLA	C4B-NB	-2.18	1.35	1.37
11	B	1235	CLA	C1C-NC	-2.18	1.34	1.37
11	2	1229	CLA	C3B-C4B	2.18	1.49	1.42
11	a	1012	CLA	C1D-C2D	2.18	1.49	1.45
11	a	1120	CLA	C4C-C3C	2.18	1.48	1.45
11	1	1113	CLA	C1C-NC	-2.18	1.34	1.37
11	a	1118	CLA	C4B-NB	-2.18	1.35	1.37
11	b	1226	CLA	C4C-C3C	2.18	1.48	1.45
11	b	1202	CLA	C3B-C4B	2.18	1.49	1.42
11	1	1130	CLA	C4B-NB	-2.18	1.35	1.37
11	A	1102	CLA	C4B-NB	-2.18	1.35	1.37
11	1	1801	CLA	C4B-NB	-2.18	1.35	1.37
11	2	1232	CLA	C4B-NB	-2.18	1.35	1.37
11	A	1101	CLA	C3B-C4B	2.18	1.49	1.42
11	b	1225	CLA	C1C-NC	-2.18	1.34	1.37
11	a	1132	CLA	C4C-C3C	2.18	1.48	1.45
11	a	1114	CLA	C4B-NB	-2.18	1.35	1.37
11	1	1140	CLA	C4B-NB	-2.18	1.35	1.37
11	a	1127	CLA	C3B-C4B	2.18	1.49	1.42
11	b	1234	CLA	C4B-NB	-2.18	1.35	1.37
11	l	1501	CLA	C4B-NB	-2.18	1.35	1.37
11	b	1023	CLA	C4C-C3C	2.18	1.48	1.45
11	A	1134	CLA	C4B-NB	-2.18	1.35	1.37
11	A	1011	CLA	C1D-C2D	2.18	1.49	1.45
11	2	1230	CLA	C1D-C2D	2.18	1.49	1.45
11	A	1126	CLA	C1C-C2C	2.18	1.48	1.44
11	A	1109	CLA	C4C-C3C	2.18	1.48	1.45
11	b	1232	CLA	C1C-NC	-2.18	1.34	1.37
11	A	1127	CLA	C4C-C3C	2.18	1.48	1.45
11	A	1012	CLA	C4C-C3C	2.18	1.48	1.45
11	2	1240	CLA	C4B-NB	-2.18	1.35	1.37
11	B	1214	CLA	C3B-C4B	2.17	1.49	1.42
11	B	1240	CLA	C1C-NC	-2.17	1.34	1.37
11	B	1208	CLA	C3B-C4B	2.17	1.49	1.42
11	a	1237	CLA	C3B-C4B	2.17	1.49	1.42
11	b	1021	CLA	C4B-NB	-2.17	1.35	1.37
11	a	1117	CLA	C4C-C3C	2.17	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1113	CLA	C1C-NC	-2.17	1.34	1.37
11	2	1210	CLA	C4C-C3C	2.17	1.48	1.45
11	K	1402	CLA	C3B-C4B	2.17	1.49	1.42
11	b	1226	CLA	C4B-NB	-2.17	1.35	1.37
11	b	1235	CLA	C3B-C4B	2.17	1.49	1.42
11	1	1107	CLA	C3B-C4B	2.17	1.49	1.42
11	B	1021	CLA	C1D-C2D	2.17	1.49	1.45
11	1	1112	CLA	C1C-NC	-2.17	1.34	1.37
11	b	1231	CLA	C4B-NB	-2.17	1.35	1.37
11	2	1013	CLA	C4C-C3C	2.17	1.48	1.45
11	b	1216	CLA	C1C-NC	-2.17	1.34	1.37
11	b	1221	CLA	C1C-C2C	2.17	1.48	1.44
11	1	1107	CLA	C4C-C3C	2.17	1.48	1.45
11	b	1228	CLA	C3B-C4B	2.17	1.49	1.42
11	b	1208	CLA	C4B-NB	-2.17	1.35	1.37
11	2	1204	CLA	C4B-NB	-2.17	1.35	1.37
11	b	1229	CLA	C4C-C3C	2.17	1.48	1.45
11	A	1119	CLA	C3B-C4B	2.17	1.49	1.42
11	A	1106	CLA	C1B-NB	-2.17	1.35	1.37
11	a	1120	CLA	C4B-NB	-2.17	1.35	1.37
11	1	1118	CLA	C1D-C2D	2.16	1.49	1.45
11	A	1116	CLA	C1C-NC	-2.16	1.34	1.37
11	1	1126	CLA	C4C-C3C	2.16	1.48	1.45
11	2	1021	CLA	C1D-C2D	2.16	1.49	1.45
11	2	1216	CLA	C1D-C2D	2.16	1.49	1.45
11	a	1012	CLA	C4C-C3C	2.16	1.48	1.45
11	2	1228	CLA	C4C-C3C	2.16	1.48	1.45
11	1	1022	CLA	C4B-NB	-2.16	1.35	1.37
11	a	1139	CLA	C4B-NB	-2.16	1.35	1.37
11	A	1140	CLA	C4B-NB	-2.16	1.35	1.37
11	b	1013	CLA	C3B-C4B	2.16	1.49	1.42
11	1	1125	CLA	C3B-C4B	2.16	1.49	1.42
11	1	1121	CLA	C4B-NB	-2.16	1.35	1.37
11	1	1116	CLA	C1C-NC	-2.16	1.34	1.37
11	A	1105	CLA	C4B-NB	-2.16	1.35	1.37
11	A	1139	CLA	C3B-C4B	2.16	1.49	1.42
11	1	1124	CLA	C4C-C3C	2.16	1.48	1.45
11	a	1109	CLA	C4B-NB	-2.15	1.35	1.37
11	b	1203	CLA	C4B-NB	-2.15	1.35	1.37
11	b	1203	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1126	CLA	C1C-NC	-2.15	1.34	1.37
11	A	1109	CLA	C3B-C4B	2.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1226	CLA	C3B-C4B	2.15	1.49	1.42
11	a	1110	CLA	C4B-NB	-2.15	1.35	1.37
11	B	1013	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1111	CLA	C4B-NB	-2.15	1.35	1.37
11	a	1104	CLA	C3B-C4B	2.15	1.49	1.42
11	2	1235	CLA	C3B-C4B	2.15	1.49	1.42
11	b	1213	CLA	C3B-C4B	2.15	1.49	1.42
11	B	1222	CLA	C1C-C2C	2.15	1.48	1.44
11	K	1402	CLA	C4C-C3C	2.15	1.48	1.45
11	A	1118	CLA	C4B-NB	-2.15	1.35	1.37
11	a	1801	CLA	C3B-C4B	2.15	1.49	1.42
11	b	1204	CLA	C4C-C3C	2.15	1.48	1.45
11	A	1130	CLA	C4C-C3C	2.15	1.48	1.45
11	1	1135	CLA	C4C-C3C	2.15	1.48	1.45
14	b	4014	BCR	C30-C25	-2.14	1.51	1.53
11	A	1119	CLA	C4B-NB	-2.14	1.35	1.37
11	2	1216	CLA	C1C-NC	-2.14	1.34	1.37
11	2	1218	CLA	C4C-C3C	2.14	1.48	1.45
11	2	1225	CLA	C3B-C4B	2.14	1.49	1.42
11	2	1206	CLA	C4B-NB	-2.14	1.35	1.37
11	2	1240	CLA	C3B-C4B	2.14	1.49	1.42
11	b	1215	CLA	C3B-C4B	2.14	1.49	1.42
11	a	1801	CLA	C4B-NB	-2.14	1.35	1.37
11	L	1501	CLA	C4B-NB	-2.14	1.35	1.37
11	1	1139	CLA	C3B-C4B	2.14	1.49	1.42
11	A	1112	CLA	C1C-NC	-2.14	1.34	1.37
11	B	1240	CLA	C4B-NB	-2.14	1.35	1.37
11	1	1122	CLA	C3B-C4B	2.14	1.49	1.42
11	A	1108	CLA	C4C-C3C	2.14	1.48	1.45
11	a	1122	CLA	C3B-C4B	2.14	1.49	1.42
11	2	1224	CLA	C4C-C3C	2.14	1.48	1.45
11	1	1137	CLA	C4C-C3C	2.14	1.48	1.45
11	2	1207	CLA	C4C-C3C	2.14	1.48	1.45
11	2	1222	CLA	C4C-C3C	2.14	1.48	1.45
11	a	1123	CLA	C1C-NC	-2.14	1.34	1.37
11	a	1237	CLA	C4B-NB	-2.14	1.35	1.37
11	a	1140	CLA	C4B-NB	-2.14	1.35	1.37
11	a	1123	CLA	C3B-C4B	2.13	1.49	1.42
11	2	1202	CLA	C3B-C4B	2.13	1.49	1.42
11	A	1109	CLA	C4B-NB	-2.13	1.35	1.37
11	1	1112	CLA	C4B-NB	-2.13	1.35	1.37
11	a	1111	CLA	C4C-C3C	2.13	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1227	CLA	C4B-NB	-2.13	1.35	1.37
11	2	1235	CLA	C4C-C3C	2.13	1.48	1.45
11	A	1022	CLA	C3B-C4B	2.13	1.49	1.42
11	b	1236	CLA	C1C-NC	-2.13	1.34	1.37
11	A	1105	CLA	C4C-C3C	2.13	1.48	1.45
11	A	1111	CLA	C3B-C4B	2.13	1.49	1.42
11	b	1215	CLA	C4B-NB	-2.13	1.35	1.37
11	1	1105	CLA	C1B-NB	-2.13	1.35	1.37
11	B	1229	CLA	C3B-C4B	2.13	1.48	1.42
11	b	1221	CLA	C4C-C3C	2.13	1.48	1.45
11	1	1138	CLA	C4C-C3C	2.13	1.48	1.45
11	1	1134	CLA	C3B-C4B	2.13	1.48	1.42
11	1	1126	CLA	C1C-C2C	2.13	1.48	1.44
11	B	1212	CLA	C3B-C4B	2.13	1.48	1.42
11	2	1226	CLA	C3B-C4B	2.13	1.48	1.42
11	b	1216	CLA	C3B-C4B	2.13	1.48	1.42
11	2	1223	CLA	C1C-C2C	2.13	1.48	1.44
11	2	1202	CLA	C4C-C3C	2.13	1.48	1.45
11	2	1213	CLA	C3B-C4B	2.13	1.48	1.42
11	A	1122	CLA	C3B-C4B	2.12	1.48	1.42
11	1	1119	CLA	C4B-NB	-2.12	1.35	1.37
11	1	1124	CLA	C3B-C4B	2.12	1.48	1.42
11	a	1112	CLA	C1C-NC	-2.12	1.34	1.37
11	2	1225	CLA	C1C-NC	-2.12	1.34	1.37
11	8	1501	CLA	C4B-NB	-2.12	1.35	1.37
11	1	1102	CLA	C3B-C4B	2.12	1.48	1.42
11	a	1011	CLA	C1A-CHA	2.12	1.51	1.43
11	2	1203	CLA	C4C-C3C	2.12	1.48	1.45
11	1	1123	CLA	C4B-NB	-2.12	1.35	1.37
11	B	1210	CLA	C3B-C4B	2.12	1.48	1.42
11	B	1023	CLA	C1D-C2D	2.12	1.49	1.45
11	B	1212	CLA	C4C-C3C	2.12	1.48	1.45
11	a	1012	CLA	C1C-C2C	2.12	1.48	1.44
11	A	1108	CLA	C3B-C4B	2.12	1.48	1.42
11	A	1139	CLA	C4C-C3C	2.12	1.48	1.45
11	A	1139	CLA	C1C-NC	-2.11	1.34	1.37
11	1	1012	CLA	C1C-C2C	2.11	1.48	1.44
11	1	1801	CLA	C3B-C4B	2.11	1.48	1.42
11	B	1013	CLA	C3B-C4B	2.11	1.48	1.42
11	b	1203	CLA	C3B-C4B	2.11	1.48	1.42
11	b	1205	CLA	C1D-C2D	2.11	1.49	1.45
11	1	1110	CLA	C4B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1113	CLA	C4C-C3C	2.11	1.48	1.45
14	B	4017	BCR	C30-C25	-2.11	1.51	1.53
11	2	1212	CLA	C3B-C4B	2.11	1.48	1.42
11	a	1107	CLA	C1A-CHA	2.11	1.51	1.43
11	B	1239	CLA	C4B-NB	-2.11	1.35	1.37
11	2	1231	CLA	C4B-NB	-2.11	1.35	1.37
11	B	1217	CLA	C3B-C4B	2.11	1.48	1.42
11	A	1101	CLA	C1C-C2C	2.11	1.48	1.44
11	A	1124	CLA	C3B-C4B	2.11	1.48	1.42
11	a	1122	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1219	CLA	C4C-C3C	2.11	1.48	1.45
11	A	1116	CLA	C3B-C4B	2.11	1.48	1.42
11	1	1122	CLA	C4C-C3C	2.11	1.48	1.45
11	b	1212	CLA	C4B-NB	-2.11	1.35	1.37
11	1	1102	CLA	C1C-NC	-2.11	1.34	1.37
14	A	4002	BCR	C30-C25	-2.11	1.51	1.53
11	2	1021	CLA	C3B-C4B	2.11	1.48	1.42
14	b	4011	BCR	C1-C6	-2.10	1.51	1.53
11	2	1204	CLA	C3B-C4B	2.10	1.48	1.42
11	2	1205	CLA	C4B-NB	-2.10	1.35	1.37
11	A	1132	CLA	C1B-NB	-2.10	1.35	1.37
11	1	1126	CLA	C4B-NB	-2.10	1.35	1.37
11	b	1221	CLA	C1C-NC	-2.10	1.34	1.37
11	2	1239	CLA	C4B-NB	-2.10	1.35	1.37
11	2	1239	CLA	C3B-C4B	2.10	1.48	1.42
11	1	1129	CLA	C3B-C4B	2.10	1.48	1.42
11	A	1120	CLA	C3B-C4B	2.10	1.48	1.42
11	A	1104	CLA	C4B-NB	-2.10	1.35	1.37
11	b	1229	CLA	C4B-NB	-2.10	1.35	1.37
11	b	1213	CLA	C1C-NC	-2.10	1.34	1.37
11	1	1135	CLA	C3B-C4B	2.10	1.48	1.42
11	2	1229	CLA	C4B-NB	-2.10	1.35	1.37
14	2	4011	BCR	C1-C6	-2.09	1.51	1.53
11	2	1208	CLA	C4C-C3C	2.09	1.48	1.45
11	A	1110	CLA	C4B-NB	-2.09	1.35	1.37
11	B	1215	CLA	C3B-C4B	2.09	1.48	1.42
11	A	1102	CLA	C3B-C4B	2.09	1.48	1.42
11	a	1115	CLA	C1C-C2C	2.09	1.48	1.44
11	B	1239	CLA	C3B-C4B	2.09	1.48	1.42
11	l	1501	CLA	C3B-C4B	2.09	1.48	1.42
11	l	1501	CLA	C4C-C3C	2.09	1.48	1.45
11	A	1237	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1119	CLA	C3B-C4B	2.09	1.48	1.42
11	2	1238	CLA	C3B-C4B	2.09	1.48	1.42
11	a	1134	CLA	C4B-NB	-2.09	1.35	1.37
11	1	1011	CLA	C4C-C3C	2.09	1.48	1.45
11	b	1221	CLA	C3B-C4B	2.09	1.48	1.42
11	1	1116	CLA	C3B-C4B	2.09	1.48	1.42
11	a	1115	CLA	C4B-NB	-2.09	1.35	1.37
11	L	1501	CLA	C3B-C4B	2.09	1.48	1.42
11	b	1217	CLA	C4B-NB	-2.08	1.35	1.37
11	A	1113	CLA	C3B-C4B	2.08	1.48	1.42
11	a	1125	CLA	C4C-C3C	2.08	1.48	1.45
11	a	1117	CLA	C3B-C4B	2.08	1.48	1.42
11	a	1102	CLA	C3B-C4B	2.08	1.48	1.42
11	a	1130	CLA	C3B-C4B	2.08	1.48	1.42
11	2	1218	CLA	C4B-NB	-2.08	1.35	1.37
11	b	1219	CLA	C3B-C4B	2.08	1.48	1.42
11	B	1021	CLA	C4C-C3C	2.08	1.48	1.45
11	b	1203	CLA	C1C-C2C	2.08	1.48	1.44
11	2	1221	CLA	C4C-C3C	2.08	1.48	1.45
11	B	1209	CLA	C3B-C4B	2.08	1.48	1.42
11	a	1108	CLA	C3B-C4B	2.08	1.48	1.42
11	B	1236	CLA	C1C-C2C	2.08	1.48	1.44
11	b	1209	CLA	C3B-C4B	2.08	1.48	1.42
11	2	1228	CLA	C3B-C4B	2.08	1.48	1.42
11	1	1120	CLA	C3B-C4B	2.08	1.48	1.42
11	2	1232	CLA	C3B-C4B	2.08	1.48	1.42
11	8	1501	CLA	C3B-C4B	2.08	1.48	1.42
11	A	1237	CLA	C4C-C3C	2.08	1.48	1.45
11	B	1221	CLA	C4C-C3C	2.08	1.48	1.45
11	a	1104	CLA	C1C-C2C	2.07	1.48	1.44
11	1	1127	CLA	C3B-C4B	2.07	1.48	1.42
11	l	1501	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1119	CLA	C3B-C4B	2.07	1.48	1.42
11	a	1121	CLA	C3B-C4B	2.07	1.48	1.42
11	b	1236	CLA	C4C-C3C	2.07	1.48	1.45
11	b	1236	CLA	C3B-C4B	2.07	1.48	1.42
11	a	1129	CLA	C4C-C3C	2.07	1.48	1.45
11	A	1107	CLA	C3B-C4B	2.07	1.48	1.42
14	a	4002	BCR	C30-C25	-2.07	1.51	1.53
11	b	1202	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1218	CLA	C4B-NB	-2.07	1.35	1.37
11	b	1201	CLA	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1225	CLA	C3B-C4B	2.07	1.48	1.42
11	a	1138	CLA	C3B-C4B	2.06	1.48	1.42
11	B	1212	CLA	C1C-C2C	2.06	1.48	1.44
11	a	1012	CLA	C3B-C4B	2.06	1.48	1.42
14	1	4002	BCR	C30-C25	-2.06	1.51	1.53
11	1	1121	CLA	C3B-C4B	2.06	1.48	1.42
11	B	1223	CLA	C1C-C2C	2.06	1.48	1.44
11	A	1112	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1108	CLA	C3B-C4B	2.06	1.48	1.42
11	B	1219	CLA	C3B-C4B	2.06	1.48	1.42
11	2	1223	CLA	C4C-C3C	2.06	1.48	1.45
11	b	1224	CLA	C3B-C4B	2.06	1.48	1.42
14	1	4008	BCR	C30-C25	-2.06	1.51	1.53
11	1	1104	CLA	C4B-NB	-2.06	1.35	1.37
11	B	1216	CLA	C3B-C4B	2.06	1.48	1.42
11	b	1238	CLA	C3B-C4B	2.06	1.48	1.42
14	2	4005	BCR	C30-C25	-2.06	1.51	1.53
11	B	1236	CLA	C3B-C4B	2.06	1.48	1.42
11	l	1503	CLA	C4C-C3C	2.06	1.48	1.45
11	B	1221	CLA	C3B-C4B	2.06	1.48	1.42
11	A	1136	CLA	C3B-C4B	2.06	1.48	1.42
11	a	1011	CLA	C3B-C4B	2.06	1.48	1.42
11	2	1213	CLA	C1C-C2C	2.06	1.48	1.44
11	B	1023	CLA	C4C-C3C	2.06	1.48	1.45
11	a	1101	CLA	C3B-C4B	2.06	1.48	1.42
11	B	1239	CLA	C4C-C3C	2.06	1.48	1.45
11	A	1105	CLA	C3B-C4B	2.06	1.48	1.42
11	A	1123	CLA	C3B-C4B	2.06	1.48	1.42
11	B	1224	CLA	C3B-C4B	2.06	1.48	1.42
11	2	1221	CLA	C3B-C4B	2.06	1.48	1.42
11	1	1011	CLA	C1A-CHA	2.05	1.51	1.43
11	a	1132	CLA	C3B-C4B	2.05	1.48	1.42
11	b	1205	CLA	C4C-C3C	2.05	1.48	1.45
11	b	1240	CLA	C3B-C4B	2.05	1.48	1.42
11	1	1117	CLA	C3B-C4B	2.05	1.48	1.42
11	2	1222	CLA	C3B-C4B	2.05	1.48	1.42
11	B	1213	CLA	C3B-C4B	2.05	1.48	1.42
11	1	1022	CLA	C3B-C4B	2.05	1.48	1.42
14	2	4010	BCR	C30-C25	-2.05	1.51	1.53
11	B	1222	CLA	C1D-C2D	2.05	1.49	1.45
11	b	1222	CLA	C3B-C4B	2.05	1.48	1.42
11	A	1116	CLA	C1C-C2C	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1124	CLA	C3B-C4B	2.05	1.48	1.42
11	A	1137	CLA	C4C-C3C	2.05	1.48	1.45
11	1	1135	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1216	CLA	C3B-C4B	2.05	1.48	1.42
11	B	1228	CLA	C3B-C4B	2.04	1.48	1.42
11	1	1139	CLA	C4B-NB	-2.04	1.35	1.37
11	A	1114	CLA	C3B-C4B	2.04	1.48	1.42
11	B	1235	CLA	C3B-C4B	2.04	1.48	1.42
11	b	1208	CLA	C3B-C4B	2.04	1.48	1.42
11	a	1129	CLA	C3B-C4B	2.04	1.48	1.42
11	b	1232	CLA	C3B-C4B	2.04	1.48	1.42
11	A	1012	CLA	C3B-C4B	2.04	1.48	1.42
11	1	1106	CLA	C4B-NB	-2.04	1.35	1.37
11	L	1501	CLA	C4C-C3C	2.04	1.48	1.45
11	2	1236	CLA	C4C-C3C	2.04	1.48	1.45
11	A	1137	CLA	C1C-C2C	2.04	1.48	1.44
11	1	1105	CLA	C3B-C4B	2.04	1.48	1.42
11	2	1023	CLA	C3B-C4B	2.04	1.48	1.42
11	b	1239	CLA	C3B-C4B	2.03	1.48	1.42
11	1	1118	CLA	C3B-C4B	2.03	1.48	1.42
11	b	1236	CLA	C1C-C2C	2.03	1.48	1.44
11	2	1229	CLA	C1C-C2C	2.03	1.48	1.44
11	b	1211	CLA	C3B-C4B	2.03	1.48	1.42
11	A	1121	CLA	C4B-NB	-2.03	1.35	1.37
11	1	1140	CLA	C1C-C2C	2.03	1.48	1.44
11	B	1211	CLA	C4C-C3C	2.03	1.48	1.45
11	2	1236	CLA	C3B-C4B	2.03	1.48	1.42
11	a	1237	CLA	C4C-C3C	2.03	1.48	1.45
11	B	1203	CLA	C3B-C4B	2.03	1.48	1.42
11	B	1208	CLA	C1C-C2C	2.03	1.48	1.44
11	1	1113	CLA	C3B-C4B	2.03	1.48	1.42
11	2	1204	CLA	C4C-C3C	2.03	1.48	1.45
11	B	1226	CLA	C4C-C3C	2.03	1.48	1.45
11	A	1139	CLA	C4B-NB	-2.03	1.35	1.37
11	1	1137	CLA	C3B-C4B	2.03	1.48	1.42
11	B	1204	CLA	C3B-C4B	2.03	1.48	1.42
11	B	1208	CLA	C4B-NB	-2.03	1.35	1.37
11	a	1126	CLA	C4B-NB	-2.03	1.35	1.37
11	2	1230	CLA	C3B-C4B	2.02	1.48	1.42
11	a	1113	CLA	C3B-C4B	2.02	1.48	1.42
11	2	1210	CLA	C3B-C4B	2.02	1.48	1.42
11	b	1212	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1118	CLA	C3B-C4B	2.02	1.48	1.42
11	1	1138	CLA	C3B-C4B	2.02	1.48	1.42
11	b	1213	CLA	C1C-C2C	2.02	1.48	1.44
11	a	1118	CLA	C4C-C3C	2.02	1.48	1.45
11	A	1104	CLA	C3B-C4B	2.02	1.48	1.42
11	A	1135	CLA	C3B-C4B	2.02	1.48	1.42
11	2	1209	CLA	C3B-C4B	2.02	1.48	1.42
11	8	1502	CLA	C1C-C2C	2.02	1.48	1.44
11	2	1208	CLA	C3B-C4B	2.02	1.48	1.42
11	2	1236	CLA	C1C-C2C	2.02	1.48	1.44
11	A	1138	CLA	C3B-C4B	2.02	1.48	1.42
11	1	1139	CLA	C1C-C2C	2.02	1.48	1.44
11	b	1235	CLA	C1C-C2C	2.02	1.48	1.44
11	2	1235	CLA	C1C-C2C	2.02	1.48	1.44
11	B	1225	CLA	C3B-C4B	2.02	1.48	1.42
11	B	1235	CLA	C1C-C2C	2.02	1.48	1.44
11	b	1204	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1126	CLA	C1C-NC	-2.01	1.34	1.37
11	B	1224	CLA	C1C-C2C	2.01	1.48	1.44
11	B	1208	CLA	C4C-C3C	2.01	1.48	1.45
11	2	1221	CLA	C1C-C2C	2.01	1.48	1.44
11	2	1232	CLA	C1C-C2C	2.01	1.48	1.44
11	a	1120	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1012	CLA	C1D-C2D	2.01	1.49	1.45
11	1	1237	CLA	C3B-C4B	2.01	1.48	1.42
11	b	1212	CLA	C3B-C4B	2.01	1.48	1.42
11	a	1115	CLA	C4C-C3C	2.01	1.48	1.45
11	1	1114	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1129	CLA	C4B-NB	-2.01	1.35	1.37
11	b	1240	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1120	CLA	C1C-C2C	2.01	1.48	1.44
11	a	1126	CLA	C4C-C3C	2.01	1.48	1.45
11	l	1502	CLA	C3B-C4B	2.01	1.48	1.42
14	A	4001	BCR	C30-C25	-2.01	1.51	1.53
11	b	1224	CLA	C1C-C2C	2.01	1.48	1.44
11	2	1211	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1103	CLA	C4C-C3C	2.01	1.48	1.45
11	a	1103	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1101	CLA	C4C-C3C	2.01	1.48	1.45
11	1	1123	CLA	C3B-C4B	2.01	1.48	1.42
11	A	1011	CLA	C1A-CHA	2.01	1.51	1.43
11	1	1132	CLA	C3B-C4B	2.01	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	1503	CLA	C3B-C4B	2.01	1.48	1.42
11	2	1205	CLA	C3B-C4B	2.01	1.48	1.42
11	B	1207	CLA	C3B-C4B	2.01	1.48	1.42
11	B	1218	CLA	C3B-C4B	2.01	1.48	1.42
11	b	1217	CLA	C1C-C2C	2.01	1.48	1.44
11	2	1216	CLA	C1C-C2C	2.00	1.48	1.44
11	a	1120	CLA	C1A-CHA	2.00	1.51	1.43
11	B	1217	CLA	C1C-C2C	2.00	1.48	1.44
14	A	4007	BCR	C30-C25	-2.00	1.51	1.53
11	1	1012	CLA	C4C-C3C	2.00	1.48	1.45
11	B	1023	CLA	C3B-C4B	2.00	1.48	1.42
11	8	1502	CLA	C4C-C3C	2.00	1.48	1.45
11	a	1111	CLA	C1C-C2C	2.00	1.48	1.44
11	B	1201	CLA	C3B-C4B	2.00	1.48	1.42
11	1	1131	CLA	C3B-C4B	2.00	1.48	1.42
11	l	1502	CLA	C1C-C2C	2.00	1.48	1.44

All (8272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	4002	BCR	C16-C17-C18	29.07	168.05	127.28
14	b	4009	BCR	C16-C17-C18	28.37	167.07	127.28
14	6	4013	BCR	C20-C21-C22	26.49	164.43	127.28
14	F	4013	BCR	C20-C21-C22	26.21	164.03	127.28
14	f	4013	BCR	C20-C21-C22	25.83	163.51	127.28
14	l	4019	BCR	C20-C21-C22	25.26	162.70	127.28
14	b	4006	BCR	C20-C21-C22	25.12	162.51	127.28
14	8	4019	BCR	C20-C21-C22	24.87	162.16	127.28
14	B	4006	BCR	C20-C21-C22	24.83	162.10	127.28
14	1	4008	BCR	C20-C21-C22	24.56	161.72	127.28
14	2	4006	BCR	C20-C21-C22	24.52	161.67	127.28
14	B	4009	BCR	C16-C17-C18	24.29	161.34	127.28
14	A	4007	BCR	C20-C21-C22	23.93	160.84	127.28
14	2	4011	BCR	C16-C17-C18	23.91	160.81	127.28
14	A	4008	BCR	C20-C21-C22	23.75	160.59	127.28
14	b	4006	BCR	C16-C17-C18	23.67	160.47	127.28
14	2	4009	BCR	C16-C17-C18	23.63	160.42	127.28
14	f	4013	BCR	C16-C17-C18	23.55	160.30	127.28
14	a	4007	BCR	C20-C21-C22	23.41	160.10	127.28
14	b	4010	BCR	C16-C17-C18	23.37	160.05	127.28
14	1	4008	BCR	C16-C17-C18	23.17	159.78	127.28
14	a	4008	BCR	C20-C21-C22	22.97	159.49	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	4019	BCR	C16-C17-C18	22.95	159.47	127.28
14	1	4002	BCR	C20-C21-C22	22.88	159.37	127.28
14	A	4007	BCR	C16-C17-C18	22.83	159.30	127.28
14	A	4002	BCR	C16-C17-C18	22.77	159.21	127.28
14	b	4017	BCR	C20-C21-C22	22.70	159.12	127.28
14	B	4009	BCR	C20-C21-C22	22.62	159.01	127.28
14	b	4010	BCR	C20-C21-C22	22.59	158.95	127.28
14	a	4002	BCR	C16-C17-C18	22.55	158.91	127.28
14	b	4011	BCR	C16-C17-C18	22.55	158.90	127.28
14	2	4017	BCR	C20-C21-C22	22.52	158.86	127.28
14	B	4011	BCR	C16-C17-C18	22.48	158.80	127.28
14	2	4009	BCR	C20-C21-C22	22.44	158.74	127.28
14	1	4007	BCR	C16-C17-C18	22.36	158.63	127.28
14	F	4013	BCR	C16-C17-C18	22.22	158.44	127.28
14	f	4020	BCR	C20-C21-C22	22.20	158.41	127.28
14	6	4013	BCR	C16-C17-C18	22.12	158.30	127.28
14	b	4011	BCR	C20-C21-C22	22.04	158.18	127.28
14	1	4007	BCR	C20-C21-C22	22.03	158.18	127.28
14	a	4007	BCR	C16-C17-C18	22.00	158.13	127.28
14	8	4019	BCR	C16-C17-C18	21.99	158.12	127.28
14	2	4005	BCR	C20-C21-C22	21.90	157.99	127.28
14	a	4008	BCR	C16-C17-C18	21.77	157.80	127.28
14	l	4019	BCR	C16-C17-C18	21.76	157.79	127.28
14	b	4004	BCR	C16-C17-C18	21.73	157.76	127.28
14	2	4017	BCR	C15-C16-C17	21.58	167.68	123.52
14	B	4006	BCR	C16-C17-C18	21.55	157.50	127.28
14	B	4004	BCR	C16-C17-C18	21.52	157.46	127.28
14	B	4010	BCR	C16-C17-C18	21.45	157.35	127.28
14	6	4020	BCR	C20-C21-C22	21.45	157.35	127.28
14	b	4014	BCR	C20-C21-C22	21.44	157.35	127.28
14	f	4018	BCR	C20-C21-C22	21.43	157.33	127.28
14	7	4021	BCR	C20-C21-C22	21.41	157.31	127.28
14	1	4001	BCR	C16-C17-C18	21.40	157.29	127.28
14	1	4003	BCR	C16-C17-C18	21.37	157.25	127.28
14	b	4005	BCR	C16-C17-C18	21.34	157.20	127.28
14	l	4022	BCR	C16-C17-C18	21.33	157.19	127.28
14	F	4018	BCR	C20-C21-C22	21.31	157.16	127.28
14	7	4021	BCR	C16-C17-C18	21.30	157.15	127.28
14	b	4014	BCR	C16-C17-C18	21.29	157.13	127.28
14	b	4005	BCR	C20-C21-C22	21.25	157.08	127.28
14	M	4021	BCR	C15-C16-C17	21.22	166.93	123.52
14	F	4018	BCR	C16-C17-C18	21.21	157.02	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4005	BCR	C16-C17-C18	21.20	157.01	127.28
14	B	4005	BCR	C20-C21-C22	21.17	156.97	127.28
14	b	4004	BCR	C20-C21-C22	21.16	156.95	127.28
14	F	4020	BCR	C15-C16-C17	21.13	166.76	123.52
14	6	4018	BCR	C20-C21-C22	21.13	156.91	127.28
14	a	4003	BCR	C16-C17-C18	21.12	156.90	127.28
14	A	4002	BCR	C20-C21-C22	21.10	156.87	127.28
14	M	4021	BCR	C20-C21-C22	21.09	156.85	127.28
14	8	4022	BCR	C16-C17-C18	21.08	156.84	127.28
14	6	4020	BCR	C16-C17-C18	21.04	156.78	127.28
14	B	4005	BCR	C16-C17-C18	21.00	156.72	127.28
14	B	4017	BCR	C20-C21-C22	20.99	156.71	127.28
14	a	4001	BCR	C16-C17-C18	20.96	156.67	127.28
14	a	4002	BCR	C20-C21-C22	20.93	156.63	127.28
14	L	4022	BCR	C16-C17-C18	20.86	156.54	127.28
14	B	4004	BCR	C20-C21-C22	20.86	156.53	127.28
14	2	4010	BCR	C16-C17-C18	20.86	156.53	127.28
14	2	4011	BCR	C20-C21-C22	20.83	156.50	127.28
14	m	4021	BCR	C20-C21-C22	20.83	156.48	127.28
14	f	4020	BCR	C15-C16-C17	20.82	166.11	123.52
14	B	4011	BCR	C20-C21-C22	20.70	156.31	127.28
14	2	4006	BCR	C16-C17-C18	20.69	156.30	127.28
14	f	4018	BCR	C16-C17-C18	20.57	156.13	127.28
14	2	4004	BCR	C16-C17-C18	20.56	156.12	127.28
14	A	4003	BCR	C16-C17-C18	20.54	156.09	127.28
14	b	4005	BCR	C15-C16-C17	20.48	165.43	123.52
14	2	4005	BCR	C15-C16-C17	20.47	165.41	123.52
14	f	4020	BCR	C16-C17-C18	20.40	155.88	127.28
14	B	4017	BCR	C15-C16-C17	20.37	165.20	123.52
14	2	4014	BCR	C16-C17-C18	20.35	155.82	127.28
14	8	4022	BCR	C20-C21-C22	20.25	155.67	127.28
14	m	4021	BCR	C15-C16-C17	20.24	164.94	123.52
14	6	4018	BCR	C16-C17-C18	20.24	155.66	127.28
14	m	4021	BCR	C16-C17-C18	20.22	155.64	127.28
14	B	4017	BCR	C16-C17-C18	20.08	155.43	127.28
14	2	4006	BCR	C15-C16-C17	20.07	164.59	123.52
14	2	4004	BCR	C20-C21-C22	20.06	155.41	127.28
14	7	4021	BCR	C15-C16-C17	20.00	164.44	123.52
14	A	4001	BCR	C16-C17-C18	19.99	155.32	127.28
14	B	4014	BCR	C16-C17-C18	19.99	155.31	127.28
14	B	4005	BCR	C15-C16-C17	19.98	164.39	123.52
14	M	4021	BCR	C16-C17-C18	19.95	155.25	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4014	BCR	C15-C16-C17	19.94	164.31	123.52
14	L	4022	BCR	C15-C16-C17	19.89	164.22	123.52
14	A	4008	BCR	C16-C17-C18	19.85	155.12	127.28
14	f	4018	BCR	C15-C16-C17	19.84	164.12	123.52
14	A	4001	BCR	C15-C16-C17	19.84	164.11	123.52
14	b	4009	BCR	C20-C21-C22	19.81	155.05	127.28
14	b	4017	BCR	C15-C16-C17	19.80	164.03	123.52
14	2	4004	BCR	C15-C16-C17	19.80	164.02	123.52
14	F	4020	BCR	C16-C17-C18	19.79	155.03	127.28
14	6	4018	BCR	C15-C16-C17	19.71	163.85	123.52
14	L	4022	BCR	C20-C21-C22	19.71	154.92	127.28
14	l	4022	BCR	C15-C16-C17	19.68	163.78	123.52
14	L	4019	BCR	C20-C21-C22	19.67	154.87	127.28
14	a	4001	BCR	C20-C21-C22	19.67	154.86	127.28
14	2	4014	BCR	C20-C21-C22	19.65	154.83	127.28
14	2	4014	BCR	C15-C16-C17	19.64	163.70	123.52
14	b	4017	BCR	C16-C17-C18	19.59	154.76	127.28
14	A	4003	BCR	C15-C16-C17	19.59	163.59	123.52
14	6	4020	BCR	C15-C16-C17	19.57	163.56	123.52
14	1	4001	BCR	C20-C21-C22	19.55	154.70	127.28
14	8	4022	BCR	C15-C16-C17	19.55	163.52	123.52
14	b	4014	BCR	C15-C16-C17	19.54	163.49	123.52
14	a	4003	BCR	C15-C16-C17	19.40	163.22	123.52
14	a	4001	BCR	C15-C16-C17	19.40	163.21	123.52
14	a	4003	BCR	C20-C21-C22	19.38	154.46	127.28
14	A	4008	BCR	C15-C16-C17	19.35	163.11	123.52
14	B	4009	BCR	C15-C16-C17	19.29	162.99	123.52
14	l	4022	BCR	C20-C21-C22	19.26	154.29	127.28
14	a	4007	BCR	C15-C16-C17	19.22	162.85	123.52
14	f	4013	BCR	C15-C16-C17	19.10	162.60	123.52
14	B	4006	BCR	C15-C16-C17	19.07	162.54	123.52
14	B	4004	BCR	C15-C16-C17	19.06	162.51	123.52
14	1	4001	BCR	C15-C16-C17	19.05	162.50	123.52
14	A	4001	BCR	C20-C21-C22	19.03	153.97	127.28
14	L	4019	BCR	C10-C11-C12	19.02	178.32	123.20
14	2	4010	BCR	C15-C16-C17	19.00	162.40	123.52
14	F	4020	BCR	C20-C21-C22	18.97	153.88	127.28
14	F	4018	BCR	C15-C16-C17	18.97	162.32	123.52
14	6	4013	BCR	C15-C16-C17	18.96	162.31	123.52
14	1	4002	BCR	C10-C11-C12	18.88	177.91	123.20
14	B	4010	BCR	C15-C16-C17	18.88	162.15	123.52
14	b	4004	BCR	C15-C16-C17	18.87	162.14	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4017	BCR	C10-C11-C12	18.87	177.86	123.20
14	1	4003	BCR	C15-C16-C17	18.82	162.03	123.52
14	B	4010	BCR	C20-C21-C22	18.79	153.63	127.28
14	b	4011	BCR	C15-C16-C17	18.76	161.90	123.52
14	F	4013	BCR	C15-C16-C17	18.75	161.88	123.52
14	2	4009	BCR	C10-C11-C12	18.73	177.49	123.20
14	F	4020	BCR	C10-C11-C12	18.72	177.45	123.20
14	1	4007	BCR	C10-C11-C12	18.72	177.44	123.20
14	1	4001	BCR	C10-C11-C12	18.71	177.43	123.20
14	f	4020	BCR	C10-C11-C12	18.71	177.41	123.20
14	l	4019	BCR	C10-C11-C12	18.69	177.36	123.20
14	a	4008	BCR	C15-C16-C17	18.67	161.73	123.52
14	B	4006	BCR	C10-C11-C12	18.66	177.28	123.20
14	7	4021	BCR	C10-C11-C12	18.66	177.26	123.20
14	b	4005	BCR	C10-C11-C12	18.66	177.26	123.20
14	1	4007	BCR	C15-C16-C17	18.64	161.66	123.52
14	6	4020	BCR	C10-C11-C12	18.61	177.12	123.20
14	B	4014	BCR	C20-C21-C22	18.60	153.36	127.28
14	A	4007	BCR	C15-C16-C17	18.60	161.57	123.52
14	B	4005	BCR	C10-C11-C12	18.60	177.09	123.20
14	2	4011	BCR	C15-C16-C17	18.52	161.42	123.52
14	2	4010	BCR	C10-C11-C12	18.51	176.83	123.20
14	b	4010	BCR	C10-C11-C12	18.44	176.63	123.20
14	m	4021	BCR	C10-C11-C12	18.44	176.62	123.20
14	2	4017	BCR	C10-C11-C12	18.43	176.60	123.20
14	B	4004	BCR	C10-C11-C12	18.41	176.55	123.20
14	F	4018	BCR	C10-C11-C12	18.39	176.48	123.20
14	2	4004	BCR	C10-C11-C12	18.36	176.40	123.20
14	b	4004	BCR	C10-C11-C12	18.36	176.39	123.20
14	a	4002	BCR	C10-C11-C12	18.35	176.38	123.20
14	a	4007	BCR	C10-C11-C12	18.32	176.27	123.20
14	a	4001	BCR	C10-C11-C12	18.32	176.27	123.20
14	8	4022	BCR	C10-C11-C12	18.31	176.26	123.20
14	b	4017	BCR	C10-C11-C12	18.30	176.24	123.20
14	l	4022	BCR	C10-C11-C12	18.28	176.17	123.20
14	M	4021	BCR	C10-C11-C12	18.28	176.16	123.20
14	2	4009	BCR	C15-C16-C17	18.27	160.90	123.52
14	2	4014	BCR	C10-C11-C12	18.20	175.94	123.20
14	b	4010	BCR	C15-C16-C17	18.13	160.61	123.52
14	A	4008	BCR	C10-C11-C12	18.12	175.70	123.20
14	b	4006	BCR	C15-C16-C17	18.12	160.59	123.52
14	b	4006	BCR	C10-C11-C12	18.10	175.65	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4007	BCR	C10-C11-C12	17.99	175.32	123.20
14	2	4010	BCR	C20-C21-C22	17.96	152.47	127.28
14	B	4011	BCR	C15-C16-C17	17.92	160.18	123.52
14	2	4017	BCR	C16-C17-C18	17.90	152.38	127.28
14	2	4006	BCR	C10-C11-C12	17.87	174.98	123.20
14	B	4010	BCR	C10-C11-C12	17.86	174.96	123.20
14	1	4008	BCR	C15-C16-C17	17.82	159.98	123.52
14	L	4019	BCR	C15-C16-C17	17.81	159.95	123.52
14	b	4009	BCR	C10-C11-C12	17.80	174.76	123.20
14	A	4003	BCR	C10-C11-C12	17.77	174.68	123.20
14	1	4003	BCR	C10-C11-C12	17.75	174.63	123.20
14	b	4014	BCR	C10-C11-C12	17.63	174.28	123.20
14	F	4013	BCR	C10-C11-C12	17.62	174.27	123.20
14	B	4009	BCR	C10-C11-C12	17.58	174.13	123.20
14	8	4019	BCR	C10-C11-C12	17.53	174.00	123.20
14	b	4011	BCR	C10-C11-C12	17.52	173.98	123.20
14	8	4019	BCR	C15-C16-C17	17.52	159.37	123.52
14	a	4008	BCR	C10-C11-C12	17.46	173.78	123.20
14	l	4019	BCR	C15-C16-C17	17.42	159.16	123.52
14	1	4008	BCR	C10-C11-C12	17.33	173.41	123.20
14	2	4011	BCR	C10-C11-C12	17.32	173.38	123.20
14	a	4002	BCR	C15-C16-C17	17.25	158.82	123.52
14	B	4011	BCR	C10-C11-C12	17.25	173.17	123.20
14	A	4002	BCR	C15-C16-C17	17.12	158.55	123.52
14	2	4005	BCR	C10-C11-C12	16.95	172.32	123.20
14	A	4001	BCR	C10-C11-C12	16.88	172.11	123.20
14	A	4003	BCR	C20-C21-C22	16.74	150.76	127.28
14	f	4018	BCR	C10-C11-C12	16.72	171.64	123.20
14	b	4011	BCR	C11-C10-C9	16.71	150.72	127.28
14	B	4014	BCR	C10-C11-C12	16.69	171.57	123.20
14	b	4009	BCR	C15-C16-C17	16.58	157.44	123.52
14	A	4002	BCR	C10-C11-C12	16.58	171.23	123.20
14	6	4013	BCR	C10-C11-C12	16.52	171.05	123.20
14	6	4018	BCR	C10-C11-C12	16.42	170.77	123.20
14	1	4003	BCR	C20-C21-C22	15.85	149.50	127.28
14	f	4013	BCR	C10-C11-C12	15.82	169.04	123.20
14	a	4003	BCR	C10-C11-C12	15.73	168.78	123.20
14	2	4011	BCR	C11-C10-C9	15.60	149.16	127.28
14	8	4019	BCR	C16-C15-C14	15.60	155.44	123.52
14	b	4009	BCR	C16-C15-C14	15.50	155.24	123.52
14	B	4011	BCR	C11-C10-C9	15.39	148.86	127.28
14	1	4008	BCR	C16-C15-C14	15.32	154.86	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4009	BCR	C16-C15-C14	15.30	154.83	123.52
14	l	4019	BCR	C16-C15-C14	15.15	154.52	123.52
14	A	4003	BCR	C21-C20-C19	15.13	167.04	123.20
14	1	4003	BCR	C21-C20-C19	15.08	166.91	123.20
14	L	4019	BCR	C16-C15-C14	14.99	154.19	123.52
14	B	4017	BCR	C21-C20-C19	14.88	166.30	123.20
14	b	4009	BCR	C21-C20-C19	14.84	166.19	123.20
14	L	4022	BCR	C10-C11-C12	14.83	166.17	123.20
14	A	4007	BCR	C11-C10-C9	14.83	148.07	127.28
14	B	4009	BCR	C16-C15-C14	14.77	153.74	123.52
14	F	4020	BCR	C21-C20-C19	14.72	165.86	123.20
14	1	4002	BCR	C15-C16-C17	14.72	153.63	123.52
14	2	4010	BCR	C21-C20-C19	14.72	165.84	123.20
14	B	4014	BCR	C21-C20-C19	14.68	165.75	123.20
14	l	4022	BCR	C21-C20-C19	14.67	165.70	123.20
14	b	4010	BCR	C16-C15-C14	14.66	153.51	123.52
14	A	4001	BCR	C21-C20-C19	14.64	165.62	123.20
14	B	4011	BCR	C16-C15-C14	14.62	153.43	123.52
14	L	4022	BCR	C21-C20-C19	14.58	165.44	123.20
14	B	4010	BCR	C21-C20-C19	14.53	165.30	123.20
14	b	4005	BCR	C11-C10-C9	14.49	147.60	127.28
14	8	4022	BCR	C21-C20-C19	14.48	165.15	123.20
14	F	4013	BCR	C16-C15-C14	14.46	153.11	123.52
14	2	4017	BCR	C21-C20-C19	14.46	165.10	123.20
14	a	4008	BCR	C16-C15-C14	14.45	153.09	123.52
14	A	4008	BCR	C16-C15-C14	14.44	153.06	123.52
14	1	4001	BCR	C16-C15-C14	14.41	153.00	123.52
14	a	4007	BCR	C11-C10-C9	14.38	147.45	127.28
14	2	4014	BCR	C21-C20-C19	14.34	164.74	123.20
14	1	4003	BCR	C16-C15-C14	14.33	152.85	123.52
14	a	4001	BCR	C21-C20-C19	14.33	164.71	123.20
14	1	4007	BCR	C16-C15-C14	14.27	152.71	123.52
14	b	4017	BCR	C11-C10-C9	14.27	147.28	127.28
14	2	4006	BCR	C11-C10-C9	14.25	147.27	127.28
14	b	4006	BCR	C16-C15-C14	14.24	152.66	123.52
14	M	4021	BCR	C11-C10-C9	14.20	147.20	127.28
14	a	4001	BCR	C11-C10-C9	14.17	147.16	127.28
14	a	4002	BCR	C16-C15-C14	14.17	152.51	123.52
14	8	4019	BCR	C21-C20-C19	14.14	164.17	123.20
14	1	4001	BCR	C21-C20-C19	14.14	164.16	123.20
14	2	4004	BCR	C21-C20-C19	14.13	164.13	123.20
14	a	4002	BCR	C21-C20-C19	14.11	164.09	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4010	BCR	C16-C15-C14	14.10	152.37	123.52
14	b	4009	BCR	C11-C10-C9	14.07	147.01	127.28
14	b	4004	BCR	C16-C15-C14	14.05	152.28	123.52
14	6	4018	BCR	C21-C20-C19	14.01	163.78	123.20
14	b	4006	BCR	C11-C10-C9	14.00	146.91	127.28
14	2	4010	BCR	C16-C15-C14	14.00	152.16	123.52
14	m	4021	BCR	C21-C20-C19	14.00	163.75	123.20
14	L	4019	BCR	C21-C20-C19	13.99	163.73	123.20
14	a	4003	BCR	C21-C20-C19	13.98	163.70	123.20
14	A	4001	BCR	C16-C15-C14	13.97	152.10	123.52
14	B	4006	BCR	C16-C15-C14	13.97	152.10	123.52
14	M	4021	BCR	C21-C20-C19	13.96	163.66	123.20
14	1	4001	BCR	C11-C10-C9	13.95	146.84	127.28
14	l	4019	BCR	C21-C20-C19	13.92	163.54	123.20
14	b	4017	BCR	C21-C20-C19	13.91	163.51	123.20
14	1	4007	BCR	C11-C10-C9	13.90	146.77	127.28
14	B	4004	BCR	C16-C15-C14	13.83	151.82	123.52
14	B	4004	BCR	C21-C20-C19	13.82	163.25	123.20
14	B	4017	BCR	C11-C10-C9	13.80	146.63	127.28
14	b	4005	BCR	C21-C20-C19	13.80	163.18	123.20
14	2	4011	BCR	C21-C20-C19	13.77	163.11	123.20
14	F	4018	BCR	C21-C20-C19	13.77	163.10	123.20
14	a	4001	BCR	C16-C15-C14	13.75	151.65	123.52
14	A	4007	BCR	C16-C15-C14	13.74	151.64	123.52
14	b	4014	BCR	C16-C15-C14	13.68	151.52	123.52
14	b	4014	BCR	C21-C20-C19	13.68	162.85	123.20
14	1	4002	BCR	C21-C20-C19	13.68	162.84	123.20
14	2	4014	BCR	C16-C15-C14	13.64	151.42	123.52
14	B	4004	BCR	C11-C10-C9	13.62	146.38	127.28
14	7	4021	BCR	C21-C20-C19	13.61	162.65	123.20
14	B	4005	BCR	C21-C20-C19	13.61	162.63	123.20
14	b	4004	BCR	C21-C20-C19	13.60	162.61	123.20
14	A	4002	BCR	C16-C15-C14	13.59	151.33	123.52
14	A	4002	BCR	C21-C20-C19	13.56	162.48	123.20
14	6	4013	BCR	C16-C15-C14	13.55	151.24	123.52
14	f	4020	BCR	C21-C20-C19	13.52	162.37	123.20
14	b	4011	BCR	C16-C15-C14	13.52	151.18	123.52
14	a	4007	BCR	C16-C15-C14	13.51	151.17	123.52
14	f	4020	BCR	C11-C10-C9	13.49	146.20	127.28
14	2	4005	BCR	C21-C20-C19	13.46	162.19	123.20
14	b	4011	BCR	C21-C20-C19	13.44	162.14	123.20
14	F	4020	BCR	C11-C10-C9	13.43	146.12	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4011	BCR	C16-C15-C14	13.41	150.96	123.52
14	A	4007	BCR	C21-C20-C19	13.36	161.90	123.20
14	B	4014	BCR	C16-C15-C14	13.36	150.85	123.52
14	B	4006	BCR	C11-C10-C9	13.34	145.98	127.28
14	f	4018	BCR	C21-C20-C19	13.33	161.82	123.20
14	7	4021	BCR	C16-C15-C14	13.32	150.77	123.52
14	a	4003	BCR	C16-C15-C14	13.30	150.73	123.52
14	b	4010	BCR	C11-C10-C9	13.30	145.93	127.28
14	2	4017	BCR	C11-C10-C9	13.28	145.91	127.28
14	2	4004	BCR	C16-C15-C14	13.27	150.67	123.52
14	2	4006	BCR	C21-C20-C19	13.26	161.63	123.20
14	F	4018	BCR	C16-C15-C14	13.24	150.62	123.52
14	B	4009	BCR	C21-C20-C19	13.22	161.52	123.20
14	a	4002	BCR	C11-C10-C9	13.19	145.77	127.28
14	B	4011	BCR	C21-C20-C19	13.18	161.40	123.20
14	A	4003	BCR	C16-C15-C14	13.18	150.48	123.52
14	b	4004	BCR	C11-C10-C9	13.17	145.75	127.28
14	A	4001	BCR	C11-C10-C9	13.16	145.73	127.28
14	b	4017	BCR	C16-C15-C14	13.10	150.33	123.52
14	a	4007	BCR	C21-C20-C19	13.09	161.12	123.20
14	7	4021	BCR	C11-C10-C9	13.07	145.61	127.28
14	8	4022	BCR	C16-C15-C14	13.05	150.22	123.52
14	F	4018	BCR	C11-C10-C9	13.04	145.57	127.28
14	2	4006	BCR	C16-C15-C14	13.03	150.17	123.52
14	8	4022	BCR	C11-C10-C9	13.02	145.54	127.28
14	f	4013	BCR	C16-C15-C14	13.02	150.16	123.52
14	B	4005	BCR	C16-C15-C14	13.02	150.15	123.52
14	6	4020	BCR	C21-C20-C19	13.00	160.86	123.20
14	A	4008	BCR	C11-C10-C9	12.96	145.45	127.28
14	6	4020	BCR	C16-C15-C14	12.95	150.02	123.52
14	2	4009	BCR	C11-C10-C9	12.95	145.44	127.28
14	B	4017	BCR	C16-C15-C14	12.82	149.76	123.52
14	6	4018	BCR	C16-C15-C14	12.79	149.69	123.52
14	B	4006	BCR	C21-C20-C19	12.77	160.19	123.20
14	2	4009	BCR	C21-C20-C19	12.74	160.13	123.20
14	m	4021	BCR	C16-C15-C14	12.72	149.55	123.52
14	l	4022	BCR	C16-C15-C14	12.72	149.55	123.52
14	b	4005	BCR	C16-C15-C14	12.68	149.47	123.52
14	1	4002	BCR	C11-C10-C9	12.64	145.01	127.28
14	b	4006	BCR	C21-C20-C19	12.62	159.78	123.20
14	a	4008	BCR	C21-C20-C19	12.61	159.75	123.20
14	2	4004	BCR	C11-C10-C9	12.57	144.90	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4010	BCR	C11-C10-C9	12.56	144.90	127.28
14	L	4022	BCR	C16-C15-C14	12.56	149.22	123.52
14	b	4010	BCR	C21-C20-C19	12.51	159.44	123.20
14	2	4005	BCR	C16-C15-C14	12.48	149.06	123.52
14	2	4011	BCR	C11-C12-C13	12.45	160.51	126.36
14	f	4018	BCR	C16-C15-C14	12.44	148.98	123.52
14	1	4003	BCR	C11-C10-C9	12.42	144.69	127.28
14	1	4007	BCR	C21-C20-C19	12.42	159.18	123.20
14	B	4011	BCR	C11-C12-C13	12.41	160.38	126.36
14	1	4008	BCR	C21-C20-C19	12.41	159.15	123.20
14	2	4014	BCR	C11-C10-C9	12.25	144.46	127.28
14	B	4010	BCR	C11-C10-C9	12.24	144.44	127.28
14	2	4017	BCR	C16-C15-C14	12.20	148.49	123.52
14	M	4021	BCR	C16-C15-C14	12.18	148.44	123.52
14	f	4013	BCR	C21-C20-C19	12.17	158.47	123.20
14	A	4008	BCR	C21-C20-C19	12.16	158.43	123.20
14	f	4020	BCR	C16-C15-C14	12.15	148.38	123.52
14	B	4005	BCR	C11-C10-C9	12.12	144.27	127.28
14	M	4021	BCR	C11-C12-C13	12.08	159.50	126.36
14	6	4013	BCR	C21-C20-C19	12.00	157.96	123.20
14	2	4006	BCR	C11-C12-C13	11.99	159.24	126.36
14	F	4020	BCR	C16-C15-C14	11.91	147.88	123.52
14	F	4013	BCR	C21-C20-C19	11.90	157.68	123.20
14	1	4002	BCR	C16-C15-C14	11.86	147.78	123.52
14	b	4011	BCR	C11-C12-C13	11.86	158.87	126.36
14	l	4019	BCR	C11-C10-C9	11.81	143.84	127.28
14	F	4018	BCR	C11-C12-C13	11.78	158.65	126.36
14	b	4014	BCR	C11-C10-C9	11.76	143.77	127.28
14	m	4021	BCR	C11-C10-C9	11.75	143.76	127.28
14	b	4006	BCR	C11-C12-C13	11.75	158.57	126.36
14	l	4022	BCR	C11-C10-C9	11.57	143.50	127.28
14	B	4005	BCR	C11-C12-C13	11.55	158.03	126.36
14	F	4013	BCR	C11-C10-C9	11.53	143.45	127.28
14	1	4008	BCR	C11-C10-C9	11.42	143.29	127.28
14	1	4008	BCR	C11-C12-C13	11.36	157.50	126.36
14	A	4007	BCR	C11-C12-C13	11.35	157.48	126.36
14	b	4009	BCR	C11-C12-C13	11.30	157.33	126.36
14	1	4002	BCR	C11-C12-C13	11.29	157.31	126.36
14	a	4007	BCR	C11-C12-C13	11.26	157.23	126.36
14	B	4006	BCR	C11-C12-C13	11.23	157.17	126.36
14	m	4021	BCR	C11-C12-C13	11.20	157.06	126.36
14	a	4001	BCR	C11-C12-C13	11.16	156.97	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	4020	BCR	C11-C12-C13	11.13	156.89	126.36
14	7	4021	BCR	C11-C12-C13	11.12	156.84	126.36
14	a	4008	BCR	C11-C12-C13	11.11	156.82	126.36
14	6	4020	BCR	C11-C10-C9	11.07	142.80	127.28
14	a	4002	BCR	C11-C12-C13	11.06	156.70	126.36
14	B	4009	BCR	C11-C12-C13	11.06	156.69	126.36
14	1	4007	BCR	C11-C12-C13	10.92	156.32	126.36
14	2	4009	BCR	C11-C12-C13	10.88	156.19	126.36
14	B	4017	BCR	C11-C12-C13	10.88	156.18	126.36
14	B	4009	BCR	C11-C10-C9	10.87	142.53	127.28
14	1	4001	BCR	C11-C12-C13	10.86	156.13	126.36
14	L	4019	BCR	C11-C12-C13	10.75	155.84	126.36
14	2	4004	BCR	C11-C12-C13	10.71	155.72	126.36
14	8	4022	BCR	C11-C12-C13	10.68	155.64	126.36
14	b	4004	BCR	C11-C12-C13	10.67	155.62	126.36
14	L	4019	BCR	C11-C10-C9	10.65	142.21	127.28
14	l	4022	BCR	C11-C12-C13	10.61	155.47	126.36
14	l	4019	BCR	C11-C12-C13	10.60	155.44	126.36
14	6	4020	BCR	C11-C12-C13	10.53	155.24	126.36
14	B	4004	BCR	C11-C12-C13	10.52	155.20	126.36
14	2	4017	BCR	C11-C12-C13	10.49	155.13	126.36
14	2	4010	BCR	C11-C12-C13	10.40	154.88	126.36
14	B	4014	BCR	C11-C10-C9	10.38	141.83	127.28
14	2	4005	BCR	C11-C12-C13	10.34	154.71	126.36
14	A	4003	BCR	C11-C12-C13	10.33	154.68	126.36
14	b	4010	BCR	C11-C12-C13	10.32	154.66	126.36
14	A	4008	BCR	C11-C12-C13	10.30	154.62	126.36
14	f	4020	BCR	C11-C12-C13	10.30	154.60	126.36
14	b	4017	BCR	C11-C12-C13	10.26	154.49	126.36
14	B	4014	BCR	C11-C12-C13	10.25	154.47	126.36
14	B	4010	BCR	C11-C12-C13	10.24	154.44	126.36
14	A	4003	BCR	C11-C10-C9	10.21	141.60	127.28
14	8	4019	BCR	C11-C10-C9	10.19	141.56	127.28
14	f	4018	BCR	C11-C10-C9	10.14	141.50	127.28
14	2	4005	BCR	C11-C10-C9	10.12	141.47	127.28
14	8	4019	BCR	C11-C12-C13	9.97	153.70	126.36
14	A	4001	BCR	C11-C12-C13	9.86	153.41	126.36
14	a	4008	BCR	C11-C10-C9	9.78	141.00	127.28
14	A	4002	BCR	C11-C12-C13	9.72	153.02	126.36
14	F	4013	BCR	C11-C12-C13	9.64	152.80	126.36
14	1	4003	BCR	C11-C12-C13	9.62	152.75	126.36
14	f	4018	BCR	C11-C12-C13	9.46	152.31	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	4014	BCR	C11-C12-C13	9.40	152.13	126.36
14	6	4018	BCR	C11-C12-C13	9.34	151.98	126.36
14	a	4003	BCR	C11-C12-C13	9.33	151.94	126.36
14	A	4007	BCR	C20-C19-C18	9.31	151.90	126.36
14	A	4002	BCR	C11-C10-C9	9.24	140.24	127.28
14	b	4005	BCR	C11-C12-C13	9.24	151.70	126.36
14	L	4022	BCR	C11-C12-C13	9.13	151.40	126.36
11	2	1225	CLA	CMD-C2D-C1D	9.09	140.73	124.73
14	6	4013	BCR	C11-C12-C13	9.06	151.21	126.36
14	L	4019	BCR	C20-C19-C18	9.04	151.16	126.36
14	a	4007	BCR	C20-C19-C18	9.03	151.12	126.36
14	2	4009	BCR	C20-C19-C18	9.00	151.04	126.36
11	A	1121	CLA	CMD-C2D-C1D	8.97	140.52	124.73
11	a	1138	CLA	CMD-C2D-C1D	8.88	140.37	124.73
11	a	1121	CLA	CMD-C2D-C1D	8.88	140.37	124.73
11	b	1236	CLA	CMD-C2D-C1D	8.87	140.35	124.73
14	2	4014	BCR	C11-C12-C13	8.87	150.67	126.36
11	A	1138	CLA	CMD-C2D-C1D	8.86	140.33	124.73
11	A	1103	CLA	CMD-C2D-C1D	8.85	140.31	124.73
11	A	1123	CLA	CMD-C2D-C1D	8.81	140.25	124.73
11	2	1202	CLA	CMD-C2D-C1D	8.81	140.24	124.73
11	2	1224	CLA	CMD-C2D-C1D	8.79	140.20	124.73
14	f	4013	BCR	C20-C19-C18	8.77	150.42	126.36
11	1	1103	CLA	CMD-C2D-C1D	8.72	140.08	124.73
11	2	1231	CLA	CMD-C2D-C1D	8.71	140.07	124.73
11	B	1203	CLA	CMD-C2D-C1D	8.66	139.97	124.73
11	2	1203	CLA	CMD-C2D-C1D	8.65	139.96	124.73
11	2	1219	CLA	CMD-C2D-C1D	8.64	139.94	124.73
11	a	1107	CLA	CMD-C2D-C1D	8.63	139.92	124.73
11	A	1120	CLA	CMD-C2D-C1D	8.62	139.91	124.73
11	1	1237	CLA	CMD-C2D-C1D	8.62	139.91	124.73
11	B	1224	CLA	CMD-C2D-C1D	8.62	139.91	124.73
11	b	1231	CLA	CMD-C2D-C1D	8.62	139.90	124.73
14	b	4006	BCR	C20-C19-C18	8.59	149.92	126.36
11	B	1218	CLA	CMD-C2D-C1D	8.54	139.76	124.73
14	6	4013	BCR	C11-C10-C9	8.52	139.23	127.28
11	2	1223	CLA	CMD-C2D-C1D	8.52	139.73	124.73
11	B	1216	CLA	CMD-C2D-C1D	8.51	139.72	124.73
11	A	1122	CLA	CMD-C2D-C1D	8.51	139.71	124.73
11	2	1218	CLA	CMD-C2D-C1D	8.50	139.69	124.73
11	1	1011	CLA	O2D-CGD-CBD	8.48	126.06	111.23
11	A	1104	CLA	CMD-C2D-C1D	8.48	139.66	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	6	4018	BCR	C11-C10-C9	8.48	139.17	127.28
14	b	4010	BCR	C20-C19-C18	8.47	149.60	126.36
11	1	1124	CLA	CMD-C2D-C1D	8.47	139.64	124.73
11	B	1201	CLA	CMD-C2D-C1D	8.46	139.62	124.73
11	A	1101	CLA	CMD-C2D-C1D	8.45	139.62	124.73
11	b	1202	CLA	CMD-C2D-C1D	8.45	139.62	124.73
11	B	1207	CLA	CMD-C2D-C1D	8.45	139.61	124.73
11	A	1112	CLA	CMD-C2D-C1D	8.45	139.61	124.73
11	2	1232	CLA	CMD-C2D-C1D	8.45	139.60	124.73
11	A	1126	CLA	CMD-C2D-C1D	8.44	139.60	124.73
11	1	1129	CLA	CMD-C2D-C1D	8.44	139.59	124.73
11	1	1121	CLA	CMD-C2D-C1D	8.44	139.59	124.73
11	B	1223	CLA	CMD-C2D-C1D	8.44	139.58	124.73
11	A	1109	CLA	CMD-C2D-C1D	8.43	139.58	124.73
11	2	1201	CLA	CMD-C2D-C1D	8.43	139.58	124.73
11	A	1125	CLA	CMD-C2D-C1D	8.42	139.55	124.73
11	A	1134	CLA	CMD-C2D-C1D	8.41	139.54	124.73
11	a	1125	CLA	CMD-C2D-C1D	8.41	139.53	124.73
11	1	1136	CLA	CMD-C2D-C1D	8.40	139.51	124.73
14	1	4008	BCR	C20-C19-C18	8.39	149.38	126.36
14	6	4013	BCR	C20-C19-C18	8.39	149.38	126.36
11	B	1220	CLA	CMD-C2D-C1D	8.39	139.50	124.73
11	B	1238	CLA	CMD-C2D-C1D	8.38	139.49	124.73
11	a	1116	CLA	CMD-C2D-C1D	8.38	139.48	124.73
11	B	1236	CLA	CMD-C2D-C1D	8.37	139.47	124.73
11	B	1215	CLA	CMD-C2D-C1D	8.37	139.47	124.73
11	A	1105	CLA	CMD-C2D-C1D	8.35	139.43	124.73
11	a	1134	CLA	CMD-C2D-C1D	8.34	139.41	124.73
11	a	1109	CLA	CMD-C2D-C1D	8.33	139.40	124.73
11	B	1208	CLA	CMD-C2D-C1D	8.33	139.40	124.73
11	b	1206	CLA	CMD-C2D-C1D	8.33	139.40	124.73
11	L	1501	CLA	CMD-C2D-C1D	8.32	139.39	124.73
11	L	1503	CLA	CMD-C2D-C1D	8.32	139.38	124.73
11	a	1123	CLA	CMD-C2D-C1D	8.32	139.38	124.73
11	B	1211	CLA	CMD-C2D-C1D	8.32	139.38	124.73
11	B	1202	CLA	CMD-C2D-C1D	8.32	139.37	124.73
11	A	1119	CLA	CMD-C2D-C1D	8.31	139.37	124.73
11	0	1401	CLA	CMD-C2D-C1D	8.30	139.34	124.73
11	1	1102	CLA	CMD-C2D-C1D	8.30	139.34	124.73
11	0	1402	CLA	CMD-C2D-C1D	8.29	139.33	124.73
11	2	1209	CLA	CMD-C2D-C1D	8.29	139.33	124.73
11	1	1123	CLA	CMD-C2D-C1D	8.28	139.32	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1222	CLA	CMD-C2D-C1D	8.28	139.32	124.73
11	b	1235	CLA	CMD-C2D-C1D	8.28	139.31	124.73
11	K	1401	CLA	CMD-C2D-C1D	8.28	139.31	124.73
11	1	1125	CLA	CMD-C2D-C1D	8.28	139.31	124.73
11	B	1204	CLA	CMD-C2D-C1D	8.28	139.31	124.73
11	1	1134	CLA	CMD-C2D-C1D	8.28	139.31	124.73
11	a	1104	CLA	CMD-C2D-C1D	8.28	139.30	124.73
11	1	1130	CLA	CMD-C2D-C1D	8.28	139.30	124.73
11	a	1101	CLA	CMD-C2D-C1D	8.28	139.30	124.73
11	a	1135	CLA	CMD-C2D-C1D	8.28	139.30	124.73
11	a	1112	CLA	CMD-C2D-C1D	8.27	139.29	124.73
11	1	1116	CLA	CMD-C2D-C1D	8.26	139.28	124.73
11	k	1401	CLA	CMD-C2D-C1D	8.26	139.28	124.73
11	b	1227	CLA	CMD-C2D-C1D	8.26	139.28	124.73
11	A	1115	CLA	CMD-C2D-C1D	8.26	139.27	124.73
11	A	1801	CLA	CMD-C2D-C1D	8.25	139.26	124.73
11	1	1108	CLA	CMD-C2D-C1D	8.25	139.26	124.73
11	A	1107	CLA	CMD-C2D-C1D	8.25	139.25	124.73
11	b	1217	CLA	CMD-C2D-C1D	8.25	139.25	124.73
11	B	1227	CLA	CMD-C2D-C1D	8.24	139.24	124.73
11	A	1132	CLA	CMD-C2D-C1D	8.24	139.24	124.73
11	1	1111	CLA	CMD-C2D-C1D	8.24	139.24	124.73
11	a	1801	CLA	CMD-C2D-C1D	8.24	139.23	124.73
11	a	1139	CLA	CMD-C2D-C1D	8.24	139.23	124.73
11	a	1108	CLA	CMD-C2D-C1D	8.23	139.23	124.73
11	b	1240	CLA	CMD-C2D-C1D	8.23	139.23	124.73
11	b	1222	CLA	CMD-C2D-C1D	8.23	139.22	124.73
14	1	4007	BCR	C20-C19-C18	8.23	148.94	126.36
11	2	1234	CLA	CMD-C2D-C1D	8.23	139.22	124.73
11	a	1105	CLA	CMD-C2D-C1D	8.23	139.22	124.73
11	a	1124	CLA	CMD-C2D-C1D	8.23	139.22	124.73
11	b	1201	CLA	CMD-C2D-C1D	8.23	139.21	124.73
11	B	1217	CLA	CMD-C2D-C1D	8.22	139.21	124.73
11	1	1112	CLA	CMD-C2D-C1D	8.22	139.20	124.73
11	B	1240	CLA	CMD-C2D-C1D	8.22	139.19	124.73
11	2	1210	CLA	CMD-C2D-C1D	8.21	139.19	124.73
11	1	1106	CLA	CMD-C2D-C1D	8.21	139.18	124.73
11	1	1115	CLA	CMD-C2D-C1D	8.21	139.18	124.73
11	A	1108	CLA	CMD-C2D-C1D	8.20	139.18	124.73
11	1	1119	CLA	CMD-C2D-C1D	8.20	139.17	124.73
11	b	1218	CLA	CMD-C2D-C1D	8.20	139.17	124.73
11	B	1228	CLA	CMD-C2D-C1D	8.20	139.17	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1223	CLA	CMD-C2D-C1D	8.20	139.17	124.73
11	L	1502	CLA	CMD-C2D-C1D	8.20	139.16	124.73
11	a	1120	CLA	CMD-C2D-C1D	8.20	139.16	124.73
11	2	1235	CLA	CMD-C2D-C1D	8.20	139.16	124.73
11	2	1220	CLA	CMD-C2D-C1D	8.19	139.16	124.73
11	b	1229	CLA	CMD-C2D-C1D	8.19	139.15	124.73
11	b	1239	CLA	CMD-C2D-C1D	8.18	139.14	124.73
11	b	1224	CLA	CMD-C2D-C1D	8.18	139.14	124.73
11	a	1115	CLA	CMD-C2D-C1D	8.18	139.14	124.73
11	A	1139	CLA	CMD-C2D-C1D	8.18	139.14	124.73
11	1	1131	CLA	CMD-C2D-C1D	8.18	139.13	124.73
14	B	4006	BCR	C20-C19-C18	8.18	148.79	126.36
11	1	1114	CLA	CMD-C2D-C1D	8.18	139.13	124.73
11	a	1129	CLA	CMD-C2D-C1D	8.18	139.13	124.73
11	1	1139	CLA	CMD-C2D-C1D	8.18	139.13	124.73
11	8	1501	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	f	4013	BCR	C11-C10-C9	8.17	138.73	127.28
11	b	1214	CLA	CMD-C2D-C1D	8.16	139.11	124.73
11	2	1227	CLA	CMD-C2D-C1D	8.16	139.11	124.73
11	A	1127	CLA	CMD-C2D-C1D	8.16	139.10	124.73
11	1	1105	CLA	CMD-C2D-C1D	8.16	139.10	124.73
11	2	1229	CLA	CMD-C2D-C1D	8.16	139.09	124.73
11	1	1127	CLA	CMD-C2D-C1D	8.15	139.09	124.73
11	A	1136	CLA	CMD-C2D-C1D	8.15	139.09	124.73
11	8	1503	CLA	CMD-C2D-C1D	8.15	139.09	124.73
11	b	1238	CLA	CMD-C2D-C1D	8.15	139.08	124.73
14	B	4011	BCR	C20-C19-C18	8.15	148.71	126.36
11	1	1101	CLA	CMD-C2D-C1D	8.15	139.08	124.73
11	1	1104	CLA	CMD-C2D-C1D	8.14	139.07	124.73
11	a	1130	CLA	CMD-C2D-C1D	8.14	139.06	124.73
11	B	1214	CLA	CMD-C2D-C1D	8.14	139.06	124.73
11	1	1801	CLA	CMD-C2D-C1D	8.14	139.06	124.73
11	b	1212	CLA	CMD-C2D-C1D	8.14	139.06	124.73
11	b	1204	CLA	CMD-C2D-C1D	8.14	139.06	124.73
11	B	1206	CLA	CMD-C2D-C1D	8.13	139.05	124.73
11	a	1102	CLA	CMD-C2D-C1D	8.13	139.04	124.73
11	b	1023	CLA	CMD-C2D-C1D	8.13	139.04	124.73
11	A	1011	CLA	CMD-C2D-C1D	8.13	139.04	124.73
14	a	4008	BCR	C20-C19-C18	8.13	148.65	126.36
11	B	1239	CLA	CMD-C2D-C1D	8.12	139.04	124.73
11	2	1228	CLA	CMD-C2D-C1D	8.12	139.04	124.73
11	B	1234	CLA	CMD-C2D-C1D	8.12	139.03	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1238	CLA	CMD-C2D-C1D	8.11	139.01	124.73
11	B	1212	CLA	CMD-C2D-C1D	8.11	139.01	124.73
11	a	1122	CLA	CMD-C2D-C1D	8.11	139.01	124.73
11	a	1103	CLA	CMD-C2D-C1D	8.11	139.01	124.73
11	B	1229	CLA	CMD-C2D-C1D	8.10	139.00	124.73
11	A	1130	CLA	CMD-C2D-C1D	8.10	139.00	124.73
11	b	1209	CLA	CMD-C2D-C1D	8.10	138.99	124.73
11	2	1214	CLA	CMD-C2D-C1D	8.10	138.99	124.73
11	a	1137	CLA	CMD-C2D-C1D	8.10	138.98	124.73
11	b	1203	CLA	CMD-C2D-C1D	8.09	138.98	124.73
11	1	1140	CLA	CMD-C2D-C1D	8.09	138.98	124.73
11	A	1118	CLA	CMD-C2D-C1D	8.09	138.98	124.73
11	1	1138	CLA	CMD-C2D-C1D	8.09	138.98	124.73
11	2	1213	CLA	CMD-C2D-C1D	8.08	138.97	124.73
11	b	1228	CLA	CMD-C2D-C1D	8.08	138.96	124.73
11	B	1235	CLA	CMD-C2D-C1D	8.08	138.95	124.73
14	b	4011	BCR	C20-C19-C18	8.07	148.50	126.36
11	A	1137	CLA	CMD-C2D-C1D	8.07	138.94	124.73
11	A	1106	CLA	CMD-C2D-C1D	8.07	138.94	124.73
11	2	1239	CLA	CMD-C2D-C1D	8.07	138.94	124.73
11	b	1213	CLA	CMD-C2D-C1D	8.07	138.94	124.73
11	a	1119	CLA	CMD-C2D-C1D	8.06	138.93	124.73
11	A	1124	CLA	CMD-C2D-C1D	8.06	138.93	124.73
11	b	1220	CLA	CMD-C2D-C1D	8.06	138.93	124.73
11	1	1122	CLA	CMD-C2D-C1D	8.05	138.91	124.73
11	A	1135	CLA	CMD-C2D-C1D	8.05	138.90	124.73
11	A	1133	CLA	CMD-C2D-C1D	8.05	138.90	124.73
11	A	1110	CLA	CMD-C2D-C1D	8.05	138.90	124.73
11	b	1234	CLA	CMD-C2D-C1D	8.04	138.89	124.73
11	B	1232	CLA	CMD-C2D-C1D	8.04	138.89	124.73
11	2	1226	CLA	CMD-C2D-C1D	8.04	138.89	124.73
11	A	1140	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	A	1129	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	1	1132	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	a	1118	CLA	CMD-C2D-C1D	8.04	138.88	124.73
14	F	4013	BCR	C20-C19-C18	8.04	148.40	126.36
11	a	1140	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	A	1114	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	a	1111	CLA	CMD-C2D-C1D	8.04	138.88	124.73
11	a	1133	CLA	CMD-C2D-C1D	8.03	138.88	124.73
11	8	1502	CLA	CMD-C2D-C1D	8.03	138.88	124.73
11	1	1113	CLA	CMD-C2D-C1D	8.03	138.87	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	6	4020	BCR	C20-C19-C18	8.03	148.39	126.36
11	a	1136	CLA	CMD-C2D-C1D	8.03	138.87	124.73
11	1	1011	CLA	CMD-C2D-C1D	8.02	138.86	124.73
11	a	1114	CLA	CMD-C2D-C1D	8.02	138.85	124.73
11	2	1215	CLA	CMD-C2D-C1D	8.02	138.85	124.73
11	b	1210	CLA	CMD-C2D-C1D	8.02	138.84	124.73
11	1	1133	CLA	CMD-C2D-C1D	8.01	138.84	124.73
11	1	1109	CLA	CMD-C2D-C1D	8.01	138.84	124.73
11	1	1135	CLA	CMD-C2D-C1D	8.01	138.83	124.73
11	B	1219	CLA	CMD-C2D-C1D	8.00	138.82	124.73
11	2	1204	CLA	CMD-C2D-C1D	8.00	138.82	124.73
11	A	1113	CLA	CMD-C2D-C1D	8.00	138.82	124.73
11	a	1117	CLA	CMD-C2D-C1D	8.00	138.81	124.73
14	b	4014	BCR	C20-C19-C18	8.00	148.29	126.36
11	2	1240	CLA	CMD-C2D-C1D	8.00	138.81	124.73
11	b	1207	CLA	CMD-C2D-C1D	7.99	138.80	124.73
11	a	1132	CLA	CMD-C2D-C1D	7.99	138.79	124.73
11	a	1113	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	A	4002	BCR	C20-C19-C18	7.98	148.24	126.36
11	1	1107	CLA	CMD-C2D-C1D	7.97	138.77	124.73
11	a	1110	CLA	CMD-C2D-C1D	7.97	138.76	124.73
11	l	1503	CLA	CMD-C2D-C1D	7.97	138.76	124.73
11	b	1215	CLA	CMD-C2D-C1D	7.97	138.76	124.73
11	B	1226	CLA	CMD-C2D-C1D	7.96	138.75	124.73
11	1	1110	CLA	CMD-C2D-C1D	7.96	138.74	124.73
11	2	1013	CLA	CMD-C2D-C1D	7.96	138.74	124.73
11	2	1216	CLA	CMD-C2D-C1D	7.95	138.73	124.73
11	A	1237	CLA	CMD-C2D-C1D	7.95	138.73	124.73
11	2	1206	CLA	CMD-C2D-C1D	7.95	138.72	124.73
11	A	1111	CLA	CMD-C2D-C1D	7.94	138.72	124.73
11	a	1131	CLA	CMD-C2D-C1D	7.94	138.71	124.73
11	b	1221	CLA	CMD-C2D-C1D	7.94	138.71	124.73
11	A	1116	CLA	CMD-C2D-C1D	7.94	138.70	124.73
11	b	1230	CLA	CMD-C2D-C1D	7.93	138.70	124.73
11	B	1231	CLA	CMD-C2D-C1D	7.93	138.69	124.73
11	1	1117	CLA	CMD-C2D-C1D	7.93	138.69	124.73
11	1	1126	CLA	CMD-C2D-C1D	7.92	138.68	124.73
11	B	1213	CLA	CMD-C2D-C1D	7.90	138.65	124.73
11	b	1216	CLA	CMD-C2D-C1D	7.90	138.64	124.73
11	b	1232	CLA	CMD-C2D-C1D	7.90	138.64	124.73
11	B	1023	CLA	CMD-C2D-C1D	7.90	138.64	124.73
11	b	1208	CLA	CMD-C2D-C1D	7.90	138.63	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1128	CLA	CMD-C2D-C1D	7.89	138.63	124.73
11	A	1102	CLA	CMD-C2D-C1D	7.89	138.63	124.73
11	2	1207	CLA	CMD-C2D-C1D	7.89	138.62	124.73
14	B	4009	BCR	C20-C19-C18	7.88	147.97	126.36
11	B	1209	CLA	CMD-C2D-C1D	7.88	138.60	124.73
14	7	4021	BCR	C20-C19-C18	7.88	147.97	126.36
11	a	1128	CLA	CMD-C2D-C1D	7.87	138.60	124.73
11	B	1210	CLA	CMD-C2D-C1D	7.86	138.57	124.73
11	b	1013	CLA	CMD-C2D-C1D	7.85	138.56	124.73
11	2	1217	CLA	CMD-C2D-C1D	7.85	138.56	124.73
11	A	1117	CLA	CMD-C2D-C1D	7.85	138.55	124.73
11	b	1225	CLA	CMD-C2D-C1D	7.85	138.55	124.73
11	k	1402	CLA	CMD-C2D-C1D	7.84	138.54	124.73
11	B	1222	CLA	CMD-C2D-C1D	7.84	138.53	124.73
11	1	1120	CLA	CMD-C2D-C1D	7.83	138.53	124.73
11	b	1211	CLA	CMD-C2D-C1D	7.83	138.51	124.73
11	a	1126	CLA	CMD-C2D-C1D	7.82	138.51	124.73
11	b	1226	CLA	CMD-C2D-C1D	7.82	138.49	124.73
11	K	1402	CLA	CMD-C2D-C1D	7.80	138.47	124.73
14	f	4018	BCR	C20-C19-C18	7.80	147.75	126.36
11	a	1011	CLA	CMD-C2D-C1D	7.80	138.46	124.73
11	2	1221	CLA	CMD-C2D-C1D	7.80	138.46	124.73
11	B	1221	CLA	CMD-C2D-C1D	7.79	138.45	124.73
11	2	1236	CLA	CMD-C2D-C1D	7.79	138.44	124.73
14	M	4021	BCR	C20-C19-C18	7.78	147.70	126.36
14	2	4005	BCR	C20-C19-C18	7.78	147.69	126.36
11	l	1502	CLA	CMD-C2D-C1D	7.78	138.43	124.73
11	l	1501	CLA	CMD-C2D-C1D	7.77	138.41	124.73
11	2	1212	CLA	CMD-C2D-C1D	7.77	138.41	124.73
11	2	1230	CLA	CMD-C2D-C1D	7.75	138.38	124.73
14	2	4006	BCR	C20-C19-C18	7.73	147.56	126.36
11	2	1023	CLA	CMD-C2D-C1D	7.73	138.34	124.73
11	b	1219	CLA	CMD-C2D-C1D	7.70	138.29	124.73
14	B	4005	BCR	C20-C19-C18	7.70	147.47	126.36
11	A	1131	CLA	CMD-C2D-C1D	7.69	138.28	124.73
11	1	1118	CLA	CMD-C2D-C1D	7.67	138.23	124.73
11	a	1237	CLA	CMD-C2D-C1D	7.66	138.23	124.73
11	2	1211	CLA	CMD-C2D-C1D	7.66	138.22	124.73
11	1	1022	CLA	CMD-C2D-C1D	7.64	138.18	124.73
11	A	1022	CLA	CMD-C2D-C1D	7.64	138.18	124.73
14	b	4005	BCR	C20-C19-C18	7.63	147.30	126.36
14	a	4003	BCR	C11-C10-C9	7.62	137.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1021	CLA	CMD-C2D-C1D	7.62	138.15	124.73
11	1	1137	CLA	CMD-C2D-C1D	7.61	138.14	124.73
11	B	1225	CLA	CMD-C2D-C1D	7.61	138.12	124.73
11	1	1011	CLA	C4A-NA-C1A	7.59	110.14	106.68
11	B	1205	CLA	C4A-NA-C1A	7.59	110.14	106.68
14	2	4011	BCR	C20-C19-C18	7.55	147.06	126.36
11	A	1128	CLA	CMD-C2D-C1D	7.54	138.01	124.73
11	a	1127	CLA	CMD-C2D-C1D	7.54	138.00	124.73
11	B	1230	CLA	CMD-C2D-C1D	7.54	138.00	124.73
11	2	1208	CLA	CMD-C2D-C1D	7.52	137.97	124.73
14	m	4021	BCR	C20-C19-C18	7.50	146.94	126.36
14	a	4002	BCR	C20-C19-C18	7.50	146.93	126.36
11	a	1106	CLA	CMD-C2D-C1D	7.49	137.92	124.73
14	a	4003	BCR	C20-C19-C18	7.48	146.87	126.36
14	2	4014	BCR	C20-C19-C18	7.47	146.86	126.36
14	1	4001	BCR	C20-C19-C18	7.47	146.83	126.36
14	f	4020	BCR	C20-C19-C18	7.46	146.83	126.36
11	2	1021	CLA	CMD-C2D-C1D	7.46	137.87	124.73
14	b	4004	BCR	C20-C19-C18	7.46	146.81	126.36
11	B	1021	CLA	CMD-C2D-C1D	7.43	137.81	124.73
14	l	4019	BCR	C20-C19-C18	7.41	146.67	126.36
14	1	4003	BCR	C24-C23-C22	-7.36	115.34	126.23
11	a	1022	CLA	CMD-C2D-C1D	7.35	137.67	124.73
11	B	1205	CLA	CMD-C2D-C1D	7.34	137.65	124.73
14	A	4008	BCR	C20-C19-C18	7.30	146.39	126.36
14	F	4018	BCR	C20-C19-C18	7.28	146.32	126.36
14	1	4002	BCR	C20-C19-C18	7.27	146.30	126.36
14	B	4004	BCR	C20-C19-C18	7.27	146.30	126.36
11	B	1013	CLA	CMD-C2D-C1D	7.23	137.47	124.73
11	2	1205	CLA	CMD-C2D-C1D	7.23	137.45	124.73
14	B	4010	BCR	C20-C19-C18	7.21	146.14	126.36
11	b	1205	CLA	CMD-C2D-C1D	7.21	137.42	124.73
11	a	1011	CLA	C4A-NA-C1A	7.20	109.96	106.68
11	2	1205	CLA	O2D-CGD-CBD	7.16	123.74	111.23
11	A	1011	CLA	C4A-NA-C1A	7.14	109.94	106.68
14	6	4018	BCR	C24-C23-C22	-7.12	115.70	126.23
14	a	4001	BCR	C20-C19-C18	7.12	145.89	126.36
14	2	4004	BCR	C20-C19-C18	7.12	145.89	126.36
14	8	4019	BCR	C20-C19-C18	7.11	145.84	126.36
11	a	1107	CLA	C4A-NA-C1A	7.08	109.91	106.68
11	B	1205	CLA	O2D-CGD-CBD	7.06	123.58	111.23
14	L	4019	BCR	C24-C23-C22	-7.03	115.83	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4010	BCR	C20-C19-C18	6.97	145.47	126.36
14	A	4001	BCR	C20-C19-C18	6.96	145.44	126.36
11	b	1207	CLA	C4A-NA-C1A	6.94	109.84	106.68
11	A	1110	CLA	O2D-CGD-CBD	6.92	123.32	111.23
14	6	4018	BCR	C20-C19-C18	6.88	145.22	126.36
11	B	1201	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	1	4003	BCR	C20-C19-C18	6.82	145.07	126.36
11	B	1221	CLA	O2D-CGD-CBD	6.82	123.15	111.23
14	B	4014	BCR	C20-C19-C18	6.80	145.00	126.36
11	a	1106	CLA	O2D-CGD-CBD	6.78	123.08	111.23
14	b	4017	BCR	C20-C19-C18	6.74	144.85	126.36
14	f	4018	BCR	C24-C23-C22	-6.74	116.26	126.23
11	1	1111	CLA	C4A-NA-C1A	6.72	109.75	106.68
11	1	1110	CLA	O2D-CGD-CBD	6.72	122.98	111.23
11	2	1207	CLA	C4A-NA-C1A	6.72	109.75	106.68
11	A	1132	CLA	O2D-CGD-CBD	6.72	122.98	111.23
14	l	4022	BCR	C20-C19-C18	6.67	144.66	126.36
11	a	1118	CLA	C4A-NA-C1A	6.67	109.72	106.68
11	2	1205	CLA	C4A-NA-C1A	6.67	109.72	106.68
11	B	1221	CLA	C4A-NA-C1A	6.62	109.70	106.68
11	1	1103	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	8	4022	BCR	C20-C19-C18	6.62	144.52	126.36
11	A	1801	CLA	C2C-C1C-NC	6.62	116.93	109.98
11	b	1221	CLA	O2D-CGD-CBD	6.59	122.75	111.23
11	a	1120	CLA	C4A-NA-C1A	6.59	109.68	106.68
11	B	1224	CLA	C1D-ND-C4D	-6.56	101.71	106.31
11	B	1207	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	7	4021	BCR	C7-C8-C9	-6.55	116.55	126.23
11	a	1012	CLA	CMD-C2D-C1D	6.55	136.26	124.73
14	A	4003	BCR	C20-C19-C18	6.54	144.29	126.36
11	1	1137	CLA	O2D-CGD-CBD	6.53	122.65	111.23
11	B	1021	CLA	C4A-NA-C1A	6.52	109.66	106.68
11	b	1201	CLA	C4A-NA-C1A	6.52	109.65	106.68
11	B	1201	CLA	O2D-CGD-CBD	6.51	122.61	111.23
11	A	1118	CLA	C4A-NA-C1A	6.50	109.64	106.68
11	A	1125	CLA	O2D-CGD-CBD	6.49	122.57	111.23
14	L	4022	BCR	C11-C10-C9	6.48	136.36	127.28
11	2	1221	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	B	1206	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	2	4011	BCR	C7-C8-C9	-6.46	116.67	126.23
11	A	1133	CLA	C2C-C1C-NC	6.46	116.77	109.98
11	A	1104	CLA	C4A-NA-C1A	6.45	109.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1237	CLA	C4A-NA-C1A	6.45	109.62	106.68
11	B	1222	CLA	O2D-CGD-CBD	6.45	122.50	111.23
14	f	4013	BCR	C11-C12-C13	6.45	144.04	126.36
11	1	1237	CLA	C4A-NA-C1A	6.44	109.62	106.68
11	A	1125	CLA	C2C-C1C-NC	6.43	116.74	109.98
14	B	4014	BCR	C7-C8-C9	-6.43	116.72	126.23
11	b	1205	CLA	C4A-NA-C1A	6.42	109.61	106.68
11	2	1201	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	L	4022	BCR	C20-C19-C18	6.42	143.97	126.36
11	8	1501	CLA	C4A-NA-C1A	6.40	109.60	106.68
11	B	1227	CLA	C4A-NA-C1A	6.40	109.60	106.68
11	a	1111	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	B	4011	BCR	C7-C8-C9	-6.39	116.79	126.23
11	B	1226	CLA	O2D-CGD-CBD	6.38	122.38	111.23
11	1	1123	CLA	O2D-CGD-CBD	6.36	122.36	111.23
11	2	1218	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	6	4020	BCR	C7-C8-C9	-6.36	116.82	126.23
11	B	1204	CLA	C4A-NA-C1A	6.36	109.58	106.68
11	A	1138	CLA	C4A-NA-C1A	6.35	109.58	106.68
11	2	1236	CLA	O2D-CGD-CBD	6.35	122.34	111.23
14	A	4003	BCR	C24-C23-C22	-6.35	116.84	126.23
14	b	4009	BCR	C20-C19-C18	6.35	143.77	126.36
11	2	1213	CLA	O2D-CGD-CBD	6.34	122.31	111.23
11	A	1140	CLA	C4A-NA-C1A	6.34	109.57	106.68
11	1	1138	CLA	C4A-NA-C1A	6.34	109.57	106.68
11	A	1237	CLA	C4A-NA-C1A	6.33	109.57	106.68
11	b	1212	CLA	C4A-NA-C1A	6.33	109.57	106.68
11	B	1227	CLA	O2D-CGD-CBD	6.31	122.27	111.23
14	F	4020	BCR	C20-C19-C18	6.31	143.68	126.36
11	B	1214	CLA	O2D-CGD-CBD	6.31	122.27	111.23
11	b	1239	CLA	C2C-C1C-NC	6.30	116.59	109.98
11	2	1226	CLA	O2D-CGD-CBD	6.29	122.23	111.23
11	b	1222	CLA	O2D-CGD-CBD	6.29	122.23	111.23
11	B	1239	CLA	C4A-NA-C1A	6.29	109.55	106.68
11	1	1133	CLA	C2C-C1C-NC	6.29	116.59	109.98
11	b	1207	CLA	C2C-C1C-NC	6.28	116.58	109.98
11	1	1011	CLA	C2C-C1C-NC	6.27	116.57	109.98
11	2	1219	CLA	C4A-NA-C1A	6.26	109.54	106.68
11	L	1501	CLA	C4A-NA-C1A	6.25	109.53	106.68
11	A	1137	CLA	C1D-ND-C4D	-6.25	101.93	106.31
11	2	1224	CLA	C4A-NA-C1A	6.25	109.53	106.68
11	A	1134	CLA	C2C-C1C-NC	6.24	116.54	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1139	CLA	C2C-C1C-NC	6.24	116.54	109.98
11	2	1226	CLA	C4A-NA-C1A	6.23	109.52	106.68
11	a	1135	CLA	C2C-C1C-NC	6.22	116.52	109.98
14	A	4001	BCR	C24-C23-C22	-6.22	117.03	126.23
11	A	1123	CLA	C2C-C1C-NC	6.22	116.51	109.98
14	B	4014	BCR	C24-C23-C22	-6.20	117.06	126.23
11	2	1206	CLA	C2C-C1C-NC	6.19	116.48	109.98
11	1	1012	CLA	CMD-C2D-C1D	6.19	135.62	124.73
11	2	1213	CLA	C2C-C1C-NC	6.18	116.47	109.98
11	L	1503	CLA	C4A-NA-C1A	6.18	109.50	106.68
11	a	1133	CLA	C2C-C1C-NC	6.18	116.47	109.98
11	b	1227	CLA	O2D-CGD-CBD	6.17	122.02	111.23
11	B	1234	CLA	C2C-C1C-NC	6.16	116.45	109.98
11	B	1236	CLA	C1D-ND-C4D	-6.16	101.99	106.31
11	b	1234	CLA	C4A-NA-C1A	6.14	109.48	106.68
11	b	1239	CLA	C4A-NA-C1A	6.14	109.48	106.68
11	B	1206	CLA	C2C-C1C-NC	6.14	116.43	109.98
11	b	1206	CLA	C4A-NA-C1A	6.13	109.48	106.68
11	l	1501	CLA	C4A-NA-C1A	6.13	109.48	106.68
11	B	1210	CLA	C4A-NA-C1A	6.12	109.47	106.68
11	a	1129	CLA	C4A-NA-C1A	6.12	109.47	106.68
11	B	1231	CLA	C2C-C1C-NC	6.12	116.41	109.98
11	L	1503	CLA	C2C-C1C-NC	6.12	116.41	109.98
11	B	1232	CLA	C2C-C1C-NC	6.11	116.40	109.98
11	A	1012	CLA	O2D-CGD-CBD	6.11	121.91	111.23
11	b	1234	CLA	C2C-C1C-NC	6.11	116.40	109.98
11	1	1115	CLA	C2C-C1C-NC	6.11	116.39	109.98
11	A	1102	CLA	C4A-NA-C1A	6.10	109.46	106.68
11	a	1137	CLA	O2D-CGD-CBD	6.10	121.89	111.23
11	a	1138	CLA	O2D-CGD-CBD	6.09	121.88	111.23
11	a	1127	CLA	C2C-C1C-NC	6.09	116.38	109.98
11	B	1227	CLA	C2C-C1C-NC	6.08	116.37	109.98
11	2	1211	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	B	1224	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	8	1501	CLA	O2D-CGD-CBD	6.08	121.86	111.23
11	a	1138	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	1	1113	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	2	1203	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	1	1129	CLA	O2D-CGD-CBD	6.08	121.85	111.23
11	1	1012	CLA	C4A-NA-C1A	6.08	109.45	106.68
11	2	1224	CLA	C1D-ND-C4D	-6.08	102.05	106.31
11	B	1021	CLA	C2C-C1C-NC	6.07	116.36	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	1502	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	L	4022	BCR	C24-C23-C22	-6.06	117.26	126.23
11	b	1236	CLA	C1D-ND-C4D	-6.06	102.06	106.31
11	1	1111	CLA	C1D-ND-C4D	-6.06	102.06	106.31
11	A	1132	CLA	C4A-NA-C1A	6.05	109.44	106.68
11	2	1227	CLA	C4A-NA-C1A	6.05	109.44	106.68
11	b	1206	CLA	C2C-C1C-NC	6.04	116.33	109.98
11	2	1239	CLA	C2C-C1C-NC	6.03	116.32	109.98
11	A	1114	CLA	C2C-C1C-NC	6.03	116.31	109.98
11	k	1401	CLA	C4A-NA-C1A	6.02	109.43	106.68
11	a	1011	CLA	C2C-C1C-NC	6.02	116.31	109.98
11	A	1012	CLA	O2A-CGA-O1A	-6.02	108.56	123.63
11	B	1240	CLA	C4A-NA-C1A	6.02	109.43	106.68
11	0	1401	CLA	C4A-NA-C1A	6.02	109.43	106.68
11	K	1401	CLA	C4A-NA-C1A	6.02	109.42	106.68
11	A	1103	CLA	C1D-ND-C4D	-6.01	102.09	106.31
11	1	1140	CLA	C4A-NA-C1A	6.01	109.42	106.68
11	a	1126	CLA	O2D-CGD-CBD	6.01	121.73	111.23
11	B	1238	CLA	C4A-NA-C1A	6.01	109.42	106.68
11	B	1224	CLA	C2D-C1D-ND	6.01	116.07	110.13
11	0	1402	CLA	C1D-ND-C4D	-6.01	102.10	106.31
11	a	1237	CLA	C1D-ND-C4D	-6.00	102.10	106.31
11	A	1107	CLA	C4A-NA-C1A	6.00	109.42	106.68
11	b	1231	CLA	C4A-NA-C1A	5.99	109.41	106.68
11	b	1219	CLA	C2C-C1C-NC	5.99	116.28	109.98
11	b	1221	CLA	C4A-NA-C1A	5.99	109.41	106.68
11	8	1502	CLA	C4A-NA-C1A	5.99	109.41	106.68
11	1	1107	CLA	C2C-C1C-NC	5.99	116.27	109.98
11	2	1212	CLA	C2C-C1C-NC	5.99	116.27	109.98
11	1	1110	CLA	C2C-C1C-NC	5.99	116.27	109.98
11	a	1103	CLA	C2C-C1C-NC	5.98	116.27	109.98
11	1	1120	CLA	O2D-CGD-CBD	5.98	121.69	111.23
14	2	4017	BCR	C20-C19-C18	5.98	142.77	126.36
11	B	1234	CLA	C4A-NA-C1A	5.98	109.41	106.68
11	2	1208	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	m	4021	BCR	C7-C8-C9	-5.98	117.39	126.23
11	k	1402	CLA	C1D-ND-C4D	-5.97	102.12	106.31
11	A	1237	CLA	C2C-C1C-NC	5.97	116.25	109.98
11	A	1126	CLA	O2D-CGD-CBD	5.97	121.66	111.23
11	B	1230	CLA	C4A-NA-C1A	5.96	109.40	106.68
11	1	1136	CLA	C4A-NA-C1A	5.96	109.40	106.68
11	a	1114	CLA	C2C-C1C-NC	5.96	116.24	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1021	CLA	C2C-C1C-NC	5.96	116.24	109.98
11	b	1208	CLA	C2C-C1C-NC	5.96	116.24	109.98
11	A	1110	CLA	C2C-C1C-NC	5.95	116.23	109.98
11	1	1801	CLA	C2C-C1C-NC	5.95	116.23	109.98
11	a	1102	CLA	C4A-NA-C1A	5.95	109.39	106.68
11	b	1219	CLA	C4A-NA-C1A	5.95	109.39	106.68
11	l	1502	CLA	C4A-NA-C1A	5.95	109.39	106.68
11	2	1206	CLA	C4A-NA-C1A	5.95	109.39	106.68
11	2	1227	CLA	C2C-C1C-NC	5.94	116.23	109.98
11	L	1503	CLA	C1C-C2C-C3C	-5.94	100.73	106.98
11	a	1111	CLA	C1D-ND-C4D	-5.94	102.14	106.31
11	A	1111	CLA	C4A-NA-C1A	5.94	109.39	106.68
11	2	1222	CLA	O2D-CGD-CBD	5.94	121.61	111.23
11	a	1107	CLA	C2C-C1C-NC	5.94	116.22	109.98
11	A	1012	CLA	C4A-NA-C1A	5.94	109.39	106.68
11	1	1136	CLA	C1D-ND-C4D	-5.93	102.15	106.31
11	A	1110	CLA	C4A-NA-C1A	5.93	109.39	106.68
11	l	1502	CLA	O2D-CGD-CBD	5.93	121.60	111.23
11	A	1136	CLA	C1D-ND-C4D	-5.93	102.15	106.31
11	A	1103	CLA	C4A-NA-C1A	5.93	109.39	106.68
11	2	1215	CLA	C2C-C1C-NC	5.93	116.21	109.98
11	2	1226	CLA	C1D-ND-C4D	-5.93	102.15	106.31
14	F	4018	BCR	C24-C23-C22	-5.93	117.46	126.23
11	A	1112	CLA	C1D-ND-C4D	-5.93	102.15	106.31
11	A	1128	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	F	4013	BCR	C15-C14-C13	-5.92	118.97	127.28
11	1	1801	CLA	C4A-NA-C1A	5.92	109.38	106.68
11	B	1229	CLA	C2C-C1C-NC	5.92	116.20	109.98
11	A	1012	CLA	CMD-C2D-C1D	5.92	135.15	124.73
11	a	1119	CLA	C2C-C1C-NC	5.92	116.20	109.98
11	a	1137	CLA	C1D-ND-C4D	-5.92	102.16	106.31
11	2	1234	CLA	C2C-C1C-NC	5.92	116.19	109.98
11	2	1021	CLA	C2C-C1C-NC	5.91	116.19	109.98
11	A	1104	CLA	C1D-ND-C4D	-5.91	102.17	106.31
11	B	1215	CLA	C2C-C1C-NC	5.91	116.19	109.98
11	1	1118	CLA	C4A-NA-C1A	5.91	109.37	106.68
11	a	1136	CLA	C1D-ND-C4D	-5.91	102.17	106.31
11	B	1207	CLA	O2D-CGD-CBD	5.90	121.55	111.23
11	b	1213	CLA	C1D-ND-C4D	-5.90	102.17	106.31
11	B	1230	CLA	C2C-C1C-NC	5.90	116.18	109.98
11	A	1126	CLA	C4A-NA-C1A	5.90	109.37	106.68
11	a	1117	CLA	C4A-NA-C1A	5.90	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	1402	CLA	C4A-NA-C1A	5.90	109.37	106.68
11	B	1023	CLA	C4A-NA-C1A	5.90	109.37	106.68
11	a	1101	CLA	C2C-C1C-NC	5.89	116.17	109.98
11	b	1226	CLA	O2D-CGD-CBD	5.89	121.53	111.23
11	2	1211	CLA	C1D-ND-C4D	-5.88	102.18	106.31
11	a	1105	CLA	C2C-C1C-NC	5.88	116.16	109.98
11	B	1213	CLA	C4A-NA-C1A	5.88	109.36	106.68
11	b	1235	CLA	C4A-NA-C1A	5.88	109.36	106.68
11	b	1222	CLA	C4A-NA-C1A	5.88	109.36	106.68
11	8	1502	CLA	O2D-CGD-CBD	5.87	121.49	111.23
11	2	1207	CLA	C2C-C1C-NC	5.87	116.14	109.98
11	2	1216	CLA	C2C-C1C-NC	5.87	116.14	109.98
11	B	1226	CLA	C2C-C1C-NC	5.86	116.14	109.98
11	a	1110	CLA	C2C-C1C-NC	5.86	116.13	109.98
11	1	1108	CLA	C4A-NA-C1A	5.85	109.35	106.68
11	A	1131	CLA	O2D-CGD-CBD	5.85	121.46	111.23
11	a	1022	CLA	C2C-C1C-NC	5.85	116.13	109.98
11	B	1214	CLA	C4A-NA-C1A	5.85	109.35	106.68
11	B	1218	CLA	C4A-NA-C1A	5.85	109.35	106.68
11	1	1012	CLA	C2C-C1C-NC	5.85	116.13	109.98
11	1	1114	CLA	C2C-C1C-NC	5.85	116.13	109.98
11	B	1225	CLA	C2C-C1C-NC	5.85	116.13	109.98
11	b	1223	CLA	C2C-C1C-NC	5.85	116.12	109.98
11	a	1012	CLA	O2D-CGD-CBD	5.84	121.45	111.23
11	b	1220	CLA	C2C-C1C-NC	5.84	116.12	109.98
11	a	1136	CLA	C4A-NA-C1A	5.84	109.34	106.68
11	b	1230	CLA	O2D-CGD-CBD	5.84	121.44	111.23
11	2	1205	CLA	O2A-CGA-O1A	-5.84	109.01	123.63
11	a	1125	CLA	C2C-C1C-NC	5.84	116.12	109.98
11	A	1123	CLA	C4A-NA-C1A	5.84	109.34	106.68
11	b	1213	CLA	C4A-NA-C1A	5.84	109.34	106.68
11	1	1134	CLA	C2C-C1C-NC	5.84	116.11	109.98
11	B	1231	CLA	O2D-CGD-CBD	5.84	121.44	111.23
11	A	1140	CLA	C2C-C1C-NC	5.84	116.11	109.98
11	B	1220	CLA	C2C-C1C-NC	5.84	116.11	109.98
11	1	1135	CLA	C4A-NA-C1A	5.84	109.34	106.68
11	A	1136	CLA	C2C-C1C-NC	5.84	116.11	109.98
11	2	1236	CLA	C1D-ND-C4D	-5.83	102.22	106.31
11	b	1230	CLA	C2C-C1C-NC	5.83	116.11	109.98
11	B	1224	CLA	O2D-CGD-CBD	5.83	121.43	111.23
11	1	1121	CLA	C4A-NA-C1A	5.83	109.34	106.68
11	k	1401	CLA	C2C-C1C-NC	5.83	116.10	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1126	CLA	O2D-CGD-CBD	5.83	121.41	111.23
11	a	1136	CLA	C2C-C1C-NC	5.82	116.10	109.98
11	A	1131	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	B	1226	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	1	1137	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	A	1011	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
11	b	1023	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	2	1240	CLA	C2C-C1C-NC	5.82	116.09	109.98
11	1	1125	CLA	O2D-CGD-CBD	5.82	121.40	111.23
11	B	1021	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
11	B	1231	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	B	1209	CLA	C2C-C1C-NC	5.82	116.09	109.98
11	1	1104	CLA	C4A-NA-C1A	5.82	109.33	106.68
11	a	1136	CLA	O2D-CGD-CBD	5.81	121.39	111.23
11	1	1107	CLA	C4A-NA-C1A	5.81	109.33	106.68
11	a	1115	CLA	C1D-ND-C4D	-5.81	102.23	106.31
11	2	1225	CLA	C2C-C1C-NC	5.81	116.08	109.98
11	A	1122	CLA	C1D-ND-C4D	-5.81	102.24	106.31
11	B	1203	CLA	C4A-NA-C1A	5.80	109.33	106.68
11	2	1216	CLA	C4A-NA-C1A	5.80	109.33	106.68
11	b	1227	CLA	C2C-C1C-NC	5.80	116.08	109.98
11	1	1123	CLA	C2C-C1C-NC	5.80	116.08	109.98
11	A	1133	CLA	C4A-NA-C1A	5.80	109.33	106.68
11	2	1013	CLA	C4A-NA-C1A	5.80	109.33	106.68
11	a	1129	CLA	C2C-C1C-NC	5.80	116.08	109.98
11	K	1402	CLA	C1D-ND-C4D	-5.80	102.24	106.31
11	b	1224	CLA	C4A-NA-C1A	5.80	109.33	106.68
14	f	4013	BCR	C24-C23-C22	-5.80	117.66	126.23
11	2	1023	CLA	C3B-C2B-C1B	-5.80	100.33	107.17
11	a	1121	CLA	C2C-C1C-NC	5.80	116.07	109.98
11	l	1503	CLA	C2C-C1C-NC	5.80	116.07	109.98
11	1	1237	CLA	C2C-C1C-NC	5.80	116.07	109.98
11	A	1106	CLA	C2C-C1C-NC	5.80	116.07	109.98
11	2	1209	CLA	C2C-C1C-NC	5.80	116.07	109.98
11	A	1109	CLA	C1D-ND-C4D	-5.79	102.25	106.31
11	2	1224	CLA	C2C-C1C-NC	5.79	116.07	109.98
14	1	4003	BCR	C23-C22-C21	5.79	128.12	119.01
11	A	1131	CLA	C2C-C1C-NC	5.79	116.06	109.98
11	0	1401	CLA	C2C-C1C-NC	5.79	116.06	109.98
11	L	1502	CLA	C2C-C1C-NC	5.78	116.06	109.98
11	a	1237	CLA	C2C-C1C-NC	5.78	116.06	109.98
11	l	1501	CLA	O2D-CGD-CBD	5.78	121.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1211	CLA	C2C-C1C-NC	5.78	116.05	109.98
11	1	1111	CLA	C2D-C1D-ND	5.78	115.84	110.13
11	2	1217	CLA	C2C-C1C-NC	5.78	116.05	109.98
11	B	1205	CLA	C2C-C1C-NC	5.78	116.05	109.98
11	8	1501	CLA	C2C-C1C-NC	5.78	116.05	109.98
11	2	1239	CLA	C4A-NA-C1A	5.78	109.31	106.68
11	b	1225	CLA	C2C-C1C-NC	5.78	116.05	109.98
11	A	1104	CLA	O2D-CGD-CBD	5.77	121.33	111.23
11	a	1116	CLA	O2D-CGD-CBD	5.77	121.32	111.23
11	B	1216	CLA	C2C-C1C-NC	5.77	116.04	109.98
11	b	1209	CLA	C2C-C1C-NC	5.77	116.04	109.98
11	2	1220	CLA	C4A-NA-C1A	5.76	109.31	106.68
11	A	1011	CLA	C2C-C1C-NC	5.76	116.04	109.98
14	B	4017	BCR	C20-C19-C18	5.76	142.16	126.36
11	a	1108	CLA	C2C-C1C-NC	5.76	116.03	109.98
11	K	1401	CLA	C2C-C1C-NC	5.76	116.03	109.98
11	B	1213	CLA	C1D-ND-C4D	-5.76	102.27	106.31
11	1	1128	CLA	C2C-C1C-NC	5.75	116.03	109.98
11	2	1240	CLA	C4A-NA-C1A	5.75	109.30	106.68
11	a	1129	CLA	O2D-CGD-CBD	5.75	121.29	111.23
11	b	1222	CLA	C2C-C1C-NC	5.75	116.02	109.98
11	L	1502	CLA	C4A-NA-C1A	5.75	109.30	106.68
11	a	1126	CLA	C4A-NA-C1A	5.75	109.30	106.68
11	a	1133	CLA	O2D-CGD-CBD	5.75	121.28	111.23
11	b	1221	CLA	C2D-C1D-ND	5.75	115.82	110.13
11	1	1121	CLA	C2C-C1C-NC	5.75	116.02	109.98
11	1	1137	CLA	C1D-ND-C4D	-5.75	102.28	106.31
11	2	1224	CLA	O2D-CGD-CBD	5.75	121.28	111.23
11	A	1112	CLA	C4A-NA-C1A	5.75	109.30	106.68
11	b	1212	CLA	C2C-C1C-NC	5.75	116.02	109.98
11	1	1112	CLA	O2D-CGD-CBD	5.75	121.27	111.23
11	1	1132	CLA	C2C-C1C-NC	5.74	116.02	109.98
11	1	1012	CLA	O2D-CGD-CBD	5.74	121.27	111.23
11	B	1236	CLA	C2D-C1D-ND	5.74	115.81	110.13
11	A	1137	CLA	C4A-NA-C1A	5.74	109.30	106.68
11	2	1226	CLA	C2C-C1C-NC	5.74	116.01	109.98
11	A	1113	CLA	C1D-ND-C4D	-5.74	102.28	106.31
11	b	1202	CLA	C1D-ND-C4D	-5.74	102.28	106.31
11	A	1132	CLA	C2C-C1C-NC	5.74	116.01	109.98
11	1	1140	CLA	O2A-CGA-O1A	-5.74	109.28	123.63
11	A	1129	CLA	C2C-C1C-NC	5.74	116.01	109.98
11	a	1137	CLA	C2C-C1C-NC	5.74	116.01	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1101	CLA	C2C-C1C-NC	5.73	116.00	109.98
11	a	1120	CLA	C2C-C1C-NC	5.72	115.99	109.98
11	1	1135	CLA	C2C-C1C-NC	5.72	115.99	109.98
11	A	1137	CLA	C2C-C1C-NC	5.72	115.99	109.98
11	B	1232	CLA	C4A-NA-C1A	5.72	109.29	106.68
11	b	1202	CLA	C4A-NA-C1A	5.72	109.29	106.68
11	A	1133	CLA	C1C-C2C-C3C	-5.72	100.97	106.98
11	1	1104	CLA	C1C-C2C-C3C	-5.72	100.97	106.98
11	2	1202	CLA	C1D-ND-C4D	-5.72	102.30	106.31
11	1	1108	CLA	C2C-C1C-NC	5.72	115.98	109.98
11	a	1139	CLA	C1C-C2C-C3C	-5.72	100.97	106.98
11	L	1502	CLA	C1D-ND-C4D	-5.71	102.30	106.31
11	b	1214	CLA	C1D-ND-C4D	-5.71	102.30	106.31
11	b	1226	CLA	C2C-C1C-NC	5.71	115.98	109.98
11	2	1213	CLA	C1D-ND-C4D	-5.71	102.31	106.31
11	a	1801	CLA	C2C-C1C-NC	5.71	115.98	109.98
11	A	1105	CLA	C4A-NA-C1A	5.71	109.28	106.68
11	l	1502	CLA	C2C-C1C-NC	5.71	115.98	109.98
11	2	1231	CLA	O2D-CGD-CBD	5.71	121.21	111.23
11	a	1124	CLA	C2C-C1C-NC	5.71	115.98	109.98
11	2	1217	CLA	C4A-NA-C1A	5.71	109.28	106.68
11	a	1012	CLA	C2C-C1C-NC	5.71	115.98	109.98
11	B	1222	CLA	C4A-NA-C1A	5.71	109.28	106.68
11	A	1106	CLA	O2D-CGD-CBD	5.71	121.20	111.23
11	b	1221	CLA	C1D-ND-C4D	-5.71	102.31	106.31
11	1	1137	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	8	1502	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	2	1221	CLA	O2D-CGD-CBD	5.70	121.20	111.23
11	1	1129	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	A	1115	CLA	C1D-ND-C4D	-5.70	102.31	106.31
11	2	1228	CLA	C4A-NA-C1A	5.70	109.28	106.68
11	2	1220	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	B	1213	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	A	1134	CLA	C4A-NA-C1A	5.70	109.28	106.68
11	a	1131	CLA	C2C-C1C-NC	5.70	115.97	109.98
11	b	1239	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
11	a	1114	CLA	C4A-NA-C1A	5.69	109.28	106.68
11	2	1023	CLA	C2C-C1C-NC	5.69	115.96	109.98
11	1	1011	CLA	C1C-C2C-C3C	-5.69	100.99	106.98
11	2	1215	CLA	O2D-CGD-CBD	5.69	121.18	111.23
11	A	1108	CLA	C1D-ND-C4D	-5.69	102.32	106.31
11	1	1120	CLA	C2C-C1C-NC	5.69	115.96	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1217	CLA	C4A-NA-C1A	5.69	109.27	106.68
11	1	1132	CLA	C4A-NA-C1A	5.69	109.27	106.68
11	a	1113	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	b	1203	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	1	1140	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	2	1023	CLA	C4A-NA-C1A	5.68	109.27	106.68
11	2	1229	CLA	C4A-NA-C1A	5.68	109.27	106.68
11	1	1012	CLA	O2A-CGA-O1A	-5.68	109.42	123.63
11	b	1211	CLA	O2D-CGD-CBD	5.68	121.16	111.23
11	1	1012	CLA	C2D-C1D-ND	5.68	115.75	110.13
11	a	1106	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	2	1201	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	a	1135	CLA	C4A-NA-C1A	5.68	109.27	106.68
11	A	1135	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	2	1238	CLA	C2C-C1C-NC	5.68	115.95	109.98
11	a	1012	CLA	C4A-NA-C1A	5.68	109.27	106.68
11	a	1124	CLA	O2D-CGD-CBD	5.68	121.15	111.23
11	b	1216	CLA	C2C-C1C-NC	5.68	115.94	109.98
11	2	1224	CLA	C2D-C1D-ND	5.68	115.74	110.13
11	a	1103	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
11	1	1120	CLA	C4A-NA-C1A	5.67	109.27	106.68
11	2	1203	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	2	1227	CLA	O2D-CGD-CBD	5.67	121.15	111.23
11	A	1124	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	b	1205	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	1	1104	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	1	1122	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	1	1101	CLA	O2D-CGD-CBD	5.67	121.14	111.23
11	A	1118	CLA	C1C-C2C-C3C	-5.67	101.02	106.98
11	1	1103	CLA	C2C-C1C-NC	5.67	115.94	109.98
11	B	1013	CLA	C4A-NA-C1A	5.67	109.26	106.68
11	A	1112	CLA	O2D-CGD-CBD	5.67	121.14	111.23
14	2	4014	BCR	C24-C23-C22	-5.67	117.85	126.23
11	a	1118	CLA	C2C-C1C-NC	5.66	115.93	109.98
11	1	1116	CLA	O2D-CGD-CBD	5.66	121.13	111.23
11	1	1106	CLA	C2C-C1C-NC	5.66	115.93	109.98
11	1	1139	CLA	C2C-C1C-NC	5.66	115.93	109.98
11	A	1130	CLA	C2C-C1C-NC	5.66	115.93	109.98
11	2	1218	CLA	O2D-CGD-CBD	5.66	121.13	111.23
11	a	1133	CLA	C4A-NA-C1A	5.66	109.26	106.68
11	2	1210	CLA	C4A-NA-C1A	5.66	109.26	106.68
11	a	1128	CLA	C2C-C1C-NC	5.66	115.93	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1210	CLA	O2D-CGD-CBD	5.66	121.12	111.23
11	1	1113	CLA	C2C-C1C-NC	5.66	115.92	109.98
11	1	1134	CLA	O2D-CGD-CBD	5.66	121.12	111.23
14	A	4003	BCR	C7-C8-C9	-5.66	117.87	126.23
11	B	1221	CLA	C2C-C1C-NC	5.66	115.92	109.98
11	a	1134	CLA	C1D-ND-C4D	-5.66	102.34	106.31
11	a	1140	CLA	C4A-NA-C1A	5.66	109.26	106.68
11	b	1023	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	2	1204	CLA	O2D-CGD-CBD	5.65	121.11	111.23
11	A	1127	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	2	1021	CLA	C4A-NA-C1A	5.65	109.26	106.68
11	B	1211	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	1	1109	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	B	1201	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	B	1239	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	a	1106	CLA	C4A-NA-C1A	5.65	109.26	106.68
11	a	1134	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	1	1117	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	B	1204	CLA	C2C-C1C-NC	5.65	115.92	109.98
11	1	1107	CLA	C1D-ND-C4D	-5.65	102.35	106.31
11	1	1137	CLA	C2D-C1D-ND	5.65	115.72	110.13
11	1	1119	CLA	O2A-CGA-O1A	-5.65	109.50	123.63
11	2	1213	CLA	C1C-C2C-C3C	-5.65	101.04	106.98
11	B	1223	CLA	O2D-CGD-CBD	5.65	121.10	111.23
11	1	1124	CLA	C4A-NA-C1A	5.64	109.25	106.68
11	b	1228	CLA	C2C-C1C-NC	5.64	115.91	109.98
11	2	1210	CLA	C1D-ND-C4D	-5.64	102.36	106.31
11	b	1232	CLA	C2C-C1C-NC	5.64	115.90	109.98
14	a	4001	BCR	C24-C23-C22	-5.64	117.90	126.23
14	b	4017	BCR	C7-C8-C9	-5.63	117.90	126.23
11	1	1123	CLA	C4A-NA-C1A	5.63	109.25	106.68
11	a	1123	CLA	C2C-C1C-NC	5.63	115.90	109.98
11	A	1102	CLA	C2C-C1C-NC	5.63	115.90	109.98
11	A	1012	CLA	C2C-C1C-NC	5.63	115.89	109.98
11	b	1215	CLA	C2C-C1C-NC	5.63	115.89	109.98
11	A	1101	CLA	C1D-ND-C4D	-5.63	102.36	106.31
14	l	4022	BCR	C24-C23-C22	-5.63	117.91	126.23
11	b	1238	CLA	C2C-C1C-NC	5.63	115.89	109.98
11	2	1211	CLA	C2C-C1C-NC	5.63	115.89	109.98
11	B	1211	CLA	C1D-ND-C4D	-5.63	102.36	106.31
11	A	1136	CLA	C4A-NA-C1A	5.63	109.25	106.68
11	1	1129	CLA	C4A-NA-C1A	5.63	109.25	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1229	CLA	C2C-C1C-NC	5.63	115.89	109.98
11	B	1207	CLA	O2A-CGA-O1A	-5.63	109.56	123.63
11	l	1503	CLA	C1C-C2C-C3C	-5.62	101.06	106.98
11	b	1203	CLA	C4A-NA-C1A	5.62	109.25	106.68
11	b	1228	CLA	C4A-NA-C1A	5.62	109.25	106.68
11	A	1116	CLA	O2D-CGD-CBD	5.62	121.06	111.23
11	b	1217	CLA	C2C-C1C-NC	5.62	115.89	109.98
11	B	1204	CLA	O2D-CGD-CBD	5.62	121.06	111.23
11	B	1236	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
11	b	1207	CLA	O2A-CGA-O1A	-5.62	109.57	123.63
11	A	1121	CLA	C2C-C1C-NC	5.62	115.89	109.98
11	1	1131	CLA	C2C-C1C-NC	5.62	115.89	109.98
11	2	1234	CLA	C4A-NA-C1A	5.62	109.24	106.68
11	a	1119	CLA	O2A-CGA-O1A	-5.62	109.57	123.63
11	2	1232	CLA	C2C-C1C-NC	5.62	115.88	109.98
11	A	1107	CLA	C1D-ND-C4D	-5.62	102.37	106.31
11	B	1208	CLA	C1D-ND-C4D	-5.62	102.37	106.31
11	1	1801	CLA	O2D-CGD-CBD	5.62	121.05	111.23
11	8	1503	CLA	C2C-C1C-NC	5.62	115.88	109.98
11	B	1203	CLA	C2C-C1C-NC	5.62	115.88	109.98
11	b	1204	CLA	C2C-C1C-NC	5.62	115.88	109.98
11	2	1222	CLA	C2C-C1C-NC	5.62	115.88	109.98
11	b	1224	CLA	C2C-C1C-NC	5.61	115.88	109.98
11	2	1221	CLA	C2C-C1C-NC	5.61	115.88	109.98
11	A	1102	CLA	O2D-CGD-CBD	5.61	121.04	111.23
11	a	1105	CLA	C4A-NA-C1A	5.61	109.24	106.68
11	B	1235	CLA	C1D-ND-C4D	-5.61	102.37	106.31
11	2	1208	CLA	C2C-C1C-NC	5.61	115.88	109.98
11	1	1102	CLA	C2C-C1C-NC	5.61	115.87	109.98
11	a	1110	CLA	O2D-CGD-CBD	5.61	121.04	111.23
11	2	1214	CLA	C2C-C1C-NC	5.61	115.87	109.98
11	B	1203	CLA	C1D-ND-C4D	-5.61	102.38	106.31
11	1	1237	CLA	C1D-ND-C4D	-5.61	102.38	106.31
11	1	1112	CLA	C1D-ND-C4D	-5.61	102.38	106.31
11	a	1140	CLA	C2C-C1C-NC	5.61	115.87	109.98
11	a	1118	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
11	l	1502	CLA	C1D-ND-C4D	-5.61	102.38	106.31
11	B	1214	CLA	C1D-ND-C4D	-5.60	102.38	106.31
11	A	1138	CLA	C2C-C1C-NC	5.60	115.87	109.98
11	B	1209	CLA	O2D-CGD-CBD	5.60	121.03	111.23
11	1	1116	CLA	C4A-NA-C1A	5.60	109.23	106.68
11	A	1104	CLA	C1C-C2C-C3C	-5.60	101.09	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1801	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
11	B	1228	CLA	C2C-C1C-NC	5.60	115.86	109.98
11	2	1211	CLA	O2D-CGD-CBD	5.60	121.01	111.23
11	B	1205	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
11	B	1236	CLA	C4A-NA-C1A	5.60	109.23	106.68
11	a	1113	CLA	C4A-NA-C1A	5.60	109.23	106.68
11	1	1134	CLA	C4A-NA-C1A	5.60	109.23	106.68
11	A	1137	CLA	C2D-C1D-ND	5.59	115.66	110.13
11	b	1210	CLA	C1D-ND-C4D	-5.59	102.39	106.31
11	A	1113	CLA	C4A-NA-C1A	5.59	109.23	106.68
11	2	1230	CLA	C2C-C1C-NC	5.59	115.86	109.98
11	b	1204	CLA	C4A-NA-C1A	5.59	109.23	106.68
11	a	1102	CLA	C2C-C1C-NC	5.59	115.85	109.98
11	A	1135	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
11	a	1137	CLA	C4A-NA-C1A	5.59	109.23	106.68
11	a	1130	CLA	C2C-C1C-NC	5.59	115.85	109.98
11	1	1104	CLA	C1D-ND-C4D	-5.59	102.39	106.31
11	a	1011	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
11	1	1122	CLA	C1D-ND-C4D	-5.58	102.39	106.31
11	a	1125	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
11	2	1221	CLA	C2D-C1D-ND	5.58	115.65	110.13
11	B	1202	CLA	C1D-ND-C4D	-5.58	102.40	106.31
11	a	1120	CLA	O2D-CGD-CBD	5.58	120.98	111.23
11	b	1224	CLA	O2D-CGD-CBD	5.58	120.98	111.23
11	1	1102	CLA	C4A-NA-C1A	5.58	109.22	106.68
11	B	1215	CLA	C4-C3-C5	5.57	124.90	115.23
11	1	1138	CLA	C1D-ND-C4D	-5.57	102.40	106.31
11	2	1235	CLA	C1D-ND-C4D	-5.57	102.41	106.31
11	L	1503	CLA	O2D-CGD-CBD	5.57	120.96	111.23
11	B	1219	CLA	C4A-NA-C1A	5.56	109.22	106.68
11	1	1105	CLA	C4A-NA-C1A	5.56	109.22	106.68
11	1	1117	CLA	C4A-NA-C1A	5.56	109.22	106.68
11	2	1235	CLA	C4A-NA-C1A	5.56	109.22	106.68
11	1	1134	CLA	C1D-ND-C4D	-5.56	102.41	106.31
11	2	1216	CLA	O2D-CGD-CBD	5.56	120.95	111.23
11	B	1013	CLA	O2A-CGA-O1A	-5.56	109.72	123.63
11	1	1124	CLA	C2C-C1C-NC	5.56	115.82	109.98
11	A	1112	CLA	C2D-C1D-ND	5.56	115.63	110.13
11	2	1224	CLA	O2A-CGA-O1A	-5.56	109.73	123.63
11	1	1133	CLA	C1C-C2C-C3C	-5.56	101.14	106.98
11	B	1207	CLA	C1D-ND-C4D	-5.55	102.42	106.31
11	2	1208	CLA	C1D-ND-C4D	-5.55	102.42	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1206	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
11	2	1231	CLA	C4A-NA-C1A	5.55	109.21	106.68
11	B	1222	CLA	C2C-C1C-NC	5.55	115.81	109.98
11	2	1207	CLA	O2A-CGA-O1A	-5.55	109.75	123.63
11	B	1234	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
11	K	1402	CLA	C2C-C1C-NC	5.55	115.81	109.98
11	B	1224	CLA	O2A-CGA-O1A	-5.55	109.75	123.63
11	B	1023	CLA	C1D-ND-C4D	-5.55	102.42	106.31
11	a	1139	CLA	C4A-NA-C1A	5.55	109.21	106.68
11	l	1503	CLA	O2D-CGD-CBD	5.55	120.93	111.23
11	a	1129	CLA	C1D-ND-C4D	-5.55	102.42	106.31
11	1	1109	CLA	C4A-NA-C1A	5.55	109.21	106.68
11	A	1122	CLA	C4A-NA-C1A	5.54	109.21	106.68
11	a	1128	CLA	C4A-NA-C1A	5.54	109.21	106.68
11	2	1230	CLA	O2D-CGD-CBD	5.54	120.92	111.23
11	1	1022	CLA	C2C-C1C-NC	5.54	115.80	109.98
11	8	1502	CLA	C1D-ND-C4D	-5.54	102.42	106.31
11	b	1013	CLA	O2A-CGA-O1A	-5.54	109.77	123.63
11	A	1118	CLA	C2C-C1C-NC	5.54	115.80	109.98
11	B	1235	CLA	C2C-C1C-NC	5.54	115.80	109.98
11	2	1225	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	b	4017	BCR	C34-C9-C10	-5.54	113.84	122.82
11	1	1111	CLA	O2D-CGD-CBD	5.54	120.91	111.23
11	1	1115	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
11	1	1112	CLA	C4A-NA-C1A	5.54	109.21	106.68
11	b	1235	CLA	C1D-ND-C4D	-5.54	102.43	106.31
11	1	1106	CLA	C1D-ND-C4D	-5.54	102.43	106.31
11	L	1501	CLA	C2C-C1C-NC	5.54	115.80	109.98
11	b	1220	CLA	C4A-NA-C1A	5.54	109.20	106.68
11	a	1112	CLA	C1D-ND-C4D	-5.54	102.43	106.31
11	a	1108	CLA	C4A-NA-C1A	5.53	109.20	106.68
11	b	1209	CLA	C4A-NA-C1A	5.53	109.20	106.68
11	b	1215	CLA	O2D-CGD-CBD	5.53	120.90	111.23
11	1	1116	CLA	C2C-C1C-NC	5.53	115.79	109.98
11	b	1213	CLA	C2C-C1C-NC	5.53	115.79	109.98
11	2	1215	CLA	C1C-C2C-C3C	-5.53	101.16	106.98
11	0	1402	CLA	C4A-NA-C1A	5.53	109.20	106.68
11	a	1109	CLA	C2C-C1C-NC	5.53	115.79	109.98
11	b	1021	CLA	C4A-NA-C1A	5.53	109.20	106.68
11	b	1240	CLA	C2C-C1C-NC	5.53	115.79	109.98
11	A	1129	CLA	C4A-NA-C1A	5.53	109.20	106.68
11	1	1130	CLA	C2C-C1C-NC	5.52	115.78	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1228	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	A	1107	CLA	C2D-C1D-ND	5.52	115.59	110.13
11	a	1111	CLA	C2D-C1D-ND	5.52	115.59	110.13
14	1	4008	BCR	C15-C14-C13	-5.52	119.53	127.28
11	B	1240	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	B	1236	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
11	b	1214	CLA	O2D-CGD-CBD	5.52	120.88	111.23
11	A	1129	CLA	C1D-ND-C4D	-5.52	102.44	106.31
11	b	1224	CLA	C1D-ND-C4D	-5.52	102.44	106.31
11	A	1113	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	2	1217	CLA	O2D-CGD-CBD	5.52	120.88	111.23
11	B	1207	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	l	1501	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	a	1801	CLA	O2D-CGD-CBD	5.52	120.88	111.23
11	8	1502	CLA	C2D-C1D-ND	5.52	115.59	110.13
11	l	1501	CLA	C1D-ND-C4D	-5.52	102.44	106.31
11	A	1122	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	B	1223	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	1	1127	CLA	C2C-C1C-NC	5.52	115.78	109.98
11	b	1239	CLA	O2D-CGD-CBD	5.52	120.87	111.23
11	A	1137	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
11	2	1013	CLA	O2A-CGA-O1A	-5.51	109.83	123.63
11	B	1235	CLA	O2D-CGD-CBD	5.51	120.87	111.23
11	A	1106	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
11	B	1219	CLA	C2C-C1C-NC	5.51	115.77	109.98
11	a	1135	CLA	O2D-CGD-CBD	5.51	120.86	111.23
11	b	1212	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
11	A	1101	CLA	C2C-C1C-NC	5.51	115.77	109.98
11	b	1226	CLA	C1D-ND-C4D	-5.51	102.45	106.31
11	1	1105	CLA	C2C-C1C-NC	5.51	115.77	109.98
11	B	1224	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
11	1	1108	CLA	C1D-ND-C4D	-5.51	102.45	106.31
11	2	1225	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
11	B	1023	CLA	C2C-C1C-NC	5.51	115.77	109.98
11	a	1138	CLA	C2C-C1C-NC	5.51	115.77	109.98
11	2	1204	CLA	C2C-C1C-NC	5.50	115.76	109.98
11	B	1217	CLA	C2C-C1C-NC	5.50	115.76	109.98
11	A	1107	CLA	C2C-C1C-NC	5.50	115.76	109.98
11	1	1129	CLA	C1D-ND-C4D	-5.50	102.45	106.31
11	b	1213	CLA	O2D-CGD-CBD	5.50	120.84	111.23
11	b	1021	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
11	2	1211	CLA	C2D-C1D-ND	5.50	115.57	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1106	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
11	A	1108	CLA	C2C-C1C-NC	5.50	115.75	109.98
11	B	1231	CLA	C1C-C2C-C3C	-5.49	101.20	106.98
11	A	1111	CLA	C1D-ND-C4D	-5.49	102.46	106.31
11	1	1127	CLA	C1D-ND-C4D	-5.49	102.46	106.31
11	b	1202	CLA	O2D-CGD-CBD	5.49	120.83	111.23
11	A	1012	CLA	C2D-C1D-ND	5.49	115.56	110.13
11	A	1106	CLA	C4A-NA-C1A	5.49	109.18	106.68
11	b	1235	CLA	C2C-C1C-NC	5.49	115.75	109.98
11	A	1237	CLA	C1D-ND-C4D	-5.49	102.46	106.31
11	1	1115	CLA	O2D-CGD-CBD	5.49	120.83	111.23
11	A	1109	CLA	C4A-NA-C1A	5.49	109.18	106.68
11	2	1230	CLA	C4A-NA-C1A	5.49	109.18	106.68
11	b	1202	CLA	C2D-C1D-ND	5.49	115.56	110.13
11	B	1239	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
11	a	1104	CLA	C1D-ND-C4D	-5.49	102.46	106.31
11	b	1218	CLA	C2C-C1C-NC	5.49	115.75	109.98
11	b	1227	CLA	C4A-NA-C1A	5.49	109.18	106.68
11	1	1131	CLA	C4A-NA-C1A	5.49	109.18	106.68
11	1	1130	CLA	O2D-CGD-CBD	5.49	120.82	111.23
11	2	1023	CLA	O2A-CGA-O1A	-5.49	109.91	123.63
11	b	1222	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
11	B	1207	CLA	C2D-C1D-ND	5.48	115.55	110.13
11	b	1217	CLA	C4A-NA-C1A	5.48	109.18	106.68
11	A	1109	CLA	C1C-C2C-C3C	-5.48	101.21	106.98
11	2	1021	CLA	C1C-C2C-C3C	-5.48	101.21	106.98
11	A	1105	CLA	C2C-C1C-NC	5.48	115.74	109.98
11	l	1503	CLA	C4A-NA-C1A	5.48	109.18	106.68
11	b	1229	CLA	C1D-ND-C4D	-5.48	102.47	106.31
11	a	1133	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
11	B	1204	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
11	B	1236	CLA	C2C-C1C-NC	5.48	115.73	109.98
11	B	1226	CLA	C1D-ND-C4D	-5.48	102.47	106.31
11	1	1118	CLA	O2D-CGD-CBD	5.48	120.81	111.23
11	l	1501	CLA	O2A-CGA-O1A	-5.48	109.93	123.63
11	0	1402	CLA	C2C-C1C-NC	5.48	115.73	109.98
11	a	1130	CLA	O2D-CGD-CBD	5.47	120.80	111.23
11	b	1203	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
11	B	1238	CLA	C2C-C1C-NC	5.47	115.73	109.98
11	B	1238	CLA	C1D-ND-C4D	-5.47	102.47	106.31
11	B	1203	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
11	1	1801	CLA	C1C-C2C-C3C	-5.47	101.22	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1231	CLA	C2C-C1C-NC	5.47	115.73	109.98
11	2	1227	CLA	C1D-ND-C4D	-5.47	102.47	106.31
14	a	4003	BCR	C24-C23-C22	-5.47	118.14	126.23
11	A	1137	CLA	O2D-CGD-CBD	5.47	120.79	111.23
11	B	1209	CLA	C4A-NA-C1A	5.47	109.17	106.68
11	a	1131	CLA	C4A-NA-C1A	5.47	109.17	106.68
11	a	1109	CLA	C1D-ND-C4D	-5.47	102.47	106.31
11	1	1135	CLA	O2D-CGD-CBD	5.47	120.79	111.23
11	b	1227	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
11	b	1209	CLA	O2D-CGD-CBD	5.46	120.78	111.23
11	2	1236	CLA	C4A-NA-C1A	5.46	109.17	106.68
11	a	1102	CLA	O2A-CGA-O1A	-5.46	109.96	123.63
11	A	1134	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
11	B	1210	CLA	C1D-ND-C4D	-5.46	102.48	106.31
11	a	1113	CLA	C1D-ND-C4D	-5.46	102.48	106.31
11	a	1105	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
11	a	1132	CLA	C4A-NA-C1A	5.46	109.17	106.68
11	K	1401	CLA	C1D-ND-C4D	-5.46	102.48	106.31
11	1	1112	CLA	C2C-C1C-NC	5.46	115.72	109.98
11	l	1501	CLA	C2D-C1D-ND	5.46	115.53	110.13
11	1	1102	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
11	1	1131	CLA	O2D-CGD-CBD	5.46	120.77	111.23
11	A	1122	CLA	O2D-CGD-CBD	5.46	120.77	111.23
11	a	1122	CLA	C1D-ND-C4D	-5.46	102.48	106.31
11	k	1401	CLA	C1D-ND-C4D	-5.46	102.48	106.31
11	a	1122	CLA	C4A-NA-C1A	5.46	109.17	106.68
11	b	1235	CLA	O2D-CGD-CBD	5.45	120.77	111.23
14	1	4002	BCR	C33-C5-C6	-5.45	118.53	124.48
11	8	1501	CLA	O2A-CGA-O1A	-5.45	109.98	123.63
11	k	1402	CLA	C2C-C1C-NC	5.45	115.71	109.98
11	1	1136	CLA	C2C-C1C-NC	5.45	115.71	109.98
11	A	1116	CLA	C4A-NA-C1A	5.45	109.17	106.68
11	b	1211	CLA	C1D-ND-C4D	-5.45	102.49	106.31
11	a	1116	CLA	C2C-C1C-NC	5.45	115.71	109.98
11	b	1210	CLA	C4A-NA-C1A	5.45	109.17	106.68
11	B	1234	CLA	O2A-CGA-O1A	-5.45	109.99	123.63
11	a	1107	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
11	B	1202	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
11	a	1132	CLA	O2D-CGD-CBD	5.45	120.75	111.23
11	B	1232	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
11	b	1236	CLA	C4A-NA-C1A	5.44	109.16	106.68
11	b	1219	CLA	C1C-C2C-C3C	-5.44	101.25	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1023	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
11	A	1130	CLA	C4A-NA-C1A	5.44	109.16	106.68
11	A	1139	CLA	C4A-NA-C1A	5.44	109.16	106.68
11	B	1228	CLA	C4A-NA-C1A	5.44	109.16	106.68
11	1	1105	CLA	C1D-ND-C4D	-5.44	102.49	106.31
11	A	1138	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
11	L	1502	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
11	l	1502	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
11	1	1119	CLA	C2C-C1C-NC	5.44	115.70	109.98
11	2	1211	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
11	b	1231	CLA	C2C-C1C-NC	5.44	115.69	109.98
11	B	1021	CLA	O2A-CGA-O1A	-5.44	110.03	123.63
11	B	1230	CLA	O2D-CGD-CBD	5.44	120.74	111.23
11	b	1205	CLA	O2D-CGD-CBD	5.44	120.73	111.23
11	2	1236	CLA	C2D-C1D-ND	5.44	115.51	110.13
11	2	1205	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
11	a	1129	CLA	C1C-C2C-C3C	-5.43	101.26	106.98
11	b	1201	CLA	C2C-C1C-NC	5.43	115.69	109.98
11	a	1116	CLA	C1D-ND-C4D	-5.43	102.50	106.31
11	A	1126	CLA	C1D-ND-C4D	-5.43	102.50	106.31
11	0	1401	CLA	C1D-ND-C4D	-5.43	102.50	106.31
11	a	1137	CLA	C2D-C1D-ND	5.43	115.50	110.13
11	b	1224	CLA	O2A-CGA-O1A	-5.43	110.04	123.63
11	a	1104	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
11	1	1109	CLA	O2A-CGA-O1A	-5.43	110.04	123.63
11	A	1115	CLA	C4A-NA-C1A	5.43	109.16	106.68
11	b	1230	CLA	C4A-NA-C1A	5.43	109.16	106.68
11	a	1101	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	1	1114	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	2	1212	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	A	1113	CLA	C2D-C1D-ND	5.43	115.50	110.13
11	B	1208	CLA	C4A-NA-C1A	5.43	109.16	106.68
11	b	1216	CLA	C1D-ND-C4D	-5.43	102.50	106.31
11	2	1221	CLA	C1D-ND-C4D	-5.43	102.50	106.31
11	a	1109	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	2	1208	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	2	1236	CLA	C2C-C1C-NC	5.43	115.68	109.98
11	A	1012	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
11	b	1207	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	2	1227	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
11	B	1228	CLA	O2D-CGD-CBD	5.43	120.71	111.23
11	B	1226	CLA	C1C-C2C-C3C	-5.42	101.28	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	4013	BCR	C7-C8-C9	-5.42	118.21	126.23
11	b	1227	CLA	C1D-ND-C4D	-5.42	102.51	106.31
11	a	1112	CLA	O2D-CGD-CBD	5.42	120.71	111.23
11	b	1205	CLA	O2A-CGA-O1A	-5.42	110.06	123.63
11	b	1206	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
11	a	1108	CLA	C1D-ND-C4D	-5.42	102.51	106.31
11	2	1226	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
11	2	1229	CLA	C2C-C1C-NC	5.42	115.67	109.98
11	1	1109	CLA	C1D-ND-C4D	-5.42	102.51	106.31
11	1	1113	CLA	C1D-ND-C4D	-5.42	102.51	106.31
11	a	1104	CLA	O2D-CGD-CBD	5.42	120.70	111.23
11	A	1135	CLA	O2A-CGA-O1A	-5.41	110.08	123.63
11	B	1211	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
11	A	1118	CLA	C1D-ND-C4D	-5.41	102.51	106.31
11	A	1114	CLA	C4A-NA-C1A	5.41	109.15	106.68
11	b	1212	CLA	C1D-ND-C4D	-5.41	102.52	106.31
11	b	1218	CLA	C1D-ND-C4D	-5.41	102.52	106.31
11	b	1221	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
11	a	1110	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
11	a	1114	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
11	2	1203	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
11	2	1234	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
11	a	1107	CLA	C2D-C1D-ND	5.41	115.48	110.13
11	1	1111	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
11	B	1218	CLA	C2C-C1C-NC	5.41	115.66	109.98
11	B	1218	CLA	C1D-ND-C4D	-5.40	102.52	106.31
11	B	1221	CLA	C2D-C1D-ND	5.40	115.47	110.13
11	A	1801	CLA	O2A-CGA-O1A	-5.40	110.11	123.63
11	2	1224	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	a	1104	CLA	C4A-NA-C1A	5.40	109.14	106.68
11	b	1211	CLA	C4A-NA-C1A	5.40	109.14	106.68
11	1	1128	CLA	C4A-NA-C1A	5.40	109.14	106.68
11	1	1110	CLA	O2A-CGA-O1A	-5.40	110.11	123.63
11	b	1210	CLA	C2D-C1D-ND	5.40	115.47	110.13
11	a	1137	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	b	1238	CLA	C1D-ND-C4D	-5.40	102.52	106.31
11	B	1215	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	1	1107	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	1	1101	CLA	C4A-NA-C1A	5.40	109.14	106.68
11	2	1222	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	2	1239	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	B	4017	BCR	C24-C23-C22	-5.40	118.25	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1213	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	a	1135	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
11	B	1021	CLA	O2D-CGD-CBD	5.40	120.66	111.23
11	A	1138	CLA	C1D-ND-C4D	-5.39	102.53	106.31
11	a	1115	CLA	C4A-NA-C1A	5.39	109.14	106.68
11	a	1109	CLA	O2A-CGA-O1A	-5.39	110.14	123.63
11	1	1125	CLA	C1D-ND-C4D	-5.39	102.53	106.31
11	l	1502	CLA	C2D-C1D-ND	5.39	115.46	110.13
11	A	1136	CLA	O2D-CGD-CBD	5.39	120.66	111.23
11	b	1221	CLA	C4-C3-C5	5.39	124.59	115.23
11	2	1224	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
11	A	1121	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
11	2	1214	CLA	C1D-ND-C4D	-5.39	102.53	106.31
11	A	1111	CLA	O2D-CGD-CBD	5.39	120.65	111.23
11	a	1125	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	2	4005	BCR	C24-C23-C22	-5.39	118.27	126.23
11	A	1114	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
11	A	1101	CLA	C4A-NA-C1A	5.39	109.14	106.68
11	2	1222	CLA	C4A-NA-C1A	5.39	109.14	106.68
11	a	1117	CLA	C2C-C1C-NC	5.39	115.64	109.98
11	A	1103	CLA	C2D-C1D-ND	5.38	115.45	110.13
11	2	1204	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
11	b	1204	CLA	O2D-CGD-CBD	5.38	120.64	111.23
11	b	1238	CLA	C4A-NA-C1A	5.38	109.14	106.68
11	A	1133	CLA	O2D-CGD-CBD	5.38	120.64	111.23
11	b	1229	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
11	b	1234	CLA	O2A-CGA-O1A	-5.38	110.17	123.63
11	2	1235	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
11	A	1104	CLA	C2D-C1D-ND	5.38	115.45	110.13
11	A	1118	CLA	O2D-CGD-CBD	5.38	120.63	111.23
11	a	1118	CLA	O2D-CGD-CBD	5.38	120.63	111.23
11	a	1132	CLA	C2C-C1C-NC	5.38	115.63	109.98
11	B	1205	CLA	C2D-C1D-ND	5.38	115.45	110.13
11	a	1123	CLA	O2D-CGD-CBD	5.38	120.63	111.23
11	1	1125	CLA	C3D-C2D-C1D	-5.38	98.50	105.83
11	a	1127	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
11	1	1125	CLA	C2C-C1C-NC	5.37	115.63	109.98
11	1	1138	CLA	C2C-C1C-NC	5.37	115.63	109.98
11	a	1012	CLA	C2D-C1D-ND	5.37	115.44	110.13
11	1	1022	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
11	B	1208	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
11	b	1224	CLA	C2D-C1D-ND	5.37	115.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1236	CLA	C2D-C1D-ND	5.37	115.44	110.13
11	a	1107	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
11	8	1501	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
11	A	1128	CLA	C2C-C1C-NC	5.37	115.62	109.98
11	b	1209	CLA	C1D-ND-C4D	-5.37	102.54	106.31
11	a	1237	CLA	C2D-C1D-ND	5.37	115.44	110.13
11	b	1021	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
11	A	1129	CLA	C2D-C1D-ND	5.37	115.44	110.13
11	B	1207	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
11	1	1122	CLA	C4A-NA-C1A	5.37	109.13	106.68
11	A	1104	CLA	C2C-C1C-NC	5.37	115.62	109.98
11	2	1202	CLA	C2C-C1C-NC	5.37	115.62	109.98
11	a	1133	CLA	C1D-ND-C4D	-5.37	102.55	106.31
11	1	1105	CLA	O2D-CGD-CBD	5.37	120.61	111.23
11	A	1101	CLA	C2D-C1D-ND	5.37	115.44	110.13
11	B	1227	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
11	A	1116	CLA	C2D-C1D-ND	5.36	115.44	110.13
11	2	1210	CLA	C2D-C1D-ND	5.36	115.44	110.13
11	1	1104	CLA	O2D-CGD-CBD	5.36	120.61	111.23
11	A	1108	CLA	C4A-NA-C1A	5.36	109.13	106.68
11	a	1106	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	b	1208	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	1	1137	CLA	O2A-CGA-O1A	-5.36	110.21	123.63
14	a	4008	BCR	C24-C23-C22	-5.36	118.30	126.23
11	A	1140	CLA	O2D-CGD-CBD	5.36	120.60	111.23
11	a	1117	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
11	A	1125	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
11	A	1137	CLA	O2A-CGA-O1A	-5.36	110.22	123.63
11	a	1118	CLA	C1D-ND-C4D	-5.36	102.55	106.31
11	1	1119	CLA	C1D-ND-C4D	-5.36	102.55	106.31
11	2	1238	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	b	1236	CLA	C2C-C1C-NC	5.36	115.61	109.98
11	a	1136	CLA	C2D-C1D-ND	5.36	115.43	110.13
11	1	1108	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	1	1118	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	1	1134	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
11	1	1116	CLA	C1D-ND-C4D	-5.36	102.55	106.31
11	A	1119	CLA	C2C-C1C-NC	5.36	115.61	109.98
11	L	1501	CLA	O2A-CGA-O1A	-5.36	110.23	123.63
11	a	1120	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
11	b	1214	CLA	C2D-C1D-ND	5.36	115.43	110.13
11	B	1208	CLA	C2C-C1C-NC	5.35	115.61	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1202	CLA	C3D-C2D-C1D	-5.35	98.52	105.83
11	1	1125	CLA	C2D-C1D-ND	5.35	115.42	110.13
11	A	1136	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
11	b	1236	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
11	1	1012	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
11	1	1104	CLA	C2D-C1D-ND	5.35	115.42	110.13
11	1	1103	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
11	A	1139	CLA	C2C-C1C-NC	5.35	115.60	109.98
11	B	1205	CLA	O2A-CGA-O1A	-5.35	110.24	123.63
11	a	1101	CLA	C4A-NA-C1A	5.35	109.12	106.68
11	1	1119	CLA	C4A-NA-C1A	5.35	109.12	106.68
11	B	1212	CLA	C2C-C1C-NC	5.35	115.60	109.98
11	A	1237	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
11	b	1201	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
11	2	1219	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
14	8	4022	BCR	C24-C23-C22	-5.35	118.33	126.23
11	b	1218	CLA	O2D-CGD-CBD	5.35	120.58	111.23
11	B	1212	CLA	O2D-CGD-CBD	5.35	120.58	111.23
11	b	1201	CLA	O2D-CGD-CBD	5.35	120.58	111.23
11	A	1130	CLA	C1C-C2C-C3C	-5.35	101.36	106.98
11	A	1116	CLA	C1D-ND-C4D	-5.34	102.56	106.31
11	b	1208	CLA	O2D-CGD-CBD	5.34	120.57	111.23
11	A	1120	CLA	C2C-C1C-NC	5.34	115.59	109.98
11	B	1225	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	2	1235	CLA	C2D-C1D-ND	5.34	115.41	110.13
11	A	1110	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	B	1222	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	A	1109	CLA	C2C-C1C-NC	5.34	115.59	109.98
11	B	1224	CLA	C2C-C1C-NC	5.34	115.59	109.98
11	2	1208	CLA	C2D-C1D-ND	5.34	115.41	110.13
11	a	1022	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	b	1203	CLA	O2D-CGD-CBD	5.34	120.56	111.23
11	A	1102	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	1	1109	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	1	1132	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
11	a	1122	CLA	C2C-C1C-NC	5.34	115.59	109.98
11	A	1115	CLA	C2D-C1D-ND	5.34	115.41	110.13
11	a	1125	CLA	C2D-C1D-ND	5.34	115.41	110.13
11	2	1205	CLA	C1D-ND-C4D	-5.34	102.57	106.31
11	B	1215	CLA	O2D-CGD-CBD	5.34	120.56	111.23
11	B	1238	CLA	C1C-C2C-C3C	-5.34	101.37	106.98
11	B	1223	CLA	C3D-C2D-C1D	-5.34	98.55	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1131	CLA	O2D-CGD-CBD	5.34	120.56	111.23
11	A	1139	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
11	a	1125	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
11	B	1216	CLA	C1D-ND-C4D	-5.33	102.57	106.31
11	B	1214	CLA	C2D-C1D-ND	5.33	115.40	110.13
11	b	1213	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
11	1	1121	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
11	1	1137	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
11	b	1023	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
11	2	1238	CLA	C4A-NA-C1A	5.33	109.11	106.68
11	B	1023	CLA	O2A-CGA-O1A	-5.33	110.30	123.63
11	A	1107	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
11	a	1126	CLA	C2D-C1D-ND	5.33	115.40	110.13
11	b	1205	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
11	2	1221	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
11	1	1136	CLA	O2D-CGD-CBD	5.33	120.54	111.23
11	2	1214	CLA	O2D-CGD-CBD	5.32	120.54	111.23
11	b	1228	CLA	O2D-CGD-CBD	5.32	120.54	111.23
11	B	1235	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
11	1	1124	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
11	1	1135	CLA	C2D-C1D-ND	5.32	115.39	110.13
11	A	1137	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
11	1	1137	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	b	4014	BCR	C24-C23-C22	-5.32	118.36	126.23
11	2	1207	CLA	C1D-ND-C4D	-5.32	102.58	106.31
11	2	1205	CLA	C2C-C1C-NC	5.32	115.57	109.98
11	A	1801	CLA	C4A-NA-C1A	5.32	109.11	106.68
11	a	1127	CLA	C4A-NA-C1A	5.32	109.11	106.68
11	b	1215	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
11	1	1135	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
11	b	1236	CLA	O2D-CGD-CBD	5.32	120.53	111.23
11	a	1104	CLA	C2D-C1D-ND	5.32	115.39	110.13
11	b	1218	CLA	C4A-NA-C1A	5.32	109.11	106.68
11	1	1139	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
11	1	1129	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
11	A	1115	CLA	C2C-C1C-NC	5.32	115.57	109.98
11	8	1503	CLA	C4A-NA-C1A	5.32	109.10	106.68
11	a	1131	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
11	1	1117	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
11	1	1130	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
11	a	1124	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
11	b	1235	CLA	C1C-C2C-C3C	-5.31	101.39	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1217	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
11	b	1222	CLA	O2A-CGA-O1A	-5.31	110.34	123.63
11	0	1402	CLA	C2D-C1D-ND	5.31	115.38	110.13
11	1	1011	CLA	C2D-C1D-ND	5.31	115.38	110.13
11	2	1210	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
11	1	1113	CLA	C2D-C1D-ND	5.31	115.38	110.13
11	a	1801	CLA	O2A-CGA-O1A	-5.31	110.35	123.63
11	B	1023	CLA	C2D-C1D-ND	5.31	115.38	110.13
11	b	1212	CLA	C2D-C1D-ND	5.31	115.38	110.13
11	1	1114	CLA	C4A-NA-C1A	5.31	109.10	106.68
11	2	1013	CLA	C3B-C2B-C1B	-5.31	100.92	107.17
11	B	1218	CLA	O2D-CGD-CBD	5.30	120.50	111.23
11	k	1401	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
11	A	1102	CLA	O2A-CGA-O1A	-5.30	110.36	123.63
11	B	1227	CLA	C1D-ND-C4D	-5.30	102.59	106.31
11	B	1211	CLA	C4A-NA-C1A	5.30	109.10	106.68
11	2	1209	CLA	C4A-NA-C1A	5.30	109.10	106.68
11	B	1239	CLA	O2D-CGD-CBD	5.30	120.50	111.23
11	a	1105	CLA	O2D-CGD-CBD	5.30	120.50	111.23
11	B	1223	CLA	C4A-NA-C1A	5.30	109.10	106.68
11	2	1212	CLA	C4A-NA-C1A	5.30	109.10	106.68
11	B	1222	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
11	a	1237	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
11	a	1136	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
11	b	1232	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
11	a	1120	CLA	C2D-C1D-ND	5.30	115.37	110.13
11	A	1102	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
11	B	1216	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
11	1	1140	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
11	A	1124	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
11	a	1132	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
11	b	1229	CLA	C4A-NA-C1A	5.30	109.09	106.68
11	b	1229	CLA	C2D-C1D-ND	5.30	115.37	110.13
11	A	1104	CLA	O2A-CGA-O1A	-5.30	110.38	123.63
11	2	1218	CLA	C1D-ND-C4D	-5.29	102.60	106.31
11	2	1238	CLA	C1D-ND-C4D	-5.29	102.60	106.31
11	1	1107	CLA	O2D-CGD-CBD	5.29	120.48	111.23
11	2	1229	CLA	O2D-CGD-CBD	5.29	120.48	111.23
11	A	1135	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
11	b	1208	CLA	C4A-NA-C1A	5.29	109.09	106.68
11	a	1102	CLA	C3B-C2B-C1B	-5.29	100.93	107.17
11	2	1207	CLA	C2D-C1D-ND	5.29	115.36	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1213	CLA	C2D-C1D-ND	5.29	115.36	110.13
11	0	1401	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
11	b	1235	CLA	C3B-C2B-C1B	-5.29	100.93	107.17
11	b	1240	CLA	C1D-ND-C4D	-5.29	102.60	106.31
11	a	1121	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
11	b	1023	CLA	O2A-CGA-O1A	-5.29	110.40	123.63
11	1	1118	CLA	C2C-C1C-NC	5.29	115.54	109.98
11	b	1201	CLA	C1D-ND-C4D	-5.29	102.60	106.31
11	L	1501	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
11	b	1013	CLA	C4A-NA-C1A	5.29	109.09	106.68
11	2	1210	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
11	1	1106	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
11	A	1135	CLA	C4A-NA-C1A	5.28	109.09	106.68
11	b	1226	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	2	1223	CLA	O2D-CGD-CBD	5.28	120.47	111.23
11	a	1108	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	a	1130	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	1	1119	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	a	1115	CLA	C2D-C1D-ND	5.28	115.36	110.13
11	A	1132	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	b	1204	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	1	1108	CLA	C2D-C1D-ND	5.28	115.35	110.13
11	b	1236	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
11	1	1126	CLA	C1D-ND-C4D	-5.28	102.61	106.31
11	1	1131	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
11	b	1211	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
11	B	1212	CLA	C1D-ND-C4D	-5.28	102.61	106.31
11	B	1214	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
11	b	1221	CLA	C2C-C1C-NC	5.28	115.53	109.98
11	a	1121	CLA	C4A-NA-C1A	5.28	109.09	106.68
11	2	1221	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
11	A	1111	CLA	C2D-C1D-ND	5.28	115.35	110.13
11	b	1217	CLA	O2A-CGA-O1A	-5.28	110.42	123.63
11	8	1503	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
11	B	1215	CLA	C4A-NA-C1A	5.28	109.09	106.68
11	2	1215	CLA	C4A-NA-C1A	5.28	109.09	106.68
11	A	1122	CLA	C2D-C1D-ND	5.28	115.35	110.13
11	b	1227	CLA	C2D-C1D-ND	5.28	115.35	110.13
11	A	1136	CLA	C2D-C1D-ND	5.27	115.35	110.13
11	2	1226	CLA	C2D-C1D-ND	5.27	115.35	110.13
11	2	1213	CLA	C4A-NA-C1A	5.27	109.08	106.68
11	1	1115	CLA	C3B-C2B-C1B	-5.27	100.95	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	1402	CLA	C2D-C1D-ND	5.27	115.34	110.13
11	K	1401	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	8	1502	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
11	A	1124	CLA	C4A-NA-C1A	5.27	109.08	106.68
11	B	1206	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	1	1135	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	b	1013	CLA	C2C-C1C-NC	5.27	115.52	109.98
11	B	1225	CLA	C4A-NA-C1A	5.27	109.08	106.68
11	2	1236	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	1	1102	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
11	8	1502	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	A	1130	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
11	b	1203	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
11	0	1401	CLA	C2D-C1D-ND	5.27	115.34	110.13
11	A	1115	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	A	1131	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	b	1224	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
11	b	1217	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
11	A	1128	CLA	C1D-ND-C4D	-5.26	102.62	106.31
11	L	1503	CLA	C1D-ND-C4D	-5.26	102.62	106.31
11	a	1140	CLA	O2D-CGD-CBD	5.26	120.43	111.23
11	a	1130	CLA	C3B-C2B-C1B	-5.26	100.96	107.17
11	0	1402	CLA	O2A-CGA-O1A	-5.26	110.46	123.63
11	B	1213	CLA	O2D-CGD-CBD	5.26	120.43	111.23
11	B	1235	CLA	C4A-NA-C1A	5.26	109.08	106.68
11	A	1116	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
11	B	1222	CLA	C2D-C1D-ND	5.26	115.33	110.13
11	a	1134	CLA	C4A-NA-C1A	5.26	109.08	106.68
11	B	1202	CLA	O2D-CGD-CBD	5.26	120.43	111.23
11	1	1012	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
11	2	1228	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
11	L	1501	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
11	B	1238	CLA	O2D-CGD-CBD	5.26	120.42	111.23
11	k	1402	CLA	C2D-C1D-ND	5.26	115.33	110.13
11	A	1137	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
11	B	1202	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
11	2	1238	CLA	O2D-CGD-CBD	5.26	120.42	111.23
11	a	1103	CLA	C1D-ND-C4D	-5.26	102.62	106.31
11	a	1119	CLA	C4A-NA-C1A	5.26	109.08	106.68
11	B	1210	CLA	C2D-C1D-ND	5.26	115.33	110.13
11	1	1140	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
11	b	1225	CLA	C1C-C2C-C3C	-5.26	101.45	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1110	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
11	A	1117	CLA	C2C-C1C-NC	5.25	115.50	109.98
11	B	1203	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
11	A	1112	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
11	b	1210	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
11	l	1501	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
11	a	1117	CLA	C1D-ND-C4D	-5.25	102.63	106.31
11	a	1102	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
11	K	1401	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	1	1115	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
11	A	1022	CLA	C2C-C1C-NC	5.25	115.50	109.98
11	b	1207	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
11	L	1503	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
11	B	1240	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
11	1	1114	CLA	O2D-CGD-CBD	5.25	120.41	111.23
11	1	1112	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	2	1219	CLA	C2C-C1C-NC	5.25	115.50	109.98
11	A	1123	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
11	1	1120	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
11	b	1208	CLA	C1D-ND-C4D	-5.25	102.63	106.31
11	L	1502	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	a	1113	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	b	1207	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	1	1140	CLA	C2D-C1D-ND	5.25	115.32	110.13
11	b	1231	CLA	C3B-C2B-C1B	-5.25	100.99	107.17
11	a	1124	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
11	1	1102	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
11	1	1137	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	b	1222	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
11	L	1501	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	1	1122	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	2	1202	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	2	1214	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	2	1223	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
11	a	1104	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
11	a	1113	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	2	1231	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	a	1122	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
11	1	1131	CLA	C1D-ND-C4D	-5.24	102.64	106.31
14	B	4005	BCR	C24-C23-C22	-5.24	118.48	126.23
11	B	1226	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	a	1140	CLA	C1D-ND-C4D	-5.24	102.64	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1215	CLA	C4-C3-C5	5.24	124.32	115.23
11	2	1227	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	L	1503	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	1	1133	CLA	C1D-ND-C4D	-5.24	102.64	106.31
11	A	1101	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
11	1	1107	CLA	C2D-C1D-ND	5.24	115.31	110.13
11	B	1240	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
11	1	1104	CLA	C3D-C2D-C1D	-5.24	98.69	105.83
11	b	1216	CLA	O2D-CGD-CBD	5.24	120.38	111.23
11	a	1120	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	2	1207	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	A	1129	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	A	1130	CLA	O2D-CGD-CBD	5.23	120.38	111.23
11	a	1137	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	a	1129	CLA	C2D-C1D-ND	5.23	115.30	110.13
11	a	1110	CLA	C4A-NA-C1A	5.23	109.06	106.68
11	2	1219	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	1	1118	CLA	C1D-ND-C4D	-5.23	102.64	106.31
11	A	1103	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
11	A	1105	CLA	C1D-ND-C4D	-5.23	102.64	106.31
11	2	1023	CLA	C1D-ND-C4D	-5.23	102.64	106.31
11	B	1229	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	A	4008	BCR	C15-C14-C13	-5.23	119.95	127.28
11	B	1212	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
11	B	1211	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
11	8	1503	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
11	b	1238	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
11	B	1203	CLA	C2D-C1D-ND	5.23	115.30	110.13
11	8	1503	CLA	O2D-CGD-CBD	5.23	120.36	111.23
11	A	1101	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
11	b	1201	CLA	C1C-C2C-C3C	-5.22	101.48	106.98
11	A	1134	CLA	C1D-ND-C4D	-5.22	102.65	106.31
11	b	1223	CLA	C1D-ND-C4D	-5.22	102.65	106.31
11	a	1119	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	2	1218	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
11	A	1107	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	A	1105	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	a	1801	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	a	1012	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	b	1230	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
11	a	1124	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	1	1120	CLA	C2D-C1D-ND	5.22	115.29	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1232	CLA	O2D-CGD-CBD	5.22	120.35	111.23
11	a	1134	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	A	1117	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
11	b	1214	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
11	a	1126	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
11	k	1401	CLA	C2D-C1D-ND	5.22	115.29	110.13
14	b	4011	BCR	C7-C8-C9	-5.22	118.52	126.23
11	b	1216	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	B	1220	CLA	C4A-NA-C1A	5.22	109.06	106.68
11	b	1240	CLA	C4A-NA-C1A	5.22	109.06	106.68
11	B	1202	CLA	C2C-C1C-NC	5.22	115.46	109.98
11	b	1228	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
11	2	1230	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
11	A	1126	CLA	C2D-C1D-ND	5.22	115.29	110.13
11	b	1203	CLA	C2D-C1D-ND	5.22	115.29	110.13
11	A	1109	CLA	C2D-C1D-ND	5.21	115.29	110.13
11	1	1136	CLA	C2D-C1D-ND	5.21	115.29	110.13
11	1	1113	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
11	b	1229	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
11	b	1204	CLA	C1D-ND-C4D	-5.21	102.65	106.31
11	1	1103	CLA	C1D-ND-C4D	-5.21	102.65	106.31
11	A	1122	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
11	B	1227	CLA	C2D-C1D-ND	5.21	115.28	110.13
11	a	1011	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
11	a	1140	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
11	1	1103	CLA	O2D-CGD-CBD	5.21	120.34	111.23
11	1	1022	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
11	B	1021	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
11	2	1235	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
11	b	1023	CLA	C1D-ND-C4D	-5.21	102.66	106.31
11	2	1223	CLA	C1D-ND-C4D	-5.21	102.66	106.31
11	1	1111	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
11	2	1228	CLA	O2A-CGA-O1A	-5.21	110.60	123.63
11	b	1232	CLA	C4A-NA-C1A	5.21	109.06	106.68
11	A	1124	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
11	a	1111	CLA	C2C-C1C-NC	5.21	115.45	109.98
11	1	1119	CLA	O2D-CGD-CBD	5.20	120.33	111.23
11	L	1501	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
11	1	1101	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
11	A	1132	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
11	a	1111	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
11	B	1214	CLA	C2C-C1C-NC	5.20	115.44	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1101	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
11	a	1011	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
11	a	1105	CLA	O2A-CGA-O1A	-5.20	110.62	123.63
11	a	1112	CLA	C4A-NA-C1A	5.20	109.05	106.68
11	b	1212	CLA	O2D-CGD-CBD	5.20	120.32	111.23
14	1	4003	BCR	C15-C14-C13	-5.20	119.99	127.28
11	1	1138	CLA	C2D-C1D-ND	5.20	115.27	110.13
11	2	1236	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
11	B	1204	CLA	C1D-ND-C4D	-5.20	102.67	106.31
11	a	1126	CLA	C1D-ND-C4D	-5.20	102.67	106.31
11	B	1229	CLA	C4A-NA-C1A	5.20	109.05	106.68
11	1	1108	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
11	A	1113	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
11	a	1117	CLA	C2D-C1D-ND	5.20	115.27	110.13
11	B	1236	CLA	O2D-CGD-CBD	5.20	120.31	111.23
11	B	1221	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
11	1	1127	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
14	6	4013	BCR	C7-C8-C9	-5.19	118.55	126.23
11	2	1013	CLA	C2C-C1C-NC	5.19	115.44	109.98
11	1	1124	CLA	C1D-ND-C4D	-5.19	102.67	106.31
11	b	1212	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
11	2	1204	CLA	C4A-NA-C1A	5.19	109.05	106.68
11	b	1223	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
11	1	1116	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
11	2	1203	CLA	C1D-ND-C4D	-5.19	102.67	106.31
11	1	1120	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
11	A	1133	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
11	A	1128	CLA	C2D-C1D-ND	5.19	115.26	110.13
11	1	1124	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
11	2	1220	CLA	C1D-ND-C4D	-5.19	102.67	106.31
11	a	1109	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
11	1	1123	CLA	C1C-C2C-C3C	-5.19	101.53	106.98
11	B	1235	CLA	C2D-C1D-ND	5.19	115.26	110.13
11	A	1115	CLA	O2D-CGD-CBD	5.18	120.29	111.23
11	b	1202	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
11	1	1801	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	2	1219	CLA	C2D-C1D-ND	5.18	115.26	110.13
11	b	1227	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	a	1109	CLA	C4A-NA-C1A	5.18	109.04	106.68
11	A	1119	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	B	1221	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	1	1111	CLA	O2A-CGA-O1A	-5.18	110.66	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	0	1401	CLA	O2A-CGA-O1A	-5.18	110.66	123.63
11	B	1202	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	A	1116	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	a	1128	CLA	C1D-ND-C4D	-5.18	102.68	106.31
11	B	1212	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	B	1240	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	a	1104	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	l	1503	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
11	A	1115	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	a	1101	CLA	O2D-CGD-CBD	5.18	120.29	111.23
11	0	1402	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	a	1134	CLA	C2D-C1D-ND	5.18	115.25	110.13
11	b	1213	CLA	C2D-C1D-ND	5.18	115.25	110.13
11	K	1401	CLA	O2A-CGA-O1A	-5.18	110.67	123.63
11	A	1127	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	2	1207	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
11	a	1012	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	B	1240	CLA	C2D-C1D-ND	5.18	115.25	110.13
11	2	1230	CLA	C2D-C1D-ND	5.18	115.25	110.13
11	A	1111	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
11	1	1103	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
11	2	1021	CLA	O2A-CGA-CBA	5.18	127.62	111.83
11	b	1205	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
11	A	1011	CLA	O2A-CGA-O1A	-5.18	110.68	123.63
11	b	1240	CLA	O2D-CGD-CBD	5.18	120.28	111.23
11	k	1401	CLA	O2A-CGA-O1A	-5.17	110.68	123.63
11	A	1126	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
11	b	1217	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
11	2	1203	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
11	1	1123	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
11	B	1212	CLA	C4A-NA-C1A	5.17	109.04	106.68
11	b	1214	CLA	C2C-C1C-NC	5.17	115.42	109.98
11	A	1107	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
11	A	1110	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
11	2	1216	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
11	1	1134	CLA	C2D-C1D-ND	5.17	115.24	110.13
11	1	1102	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
11	B	1214	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
11	2	1223	CLA	C2C-C1C-NC	5.17	115.41	109.98
11	b	1231	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
11	a	1109	CLA	C2D-C1D-ND	5.17	115.24	110.13
11	a	1136	CLA	C3D-C2D-C1D	-5.17	98.78	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1121	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
11	2	1225	CLA	C4A-NA-C1A	5.17	109.04	106.68
11	1	1237	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
11	A	1127	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
11	a	1102	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
11	1	1128	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
11	2	1021	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
11	1	1119	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
11	2	1219	CLA	C1D-ND-C4D	-5.17	102.69	106.31
11	1	1113	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
11	A	1022	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
11	A	1118	CLA	O2A-CGA-O1A	-5.16	110.71	123.63
11	B	1227	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
11	b	1021	CLA	O2D-CGD-CBD	5.16	120.26	111.23
11	2	1223	CLA	C4A-NA-C1A	5.16	109.03	106.68
11	2	1235	CLA	O2D-CGD-CBD	5.16	120.26	111.23
11	a	1104	CLA	C2C-C1C-NC	5.16	115.41	109.98
11	a	1140	CLA	C2D-C1D-ND	5.16	115.24	110.13
11	2	1239	CLA	O2D-CGD-CBD	5.16	120.26	111.23
11	a	1128	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
11	B	1217	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	B	1238	CLA	C2D-C1D-ND	5.16	115.23	110.13
11	B	1210	CLA	CAC-C3C-C4C	5.16	131.51	124.79
11	B	1210	CLA	C2C-C1C-NC	5.16	115.40	109.98
11	2	1218	CLA	C2D-C1D-ND	5.16	115.23	110.13
11	A	1130	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	b	1218	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
11	B	1229	CLA	C1D-ND-C4D	-5.16	102.69	106.31
11	k	1402	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
11	1	1011	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	b	1238	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
11	2	1240	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	B	1235	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
11	B	1208	CLA	C2D-C1D-ND	5.16	115.23	110.13
11	a	1112	CLA	C2D-C1D-ND	5.16	115.23	110.13
11	1	1103	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	f	4013	BCR	C15-C14-C13	-5.16	120.05	127.28
11	a	1117	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	0	1401	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	1	1125	CLA	C4A-NA-C1A	5.16	109.03	106.68
11	a	1132	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
11	A	1022	CLA	C1C-C2C-C3C	-5.16	101.56	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	l	1501	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
11	K	1401	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
11	2	1222	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
11	a	1122	CLA	O2D-CGD-CBD	5.15	120.23	111.23
11	1	1134	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
11	a	1123	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
11	A	1127	CLA	C1D-ND-C4D	-5.15	102.70	106.31
11	2	1222	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
14	7	4021	BCR	C33-C5-C6	-5.15	118.87	124.48
11	b	1230	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
11	A	1127	CLA	C2D-C1D-ND	5.15	115.22	110.13
11	A	1139	CLA	C1D-ND-C4D	-5.15	102.70	106.31
11	1	1112	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
11	B	1217	CLA	O2A-CGA-O1A	-5.15	110.76	123.63
11	B	1239	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
11	B	1218	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
11	a	1123	CLA	C4A-NA-C1A	5.14	109.03	106.68
11	1	1135	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
11	A	1120	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	b	1209	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	1	1105	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	B	1221	CLA	C1D-ND-C4D	-5.14	102.70	106.31
11	2	1234	CLA	O2A-CGA-O1A	-5.14	110.76	123.63
11	a	1011	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
11	B	1220	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	a	1132	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	2	1236	CLA	O2A-CGA-O1A	-5.14	110.76	123.63
11	b	1225	CLA	O2D-CGD-CBD	5.14	120.22	111.23
11	B	1205	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
11	b	1235	CLA	C2D-C1D-ND	5.14	115.22	110.13
11	A	1123	CLA	O2D-CGD-CBD	5.14	120.22	111.23
11	A	1117	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	b	1023	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	b	1013	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
11	1	1139	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
11	2	1227	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
11	b	1214	CLA	C4A-NA-C1A	5.14	109.02	106.68
11	1	1122	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
11	k	1401	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
11	1	1127	CLA	O2A-CGA-O1A	-5.14	110.78	123.63
11	A	1140	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
11	1	1126	CLA	C2D-C1D-ND	5.14	115.21	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1126	CLA	C4A-NA-C1A	5.14	109.02	106.68
11	b	1239	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
11	A	1111	CLA	O2A-CGA-O1A	-5.14	110.78	123.63
11	A	1120	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
11	A	1116	CLA	C2C-C1C-NC	5.13	115.38	109.98
11	0	1402	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
11	1	1101	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
11	2	1222	CLA	O2A-CGA-O1A	-5.13	110.79	123.63
11	B	1219	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	B	1021	CLA	C1D-ND-C4D	-5.13	102.71	106.31
11	b	1226	CLA	C4A-NA-C1A	5.13	109.02	106.68
11	K	1402	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	a	1801	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
11	a	1124	CLA	C1D-ND-C4D	-5.13	102.71	106.31
11	l	1503	CLA	C1D-ND-C4D	-5.13	102.71	106.31
11	a	1138	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
11	a	1140	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	A	1109	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	B	1222	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	a	1129	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	b	1238	CLA	O2D-CGD-CBD	5.13	120.19	111.23
11	b	1215	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
11	b	1234	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
11	B	1232	CLA	O2D-CGD-CBD	5.13	120.19	111.23
11	a	1125	CLA	C1D-ND-C4D	-5.13	102.72	106.31
11	1	1126	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
11	B	1208	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
11	A	1125	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
11	b	1240	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
11	a	1112	CLA	C2C-C1C-NC	5.13	115.36	109.98
11	B	1238	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
11	A	1124	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
11	A	1127	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
11	k	1401	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
11	A	1113	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
11	b	1224	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
11	2	1213	CLA	C2D-C1D-ND	5.12	115.20	110.13
11	A	1111	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
11	0	1401	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
11	B	1202	CLA	C2D-C1D-ND	5.12	115.20	110.13
11	A	1022	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
11	a	1107	CLA	C3B-C2B-C1B	-5.12	101.13	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1133	CLA	C4A-NA-C1A	5.12	109.02	106.68
11	A	1138	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
11	l	1503	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
11	a	1119	CLA	O2D-CGD-CBD	5.12	120.18	111.23
11	1	1022	CLA	O2D-CGD-CBD	5.12	120.18	111.23
11	A	1012	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
11	K	1401	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
11	B	1223	CLA	C2D-C1D-ND	5.12	115.19	110.13
11	1	1116	CLA	O2A-CGA-O1A	-5.12	110.82	123.63
11	b	1231	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
11	a	1127	CLA	O2D-CGD-CBD	5.12	120.18	111.23
11	2	1234	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
11	b	1203	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
11	2	1232	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
11	1	1140	CLA	C1D-ND-C4D	-5.12	102.72	106.31
11	2	1229	CLA	C1D-ND-C4D	-5.12	102.72	106.31
11	b	1220	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
11	B	1207	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
11	1	1118	CLA	C2D-C1D-ND	5.12	115.19	110.13
11	b	1234	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
11	1	1132	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
11	b	1210	CLA	O2D-CGD-CBD	5.12	120.17	111.23
11	a	1113	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
11	a	1137	CLA	O2A-CGA-O1A	-5.11	110.83	123.63
11	1	1138	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
11	1	1132	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
11	1	1128	CLA	O2D-CGD-CBD	5.11	120.17	111.23
11	2	1205	CLA	C2D-C1D-ND	5.11	115.19	110.13
11	1	1120	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
11	B	1224	CLA	C1C-C2C-C3C	-5.11	101.60	106.98
11	b	1222	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
11	A	1126	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
11	1	1124	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
11	b	1240	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
11	A	1123	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
11	B	1226	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
11	1	1105	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
11	1	1125	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
11	1	1106	CLA	C2D-C1D-ND	5.11	115.18	110.13
11	1	1115	CLA	C4A-NA-C1A	5.11	109.01	106.68
11	a	1104	CLA	O2A-CGA-O1A	-5.11	110.85	123.63
11	A	1105	CLA	C3D-C2D-C1D	-5.11	98.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1117	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
11	B	1211	CLA	O2D-CGD-CBD	5.11	120.16	111.23
11	B	1217	CLA	C1D-ND-C4D	-5.11	102.73	106.31
11	b	1210	CLA	C2C-C1C-NC	5.11	115.35	109.98
11	a	1012	CLA	O2A-CGA-O1A	-5.11	110.85	123.63
11	A	1128	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
11	A	1114	CLA	C1D-ND-C4D	-5.11	102.73	106.31
11	2	1220	CLA	C2D-C1D-ND	5.11	115.18	110.13
11	2	1217	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
11	1	1106	CLA	O2A-CGA-O1A	-5.11	110.86	123.63
11	L	1502	CLA	C3D-C2D-C1D	-5.10	98.86	105.83
11	b	1218	CLA	C2D-C1D-ND	5.10	115.18	110.13
11	1	1124	CLA	O2A-CGA-O1A	-5.10	110.86	123.63
11	a	1134	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	a	1122	CLA	C2D-C1D-ND	5.10	115.18	110.13
11	1	1112	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
11	1	1110	CLA	C4A-NA-C1A	5.10	109.01	106.68
11	B	1210	CLA	O2A-CGA-O1A	-5.10	110.86	123.63
11	B	1222	CLA	O2A-CGA-O1A	-5.10	110.86	123.63
11	A	1011	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	1	1133	CLA	O2D-CGD-CBD	5.10	120.15	111.23
11	2	1208	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	1	1121	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	a	1107	CLA	C1D-ND-C4D	-5.10	102.73	106.31
11	b	1222	CLA	C2D-C1D-ND	5.10	115.17	110.13
11	1	1119	CLA	C2D-C1D-ND	5.10	115.17	110.13
11	B	1013	CLA	C2C-C1C-NC	5.10	115.34	109.98
11	1	1132	CLA	O2D-CGD-CBD	5.10	120.15	111.23
11	B	1207	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
11	2	1229	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	8	1502	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
11	a	1130	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	b	1238	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	B	1228	CLA	C1D-ND-C4D	-5.10	102.73	106.31
11	b	1218	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	a	1121	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
11	b	1235	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
11	A	1012	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
11	A	1108	CLA	C2D-C1D-ND	5.10	115.17	110.13
11	B	1212	CLA	C2D-C1D-ND	5.10	115.17	110.13
11	B	1013	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
11	2	1240	CLA	C1C-C2C-C3C	-5.10	101.62	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1238	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
11	1	1022	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
11	b	1223	CLA	C2D-C1D-ND	5.10	115.17	110.13
11	B	1201	CLA	C3B-C2B-C1B	-5.09	101.16	107.17
11	A	1022	CLA	C2D-C1D-ND	5.09	115.17	110.13
11	1	1801	CLA	C2D-C1D-ND	5.09	115.17	110.13
11	A	1109	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
11	B	1225	CLA	C1D-ND-C4D	-5.09	102.74	106.31
11	1	1126	CLA	C2C-C1C-NC	5.09	115.33	109.98
11	2	1235	CLA	C2C-C1C-NC	5.09	115.33	109.98
11	l	1502	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
11	B	1239	CLA	C2D-C1D-ND	5.09	115.17	110.13
11	2	1201	CLA	O2D-CGD-CBD	5.09	120.13	111.23
11	2	1203	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
11	b	1225	CLA	C4A-NA-C1A	5.09	109.00	106.68
11	A	1131	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
11	B	1239	CLA	C1D-ND-C4D	-5.09	102.74	106.31
11	1	1101	CLA	C1D-ND-C4D	-5.09	102.74	106.31
11	B	1215	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
11	B	1226	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
11	a	1128	CLA	O2D-CGD-CBD	5.09	120.13	111.23
11	b	1228	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
11	b	1223	CLA	C4A-NA-C1A	5.09	109.00	106.68
11	1	1237	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
11	1	1011	CLA	O2A-CGA-O1A	-5.09	110.90	123.63
11	1	1102	CLA	C2D-C1D-ND	5.09	115.16	110.13
11	A	1125	CLA	CAC-C3C-C4C	5.09	131.41	124.79
14	M	4021	BCR	C33-C5-C6	-5.09	118.93	124.48
11	2	1202	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
11	2	1211	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
11	2	1202	CLA	O2A-CGA-O1A	-5.09	110.91	123.63
11	a	1102	CLA	C2D-C1D-ND	5.09	115.16	110.13
11	A	1108	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
11	2	1203	CLA	C2D-C1D-ND	5.09	115.16	110.13
11	B	1204	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
11	b	1021	CLA	C1D-ND-C4D	-5.09	102.74	106.31
11	B	1235	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
11	a	1127	CLA	O2A-CGA-O1A	-5.08	110.91	123.63
11	2	1210	CLA	C2C-C1C-NC	5.08	115.32	109.98
11	b	1219	CLA	O2A-CGA-O1A	-5.08	110.91	123.63
11	A	1124	CLA	C2D-C1D-ND	5.08	115.16	110.13
11	b	1240	CLA	C3B-C2B-C1B	-5.08	101.18	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1126	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
11	B	1210	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
11	b	1023	CLA	C2D-C1D-ND	5.08	115.16	110.13
11	A	1122	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
11	8	1501	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
11	a	1114	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
11	a	1120	CLA	C1D-ND-C4D	-5.08	102.75	106.31
11	2	1216	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
11	2	1207	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
11	1	1106	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
11	2	1240	CLA	C2D-C1D-ND	5.08	115.15	110.13
11	b	1201	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
11	A	1112	CLA	C2C-C1C-NC	5.08	115.31	109.98
11	B	1214	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
11	2	1219	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
11	b	1203	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
11	2	1204	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
11	a	1101	CLA	C2D-C1D-ND	5.07	115.15	110.13
11	1	1124	CLA	C2D-C1D-ND	5.07	115.15	110.13
11	B	1229	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	2	1213	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	A	1111	CLA	C2C-C1C-NC	5.07	115.31	109.98
11	B	1209	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
11	b	1223	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
11	B	1217	CLA	C2D-C1D-ND	5.07	115.15	110.13
11	a	1124	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
11	a	1012	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
11	b	1236	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
11	2	1215	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	2	1229	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
11	1	1105	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
11	A	1131	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	1	1117	CLA	O2D-CGD-CBD	5.07	120.09	111.23
11	B	1220	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	B	1204	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	B	1213	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	m	4021	BCR	C33-C5-C6	-5.07	118.95	124.48
11	A	1107	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
11	L	1502	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
11	2	1223	CLA	C2D-C1D-ND	5.07	115.14	110.13
11	8	1501	CLA	C2D-C1D-ND	5.07	115.14	110.13
11	2	1220	CLA	C3D-C2D-C1D	-5.07	98.91	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1127	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
11	A	1140	CLA	C2D-C1D-ND	5.07	115.14	110.13
11	a	1112	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
11	B	1202	CLA	C4A-NA-C1A	5.07	108.99	106.68
11	1	1135	CLA	C1D-ND-C4D	-5.07	102.76	106.31
11	a	1124	CLA	C2D-C1D-ND	5.07	115.14	110.13
11	a	1109	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
11	2	1228	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
11	1	1117	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
11	2	1229	CLA	C2D-C1D-ND	5.06	115.14	110.13
11	b	1204	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
11	b	1222	CLA	C1D-ND-C4D	-5.06	102.76	106.31
11	A	1134	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
11	1	1129	CLA	C2D-C1D-ND	5.06	115.14	110.13
14	b	4006	BCR	C7-C8-C9	-5.06	118.75	126.23
11	a	1110	CLA	C1D-ND-C4D	-5.06	102.76	106.31
11	2	1232	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
11	B	1212	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
11	2	1204	CLA	C1D-ND-C4D	-5.06	102.76	106.31
11	2	1232	CLA	C1D-ND-C4D	-5.06	102.76	106.31
11	2	1023	CLA	O2D-CGD-CBD	5.06	120.08	111.23
11	a	1106	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
11	1	1110	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
14	6	4020	BCR	C24-C23-C22	-5.06	118.75	126.23
11	B	1202	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
11	b	1217	CLA	C1D-ND-C4D	-5.06	102.76	106.31
11	B	1219	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
11	b	1205	CLA	C2D-C1D-ND	5.06	115.13	110.13
11	A	1139	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
14	M	4021	BCR	C7-C8-C9	-5.06	118.75	126.23
11	2	1209	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
11	1	1131	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
11	A	1136	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
11	a	1123	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
11	l	1503	CLA	C2D-C1D-ND	5.06	115.13	110.13
11	A	1011	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
11	k	1402	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	7	4021	BCR	C38-C26-C25	-5.05	118.97	124.48
11	A	1139	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
11	A	1104	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
11	B	1225	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
14	2	4014	BCR	C15-C14-C13	-5.05	120.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1011	CLA	C1D-ND-C4D	-5.05	102.77	106.31
11	a	1022	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
11	b	1204	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
11	1	1128	CLA	C1D-ND-C4D	-5.05	102.77	106.31
11	B	1234	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
11	1	1801	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
11	1	1101	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
11	B	1228	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
11	2	1213	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
11	a	1116	CLA	C4A-NA-C1A	5.05	108.98	106.68
11	1	1103	CLA	C2D-C1D-ND	5.05	115.12	110.13
11	2	1023	CLA	C2D-C1D-ND	5.05	115.12	110.13
11	2	1232	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
11	B	1223	CLA	C1D-ND-C4D	-5.05	102.77	106.31
11	2	1240	CLA	C1D-ND-C4D	-5.05	102.77	106.31
11	A	1125	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
11	1	1237	CLA	C2D-C1D-ND	5.05	115.12	110.13
11	A	1110	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
11	B	1224	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
11	A	1237	CLA	C2D-C1D-ND	5.05	115.12	110.13
11	a	1108	CLA	C2D-C1D-ND	5.05	115.12	110.13
11	a	1022	CLA	C4A-NA-C1A	5.05	108.98	106.68
11	b	1211	CLA	C2D-C1D-ND	5.04	115.12	110.13
11	2	1021	CLA	O2D-CGD-CBD	5.04	120.05	111.23
11	A	1122	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
11	A	1108	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
11	A	1128	CLA	O2D-CGD-CBD	5.04	120.05	111.23
11	2	1217	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
11	k	1402	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
11	b	1205	CLA	C1D-ND-C4D	-5.04	102.77	106.31
11	2	1201	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
11	2	1206	CLA	O2D-CGD-CBD	5.04	120.04	111.23
11	B	1219	CLA	O2A-CGA-O1A	-5.04	111.02	123.63
11	a	1123	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
11	a	1131	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
11	b	1238	CLA	C2D-C1D-ND	5.04	115.11	110.13
11	b	1023	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
11	a	1137	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
11	b	1228	CLA	O2A-CGA-O1A	-5.04	111.02	123.63
11	2	1226	CLA	O2A-CGA-O1A	-5.04	111.02	123.63
11	A	1122	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
11	a	1101	CLA	C3B-C2B-C1B	-5.04	101.23	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1240	CLA	C2D-C1D-ND	5.04	115.11	110.13
11	B	1228	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
11	2	1224	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
11	1	1109	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
11	A	1114	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
11	a	1133	CLA	C2D-C1D-ND	5.04	115.11	110.13
11	b	1207	CLA	C1D-ND-C4D	-5.03	102.78	106.31
11	8	1503	CLA	C1D-ND-C4D	-5.03	102.78	106.31
11	l	1503	CLA	O2A-CGA-O1A	-5.03	111.04	123.63
11	2	1238	CLA	C2D-C1D-ND	5.03	115.11	110.13
11	1	1114	CLA	C1D-ND-C4D	-5.03	102.78	106.31
11	a	1101	CLA	O2A-CGA-O1A	-5.03	111.04	123.63
11	a	1108	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
11	B	1218	CLA	C2D-C1D-ND	5.03	115.11	110.13
11	A	1108	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
11	A	1107	CLA	O2D-CGD-CBD	5.03	120.03	111.23
11	A	1129	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
11	A	1123	CLA	C1D-ND-C4D	-5.03	102.78	106.31
11	a	1103	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
14	2	4014	BCR	C7-C8-C9	-5.03	118.80	126.23
11	B	1228	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
11	1	1122	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	B	4004	BCR	C7-C8-C9	-5.03	118.80	126.23
11	A	1139	CLA	C2D-C1D-ND	5.03	115.10	110.13
11	a	1132	CLA	C2D-C1D-ND	5.03	115.10	110.13
11	b	1013	CLA	C1D-ND-C4D	-5.03	102.78	106.31
11	b	1228	CLA	C1D-ND-C4D	-5.03	102.79	106.31
11	a	1022	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
11	A	1106	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
11	2	1223	CLA	O2A-CGA-O1A	-5.02	111.06	123.63
11	2	1204	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
11	a	1101	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	a	1119	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	2	1222	CLA	C2D-C1D-ND	5.02	115.10	110.13
11	2	1239	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
16	B	5002	LMG	O7-C10-C11	5.02	122.35	111.48
11	B	1223	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
11	a	1116	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
11	2	1230	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	A	1109	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
11	A	1140	CLA	O2A-CGA-O1A	-5.02	111.06	123.63
11	A	1124	CLA	O2D-CGD-CBD	5.02	120.01	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1219	CLA	C2D-C1D-ND	5.02	115.10	110.13
11	b	1223	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
11	b	1203	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	B	1205	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
11	A	1124	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
11	A	1140	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	K	1402	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
11	8	1503	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	2	1229	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
11	A	1132	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	A	1801	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	a	1118	CLA	C2D-C1D-ND	5.02	115.09	110.13
11	a	1115	CLA	C2C-C1C-NC	5.02	115.25	109.98
11	a	1116	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	1	1139	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	b	1210	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
11	A	1121	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	b	1202	CLA	O2A-CGA-O1A	-5.02	111.08	123.63
11	a	1133	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
11	B	1021	CLA	C2D-C1D-ND	5.02	115.09	110.13
11	1	1136	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
11	a	1115	CLA	O2D-CGD-CBD	5.02	120.00	111.23
11	2	1222	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	2	1230	CLA	C1D-ND-C4D	-5.02	102.79	106.31
11	B	1023	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
11	A	1105	CLA	C2D-C1D-ND	5.01	115.09	110.13
11	b	1226	CLA	C2D-C1D-ND	5.01	115.09	110.13
11	A	1127	CLA	C4A-NA-C1A	5.01	108.97	106.68
11	B	1205	CLA	C1D-ND-C4D	-5.01	102.80	106.31
11	1	1107	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
11	a	1117	CLA	O2D-CGD-CBD	5.01	119.99	111.23
11	B	1230	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
11	a	1105	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
11	2	1211	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
11	a	1138	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
11	B	1229	CLA	C2D-C1D-ND	5.01	115.08	110.13
11	a	1106	CLA	C2D-C1D-ND	5.01	115.08	110.13
11	1	1139	CLA	C4A-NA-C1A	5.01	108.96	106.68
11	B	1209	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
11	A	1022	CLA	C1D-ND-C4D	-5.01	102.80	106.31
11	2	1215	CLA	C1D-ND-C4D	-5.01	102.80	106.31
11	8	1501	CLA	C1D-ND-C4D	-5.01	102.80	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1116	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
11	a	1801	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
11	a	1116	CLA	C2D-C1D-ND	5.01	115.08	110.13
11	b	1236	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
11	1	1130	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
11	b	1217	CLA	O2D-CGD-CBD	5.01	119.98	111.23
11	2	1214	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
11	a	1105	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	2	1228	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	b	1217	CLA	C2D-C1D-ND	5.00	115.08	110.13
11	L	1503	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
11	1	1108	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
11	A	1103	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
11	B	1231	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
11	1	1131	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
11	b	1231	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	b	1239	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	b	1234	CLA	C2D-C1D-ND	5.00	115.08	110.13
11	1	1117	CLA	O2A-CGA-O1A	-5.00	111.12	123.63
11	1	1139	CLA	O2D-CGD-CBD	5.00	119.97	111.23
11	B	1240	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	1	1117	CLA	C1D-ND-C4D	-5.00	102.80	106.31
11	2	1202	CLA	C2D-C1D-ND	5.00	115.07	110.13
11	2	1215	CLA	C2D-C1D-ND	5.00	115.07	110.13
11	b	1220	CLA	O2D-CGD-CBD	5.00	119.97	111.23
14	6	4018	BCR	C7-C8-C9	-5.00	118.84	126.23
11	B	1236	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
11	2	1218	CLA	C2C-C1C-NC	5.00	115.23	109.98
11	1	1116	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
11	B	1201	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
11	1	1109	CLA	C2D-C1D-ND	5.00	115.07	110.13
11	2	1228	CLA	C2D-C1D-ND	5.00	115.07	110.13
11	2	1231	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
11	2	1212	CLA	O2D-CGD-CBD	5.00	119.96	111.23
11	b	1228	CLA	C2D-C1D-ND	5.00	115.07	110.13
11	b	1211	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
11	1	1138	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
11	2	1013	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
11	1	1105	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
11	L	1503	CLA	O2A-CGA-O1A	-4.99	111.14	123.63
14	1	4007	BCR	C24-C23-C22	-4.99	118.85	126.23
11	B	1207	CLA	O2A-CGA-CBA	4.99	127.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1219	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
11	A	1121	CLA	C1D-ND-C4D	-4.99	102.81	106.31
11	1	1022	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
11	b	1201	CLA	C2D-C1D-ND	4.99	115.06	110.13
11	B	1219	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
11	a	1105	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
11	a	1022	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
11	2	1231	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
11	B	1013	CLA	C2D-C1D-ND	4.99	115.06	110.13
14	B	4004	BCR	C33-C5-C6	-4.99	119.04	124.48
11	a	1106	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
11	A	1132	CLA	C1D-ND-C4D	-4.99	102.81	106.31
11	B	1217	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
11	b	1232	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
11	A	1130	CLA	C1D-ND-C4D	-4.98	102.81	106.31
11	b	1232	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
11	1	1140	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
11	A	1102	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
11	1	1114	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
11	b	1239	CLA	C2D-C1D-ND	4.98	115.06	110.13
11	a	1126	CLA	C2C-C1C-NC	4.98	115.21	109.98
11	1	1116	CLA	C2D-C1D-ND	4.98	115.06	110.13
11	1	1131	CLA	C2D-C1D-ND	4.98	115.06	110.13
11	L	1501	CLA	C1D-ND-C4D	-4.98	102.82	106.31
11	B	1232	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
11	2	1220	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
11	K	1402	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
11	2	1202	CLA	C4A-NA-C1A	4.98	108.95	106.68
11	2	1232	CLA	C4A-NA-C1A	4.98	108.95	106.68
11	a	1132	CLA	C1D-ND-C4D	-4.98	102.82	106.31
11	B	1021	CLA	O2A-CGA-CBA	4.98	127.01	111.83
11	a	1139	CLA	O2A-CGA-O1A	-4.98	111.18	123.63
11	A	1130	CLA	C2D-C1D-ND	4.97	115.05	110.13
11	1	1105	CLA	C2D-C1D-ND	4.97	115.05	110.13
11	1	1120	CLA	C1D-ND-C4D	-4.97	102.82	106.31
11	1	1121	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
11	A	1128	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
11	B	1216	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
11	A	1120	CLA	C1D-ND-C4D	-4.97	102.82	106.31
11	B	1204	CLA	C2D-C1D-ND	4.97	115.05	110.13
11	a	1103	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
11	2	1210	CLA	O2A-CGA-O1A	-4.97	111.19	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1204	CLA	C2D-C1D-ND	4.97	115.05	110.13
14	a	4002	BCR	C7-C8-C9	-4.97	118.88	126.23
11	A	1105	CLA	O2D-CGD-CBD	4.97	119.92	111.23
11	2	1212	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
11	b	1219	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
11	b	1021	CLA	C2D-C1D-ND	4.97	115.04	110.13
11	1	1129	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
11	A	1120	CLA	O2D-CGD-CBD	4.97	119.91	111.23
11	B	1215	CLA	O2A-CGA-O1A	-4.97	111.21	123.63
11	A	1115	CLA	C3B-C2B-C1B	-4.97	101.32	107.17
11	B	1013	CLA	C1D-ND-C4D	-4.97	102.83	106.31
11	a	1237	CLA	O2A-CGA-O1A	-4.97	111.21	123.63
11	B	1209	CLA	C1D-ND-C4D	-4.96	102.83	106.31
11	A	1138	CLA	C2D-C1D-ND	4.96	115.04	110.13
11	B	1239	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
11	B	1236	CLA	O2A-CGA-O1A	-4.96	111.21	123.63
11	1	1127	CLA	C2D-C1D-ND	4.96	115.04	110.13
11	1	1012	CLA	C1D-ND-C4D	-4.96	102.83	106.31
11	B	1206	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
11	a	1111	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
11	a	1140	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
11	A	1117	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
11	a	1135	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
11	2	1013	CLA	C1D-ND-C4D	-4.96	102.83	106.31
11	A	1117	CLA	O2D-CGD-CBD	4.96	119.90	111.23
11	b	1215	CLA	C4A-NA-C1A	4.96	108.94	106.68
11	2	1203	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
11	A	1131	CLA	C2D-C1D-ND	4.96	115.03	110.13
11	A	1113	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
11	b	1221	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
11	a	1110	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
11	b	1215	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
11	b	1230	CLA	C1C-C2C-C3C	-4.96	101.77	106.98
11	2	1234	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
11	2	1226	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
11	B	1218	CLA	C1C-C2C-C3C	-4.96	101.77	106.98
11	a	1119	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
11	l	1501	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
11	a	1116	CLA	O2A-CGA-O1A	-4.95	111.23	123.63
11	A	1237	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
11	1	1104	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
11	A	1119	CLA	C1D-ND-C4D	-4.95	102.84	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	1402	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
11	b	1230	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
11	A	1104	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
11	2	1217	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
11	a	1115	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
11	B	1230	CLA	C2D-C1D-ND	4.95	115.03	110.13
11	b	1230	CLA	C2D-C1D-ND	4.95	115.03	110.13
11	B	1234	CLA	C1D-ND-C4D	-4.95	102.84	106.31
11	b	1220	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
11	a	1125	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
11	A	1138	CLA	O2D-CGD-CBD	4.95	119.88	111.23
11	b	1207	CLA	O2A-CGA-CBA	4.95	126.92	111.83
11	1	1115	CLA	C2D-C1D-ND	4.95	115.02	110.13
11	2	1204	CLA	C2D-C1D-ND	4.95	115.02	110.13
11	a	1102	CLA	C1D-ND-C4D	-4.95	102.84	106.31
11	b	1232	CLA	C1D-ND-C4D	-4.95	102.84	106.31
11	B	1215	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
11	A	1134	CLA	C2D-C1D-ND	4.95	115.02	110.13
11	b	1209	CLA	C2D-C1D-ND	4.95	115.02	110.13
11	8	1503	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
11	B	1216	CLA	O2D-CGD-CBD	4.94	119.87	111.23
11	0	1401	CLA	O2D-CGD-CBD	4.94	119.87	111.23
11	1	1138	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
11	B	1210	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
11	2	1228	CLA	O2D-CGD-CBD	4.94	119.87	111.23
11	B	1219	CLA	C1D-ND-C4D	-4.94	102.85	106.31
11	2	1209	CLA	C1D-ND-C4D	-4.94	102.85	106.31
11	a	1122	CLA	C1C-C2C-C3C	-4.94	101.79	106.98
11	A	1135	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
11	2	1212	CLA	C2D-C1D-ND	4.94	115.01	110.13
11	b	1224	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
11	1	1127	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
11	B	1231	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
11	a	1111	CLA	O2D-CGD-CBD	4.94	119.86	111.23
11	1	1122	CLA	O2A-CGA-O1A	-4.93	111.28	123.63
11	b	1221	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
11	a	1120	CLA	C3B-C2B-C1B	-4.93	101.35	107.17
11	b	1213	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	a	1128	CLA	C2D-C1D-ND	4.93	115.01	110.13
11	1	1101	CLA	C2D-C1D-ND	4.93	115.01	110.13
11	a	1237	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	B	1216	CLA	C3D-C2D-C1D	-4.93	99.10	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1013	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
11	b	1209	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	a	1131	CLA	C1D-ND-C4D	-4.93	102.85	106.31
11	B	1013	CLA	O2D-CGD-CBD	4.93	119.85	111.23
11	A	1117	CLA	O2A-CGA-O1A	-4.93	111.29	123.63
11	A	1114	CLA	C2D-C1D-ND	4.93	115.01	110.13
11	1	1118	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
11	b	1226	CLA	O2A-CGA-O1A	-4.93	111.29	123.63
11	2	1220	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
11	2	1225	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	1	1139	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	K	1401	CLA	O2D-CGD-CBD	4.93	119.85	111.23
11	A	1121	CLA	C4A-NA-C1A	4.93	108.93	106.68
11	b	1201	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
11	a	1127	CLA	C1D-ND-C4D	-4.93	102.85	106.31
11	1	1801	CLA	C1D-ND-C4D	-4.93	102.85	106.31
11	b	1210	CLA	O2A-CGA-O1A	-4.93	111.30	123.63
11	b	1202	CLA	C2C-C1C-NC	4.93	115.16	109.98
11	b	1219	CLA	C2D-C1D-ND	4.93	115.00	110.13
11	1	1117	CLA	C2D-C1D-ND	4.93	115.00	110.13
11	1	1132	CLA	C2D-C1D-ND	4.93	115.00	110.13
11	2	1236	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
11	2	1214	CLA	C2D-C1D-ND	4.93	115.00	110.13
14	b	4004	BCR	C7-C8-C9	-4.93	118.95	126.23
14	A	4002	BCR	C33-C5-C6	-4.93	119.11	124.48
11	2	1207	CLA	O2D-CGD-CBD	4.93	119.84	111.23
11	k	1401	CLA	O2D-CGD-CBD	4.93	119.84	111.23
11	2	1214	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
11	2	1227	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
11	2	1213	CLA	O2A-CGA-O1A	-4.92	111.31	123.63
14	2	4004	BCR	C33-C5-C6	-4.92	119.11	124.48
11	A	1126	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
11	a	1131	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
11	1	1126	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
11	A	1022	CLA	C4A-NA-C1A	4.92	108.92	106.68
11	a	1113	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
11	B	1209	CLA	C2D-C1D-ND	4.92	115.00	110.13
11	a	1115	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
11	b	1217	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
11	8	1501	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
11	1	1123	CLA	C2D-C1D-ND	4.92	115.00	110.13
11	B	1229	CLA	O2D-CGD-CBD	4.92	119.83	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1126	CLA	C4-C3-C5	4.92	123.76	115.23
11	A	1120	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
11	2	1221	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
11	2	1239	CLA	C1D-ND-C4D	-4.92	102.86	106.31
11	a	1103	CLA	C2D-C1D-ND	4.92	114.99	110.13
11	a	1114	CLA	C2D-C1D-ND	4.92	114.99	110.13
11	2	1023	CLA	C1C-C2C-C3C	-4.92	101.81	106.98
11	2	1207	CLA	O2A-CGA-CBA	4.92	126.82	111.83
11	A	1012	CLA	C1D-ND-C4D	-4.92	102.86	106.31
11	B	1230	CLA	C3B-C2B-C1B	-4.92	101.38	107.17
14	A	4008	BCR	C24-C23-C22	-4.92	118.96	126.23
14	b	4014	BCR	C7-C8-C9	-4.91	118.96	126.23
11	B	1228	CLA	O2A-CGA-O1A	-4.91	111.33	123.63
11	2	1225	CLA	C1D-ND-C4D	-4.91	102.86	106.31
11	b	1208	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	a	1122	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	a	1126	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	2	1206	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	b	1231	CLA	C2D-C1D-ND	4.91	114.99	110.13
11	1	1136	CLA	C1C-C2C-C3C	-4.91	101.81	106.98
11	A	1140	CLA	C1C-C2C-C3C	-4.91	101.81	106.98
11	1	1101	CLA	O2A-CGA-O1A	-4.91	111.34	123.63
11	A	1124	CLA	C1D-ND-C4D	-4.91	102.87	106.31
11	B	1203	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	B	1218	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	a	1122	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	1	1801	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	1	1118	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	a	1801	CLA	C4A-NA-C1A	4.91	108.92	106.68
11	a	1138	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
11	2	1229	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
14	2	4006	BCR	C1-C6-C5	-4.91	115.93	122.64
11	2	1013	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
11	A	1101	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
11	A	1117	CLA	C1D-ND-C4D	-4.91	102.87	106.31
11	1	1130	CLA	C1D-ND-C4D	-4.91	102.87	106.31
11	1	1135	CLA	C4-C3-C5	4.91	121.91	116.13
11	1	1121	CLA	C2D-C1D-ND	4.91	114.98	110.13
11	b	1211	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	2	1201	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
11	A	1110	CLA	C2D-C1D-ND	4.91	114.98	110.13
11	A	1138	CLA	C3B-C2B-C1B	-4.91	101.39	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4010	BCR	C33-C5-C6	-4.90	119.13	124.48
11	A	1116	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
11	2	1209	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
11	1	1122	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
11	1	1121	CLA	C1D-ND-C4D	-4.90	102.87	106.31
11	a	1128	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
11	a	1118	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
11	B	1235	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
11	8	1503	CLA	C2D-C1D-ND	4.90	114.97	110.13
11	b	1216	CLA	C4A-NA-C1A	4.90	108.91	106.68
11	2	1208	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
11	B	1228	CLA	C2D-C1D-ND	4.90	114.97	110.13
11	a	1801	CLA	C1D-ND-C4D	-4.90	102.88	106.31
11	2	1023	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
14	A	4008	BCR	C33-C5-C6	-4.90	119.14	124.48
11	b	1013	CLA	C2D-C1D-ND	4.90	114.97	110.13
11	1	1109	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
11	b	1234	CLA	O2D-CGD-CBD	4.89	119.78	111.23
11	2	1013	CLA	C2D-C1D-ND	4.89	114.97	110.13
11	b	1202	CLA	C1C-C2C-C3C	-4.89	101.84	106.98
11	1	1127	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
14	a	4007	BCR	C33-C5-C6	-4.89	119.15	124.48
11	2	1238	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
11	b	1013	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
11	2	1225	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
11	b	1226	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
11	B	1221	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
11	a	1124	CLA	C4A-NA-C1A	4.88	108.91	106.68
11	B	1234	CLA	C2D-C1D-ND	4.88	114.96	110.13
11	2	1021	CLA	O2A-CGA-O1A	-4.88	111.41	123.63
11	B	1201	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
11	b	1215	CLA	C4-C3-C5	4.88	123.70	115.23
11	1	1012	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
11	a	1118	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
11	a	1129	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
11	B	1023	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
11	b	1209	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
11	A	1119	CLA	C4A-NA-C1A	4.88	108.90	106.68
11	B	1216	CLA	C4A-NA-C1A	4.88	108.90	106.68
11	A	1237	CLA	O2A-CGA-O1A	-4.87	111.44	123.63
11	a	1121	CLA	O2D-CGD-CBD	4.87	119.75	111.23
11	b	1225	CLA	C3B-C2B-C1B	-4.87	101.43	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1114	CLA	C1D-ND-C4D	-4.87	102.89	106.31
11	b	1206	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
11	B	1223	CLA	O2A-CGA-O1A	-4.87	111.45	123.63
11	b	1225	CLA	C1D-ND-C4D	-4.87	102.89	106.31
11	A	1132	CLA	C2D-C1D-ND	4.87	114.94	110.13
11	A	1106	CLA	O2A-CGA-O1A	-4.87	111.45	123.63
14	A	4002	BCR	C24-C23-C22	-4.87	119.03	126.23
11	2	1228	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
11	B	1208	CLA	O2D-CGD-CBD	4.87	119.74	111.23
11	a	1111	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
11	B	1213	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
11	A	1103	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
11	a	1110	CLA	C2D-C1D-ND	4.87	114.94	110.13
11	b	1208	CLA	C2D-C1D-ND	4.87	114.94	110.13
11	b	1213	CLA	O2A-CGA-O1A	-4.87	111.46	123.63
11	1	1133	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
11	b	1213	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	B	1222	CLA	C1D-ND-C4D	-4.86	102.90	106.31
11	2	1216	CLA	C1D-ND-C4D	-4.86	102.90	106.31
11	a	1113	CLA	O2D-CGD-CBD	4.86	119.73	111.23
11	a	1112	CLA	C1C-C2C-C3C	-4.86	101.87	106.98
11	l	1502	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	2	1239	CLA	C2D-C1D-ND	4.86	114.94	110.13
11	b	1205	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
16	2	5002	LMG	O7-C10-C11	4.86	122.00	111.48
11	b	1227	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	1	1119	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
14	F	4020	BCR	C33-C5-C6	-4.86	119.18	124.48
11	1	1113	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	2	1201	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
11	2	1217	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
11	2	1212	CLA	C1D-ND-C4D	-4.86	102.90	106.31
11	B	1206	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	A	1022	CLA	O2A-CGA-O1A	-4.86	111.48	123.63
11	2	1239	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
11	1	1112	CLA	C3B-C2B-C1B	-4.86	101.45	107.17
11	2	1201	CLA	C3B-C2B-C1B	-4.86	101.45	107.17
11	A	1123	CLA	C2D-C1D-ND	4.85	114.93	110.13
11	1	1115	CLA	C1D-ND-C4D	-4.85	102.91	106.31
11	A	1125	CLA	O2A-CGA-O1A	-4.85	111.49	123.63
11	A	1801	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
11	1	1012	CLA	O2A-CGA-CBA	4.85	126.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1139	CLA	O2D-CGD-CBD	4.85	119.71	111.23
14	A	4008	BCR	C7-C8-C9	-4.85	119.06	126.23
11	A	1125	CLA	C4A-NA-C1A	4.85	108.89	106.68
11	b	1238	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	F	4018	BCR	C7-C8-C9	-4.85	119.06	126.23
11	B	1215	CLA	C1D-ND-C4D	-4.85	102.91	106.31
11	1	1110	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
11	2	1223	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
11	2	1206	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
11	2	1209	CLA	O2D-CGD-CBD	4.84	119.70	111.23
11	2	1209	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
11	B	1215	CLA	C2D-C1D-ND	4.84	114.92	110.13
11	A	1120	CLA	C4A-NA-C1A	4.84	108.89	106.68
11	A	1133	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
11	B	1221	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
11	2	1232	CLA	C2D-C1D-ND	4.84	114.92	110.13
14	b	4010	BCR	C7-C8-C9	-4.84	119.07	126.23
11	1	1117	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
11	A	1237	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
11	2	1205	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
11	A	1119	CLA	C2D-C1D-ND	4.84	114.91	110.13
11	B	1238	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
11	1	1134	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
11	b	1232	CLA	C2D-C1D-ND	4.83	114.91	110.13
11	2	1234	CLA	C2D-C1D-ND	4.83	114.91	110.13
11	1	1138	CLA	O2D-CGD-CBD	4.83	119.68	111.23
11	a	1106	CLA	C1D-ND-C4D	-4.83	102.92	106.31
11	b	1234	CLA	C1D-ND-C4D	-4.83	102.92	106.31
11	b	1207	CLA	O2D-CGD-CBD	4.83	119.67	111.23
11	A	1135	CLA	C1D-ND-C4D	-4.83	102.92	106.31
11	2	1212	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
11	a	1131	CLA	C2D-C1D-ND	4.83	114.91	110.13
11	b	1216	CLA	C2D-C1D-ND	4.83	114.90	110.13
11	a	1106	CLA	O2A-CGA-O1A	-4.83	111.56	123.63
14	1	4003	BCR	C37-C22-C21	-4.83	115.00	122.82
11	B	1201	CLA	C1D-ND-C4D	-4.83	102.93	106.31
11	A	1011	CLA	C2D-C1D-ND	4.82	114.90	110.13
11	a	1117	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
11	a	1135	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
11	A	1117	CLA	C2D-C1D-ND	4.82	114.90	110.13
11	A	1103	CLA	C2C-C1C-NC	4.82	115.05	109.98
11	a	1116	CLA	C3B-C2B-C1B	-4.82	101.48	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1136	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
11	2	1217	CLA	C2D-C1D-ND	4.82	114.90	110.13
11	b	1212	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
11	b	1207	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
11	B	1217	CLA	O2D-CGD-CBD	4.82	119.66	111.23
11	a	1135	CLA	C1D-ND-C4D	-4.82	102.93	106.31
11	b	1021	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
11	b	1215	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
11	a	1121	CLA	C2D-C1D-ND	4.82	114.89	110.13
11	2	1021	CLA	C2D-C1D-ND	4.82	114.89	110.13
11	1	1132	CLA	C1D-ND-C4D	-4.82	102.93	106.31
14	f	4020	BCR	C7-C8-C9	-4.82	119.11	126.23
11	b	1214	CLA	C3B-C2B-C1B	-4.81	101.49	107.17
11	1	1118	CLA	O2A-CGA-O1A	-4.81	111.58	123.63
11	2	1230	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
11	A	1118	CLA	C2D-C1D-ND	4.81	114.89	110.13
11	a	1105	CLA	C2D-C1D-ND	4.81	114.89	110.13
11	1	1114	CLA	C2D-C1D-ND	4.81	114.89	110.13
11	B	1232	CLA	C1D-ND-C4D	-4.81	102.94	106.31
11	1	1110	CLA	C2D-C1D-ND	4.81	114.89	110.13
11	B	1230	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
11	a	1114	CLA	O2D-CGD-CBD	4.81	119.64	111.23
11	a	1108	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
11	B	1220	CLA	C1D-ND-C4D	-4.81	102.94	106.31
14	b	4010	BCR	C38-C26-C25	-4.81	119.24	124.48
11	A	1139	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
11	a	1801	CLA	C2D-C1D-ND	4.81	114.89	110.13
11	A	1112	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
11	a	1107	CLA	O2D-CGD-CBD	4.81	119.64	111.23
11	1	1140	CLA	O2D-CGD-CBD	4.81	119.64	111.23
11	1	1126	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
11	a	1118	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
11	a	1103	CLA	O2D-CGD-CBD	4.80	119.63	111.23
11	B	1021	CLA	C3D-C2D-C1D	-4.80	99.27	105.83
14	f	4018	BCR	C7-C8-C9	-4.80	119.13	126.23
11	1	1133	CLA	C2D-C1D-ND	4.80	114.88	110.13
14	F	4013	BCR	C24-C23-C22	-4.80	119.13	126.23
11	A	1105	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
11	B	1213	CLA	O2A-CGA-O1A	-4.80	111.62	123.63
14	b	4009	BCR	C19-C18-C17	4.80	126.56	119.01
11	b	1240	CLA	O2A-CGA-O1A	-4.80	110.99	123.33
11	A	1105	CLA	O2A-CGA-O1A	-4.80	111.62	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1119	CLA	O2D-CGD-CBD	4.80	119.62	111.23
11	b	1216	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
11	2	1215	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
11	a	1103	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
11	a	1126	CLA	C1C-C2C-C3C	-4.80	101.94	106.98
11	b	1228	CLA	C3B-C2B-C1B	-4.80	101.52	107.17
11	a	1126	CLA	O2A-CGA-O1A	-4.79	111.63	123.63
11	B	1013	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
11	A	1102	CLA	C2D-C1D-ND	4.79	114.87	110.13
11	1	1130	CLA	C2D-C1D-ND	4.79	114.87	110.13
11	B	1214	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
11	2	1235	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
11	B	1220	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	1	4007	BCR	C33-C5-C6	-4.79	119.25	124.48
11	A	1022	CLA	O2D-CGD-CBD	4.79	119.61	111.23
11	a	1131	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
11	b	1220	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
11	1	1139	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
11	B	1210	CLA	O2D-CGD-CBD	4.79	119.60	111.23
11	1	1128	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
11	2	1216	CLA	C2D-C1D-ND	4.79	114.87	110.13
11	1	1126	CLA	C4-C3-C5	4.79	123.54	115.23
14	a	4002	BCR	C33-C5-C6	-4.79	119.26	124.48
11	a	1112	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
11	L	1501	CLA	O2D-CGD-CBD	4.79	119.60	111.23
11	a	1011	CLA	O2A-CGA-CBA	4.79	126.43	111.83
11	B	1230	CLA	C1D-ND-C4D	-4.79	102.95	106.31
11	2	1240	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
11	A	1128	CLA	O2A-CGA-O1A	-4.79	111.66	123.63
11	A	1126	CLA	C2C-C1C-NC	4.79	115.01	109.98
11	a	1110	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
11	B	1222	CLA	C4-C3-C5	4.78	123.53	115.23
11	A	1125	CLA	C2D-C1D-ND	4.78	114.86	110.13
11	B	1234	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
11	a	1130	CLA	C2D-C1D-ND	4.78	114.86	110.13
11	B	1216	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
11	a	1108	CLA	O2A-CGA-O1A	-4.78	111.04	123.33
11	B	1013	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
11	a	1121	CLA	C1D-ND-C4D	-4.78	102.96	106.31
11	1	1128	CLA	C2D-C1D-ND	4.78	114.86	110.13
11	a	1110	CLA	O2A-CGA-O1A	-4.78	111.67	123.63
11	a	1011	CLA	C2D-C1D-ND	4.78	114.86	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1131	CLA	C1D-ND-C4D	-4.78	102.96	106.31
11	0	1402	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
11	b	1215	CLA	C2D-C1D-ND	4.78	114.85	110.13
11	A	1132	CLA	O2A-CGA-O1A	-4.78	111.68	123.63
11	b	1239	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
11	B	1209	CLA	O2A-CGA-O1A	-4.78	111.05	123.33
11	1	1139	CLA	C2D-C1D-ND	4.77	114.85	110.13
11	A	1135	CLA	C2D-C1D-ND	4.77	114.85	110.13
11	2	1219	CLA	O2A-CGA-O1A	-4.77	111.69	123.63
11	a	1022	CLA	C2D-C1D-ND	4.77	114.85	110.13
11	a	1130	CLA	C4A-NA-C1A	4.77	108.86	106.68
11	2	1201	CLA	C1D-ND-C4D	-4.77	102.96	106.31
14	B	4005	BCR	C7-C8-C9	-4.77	119.18	126.23
11	A	1121	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
11	A	1121	CLA	O2D-CGD-CBD	4.77	119.57	111.23
11	b	1221	CLA	O2A-CGA-O1A	-4.77	111.70	123.63
11	b	1215	CLA	C1D-ND-C4D	-4.77	102.97	106.31
11	b	1013	CLA	O2D-CGD-CBD	4.77	119.56	111.23
11	A	1801	CLA	C2D-C1D-ND	4.77	114.84	110.13
11	K	1402	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
11	a	1102	CLA	O2D-CGD-CBD	4.77	119.56	111.23
11	a	1130	CLA	C1D-ND-C4D	-4.76	102.97	106.31
11	a	1138	CLA	C1D-ND-C4D	-4.76	102.97	106.31
11	A	1801	CLA	O2A-CGA-CBA	4.76	126.35	111.83
11	2	1217	CLA	C1D-ND-C4D	-4.76	102.97	106.31
11	a	1801	CLA	O2A-CGA-CBA	4.76	126.34	111.83
11	a	1135	CLA	C2D-C1D-ND	4.76	114.83	110.13
11	1	1122	CLA	O2D-CGD-CBD	4.76	119.55	111.23
11	2	1218	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
11	2	1209	CLA	O2A-CGA-O1A	-4.75	111.10	123.33
11	b	1218	CLA	C3B-C2B-C1B	-4.75	101.56	107.17
11	b	1214	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
11	2	1216	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
11	b	1208	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
11	a	1123	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	2	1231	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	1	1123	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	1	1104	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
11	B	1232	CLA	C2D-C1D-ND	4.75	114.83	110.13
11	1	1112	CLA	O2A-CGA-O1A	-4.75	111.12	123.33
11	a	1012	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	A	1120	CLA	C2D-C1D-ND	4.75	114.83	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1106	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	A	1133	CLA	C1D-ND-C4D	-4.75	102.98	106.31
11	a	1112	CLA	O2A-CGA-O1A	-4.75	111.12	123.33
11	a	1114	CLA	C3B-C2B-C1B	-4.75	101.58	107.17
11	1	1022	CLA	C2D-C1D-ND	4.74	114.82	110.13
11	B	1225	CLA	O2A-CGA-O1A	-4.74	111.76	123.63
11	b	1223	CLA	O2D-CGD-CBD	4.74	119.52	111.23
11	0	1402	CLA	O2D-CGD-CBD	4.74	119.52	111.23
11	b	1206	CLA	C1D-ND-C4D	-4.74	102.98	106.31
11	a	1119	CLA	C2D-C1D-ND	4.74	114.82	110.13
11	2	1231	CLA	C2D-C1D-ND	4.74	114.82	110.13
11	B	1217	CLA	O2A-CGA-CBA	4.74	126.30	111.83
11	A	1110	CLA	C1D-ND-C4D	-4.74	102.98	106.31
11	A	1012	CLA	O2A-CGA-CBA	4.74	126.29	111.83
11	2	1021	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
11	A	1108	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
11	a	1128	CLA	O2A-CGA-O1A	-4.74	111.78	123.63
11	2	1209	CLA	C2D-C1D-ND	4.74	114.81	110.13
11	B	1229	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
11	2	1225	CLA	O2A-CGA-O1A	-4.73	111.79	123.63
14	b	4005	BCR	C24-C23-C22	-4.73	119.23	126.23
11	1	1121	CLA	O2D-CGD-CBD	4.73	119.50	111.23
11	1	1102	CLA	C1D-ND-C4D	-4.73	102.99	106.31
11	1	1129	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
11	B	1206	CLA	C2D-C1D-ND	4.73	114.81	110.13
11	B	1203	CLA	O2A-CGA-O1A	-4.73	111.81	123.63
11	1	1113	CLA	O2D-CGD-CBD	4.73	119.49	111.23
11	2	1205	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
11	1	1123	CLA	O2A-CGA-O1A	-4.72	111.81	123.63
11	A	1011	CLA	O2A-CGA-CBA	4.72	126.24	111.83
11	1	1114	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
11	B	1209	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
11	a	1123	CLA	C2D-C1D-ND	4.72	114.80	110.13
11	A	1106	CLA	C2D-C1D-ND	4.72	114.80	110.13
11	B	1201	CLA	C2D-C1D-ND	4.72	114.80	110.13
11	1	1111	CLA	C2C-C1C-NC	4.72	114.94	109.98
11	a	1125	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
11	1	1113	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
11	b	1229	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
11	2	1202	CLA	O2D-CGD-CBD	4.71	119.47	111.23
11	A	1133	CLA	C2D-C1D-ND	4.71	114.79	110.13
14	8	4019	BCR	C15-C14-C13	-4.71	120.67	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1225	CLA	C2D-C1D-ND	4.71	114.79	110.13
11	A	1116	CLA	C1C-C2C-C3C	-4.71	102.03	106.98
11	B	1216	CLA	C2D-C1D-ND	4.71	114.79	110.13
11	2	1223	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
11	2	1240	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
11	2	1234	CLA	C1D-ND-C4D	-4.71	103.01	106.31
11	a	1139	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
11	b	1216	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
11	A	1113	CLA	O2A-CGA-O1A	-4.70	111.23	123.33
11	A	1113	CLA	O2D-CGD-CBD	4.70	119.45	111.23
11	2	1227	CLA	O2A-CGA-O1A	-4.70	111.23	123.33
11	A	1110	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
11	b	1220	CLA	C2D-C1D-ND	4.70	114.78	110.13
11	a	1113	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
11	2	1206	CLA	C2D-C1D-ND	4.70	114.78	110.13
11	A	1112	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
11	k	1402	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
11	A	1129	CLA	O2D-CGD-CBD	4.70	119.44	111.23
11	b	1230	CLA	C1D-ND-C4D	-4.69	103.02	106.31
11	b	1220	CLA	C1D-ND-C4D	-4.69	103.02	106.31
11	B	1229	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
11	1	1107	CLA	O2A-CGA-O1A	-4.69	111.89	123.63
11	B	1208	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
14	A	4002	BCR	C38-C26-C25	-4.69	119.36	124.48
11	a	1108	CLA	O2D-CGD-CBD	4.69	119.43	111.23
11	b	1219	CLA	C1D-ND-C4D	-4.69	103.02	106.31
11	A	1134	CLA	O2D-CGD-CBD	4.69	119.43	111.23
11	b	1206	CLA	O2D-CGD-CBD	4.69	119.42	111.23
11	A	1118	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
11	B	1240	CLA	O2A-CGA-O1A	-4.69	111.28	123.33
11	B	1208	CLA	O2A-CGA-O1A	-4.68	111.28	123.33
11	A	1114	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
11	1	1135	CLA	O2A-CGA-O1A	-4.68	111.91	123.63
11	b	1232	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
11	k	1402	CLA	O2D-CGD-CBD	4.68	119.41	111.23
11	2	1013	CLA	O2D-CGD-CBD	4.68	119.41	111.23
11	2	1212	CLA	O2A-CGA-O1A	-4.68	111.31	123.33
11	1	1128	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
11	b	1231	CLA	O2A-CGA-O1A	-4.68	111.31	123.33
11	2	1201	CLA	C2D-C1D-ND	4.68	114.75	110.13
11	1	1125	CLA	C1C-C2C-C3C	-4.67	102.06	106.98
11	1	1237	CLA	C3B-C2B-C1B	-4.67	101.66	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1224	CLA	O2A-CGA-CBA	4.67	126.09	111.83
11	1	1022	CLA	C4A-NA-C1A	4.67	108.81	106.68
11	A	1111	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
11	1	1123	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
11	1	1131	CLA	O2A-CGA-O1A	-4.67	111.95	123.63
11	a	1107	CLA	O2A-CGA-O1A	-4.67	111.96	123.63
11	B	1204	CLA	O2A-CGA-O1A	-4.66	111.96	123.63
11	a	1115	CLA	C1C-C2C-C3C	-4.66	102.07	106.98
14	f	4013	BCR	C38-C26-C25	-4.66	119.40	124.48
11	a	1140	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
14	A	4007	BCR	C38-C26-C25	-4.66	119.40	124.48
11	b	1021	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
11	1	1107	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
11	B	1230	CLA	O2A-C1-C2	4.66	126.03	108.11
11	b	1209	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
11	b	1219	CLA	O2D-CGD-CBD	4.65	119.37	111.23
14	1	4002	BCR	C24-C23-C22	-4.65	119.35	126.23
11	b	1227	CLA	O2A-CGA-O1A	-4.65	111.37	123.33
11	A	1801	CLA	C1D-ND-C4D	-4.65	103.05	106.31
11	B	1232	CLA	O2A-CGA-O1A	-4.65	111.37	123.33
11	B	1231	CLA	O2A-CGA-O1A	-4.65	111.37	123.33
11	2	1221	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
11	a	1135	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
11	a	1125	CLA	O2D-CGD-CBD	4.65	119.35	111.23
11	B	1206	CLA	O2A-CGA-O1A	-4.64	112.01	123.63
11	2	1230	CLA	O2A-CGA-O1A	-4.64	112.01	123.63
11	1	1133	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
11	1	1108	CLA	O2D-CGD-CBD	4.64	119.34	111.23
11	b	1206	CLA	C2D-C1D-ND	4.64	114.72	110.13
11	2	1232	CLA	O2A-CGA-O1A	-4.64	111.40	123.33
11	1	1125	CLA	O2A-CGA-O1A	-4.64	112.02	123.63
11	A	1126	CLA	O2A-CGA-O1A	-4.64	112.02	123.63
11	B	1232	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
11	1	1127	CLA	O2D-CGD-CBD	4.64	119.34	111.23
15	B	5004	LHG	O7-C7-C8	4.64	121.51	111.48
11	1	1130	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
14	1	4008	BCR	C33-C5-C6	-4.64	119.42	124.48
11	A	1112	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
11	2	1218	CLA	O2A-CGA-O1A	-4.63	111.42	123.33
11	a	1139	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
11	K	1401	CLA	O2A-CGA-CBA	4.63	125.96	111.83
11	0	1401	CLA	O2A-CGA-CBA	4.63	125.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1105	CLA	O2A-CGA-CBA	4.63	125.95	111.83
11	k	1401	CLA	O2A-CGA-CBA	4.63	125.95	111.83
11	A	1127	CLA	O2D-CGD-CBD	4.63	119.32	111.23
14	1	4002	BCR	C7-C8-C9	-4.63	119.39	126.23
14	2	4010	BCR	C7-C8-C9	-4.63	119.39	126.23
11	1	1108	CLA	O2A-CGA-O1A	-4.63	111.43	123.33
11	b	1218	CLA	O2A-CGA-O1A	-4.63	111.43	123.33
11	K	1402	CLA	O2D-CGD-CBD	4.62	119.31	111.23
11	2	1204	CLA	O2A-CGA-O1A	-4.62	112.06	123.63
11	2	1021	CLA	C1D-ND-C4D	-4.62	103.07	106.31
11	2	1208	CLA	O2D-CGD-CBD	4.62	119.31	111.23
11	1	1109	CLA	O2D-CGD-CBD	4.62	119.31	111.23
11	B	1231	CLA	C2D-C1D-ND	4.62	114.70	110.13
11	a	1111	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
14	F	4013	BCR	C7-C8-C9	-4.62	119.40	126.23
11	1	1106	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
11	A	1140	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
11	2	1215	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
14	A	4007	BCR	C33-C5-C6	-4.61	119.45	124.48
11	2	1220	CLA	CAC-C3C-C4C	4.61	130.79	124.79
14	B	4010	BCR	C7-C8-C9	-4.61	119.41	126.23
14	8	4019	BCR	C33-C5-C6	-4.61	119.45	124.48
11	b	1208	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
11	b	1204	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
11	1	1137	CLA	O2A-CGA-CBA	4.61	125.88	111.83
11	1	1110	CLA	C1D-ND-C4D	-4.60	103.08	106.31
11	2	1240	CLA	O2D-CGD-CBD	4.60	119.28	111.23
11	2	1218	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
11	A	1137	CLA	O2A-CGA-CBA	4.60	125.86	111.83
11	b	1225	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
11	A	1109	CLA	O2D-CGD-CBD	4.60	119.26	111.23
11	b	1217	CLA	O2A-CGA-CBA	4.59	125.84	111.83
11	B	1220	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
11	1	1237	CLA	O2A-CGA-O1A	-4.59	112.14	123.63
14	6	4013	BCR	C38-C26-C25	-4.59	119.47	124.48
11	a	1136	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
14	f	4020	BCR	C33-C5-C6	-4.59	119.47	124.48
11	2	1226	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
11	b	1212	CLA	O2A-CGA-O1A	-4.59	111.53	123.33
11	B	1227	CLA	O2A-CGA-O1A	-4.59	111.53	123.33
11	1	1124	CLA	O2D-CGD-CBD	4.58	119.25	111.23
11	B	1225	CLA	C3D-C2D-C1D	-4.58	99.58	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1231	CLA	O2A-CGA-O1A	-4.58	111.54	123.33
14	l	4019	BCR	C15-C14-C13	-4.58	120.85	127.28
11	B	1218	CLA	O2A-CGA-O1A	-4.58	111.55	123.33
11	A	1102	CLA	C1D-ND-C4D	-4.58	103.10	106.31
11	2	1023	CLA	O2A-CGA-CBA	4.58	125.80	111.83
14	A	4008	BCR	C34-C9-C10	-4.58	115.40	122.82
11	b	1230	CLA	O2A-CGA-CBA	4.58	125.79	111.83
11	B	1234	CLA	O2A-CGA-CBA	4.57	125.78	111.83
14	2	4010	BCR	C38-C26-C25	-4.57	119.49	124.48
11	B	1212	CLA	O2A-CGA-O1A	-4.57	111.58	123.33
14	b	4010	BCR	C33-C5-C6	-4.57	119.50	124.48
11	A	1122	CLA	O2A-CGA-CBA	4.57	125.77	111.83
11	A	1123	CLA	O2A-CGA-O1A	-4.57	112.20	123.63
11	a	1138	CLA	C2D-C1D-ND	4.56	114.64	110.13
11	1	1132	CLA	O2A-CGA-O1A	-4.56	112.22	123.63
15	A	5003	LHG	O7-C7-C8	4.56	121.35	111.48
11	b	1235	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
11	b	1230	CLA	C4-C3-C5	4.55	123.13	115.23
11	2	1202	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
11	B	1201	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
11	A	1109	CLA	O2A-CGA-CBA	4.55	125.72	111.83
11	B	1013	CLA	O2A-CGA-CBA	4.55	125.71	111.83
11	B	1224	CLA	O2A-CGA-CBA	4.55	125.71	111.83
11	A	1118	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
11	a	1133	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
11	B	1230	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
11	a	1119	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
11	2	1208	CLA	O2A-CGA-O1A	-4.54	111.65	123.33
11	A	1011	CLA	C1-C2-C3	-4.54	118.76	126.20
11	B	1206	CLA	C1D-ND-C4D	-4.54	103.13	106.31
11	1	1103	CLA	O2A-CGA-O1A	-4.54	112.27	123.63
11	A	1121	CLA	C2D-C1D-ND	4.54	114.62	110.13
11	b	1214	CLA	O2A-CGA-O1A	-4.53	112.29	123.63
11	a	1022	CLA	O2D-CGD-CBD	4.53	119.16	111.23
11	A	1119	CLA	O2A-CGA-O1A	-4.53	112.29	123.63
11	1	1012	CLA	C4-C3-C5	4.53	123.09	115.23
11	1	1109	CLA	O2A-CGA-CBA	4.53	125.65	111.83
11	b	1225	CLA	O2A-CGA-O1A	-4.53	112.30	123.63
14	6	4013	BCR	C33-C5-C6	-4.53	119.54	124.48
14	L	4019	BCR	C33-C5-C6	-4.53	119.54	124.48
11	2	1238	CLA	O2A-CGA-O1A	-4.53	112.30	123.63
14	a	4003	BCR	C7-C8-C9	-4.53	119.54	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1223	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
11	a	1127	CLA	C2D-C1D-ND	4.52	114.60	110.13
11	a	1127	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	b	1229	CLA	O2D-CGD-CBD	4.52	119.13	111.23
11	a	1109	CLA	O2D-CGD-CBD	4.52	119.12	111.23
11	a	1132	CLA	O2A-CGA-O1A	-4.51	112.33	123.63
11	1	1109	CLA	C4-C3-C5	4.51	123.06	115.23
11	a	1022	CLA	C1D-ND-C4D	-4.51	103.14	106.31
11	a	1102	CLA	O2A-CGA-CBA	4.51	125.60	111.83
14	a	4002	BCR	C24-C23-C22	-4.51	119.56	126.23
11	A	1131	CLA	O2A-CGA-O1A	-4.51	112.35	123.63
11	B	1227	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
11	A	1136	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
11	2	1214	CLA	O2A-CGA-O1A	-4.51	112.36	123.63
11	a	1122	CLA	O2A-CGA-CBA	4.50	125.57	111.83
11	B	1219	CLA	O2D-CGD-CBD	4.50	119.10	111.23
11	2	1216	CLA	O2A-CGA-CBA	4.50	125.57	111.83
11	A	1102	CLA	O2A-CGA-CBA	4.50	125.56	111.83
14	2	4006	BCR	C38-C26-C25	-4.50	119.57	124.48
11	A	1139	CLA	O2D-CGD-CBD	4.50	119.10	111.23
11	b	1236	CLA	O2A-CGA-CBA	4.50	125.56	111.83
11	B	1234	CLA	O2D-CGD-CBD	4.50	119.09	111.23
11	1	1130	CLA	C4A-NA-C1A	4.49	108.73	106.68
11	A	1114	CLA	O2D-CGD-CBD	4.49	119.08	111.23
11	b	1234	CLA	O2A-CGA-CBA	4.49	125.53	111.83
11	b	1023	CLA	O2D-CGD-CBD	4.49	119.07	111.23
11	1	1111	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
11	b	1224	CLA	O2A-CGA-CBA	4.49	125.51	111.83
11	B	1238	CLA	O2A-CGA-O1A	-4.48	112.41	123.63
11	b	1225	CLA	C2D-C1D-ND	4.48	114.56	110.13
11	b	1210	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
11	b	1222	CLA	C4-C3-C5	4.48	123.00	115.23
11	2	1013	CLA	O2A-CGA-CBA	4.48	125.49	111.83
11	1	1111	CLA	O2A-CGA-CBA	4.48	125.49	111.83
11	2	1216	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
11	b	1213	CLA	C4-C3-C5	4.47	122.99	115.23
11	B	1211	CLA	C2D-C1D-ND	4.47	114.55	110.13
11	A	1119	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
14	F	4013	BCR	C38-C26-C25	-4.47	119.60	124.48
11	B	1226	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
14	6	4020	BCR	C33-C5-C6	-4.47	119.61	124.48
11	a	1137	CLA	O2A-CGA-CBA	4.47	125.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1225	CLA	C2D-C1D-ND	4.47	114.55	110.13
11	b	1231	CLA	O2D-CGD-CBD	4.46	119.03	111.23
14	6	4013	BCR	C24-C23-C22	-4.46	119.64	126.23
11	1	1106	CLA	O2D-CGD-CBD	4.46	119.03	111.23
11	A	1135	CLA	O2A-CGA-CBA	4.46	125.43	111.83
11	1	1119	CLA	O2A-CGA-CBA	4.45	125.41	111.83
11	b	1229	CLA	O2A-CGA-O1A	-4.45	112.49	123.63
11	1	1022	CLA	C1D-ND-C4D	-4.45	103.19	106.31
11	B	1230	CLA	C1-O2A-CGA	4.45	127.41	116.65
16	b	5002	LMG	O7-C10-C11	4.44	121.08	111.48
14	2	4017	BCR	C24-C23-C22	-4.43	119.67	126.23
14	1	4001	BCR	C24-C23-C22	-4.43	119.68	126.23
11	b	1205	CLA	O2A-CGA-CBA	4.43	125.35	111.83
14	A	4001	BCR	C15-C14-C13	-4.43	121.07	127.28
11	b	1206	CLA	O2A-CGA-O1A	-4.43	112.55	123.63
15	A	5001	LHG	O7-C7-C8	4.42	121.05	111.48
14	A	4001	BCR	C1-C6-C5	-4.42	116.59	122.64
11	A	1117	CLA	C4A-NA-C1A	4.42	108.70	106.68
11	B	1205	CLA	O2A-CGA-CBA	4.42	125.32	111.83
11	B	1240	CLA	O2D-CGD-CBD	4.42	118.96	111.23
11	a	1134	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
11	b	1013	CLA	O2A-CGA-CBA	4.42	125.31	111.83
11	A	1103	CLA	O2D-CGD-CBD	4.42	118.95	111.23
11	a	1107	CLA	C4-C3-C5	4.41	122.89	115.23
11	2	1230	CLA	O2A-C1-C2	4.41	125.09	108.11
11	b	1226	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
11	1	1011	CLA	O2A-CGA-CBA	4.41	125.29	111.83
11	b	1222	CLA	O2A-CGA-CBA	4.41	125.28	111.83
11	1	1011	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
11	A	1801	CLA	O2D-CGD-CBD	4.40	118.92	111.23
11	A	1140	CLA	O2A-CGA-CBA	4.40	125.25	111.83
11	a	1139	CLA	C1D-ND-C4D	-4.40	103.22	106.31
11	2	1206	CLA	C1D-ND-C4D	-4.40	103.22	106.31
11	b	1021	CLA	O2A-CGA-CBA	4.40	125.24	111.83
11	b	1206	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
11	a	1134	CLA	O2D-CGD-CBD	4.39	118.91	111.23
14	b	4014	BCR	C15-C14-C13	-4.39	121.12	127.28
11	A	1104	CLA	O2A-CGA-CBA	4.39	125.22	111.83
14	B	4006	BCR	C7-C8-C9	-4.39	119.74	126.23
11	2	1232	CLA	O2D-CGD-CBD	4.39	118.90	111.23
11	1	1121	CLA	O2A-CGA-O1A	-4.39	110.11	123.20
11	0	1402	CLA	O2A-CGA-CBA	4.39	125.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1116	CLA	O2A-CGA-CBA	4.38	125.20	111.83
11	A	1123	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
11	A	1116	CLA	O2A-CGA-CBA	4.38	125.20	111.83
11	1	1116	CLA	O2A-CGA-CBA	4.38	125.20	111.83
11	1	1127	CLA	C4A-NA-C1A	4.38	108.68	106.68
11	2	1219	CLA	O2D-CGD-CBD	4.38	118.89	111.23
14	2	4006	BCR	C7-C8-C9	-4.38	119.76	126.23
11	1	1137	CLA	C4-C3-C5	4.37	122.82	115.23
11	2	1210	CLA	C1C-C2C-C3C	-4.37	102.38	106.98
14	a	4002	BCR	C38-C26-C25	-4.37	119.72	124.48
14	b	4010	BCR	C15-C14-C13	-4.37	121.15	127.28
11	A	1124	CLA	O2A-CGA-CBA	4.37	125.15	111.83
11	A	1103	CLA	O2A-CGA-O1A	-4.36	112.72	123.63
11	a	1115	CLA	O2A-CGA-O1A	-4.36	110.19	123.20
11	2	1236	CLA	O2A-CGA-CBA	4.36	125.12	111.83
11	B	1211	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
11	A	1120	CLA	O2A-CGA-O1A	-4.35	110.21	123.20
11	A	1117	CLA	O2A-CGA-CBA	4.35	125.09	111.83
11	B	1013	CLA	O2A-C1-C2	4.35	124.83	108.11
11	B	1214	CLA	C4-C3-C5	4.35	122.77	115.23
11	b	1216	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
14	b	4011	BCR	C34-C9-C10	-4.34	115.78	122.82
11	A	1119	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
11	a	1127	CLA	O2A-CGA-CBA	4.34	125.07	111.83
11	2	1203	CLA	O2D-CGD-CBD	4.34	118.81	111.23
11	a	1127	CLA	C3B-C2B-C1B	-4.34	102.06	107.17
14	b	4017	BCR	C24-C23-C22	-4.34	119.82	126.23
11	B	1231	CLA	C1D-ND-C4D	-4.34	103.27	106.31
11	k	1402	CLA	O2A-CGA-CBA	4.33	125.05	111.83
11	A	1108	CLA	O2D-CGD-CBD	4.33	118.80	111.23
11	2	1205	CLA	O2A-CGA-CBA	4.33	125.04	111.83
14	A	4003	BCR	C37-C22-C21	-4.33	115.81	122.82
11	1	1110	CLA	O2A-CGA-CBA	4.33	125.02	111.83
11	2	1235	CLA	O2A-CGA-O1A	-4.33	112.81	123.63
11	l	1501	CLA	O2A-CGA-CBA	4.32	124.99	111.83
14	L	4022	BCR	C33-C5-C6	-4.31	119.78	124.48
11	2	1234	CLA	O2A-CGA-CBA	4.31	124.99	111.83
11	A	1125	CLA	C1D-ND-C4D	-4.31	103.29	106.31
11	A	1115	CLA	O2A-CGA-O1A	-4.31	110.33	123.20
11	A	1012	CLA	C4-C3-C5	4.30	122.70	115.23
11	B	1219	CLA	O2A-CGA-CBA	4.30	124.94	111.83
14	b	4004	BCR	C33-C5-C6	-4.29	119.80	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1118	CLA	O2A-CGA-CBA	4.29	124.93	111.83
11	2	1222	CLA	O2A-CGA-CBA	4.29	124.92	111.83
11	b	1234	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
14	L	4022	BCR	C38-C26-C25	-4.29	119.80	124.48
11	B	1228	CLA	O2A-CGA-CBA	4.29	124.92	111.83
11	a	1128	CLA	C3B-C2B-C1B	-4.29	102.12	107.17
11	B	1222	CLA	O2A-CGA-CBA	4.28	124.90	111.83
14	2	4009	BCR	C15-C14-C13	-4.28	121.27	127.28
11	a	1139	CLA	C2D-C1D-ND	4.28	114.36	110.13
11	b	1219	CLA	O2A-CGA-CBA	4.27	124.87	111.83
11	A	1129	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
11	b	1214	CLA	O2A-CGA-CBA	4.27	124.86	111.83
11	1	1801	CLA	O2A-CGA-CBA	4.27	124.85	111.83
11	b	1223	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
11	a	1237	CLA	C3B-C2B-C1B	-4.26	102.14	107.17
11	1	1102	CLA	O2A-CGA-CBA	4.26	124.83	111.83
11	2	1228	CLA	O2A-CGA-CBA	4.26	124.82	111.83
11	1	1125	CLA	CAC-C3C-C4C	4.26	130.33	124.79
11	A	1111	CLA	O2A-CGA-CBA	4.25	124.81	111.83
14	l	4022	BCR	C38-C26-C25	-4.25	119.84	124.48
15	a	5001	LHG	O7-C7-C8	4.25	120.68	111.48
11	a	1123	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
11	A	1135	CLA	O2D-CGD-CBD	4.25	118.66	111.23
14	A	4007	BCR	C24-C23-C22	-4.25	119.95	126.23
11	A	1127	CLA	O2A-CGA-CBA	4.25	124.79	111.83
14	L	4019	BCR	C7-C8-C9	-4.25	119.95	126.23
14	2	4017	BCR	C19-C18-C17	4.25	125.69	119.01
14	b	4009	BCR	C38-C26-C25	-4.24	119.86	124.48
11	B	1226	CLA	O2A-CGA-CBA	4.24	124.76	111.83
11	a	1120	CLA	O2A-CGA-O1A	-4.23	110.57	123.20
14	L	4019	BCR	C15-C14-C13	-4.23	121.35	127.28
11	A	1134	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
14	f	4018	BCR	C15-C14-C13	-4.22	121.36	127.28
14	1	4002	BCR	C19-C18-C17	4.22	125.65	119.01
11	B	1210	CLA	O2A-CGA-CBA	4.22	124.71	111.83
11	1	1140	CLA	O2A-CGA-CBA	4.22	124.71	111.83
11	B	1235	CLA	O2A-C1-C2	4.22	124.35	108.11
11	b	1223	CLA	O2A-CGA-CBA	4.21	124.69	111.83
11	A	1126	CLA	C4-C3-C5	4.21	122.54	115.23
11	2	1217	CLA	O2A-CGA-CBA	4.21	124.68	111.83
11	2	1239	CLA	O2A-CGA-O1A	-4.21	110.63	123.20
11	A	1101	CLA	O2A-CGA-O1A	-4.21	113.09	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1109	CLA	C4-C3-C5	4.21	122.53	115.23
14	6	4020	BCR	C34-C9-C10	-4.21	116.00	122.82
11	a	1111	CLA	O2A-CGA-CBA	4.21	124.67	111.83
14	f	4018	BCR	C3-C4-C5	-4.21	106.55	114.06
14	1	4002	BCR	C36-C18-C17	-4.20	116.00	122.82
11	1	1102	CLA	O2D-CGD-CBD	4.20	118.58	111.23
15	1	5001	LHG	O7-C7-C8	4.20	120.57	111.48
11	8	1502	CLA	O2A-CGA-O1A	-4.19	110.68	123.20
15	1	5003	LHG	O7-C7-C8	4.19	120.55	111.48
11	A	1110	CLA	O2A-CGA-CBA	4.18	124.59	111.83
11	1	1117	CLA	O2A-CGA-CBA	4.18	124.59	111.83
14	a	4003	BCR	C3-C4-C5	-4.18	106.60	114.06
11	1	1237	CLA	C1-C2-C3	-4.18	119.35	126.20
11	b	1215	CLA	O2A-CGA-CBA	4.18	124.58	111.83
11	B	1203	CLA	O2D-CGD-CBD	4.18	118.53	111.23
11	2	1234	CLA	O2D-CGD-CBD	4.18	118.53	111.23
14	8	4019	BCR	C24-C23-C22	-4.18	120.06	126.23
14	8	4019	BCR	C7-C8-C9	-4.17	120.07	126.23
14	m	4021	BCR	C28-C27-C26	-4.17	106.63	114.06
14	f	4013	BCR	C33-C5-C6	-4.17	119.94	124.48
14	1	4001	BCR	C15-C14-C13	-4.16	121.44	127.28
11	1	1120	CLA	O2A-CGA-O1A	-4.16	110.78	123.20
11	a	1110	CLA	O2A-CGA-CBA	4.16	124.52	111.83
11	B	1023	CLA	O2D-CGD-CBD	4.16	118.50	111.23
14	B	4014	BCR	C33-C5-C6	-4.16	119.95	124.48
11	A	1133	CLA	O2A-CGA-O1A	-4.16	110.79	123.20
11	a	1012	CLA	C4-C3-C5	4.16	122.44	115.23
11	l	1503	CLA	O2A-CGA-CBA	4.15	124.49	111.83
15	b	5004	LHG	O7-C7-C8	4.15	120.46	111.48
11	a	1012	CLA	O2A-CGA-CBA	4.15	124.48	111.83
14	6	4018	BCR	C3-C4-C5	-4.15	106.66	114.06
14	F	4020	BCR	C7-C8-C9	-4.14	120.10	126.23
11	B	1236	CLA	O2A-CGA-CBA	4.14	124.47	111.83
11	A	1121	CLA	O2A-CGA-O1A	-4.14	110.83	123.20
11	B	1210	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
11	a	1124	CLA	O2A-CGA-CBA	4.14	124.45	111.83
11	a	1134	CLA	O2A-CGA-O1A	-4.14	110.85	123.20
11	2	1210	CLA	O2A-CGA-CBA	4.14	124.45	111.83
11	a	1121	CLA	O2A-CGA-O1A	-4.14	110.86	123.20
11	2	1230	CLA	C4-C3-C5	4.13	122.40	115.23
14	F	4013	BCR	C33-C5-C6	-4.13	119.97	124.48
11	B	1021	CLA	C4-C3-C5	4.13	122.40	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1140	CLA	C1-C2-C3	-4.13	119.43	126.20
14	b	4006	BCR	C38-C26-C25	-4.13	119.98	124.48
14	1	4003	BCR	C7-C8-C9	-4.13	120.13	126.23
11	L	1501	CLA	O2A-CGA-CBA	4.12	124.41	111.83
14	a	4008	BCR	C15-C14-C13	-4.12	121.49	127.28
11	a	1130	CLA	O2A-CGA-O1A	-4.12	110.89	123.20
11	a	1104	CLA	O2A-CGA-CBA	4.12	124.40	111.83
11	a	1109	CLA	O2A-CGA-CBA	4.12	124.39	111.83
11	2	1023	CLA	O2A-C1-C2	4.12	123.95	108.11
11	B	1239	CLA	O2A-CGA-O1A	-4.11	110.92	123.20
11	1	1237	CLA	O2D-CGD-CBD	4.11	118.42	111.23
14	B	4006	BCR	C1-C6-C5	-4.11	117.02	122.64
11	1	1140	CLA	O2A-C1-C2	4.11	123.92	108.11
14	B	4011	BCR	C15-C14-C13	-4.11	121.52	127.28
11	A	1011	CLA	C1D-ND-C4D	-4.10	103.43	106.31
11	a	1119	CLA	O2A-CGA-CBA	4.10	124.35	111.83
11	2	1220	CLA	O2D-CGD-CBD	4.10	118.40	111.23
11	a	1117	CLA	O2A-CGA-CBA	4.10	124.34	111.83
11	B	1023	CLA	O2A-C1-C2	4.10	123.89	108.11
11	A	1128	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
14	1	4007	BCR	C38-C26-C25	-4.10	120.01	124.48
11	2	1220	CLA	O2A-CGA-O1A	-4.10	110.97	123.20
14	2	4010	BCR	C15-C14-C13	-4.09	121.54	127.28
11	A	1109	CLA	CHD-C1D-ND	-4.09	119.04	124.80
11	a	1133	CLA	O2A-CGA-O1A	-4.09	110.99	123.20
11	b	1203	CLA	O2A-CGA-CBA	4.09	124.30	111.83
15	2	5004	LHG	O7-C7-C8	4.09	120.32	111.48
14	A	4003	BCR	C23-C22-C21	4.09	125.44	119.01
11	1	1134	CLA	O2A-CGA-O1A	-4.09	111.00	123.20
11	1	1106	CLA	C4A-NA-C1A	4.09	108.54	106.68
11	a	1140	CLA	O2A-CGA-CBA	4.08	124.29	111.83
11	2	1213	CLA	C4-C3-C5	4.08	122.31	115.23
14	L	4022	BCR	C7-C8-C9	-4.07	120.21	126.23
11	b	1210	CLA	O2A-CGA-CBA	4.07	124.25	111.83
11	2	1229	CLA	O2A-CGA-CBA	4.07	124.25	111.83
11	A	1237	CLA	O2D-CGD-CBD	4.07	118.34	111.23
14	2	4011	BCR	C34-C9-C10	-4.07	116.22	122.82
14	6	4018	BCR	C33-C5-C6	-4.07	120.05	124.48
11	1	1104	CLA	O2A-CGA-CBA	4.06	124.23	111.83
11	1	1136	CLA	O2A-CGA-O1A	-4.06	111.07	123.20
11	B	1214	CLA	O2A-CGA-CBA	4.06	124.22	111.83
11	1	1122	CLA	O2A-CGA-CBA	4.06	124.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1133	CLA	O2A-CGA-O1A	-4.06	111.08	123.20
11	1	1124	CLA	O2A-CGA-CBA	4.06	124.21	111.83
11	1	1022	CLA	O2A-CGA-CBA	4.06	124.20	111.83
11	2	1206	CLA	O2A-CGA-CBA	4.05	124.19	111.83
11	a	1114	CLA	O2A-CGA-O1A	-4.05	111.10	123.20
11	2	1206	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
11	b	1013	CLA	O2A-C1-C2	4.05	123.69	108.11
14	6	4018	BCR	C15-C14-C13	-4.05	121.60	127.28
11	a	1237	CLA	O2D-CGD-CBD	4.04	118.29	111.23
11	L	1503	CLA	O2A-CGA-CBA	4.04	124.15	111.83
11	B	1220	CLA	O2A-CGA-O1A	-4.04	111.15	123.20
11	a	1136	CLA	O2A-CGA-O1A	-4.04	111.15	123.20
14	2	4010	BCR	C23-C22-C21	4.03	125.35	119.01
11	B	1215	CLA	O2A-CGA-CBA	4.03	124.12	111.83
14	1	4002	BCR	C38-C26-C25	-4.03	120.09	124.48
11	A	1129	CLA	O2A-CGA-O1A	-4.03	111.18	123.20
11	2	1213	CLA	O2A-CGA-CBA	4.02	124.10	111.83
11	8	1503	CLA	O2A-CGA-CBA	4.02	124.10	111.83
11	8	1501	CLA	C4-C3-C5	4.02	122.20	115.23
11	b	1023	CLA	O2A-CGA-CBA	4.01	124.08	111.83
11	b	1021	CLA	C4-C3-C5	4.01	122.19	115.23
14	2	4014	BCR	C33-C5-C6	-4.01	120.11	124.48
14	2	4005	BCR	C7-C8-C9	-4.01	120.31	126.23
14	l	4019	BCR	C33-C5-C6	-4.01	120.11	124.48
11	a	1138	CLA	O2A-CGA-O1A	-4.01	111.24	123.20
11	b	1239	CLA	O2A-CGA-O1A	-4.01	111.24	123.20
11	a	1129	CLA	O2A-CGA-O1A	-4.01	111.24	123.20
14	m	4021	BCR	C24-C23-C22	-4.01	120.31	126.23
11	2	1219	CLA	C2B-C1B-NB	4.00	114.47	110.33
11	K	1402	CLA	O2A-CGA-CBA	4.00	124.02	111.83
11	2	1021	CLA	C4-C3-C5	4.00	122.17	115.23
15	a	5003	LHG	O7-C7-C8	4.00	120.13	111.48
11	B	1229	CLA	O2A-CGA-CBA	3.99	124.01	111.83
11	b	1228	CLA	O2A-CGA-CBA	3.99	124.00	111.83
11	B	1206	CLA	O2D-CGD-CBD	3.99	118.21	111.23
11	a	1139	CLA	O2A-CGA-CBA	3.99	124.00	111.83
11	A	1105	CLA	O2A-CGA-CBA	3.99	123.99	111.83
11	2	1226	CLA	O2A-CGA-CBA	3.99	123.99	111.83
11	A	1138	CLA	O2A-CGA-O1A	-3.98	111.31	123.20
14	B	4010	BCR	C23-C22-C21	3.98	125.27	119.01
11	B	1220	CLA	O2D-CGD-CBD	3.98	118.19	111.23
11	b	1202	CLA	O2A-CGA-CBA	3.98	123.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1136	CLA	O2A-CGA-O1A	-3.98	111.33	123.20
11	b	1213	CLA	O2A-CGA-CBA	3.98	123.96	111.83
11	b	1220	CLA	O2A-CGA-O1A	-3.97	111.34	123.20
14	B	4011	BCR	C28-C27-C26	-3.97	106.97	114.06
11	1	1127	CLA	O2A-CGA-CBA	3.97	123.94	111.83
11	A	1114	CLA	O2A-CGA-O1A	-3.97	111.35	123.20
14	a	4007	BCR	C38-C26-C25	-3.97	120.16	124.48
11	A	1109	CLA	C4-C3-C5	3.97	122.11	115.23
11	1	1106	CLA	O2A-CGA-CBA	3.97	123.93	111.83
11	a	1103	CLA	O2A-CGA-CBA	3.96	123.92	111.83
11	1	1138	CLA	O2A-CGA-O1A	-3.96	111.37	123.20
11	2	1223	CLA	O2A-CGA-CBA	3.96	123.91	111.83
11	L	1503	CLA	CHD-C1D-ND	-3.96	119.23	124.80
14	l	4019	BCR	C38-C26-C25	-3.96	120.17	124.48
11	B	1202	CLA	O2A-CGA-CBA	3.95	123.89	111.83
11	1	1128	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
11	1	1139	CLA	C1-C2-C3	-3.95	120.37	126.76
11	A	1134	CLA	O2A-CGA-O1A	-3.95	111.40	123.20
11	a	1118	CLA	O2A-CGA-CBA	3.95	123.88	111.83
11	A	1101	CLA	O2D-CGD-CBD	3.95	118.13	111.23
11	1	1130	CLA	O2A-CGA-O1A	-3.95	111.41	123.20
11	B	1225	CLA	O2D-CGD-CBD	3.95	118.13	111.23
11	2	1021	CLA	C1-C2-C3	-3.95	119.73	126.20
11	2	1215	CLA	O2A-C1-C2	3.94	123.29	108.11
14	F	4018	BCR	C3-C4-C5	-3.94	107.02	114.06
11	B	1208	CLA	CHD-C1D-ND	-3.94	119.26	124.80
11	2	1230	CLA	C1-O2A-CGA	3.93	126.17	116.65
11	A	1106	CLA	CMB-C2B-C1B	3.93	131.41	125.42
11	A	1117	CLA	C2B-C1B-NB	3.93	114.40	110.33
11	2	1202	CLA	O2A-CGA-CBA	3.93	123.82	111.83
14	2	4011	BCR	C38-C26-C25	-3.93	120.20	124.48
11	1	1139	CLA	O2A-CGA-CBA	3.92	123.80	111.83
14	A	4003	BCR	C3-C4-C5	-3.92	107.06	114.06
11	1	1114	CLA	O2A-CGA-O1A	-3.92	111.49	123.20
11	2	1214	CLA	C4A-NA-C1A	3.92	108.47	106.68
11	2	1235	CLA	O2A-CGA-CBA	3.92	123.79	111.83
14	2	4014	BCR	C30-C25-C26	-3.92	117.28	122.64
11	B	1222	CLA	C2B-C1B-NB	3.91	114.39	110.33
11	2	1013	CLA	O2A-C1-C2	3.91	123.17	108.11
11	1	1118	CLA	O2A-CGA-CBA	3.91	123.77	111.83
11	B	1013	CLA	C1-O2A-CGA	3.91	126.12	116.65
14	a	4003	BCR	C15-C14-C13	-3.91	121.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1130	CLA	O2A-CGA-O1A	-3.91	111.54	123.20
14	f	4018	BCR	C33-C5-C6	-3.91	120.22	124.48
14	B	4009	BCR	C38-C26-C25	-3.90	120.22	124.48
11	1	1105	CLA	O2A-CGA-CBA	3.90	123.73	111.83
11	b	1211	CLA	O2A-CGA-O1A	-3.90	111.55	123.20
11	A	1103	CLA	C1-C2-C3	-3.90	119.81	126.20
11	1	1101	CLA	O2A-CGA-CBA	3.90	123.72	111.83
14	1	4001	BCR	C1-C6-C5	-3.90	117.31	122.64
11	b	1226	CLA	O2A-CGA-CBA	3.90	123.72	111.83
11	A	1106	CLA	O2A-CGA-CBA	3.90	123.72	111.83
11	1	1129	CLA	O2A-CGA-O1A	-3.90	111.57	123.20
11	B	1206	CLA	O2A-CGA-CBA	3.90	123.72	111.83
14	a	4007	BCR	C24-C23-C22	-3.89	120.48	126.23
14	l	4019	BCR	C24-C23-C22	-3.89	120.48	126.23
11	b	1215	CLA	O2A-C1-C2	3.89	123.08	108.11
11	l	1502	CLA	O2A-CGA-O1A	-3.89	111.58	123.20
11	b	1229	CLA	CHD-C1D-ND	-3.89	119.33	124.80
11	A	1139	CLA	O2A-CGA-CBA	3.89	123.68	111.83
11	b	1023	CLA	O2A-C1-C2	3.88	123.06	108.11
11	B	1203	CLA	CHD-C1D-ND	-3.88	119.34	124.80
14	l	4022	BCR	C33-C5-C6	-3.88	120.25	124.48
11	1	1115	CLA	O2A-CGA-O1A	-3.88	111.61	123.20
11	B	1023	CLA	O2A-CGA-CBA	3.88	123.67	111.83
11	B	1223	CLA	O2A-CGA-CBA	3.88	123.67	111.83
11	b	1227	CLA	CHD-C1D-ND	-3.88	119.34	124.80
11	b	1216	CLA	O2A-CGA-CBA	3.88	123.66	111.83
11	L	1502	CLA	O2A-CGA-O1A	-3.88	111.63	123.20
11	b	1229	CLA	O2A-CGA-CBA	3.88	123.66	111.83
11	A	1121	CLA	CHD-C1D-ND	-3.88	119.35	124.80
11	2	1211	CLA	O2A-CGA-O1A	-3.87	111.63	123.20
14	F	4020	BCR	C38-C26-C25	-3.87	120.26	124.48
14	A	4003	BCR	C15-C14-C13	-3.87	121.86	127.28
14	f	4020	BCR	C24-C23-C22	-3.87	120.52	126.23
14	b	4017	BCR	C27-C26-C25	-3.87	117.48	122.70
11	a	1011	CLA	C2B-C1B-NB	3.87	114.33	110.33
11	A	1104	CLA	C1-C2-C3	-3.86	119.87	126.20
11	A	1011	CLA	C2B-C1B-NB	3.86	114.33	110.33
11	a	1109	CLA	CHD-C1D-ND	-3.86	119.37	124.80
14	B	4006	BCR	C38-C26-C25	-3.86	120.27	124.48
14	b	4017	BCR	C15-C14-C13	-3.86	121.87	127.28
11	a	1011	CLA	C1D-ND-C4D	-3.86	103.61	106.31
11	2	1219	CLA	O2A-CGA-CBA	3.85	123.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	4003	BCR	C38-C26-C25	-3.85	120.28	124.48
11	B	1211	CLA	O2A-CGA-O1A	-3.85	111.70	123.20
14	2	4009	BCR	C38-C26-C25	-3.85	120.28	124.48
11	A	1132	CLA	O2A-CGA-CBA	3.85	123.58	111.83
11	a	1022	CLA	O2A-CGA-CBA	3.85	123.58	111.83
11	1	1107	CLA	O2A-C1-C2	3.85	122.93	108.11
11	b	1210	CLA	CAC-C3C-C4C	3.85	129.80	124.79
11	A	1138	CLA	CHD-C1D-ND	-3.85	119.39	124.80
11	a	1103	CLA	C4A-NA-C1A	3.84	108.43	106.68
11	1	1107	CLA	O2A-CGA-CBA	3.84	123.55	111.83
11	B	1238	CLA	CHD-C1D-ND	-3.84	119.40	124.80
11	A	1120	CLA	CHD-C1D-ND	-3.84	119.40	124.80
14	2	4010	BCR	C33-C5-C6	-3.84	120.30	124.48
11	b	1236	CLA	CHD-C1D-ND	-3.84	119.40	124.80
14	f	4020	BCR	C38-C26-C25	-3.84	120.30	124.48
11	B	1205	CLA	CMB-C2B-C1B	3.83	131.25	125.42
11	1	1104	CLA	CHD-C1D-ND	-3.83	119.42	124.80
11	A	1126	CLA	CHD-C1D-ND	-3.83	119.42	124.80
11	b	1206	CLA	O2A-CGA-CBA	3.83	123.50	111.83
14	b	4006	BCR	C3-C4-C5	-3.82	107.24	114.06
11	a	1104	CLA	CHD-C1D-ND	-3.82	119.42	124.80
11	B	1202	CLA	C2B-C1B-NB	3.82	114.29	110.33
11	A	1107	CLA	O2A-CGA-CBA	3.82	123.48	111.83
11	a	1101	CLA	O2A-CGA-CBA	3.82	123.47	111.83
14	8	4019	BCR	C38-C26-C25	-3.82	120.32	124.48
11	l	1501	CLA	C4-C3-C5	3.81	121.85	115.23
14	2	4010	BCR	C37-C22-C21	-3.81	116.64	122.82
11	b	1235	CLA	O2A-CGA-CBA	3.81	123.45	111.83
11	A	1137	CLA	CHD-C1D-ND	-3.81	119.44	124.80
11	2	1227	CLA	CHD-C1D-ND	-3.81	119.44	124.80
11	a	1107	CLA	CAA-C2A-C3A	-3.81	102.71	113.00
11	A	1128	CLA	O2A-CGA-CBA	3.81	123.44	111.83
11	1	1101	CLA	CHD-C1D-ND	-3.81	119.45	124.80
11	2	1232	CLA	CHD-C1D-ND	-3.80	119.45	124.80
11	B	1216	CLA	O2A-CGA-CBA	3.80	123.43	111.83
11	1	1135	CLA	O2A-CGA-CBA	3.80	123.41	111.83
11	b	1231	CLA	CHD-C1D-ND	-3.80	119.46	124.80
14	1	4008	BCR	C34-C9-C10	-3.79	116.67	122.82
11	A	1122	CLA	C4-C3-C5	3.79	121.81	115.23
14	B	4009	BCR	C15-C14-C13	-3.79	121.97	127.28
14	B	4014	BCR	C15-C14-C13	-3.79	121.97	127.28
11	1	1119	CLA	CHD-C1D-ND	-3.78	119.48	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1213	CLA	O2A-CGA-CBA	3.78	123.37	111.83
11	1	1011	CLA	O1D-CGD-CBD	-3.78	117.06	124.52
14	B	4017	BCR	C7-C8-C9	-3.78	120.64	126.23
14	F	4018	BCR	C15-C14-C13	-3.78	121.98	127.28
11	1	1127	CLA	CHD-C1D-ND	-3.78	119.49	124.80
14	B	4017	BCR	C1-C6-C5	-3.78	117.47	122.64
11	2	1202	CLA	CHD-C1D-ND	-3.77	119.49	124.80
11	b	1013	CLA	CHD-C1D-ND	-3.77	119.50	124.80
11	A	1237	CLA	O2A-C1-C2	3.77	122.62	108.11
11	1	1126	CLA	O2A-CGA-CBA	3.77	123.33	111.83
11	B	1216	CLA	CHD-C1D-ND	-3.77	119.50	124.80
11	2	1228	CLA	C1-C2-C3	-3.77	120.66	126.76
11	2	1203	CLA	O2A-CGA-CBA	3.77	123.32	111.83
11	a	1122	CLA	O2A-C1-C2	3.77	122.60	108.11
14	7	4021	BCR	C24-C23-C22	-3.77	120.67	126.23
11	a	1128	CLA	O2A-CGA-CBA	3.76	123.31	111.83
11	A	1022	CLA	CHD-C1D-ND	-3.76	119.51	124.80
11	8	1501	CLA	O2A-CGA-CBA	3.76	123.31	111.83
11	B	1224	CLA	CHD-C1D-ND	-3.76	119.51	124.80
11	1	1125	CLA	CHD-C1D-ND	-3.76	119.51	124.80
11	B	1204	CLA	CHD-C1D-ND	-3.75	119.52	124.80
11	B	1227	CLA	CHD-C1D-ND	-3.75	119.52	124.80
11	b	1201	CLA	C2B-C1B-NB	3.75	114.22	110.33
11	l	1503	CLA	CHD-C1D-ND	-3.75	119.52	124.80
11	B	1215	CLA	O2A-C1-C2	3.75	122.54	108.11
14	B	4009	BCR	C7-C8-C9	-3.75	120.69	126.23
11	2	1201	CLA	O2A-CGA-CBA	3.75	123.27	111.83
11	b	1238	CLA	CHD-C1D-ND	-3.75	119.53	124.80
11	B	1230	CLA	C4-C3-C5	3.74	121.72	115.23
11	2	1213	CLA	CHD-C1D-ND	-3.74	119.53	124.80
14	a	4008	BCR	C38-C26-C25	-3.74	120.40	124.48
14	1	4003	BCR	C3-C4-C5	-3.74	107.39	114.06
11	1	1130	CLA	CHD-C1D-ND	-3.74	119.54	124.80
11	a	1131	CLA	O2A-CGA-CBA	3.74	123.23	111.83
11	B	1203	CLA	O2A-CGA-CBA	3.74	123.23	111.83
11	A	1124	CLA	C1-C2-C3	-3.74	120.08	126.20
14	B	4004	BCR	C38-C26-C25	-3.73	120.41	124.48
11	B	1220	CLA	CHD-C1D-ND	-3.73	119.55	124.80
11	b	1218	CLA	CHD-C1D-ND	-3.73	119.55	124.80
11	a	1237	CLA	O2A-C1-C2	3.73	122.47	108.11
11	a	1122	CLA	C1-O2A-CGA	3.73	125.68	116.65
11	2	1023	CLA	C2B-C1B-NB	3.73	114.19	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1131	CLA	CHD-C1D-ND	-3.73	119.56	124.80
11	2	1013	CLA	CHD-C1D-ND	-3.73	119.56	124.80
14	F	4018	BCR	C38-C26-C25	-3.73	120.42	124.48
14	1	4007	BCR	C7-C8-C9	-3.73	120.72	126.23
11	A	1135	CLA	C2B-C1B-NB	3.73	114.19	110.33
11	a	1130	CLA	CHD-C1D-ND	-3.72	119.56	124.80
11	A	1130	CLA	CHD-C1D-ND	-3.72	119.56	124.80
11	A	1119	CLA	CHD-C1D-ND	-3.72	119.57	124.80
11	A	1135	CLA	CHD-C1D-ND	-3.72	119.57	124.80
14	B	4011	BCR	C33-C5-C6	-3.72	120.43	124.48
11	A	1135	CLA	C1-C2-C3	-3.72	120.11	126.20
11	a	1124	CLA	C1-C2-C3	-3.71	120.11	126.20
11	1	1124	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	1	4007	BCR	C15-C14-C13	-3.71	122.07	127.28
11	b	1231	CLA	C2B-C1B-NB	3.71	114.18	110.33
14	1	4008	BCR	C7-C8-C9	-3.71	120.74	126.23
11	B	1228	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	2	4009	BCR	C24-C23-C22	-3.71	120.75	126.23
11	A	1117	CLA	CHD-C1D-ND	-3.71	119.58	124.80
11	1	1111	CLA	O2A-C1-C2	3.71	122.38	108.11
14	2	4006	BCR	C4-C5-C6	-3.71	117.69	122.70
11	2	1208	CLA	CHD-C1D-ND	-3.71	119.59	124.80
14	6	4018	BCR	C27-C26-C25	-3.71	117.70	122.70
11	B	1215	CLA	CHD-C1D-ND	-3.71	119.59	124.80
14	b	4011	BCR	C38-C26-C25	-3.71	120.44	124.48
11	1	1121	CLA	O2A-CGA-CBA	3.70	126.13	112.14
14	6	4020	BCR	C38-C26-C25	-3.70	120.44	124.48
14	6	4020	BCR	C15-C14-C13	-3.70	122.08	127.28
11	B	1221	CLA	O2A-CGA-CBA	3.70	123.13	111.83
11	2	1013	CLA	C2B-C1B-NB	3.70	114.17	110.33
11	2	1231	CLA	C2B-C1B-NB	3.70	114.17	110.33
14	a	4001	BCR	C33-C5-C6	-3.70	120.44	124.48
11	1	1106	CLA	CHD-C1D-ND	-3.70	119.59	124.80
11	8	1503	CLA	C2B-C1B-NB	3.70	114.16	110.33
11	A	1104	CLA	CHD-C1D-ND	-3.70	119.60	124.80
14	2	4004	BCR	C38-C26-C25	-3.70	120.45	124.48
11	8	1503	CLA	CHD-C1D-ND	-3.70	119.60	124.80
11	a	1132	CLA	CHD-C1D-ND	-3.69	119.60	124.80
11	1	1126	CLA	CHD-C1D-ND	-3.69	119.60	124.80
14	2	4014	BCR	C27-C26-C25	-3.69	117.71	122.70
11	1	1128	CLA	O2A-CGA-CBA	3.69	123.09	111.83
11	2	1224	CLA	CHD-C1D-ND	-3.69	119.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1115	CLA	CHD-C1D-ND	-3.69	119.61	124.80
11	A	1118	CLA	CHD-C1D-ND	-3.69	119.61	124.80
11	b	1240	CLA	CHD-C1D-ND	-3.69	119.61	124.80
11	b	1201	CLA	O2A-CGA-CBA	3.69	123.08	111.83
11	B	1218	CLA	CHD-C1D-ND	-3.69	119.61	124.80
11	A	1022	CLA	O2A-CGA-CBA	3.69	123.08	111.83
11	2	1204	CLA	CHD-C1D-ND	-3.69	119.61	124.80
11	A	1123	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	b	4014	BCR	C33-C5-C6	-3.69	120.46	124.48
14	M	4021	BCR	C38-C26-C25	-3.69	120.46	124.48
14	B	4005	BCR	C33-C5-C6	-3.68	120.47	124.48
11	a	1121	CLA	CHD-C1D-ND	-3.68	119.62	124.80
11	1	1131	CLA	O2A-CGA-CBA	3.68	123.06	111.83
11	A	1132	CLA	O2A-C1-C2	3.68	122.27	108.11
11	1	1103	CLA	O2A-CGA-CBA	3.68	123.06	111.83
14	A	4001	BCR	C23-C22-C21	3.68	124.80	119.01
14	2	4009	BCR	C33-C5-C6	-3.68	120.47	124.48
11	a	1137	CLA	CHD-C1D-ND	-3.68	119.63	124.80
11	A	1108	CLA	CHD-C1D-ND	-3.67	119.63	124.80
11	a	1801	CLA	CHD-C1D-ND	-3.67	119.63	124.80
11	A	1102	CLA	C2B-C1B-NB	3.67	114.13	110.33
11	a	1132	CLA	O2A-CGA-CBA	3.67	123.03	111.83
11	a	1132	CLA	C1-O2A-CGA	3.67	125.53	116.65
14	B	4006	BCR	C3-C4-C5	-3.67	107.52	114.06
11	1	1123	CLA	O2A-CGA-CBA	3.67	123.02	111.83
14	1	4003	BCR	C33-C5-C6	-3.67	120.48	124.48
11	b	1208	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	2	4005	BCR	C33-C5-C6	-3.66	120.49	124.48
11	b	1215	CLA	CHD-C1D-ND	-3.66	119.65	124.80
11	1	1121	CLA	CHD-C1D-ND	-3.66	119.65	124.80
11	1	1114	CLA	CHD-C1D-ND	-3.66	119.65	124.80
11	2	1225	CLA	CHD-C1D-ND	-3.66	119.65	124.80
11	2	1223	CLA	CHD-C1D-ND	-3.66	119.65	124.80
11	a	1124	CLA	CHD-C1D-ND	-3.66	119.66	124.80
14	A	4002	BCR	C7-C8-C9	-3.66	120.83	126.23
11	A	1132	CLA	CMB-C2B-C1B	3.66	130.99	125.42
11	B	1236	CLA	CHD-C1D-ND	-3.65	119.66	124.80
11	a	1135	CLA	O2A-CGA-CBA	3.65	122.97	111.83
11	a	1101	CLA	CHD-C1D-ND	-3.65	119.67	124.80
11	A	1123	CLA	CAC-C3C-C4C	3.65	129.54	124.79
11	b	1204	CLA	CHD-C1D-ND	-3.65	119.67	124.80
11	b	1220	CLA	CAC-C3C-C4C	3.65	129.53	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1127	CLA	C1-C2-C3	-3.65	120.22	126.20
14	F	4018	BCR	C33-C5-C6	-3.64	120.51	124.48
11	A	1125	CLA	O2A-CGA-CBA	3.64	122.94	111.83
11	b	1238	CLA	O2A-CGA-CBA	3.64	122.94	111.83
11	2	1215	CLA	O2A-CGA-CBA	3.64	122.94	111.83
11	1	1132	CLA	CHD-C1D-ND	-3.64	119.68	124.80
11	a	1120	CLA	O2A-CGA-CBA	3.64	125.88	112.14
11	A	1123	CLA	O2A-CGA-CBA	3.64	122.93	111.83
11	1	1011	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
11	A	1105	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	B	4017	BCR	C27-C26-C25	-3.64	117.79	122.70
11	A	1122	CLA	CHD-C1D-ND	-3.64	119.69	124.80
14	b	4011	BCR	C33-C5-C6	-3.64	120.52	124.48
14	B	4017	BCR	C19-C18-C17	3.64	124.73	119.01
11	2	1234	CLA	C1-C2-C3	-3.63	120.24	126.20
11	1	1012	CLA	O2A-C1-C2	3.63	122.09	108.11
11	B	1230	CLA	O2A-CGA-CBA	3.63	122.91	111.83
11	a	1117	CLA	CHD-C1D-ND	-3.63	119.69	124.80
11	a	1123	CLA	CHD-C1D-ND	-3.63	119.69	124.80
11	1	1105	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	6	4020	BCR	C38-C26-C27	3.63	121.33	113.60
11	A	1124	CLA	CHD-C1D-ND	-3.63	119.69	124.80
11	a	1115	CLA	O2A-CGA-CBA	3.63	125.84	112.14
14	8	4022	BCR	C33-C5-C6	-3.63	120.53	124.48
11	B	1223	CLA	CHD-C1D-ND	-3.63	119.70	124.80
11	2	1229	CLA	CHD-C1D-ND	-3.63	119.70	124.80
11	1	1117	CLA	CHD-C1D-ND	-3.63	119.70	124.80
11	2	1202	CLA	C1-C2-C3	-3.62	120.26	126.20
11	a	1140	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	B	1207	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	B	1212	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	A	1139	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	b	1232	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	2	1218	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	0	1402	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	B	1202	CLA	CHD-C1D-ND	-3.62	119.70	124.80
11	2	1215	CLA	C1-O2A-CGA	3.62	125.42	116.65
14	b	4006	BCR	C33-C5-C4	3.62	121.31	113.60
14	B	4011	BCR	C24-C23-C22	-3.62	120.88	126.23
14	B	4011	BCR	C34-C9-C10	-3.62	116.95	122.82
14	A	4003	BCR	C33-C5-C6	-3.62	120.53	124.48
11	A	1126	CLA	O2A-CGA-CBA	3.62	122.87	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1111	CLA	CMC-C2C-C1C	3.62	130.69	125.03
11	B	1239	CLA	CHD-C1D-ND	-3.62	119.71	124.80
11	L	1501	CLA	CHD-C1D-ND	-3.62	119.71	124.80
11	A	1111	CLA	C1-C2-C3	-3.62	120.27	126.20
11	2	1210	CLA	C1-C2-C3	-3.62	120.27	126.20
11	2	1021	CLA	C2B-C1B-NB	3.62	114.08	110.33
11	1	1109	CLA	CHD-C1D-ND	-3.61	119.72	124.80
11	B	1021	CLA	CMB-C2B-C1B	3.61	130.92	125.42
14	2	4011	BCR	C33-C5-C6	-3.61	120.54	124.48
11	B	1231	CLA	C2B-C1B-NB	3.61	114.07	110.33
11	1	1139	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	B	4010	BCR	C38-C26-C25	-3.61	120.55	124.48
11	a	1106	CLA	O2A-CGA-CBA	3.61	122.84	111.83
11	1	1124	CLA	C1-C2-C3	-3.61	120.28	126.20
11	a	1237	CLA	O2A-CGA-CBA	3.61	122.84	111.83
11	1	1801	CLA	CHD-C1D-ND	-3.60	119.73	124.80
11	a	1123	CLA	O2A-CGA-CBA	3.60	122.82	111.83
14	a	4003	BCR	C33-C5-C6	-3.60	120.55	124.48
14	2	4017	BCR	C1-C6-C5	-3.60	117.72	122.64
11	a	1103	CLA	CHD-C1D-ND	-3.60	119.74	124.80
11	a	1137	CLA	C4-C3-C5	3.60	121.47	115.23
11	A	1103	CLA	CHD-C1D-ND	-3.60	119.74	124.80
11	b	1206	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	A	4003	BCR	C38-C26-C25	-3.60	120.56	124.48
11	b	1217	CLA	CHD-C1D-ND	-3.59	119.74	124.80
11	2	1220	CLA	CHD-C1D-ND	-3.59	119.75	124.80
11	1	1237	CLA	CHD-C1D-ND	-3.59	119.75	124.80
11	A	1101	CLA	O2A-CGA-CBA	3.59	122.78	111.83
14	b	4009	BCR	C24-C23-C22	-3.59	120.92	126.23
14	B	4006	BCR	C4-C5-C6	-3.59	117.85	122.70
14	b	4006	BCR	C1-C6-C5	-3.59	117.73	122.64
11	B	1229	CLA	CHD-C1D-ND	-3.59	119.75	124.80
11	A	1140	CLA	C1-C2-C3	-3.59	120.32	126.20
14	b	4005	BCR	C33-C5-C6	-3.59	120.57	124.48
14	b	4005	BCR	C15-C14-C13	-3.59	122.25	127.28
11	A	1101	CLA	CHD-C1D-ND	-3.58	119.76	124.80
11	2	1013	CLA	C1-O2A-CGA	3.58	125.33	116.65
11	b	1203	CLA	CHD-C1D-ND	-3.58	119.76	124.80
14	b	4009	BCR	C33-C5-C6	-3.58	120.58	124.48
11	b	1239	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	F	4018	BCR	C34-C9-C10	-3.58	117.02	122.82
11	A	1137	CLA	C2B-C1B-NB	3.58	114.04	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1107	CLA	O2A-CGA-CBA	3.58	122.75	111.83
11	b	1228	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	L	4019	BCR	C23-C22-C21	3.58	124.64	119.01
11	2	1201	CLA	O2A-C1-C2	3.58	121.87	108.11
11	2	1238	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	b	4005	BCR	C38-C26-C25	-3.57	120.58	124.48
11	k	1401	CLA	CMB-C2B-C1B	3.57	130.86	125.42
11	a	1135	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	2	4014	BCR	C36-C18-C17	-3.57	117.04	122.82
14	B	4014	BCR	C23-C22-C21	3.57	124.62	119.01
11	2	1214	CLA	CHD-C1D-ND	-3.57	119.78	124.80
11	a	1116	CLA	CHD-C1D-ND	-3.56	119.79	124.80
11	L	1502	CLA	CHD-C1D-ND	-3.56	119.79	124.80
14	b	4006	BCR	C4-C5-C6	-3.56	117.89	122.70
11	B	1232	CLA	CHD-C1D-ND	-3.56	119.79	124.80
11	B	1217	CLA	CHD-C1D-ND	-3.56	119.79	124.80
11	K	1401	CLA	CMB-C2B-C1B	3.56	130.84	125.42
11	a	1105	CLA	CHD-C1D-ND	-3.56	119.79	124.80
11	a	1138	CLA	CHD-C1D-ND	-3.56	119.80	124.80
11	2	1215	CLA	CHD-C1D-ND	-3.56	119.80	124.80
11	A	1131	CLA	O2A-CGA-CBA	3.56	122.68	111.83
11	k	1402	CLA	CHD-C1D-ND	-3.55	119.80	124.80
11	A	1124	CLA	C2B-C1B-NB	3.55	114.01	110.33
11	0	1401	CLA	CMB-C2B-C1B	3.55	130.83	125.42
11	b	1225	CLA	O2A-CGA-CBA	3.55	122.66	111.83
11	A	1114	CLA	CHD-C1D-ND	-3.55	119.81	124.80
11	a	1126	CLA	O2A-CGA-CBA	3.55	122.66	111.83
11	a	1136	CLA	CHD-C1D-ND	-3.55	119.81	124.80
11	a	1110	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	b	4004	BCR	C38-C26-C25	-3.55	120.61	124.48
11	B	1234	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	L	4019	BCR	C38-C26-C25	-3.55	120.61	124.48
11	2	1203	CLA	CHD-C1D-ND	-3.55	119.81	124.80
11	1	1112	CLA	CHD-C1D-ND	-3.54	119.82	124.80
11	1	1138	CLA	CHD-C1D-ND	-3.54	119.82	124.80
11	1	1134	CLA	CHD-C1D-ND	-3.54	119.82	124.80
14	a	4008	BCR	C7-C8-C9	-3.54	121.00	126.23
11	B	1213	CLA	CHD-C1D-ND	-3.54	119.82	124.80
11	a	1134	CLA	CHD-C1D-ND	-3.54	119.82	124.80
14	B	4004	BCR	C15-C14-C13	-3.54	122.32	127.28
11	B	1211	CLA	C4D-C3D-CAD	3.54	111.95	108.11
11	a	1125	CLA	O2A-CGA-CBA	3.54	122.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1115	CLA	CHD-C1D-ND	-3.54	119.83	124.80
14	2	4014	BCR	C23-C22-C21	3.53	124.57	119.01
11	B	1240	CLA	CHD-C1D-ND	-3.53	119.83	124.80
11	2	1239	CLA	O2A-CGA-CBA	3.53	125.48	112.14
11	A	1107	CLA	C4-C3-C5	3.53	121.36	115.23
11	A	1132	CLA	CHD-C1D-ND	-3.53	119.83	124.80
11	2	1234	CLA	CHD-C1D-ND	-3.53	119.83	124.80
11	a	1129	CLA	CHD-C1D-ND	-3.53	119.83	124.80
14	2	4006	BCR	C33-C5-C4	3.53	121.12	113.60
11	a	1102	CLA	CHD-C1D-ND	-3.53	119.83	124.80
11	a	1105	CLA	O2A-C1-C2	3.53	121.25	109.44
11	a	1011	CLA	O2D-CGD-CBD	3.53	117.40	111.23
11	1	1102	CLA	CHD-C1D-ND	-3.53	119.84	124.80
11	l	1501	CLA	CHD-C1D-ND	-3.53	119.84	124.80
11	1	1107	CLA	C1-O2A-CGA	3.53	125.19	116.65
11	1	1110	CLA	CHD-C1D-ND	-3.53	119.84	124.80
11	b	1204	CLA	O2A-CGA-CBA	3.53	122.58	111.83
11	B	1240	CLA	C2B-C1B-NB	3.52	113.98	110.33
11	a	1128	CLA	CHD-C1D-ND	-3.52	119.84	124.80
11	A	1140	CLA	O2A-C1-C2	3.52	121.66	108.11
11	2	1238	CLA	O2A-CGA-CBA	3.52	122.57	111.83
11	2	1211	CLA	CHD-C1D-ND	-3.52	119.85	124.80
11	a	1104	CLA	C2B-C1B-NB	3.52	113.97	110.33
11	2	1207	CLA	C1-O2A-CGA	3.52	125.17	116.65
14	b	4004	BCR	C15-C14-C13	-3.52	122.34	127.28
11	a	1118	CLA	CHD-C1D-ND	-3.51	119.86	124.80
14	a	4002	BCR	C34-C9-C10	-3.51	117.12	122.82
11	b	1230	CLA	O2A-C1-C2	3.51	121.63	108.11
14	B	4009	BCR	C33-C5-C6	-3.51	120.65	124.48
11	a	1112	CLA	CHD-C1D-ND	-3.51	119.86	124.80
11	b	1213	CLA	CHD-C1D-ND	-3.51	119.86	124.80
11	b	1234	CLA	C1-C2-C3	-3.51	120.44	126.20
11	A	1126	CLA	C2B-C1B-NB	3.51	113.97	110.33
11	a	1119	CLA	CHD-C1D-ND	-3.51	119.86	124.80
11	2	1226	CLA	CHD-C1D-ND	-3.51	119.86	124.80
11	A	1140	CLA	C4-C3-C5	3.51	121.32	115.23
11	A	1138	CLA	CMC-C2C-C1C	3.51	130.52	125.03
11	a	1120	CLA	CHD-C1D-ND	-3.51	119.86	124.80
11	A	1120	CLA	O2A-CGA-CBA	3.51	125.38	112.14
11	a	1114	CLA	CHD-C1D-ND	-3.51	119.87	124.80
11	1	1123	CLA	CHD-C1D-ND	-3.51	119.87	124.80
11	b	1222	CLA	CHD-C1D-ND	-3.50	119.87	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1201	CLA	O2A-CGA-CBA	3.50	122.52	111.83
11	1	1022	CLA	CHD-C1D-ND	-3.50	119.87	124.80
11	B	1235	CLA	CHD-C1D-ND	-3.50	119.87	124.80
11	A	1135	CLA	O2A-C1-C2	3.50	121.59	108.11
11	A	1012	CLA	C1-C2-C3	-3.50	120.46	126.20
11	A	1102	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	A	4003	BCR	C30-C25-C26	-3.50	117.85	122.64
11	B	1227	CLA	CAC-C3C-C4C	3.50	129.34	124.79
11	B	1235	CLA	O2A-CGA-CBA	3.50	122.50	111.83
11	2	1231	CLA	CHD-C1D-ND	-3.50	119.88	124.80
11	B	1234	CLA	CMB-C2B-C1B	3.50	130.74	125.42
11	b	1221	CLA	O2A-CGA-CBA	3.50	122.49	111.83
11	A	1107	CLA	CAA-C2A-C3A	-3.49	103.56	113.00
11	A	1237	CLA	O2A-CGA-CBA	3.49	122.48	111.83
11	A	1113	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	b	4009	BCR	C15-C14-C13	-3.49	122.38	127.28
11	A	1139	CLA	CMC-C2C-C1C	3.49	130.49	125.03
11	2	1219	CLA	CHD-C1D-ND	-3.49	119.89	124.80
11	2	1023	CLA	C1-O2A-CGA	3.49	125.10	116.65
14	B	4009	BCR	C24-C23-C22	-3.49	121.07	126.23
11	1	1135	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	2	4006	BCR	C3-C4-C5	-3.49	107.84	114.06
11	b	1013	CLA	C2B-C1B-NB	3.49	113.94	110.33
11	2	1228	CLA	CHD-C1D-ND	-3.49	119.90	124.80
11	2	1209	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	b	4017	BCR	C1-C6-C5	-3.48	117.88	122.64
11	1	1120	CLA	CHD-C1D-ND	-3.48	119.90	124.80
11	a	1111	CLA	CMB-C2B-C1B	3.48	130.72	125.42
11	b	1212	CLA	CMB-C2B-C1B	3.48	130.72	125.42
11	2	1239	CLA	CHD-C1D-ND	-3.48	119.90	124.80
11	B	1238	CLA	O2A-CGA-CBA	3.48	122.44	111.83
11	B	1219	CLA	CHD-C1D-ND	-3.48	119.91	124.80
11	1	1011	CLA	CHD-C1D-ND	-3.48	119.91	124.80
11	2	1221	CLA	O2A-C1-C2	3.48	121.49	108.11
11	a	1125	CLA	CHD-C1D-ND	-3.48	119.91	124.80
11	A	1131	CLA	CHD-C1D-ND	-3.48	119.91	124.80
11	a	1131	CLA	CHD-C1D-ND	-3.48	119.91	124.80
14	1	4001	BCR	C23-C22-C21	3.48	124.48	119.01
14	A	4001	BCR	C4-C5-C6	-3.48	118.01	122.70
11	A	1112	CLA	CHD-C1D-ND	-3.47	119.91	124.80
14	b	4004	BCR	C30-C25-C26	-3.47	117.89	122.64
11	2	1221	CLA	O2A-CGA-CBA	3.47	122.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1111	CLA	O2A-C1-C2	3.47	121.47	108.11
11	A	1106	CLA	CHD-C1D-ND	-3.47	119.92	124.80
11	1	1116	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	a	4008	BCR	C33-C5-C6	-3.47	120.70	124.48
11	a	1801	CLA	C2B-C1B-NB	3.47	113.92	110.33
11	A	1122	CLA	O2A-C1-C2	3.47	121.46	108.11
14	F	4013	BCR	C23-C22-C21	3.47	124.47	119.01
11	a	1119	CLA	O2A-C1-C2	3.47	121.45	108.11
11	a	1132	CLA	O2A-C1-C2	3.47	121.45	108.11
11	A	1138	CLA	CAC-C3C-C4C	3.46	129.30	124.79
11	1	1140	CLA	CHD-C1D-ND	-3.46	119.93	124.80
11	A	1124	CLA	O2A-C1-C2	3.46	121.44	108.11
15	A	5003	LHG	C5-O7-C7	-3.46	109.52	117.80
11	2	1222	CLA	CHD-C1D-ND	-3.46	119.93	124.80
11	2	1236	CLA	CHD-C1D-ND	-3.46	119.93	124.80
11	2	1230	CLA	O2A-CGA-CBA	3.46	122.37	111.83
11	b	1210	CLA	C1-C2-C3	-3.45	120.54	126.20
11	B	1203	CLA	C4-C3-C5	3.45	121.22	115.23
11	A	1115	CLA	O2A-CGA-CBA	3.45	125.18	112.14
11	a	1102	CLA	C2B-C1B-NB	3.45	113.91	110.33
11	b	1201	CLA	CHD-C1D-ND	-3.45	119.94	124.80
11	B	1021	CLA	CHB-C4A-NA	3.45	129.38	124.40
11	1	1103	CLA	C1-C2-C3	-3.45	120.55	126.20
11	A	1128	CLA	CHD-C1D-ND	-3.45	119.95	124.80
11	A	1012	CLA	C2B-C1B-NB	3.45	113.90	110.33
11	B	1239	CLA	O2A-CGA-CBA	3.44	125.14	112.14
11	a	1108	CLA	CHD-C1D-ND	-3.44	119.96	124.80
11	A	1140	CLA	CHD-C1D-ND	-3.44	119.96	124.80
11	2	1210	CLA	CHD-C1D-ND	-3.44	119.96	124.80
11	1	1106	CLA	C1-O2A-CGA	3.44	124.97	116.65
14	L	4019	BCR	C37-C22-C21	-3.44	117.25	122.82
11	A	1801	CLA	CHD-C1D-ND	-3.44	119.97	124.80
11	b	1223	CLA	CHD-C1D-ND	-3.44	119.97	124.80
14	l	4022	BCR	C37-C22-C21	-3.43	117.25	122.82
11	1	1111	CLA	CHD-C1D-ND	-3.43	119.97	124.80
11	b	1235	CLA	C2B-C1B-NB	3.43	113.89	110.33
11	k	1402	CLA	C3D-C4D-ND	3.43	115.56	109.99
11	a	1022	CLA	CHD-C1D-ND	-3.43	119.97	124.80
11	b	1235	CLA	CHD-C1D-ND	-3.43	119.97	124.80
11	1	1125	CLA	O2A-CGA-CBA	3.43	122.29	111.83
11	2	1217	CLA	CHD-C1D-ND	-3.43	119.98	124.80
11	b	1013	CLA	C1-O2A-CGA	3.43	124.95	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1136	CLA	CHD-C1D-ND	-3.43	119.98	124.80
11	b	1202	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	A	4008	BCR	C27-C26-C25	-3.42	118.08	122.70
11	A	1104	CLA	O2A-C1-C2	3.42	121.27	108.11
14	f	4013	BCR	C23-C22-C21	3.42	124.39	119.01
14	A	4008	BCR	C38-C26-C27	3.42	120.89	113.60
11	1	1102	CLA	C2B-C1B-NB	3.42	113.87	110.33
11	B	1214	CLA	C1-C2-C3	-3.41	120.60	126.20
11	b	1211	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	8	4022	BCR	C38-C26-C25	-3.41	120.76	124.48
11	B	1231	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	b	4009	BCR	C36-C18-C17	-3.41	117.29	122.82
11	1	1120	CLA	O2A-CGA-CBA	3.41	125.02	112.14
11	A	1134	CLA	CHD-C1D-ND	-3.41	120.01	124.80
11	1	1106	CLA	O2A-C1-C2	3.41	121.22	108.11
11	1	1108	CLA	CHD-C1D-ND	-3.41	120.01	124.80
11	A	1107	CLA	CHD-C1D-ND	-3.41	120.01	124.80
11	2	1240	CLA	CHD-C1D-ND	-3.41	120.01	124.80
11	1	1129	CLA	CHD-C1D-ND	-3.41	120.01	124.80
11	b	1219	CLA	CHD-C1D-ND	-3.40	120.01	124.80
11	A	1022	CLA	C2B-C1B-NB	3.40	113.86	110.33
11	2	1214	CLA	O2A-CGA-CBA	3.40	122.21	111.83
11	2	1236	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
11	b	1214	CLA	CHD-C1D-ND	-3.40	120.02	124.80
11	0	1401	CLA	CHD-C1D-ND	-3.40	120.02	124.80
11	B	1204	CLA	CMB-C2B-C1B	3.40	130.59	125.42
14	b	4017	BCR	C19-C18-C17	3.40	124.36	119.01
11	A	1237	CLA	CHD-C1D-ND	-3.40	120.02	124.80
11	a	1118	CLA	O2A-C1-C2	3.40	121.19	108.11
14	1	4003	BCR	C30-C25-C24	3.40	124.86	115.65
11	B	1211	CLA	C3D-C4D-ND	3.39	115.50	109.99
11	A	1123	CLA	O2A-C1-C2	3.39	121.17	108.11
11	1	1122	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	A	4001	BCR	C19-C18-C17	3.39	124.34	119.01
11	A	1127	CLA	CHD-C1D-ND	-3.39	120.03	124.80
11	k	1402	CLA	O2A-C1-C2	3.39	121.15	108.11
11	B	1229	CLA	O2A-C1-C2	3.39	121.14	108.11
11	A	1127	CLA	C9-C8-C10	3.39	123.35	111.27
14	m	4021	BCR	C38-C26-C25	-3.39	120.79	124.48
11	a	1128	CLA	C4-C3-C5	3.39	121.11	115.23
11	K	1401	CLA	CHD-C1D-ND	-3.39	120.04	124.80
11	B	1226	CLA	CHD-C1D-ND	-3.38	120.04	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1138	CLA	C2B-C1B-NB	3.38	113.83	110.33
14	b	4006	BCR	C33-C5-C6	-3.38	120.79	124.48
11	b	1235	CLA	C9-C8-C7	3.38	123.32	111.27
11	L	1501	CLA	C2B-C1B-NB	3.38	113.83	110.33
11	a	1126	CLA	CHD-C1D-ND	-3.38	120.05	124.80
11	b	1239	CLA	O2A-CGA-CBA	3.38	124.89	112.14
11	b	1205	CLA	O2A-C1-C2	3.38	121.10	108.11
14	B	4014	BCR	C30-C25-C26	-3.38	118.02	122.64
11	B	1229	CLA	CMB-C2B-C1B	3.38	130.56	125.42
11	b	1223	CLA	O2A-C1-C2	3.37	121.10	108.11
11	A	1121	CLA	O2A-CGA-CBA	3.37	124.89	112.14
11	b	1212	CLA	CHD-C1D-ND	-3.37	120.05	124.80
11	1	1124	CLA	O2A-C1-C2	3.37	121.09	108.11
11	a	1130	CLA	C2B-C1B-NB	3.37	113.83	110.33
11	A	1125	CLA	CHD-C1D-ND	-3.37	120.05	124.80
11	K	1402	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	2	4009	BCR	C3-C4-C5	-3.37	108.04	114.06
11	2	1235	CLA	CHD-C1D-ND	-3.37	120.06	124.80
11	a	1139	CLA	CHD-C1D-ND	-3.37	120.06	124.80
11	1	1136	CLA	CHD-C1D-ND	-3.37	120.06	124.80
11	b	1228	CLA	C1-C2-C3	-3.37	121.31	126.76
11	2	1227	CLA	CMB-C2B-C1B	3.37	130.54	125.42
11	k	1401	CLA	CHD-C1D-ND	-3.37	120.07	124.80
11	b	1240	CLA	O2A-CGA-CBA	3.36	124.62	114.00
11	1	1111	CLA	C2B-C1B-NB	3.36	113.81	110.33
11	B	1013	CLA	CHD-C1D-ND	-3.36	120.07	124.80
11	b	1207	CLA	C1-O2A-CGA	3.36	124.79	116.65
11	B	1225	CLA	O2A-CGA-CBA	3.36	122.08	111.83
11	a	1135	CLA	O2A-C1-C2	3.36	121.04	108.11
14	1	4001	BCR	C33-C5-C6	-3.36	120.82	124.48
11	k	1402	CLA	C1-C2-C3	-3.36	121.33	126.76
14	A	4003	BCR	C30-C25-C24	3.36	124.76	115.65
11	0	1402	CLA	C3D-C4D-ND	3.36	115.45	109.99
11	8	1501	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	A	4001	BCR	C30-C25-C26	-3.35	118.05	122.64
11	2	1213	CLA	C3D-C4D-ND	3.35	115.44	109.99
11	8	1502	CLA	O2A-CGA-CBA	3.35	124.80	112.14
11	A	1109	CLA	C3D-C4D-ND	3.35	115.44	109.99
11	A	1111	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	b	1226	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	l	1502	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	2	1209	CLA	O2A-CGA-CBA	3.35	124.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1023	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	B	1236	CLA	O2A-C1-C2	3.35	120.41	108.40
11	a	1126	CLA	O2A-C1-C2	3.35	120.99	108.11
11	a	1115	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	b	1216	CLA	CHD-C1D-ND	-3.35	120.09	124.80
11	2	1204	CLA	O2A-CGA-CBA	3.35	122.04	111.83
14	a	4003	BCR	C37-C22-C21	-3.35	117.40	122.82
11	1	1118	CLA	CHD-C1D-ND	-3.34	120.09	124.80
14	a	4008	BCR	C33-C5-C4	3.34	120.73	113.60
11	A	1801	CLA	C2B-C1B-NB	3.34	113.79	110.33
11	A	1117	CLA	O2A-C1-C2	3.34	120.97	108.11
11	a	1132	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	f	4018	BCR	C33-C5-C4	3.34	120.72	113.60
11	k	1401	CLA	C4-C3-C5	3.34	121.03	115.23
14	a	4007	BCR	C7-C8-C9	-3.34	121.30	126.23
11	8	1501	CLA	C1-C2-C3	-3.34	120.73	126.20
11	A	1137	CLA	C3D-C4D-ND	3.34	115.41	109.99
11	B	1206	CLA	C4D-C3D-CAD	3.34	111.73	108.11
11	a	1121	CLA	O2A-CGA-CBA	3.34	124.75	112.14
14	2	4011	BCR	C28-C27-C26	-3.34	108.11	114.06
14	8	4022	BCR	C34-C9-C10	-3.34	117.41	122.82
11	b	1236	CLA	O2A-C1-C2	3.34	120.36	108.40
11	K	1401	CLA	C4-C3-C5	3.33	121.02	115.23
11	a	1122	CLA	CHD-C1D-ND	-3.33	120.12	124.80
11	2	1231	CLA	O2A-CGA-CBA	3.33	124.52	114.00
11	B	1225	CLA	C4D-C3D-CAD	3.33	111.72	108.11
14	2	4014	BCR	C37-C22-C21	-3.33	117.42	122.82
11	b	1203	CLA	C2B-C1B-NB	3.33	113.78	110.33
11	1	1127	CLA	O2A-C1-C2	3.33	120.91	108.11
14	2	4004	BCR	C7-C8-C9	-3.33	121.31	126.23
14	A	4001	BCR	C36-C18-C17	-3.33	117.43	122.82
11	0	1401	CLA	C4-C3-C5	3.33	121.00	115.23
11	2	1207	CLA	CHD-C1D-ND	-3.33	120.12	124.80
14	b	4011	BCR	C28-C27-C26	-3.33	108.13	114.06
11	B	1204	CLA	O2A-CGA-CBA	3.32	121.97	111.83
11	a	1117	CLA	C2B-C1B-NB	3.32	113.77	110.33
11	2	1223	CLA	O2A-C1-C2	3.32	120.89	108.11
11	1	1128	CLA	CHD-C1D-ND	-3.32	120.13	124.80
11	A	1123	CLA	CMB-C2B-C1B	3.32	130.47	125.42
11	1	1137	CLA	CHD-C1D-ND	-3.32	120.13	124.80
11	a	1127	CLA	O2A-C1-C2	3.32	120.88	108.11
11	1	1105	CLA	O2A-C1-C2	3.32	120.55	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	4008	BCR	C38-C26-C27	3.32	120.67	113.60
11	b	1221	CLA	CMC-C2C-C1C	3.32	130.22	125.03
11	a	1113	CLA	CHD-C1D-ND	-3.32	120.14	124.80
14	6	4020	BCR	C27-C26-C25	-3.32	118.22	122.70
11	2	1213	CLA	O2A-C1-C2	3.32	120.87	108.11
11	B	1201	CLA	CHD-C1D-ND	-3.31	120.14	124.80
11	A	1129	CLA	CHD-C1D-ND	-3.31	120.14	124.80
11	2	1235	CLA	C2B-C1B-NB	3.31	113.76	110.33
11	A	1116	CLA	CHD-C1D-ND	-3.31	120.14	124.80
11	B	1206	CLA	CHD-C1D-ND	-3.31	120.14	124.80
11	a	1133	CLA	CHD-C1D-ND	-3.31	120.15	124.80
11	B	1209	CLA	O2A-CGA-CBA	3.31	124.45	114.00
14	b	4014	BCR	C30-C25-C26	-3.31	118.12	122.64
11	1	1127	CLA	C3D-C4D-ND	3.31	115.36	109.99
11	a	1133	CLA	O2A-CGA-CBA	3.31	124.63	112.14
11	B	1220	CLA	CAC-C3C-C4C	3.31	129.09	124.79
11	a	1135	CLA	C1-C2-C3	-3.31	120.78	126.20
11	A	1012	CLA	C9-C8-C10	3.30	123.06	111.27
14	1	4008	BCR	C27-C26-C25	-3.30	118.24	122.70
11	A	1112	CLA	O2A-CGA-CBA	3.30	124.43	114.00
14	2	4006	BCR	C23-C24-C25	-3.30	118.18	127.00
11	A	1137	CLA	C4-C3-C5	3.30	120.96	115.23
11	A	1122	CLA	C3D-C4D-ND	3.30	115.35	109.99
11	1	1103	CLA	CHD-C1D-ND	-3.30	120.16	124.80
11	a	1109	CLA	C2B-C1B-NB	3.30	113.75	110.33
11	b	1023	CLA	CHD-C1D-ND	-3.30	120.16	124.80
11	1	1237	CLA	O2A-CGA-CBA	3.30	121.89	111.83
11	B	1214	CLA	O2A-C1-C2	3.30	120.80	108.11
11	K	1402	CLA	C3D-C4D-ND	3.30	115.34	109.99
11	2	1205	CLA	CMB-C2B-C1B	3.30	130.44	125.42
11	B	1209	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	2	4017	BCR	C36-C18-C17	-3.29	117.48	122.82
11	A	1011	CLA	CHD-C1D-ND	-3.29	120.17	124.80
11	a	1106	CLA	C2B-C1B-NB	3.29	113.74	110.33
11	1	1105	CLA	CMB-C2B-C1B	3.29	130.43	125.42
11	1	1117	CLA	O2A-C1-C2	3.29	120.78	108.11
14	b	4017	BCR	C4-C5-C6	-3.29	118.25	122.70
11	B	1013	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	2	4017	BCR	C27-C26-C25	-3.29	118.26	122.70
11	1	1124	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	6	4013	BCR	C23-C22-C21	3.29	124.19	119.01
11	2	1229	CLA	CMB-C2B-C1B	3.29	130.43	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	4017	BCR	C34-C9-C8	3.29	123.11	118.09
11	b	1234	CLA	CHD-C1D-ND	-3.29	120.18	124.80
14	A	4001	BCR	C37-C22-C21	-3.28	117.49	122.82
11	2	1225	CLA	CMD-C2D-C3D	-3.28	120.16	127.69
11	b	1218	CLA	O2A-CGA-CBA	3.28	124.38	114.00
11	A	1106	CLA	C2B-C1B-NB	3.28	113.73	110.33
11	A	1126	CLA	O2A-C1-C2	3.28	120.74	108.11
11	B	1211	CLA	CHD-C1D-ND	-3.28	120.18	124.80
11	b	1224	CLA	CHD-C1D-ND	-3.28	120.18	124.80
11	a	1123	CLA	CMC-C2C-C1C	3.28	130.16	125.03
11	B	1216	CLA	C3D-C4D-ND	3.28	115.32	109.99
11	A	1136	CLA	C3D-C4D-ND	3.28	115.32	109.99
11	B	1214	CLA	CHD-C1D-ND	-3.28	120.19	124.80
14	2	4004	BCR	C30-C25-C26	-3.28	118.16	122.64
11	b	1213	CLA	C3D-C4D-ND	3.28	115.32	109.99
11	b	1208	CLA	O2A-CGA-CBA	3.28	124.36	114.00
11	b	1222	CLA	C2B-C1B-NB	3.28	113.73	110.33
11	1	1136	CLA	C3D-C4D-ND	3.28	115.32	109.99
11	b	1210	CLA	CHD-C1D-ND	-3.28	120.19	124.80
11	2	1207	CLA	O2A-C1-C2	3.28	120.71	108.11
11	a	1124	CLA	C2B-C1B-NB	3.28	113.72	110.33
14	2	4006	BCR	C34-C9-C10	-3.28	117.51	122.82
11	A	1125	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
11	a	1012	CLA	CHD-C1D-ND	-3.27	120.20	124.80
11	A	1137	CLA	O2A-C1-C2	3.27	120.70	108.11
11	2	1212	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	6	4020	BCR	C28-C27-C26	-3.27	108.22	114.06
11	2	1234	CLA	CMB-C2B-C1B	3.27	130.40	125.42
11	A	1119	CLA	C1-O2A-CGA	3.27	124.57	116.65
11	a	1112	CLA	O2A-CGA-CBA	3.27	124.33	114.00
11	A	1108	CLA	C3D-C4D-ND	3.27	115.30	109.99
14	b	4009	BCR	C7-C8-C9	-3.27	121.40	126.23
11	8	1501	CLA	C2B-C1B-NB	3.27	113.72	110.33
11	a	1012	CLA	O2A-C1-C2	3.27	120.69	108.11
11	B	1201	CLA	C2B-C1B-NB	3.27	113.72	110.33
14	1	4008	BCR	C33-C5-C4	3.27	120.56	113.60
11	8	1502	CLA	CHD-C1D-ND	-3.27	120.20	124.80
11	2	1224	CLA	C1-C2-C3	-3.27	120.84	126.20
14	2	4017	BCR	C34-C9-C8	3.27	123.08	118.09
11	b	1228	CLA	O2A-C1-C2	3.27	120.68	108.11
11	a	1237	CLA	C3D-C4D-ND	3.27	115.30	109.99
11	1	1126	CLA	C2B-C1B-NB	3.27	113.71	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1228	CLA	O2A-C1-C2	3.26	120.67	108.11
11	b	1209	CLA	CHD-C1D-ND	-3.26	120.21	124.80
14	2	4009	BCR	C1-C6-C5	-3.26	118.17	122.64
11	A	1110	CLA	CHD-C1D-ND	-3.26	120.21	124.80
11	a	1126	CLA	CMC-C2C-C1C	3.26	130.13	125.03
11	a	1011	CLA	CHB-C4A-NA	3.26	129.11	124.40
14	A	4008	BCR	C19-C18-C17	3.26	124.14	119.01
11	1	1105	CLA	C3D-C4D-ND	3.26	115.29	109.99
11	B	1223	CLA	OBD-CAD-C3D	-3.26	120.80	128.42
11	b	1219	CLA	C2B-C1B-NB	3.26	113.70	110.33
14	1	4008	BCR	C38-C26-C27	3.26	120.54	113.60
11	1	1123	CLA	CAC-C3C-C4C	3.26	129.03	124.79
11	a	1140	CLA	C1-O2A-CGA	3.26	124.53	116.65
14	b	4011	BCR	C8-C9-C10	3.26	124.13	119.01
11	2	1221	CLA	C4-C3-C5	3.26	120.88	115.23
11	1	1133	CLA	CHD-C1D-ND	-3.25	120.22	124.80
11	1	1107	CLA	CHD-C1D-ND	-3.25	120.22	124.80
14	1	4008	BCR	C30-C25-C26	-3.25	118.19	122.64
11	B	1231	CLA	O2A-CGA-CBA	3.25	124.28	114.00
11	A	1111	CLA	CAC-C3C-C4C	3.25	129.02	124.79
11	A	1119	CLA	O2A-CGA-CBA	3.25	121.75	111.83
11	1	1102	CLA	CMC-C2C-C1C	3.25	130.12	125.03
11	a	1140	CLA	O2A-C1-C2	3.25	120.62	108.11
14	b	4009	BCR	C23-C22-C21	3.25	124.12	119.01
11	2	1210	CLA	CAC-C3C-C4C	3.25	129.02	124.79
11	1	1112	CLA	O2A-CGA-CBA	3.25	124.27	114.00
12	B	2002	PQN	C24-C23-C25	3.25	122.86	111.27
14	B	4006	BCR	C33-C5-C4	3.25	120.53	113.60
11	a	1123	CLA	CAC-C3C-C4C	3.25	129.02	124.79
11	A	1011	CLA	CHB-C4A-NA	3.25	129.09	124.40
11	b	1216	CLA	C3D-C4D-ND	3.25	115.27	109.99
11	a	1126	CLA	C1-C2-C3	-3.25	120.87	126.20
11	B	1023	CLA	C2B-C1B-NB	3.25	113.70	110.33
14	b	4011	BCR	C38-C26-C27	3.25	120.53	113.60
11	A	1011	CLA	O2D-CGD-CBD	3.25	116.91	111.23
11	1	1137	CLA	C4-C3-C2	-3.25	115.28	123.63
14	a	4002	BCR	C38-C26-C27	3.25	120.52	113.60
14	B	4004	BCR	C30-C25-C26	-3.25	118.20	122.64
11	B	1215	CLA	C2B-C1B-NB	3.25	113.69	110.33
11	b	1224	CLA	O2A-C1-C2	3.25	120.60	108.11
14	m	4021	BCR	C38-C26-C27	3.25	120.52	113.60
11	B	1208	CLA	C3D-C4D-ND	3.25	115.26	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1021	CLA	C2B-C1B-NB	3.24	113.69	110.33
11	b	1207	CLA	CMB-C2B-C1B	3.24	130.36	125.42
11	2	1021	CLA	CHB-C4A-NA	3.24	129.08	124.40
11	b	1202	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
11	b	1023	CLA	C1-C2-C3	-3.24	120.89	126.20
11	B	1204	CLA	C2B-C1B-NB	3.24	113.69	110.33
11	A	1126	CLA	C1-C2-C3	-3.24	120.89	126.20
11	B	1212	CLA	C2B-C1B-NB	3.24	113.69	110.33
11	1	1125	CLA	C2B-C1B-NB	3.24	113.68	110.33
11	a	1130	CLA	O2A-CGA-CBA	3.24	124.37	112.14
11	a	1114	CLA	O2A-CGA-CBA	3.24	124.37	112.14
11	2	1202	CLA	O2A-C1-C2	3.24	120.56	108.11
11	2	1234	CLA	O2A-C1-C2	3.24	120.56	108.11
11	b	1023	CLA	C2B-C1B-NB	3.24	113.68	110.33
11	B	1221	CLA	O2A-C1-C2	3.24	120.56	108.11
11	2	1214	CLA	C1-C2-C3	-3.23	120.90	126.20
11	1	1113	CLA	O2A-CGA-CBA	3.23	124.21	114.00
11	2	1230	CLA	CHD-C1D-ND	-3.23	120.25	124.80
11	1	1120	CLA	C2B-C1B-NB	3.23	113.68	110.33
11	B	1201	CLA	O2A-C1-C2	3.23	120.53	108.11
14	b	4014	BCR	C38-C26-C25	-3.23	120.96	124.48
11	a	1139	CLA	CMC-C2C-C1C	3.23	130.08	125.03
11	b	1208	CLA	C3D-C4D-ND	3.23	115.23	109.99
11	a	1127	CLA	CAC-C3C-C4C	3.23	128.99	124.79
11	a	1109	CLA	CMC-C2C-C1C	3.22	130.07	125.03
14	B	4009	BCR	C34-C9-C10	-3.22	117.59	122.82
11	a	1137	CLA	C3D-C4D-ND	3.22	115.23	109.99
11	1	1113	CLA	CHD-C1D-ND	-3.22	120.27	124.80
11	2	1212	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	8	4022	BCR	C38-C26-C27	3.22	120.46	113.60
11	B	1023	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	2	4010	BCR	C23-C24-C25	-3.22	118.40	127.00
11	a	1111	CLA	CHD-C1D-ND	-3.22	120.27	124.80
11	a	1116	CLA	C2B-C1B-NB	3.22	113.66	110.33
14	2	4014	BCR	C19-C18-C17	3.22	124.07	119.01
11	A	1104	CLA	C3D-C4D-ND	3.22	115.22	109.99
11	b	1238	CLA	C3D-C4D-ND	3.22	115.22	109.99
11	B	1225	CLA	CHD-C1D-ND	-3.22	120.28	124.80
11	b	1234	CLA	O2A-C1-C2	3.22	120.49	108.11
14	2	4004	BCR	C24-C23-C22	-3.22	121.48	126.23
14	B	4011	BCR	C38-C26-C27	3.22	120.45	113.60
11	B	1213	CLA	C3D-C4D-ND	3.22	115.21	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1104	CLA	C2B-C1B-NB	3.21	113.66	110.33
11	b	1207	CLA	CHD-C1D-ND	-3.21	120.28	124.80
11	B	1235	CLA	C1-O2A-CGA	3.21	124.43	116.65
14	1	4008	BCR	C24-C23-C22	-3.21	121.48	126.23
11	a	1801	CLA	C1-O2A-CGA	3.21	124.43	116.65
14	b	4009	BCR	C37-C22-C21	-3.21	117.61	122.82
11	1	1127	CLA	C1-C2-C3	-3.21	120.94	126.20
11	2	1220	CLA	O2A-CGA-CBA	3.21	124.27	112.14
11	a	1115	CLA	C3D-C4D-ND	3.21	115.21	109.99
14	A	4007	BCR	C34-C9-C8	3.21	122.99	118.09
11	1	1123	CLA	CMC-C2C-C1C	3.21	130.05	125.03
11	A	1131	CLA	O2A-C1-C2	3.21	120.46	108.11
11	2	1240	CLA	O2A-CGA-CBA	3.21	124.14	114.00
11	2	1206	CLA	CHD-C1D-ND	-3.21	120.29	124.80
11	b	1215	CLA	C2B-C1B-NB	3.21	113.65	110.33
11	b	1236	CLA	C3D-C4D-ND	3.21	115.20	109.99
11	1	1122	CLA	C9-C8-C10	3.21	122.71	111.27
11	2	1235	CLA	CMC-C2C-C1C	3.21	130.05	125.03
11	B	1222	CLA	C4-C3-C2	-3.21	115.39	123.63
11	b	1235	CLA	O2A-C1-C2	3.21	120.45	108.11
11	2	1214	CLA	C3D-C4D-ND	3.21	115.20	109.99
11	B	1207	CLA	CMB-C2B-C1B	3.20	130.30	125.42
14	A	4008	BCR	C36-C18-C17	-3.20	117.62	122.82
11	1	1110	CLA	C2B-C1B-NB	3.20	113.65	110.33
11	A	1118	CLA	C3D-C4D-ND	3.20	115.19	109.99
11	b	1220	CLA	O2A-CGA-CBA	3.20	124.23	112.14
11	b	1217	CLA	C2B-C1B-NB	3.20	113.65	110.33
11	1	1801	CLA	C2B-C1B-NB	3.20	113.65	110.33
11	B	1232	CLA	O2A-CGA-CBA	3.20	124.11	114.00
11	2	1208	CLA	C3D-C4D-ND	3.20	115.19	109.99
11	b	1214	CLA	O2A-C1-C2	3.20	120.43	108.11
14	B	4004	BCR	C38-C26-C27	3.20	120.42	113.60
11	2	1222	CLA	C2B-C1B-NB	3.20	113.64	110.33
11	2	1217	CLA	CAC-C3C-C4C	3.20	128.95	124.79
11	A	1120	CLA	C2B-C1B-NB	3.20	113.64	110.33
11	b	1238	CLA	C2B-C1B-NB	3.20	113.64	110.33
11	2	1226	CLA	C3D-C4D-ND	3.20	115.18	109.99
11	2	1211	CLA	C3D-C4D-ND	3.20	115.18	109.99
11	2	1201	CLA	CHD-C1D-ND	-3.20	120.30	124.80
11	a	1137	CLA	O2A-C1-C2	3.20	120.41	108.11
11	a	1136	CLA	C3D-C4D-ND	3.20	115.18	109.99
11	2	1236	CLA	O2A-C1-C2	3.20	119.86	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1109	CLA	C2B-C1B-NB	3.20	113.64	110.33
14	b	4004	BCR	C38-C26-C27	3.19	120.41	113.60
11	A	1116	CLA	C2B-C1B-NB	3.19	113.64	110.33
11	a	1103	CLA	O2A-C1-C2	3.19	120.40	108.11
11	a	1106	CLA	CHD-C1D-ND	-3.19	120.31	124.80
11	a	1108	CLA	O2A-CGA-CBA	3.19	124.08	114.00
11	B	1205	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
11	A	1110	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
11	A	1133	CLA	CHD-C1D-ND	-3.19	120.32	124.80
11	B	1222	CLA	CHD-C1D-ND	-3.19	120.32	124.80
11	A	1119	CLA	O2A-C1-C2	3.19	120.37	108.11
14	a	4003	BCR	C33-C5-C4	3.19	120.39	113.60
11	1	1801	CLA	O2A-C1-C2	3.19	120.37	108.11
11	b	1211	CLA	C3D-C4D-ND	3.19	115.17	109.99
11	L	1502	CLA	C3D-C4D-ND	3.19	115.17	109.99
11	2	1216	CLA	C9-C8-C10	3.19	122.63	111.27
11	b	1209	CLA	O2A-CGA-CBA	3.18	124.06	114.00
11	a	1125	CLA	C1-C2-C3	-3.18	120.98	126.20
11	2	1203	CLA	O2A-C1-C2	3.18	120.36	108.11
11	B	1205	CLA	O2A-C1-C2	3.18	120.36	108.11
11	B	1223	CLA	O2A-C1-C2	3.18	120.35	108.11
11	1	1101	CLA	CMB-C2B-C1B	3.18	130.26	125.42
14	B	4010	BCR	C33-C5-C4	3.18	120.38	113.60
11	1	1106	CLA	C3D-C4D-ND	3.18	115.16	109.99
11	a	1117	CLA	O2A-C1-C2	3.18	120.35	108.11
11	A	1012	CLA	CHD-C1D-ND	-3.18	120.33	124.80
11	b	1220	CLA	CHD-C1D-ND	-3.18	120.33	124.80
14	B	4005	BCR	C27-C26-C25	-3.18	118.41	122.70
11	A	1012	CLA	O2A-C1-C2	3.18	120.34	108.11
11	A	1132	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
11	B	1214	CLA	C2B-C1B-NB	3.18	113.62	110.33
11	A	1112	CLA	C4D-C3D-CAD	3.18	111.56	108.11
11	B	1228	CLA	C2B-C1B-NB	3.18	113.62	110.33
11	B	1235	CLA	C3D-C4D-ND	3.18	115.15	109.99
14	a	4001	BCR	C23-C22-C21	3.18	124.00	119.01
11	A	1129	CLA	O2A-CGA-CBA	3.18	124.14	112.14
11	2	1221	CLA	C1-O2A-CGA	3.18	124.34	116.65
11	l	1503	CLA	C2B-C1B-NB	3.18	113.62	110.33
11	2	1230	CLA	C2B-C1B-NB	3.18	113.62	110.33
11	a	1237	CLA	CHD-C1D-ND	-3.18	120.33	124.80
11	1	1136	CLA	CMB-C2B-C1B	3.17	130.25	125.42
11	B	1206	CLA	CMB-C2B-C1B	3.17	130.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1205	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	l	4022	BCR	C7-C8-C9	-3.17	121.54	126.23
11	1	1237	CLA	C4-C3-C5	3.17	120.73	115.23
11	0	1401	CLA	O2A-C1-C2	3.17	120.32	108.11
11	a	1101	CLA	C2B-C1B-NB	3.17	113.61	110.33
11	b	1228	CLA	C2B-C1B-NB	3.17	113.61	110.33
11	K	1401	CLA	O2A-C1-C2	3.17	120.31	108.11
11	1	1110	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
11	2	1202	CLA	C3D-C4D-ND	3.17	115.14	109.99
11	k	1401	CLA	O2A-C1-C2	3.17	120.31	108.11
14	B	4011	BCR	C27-C26-C25	-3.17	118.42	122.70
11	A	1022	CLA	O2A-C1-C2	3.17	120.31	108.11
11	1	1135	CLA	O2A-C1-C2	3.17	120.30	108.11
11	A	1118	CLA	C4D-C3D-CAD	3.17	111.55	108.11
11	2	1232	CLA	CMB-C2B-C1B	3.17	130.24	125.42
14	L	4022	BCR	C33-C5-C4	3.17	120.35	113.60
11	a	1123	CLA	O2A-C1-C2	3.17	120.30	108.11
11	b	1221	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	B	4017	BCR	C15-C14-C13	-3.17	122.84	127.28
11	2	1236	CLA	C3D-C4D-ND	3.16	115.13	109.99
14	A	4008	BCR	C38-C26-C25	-3.16	121.03	124.48
11	A	1112	CLA	C2B-C1B-NB	3.16	113.61	110.33
11	b	1226	CLA	C3D-C4D-ND	3.16	115.13	109.99
11	a	1137	CLA	C4-C3-C2	-3.16	115.50	123.63
11	K	1402	CLA	O2A-C1-C2	3.16	120.28	108.11
11	a	1106	CLA	O2A-C1-C2	3.16	120.27	108.11
11	a	1118	CLA	C4D-C3D-CAD	3.16	111.54	108.11
14	a	4002	BCR	C23-C22-C21	3.16	123.98	119.01
11	a	1134	CLA	O2A-CGA-CBA	3.16	124.07	112.14
11	B	1222	CLA	O2A-C1-C2	3.16	120.26	108.11
11	b	1227	CLA	O2A-CGA-CBA	3.16	123.97	114.00
11	a	1103	CLA	C4-C3-C5	3.16	120.71	115.23
11	1	1107	CLA	C4-C3-C5	3.16	120.71	115.23
11	B	1232	CLA	CMB-C2B-C1B	3.16	130.23	125.42
11	B	1220	CLA	O2A-CGA-CBA	3.16	124.06	112.14
11	b	1202	CLA	C2B-C1B-NB	3.16	113.60	110.33
11	b	1231	CLA	O2A-CGA-CBA	3.15	123.97	114.00
11	a	1112	CLA	C2B-C1B-NB	3.15	113.60	110.33
11	a	1113	CLA	O2A-CGA-CBA	3.15	123.97	114.00
11	1	1137	CLA	C2B-C1B-NB	3.15	113.60	110.33
11	b	1221	CLA	O2A-C1-C2	3.15	120.24	108.11
11	a	1107	CLA	C4-C3-C2	-3.15	115.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1138	CLA	CAC-C3C-C4C	3.15	128.89	124.79
11	1	1135	CLA	C2B-C1B-NB	3.15	113.59	110.33
11	A	1111	CLA	O2A-C1-C2	3.15	120.23	108.11
11	A	1134	CLA	O2A-CGA-CBA	3.15	124.04	112.14
11	2	1214	CLA	O2A-C1-C2	3.15	120.23	108.11
11	1	1140	CLA	C9-C8-C7	3.15	122.50	111.27
11	A	1118	CLA	CMC-C2C-C1C	3.15	129.95	125.03
11	B	1224	CLA	C3D-C4D-ND	3.15	115.10	109.99
11	1	1122	CLA	O2A-C1-C2	3.15	120.22	108.11
11	1	1109	CLA	C3D-C4D-ND	3.15	115.10	109.99
11	2	1232	CLA	O2A-CGA-CBA	3.15	123.94	114.00
11	A	1113	CLA	O2A-CGA-CBA	3.14	123.94	114.00
11	2	1221	CLA	CHD-C1D-ND	-3.14	120.38	124.80
11	B	1210	CLA	CHD-C1D-ND	-3.14	120.38	124.80
11	2	1204	CLA	C1-C2-C3	-3.14	121.05	126.20
11	2	1225	CLA	C2B-C1B-NB	3.14	113.58	110.33
11	B	1210	CLA	O2A-C1-C2	3.14	120.20	108.11
11	A	1139	CLA	O2A-C1-C2	3.14	120.19	108.11
11	1	1132	CLA	C2B-C1B-NB	3.14	113.58	110.33
11	A	1121	CLA	CMD-C2D-C3D	-3.14	120.49	127.69
11	b	1229	CLA	C3D-C4D-ND	3.14	115.09	109.99
14	F	4020	BCR	C23-C24-C25	-3.14	118.62	127.00
11	B	1217	CLA	O2A-C1-C2	3.14	119.65	108.40
11	B	1205	CLA	C1-C2-C3	-3.14	121.06	126.20
11	A	1022	CLA	OBD-CAD-C3D	-3.14	121.08	128.42
11	A	1103	CLA	O2A-CGA-CBA	3.14	121.40	111.83
11	B	1221	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
11	1	1237	CLA	C3D-C4D-ND	3.14	115.08	109.99
11	A	1126	CLA	C9-C8-C10	3.13	122.45	111.27
11	A	1122	CLA	C1-O2A-CGA	3.13	124.24	116.65
11	1	1134	CLA	O2A-CGA-CBA	3.13	123.98	112.14
11	a	1134	CLA	C3D-C4D-ND	3.13	115.08	109.99
11	B	1236	CLA	C3D-C4D-ND	3.13	115.08	109.99
11	B	1219	CLA	C2B-C1B-NB	3.13	113.58	110.33
11	2	1222	CLA	O2A-C1-C2	3.13	120.16	108.11
11	B	1231	CLA	CAC-C3C-C4C	3.13	128.86	124.79
11	A	1115	CLA	C3D-C4D-ND	3.13	115.08	109.99
11	A	1105	CLA	CMC-C2C-C1C	3.13	129.93	125.03
11	2	1231	CLA	CMA-C3A-C4A	-3.13	103.36	111.77
11	b	1225	CLA	CHD-C1D-ND	-3.13	120.40	124.80
11	1	1119	CLA	C3D-C4D-ND	3.13	115.07	109.99
11	1	1132	CLA	O2A-CGA-CBA	3.13	121.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1214	CLA	C3D-C4D-ND	3.13	115.07	109.99
11	a	1022	CLA	OBD-CAD-C3D	-3.13	121.11	128.42
11	A	1139	CLA	C1-C2-C3	-3.13	121.70	126.76
11	b	1216	CLA	C9-C8-C10	3.13	122.42	111.27
11	1	1133	CLA	C3D-C4D-ND	3.13	115.07	109.99
11	b	1223	CLA	CAC-C3C-C4C	3.13	128.86	124.79
14	a	4003	BCR	C23-C22-C21	3.12	123.92	119.01
11	A	1106	CLA	O2A-C1-C2	3.12	120.13	108.11
11	A	1121	CLA	C3D-C4D-ND	3.12	115.06	109.99
11	a	1122	CLA	C3D-C4D-ND	3.12	115.06	109.99
11	B	1021	CLA	CHD-C1D-ND	-3.12	120.41	124.80
11	a	1107	CLA	CHD-C1D-ND	-3.12	120.41	124.80
14	1	4003	BCR	C30-C25-C26	-3.12	118.37	122.64
11	a	1106	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
11	a	1121	CLA	C2B-C1B-NB	3.12	113.56	110.33
11	B	1208	CLA	O2A-CGA-CBA	3.12	123.86	114.00
11	a	1237	CLA	C4D-C3D-CAD	3.12	111.50	108.11
11	b	1206	CLA	C4D-C3D-CAD	3.12	111.50	108.11
11	1	1113	CLA	CMB-C2B-C1B	3.12	130.17	125.42
11	a	1139	CLA	O2A-C1-C2	3.12	120.12	108.11
11	2	1229	CLA	C2B-C1B-NB	3.12	113.56	110.33
11	2	1205	CLA	C4D-C3D-CAD	3.12	111.49	108.11
14	B	4017	BCR	C38-C26-C27	3.12	120.25	113.60
11	a	1109	CLA	C3D-C4D-ND	3.12	115.06	109.99
11	8	1501	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	F	4020	BCR	C24-C23-C22	-3.12	121.62	126.23
14	L	4022	BCR	C3-C4-C5	-3.12	108.50	114.06
14	6	4013	BCR	C37-C22-C21	-3.12	117.76	122.82
11	A	1139	CLA	C2B-C1B-NB	3.12	113.56	110.33
11	1	1128	CLA	C3D-C4D-ND	3.12	115.05	109.99
11	2	1219	CLA	C4D-C3D-CAD	3.12	111.49	108.11
11	A	1128	CLA	C1-C2-C3	-3.12	121.09	126.20
14	a	4008	BCR	C1-C6-C5	-3.12	118.38	122.64
11	B	1214	CLA	C4D-C3D-CAD	3.12	111.49	108.11
11	a	1012	CLA	C2B-C1B-NB	3.12	113.56	110.33
11	A	1237	CLA	C3D-C4D-ND	3.11	115.05	109.99
11	a	1124	CLA	O2A-C1-C2	3.11	120.09	108.11
14	1	4001	BCR	C37-C22-C21	-3.11	117.77	122.82
11	2	1217	CLA	C2B-C1B-NB	3.11	113.56	110.33
11	b	1218	CLA	C3D-C4D-ND	3.11	115.05	109.99
11	B	1238	CLA	C3D-C4D-ND	3.11	115.05	109.99
11	a	1128	CLA	C3D-C4D-ND	3.11	115.05	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1227	CLA	C3D-C4D-ND	3.11	115.05	109.99
11	2	1023	CLA	C4-C3-C5	3.11	120.63	115.23
14	b	4010	BCR	C28-C27-C26	-3.11	108.51	114.06
11	1	1133	CLA	O2A-CGA-CBA	3.11	123.89	112.14
11	B	1240	CLA	O2A-CGA-CBA	3.11	123.82	114.00
11	2	1205	CLA	O1D-CGD-CBD	-3.11	118.39	124.52
11	1	1128	CLA	C9-C8-C7	3.11	122.36	111.27
11	b	1205	CLA	CMB-C2B-C1B	3.11	130.15	125.42
11	b	1230	CLA	CHD-C1D-ND	-3.11	120.43	124.80
11	b	1013	CLA	C3D-C4D-ND	3.11	115.04	109.99
11	b	1210	CLA	O2A-C1-C2	3.11	120.06	108.11
11	B	1224	CLA	C4D-C3D-CAD	3.11	111.48	108.11
11	1	1122	CLA	C3D-C4D-ND	3.11	115.04	109.99
11	1	1137	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
11	A	1138	CLA	C4D-C3D-CAD	3.11	111.48	108.11
11	a	1127	CLA	C3D-C4D-ND	3.10	115.03	109.99
14	2	4017	BCR	C34-C9-C10	-3.10	117.79	122.82
11	a	1119	CLA	C3D-C4D-ND	3.10	115.03	109.99
11	b	1240	CLA	C3D-C4D-ND	3.10	115.03	109.99
11	A	1135	CLA	C4-C3-C5	3.10	119.78	116.13
11	a	1126	CLA	C2B-C1B-NB	3.10	113.54	110.33
11	a	1118	CLA	C3D-C4D-ND	3.10	115.03	109.99
11	a	1103	CLA	C11-C12-C13	-3.10	105.66	115.97
11	B	1223	CLA	C4D-C3D-CAD	3.10	111.47	108.11
11	B	1212	CLA	C3D-C4D-ND	3.10	115.02	109.99
14	A	4002	BCR	C31-C1-C6	-3.10	105.39	110.24
11	B	1218	CLA	O2A-CGA-CBA	3.09	123.78	114.00
11	B	1217	CLA	C2B-C1B-NB	3.09	113.53	110.33
11	2	1210	CLA	C2B-C1B-NB	3.09	113.53	110.33
11	2	1210	CLA	O2A-C1-C2	3.09	120.01	108.11
11	2	1223	CLA	C1-C2-C3	-3.09	121.13	126.20
11	b	1212	CLA	O2A-CGA-CBA	3.09	123.77	114.00
11	1	1138	CLA	C3D-C4D-ND	3.09	115.01	109.99
11	b	1206	CLA	O2A-C1-C2	3.09	120.01	108.11
11	1	1022	CLA	OBD-CAD-C3D	-3.09	121.19	128.42
11	2	1203	CLA	C2B-C1B-NB	3.09	113.53	110.33
11	a	1138	CLA	O2A-CGA-CBA	3.09	123.82	112.14
11	l	1503	CLA	C3D-C4D-ND	3.09	115.01	109.99
11	1	1114	CLA	C3D-C4D-ND	3.09	115.01	109.99
11	1	1136	CLA	O2A-CGA-CBA	3.09	123.81	112.14
11	A	1123	CLA	C4D-C3D-CAD	3.09	111.46	108.11
11	1	1131	CLA	C3D-C4D-ND	3.09	115.01	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1011	CLA	CHD-C1D-ND	-3.09	120.45	124.80
11	a	1132	CLA	C1-C2-C3	-3.09	121.14	126.20
11	a	1022	CLA	O2A-C1-C2	3.09	119.99	108.11
14	A	4008	BCR	C33-C5-C4	3.09	120.18	113.60
11	1	1012	CLA	CHD-C1D-ND	-3.09	120.46	124.80
11	2	1021	CLA	CHD-C1D-ND	-3.09	120.46	124.80
11	a	1121	CLA	CMC-C2C-C1C	3.09	129.86	125.03
11	1	1022	CLA	O2A-C1-C2	3.09	119.99	108.11
11	A	1801	CLA	C1-C2-C3	-3.09	121.14	126.20
11	1	1114	CLA	O2A-CGA-CBA	3.09	123.80	112.14
11	A	1105	CLA	O2A-C1-C2	3.09	119.77	109.44
11	A	1117	CLA	CMB-C2B-C3B	3.09	133.81	126.55
14	b	4014	BCR	C36-C18-C17	-3.09	117.82	122.82
14	B	4004	BCR	C24-C23-C22	-3.09	121.67	126.23
11	A	1120	CLA	C4D-C3D-CAD	3.08	111.46	108.11
11	2	1201	CLA	C1-O2A-CGA	3.08	124.11	116.65
11	2	1228	CLA	O2A-C1-C2	3.08	119.96	108.11
14	6	4013	BCR	C30-C25-C24	3.08	124.00	115.65
11	b	1203	CLA	C9-C8-C7	3.08	122.25	111.27
11	a	1138	CLA	CMD-C2D-C3D	-3.08	120.63	127.69
11	1	1123	CLA	O2A-C1-C2	3.08	119.95	108.11
11	B	1212	CLA	O2A-CGA-CBA	3.08	123.72	114.00
11	b	1204	CLA	C3D-C4D-ND	3.08	114.99	109.99
11	b	1207	CLA	O2A-C1-C2	3.08	119.95	108.11
14	B	4011	BCR	C38-C26-C25	-3.08	121.13	124.48
11	A	1128	CLA	C3D-C4D-ND	3.08	114.99	109.99
11	a	1109	CLA	O2A-C1-C2	3.08	119.95	108.11
14	1	4002	BCR	C3-C4-C5	-3.08	108.57	114.06
11	2	1219	CLA	CMB-C2B-C3B	3.08	133.78	126.55
11	2	1238	CLA	C2B-C1B-NB	3.08	113.52	110.33
11	2	1218	CLA	O2A-CGA-CBA	3.08	123.72	114.00
11	B	1227	CLA	O2A-CGA-CBA	3.07	123.71	114.00
11	2	1217	CLA	O2A-C1-C2	3.07	119.42	108.40
11	B	1207	CLA	C2B-C1B-NB	3.07	113.51	110.33
11	1	1103	CLA	C2B-C1B-NB	3.07	113.51	110.33
11	2	1205	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
11	2	1227	CLA	O2A-CGA-CBA	3.07	123.71	114.00
14	B	4006	BCR	C23-C24-C25	-3.07	118.79	127.00
11	A	1103	CLA	C3D-C4D-ND	3.07	114.98	109.99
11	B	1224	CLA	C1-C2-C3	-3.07	121.17	126.20
11	b	1211	CLA	O2A-CGA-CBA	3.07	123.74	112.14
11	1	1112	CLA	C3D-C4D-ND	3.07	114.98	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1118	CLA	CMB-C2B-C1B	3.07	130.09	125.42
14	F	4020	BCR	C19-C18-C17	3.07	123.84	119.01
11	a	1110	CLA	C3D-C4D-ND	3.07	114.98	109.99
14	2	4004	BCR	C38-C26-C27	3.07	120.14	113.60
11	a	1108	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	b	1209	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	A	1022	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	2	1210	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	0	1402	CLA	O2A-C1-C2	3.07	119.91	108.11
11	B	1023	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	1	1104	CLA	C3D-C4D-ND	3.07	114.97	109.99
11	A	1114	CLA	O2A-CGA-CBA	3.07	123.72	112.14
11	1	1134	CLA	C3D-C4D-ND	3.06	114.97	109.99
11	B	1204	CLA	C3D-C4D-ND	3.06	114.97	109.99
11	2	1218	CLA	C2B-C1B-NB	3.06	113.50	110.33
11	A	1113	CLA	C3D-C4D-ND	3.06	114.97	109.99
11	2	1205	CLA	CMC-C2C-C1C	3.06	129.82	125.03
11	1	1012	CLA	C9-C8-C7	3.06	122.19	111.27
11	a	1012	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	b	4017	BCR	C38-C26-C27	3.06	120.12	113.60
11	b	1240	CLA	C2B-C1B-NB	3.06	113.50	110.33
11	B	1229	CLA	C1-C2-C3	-3.06	121.18	126.20
11	A	1101	CLA	C2B-C1B-NB	3.06	113.50	110.33
11	1	1118	CLA	CMC-C2C-C1C	3.06	129.81	125.03
11	a	1101	CLA	O2A-C1-C2	3.06	119.88	108.11
14	B	4014	BCR	C38-C26-C25	-3.06	121.15	124.48
14	b	4017	BCR	C30-C25-C26	-3.06	118.46	122.64
11	A	1107	CLA	C2B-C1B-NB	3.06	113.50	110.33
11	B	1202	CLA	C3D-C4D-ND	3.06	114.96	109.99
11	2	1209	CLA	CAC-C3C-C4C	3.06	128.77	124.79
11	1	1101	CLA	C3D-C4D-ND	3.06	114.96	109.99
11	2	1238	CLA	C3D-C4D-ND	3.06	114.96	109.99
11	B	1225	CLA	C2B-C1B-NB	3.06	113.50	110.33
11	a	1117	CLA	C9-C8-C7	3.06	122.17	111.27
14	a	4008	BCR	C4-C5-C6	-3.06	118.57	122.70
11	A	1107	CLA	C4D-C3D-CAD	3.06	111.42	108.11
14	m	4021	BCR	C36-C18-C17	-3.06	117.87	122.82
11	1	1103	CLA	O2A-C1-C2	3.06	119.86	108.11
14	B	4010	BCR	C37-C22-C21	-3.05	117.87	122.82
11	B	1229	CLA	C3D-C4D-ND	3.05	114.95	109.99
11	2	1217	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
15	A	5001	LHG	C5-O7-C7	-3.05	110.49	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1130	CLA	O2A-CGA-CBA	3.05	123.67	112.14
11	a	1111	CLA	CAC-C3C-C4C	3.05	128.76	124.79
11	A	1117	CLA	C3D-C4D-ND	3.05	114.95	109.99
11	2	1204	CLA	C3D-C4D-ND	3.05	114.95	109.99
11	a	1134	CLA	C4D-C3D-CAD	3.05	111.42	108.11
11	B	1219	CLA	C1-C2-C3	-3.05	121.20	126.20
11	B	1222	CLA	CMB-C2B-C3B	3.05	133.72	126.55
11	a	1103	CLA	C2B-C1B-NB	3.05	113.49	110.33
11	b	1232	CLA	C3D-C4D-ND	3.05	114.94	109.99
14	A	4002	BCR	C38-C26-C27	3.05	120.10	113.60
11	a	1103	CLA	C3D-C4D-ND	3.05	114.94	109.99
14	2	4006	BCR	C1-C6-C7	3.05	123.92	115.65
11	A	1101	CLA	C1-C2-C3	-3.05	121.20	126.20
11	1	1111	CLA	CHB-C4A-NA	3.05	128.80	124.40
11	A	1108	CLA	O2A-CGA-CBA	3.05	123.63	114.00
11	1	1104	CLA	O2A-C1-C2	3.05	119.83	108.11
11	b	1205	CLA	C1-C2-C3	-3.05	121.21	126.20
11	a	1237	CLA	CMC-C2C-C1C	3.05	129.79	125.03
11	A	1108	CLA	C2B-C1B-NB	3.05	113.48	110.33
11	A	1138	CLA	C2B-C1B-NB	3.05	113.48	110.33
11	l	1502	CLA	CMC-C2C-C1C	3.04	129.79	125.03
11	B	1218	CLA	C3D-C4D-ND	3.04	114.94	109.99
14	2	4017	BCR	C7-C8-C9	-3.04	121.73	126.23
14	1	4008	BCR	C23-C24-C25	-3.04	118.87	127.00
11	A	1137	CLA	C4D-C3D-CAD	3.04	111.41	108.11
14	b	4005	BCR	C38-C26-C27	3.04	120.08	113.60
11	2	1231	CLA	CMC-C2C-C1C	3.04	129.79	125.03
11	a	1116	CLA	C3D-C4D-ND	3.04	114.93	109.99
11	a	1129	CLA	C3D-C4D-ND	3.04	114.93	109.99
11	b	1021	CLA	CHD-C1D-ND	-3.04	120.52	124.80
11	B	1210	CLA	C1-C2-C3	-3.04	121.22	126.20
11	a	1133	CLA	C3D-C4D-ND	3.04	114.93	109.99
11	1	1107	CLA	C3D-C4D-ND	3.04	114.93	109.99
11	l	1502	CLA	O2A-CGA-CBA	3.04	123.62	112.14
11	B	1211	CLA	CMD-C2D-C3D	-3.04	120.72	127.69
11	B	1203	CLA	C3D-C4D-ND	3.04	114.92	109.99
11	1	1115	CLA	C2B-C1B-NB	3.04	113.48	110.33
14	a	4001	BCR	C37-C22-C21	-3.04	117.90	122.82
11	l	1502	CLA	C3D-C4D-ND	3.04	114.92	109.99
11	A	1107	CLA	O2A-C1-C2	3.04	119.79	108.11
11	2	1203	CLA	CMB-C2B-C1B	3.03	130.04	125.42
11	a	1131	CLA	O2A-C1-C2	3.03	119.78	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	2002	PQN	C24-C23-C25	3.03	122.09	111.27
11	B	1228	CLA	C3D-C4D-ND	3.03	114.92	109.99
14	2	4006	BCR	C33-C5-C6	-3.03	121.17	124.48
11	A	1128	CLA	O2A-C1-C2	3.03	119.78	108.11
11	A	1138	CLA	C3D-C4D-ND	3.03	114.92	109.99
11	A	1135	CLA	C3D-C4D-ND	3.03	114.92	109.99
14	b	4017	BCR	C33-C5-C4	3.03	120.06	113.60
11	b	1232	CLA	C2B-C1B-NB	3.03	113.47	110.33
11	2	1228	CLA	C2B-C1B-NB	3.03	113.47	110.33
14	B	4014	BCR	C3-C4-C5	-3.03	108.65	114.06
11	B	1224	CLA	O2A-C1-C2	3.03	119.77	108.11
11	2	1208	CLA	O2A-CGA-CBA	3.03	123.57	114.00
11	b	1213	CLA	CMC-C2C-C1C	3.03	129.77	125.03
11	1	1126	CLA	C9-C8-C10	3.03	122.07	111.27
14	A	4008	BCR	C30-C25-C26	-3.03	118.50	122.64
11	2	1206	CLA	O2A-C1-C2	3.03	119.76	108.11
14	2	4011	BCR	C8-C9-C10	3.03	123.77	119.01
14	a	4003	BCR	C30-C25-C24	3.03	123.86	115.65
11	a	1111	CLA	C9-C8-C7	3.03	122.07	111.27
14	B	4014	BCR	C38-C26-C27	3.03	120.05	113.60
11	1	1129	CLA	C3D-C4D-ND	3.03	114.91	109.99
11	2	1238	CLA	O2A-C1-C2	3.03	119.76	108.11
11	1	1103	CLA	C4D-C3D-CAD	3.03	111.39	108.11
11	1	1103	CLA	CMB-C2B-C1B	3.03	130.03	125.42
11	a	1022	CLA	C2B-C1B-NB	3.03	113.46	110.33
11	A	1134	CLA	CAC-C3C-C4C	3.03	128.73	124.79
11	a	1137	CLA	C9-C8-C7	3.03	122.06	111.27
11	a	1111	CLA	C3D-C4D-ND	3.03	114.91	109.99
14	f	4018	BCR	C38-C26-C25	-3.03	121.18	124.48
11	2	1223	CLA	C2B-C1B-NB	3.02	113.46	110.33
11	B	1013	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	1	1126	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	a	1128	CLA	O2A-C1-C2	3.02	119.74	108.11
11	A	1133	CLA	O2A-CGA-CBA	3.02	123.56	112.14
11	b	1227	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	2	1023	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	1	1117	CLA	C2B-C1B-NB	3.02	113.46	110.33
11	1	1121	CLA	C2B-C1B-NB	3.02	113.46	110.33
11	a	1127	CLA	C4D-C3D-CAD	3.02	111.39	108.11
11	1	1126	CLA	O2A-C1-C2	3.02	119.73	108.11
11	A	1101	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	b	1201	CLA	C3D-C4D-ND	3.02	114.90	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	4004	BCR	C24-C23-C22	-3.02	121.77	126.23
11	1	1139	CLA	C3D-C4D-ND	3.02	114.90	109.99
11	1	1115	CLA	O2A-CGA-CBA	3.02	123.55	112.14
11	A	1114	CLA	C3D-C4D-ND	3.02	114.89	109.99
11	2	1232	CLA	C3D-C4D-ND	3.02	114.89	109.99
11	A	1115	CLA	CMC-C2C-C1C	3.02	129.75	125.03
11	1	1118	CLA	C3D-C4D-ND	3.02	114.89	109.99
11	1	1126	CLA	C1-C2-C3	-3.02	121.25	126.20
11	A	1139	CLA	C4D-C3D-CAD	3.02	111.38	108.11
14	1	4001	BCR	C38-C26-C25	-3.02	121.19	124.48
11	1	1112	CLA	CMB-C2B-C1B	3.02	130.01	125.42
11	1	1119	CLA	C4-C3-C5	3.01	120.46	115.23
11	a	1120	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	1	1022	CLA	C2B-C1B-NB	3.01	113.45	110.33
14	2	4004	BCR	C33-C5-C4	3.01	120.02	113.60
11	a	1112	CLA	C3D-C4D-ND	3.01	114.89	109.99
14	a	4001	BCR	C1-C6-C5	-3.01	118.52	122.64
11	2	1204	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	B	1201	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
11	1	1121	CLA	CMB-C2B-C1B	3.01	130.01	125.42
11	1	1138	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	a	1104	CLA	C3D-C4D-ND	3.01	114.88	109.99
11	a	1139	CLA	C4D-C3D-CAD	3.01	111.38	108.11
11	a	1119	CLA	C1-C2-C3	-3.01	121.26	126.20
11	a	1128	CLA	C9-C8-C7	3.01	122.00	111.27
11	2	1224	CLA	C4D-C3D-CAD	3.01	111.38	108.11
11	2	1225	CLA	O2A-CGA-CBA	3.01	121.01	111.83
14	B	4014	BCR	C36-C18-C17	-3.01	117.94	122.82
11	A	1105	CLA	C3D-C4D-ND	3.01	114.88	109.99
11	b	1217	CLA	O2A-C1-C2	3.01	119.19	108.40
11	1	1126	CLA	CMC-C2C-C1C	3.01	129.74	125.03
11	a	1107	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	2	1207	CLA	C2B-C1B-NB	3.01	113.45	110.33
11	2	1023	CLA	CHB-C4A-NA	3.01	128.74	124.40
11	a	1136	CLA	O2A-CGA-CBA	3.01	123.50	112.14
11	B	1225	CLA	C3D-C4D-ND	3.01	114.88	109.99
11	1	1130	CLA	C3D-C4D-ND	3.01	114.88	109.99
11	A	1130	CLA	O2A-CGA-CBA	3.01	123.50	112.14
11	b	1221	CLA	CHD-C1D-ND	-3.01	120.57	124.80
11	1	1128	CLA	O2A-C1-C2	3.01	119.67	108.11
11	b	1204	CLA	C2B-C1B-NB	3.00	113.44	110.33
14	a	4008	BCR	C34-C9-C10	-3.00	117.95	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1105	CLA	C3D-C4D-ND	3.00	114.87	109.99
11	b	1201	CLA	O2A-C1-C2	3.00	119.67	108.11
11	1	1116	CLA	C3D-C4D-ND	3.00	114.87	109.99
11	L	1503	CLA	C2B-C1B-NB	3.00	113.44	110.33
11	B	1013	CLA	C9-C8-C10	3.00	121.97	111.27
11	a	1117	CLA	C3D-C4D-ND	3.00	114.86	109.99
11	B	1203	CLA	C2B-C1B-NB	3.00	113.44	110.33
11	A	1801	CLA	O2A-C1-C2	3.00	119.65	108.11
11	b	1230	CLA	C2B-C1B-NB	3.00	113.44	110.33
14	B	4014	BCR	C37-C22-C21	-3.00	117.96	122.82
11	A	1118	CLA	O2A-C1-C2	3.00	119.64	108.11
11	b	1021	CLA	C1-O2A-CGA	3.00	123.90	116.65
14	2	4017	BCR	C33-C5-C6	-3.00	121.22	124.48
11	A	1136	CLA	O2A-CGA-CBA	3.00	123.46	112.14
11	A	1113	CLA	CMC-C2C-C1C	3.00	129.72	125.03
11	b	1235	CLA	C3D-C4D-ND	3.00	114.86	109.99
11	l	1503	CLA	C4-C3-C5	3.00	120.43	115.23
11	1	1103	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
11	a	1107	CLA	C4D-C3D-CAD	2.99	111.36	108.11
11	2	1226	CLA	C4D-C3D-CAD	2.99	111.36	108.11
11	A	1130	CLA	C2B-C1B-NB	2.99	113.43	110.33
11	1	1108	CLA	O2A-CGA-CBA	2.99	123.46	114.00
11	A	1127	CLA	O2A-C1-C2	2.99	119.63	108.11
14	1	4008	BCR	C38-C26-C25	-2.99	121.22	124.48
11	1	1139	CLA	C4D-C3D-CAD	2.99	111.36	108.11
14	1	4003	BCR	C38-C26-C25	-2.99	121.22	124.48
11	1	1109	CLA	O2A-C1-C2	2.99	119.62	108.11
11	A	1237	CLA	C4-C3-C5	2.99	120.42	115.23
11	1	1129	CLA	O2A-CGA-CBA	2.99	123.44	112.14
11	B	1207	CLA	O2A-C1-C2	2.99	119.61	108.11
11	a	1801	CLA	O2A-C1-C2	2.99	119.61	108.11
11	A	1138	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
11	a	1110	CLA	C2B-C1B-NB	2.99	113.43	110.33
14	B	4017	BCR	C34-C9-C8	2.99	122.65	118.09
11	A	1137	CLA	C4-C3-C2	-2.99	115.95	123.63
11	a	1136	CLA	CMB-C2B-C1B	2.99	129.97	125.42
11	A	1104	CLA	C2B-C1B-NB	2.99	113.42	110.33
11	b	1021	CLA	C2B-C1B-NB	2.99	113.42	110.33
11	2	1232	CLA	C2B-C1B-NB	2.99	113.42	110.33
11	a	1133	CLA	CMB-C2B-C1B	2.99	129.97	125.42
11	2	1235	CLA	C3D-C4D-ND	2.99	114.84	109.99
11	2	1225	CLA	C4D-C3D-CAD	2.99	111.35	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1214	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
11	A	1119	CLA	C2B-C1B-NB	2.99	113.42	110.33
11	l	1501	CLA	C2B-C1B-NB	2.99	113.42	110.33
11	A	1127	CLA	C3D-C4D-ND	2.98	114.84	109.99
11	1	1122	CLA	C4-C3-C5	2.98	120.41	115.23
11	a	1121	CLA	CMD-C2D-C3D	-2.98	120.85	127.69
11	2	1225	CLA	C3D-C4D-ND	2.98	114.84	109.99
11	A	1109	CLA	O2A-C1-C2	2.98	119.59	108.11
11	B	1207	CLA	C1-O2A-CGA	2.98	123.87	116.65
15	2	5004	LHG	O8-C23-C24	2.98	120.93	111.83
11	2	1013	CLA	C3D-C4D-ND	2.98	114.83	109.99
11	1	1109	CLA	C2B-C1B-NB	2.98	113.42	110.33
11	2	1224	CLA	C3D-C4D-ND	2.98	114.83	109.99
11	A	1116	CLA	CMC-C2C-C1C	2.98	129.69	125.03
11	b	1232	CLA	CMC-C2C-C1C	2.98	129.69	125.03
11	2	1023	CLA	CMB-C2B-C1B	2.98	129.95	125.42
11	A	1131	CLA	CMB-C2B-C1B	2.98	129.95	125.42
11	a	1105	CLA	C1-O2A-CGA	2.97	123.85	116.65
11	B	1201	CLA	C4D-C3D-CAD	2.97	111.34	108.11
11	1	1138	CLA	O2A-CGA-CBA	2.97	123.37	112.14
11	1	1102	CLA	O2A-C1-C2	2.97	119.55	108.11
11	b	1225	CLA	C3D-C4D-ND	2.97	114.82	109.99
11	2	1202	CLA	CMD-C2D-C3D	-2.97	120.87	127.69
11	2	1229	CLA	O2A-C1-C2	2.97	119.55	108.11
11	a	1130	CLA	C3D-C4D-ND	2.97	114.82	109.99
14	2	4014	BCR	C3-C4-C5	-2.97	108.76	114.06
11	A	1126	CLA	CMC-C2C-C1C	2.97	129.68	125.03
11	A	1103	CLA	C4D-C3D-CAD	2.97	111.33	108.11
11	b	1218	CLA	C2B-C1B-NB	2.97	113.41	110.33
11	l	1501	CLA	C3D-C4D-ND	2.97	114.81	109.99
14	M	4021	BCR	C19-C18-C17	2.97	123.68	119.01
11	1	1139	CLA	CMC-C2C-C1C	2.97	129.67	125.03
11	A	1011	CLA	O2A-C1-C2	2.97	119.53	108.11
15	1	5003	LHG	O8-C23-C24	2.97	120.89	111.83
11	B	1202	CLA	CMB-C2B-C3B	2.97	133.53	126.55
11	b	1210	CLA	C2B-C1B-NB	2.97	113.40	110.33
11	b	1220	CLA	C2B-C1B-NB	2.97	113.40	110.33
11	1	1139	CLA	C2B-C1B-NB	2.97	113.40	110.33
14	L	4019	BCR	C34-C9-C10	-2.97	118.01	122.82
11	B	1211	CLA	O2A-CGA-CBA	2.97	123.35	112.14
14	m	4021	BCR	C27-C26-C25	-2.97	118.69	122.70
11	a	1131	CLA	C1-C2-C3	-2.97	121.33	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1117	CLA	C3D-C4D-ND	2.97	114.81	109.99
11	b	1235	CLA	C1-O2A-CGA	2.97	123.83	116.65
11	2	1213	CLA	CAC-C3C-C2C	2.97	133.01	127.56
11	8	1503	CLA	C3D-C4D-ND	2.97	114.81	109.99
11	1	1012	CLA	C3C-C4C-NC	2.97	114.23	110.43
11	L	1503	CLA	C3D-C4D-ND	2.96	114.81	109.99
11	b	1205	CLA	C2B-C1B-NB	2.96	113.40	110.33
11	A	1130	CLA	C3D-C4D-ND	2.96	114.81	109.99
11	1	1123	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
11	a	1129	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
11	A	1111	CLA	C2B-C1B-NB	2.96	113.40	110.33
11	B	1239	CLA	C2B-C1B-NB	2.96	113.40	110.33
11	1	1118	CLA	C4D-C3D-CAD	2.96	111.32	108.11
11	b	1232	CLA	O2A-CGA-CBA	2.96	123.36	114.00
11	A	1123	CLA	CMD-C2D-C3D	-2.96	120.90	127.69
11	a	1127	CLA	CHD-C1D-ND	-2.96	120.64	124.80
14	a	4001	BCR	C15-C14-C13	-2.96	123.13	127.28
11	b	1216	CLA	C1-C2-C3	-2.96	121.35	126.20
11	a	1106	CLA	C4-C3-C5	2.96	120.36	115.23
11	2	1240	CLA	C2B-C1B-NB	2.96	113.39	110.33
11	A	1137	CLA	C9-C8-C10	2.96	121.82	111.27
11	a	1140	CLA	C3D-C4D-ND	2.96	114.80	109.99
11	B	1234	CLA	C1-C2-C3	-2.96	121.35	126.20
11	8	1503	CLA	O2A-C1-C2	2.96	119.50	108.11
15	a	5001	LHG	O8-C23-C24	2.96	120.86	111.83
11	a	1012	CLA	CMC-C2C-C1C	2.96	129.66	125.03
11	B	1234	CLA	O2A-C1-C2	2.96	119.49	108.11
11	b	1225	CLA	C4D-C3D-CAD	2.96	111.32	108.11
11	a	1124	CLA	C3D-C4D-ND	2.96	114.79	109.99
11	2	1222	CLA	CMC-C2C-C1C	2.96	129.65	125.03
11	B	1227	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
11	B	1226	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
11	B	1232	CLA	CAC-C3C-C4C	2.95	128.63	124.79
11	2	1205	CLA	C3D-C4D-ND	2.95	114.79	109.99
11	2	1231	CLA	CMD-C2D-C3D	-2.95	120.92	127.69
14	B	4006	BCR	C15-C14-C13	-2.95	123.14	127.28
11	A	1103	CLA	C2B-C1B-NB	2.95	113.39	110.33
11	1	1101	CLA	C2B-C1B-NB	2.95	113.39	110.33
14	M	4021	BCR	C34-C9-C10	-2.95	118.03	122.82
14	8	4022	BCR	C33-C5-C4	2.95	119.89	113.60
15	A	5003	LHG	O8-C23-C24	2.95	120.83	111.83
11	B	1205	CLA	CHD-C1D-ND	-2.95	120.65	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1235	CLA	C9-C8-C7	2.95	121.79	111.27
11	2	1209	CLA	C2B-C1B-NB	2.95	113.39	110.33
11	k	1401	CLA	C2B-C1B-NB	2.95	113.39	110.33
15	B	5004	LHG	C5-O7-C7	-2.95	110.74	117.80
11	A	1119	CLA	C3D-C4D-ND	2.95	114.78	109.99
11	B	1214	CLA	C3D-C4D-ND	2.95	114.78	109.99
11	b	1023	CLA	C3D-C4D-ND	2.95	114.78	109.99
11	2	1211	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
11	b	1214	CLA	C2B-C1B-NB	2.95	113.38	110.33
11	a	1122	CLA	C4-C3-C5	2.95	120.34	115.23
11	a	1801	CLA	C3D-C4D-ND	2.95	114.78	109.99
11	1	1011	CLA	CHA-C1A-NA	-2.95	119.72	126.39
11	1	1132	CLA	O2A-C1-C2	2.95	119.44	108.11
14	a	4002	BCR	C3-C4-C5	-2.95	108.80	114.06
11	A	1111	CLA	C3D-C4D-ND	2.95	114.77	109.99
11	b	1214	CLA	C1-C2-C3	-2.94	121.37	126.20
11	A	1115	CLA	C2B-C1B-NB	2.94	113.38	110.33
14	b	4005	BCR	C30-C25-C26	-2.94	118.61	122.64
11	b	1210	CLA	C3D-C4D-ND	2.94	114.77	109.99
11	B	1210	CLA	C3D-C4D-ND	2.94	114.77	109.99
11	A	1127	CLA	C2B-C1B-NB	2.94	113.38	110.33
11	B	1226	CLA	C3D-C4D-ND	2.94	114.77	109.99
11	1	1137	CLA	C3D-C4D-ND	2.94	114.77	109.99
11	A	1133	CLA	CMB-C2B-C1B	2.94	129.90	125.42
11	1	1108	CLA	C3D-C4D-ND	2.94	114.77	109.99
11	B	1235	CLA	C2B-C1B-NB	2.94	113.38	110.33
11	b	1212	CLA	CMC-C2C-C1C	2.94	129.63	125.03
11	2	1236	CLA	CMC-C2C-C1C	2.94	129.63	125.03
11	b	1213	CLA	O2A-C1-C2	2.94	119.42	108.11
11	B	1227	CLA	C3D-C4D-ND	2.94	114.76	109.99
11	a	1022	CLA	C3D-C4D-ND	2.94	114.76	109.99
11	B	1202	CLA	O2A-C1-C2	2.94	119.42	108.11
11	1	1132	CLA	C1-O2A-CGA	2.94	123.76	116.65
11	b	1229	CLA	C2B-C1B-NB	2.94	113.37	110.33
11	B	1203	CLA	O2A-C1-C2	2.94	119.42	108.11
14	b	4010	BCR	C24-C23-C22	-2.94	121.89	126.23
11	a	1131	CLA	C3D-C4D-ND	2.94	114.76	109.99
11	b	1202	CLA	C4D-C3D-CAD	2.94	111.30	108.11
11	2	1223	CLA	C4D-C3D-CAD	2.94	111.30	108.11
11	B	1215	CLA	C4-C3-C2	-2.94	116.08	123.63
11	A	1101	CLA	O2A-C1-C2	2.94	119.41	108.11
11	1	1129	CLA	C4D-C3D-CAD	2.94	111.30	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1219	CLA	C4-C3-C5	2.94	120.32	115.23
11	A	1126	CLA	C3D-C4D-ND	2.94	114.76	109.99
11	1	1111	CLA	C3D-C4D-ND	2.94	114.76	109.99
14	A	4001	BCR	C7-C8-C9	-2.94	121.89	126.23
11	2	1207	CLA	C3D-C4D-ND	2.93	114.75	109.99
11	B	1219	CLA	O2A-C1-C2	2.93	119.40	108.11
11	b	1214	CLA	C4-C3-C5	2.93	120.32	115.23
11	A	1103	CLA	O2A-C1-C2	2.93	119.39	108.11
11	a	1125	CLA	O2A-C1-C2	2.93	119.39	108.11
11	B	1207	CLA	C4D-C3D-CAD	2.93	111.29	108.11
11	1	1105	CLA	C4D-C3D-CAD	2.93	111.29	108.11
11	b	1201	CLA	C1-C2-C3	-2.93	121.39	126.20
11	a	1109	CLA	C9-C8-C10	2.93	121.72	111.27
11	2	1235	CLA	C4-C3-C5	2.93	120.31	115.23
11	1	1118	CLA	C2B-C1B-NB	2.93	113.36	110.33
11	A	1120	CLA	CMD-C2D-C3D	-2.93	120.97	127.69
11	2	1220	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	B	4010	BCR	C15-C14-C13	-2.93	123.17	127.28
11	A	1129	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	M	4021	BCR	C36-C18-C17	-2.93	118.07	122.82
11	1	1105	CLA	C2B-C1B-NB	2.93	113.36	110.33
11	b	1206	CLA	C3D-C4D-ND	2.93	114.75	109.99
11	a	1122	CLA	C4D-C3D-CAD	2.93	111.29	108.11
11	b	1223	CLA	C1-C2-C3	-2.93	121.40	126.20
14	b	4004	BCR	C3-C4-C5	-2.93	108.83	114.06
11	B	1214	CLA	C9-C8-C7	2.93	121.71	111.27
11	1	1111	CLA	C9-C8-C7	2.93	121.71	111.27
11	1	1112	CLA	C2B-C1B-NB	2.93	113.36	110.33
11	A	1012	CLA	OBD-CAD-C3D	-2.93	121.57	128.42
14	2	4009	BCR	C33-C5-C4	2.93	119.84	113.60
11	2	1214	CLA	C2B-C1B-NB	2.93	113.36	110.33
11	a	1131	CLA	C2B-C1B-NB	2.93	113.36	110.33
11	A	1139	CLA	C3D-C4D-ND	2.93	114.74	109.99
11	b	1224	CLA	C1-O2A-CGA	2.93	123.73	116.65
11	B	1209	CLA	CAC-C3C-C4C	2.93	128.60	124.79
15	1	5001	LHG	O8-C23-C24	2.93	120.75	111.83
11	A	1112	CLA	CMB-C2B-C1B	2.93	129.87	125.42
11	A	1138	CLA	O2A-CGA-CBA	2.93	123.19	112.14
14	A	4008	BCR	C3-C4-C5	-2.92	108.84	114.06
11	A	1134	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	b	1215	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	2	1209	CLA	C3D-C4D-ND	2.92	114.74	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1012	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	B	1232	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	a	1113	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	b	1204	CLA	CMB-C2B-C1B	2.92	129.87	125.42
14	L	4022	BCR	C38-C26-C27	2.92	119.83	113.60
11	L	1502	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
11	1	1137	CLA	C9-C8-C10	2.92	121.69	111.27
11	2	1212	CLA	C3D-C4D-ND	2.92	114.74	109.99
11	2	1226	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
11	B	1236	CLA	C4D-C3D-CAD	2.92	111.28	108.11
14	F	4020	BCR	C28-C27-C26	-2.92	108.85	114.06
14	8	4019	BCR	C28-C27-C26	-2.92	108.85	114.06
11	a	1137	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
11	1	1103	CLA	CHB-C4A-NA	2.92	128.61	124.40
11	8	1502	CLA	C2B-C1B-NB	2.92	113.35	110.33
11	A	1133	CLA	C3D-C4D-ND	2.92	114.73	109.99
11	b	1234	CLA	CAC-C3C-C4C	2.92	128.59	124.79
11	B	1209	CLA	C2B-C1B-NB	2.92	113.35	110.33
11	2	1223	CLA	C3D-C4D-ND	2.92	114.73	109.99
11	b	1228	CLA	C3D-C4D-ND	2.92	114.73	109.99
11	a	1129	CLA	O2A-CGA-CBA	2.92	123.16	112.14
14	2	4004	BCR	C37-C22-C21	-2.92	118.09	122.82
11	2	1220	CLA	C2B-C1B-NB	2.92	113.35	110.33
11	1	1137	CLA	O2A-C1-C2	2.92	119.33	108.11
11	A	1103	CLA	CMD-C2D-C3D	-2.92	121.00	127.69
11	B	1220	CLA	C3D-C4D-ND	2.92	114.73	109.99
11	a	1103	CLA	C1-C2-C3	-2.92	121.42	126.20
11	K	1401	CLA	C2B-C1B-NB	2.92	113.35	110.33
11	b	1202	CLA	O2A-C1-C2	2.92	119.33	108.11
14	B	4017	BCR	C34-C9-C10	-2.92	118.09	122.82
11	1	1140	CLA	C4-C3-C5	2.92	120.29	115.23
11	B	1023	CLA	C4D-C3D-CAD	2.92	111.27	108.11
11	A	1132	CLA	C1-O2A-CGA	2.92	123.71	116.65
11	a	1126	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
11	b	1212	CLA	C3D-C4D-ND	2.91	114.72	109.99
11	A	1120	CLA	CMC-C2C-C1C	2.91	129.59	125.03
11	B	1222	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
11	b	1212	CLA	C4D-C3D-CAD	2.91	111.27	108.11
11	8	1502	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
11	a	1104	CLA	CMB-C2B-C1B	2.91	129.85	125.42
11	b	1219	CLA	O2A-C1-C2	2.91	119.32	108.11
11	a	1140	CLA	CMC-C2C-C1C	2.91	129.59	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	0	1401	CLA	C2B-C1B-NB	2.91	113.35	110.33
14	B	4006	BCR	C34-C9-C10	-2.91	118.10	122.82
11	2	1013	CLA	C9-C8-C10	2.91	121.65	111.27
11	a	1121	CLA	C4D-C3D-CAD	2.91	111.27	108.11
11	1	1131	CLA	C4D-C3D-CAD	2.91	111.27	108.11
11	2	1215	CLA	C3D-C4D-ND	2.91	114.72	109.99
11	1	1139	CLA	O2A-C1-C2	2.91	119.31	108.11
11	a	1138	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
11	1	1129	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
11	a	1107	CLA	CMB-C2B-C1B	2.91	129.85	125.42
11	A	1112	CLA	C3D-C4D-ND	2.91	114.72	109.99
11	A	1123	CLA	C3D-C4D-ND	2.91	114.72	109.99
11	A	1120	CLA	C3D-C4D-ND	2.91	114.72	109.99
11	B	1205	CLA	O1D-CGD-CBD	-2.91	118.78	124.52
14	b	4014	BCR	C38-C26-C27	2.91	119.80	113.60
11	b	1222	CLA	O2A-C1-C2	2.91	119.30	108.11
11	2	1214	CLA	C1-O2A-CGA	2.91	123.69	116.65
11	1	1132	CLA	CMB-C2B-C1B	2.91	129.85	125.42
11	b	1236	CLA	CMD-C2D-C3D	-2.91	121.02	127.69
14	8	4022	BCR	C27-C26-C25	-2.91	118.78	122.70
11	b	1229	CLA	O2A-C1-C2	2.91	119.29	108.11
11	b	1225	CLA	O2A-C1-C2	2.91	119.29	108.11
11	a	1107	CLA	O2A-C1-C2	2.91	119.29	108.11
11	a	1101	CLA	C3D-C4D-ND	2.91	114.71	109.99
11	1	1125	CLA	C3D-C4D-ND	2.91	114.71	109.99
11	A	1106	CLA	C3D-C4D-ND	2.90	114.71	109.99
11	L	1502	CLA	O2A-CGA-CBA	2.90	123.11	112.14
14	B	4010	BCR	C30-C25-C26	-2.90	118.67	122.64
11	A	1121	CLA	C2B-C1B-NB	2.90	113.34	110.33
11	2	1207	CLA	CMB-C2B-C1B	2.90	129.84	125.42
11	A	1801	CLA	CMB-C2B-C1B	2.90	129.84	125.42
14	a	4003	BCR	C30-C25-C26	-2.90	118.67	122.64
11	B	1227	CLA	CMB-C2B-C1B	2.90	129.84	125.42
11	B	1230	CLA	CHD-C1D-ND	-2.90	120.72	124.80
11	2	1231	CLA	CAC-C3C-C4C	2.90	128.56	124.79
11	A	1801	CLA	CMC-C2C-C3C	2.90	134.00	126.15
11	b	1203	CLA	CMC-C2C-C1C	2.90	129.57	125.03
11	2	1239	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	2	1212	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	a	1132	CLA	C3D-C4D-ND	2.90	114.70	109.99
11	2	1229	CLA	C3D-C4D-ND	2.90	114.70	109.99
11	A	1137	CLA	CMC-C2C-C1C	2.90	129.56	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1218	CLA	C4D-C3D-CAD	2.90	111.25	108.11
11	2	1231	CLA	C4D-C3D-CAD	2.90	111.25	108.11
11	1	1106	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	1	1140	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	1	1112	CLA	CMC-C2C-C1C	2.90	129.56	125.03
11	b	1225	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	2	1221	CLA	C2B-C1B-NB	2.90	113.33	110.33
11	k	1402	CLA	C2B-C1B-NB	2.90	113.33	110.33
14	2	4010	BCR	C33-C5-C4	2.90	119.77	113.60
11	A	1113	CLA	C4D-C3D-CAD	2.90	111.25	108.11
11	b	1217	CLA	C3D-C4D-ND	2.90	114.69	109.99
11	2	1224	CLA	O2A-C1-C2	2.89	119.25	108.11
11	A	1136	CLA	C4D-C3D-CAD	2.89	111.25	108.11
14	6	4013	BCR	C15-C14-C13	-2.89	123.22	127.28
11	B	1234	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	A	4002	BCR	C34-C9-C10	-2.89	118.13	122.82
11	a	1111	CLA	C4D-C3D-CAD	2.89	111.25	108.11
11	a	1120	CLA	CMB-C2B-C1B	2.89	129.82	125.42
11	b	1214	CLA	C1-O2A-CGA	2.89	123.65	116.65
11	a	1134	CLA	C2B-C1B-NB	2.89	113.33	110.33
11	k	1401	CLA	C3D-C4D-ND	2.89	114.69	109.99
11	a	1011	CLA	CED-O2D-CGD	2.89	122.47	115.92
11	L	1503	CLA	CMB-C2B-C1B	2.89	129.82	125.42
11	B	1207	CLA	C3D-C4D-ND	2.89	114.69	109.99
11	8	1502	CLA	C3D-C4D-ND	2.89	114.68	109.99
11	A	1012	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
11	b	1216	CLA	C4D-C3D-CAD	2.89	111.24	108.11
11	B	1226	CLA	C9-C8-C7	2.89	121.57	111.27
11	1	1107	CLA	C4D-C3D-CAD	2.89	111.24	108.11
11	A	1122	CLA	C2B-C1B-NB	2.89	113.32	110.33
11	b	1222	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	B	4014	BCR	C27-C26-C25	-2.89	118.80	122.70
14	a	4001	BCR	C19-C18-C17	2.89	123.55	119.01
11	a	1105	CLA	C2B-C1B-NB	2.89	113.32	110.33
11	1	1124	CLA	C3D-C4D-ND	2.89	114.68	109.99
11	1	1117	CLA	C1-C2-C3	-2.89	121.47	126.20
11	A	1125	CLA	OBD-CAD-C3D	-2.88	121.67	128.42
14	6	4020	BCR	C8-C9-C10	2.88	123.55	119.01
11	2	1217	CLA	C4D-C3D-CAD	2.88	111.24	108.11
11	B	1207	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
14	6	4018	BCR	C33-C5-C4	2.88	119.74	113.60
11	A	1124	CLA	CMB-C2B-C1B	2.88	129.81	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1216	CLA	C2B-C1B-NB	2.88	113.31	110.33
11	1	1119	CLA	C2B-C1B-NB	2.88	113.31	110.33
11	A	1140	CLA	C4D-C3D-CAD	2.88	111.24	108.11
14	2	4010	BCR	C38-C26-C27	2.88	119.74	113.60
11	B	1218	CLA	C2B-C1B-NB	2.88	113.31	110.33
11	B	1220	CLA	C2B-C1B-NB	2.88	113.31	110.33
11	A	1102	CLA	CMC-C2C-C1C	2.88	129.54	125.03
11	1	1130	CLA	C2B-C1B-NB	2.88	113.31	110.33
11	2	1235	CLA	CAC-C3C-C4C	2.88	128.54	124.79
11	a	1123	CLA	C3D-C4D-ND	2.88	114.67	109.99
11	b	1204	CLA	CMC-C2C-C1C	2.88	129.53	125.03
11	2	1218	CLA	C3D-C4D-ND	2.88	114.67	109.99
11	A	1118	CLA	CBC-CAC-C3C	-2.88	104.62	112.42
11	b	1223	CLA	C3D-C4D-ND	2.88	114.67	109.99
11	b	1207	CLA	C4D-C3D-CAD	2.88	111.23	108.11
14	2	4004	BCR	C3-C4-C5	-2.88	108.92	114.06
11	a	1113	CLA	CMC-C2C-C1C	2.88	129.53	125.03
14	1	4002	BCR	C38-C26-C27	2.88	119.73	113.60
11	2	1228	CLA	C3D-C4D-ND	2.88	114.66	109.99
11	a	1104	CLA	O2A-C1-C2	2.87	119.17	108.11
11	a	1114	CLA	C3D-C4D-ND	2.87	114.66	109.99
11	a	1138	CLA	C4D-C3D-CAD	2.87	111.23	108.11
11	1	1127	CLA	C4D-C3D-CAD	2.87	111.23	108.11
11	2	1201	CLA	C4D-C3D-CAD	2.87	111.23	108.11
11	a	1125	CLA	C2B-C1B-NB	2.87	113.31	110.33
11	2	1208	CLA	CMB-C2B-C1B	2.87	129.79	125.42
11	b	1227	CLA	C2B-C1B-NB	2.87	113.30	110.33
11	2	1213	CLA	C3C-C4C-NC	2.87	114.11	110.43
14	a	4002	BCR	C37-C22-C21	-2.87	118.17	122.82
11	A	1102	CLA	O2A-C1-C2	2.87	119.15	108.11
11	B	1239	CLA	C3D-C4D-ND	2.87	114.65	109.99
11	2	1023	CLA	C4D-C3D-CAD	2.87	111.22	108.11
11	B	1204	CLA	CMC-C2C-C1C	2.87	129.52	125.03
11	b	1222	CLA	CMB-C2B-C1B	2.87	129.79	125.42
11	A	1116	CLA	C3D-C4D-ND	2.87	114.65	109.99
11	b	1236	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
11	K	1401	CLA	C3D-C4D-ND	2.87	114.65	109.99
11	B	1226	CLA	C4D-C3D-CAD	2.87	111.22	108.11
11	a	1108	CLA	C4D-C3D-CAD	2.87	111.22	108.11
11	2	1222	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
11	1	1103	CLA	CMD-C2D-C3D	-2.86	121.12	127.69
11	1	1125	CLA	CMB-C2B-C1B	2.86	129.78	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1116	CLA	C2B-C1B-NB	2.86	113.30	110.33
11	2	1239	CLA	C3D-C4D-ND	2.86	114.64	109.99
11	A	1122	CLA	C4D-C3D-CAD	2.86	111.22	108.11
14	a	4001	BCR	C36-C18-C17	-2.86	118.18	122.82
14	M	4021	BCR	C24-C23-C22	-2.86	122.00	126.23
11	b	1239	CLA	C2B-C1B-NB	2.86	113.30	110.33
11	b	1236	CLA	CMC-C2C-C1C	2.86	129.51	125.03
11	B	1225	CLA	O2A-C1-C2	2.86	119.12	108.11
14	B	4005	BCR	C38-C26-C27	2.86	119.70	113.60
14	b	4011	BCR	C24-C23-C22	-2.86	122.00	126.23
11	A	1104	CLA	C4D-C3D-CAD	2.86	111.21	108.11
11	1	1136	CLA	C4D-C3D-CAD	2.86	111.21	108.11
11	2	1217	CLA	CMB-C2B-C1B	2.86	129.77	125.42
11	2	1216	CLA	CMC-C2C-C1C	2.86	129.50	125.03
11	b	1236	CLA	C2B-C1B-NB	2.86	113.29	110.33
14	2	4004	BCR	C23-C22-C21	2.86	123.51	119.01
11	A	1132	CLA	C3D-C4D-ND	2.86	114.63	109.99
11	B	1209	CLA	C3D-C4D-ND	2.86	114.63	109.99
14	B	4010	BCR	C38-C26-C27	2.86	119.69	113.60
11	B	1209	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
11	a	1801	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
11	b	1207	CLA	C2B-C1B-NB	2.86	113.29	110.33
11	0	1401	CLA	C3D-C4D-ND	2.86	114.63	109.99
14	B	4017	BCR	C4-C5-C6	-2.86	118.84	122.70
11	a	1140	CLA	C1-C2-C3	-2.86	121.52	126.20
11	1	1011	CLA	CHB-C4A-NA	2.85	128.52	124.40
11	2	1234	CLA	CMC-C2C-C1C	2.85	129.50	125.03
15	1	5001	LHG	C5-O7-C7	-2.85	110.96	117.80
11	1	1140	CLA	C1-O2A-CGA	2.85	123.56	116.65
14	a	4001	BCR	C7-C8-C9	-2.85	122.01	126.23
11	A	1110	CLA	C1-C2-C3	-2.85	121.52	126.20
11	B	1238	CLA	C2B-C1B-NB	2.85	113.28	110.33
11	1	1113	CLA	C3D-C4D-ND	2.85	114.62	109.99
11	B	1215	CLA	C3D-C4D-ND	2.85	114.62	109.99
11	b	1239	CLA	C3D-C4D-ND	2.85	114.62	109.99
11	b	1202	CLA	CMC-C2C-C1C	2.85	129.49	125.03
11	1	1116	CLA	C4D-C3D-CAD	2.85	111.20	108.11
11	a	1117	CLA	C1-C2-C3	-2.85	121.53	126.20
11	A	1106	CLA	CMC-C2C-C1C	2.85	129.49	125.03
11	A	1237	CLA	C2B-C1B-NB	2.85	113.28	110.33
11	1	1110	CLA	C1-C2-C3	-2.85	121.53	126.20
11	2	1211	CLA	O2A-CGA-CBA	2.85	122.90	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1216	CLA	C4D-C3D-CAD	2.85	111.20	108.11
11	2	1211	CLA	CMC-C2C-C1C	2.85	129.48	125.03
11	2	1239	CLA	C4D-C3D-CAD	2.85	111.20	108.11
11	a	1102	CLA	CMC-C2C-C1C	2.85	129.48	125.03
11	A	1136	CLA	CMB-C2B-C1B	2.85	129.75	125.42
11	B	1023	CLA	C1-O2A-CGA	2.85	123.54	116.65
11	B	1226	CLA	O2A-C1-C2	2.85	119.06	108.11
11	2	1203	CLA	C3D-C4D-ND	2.85	114.61	109.99
11	a	1140	CLA	C4D-C3D-CAD	2.85	111.20	108.11
11	1	1113	CLA	C4D-C3D-CAD	2.85	111.20	108.11
11	b	1211	CLA	CMC-C2C-C1C	2.84	129.48	125.03
11	A	1131	CLA	C3D-C4D-ND	2.84	114.61	109.99
11	a	1135	CLA	C3D-C4D-ND	2.84	114.61	109.99
11	a	1123	CLA	C1-C2-C3	-2.84	121.54	126.20
11	1	1127	CLA	C2B-C1B-NB	2.84	113.27	110.33
11	K	1402	CLA	C2B-C1B-NB	2.84	113.27	110.33
11	a	1104	CLA	CMC-C2C-C1C	2.84	129.48	125.03
14	f	4013	BCR	C37-C22-C21	-2.84	118.21	122.82
11	2	1207	CLA	C4D-C3D-CAD	2.84	111.19	108.11
11	b	1202	CLA	C3D-C4D-ND	2.84	114.61	109.99
11	b	1205	CLA	C3D-C4D-ND	2.84	114.61	109.99
14	1	4001	BCR	C36-C18-C17	-2.84	118.21	122.82
11	2	1210	CLA	C9-C8-C7	2.84	121.40	111.27
11	B	1221	CLA	CMB-C2B-C1B	2.84	129.74	125.42
11	1	1138	CLA	CED-O2D-CGD	2.84	122.36	115.92
11	1	1115	CLA	C3D-C4D-ND	2.84	114.60	109.99
11	b	1023	CLA	CMB-C2B-C1B	2.84	129.74	125.42
11	b	1213	CLA	C4D-C3D-CAD	2.84	111.19	108.11
11	1	1132	CLA	C3D-C4D-ND	2.84	114.60	109.99
11	1	1125	CLA	CMC-C2C-C1C	2.84	129.47	125.03
11	1	1127	CLA	CMC-C2C-C1C	2.84	129.47	125.03
11	B	1216	CLA	CMD-C2D-C3D	-2.84	121.18	127.69
11	1	1140	CLA	CMB-C2B-C1B	2.84	129.74	125.42
11	2	1228	CLA	C4D-C3D-CAD	2.84	111.19	108.11
15	A	5001	LHG	O8-C23-C24	2.83	120.48	111.83
11	B	1217	CLA	C3D-C4D-ND	2.83	114.59	109.99
11	B	1205	CLA	C2B-C1B-NB	2.83	113.27	110.33
11	2	1211	CLA	C2B-C1B-NB	2.83	113.27	110.33
11	A	1105	CLA	C4D-C3D-CAD	2.83	111.18	108.11
11	a	1112	CLA	CMB-C2B-C1B	2.83	129.73	125.42
11	2	1218	CLA	CMB-C2B-C1B	2.83	129.73	125.42
14	l	4022	BCR	C33-C5-C4	2.83	119.64	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1224	CLA	C3D-C4D-ND	2.83	114.59	109.99
11	2	1204	CLA	CMC-C2C-C1C	2.83	129.46	125.03
11	A	1101	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	2	4017	BCR	C38-C26-C27	2.83	119.64	113.60
11	B	1210	CLA	C9-C8-C7	2.83	121.37	111.27
11	B	1229	CLA	C4D-C3D-CAD	2.83	111.18	108.11
11	A	1132	CLA	C1-C2-C3	-2.83	121.56	126.20
14	2	4004	BCR	C19-C18-C17	2.83	123.46	119.01
11	b	1231	CLA	C3D-C4D-ND	2.83	114.59	109.99
11	2	1240	CLA	C3D-C4D-ND	2.83	114.59	109.99
11	B	1239	CLA	CMC-C2C-C1C	2.83	129.46	125.03
11	A	1116	CLA	O2A-C1-C2	2.83	119.00	108.11
14	8	4022	BCR	C3-C4-C5	-2.83	109.01	114.06
11	2	1216	CLA	CHD-C1D-ND	-2.83	120.82	124.80
15	a	5003	LHG	O8-C23-C24	2.83	120.46	111.83
11	a	1129	CLA	CMB-C2B-C1B	2.83	129.73	125.42
11	2	1205	CLA	CHD-C1D-ND	-2.83	120.82	124.80
11	A	1134	CLA	C4D-C3D-CAD	2.83	111.18	108.11
11	A	1131	CLA	C2B-C1B-NB	2.83	113.26	110.33
11	1	1012	CLA	C2B-C1B-NB	2.83	113.26	110.33
11	b	1220	CLA	C3D-C4D-ND	2.83	114.58	109.99
11	1	1124	CLA	C4D-C3D-CAD	2.83	111.18	108.11
11	b	1209	CLA	CAC-C3C-C4C	2.83	128.47	124.79
11	B	1212	CLA	CMC-C2C-C1C	2.83	129.45	125.03
11	a	1801	CLA	C4D-C3D-CAD	2.83	111.18	108.11
11	1	1237	CLA	CMD-C2D-C3D	-2.83	121.20	127.69
11	a	1011	CLA	O2A-C1-C2	2.83	118.99	108.11
11	b	1210	CLA	CMC-C2C-C1C	2.83	129.45	125.03
11	A	1140	CLA	C2B-C1B-NB	2.83	113.26	110.33
11	B	1201	CLA	CMD-C2D-C3D	-2.83	121.21	127.69
14	2	4011	BCR	C24-C23-C22	-2.82	122.06	126.23
11	L	1502	CLA	C2B-C1B-NB	2.82	113.25	110.33
11	l	1502	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
14	b	4014	BCR	C3-C4-C5	-2.82	109.02	114.06
11	a	1122	CLA	CMC-C2C-C1C	2.82	129.45	125.03
14	a	4001	BCR	C38-C26-C25	-2.82	121.40	124.48
11	2	1230	CLA	C3D-C4D-ND	2.82	114.58	109.99
11	L	1502	CLA	C4D-C3D-CAD	2.82	111.17	108.11
14	A	4001	BCR	C27-C26-C25	-2.82	118.89	122.70
14	6	4018	BCR	C34-C9-C10	-2.82	118.25	122.82
11	A	1109	CLA	CMC-C2C-C1C	2.82	129.44	125.03
11	1	1012	CLA	O2D-CGD-O1D	-2.82	118.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	1501	CLA	CMB-C2B-C1B	2.82	129.71	125.42
11	B	1222	CLA	CMC-C2C-C1C	2.82	129.44	125.03
11	B	1236	CLA	CMC-C2C-C1C	2.82	129.44	125.03
11	1	1131	CLA	CMC-C2C-C1C	2.82	129.44	125.03
11	a	1139	CLA	CMB-C2B-C1B	2.82	129.71	125.42
11	a	1115	CLA	C2B-C1B-NB	2.82	113.25	110.33
11	B	1213	CLA	C4D-C3D-CAD	2.82	111.17	108.11
11	a	1121	CLA	CAC-C3C-C4C	2.82	128.46	124.79
14	8	4019	BCR	C19-C18-C17	2.82	123.44	119.01
11	a	1114	CLA	CMC-C2C-C1C	2.82	129.44	125.03
11	b	1227	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
11	1	1011	CLA	CAA-C2A-C3A	-2.82	105.39	113.00
11	b	1204	CLA	C1-C2-C3	-2.82	121.58	126.20
11	B	1210	CLA	C2B-C1B-NB	2.82	113.25	110.33
11	1	1133	CLA	CAC-C3C-C4C	2.82	128.45	124.79
14	A	4007	BCR	C3-C4-C5	-2.81	109.04	114.06
11	2	1217	CLA	C3D-C4D-ND	2.81	114.56	109.99
11	A	1113	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	B	1223	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	a	1112	CLA	C4D-C3D-CAD	2.81	111.16	108.11
14	F	4018	BCR	C33-C5-C4	2.81	119.59	113.60
14	b	4006	BCR	C23-C24-C25	-2.81	119.48	127.00
14	a	4001	BCR	C30-C25-C26	-2.81	118.79	122.64
11	A	1121	CLA	C4D-C3D-CAD	2.81	111.16	108.11
11	2	1202	CLA	C4D-C3D-CAD	2.81	111.16	108.11
11	B	1224	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	b	1219	CLA	CMB-C2B-C3B	2.81	133.16	126.55
11	b	1208	CLA	CMB-C2B-C1B	2.81	129.70	125.42
11	a	1116	CLA	O2A-C1-C2	2.81	118.93	108.11
11	a	1134	CLA	CED-O2D-CGD	2.81	122.29	115.92
11	1	1131	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	1	1105	CLA	CMC-C2C-C1C	2.81	129.43	125.03
11	b	1201	CLA	C4D-C3D-CAD	2.81	111.16	108.11
11	1	1123	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	2	1224	CLA	CMB-C2B-C1B	2.81	129.69	125.42
11	B	1231	CLA	C4D-C3D-CAD	2.81	111.16	108.11
11	a	1128	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	2	1202	CLA	CMC-C2C-C1C	2.81	129.42	125.03
14	l	4022	BCR	C38-C26-C27	2.81	119.58	113.60
11	l	1503	CLA	CMC-C2C-C1C	2.81	129.42	125.03
11	2	1214	CLA	C4D-C3D-CAD	2.81	111.16	108.11
11	A	1107	CLA	C3D-C4D-ND	2.81	114.55	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1123	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
11	B	1208	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	2	1234	CLA	C2B-C1B-NB	2.81	113.24	110.33
11	a	1135	CLA	C4-C3-C5	2.81	119.43	116.13
11	A	1111	CLA	CMC-C2C-C1C	2.81	129.42	125.03
11	a	1126	CLA	C3D-C4D-ND	2.81	114.55	109.99
11	1	1237	CLA	O2A-C1-C2	2.81	118.91	108.11
11	1	1022	CLA	C3D-C4D-ND	2.81	114.55	109.99
11	2	1222	CLA	C3D-C4D-ND	2.81	114.55	109.99
14	a	4001	BCR	C38-C26-C27	2.81	119.58	113.60
11	b	1231	CLA	CMD-C2D-C3D	-2.81	121.26	127.69
11	a	1106	CLA	CMB-C2B-C1B	2.80	129.69	125.42
11	2	1201	CLA	C2B-C1B-NB	2.80	113.23	110.33
14	b	4010	BCR	C33-C5-C4	2.80	119.57	113.60
14	2	4006	BCR	C8-C9-C10	2.80	123.42	119.01
14	2	4014	BCR	C33-C5-C4	2.80	119.57	113.60
11	1	1134	CLA	C2B-C1B-NB	2.80	113.23	110.33
11	1	1012	CLA	C9-C8-C10	2.80	121.27	111.27
11	1	1801	CLA	C3D-C4D-ND	2.80	114.54	109.99
14	B	4014	BCR	C33-C5-C4	2.80	119.57	113.60
14	2	4004	BCR	C34-C9-C10	-2.80	118.28	122.82
11	A	1114	CLA	CMB-C2B-C1B	2.80	129.69	125.42
11	2	1229	CLA	CMC-C2C-C1C	2.80	129.41	125.03
11	A	1012	CLA	CMB-C2B-C1B	2.80	129.68	125.42
11	1	1011	CLA	O2A-C1-C2	2.80	118.89	108.11
11	1	1125	CLA	C1-C2-C3	-2.80	121.61	126.20
11	b	1214	CLA	C9-C8-C10	2.80	121.26	111.27
11	b	1226	CLA	C9-C8-C7	2.80	121.25	111.27
11	a	1110	CLA	O2A-C1-C2	2.80	118.88	108.11
11	B	1210	CLA	C4D-C3D-CAD	2.80	111.15	108.11
11	a	1116	CLA	C4D-C3D-CAD	2.80	111.15	108.11
11	a	1106	CLA	CMC-C2C-C1C	2.80	129.41	125.03
14	6	4018	BCR	C38-C26-C27	2.80	119.56	113.60
11	2	1224	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	B	4017	BCR	C1-C6-C7	2.80	123.24	115.65
14	2	4011	BCR	C23-C24-C25	-2.80	119.52	127.00
11	2	1222	CLA	C4D-C3D-CAD	2.80	111.14	108.11
14	b	4006	BCR	C34-C9-C10	-2.80	118.28	122.82
11	b	1218	CLA	CMC-C2C-C1C	2.80	129.41	125.03
11	2	1203	CLA	CMD-C2D-C3D	-2.80	121.27	127.69
11	2	1023	CLA	C9-C8-C7	2.80	121.25	111.27
11	B	1021	CLA	C3D-C4D-ND	2.80	114.53	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1213	CLA	O1D-CGD-CBD	-2.80	119.00	124.52
14	a	4008	BCR	C30-C25-C26	-2.80	118.82	122.64
11	1	1125	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
14	B	4011	BCR	C35-C13-C12	2.79	122.36	118.09
11	2	1227	CLA	C2B-C1B-NB	2.79	113.22	110.33
14	a	4008	BCR	C27-C26-C25	-2.79	118.93	122.70
11	A	1011	CLA	C4-C3-C5	2.79	120.08	115.23
11	A	1118	CLA	C1-C2-C3	-2.79	121.62	126.20
11	A	1110	CLA	C2B-C1B-NB	2.79	113.22	110.33
11	2	1201	CLA	CMD-C2D-C3D	-2.79	121.29	127.69
14	a	4007	BCR	C28-C27-C26	-2.79	109.08	114.06
11	B	1221	CLA	C2B-C1B-NB	2.79	113.22	110.33
14	2	4017	BCR	C15-C14-C13	-2.79	123.36	127.28
11	a	1109	CLA	CMB-C2B-C1B	2.79	129.67	125.42
11	1	1121	CLA	C3D-C4D-ND	2.79	114.52	109.99
11	L	1501	CLA	C1-O2A-CGA	2.79	123.40	116.65
11	2	1220	CLA	CMC-C2C-C1C	2.79	129.39	125.03
14	6	4020	BCR	C23-C24-C25	-2.79	119.55	127.00
11	A	1132	CLA	C4D-C3D-CAD	2.79	111.13	108.11
11	1	1111	CLA	CMB-C2B-C1B	2.79	129.66	125.42
11	B	1235	CLA	CMC-C2C-C1C	2.79	129.39	125.03
11	2	1226	CLA	O2A-C1-C2	2.79	118.83	108.11
11	A	1106	CLA	C1-O2A-CGA	2.79	123.39	116.65
11	2	1221	CLA	C4D-C3D-CAD	2.79	111.13	108.11
14	A	4002	BCR	C15-C14-C13	-2.79	123.37	127.28
11	A	1101	CLA	CMC-C2C-C1C	2.78	129.39	125.03
14	2	4011	BCR	C38-C26-C27	2.78	119.53	113.60
11	a	1122	CLA	C2B-C1B-NB	2.78	113.21	110.33
11	b	1222	CLA	C3D-C4D-ND	2.78	114.51	109.99
11	A	1127	CLA	CMC-C2C-C1C	2.78	129.38	125.03
11	a	1110	CLA	C1-C2-C3	-2.78	121.64	126.20
11	b	1204	CLA	C4D-C3D-CAD	2.78	111.13	108.11
11	1	1114	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	2	4010	BCR	C36-C18-C17	-2.78	118.31	122.82
11	1	1111	CLA	C1-O2A-CGA	2.78	123.38	116.65
16	2	5002	LMG	C8-O7-C10	-2.78	111.14	117.80
11	a	1102	CLA	O2A-C1-C2	2.78	118.81	108.11
11	2	1224	CLA	C2B-C1B-NB	2.78	113.21	110.33
11	A	1122	CLA	CMB-C2B-C1B	2.78	129.65	125.42
11	1	1106	CLA	C4D-C3D-CAD	2.78	111.12	108.11
11	b	1021	CLA	C3D-C4D-ND	2.78	114.50	109.99
14	2	4017	BCR	C33-C5-C4	2.78	119.52	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1138	CLA	C3D-C4D-ND	2.78	114.50	109.99
11	8	1502	CLA	C3C-C4C-NC	2.78	113.99	110.43
11	1	1101	CLA	CMC-C2C-C1C	2.78	129.38	125.03
11	2	1021	CLA	O2A-C1-C2	2.78	118.80	108.11
11	A	1110	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
11	B	1206	CLA	C3D-C4D-ND	2.78	114.50	109.99
11	A	1801	CLA	C3D-C4D-ND	2.78	114.50	109.99
11	A	1135	CLA	CMC-C2C-C1C	2.78	129.37	125.03
14	B	4011	BCR	C8-C9-C10	2.78	123.38	119.01
11	1	1108	CLA	C2B-C1B-NB	2.78	113.20	110.33
11	1	1104	CLA	C9-C8-C7	2.78	121.17	111.27
11	2	1214	CLA	CMB-C2B-C1B	2.78	129.65	125.42
11	B	1234	CLA	C4D-C3D-CAD	2.78	111.12	108.11
11	2	1206	CLA	C4D-C3D-CAD	2.78	111.12	108.11
11	2	1224	CLA	CMD-C2D-C3D	-2.78	121.32	127.69
11	b	1239	CLA	CMB-C2B-C1B	2.78	129.65	125.42
11	a	1140	CLA	C9-C8-C7	2.77	121.17	111.27
11	A	1104	CLA	CMB-C2B-C1B	2.77	129.64	125.42
11	1	1120	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
11	b	1203	CLA	C3D-C4D-ND	2.77	114.50	109.99
11	A	1116	CLA	C4D-C3D-CAD	2.77	111.12	108.11
11	B	1201	CLA	C3D-C4D-ND	2.77	114.50	109.99
11	B	1230	CLA	C3D-C4D-ND	2.77	114.50	109.99
14	2	4006	BCR	C19-C18-C17	2.77	123.37	119.01
11	2	1201	CLA	CMB-C2B-C1B	2.77	129.64	125.42
11	B	1208	CLA	CMC-C2C-C1C	2.77	129.37	125.03
11	1	1116	CLA	O2A-C1-C2	2.77	118.78	108.11
14	b	4009	BCR	C34-C9-C10	-2.77	118.32	122.82
14	m	4021	BCR	C19-C18-C17	2.77	123.37	119.01
11	a	1135	CLA	C2B-C1B-NB	2.77	113.20	110.33
11	1	1112	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
11	B	1214	CLA	CMB-C2B-C1B	2.77	129.64	125.42
11	2	1215	CLA	C4-C3-C2	-2.77	116.51	123.63
11	b	1211	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
11	B	1219	CLA	C3D-C4D-ND	2.77	114.49	109.99
11	A	1103	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
11	A	1131	CLA	C1-C2-C3	-2.77	121.66	126.20
11	a	1112	CLA	CMC-C2C-C1C	2.77	129.36	125.03
11	1	1114	CLA	C2B-C1B-NB	2.77	113.20	110.33
11	A	1140	CLA	C3D-C4D-ND	2.77	114.49	109.99
11	b	1226	CLA	O2A-C1-C2	2.77	118.76	108.11
11	2	1209	CLA	C4D-C3D-CAD	2.77	111.11	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	8	1502	CLA	C4D-C3D-CAD	2.77	111.11	108.11
11	a	1118	CLA	C2B-C1B-NB	2.77	113.20	110.33
11	1	1111	CLA	C4D-C3D-CAD	2.77	111.11	108.11
11	B	1238	CLA	C4-C3-C5	2.77	120.03	115.23
11	a	1012	CLA	C3D-C4D-ND	2.77	114.48	109.99
11	a	1119	CLA	C2B-C1B-NB	2.77	113.19	110.33
11	2	1225	CLA	CMC-C2C-C1C	2.77	129.36	125.03
11	A	1122	CLA	CMD-C2D-C3D	-2.77	121.34	127.69
11	a	1115	CLA	C4D-C3D-CAD	2.77	111.11	108.11
14	B	4017	BCR	C33-C5-C4	2.77	119.49	113.60
11	2	1238	CLA	CMC-C2C-C1C	2.76	129.35	125.03
11	A	1102	CLA	C3D-C4D-ND	2.76	114.48	109.99
11	a	1011	CLA	CMB-C2B-C3B	2.76	133.05	126.55
14	m	4021	BCR	C37-C22-C21	-2.76	118.34	122.82
11	1	1119	CLA	O2A-C1-C2	2.76	118.74	108.11
11	b	1209	CLA	C4D-C3D-CAD	2.76	111.11	108.11
11	b	1211	CLA	CMB-C2B-C1B	2.76	129.63	125.42
11	1	1129	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
11	a	1139	CLA	C3D-C4D-ND	2.76	114.48	109.99
11	1	1138	CLA	CMB-C2B-C1B	2.76	129.62	125.42
11	K	1402	CLA	C4D-C3D-CAD	2.76	111.11	108.11
11	a	1139	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
11	1	1111	CLA	CMC-C2C-C1C	2.76	129.35	125.03
14	1	4002	BCR	C31-C1-C6	-2.76	105.91	110.24
11	A	1111	CLA	CMB-C2B-C1B	2.76	129.62	125.42
11	b	1222	CLA	C4D-C3D-CAD	2.76	111.10	108.11
11	2	1201	CLA	C3D-C4D-ND	2.76	114.47	109.99
14	A	4003	BCR	C34-C9-C10	-2.76	118.35	122.82
11	A	1137	CLA	C9-C8-C7	2.76	121.11	111.27
11	b	1219	CLA	CMC-C2C-C1C	2.76	129.34	125.03
11	2	1219	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
11	2	1221	CLA	CMC-C2C-C1C	2.76	129.34	125.03
11	b	1224	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	b	4004	BCR	C27-C26-C25	-2.76	118.98	122.70
11	B	1203	CLA	CMD-C2D-C3D	-2.76	121.37	127.69
11	1	1110	CLA	CAC-C3C-C4C	2.76	128.38	124.79
11	B	1213	CLA	C9-C8-C7	2.75	121.09	111.27
11	2	1222	CLA	CMB-C2B-C1B	2.75	129.61	125.42
11	A	1107	CLA	C4-C3-C2	-2.75	116.56	123.63
11	A	1237	CLA	C4D-C3D-CAD	2.75	111.10	108.11
11	B	1226	CLA	C1-C2-C3	-2.75	121.69	126.20
11	B	1213	CLA	CMB-C2B-C1B	2.75	129.61	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1227	CLA	CMC-C2C-C1C	2.75	129.33	125.03
11	l	1501	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
11	B	1240	CLA	CMC-C2C-C1C	2.75	129.33	125.03
11	2	1214	CLA	CAA-CBA-CGA	-2.75	105.40	113.21
11	1	1104	CLA	CMC-C2C-C1C	2.75	129.33	125.03
11	A	1118	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
11	b	1219	CLA	C3D-C4D-ND	2.75	114.45	109.99
14	2	4005	BCR	C38-C26-C25	-2.75	121.48	124.48
11	A	1115	CLA	C4D-C3D-CAD	2.75	111.09	108.11
11	A	1107	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
11	a	1117	CLA	CMB-C2B-C1B	2.75	129.60	125.42
11	b	1227	CLA	C4D-C3D-CAD	2.75	111.09	108.11
11	2	1236	CLA	C4D-C3D-CAD	2.75	111.09	108.11
11	A	1130	CLA	CMB-C2B-C1B	2.75	129.60	125.42
11	b	1215	CLA	C4-C3-C2	-2.75	116.57	123.63
11	B	1230	CLA	C2B-C1B-NB	2.75	113.17	110.33
11	a	1110	CLA	C4D-C3D-CAD	2.75	111.09	108.11
14	F	4013	BCR	C36-C18-C17	-2.75	118.37	122.82
11	b	1208	CLA	CMC-C2C-C1C	2.75	129.32	125.03
11	b	1235	CLA	C4D-C3D-CAD	2.74	111.09	108.11
11	b	1231	CLA	CMC-C2C-C1C	2.74	129.32	125.03
11	B	1223	CLA	C3D-C4D-ND	2.74	114.45	109.99
11	2	1234	CLA	C3D-C4D-ND	2.74	114.45	109.99
11	l	1501	CLA	C4D-C3D-CAD	2.74	111.09	108.11
11	b	1216	CLA	O2A-C1-C2	2.74	118.67	108.11
11	B	1221	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
11	B	1238	CLA	C4D-C3D-CAD	2.74	111.08	108.11
14	B	4011	BCR	C33-C5-C4	2.74	119.44	113.60
14	L	4022	BCR	C34-C9-C10	-2.74	118.37	122.82
11	2	1203	CLA	C4-C3-C5	2.74	119.99	115.23
11	2	1208	CLA	CMC-C2C-C1C	2.74	129.32	125.03
11	A	1104	CLA	CMD-C2D-C3D	-2.74	121.40	127.69
14	f	4020	BCR	C3-C4-C5	-2.74	109.17	114.06
11	2	1203	CLA	C4D-C3D-CAD	2.74	111.08	108.11
11	1	1109	CLA	C9-C8-C10	2.74	121.04	111.27
11	1	1120	CLA	C3D-C4D-ND	2.74	114.44	109.99
11	2	1208	CLA	C2B-C1B-NB	2.74	113.17	110.33
14	B	4005	BCR	C15-C14-C13	-2.74	123.44	127.28
11	A	1124	CLA	CAC-C3C-C4C	2.74	128.35	124.79
11	b	1230	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
11	a	1107	CLA	CHB-C4A-NA	2.74	128.35	124.40
11	a	1121	CLA	C3D-C4D-ND	2.74	114.44	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	0	1402	CLA	C2B-C1B-NB	2.74	113.17	110.33
14	F	4020	BCR	C38-C26-C27	2.74	119.44	113.60
11	A	1119	CLA	CAC-C3C-C4C	2.74	128.35	124.79
11	1	1131	CLA	O2A-C1-C2	2.74	118.65	108.11
11	A	1135	CLA	C4D-C3D-CAD	2.74	111.08	108.11
11	a	1138	CLA	CMB-C2B-C1B	2.74	129.59	125.42
11	1	1801	CLA	C1-O2A-CGA	2.74	123.28	116.65
11	L	1501	CLA	C4D-C3D-CAD	2.74	111.08	108.11
11	1	1012	CLA	C3D-C4D-ND	2.74	114.44	109.99
11	B	1205	CLA	C4D-C3D-CAD	2.74	111.08	108.11
11	a	1135	CLA	C4D-C3D-CAD	2.74	111.08	108.11
11	B	1013	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
11	a	1102	CLA	C3D-C4D-ND	2.74	114.43	109.99
14	f	4020	BCR	C38-C26-C27	2.74	119.43	113.60
11	1	1116	CLA	CMB-C2B-C1B	2.73	129.58	125.42
11	b	1211	CLA	C4D-C3D-CAD	2.73	111.08	108.11
11	b	1206	CLA	CMD-C2D-C3D	-2.73	121.42	127.69
11	b	1234	CLA	C3D-C4D-ND	2.73	114.43	109.99
11	2	1238	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
11	2	1226	CLA	C9-C8-C10	2.73	121.01	111.27
11	b	1208	CLA	C4D-C3D-CAD	2.73	111.07	108.11
11	B	1218	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
14	1	4007	BCR	C33-C5-C4	2.73	119.42	113.60
11	A	1122	CLA	C9-C8-C10	2.73	121.01	111.27
11	1	1108	CLA	C4D-C3D-CAD	2.73	111.07	108.11
11	1	1110	CLA	CMC-C2C-C1C	2.73	129.30	125.03
11	1	1140	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	b	4010	BCR	C23-C24-C25	-2.73	119.71	127.00
11	A	1124	CLA	C3D-C4D-ND	2.73	114.42	109.99
11	a	1127	CLA	CED-O2D-CGD	2.73	122.11	115.92
14	2	4006	BCR	C24-C23-C22	-2.73	122.20	126.23
11	B	1021	CLA	C4D-C3D-CAD	2.73	111.07	108.11
11	1	1237	CLA	C4D-C3D-CAD	2.73	111.07	108.11
11	1	1134	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
11	b	1023	CLA	C9-C8-C7	2.73	121.00	111.27
11	a	1111	CLA	C1-C2-C3	-2.73	121.73	126.20
14	a	4001	BCR	C27-C26-C25	-2.73	119.02	122.70
11	1	1011	CLA	C2B-C1B-NB	2.73	113.15	110.33
11	b	1236	CLA	C4D-C3D-CAD	2.73	111.07	108.11
11	L	1503	CLA	CMC-C2C-C1C	2.73	129.29	125.03
11	a	1012	CLA	CMB-C2B-C1B	2.73	129.57	125.42
14	A	4008	BCR	C8-C9-C10	2.73	123.30	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1021	CLA	C9-C8-C7	2.73	120.99	111.27
14	B	4017	BCR	C30-C25-C26	-2.73	118.91	122.64
11	b	1215	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
14	1	4008	BCR	C3-C4-C5	-2.72	109.20	114.06
14	1	4001	BCR	C35-C13-C14	-2.72	118.40	122.82
11	b	1021	CLA	CBA-CAA-C2A	2.72	121.90	113.79
11	2	1023	CLA	CAC-C3C-C4C	2.72	128.33	124.79
14	m	4021	BCR	C15-C14-C13	-2.72	123.46	127.28
11	1	1129	CLA	CMC-C2C-C1C	2.72	129.29	125.03
11	A	1801	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	a	1139	CLA	CAC-C3C-C4C	2.72	128.33	124.79
14	6	4020	BCR	C33-C5-C4	2.72	119.40	113.60
11	8	1501	CLA	C3D-C4D-ND	2.72	114.41	109.99
11	a	1106	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
11	a	1129	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	1	1135	CLA	C3D-C4D-ND	2.72	114.41	109.99
11	2	1203	CLA	CMC-C2C-C1C	2.72	129.29	125.03
14	6	4018	BCR	C30-C25-C26	-2.72	118.92	122.64
11	2	1204	CLA	C1-O2A-CGA	2.72	123.24	116.65
14	b	4006	BCR	C15-C14-C13	-2.72	123.46	127.28
11	B	1202	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	b	1224	CLA	C2B-C1B-NB	2.72	113.15	110.33
11	1	1135	CLA	CMB-C2B-C1B	2.72	129.56	125.42
11	a	1133	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
11	B	1225	CLA	CMC-C2C-C1C	2.72	129.28	125.03
11	a	1114	CLA	C2B-C1B-NB	2.72	113.15	110.33
11	a	1136	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
11	a	1105	CLA	CMC-C2C-C1C	2.72	129.28	125.03
11	2	1216	CLA	C3D-C4D-ND	2.72	114.41	109.99
11	B	1221	CLA	C4-C3-C5	2.72	119.95	115.23
14	B	4010	BCR	C19-C18-C17	2.72	123.29	119.01
11	B	1221	CLA	CHD-C1D-ND	-2.72	120.98	124.80
11	b	1215	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	l	1502	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	b	1208	CLA	CAC-C3C-C4C	2.72	128.33	124.79
14	B	4005	BCR	C3-C4-C5	-2.72	109.21	114.06
11	b	1226	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	b	4011	BCR	C27-C26-C25	-2.72	119.03	122.70
11	B	1221	CLA	C3C-C4C-NC	2.72	113.91	110.43
11	8	1501	CLA	O2A-C1-C2	2.72	118.57	108.11
11	1	1106	CLA	CMC-C2C-C1C	2.72	129.28	125.03
11	A	1137	CLA	CMB-C2B-C3B	2.72	132.94	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1123	CLA	C3D-C4D-ND	2.72	114.40	109.99
11	b	1226	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	b	1222	CLA	C4-C3-C2	-2.72	116.65	123.63
11	b	1235	CLA	CMC-C2C-C1C	2.72	129.28	125.03
11	B	1013	CLA	CED-O2D-CGD	2.72	122.08	115.92
11	b	1209	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
11	a	1128	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	A	4001	BCR	C38-C26-C27	2.72	119.39	113.60
14	l	4019	BCR	C7-C8-C9	-2.72	122.22	126.23
11	a	1106	CLA	C4D-C3D-CAD	2.72	111.06	108.11
11	b	1239	CLA	C4D-C3D-CAD	2.71	111.05	108.11
11	a	1127	CLA	C9-C8-C10	2.71	120.95	111.27
11	b	1240	CLA	CMB-C2B-C1B	2.71	129.55	125.42
11	b	1209	CLA	C2B-C1B-NB	2.71	113.14	110.33
11	A	1108	CLA	C4D-C3D-CAD	2.71	111.05	108.11
11	1	1011	CLA	C3D-C4D-ND	2.71	114.40	109.99
11	B	1240	CLA	C3D-C4D-ND	2.71	114.39	109.99
11	1	1122	CLA	C2B-C1B-NB	2.71	113.14	110.33
11	2	1214	CLA	CMC-C2C-C1C	2.71	129.27	125.03
11	B	1221	CLA	C1-O2A-CGA	2.71	123.21	116.65
14	a	4002	BCR	C33-C5-C4	2.71	119.38	113.60
11	1	1022	CLA	CMB-C2B-C1B	2.71	129.55	125.42
11	1	1120	CLA	CMB-C2B-C1B	2.71	129.55	125.42
11	B	1206	CLA	C2B-C1B-NB	2.71	113.14	110.33
11	B	1218	CLA	C4D-C3D-CAD	2.71	111.05	108.11
11	2	1232	CLA	CMD-C2D-C3D	-2.71	121.47	127.69
15	B	5004	LHG	O8-C23-C24	2.71	120.10	111.83
11	a	1120	CLA	C4D-C3D-CAD	2.71	111.05	108.11
11	B	1023	CLA	C9-C8-C7	2.71	120.93	111.27
11	1	1109	CLA	C1-C2-C3	-2.71	121.76	126.20
11	1	1115	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	L	4022	BCR	C37-C22-C21	-2.71	118.43	122.82
14	L	4022	BCR	C19-C18-C17	2.71	123.27	119.01
11	B	1213	CLA	CMC-C2C-C1C	2.71	129.27	125.03
11	b	1218	CLA	CMB-C2B-C1B	2.71	129.54	125.42
11	1	1106	CLA	C4-C3-C5	2.71	119.93	115.23
11	2	1013	CLA	C1-C2-C3	-2.71	121.76	126.20
11	1	1138	CLA	C4D-C3D-CAD	2.71	111.05	108.11
11	A	1122	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
11	B	1229	CLA	C2B-C1B-NB	2.71	113.13	110.33
11	A	1125	CLA	O2A-C1-C2	2.71	118.52	108.11
11	b	1231	CLA	C4D-C3D-CAD	2.71	111.04	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1121	CLA	C4D-C3D-CAD	2.71	111.04	108.11
11	1	1132	CLA	C1-C2-C3	-2.70	121.77	126.20
16	2	5002	LMG	O8-C28-C29	2.70	120.08	111.83
11	a	1140	CLA	C2B-C1B-NB	2.70	113.13	110.33
11	1	1110	CLA	C3D-C4D-ND	2.70	114.38	109.99
11	a	1113	CLA	C4D-C3D-CAD	2.70	111.04	108.11
14	8	4022	BCR	C34-C9-C8	2.70	122.22	118.09
11	b	1230	CLA	CAC-C3C-C4C	2.70	128.31	124.79
11	2	1213	CLA	C2B-C1B-NB	2.70	113.13	110.33
11	1	1125	CLA	C4-C3-C5	2.70	119.92	115.23
11	a	1121	CLA	CMB-C2B-C1B	2.70	129.53	125.42
14	a	4003	BCR	C4-C5-C6	-2.70	119.06	122.70
11	A	1103	CLA	C9-C8-C7	2.70	120.90	111.27
11	b	1213	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	f	4018	BCR	C4-C5-C6	-2.70	119.06	122.70
11	B	1213	CLA	O2A-C1-C2	2.70	118.50	108.11
11	2	1216	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
11	1	1136	CLA	CMD-C2D-C3D	-2.70	121.50	127.69
11	b	1021	CLA	CED-O2D-CGD	2.70	122.04	115.92
11	1	1112	CLA	C4D-C3D-CAD	2.70	111.04	108.11
11	A	1105	CLA	C2B-C1B-NB	2.70	113.12	110.33
11	B	1226	CLA	C2B-C1B-NB	2.70	113.12	110.33
11	a	1139	CLA	C2B-C1B-NB	2.70	113.12	110.33
11	b	1021	CLA	C9-C8-C7	2.70	120.89	111.27
11	1	1131	CLA	C9-C8-C10	2.70	120.89	111.27
11	b	1224	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
11	B	1202	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	b	4010	BCR	C38-C26-C27	2.70	119.34	113.60
11	1	1110	CLA	O2A-C1-C2	2.70	118.48	108.11
11	a	1113	CLA	C2B-C1B-NB	2.70	113.12	110.33
11	A	1127	CLA	C4D-C3D-CAD	2.69	111.03	108.11
11	1	1135	CLA	CMC-C2C-C1C	2.69	129.24	125.03
11	a	1237	CLA	C4-C3-C5	2.69	119.90	115.23
11	b	1230	CLA	C3D-C4D-ND	2.69	114.36	109.99
11	B	1211	CLA	C2B-C1B-NB	2.69	113.12	110.33
14	b	4004	BCR	C33-C5-C4	2.69	119.34	113.60
11	a	1104	CLA	C4-C3-C5	2.69	119.90	115.23
14	b	4014	BCR	C33-C5-C4	2.69	119.33	113.60
11	a	1103	CLA	CMC-C2C-C1C	2.69	129.24	125.03
11	2	1223	CLA	CMB-C2B-C1B	2.69	129.52	125.42
11	A	1134	CLA	C2B-C1B-NB	2.69	113.12	110.33
11	b	1201	CLA	CMB-C2B-C3B	2.69	132.88	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1022	CLA	C4D-C3D-CAD	2.69	111.03	108.11
11	1	1115	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
11	a	1111	CLA	C4-C3-C5	2.69	119.90	115.23
11	2	1226	CLA	C2B-C1B-NB	2.69	113.12	110.33
11	B	1023	CLA	CMB-C2B-C1B	2.69	129.51	125.42
11	b	1221	CLA	C3D-C4D-ND	2.69	114.36	109.99
11	2	1232	CLA	CMC-C2C-C1C	2.69	129.24	125.03
11	b	1212	CLA	C2B-C1B-NB	2.69	113.11	110.33
11	2	1206	CLA	C3D-C4D-ND	2.69	114.36	109.99
11	A	1110	CLA	C3D-C4D-ND	2.69	114.36	109.99
11	B	1228	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
11	0	1402	CLA	C4D-C3D-CAD	2.69	111.02	108.11
11	B	1239	CLA	CMB-C2B-C1B	2.69	129.51	125.42
11	b	1221	CLA	C3C-C4C-NC	2.69	113.87	110.43
11	2	1221	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
11	2	1227	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
11	B	1201	CLA	C1-O2A-CGA	2.69	123.15	116.65
11	2	1234	CLA	CBB-CAB-C3B	-2.69	114.11	127.53
11	a	1137	CLA	C2B-C1B-NB	2.69	113.11	110.33
11	A	1112	CLA	CMC-C2C-C1C	2.68	129.23	125.03
11	2	1209	CLA	CMD-C2D-C3D	-2.68	121.53	127.69
11	b	1023	CLA	C1-O2A-CGA	2.68	123.15	116.65
11	A	1132	CLA	C2B-C1B-NB	2.68	113.11	110.33
11	A	1134	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
11	A	1104	CLA	C9-C8-C7	2.68	120.84	111.27
11	a	1116	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
11	A	1109	CLA	C4D-C3D-CAD	2.68	111.02	108.11
11	1	1116	CLA	CMC-C2C-C1C	2.68	129.22	125.03
11	B	1225	CLA	CMB-C2B-C1B	2.68	129.50	125.42
11	B	1203	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	2	4009	BCR	C23-C24-C25	-2.68	119.84	127.00
11	1	1121	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
11	b	1232	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
11	B	1239	CLA	C4D-C3D-CAD	2.68	111.02	108.11
11	A	1137	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
11	b	1211	CLA	C2B-C1B-NB	2.68	113.10	110.33
11	B	1226	CLA	CMC-C2C-C1C	2.68	129.22	125.03
11	b	1226	CLA	CMC-C2C-C1C	2.68	129.22	125.03
11	b	1206	CLA	C2B-C1B-NB	2.68	113.10	110.33
11	a	1101	CLA	CMB-C2B-C1B	2.68	129.50	125.42
11	2	1211	CLA	C4D-C3D-CAD	2.68	111.01	108.11
11	a	1140	CLA	O2D-CGD-O1D	-2.68	118.64	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1126	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
12	a	2001	PQN	C2M-C2-C3	-2.68	120.05	124.45
14	b	4014	BCR	C23-C22-C21	2.68	123.22	119.01
11	L	1501	CLA	C3D-C4D-ND	2.68	114.33	109.99
11	1	1104	CLA	C4-C3-C5	2.67	119.87	115.23
11	2	1219	CLA	C3D-C4D-ND	2.67	114.33	109.99
11	2	1221	CLA	C3D-C4D-ND	2.67	114.33	109.99
11	a	1106	CLA	C3D-C4D-ND	2.67	114.33	109.99
11	l	1503	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	f	4018	BCR	C35-C13-C12	2.67	122.17	118.09
11	2	1215	CLA	C2B-C1B-NB	2.67	113.10	110.33
11	2	1232	CLA	C4D-C3D-CAD	2.67	111.01	108.11
11	b	1209	CLA	CMB-C2B-C1B	2.67	129.49	125.42
12	b	2002	PQN	C2M-C2-C3	-2.67	120.06	124.45
11	b	1223	CLA	C4D-C3D-CAD	2.67	111.01	108.11
11	2	1021	CLA	C4D-C3D-CAD	2.67	111.01	108.11
11	b	1229	CLA	CMB-C2B-C1B	2.67	129.49	125.42
11	a	1120	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	2	1230	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	2	1223	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	1	4007	BCR	C28-C27-C26	-2.67	109.29	114.06
11	A	1116	CLA	CAC-C3C-C4C	2.67	128.26	124.79
11	a	1103	CLA	C4D-C3D-CAD	2.67	111.01	108.11
11	a	1123	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	f	4020	BCR	C33-C5-C4	2.67	119.29	113.60
11	k	1401	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	l	1501	CLA	CMC-C2C-C1C	2.67	129.21	125.03
11	2	1231	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	A	1126	CLA	C4D-C3D-CAD	2.67	111.00	108.11
11	a	1118	CLA	CMC-C2C-C1C	2.67	129.21	125.03
11	A	1127	CLA	C1-C2-C3	-2.67	121.82	126.20
11	2	1209	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	0	1401	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
11	A	1110	CLA	CMC-C2C-C1C	2.67	129.20	125.03
11	1	1110	CLA	C4-C3-C5	2.67	119.86	115.23
14	A	4008	BCR	C35-C13-C14	-2.67	118.50	122.82
11	1	1133	CLA	C4D-C3D-CAD	2.67	111.00	108.11
11	A	1109	CLA	CMD-C2D-C3D	-2.67	121.58	127.69
11	1	1121	CLA	CMC-C2C-C1C	2.67	129.20	125.03
11	A	1105	CLA	CMB-C2B-C1B	2.67	129.48	125.42
11	2	1221	CLA	CMB-C2B-C1B	2.67	129.48	125.42
11	2	1207	CLA	CAC-C3C-C4C	2.66	128.26	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1021	CLA	CMC-C2C-C1C	2.66	129.20	125.03
11	a	1110	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
11	1	1114	CLA	CMB-C2B-C1B	2.66	129.47	125.42
11	A	1118	CLA	CMD-C2D-C3D	-2.66	121.58	127.69
11	b	1225	CLA	CAC-C3C-C4C	2.66	128.25	124.79
11	A	1125	CLA	C4D-C3D-CAD	2.66	111.00	108.11
11	8	1503	CLA	CMC-C2C-C1C	2.66	129.19	125.03
11	b	1207	CLA	C3D-C4D-ND	2.66	114.31	109.99
11	A	1140	CLA	CMB-C2B-C1B	2.66	129.47	125.42
11	a	1012	CLA	OBD-CAD-C3D	-2.66	122.19	128.42
11	2	1013	CLA	CHB-C4A-NA	2.66	128.24	124.40
11	a	1127	CLA	C4-C3-C5	2.66	119.85	115.23
14	f	4020	BCR	C36-C18-C17	-2.66	118.50	122.82
14	2	4006	BCR	C38-C26-C27	2.66	119.27	113.60
11	a	1118	CLA	CMB-C2B-C1B	2.66	129.47	125.42
11	a	1124	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
11	l	1501	CLA	C1-O2A-CGA	2.66	123.09	116.65
11	B	1220	CLA	CMD-C2D-C3D	-2.66	121.59	127.69
11	l	1501	CLA	CMB-C2B-C1B	2.66	129.47	125.42
11	B	1222	CLA	C3C-C4C-NC	2.66	113.84	110.43
11	b	1213	CLA	C4-C3-C2	-2.66	116.79	123.63
11	K	1401	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
11	B	1217	CLA	C4D-C3D-CAD	2.66	111.00	108.11
11	1	1122	CLA	C4D-C3D-CAD	2.66	111.00	108.11
11	a	1129	CLA	C2B-C1B-NB	2.66	113.08	110.33
11	b	1224	CLA	C1-C2-C3	-2.66	121.84	126.20
11	2	1223	CLA	CMD-C2D-C3D	-2.66	121.59	127.69
11	k	1402	CLA	C4D-C3D-CAD	2.66	110.99	108.11
12	A	2001	PQN	C2M-C2-C3	-2.66	120.08	124.45
11	A	1104	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
11	B	1236	CLA	CMB-C2B-C1B	2.66	129.47	125.42
11	B	1234	CLA	CMC-C2C-C1C	2.66	129.19	125.03
11	2	1213	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
11	A	1110	CLA	O2A-C1-C2	2.66	118.33	108.11
11	a	1012	CLA	C3C-C4C-NC	2.66	113.83	110.43
11	B	1227	CLA	C4D-C3D-CAD	2.66	110.99	108.11
11	2	1219	CLA	C1-C2-C3	-2.66	121.84	126.20
11	B	1235	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
11	1	1108	CLA	CMC-C2C-C1C	2.66	129.18	125.03
11	a	1108	CLA	C2B-C1B-NB	2.65	113.08	110.33
11	A	1109	CLA	CMB-C2B-C1B	2.65	129.46	125.42
11	2	1218	CLA	CMD-C2D-C3D	-2.65	121.60	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1125	CLA	C3D-C4D-ND	2.65	114.30	109.99
11	1	1124	CLA	CMD-C2D-C3D	-2.65	121.60	127.69
11	A	1138	CLA	CMB-C2B-C1B	2.65	129.46	125.42
14	l	4022	BCR	C23-C22-C21	2.65	123.18	119.01
11	a	1011	CLA	CMC-C2C-C1C	2.65	129.18	125.03
14	A	4007	BCR	C15-C14-C13	-2.65	123.56	127.28
11	1	1101	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
11	8	1501	CLA	C4D-C3D-CAD	2.65	110.98	108.11
11	B	1204	CLA	C1-O2A-CGA	2.65	123.07	116.65
11	a	1022	CLA	CMC-C2C-C1C	2.65	129.18	125.03
11	b	1230	CLA	C1-O2A-CGA	2.65	123.07	116.65
11	A	1801	CLA	C3C-C4C-NC	2.65	113.83	110.43
11	a	1140	CLA	CMB-C2B-C1B	2.65	129.45	125.42
11	b	1221	CLA	C2B-C1B-NB	2.65	113.07	110.33
11	A	1111	CLA	C4-C3-C5	2.65	119.83	115.23
11	b	1225	CLA	CMC-C2C-C1C	2.65	129.17	125.03
11	a	1112	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
11	A	1114	CLA	C4D-C3D-CAD	2.65	110.98	108.11
11	b	1218	CLA	C4D-C3D-CAD	2.65	110.98	108.11
11	a	1011	CLA	C1-C2-C3	-2.65	121.86	126.20
11	b	1224	CLA	CMB-C2B-C1B	2.65	129.45	125.42
11	B	1203	CLA	CMB-C2B-C1B	2.65	129.45	125.42
11	B	1212	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
11	l	1502	CLA	C3C-C4C-NC	2.65	113.82	110.43
11	b	1210	CLA	C4D-C3D-CAD	2.65	110.98	108.11
11	B	1238	CLA	CMC-C2C-C1C	2.65	129.17	125.03
11	a	1131	CLA	CMC-C2C-C1C	2.65	129.17	125.03
11	L	1502	CLA	CMB-C2B-C1B	2.65	129.45	125.42
14	A	4003	BCR	C33-C5-C4	2.65	119.24	113.60
11	B	1224	CLA	C3C-C4C-NC	2.65	113.82	110.43
11	1	1132	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
14	1	4002	BCR	C30-C25-C26	-2.64	119.02	122.64
11	a	1134	CLA	CMC-C2C-C1C	2.64	129.17	125.03
14	B	4009	BCR	C37-C22-C21	-2.64	118.53	122.82
11	B	1214	CLA	CMC-C2C-C1C	2.64	129.16	125.03
11	2	1216	CLA	C3C-C4C-NC	2.64	113.82	110.43
11	b	1227	CLA	CMB-C2B-C1B	2.64	129.44	125.42
11	b	1220	CLA	C4D-C3D-CAD	2.64	110.98	108.11
11	B	1232	CLA	CMC-C2C-C1C	2.64	129.16	125.03
11	2	1215	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
11	b	1203	CLA	CMB-C2B-C1B	2.64	129.44	125.42
14	B	4010	BCR	C36-C18-C17	-2.64	118.54	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1105	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	a	4007	BCR	C3-C4-C5	-2.64	109.35	114.06
11	A	1109	CLA	CED-O2D-CGD	2.64	121.91	115.92
11	A	1101	CLA	C6-C5-C3	-2.64	107.04	113.47
11	b	1021	CLA	C9-C8-C10	2.64	120.69	111.27
11	2	1212	CLA	CMC-C2C-C1C	2.64	129.16	125.03
14	1	4007	BCR	C38-C26-C27	2.64	119.22	113.60
11	A	1137	CLA	C3C-C4C-NC	2.64	113.81	110.43
11	A	1126	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
14	B	4005	BCR	C35-C13-C12	2.64	122.12	118.09
11	a	1135	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
11	A	1135	CLA	CMB-C2B-C1B	2.64	129.44	125.42
11	b	1230	CLA	C3C-C4C-NC	2.64	113.81	110.43
11	a	1105	CLA	CMB-C2B-C1B	2.64	129.44	125.42
11	B	1215	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
11	1	1801	CLA	C1-C2-C3	-2.64	121.88	126.20
11	B	1235	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	b	4004	BCR	C19-C18-C17	2.64	123.16	119.01
11	2	1216	CLA	O2A-C1-C2	2.64	118.26	108.11
11	b	1234	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	l	4022	BCR	C29-C30-C25	-2.64	106.61	110.44
11	A	1102	CLA	CHB-C4A-NA	2.64	128.21	124.40
11	B	1222	CLA	O1D-CGD-CBD	-2.64	119.32	124.52
14	1	4001	BCR	C38-C26-C27	2.64	119.22	113.60
11	2	1218	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
11	2	1203	CLA	C9-C8-C7	2.63	120.67	111.27
14	2	4004	BCR	C36-C18-C17	-2.63	118.55	122.82
11	b	1214	CLA	CMC-C2C-C1C	2.63	129.15	125.03
11	2	1210	CLA	C4D-C3D-CAD	2.63	110.97	108.11
11	2	1227	CLA	C4D-C3D-CAD	2.63	110.97	108.11
14	B	4006	BCR	C33-C5-C6	-2.63	121.61	124.48
11	A	1117	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
11	A	1125	CLA	C2B-C1B-NB	2.63	113.06	110.33
11	2	1223	CLA	C9-C8-C10	2.63	120.66	111.27
14	6	4020	BCR	C3-C4-C5	-2.63	109.36	114.06
11	B	1219	CLA	CMC-C2C-C1C	2.63	129.15	125.03
11	2	1235	CLA	C4D-C3D-CAD	2.63	110.96	108.11
11	1	1103	CLA	C3D-C4D-ND	2.63	114.26	109.99
11	A	1114	CLA	C2B-C1B-NB	2.63	113.05	110.33
11	b	1223	CLA	C2B-C1B-NB	2.63	113.05	110.33
11	b	1203	CLA	O2A-C1-C2	2.63	118.23	108.11
11	2	1201	CLA	O2D-CGD-O1D	-2.63	118.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1206	CLA	CAC-C3C-C4C	2.63	128.21	124.79
11	1	1107	CLA	CMB-C2B-C1B	2.63	129.42	125.42
11	b	1229	CLA	C4D-C3D-CAD	2.63	110.96	108.11
11	1	1140	CLA	C4D-C3D-CAD	2.63	110.96	108.11
11	1	1012	CLA	CMC-C2C-C1C	2.63	129.14	125.03
11	A	1012	CLA	C3C-C4C-NC	2.63	113.80	110.43
11	1	1134	CLA	CMC-C2C-C1C	2.63	129.14	125.03
11	2	1218	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	1	4003	BCR	C38-C26-C27	2.63	119.20	113.60
11	b	1222	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	1	4003	BCR	C33-C5-C4	2.63	119.20	113.60
11	a	1120	CLA	C3D-C4D-ND	2.63	114.26	109.99
11	a	1108	CLA	CMC-C2C-C1C	2.63	129.14	125.03
11	2	1229	CLA	C4D-C3D-CAD	2.63	110.96	108.11
11	b	1213	CLA	C2B-C1B-NB	2.63	113.05	110.33
11	1	1110	CLA	O1D-CGD-CBD	-2.63	119.34	124.52
11	a	1135	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
15	b	5004	LHG	O8-C23-C24	2.63	119.84	111.83
11	a	1123	CLA	CMD-C2D-C3D	-2.63	121.67	127.69
14	b	4005	BCR	C3-C4-C5	-2.63	109.37	114.06
14	2	4010	BCR	C3-C4-C5	-2.62	109.38	114.06
11	1	1117	CLA	C9-C8-C7	2.62	120.63	111.27
11	B	1238	CLA	CMD-C2D-C3D	-2.62	121.67	127.69
11	a	1123	CLA	C2B-C1B-NB	2.62	113.05	110.33
11	A	1131	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
11	1	1122	CLA	C3C-C4C-NC	2.62	113.79	110.43
14	b	4004	BCR	C34-C9-C10	-2.62	118.57	122.82
14	B	4010	BCR	C3-C4-C5	-2.62	109.38	114.06
11	b	1023	CLA	CBB-CAB-C3B	-2.62	114.42	127.53
11	A	1136	CLA	CMC-C2C-C1C	2.62	129.13	125.03
11	a	1114	CLA	C4D-C3D-CAD	2.62	110.95	108.11
11	b	1228	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
11	A	1106	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
14	f	4020	BCR	C28-C27-C26	-2.62	109.38	114.06
11	a	1124	CLA	CED-O2D-CGD	2.62	121.86	115.92
11	b	1232	CLA	CMB-C2B-C1B	2.62	129.41	125.42
11	1	1123	CLA	CMB-C2B-C1B	2.62	129.41	125.42
11	b	1201	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
14	8	4022	BCR	C19-C18-C17	2.62	123.13	119.01
11	b	1230	CLA	CMB-C2B-C1B	2.62	129.41	125.42
11	b	1214	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
11	b	1239	CLA	O2D-CGD-O1D	-2.62	118.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1101	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
11	a	1101	CLA	C4-C3-C2	-2.62	116.90	123.63
11	b	1238	CLA	C4D-C3D-CAD	2.62	110.95	108.11
11	2	1021	CLA	C3D-C4D-ND	2.62	114.24	109.99
11	a	1109	CLA	C1-C2-C3	-2.62	121.91	126.20
11	A	1132	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
14	F	4020	BCR	C33-C5-C4	2.62	119.18	113.60
11	1	1135	CLA	C1-C2-C3	-2.62	121.91	126.20
11	2	1239	CLA	CMB-C2B-C1B	2.62	129.41	125.42
11	B	1202	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
11	B	1240	CLA	C4D-C3D-CAD	2.62	110.95	108.11
11	2	1230	CLA	C3C-C4C-NC	2.62	113.78	110.43
11	B	1204	CLA	CBC-CAC-C3C	-2.62	105.33	112.42
11	a	1107	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
11	A	1103	CLA	C1-O2A-CGA	2.62	122.99	116.65
11	B	1213	CLA	C2B-C1B-NB	2.62	113.04	110.33
11	A	1122	CLA	C3C-C4C-NC	2.62	113.78	110.43
11	2	1214	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
11	1	1801	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
14	B	4004	BCR	C27-C26-C25	-2.61	119.17	122.70
11	b	1216	CLA	CMC-C2C-C1C	2.61	129.12	125.03
11	A	1111	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
11	2	1231	CLA	C3D-C4D-ND	2.61	114.23	109.99
11	a	1110	CLA	CMC-C2C-C1C	2.61	129.12	125.03
11	a	1108	CLA	CAC-C3C-C4C	2.61	128.19	124.79
11	B	1013	CLA	CHB-C4A-NA	2.61	128.17	124.40
11	2	1013	CLA	C4-C3-C5	2.61	119.76	115.23
11	1	1130	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
11	2	1215	CLA	CMB-C2B-C1B	2.61	129.40	125.42
14	b	4006	BCR	C35-C13-C12	2.61	122.08	118.09
11	1	1118	CLA	C1-O2A-CGA	2.61	122.97	116.65
11	a	1131	CLA	CMB-C2B-C1B	2.61	129.39	125.42
11	B	1224	CLA	C4-C3-C5	2.61	119.76	115.23
11	1	1132	CLA	C4D-C3D-CAD	2.61	110.94	108.11
11	b	1220	CLA	C3C-C4C-NC	2.61	113.77	110.43
11	l	1502	CLA	C2B-C1B-NB	2.61	113.03	110.33
11	A	1105	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
11	1	1108	CLA	CMB-C2B-C1B	2.61	129.39	125.42
11	a	1105	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
11	B	1231	CLA	C3D-C4D-ND	2.61	114.23	109.99
11	1	1116	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
11	1	1129	CLA	CMB-C2B-C1B	2.61	129.39	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1216	CLA	C4D-C3D-CAD	2.61	110.94	108.11
11	B	1215	CLA	CMB-C2B-C1B	2.61	129.39	125.42
11	B	1206	CLA	CAC-C3C-C4C	2.61	128.18	124.79
11	B	1204	CLA	C1-C2-C3	-2.61	121.93	126.20
11	2	1204	CLA	CMB-C2B-C1B	2.61	129.39	125.42
11	1	1130	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
11	a	1124	CLA	C4D-C3D-CAD	2.61	110.94	108.11
11	1	1118	CLA	CMB-C2B-C1B	2.61	129.39	125.42
11	a	1123	CLA	C9-C8-C10	2.60	120.56	111.27
11	1	1139	CLA	CAC-C3C-C4C	2.60	128.18	124.79
14	L	4019	BCR	C7-C6-C5	-2.60	115.56	121.56
11	1	1102	CLA	C4D-C3D-CAD	2.60	110.93	108.11
11	a	1134	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
11	b	1021	CLA	O2A-C1-C2	2.60	118.13	108.11
11	a	1022	CLA	CMB-C2B-C1B	2.60	129.38	125.42
14	2	4005	BCR	C38-C26-C27	2.60	119.14	113.60
11	A	1101	CLA	C9-C8-C7	2.60	120.55	111.27
14	1	4001	BCR	C30-C25-C26	-2.60	119.08	122.64
11	A	1128	CLA	CMB-C2B-C1B	2.60	129.38	125.42
11	a	1126	CLA	C4D-C3D-CAD	2.60	110.93	108.11
11	B	1236	CLA	C2B-C1B-NB	2.60	113.02	110.33
11	1	1022	CLA	CMC-C2C-C1C	2.60	129.10	125.03
11	b	1219	CLA	C4D-C3D-CAD	2.60	110.93	108.11
11	1	1135	CLA	C3C-C4C-NC	2.60	113.76	110.43
11	a	1114	CLA	CMB-C2B-C1B	2.60	129.38	125.42
14	8	4022	BCR	C37-C22-C21	-2.60	118.60	122.82
14	B	4009	BCR	C38-C26-C27	2.60	119.14	113.60
14	a	4002	BCR	C30-C25-C26	-2.60	119.08	122.64
11	1	1801	CLA	CMB-C2B-C1B	2.60	129.38	125.42
11	B	1231	CLA	CMC-C2C-C1C	2.60	129.10	125.03
11	2	1223	CLA	C3C-C4C-NC	2.60	113.76	110.43
11	A	1112	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
11	b	1205	CLA	C4D-C3D-CAD	2.60	110.93	108.11
11	1	1102	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	2	4014	BCR	C38-C26-C27	2.60	119.13	113.60
11	A	1104	CLA	C4-C3-C5	2.60	119.73	115.23
11	1	1140	CLA	CMC-C2C-C1C	2.60	129.09	125.03
11	2	1236	CLA	C2B-C1B-NB	2.60	113.02	110.33
11	a	1126	CLA	C3C-C4C-NC	2.60	113.75	110.43
11	a	1102	CLA	C4D-C3D-CAD	2.60	110.92	108.11
12	1	2001	PQN	C24-C23-C25	2.60	120.53	111.27
11	1	1103	CLA	CMC-C2C-C1C	2.59	129.09	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1204	CLA	C4-C3-C5	2.59	119.73	115.23
11	a	1108	CLA	CMB-C2B-C1B	2.59	129.37	125.42
11	A	1112	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
11	1	1237	CLA	CMB-C2B-C1B	2.59	129.37	125.42
14	1	4008	BCR	C1-C6-C5	-2.59	119.09	122.64
11	2	1206	CLA	CMC-C2C-C1C	2.59	129.09	125.03
11	2	1226	CLA	C9-C8-C7	2.59	120.52	111.27
11	a	1122	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
11	b	1235	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
11	B	1218	CLA	CMC-C2C-C1C	2.59	129.09	125.03
11	B	1201	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
11	b	1208	CLA	C2B-C1B-NB	2.59	113.01	110.33
14	B	4017	BCR	C33-C5-C6	-2.59	121.66	124.48
11	a	1107	CLA	C9-C8-C7	2.59	120.51	111.27
11	1	1133	CLA	CMB-C2B-C1B	2.59	129.36	125.42
14	8	4019	BCR	C38-C26-C27	2.59	119.12	113.60
11	B	1238	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
11	B	1224	CLA	CMC-C2C-C1C	2.59	129.08	125.03
11	1	1124	CLA	CMC-C2C-C1C	2.59	129.08	125.03
11	2	1202	CLA	C4-C3-C5	2.59	119.72	115.23
11	a	1133	CLA	C4D-C3D-CAD	2.59	110.92	108.11
11	A	1117	CLA	C1-O2A-CGA	2.59	122.92	116.65
11	1	1113	CLA	C2B-C1B-NB	2.59	113.01	110.33
11	b	1221	CLA	C4D-C3D-CAD	2.59	110.92	108.11
11	1	1104	CLA	C9-C8-C10	2.59	120.50	111.27
11	A	1801	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
11	1	1127	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
11	k	1401	CLA	C4D-C3D-CAD	2.59	110.92	108.11
11	a	1134	CLA	CAC-C3C-C4C	2.59	128.16	124.79
11	a	1125	CLA	CMC-C2C-C1C	2.59	129.08	125.03
11	1	1119	CLA	CMC-C2C-C1C	2.59	129.08	125.03
11	A	1128	CLA	C9-C8-C7	2.59	120.50	111.27
11	A	1122	CLA	C1-C2-C3	-2.59	121.96	126.20
11	b	1219	CLA	C1-C2-C3	-2.59	121.96	126.20
11	a	1132	CLA	CMC-C2C-C1C	2.59	129.07	125.03
11	a	1105	CLA	CMD-C2D-C3D	-2.59	121.76	127.69
14	A	4002	BCR	C23-C22-C21	2.59	123.08	119.01
14	B	4004	BCR	C30-C25-C24	2.59	122.66	115.65
14	B	4010	BCR	C30-C25-C24	2.59	122.66	115.65
11	A	1133	CLA	C4D-C3D-CAD	2.59	110.91	108.11
11	0	1401	CLA	C4D-C3D-CAD	2.59	110.91	108.11
11	A	1102	CLA	O2D-CGD-O1D	-2.59	118.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1118	CLA	O2D-CGD-O1D	-2.59	118.82	123.85
11	B	1222	CLA	C3D-C4D-ND	2.58	114.19	109.99
11	1	1801	CLA	C3C-C4C-NC	2.58	113.74	110.43
14	M	4021	BCR	C37-C22-C21	-2.58	118.63	122.82
14	2	4017	BCR	C1-C6-C7	2.58	122.66	115.65
11	a	1115	CLA	C3C-C4C-NC	2.58	113.74	110.43
11	B	1208	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
11	2	1220	CLA	C4D-C3D-CAD	2.58	110.91	108.11
11	a	1127	CLA	C2B-C1B-NB	2.58	113.00	110.33
11	b	1215	CLA	CMB-C2B-C1B	2.58	129.35	125.42
11	2	1219	CLA	CMC-C2C-C1C	2.58	129.07	125.03
11	l	1503	CLA	O2A-C1-C2	2.58	118.05	108.11
11	A	1128	CLA	C4D-C3D-CAD	2.58	110.91	108.11
11	A	1133	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	4005	BCR	C36-C18-C17	-2.58	118.63	122.82
14	b	4011	BCR	C23-C24-C25	-2.58	120.10	127.00
11	l	1501	CLA	O2A-C1-C2	2.58	118.04	108.11
11	a	1801	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
11	a	1128	CLA	CMB-C2B-C1B	2.58	129.35	125.42
11	b	1208	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
11	B	1234	CLA	C9-C8-C10	2.58	120.47	111.27
14	L	4019	BCR	C8-C9-C10	2.58	123.07	119.01
11	A	1108	CLA	CMB-C2B-C1B	2.58	129.35	125.42
11	1	1139	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
11	B	1228	CLA	C4D-C3D-CAD	2.58	110.91	108.11
11	1	1137	CLA	C4D-C3D-CAD	2.58	110.91	108.11
11	A	1101	CLA	C3C-C4C-NC	2.58	113.74	110.43
11	2	1202	CLA	C2B-C1B-NB	2.58	113.00	110.33
11	2	1217	CLA	C1-O2A-CGA	2.58	124.00	116.67
11	a	1237	CLA	CMB-C2B-C1B	2.58	129.35	125.42
11	A	1104	CLA	C9-C8-C10	2.58	120.47	111.27
11	A	1119	CLA	C9-C8-C10	2.58	120.47	111.27
11	A	1132	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
11	a	1107	CLA	C3C-C4C-NC	2.58	113.73	110.43
11	1	1106	CLA	CMB-C2B-C1B	2.58	129.35	125.42
11	b	1203	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
11	b	1220	CLA	CMD-C2D-C3D	-2.58	121.78	127.69
11	A	1103	CLA	CMC-C2C-C1C	2.58	129.06	125.03
11	A	1123	CLA	CMC-C2C-C1C	2.58	129.06	125.03
11	a	1117	CLA	CMC-C2C-C1C	2.58	129.06	125.03
11	2	1238	CLA	C4D-C3D-CAD	2.58	110.91	108.11
11	B	1224	CLA	CMD-C2D-C3D	-2.58	121.78	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1128	CLA	C1-C2-C3	-2.58	121.97	126.20
11	b	1221	CLA	CMB-C2B-C1B	2.58	129.34	125.42
11	2	1216	CLA	CAC-C3C-C4C	2.58	128.14	124.79
14	l	4022	BCR	C3-C4-C5	-2.58	109.46	114.06
11	B	1204	CLA	CMD-C2D-C3D	-2.58	121.78	127.69
11	8	1503	CLA	C4-C3-C5	2.58	119.70	115.23
11	1	1114	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
11	B	1013	CLA	C4D-C3D-CAD	2.58	110.90	108.11
14	b	4017	BCR	C33-C5-C6	-2.58	121.67	124.48
11	2	1221	CLA	C3C-C4C-NC	2.58	113.73	110.43
11	B	1218	CLA	CMB-C2B-C1B	2.57	129.34	125.42
11	b	1238	CLA	CMC-C2C-C1C	2.57	129.06	125.03
11	1	1107	CLA	C4-C3-C2	-2.57	117.02	123.63
14	B	4017	BCR	C23-C24-C25	-2.57	120.12	127.00
11	a	1115	CLA	CMD-C2D-C3D	-2.57	121.79	127.69
14	b	4017	BCR	C36-C18-C17	-2.57	118.65	122.82
11	K	1401	CLA	C4D-C3D-CAD	2.57	110.90	108.11
11	k	1401	CLA	CMC-C2C-C1C	2.57	129.05	125.03
11	a	1112	CLA	CMD-C2D-C3D	-2.57	121.79	127.69
11	1	1104	CLA	C4D-C3D-CAD	2.57	110.90	108.11
11	B	1223	CLA	C3C-C4C-NC	2.57	113.72	110.43
11	b	1021	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
11	A	1110	CLA	C4D-C3D-CAD	2.57	110.90	108.11
11	A	1140	CLA	C1-O2A-CGA	2.57	122.87	116.65
11	2	1205	CLA	C2B-C1B-NB	2.57	112.99	110.33
11	b	1214	CLA	C4D-C3D-CAD	2.57	110.90	108.11
12	B	2002	PQN	C2M-C2-C3	-2.57	120.23	124.45
11	2	1234	CLA	C4-C3-C5	2.57	119.69	115.23
11	B	1218	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	M	4021	BCR	C23-C22-C21	2.57	123.05	119.01
14	B	4004	BCR	C33-C5-C4	2.57	119.07	113.60
11	1	1128	CLA	C2B-C1B-NB	2.57	112.99	110.33
11	1	1103	CLA	C9-C8-C7	2.57	120.42	111.27
14	6	4013	BCR	C33-C5-C4	2.57	119.07	113.60
11	a	1108	CLA	CMD-C2D-C3D	-2.57	121.81	127.69
11	A	1129	CLA	C3C-C4C-NC	2.56	113.72	110.43
11	b	1201	CLA	C4-C3-C5	2.56	119.68	115.23
11	1	1125	CLA	C4D-C3D-CAD	2.56	110.89	108.11
11	1	1129	CLA	C2B-C1B-NB	2.56	112.98	110.33
11	1	1107	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
11	B	1021	CLA	C9-C8-C7	2.56	120.41	111.27
14	b	4014	BCR	C27-C26-C25	-2.56	119.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	4020	BCR	C36-C18-C17	-2.56	118.66	122.82
11	a	1104	CLA	C4D-C3D-CAD	2.56	110.89	108.11
11	b	1235	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
11	B	1216	CLA	O2A-C1-C2	2.56	117.97	108.11
11	1	1126	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
11	b	1223	CLA	CMC-C2C-C1C	2.56	129.04	125.03
11	B	1227	CLA	C2B-C1B-NB	2.56	112.98	110.33
11	1	1117	CLA	C4-C3-C5	2.56	119.67	115.23
11	b	1203	CLA	C4-C3-C5	2.56	119.67	115.23
11	b	1204	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
11	1	1109	CLA	CMB-C2B-C1B	2.56	129.32	125.42
11	1	1130	CLA	CMC-C2C-C1C	2.56	129.03	125.03
11	A	1110	CLA	C4-C3-C5	2.56	119.67	115.23
11	B	1206	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
14	f	4018	BCR	C32-C1-C6	-2.56	106.23	110.24
14	M	4021	BCR	C23-C24-C25	-2.56	120.17	127.00
11	B	1214	CLA	CAC-C3C-C4C	2.56	128.12	124.79
11	A	1136	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
14	b	4009	BCR	C3-C4-C5	-2.56	109.50	114.06
11	B	1226	CLA	CMB-C2B-C1B	2.56	129.31	125.42
14	1	4003	BCR	C36-C18-C17	-2.56	118.67	122.82
14	a	4002	BCR	C30-C25-C24	2.56	122.58	115.65
11	2	1203	CLA	CBC-CAC-C3C	-2.56	105.49	112.42
11	2	1230	CLA	CMB-C2B-C1B	2.56	129.31	125.42
11	B	1239	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
11	a	1116	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
11	A	1102	CLA	C9-C8-C7	2.56	120.38	111.27
11	b	1210	CLA	CMB-C2B-C1B	2.55	129.31	125.42
11	a	1130	CLA	CMC-C2C-C1C	2.55	129.03	125.03
11	b	1228	CLA	C4D-C3D-CAD	2.55	110.88	108.11
11	B	1224	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
11	B	1206	CLA	O2A-C1-C2	2.55	117.94	108.11
11	B	1223	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
11	2	1021	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
14	2	4017	BCR	C4-C5-C6	-2.55	119.25	122.70
11	0	1401	CLA	CMC-C2C-C1C	2.55	129.02	125.03
14	b	4017	BCR	C8-C9-C10	2.55	123.02	119.01
14	b	4006	BCR	C37-C22-C21	-2.55	118.68	122.82
11	A	1111	CLA	C4D-C3D-CAD	2.55	110.88	108.11
11	a	1109	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
14	f	4013	BCR	C33-C5-C4	2.55	119.04	113.60
11	1	1106	CLA	C1-C2-C3	-2.55	122.02	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1114	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
11	1	1237	CLA	C2B-C1B-NB	2.55	112.97	110.33
11	b	1021	CLA	C4D-C3D-CAD	2.55	110.88	108.11
11	b	1226	CLA	C1-C2-C3	-2.55	122.02	126.20
11	B	1232	CLA	C2B-C1B-NB	2.55	112.97	110.33
11	a	1109	CLA	C4D-C3D-CAD	2.55	110.88	108.11
11	1	1134	CLA	C4D-C3D-CAD	2.55	110.88	108.11
14	A	4007	BCR	C35-C13-C12	2.55	121.98	118.09
11	1	1135	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
11	1	1136	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
14	l	4022	BCR	C35-C13-C12	2.55	121.98	118.09
11	A	1102	CLA	CMB-C2B-C1B	2.55	129.30	125.42
11	b	1205	CLA	CMC-C2C-C1C	2.55	129.02	125.03
14	2	4011	BCR	C37-C22-C21	-2.55	118.69	122.82
11	B	1236	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
11	B	1213	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
11	1	1127	CLA	CMB-C2B-C1B	2.55	129.30	125.42
11	1	1120	CLA	CMC-C2C-C1C	2.55	129.01	125.03
11	A	1125	CLA	CMB-C2B-C1B	2.55	129.30	125.42
11	0	1402	CLA	CMD-C2D-C3D	-2.55	121.85	127.69
11	K	1401	CLA	CMC-C2C-C1C	2.55	129.01	125.03
11	1	1139	CLA	CMB-C2B-C1B	2.55	129.30	125.42
14	B	4006	BCR	C23-C22-C21	2.55	123.02	119.01
11	B	1234	CLA	CBB-CAB-C3B	-2.55	114.80	127.53
11	1	1113	CLA	CMC-C2C-C1C	2.55	129.01	125.03
14	2	4006	BCR	C36-C18-C17	-2.55	118.69	122.82
11	1	1111	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
11	2	1013	CLA	CED-O2D-CGD	2.55	121.69	115.92
11	B	1223	CLA	C1-C2-C3	-2.55	122.03	126.20
11	a	1101	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	b	4011	BCR	C1-C6-C5	-2.54	119.16	122.64
11	2	1023	CLA	O2D-CGD-O1D	-2.54	118.89	123.85
11	1	1107	CLA	C2B-C1B-NB	2.54	112.96	110.33
11	2	1224	CLA	CMC-C2C-C1C	2.54	129.01	125.03
14	8	4022	BCR	C7-C8-C9	-2.54	122.47	126.23
11	B	1221	CLA	C4D-C3D-CAD	2.54	110.87	108.11
11	2	1235	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
11	1	1119	CLA	C9-C8-C10	2.54	120.34	111.27
11	b	1202	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
11	1	1103	CLA	CAC-C3C-C4C	2.54	128.10	124.79
11	B	1224	CLA	C1-O2A-CGA	2.54	122.81	116.65
11	a	1116	CLA	C1-O2A-CGA	2.54	122.81	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1116	CLA	CMB-C2B-C1B	2.54	129.29	125.42
11	8	1503	CLA	C4D-C3D-CAD	2.54	110.87	108.11
11	A	1108	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
11	2	1213	CLA	CMC-C2C-C3C	2.54	133.02	126.15
11	L	1503	CLA	C4D-C3D-CAD	2.54	110.87	108.11
11	a	1122	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
11	A	1123	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
11	2	1207	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
11	B	1228	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
12	2	2002	PQN	C2M-C2-C3	-2.54	120.28	124.45
11	A	1119	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
11	0	1401	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
11	b	1229	CLA	CMC-C2C-C1C	2.54	129.00	125.03
11	L	1503	CLA	O2A-C1-C2	2.54	117.88	108.11
11	a	1136	CLA	C4D-C3D-CAD	2.54	110.86	108.11
11	2	1215	CLA	C4D-C3D-CAD	2.54	110.86	108.11
11	1	1115	CLA	CMC-C2C-C1C	2.54	129.00	125.03
11	B	1205	CLA	C3D-C4D-ND	2.54	114.11	109.99
11	B	1220	CLA	C4D-C3D-CAD	2.54	110.86	108.11
11	b	1215	CLA	C9-C8-C10	2.54	120.32	111.27
11	1	1104	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
11	B	1223	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
11	b	1224	CLA	C3C-C4C-NC	2.54	113.68	110.43
11	1	1137	CLA	C3C-C4C-NC	2.54	113.68	110.43
11	2	1219	CLA	C3C-C4C-NC	2.54	113.68	110.43
11	B	1209	CLA	C4D-C3D-CAD	2.54	110.86	108.11
11	1	1128	CLA	C4D-C3D-CAD	2.54	110.86	108.11
11	B	1230	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
11	A	1101	CLA	CMB-C2B-C1B	2.54	129.28	125.42
11	A	1133	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
14	L	4019	BCR	C1-C6-C7	2.54	122.53	115.65
11	B	1228	CLA	C1-C2-C3	-2.53	122.66	126.76
11	B	1203	CLA	C4D-C3D-CAD	2.53	110.86	108.11
11	a	1115	CLA	CMC-C2C-C1C	2.53	129.00	125.03
11	b	1215	CLA	CMC-C2C-C1C	2.53	129.00	125.03
11	A	1107	CLA	C3C-C4C-NC	2.53	113.68	110.43
11	A	1116	CLA	C3C-C4C-NC	2.53	113.68	110.43
11	B	1230	CLA	C3C-C4C-NC	2.53	113.68	110.43
11	1	1123	CLA	C4D-C3D-CAD	2.53	110.86	108.11
11	B	1231	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
11	a	1101	CLA	CMC-C2C-C1C	2.53	128.99	125.03
11	a	1119	CLA	C9-C8-C10	2.53	120.30	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	4021	BCR	C37-C22-C21	-2.53	118.71	122.82
14	A	4001	BCR	C38-C26-C25	-2.53	121.72	124.48
11	2	1222	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
11	B	1226	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
11	2	1240	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	B	4004	BCR	C3-C4-C5	-2.53	109.54	114.06
11	A	1134	CLA	CED-O2D-CGD	2.53	121.66	115.92
11	B	1236	CLA	OBD-CAD-C3D	-2.53	122.50	128.42
11	1	1140	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
11	B	1207	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
11	b	1238	CLA	O2A-C1-C2	2.53	117.85	108.11
11	b	1225	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
14	m	4021	BCR	C23-C22-C21	2.53	122.99	119.01
11	1	1105	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
11	1	1131	CLA	CMB-C2B-C1B	2.53	129.27	125.42
11	B	1206	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
14	A	4002	BCR	C37-C22-C21	-2.53	118.72	122.82
14	1	4001	BCR	C35-C13-C12	2.53	121.95	118.09
11	B	1204	CLA	C4D-C3D-CAD	2.53	110.85	108.11
11	B	1208	CLA	C4D-C3D-CAD	2.53	110.85	108.11
11	B	1215	CLA	C4D-C3D-CAD	2.53	110.85	108.11
11	2	1229	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
11	K	1401	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
14	F	4013	BCR	C33-C5-C4	2.53	118.99	113.60
11	A	1140	CLA	CAC-C3C-C4C	2.53	128.08	124.79
11	B	1203	CLA	C9-C8-C7	2.53	120.29	111.27
11	b	1211	CLA	CAC-C3C-C4C	2.53	128.08	124.79
11	1	1134	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
11	B	1221	CLA	CMC-C2C-C1C	2.53	128.98	125.03
11	B	1234	CLA	C2B-C1B-NB	2.53	112.95	110.33
11	k	1402	CLA	C1-O2A-CGA	2.53	122.77	116.65
11	A	1133	CLA	C2B-C1B-NB	2.53	112.94	110.33
11	1	1137	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
11	2	1214	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
11	A	1106	CLA	C4D-C3D-CAD	2.52	110.85	108.11
11	a	1113	CLA	CMB-C2B-C1B	2.52	129.26	125.42
11	A	1108	CLA	CMC-C2C-C1C	2.52	128.98	125.03
14	A	4001	BCR	C3-C4-C5	-2.52	109.55	114.06
11	A	1011	CLA	CMC-C2C-C1C	2.52	128.98	125.03
11	b	1240	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
11	b	1206	CLA	C1-O2A-CGA	2.52	122.76	116.65
11	2	1225	CLA	CAC-C3C-C4C	2.52	128.07	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1232	CLA	CAC-C3C-C4C	2.52	128.07	124.79
11	1	1122	CLA	CMC-C2C-C1C	2.52	128.98	125.03
11	1	1114	CLA	CMC-C2C-C1C	2.52	128.98	125.03
11	B	1224	CLA	CMB-C2B-C1B	2.52	129.26	125.42
11	k	1401	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
11	a	1104	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
11	a	1132	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
11	A	1012	CLA	CHB-C4A-NA	2.52	128.04	124.40
11	1	1104	CLA	C1-C2-C3	-2.52	122.07	126.20
11	b	1222	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
11	B	1232	CLA	C4D-C3D-CAD	2.52	110.84	108.11
11	b	1023	CLA	CHB-C4A-NA	2.52	128.04	124.40
11	B	1208	CLA	CMB-C2B-C1B	2.52	129.26	125.42
11	a	1118	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
11	b	1209	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
14	b	4005	BCR	C8-C7-C6	-2.52	120.27	127.00
11	2	1210	CLA	CMC-C2C-C1C	2.52	128.97	125.03
11	1	1120	CLA	C4D-C3D-CAD	2.52	110.84	108.11
11	1	1123	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
14	B	4011	BCR	C23-C24-C25	-2.52	120.27	127.00
11	A	1139	CLA	CMB-C2B-C1B	2.52	129.25	125.42
11	1	1119	CLA	CMB-C2B-C1B	2.52	129.25	125.42
11	b	1240	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
11	1	1106	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
14	l	4022	BCR	C34-C9-C10	-2.52	118.74	122.82
14	b	4011	BCR	C15-C14-C13	-2.52	123.75	127.28
11	a	1103	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
11	a	1127	CLA	CMC-C2C-C1C	2.52	128.97	125.03
11	L	1503	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
11	b	1205	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
11	1	1117	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
15	b	5004	LHG	C5-O7-C7	-2.52	111.78	117.80
11	b	1221	CLA	O1D-CGD-CBD	-2.52	119.56	124.52
11	b	1222	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
11	2	1216	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
14	1	4002	BCR	C33-C5-C4	2.52	118.96	113.60
11	B	1023	CLA	CAC-C3C-C4C	2.51	128.06	124.79
11	B	1023	CLA	C3C-C4C-NC	2.51	113.65	110.43
11	l	1501	CLA	C3C-C4C-NC	2.51	113.65	110.43
11	2	1226	CLA	C3C-C4C-NC	2.51	113.65	110.43
11	a	1130	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
11	b	1223	CLA	C4-C3-C5	2.51	119.59	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1117	CLA	C4D-C3D-CAD	2.51	110.84	108.11
11	A	1113	CLA	C3C-C4C-NC	2.51	113.65	110.43
14	7	4021	BCR	C36-C18-C17	-2.51	118.74	122.82
12	A	2001	PQN	C24-C23-C22	2.51	120.23	111.27
11	b	1212	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
11	2	1225	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
11	2	1225	CLA	O2A-C1-C2	2.51	117.78	108.11
11	a	1104	CLA	C9-C8-C10	2.51	120.23	111.27
11	a	1137	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	2	4010	BCR	C34-C9-C10	-2.51	118.75	122.82
14	f	4020	BCR	C23-C24-C25	-2.51	120.29	127.00
14	b	4010	BCR	C3-C4-C5	-2.51	109.58	114.06
14	6	4018	BCR	C32-C1-C6	-2.51	106.31	110.24
11	1	1128	CLA	C1-C2-C3	-2.51	122.08	126.20
11	2	1220	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
11	1	1123	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
11	2	1207	CLA	CMC-C2C-C1C	2.51	128.96	125.03
11	8	1503	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
11	a	1114	CLA	CAC-C3C-C4C	2.51	128.06	124.79
14	A	4001	BCR	C33-C5-C4	2.51	118.95	113.60
11	a	1103	CLA	CMB-C2B-C1B	2.51	129.24	125.42
11	A	1125	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
14	L	4022	BCR	C35-C13-C12	2.51	121.92	118.09
14	b	4005	BCR	C36-C18-C17	-2.51	118.75	122.82
11	2	1210	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
11	A	1139	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
11	L	1501	CLA	CMC-C2C-C1C	2.51	128.96	125.03
11	2	1234	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
11	a	1119	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
11	a	1131	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
11	1	1131	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
11	A	1127	CLA	C3C-C4C-NC	2.51	113.64	110.43
11	B	1219	CLA	C4D-C3D-CAD	2.51	110.83	108.11
11	2	1230	CLA	C4D-C3D-CAD	2.51	110.83	108.11
11	2	1229	CLA	C9-C8-C7	2.51	120.21	111.27
14	2	4011	BCR	C33-C5-C4	2.51	118.94	113.60
11	a	1118	CLA	C1-C2-C3	-2.51	122.09	126.20
14	1	4007	BCR	C3-C4-C5	-2.51	109.58	114.06
11	2	1222	CLA	C9-C8-C7	2.51	120.21	111.27
11	a	1131	CLA	C4-C3-C5	2.51	119.58	115.23
12	a	2001	PQN	C14-C13-C15	2.51	119.58	115.23
11	B	1013	CLA	CMB-C2B-C1B	2.51	129.23	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1217	CLA	CMB-C2B-C1B	2.51	129.23	125.42
11	a	1102	CLA	CMB-C2B-C1B	2.51	129.23	125.42
11	a	1131	CLA	C4D-C3D-CAD	2.51	110.83	108.11
11	a	1103	CLA	CED-O2D-CGD	2.51	121.60	115.92
11	b	1226	CLA	C3C-C4C-NC	2.50	113.64	110.43
11	2	1235	CLA	O2A-C1-C2	2.50	117.75	108.11
11	a	1103	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
11	a	1118	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
11	2	1204	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
11	1	1107	CLA	C3C-C4C-NC	2.50	113.64	110.43
11	1	1132	CLA	CMC-C2C-C1C	2.50	128.95	125.03
11	L	1503	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
11	B	1221	CLA	C3D-C4D-ND	2.50	114.06	109.99
11	A	1131	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	b	1224	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	b	1216	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
11	A	1119	CLA	C1-C2-C3	-2.50	122.10	126.20
11	8	1501	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	a	1115	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
11	a	1129	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	2	1239	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	B	4010	BCR	C23-C24-C25	-2.50	120.32	127.00
11	b	1218	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
11	1	1101	CLA	C4D-C3D-CAD	2.50	110.82	108.11
11	A	1130	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
11	b	1232	CLA	CAC-C3C-C4C	2.50	128.04	124.79
14	6	4018	BCR	C28-C27-C26	-2.50	109.60	114.06
11	A	1122	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	B	1234	CLA	C4-C3-C5	2.50	119.56	115.23
11	A	1115	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
11	1	1801	CLA	CMC-C2C-C3C	2.50	132.90	126.15
11	a	1105	CLA	CAC-C3C-C4C	2.50	128.04	124.79
11	B	1213	CLA	C9-C8-C10	2.50	120.18	111.27
11	a	1122	CLA	C3C-C4C-NC	2.50	113.63	110.43
11	A	1121	CLA	CMC-C2C-C1C	2.50	128.94	125.03
11	a	1125	CLA	CMB-C2B-C1B	2.50	129.22	125.42
11	a	1101	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
11	1	1105	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
11	b	1213	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
11	b	1227	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
11	1	1133	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
11	B	1208	CLA	O2D-CGD-O1D	-2.49	118.99	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	4005	BCR	C27-C26-C25	-2.49	119.33	122.70
11	A	1116	CLA	C4-C3-C5	2.49	119.56	115.23
11	1	1117	CLA	C4D-C3D-CAD	2.49	110.81	108.11
11	A	1117	CLA	CHB-C1B-C2B	-2.49	120.19	127.43
11	k	1401	CLA	CAA-C2A-C3A	2.49	119.74	113.00
11	a	1120	CLA	C3C-C4C-NC	2.49	113.62	110.43
11	b	1210	CLA	C9-C8-C10	2.49	120.16	111.27
11	L	1502	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
11	A	1140	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	2	4017	BCR	C30-C25-C26	-2.49	119.23	122.64
11	B	1227	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
11	A	1112	CLA	C3C-C4C-NC	2.49	113.62	110.43
11	A	1125	CLA	C3D-C4D-ND	2.49	114.04	109.99
11	a	1107	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
11	b	1210	CLA	C1-O2A-CGA	2.49	122.68	116.65
15	a	5003	LHG	C5-O7-C7	-2.49	111.83	117.80
11	A	1129	CLA	C2B-C1B-NB	2.49	112.91	110.33
11	a	1119	CLA	C9-C8-C7	2.49	120.15	111.27
11	2	1210	CLA	C4-C3-C5	2.49	119.55	115.23
11	b	1217	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
11	A	1801	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
11	A	1136	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
11	B	1023	CLA	CBB-CAB-C3B	-2.49	115.09	127.53
11	8	1501	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
11	l	1503	CLA	CMB-C2B-C1B	2.49	129.21	125.42
11	2	1226	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
11	b	1216	CLA	C4-C3-C5	2.49	119.55	115.23
11	A	1131	CLA	C9-C8-C10	2.49	120.14	111.27
11	1	1101	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
11	B	1228	CLA	CMB-C2B-C1B	2.49	129.21	125.42
11	b	1217	CLA	CMC-C2C-C1C	2.49	128.92	125.03
11	2	1220	CLA	CMB-C2B-C1B	2.49	129.20	125.42
11	1	1131	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
14	A	4003	BCR	C38-C26-C27	2.49	118.89	113.60
14	a	4007	BCR	C38-C26-C27	2.49	118.89	113.60
14	b	4006	BCR	C1-C6-C7	2.49	122.39	115.65
14	2	4010	BCR	C19-C18-C17	2.49	122.92	119.01
11	b	1227	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
11	1	1137	CLA	C9-C8-C7	2.48	120.13	111.27
11	A	1124	CLA	C4D-C3D-CAD	2.48	110.80	108.11
11	a	1137	CLA	C4D-C3D-CAD	2.48	110.80	108.11
11	1	1112	CLA	CMD-C2D-C3D	-2.48	122.00	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1210	CLA	CMB-C2B-C1B	2.48	129.20	125.42
11	a	1127	CLA	C6-C5-C3	-2.48	107.42	113.47
11	L	1501	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
11	2	1239	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
15	A	5003	LHG	O7-C7-O9	-2.48	117.90	123.70
14	B	4011	BCR	C37-C22-C21	-2.48	118.80	122.82
11	A	1115	CLA	CMB-C2B-C1B	2.48	129.20	125.42
14	7	4021	BCR	C38-C26-C27	2.48	118.89	113.60
11	b	1235	CLA	CMB-C2B-C3B	2.48	132.38	126.55
11	a	1119	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
11	1	1108	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
14	6	4018	BCR	C8-C7-C6	-2.48	120.38	127.00
11	1	1113	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	l	4019	BCR	C28-C27-C26	-2.48	109.64	114.06
11	B	1227	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
11	A	1135	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
11	1	1128	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
11	B	1217	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
11	b	1023	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
11	b	1204	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
11	A	1114	CLA	CAC-C3C-C4C	2.48	128.01	124.79
11	2	1203	CLA	CED-O2D-CGD	2.48	121.54	115.92
11	a	1132	CLA	CMB-C2B-C1B	2.48	129.19	125.42
11	b	1231	CLA	CMB-C2B-C1B	2.48	129.19	125.42
11	l	1502	CLA	CMB-C2B-C1B	2.48	129.19	125.42
11	b	1240	CLA	C4D-C3D-CAD	2.48	110.80	108.11
11	B	1238	CLA	CMB-C2B-C1B	2.48	129.19	125.42
11	a	1111	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
11	K	1401	CLA	CAA-C2A-C3A	2.48	119.69	113.00
11	b	1222	CLA	C9-C8-C7	2.48	120.10	111.27
11	b	1216	CLA	C2B-C1B-NB	2.48	112.89	110.33
11	b	1207	CLA	C3C-C4C-NC	2.48	113.60	110.43
11	b	1218	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
14	b	4011	BCR	C33-C5-C4	2.47	118.87	113.60
11	B	1231	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
12	A	2001	PQN	C14-C13-C15	2.47	119.52	115.23
12	1	2001	PQN	C14-C13-C15	2.47	119.52	115.23
11	0	1401	CLA	CAA-C2A-C3A	2.47	119.69	113.00
11	A	1116	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
11	a	1124	CLA	CMB-C2B-C1B	2.47	129.19	125.42
11	A	1124	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
11	A	1123	CLA	C2B-C1B-NB	2.47	112.89	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1104	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	2	4006	BCR	C29-C28-C27	2.47	116.71	111.28
11	A	1130	CLA	CMC-C2C-C1C	2.47	128.90	125.03
11	A	1115	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
11	1	1102	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	B	4017	BCR	C3-C4-C5	-2.47	109.65	114.06
11	b	1230	CLA	C4D-C3D-CAD	2.47	110.79	108.11
11	b	1225	CLA	C9-C8-C7	2.47	120.09	111.27
11	1	1116	CLA	C1-O2A-CGA	2.47	122.63	116.65
11	A	1103	CLA	CHB-C4A-NA	2.47	127.97	124.40
11	B	1226	CLA	C3C-C4C-NC	2.47	113.60	110.43
11	B	1215	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	6	4018	BCR	C37-C22-C21	-2.47	118.81	122.82
11	8	1503	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	1	4001	BCR	C33-C5-C4	2.47	118.86	113.60
11	b	1221	CLA	C1-O2A-CGA	2.47	122.63	116.65
11	B	1225	CLA	C3C-C4C-NC	2.47	113.59	110.43
11	b	1202	CLA	CHB-C4A-NA	2.47	127.96	124.40
11	B	1204	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
11	b	1216	CLA	C9-C8-C7	2.47	120.08	111.27
14	2	4005	BCR	C27-C26-C25	-2.47	119.37	122.70
11	b	1202	CLA	C1-C2-C3	-2.47	122.15	126.20
11	b	1201	CLA	CMC-C2C-C1C	2.47	128.89	125.03
11	1	1136	CLA	CMC-C2C-C1C	2.47	128.89	125.03
11	b	1225	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
11	b	1217	CLA	C4D-C3D-CAD	2.47	110.79	108.11
11	2	1206	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
11	1	1104	CLA	CMB-C2B-C1B	2.47	129.18	125.42
11	1	1237	CLA	CAC-C3C-C4C	2.47	128.00	124.79
11	2	1229	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
11	2	1224	CLA	C3C-C4C-NC	2.47	113.59	110.43
11	2	1210	CLA	CMB-C2B-C1B	2.47	129.17	125.42
11	2	1211	CLA	CMB-C2B-C1B	2.47	129.17	125.42
11	B	1234	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
11	b	1201	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
11	a	1137	CLA	C1-O2A-CGA	2.47	122.62	116.65
11	a	1129	CLA	CMD-C2D-C3D	-2.47	122.04	127.69
14	a	4008	BCR	C8-C7-C6	-2.46	120.41	127.00
11	b	1239	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
14	A	4008	BCR	C23-C24-C25	-2.46	120.42	127.00
11	A	1133	CLA	CAC-C3C-C4C	2.46	128.00	124.79
14	B	4011	BCR	C32-C1-C6	-2.46	106.38	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1240	CLA	C3C-C4C-NC	2.46	113.59	110.43
14	1	4001	BCR	C19-C18-C17	2.46	122.88	119.01
11	a	1135	CLA	CMB-C2B-C1B	2.46	129.17	125.42
11	1	1125	CLA	O2A-C1-C2	2.46	117.59	108.11
11	B	1224	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
11	A	1112	CLA	CHB-C4A-NA	2.46	127.95	124.40
11	2	1226	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
11	A	1126	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
14	B	4006	BCR	C36-C18-C17	-2.46	118.83	122.82
14	a	4003	BCR	C29-C30-C25	-2.46	106.86	110.44
14	B	4014	BCR	C19-C18-C17	2.46	122.88	119.01
11	B	1230	CLA	C4D-C3D-CAD	2.46	110.78	108.11
11	b	1238	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
11	2	1228	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
11	a	1102	CLA	C1-O2A-CGA	2.46	122.61	116.65
11	k	1401	CLA	CHB-C4A-NA	2.46	127.95	124.40
11	A	1135	CLA	CAC-C3C-C4C	2.46	127.99	124.79
11	1	1119	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
11	b	1240	CLA	CMC-C2C-C1C	2.46	128.88	125.03
11	1	1109	CLA	CMC-C2C-C1C	2.46	128.88	125.03
11	A	1127	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
11	1	1133	CLA	C2B-C1B-NB	2.46	112.88	110.33
11	1	1115	CLA	CMB-C2B-C1B	2.46	129.16	125.42
11	2	1236	CLA	CMB-C2B-C1B	2.46	129.16	125.42
14	a	4007	BCR	C15-C14-C13	-2.46	123.83	127.28
11	a	1115	CLA	CMB-C2B-C1B	2.46	129.16	125.42
11	B	1225	CLA	C1-O2A-CGA	2.46	122.60	116.65
12	2	2002	PQN	C11-C3-C2	-2.46	120.68	124.89
11	B	1201	CLA	C4-C3-C5	2.46	119.49	115.23
11	A	1237	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	A	4003	BCR	C36-C18-C17	-2.46	118.84	122.82
11	B	1207	CLA	C3C-C4C-NC	2.46	113.58	110.43
11	L	1501	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	2	4010	BCR	C30-C25-C26	-2.45	119.28	122.64
11	0	1402	CLA	CMC-C2C-C1C	2.45	128.87	125.03
11	l	1503	CLA	C4D-C3D-CAD	2.45	110.77	108.11
11	a	1130	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
11	2	1231	CLA	CHB-C4A-NA	2.45	127.94	124.40
11	1	1110	CLA	C4D-C3D-CAD	2.45	110.77	108.11
11	B	1212	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
11	B	1023	CLA	CMC-C2C-C1C	2.45	128.87	125.03
11	2	1216	CLA	C2B-C1B-NB	2.45	112.87	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1226	CLA	C4-C3-C5	2.45	119.48	115.23
11	b	1021	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
11	a	1101	CLA	C4D-C3D-CAD	2.45	110.77	108.11
11	B	1214	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
11	B	1023	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	2	4017	BCR	C23-C24-C25	-2.45	120.45	127.00
14	B	4005	BCR	C30-C25-C26	-2.45	119.29	122.64
11	2	1021	CLA	C9-C8-C10	2.45	120.01	111.27
11	A	1119	CLA	C4D-C3D-CAD	2.45	110.77	108.11
11	1	1128	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
11	A	1111	CLA	CHB-C4A-NA	2.45	127.93	124.40
11	1	1133	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
11	B	1232	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
11	2	1227	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
11	A	1106	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
11	a	1109	CLA	CAC-C3C-C4C	2.45	127.97	124.79
11	b	1234	CLA	C2B-C1B-NB	2.45	112.86	110.33
11	A	1127	CLA	CMB-C2B-C1B	2.45	129.14	125.42
11	K	1401	CLA	CHB-C4A-NA	2.45	127.93	124.40
11	B	1232	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
11	b	1203	CLA	C4D-C3D-CAD	2.44	110.76	108.11
14	1	4002	BCR	C35-C13-C12	2.44	121.82	118.09
11	B	1216	CLA	CAC-C3C-C4C	2.44	127.97	124.79
11	b	1223	CLA	CMD-C2D-C3D	-2.44	122.08	127.69
11	2	1239	CLA	CMD-C2D-C3D	-2.44	122.08	127.69
11	A	1128	CLA	C2B-C1B-NB	2.44	112.86	110.33
11	0	1401	CLA	CHB-C4A-NA	2.44	127.93	124.40
14	b	4009	BCR	C1-C6-C5	-2.44	119.30	122.64
14	a	4001	BCR	C33-C5-C4	2.44	118.80	113.60
11	1	1101	CLA	C9-C8-C7	2.44	119.98	111.27
11	1	1109	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
11	2	1228	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
11	A	1128	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
11	B	1212	CLA	C4D-C3D-CAD	2.44	110.76	108.11
11	A	1011	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
11	1	1139	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
11	1	1140	CLA	C3C-C4C-NC	2.44	113.56	110.43
11	A	1125	CLA	CMC-C2C-C1C	2.44	128.85	125.03
11	L	1503	CLA	C4-C3-C5	2.44	119.46	115.23
11	a	1128	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
11	1	1116	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
11	B	1222	CLA	C4D-C3D-CAD	2.44	110.75	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1230	CLA	CMB-C2B-C1B	2.44	129.13	125.42
11	B	1229	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
11	2	1226	CLA	C1-C2-C3	-2.44	122.20	126.20
14	2	4004	BCR	C27-C26-C25	-2.44	119.41	122.70
11	a	1110	CLA	C4-C3-C5	2.44	119.46	115.23
11	2	1228	CLA	CMC-C2C-C1C	2.44	128.84	125.03
11	2	1214	CLA	CAC-C3C-C4C	2.44	127.96	124.79
11	A	1129	CLA	C4D-C3D-CAD	2.44	110.75	108.11
11	a	1125	CLA	C3C-C4C-NC	2.44	113.55	110.43
11	b	1223	CLA	C3C-C4C-NC	2.44	113.55	110.43
11	1	1122	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
11	B	1214	CLA	C3C-C4C-NC	2.44	113.55	110.43
11	B	1021	CLA	O2A-C1-C2	2.44	117.48	108.11
14	8	4019	BCR	C1-C6-C7	2.44	122.25	115.65
11	8	1503	CLA	CMB-C2B-C3B	2.43	132.28	126.55
11	A	1136	CLA	CAC-C3C-C4C	2.43	127.96	124.79
11	B	1202	CLA	C1-O2A-CGA	2.43	122.54	116.65
11	a	1124	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
11	A	1124	CLA	CMC-C2C-C1C	2.43	128.84	125.03
14	2	4011	BCR	C32-C1-C6	-2.43	106.43	110.24
11	1	1012	CLA	CMB-C2B-C1B	2.43	129.12	125.42
14	a	4007	BCR	C34-C9-C8	2.43	121.81	118.09
11	a	1129	CLA	C3C-C4C-NC	2.43	113.55	110.43
11	B	1236	CLA	C3C-C4C-NC	2.43	113.55	110.43
11	2	1223	CLA	C9-C8-C7	2.43	119.94	111.27
11	2	1238	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
11	2	1021	CLA	CMC-C2C-C1C	2.43	128.83	125.03
11	2	1235	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
11	1	1129	CLA	C3C-C4C-NC	2.43	113.54	110.43
11	1	1130	CLA	C4D-C3D-CAD	2.43	110.74	108.11
11	1	1119	CLA	C9-C8-C7	2.43	119.93	111.27
11	a	1022	CLA	C3C-C4C-NC	2.43	113.54	110.43
11	1	1126	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
11	1	1122	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
11	2	1013	CLA	C4D-C3D-CAD	2.43	110.74	108.11
11	B	1201	CLA	C1-C2-C3	-2.43	122.22	126.20
11	L	1501	CLA	O2A-C1-C2	2.43	117.44	108.11
11	b	1232	CLA	C4D-C3D-CAD	2.43	110.74	108.11
14	B	4004	BCR	C37-C22-C21	-2.43	118.89	122.82
11	2	1213	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
11	A	1237	CLA	CMC-C2C-C1C	2.42	128.82	125.03
11	a	1120	CLA	CHB-C4A-NA	2.42	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1234	CLA	C9-C8-C7	2.42	119.91	111.27
11	b	1229	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
11	B	1210	CLA	C4-C3-C5	2.42	119.43	115.23
11	a	1125	CLA	C4-C3-C5	2.42	119.43	115.23
11	a	1104	CLA	C1-C2-C3	-2.42	122.23	126.20
11	a	1133	CLA	CAC-C3C-C4C	2.42	127.94	124.79
11	B	1240	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
11	a	1133	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
11	A	1128	CLA	C4-C3-C5	2.42	119.43	115.23
11	1	1011	CLA	C3C-C4C-NC	2.42	113.53	110.43
11	2	1204	CLA	O2A-C1-C2	2.42	117.42	108.11
11	b	1214	CLA	CAC-C3C-C4C	2.42	127.94	124.79
11	2	1211	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	F	4018	BCR	C32-C1-C6	-2.42	106.45	110.24
11	B	1229	CLA	C9-C8-C10	2.42	119.89	111.27
14	b	4005	BCR	C19-C18-C17	2.42	122.81	119.01
14	2	4011	BCR	C35-C13-C12	2.42	121.78	118.09
11	A	1120	CLA	CMB-C2B-C1B	2.42	129.10	125.42
11	A	1104	CLA	C6-C5-C3	-2.42	107.58	113.47
11	b	1013	CLA	C4D-C3D-CAD	2.42	110.73	108.11
11	b	1013	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
11	B	1229	CLA	C1-O2A-CGA	2.42	122.50	116.65
11	2	1234	CLA	C9-C8-C10	2.42	119.89	111.27
11	a	1138	CLA	CMC-C2C-C1C	2.42	128.81	125.03
11	b	1234	CLA	C3C-C4C-NC	2.42	113.52	110.43
11	1	1109	CLA	C4D-C3D-CAD	2.42	110.73	108.11
11	a	1120	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
11	2	1206	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
11	A	1105	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
11	1	1115	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
11	2	1209	CLA	CMB-C2B-C1B	2.41	129.09	125.42
11	2	1013	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
14	b	4014	BCR	C37-C22-C21	-2.41	118.91	122.82
11	1	1237	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
11	B	1239	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
11	B	1235	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
11	b	1213	CLA	CMB-C2B-C1B	2.41	129.09	125.42
11	A	1110	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
11	B	1021	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
11	2	1213	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	1	4003	BCR	C8-C7-C6	-2.41	120.56	127.00
11	b	1228	CLA	CMD-C2D-C3D	-2.41	122.16	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1135	CLA	C4D-C3D-CAD	2.41	110.72	108.11
11	1	1101	CLA	O2A-C1-C2	2.41	117.38	108.11
11	2	1208	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
11	8	1502	CLA	CMC-C2C-C1C	2.41	128.80	125.03
11	A	1114	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
11	B	1214	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
11	1	1110	CLA	CMB-C2B-C1B	2.41	129.09	125.42
11	B	1202	CLA	CMC-C2C-C1C	2.41	128.80	125.03
11	a	1121	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
11	b	1207	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
11	1	1116	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
14	l	4022	BCR	C19-C18-C17	2.41	122.80	119.01
11	A	1237	CLA	CED-O2D-CGD	2.41	121.38	115.92
11	B	1216	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
11	A	1801	CLA	C1-O2A-CGA	2.41	122.48	116.65
11	1	1125	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	F	4020	BCR	C34-C9-C10	-2.41	118.92	122.82
11	A	1118	CLA	C2B-C1B-NB	2.41	112.82	110.33
11	1	1138	CLA	CMC-C2C-C1C	2.41	128.79	125.03
11	a	1237	CLA	C3C-C4C-NC	2.41	113.51	110.43
11	1	1138	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
11	k	1401	CLA	C1-O2A-CGA	2.41	122.48	116.65
15	1	5003	LHG	C5-O7-C7	-2.41	112.04	117.80
11	a	1110	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
11	B	1223	CLA	CMC-C2C-C1C	2.41	128.79	125.03
14	A	4002	BCR	C3-C4-C5	-2.41	109.77	114.06
11	a	1111	CLA	C2B-C1B-NB	2.41	112.82	110.33
11	b	1234	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
11	A	1129	CLA	CAC-C3C-C4C	2.41	127.92	124.79
11	a	1131	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
11	2	1228	CLA	CED-O2D-CGD	2.41	121.37	115.92
11	B	1210	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
11	L	1502	CLA	C3C-C4C-NC	2.41	113.51	110.43
11	2	1204	CLA	C4D-C3D-CAD	2.40	110.72	108.11
11	B	1231	CLA	CHB-C4A-NA	2.40	127.87	124.40
11	A	1109	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
11	A	1126	CLA	CHB-C1B-C2B	-2.40	120.45	127.43
14	b	4005	BCR	C37-C22-C21	-2.40	118.92	122.82
11	b	1215	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
11	k	1402	CLA	CMC-C2C-C1C	2.40	128.79	125.03
11	1	1127	CLA	CAC-C3C-C4C	2.40	127.92	124.79
11	b	1202	CLA	C3C-C4C-NC	2.40	113.51	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1102	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
11	K	1401	CLA	C1-O2A-CGA	2.40	122.47	116.65
11	0	1401	CLA	C1-O2A-CGA	2.40	122.47	116.65
11	1	1801	CLA	C4D-C3D-CAD	2.40	110.72	108.11
11	a	1011	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
11	1	1101	CLA	C4-C3-C2	-2.40	117.46	123.63
11	b	1214	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
11	1	1801	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
11	A	1130	CLA	C4D-C3D-CAD	2.40	110.71	108.11
11	A	1117	CLA	C9-C8-C10	2.40	119.83	111.27
11	A	1107	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
11	b	1240	CLA	C3C-C4C-NC	2.40	113.50	110.43
11	1	1124	CLA	CMB-C2B-C1B	2.40	129.07	125.42
11	1	1119	CLA	C4D-C3D-CAD	2.40	110.71	108.11
11	b	1220	CLA	CMC-C2C-C1C	2.40	128.78	125.03
14	l	4019	BCR	C19-C18-C17	2.40	122.78	119.01
11	A	1128	CLA	C3C-C4C-NC	2.40	113.50	110.43
11	b	1220	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	2	4009	BCR	C34-C9-C10	-2.40	118.93	122.82
11	A	1129	CLA	CMB-C2B-C1B	2.40	129.07	125.42
11	a	1101	CLA	CED-O2D-CGD	2.40	121.35	115.92
11	A	1131	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
11	b	1212	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
11	B	1217	CLA	C3C-C4C-NC	2.40	113.50	110.43
11	B	1238	CLA	O2A-C1-C2	2.40	117.33	108.11
11	B	1202	CLA	CHB-C4A-NA	2.40	127.86	124.40
11	b	1238	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
11	a	1237	CLA	CAC-C3C-C4C	2.40	127.91	124.79
11	b	1225	CLA	C1-O2A-CGA	2.40	122.45	116.65
11	2	1238	CLA	C1-O2A-CGA	2.40	122.45	116.65
11	1	1126	CLA	C4D-C3D-CAD	2.40	110.71	108.11
11	0	1401	CLA	CBA-CAA-C2A	2.40	120.92	113.79
11	1	1125	CLA	CMD-C2D-C3D	-2.40	122.20	127.69
11	A	1237	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
14	a	4007	BCR	C23-C24-C25	-2.39	120.60	127.00
11	B	1013	CLA	C1-C2-C3	-2.39	122.28	126.20
11	b	1214	CLA	C3C-C4C-NC	2.39	113.50	110.43
11	1	1117	CLA	CMC-C2C-C1C	2.39	128.77	125.03
14	b	4004	BCR	C36-C18-C17	-2.39	118.94	122.82
11	a	1012	CLA	C4D-C3D-CAD	2.39	110.70	108.11
11	2	1201	CLA	CAC-C3C-C4C	2.39	127.90	124.79
11	2	1204	CLA	CMD-C2D-C3D	-2.39	122.20	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1131	CLA	CAC-C3C-C4C	2.39	127.90	124.79
11	k	1401	CLA	CAC-C3C-C4C	2.39	127.90	124.79
11	1	1123	CLA	C9-C8-C10	2.39	119.80	111.27
11	1	1109	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
11	A	1011	CLA	CHA-C1A-NA	-2.39	120.98	126.39
11	a	1116	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
14	b	4004	BCR	C30-C25-C24	2.39	122.14	115.65
14	B	4004	BCR	C19-C18-C17	2.39	122.77	119.01
14	2	4004	BCR	C15-C14-C13	-2.39	123.93	127.28
15	a	5001	LHG	C5-O7-C7	-2.39	112.08	117.80
14	b	4004	BCR	C28-C27-C26	-2.39	109.79	114.06
11	B	1211	CLA	CMC-C2C-C1C	2.39	128.77	125.03
11	1	1107	CLA	CMC-C2C-C1C	2.39	128.77	125.03
11	A	1130	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
14	F	4018	BCR	C8-C9-C10	2.39	122.77	119.01
11	a	1113	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
11	B	1231	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
11	b	1224	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
14	f	4020	BCR	C19-C18-C17	2.39	122.76	119.01
11	B	1216	CLA	C4-C3-C5	2.39	119.37	115.23
11	1	1011	CLA	CAA-C2A-C1A	2.39	119.80	111.97
11	a	1139	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
11	2	1210	CLA	C3C-C4C-NC	2.39	113.49	110.43
11	B	1234	CLA	CAC-C3C-C4C	2.39	127.89	124.79
11	K	1401	CLA	CBA-CAA-C2A	2.39	120.89	113.79
11	1	1120	CLA	C3C-C4C-NC	2.39	113.49	110.43
11	B	1229	CLA	C9-C8-C7	2.38	119.77	111.27
11	b	1226	CLA	CMB-C2B-C1B	2.38	129.05	125.42
11	B	1205	CLA	CMC-C2C-C1C	2.38	128.76	125.03
11	1	1115	CLA	OBD-CAD-C3D	-2.38	122.84	128.42
16	B	5002	LMG	O7-C10-O9	-2.38	118.13	123.70
11	1	1012	CLA	C4D-C3D-CAD	2.38	110.69	108.11
11	2	1240	CLA	CAC-C3C-C4C	2.38	127.89	124.79
11	8	1502	CLA	CMB-C2B-C1B	2.38	129.05	125.42
11	b	1230	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
11	2	1210	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
11	A	1104	CLA	CMC-C2C-C1C	2.38	128.76	125.03
11	b	1013	CLA	CHB-C4A-NA	2.38	127.84	124.40
11	b	1210	CLA	C3C-C4C-NC	2.38	113.48	110.43
11	A	1022	CLA	C4-C3-C5	2.38	119.36	115.23
11	B	1204	CLA	O2A-C1-C2	2.38	117.27	108.11
14	B	4006	BCR	C38-C26-C27	2.38	118.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4005	BCR	C38-C26-C25	-2.38	121.89	124.48
11	k	1402	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
11	a	1120	CLA	CMC-C2C-C1C	2.38	128.75	125.03
11	2	1227	CLA	CAC-C3C-C4C	2.38	127.89	124.79
11	B	1236	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
11	A	1110	CLA	CMB-C2B-C1B	2.38	129.04	125.42
11	b	1229	CLA	C1-O2A-CGA	2.38	122.41	116.65
11	b	1023	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	b	4011	BCR	C37-C22-C21	-2.38	118.96	122.82
14	2	4005	BCR	C36-C18-C17	-2.38	118.96	122.82
11	1	1107	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
11	k	1401	CLA	CBA-CAA-C2A	2.38	120.87	113.79
14	A	4008	BCR	C1-C6-C7	2.38	122.10	115.65
12	A	2001	PQN	C11-C3-C2	-2.38	120.81	124.89
14	L	4019	BCR	C38-C26-C27	2.38	118.66	113.60
11	1	1101	CLA	CAC-C3C-C4C	2.38	127.88	124.79
11	2	1215	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
11	a	1119	CLA	C4D-C3D-CAD	2.38	110.69	108.11
11	b	1208	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
11	a	1125	CLA	C4D-C3D-CAD	2.38	110.69	108.11
11	B	1220	CLA	CMC-C2C-C1C	2.38	128.75	125.03
11	2	1013	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
11	A	1123	CLA	C9-C8-C10	2.37	119.74	111.27
14	8	4022	BCR	C28-C27-C26	-2.37	109.82	114.06
11	B	1215	CLA	CMC-C2C-C1C	2.37	128.74	125.03
11	1	1104	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
11	1	1801	CLA	CAC-C3C-C2C	2.37	131.92	127.56
11	A	1114	CLA	CMC-C2C-C1C	2.37	128.74	125.03
11	A	1132	CLA	CMC-C2C-C1C	2.37	128.74	125.03
11	1	1114	CLA	CAC-C3C-C4C	2.37	127.88	124.79
11	a	1125	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
14	2	4004	BCR	C30-C25-C24	2.37	122.08	115.65
11	B	1217	CLA	CMC-C2C-C1C	2.37	128.74	125.03
11	a	1114	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
11	2	1219	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
11	A	1125	CLA	C3C-C4C-NC	2.37	113.47	110.43
11	1	1115	CLA	C3C-C4C-NC	2.37	113.47	110.43
11	K	1401	CLA	CAC-C3C-C4C	2.37	127.87	124.79
11	A	1138	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
11	b	1216	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
11	b	1013	CLA	CED-O2D-CGD	2.37	121.29	115.92
14	a	4003	BCR	C36-C18-C17	-2.37	118.98	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1127	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
11	b	1229	CLA	C9-C8-C7	2.37	119.72	111.27
11	a	1107	CLA	C3D-C4D-ND	2.37	113.84	109.99
11	2	1236	CLA	C3C-C4C-NC	2.37	113.47	110.43
11	a	1116	CLA	CMC-C2C-C1C	2.37	128.74	125.03
11	b	1205	CLA	C4-C3-C5	2.37	119.34	115.23
12	2	2002	PQN	C24-C23-C25	2.37	119.72	111.27
11	a	1119	CLA	CAC-C3C-C4C	2.37	127.87	124.79
11	A	1801	CLA	C4B-CHC-C1C	2.37	131.81	126.25
11	A	1125	CLA	C1-O2A-CGA	2.37	122.38	116.65
11	b	1215	CLA	C9-C8-C7	2.37	119.71	111.27
11	B	1219	CLA	C3C-C4C-NC	2.37	113.46	110.43
11	A	1123	CLA	C4-C3-C5	2.37	119.34	115.23
14	F	4013	BCR	C37-C22-C21	-2.37	118.98	122.82
11	a	1128	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
11	A	1113	CLA	CMB-C2B-C1B	2.37	129.02	125.42
11	1	1011	CLA	CMB-C2B-C1B	2.37	129.02	125.42
11	a	1113	CLA	CAC-C3C-C4C	2.37	127.87	124.79
14	B	4010	BCR	C24-C23-C22	-2.37	122.73	126.23
11	a	1102	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
11	1	1132	CLA	CMD-C2D-C3D	-2.37	122.27	127.69
14	1	4007	BCR	C34-C9-C8	2.37	121.70	118.09
11	A	1118	CLA	C4-C3-C5	2.36	119.33	115.23
11	2	1227	CLA	CMC-C2C-C1C	2.36	128.73	125.03
14	B	4006	BCR	C19-C18-C17	2.36	122.73	119.01
11	B	1223	CLA	CMB-C2B-C1B	2.36	129.02	125.42
11	a	1110	CLA	CMB-C2B-C1B	2.36	129.02	125.42
11	A	1138	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
11	2	1223	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
11	b	1234	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
14	8	4022	BCR	C23-C24-C25	-2.36	120.69	127.00
11	b	1217	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
14	8	4019	BCR	C36-C18-C17	-2.36	118.99	122.82
11	b	1226	CLA	C2B-C1B-NB	2.36	112.77	110.33
14	1	4001	BCR	C3-C4-C5	-2.36	109.85	114.06
11	B	1229	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	f	4018	BCR	C8-C7-C6	-2.36	120.70	127.00
11	1	1120	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
11	a	1011	CLA	C3C-C4C-NC	2.36	113.45	110.43
11	2	1240	CLA	C3C-C4C-NC	2.36	113.45	110.43
11	1	1136	CLA	C2B-C1B-NB	2.36	112.77	110.33
11	b	1013	CLA	CMD-C2D-C3D	-2.36	122.28	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1012	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
11	2	1212	CLA	C3C-C4C-NC	2.36	113.45	110.43
11	L	1502	CLA	CMC-C2C-C1C	2.36	128.72	125.03
12	A	2001	PQN	C24-C23-C25	2.36	119.67	111.27
11	a	1132	CLA	C4D-C3D-CAD	2.36	110.67	108.11
11	8	1501	CLA	CHB-C4A-NA	2.36	127.80	124.40
11	1	1108	CLA	C3C-C4C-NC	2.36	113.45	110.43
14	L	4019	BCR	C3-C4-C5	-2.36	109.86	114.06
11	2	1023	CLA	CBB-CAB-C3B	-2.36	115.76	127.53
11	b	1227	CLA	CAC-C3C-C4C	2.36	127.85	124.79
11	B	1220	CLA	CMB-C2B-C1B	2.35	129.00	125.42
11	A	1112	CLA	CAC-C3C-C4C	2.35	127.85	124.79
11	a	1140	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
11	b	1021	CLA	C11-C10-C8	-2.35	108.14	115.97
11	B	1209	CLA	CMC-C2C-C1C	2.35	128.71	125.03
11	0	1401	CLA	CAC-C3C-C4C	2.35	127.85	124.79
11	A	1140	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
11	b	1219	CLA	C3C-C4C-NC	2.35	113.44	110.43
11	b	1229	CLA	C9-C8-C10	2.35	119.65	111.27
11	b	1230	CLA	CMC-C2C-C1C	2.35	128.71	125.03
11	A	1237	CLA	CHB-C4A-NA	2.35	127.79	124.40
11	B	1225	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
11	1	1111	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
11	B	1235	CLA	CMB-C2B-C1B	2.35	128.99	125.42
11	b	1023	CLA	C3C-C4C-NC	2.35	113.44	110.43
11	a	1106	CLA	C4-C3-C2	-2.35	117.60	123.63
11	A	1127	CLA	OBD-CAD-C3D	-2.34	122.94	128.42
16	2	5002	LMG	O7-C10-O9	-2.34	118.22	123.70
11	1	1011	CLA	CMC-C2C-C1C	2.34	128.70	125.03
11	1	1134	CLA	CAC-C3C-C4C	2.34	127.84	124.79
11	a	1101	CLA	C3C-C4C-NC	2.34	113.43	110.43
11	b	1234	CLA	C4-C3-C5	2.34	119.30	115.23
11	B	1221	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	l	4022	BCR	C30-C25-C24	2.34	122.01	115.65
11	B	1217	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
16	b	5002	LMG	O7-C10-O9	-2.34	118.23	123.70
14	l	4019	BCR	C36-C18-C17	-2.34	119.02	122.82
11	b	1209	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	2	4005	BCR	C19-C18-C17	2.34	122.69	119.01
11	L	1501	CLA	C4-C3-C5	2.34	119.29	115.23
11	2	1212	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
14	6	4013	BCR	C30-C25-C26	-2.34	119.44	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1124	CLA	CMC-C2C-C1C	2.34	128.69	125.03
11	a	1137	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
11	B	1204	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
11	A	1117	CLA	C4-C3-C5	2.34	119.29	115.23
14	B	4006	BCR	C37-C22-C21	-2.34	119.03	122.82
11	1	1118	CLA	C4-C3-C5	2.34	119.29	115.23
11	8	1501	CLA	CMB-C2B-C1B	2.34	128.98	125.42
11	b	1221	CLA	CAC-C3C-C4C	2.34	127.83	124.79
11	2	1215	CLA	C6-C5-C3	2.34	119.17	113.47
11	A	1116	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
11	a	1114	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
11	B	1212	CLA	C3C-C4C-NC	2.34	113.42	110.43
11	A	1129	CLA	CMC-C2C-C1C	2.34	128.69	125.03
11	2	1215	CLA	CMC-C2C-C1C	2.34	128.69	125.03
11	1	1111	CLA	CAC-C3C-C4C	2.34	127.83	124.79
11	2	1204	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
11	b	1232	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
11	b	1210	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
11	a	1127	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
11	1	1137	CLA	CMC-C2C-C1C	2.34	128.69	125.03
11	A	1106	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	2	4010	BCR	C30-C25-C24	2.34	121.99	115.65
14	b	4006	BCR	C38-C26-C27	2.34	118.58	113.60
14	l	4022	BCR	C30-C25-C26	-2.34	119.44	122.64
11	1	1102	CLA	C3C-C4C-NC	2.34	113.42	110.43
11	1	1110	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
14	2	4009	BCR	C7-C8-C9	-2.34	122.78	126.23
11	b	1220	CLA	CMB-C2B-C1B	2.34	128.97	125.42
11	B	1229	CLA	C4-C3-C5	2.33	119.28	115.23
11	2	1235	CLA	C3C-C4C-NC	2.33	113.42	110.43
11	2	1210	CLA	O1D-CGD-CBD	-2.33	119.91	124.52
11	1	1122	CLA	CMB-C2B-C1B	2.33	128.97	125.42
11	B	1229	CLA	CMC-C2C-C1C	2.33	128.68	125.03
14	2	4009	BCR	C36-C18-C17	-2.33	119.03	122.82
11	B	1021	CLA	C9-C8-C10	2.33	119.59	111.27
11	A	1102	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
11	2	1212	CLA	C4D-C3D-CAD	2.33	110.64	108.11
11	a	1801	CLA	CMB-C2B-C1B	2.33	128.97	125.42
14	2	4004	BCR	C28-C27-C26	-2.33	109.90	114.06
14	1	4003	BCR	C27-C26-C25	-2.33	119.55	122.70
11	b	1211	CLA	C3C-C4C-NC	2.33	113.42	110.43
11	b	1226	CLA	O1D-CGD-CBD	-2.33	119.92	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1012	CLA	C4D-C3D-CAD	2.33	110.64	108.11
11	a	1131	CLA	CAC-C3C-C4C	2.33	127.82	124.79
11	a	1117	CLA	C4-C3-C5	2.33	119.28	115.23
11	b	1226	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
11	B	1021	CLA	C1-C2-C3	-2.33	122.38	126.20
11	A	1133	CLA	CHB-C4A-NA	2.33	127.76	124.40
11	A	1022	CLA	CMB-C2B-C1B	2.33	128.97	125.42
11	A	1124	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
11	a	1012	CLA	C1-O2A-CGA	2.33	122.29	116.65
11	a	1801	CLA	C3C-C4C-NC	2.33	113.41	110.43
11	b	1216	CLA	C3C-C4C-NC	2.33	113.41	110.43
11	B	1211	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
11	a	1136	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
11	1	1011	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
11	A	1120	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
11	B	1219	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
11	a	1121	CLA	C3C-C4C-NC	2.33	113.41	110.43
11	b	1013	CLA	CMB-C2B-C1B	2.33	128.96	125.42
11	a	1138	CLA	CED-O2D-CGD	2.33	121.19	115.92
11	1	1138	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
11	a	1113	CLA	C3C-C4C-NC	2.33	113.41	110.43
12	1	2001	PQN	C2M-C2-C3	-2.33	120.63	124.45
11	A	1108	CLA	CED-O2D-CGD	2.33	121.19	115.92
11	B	1214	CLA	CHB-C4A-NA	2.33	127.76	124.40
11	b	1211	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
11	b	1217	CLA	C3C-C4C-NC	2.33	113.41	110.43
11	2	1228	CLA	C3C-C4C-NC	2.33	113.41	110.43
11	a	1122	CLA	CAC-C3C-C4C	2.33	127.81	124.79
11	2	1021	CLA	CHA-C1A-NA	-2.33	121.13	126.39
11	a	1138	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
14	A	4002	BCR	C33-C5-C4	2.32	118.55	113.60
11	A	1136	CLA	C2B-C1B-NB	2.32	112.74	110.33
14	B	4004	BCR	C36-C18-C17	-2.32	119.05	122.82
11	a	1136	CLA	CMC-C2C-C1C	2.32	128.66	125.03
11	2	1224	CLA	C4-C3-C5	2.32	119.26	115.23
11	B	1212	CLA	CMB-C2B-C1B	2.32	128.96	125.42
11	1	1140	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
11	a	1101	CLA	C9-C8-C7	2.32	119.55	111.27
14	F	4020	BCR	C31-C1-C6	-2.32	106.60	110.24
11	B	1211	CLA	C3C-C4C-NC	2.32	113.41	110.43
11	a	1113	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
11	B	1230	CLA	CAC-C3C-C4C	2.32	127.81	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1224	CLA	CAC-C3C-C4C	2.32	127.81	124.79
11	2	1238	CLA	C1-C2-C3	-2.32	122.39	126.20
11	1	1127	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
11	A	1107	CLA	CMC-C2C-C1C	2.32	128.66	125.03
11	B	1216	CLA	CMC-C2C-C1C	2.32	128.66	125.03
11	a	1111	CLA	C3C-C4C-NC	2.32	113.40	110.43
11	2	1217	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	F	4013	BCR	C40-C30-C25	-2.32	106.60	110.24
11	A	1140	CLA	C3C-C4C-NC	2.32	113.40	110.43
11	a	1108	CLA	CED-O2D-CGD	2.32	121.18	115.92
11	2	1234	CLA	C4D-C3D-CAD	2.32	110.62	108.11
11	a	1137	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
11	b	1203	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
11	B	1210	CLA	C3C-C4C-NC	2.32	113.40	110.43
11	a	1116	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	b	4009	BCR	C33-C5-C4	2.32	118.54	113.60
11	B	1023	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	B	4017	BCR	C28-C27-C26	-2.32	109.92	114.06
14	a	4001	BCR	C35-C13-C12	2.32	121.63	118.09
11	1	1119	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
11	2	1229	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	f	4018	BCR	C34-C9-C10	-2.32	119.06	122.82
11	a	1134	CLA	CMB-C2B-C1B	2.32	128.95	125.42
11	2	1235	CLA	C1-C2-C3	-2.32	122.40	126.20
11	A	1117	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
11	A	1117	CLA	C4D-C3D-CAD	2.32	110.62	108.11
11	A	1125	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
11	2	1205	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	a	4007	BCR	C33-C5-C4	2.32	118.53	113.60
11	A	1116	CLA	C1-O2A-CGA	2.31	122.25	116.65
11	a	1130	CLA	C4D-C3D-CAD	2.31	110.62	108.11
11	1	1101	CLA	C9-C8-C10	2.31	119.53	111.27
11	b	1202	CLA	C4-C3-C5	2.31	119.25	115.23
14	1	4008	BCR	C30-C25-C24	2.31	121.93	115.65
11	A	1134	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
11	2	1214	CLA	C4-C3-C5	2.31	119.24	115.23
11	A	1102	CLA	C1-O2A-CGA	2.31	122.25	116.65
11	1	1102	CLA	CMB-C2B-C1B	2.31	128.94	125.42
11	1	1128	CLA	CMB-C2B-C1B	2.31	128.94	125.42
11	a	1117	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
14	a	4008	BCR	C34-C9-C8	2.31	121.62	118.09
11	A	1012	CLA	CMC-C2C-C1C	2.31	128.65	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1013	CLA	CMB-C2B-C1B	2.31	128.94	125.42
11	2	1239	CLA	C3C-C4C-NC	2.31	113.39	110.43
11	a	1130	CLA	CAC-C3C-C4C	2.31	127.80	124.79
11	1	1117	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
11	1	1108	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
11	2	1221	CLA	CHB-C4A-NA	2.31	127.74	124.40
14	B	4011	BCR	C1-C6-C5	-2.31	119.48	122.64
11	2	1217	CLA	CMC-C2C-C1C	2.31	128.65	125.03
11	b	1203	CLA	C3C-C4C-NC	2.31	113.39	110.43
11	b	1219	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
11	a	1131	CLA	C9-C8-C7	2.31	119.51	111.27
11	1	1129	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
11	2	1226	CLA	CMC-C2C-C1C	2.31	128.65	125.03
11	B	1219	CLA	CAC-C3C-C4C	2.31	127.80	124.79
11	k	1402	CLA	C4B-CHC-C1C	2.31	131.68	126.25
14	B	4017	BCR	C38-C26-C25	-2.31	121.96	124.48
11	a	1111	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
11	B	1226	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
11	2	1212	CLA	CMB-C2B-C1B	2.31	128.94	125.42
14	B	4005	BCR	C33-C5-C4	2.31	118.52	113.60
11	B	1214	CLA	C9-C8-C10	2.31	119.50	111.27
11	l	1503	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
11	2	1208	CLA	C4D-C3D-CAD	2.31	110.61	108.11
14	8	4022	BCR	C4-C5-C6	-2.31	119.58	122.70
14	1	4001	BCR	C27-C26-C25	-2.31	119.59	122.70
11	1	1022	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
11	B	1209	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
11	b	1215	CLA	C1-C2-C3	-2.31	122.42	126.20
14	a	4003	BCR	C8-C7-C6	-2.31	120.84	127.00
11	b	1206	CLA	CMC-C2C-C1C	2.31	128.64	125.03
11	2	1240	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
11	2	1207	CLA	CHB-C4A-NA	2.31	127.73	124.40
11	A	1137	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
11	1	1126	CLA	CAC-C3C-C4C	2.31	127.79	124.79
11	1	1237	CLA	CBA-CAA-C2A	2.30	120.65	113.79
11	1	1105	CLA	CAC-C3C-C4C	2.30	127.79	124.79
11	a	1139	CLA	C1-C2-C3	-2.30	123.03	126.76
11	A	1109	CLA	C9-C8-C7	2.30	119.49	111.27
11	A	1107	CLA	CHB-C4A-NA	2.30	127.72	124.40
11	a	1132	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
14	f	4018	BCR	C36-C18-C17	-2.30	119.09	122.82
11	A	1127	CLA	O2D-CGD-O1D	-2.30	119.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1110	CLA	C3C-C4C-NC	2.30	113.38	110.43
11	A	1237	CLA	CMB-C2B-C1B	2.30	128.92	125.42
11	1	1113	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
11	8	1501	CLA	CAC-C3C-C4C	2.30	127.78	124.79
11	a	1107	CLA	CMC-C2C-C1C	2.30	128.63	125.03
11	1	1134	CLA	CMB-C2B-C1B	2.30	128.92	125.42
14	6	4013	BCR	C36-C18-C17	-2.30	119.09	122.82
11	A	1131	CLA	C3C-C4C-NC	2.30	113.38	110.43
11	a	1131	CLA	C9-C8-C10	2.30	119.47	111.27
11	a	1112	CLA	CAC-C3C-C4C	2.30	127.78	124.79
11	1	1122	CLA	C1-O2A-CGA	2.30	122.21	116.65
11	b	1229	CLA	C4-C3-C5	2.30	119.22	115.23
11	A	1022	CLA	CMC-C2C-C1C	2.30	128.62	125.03
11	a	1104	CLA	C3C-C4C-NC	2.30	113.37	110.43
11	2	1202	CLA	C1-O2A-CGA	2.30	122.21	116.65
11	b	1202	CLA	CMB-C2B-C1B	2.30	128.91	125.42
11	1	1117	CLA	CMB-C2B-C1B	2.30	128.91	125.42
11	A	1129	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
11	a	1237	CLA	C1-O2A-CGA	2.30	122.21	116.65
11	a	1106	CLA	CHB-C4A-NA	2.30	127.71	124.40
14	B	4009	BCR	C3-C4-C5	-2.30	109.96	114.06
11	A	1119	CLA	C3C-C4C-NC	2.29	113.37	110.43
14	b	4004	BCR	C37-C22-C21	-2.29	119.10	122.82
11	A	1130	CLA	C3C-C4C-NC	2.29	113.37	110.43
11	2	1213	CLA	C4-C3-C2	-2.29	117.73	123.63
11	1	1801	CLA	CHB-C4A-NA	2.29	127.71	124.40
11	A	1011	CLA	C4D-C3D-CAD	2.29	110.60	108.11
11	2	1240	CLA	CMC-C2C-C1C	2.29	128.62	125.03
11	b	1023	CLA	C4-C3-C5	2.29	119.21	115.23
11	A	1129	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
11	a	1117	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
11	2	1220	CLA	C3C-C4C-NC	2.29	113.36	110.43
11	A	1102	CLA	C9-C8-C10	2.29	119.44	111.27
11	A	1104	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
11	A	1139	CLA	C3C-C4C-NC	2.29	113.36	110.43
11	A	1128	CLA	CMC-C2C-C1C	2.29	128.61	125.03
11	B	1238	CLA	C1-O2A-CGA	2.29	122.19	116.65
11	A	1102	CLA	C4D-C3D-CAD	2.29	110.59	108.11
11	1	1121	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
11	L	1502	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
11	a	1102	CLA	C3C-C4C-NC	2.29	113.36	110.43
11	a	1022	CLA	C1-O2A-CGA	2.29	122.19	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1216	CLA	CAC-C3C-C4C	2.29	127.77	124.79
11	B	1213	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
11	a	1124	CLA	C4-C3-C5	2.29	119.20	115.23
11	A	1113	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
11	2	1206	CLA	C2B-C1B-NB	2.29	112.70	110.33
11	2	1232	CLA	C3C-C4C-NC	2.28	113.36	110.43
14	6	4018	BCR	C35-C13-C12	2.28	121.58	118.09
14	l	4019	BCR	C38-C26-C27	2.28	118.47	113.60
11	a	1109	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
11	B	1222	CLA	C9-C8-C7	2.28	119.41	111.27
11	b	1229	CLA	C3C-C4C-NC	2.28	113.36	110.43
14	a	4002	BCR	C15-C14-C13	-2.28	124.08	127.28
11	b	1214	CLA	CMB-C2B-C1B	2.28	128.90	125.42
12	B	2002	PQN	C11-C3-C2	-2.28	120.98	124.89
11	b	1021	CLA	C3C-C4C-NC	2.28	113.35	110.43
11	a	1136	CLA	C2B-C1B-NB	2.28	112.69	110.33
14	2	4004	BCR	C34-C9-C8	2.28	121.57	118.09
14	f	4013	BCR	C30-C25-C24	2.28	121.84	115.65
11	B	1223	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
11	B	1235	CLA	C3C-C4C-NC	2.28	113.35	110.43
11	a	1126	CLA	C4-C3-C2	-2.28	117.77	123.63
11	b	1206	CLA	CMB-C2B-C1B	2.28	128.89	125.42
11	2	1201	CLA	CMC-C2C-C1C	2.28	128.60	125.03
14	A	4002	BCR	C34-C9-C8	2.28	121.57	118.09
11	b	1021	CLA	CHB-C4A-NA	2.28	127.69	124.40
11	1	1131	CLA	CAC-C3C-C4C	2.28	127.76	124.79
11	A	1103	CLA	CMB-C2B-C1B	2.28	128.89	125.42
11	a	1135	CLA	CAC-C3C-C4C	2.28	127.75	124.79
11	A	1131	CLA	C4D-C3D-CAD	2.28	110.58	108.11
11	a	1122	CLA	C9-C8-C7	2.28	119.40	111.27
11	1	1122	CLA	CED-O2D-CGD	2.28	121.08	115.92
11	a	1133	CLA	C2B-C1B-NB	2.28	112.69	110.33
14	1	4007	BCR	C37-C22-C21	-2.28	119.13	122.82
11	1	1022	CLA	CBB-CAB-C3B	-2.28	116.15	127.53
11	a	1102	CLA	CHB-C4A-NA	2.28	127.69	124.40
11	2	1235	CLA	C9-C8-C10	2.28	119.39	111.27
11	a	1137	CLA	CMB-C2B-C1B	2.28	128.89	125.42
11	B	1225	CLA	C6-C5-C3	-2.28	107.92	113.47
14	f	4013	BCR	C3-C4-C5	-2.28	110.00	114.06
14	2	4011	BCR	C23-C22-C21	2.28	122.59	119.01
11	a	1107	CLA	C9-C8-C10	2.28	119.39	111.27
11	A	1121	CLA	CMB-C2B-C1B	2.28	128.88	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1136	CLA	CAC-C3C-C4C	2.28	127.75	124.79
11	a	1011	CLA	CHA-C1A-NA	-2.28	121.24	126.39
11	A	1135	CLA	CHB-C4A-NA	2.27	127.68	124.40
11	b	1023	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
14	A	4008	BCR	C28-C27-C26	-2.27	110.00	114.06
11	A	1022	CLA	C1-O2A-CGA	2.27	122.16	116.65
11	a	1124	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	B	4011	BCR	C36-C18-C17	-2.27	119.13	122.82
11	2	1230	CLA	CAC-C3C-C4C	2.27	127.75	124.79
11	b	1235	CLA	C9-C8-C10	2.27	119.38	111.27
11	1	1022	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	l	4022	BCR	C1-C6-C5	-2.27	119.53	122.64
11	a	1110	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	1	1112	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	A	1022	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
11	1	1012	CLA	OBD-CAD-C3D	-2.27	123.10	128.42
11	a	1137	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	a	1136	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	a	1137	CLA	C9-C8-C10	2.27	119.37	111.27
11	a	1117	CLA	C1-O2A-CGA	2.27	122.15	116.65
11	A	1116	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	2	4006	BCR	C23-C22-C21	2.27	122.58	119.01
11	2	1023	CLA	C1-C2-C3	-2.27	122.47	126.20
11	b	1210	CLA	C4-C3-C5	2.27	119.17	115.23
11	A	1120	CLA	CAC-C3C-C4C	2.27	127.75	124.79
11	A	1119	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
11	b	1230	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
14	2	4005	BCR	C30-C25-C26	-2.27	119.53	122.64
14	a	4008	BCR	C3-C4-C5	-2.27	110.01	114.06
11	2	1234	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	L	1501	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
11	8	1502	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	m	4021	BCR	C23-C24-C25	-2.27	120.94	127.00
11	1	1126	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
11	2	1206	CLA	C3C-C4C-NC	2.27	113.34	110.43
11	b	1234	CLA	CMB-C2B-C1B	2.27	128.87	125.42
11	2	1240	CLA	CMB-C2B-C1B	2.27	128.87	125.42
11	l	1502	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
11	B	1210	CLA	CMC-C2C-C1C	2.27	128.58	125.03
11	a	1114	CLA	C3C-C4C-NC	2.27	113.33	110.43
14	B	4004	BCR	C28-C27-C26	-2.27	110.01	114.06
11	b	1239	CLA	CAC-C3C-C4C	2.27	127.74	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1117	CLA	CMC-C2C-C1C	2.27	128.57	125.03
11	b	1210	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
11	L	1503	CLA	C3C-C4C-NC	2.27	113.33	110.43
11	A	1106	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
11	b	1224	CLA	C4-C3-C5	2.27	119.16	115.23
11	B	1229	CLA	C3C-C4C-NC	2.26	113.33	110.43
11	a	1136	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
14	a	4008	BCR	C36-C18-C17	-2.26	119.15	122.82
11	2	1210	CLA	C1-O2A-CGA	2.26	122.13	116.65
14	b	4006	BCR	C23-C22-C21	2.26	122.57	119.01
14	7	4021	BCR	C23-C24-C25	-2.26	120.95	127.00
14	b	4017	BCR	C3-C4-C5	-2.26	110.02	114.06
12	a	2001	PQN	C11-C3-C2	-2.26	121.01	124.89
14	6	4013	BCR	C38-C26-C27	2.26	118.42	113.60
14	a	4007	BCR	C36-C18-C17	-2.26	119.15	122.82
11	A	1134	CLA	CMC-C2C-C1C	2.26	128.57	125.03
16	b	5002	LMG	O8-C28-C29	2.26	118.73	111.83
11	A	1101	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
11	1	1126	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	7	4021	BCR	C34-C9-C10	-2.26	119.15	122.82
11	A	1137	CLA	OBD-CAD-C3D	-2.26	123.13	128.42
14	a	4003	BCR	C34-C9-C10	-2.26	119.15	122.82
11	B	1021	CLA	CMC-C2C-C1C	2.26	128.57	125.03
11	A	1131	CLA	C1-O2A-CGA	2.26	122.12	116.65
11	A	1110	CLA	CAC-C3C-C4C	2.26	127.73	124.79
11	1	1139	CLA	C5-C3-C4	2.26	119.79	114.59
14	2	4011	BCR	C1-C6-C5	-2.26	119.55	122.64
14	L	4022	BCR	C29-C30-C25	-2.26	107.16	110.44
14	L	4022	BCR	C23-C22-C21	2.26	122.56	119.01
11	B	1228	CLA	C1-O2A-CGA	2.26	122.12	116.65
11	A	1108	CLA	C3C-C4C-NC	2.26	113.33	110.43
11	A	1126	CLA	C3C-C4C-NC	2.26	113.33	110.43
11	1	1136	CLA	C3C-C4C-NC	2.26	113.33	110.43
11	b	1206	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
11	A	1112	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
11	a	1126	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
11	a	1140	CLA	C3C-C4C-NC	2.26	113.32	110.43
11	2	1023	CLA	C3C-C4C-NC	2.26	113.32	110.43
11	b	1215	CLA	C1-O2A-CGA	2.26	122.12	116.65
11	K	1402	CLA	C3C-C4C-NC	2.26	113.32	110.43
11	1	1116	CLA	CAC-C3C-C4C	2.26	127.73	124.79
11	0	1402	CLA	O2D-CGD-O1D	-2.26	119.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1119	CLA	C3C-C4C-NC	2.26	113.32	110.43
11	2	1023	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
11	b	1228	CLA	C1-O2A-CGA	2.26	122.11	116.65
11	k	1402	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
14	6	4018	BCR	C29-C30-C25	-2.26	107.16	110.44
11	b	1223	CLA	CMB-C2B-C1B	2.26	128.85	125.42
14	2	4004	BCR	C1-C6-C5	-2.26	119.55	122.64
11	1	1113	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
11	a	1104	CLA	C9-C8-C7	2.26	119.31	111.27
11	1	1118	CLA	CBC-CAC-C3C	-2.26	106.31	112.42
11	b	1219	CLA	C4-C3-C5	2.26	119.14	115.23
11	K	1401	CLA	C3C-C4C-NC	2.26	113.32	110.43
11	B	1210	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
11	A	1111	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
14	8	4022	BCR	C30-C25-C24	2.25	121.77	115.65
11	a	1122	CLA	CMB-C2B-C1B	2.25	128.85	125.42
11	b	1213	CLA	C3C-C4C-NC	2.25	113.32	110.43
11	1	1110	CLA	C3C-C4C-NC	2.25	113.32	110.43
11	2	1222	CLA	C3C-C4C-NC	2.25	113.32	110.43
11	A	1119	CLA	C4C-C3C-C2C	-2.25	103.61	106.89
11	2	1215	CLA	C9-C8-C7	2.25	119.30	111.27
11	1	1106	CLA	CAC-C3C-C4C	2.25	127.72	124.79
11	2	1206	CLA	CAC-C3C-C4C	2.25	127.72	124.79
11	B	1229	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
11	1	1121	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	1	4001	BCR	C34-C9-C10	-2.25	119.17	122.82
11	1	1111	CLA	C3C-C4C-NC	2.25	113.31	110.43
11	B	1219	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
11	b	1207	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
14	1	4003	BCR	C19-C18-C17	2.25	122.55	119.01
14	B	4017	BCR	C36-C18-C17	-2.25	119.17	122.82
11	L	1503	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
11	B	1213	CLA	C3C-C4C-NC	2.25	113.31	110.43
11	b	1235	CLA	CHB-C4A-NA	2.25	127.64	124.40
11	B	1210	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
11	2	1229	CLA	C1-C2-C3	-2.25	122.51	126.20
11	A	1116	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
11	B	1209	CLA	C3C-C4C-NC	2.25	113.31	110.43
12	b	2002	PQN	C11-C12-C13	-2.25	122.96	126.83
11	2	1021	CLA	CMB-C2B-C1B	2.25	128.84	125.42
11	A	1115	CLA	C3C-C4C-NC	2.25	113.31	110.43
11	2	1240	CLA	O2D-CGD-O1D	-2.25	119.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1219	CLA	O2A-C1-C2	2.24	116.75	108.11
16	B	5002	LMG	O8-C28-C29	2.24	118.68	111.83
11	2	1206	CLA	C1-C2-C3	-2.24	122.52	126.20
11	b	1228	CLA	CMC-C2C-C1C	2.24	128.54	125.03
11	2	1213	CLA	CMB-C2B-C1B	2.24	128.84	125.42
11	a	1111	CLA	CHB-C4A-NA	2.24	127.64	124.40
11	A	1109	CLA	C9-C8-C10	2.24	119.27	111.27
11	2	1212	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
11	2	1023	CLA	C11-C10-C8	-2.24	108.51	115.97
11	a	1116	CLA	C4B-CHC-C1C	2.24	131.52	126.25
11	B	1205	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	1	4008	BCR	C1-C6-C7	2.24	121.73	115.65
11	A	1011	CLA	C3D-C4D-ND	2.24	113.63	109.99
11	a	1139	CLA	C1-O2A-CGA	2.24	122.08	116.65
11	a	1135	CLA	C3C-C4C-NC	2.24	113.30	110.43
11	k	1401	CLA	C3C-C4C-NC	2.24	113.30	110.43
11	b	1231	CLA	CHB-C4A-NA	2.24	127.63	124.40
11	B	1021	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
11	2	1206	CLA	CMB-C2B-C1B	2.24	128.83	125.42
11	a	1116	CLA	C3C-C4C-NC	2.24	113.30	110.43
11	B	1236	CLA	C1-O2A-CGA	2.24	123.03	116.67
14	B	4005	BCR	C23-C24-C25	-2.24	121.02	127.00
11	B	1201	CLA	CHB-C4A-NA	2.24	127.63	124.40
11	A	1139	CLA	CED-O2D-CGD	2.24	120.99	115.92
11	B	1206	CLA	CED-O2D-CGD	2.24	120.99	115.92
11	A	1124	CLA	C3C-C4C-NC	2.24	113.30	110.43
11	2	1215	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
11	A	1022	CLA	C3C-C4C-NC	2.24	113.30	110.43
15	A	5001	LHG	O7-C7-O9	-2.24	118.48	123.70
11	a	1101	CLA	C9-C8-C10	2.24	119.24	111.27
11	1	1118	CLA	O2A-C1-C2	2.24	116.71	108.11
14	1	4008	BCR	C28-C27-C26	-2.24	110.07	114.06
11	b	1222	CLA	CHB-C4A-NA	2.23	127.62	124.40
11	B	1234	CLA	C6-C7-C8	-2.23	108.54	115.97
11	b	1235	CLA	C11-C10-C8	-2.23	108.54	115.97
11	A	1108	CLA	CHB-C4A-NA	2.23	127.62	124.40
11	A	1135	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
11	2	1212	CLA	CAC-C3C-C4C	2.23	127.70	124.79
11	A	1133	CLA	CMC-C2C-C1C	2.23	128.52	125.03
11	B	1219	CLA	C4-C3-C5	2.23	119.10	115.23
11	a	1125	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
14	2	4009	BCR	C8-C7-C6	-2.23	121.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	0	1401	CLA	C3C-C4C-NC	2.23	113.29	110.43
11	a	1801	CLA	C1-C2-C3	-2.23	122.54	126.20
11	a	1111	CLA	C4B-CHC-C1C	2.23	131.49	126.25
11	1	1101	CLA	C4-C3-C5	2.23	119.10	115.23
11	1	1128	CLA	C4-C3-C5	2.23	119.10	115.23
11	1	1101	CLA	C3C-C4C-NC	2.23	113.29	110.43
11	2	1222	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
14	2	4009	BCR	C4-C5-C6	-2.23	119.69	122.70
11	k	1402	CLA	CAC-C3C-C4C	2.23	127.69	124.79
11	b	1210	CLA	C9-C8-C7	2.23	119.22	111.27
11	A	1105	CLA	CED-O2D-CGD	2.23	120.97	115.92
11	B	1013	CLA	C3C-C4C-NC	2.23	113.28	110.43
14	m	4021	BCR	C34-C9-C10	-2.23	119.21	122.82
11	b	1222	CLA	C3C-C4C-NC	2.23	113.28	110.43
11	2	1021	CLA	C3C-C4C-NC	2.23	113.28	110.43
11	a	1237	CLA	C4B-CHC-C1C	2.23	131.48	126.25
11	b	1216	CLA	C6-C7-C8	-2.23	108.56	115.97
11	B	1207	CLA	CMC-C2C-C1C	2.23	128.51	125.03
11	A	1102	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	f	4018	BCR	C38-C26-C27	2.23	118.34	113.60
11	B	1201	CLA	CMB-C2B-C1B	2.23	128.81	125.42
14	a	4001	BCR	C3-C4-C5	-2.23	110.09	114.06
11	A	1022	CLA	CHB-C1B-C2B	-2.23	120.97	127.43
11	a	1129	CLA	CHB-C4A-NA	2.23	127.61	124.40
11	2	1225	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
11	B	1206	CLA	C3C-C4C-NC	2.23	113.28	110.43
11	b	1212	CLA	C3C-C4C-NC	2.23	113.28	110.43
14	b	4017	BCR	C23-C24-C25	-2.23	121.05	127.00
11	b	1204	CLA	O2A-C1-C2	2.23	116.67	108.11
11	a	1132	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	1	1237	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	1	1123	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	1	1134	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	b	1013	CLA	C1-C2-C3	-2.22	122.55	126.20
11	8	1503	CLA	C3C-C4C-NC	2.22	113.28	110.43
14	A	4007	BCR	C33-C5-C4	2.22	118.33	113.60
11	1	1132	CLA	CBB-CAB-C3B	-2.22	116.42	127.53
11	A	1119	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
11	1	1128	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	A	1102	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
11	2	1218	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
11	B	1203	CLA	C3C-C4C-NC	2.22	113.28	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1106	CLA	C3C-C4C-NC	2.22	113.28	110.43
11	2	1231	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
11	2	1211	CLA	CHB-C4A-NA	2.22	127.61	124.40
14	b	4011	BCR	C1-C6-C7	2.22	121.67	115.65
11	b	1021	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
11	a	1111	CLA	C9-C8-C10	2.22	119.19	111.27
11	b	1215	CLA	CAC-C3C-C4C	2.22	127.68	124.79
11	a	1108	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
11	b	1225	CLA	C3C-C4C-NC	2.22	113.27	110.43
11	b	1227	CLA	C3C-C4C-NC	2.22	113.27	110.43
11	1	1135	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
11	2	1212	CLA	CED-O2D-CGD	2.22	120.95	115.92
14	F	4013	BCR	C30-C25-C24	2.22	121.67	115.65
11	2	1217	CLA	C3C-C4C-NC	2.22	113.27	110.43
11	B	1206	CLA	C4-C3-C5	2.22	119.08	115.23
11	B	1228	CLA	CAC-C3C-C4C	2.22	127.67	124.79
11	2	1021	CLA	CAC-C3C-C4C	2.22	127.67	124.79
11	2	1222	CLA	C4-C3-C2	-2.22	117.93	123.63
14	B	4017	BCR	C35-C13-C12	2.22	121.47	118.09
11	A	1115	CLA	CAC-C3C-C4C	2.22	127.67	124.79
14	L	4019	BCR	C36-C18-C17	-2.22	119.22	122.82
11	A	1105	CLA	C3C-C4C-NC	2.21	113.27	110.43
14	b	4009	BCR	C1-C6-C7	2.21	121.66	115.65
11	1	1126	CLA	CHB-C1B-C2B	-2.21	121.00	127.43
11	2	1223	CLA	OBD-CAD-C3D	-2.21	123.24	128.42
14	l	4019	BCR	C8-C7-C6	-2.21	121.08	127.00
14	f	4013	BCR	C35-C13-C12	2.21	121.47	118.09
11	2	1203	CLA	C1-O2A-CGA	2.21	122.01	116.65
14	6	4020	BCR	C36-C18-C17	-2.21	119.23	122.82
11	A	1108	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
11	b	1238	CLA	CMB-C2B-C1B	2.21	128.79	125.42
11	B	1215	CLA	C11-C10-C8	-2.21	108.61	115.97
11	2	1221	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	f	4013	BCR	C40-C30-C25	-2.21	106.78	110.24
11	b	1219	CLA	CAC-C3C-C4C	2.21	127.67	124.79
11	B	1227	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	L	4022	BCR	C34-C9-C8	2.21	121.46	118.09
11	a	1133	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
11	a	1132	CLA	CBB-CAB-C3B	-2.21	116.49	127.53
11	2	1225	CLA	C4-C3-C5	2.21	119.06	115.23
11	b	1207	CLA	CED-O2D-CGD	2.21	120.92	115.92
11	b	1231	CLA	CAC-C3C-C4C	2.21	127.66	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	l	1501	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
11	B	1222	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
11	2	1021	CLA	CED-O2D-CGD	2.21	120.92	115.92
11	l	1503	CLA	C3C-C4C-NC	2.21	113.26	110.43
11	a	1128	CLA	CMC-C2C-C1C	2.21	128.48	125.03
11	2	1209	CLA	CMC-C2C-C1C	2.21	128.48	125.03
11	2	1235	CLA	C6-C5-C3	-2.21	108.09	113.47
11	1	1126	CLA	CMB-C2B-C1B	2.21	128.78	125.42
11	a	1140	CLA	C4-C3-C5	2.21	119.06	115.23
11	A	1113	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
11	A	1124	CLA	C6-C5-C3	-2.20	108.10	113.47
11	1	1101	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
14	A	4007	BCR	C36-C18-C17	-2.20	119.25	122.82
14	m	4021	BCR	C33-C5-C4	2.20	118.30	113.60
11	a	1134	CLA	CHB-C4A-NA	2.20	127.58	124.40
14	6	4018	BCR	C36-C18-C17	-2.20	119.25	122.82
14	l	4019	BCR	C33-C5-C4	2.20	118.29	113.60
11	A	1133	CLA	C3C-C4C-NC	2.20	113.25	110.43
14	8	4022	BCR	C35-C13-C12	2.20	121.45	118.09
11	A	1132	CLA	C3C-C4C-NC	2.20	113.25	110.43
11	1	1118	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
11	b	1207	CLA	CMC-C2C-C1C	2.20	128.47	125.03
11	B	1234	CLA	C9-C8-C7	2.20	119.12	111.27
11	1	1117	CLA	C9-C8-C10	2.20	119.12	111.27
11	a	1124	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
11	1	1128	CLA	C11-C12-C13	-2.20	108.65	115.97
11	a	1127	CLA	CMB-C2B-C1B	2.20	128.77	125.42
11	1	1130	CLA	CHB-C1B-C2B	-2.20	121.04	127.43
14	a	4007	BCR	C31-C1-C6	-2.20	106.79	110.24
11	a	1108	CLA	C3C-C4C-NC	2.20	113.25	110.43
11	A	1103	CLA	C9-C8-C10	2.20	119.12	111.27
11	B	1021	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
11	2	1230	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
11	A	1113	CLA	CAC-C3C-C4C	2.20	127.65	124.79
11	1	1116	CLA	C3C-C4C-NC	2.20	113.25	110.43
11	b	1217	CLA	CMB-C2B-C1B	2.20	128.77	125.42
11	2	1203	CLA	CHB-C4A-NA	2.20	127.57	124.40
11	1	1112	CLA	CAC-C3C-C4C	2.20	127.65	124.79
11	2	1228	CLA	CMB-C2B-C1B	2.20	128.77	125.42
11	2	1210	CLA	C11-C10-C8	-2.20	108.66	115.97
11	2	1207	CLA	C3C-C4C-NC	2.20	113.25	110.43
14	B	4005	BCR	C37-C22-C21	-2.20	119.26	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1111	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
16	B	5002	LMG	C8-O7-C10	-2.20	112.54	117.80
14	7	4021	BCR	C35-C13-C12	2.20	121.44	118.09
11	2	1219	CLA	CHB-C4A-NA	2.20	127.57	124.40
14	F	4018	BCR	C38-C26-C27	2.20	118.28	113.60
11	a	1127	CLA	C10-C8-C7	2.20	123.19	112.07
11	1	1125	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
11	B	1223	CLA	C1-O2A-CGA	2.19	121.96	116.65
11	B	1230	CLA	CHB-C4A-NA	2.19	127.57	124.40
11	B	1021	CLA	CHA-C1A-NA	-2.19	121.42	126.39
15	B	5004	LHG	O7-C7-O9	-2.19	118.58	123.70
11	A	1114	CLA	C3C-C4C-NC	2.19	113.24	110.43
11	k	1402	CLA	C3C-C4C-NC	2.19	113.24	110.43
11	1	1801	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
11	1	1127	CLA	C4-C3-C5	2.19	119.03	115.23
11	b	1235	CLA	C3C-C4C-NC	2.19	113.24	110.43
11	1	1124	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
14	F	4018	BCR	C8-C7-C6	-2.19	121.14	127.00
11	a	1128	CLA	C11-C10-C8	-2.19	108.68	115.97
11	1	1237	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	2	5004	LHG	C5-O7-C7	-2.19	112.55	117.80
14	1	4003	BCR	C34-C9-C10	-2.19	119.27	122.82
11	2	1209	CLA	C3C-C4C-NC	2.19	113.23	110.43
14	2	4005	BCR	C3-C4-C5	-2.19	110.15	114.06
14	b	4006	BCR	C8-C7-C6	-2.19	121.15	127.00
11	0	1402	CLA	C4B-CHC-C1C	2.19	131.39	126.25
14	2	4010	BCR	C1-C6-C5	-2.19	119.65	122.64
11	a	1237	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
14	8	4019	BCR	C34-C9-C10	-2.19	119.27	122.82
14	A	4008	BCR	C1-C6-C5	-2.19	119.65	122.64
11	B	1207	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
11	2	1205	CLA	C1-O2A-CGA	2.19	121.94	116.65
11	1	1131	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
11	a	1117	CLA	C3C-C4C-NC	2.18	113.23	110.43
11	b	1013	CLA	C3C-C4C-NC	2.18	113.23	110.43
11	b	1218	CLA	C3C-C4C-NC	2.18	113.23	110.43
11	B	1216	CLA	C1-C2-C3	-2.18	122.62	126.20
11	L	1501	CLA	CHB-C4A-NA	2.18	127.55	124.40
11	B	1206	CLA	CMC-C2C-C1C	2.18	128.45	125.03
11	2	1216	CLA	C9-C8-C7	2.18	119.06	111.27
14	1	4002	BCR	C34-C9-C10	-2.18	119.28	122.82
14	F	4020	BCR	C3-C4-C5	-2.18	110.16	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	4017	BCR	C38-C26-C25	-2.18	122.10	124.48
11	1	1117	CLA	C1-O2A-CGA	2.18	121.93	116.65
11	A	1136	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	2	1229	CLA	C9-C8-C10	2.18	119.05	111.27
11	B	1223	CLA	C4-C3-C5	2.18	119.01	115.23
11	B	1215	CLA	C9-C8-C10	2.18	119.05	111.27
11	B	1211	CLA	CMB-C2B-C1B	2.18	128.74	125.42
11	a	1124	CLA	C10-C8-C9	2.18	120.26	110.53
11	B	1215	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	a	1112	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	a	1133	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	b	1201	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	a	1133	CLA	CMC-C2C-C1C	2.18	128.44	125.03
11	A	1121	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
11	2	1207	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	f	4020	BCR	C34-C9-C10	-2.18	119.29	122.82
14	B	4006	BCR	C29-C30-C25	2.18	113.60	110.44
11	b	1219	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
11	l	1502	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
11	a	1128	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	b	1207	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	a	4002	BCR	C27-C26-C25	-2.18	119.76	122.70
11	B	1234	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	A	1101	CLA	C9-C8-C10	2.18	119.03	111.27
11	b	1204	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	b	1238	CLA	C3C-C4C-NC	2.18	113.22	110.43
11	B	1222	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
14	B	4010	BCR	C27-C26-C25	-2.17	119.77	122.70
11	1	1112	CLA	CED-O2D-CGD	2.17	120.85	115.92
11	K	1402	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
11	2	1227	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
14	6	4013	BCR	C35-C13-C12	2.17	121.41	118.09
14	2	4011	BCR	C36-C18-C17	-2.17	119.29	122.82
11	2	1217	CLA	CHB-C4A-NA	2.17	127.54	124.40
11	b	1226	CLA	C1-O2A-CGA	2.17	121.91	116.65
11	a	1022	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
11	a	1119	CLA	C4-C3-C5	2.17	119.00	115.23
11	a	1103	CLA	C3C-C4C-NC	2.17	113.21	110.43
14	a	4008	BCR	C23-C24-C25	-2.17	121.19	127.00
12	B	2002	PQN	C11-C12-C13	-2.17	123.09	126.83
11	1	1116	CLA	C4-C3-C5	2.17	119.00	115.23
11	B	1202	CLA	C1-C2-C3	-2.17	122.64	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1219	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
14	F	4020	BCR	C34-C9-C8	2.17	121.41	118.09
11	b	1214	CLA	C4B-CHC-C1C	2.17	131.35	126.25
14	1	4007	BCR	C34-C9-C10	-2.17	119.30	122.82
11	b	1205	CLA	C3C-C4C-NC	2.17	113.21	110.43
11	B	1205	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	a	4003	BCR	C38-C26-C27	2.17	118.22	113.60
11	1	1118	CLA	C3C-C4C-NC	2.17	113.21	110.43
14	7	4021	BCR	C33-C5-C4	2.17	118.22	113.60
14	6	4013	BCR	C24-C25-C26	-2.17	116.56	121.56
11	1	1131	CLA	C3C-C4C-NC	2.17	113.21	110.43
11	1	1124	CLA	C4-C3-C5	2.17	118.99	115.23
11	1	1116	CLA	CHB-C4A-NA	2.17	127.53	124.40
11	B	1209	CLA	CHB-C4A-NA	2.17	127.53	124.40
11	2	1222	CLA	C1-C2-C3	-2.17	122.65	126.20
11	b	1021	CLA	CAC-C3C-C4C	2.17	127.61	124.79
11	A	1110	CLA	C4B-CHC-C1C	2.17	131.34	126.25
11	a	1130	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
11	1	1140	CLA	C9-C8-C10	2.17	119.00	111.27
12	b	2002	PQN	C11-C3-C2	-2.17	121.18	124.89
11	A	1127	CLA	CED-O2D-CGD	2.17	120.83	115.92
14	2	4006	BCR	C35-C13-C12	2.17	121.40	118.09
11	A	1126	CLA	C9-C8-C7	2.17	119.00	111.27
11	B	1023	CLA	C4-C3-C5	2.17	118.99	115.23
11	1	1133	CLA	CMC-C2C-C1C	2.17	128.42	125.03
11	1	1120	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
11	a	1110	CLA	C4B-CHC-C1C	2.16	131.34	126.25
11	a	1123	CLA	C3C-C4C-NC	2.16	113.20	110.43
11	a	1011	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
14	f	4018	BCR	C37-C22-C21	-2.16	119.31	122.82
11	B	1230	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
11	B	1216	CLA	CBB-CAB-C3B	-2.16	116.72	127.53
14	2	4004	BCR	C1-C6-C7	2.16	121.52	115.65
11	b	1013	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
11	2	1205	CLA	C4-C3-C5	2.16	118.98	115.23
11	2	1229	CLA	C4-C3-C5	2.16	118.98	115.23
11	b	1013	CLA	CMC-C2C-C1C	2.16	128.41	125.03
11	A	1127	CLA	CAC-C3C-C4C	2.16	127.60	124.79
11	1	1119	CLA	C7-C6-C5	-2.16	107.50	113.26
11	b	1013	CLA	C4-C3-C5	2.16	118.98	115.23
11	A	1134	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
11	2	1023	CLA	OBD-CAD-C3D	-2.16	123.37	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1140	CLA	C4-C3-C2	-2.16	118.08	123.63
11	a	1106	CLA	C1-O2A-CGA	2.16	121.87	116.65
11	2	1224	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
11	b	1221	CLA	C1-C2-C3	-2.16	122.66	126.20
11	B	1206	CLA	C1-O2A-CGA	2.16	121.87	116.65
14	b	4005	BCR	C33-C5-C4	2.16	118.19	113.60
11	A	1137	CLA	CAA-CBA-CGA	-2.16	107.09	113.21
11	B	1204	CLA	C6-C5-C3	-2.16	108.22	113.47
11	b	1236	CLA	C3C-C4C-NC	2.16	113.19	110.43
11	1	1124	CLA	C3C-C4C-NC	2.16	113.19	110.43
11	0	1402	CLA	C3C-C4C-NC	2.16	113.19	110.43
11	B	1207	CLA	CHB-C4A-NA	2.16	127.51	124.40
14	a	4008	BCR	C1-C6-C7	2.15	121.49	115.65
11	B	1201	CLA	C3C-C4C-NC	2.15	113.19	110.43
11	1	1130	CLA	C3C-C4C-NC	2.15	113.19	110.43
11	2	1201	CLA	C3C-C4C-NC	2.15	113.19	110.43
11	B	1219	CLA	CED-O2D-CGD	2.15	120.80	115.92
11	1	1112	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
11	2	1234	CLA	CAC-C3C-C4C	2.15	127.59	124.79
14	b	4006	BCR	C28-C27-C26	-2.15	110.22	114.06
11	B	1230	CLA	CMC-C2C-C1C	2.15	128.39	125.03
11	b	1216	CLA	CED-O2D-CGD	2.15	120.79	115.92
11	a	1131	CLA	CHB-C4A-NA	2.15	127.50	124.40
11	2	1235	CLA	CHB-C4A-NA	2.15	127.50	124.40
11	2	1231	CLA	CMB-C2B-C1B	2.15	128.69	125.42
11	A	1135	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
11	b	1235	CLA	C4-C3-C5	2.15	118.96	115.23
11	B	1227	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
11	a	1107	CLA	C1-O2A-CGA	2.15	121.85	116.65
14	B	4004	BCR	C34-C9-C10	-2.15	119.34	122.82
11	2	1021	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
11	2	1238	CLA	CMB-C2B-C1B	2.15	128.69	125.42
11	a	1127	CLA	C3C-C4C-NC	2.15	113.18	110.43
11	b	1228	CLA	C3C-C4C-NC	2.15	113.18	110.43
11	2	1223	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
11	A	1801	CLA	C4C-C3C-C2C	-2.15	103.77	106.89
11	a	1237	CLA	C2B-C1B-NB	2.15	112.55	110.33
11	1	1237	CLA	CMC-C2C-C1C	2.15	128.39	125.03
11	1	1131	CLA	C9-C8-C7	2.15	118.92	111.27
14	8	4019	BCR	C33-C5-C4	2.15	118.17	113.60
11	1	1132	CLA	C3C-C4C-NC	2.15	113.18	110.43
11	B	1238	CLA	C3C-C4C-NC	2.14	113.18	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1013	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
11	2	1231	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
11	B	1239	CLA	C3C-C4C-NC	2.14	113.18	110.43
11	a	1011	CLA	C4-C3-C5	2.14	118.95	115.23
11	K	1402	CLA	C1-C2-C3	-2.14	123.30	126.76
11	2	1222	CLA	C1-O2A-CGA	2.14	121.84	116.65
11	A	1119	CLA	C9-C8-C7	2.14	118.91	111.27
14	A	4003	BCR	C19-C18-C17	2.14	122.38	119.01
11	b	1206	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
11	B	1222	CLA	C1-O2A-CGA	2.14	121.83	116.65
14	8	4022	BCR	C30-C25-C26	-2.14	119.71	122.64
11	2	1218	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	B	4006	BCR	C1-C6-C7	2.14	121.46	115.65
11	1	1103	CLA	CED-O2D-CGD	2.14	120.77	115.92
11	8	1501	CLA	C3C-C4C-NC	2.14	113.17	110.43
11	b	1229	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
11	a	1126	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
11	a	1128	CLA	C1-O2A-CGA	2.14	121.83	116.65
11	b	1203	CLA	CHB-C4A-NA	2.14	127.49	124.40
11	a	1116	CLA	CMB-C2B-C1B	2.14	128.68	125.42
11	a	1110	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
11	B	1205	CLA	C4-C3-C5	2.14	118.94	115.23
11	B	1218	CLA	C3C-C4C-NC	2.14	113.17	110.43
11	b	1231	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
11	l	1501	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
11	1	1106	CLA	CED-O2D-CGD	2.14	120.76	115.92
11	2	1238	CLA	C3C-C4C-NC	2.14	113.17	110.43
11	A	1124	CLA	CHB-C4A-NA	2.14	127.48	124.40
14	b	4005	BCR	C28-C27-C26	-2.14	110.25	114.06
11	2	1223	CLA	C4-C3-C5	2.14	118.94	115.23
11	a	1131	CLA	C3C-C4C-NC	2.13	113.17	110.43
14	1	4001	BCR	C8-C7-C6	-2.13	121.30	127.00
14	7	4021	BCR	C19-C18-C17	2.13	122.37	119.01
11	a	1132	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
11	1	1111	CLA	C1-C2-C3	-2.13	122.70	126.20
11	2	1207	CLA	CAA-C2A-C1A	2.13	118.97	111.97
11	B	1208	CLA	C3C-C4C-NC	2.13	113.16	110.43
11	B	1221	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
14	b	4010	BCR	C1-C6-C5	-2.13	119.72	122.64
11	A	1135	CLA	C3C-C4C-NC	2.13	113.16	110.43
11	8	1503	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
11	a	1127	CLA	C4B-CHC-C1C	2.13	131.26	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4007	BCR	C37-C22-C21	-2.13	119.36	122.82
14	b	4009	BCR	C8-C9-C10	2.13	122.36	119.01
11	b	1205	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
11	B	1222	CLA	CHB-C4A-NA	2.13	127.47	124.40
11	B	1204	CLA	CBB-CAB-C3B	-2.13	116.88	127.53
11	A	1140	CLA	C4B-CHC-C1C	2.13	131.26	126.25
11	a	1127	CLA	OBD-CAD-C3D	-2.13	123.44	128.42
11	A	1131	CLA	C4-C3-C5	2.13	118.92	115.23
11	A	1131	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
11	1	1135	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
11	a	1111	CLA	C11-C10-C8	-2.12	108.90	115.97
14	1	4003	BCR	C24-C25-C26	-2.12	116.66	121.56
11	A	1129	CLA	C4B-CHC-C1C	2.12	131.24	126.25
11	8	1502	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
11	2	1013	CLA	C3C-C4C-NC	2.12	113.15	110.43
11	A	1237	CLA	C1-O2A-CGA	2.12	121.79	116.65
11	b	1223	CLA	C1-O2A-CGA	2.12	121.79	116.65
11	1	1022	CLA	C11-C10-C8	-2.12	108.91	115.97
11	B	1208	CLA	CED-O2D-CGD	2.12	120.73	115.92
11	1	1119	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
11	A	1114	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
11	2	1239	CLA	CED-O2D-CGD	2.12	120.73	115.92
11	A	1128	CLA	C9-C8-C10	2.12	118.83	111.27
11	2	1236	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
11	b	1219	CLA	CED-O2D-CGD	2.12	120.73	115.92
14	F	4013	BCR	C1-C6-C5	-2.12	119.74	122.64
11	a	1116	CLA	CHB-C1B-C2B	-2.12	121.27	127.43
11	a	1132	CLA	CHB-C1B-C2B	-2.12	121.27	127.43
11	B	1013	CLA	CMC-C2C-C1C	2.12	128.35	125.03
11	2	1229	CLA	CAC-C3C-C4C	2.12	127.55	124.79
11	A	1138	CLA	CED-O2D-CGD	2.12	120.72	115.92
11	A	1123	CLA	C3C-C4C-NC	2.12	113.14	110.43
11	2	1202	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
11	1	1134	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
11	A	1123	CLA	C9-C8-C7	2.12	118.83	111.27
11	a	1134	CLA	C3C-C4C-NC	2.12	113.14	110.43
11	2	1235	CLA	CED-O2D-CGD	2.12	120.72	115.92
11	2	1232	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
11	B	1206	CLA	CHC-C1C-C2C	-2.12	120.93	126.95
11	A	1801	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
11	2	1209	CLA	CHB-C4A-NA	2.12	127.45	124.40
11	b	1221	CLA	CMD-C2D-C3D	-2.12	122.84	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1111	CLA	C4-C3-C5	2.12	118.90	115.23
11	b	1201	CLA	CED-O2D-CGD	2.12	120.71	115.92
11	A	1105	CLA	CAC-C3C-C4C	2.11	127.54	124.79
11	a	1125	CLA	C4B-CHC-C1C	2.11	131.22	126.25
11	1	1110	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
11	B	1230	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
11	a	1120	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
11	b	1210	CLA	CHB-C4A-NA	2.11	127.45	124.40
11	2	1230	CLA	CED-O2D-CGD	2.11	120.70	115.92
11	b	1023	CLA	C9-C8-C10	2.11	118.80	111.27
16	b	5002	LMG	C8-O7-C10	-2.11	112.74	117.80
11	A	1104	CLA	C3C-C4C-NC	2.11	113.13	110.43
14	a	4007	BCR	C35-C13-C12	2.11	121.31	118.09
11	1	1103	CLA	C1-O2A-CGA	2.11	121.76	116.65
11	a	1104	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
11	b	1235	CLA	CAC-C3C-C4C	2.11	127.53	124.79
11	A	1139	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
11	B	1216	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
11	8	1501	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
11	a	1134	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
11	B	1225	CLA	CHB-C4A-NA	2.11	127.44	124.40
11	b	1216	CLA	C1-O2A-CGA	2.11	121.75	116.65
11	1	1135	CLA	C1-O2A-CGA	2.11	121.75	116.65
11	B	1220	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
11	2	1214	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	2	2002	PQN	C25-C23-C22	2.11	122.75	112.07
14	B	4014	BCR	C31-C1-C6	-2.11	106.94	110.24
11	a	1801	CLA	CHB-C4A-NA	2.11	127.44	124.40
11	a	1011	CLA	CHA-C4D-ND	2.11	136.89	132.55
11	2	1207	CLA	OBD-CAD-C3D	-2.11	123.49	128.42
11	a	1104	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
11	b	1214	CLA	O1D-CGD-CBD	-2.11	120.37	124.52
14	A	4008	BCR	C34-C9-C8	2.10	121.30	118.09
11	b	1201	CLA	CHB-C4A-NA	2.10	127.44	124.40
11	A	1012	CLA	C5-C3-C2	-2.10	116.44	121.17
11	B	1203	CLA	CHB-C4A-NA	2.10	127.44	124.40
11	A	1102	CLA	C3C-C4C-NC	2.10	113.12	110.43
11	b	1232	CLA	C3C-C4C-NC	2.10	113.12	110.43
11	1	1012	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
11	2	1204	CLA	CBB-CAB-C3B	-2.10	117.02	127.53
11	A	1022	CLA	CBB-CAB-C3B	-2.10	117.02	127.53
11	B	1230	CLA	CED-O2D-CGD	2.10	120.69	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1022	CLA	C4-C3-C5	2.10	118.88	115.23
11	b	1201	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
11	B	1223	CLA	C9-C8-C7	2.10	118.77	111.27
11	b	1239	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
11	2	1202	CLA	CED-O2D-CGD	2.10	120.68	115.92
11	B	1023	CLA	C1-C2-C3	-2.10	122.75	126.20
11	1	1011	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
11	2	1220	CLA	CED-O2D-CGD	2.10	120.68	115.92
11	B	1212	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
11	a	1126	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
11	B	1217	CLA	CHB-C4A-NA	2.10	127.43	124.40
11	2	1224	CLA	CHB-C4A-NA	2.10	127.43	124.40
11	b	1208	CLA	C3C-C4C-NC	2.10	113.12	110.43
11	A	1011	CLA	CED-O2D-CGD	2.10	120.68	115.92
11	A	1107	CLA	C1-O2A-CGA	2.10	121.73	116.65
11	b	1228	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
11	1	1118	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
11	b	1211	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
11	1	1106	CLA	C3C-C4C-NC	2.10	113.12	110.43
11	2	1230	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
11	b	1216	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
14	8	4022	BCR	C1-C6-C5	-2.10	119.77	122.64
11	2	1215	CLA	C9-C8-C10	2.10	118.75	111.27
14	B	4005	BCR	C19-C18-C17	2.10	122.31	119.01
11	A	1022	CLA	C1-C2-C3	-2.10	122.76	126.20
15	1	5001	LHG	O7-C7-O9	-2.10	118.81	123.70
14	L	4022	BCR	C4-C5-C6	-2.10	119.87	122.70
15	a	5001	LHG	O7-C7-O9	-2.10	118.81	123.70
11	1	1139	CLA	C3C-C4C-NC	2.10	113.11	110.43
11	2	1204	CLA	C3C-C4C-NC	2.10	113.11	110.43
12	2	2002	PQN	C14-C13-C15	2.09	118.86	115.23
11	b	1234	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
11	B	1220	CLA	C3C-C4C-NC	2.09	113.11	110.43
11	b	1228	CLA	CMB-C2B-C1B	2.09	128.61	125.42
14	1	4007	BCR	C31-C1-C6	-2.09	106.96	110.24
11	1	1133	CLA	C3C-C4C-NC	2.09	113.11	110.43
11	a	1134	CLA	C4B-CHC-C1C	2.09	131.17	126.25
11	2	1230	CLA	CHB-C4A-NA	2.09	127.42	124.40
11	K	1402	CLA	C4B-CHC-C1C	2.09	131.17	126.25
11	a	1237	CLA	CED-O2D-CGD	2.09	120.66	115.92
11	1	1104	CLA	C3C-C4C-NC	2.09	113.11	110.43
11	b	1239	CLA	CHC-C1C-C2C	-2.09	121.00	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	2	1211	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
14	b	4005	BCR	C7-C8-C9	-2.09	123.14	126.23
11	b	1218	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
11	1	1127	CLA	CED-O2D-CGD	2.09	120.66	115.92
11	B	1231	CLA	CMB-C2B-C1B	2.09	128.60	125.42
11	B	1226	CLA	C4-C3-C5	2.09	118.86	115.23
11	2	1224	CLA	C1-O2A-CGA	2.09	121.71	116.65
11	B	1201	CLA	CAC-C3C-C4C	2.09	127.51	124.79
11	a	1112	CLA	CHB-C4A-NA	2.09	127.42	124.40
11	1	1105	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	A	1133	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
11	2	1234	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
11	B	1215	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	2	1238	CLA	CAC-C3C-C4C	2.09	127.51	124.79
11	0	1402	CLA	CMB-C2B-C1B	2.09	128.60	125.42
11	A	1140	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	a	1135	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	b	1224	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	B	1228	CLA	C3C-C4C-NC	2.09	113.11	110.43
11	B	1225	CLA	C4-C3-C5	2.09	118.85	115.23
11	a	1130	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
14	1	4007	BCR	C23-C24-C25	-2.09	121.42	127.00
11	b	1230	CLA	CHB-C4A-NA	2.09	127.41	124.40
11	1	1130	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
11	b	1236	CLA	CMB-C2B-C1B	2.09	128.59	125.42
11	A	1118	CLA	CHB-C4A-NA	2.09	127.41	124.40
14	F	4018	BCR	C37-C22-C21	-2.09	119.44	122.82
11	1	1127	CLA	C3C-C4C-NC	2.09	113.10	110.43
11	b	1229	CLA	CED-O2D-CGD	2.08	120.64	115.92
11	b	1221	CLA	C4-C3-C2	-2.08	118.28	123.63
11	B	1213	CLA	C4-C3-C5	2.08	118.84	115.23
11	a	1022	CLA	C4D-C3D-CAD	2.08	110.37	108.11
11	1	1137	CLA	CHB-C4A-NA	2.08	127.41	124.40
11	B	1021	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
11	b	1231	CLA	C3C-C4C-NC	2.08	113.10	110.43
11	B	1231	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
11	A	1116	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
14	B	4009	BCR	C33-C5-C4	2.08	118.03	113.60
11	B	1201	CLA	CMC-C2C-C1C	2.08	128.29	125.03
11	a	1118	CLA	C1-O2A-CGA	2.08	121.69	116.65
11	B	1210	CLA	CHB-C4A-NA	2.08	127.40	124.40
11	B	1231	CLA	CHB-C1B-C2B	-2.08	121.39	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1	1113	CLA	CAC-C3C-C4C	2.08	127.50	124.79
11	1	1105	CLA	C3C-C4C-NC	2.08	113.09	110.43
11	2	1208	CLA	C3C-C4C-NC	2.08	113.09	110.43
11	B	1023	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
11	B	1021	CLA	C3C-C4C-NC	2.08	113.09	110.43
11	B	1202	CLA	C3C-C4C-NC	2.08	113.09	110.43
14	f	4013	BCR	C24-C25-C26	-2.08	116.77	121.56
14	F	4018	BCR	C4-C5-C6	-2.08	119.90	122.70
11	a	1123	CLA	C9-C8-C7	2.08	118.68	111.27
14	f	4018	BCR	C29-C30-C25	-2.08	107.42	110.44
11	2	1203	CLA	C3C-C4C-NC	2.08	113.09	110.43
11	a	1118	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
11	A	1135	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
11	B	1240	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
11	2	1210	CLA	CHB-C4A-NA	2.08	127.39	124.40
11	1	1022	CLA	C1-C2-C3	-2.08	122.80	126.20
11	l	1503	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
11	B	1232	CLA	CHC-C1C-C2C	-2.07	121.05	126.95
11	a	1106	CLA	C4B-CHC-C1C	2.07	131.13	126.25
11	A	1123	CLA	C1-O2A-CGA	2.07	121.67	116.65
14	A	4007	BCR	C8-C7-C6	-2.07	121.46	127.00
11	1	1106	CLA	C7-C6-C5	-2.07	107.74	113.26
11	2	1221	CLA	C1-C2-C3	-2.07	122.80	126.20
11	a	1110	CLA	CAC-C3C-C4C	2.07	127.49	124.79
14	B	4005	BCR	C34-C9-C10	-2.07	119.46	122.82
11	2	1230	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
11	2	1205	CLA	O2A-C1-C2	2.07	116.08	108.11
11	B	1215	CLA	C9-C8-C7	2.07	118.66	111.27
11	2	1215	CLA	C3C-C4C-NC	2.07	113.08	110.43
11	b	1235	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
11	A	1122	CLA	C9-C8-C7	2.07	118.66	111.27
11	b	1021	CLA	CMB-C2B-C1B	2.07	128.57	125.42
11	1	1022	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
11	b	1220	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
14	B	4004	BCR	C23-C22-C21	2.07	122.27	119.01
11	b	1234	CLA	CMC-C2C-C1C	2.07	128.27	125.03
11	2	1236	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
11	A	1128	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
11	a	1104	CLA	CHB-C4A-NA	2.07	127.39	124.40
11	2	1201	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	l	4022	BCR	C36-C18-C17	-2.07	119.46	122.82
11	a	1115	CLA	CAC-C3C-C4C	2.07	127.48	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	6	4020	BCR	C35-C13-C12	2.07	121.25	118.09
11	1	1126	CLA	C9-C8-C7	2.07	118.65	111.27
14	b	4011	BCR	C32-C1-C6	-2.07	107.00	110.24
11	A	1111	CLA	C3C-C4C-NC	2.07	113.08	110.43
11	1	1111	CLA	CHA-C1A-NA	-2.07	121.71	126.39
11	2	1013	CLA	CBB-CAB-C3B	-2.07	117.19	127.53
11	b	1215	CLA	C3C-C4C-NC	2.07	113.08	110.43
11	A	1134	CLA	C4B-CHC-C1C	2.07	131.11	126.25
11	l	1503	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
14	b	4017	BCR	C28-C27-C26	-2.07	110.37	114.06
11	A	1125	CLA	C4-C3-C5	2.07	118.81	115.23
11	2	1225	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
11	b	1023	CLA	CAC-C3C-C4C	2.07	127.48	124.79
11	1	1133	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
11	b	1214	CLA	C9-C8-C7	2.07	118.64	111.27
11	A	1011	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
14	b	4010	BCR	C34-C9-C10	-2.07	119.47	122.82
11	a	1138	CLA	CHB-C4A-NA	2.07	127.38	124.40
11	1	1107	CLA	C4B-CHC-C1C	2.07	131.10	126.25
11	B	1013	CLA	CAC-C3C-C4C	2.06	127.47	124.79
11	b	1213	CLA	CAC-C3C-C4C	2.06	127.47	124.79
11	b	1210	CLA	C4B-CHC-C1C	2.06	131.10	126.25
11	8	1502	CLA	CHB-C4A-NA	2.06	127.38	124.40
11	l	1501	CLA	C4-C3-C2	-2.06	118.33	123.63
11	B	1234	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
11	2	1216	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
11	1	1128	CLA	CMC-C2C-C1C	2.06	128.26	125.03
11	a	1011	CLA	C3D-C4D-ND	2.06	113.34	109.99
11	1	1012	CLA	CHB-C4A-NA	2.06	127.38	124.40
11	B	1235	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
14	L	4019	BCR	C28-C27-C26	-2.06	110.38	114.06
11	2	1228	CLA	C5-C3-C4	2.06	119.33	114.59
11	1	1102	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
11	1	1102	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
11	A	1108	CLA	CAC-C3C-C4C	2.06	127.47	124.79
11	A	1118	CLA	C1-O2A-CGA	2.06	121.64	116.65
11	B	1021	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
11	1	1126	CLA	C4-C3-C2	-2.06	118.34	123.63
14	B	4004	BCR	C23-C24-C25	-2.06	121.50	127.00
11	A	1137	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
11	B	1225	CLA	CBA-CAA-C2A	2.06	119.91	113.79
11	1	1022	CLA	O2D-CGD-O1D	-2.06	119.84	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4007	BCR	C7-C8-C9	-2.06	123.19	126.23
11	A	1120	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
11	1	1109	CLA	CED-O2D-CGD	2.06	120.58	115.92
11	a	1119	CLA	C3C-C4C-NC	2.06	113.06	110.43
14	F	4018	BCR	C40-C30-C25	-2.06	107.02	110.24
11	1	1022	CLA	C4D-C3D-CAD	2.06	110.34	108.11
11	a	1102	CLA	C6-C5-C3	-2.06	108.46	113.47
14	f	4020	BCR	C35-C13-C12	2.05	121.23	118.09
11	A	1022	CLA	CHB-C4A-NA	2.05	127.36	124.40
11	2	1221	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
11	B	1202	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
11	a	1112	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
14	L	4022	BCR	C23-C24-C25	-2.05	121.52	127.00
11	b	1238	CLA	C1-O2A-CGA	2.05	121.62	116.65
11	B	1213	CLA	C1-C2-C3	-2.05	122.84	126.20
11	A	1136	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
11	A	1101	CLA	CED-O2D-CGD	2.05	120.57	115.92
11	B	1209	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
11	a	1131	CLA	C1-O2A-CGA	2.05	121.61	116.65
11	A	1011	CLA	CHA-C4D-ND	2.05	136.78	132.55
14	2	4010	BCR	C4-C5-C6	-2.05	119.93	122.70
14	2	4006	BCR	C37-C22-C21	-2.05	119.49	122.82
11	A	1124	CLA	CED-O2D-CGD	2.05	120.57	115.92
11	b	1214	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
11	B	1226	CLA	C1-O2A-CGA	2.05	121.61	116.65
14	8	4022	BCR	C36-C18-C17	-2.05	119.50	122.82
11	B	1218	CLA	CAC-C3C-C4C	2.05	127.46	124.79
12	2	2002	PQN	C11-C12-C13	-2.05	123.30	126.83
14	B	4011	BCR	C23-C22-C21	2.05	122.23	119.01
11	A	1112	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
11	B	1234	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
11	a	1131	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
11	1	1103	CLA	CHA-C4D-ND	2.05	136.77	132.55
11	A	1121	CLA	C3C-C4C-NC	2.05	113.05	110.43
14	a	4002	BCR	C28-C27-C26	-2.05	110.41	114.06
11	1	1109	CLA	CAC-C3C-C4C	2.05	127.45	124.79
11	1	1102	CLA	C1-O2A-CGA	2.05	121.60	116.65
11	1	1104	CLA	O1D-CGD-CBD	-2.04	120.48	124.52
11	2	1203	CLA	CAC-C3C-C4C	2.04	127.45	124.79
11	A	1120	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
11	2	1203	CLA	C1-C2-C3	-2.04	122.85	126.20
11	b	1240	CLA	CAC-C3C-C4C	2.04	127.45	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	2001	PQN	C11-C12-C13	-2.04	123.31	126.83
11	2	1227	CLA	C3C-C4C-NC	2.04	113.05	110.43
11	A	1132	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
11	8	1503	CLA	C1-O2A-CGA	2.04	121.59	116.65
11	b	1209	CLA	C3C-C4C-NC	2.04	113.05	110.43
11	a	1119	CLA	CHC-C1C-C2C	-2.04	121.14	126.95
11	1	1125	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
11	1	1117	CLA	C3C-C4C-NC	2.04	113.05	110.43
11	a	1124	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
11	b	1204	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
11	A	1124	CLA	CBB-CAB-C3B	-2.04	117.33	127.53
11	b	1206	CLA	CHB-C4A-NA	2.04	127.34	124.40
11	B	1023	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
14	8	4022	BCR	C23-C22-C21	2.04	122.22	119.01
15	b	5004	LHG	O7-C7-O9	-2.04	118.93	123.70
11	1	1111	CLA	C9-C8-C10	2.04	118.55	111.27
11	2	1238	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
11	A	1125	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	B	4009	BCR	C23-C24-C25	-2.04	121.55	127.00
11	2	1023	CLA	CED-O2D-CGD	2.04	120.54	115.92
11	8	1501	CLA	C4-C3-C2	-2.04	118.39	123.63
11	A	1103	CLA	C3C-C4C-NC	2.04	113.04	110.43
11	a	1105	CLA	C3C-C4C-NC	2.04	113.04	110.43
11	B	1216	CLA	C1-O2A-CGA	2.04	121.59	116.65
14	b	4014	BCR	C8-C7-C6	-2.04	121.55	127.00
11	2	1239	CLA	CAC-C3C-C4C	2.04	127.44	124.79
11	a	1121	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
11	b	1239	CLA	CMC-C2C-C1C	2.04	128.22	125.03
11	A	1107	CLA	CHA-C1A-NA	-2.04	121.78	126.39
11	a	1101	CLA	C4-C3-C5	2.04	118.76	115.23
11	A	1139	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
11	1	1101	CLA	CED-O2D-CGD	2.04	120.53	115.92
11	1	1125	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
11	1	1113	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	a	4003	BCR	C35-C13-C12	2.04	121.20	118.09
11	B	1240	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
11	b	1223	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
11	a	1107	CLA	CHA-C1A-NA	-2.03	121.78	126.39
11	b	1206	CLA	C4-C3-C5	2.03	118.76	115.23
11	1	1237	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
11	K	1402	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
11	2	1218	CLA	CHB-C4A-NA	2.03	127.33	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4001	BCR	C8-C7-C6	-2.03	121.57	127.00
11	b	1223	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
11	a	1116	CLA	C4-C3-C5	2.03	118.76	115.23
11	b	1231	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
11	K	1402	CLA	CMB-C2B-C1B	2.03	128.51	125.42
14	1	4007	BCR	C35-C13-C12	2.03	121.19	118.09
11	B	1219	CLA	CHB-C4A-NA	2.03	127.33	124.40
11	2	1213	CLA	C7-C6-C5	-2.03	107.84	113.26
11	1	1022	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
11	a	1140	CLA	C9-C8-C10	2.03	118.52	111.27
11	a	1022	CLA	C4-C3-C5	2.03	118.75	115.23
11	b	1013	CLA	CBB-CAB-C3B	-2.03	117.38	127.53
14	b	4005	BCR	C23-C24-C25	-2.03	121.57	127.00
11	1	1124	CLA	CHB-C4A-NA	2.03	127.33	124.40
11	k	1401	CLA	CHA-C1A-NA	-2.03	121.79	126.39
11	A	1801	CLA	CAC-C3C-C2C	2.03	131.29	127.56
11	B	1223	CLA	C9-C8-C10	2.03	118.50	111.27
11	2	1228	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
14	2	4017	BCR	C3-C4-C5	-2.03	110.44	114.06
11	a	1118	CLA	C3C-C4C-NC	2.03	113.03	110.43
11	2	1223	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
11	b	1239	CLA	C3C-C4C-NC	2.03	113.03	110.43
11	A	1022	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
11	2	1231	CLA	C4B-CHC-C1C	2.03	131.01	126.25
11	1	1118	CLA	OBD-CAD-C3D	-2.03	123.68	128.42
14	a	4008	BCR	C37-C22-C21	-2.03	119.53	122.82
11	2	1205	CLA	C1-C2-C3	-2.03	122.88	126.20
11	a	1123	CLA	C4-C3-C5	2.03	118.75	115.23
11	B	1211	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
11	b	1210	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
11	A	1134	CLA	C3C-C4C-NC	2.03	113.03	110.43
11	K	1401	CLA	CHA-C1A-NA	-2.03	121.80	126.39
11	A	1104	CLA	CHB-C4A-NA	2.02	127.32	124.40
11	a	1801	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
14	A	4002	BCR	C30-C25-C24	2.02	121.14	115.65
11	2	1209	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
11	B	1240	CLA	CMB-C2B-C3B	2.02	131.31	126.55
11	b	1230	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
11	1	1121	CLA	CED-O2D-CGD	2.02	120.50	115.92
11	b	1205	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
14	B	4010	BCR	C1-C6-C5	-2.02	119.87	122.64
11	B	1201	CLA	CHC-C1C-C2C	-2.02	121.20	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1217	CLA	C1-O2A-CGA	2.02	122.41	116.67
11	b	1207	CLA	CAC-C3C-C4C	2.02	127.42	124.79
11	A	1801	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
11	B	1226	CLA	CHB-C4A-NA	2.02	127.32	124.40
11	1	1112	CLA	CHB-C4A-NA	2.02	127.32	124.40
11	a	1106	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
11	2	1231	CLA	CHA-C4D-ND	2.02	136.72	132.55
11	1	1120	CLA	CHB-C4A-NA	2.02	127.32	124.40
11	2	1229	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
11	A	1125	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
11	b	1023	CLA	CMC-C2C-C1C	2.02	128.19	125.03
14	2	4014	BCR	C8-C7-C6	-2.02	121.60	127.00
11	A	1129	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
11	a	1022	CLA	CBB-CAB-C3B	-2.02	117.44	127.53
11	A	1117	CLA	C9-C8-C7	2.02	118.47	111.27
11	A	1133	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
14	B	4009	BCR	C30-C25-C26	-2.02	119.88	122.64
11	a	1127	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
11	b	1209	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
11	1	1121	CLA	CHB-C4A-NA	2.02	127.31	124.40
11	2	1216	CLA	C4-C3-C5	2.02	118.73	115.23
11	B	1023	CLA	C9-C8-C10	2.02	118.47	111.27
11	a	1118	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
11	a	1122	CLA	C9-C8-C10	2.02	118.47	111.27
11	2	1204	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
11	a	1110	CLA	C1-O2A-CGA	2.02	121.53	116.65
11	A	1123	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
11	0	1401	CLA	CHA-C1A-NA	-2.02	121.82	126.39
14	8	4019	BCR	C35-C13-C14	-2.02	119.55	122.82
11	B	1240	CLA	CAC-C3C-C4C	2.02	127.41	124.79
14	2	4009	BCR	C32-C1-C6	-2.02	107.08	110.24
11	L	1501	CLA	C1-C2-C3	-2.02	122.89	126.20
11	A	1124	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
14	1	4008	BCR	C34-C9-C8	2.02	121.17	118.09
11	2	1217	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
11	1	1119	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
11	a	1109	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
11	2	1223	CLA	C1-O2A-CGA	2.01	121.53	116.65
14	2	4005	BCR	C33-C5-C4	2.01	117.89	113.60
11	2	1207	CLA	C11-C10-C8	-2.01	109.27	115.97
11	A	1115	CLA	C4B-CHC-C1C	2.01	130.99	126.25
11	a	1135	CLA	CHC-C1C-C2C	-2.01	121.22	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	b	1238	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
11	b	1225	CLA	CMB-C2B-C1B	2.01	128.49	125.42
11	A	1124	CLA	C1-O2A-CGA	2.01	121.53	116.65
11	2	1206	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
11	2	1224	CLA	C10-C8-C9	2.01	119.52	110.53
12	1	2001	PQN	C11-C3-C2	-2.01	121.44	124.89
12	2	2002	PQN	C12-C11-C3	-2.01	107.12	112.08
11	B	1229	CLA	C4B-CHC-C1C	2.01	130.98	126.25
11	k	1401	CLA	C9-C8-C7	2.01	118.45	111.27
12	b	2002	PQN	C24-C23-C22	2.01	118.45	111.27
14	1	4007	BCR	C36-C18-C17	-2.01	119.56	122.82
11	a	1133	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
11	a	1118	CLA	C4-C3-C5	2.01	118.72	115.23
11	A	1136	CLA	C4B-CHC-C1C	2.01	130.98	126.25
11	b	1215	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
11	2	1225	CLA	CMB-C2B-C1B	2.01	128.48	125.42
11	A	1125	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
11	b	1210	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
11	2	1021	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
11	2	1222	CLA	CHB-C4A-NA	2.01	127.30	124.40
11	b	1205	CLA	CAC-C3C-C4C	2.01	127.40	124.79
11	a	1117	CLA	C6-C5-C3	-2.01	108.57	113.47
11	K	1402	CLA	CHB-C4A-NA	2.01	127.30	124.40
11	A	1119	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
11	2	1235	CLA	C1-O2A-CGA	2.01	121.51	116.65
11	a	1113	CLA	CHB-C4A-NA	2.01	127.30	124.40
11	b	1238	CLA	C11-C10-C8	-2.01	109.29	115.97
11	2	1232	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
11	1	1114	CLA	C3C-C4C-NC	2.01	113.00	110.43
11	A	1113	CLA	CHB-C4A-NA	2.01	127.30	124.40
11	a	1115	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
11	B	1013	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
11	K	1401	CLA	C9-C8-C7	2.01	118.43	111.27
11	1	1104	CLA	C4B-CHC-C1C	2.01	130.97	126.25
11	b	1226	CLA	CAC-C3C-C4C	2.01	127.40	124.79
11	b	1213	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
11	2	1202	CLA	C3C-C4C-NC	2.01	113.00	110.43
11	b	1238	CLA	CAC-C3C-C4C	2.01	127.40	124.79
11	B	1216	CLA	CED-O2D-CGD	2.00	120.46	115.92
11	1	1115	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
11	0	1401	CLA	C9-C8-C7	2.00	118.42	111.27
11	b	1207	CLA	CHC-C1C-C2C	-2.00	121.25	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	1121	CLA	C1-O2A-CGA	2.00	122.49	116.07
11	A	1119	CLA	CED-O2D-CGD	2.00	120.46	115.92
11	a	1115	CLA	C4B-CHC-C1C	2.00	130.96	126.25
11	1	1118	CLA	CHB-C4A-NA	2.00	127.29	124.40
14	2	4010	BCR	C8-C7-C6	-2.00	121.65	127.00
11	A	1115	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
11	1	1124	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
11	a	1119	CLA	CMB-C2B-C1B	2.00	128.47	125.42
11	b	1021	CLA	C5-C3-C2	-2.00	116.67	121.17
11	B	1216	CLA	C3C-C4C-NC	2.00	113.00	110.43
11	b	1218	CLA	CED-O2D-CGD	2.00	120.46	115.92
11	2	1225	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
11	2	1213	CLA	C4B-CHC-C1C	2.00	130.96	126.25
11	A	1123	CLA	C4B-CHC-C1C	2.00	130.95	126.25
11	B	1240	CLA	CHB-C4A-NA	2.00	127.29	124.40
11	a	1102	CLA	CED-O2D-CGD	2.00	120.45	115.92
11	1	1136	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
11	A	1237	CLA	O2D-CGD-O1D	-2.00	119.95	123.85

There are no chirality outliers.

All (4221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1237	CLA	C1A-C2A-CAA-CBA
11	A	1237	CLA	O2A-C1-C2-C3
11	A	1022	CLA	C2-C1-O2A-CGA
11	A	1022	CLA	CBD-CGD-O2D-CED
11	A	1101	CLA	C3A-C2A-CAA-CBA
11	A	1101	CLA	C2-C1-O2A-CGA
11	A	1102	CLA	C1A-C2A-CAA-CBA
11	A	1102	CLA	C3A-C2A-CAA-CBA
11	A	1102	CLA	O1A-CGA-O2A-C1
11	A	1102	CLA	CBD-CGD-O2D-CED
11	A	1103	CLA	C3A-C2A-CAA-CBA
11	A	1103	CLA	CAD-CBD-CGD-O1D
11	A	1103	CLA	CAD-CBD-CGD-O2D
11	A	1104	CLA	CBD-CGD-O2D-CED
11	A	1105	CLA	CBD-CGD-O2D-CED
11	A	1106	CLA	C3A-C2A-CAA-CBA
11	A	1106	CLA	CHA-CBD-CGD-O1D
11	A	1106	CLA	CHA-CBD-CGD-O2D
11	A	1107	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	A	1107	CLA	C2-C3-C5-C6
11	A	1107	CLA	C4-C3-C5-C6
11	A	1108	CLA	C1A-C2A-CAA-CBA
11	A	1108	CLA	C3A-C2A-CAA-CBA
11	A	1110	CLA	CBA-CGA-O2A-C1
11	A	1110	CLA	O1A-CGA-O2A-C1
11	A	1110	CLA	CHA-CBD-CGD-O1D
11	A	1110	CLA	CHA-CBD-CGD-O2D
11	A	1112	CLA	C1A-C2A-CAA-CBA
11	A	1112	CLA	C3A-C2A-CAA-CBA
11	A	1113	CLA	C2B-C3B-CAB-CBB
11	A	1113	CLA	C4B-C3B-CAB-CBB
11	A	1113	CLA	CBD-CGD-O2D-CED
11	A	1116	CLA	C3A-C2A-CAA-CBA
11	A	1116	CLA	CBD-CGD-O2D-CED
11	A	1117	CLA	CBD-CGD-O2D-CED
11	A	1118	CLA	C2B-C3B-CAB-CBB
11	A	1118	CLA	C4B-C3B-CAB-CBB
11	A	1118	CLA	CAD-CBD-CGD-O1D
11	A	1118	CLA	CAD-CBD-CGD-O2D
11	A	1122	CLA	CBA-CGA-O2A-C1
11	A	1122	CLA	C2B-C3B-CAB-CBB
11	A	1122	CLA	C4B-C3B-CAB-CBB
11	A	1123	CLA	C2-C1-O2A-CGA
11	A	1124	CLA	C2-C1-O2A-CGA
11	A	1125	CLA	C2C-C3C-CAC-CBC
11	A	1125	CLA	C4C-C3C-CAC-CBC
11	A	1126	CLA	C2B-C3B-CAB-CBB
11	A	1126	CLA	C4B-C3B-CAB-CBB
11	A	1126	CLA	CBD-CGD-O2D-CED
11	A	1128	CLA	C2B-C3B-CAB-CBB
11	A	1128	CLA	C4B-C3B-CAB-CBB
11	A	1128	CLA	C6-C7-C8-C9
11	A	1130	CLA	C2B-C3B-CAB-CBB
11	A	1130	CLA	C4B-C3B-CAB-CBB
11	A	1131	CLA	C1A-C2A-CAA-CBA
11	A	1131	CLA	C3A-C2A-CAA-CBA
11	A	1131	CLA	C2B-C3B-CAB-CBB
11	A	1131	CLA	C4B-C3B-CAB-CBB
11	A	1131	CLA	CBD-CGD-O2D-CED
11	A	1139	CLA	C1A-C2A-CAA-CBA
11	A	1139	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	A	1139	CLA	CBD-CGD-O2D-CED
11	A	1011	CLA	C1A-C2A-CAA-CBA
11	A	1011	CLA	C3A-C2A-CAA-CBA
11	A	1011	CLA	CBD-CGD-O2D-CED
11	A	1012	CLA	C2B-C3B-CAB-CBB
11	A	1012	CLA	C4B-C3B-CAB-CBB
11	A	1012	CLA	C4-C3-C5-C6
11	A	1114	CLA	CBA-CGA-O2A-C1
11	A	1114	CLA	CBD-CGD-O2D-CED
11	A	1120	CLA	C3A-C2A-CAA-CBA
11	A	1120	CLA	CHA-CBD-CGD-O1D
11	A	1120	CLA	CHA-CBD-CGD-O2D
11	A	1121	CLA	CBD-CGD-O2D-CED
11	A	1132	CLA	CHA-CBD-CGD-O1D
11	A	1132	CLA	CHA-CBD-CGD-O2D
11	B	1013	CLA	CBD-CGD-O2D-CED
11	B	1021	CLA	CBD-CGD-O2D-CED
11	B	1023	CLA	C2-C1-O2A-CGA
11	B	1023	CLA	C2B-C3B-CAB-CBB
11	B	1023	CLA	C4B-C3B-CAB-CBB
11	B	1023	CLA	CBD-CGD-O2D-CED
11	B	1023	CLA	C6-C7-C8-C9
11	B	1201	CLA	CHA-CBD-CGD-O2D
11	B	1202	CLA	C3A-C2A-CAA-CBA
11	B	1202	CLA	CAD-CBD-CGD-O1D
11	B	1202	CLA	CAD-CBD-CGD-O2D
11	B	1203	CLA	C6-C7-C8-C9
11	B	1205	CLA	C2B-C3B-CAB-CBB
11	B	1205	CLA	C4B-C3B-CAB-CBB
11	B	1205	CLA	CHA-CBD-CGD-O1D
11	B	1205	CLA	CHA-CBD-CGD-O2D
11	B	1208	CLA	CBD-CGD-O2D-CED
11	B	1209	CLA	C1A-C2A-CAA-CBA
11	B	1209	CLA	C3A-C2A-CAA-CBA
11	B	1210	CLA	CAD-CBD-CGD-O1D
11	B	1210	CLA	CAD-CBD-CGD-O2D
11	B	1210	CLA	CBD-CGD-O2D-CED
11	B	1212	CLA	C2B-C3B-CAB-CBB
11	B	1212	CLA	C4B-C3B-CAB-CBB
11	B	1213	CLA	C2B-C3B-CAB-CBB
11	B	1213	CLA	C4B-C3B-CAB-CBB
11	B	1214	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	B	1215	CLA	C1A-C2A-CAA-CBA
11	B	1215	CLA	C3A-C2A-CAA-CBA
11	B	1215	CLA	CBD-CGD-O2D-CED
11	B	1216	CLA	C2B-C3B-CAB-CBB
11	B	1216	CLA	C4B-C3B-CAB-CBB
11	B	1217	CLA	C3A-C2A-CAA-CBA
11	B	1217	CLA	CAD-CBD-CGD-O1D
11	B	1217	CLA	CAD-CBD-CGD-O2D
11	B	1221	CLA	C2B-C3B-CAB-CBB
11	B	1221	CLA	C4B-C3B-CAB-CBB
11	B	1221	CLA	CHA-CBD-CGD-O1D
11	B	1221	CLA	CHA-CBD-CGD-O2D
11	B	1222	CLA	CHA-CBD-CGD-O1D
11	B	1222	CLA	CHA-CBD-CGD-O2D
11	B	1225	CLA	C1A-C2A-CAA-CBA
11	B	1225	CLA	C3A-C2A-CAA-CBA
11	B	1225	CLA	C11-C10-C8-C7
11	B	1226	CLA	CHA-CBD-CGD-O1D
11	B	1226	CLA	CHA-CBD-CGD-O2D
11	B	1228	CLA	C2B-C3B-CAB-CBB
11	B	1228	CLA	C4B-C3B-CAB-CBB
11	B	1228	CLA	CBD-CGD-O2D-CED
11	B	1230	CLA	C2-C1-O2A-CGA
11	B	1230	CLA	CHA-CBD-CGD-O1D
11	B	1230	CLA	CHA-CBD-CGD-O2D
11	B	1230	CLA	C2-C3-C5-C6
11	B	1231	CLA	CHA-CBD-CGD-O1D
11	B	1231	CLA	CHA-CBD-CGD-O2D
11	B	1231	CLA	CBD-CGD-O2D-CED
11	B	1232	CLA	CBD-CGD-O2D-CED
11	B	1236	CLA	C2B-C3B-CAB-CBB
11	B	1236	CLA	C4B-C3B-CAB-CBB
11	B	1236	CLA	CBD-CGD-O2D-CED
11	B	1240	CLA	C1A-C2A-CAA-CBA
11	B	1240	CLA	CBD-CGD-O2D-CED
11	B	1211	CLA	CBA-CGA-O2A-C1
11	B	1211	CLA	C4B-C3B-CAB-CBB
11	L	1501	CLA	C1A-C2A-CAA-CBA
11	L	1503	CLA	C2-C1-O2A-CGA
11	a	1801	CLA	C1A-C2A-CAA-CBA
11	a	1801	CLA	C3A-C2A-CAA-CBA
11	a	1801	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	a	1801	CLA	O1A-CGA-O2A-C1
11	a	1801	CLA	C2B-C3B-CAB-CBB
11	a	1801	CLA	C4B-C3B-CAB-CBB
11	a	1801	CLA	CBD-CGD-O2D-CED
11	a	1237	CLA	C1A-C2A-CAA-CBA
11	a	1237	CLA	O2A-C1-C2-C3
11	a	1022	CLA	C2B-C3B-CAB-CBB
11	a	1022	CLA	C4B-C3B-CAB-CBB
11	a	1022	CLA	CBD-CGD-O2D-CED
11	a	1101	CLA	C1A-C2A-CAA-CBA
11	a	1101	CLA	C2-C1-O2A-CGA
11	a	1101	CLA	CHA-CBD-CGD-O1D
11	a	1101	CLA	CHA-CBD-CGD-O2D
11	a	1102	CLA	C1A-C2A-CAA-CBA
11	a	1102	CLA	C3A-C2A-CAA-CBA
11	a	1102	CLA	CBD-CGD-O2D-CED
11	a	1103	CLA	C2-C1-O2A-CGA
11	a	1103	CLA	C2B-C3B-CAB-CBB
11	a	1103	CLA	C4B-C3B-CAB-CBB
11	a	1103	CLA	CAD-CBD-CGD-O1D
11	a	1103	CLA	CAD-CBD-CGD-O2D
11	a	1104	CLA	C1A-C2A-CAA-CBA
11	a	1104	CLA	CBD-CGD-O2D-CED
11	a	1105	CLA	C2-C1-O2A-CGA
11	a	1105	CLA	CBD-CGD-O2D-CED
11	a	1106	CLA	CHA-CBD-CGD-O1D
11	a	1106	CLA	CHA-CBD-CGD-O2D
11	a	1107	CLA	C2B-C3B-CAB-CBB
11	a	1107	CLA	C4B-C3B-CAB-CBB
11	a	1109	CLA	CBD-CGD-O2D-CED
11	a	1113	CLA	CBD-CGD-O2D-CED
11	a	1116	CLA	C3A-C2A-CAA-CBA
11	a	1116	CLA	CBD-CGD-O2D-CED
11	a	1118	CLA	CBD-CGD-O2D-CED
11	a	1119	CLA	C2-C1-O2A-CGA
11	a	1119	CLA	CBD-CGD-O2D-CED
11	a	1122	CLA	C2-C1-O2A-CGA
11	a	1122	CLA	C4B-C3B-CAB-CBB
11	a	1123	CLA	C2-C1-O2A-CGA
11	a	1123	CLA	C2B-C3B-CAB-CBB
11	a	1123	CLA	C4B-C3B-CAB-CBB
11	a	1124	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
11	a	1124	CLA	CBD-CGD-O2D-CED
11	a	1125	CLA	CBD-CGD-O2D-CED
11	a	1126	CLA	C2B-C3B-CAB-CBB
11	a	1126	CLA	C4B-C3B-CAB-CBB
11	a	1126	CLA	CBD-CGD-O2D-CED
11	a	1127	CLA	C11-C10-C8-C9
11	a	1131	CLA	C4B-C3B-CAB-CBB
11	a	1131	CLA	CBD-CGD-O2D-CED
11	a	1137	CLA	C2-C1-O2A-CGA
11	a	1137	CLA	C11-C10-C8-C9
11	a	1138	CLA	CBD-CGD-O2D-CED
11	a	1140	CLA	CBD-CGD-O2D-CED
11	a	1011	CLA	C1A-C2A-CAA-CBA
11	a	1011	CLA	C3A-C2A-CAA-CBA
11	a	1011	CLA	CBD-CGD-O2D-CED
11	a	1012	CLA	C2B-C3B-CAB-CBB
11	a	1012	CLA	C4B-C3B-CAB-CBB
11	a	1012	CLA	CAD-CBD-CGD-O1D
11	a	1012	CLA	CAD-CBD-CGD-O2D
11	a	1012	CLA	C4-C3-C5-C6
11	a	1114	CLA	CBD-CGD-O2D-CED
11	a	1120	CLA	C3A-C2A-CAA-CBA
11	a	1129	CLA	C4B-C3B-CAB-CBB
11	a	1129	CLA	CAD-CBD-CGD-O2D
11	a	1132	CLA	C2B-C3B-CAB-CBB
11	a	1132	CLA	C4B-C3B-CAB-CBB
11	a	1132	CLA	CHA-CBD-CGD-O1D
11	a	1132	CLA	CHA-CBD-CGD-O2D
11	a	1133	CLA	CBA-CGA-O2A-C1
11	a	1134	CLA	C3A-C2A-CAA-CBA
11	a	1135	CLA	CHA-CBD-CGD-O1D
11	a	1135	CLA	CHA-CBD-CGD-O2D
11	b	1013	CLA	CBD-CGD-O2D-CED
11	b	1021	CLA	C1A-C2A-CAA-CBA
11	b	1021	CLA	C3A-C2A-CAA-CBA
11	b	1021	CLA	CBD-CGD-O2D-CED
11	b	1021	CLA	O1D-CGD-O2D-CED
11	b	1023	CLA	C2B-C3B-CAB-CBB
11	b	1023	CLA	C4B-C3B-CAB-CBB
11	b	1023	CLA	C6-C7-C8-C9
11	b	1201	CLA	CBD-CGD-O2D-CED
11	b	1202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	b	1202	CLA	C3A-C2A-CAA-CBA
11	b	1202	CLA	CAD-CBD-CGD-O1D
11	b	1202	CLA	CAD-CBD-CGD-O2D
11	b	1203	CLA	C6-C7-C8-C9
11	b	1204	CLA	C2B-C3B-CAB-CBB
11	b	1204	CLA	C4B-C3B-CAB-CBB
11	b	1205	CLA	CHA-CBD-CGD-O1D
11	b	1205	CLA	CHA-CBD-CGD-O2D
11	b	1212	CLA	CBD-CGD-O2D-CED
11	b	1213	CLA	C2B-C3B-CAB-CBB
11	b	1213	CLA	C4B-C3B-CAB-CBB
11	b	1214	CLA	CBD-CGD-O2D-CED
11	b	1215	CLA	C1A-C2A-CAA-CBA
11	b	1215	CLA	C3A-C2A-CAA-CBA
11	b	1216	CLA	C2B-C3B-CAB-CBB
11	b	1216	CLA	C4B-C3B-CAB-CBB
11	b	1217	CLA	C1A-C2A-CAA-CBA
11	b	1217	CLA	C3A-C2A-CAA-CBA
11	b	1220	CLA	CBD-CGD-O2D-CED
11	b	1221	CLA	CHA-CBD-CGD-O1D
11	b	1221	CLA	CHA-CBD-CGD-O2D
11	b	1222	CLA	CHA-CBD-CGD-O1D
11	b	1222	CLA	CHA-CBD-CGD-O2D
11	b	1223	CLA	C2B-C3B-CAB-CBB
11	b	1223	CLA	C4B-C3B-CAB-CBB
11	b	1223	CLA	CAD-CBD-CGD-O1D
11	b	1223	CLA	CAD-CBD-CGD-O2D
11	b	1224	CLA	CBA-CGA-O2A-C1
11	b	1224	CLA	CBD-CGD-O2D-CED
11	b	1225	CLA	C6-C7-C8-C9
11	b	1226	CLA	CHA-CBD-CGD-O1D
11	b	1226	CLA	CHA-CBD-CGD-O2D
11	b	1229	CLA	C2-C1-O2A-CGA
11	b	1230	CLA	C2-C1-O2A-CGA
11	b	1230	CLA	CHA-CBD-CGD-O1D
11	b	1230	CLA	CHA-CBD-CGD-O2D
11	b	1231	CLA	CHA-CBD-CGD-O1D
11	b	1231	CLA	CHA-CBD-CGD-O2D
11	b	1232	CLA	CBD-CGD-O2D-CED
11	b	1234	CLA	CAD-CBD-CGD-O1D
11	b	1234	CLA	CAD-CBD-CGD-O2D
11	b	1235	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1240	CLA	C1A-C2A-CAA-CBA
11	b	1240	CLA	C3A-C2A-CAA-CBA
11	b	1211	CLA	C2B-C3B-CAB-CBB
11	b	1211	CLA	C4B-C3B-CAB-CBB
11	b	1211	CLA	CBD-CGD-O2D-CED
11	b	1238	CLA	CBD-CGD-O2D-CED
11	b	1239	CLA	CBA-CGA-O2A-C1
11	l	1503	CLA	C2-C1-O2A-CGA
11	l	1503	CLA	C2B-C3B-CAB-CBB
11	l	1503	CLA	C4B-C3B-CAB-CBB
11	1	1801	CLA	C1A-C2A-CAA-CBA
11	1	1801	CLA	C3A-C2A-CAA-CBA
11	1	1801	CLA	CBA-CGA-O2A-C1
11	1	1801	CLA	O1A-CGA-O2A-C1
11	1	1237	CLA	C1A-C2A-CAA-CBA
11	1	1237	CLA	CBD-CGD-O2D-CED
11	1	1022	CLA	CBD-CGD-O2D-CED
11	1	1101	CLA	C2-C1-O2A-CGA
11	1	1101	CLA	C2B-C3B-CAB-CBB
11	1	1101	CLA	C4B-C3B-CAB-CBB
11	1	1102	CLA	C1A-C2A-CAA-CBA
11	1	1102	CLA	C3A-C2A-CAA-CBA
11	1	1102	CLA	CBD-CGD-O2D-CED
11	1	1103	CLA	C1A-C2A-CAA-CBA
11	1	1103	CLA	C3A-C2A-CAA-CBA
11	1	1103	CLA	CAD-CBD-CGD-O1D
11	1	1103	CLA	CAD-CBD-CGD-O2D
11	1	1104	CLA	C1A-C2A-CAA-CBA
11	1	1104	CLA	CBD-CGD-O2D-CED
11	1	1106	CLA	C1A-C2A-CAA-CBA
11	1	1106	CLA	C3A-C2A-CAA-CBA
11	1	1106	CLA	CHA-CBD-CGD-O1D
11	1	1106	CLA	CHA-CBD-CGD-O2D
11	1	1106	CLA	C4-C3-C5-C6
11	1	1107	CLA	C1A-C2A-CAA-CBA
11	1	1107	CLA	CBD-CGD-O2D-CED
11	1	1109	CLA	C4-C3-C5-C6
11	1	1110	CLA	CHA-CBD-CGD-O1D
11	1	1110	CLA	CHA-CBD-CGD-O2D
11	1	1111	CLA	CHA-CBD-CGD-O1D
11	1	1111	CLA	CHA-CBD-CGD-O2D
11	1	1111	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	1	1113	CLA	CBD-CGD-O2D-CED
11	1	1116	CLA	C3A-C2A-CAA-CBA
11	1	1116	CLA	CBD-CGD-O2D-CED
11	1	1118	CLA	C2B-C3B-CAB-CBB
11	1	1118	CLA	C4B-C3B-CAB-CBB
11	1	1119	CLA	C2-C1-O2A-CGA
11	1	1119	CLA	CBD-CGD-O2D-CED
11	1	1122	CLA	C2B-C3B-CAB-CBB
11	1	1122	CLA	C4B-C3B-CAB-CBB
11	1	1123	CLA	C2-C1-O2A-CGA
11	1	1123	CLA	C2B-C3B-CAB-CBB
11	1	1123	CLA	C4B-C3B-CAB-CBB
11	1	1124	CLA	C4B-C3B-CAB-CBB
11	1	1126	CLA	C4B-C3B-CAB-CBB
11	1	1126	CLA	CBD-CGD-O2D-CED
11	1	1128	CLA	CBD-CGD-O2D-CED
11	1	1128	CLA	C6-C7-C8-C9
11	1	1130	CLA	CBA-CGA-O2A-C1
11	1	1137	CLA	C2-C1-O2A-CGA
11	1	1137	CLA	CHA-CBD-CGD-O1D
11	1	1137	CLA	CHA-CBD-CGD-O2D
11	1	1137	CLA	CBD-CGD-O2D-CED
11	1	1139	CLA	CBD-CGD-O2D-CED
11	1	1140	CLA	C2-C1-O2A-CGA
11	1	1140	CLA	C6-C7-C8-C9
11	1	1120	CLA	C1A-C2A-CAA-CBA
11	1	1120	CLA	C3A-C2A-CAA-CBA
11	1	1121	CLA	C3A-C2A-CAA-CBA
11	1	1121	CLA	CBA-CGA-O2A-C1
11	1	1121	CLA	C2B-C3B-CAB-CBB
11	1	1121	CLA	C4B-C3B-CAB-CBB
11	1	1132	CLA	C2B-C3B-CAB-CBB
11	1	1132	CLA	C4B-C3B-CAB-CBB
11	1	1135	CLA	CHA-CBD-CGD-O1D
11	1	1135	CLA	CHA-CBD-CGD-O2D
11	1	1135	CLA	C2-C3-C5-C6
11	1	1135	CLA	C4-C3-C5-C6
11	2	1021	CLA	C3A-C2A-CAA-CBA
11	2	1021	CLA	CBD-CGD-O2D-CED
11	2	1021	CLA	O1D-CGD-O2D-CED
11	2	1023	CLA	CBD-CGD-O2D-CED
11	2	1201	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	2	1201	CLA	CAD-CBD-CGD-O2D
11	2	1202	CLA	C3A-C2A-CAA-CBA
11	2	1203	CLA	C2-C1-O2A-CGA
11	2	1203	CLA	C2B-C3B-CAB-CBB
11	2	1203	CLA	C4B-C3B-CAB-CBB
11	2	1205	CLA	CHA-CBD-CGD-O1D
11	2	1205	CLA	CHA-CBD-CGD-O2D
11	2	1206	CLA	C2B-C3B-CAB-CBB
11	2	1206	CLA	C4B-C3B-CAB-CBB
11	2	1206	CLA	CBD-CGD-O2D-CED
11	2	1208	CLA	CBD-CGD-O2D-CED
11	2	1210	CLA	C2B-C3B-CAB-CBB
11	2	1210	CLA	C4B-C3B-CAB-CBB
11	2	1213	CLA	C6-C7-C8-C9
11	2	1214	CLA	C2B-C3B-CAB-CBB
11	2	1214	CLA	C4B-C3B-CAB-CBB
11	2	1215	CLA	C3A-C2A-CAA-CBA
11	2	1216	CLA	C2-C1-O2A-CGA
11	2	1216	CLA	C2B-C3B-CAB-CBB
11	2	1216	CLA	C4B-C3B-CAB-CBB
11	2	1216	CLA	CBD-CGD-O2D-CED
11	2	1217	CLA	C1A-C2A-CAA-CBA
11	2	1217	CLA	C3A-C2A-CAA-CBA
11	2	1217	CLA	C2B-C3B-CAB-CBB
11	2	1217	CLA	C4B-C3B-CAB-CBB
11	2	1217	CLA	CAD-CBD-CGD-O1D
11	2	1217	CLA	CAD-CBD-CGD-O2D
11	2	1219	CLA	C1A-C2A-CAA-CBA
11	2	1219	CLA	C3A-C2A-CAA-CBA
11	2	1221	CLA	C4B-C3B-CAB-CBB
11	2	1221	CLA	CHA-CBD-CGD-O1D
11	2	1221	CLA	CHA-CBD-CGD-O2D
11	2	1222	CLA	C2B-C3B-CAB-CBB
11	2	1222	CLA	C4B-C3B-CAB-CBB
11	2	1222	CLA	CHA-CBD-CGD-O1D
11	2	1222	CLA	CHA-CBD-CGD-O2D
11	2	1223	CLA	C4B-C3B-CAB-CBB
11	2	1224	CLA	C2B-C3B-CAB-CBB
11	2	1224	CLA	C4B-C3B-CAB-CBB
11	2	1224	CLA	CBD-CGD-O2D-CED
11	2	1225	CLA	C1A-C2A-CAA-CBA
11	2	1225	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	2	1225	CLA	C2B-C3B-CAB-CBB
11	2	1225	CLA	C4B-C3B-CAB-CBB
11	2	1228	CLA	C2B-C3B-CAB-CBB
11	2	1228	CLA	C4B-C3B-CAB-CBB
11	2	1229	CLA	C2-C1-O2A-CGA
11	2	1230	CLA	CHA-CBD-CGD-O1D
11	2	1230	CLA	CHA-CBD-CGD-O2D
11	2	1231	CLA	CHA-CBD-CGD-O1D
11	2	1231	CLA	CHA-CBD-CGD-O2D
11	2	1232	CLA	CBD-CGD-O2D-CED
11	2	1234	CLA	C1A-C2A-CAA-CBA
11	2	1234	CLA	C2B-C3B-CAB-CBB
11	2	1234	CLA	C4B-C3B-CAB-CBB
11	2	1234	CLA	CAD-CBD-CGD-O1D
11	2	1234	CLA	CAD-CBD-CGD-O2D
11	2	1236	CLA	CAD-CBD-CGD-O1D
11	2	1236	CLA	CAD-CBD-CGD-O2D
11	2	1240	CLA	CBD-CGD-O2D-CED
11	2	1211	CLA	CBA-CGA-O2A-C1
11	2	1211	CLA	C4B-C3B-CAB-CBB
11	2	1211	CLA	CAD-CBD-CGD-O1D
11	2	1211	CLA	CAD-CBD-CGD-O2D
11	2	1239	CLA	C1A-C2A-CAA-CBA
11	2	1239	CLA	C3A-C2A-CAA-CBA
11	2	1239	CLA	CBD-CGD-O2D-CED
11	8	1501	CLA	C1A-C2A-CAA-CBA
11	8	1501	CLA	C3A-C2A-CAA-CBA
11	8	1501	CLA	CAD-CBD-CGD-O1D
11	8	1501	CLA	CAD-CBD-CGD-O2D
11	8	1503	CLA	C2-C1-O2A-CGA
11	K	1401	CLA	C3A-C2A-CAA-CBA
11	K	1401	CLA	C2B-C3B-CAB-CBB
11	K	1401	CLA	C4B-C3B-CAB-CBB
11	K	1401	CLA	CAD-CBD-CGD-O1D
11	K	1401	CLA	CAD-CBD-CGD-O2D
11	K	1401	CLA	CBD-CGD-O2D-CED
11	K	1402	CLA	C1A-C2A-CAA-CBA
11	K	1402	CLA	CBD-CGD-O2D-CED
11	k	1401	CLA	C3A-C2A-CAA-CBA
11	k	1401	CLA	C2B-C3B-CAB-CBB
11	k	1401	CLA	C4B-C3B-CAB-CBB
11	k	1401	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	k	1401	CLA	CAD-CBD-CGD-O2D
11	k	1401	CLA	CBD-CGD-O2D-CED
11	k	1402	CLA	CBD-CGD-O2D-CED
11	0	1401	CLA	C3A-C2A-CAA-CBA
11	0	1401	CLA	C2B-C3B-CAB-CBB
11	0	1401	CLA	C4B-C3B-CAB-CBB
11	0	1401	CLA	CAD-CBD-CGD-O1D
11	0	1401	CLA	CAD-CBD-CGD-O2D
11	0	1401	CLA	CBD-CGD-O2D-CED
11	0	1402	CLA	CBD-CGD-O2D-CED
14	A	4002	BCR	C11-C10-C9-C8
14	A	4002	BCR	C11-C10-C9-C34
14	A	4002	BCR	C10-C11-C12-C13
14	A	4002	BCR	C23-C24-C25-C26
14	A	4002	BCR	C23-C24-C25-C30
14	A	4003	BCR	C10-C11-C12-C13
14	A	4007	BCR	C10-C11-C12-C13
14	A	4007	BCR	C21-C22-C23-C24
14	A	4007	BCR	C37-C22-C23-C24
14	A	4008	BCR	C7-C8-C9-C10
14	A	4008	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	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C11-C10-C9-C34
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C21-C22-C23-C24
14	B	4005	BCR	C37-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	C5-C6-C7-C8
14	B	4009	BCR	C11-C12-C13-C14
14	B	4009	BCR	C13-C14-C15-C16
14	B	4009	BCR	C21-C22-C23-C24
14	B	4010	BCR	C7-C8-C9-C10
14	B	4010	BCR	C7-C8-C9-C34
14	B	4010	BCR	C11-C10-C9-C8
14	B	4010	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
14	B	4010	BCR	C10-C11-C12-C13
14	B	4010	BCR	C17-C18-C19-C20
14	B	4010	BCR	C23-C24-C25-C26
14	B	4011	BCR	C1-C6-C7-C8
14	B	4011	BCR	C5-C6-C7-C8
14	B	4011	BCR	C11-C10-C9-C8
14	B	4011	BCR	C11-C10-C9-C34
14	B	4011	BCR	C23-C24-C25-C26
14	B	4011	BCR	C23-C24-C25-C30
14	B	4014	BCR	C11-C10-C9-C8
14	B	4014	BCR	C11-C10-C9-C34
14	B	4014	BCR	C10-C11-C12-C13
14	B	4014	BCR	C17-C18-C19-C20
14	B	4014	BCR	C36-C18-C19-C20
14	B	4017	BCR	C11-C10-C9-C8
14	B	4017	BCR	C11-C10-C9-C34
14	B	4017	BCR	C9-C10-C11-C12
14	B	4017	BCR	C10-C11-C12-C13
14	F	4018	BCR	C11-C10-C9-C8
14	F	4018	BCR	C11-C10-C9-C34
14	F	4018	BCR	C10-C11-C12-C13
14	F	4020	BCR	C7-C8-C9-C10
14	F	4020	BCR	C7-C8-C9-C34
14	F	4020	BCR	C11-C10-C9-C8
14	F	4020	BCR	C11-C10-C9-C34
14	F	4020	BCR	C10-C11-C12-C13
14	F	4020	BCR	C21-C22-C23-C24
14	F	4013	BCR	C1-C6-C7-C8
14	F	4013	BCR	C5-C6-C7-C8
14	F	4013	BCR	C11-C10-C9-C8
14	F	4013	BCR	C11-C10-C9-C34
14	F	4013	BCR	C11-C12-C13-C35
14	L	4019	BCR	C10-C11-C12-C13
14	L	4019	BCR	C23-C24-C25-C26
14	L	4019	BCR	C23-C24-C25-C30
14	L	4022	BCR	C11-C10-C9-C8
14	L	4022	BCR	C11-C10-C9-C34
14	L	4022	BCR	C10-C11-C12-C13
14	L	4022	BCR	C17-C18-C19-C20
14	L	4022	BCR	C21-C22-C23-C24
14	M	4021	BCR	C5-C6-C7-C8
14	M	4021	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	M	4021	BCR	C11-C10-C9-C34
14	M	4021	BCR	C21-C22-C23-C24
14	M	4021	BCR	C37-C22-C23-C24
14	a	4001	BCR	C11-C10-C9-C8
14	a	4001	BCR	C11-C10-C9-C34
14	a	4001	BCR	C10-C11-C12-C13
14	a	4002	BCR	C7-C8-C9-C10
14	a	4002	BCR	C7-C8-C9-C34
14	a	4002	BCR	C11-C10-C9-C8
14	a	4002	BCR	C11-C10-C9-C34
14	a	4002	BCR	C17-C18-C19-C20
14	a	4002	BCR	C21-C22-C23-C24
14	a	4002	BCR	C23-C24-C25-C26
14	a	4002	BCR	C23-C24-C25-C30
14	a	4003	BCR	C10-C11-C12-C13
14	a	4003	BCR	C21-C22-C23-C24
14	a	4003	BCR	C23-C24-C25-C26
14	a	4003	BCR	C23-C24-C25-C30
14	a	4007	BCR	C7-C8-C9-C10
14	a	4007	BCR	C23-C24-C25-C26
14	a	4007	BCR	C23-C24-C25-C30
14	a	4008	BCR	C7-C8-C9-C10
14	a	4008	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	4008	BCR	C11-C12-C13-C14
14	a	4008	BCR	C11-C12-C13-C35
14	a	4008	BCR	C21-C22-C23-C24
14	a	4008	BCR	C37-C22-C23-C24
14	b	4004	BCR	C11-C10-C9-C8
14	b	4004	BCR	C11-C10-C9-C34
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	C9-C10-C11-C12
14	b	4005	BCR	C10-C11-C12-C13
14	b	4005	BCR	C11-C12-C13-C14
14	b	4006	BCR	C11-C10-C9-C8
14	b	4006	BCR	C11-C10-C9-C34
14	b	4006	BCR	C11-C12-C13-C14
14	b	4006	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	b	4006	BCR	C23-C24-C25-C30
14	b	4009	BCR	C1-C6-C7-C8
14	b	4009	BCR	C5-C6-C7-C8
14	b	4009	BCR	C7-C8-C9-C10
14	b	4009	BCR	C7-C8-C9-C34
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	4009	BCR	C21-C22-C23-C24
14	b	4009	BCR	C37-C22-C23-C24
14	b	4010	BCR	C11-C10-C9-C8
14	b	4010	BCR	C11-C10-C9-C34
14	b	4010	BCR	C19-C20-C21-C22
14	b	4010	BCR	C23-C24-C25-C26
14	b	4010	BCR	C23-C24-C25-C30
14	b	4011	BCR	C1-C6-C7-C8
14	b	4011	BCR	C5-C6-C7-C8
14	b	4011	BCR	C7-C8-C9-C10
14	b	4011	BCR	C7-C8-C9-C34
14	b	4011	BCR	C17-C18-C19-C20
14	b	4011	BCR	C23-C24-C25-C26
14	b	4011	BCR	C23-C24-C25-C30
14	b	4014	BCR	C11-C10-C9-C8
14	b	4014	BCR	C11-C10-C9-C34
14	b	4014	BCR	C10-C11-C12-C13
14	b	4014	BCR	C11-C12-C13-C35
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	b	4017	BCR	C11-C12-C13-C14
14	b	4017	BCR	C11-C12-C13-C35
14	f	4018	BCR	C11-C10-C9-C8
14	f	4018	BCR	C11-C10-C9-C34
14	f	4018	BCR	C11-C12-C13-C14
14	f	4018	BCR	C11-C12-C13-C35
14	f	4020	BCR	C7-C8-C9-C34
14	f	4020	BCR	C11-C10-C9-C8
14	f	4020	BCR	C11-C10-C9-C34
14	f	4020	BCR	C10-C11-C12-C13
14	f	4020	BCR	C37-C22-C23-C24
14	f	4013	BCR	C5-C6-C7-C8
14	f	4013	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	f	4013	BCR	C11-C10-C9-C34
14	f	4013	BCR	C21-C22-C23-C24
14	f	4013	BCR	C23-C24-C25-C26
14	f	4013	BCR	C23-C24-C25-C30
14	l	4019	BCR	C1-C6-C7-C8
14	l	4019	BCR	C5-C6-C7-C8
14	l	4019	BCR	C11-C10-C9-C8
14	l	4019	BCR	C11-C10-C9-C34
14	l	4019	BCR	C10-C11-C12-C13
14	l	4019	BCR	C11-C12-C13-C14
14	l	4019	BCR	C11-C12-C13-C35
14	l	4019	BCR	C23-C24-C25-C26
14	l	4019	BCR	C23-C24-C25-C30
14	l	4022	BCR	C7-C8-C9-C10
14	l	4022	BCR	C7-C8-C9-C34
14	l	4022	BCR	C11-C10-C9-C8
14	l	4022	BCR	C11-C10-C9-C34
14	l	4022	BCR	C17-C18-C19-C20
14	l	4022	BCR	C21-C22-C23-C24
14	l	4022	BCR	C37-C22-C23-C24
14	m	4021	BCR	C11-C10-C9-C8
14	m	4021	BCR	C11-C10-C9-C34
14	m	4021	BCR	C10-C11-C12-C13
14	1	4001	BCR	C7-C8-C9-C10
14	1	4001	BCR	C7-C8-C9-C34
14	1	4001	BCR	C11-C10-C9-C8
14	1	4001	BCR	C11-C10-C9-C34
14	1	4001	BCR	C10-C11-C12-C13
14	1	4002	BCR	C7-C8-C9-C10
14	1	4002	BCR	C7-C8-C9-C34
14	1	4002	BCR	C11-C10-C9-C8
14	1	4002	BCR	C11-C10-C9-C34
14	1	4002	BCR	C9-C10-C11-C12
14	1	4002	BCR	C17-C18-C19-C20
14	1	4002	BCR	C23-C24-C25-C26
14	1	4002	BCR	C23-C24-C25-C30
14	1	4003	BCR	C1-C6-C7-C8
14	1	4003	BCR	C5-C6-C7-C8
14	1	4003	BCR	C11-C10-C9-C8
14	1	4003	BCR	C11-C10-C9-C34
14	1	4003	BCR	C10-C11-C12-C13
14	1	4007	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	1	4007	BCR	C7-C8-C9-C34
14	1	4007	BCR	C11-C10-C9-C8
14	1	4007	BCR	C11-C10-C9-C34
14	1	4007	BCR	C10-C11-C12-C13
14	1	4007	BCR	C19-C20-C21-C22
14	1	4007	BCR	C23-C24-C25-C26
14	1	4008	BCR	C7-C8-C9-C34
14	1	4008	BCR	C11-C10-C9-C8
14	1	4008	BCR	C11-C10-C9-C34
14	1	4008	BCR	C10-C11-C12-C13
14	1	4008	BCR	C11-C12-C13-C14
14	1	4008	BCR	C11-C12-C13-C35
14	1	4008	BCR	C21-C22-C23-C24
14	1	4008	BCR	C37-C22-C23-C24
14	2	4004	BCR	C7-C8-C9-C10
14	2	4004	BCR	C7-C8-C9-C34
14	2	4004	BCR	C11-C10-C9-C8
14	2	4004	BCR	C11-C10-C9-C34
14	2	4004	BCR	C10-C11-C12-C13
14	2	4004	BCR	C21-C22-C23-C24
14	2	4004	BCR	C37-C22-C23-C24
14	2	4005	BCR	C1-C6-C7-C8
14	2	4005	BCR	C5-C6-C7-C8
14	2	4005	BCR	C7-C8-C9-C10
14	2	4005	BCR	C7-C8-C9-C34
14	2	4006	BCR	C11-C10-C9-C8
14	2	4006	BCR	C11-C10-C9-C34
14	2	4006	BCR	C23-C24-C25-C26
14	2	4006	BCR	C23-C24-C25-C30
14	2	4009	BCR	C1-C6-C7-C8
14	2	4009	BCR	C5-C6-C7-C8
14	2	4009	BCR	C7-C8-C9-C10
14	2	4009	BCR	C7-C8-C9-C34
14	2	4009	BCR	C11-C10-C9-C8
14	2	4009	BCR	C11-C10-C9-C34
14	2	4009	BCR	C15-C16-C17-C18
14	2	4009	BCR	C21-C22-C23-C24
14	2	4009	BCR	C37-C22-C23-C24
14	2	4010	BCR	C7-C8-C9-C10
14	2	4010	BCR	C7-C8-C9-C34
14	2	4010	BCR	C11-C10-C9-C8
14	2	4010	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
14	2	4010	BCR	C9-C10-C11-C12
14	2	4010	BCR	C23-C24-C25-C26
14	2	4010	BCR	C23-C24-C25-C30
14	2	4011	BCR	C1-C6-C7-C8
14	2	4011	BCR	C5-C6-C7-C8
14	2	4011	BCR	C11-C10-C9-C8
14	2	4011	BCR	C11-C10-C9-C34
14	2	4011	BCR	C21-C22-C23-C24
14	2	4011	BCR	C23-C24-C25-C26
14	2	4014	BCR	C11-C10-C9-C8
14	2	4014	BCR	C11-C10-C9-C34
14	2	4014	BCR	C9-C10-C11-C12
14	2	4014	BCR	C17-C18-C19-C20
14	2	4014	BCR	C21-C22-C23-C24
14	2	4014	BCR	C37-C22-C23-C24
14	2	4017	BCR	C11-C10-C9-C8
14	2	4017	BCR	C11-C10-C9-C34
14	2	4017	BCR	C10-C11-C12-C13
14	6	4018	BCR	C11-C10-C9-C8
14	6	4018	BCR	C11-C10-C9-C34
14	6	4018	BCR	C11-C12-C13-C14
14	6	4018	BCR	C11-C12-C13-C35
14	6	4018	BCR	C21-C22-C23-C24
14	6	4018	BCR	C23-C24-C25-C26
14	6	4020	BCR	C7-C8-C9-C10
14	6	4020	BCR	C7-C8-C9-C34
14	6	4020	BCR	C11-C10-C9-C8
14	6	4020	BCR	C11-C10-C9-C34
14	6	4020	BCR	C9-C10-C11-C12
14	6	4020	BCR	C10-C11-C12-C13
14	6	4020	BCR	C21-C22-C23-C24
14	6	4020	BCR	C37-C22-C23-C24
14	6	4013	BCR	C11-C10-C9-C8
14	6	4013	BCR	C11-C10-C9-C34
14	6	4013	BCR	C21-C22-C23-C24
14	6	4013	BCR	C37-C22-C23-C24
14	8	4019	BCR	C7-C8-C9-C10
14	8	4019	BCR	C7-C8-C9-C34
14	8	4019	BCR	C9-C10-C11-C12
14	8	4019	BCR	C11-C12-C13-C14
14	8	4019	BCR	C19-C20-C21-C22
14	8	4019	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	8	4019	BCR	C23-C24-C25-C26
14	8	4019	BCR	C23-C24-C25-C30
14	8	4022	BCR	C11-C10-C9-C8
14	8	4022	BCR	C11-C10-C9-C34
14	8	4022	BCR	C17-C18-C19-C20
14	7	4021	BCR	C11-C10-C9-C8
14	7	4021	BCR	C11-C10-C9-C34
14	7	4021	BCR	C10-C11-C12-C13
14	7	4021	BCR	C21-C22-C23-C24
14	7	4021	BCR	C37-C22-C23-C24
15	A	5001	LHG	O1-C1-C2-C3
15	A	5001	LHG	C1-C2-C3-O3
15	A	5001	LHG	C4-O6-P-O5
15	A	5001	LHG	O7-C5-C6-O8
15	A	5003	LHG	O1-C1-C2-C3
15	A	5003	LHG	C3-O3-P-O5
15	A	5003	LHG	C4-O6-P-O3
15	A	5003	LHG	C4-O6-P-O4
15	A	5003	LHG	C4-O6-P-O5
15	a	5001	LHG	O1-C1-C2-O2
15	a	5001	LHG	O1-C1-C2-C3
15	a	5001	LHG	C3-O3-P-O4
15	a	5001	LHG	C3-O3-P-O6
15	a	5001	LHG	C4-O6-P-O3
15	a	5001	LHG	C4-O6-P-O5
15	a	5001	LHG	O7-C5-C6-O8
15	a	5003	LHG	C3-O3-P-O5
15	a	5003	LHG	C3-O3-P-O6
15	a	5003	LHG	C4-O6-P-O3
15	a	5003	LHG	C4-O6-P-O4
15	a	5003	LHG	C4-O6-P-O5
15	b	5004	LHG	C3-O3-P-O4
15	b	5004	LHG	C4-O6-P-O3
15	b	5004	LHG	C4-O6-P-O4
15	1	5001	LHG	C4-O6-P-O3
15	1	5001	LHG	C4-O6-P-O4
15	1	5003	LHG	O1-C1-C2-C3
15	1	5003	LHG	C3-O3-P-O5
15	1	5003	LHG	C4-O6-P-O3
15	1	5003	LHG	C4-O6-P-O4
15	1	5003	LHG	C4-O6-P-O5
15	2	5004	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
15	2	5004	LHG	C3-O3-P-O6
15	2	5004	LHG	C4-O6-P-O3
15	2	5004	LHG	C4-O6-P-O4
15	2	5004	LHG	C8-C7-O7-C5
11	A	1801	CLA	C4C-C3C-CAC-CBC
11	1	1801	CLA	C4C-C3C-CAC-CBC
11	1	1125	CLA	C4C-C3C-CAC-CBC
11	1	1125	CLA	C2C-C3C-CAC-CBC
11	A	1105	CLA	O1D-CGD-O2D-CED
11	A	1109	CLA	O1D-CGD-O2D-CED
11	B	1023	CLA	O1D-CGD-O2D-CED
11	B	1210	CLA	O1D-CGD-O2D-CED
11	a	1022	CLA	O1D-CGD-O2D-CED
11	a	1108	CLA	O1D-CGD-O2D-CED
11	a	1011	CLA	O1D-CGD-O2D-CED
11	a	1121	CLA	O1D-CGD-O2D-CED
11	1	1108	CLA	O1D-CGD-O2D-CED
11	1	1109	CLA	O1D-CGD-O2D-CED
11	1	1133	CLA	O1D-CGD-O2D-CED
11	A	1801	CLA	C2C-C3C-CAC-CBC
11	2	1220	CLA	C2C-C3C-CAC-CBC
11	A	1801	CLA	O1D-CGD-O2D-CED
11	A	1104	CLA	O1D-CGD-O2D-CED
11	A	1107	CLA	O1D-CGD-O2D-CED
11	A	1113	CLA	O1D-CGD-O2D-CED
11	A	1130	CLA	O1D-CGD-O2D-CED
11	A	1139	CLA	O1D-CGD-O2D-CED
11	A	1011	CLA	O1D-CGD-O2D-CED
11	A	1114	CLA	O1D-CGD-O2D-CED
11	A	1121	CLA	O1D-CGD-O2D-CED
11	B	1021	CLA	O1D-CGD-O2D-CED
11	B	1208	CLA	O1D-CGD-O2D-CED
11	B	1219	CLA	O1D-CGD-O2D-CED
11	B	1231	CLA	O1D-CGD-O2D-CED
11	B	1240	CLA	O1D-CGD-O2D-CED
11	a	1109	CLA	O1D-CGD-O2D-CED
11	a	1124	CLA	O1D-CGD-O2D-CED
11	a	1131	CLA	O1D-CGD-O2D-CED
11	a	1138	CLA	O1D-CGD-O2D-CED
11	a	1139	CLA	O1D-CGD-O2D-CED
11	b	1210	CLA	O1D-CGD-O2D-CED
11	b	1216	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1220	CLA	O1D-CGD-O2D-CED
11	b	1240	CLA	O1D-CGD-O2D-CED
11	1	1022	CLA	O1D-CGD-O2D-CED
11	1	1102	CLA	O1D-CGD-O2D-CED
11	1	1104	CLA	O1D-CGD-O2D-CED
11	1	1113	CLA	O1D-CGD-O2D-CED
11	1	1139	CLA	O1D-CGD-O2D-CED
11	1	1121	CLA	O1D-CGD-O2D-CED
11	2	1208	CLA	O1D-CGD-O2D-CED
11	2	1219	CLA	O1D-CGD-O2D-CED
11	2	1232	CLA	O1D-CGD-O2D-CED
11	K	1402	CLA	O1D-CGD-O2D-CED
11	A	1801	CLA	CBD-CGD-O2D-CED
11	A	1103	CLA	CBD-CGD-O2D-CED
11	A	1107	CLA	CBD-CGD-O2D-CED
11	A	1109	CLA	CBD-CGD-O2D-CED
11	A	1112	CLA	CBD-CGD-O2D-CED
11	A	1123	CLA	CBD-CGD-O2D-CED
11	A	1128	CLA	CBD-CGD-O2D-CED
11	A	1130	CLA	CBD-CGD-O2D-CED
11	B	1212	CLA	CBD-CGD-O2D-CED
11	B	1219	CLA	CBD-CGD-O2D-CED
11	B	1222	CLA	CBD-CGD-O2D-CED
11	B	1224	CLA	CBD-CGD-O2D-CED
11	B	1238	CLA	CBD-CGD-O2D-CED
11	B	1239	CLA	CBD-CGD-O2D-CED
11	L	1503	CLA	CBD-CGD-O2D-CED
11	a	1101	CLA	CBD-CGD-O2D-CED
11	a	1106	CLA	CBD-CGD-O2D-CED
11	a	1107	CLA	CBD-CGD-O2D-CED
11	a	1108	CLA	CBD-CGD-O2D-CED
11	a	1111	CLA	CBD-CGD-O2D-CED
11	a	1117	CLA	CBD-CGD-O2D-CED
11	a	1127	CLA	CBD-CGD-O2D-CED
11	a	1130	CLA	CBD-CGD-O2D-CED
11	a	1139	CLA	CBD-CGD-O2D-CED
11	a	1121	CLA	CBD-CGD-O2D-CED
11	b	1023	CLA	CBD-CGD-O2D-CED
11	b	1205	CLA	CBD-CGD-O2D-CED
11	b	1207	CLA	CBD-CGD-O2D-CED
11	b	1210	CLA	CBD-CGD-O2D-CED
11	b	1216	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1218	CLA	CBD-CGD-O2D-CED
11	b	1219	CLA	CBD-CGD-O2D-CED
11	b	1234	CLA	CBD-CGD-O2D-CED
11	b	1240	CLA	CBD-CGD-O2D-CED
11	b	1206	CLA	CBD-CGD-O2D-CED
11	b	1239	CLA	CBD-CGD-O2D-CED
11	l	1501	CLA	CBD-CGD-O2D-CED
11	l	1503	CLA	CBD-CGD-O2D-CED
11	1	1103	CLA	CBD-CGD-O2D-CED
11	1	1108	CLA	CBD-CGD-O2D-CED
11	1	1109	CLA	CBD-CGD-O2D-CED
11	1	1117	CLA	CBD-CGD-O2D-CED
11	1	1130	CLA	CBD-CGD-O2D-CED
11	1	1131	CLA	CBD-CGD-O2D-CED
11	1	1138	CLA	CBD-CGD-O2D-CED
11	1	1140	CLA	CBD-CGD-O2D-CED
11	1	1114	CLA	CBD-CGD-O2D-CED
11	1	1121	CLA	CBD-CGD-O2D-CED
11	1	1133	CLA	CBD-CGD-O2D-CED
11	1	1135	CLA	CBD-CGD-O2D-CED
11	1	1136	CLA	CBD-CGD-O2D-CED
11	2	1013	CLA	CBD-CGD-O2D-CED
11	2	1218	CLA	CBD-CGD-O2D-CED
11	2	1219	CLA	CBD-CGD-O2D-CED
11	2	1222	CLA	CBD-CGD-O2D-CED
11	2	1223	CLA	CBD-CGD-O2D-CED
11	2	1225	CLA	CBD-CGD-O2D-CED
11	2	1231	CLA	CBD-CGD-O2D-CED
11	2	1234	CLA	CBD-CGD-O2D-CED
11	2	1238	CLA	CBD-CGD-O2D-CED
11	8	1503	CLA	CBD-CGD-O2D-CED
11	A	1122	CLA	O1A-CGA-O2A-C1
11	B	1013	CLA	O1A-CGA-O2A-C1
11	B	1224	CLA	O1A-CGA-O2A-C1
11	L	1501	CLA	O1A-CGA-O2A-C1
11	b	1223	CLA	O1A-CGA-O2A-C1
11	b	1224	CLA	O1A-CGA-O2A-C1
11	1	1237	CLA	O1A-CGA-O2A-C1
11	1	1102	CLA	O1A-CGA-O2A-C1
11	1	1104	CLA	O1A-CGA-O2A-C1
11	1	1122	CLA	O1A-CGA-O2A-C1
11	1	1140	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	2	1013	CLA	O1A-CGA-O2A-C1
11	2	1224	CLA	O1A-CGA-O2A-C1
11	A	1130	CLA	O1A-CGA-O2A-C1
11	A	1120	CLA	O1A-CGA-O2A-C1
11	A	1129	CLA	O1A-CGA-O2A-C1
11	B	1211	CLA	O1A-CGA-O2A-C1
11	a	1133	CLA	O1A-CGA-O2A-C1
11	1	1130	CLA	O1A-CGA-O2A-C1
11	b	1236	CLA	C2-C1-O2A-CGA
11	B	1210	CLA	C2C-C3C-CAC-CBC
11	B	1227	CLA	C2C-C3C-CAC-CBC
11	a	1104	CLA	O1D-CGD-O2D-CED
11	a	1111	CLA	O1D-CGD-O2D-CED
11	a	1113	CLA	O1D-CGD-O2D-CED
11	a	1114	CLA	O1D-CGD-O2D-CED
11	2	1023	CLA	O1D-CGD-O2D-CED
11	2	1240	CLA	O1D-CGD-O2D-CED
11	k	1402	CLA	O1D-CGD-O2D-CED
11	0	1402	CLA	O1D-CGD-O2D-CED
11	A	1115	CLA	CBA-CGA-O2A-C1
11	A	1130	CLA	CBA-CGA-O2A-C1
11	A	1120	CLA	CBA-CGA-O2A-C1
11	A	1129	CLA	CBA-CGA-O2A-C1
11	B	1239	CLA	CBA-CGA-O2A-C1
11	L	1502	CLA	CBA-CGA-O2A-C1
11	a	1129	CLA	CBA-CGA-O2A-C1
11	a	1136	CLA	CBA-CGA-O2A-C1
11	1	1129	CLA	CBA-CGA-O2A-C1
11	2	1220	CLA	C4C-C3C-CAC-CBC
11	1	1801	CLA	C2C-C3C-CAC-CBC
11	a	1107	CLA	O1D-CGD-O2D-CED
11	a	1117	CLA	O1D-CGD-O2D-CED
11	b	1023	CLA	O1D-CGD-O2D-CED
11	b	1219	CLA	O1D-CGD-O2D-CED
11	1	1131	CLA	O1D-CGD-O2D-CED
11	2	1231	CLA	O1D-CGD-O2D-CED
11	A	1102	CLA	CBA-CGA-O2A-C1
11	B	1013	CLA	CBA-CGA-O2A-C1
11	B	1224	CLA	CBA-CGA-O2A-C1
11	1	1237	CLA	CBA-CGA-O2A-C1
11	1	1102	CLA	CBA-CGA-O2A-C1
11	2	1013	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	2	1224	CLA	CBA-CGA-O2A-C1
11	A	1118	CLA	CBD-CGD-O2D-CED
11	b	1225	CLA	CBD-CGD-O2D-CED
11	1	1101	CLA	CBD-CGD-O2D-CED
11	2	1236	CLA	C2-C1-O2A-CGA
11	A	1801	CLA	O1A-CGA-O2A-C1
11	A	1237	CLA	O1A-CGA-O2A-C1
11	A	1118	CLA	O1A-CGA-O2A-C1
11	B	1228	CLA	O1A-CGA-O2A-C1
11	L	1503	CLA	O1A-CGA-O2A-C1
11	a	1237	CLA	O1A-CGA-O2A-C1
11	a	1102	CLA	O1A-CGA-O2A-C1
11	a	1122	CLA	O1A-CGA-O2A-C1
11	a	1123	CLA	O1A-CGA-O2A-C1
11	a	1140	CLA	O1A-CGA-O2A-C1
11	b	1013	CLA	O1A-CGA-O2A-C1
11	b	1021	CLA	O1A-CGA-O2A-C1
11	b	1023	CLA	O1A-CGA-O2A-C1
11	b	1228	CLA	O1A-CGA-O2A-C1
11	l	1501	CLA	O1A-CGA-O2A-C1
11	l	1503	CLA	O1A-CGA-O2A-C1
11	1	1109	CLA	O1A-CGA-O2A-C1
11	1	1110	CLA	O1A-CGA-O2A-C1
11	1	1111	CLA	O1A-CGA-O2A-C1
11	2	1021	CLA	O1A-CGA-O2A-C1
11	2	1023	CLA	O1A-CGA-O2A-C1
11	2	1226	CLA	O1A-CGA-O2A-C1
11	2	1228	CLA	O1A-CGA-O2A-C1
11	K	1401	CLA	O1A-CGA-O2A-C1
11	k	1401	CLA	O1A-CGA-O2A-C1
11	0	1401	CLA	O1A-CGA-O2A-C1
11	A	1115	CLA	O1A-CGA-O2A-C1
11	A	1114	CLA	O1A-CGA-O2A-C1
11	A	1121	CLA	O1A-CGA-O2A-C1
11	a	1115	CLA	O1A-CGA-O2A-C1
11	a	1130	CLA	O1A-CGA-O2A-C1
11	a	1121	CLA	O1A-CGA-O2A-C1
11	b	1239	CLA	O1A-CGA-O2A-C1
11	1	1121	CLA	O1A-CGA-O2A-C1
11	2	1211	CLA	O1A-CGA-O2A-C1
11	B	1210	CLA	C4C-C3C-CAC-CBC
11	A	1128	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1013	CLA	O1D-CGD-O2D-CED
11	L	1503	CLA	O1D-CGD-O2D-CED
11	a	1118	CLA	O1D-CGD-O2D-CED
11	a	1125	CLA	O1D-CGD-O2D-CED
11	a	1140	CLA	O1D-CGD-O2D-CED
11	b	1013	CLA	O1D-CGD-O2D-CED
11	b	1214	CLA	O1D-CGD-O2D-CED
11	b	1232	CLA	O1D-CGD-O2D-CED
11	1	1103	CLA	O1D-CGD-O2D-CED
11	1	1111	CLA	O1D-CGD-O2D-CED
11	1	1119	CLA	O1D-CGD-O2D-CED
11	1	1140	CLA	O1D-CGD-O2D-CED
11	2	1206	CLA	O1D-CGD-O2D-CED
11	8	1503	CLA	O1D-CGD-O2D-CED
11	K	1401	CLA	O1D-CGD-O2D-CED
11	k	1401	CLA	O1D-CGD-O2D-CED
11	0	1401	CLA	O1D-CGD-O2D-CED
11	A	1116	CLA	O1D-CGD-O2D-CED
11	A	1131	CLA	O1D-CGD-O2D-CED
11	B	1215	CLA	O1D-CGD-O2D-CED
11	B	1232	CLA	O1D-CGD-O2D-CED
11	a	1801	CLA	O1D-CGD-O2D-CED
11	a	1102	CLA	O1D-CGD-O2D-CED
11	a	1119	CLA	O1D-CGD-O2D-CED
11	a	1126	CLA	O1D-CGD-O2D-CED
11	b	1201	CLA	O1D-CGD-O2D-CED
11	b	1211	CLA	O1D-CGD-O2D-CED
11	1	1107	CLA	O1D-CGD-O2D-CED
11	1	1116	CLA	O1D-CGD-O2D-CED
11	1	1128	CLA	O1D-CGD-O2D-CED
11	A	1132	CLA	CBD-CGD-O2D-CED
11	b	1209	CLA	CBD-CGD-O2D-CED
11	b	1228	CLA	CBD-CGD-O2D-CED
11	2	1212	CLA	CBD-CGD-O2D-CED
11	A	1124	CLA	O1A-CGA-O2A-C1
11	a	1125	CLA	O1A-CGA-O2A-C1
11	2	1203	CLA	O1A-CGA-O2A-C1
11	2	1213	CLA	C4C-C3C-CAC-CBC
11	2	1213	CLA	C2C-C3C-CAC-CBC
15	2	5004	LHG	O9-C7-O7-C5
11	A	1022	CLA	O1D-CGD-O2D-CED
11	B	1228	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1224	CLA	O1D-CGD-O2D-CED
11	b	1238	CLA	O1D-CGD-O2D-CED
11	2	1216	CLA	O1D-CGD-O2D-CED
11	A	1121	CLA	CBA-CGA-O2A-C1
11	a	1115	CLA	CBA-CGA-O2A-C1
11	a	1130	CLA	CBA-CGA-O2A-C1
11	a	1121	CLA	CBA-CGA-O2A-C1
11	a	1134	CLA	CBA-CGA-O2A-C1
11	b	1211	CLA	CBA-CGA-O2A-C1
11	1	1120	CLA	CBA-CGA-O2A-C1
11	A	1134	CLA	O1A-CGA-O2A-C1
11	L	1502	CLA	O1A-CGA-O2A-C1
11	a	1134	CLA	O1A-CGA-O2A-C1
11	b	1211	CLA	O1A-CGA-O2A-C1
11	1	1115	CLA	O1A-CGA-O2A-C1
11	1	1120	CLA	O1A-CGA-O2A-C1
11	1	1134	CLA	O1A-CGA-O2A-C1
11	A	1022	CLA	C3-C5-C6-C7
11	A	1119	CLA	C3-C5-C6-C7
11	B	1216	CLA	C3-C5-C6-C7
11	B	1223	CLA	C3-C5-C6-C7
11	B	1235	CLA	C3-C5-C6-C7
11	B	1206	CLA	C3-C5-C6-C7
11	L	1501	CLA	C3-C5-C6-C7
11	L	1503	CLA	C3-C5-C6-C7
11	a	1237	CLA	C3-C5-C6-C7
11	a	1110	CLA	C3-C5-C6-C7
11	a	1117	CLA	C3-C5-C6-C7
11	a	1119	CLA	C3-C5-C6-C7
11	a	1131	CLA	C3-C5-C6-C7
11	a	1140	CLA	C3-C5-C6-C7
11	a	1011	CLA	C3-C5-C6-C7
11	b	1207	CLA	C3-C5-C6-C7
11	b	1210	CLA	C3-C5-C6-C7
11	b	1223	CLA	C3-C5-C6-C7
11	l	1503	CLA	C3-C5-C6-C7
11	1	1022	CLA	C3-C5-C6-C7
11	1	1117	CLA	C3-C5-C6-C7
11	2	1202	CLA	C3-C5-C6-C7
11	2	1215	CLA	C3-C5-C6-C7
11	2	1234	CLA	C3-C5-C6-C7
12	B	2002	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	B	1227	CLA	C4C-C3C-CAC-CBC
11	a	1105	CLA	O1D-CGD-O2D-CED
11	a	1116	CLA	O1D-CGD-O2D-CED
11	2	1239	CLA	O1D-CGD-O2D-CED
11	A	1118	CLA	CBA-CGA-O2A-C1
11	B	1021	CLA	CBA-CGA-O2A-C1
11	B	1226	CLA	CBA-CGA-O2A-C1
11	L	1501	CLA	CBA-CGA-O2A-C1
11	L	1503	CLA	CBA-CGA-O2A-C1
11	a	1237	CLA	CBA-CGA-O2A-C1
11	a	1102	CLA	CBA-CGA-O2A-C1
11	a	1119	CLA	CBA-CGA-O2A-C1
11	a	1122	CLA	CBA-CGA-O2A-C1
11	b	1013	CLA	CBA-CGA-O2A-C1
11	b	1021	CLA	CBA-CGA-O2A-C1
11	b	1223	CLA	CBA-CGA-O2A-C1
11	l	1501	CLA	CBA-CGA-O2A-C1
11	l	1503	CLA	CBA-CGA-O2A-C1
11	1	1104	CLA	CBA-CGA-O2A-C1
11	1	1109	CLA	CBA-CGA-O2A-C1
11	1	1110	CLA	CBA-CGA-O2A-C1
11	1	1122	CLA	CBA-CGA-O2A-C1
11	1	1140	CLA	CBA-CGA-O2A-C1
11	2	1021	CLA	CBA-CGA-O2A-C1
11	2	1216	CLA	CBA-CGA-O2A-C1
11	2	1226	CLA	CBA-CGA-O2A-C1
11	K	1401	CLA	CBA-CGA-O2A-C1
11	k	1401	CLA	CBA-CGA-O2A-C1
11	0	1401	CLA	CBA-CGA-O2A-C1
11	0	1402	CLA	CBA-CGA-O2A-C1
11	A	1106	CLA	CBD-CGD-O2D-CED
11	A	1140	CLA	CBD-CGD-O2D-CED
11	A	1136	CLA	CBD-CGD-O2D-CED
11	B	1201	CLA	CBD-CGD-O2D-CED
11	B	1209	CLA	CBD-CGD-O2D-CED
11	B	1213	CLA	CBD-CGD-O2D-CED
11	B	1218	CLA	CBD-CGD-O2D-CED
11	B	1226	CLA	CBD-CGD-O2D-CED
11	B	1234	CLA	CBD-CGD-O2D-CED
11	a	1103	CLA	CBD-CGD-O2D-CED
11	a	1132	CLA	CBD-CGD-O2D-CED
11	a	1135	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1202	CLA	CBD-CGD-O2D-CED
11	b	1208	CLA	CBD-CGD-O2D-CED
11	1	1801	CLA	CBD-CGD-O2D-CED
11	1	1112	CLA	CBD-CGD-O2D-CED
11	1	1120	CLA	CBD-CGD-O2D-CED
11	2	1203	CLA	CBD-CGD-O2D-CED
11	2	1215	CLA	CBD-CGD-O2D-CED
11	2	1217	CLA	CBD-CGD-O2D-CED
11	A	1102	CLA	O1D-CGD-O2D-CED
11	A	1117	CLA	O1D-CGD-O2D-CED
11	A	1126	CLA	O1D-CGD-O2D-CED
11	B	1236	CLA	O1D-CGD-O2D-CED
11	b	1212	CLA	O1D-CGD-O2D-CED
11	b	1235	CLA	O1D-CGD-O2D-CED
11	1	1237	CLA	O1D-CGD-O2D-CED
11	1	1117	CLA	O1D-CGD-O2D-CED
11	1	1126	CLA	O1D-CGD-O2D-CED
11	1	1137	CLA	O1D-CGD-O2D-CED
11	1	1138	CLA	O1D-CGD-O2D-CED
11	2	1224	CLA	O1D-CGD-O2D-CED
11	a	1104	CLA	O1A-CGA-O2A-C1
11	1	1125	CLA	O1A-CGA-O2A-C1
11	8	1503	CLA	O1A-CGA-O2A-C1
11	B	1239	CLA	O1A-CGA-O2A-C1
11	a	1129	CLA	O1A-CGA-O2A-C1
11	a	1136	CLA	O1A-CGA-O2A-C1
11	B	1236	CLA	C2-C1-O2A-CGA
11	2	1222	CLA	O1D-CGD-O2D-CED
11	A	1109	CLA	C4-C3-C5-C6
11	A	1122	CLA	C4-C3-C5-C6
11	A	1126	CLA	C4-C3-C5-C6
11	B	1222	CLA	C4-C3-C5-C6
11	B	1230	CLA	C4-C3-C5-C6
11	a	1107	CLA	C4-C3-C5-C6
11	a	1109	CLA	C4-C3-C5-C6
11	b	1213	CLA	C4-C3-C5-C6
11	b	1230	CLA	C4-C3-C5-C6
11	l	1501	CLA	C4-C3-C5-C6
11	1	1126	CLA	C4-C3-C5-C6
11	2	1213	CLA	C4-C3-C5-C6
11	2	1215	CLA	C4-C3-C5-C6
11	A	1109	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	A	1122	CLA	C2-C3-C5-C6
11	A	1126	CLA	C2-C3-C5-C6
11	A	1012	CLA	C2-C3-C5-C6
11	B	1214	CLA	C2-C3-C5-C6
11	B	1222	CLA	C2-C3-C5-C6
11	a	1107	CLA	C2-C3-C5-C6
11	a	1109	CLA	C2-C3-C5-C6
11	a	1012	CLA	C2-C3-C5-C6
11	1	1106	CLA	C2-C3-C5-C6
11	1	1109	CLA	C2-C3-C5-C6
11	1	1126	CLA	C2-C3-C5-C6
11	2	1213	CLA	C2-C3-C5-C6
11	A	1134	CLA	CBA-CGA-O2A-C1
11	a	1120	CLA	CBA-CGA-O2A-C1
11	1	1134	CLA	CBA-CGA-O2A-C1
11	a	1122	CLA	CBD-CGD-O2D-CED
11	b	1230	CLA	CBD-CGD-O2D-CED
11	B	1239	CLA	O1D-CGD-O2D-CED
11	a	1127	CLA	O1D-CGD-O2D-CED
11	b	1207	CLA	O1D-CGD-O2D-CED
11	1	1114	CLA	O1D-CGD-O2D-CED
11	1	1105	CLA	C2A-CAA-CBA-CGA
11	2	1232	CLA	C2A-CAA-CBA-CGA
11	A	1101	CLA	O1A-CGA-O2A-C1
11	a	1118	CLA	O1A-CGA-O2A-C1
11	A	1106	CLA	C3-C5-C6-C7
11	A	1011	CLA	C3-C5-C6-C7
11	B	1222	CLA	C3-C5-C6-C7
11	B	1238	CLA	C3-C5-C6-C7
11	b	1206	CLA	C3-C5-C6-C7
11	1	1237	CLA	C3-C5-C6-C7
11	1	1118	CLA	C3-C5-C6-C7
11	2	1210	CLA	C3-C5-C6-C7
11	A	1801	CLA	CBA-CGA-O2A-C1
11	A	1237	CLA	CBA-CGA-O2A-C1
11	A	1104	CLA	CBA-CGA-O2A-C1
11	A	1107	CLA	CBA-CGA-O2A-C1
11	A	1124	CLA	CBA-CGA-O2A-C1
11	B	1219	CLA	CBA-CGA-O2A-C1
11	B	1228	CLA	CBA-CGA-O2A-C1
11	B	1229	CLA	CBA-CGA-O2A-C1
11	a	1101	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	a	1105	CLA	CBA-CGA-O2A-C1
11	a	1123	CLA	CBA-CGA-O2A-C1
11	a	1125	CLA	CBA-CGA-O2A-C1
11	a	1140	CLA	CBA-CGA-O2A-C1
11	b	1023	CLA	CBA-CGA-O2A-C1
11	b	1219	CLA	CBA-CGA-O2A-C1
11	b	1226	CLA	CBA-CGA-O2A-C1
11	b	1228	CLA	CBA-CGA-O2A-C1
11	b	1234	CLA	CBA-CGA-O2A-C1
11	1	1101	CLA	CBA-CGA-O2A-C1
11	1	1103	CLA	CBA-CGA-O2A-C1
11	1	1111	CLA	CBA-CGA-O2A-C1
11	1	1119	CLA	CBA-CGA-O2A-C1
11	1	1123	CLA	CBA-CGA-O2A-C1
11	1	1124	CLA	CBA-CGA-O2A-C1
11	2	1023	CLA	CBA-CGA-O2A-C1
11	2	1213	CLA	CBA-CGA-O2A-C1
11	2	1228	CLA	CBA-CGA-O2A-C1
11	k	1402	CLA	CBA-CGA-O2A-C1
11	2	1230	CLA	CBD-CGD-O2D-CED
14	A	4002	BCR	C15-C16-C17-C18
14	A	4007	BCR	C19-C20-C21-C22
14	L	4019	BCR	C15-C16-C17-C18
14	a	4002	BCR	C15-C16-C17-C18
14	a	4007	BCR	C19-C20-C21-C22
14	b	4004	BCR	C9-C10-C11-C12
14	f	4013	BCR	C9-C10-C11-C12
14	2	4009	BCR	C13-C14-C15-C16
14	8	4019	BCR	C13-C14-C15-C16
11	B	1226	CLA	O1A-CGA-O2A-C1
11	a	1119	CLA	O1A-CGA-O2A-C1
11	a	1127	CLA	O1A-CGA-O2A-C1
11	b	1219	CLA	O1A-CGA-O2A-C1
11	1	1101	CLA	O1A-CGA-O2A-C1
11	2	1213	CLA	O1A-CGA-O2A-C1
11	2	1216	CLA	O1A-CGA-O2A-C1
11	a	1801	CLA	C2C-C3C-CAC-CBC
11	b	1220	CLA	C2C-C3C-CAC-CBC
11	A	1103	CLA	O1D-CGD-O2D-CED
11	A	1011	CLA	C5-C6-C7-C8
11	1	1115	CLA	CBA-CGA-O2A-C1
11	a	1120	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	1	1129	CLA	O1A-CGA-O2A-C1
11	B	1224	CLA	O1D-CGD-O2D-CED
11	1	1135	CLA	O1D-CGD-O2D-CED
11	2	1234	CLA	O1D-CGD-O2D-CED
11	A	1107	CLA	C3-C5-C6-C7
11	A	1110	CLA	C3-C5-C6-C7
11	B	1202	CLA	C3-C5-C6-C7
11	b	1216	CLA	C3-C5-C6-C7
11	b	1235	CLA	C3-C5-C6-C7
11	l	1501	CLA	C3-C5-C6-C7
11	1	1107	CLA	C3-C5-C6-C7
11	1	1124	CLA	C3-C5-C6-C7
11	2	1203	CLA	C3-C5-C6-C7
11	2	1225	CLA	C3-C5-C6-C7
11	2	1238	CLA	C3-C5-C6-C7
11	8	1503	CLA	C3-C5-C6-C7
11	A	1237	CLA	CBD-CGD-O2D-CED
11	A	1115	CLA	CBD-CGD-O2D-CED
11	A	1125	CLA	CBD-CGD-O2D-CED
11	B	1230	CLA	CBD-CGD-O2D-CED
11	a	1112	CLA	CBD-CGD-O2D-CED
11	a	1136	CLA	CBD-CGD-O2D-CED
11	b	1227	CLA	CBD-CGD-O2D-CED
11	1	1115	CLA	CBD-CGD-O2D-CED
11	2	1220	CLA	CBD-CGD-O2D-CED
11	2	1227	CLA	CBD-CGD-O2D-CED
15	A	5001	LHG	O2-C2-C3-O3
15	A	5003	LHG	O2-C2-C3-O3
15	a	5003	LHG	O2-C2-C3-O3
15	1	5001	LHG	O2-C2-C3-O3
11	B	1212	CLA	O1D-CGD-O2D-CED
11	B	1222	CLA	O1D-CGD-O2D-CED
11	a	1101	CLA	O1D-CGD-O2D-CED
11	b	1218	CLA	O1D-CGD-O2D-CED
11	b	1239	CLA	O1D-CGD-O2D-CED
11	1	1130	CLA	O1D-CGD-O2D-CED
11	1	1136	CLA	O1D-CGD-O2D-CED
11	A	1101	CLA	CBA-CGA-O2A-C1
11	A	1105	CLA	CBA-CGA-O2A-C1
11	A	1111	CLA	CBA-CGA-O2A-C1
11	A	1127	CLA	CBA-CGA-O2A-C1
11	B	1202	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	a	1104	CLA	CBA-CGA-O2A-C1
11	a	1118	CLA	CBA-CGA-O2A-C1
11	a	1124	CLA	CBA-CGA-O2A-C1
11	a	1131	CLA	CBA-CGA-O2A-C1
11	1	1137	CLA	CBA-CGA-O2A-C1
11	2	1203	CLA	CBA-CGA-O2A-C1
11	8	1503	CLA	CBA-CGA-O2A-C1
11	K	1402	CLA	CBA-CGA-O2A-C1
11	A	1104	CLA	O1A-CGA-O2A-C1
11	A	1140	CLA	O1A-CGA-O2A-C1
11	a	1105	CLA	O1A-CGA-O2A-C1
11	a	1109	CLA	O1A-CGA-O2A-C1
11	a	1135	CLA	O1A-CGA-O2A-C1
11	b	1226	CLA	O1A-CGA-O2A-C1
11	1	1123	CLA	O1A-CGA-O2A-C1
11	0	1402	CLA	O1A-CGA-O2A-C1
11	a	1106	CLA	O1D-CGD-O2D-CED
11	l	1501	CLA	O1D-CGD-O2D-CED
11	B	1203	CLA	CBD-CGD-O2D-CED
11	B	1211	CLA	CBD-CGD-O2D-CED
11	2	1204	CLA	CBD-CGD-O2D-CED
16	B	5002	LMG	C11-C10-O7-C8
11	1	1136	CLA	CBA-CGA-O2A-C1
11	a	1130	CLA	O1D-CGD-O2D-CED
11	b	1206	CLA	O1D-CGD-O2D-CED
11	2	1225	CLA	O1D-CGD-O2D-CED
11	B	1021	CLA	O1A-CGA-O2A-C1
11	k	1402	CLA	O1A-CGA-O2A-C1
11	b	1223	CLA	C2C-C3C-CAC-CBC
11	2	1013	CLA	O1D-CGD-O2D-CED
11	b	1224	CLA	C3-C5-C6-C7
11	2	1206	CLA	C3-C5-C6-C7
12	2	2002	PQN	C13-C15-C16-C17
11	A	1133	CLA	CBD-CGD-O2D-CED
11	B	1220	CLA	CBD-CGD-O2D-CED
11	B	1227	CLA	CBD-CGD-O2D-CED
11	B	1206	CLA	CBD-CGD-O2D-CED
11	b	1215	CLA	CBD-CGD-O2D-CED
11	1	1118	CLA	CBD-CGD-O2D-CED
11	2	1207	CLA	CBD-CGD-O2D-CED
11	A	1112	CLA	O1D-CGD-O2D-CED
11	A	1123	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1234	CLA	O1D-CGD-O2D-CED
11	l	1503	CLA	O1D-CGD-O2D-CED
11	2	1218	CLA	O1D-CGD-O2D-CED
11	2	1223	CLA	O1D-CGD-O2D-CED
11	2	1238	CLA	O1D-CGD-O2D-CED
11	A	1109	CLA	CBA-CGA-O2A-C1
11	A	1140	CLA	CBA-CGA-O2A-C1
11	a	1109	CLA	CBA-CGA-O2A-C1
11	a	1127	CLA	CBA-CGA-O2A-C1
11	a	1135	CLA	CBA-CGA-O2A-C1
11	1	1125	CLA	CBA-CGA-O2A-C1
11	B	1215	CLA	C4-C3-C5-C6
11	a	1126	CLA	C4-C3-C5-C6
11	b	1215	CLA	C4-C3-C5-C6
11	b	1221	CLA	C4-C3-C5-C6
11	B	1215	CLA	C2-C3-C5-C6
11	a	1126	CLA	C2-C3-C5-C6
11	b	1215	CLA	C2-C3-C5-C6
11	b	1221	CLA	C2-C3-C5-C6
11	l	1501	CLA	C2-C3-C5-C6
11	1	1012	CLA	C2-C3-C5-C6
11	2	1215	CLA	C2-C3-C5-C6
11	2	1230	CLA	C2-C3-C5-C6
11	A	1107	CLA	O1A-CGA-O2A-C1
11	A	1111	CLA	O1A-CGA-O2A-C1
11	A	1127	CLA	O1A-CGA-O2A-C1
11	B	1202	CLA	O1A-CGA-O2A-C1
11	B	1219	CLA	O1A-CGA-O2A-C1
11	B	1229	CLA	O1A-CGA-O2A-C1
11	a	1101	CLA	O1A-CGA-O2A-C1
11	b	1234	CLA	O1A-CGA-O2A-C1
11	1	1103	CLA	O1A-CGA-O2A-C1
11	1	1124	CLA	O1A-CGA-O2A-C1
11	1	1137	CLA	O1A-CGA-O2A-C1
16	2	5002	LMG	O6-C5-C6-O5
11	b	1205	CLA	O1D-CGD-O2D-CED
11	l	1502	CLA	CBA-CGA-O2A-C1
11	B	1205	CLA	CBD-CGD-O2D-CED
11	b	1236	CLA	CBD-CGD-O2D-CED
11	A	1135	CLA	C2A-CAA-CBA-CGA
11	B	1222	CLA	C2A-CAA-CBA-CGA
11	b	1232	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	1	1132	CLA	C2A-CAA-CBA-CGA
11	2	1222	CLA	C2A-CAA-CBA-CGA
11	b	1217	CLA	C2-C1-O2A-CGA
11	B	1238	CLA	O1D-CGD-O2D-CED
11	1	1101	CLA	O1D-CGD-O2D-CED
11	a	1124	CLA	O1A-CGA-O2A-C1
11	a	1131	CLA	O1A-CGA-O2A-C1
11	1	1119	CLA	O1A-CGA-O2A-C1
11	A	1119	CLA	C2C-C3C-CAC-CBC
11	b	1227	CLA	C2C-C3C-CAC-CBC
11	A	1118	CLA	O1D-CGD-O2D-CED
11	b	1225	CLA	O1D-CGD-O2D-CED
11	b	1202	CLA	CBA-CGA-O2A-C1
11	1	1139	CLA	CBA-CGA-O2A-C1
11	1	1011	CLA	CBA-CGA-O2A-C1
11	2	1205	CLA	CBA-CGA-O2A-C1
11	2	1222	CLA	CBA-CGA-O2A-C1
16	b	5002	LMG	C29-C28-O8-C9
11	A	1124	CLA	CBD-CGD-O2D-CED
11	A	1135	CLA	CBD-CGD-O2D-CED
11	B	1235	CLA	CBD-CGD-O2D-CED
11	a	1237	CLA	CBD-CGD-O2D-CED
11	b	1203	CLA	CBD-CGD-O2D-CED
11	1	1106	CLA	CBD-CGD-O2D-CED
11	1	1129	CLA	CBD-CGD-O2D-CED
11	2	1235	CLA	CBD-CGD-O2D-CED
11	a	1801	CLA	C4C-C3C-CAC-CBC
11	A	1105	CLA	O1A-CGA-O2A-C1
11	1	1011	CLA	O1A-CGA-O2A-C1
11	2	1205	CLA	O1A-CGA-O2A-C1
11	K	1402	CLA	O1A-CGA-O2A-C1
16	b	5002	LMG	O6-C5-C6-O5
11	a	1133	CLA	CBD-CGD-O2D-CED
11	1	1105	CLA	CBD-CGD-O2D-CED
15	b	5004	LHG	C8-C7-O7-C5
11	b	1209	CLA	O1D-CGD-O2D-CED
11	b	1228	CLA	O1D-CGD-O2D-CED
14	B	4004	BCR	C9-C10-C11-C12
11	A	1109	CLA	O1A-CGA-O2A-C1
11	a	1111	CLA	O1A-CGA-O2A-C1
11	1	1139	CLA	O1A-CGA-O2A-C1
16	b	5002	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
16	B	5002	LMG	O9-C10-O7-C8
15	B	5004	LHG	C1-C2-C3-O3
15	1	5001	LHG	C1-C2-C3-O3
11	2	1212	CLA	O1D-CGD-O2D-CED
11	A	1022	CLA	CBA-CGA-O2A-C1
11	A	1123	CLA	CBA-CGA-O2A-C1
11	A	1131	CLA	CBA-CGA-O2A-C1
11	A	1011	CLA	CBA-CGA-O2A-C1
11	B	1023	CLA	CBA-CGA-O2A-C1
11	B	1207	CLA	CBA-CGA-O2A-C1
11	B	1213	CLA	CBA-CGA-O2A-C1
11	B	1222	CLA	CBA-CGA-O2A-C1
11	B	1234	CLA	CBA-CGA-O2A-C1
11	B	1236	CLA	CBA-CGA-O2A-C1
11	B	1238	CLA	CBA-CGA-O2A-C1
11	a	1111	CLA	CBA-CGA-O2A-C1
11	a	1128	CLA	CBA-CGA-O2A-C1
11	a	1137	CLA	CBA-CGA-O2A-C1
11	a	1011	CLA	CBA-CGA-O2A-C1
11	b	1203	CLA	CBA-CGA-O2A-C1
11	b	1207	CLA	CBA-CGA-O2A-C1
11	b	1217	CLA	CBA-CGA-O2A-C1
11	b	1222	CLA	CBA-CGA-O2A-C1
11	b	1230	CLA	CBA-CGA-O2A-C1
11	1	1128	CLA	CBA-CGA-O2A-C1
11	1	1131	CLA	CBA-CGA-O2A-C1
11	2	1202	CLA	CBA-CGA-O2A-C1
11	2	1206	CLA	CBA-CGA-O2A-C1
11	2	1236	CLA	CBA-CGA-O2A-C1
16	2	5002	LMG	C29-C28-O8-C9
11	B	1214	CLA	CBD-CGD-O2D-CED
11	A	1115	CLA	C2C-C3C-CAC-CBC
11	b	1210	CLA	C2C-C3C-CAC-CBC
11	A	1132	CLA	O1D-CGD-O2D-CED
11	B	1218	CLA	O1D-CGD-O2D-CED
11	a	1103	CLA	O1D-CGD-O2D-CED
11	b	1202	CLA	O1D-CGD-O2D-CED
11	2	1203	CLA	O1D-CGD-O2D-CED
11	b	1217	CLA	O1A-CGA-O2A-C1
11	B	1021	CLA	C4-C3-C5-C6
11	b	1222	CLA	C4-C3-C5-C6
11	1	1107	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	1	1012	CLA	C4-C3-C5-C6
11	B	1021	CLA	C2-C3-C5-C6
11	b	1213	CLA	C2-C3-C5-C6
11	b	1222	CLA	C2-C3-C5-C6
11	b	1230	CLA	C2-C3-C5-C6
11	2	1201	CLA	C3-C5-C6-C7
12	b	2002	PQN	C13-C15-C16-C17
11	b	1231	CLA	CBD-CGD-O2D-CED
11	2	1226	CLA	CBD-CGD-O2D-CED
11	A	1022	CLA	C6-C7-C8-C9
11	A	1126	CLA	C6-C7-C8-C9
11	A	1126	CLA	C11-C10-C8-C9
11	A	1127	CLA	C11-C10-C8-C9
11	A	1137	CLA	C6-C7-C8-C9
11	A	1137	CLA	C11-C10-C8-C9
11	A	1140	CLA	C6-C7-C8-C9
11	A	1011	CLA	C11-C10-C8-C9
11	A	1012	CLA	C11-C10-C8-C9
11	A	1132	CLA	C11-C10-C8-C9
11	B	1023	CLA	C11-C12-C13-C14
11	B	1202	CLA	C6-C7-C8-C9
11	B	1204	CLA	C11-C12-C13-C14
11	B	1213	CLA	C6-C7-C8-C9
11	B	1213	CLA	C11-C10-C8-C9
11	B	1226	CLA	C6-C7-C8-C9
11	L	1501	CLA	C6-C7-C8-C9
11	a	1022	CLA	C6-C7-C8-C9
11	a	1102	CLA	C6-C7-C8-C9
11	a	1109	CLA	C11-C12-C13-C14
11	a	1117	CLA	C6-C7-C8-C9
11	a	1128	CLA	C6-C7-C8-C9
11	a	1140	CLA	C6-C7-C8-C9
11	a	1012	CLA	C11-C10-C8-C9
11	a	1132	CLA	C11-C10-C8-C9
11	b	1023	CLA	C11-C12-C13-C14
11	b	1214	CLA	C11-C10-C8-C9
11	b	1216	CLA	C11-C10-C8-C9
11	b	1226	CLA	C6-C7-C8-C9
11	b	1226	CLA	C11-C12-C13-C14
11	b	1234	CLA	C11-C10-C8-C9
11	b	1235	CLA	C6-C7-C8-C9
11	l	1501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	1	1022	CLA	C6-C7-C8-C9
11	1	1022	CLA	C14-C13-C15-C16
11	1	1102	CLA	C6-C7-C8-C9
11	1	1103	CLA	C6-C7-C8-C9
11	1	1106	CLA	C11-C10-C8-C9
11	1	1109	CLA	C11-C12-C13-C14
11	1	1111	CLA	C6-C7-C8-C9
11	1	1122	CLA	C11-C10-C8-C9
11	1	1126	CLA	C11-C10-C8-C9
11	1	1127	CLA	C11-C10-C8-C9
11	1	1137	CLA	C6-C7-C8-C9
11	1	1137	CLA	C11-C10-C8-C9
11	1	1011	CLA	C11-C10-C8-C9
11	1	1012	CLA	C6-C7-C8-C9
11	1	1012	CLA	C11-C10-C8-C9
11	2	1013	CLA	C11-C10-C8-C9
11	2	1013	CLA	C11-C12-C13-C14
11	2	1023	CLA	C6-C7-C8-C9
11	2	1203	CLA	C6-C7-C8-C9
11	2	1210	CLA	C11-C12-C13-C14
11	2	1214	CLA	C11-C10-C8-C9
11	2	1216	CLA	C11-C10-C8-C9
11	2	1226	CLA	C6-C7-C8-C9
11	K	1401	CLA	C11-C12-C13-C14
11	k	1401	CLA	C11-C12-C13-C14
11	0	1401	CLA	C11-C12-C13-C14
12	B	2002	PQN	C24-C23-C25-C26
12	b	2002	PQN	C24-C23-C25-C26
12	2	2002	PQN	C24-C23-C25-C26
11	A	1106	CLA	O1D-CGD-O2D-CED
11	A	1136	CLA	O1D-CGD-O2D-CED
11	2	1217	CLA	O1D-CGD-O2D-CED
15	1	5003	LHG	O2-C2-C3-O3
11	A	1140	CLA	O1D-CGD-O2D-CED
11	b	1208	CLA	O1D-CGD-O2D-CED
11	A	1123	CLA	O1A-CGA-O2A-C1
11	B	1023	CLA	O1A-CGA-O2A-C1
11	B	1207	CLA	O1A-CGA-O2A-C1
11	B	1234	CLA	O1A-CGA-O2A-C1
11	a	1128	CLA	O1A-CGA-O2A-C1
11	2	1202	CLA	O1A-CGA-O2A-C1
16	2	5002	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
16	2	5002	LMG	C4-C5-C6-O5
11	B	1234	CLA	O1D-CGD-O2D-CED
11	1	1801	CLA	O1D-CGD-O2D-CED
14	A	4001	BCR	C7-C8-C9-C34
14	A	4001	BCR	C37-C22-C23-C24
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C37-C22-C23-C24
14	A	4003	BCR	C7-C8-C9-C34
14	A	4003	BCR	C37-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C34
14	B	4005	BCR	C7-C8-C9-C34
14	B	4006	BCR	C7-C8-C9-C34
14	B	4006	BCR	C37-C22-C23-C24
14	B	4009	BCR	C7-C8-C9-C34
14	B	4009	BCR	C11-C12-C13-C35
14	B	4009	BCR	C37-C22-C23-C24
14	B	4010	BCR	C36-C18-C19-C20
14	B	4011	BCR	C7-C8-C9-C34
14	B	4011	BCR	C37-C22-C23-C24
14	F	4018	BCR	C7-C8-C9-C34
14	F	4020	BCR	C37-C22-C23-C24
14	F	4013	BCR	C7-C8-C9-C34
14	L	4019	BCR	C37-C22-C23-C24
14	L	4022	BCR	C11-C12-C13-C35
14	L	4022	BCR	C36-C18-C19-C20
14	L	4022	BCR	C37-C22-C23-C24
14	M	4021	BCR	C7-C8-C9-C34
14	a	4001	BCR	C7-C8-C9-C34
14	a	4002	BCR	C11-C12-C13-C35
14	a	4002	BCR	C36-C18-C19-C20
14	a	4002	BCR	C37-C22-C23-C24
14	a	4003	BCR	C7-C8-C9-C34
14	a	4003	BCR	C11-C12-C13-C35
14	a	4007	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	C11-C12-C13-C35
14	b	4005	BCR	C37-C22-C23-C24
14	b	4006	BCR	C7-C8-C9-C34
14	b	4006	BCR	C11-C12-C13-C35
14	b	4006	BCR	C37-C22-C23-C24
14	b	4010	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
14	b	4011	BCR	C36-C18-C19-C20
14	b	4014	BCR	C7-C8-C9-C34
14	b	4014	BCR	C36-C18-C19-C20
14	b	4014	BCR	C37-C22-C23-C24
14	f	4018	BCR	C7-C8-C9-C34
14	f	4013	BCR	C37-C22-C23-C24
14	l	4019	BCR	C7-C8-C9-C34
14	l	4022	BCR	C36-C18-C19-C20
14	m	4021	BCR	C37-C22-C23-C24
14	1	4002	BCR	C36-C18-C19-C20
14	1	4002	BCR	C37-C22-C23-C24
14	1	4007	BCR	C37-C22-C23-C24
14	2	4005	BCR	C37-C22-C23-C24
14	2	4006	BCR	C7-C8-C9-C34
14	2	4006	BCR	C37-C22-C23-C24
14	2	4009	BCR	C11-C12-C13-C35
14	2	4011	BCR	C7-C8-C9-C34
14	2	4011	BCR	C37-C22-C23-C24
14	2	4014	BCR	C11-C12-C13-C35
14	2	4014	BCR	C36-C18-C19-C20
14	6	4018	BCR	C7-C8-C9-C34
14	6	4020	BCR	C11-C12-C13-C35
14	8	4019	BCR	C11-C12-C13-C35
14	8	4022	BCR	C36-C18-C19-C20
14	7	4021	BCR	C7-C8-C9-C34
14	A	4001	BCR	C21-C22-C23-C24
14	A	4002	BCR	C21-C22-C23-C24
14	A	4003	BCR	C21-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C10
14	B	4005	BCR	C7-C8-C9-C10
14	B	4006	BCR	C7-C8-C9-C10
14	B	4009	BCR	C7-C8-C9-C10
14	B	4011	BCR	C7-C8-C9-C10
14	B	4011	BCR	C21-C22-C23-C24
14	F	4018	BCR	C7-C8-C9-C10
14	F	4013	BCR	C7-C8-C9-C10
14	F	4013	BCR	C11-C12-C13-C14
14	L	4019	BCR	C7-C8-C9-C10
14	L	4019	BCR	C21-C22-C23-C24
14	M	4021	BCR	C7-C8-C9-C10
14	a	4001	BCR	C7-C8-C9-C10
14	a	4003	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	a	4003	BCR	C11-C12-C13-C14
14	a	4007	BCR	C21-C22-C23-C24
14	b	4004	BCR	C7-C8-C9-C10
14	b	4006	BCR	C7-C8-C9-C10
14	b	4010	BCR	C7-C8-C9-C10
14	b	4011	BCR	C21-C22-C23-C24
14	b	4014	BCR	C7-C8-C9-C10
14	b	4014	BCR	C11-C12-C13-C14
14	b	4014	BCR	C17-C18-C19-C20
14	b	4014	BCR	C21-C22-C23-C24
14	f	4020	BCR	C7-C8-C9-C10
14	f	4020	BCR	C21-C22-C23-C24
14	f	4013	BCR	C7-C8-C9-C10
14	f	4013	BCR	C11-C12-C13-C14
14	l	4019	BCR	C7-C8-C9-C10
14	m	4021	BCR	C21-C22-C23-C24
14	1	4001	BCR	C21-C22-C23-C24
14	1	4002	BCR	C21-C22-C23-C24
14	1	4007	BCR	C21-C22-C23-C24
14	1	4008	BCR	C7-C8-C9-C10
14	2	4006	BCR	C21-C22-C23-C24
14	2	4011	BCR	C7-C8-C9-C10
14	2	4014	BCR	C11-C12-C13-C14
14	6	4018	BCR	C7-C8-C9-C10
14	6	4020	BCR	C11-C12-C13-C14
14	8	4019	BCR	C21-C22-C23-C24
11	A	1113	CLA	C2A-CAA-CBA-CGA
11	b	1021	CLA	C2A-CAA-CBA-CGA
11	b	1214	CLA	C2A-CAA-CBA-CGA
15	B	5004	LHG	C23-C24-C25-C26
11	B	1226	CLA	O1D-CGD-O2D-CED
11	1	1136	CLA	O1A-CGA-O2A-C1
11	A	1131	CLA	O1A-CGA-O2A-C1
11	b	1203	CLA	O1A-CGA-O2A-C1
11	1	1131	CLA	O1A-CGA-O2A-C1
11	2	1236	CLA	O1A-CGA-O2A-C1
11	B	1203	CLA	C3-C5-C6-C7
11	a	1103	CLA	C8-C10-C11-C12
11	2	1203	CLA	C10-C11-C12-C13
16	b	5002	LMG	C4-C5-C6-O5
11	a	1138	CLA	CBA-CGA-O2A-C1
15	B	5004	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
11	2	1238	CLA	CBA-CGA-O2A-C1
16	B	5002	LMG	C29-C28-O8-C9
11	1	1126	CLA	C8-C10-C11-C12
11	A	1104	CLA	C2-C1-O2A-CGA
11	A	1139	CLA	C2-C1-O2A-CGA
11	a	1022	CLA	C2-C1-O2A-CGA
11	a	1104	CLA	C2-C1-O2A-CGA
11	b	1013	CLA	C2-C1-O2A-CGA
11	b	1023	CLA	C2-C1-O2A-CGA
11	b	1203	CLA	C2-C1-O2A-CGA
11	b	1235	CLA	C2-C1-O2A-CGA
11	1	1022	CLA	C2-C1-O2A-CGA
11	1	1103	CLA	C2-C1-O2A-CGA
11	1	1122	CLA	C2-C1-O2A-CGA
11	1	1124	CLA	C2-C1-O2A-CGA
11	2	1214	CLA	C2-C1-O2A-CGA
11	2	1223	CLA	C2-C1-O2A-CGA
11	2	1230	CLA	C2-C1-O2A-CGA
11	B	1209	CLA	O1D-CGD-O2D-CED
11	a	1132	CLA	O1D-CGD-O2D-CED
11	1	1120	CLA	O1D-CGD-O2D-CED
11	B	1220	CLA	C2C-C3C-CAC-CBC
11	A	1109	CLA	C5-C6-C7-C8
11	A	1140	CLA	C8-C10-C11-C12
11	B	1021	CLA	C13-C15-C16-C17
11	a	1132	CLA	C5-C6-C7-C8
11	1	1102	CLA	C13-C15-C16-C17
11	1	1132	CLA	C10-C11-C12-C13
11	2	1223	CLA	C8-C10-C11-C12
11	A	1237	CLA	C3-C5-C6-C7
11	B	1201	CLA	O1D-CGD-O2D-CED
11	1	1112	CLA	O1D-CGD-O2D-CED
11	a	1137	CLA	O1A-CGA-O2A-C1
11	b	1207	CLA	O1A-CGA-O2A-C1
11	B	1204	CLA	C15-C16-C17-C18
11	1	1140	CLA	C8-C10-C11-C12
11	2	1023	CLA	C10-C11-C12-C13
11	2	1214	CLA	CBD-CGD-O2D-CED
11	A	1103	CLA	C11-C10-C8-C7
11	A	1107	CLA	C6-C7-C8-C10
11	A	1117	CLA	C11-C10-C8-C7
11	B	1013	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
11	B	1203	CLA	C11-C10-C8-C7
11	L	1503	CLA	C6-C7-C8-C10
11	a	1109	CLA	C6-C7-C8-C10
11	a	1127	CLA	C6-C7-C8-C10
11	b	1013	CLA	C6-C7-C8-C10
11	b	1225	CLA	C11-C10-C8-C7
11	l	1503	CLA	C6-C7-C8-C10
11	1	1131	CLA	C11-C12-C13-C15
11	2	1013	CLA	C6-C7-C8-C10
11	8	1503	CLA	C6-C7-C8-C10
12	a	2001	PQN	C21-C22-C23-C25
12	2	2002	PQN	C21-C22-C23-C25
11	a	1110	CLA	CBA-CGA-O2A-C1
11	1	1137	CLA	C4-C3-C5-C6
11	2	1230	CLA	C4-C3-C5-C6
11	1	1011	CLA	C5-C6-C7-C8
11	2	1215	CLA	O1D-CGD-O2D-CED
14	A	4008	BCR	C9-C10-C11-C12
14	B	4009	BCR	C15-C16-C17-C18
14	b	4014	BCR	C9-C10-C11-C12
14	b	4017	BCR	C9-C10-C11-C12
14	f	4020	BCR	C9-C10-C11-C12
14	8	4019	BCR	C15-C16-C17-C18
11	A	1012	CLA	C15-C16-C17-C18
11	b	1021	CLA	C13-C15-C16-C17
11	b	1214	CLA	C5-C6-C7-C8
12	B	2002	PQN	C20-C21-C22-C23
16	B	5002	LMG	O6-C5-C6-O5
15	A	5003	LHG	C7-C8-C9-C10
15	A	5003	LHG	C23-C24-C25-C26
15	b	5004	LHG	C23-C24-C25-C26
15	1	5003	LHG	C7-C8-C9-C10
15	2	5004	LHG	C23-C24-C25-C26
11	A	1022	CLA	O1A-CGA-O2A-C1
11	B	1222	CLA	O1A-CGA-O2A-C1
11	b	1230	CLA	O1A-CGA-O2A-C1
11	1	1128	CLA	O1A-CGA-O2A-C1
11	2	1222	CLA	O1A-CGA-O2A-C1
11	B	1203	CLA	C10-C11-C12-C13
11	B	1210	CLA	C8-C10-C11-C12
11	B	1226	CLA	C15-C16-C17-C18
11	a	1107	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	b	1013	CLA	C13-C15-C16-C17
11	1	1103	CLA	C8-C10-C11-C12
11	1	1118	CLA	C8-C10-C11-C12
11	1	1123	CLA	C13-C15-C16-C17
11	2	1206	CLA	C8-C10-C11-C12
12	1	2001	PQN	C20-C21-C22-C23
11	A	1107	CLA	C2A-CAA-CBA-CGA
11	A	1119	CLA	C2A-CAA-CBA-CGA
11	B	1232	CLA	C2A-CAA-CBA-CGA
11	B	1238	CLA	C2A-CAA-CBA-CGA
11	a	1110	CLA	C2A-CAA-CBA-CGA
11	a	1123	CLA	C2A-CAA-CBA-CGA
11	a	1140	CLA	C2A-CAA-CBA-CGA
11	a	1012	CLA	C2A-CAA-CBA-CGA
11	b	1209	CLA	C2A-CAA-CBA-CGA
11	b	1222	CLA	C2A-CAA-CBA-CGA
11	b	1223	CLA	C2A-CAA-CBA-CGA
11	b	1228	CLA	C2A-CAA-CBA-CGA
11	b	1240	CLA	C2A-CAA-CBA-CGA
11	b	1238	CLA	C2A-CAA-CBA-CGA
11	1	1101	CLA	C2A-CAA-CBA-CGA
11	2	1214	CLA	C2A-CAA-CBA-CGA
11	2	1225	CLA	C2A-CAA-CBA-CGA
11	2	1227	CLA	C2A-CAA-CBA-CGA
11	B	1224	CLA	C2C-C3C-CAC-CBC
14	B	4009	BCR	C10-C11-C12-C13
14	6	4013	BCR	C10-C11-C12-C13
11	A	1111	CLA	C5-C6-C7-C8
11	B	1021	CLA	C5-C6-C7-C8
11	B	1203	CLA	C15-C16-C17-C18
11	L	1503	CLA	C15-C16-C17-C18
11	b	1203	CLA	C13-C15-C16-C17
11	b	1207	CLA	C15-C16-C17-C18
11	b	1238	CLA	C10-C11-C12-C13
11	1	1103	CLA	C15-C16-C17-C18
11	1	1106	CLA	C8-C10-C11-C12
11	1	1127	CLA	C10-C11-C12-C13
11	1	1132	CLA	C15-C16-C17-C18
11	2	1021	CLA	C5-C6-C7-C8
12	A	2001	PQN	C15-C16-C17-C18
12	1	2001	PQN	C18-C20-C21-C22
12	2	2002	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
15	B	5004	LHG	C7-C8-C9-C10
15	a	5003	LHG	C23-C24-C25-C26
15	1	5003	LHG	C23-C24-C25-C26
11	b	1202	CLA	O1A-CGA-O2A-C1
11	b	1222	CLA	O1A-CGA-O2A-C1
11	2	1206	CLA	O1A-CGA-O2A-C1
11	A	1117	CLA	C3-C5-C6-C7
16	b	5002	LMG	O6-C1-O1-C7
11	B	1213	CLA	O1D-CGD-O2D-CED
11	a	1135	CLA	O1D-CGD-O2D-CED
11	b	1230	CLA	O1D-CGD-O2D-CED
11	A	1102	CLA	C10-C11-C12-C13
11	A	1118	CLA	C10-C11-C12-C13
11	A	1131	CLA	C10-C11-C12-C13
11	B	1214	CLA	C5-C6-C7-C8
11	B	1235	CLA	C5-C6-C7-C8
11	a	1111	CLA	C10-C11-C12-C13
11	a	1122	CLA	C8-C10-C11-C12
11	a	1131	CLA	C10-C11-C12-C13
11	b	1207	CLA	C8-C10-C11-C12
11	b	1238	CLA	C13-C15-C16-C17
11	1	1102	CLA	C15-C16-C17-C18
11	1	1106	CLA	C15-C16-C17-C18
12	A	2001	PQN	C23-C25-C26-C27
15	B	5004	LHG	O2-C2-C3-O3
15	b	5004	LHG	O2-C2-C3-O3
15	2	5004	LHG	O2-C2-C3-O3
11	b	1213	CLA	CBA-CGA-O2A-C1
11	8	1501	CLA	CBA-CGA-O2A-C1
11	b	1229	CLA	CBD-CGD-O2D-CED
11	B	1213	CLA	O1A-CGA-O2A-C1
11	B	1236	CLA	O1A-CGA-O2A-C1
16	B	5002	LMG	C4-C5-C6-O5
11	A	1022	CLA	C15-C16-C17-C18
11	B	1013	CLA	C13-C15-C16-C17
11	b	1216	CLA	C15-C16-C17-C18
11	1	1118	CLA	C10-C11-C12-C13
11	1	1131	CLA	C5-C6-C7-C8
15	b	5004	LHG	O9-C7-O7-C5
11	a	1136	CLA	O1D-CGD-O2D-CED
11	1	1115	CLA	O1D-CGD-O2D-CED
11	A	1237	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1230	CLA	O1D-CGD-O2D-CED
11	a	1122	CLA	O1D-CGD-O2D-CED
11	b	1227	CLA	O1D-CGD-O2D-CED
11	2	1220	CLA	O1D-CGD-O2D-CED
11	2	1230	CLA	O1D-CGD-O2D-CED
11	B	1202	CLA	C8-C10-C11-C12
11	b	1229	CLA	C8-C10-C11-C12
11	1	1140	CLA	C10-C11-C12-C13
11	2	1204	CLA	C5-C6-C7-C8
11	2	1229	CLA	C8-C10-C11-C12
12	a	2001	PQN	C15-C16-C17-C18
11	b	1220	CLA	C4C-C3C-CAC-CBC
11	b	1204	CLA	CBD-CGD-O2D-CED
11	A	1115	CLA	O1D-CGD-O2D-CED
11	A	1125	CLA	O1D-CGD-O2D-CED
11	2	1227	CLA	O1D-CGD-O2D-CED
11	A	1109	CLA	C8-C10-C11-C12
11	B	1229	CLA	C13-C15-C16-C17
11	a	1128	CLA	C10-C11-C12-C13
11	b	1203	CLA	C10-C11-C12-C13
11	b	1213	CLA	C10-C11-C12-C13
11	1	1101	CLA	C10-C11-C12-C13
11	8	1503	CLA	C15-C16-C17-C18
11	A	1139	CLA	CBA-CGA-O2A-C1
11	b	1216	CLA	CBA-CGA-O2A-C1
11	b	1236	CLA	CBA-CGA-O2A-C1
11	1	1105	CLA	CBA-CGA-O2A-C1
11	1	1118	CLA	CBA-CGA-O2A-C1
11	2	1207	CLA	CBA-CGA-O2A-C1
11	1	1110	CLA	CBD-CGD-O2D-CED
11	A	1011	CLA	O1A-CGA-O2A-C1
11	B	1238	CLA	O1A-CGA-O2A-C1
11	a	1011	CLA	O1A-CGA-O2A-C1
16	B	5002	LMG	O10-C28-O8-C9
11	B	1227	CLA	O1D-CGD-O2D-CED
11	2	1213	CLA	C13-C15-C16-C17
11	8	1501	CLA	C3-C5-C6-C7
14	b	4011	BCR	C19-C20-C21-C22
11	A	1119	CLA	C5-C6-C7-C8
11	A	1123	CLA	C13-C15-C16-C17
11	b	1225	CLA	C13-C15-C16-C17
15	b	5004	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	A	5003	LHG	C1-C2-C3-O3
15	a	5003	LHG	C1-C2-C3-O3
15	b	5004	LHG	C1-C2-C3-O3
15	2	5004	LHG	C1-C2-C3-O3
11	a	1121	CLA	C2A-CAA-CBA-CGA
11	b	1201	CLA	C2A-CAA-CBA-CGA
11	1	1124	CLA	C2A-CAA-CBA-CGA
11	1	1134	CLA	C2A-CAA-CBA-CGA
11	2	1021	CLA	C2A-CAA-CBA-CGA
11	B	1211	CLA	O1D-CGD-O2D-CED
11	A	1119	CLA	CBA-CGA-O2A-C1
11	A	1125	CLA	CBA-CGA-O2A-C1
11	a	1103	CLA	CBA-CGA-O2A-C1
11	1	1127	CLA	CBA-CGA-O2A-C1
11	A	1104	CLA	C8-C10-C11-C12
11	A	1123	CLA	C10-C11-C12-C13
11	B	1203	CLA	C13-C15-C16-C17
11	a	1104	CLA	C5-C6-C7-C8
11	a	1131	CLA	C5-C6-C7-C8
11	a	1137	CLA	C5-C6-C7-C8
11	a	1137	CLA	C8-C10-C11-C12
11	a	1140	CLA	C15-C16-C17-C18
11	b	1213	CLA	C13-C15-C16-C17
11	l	1503	CLA	C5-C6-C7-C8
11	1	1104	CLA	C5-C6-C7-C8
11	1	1117	CLA	C5-C6-C7-C8
11	1	1137	CLA	C13-C15-C16-C17
11	1	1012	CLA	C5-C6-C7-C8
11	2	1203	CLA	C13-C15-C16-C17
11	2	1205	CLA	C5-C6-C7-C8
11	2	1210	CLA	C8-C10-C11-C12
11	2	1216	CLA	C13-C15-C16-C17
11	2	1219	CLA	C5-C6-C7-C8
11	K	1401	CLA	C15-C16-C17-C18
11	k	1401	CLA	C15-C16-C17-C18
11	0	1401	CLA	C15-C16-C17-C18
12	b	2002	PQN	C20-C21-C22-C23
11	1	1125	CLA	CBD-CGD-O2D-CED
11	a	1110	CLA	O1A-CGA-O2A-C1
11	B	1206	CLA	O1D-CGD-O2D-CED
11	a	1112	CLA	O1D-CGD-O2D-CED
11	2	1204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1023	CLA	C13-C15-C16-C17
11	B	1229	CLA	C10-C11-C12-C13
11	a	1101	CLA	C10-C11-C12-C13
11	a	1123	CLA	C13-C15-C16-C17
11	1	1011	CLA	C10-C11-C12-C13
11	1	1012	CLA	C13-C15-C16-C17
11	A	1104	CLA	C5-C6-C7-C8
11	A	1106	CLA	C5-C6-C7-C8
11	A	1107	CLA	C8-C10-C11-C12
11	A	1123	CLA	C8-C10-C11-C12
11	a	1101	CLA	C8-C10-C11-C12
11	a	1104	CLA	C8-C10-C11-C12
11	a	1106	CLA	C5-C6-C7-C8
11	a	1117	CLA	C5-C6-C7-C8
11	a	1137	CLA	C15-C16-C17-C18
11	b	1023	CLA	C13-C15-C16-C17
11	b	1214	CLA	C8-C10-C11-C12
11	l	1503	CLA	C8-C10-C11-C12
11	1	1109	CLA	C15-C16-C17-C18
11	1	1119	CLA	C13-C15-C16-C17
11	2	1203	CLA	C15-C16-C17-C18
11	2	1235	CLA	C8-C10-C11-C12
11	K	1401	CLA	C5-C6-C7-C8
11	k	1401	CLA	C5-C6-C7-C8
11	0	1401	CLA	C5-C6-C7-C8
11	1	1118	CLA	O1D-CGD-O2D-CED
11	A	1128	CLA	CBA-CGA-O2A-C1
11	a	1122	CLA	C4-C3-C5-C6
11	A	1119	CLA	C10-C11-C12-C13
11	a	1128	CLA	C5-C6-C7-C8
11	1	1106	CLA	C5-C6-C7-C8
11	B	1221	CLA	CBD-CGD-O2D-CED
11	a	1012	CLA	CBD-CGD-O2D-CED
11	b	1226	CLA	CBD-CGD-O2D-CED
15	B	5004	LHG	C8-C7-O7-C5
11	B	1203	CLA	O1D-CGD-O2D-CED
11	B	1220	CLA	O1D-CGD-O2D-CED
15	B	5004	LHG	O9-C7-O7-C5
16	b	5002	LMG	C2-C1-O1-C7
11	a	1012	CLA	C8-C10-C11-C12
11	b	1235	CLA	C10-C11-C12-C13
11	A	1111	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	b	1238	CLA	CBA-CGA-O2A-C1
11	2	1229	CLA	CBA-CGA-O2A-C1
11	2	1201	CLA	C2C-C3C-CAC-CBC
11	a	1012	CLA	C5-C6-C7-C8
11	1	1104	CLA	C8-C10-C11-C12
14	A	4001	BCR	C11-C10-C9-C34
14	A	4007	BCR	C11-C10-C9-C34
14	B	4005	BCR	C11-C10-C9-C34
14	a	4003	BCR	C11-C10-C9-C34
14	a	4007	BCR	C11-C10-C9-C34
11	b	1223	CLA	C4C-C3C-CAC-CBC
11	B	1205	CLA	C3-C5-C6-C7
11	b	1021	CLA	C5-C6-C7-C8
11	2	1215	CLA	C8-C10-C11-C12
11	2	1226	CLA	C5-C6-C7-C8
14	A	4003	BCR	C11-C12-C13-C35
14	A	4008	BCR	C37-C22-C23-C24
14	B	4014	BCR	C7-C8-C9-C34
14	B	4014	BCR	C11-C12-C13-C35
14	B	4014	BCR	C37-C22-C23-C24
14	B	4017	BCR	C7-C8-C9-C34
14	F	4013	BCR	C37-C22-C23-C24
14	L	4019	BCR	C7-C8-C9-C34
14	L	4019	BCR	C11-C12-C13-C35
14	a	4001	BCR	C37-C22-C23-C24
14	a	4003	BCR	C37-C22-C23-C24
14	a	4007	BCR	C37-C22-C23-C24
14	b	4011	BCR	C37-C22-C23-C24
14	f	4013	BCR	C7-C8-C9-C34
14	f	4013	BCR	C11-C12-C13-C35
14	l	4019	BCR	C37-C22-C23-C24
14	m	4021	BCR	C7-C8-C9-C34
14	1	4001	BCR	C37-C22-C23-C24
14	1	4003	BCR	C7-C8-C9-C34
14	1	4003	BCR	C11-C12-C13-C35
14	1	4003	BCR	C37-C22-C23-C24
14	2	4010	BCR	C37-C22-C23-C24
14	2	4014	BCR	C7-C8-C9-C34
14	2	4017	BCR	C7-C8-C9-C34
14	6	4018	BCR	C37-C22-C23-C24
14	6	4013	BCR	C7-C8-C9-C34
14	6	4013	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
14	A	4001	BCR	C7-C8-C9-C10
14	A	4003	BCR	C7-C8-C9-C10
14	A	4003	BCR	C11-C12-C13-C14
14	B	4006	BCR	C21-C22-C23-C24
14	B	4014	BCR	C7-C8-C9-C10
14	B	4014	BCR	C11-C12-C13-C14
14	B	4014	BCR	C21-C22-C23-C24
14	F	4013	BCR	C21-C22-C23-C24
14	a	4001	BCR	C21-C22-C23-C24
14	b	4005	BCR	C7-C8-C9-C10
14	b	4006	BCR	C21-C22-C23-C24
14	f	4018	BCR	C7-C8-C9-C10
14	l	4019	BCR	C21-C22-C23-C24
14	m	4021	BCR	C7-C8-C9-C10
14	1	4003	BCR	C7-C8-C9-C10
14	1	4003	BCR	C21-C22-C23-C24
14	2	4006	BCR	C7-C8-C9-C10
14	2	4009	BCR	C11-C12-C13-C14
14	2	4010	BCR	C21-C22-C23-C24
14	2	4014	BCR	C7-C8-C9-C10
14	6	4013	BCR	C7-C8-C9-C10
14	6	4013	BCR	C11-C12-C13-C14
14	7	4021	BCR	C7-C8-C9-C10
11	A	1125	CLA	O1A-CGA-O2A-C1
11	A	1139	CLA	O1A-CGA-O2A-C1
11	b	1236	CLA	O1A-CGA-O2A-C1
11	A	1801	CLA	C2A-CAA-CBA-CGA
11	A	1109	CLA	C2A-CAA-CBA-CGA
11	A	1140	CLA	C2A-CAA-CBA-CGA
11	B	1214	CLA	C2A-CAA-CBA-CGA
11	B	1219	CLA	C2A-CAA-CBA-CGA
11	a	1101	CLA	C2A-CAA-CBA-CGA
11	a	1109	CLA	C2A-CAA-CBA-CGA
11	2	1238	CLA	C2A-CAA-CBA-CGA
11	A	1140	CLA	C5-C6-C7-C8
11	A	1132	CLA	C5-C6-C7-C8
11	a	1140	CLA	C10-C11-C12-C13
12	a	2001	PQN	C25-C26-C27-C28
15	B	5004	LHG	O1-C1-C2-C3
11	b	1236	CLA	O1D-CGD-O2D-CED
11	l	1502	CLA	O1A-CGA-O2A-C1
14	l	4019	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	B	1021	CLA	C16-C17-C18-C19
11	B	1021	CLA	C16-C17-C18-C20
11	B	1226	CLA	C16-C17-C18-C20
11	B	1206	CLA	C16-C17-C18-C20
11	a	1126	CLA	C16-C17-C18-C19
11	b	1021	CLA	C16-C17-C18-C20
11	b	1023	CLA	C16-C17-C18-C19
11	b	1224	CLA	C6-C7-C8-C10
11	b	1238	CLA	C16-C17-C18-C19
11	l	1501	CLA	C16-C17-C18-C19
11	1	1106	CLA	C16-C17-C18-C19
11	2	1206	CLA	C16-C17-C18-C20
11	2	1235	CLA	O1D-CGD-O2D-CED
11	a	1103	CLA	O1A-CGA-O2A-C1
11	b	1213	CLA	O1A-CGA-O2A-C1
11	1	1118	CLA	O1A-CGA-O2A-C1
11	2	1238	CLA	O1A-CGA-O2A-C1
11	b	1202	CLA	C3-C5-C6-C7
14	A	4001	BCR	C11-C10-C9-C8
14	A	4007	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C8
14	a	4007	BCR	C11-C10-C9-C8
11	b	1239	CLA	C2C-C3C-CAC-CBC
11	2	1239	CLA	CBA-CGA-O2A-C1
11	A	1133	CLA	O1D-CGD-O2D-CED
11	b	1215	CLA	O1D-CGD-O2D-CED
11	2	1207	CLA	O1D-CGD-O2D-CED
11	b	1201	CLA	CBA-CGA-O2A-C1
11	B	1023	CLA	C10-C11-C12-C13
11	a	1123	CLA	C8-C10-C11-C12
11	1	1101	CLA	C8-C10-C11-C12
11	8	1503	CLA	C8-C10-C11-C12
11	A	1117	CLA	C2-C1-O2A-CGA
11	A	1131	CLA	C2-C1-O2A-CGA
11	B	1013	CLA	C2-C1-O2A-CGA
11	B	1203	CLA	C2-C1-O2A-CGA
11	B	1221	CLA	C2-C1-O2A-CGA
11	B	1223	CLA	C2-C1-O2A-CGA
11	B	1229	CLA	C2-C1-O2A-CGA
11	a	1117	CLA	C2-C1-O2A-CGA
11	a	1126	CLA	C2-C1-O2A-CGA
11	b	1021	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
11	1	1107	CLA	C2-C1-O2A-CGA
11	1	1117	CLA	C2-C1-O2A-CGA
11	1	1126	CLA	C2-C1-O2A-CGA
11	2	1023	CLA	C2-C1-O2A-CGA
11	2	1215	CLA	C2-C1-O2A-CGA
11	2	1221	CLA	C2-C1-O2A-CGA
11	2	1235	CLA	C2-C1-O2A-CGA
11	K	1401	CLA	C2-C1-O2A-CGA
11	k	1401	CLA	C2-C1-O2A-CGA
11	0	1401	CLA	C2-C1-O2A-CGA
11	A	1102	CLA	C16-C17-C18-C19
11	A	1117	CLA	C16-C17-C18-C20
11	B	1213	CLA	C16-C17-C18-C19
11	B	1206	CLA	C16-C17-C18-C19
11	a	1117	CLA	C16-C17-C18-C20
11	a	1126	CLA	C16-C17-C18-C20
11	b	1021	CLA	C16-C17-C18-C19
11	b	1204	CLA	C16-C17-C18-C19
11	b	1206	CLA	C16-C17-C18-C20
11	l	1501	CLA	C16-C17-C18-C20
11	1	1101	CLA	C16-C17-C18-C19
11	1	1137	CLA	C16-C17-C18-C20
11	1	1011	CLA	C16-C17-C18-C19
11	2	1206	CLA	C16-C17-C18-C19
11	2	1207	CLA	C16-C17-C18-C20
11	2	1224	CLA	C6-C7-C8-C10
11	b	1216	CLA	O1A-CGA-O2A-C1
11	1	1127	CLA	O1A-CGA-O2A-C1
11	2	1207	CLA	O1A-CGA-O2A-C1
11	8	1501	CLA	O1A-CGA-O2A-C1
11	l	1501	CLA	C5-C6-C7-C8
11	1	1011	CLA	C15-C16-C17-C18
12	a	2001	PQN	C18-C20-C21-C22
16	b	5002	LMG	C38-C39-C40-C41
11	8	1502	CLA	CBA-CGA-O2A-C1
15	A	5001	LHG	C28-C29-C30-C31
16	b	5002	LMG	C34-C35-C36-C37
11	B	1205	CLA	O1D-CGD-O2D-CED
11	A	1118	CLA	C5-C6-C7-C8
11	B	1204	CLA	C8-C10-C11-C12
11	a	1128	CLA	C13-C15-C16-C17
11	2	1023	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	B	5004	LHG	C13-C14-C15-C16
15	a	5003	LHG	C13-C14-C15-C16
16	2	5002	LMG	C36-C37-C38-C39
11	b	1225	CLA	CBA-CGA-O2A-C1
11	b	1227	CLA	C4C-C3C-CAC-CBC
15	b	5004	LHG	C15-C16-C17-C18
15	A	5001	LHG	O1-C1-C2-O2
15	A	5003	LHG	O1-C1-C2-O2
15	b	5004	LHG	C31-C32-C33-C34
15	2	5004	LHG	C11-C10-C9-C8
11	b	1204	CLA	C15-C16-C17-C18
11	1	1128	CLA	C5-C6-C7-C8
11	A	1022	CLA	C4B-C3B-CAB-CBB
11	A	1105	CLA	C4B-C3B-CAB-CBB
11	A	1106	CLA	C4B-C3B-CAB-CBB
11	A	1124	CLA	C4B-C3B-CAB-CBB
11	B	1013	CLA	C4B-C3B-CAB-CBB
11	B	1204	CLA	C4B-C3B-CAB-CBB
11	B	1208	CLA	C4B-C3B-CAB-CBB
11	B	1217	CLA	C4B-C3B-CAB-CBB
11	B	1224	CLA	C4B-C3B-CAB-CBB
11	B	1232	CLA	C4B-C3B-CAB-CBB
11	B	1234	CLA	C4B-C3B-CAB-CBB
11	a	1120	CLA	C4B-C3B-CAB-CBB
11	a	1135	CLA	C4B-C3B-CAB-CBB
11	b	1202	CLA	C4B-C3B-CAB-CBB
11	b	1203	CLA	C4B-C3B-CAB-CBB
11	b	1224	CLA	C4B-C3B-CAB-CBB
11	b	1225	CLA	C4B-C3B-CAB-CBB
11	b	1227	CLA	C4B-C3B-CAB-CBB
11	b	1240	CLA	C4B-C3B-CAB-CBB
11	1	1114	CLA	C4B-C3B-CAB-CBB
11	1	1120	CLA	C4B-C3B-CAB-CBB
11	2	1205	CLA	C4B-C3B-CAB-CBB
11	2	1227	CLA	C4B-C3B-CAB-CBB
15	A	5003	LHG	C29-C30-C31-C32
11	A	1137	CLA	C16-C17-C18-C19
11	A	1137	CLA	C16-C17-C18-C20
11	B	1226	CLA	C16-C17-C18-C19
11	b	1023	CLA	C16-C17-C18-C20
11	b	1204	CLA	C16-C17-C18-C20
11	2	1207	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	A	2001	PQN	C26-C27-C28-C29
11	A	1135	CLA	O1D-CGD-O2D-CED
11	1	1129	CLA	O1D-CGD-O2D-CED
11	A	1126	CLA	C2A-CAA-CBA-CGA
15	1	5003	LHG	C29-C30-C31-C32
16	2	5002	LMG	C13-C14-C15-C16
11	A	1127	CLA	C15-C16-C17-C18
11	B	1238	CLA	C5-C6-C7-C8
11	b	1226	CLA	C13-C15-C16-C17
11	1	1107	CLA	C8-C10-C11-C12
11	2	1229	CLA	C10-C11-C12-C13
11	8	1501	CLA	C5-C6-C7-C8
16	B	5002	LMG	C14-C15-C16-C17
11	B	1215	CLA	C6-C7-C8-C10
11	a	1106	CLA	C6-C7-C8-C10
11	1	1103	CLA	C11-C10-C8-C7
11	1	1107	CLA	C6-C7-C8-C10
11	1	1109	CLA	C6-C7-C8-C10
11	2	1203	CLA	C11-C10-C8-C7
12	1	2001	PQN	C21-C22-C23-C25
11	2	1201	CLA	C5-C6-C7-C8
11	L	1503	CLA	C8-C10-C11-C12
11	a	1011	CLA	C8-C10-C11-C12
11	1	1022	CLA	C15-C16-C17-C18
12	B	2002	PQN	C15-C16-C17-C18
15	a	5001	LHG	C29-C30-C31-C32
16	B	5002	LMG	C35-C36-C37-C38
11	A	1119	CLA	O1A-CGA-O2A-C1
11	b	1201	CLA	O1A-CGA-O2A-C1
11	1	1105	CLA	O1A-CGA-O2A-C1
11	2	1223	CLA	C3-C5-C6-C7
11	A	1237	CLA	C3A-C2A-CAA-CBA
11	A	1104	CLA	C3A-C2A-CAA-CBA
11	A	1135	CLA	C3A-C2A-CAA-CBA
11	B	1210	CLA	C3A-C2A-CAA-CBA
11	B	1240	CLA	C3A-C2A-CAA-CBA
11	a	1101	CLA	C3A-C2A-CAA-CBA
11	a	1104	CLA	C3A-C2A-CAA-CBA
11	a	1123	CLA	C3A-C2A-CAA-CBA
11	a	1131	CLA	C3A-C2A-CAA-CBA
11	a	1139	CLA	C3A-C2A-CAA-CBA
11	1	1237	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	1	1101	CLA	C3A-C2A-CAA-CBA
11	1	1104	CLA	C3A-C2A-CAA-CBA
11	1	1107	CLA	C3A-C2A-CAA-CBA
11	1	1131	CLA	C3A-C2A-CAA-CBA
11	1	1139	CLA	C3A-C2A-CAA-CBA
11	2	1210	CLA	C3A-C2A-CAA-CBA
11	2	1234	CLA	C3A-C2A-CAA-CBA
11	a	1237	CLA	O1D-CGD-O2D-CED
11	1	1110	CLA	C5-C6-C7-C8
15	1	5001	LHG	C28-C29-C30-C31
11	1	1107	CLA	C2-C3-C5-C6
11	A	1119	CLA	C4C-C3C-CAC-CBC
11	a	1102	CLA	C10-C11-C12-C13
11	b	1013	CLA	C8-C10-C11-C12
11	b	1023	CLA	C10-C11-C12-C13
11	b	1235	CLA	C5-C6-C7-C8
11	8	1501	CLA	C8-C10-C11-C12
16	B	5002	LMG	C37-C38-C39-C40
16	b	5002	LMG	C13-C14-C15-C16
14	A	4001	BCR	C9-C10-C11-C12
14	F	4013	BCR	C9-C10-C11-C12
14	a	4008	BCR	C9-C10-C11-C12
14	8	4022	BCR	C9-C10-C11-C12
11	b	1207	CLA	C16-C17-C18-C19
11	b	1207	CLA	C16-C17-C18-C20
11	b	1238	CLA	C16-C17-C18-C20
11	1	1101	CLA	C16-C17-C18-C20
11	1	1106	CLA	C16-C17-C18-C20
11	1	1106	CLA	O1D-CGD-O2D-CED
11	2	1211	CLA	CBD-CGD-O2D-CED
11	2	1219	CLA	CBA-CGA-O2A-C1
11	2	1225	CLA	CBA-CGA-O2A-C1
15	a	5001	LHG	C18-C19-C20-C21
16	b	5002	LMG	C40-C41-C42-C43
11	A	1124	CLA	C3-C5-C6-C7
11	b	1229	CLA	C3-C5-C6-C7
11	A	1122	CLA	C10-C11-C12-C13
15	2	5004	LHG	C15-C16-C17-C18
11	2	1229	CLA	O1A-CGA-O2A-C1
15	2	5004	LHG	C11-C12-C13-C14
15	a	5001	LHG	C11-C12-C13-C14
11	B	1235	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	a	1116	CLA	C5-C6-C7-C8
15	B	5004	LHG	C16-C17-C18-C19
11	A	1126	CLA	C16-C17-C18-C19
11	b	1206	CLA	C16-C17-C18-C19
11	1	1137	CLA	C16-C17-C18-C19
11	A	1105	CLA	C2B-C3B-CAB-CBB
11	A	1106	CLA	C2B-C3B-CAB-CBB
11	A	1132	CLA	C2B-C3B-CAB-CBB
11	B	1208	CLA	C2B-C3B-CAB-CBB
11	B	1217	CLA	C2B-C3B-CAB-CBB
11	B	1211	CLA	C2B-C3B-CAB-CBB
11	a	1122	CLA	C2B-C3B-CAB-CBB
11	a	1131	CLA	C2B-C3B-CAB-CBB
11	a	1129	CLA	C2B-C3B-CAB-CBB
11	b	1203	CLA	C2B-C3B-CAB-CBB
11	1	1124	CLA	C2B-C3B-CAB-CBB
11	1	1126	CLA	C2B-C3B-CAB-CBB
11	1	1114	CLA	C2B-C3B-CAB-CBB
11	2	1205	CLA	C2B-C3B-CAB-CBB
11	2	1221	CLA	C2B-C3B-CAB-CBB
11	2	1223	CLA	C2B-C3B-CAB-CBB
11	2	1227	CLA	C2B-C3B-CAB-CBB
11	2	1211	CLA	C2B-C3B-CAB-CBB
14	A	4001	BCR	C1-C6-C7-C8
14	A	4001	BCR	C5-C6-C7-C8
14	A	4003	BCR	C1-C6-C7-C8
14	A	4003	BCR	C5-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C30
14	A	4007	BCR	C23-C24-C25-C26
14	A	4007	BCR	C23-C24-C25-C30
14	B	4006	BCR	C1-C6-C7-C8
14	B	4006	BCR	C5-C6-C7-C8
14	B	4009	BCR	C1-C6-C7-C8
14	B	4009	BCR	C23-C24-C25-C30
14	B	4010	BCR	C23-C24-C25-C30
14	M	4021	BCR	C1-C6-C7-C8
14	a	4003	BCR	C1-C6-C7-C8
14	a	4003	BCR	C5-C6-C7-C8
14	b	4005	BCR	C1-C6-C7-C8
14	f	4020	BCR	C23-C24-C25-C30
14	f	4013	BCR	C1-C6-C7-C8
14	m	4021	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	m	4021	BCR	C5-C6-C7-C8
14	1	4001	BCR	C1-C6-C7-C8
14	1	4001	BCR	C5-C6-C7-C8
14	1	4007	BCR	C23-C24-C25-C30
14	2	4004	BCR	C23-C24-C25-C26
14	2	4004	BCR	C23-C24-C25-C30
14	2	4006	BCR	C1-C6-C7-C8
14	2	4011	BCR	C23-C24-C25-C30
14	2	4014	BCR	C23-C24-C25-C26
14	2	4014	BCR	C23-C24-C25-C30
14	6	4018	BCR	C23-C24-C25-C30
14	6	4013	BCR	C1-C6-C7-C8
14	6	4013	BCR	C5-C6-C7-C8
14	8	4019	BCR	C1-C6-C7-C8
14	8	4019	BCR	C5-C6-C7-C8
14	7	4021	BCR	C1-C6-C7-C8
14	7	4021	BCR	C5-C6-C7-C8
14	7	4021	BCR	C23-C24-C25-C26
14	7	4021	BCR	C23-C24-C25-C30
11	2	1234	CLA	CBA-CGA-O2A-C1
11	B	1216	CLA	C13-C15-C16-C17
11	B	1210	CLA	C3-C5-C6-C7
16	b	5002	LMG	C11-C12-C13-C14
16	b	5002	LMG	C17-C18-C19-C20
11	A	1124	CLA	O1D-CGD-O2D-CED
11	B	1229	CLA	C2A-CAA-CBA-CGA
11	K	1401	CLA	C2A-CAA-CBA-CGA
11	k	1401	CLA	C2A-CAA-CBA-CGA
11	0	1401	CLA	C2A-CAA-CBA-CGA
11	A	1101	CLA	C5-C6-C7-C8
11	1	1109	CLA	C8-C10-C11-C12
15	A	5001	LHG	C11-C12-C13-C14
16	B	5002	LMG	C29-C30-C31-C32
11	A	1128	CLA	O1A-CGA-O2A-C1
11	b	1238	CLA	O1A-CGA-O2A-C1
11	2	1217	CLA	C2C-C3C-CAC-CBC
11	a	1138	CLA	O1A-CGA-O2A-C1
15	B	5004	LHG	C9-C10-C11-C12
11	b	1222	CLA	C11-C10-C8-C7
11	A	1137	CLA	C4-C3-C5-C6
11	2	1226	CLA	C4-C3-C5-C6
11	a	1110	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	a	4007	BCR	C10-C11-C12-C13
14	b	4004	BCR	C10-C11-C12-C13
11	a	1022	CLA	C15-C16-C17-C18
11	1	1012	CLA	C8-C10-C11-C12
11	a	1122	CLA	C2-C3-C5-C6
11	1	1137	CLA	C2-C3-C5-C6
15	B	5004	LHG	C34-C35-C36-C37
16	b	5002	LMG	C36-C37-C38-C39
11	b	1210	CLA	C4C-C3C-CAC-CBC
11	B	1210	CLA	CBA-CGA-O2A-C1
11	1	1135	CLA	CBA-CGA-O2A-C1
12	a	2001	PQN	C24-C23-C25-C26
11	b	1210	CLA	C8-C10-C11-C12
11	A	1115	CLA	C4C-C3C-CAC-CBC
16	B	5002	LMG	C13-C14-C15-C16
11	b	1203	CLA	O1D-CGD-O2D-CED
11	a	1109	CLA	C15-C16-C17-C18
11	b	1225	CLA	O1A-CGA-O2A-C1
15	A	5003	LHG	C24-C25-C26-C27
15	1	5001	LHG	C18-C19-C20-C21
15	B	5004	LHG	C28-C29-C30-C31
14	b	4009	BCR	C9-C10-C11-C12
14	l	4019	BCR	C9-C10-C11-C12
11	A	1102	CLA	C16-C17-C18-C20
11	B	1207	CLA	C16-C17-C18-C19
11	a	1117	CLA	C16-C17-C18-C19
11	1	1011	CLA	C16-C17-C18-C20
15	a	5001	LHG	C8-C7-O7-C5
16	b	5002	LMG	C11-C10-O7-C8
16	2	5002	LMG	C11-C10-O7-C8
16	2	5002	LMG	C21-C22-C23-C24
16	2	5002	LMG	O9-C10-O7-C8
15	1	5003	LHG	C18-C19-C20-C21
16	B	5002	LMG	C21-C22-C23-C24
16	b	5002	LMG	C14-C15-C16-C17
15	A	5003	LHG	C32-C33-C34-C35
14	b	4010	BCR	C37-C22-C23-C24
14	f	4020	BCR	C11-C12-C13-C35
11	A	1116	CLA	C3-C5-C6-C7
11	a	1103	CLA	C3-C5-C6-C7
11	1	1109	CLA	C3-C5-C6-C7
11	2	1222	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	L	4022	BCR	C11-C12-C13-C14
14	a	4002	BCR	C11-C12-C13-C14
14	b	4005	BCR	C21-C22-C23-C24
14	b	4010	BCR	C21-C22-C23-C24
14	2	4005	BCR	C21-C22-C23-C24
15	1	5001	LHG	C12-C13-C14-C15
11	A	1131	CLA	C5-C6-C7-C8
11	A	1115	CLA	C2A-CAA-CBA-CGA
11	B	1240	CLA	C2A-CAA-CBA-CGA
11	a	1115	CLA	C2A-CAA-CBA-CGA
11	a	1127	CLA	C2A-CAA-CBA-CGA
11	A	1117	CLA	C16-C17-C18-C19
11	A	1119	CLA	C16-C17-C18-C19
11	A	1119	CLA	C16-C17-C18-C20
11	A	1126	CLA	C16-C17-C18-C20
11	B	1224	CLA	C6-C7-C8-C10
12	A	2001	PQN	C26-C27-C28-C30
11	1	1122	CLA	C2C-C3C-CAC-CBC
11	1	1116	CLA	C5-C6-C7-C8
15	1	5003	LHG	C30-C31-C32-C33
11	a	1801	CLA	C4-C3-C5-C6
11	1	1122	CLA	C4-C3-C5-C6
11	a	1801	CLA	C2-C3-C5-C6
15	1	5001	LHG	C11-C12-C13-C14
11	1	1105	CLA	O1D-CGD-O2D-CED
11	B	1204	CLA	C5-C6-C7-C8
11	a	1140	CLA	C13-C15-C16-C17
11	b	1203	CLA	C8-C10-C11-C12
16	B	5002	LMG	C39-C40-C41-C42
11	A	1124	CLA	C2C-C3C-CAC-CBC
11	b	1203	CLA	C3-C5-C6-C7
11	1	1127	CLA	C3-C5-C6-C7
11	A	1137	CLA	C5-C6-C7-C8
11	A	1011	CLA	C10-C11-C12-C13
11	B	1223	CLA	C15-C16-C17-C18
11	a	1127	CLA	C15-C16-C17-C18
11	2	1204	CLA	C8-C10-C11-C12
11	2	1214	CLA	C10-C11-C12-C13
11	2	1221	CLA	C5-C6-C7-C8
11	A	1022	CLA	C10-C11-C12-C13
11	A	1102	CLA	C13-C15-C16-C17
11	A	1104	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	A	1106	CLA	C13-C15-C16-C17
11	B	1210	CLA	C15-C16-C17-C18
11	a	1022	CLA	C13-C15-C16-C17
11	b	1205	CLA	C5-C6-C7-C8
11	1	1117	CLA	C16-C17-C18-C20
15	A	5003	LHG	C18-C19-C20-C21
15	b	5004	LHG	C33-C34-C35-C36
16	b	5002	LMG	C21-C22-C23-C24
16	2	5002	LMG	C14-C15-C16-C17
11	2	1219	CLA	O1A-CGA-O2A-C1
15	b	5004	LHG	C16-C17-C18-C19
15	1	5001	LHG	C25-C26-C27-C28
11	B	1225	CLA	C13-C15-C16-C17
11	1	1128	CLA	C15-C16-C17-C18
15	1	5001	LHG	O7-C5-C6-O8
15	1	5003	LHG	O7-C5-C6-O8
16	B	5002	LMG	O7-C8-C9-O8
11	a	1126	CLA	CBA-CGA-O2A-C1
15	1	5001	LHG	C26-C27-C28-C29
11	b	1202	CLA	C15-C16-C17-C18
11	2	1226	CLA	O1D-CGD-O2D-CED
11	1	1133	CLA	CBA-CGA-O2A-C1
11	B	1235	CLA	C2-C1-O2A-CGA
11	b	1221	CLA	C2-C1-O2A-CGA
11	1	1104	CLA	C2-C1-O2A-CGA
11	B	1205	CLA	C6-C7-C8-C10
11	B	1213	CLA	C16-C17-C18-C20
11	2	1229	CLA	C16-C17-C18-C19
11	B	1238	CLA	C8-C10-C11-C12
11	a	1109	CLA	C5-C6-C7-C8
11	a	1140	CLA	C8-C10-C11-C12
15	2	5004	LHG	C7-C8-C9-C10
11	1	1103	CLA	C2-C3-C5-C6
15	a	5001	LHG	O9-C7-O7-C5
15	a	5003	LHG	C28-C29-C30-C31
11	A	1134	CLA	C2A-CAA-CBA-CGA
11	b	1234	CLA	C2C-C3C-CAC-CBC
11	b	1210	CLA	C15-C16-C17-C18
15	a	5001	LHG	C28-C29-C30-C31
11	a	1133	CLA	O1D-CGD-O2D-CED
15	2	5004	LHG	C16-C17-C18-C19
16	2	5002	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
15	1	5003	LHG	O1-C1-C2-O2
11	B	1210	CLA	O1A-CGA-O2A-C1
11	2	1225	CLA	O1A-CGA-O2A-C1
11	2	1234	CLA	O1A-CGA-O2A-C1
11	B	1213	CLA	C3-C5-C6-C7
11	b	1201	CLA	C3-C5-C6-C7
11	A	1101	CLA	C1A-C2A-CAA-CBA
11	A	1103	CLA	C1A-C2A-CAA-CBA
11	A	1104	CLA	C1A-C2A-CAA-CBA
11	A	1106	CLA	C1A-C2A-CAA-CBA
11	A	1109	CLA	C1A-C2A-CAA-CBA
11	A	1110	CLA	C1A-C2A-CAA-CBA
11	A	1116	CLA	C1A-C2A-CAA-CBA
11	A	1117	CLA	C1A-C2A-CAA-CBA
11	A	1119	CLA	C1A-C2A-CAA-CBA
11	A	1130	CLA	C1A-C2A-CAA-CBA
11	A	1137	CLA	C1A-C2A-CAA-CBA
11	A	1114	CLA	C1A-C2A-CAA-CBA
11	A	1120	CLA	C1A-C2A-CAA-CBA
11	A	1121	CLA	C1A-C2A-CAA-CBA
11	A	1135	CLA	C1A-C2A-CAA-CBA
11	B	1202	CLA	C1A-C2A-CAA-CBA
11	B	1212	CLA	C1A-C2A-CAA-CBA
11	B	1213	CLA	C1A-C2A-CAA-CBA
11	B	1217	CLA	C1A-C2A-CAA-CBA
11	B	1231	CLA	C1A-C2A-CAA-CBA
11	B	1236	CLA	C1A-C2A-CAA-CBA
11	B	1211	CLA	C1A-C2A-CAA-CBA
11	a	1106	CLA	C1A-C2A-CAA-CBA
11	a	1109	CLA	C1A-C2A-CAA-CBA
11	a	1110	CLA	C1A-C2A-CAA-CBA
11	a	1116	CLA	C1A-C2A-CAA-CBA
11	a	1117	CLA	C1A-C2A-CAA-CBA
11	a	1119	CLA	C1A-C2A-CAA-CBA
11	a	1123	CLA	C1A-C2A-CAA-CBA
11	a	1128	CLA	C1A-C2A-CAA-CBA
11	a	1131	CLA	C1A-C2A-CAA-CBA
11	a	1139	CLA	C1A-C2A-CAA-CBA
11	a	1114	CLA	C1A-C2A-CAA-CBA
11	a	1120	CLA	C1A-C2A-CAA-CBA
11	a	1134	CLA	C1A-C2A-CAA-CBA
11	b	1213	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	b	1216	CLA	C1A-C2A-CAA-CBA
11	b	1225	CLA	C1A-C2A-CAA-CBA
11	b	1229	CLA	C1A-C2A-CAA-CBA
11	b	1232	CLA	C1A-C2A-CAA-CBA
11	b	1236	CLA	C1A-C2A-CAA-CBA
11	1	1101	CLA	C1A-C2A-CAA-CBA
11	1	1110	CLA	C1A-C2A-CAA-CBA
11	1	1116	CLA	C1A-C2A-CAA-CBA
11	1	1117	CLA	C1A-C2A-CAA-CBA
11	1	1119	CLA	C1A-C2A-CAA-CBA
11	1	1128	CLA	C1A-C2A-CAA-CBA
11	1	1131	CLA	C1A-C2A-CAA-CBA
11	1	1139	CLA	C1A-C2A-CAA-CBA
11	1	1114	CLA	C1A-C2A-CAA-CBA
11	1	1121	CLA	C1A-C2A-CAA-CBA
11	1	1132	CLA	C1A-C2A-CAA-CBA
11	2	1021	CLA	C1A-C2A-CAA-CBA
11	2	1202	CLA	C1A-C2A-CAA-CBA
11	2	1208	CLA	C1A-C2A-CAA-CBA
11	2	1213	CLA	C1A-C2A-CAA-CBA
11	2	1215	CLA	C1A-C2A-CAA-CBA
11	2	1218	CLA	C1A-C2A-CAA-CBA
11	2	1236	CLA	C1A-C2A-CAA-CBA
11	2	1211	CLA	C1A-C2A-CAA-CBA
11	K	1401	CLA	C1A-C2A-CAA-CBA
11	k	1401	CLA	C1A-C2A-CAA-CBA
11	k	1402	CLA	C1A-C2A-CAA-CBA
11	0	1401	CLA	C1A-C2A-CAA-CBA
11	0	1402	CLA	C1A-C2A-CAA-CBA
11	A	1128	CLA	C10-C11-C12-C13
15	a	5001	LHG	C14-C15-C16-C17
11	2	1239	CLA	C2C-C3C-CAC-CBC
11	B	1229	CLA	C8-C10-C11-C12
11	a	1117	CLA	C8-C10-C11-C12
15	a	5001	LHG	O6-C4-C5-C6
16	b	5002	LMG	O9-C10-O7-C8
15	a	5001	LHG	C31-C32-C33-C34
16	b	5002	LMG	C31-C32-C33-C34
11	A	1114	CLA	C2C-C3C-CAC-CBC
11	A	1111	CLA	C3-C5-C6-C7
11	A	1101	CLA	C6-C7-C8-C10
11	A	1102	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
11	A	1109	CLA	C6-C7-C8-C10
11	A	1118	CLA	C11-C10-C8-C7
11	A	1118	CLA	C11-C12-C13-C15
11	A	1127	CLA	C11-C12-C13-C15
11	B	1021	CLA	C12-C13-C15-C16
11	B	1023	CLA	C11-C10-C8-C7
11	B	1023	CLA	C11-C12-C13-C15
11	B	1202	CLA	C6-C7-C8-C10
11	B	1207	CLA	C6-C7-C8-C10
11	B	1238	CLA	C11-C12-C13-C15
11	a	1117	CLA	C11-C10-C8-C7
11	a	1122	CLA	C11-C10-C8-C7
11	a	1126	CLA	C11-C12-C13-C15
11	b	1021	CLA	C12-C13-C15-C16
11	b	1023	CLA	C11-C10-C8-C7
11	b	1215	CLA	C11-C10-C8-C7
11	b	1226	CLA	C11-C10-C8-C7
11	b	1234	CLA	C11-C10-C8-C7
11	1	1022	CLA	C6-C7-C8-C10
11	1	1101	CLA	C6-C7-C8-C10
11	1	1103	CLA	C11-C12-C13-C15
11	1	1106	CLA	C6-C7-C8-C10
11	1	1119	CLA	C12-C13-C15-C16
11	1	1123	CLA	C11-C10-C8-C7
11	1	1126	CLA	C11-C12-C13-C15
11	1	1131	CLA	C11-C10-C8-C7
11	1	1011	CLA	C11-C10-C8-C7
11	2	1206	CLA	C12-C13-C15-C16
11	2	1213	CLA	C6-C7-C8-C10
11	2	1215	CLA	C11-C10-C8-C7
11	2	1223	CLA	C6-C7-C8-C10
11	K	1401	CLA	C6-C7-C8-C10
11	K	1401	CLA	C11-C10-C8-C7
11	k	1401	CLA	C6-C7-C8-C10
11	k	1401	CLA	C11-C10-C8-C7
11	0	1401	CLA	C6-C7-C8-C10
11	0	1401	CLA	C11-C10-C8-C7
12	A	2001	PQN	C21-C22-C23-C25
12	A	2001	PQN	C22-C23-C25-C26
11	A	1011	CLA	C16-C17-C18-C19
11	a	1119	CLA	C16-C17-C18-C20
11	B	1210	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	A	1119	CLA	C8-C10-C11-C12
11	a	1126	CLA	C8-C10-C11-C12
11	1	1107	CLA	C15-C16-C17-C18
16	B	5002	LMG	C11-C12-C13-C14
16	B	5002	LMG	C41-C42-C43-C44
11	a	1119	CLA	C13-C15-C16-C17
11	A	1108	CLA	C2A-CAA-CBA-CGA
11	1	1106	CLA	C2A-CAA-CBA-CGA
11	1	1111	CLA	C2A-CAA-CBA-CGA
11	1	1118	CLA	C2A-CAA-CBA-CGA
11	1	1125	CLA	C3-C5-C6-C7
11	1	1129	CLA	C2A-CAA-CBA-CGA
11	A	1101	CLA	C14-C13-C15-C16
11	A	1107	CLA	C6-C7-C8-C9
11	A	1109	CLA	C6-C7-C8-C9
11	A	1122	CLA	C6-C7-C8-C9
11	A	1123	CLA	C6-C7-C8-C9
11	A	1127	CLA	C11-C12-C13-C14
11	A	1140	CLA	C14-C13-C15-C16
11	B	1021	CLA	C11-C10-C8-C9
11	B	1207	CLA	C6-C7-C8-C9
11	B	1214	CLA	C6-C7-C8-C9
11	B	1229	CLA	C6-C7-C8-C9
11	B	1206	CLA	C11-C10-C8-C9
11	a	1126	CLA	C11-C12-C13-C14
11	a	1131	CLA	C6-C7-C8-C9
11	b	1021	CLA	C11-C10-C8-C9
11	b	1214	CLA	C6-C7-C8-C9
11	b	1216	CLA	C6-C7-C8-C9
11	1	1106	CLA	C11-C12-C13-C14
11	1	1119	CLA	C11-C12-C13-C14
11	1	1119	CLA	C14-C13-C15-C16
11	1	1126	CLA	C11-C12-C13-C14
11	1	1140	CLA	C11-C10-C8-C9
11	2	1229	CLA	C11-C12-C13-C14
11	2	1235	CLA	C11-C10-C8-C9
15	a	5003	LHG	C31-C32-C33-C34
11	b	1223	CLA	C5-C6-C7-C8
11	a	1105	CLA	O2A-C1-C2-C3
15	A	5001	LHG	C4-C5-C6-O8
15	B	5004	LHG	C4-C5-C6-O8
15	b	5004	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
16	b	5002	LMG	O1-C7-C8-C9
16	2	5002	LMG	O1-C7-C8-C9
15	1	5001	LHG	C16-C17-C18-C19
15	1	5003	LHG	C33-C34-C35-C36
15	B	5004	LHG	C11-C12-C13-C14
11	a	1131	CLA	C15-C16-C17-C18
11	b	1223	CLA	C15-C16-C17-C18
11	B	1204	CLA	CBA-CGA-O2A-C1
11	B	1225	CLA	CBA-CGA-O2A-C1
15	1	5001	LHG	C7-C8-C9-C10
11	b	1229	CLA	C16-C17-C18-C19
11	1	1117	CLA	C16-C17-C18-C19
11	1	1135	CLA	O1A-CGA-O2A-C1
11	A	1123	CLA	C5-C6-C7-C8
15	1	5003	LHG	C14-C15-C16-C17
11	1	1103	CLA	C4-C3-C5-C6
11	1	1114	CLA	C2C-C3C-CAC-CBC
11	2	1227	CLA	C2C-C3C-CAC-CBC
11	2	1226	CLA	C2-C3-C5-C6
11	a	1106	CLA	C13-C15-C16-C17
11	a	1137	CLA	C13-C15-C16-C17
11	1	1140	CLA	C5-C6-C7-C8
11	2	1013	CLA	C13-C15-C16-C17
14	B	4004	BCR	C37-C22-C23-C24
14	B	4006	BCR	C11-C12-C13-C35
14	B	4010	BCR	C37-C22-C23-C24
14	b	4004	BCR	C37-C22-C23-C24
15	b	5004	LHG	C28-C29-C30-C31
14	A	4002	BCR	C7-C8-C9-C10
14	B	4004	BCR	C21-C22-C23-C24
14	B	4010	BCR	C21-C22-C23-C24
14	B	4017	BCR	C7-C8-C9-C10
14	b	4004	BCR	C21-C22-C23-C24
11	A	1140	CLA	C10-C11-C12-C13
11	A	1012	CLA	C8-C10-C11-C12
11	b	1216	CLA	C13-C15-C16-C17
11	1	1123	CLA	C8-C10-C11-C12
11	2	1207	CLA	C10-C11-C12-C13
11	a	1106	CLA	C2A-CAA-CBA-CGA
11	A	1012	CLA	C3-C5-C6-C7
11	1	1138	CLA	CBA-CGA-O2A-C1
11	A	1117	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	1	1137	CLA	C8-C10-C11-C12
11	2	1216	CLA	C5-C6-C7-C8
15	2	5004	LHG	C13-C14-C15-C16
11	a	1139	CLA	CBA-CGA-O2A-C1
11	2	1023	CLA	O2A-C1-C2-C3
16	2	5002	LMG	C18-C19-C20-C21
16	2	5002	LMG	C39-C40-C41-C42
11	a	1012	CLA	C10-C11-C12-C13
15	a	5003	LHG	C26-C27-C28-C29
14	B	4010	BCR	C9-C10-C11-C12
14	a	4002	BCR	C19-C20-C21-C22
14	b	4006	BCR	C19-C20-C21-C22
14	b	4010	BCR	C9-C10-C11-C12
14	1	4003	BCR	C19-C20-C21-C22
14	6	4020	BCR	C19-C20-C21-C22
11	B	1207	CLA	C16-C17-C18-C20
11	2	1229	CLA	C16-C17-C18-C20
11	B	1204	CLA	O1A-CGA-O2A-C1
11	B	1225	CLA	O1A-CGA-O2A-C1
11	B	1013	CLA	C3-C5-C6-C7
15	A	5001	LHG	C24-C25-C26-C27
14	a	4003	BCR	C11-C10-C9-C8
11	b	1229	CLA	O1D-CGD-O2D-CED
11	2	1214	CLA	O1D-CGD-O2D-CED
11	B	1217	CLA	CBA-CGA-O2A-C1
11	1	1126	CLA	CBA-CGA-O2A-C1
15	a	5003	LHG	C35-C36-C37-C38
15	A	5003	LHG	C10-C11-C12-C13
11	2	1201	CLA	C4C-C3C-CAC-CBC
11	1	1801	CLA	C2-C3-C5-C6
15	b	5004	LHG	C19-C20-C21-C22
15	b	5004	LHG	C11-C12-C13-C14
11	B	1220	CLA	C4C-C3C-CAC-CBC
16	B	5002	LMG	C19-C20-C21-C22
16	B	5002	LMG	C31-C32-C33-C34
16	2	5002	LMG	C23-C24-C25-C26
11	a	1125	CLA	C2C-C3C-CAC-CBC
15	b	5004	LHG	O7-C5-C6-O8
15	2	5004	LHG	C31-C32-C33-C34
11	A	1140	CLA	C2C-C3C-CAC-CBC
11	b	1231	CLA	O1D-CGD-O2D-CED
16	2	5002	LMG	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
15	2	5004	LHG	O8-C23-C24-C25
11	A	1124	CLA	C2A-CAA-CBA-CGA
11	a	1124	CLA	C2A-CAA-CBA-CGA
11	B	1215	CLA	C3-C5-C6-C7
11	1	1110	CLA	C3-C5-C6-C7
11	a	1119	CLA	C16-C17-C18-C19
11	b	1205	CLA	C6-C7-C8-C9
11	1	1122	CLA	C11-C12-C13-C14
11	B	1214	CLA	O1D-CGD-O2D-CED
11	b	1204	CLA	O1D-CGD-O2D-CED
11	A	1106	CLA	CBA-CGA-O2A-C1
11	A	1137	CLA	CBA-CGA-O2A-C1
11	2	1210	CLA	CBA-CGA-O2A-C1
15	A	5003	LHG	C24-C23-O8-C6
16	2	5002	LMG	C24-C25-C26-C27
11	B	1202	CLA	CBD-CGD-O2D-CED
15	a	5003	LHG	C15-C16-C17-C18
16	2	5002	LMG	C16-C17-C18-C19
11	A	1101	CLA	C13-C15-C16-C17
11	a	1126	CLA	O1A-CGA-O2A-C1
15	2	5004	LHG	C35-C36-C37-C38
15	a	5003	LHG	C7-C8-C9-C10
11	2	1211	CLA	O1D-CGD-O2D-CED
14	l	4019	BCR	C19-C20-C21-C22
11	A	1011	CLA	C16-C17-C18-C20
11	2	1213	CLA	CBD-CGD-O2D-CED
11	a	1022	CLA	C4-C3-C5-C6
11	a	1123	CLA	C4-C3-C5-C6
11	1	1801	CLA	C4-C3-C5-C6
11	1	1127	CLA	C4-C3-C5-C6
11	2	1207	CLA	C4-C3-C5-C6
11	A	1116	CLA	CAA-CBA-CGA-O2A
11	A	1103	CLA	C2-C3-C5-C6
15	A	5003	LHG	C26-C27-C28-C29
11	a	1114	CLA	CBA-CGA-O2A-C1
11	8	1502	CLA	O1A-CGA-O2A-C1
11	A	1102	CLA	C11-C10-C8-C9
11	A	1118	CLA	C11-C10-C8-C9
11	A	1118	CLA	C11-C12-C13-C14
11	B	1021	CLA	C6-C7-C8-C9
11	B	1021	CLA	C14-C13-C15-C16
11	B	1223	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	B	1229	CLA	C11-C12-C13-C14
11	B	1238	CLA	C11-C12-C13-C14
11	a	1101	CLA	C11-C10-C8-C9
11	a	1106	CLA	C11-C10-C8-C9
11	a	1109	CLA	C11-C10-C8-C9
11	a	1111	CLA	C11-C10-C8-C9
11	a	1123	CLA	C6-C7-C8-C9
11	a	1140	CLA	C11-C10-C8-C9
11	b	1021	CLA	C11-C12-C13-C14
11	b	1021	CLA	C14-C13-C15-C16
11	b	1202	CLA	C14-C13-C15-C16
11	b	1203	CLA	C11-C10-C8-C9
11	b	1215	CLA	C6-C7-C8-C9
11	b	1235	CLA	C11-C10-C8-C9
11	b	1238	CLA	C11-C10-C8-C9
11	l	1503	CLA	C6-C7-C8-C9
11	1	1101	CLA	C11-C10-C8-C9
11	1	1103	CLA	C11-C12-C13-C14
11	1	1107	CLA	C11-C10-C8-C9
11	1	1118	CLA	C6-C7-C8-C9
11	1	1122	CLA	C6-C7-C8-C9
11	1	1123	CLA	C6-C7-C8-C9
11	1	1127	CLA	C11-C12-C13-C14
11	2	1021	CLA	C6-C7-C8-C9
11	2	1206	CLA	C14-C13-C15-C16
11	2	1215	CLA	C6-C7-C8-C9
11	2	1223	CLA	C11-C10-C8-C9
11	2	1229	CLA	C6-C7-C8-C9
11	2	1238	CLA	C11-C12-C13-C14
12	B	2002	PQN	C21-C22-C23-C24
12	b	2002	PQN	C21-C22-C23-C24
11	a	1012	CLA	O1D-CGD-O2D-CED
11	a	1109	CLA	C13-C15-C16-C17
11	b	1222	CLA	C5-C6-C7-C8
11	8	1501	CLA	C15-C16-C17-C18
15	A	5003	LHG	C2-C3-O3-P
15	a	5003	LHG	C2-C3-O3-P
11	A	1102	CLA	C4B-C3B-CAB-CBB
11	A	1132	CLA	C4B-C3B-CAB-CBB
11	B	1021	CLA	C4B-C3B-CAB-CBB
11	b	1221	CLA	C4B-C3B-CAB-CBB
11	b	1230	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	b	1236	CLA	C4B-C3B-CAB-CBB
11	1	1022	CLA	C4B-C3B-CAB-CBB
11	1	1127	CLA	C4B-C3B-CAB-CBB
11	1	1140	CLA	C4B-C3B-CAB-CBB
11	1	1012	CLA	C4B-C3B-CAB-CBB
11	2	1220	CLA	C4B-C3B-CAB-CBB
11	2	1236	CLA	C4B-C3B-CAB-CBB
15	2	5004	LHG	C28-C29-C30-C31
11	A	1102	CLA	C15-C16-C17-C18
11	1	1111	CLA	C10-C11-C12-C13
11	B	1013	CLA	C16-C17-C18-C20
11	a	1111	CLA	C2A-CAA-CBA-CGA
11	1	1237	CLA	C2A-CAA-CBA-CGA
11	1	1012	CLA	C2A-CAA-CBA-CGA
12	2	2002	PQN	C15-C16-C17-C18
11	1	1131	CLA	C3-C5-C6-C7
15	A	5001	LHG	O6-C4-C5-C6
15	2	5004	LHG	O6-C4-C5-C6
11	A	1022	CLA	C6-C7-C8-C10
11	A	1101	CLA	C12-C13-C15-C16
11	A	1111	CLA	C11-C10-C8-C7
11	A	1119	CLA	C11-C10-C8-C7
11	A	1126	CLA	C12-C13-C15-C16
11	A	1131	CLA	C11-C10-C8-C7
11	A	1140	CLA	C12-C13-C15-C16
11	A	1132	CLA	C11-C10-C8-C7
11	A	1132	CLA	C12-C13-C15-C16
11	B	1210	CLA	C6-C7-C8-C10
11	B	1215	CLA	C11-C10-C8-C7
11	B	1215	CLA	C12-C13-C15-C16
11	B	1229	CLA	C11-C12-C13-C15
11	B	1234	CLA	C11-C10-C8-C7
11	B	1235	CLA	C11-C10-C8-C7
11	B	1206	CLA	C11-C10-C8-C7
11	L	1501	CLA	C11-C10-C8-C7
11	a	1111	CLA	C6-C7-C8-C10
11	a	1119	CLA	C11-C10-C8-C7
11	a	1127	CLA	C11-C10-C8-C7
11	a	1131	CLA	C11-C10-C8-C7
11	a	1137	CLA	C11-C10-C8-C7
11	a	1132	CLA	C12-C13-C15-C16
11	b	1021	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	b	1202	CLA	C12-C13-C15-C16
11	b	1223	CLA	C12-C13-C15-C16
11	b	1238	CLA	C11-C10-C8-C7
11	l	1501	CLA	C11-C12-C13-C15
11	l	1503	CLA	C12-C13-C15-C16
11	1	1104	CLA	C11-C10-C8-C7
11	1	1106	CLA	C11-C12-C13-C15
11	1	1117	CLA	C6-C7-C8-C10
11	1	1118	CLA	C6-C7-C8-C10
11	1	1119	CLA	C11-C12-C13-C15
11	1	1126	CLA	C6-C7-C8-C10
11	1	1127	CLA	C11-C12-C13-C15
11	1	1137	CLA	C6-C7-C8-C10
11	1	1140	CLA	C12-C13-C15-C16
11	2	1225	CLA	C11-C12-C13-C15
11	2	1229	CLA	C11-C10-C8-C7
11	2	1229	CLA	C11-C12-C13-C15
11	2	1234	CLA	C11-C10-C8-C7
11	2	1235	CLA	C6-C7-C8-C10
11	2	1238	CLA	C11-C12-C13-C15
11	A	1128	CLA	C13-C15-C16-C17
11	b	1202	CLA	C8-C10-C11-C12
11	1	1131	CLA	C16-C17-C18-C20
11	A	1801	CLA	C3A-C2A-CAA-CBA
11	A	1022	CLA	C4-C3-C5-C6
11	B	1021	CLA	C3A-C2A-CAA-CBA
11	B	1207	CLA	C4-C3-C5-C6
11	B	1214	CLA	C3A-C2A-CAA-CBA
11	B	1219	CLA	C3A-C2A-CAA-CBA
11	L	1501	CLA	C3A-C2A-CAA-CBA
11	a	1103	CLA	C4-C3-C5-C6
11	a	1106	CLA	C3A-C2A-CAA-CBA
11	b	1225	CLA	C3A-C2A-CAA-CBA
11	1	1118	CLA	C3A-C2A-CAA-CBA
11	B	1206	CLA	C8-C10-C11-C12
11	1	1012	CLA	C15-C16-C17-C18
12	b	2002	PQN	C15-C16-C17-C18
11	1	1110	CLA	O1D-CGD-O2D-CED
11	B	1239	CLA	CAA-CBA-CGA-O2A
11	b	1226	CLA	O1D-CGD-O2D-CED
11	a	1139	CLA	O1A-CGA-O2A-C1
11	a	1118	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	1	1111	CLA	C5-C6-C7-C8
11	a	1132	CLA	CBA-CGA-O2A-C1
14	A	4002	BCR	C19-C20-C21-C22
14	A	4003	BCR	C9-C10-C11-C12
14	f	4020	BCR	C19-C20-C21-C22
14	2	4004	BCR	C19-C20-C21-C22
14	2	4006	BCR	C19-C20-C21-C22
14	2	4011	BCR	C19-C20-C21-C22
14	2	4017	BCR	C9-C10-C11-C12
11	b	1239	CLA	C4C-C3C-CAC-CBC
14	A	4002	BCR	C36-C18-C19-C20
15	2	5004	LHG	C26-C27-C28-C29
11	B	1215	CLA	CAA-CBA-CGA-O2A
11	B	1217	CLA	O1A-CGA-O2A-C1
11	B	1221	CLA	C5-C6-C7-C8
11	B	1214	CLA	C8-C10-C11-C12
11	2	1238	CLA	C10-C11-C12-C13
12	2	2002	PQN	C18-C20-C21-C22
14	2	4017	BCR	C7-C8-C9-C10
11	B	1201	CLA	C2A-CAA-CBA-CGA
11	1	1113	CLA	C2A-CAA-CBA-CGA
11	2	1216	CLA	C2A-CAA-CBA-CGA
11	B	1216	CLA	CBA-CGA-O2A-C1
15	a	5001	LHG	C4-C5-C6-O8
15	1	5001	LHG	C4-C5-C6-O8
15	1	5003	LHG	C4-C5-C6-O8
16	B	5002	LMG	C7-C8-C9-O8
11	B	1214	CLA	C10-C11-C12-C13
16	B	5002	LMG	C38-C39-C40-C41
11	b	1229	CLA	C16-C17-C18-C20
11	a	1102	CLA	C15-C16-C17-C18
11	a	1106	CLA	C8-C10-C11-C12
11	a	1109	CLA	C8-C10-C11-C12
15	b	5004	LHG	C13-C14-C15-C16
12	B	2002	PQN	C18-C20-C21-C22
15	b	5004	LHG	C9-C10-C11-C12
11	A	1103	CLA	C4-C3-C5-C6
11	2	1229	CLA	CAA-CBA-CGA-O2A
11	A	1022	CLA	C2-C3-C5-C6
11	a	1103	CLA	C2-C3-C5-C6
11	a	1123	CLA	C2-C3-C5-C6
11	1	1127	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	a	1106	CLA	C3-C5-C6-C7
11	B	1221	CLA	O1D-CGD-O2D-CED
11	L	1503	CLA	C5-C6-C7-C8
11	2	1238	CLA	C8-C10-C11-C12
15	2	5004	LHG	O6-C4-C5-O7
11	1	1125	CLA	O1D-CGD-O2D-CED
11	1	1140	CLA	C2B-C3B-CAB-CBB
11	2	1232	CLA	C2B-C3B-CAB-CBB
14	A	4003	BCR	C23-C24-C25-C26
14	b	4006	BCR	C1-C6-C7-C8
14	b	4009	BCR	C23-C24-C25-C30
14	2	4009	BCR	C23-C24-C25-C30
14	6	4020	BCR	C23-C24-C25-C30
14	6	4013	BCR	C23-C24-C25-C26
11	1	1101	CLA	C5-C6-C7-C8
11	1	1128	CLA	C8-C10-C11-C12
11	a	1111	CLA	C5-C6-C7-C8
11	b	1207	CLA	C13-C15-C16-C17
11	2	1204	CLA	C10-C11-C12-C13
11	2	1206	CLA	C13-C15-C16-C17
16	b	5002	LMG	C29-C30-C31-C32
11	2	1239	CLA	O1A-CGA-O2A-C1
11	1	1110	CLA	C6-C7-C8-C9
11	A	1237	CLA	C6-C7-C8-C9
11	A	1104	CLA	C16-C17-C18-C20
11	b	1217	CLA	C2A-CAA-CBA-CGA
11	A	1112	CLA	C2C-C3C-CAC-CBC
16	b	5002	LMG	O1-C7-C8-O7
16	2	5002	LMG	O1-C7-C8-O7
11	b	1201	CLA	C5-C6-C7-C8
11	1	1122	CLA	C4C-C3C-CAC-CBC
11	B	1224	CLA	C4C-C3C-CAC-CBC
15	1	5001	LHG	C10-C11-C12-C13
11	A	1127	CLA	C13-C15-C16-C17
11	A	1128	CLA	C5-C6-C7-C8
11	1	1117	CLA	C8-C10-C11-C12
11	a	1022	CLA	C2-C3-C5-C6
11	A	1012	CLA	CBA-CGA-O2A-C1
11	b	1229	CLA	CBA-CGA-O2A-C1
11	A	1140	CLA	C3-C5-C6-C7
11	A	1103	CLA	C6-C7-C8-C9
11	A	1126	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	A	1127	CLA	C6-C7-C8-C9
11	A	1131	CLA	C6-C7-C8-C9
11	A	1132	CLA	C14-C13-C15-C16
11	B	1215	CLA	C14-C13-C15-C16
11	a	1111	CLA	C6-C7-C8-C9
11	a	1132	CLA	C14-C13-C15-C16
11	b	1215	CLA	C14-C13-C15-C16
11	1	1128	CLA	C11-C10-C8-C9
11	1	1131	CLA	C6-C7-C8-C9
11	2	1021	CLA	C11-C12-C13-C14
11	2	1023	CLA	C11-C10-C8-C9
11	2	1215	CLA	C14-C13-C15-C16
11	2	1235	CLA	C6-C7-C8-C9
11	2	1238	CLA	C5-C6-C7-C8
15	A	5001	LHG	C19-C20-C21-C22
11	B	1013	CLA	C16-C17-C18-C19
11	1	1124	CLA	C6-C7-C8-C9
15	b	5004	LHG	C26-C27-C28-C29
11	b	1235	CLA	CBA-CGA-O2A-C1
14	b	4004	BCR	C19-C20-C21-C22
14	f	4013	BCR	C13-C14-C15-C16
11	B	1207	CLA	C2-C3-C5-C6
11	B	1205	CLA	C6-C7-C8-C9
11	a	1117	CLA	C15-C16-C17-C18
15	A	5001	LHG	C11-C10-C9-C8
11	A	1103	CLA	C8-C10-C11-C12
11	b	1223	CLA	C10-C11-C12-C13
15	a	5003	LHG	C18-C19-C20-C21
14	2	4005	BCR	C11-C10-C9-C34
14	8	4019	BCR	C20-C21-C22-C37
11	B	1226	CLA	C3-C5-C6-C7
11	a	1022	CLA	C3-C5-C6-C7
11	b	1225	CLA	C3-C5-C6-C7
11	B	1021	CLA	CAA-CBA-CGA-O2A
11	B	1206	CLA	C13-C15-C16-C17
11	1	1012	CLA	C10-C11-C12-C13
15	1	5003	LHG	O6-C4-C5-C6
11	A	1111	CLA	O1D-CGD-O2D-CED
15	a	5003	LHG	C16-C17-C18-C19
16	b	5002	LMG	C32-C33-C34-C35
11	2	1202	CLA	C15-C16-C17-C18
11	A	1118	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
11	A	1128	CLA	C11-C10-C8-C7
11	A	1140	CLA	C6-C7-C8-C10
11	A	1012	CLA	C6-C7-C8-C10
11	B	1021	CLA	C11-C12-C13-C15
11	B	1226	CLA	C6-C7-C8-C10
11	B	1226	CLA	C11-C10-C8-C7
11	B	1234	CLA	C6-C7-C8-C10
11	L	1501	CLA	C6-C7-C8-C10
11	a	1101	CLA	C6-C7-C8-C10
11	a	1109	CLA	C11-C12-C13-C15
11	a	1119	CLA	C12-C13-C15-C16
11	a	1012	CLA	C11-C10-C8-C7
11	b	1204	CLA	C12-C13-C15-C16
11	b	1215	CLA	C12-C13-C15-C16
11	b	1223	CLA	C11-C12-C13-C15
11	b	1229	CLA	C11-C12-C13-C15
11	2	1021	CLA	C11-C12-C13-C15
11	2	1215	CLA	C12-C13-C15-C16
12	A	2001	PQN	C17-C18-C20-C21
12	b	2002	PQN	C22-C23-C25-C26
12	2	2002	PQN	C22-C23-C25-C26
11	2	1213	CLA	O1D-CGD-O2D-CED
11	B	1013	CLA	C10-C11-C12-C13
11	a	1111	CLA	C8-C10-C11-C12
11	b	1204	CLA	C10-C11-C12-C13
11	1	1131	CLA	C15-C16-C17-C18
11	A	1129	CLA	C2C-C3C-CAC-CBC
14	A	4002	BCR	C17-C18-C19-C20
14	A	4008	BCR	C21-C22-C23-C24
14	L	4019	BCR	C11-C12-C13-C14
14	f	4020	BCR	C11-C12-C13-C14
11	A	1106	CLA	O1A-CGA-O2A-C1
11	A	1137	CLA	O1A-CGA-O2A-C1
11	A	1012	CLA	O1A-CGA-O2A-C1
11	a	1132	CLA	O1A-CGA-O2A-C1
11	1	1116	CLA	O1A-CGA-O2A-C1
11	1	1126	CLA	O1A-CGA-O2A-C1
11	2	1210	CLA	O1A-CGA-O2A-C1
11	1	1109	CLA	C5-C6-C7-C8
11	B	1224	CLA	C2A-CAA-CBA-CGA
11	b	1013	CLA	C2A-CAA-CBA-CGA
11	1	1131	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	B	1219	CLA	C4-C3-C5-C6
11	b	1234	CLA	C4-C3-C5-C6
11	L	1503	CLA	CAA-CBA-CGA-O2A
11	2	1207	CLA	C2-C3-C5-C6
11	A	1011	CLA	O2A-C1-C2-C3
11	B	1013	CLA	O2A-C1-C2-C3
11	b	1023	CLA	O2A-C1-C2-C3
11	A	1101	CLA	C16-C17-C18-C20
11	B	1224	CLA	C6-C7-C8-C9
16	B	5002	LMG	C42-C43-C44-C45
15	A	5001	LHG	C35-C36-C37-C38
15	A	5001	LHG	C14-C15-C16-C17
11	B	1229	CLA	C15-C16-C17-C18
11	B	1217	CLA	CAA-CBA-CGA-O2A
15	A	5003	LHG	O6-C4-C5-O7
15	1	5003	LHG	O6-C4-C5-O7
16	B	5002	LMG	O1-C7-C8-C9
15	1	5001	LHG	C8-C7-O7-C5
11	B	1202	CLA	C13-C15-C16-C17
11	a	1109	CLA	C10-C11-C12-C13
11	b	1229	CLA	O1A-CGA-O2A-C1
15	A	5003	LHG	O10-C23-O8-C6
11	1	1116	CLA	CBA-CGA-O2A-C1
11	b	1202	CLA	C10-C11-C12-C13
11	2	1213	CLA	C10-C11-C12-C13
11	2	1229	CLA	C4-C3-C5-C6
11	A	1137	CLA	C2-C3-C5-C6
11	1	1122	CLA	C2-C3-C5-C6
15	2	5004	LHG	C30-C31-C32-C33
15	B	5004	LHG	C30-C31-C32-C33
11	1	1131	CLA	C10-C11-C12-C13
16	B	5002	LMG	O1-C7-C8-O7
16	2	5002	LMG	O7-C8-C9-O8
11	A	1118	CLA	C6-C7-C8-C9
11	B	1021	CLA	C11-C12-C13-C14
11	B	1215	CLA	C6-C7-C8-C9
11	B	1222	CLA	C6-C7-C8-C9
11	B	1235	CLA	C11-C10-C8-C9
11	L	1501	CLA	C11-C10-C8-C9
11	a	1137	CLA	C6-C7-C8-C9
11	b	1013	CLA	C6-C7-C8-C9
11	b	1229	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	1	1111	CLA	C11-C10-C8-C9
11	1	1131	CLA	C11-C12-C13-C14
11	2	1226	CLA	C11-C10-C8-C9
11	2	1234	CLA	C11-C10-C8-C9
11	8	1501	CLA	C14-C13-C15-C16
12	A	2001	PQN	C19-C18-C20-C21
11	A	1104	CLA	C16-C17-C18-C19
15	a	5001	LHG	C16-C17-C18-C19
11	B	1216	CLA	O1A-CGA-O2A-C1
15	1	5003	LHG	C15-C16-C17-C18
12	2	2002	PQN	C20-C21-C22-C23
15	1	5003	LHG	C10-C11-C12-C13
11	A	1116	CLA	C6-C7-C8-C9
15	a	5001	LHG	C33-C34-C35-C36
15	B	5004	LHG	C31-C32-C33-C34
11	a	1139	CLA	C2-C1-O2A-CGA
11	2	1013	CLA	C2-C1-O2A-CGA
11	A	1132	CLA	C4-C3-C5-C6
11	1	1123	CLA	C4-C3-C5-C6
11	2	1021	CLA	C4-C3-C5-C6
11	B	1219	CLA	C2-C3-C5-C6
11	2	1229	CLA	C2-C3-C5-C6
15	1	5003	LHG	C1-C2-C3-O3
11	A	1117	CLA	C8-C10-C11-C12
11	b	1210	CLA	C13-C15-C16-C17
11	2	1223	CLA	C13-C15-C16-C17
11	A	1237	CLA	C6-C7-C8-C10
11	1	1111	CLA	C11-C12-C13-C14
11	2	1213	CLA	C16-C17-C18-C20
11	b	1234	CLA	C8-C10-C11-C12
11	b	1238	CLA	C15-C16-C17-C18
11	b	1222	CLA	C3-C5-C6-C7
15	B	5004	LHG	C26-C27-C28-C29
14	2	4005	BCR	C10-C11-C12-C13
15	A	5001	LHG	C17-C18-C19-C20
15	b	5004	LHG	C34-C35-C36-C37
11	A	1114	CLA	C4C-C3C-CAC-CBC
11	2	1235	CLA	C10-C11-C12-C13
11	1	1114	CLA	CBA-CGA-O2A-C1
11	b	1235	CLA	O1A-CGA-O2A-C1
11	2	1223	CLA	C5-C6-C7-C8
14	B	4011	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
11	2	1239	CLA	C4C-C3C-CAC-CBC
11	A	1801	CLA	C1A-C2A-CAA-CBA
11	A	1109	CLA	C4B-C3B-CAB-CBB
11	A	1116	CLA	C4B-C3B-CAB-CBB
11	A	1118	CLA	C1A-C2A-CAA-CBA
11	A	1128	CLA	C1A-C2A-CAA-CBA
11	A	1139	CLA	C4B-C3B-CAB-CBB
11	B	1207	CLA	C4B-C3B-CAB-CBB
11	B	1208	CLA	C1A-C2A-CAA-CBA
11	B	1210	CLA	C1A-C2A-CAA-CBA
11	B	1214	CLA	C1A-C2A-CAA-CBA
11	B	1216	CLA	C1A-C2A-CAA-CBA
11	B	1219	CLA	C1A-C2A-CAA-CBA
11	B	1223	CLA	C4B-C3B-CAB-CBB
11	B	1225	CLA	C4B-C3B-CAB-CBB
11	B	1229	CLA	C1A-C2A-CAA-CBA
11	B	1235	CLA	C4B-C3B-CAB-CBB
11	B	1239	CLA	C4B-C3B-CAB-CBB
11	L	1501	CLA	C4B-C3B-CAB-CBB
11	a	1101	CLA	C4B-C3B-CAB-CBB
11	a	1124	CLA	C4B-C3B-CAB-CBB
11	a	1130	CLA	C1A-C2A-CAA-CBA
11	a	1138	CLA	C4B-C3B-CAB-CBB
11	a	1139	CLA	C4B-C3B-CAB-CBB
11	a	1129	CLA	C1A-C2A-CAA-CBA
11	a	1132	CLA	C1A-C2A-CAA-CBA
11	b	1205	CLA	C4B-C3B-CAB-CBB
11	b	1212	CLA	C1A-C2A-CAA-CBA
11	b	1231	CLA	C1A-C2A-CAA-CBA
11	b	1231	CLA	C4B-C3B-CAB-CBB
11	b	1232	CLA	C4B-C3B-CAB-CBB
11	l	1501	CLA	C4B-C3B-CAB-CBB
11	1	1801	CLA	C4B-C3B-CAB-CBB
11	1	1108	CLA	C4B-C3B-CAB-CBB
11	1	1116	CLA	C4B-C3B-CAB-CBB
11	1	1118	CLA	C1A-C2A-CAA-CBA
11	1	1122	CLA	C1A-C2A-CAA-CBA
11	1	1130	CLA	C1A-C2A-CAA-CBA
11	1	1131	CLA	C4B-C3B-CAB-CBB
11	1	1138	CLA	C4B-C3B-CAB-CBB
11	1	1129	CLA	C4B-C3B-CAB-CBB
11	2	1218	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	2	1230	CLA	C4B-C3B-CAB-CBB
11	2	1232	CLA	C4B-C3B-CAB-CBB
11	8	1502	CLA	C4B-C3B-CAB-CBB
15	1	5001	LHG	C30-C31-C32-C33
11	B	1221	CLA	C6-C7-C8-C9
11	1	1118	CLA	CAA-CBA-CGA-O2A
14	B	4006	BCR	C11-C12-C13-C14
14	1	4003	BCR	C11-C12-C13-C14
14	B	4004	BCR	C19-C20-C21-C22
14	a	4002	BCR	C9-C10-C11-C12
11	l	1503	CLA	C16-C17-C18-C20
11	b	1023	CLA	C2A-CAA-CBA-CGA
11	B	1013	CLA	C15-C16-C17-C18
11	2	1202	CLA	C8-C10-C11-C12
15	A	5003	LHG	O6-C4-C5-C6
15	a	5003	LHG	O6-C4-C5-C6
15	1	5001	LHG	O9-C7-O7-C5
11	B	1205	CLA	C5-C6-C7-C8
11	A	1102	CLA	C11-C12-C13-C15
11	A	1106	CLA	C11-C12-C13-C15
11	A	1109	CLA	C11-C10-C8-C7
11	A	1011	CLA	C11-C10-C8-C7
11	B	1213	CLA	C11-C10-C8-C7
11	B	1213	CLA	C12-C13-C15-C16
11	a	1103	CLA	C11-C12-C13-C15
11	a	1104	CLA	C11-C12-C13-C15
11	a	1117	CLA	C6-C7-C8-C10
11	a	1012	CLA	C11-C12-C13-C15
11	b	1214	CLA	C11-C10-C8-C7
11	1	1022	CLA	C12-C13-C15-C16
11	1	1102	CLA	C11-C12-C13-C15
11	1	1119	CLA	C11-C10-C8-C7
11	1	1126	CLA	C11-C10-C8-C7
11	1	1126	CLA	C12-C13-C15-C16
11	2	1021	CLA	C12-C13-C15-C16
11	2	1210	CLA	C11-C12-C13-C15
11	2	1216	CLA	C11-C10-C8-C7
11	2	1222	CLA	C6-C7-C8-C10
11	2	1226	CLA	C6-C7-C8-C10
11	K	1401	CLA	C11-C12-C13-C15
11	k	1401	CLA	C11-C12-C13-C15
11	0	1401	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
12	B	2002	PQN	C22-C23-C25-C26
16	b	5002	LMG	C15-C16-C17-C18
11	B	1202	CLA	O1D-CGD-O2D-CED
15	1	5003	LHG	C35-C36-C37-C38
11	2	1204	CLA	C4-C3-C5-C6
11	1	1133	CLA	O1A-CGA-O2A-C1
15	A	5001	LHG	O6-C4-C5-O7
15	a	5001	LHG	O6-C4-C5-O7
15	a	5003	LHG	O6-C4-C5-O7
11	A	1102	CLA	C3-C5-C6-C7
11	A	1104	CLA	C11-C10-C8-C9
11	A	1119	CLA	C6-C7-C8-C9
11	a	1104	CLA	C11-C10-C8-C9
11	a	1106	CLA	C6-C7-C8-C9
11	a	1119	CLA	C14-C13-C15-C16
11	a	1012	CLA	C11-C12-C13-C14
11	b	1021	CLA	C6-C7-C8-C9
11	b	1210	CLA	C11-C10-C8-C9
11	1	1104	CLA	C6-C7-C8-C9
11	1	1107	CLA	C6-C7-C8-C9
11	1	1140	CLA	C14-C13-C15-C16
11	2	1210	CLA	C11-C10-C8-C9
11	2	1225	CLA	C11-C12-C13-C14
12	a	2001	PQN	C21-C22-C23-C24
11	2	1217	CLA	O1A-CGA-O2A-C1
14	A	4003	BCR	C19-C20-C21-C22
14	B	4006	BCR	C19-C20-C21-C22
14	l	4019	BCR	C13-C14-C15-C16
11	2	1224	CLA	C6-C7-C8-C9
11	B	1222	CLA	C5-C6-C7-C8
15	1	5001	LHG	C11-C10-C9-C8
11	a	1120	CLA	C2C-C3C-CAC-CBC
11	b	1224	CLA	C6-C7-C8-C9
11	a	1132	CLA	C4-C3-C5-C6
11	b	1206	CLA	C4-C3-C5-C6
11	A	1110	CLA	C5-C6-C7-C8
11	A	1111	CLA	CAD-CBD-CGD-O2D
11	A	1012	CLA	CAD-CBD-CGD-O2D
11	A	1129	CLA	CAD-CBD-CGD-O2D
11	A	1135	CLA	CAD-CBD-CGD-O2D
11	L	1502	CLA	CAD-CBD-CGD-O2D
11	a	1111	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	a	1118	CLA	CAD-CBD-CGD-O2D
11	a	1120	CLA	CAD-CBD-CGD-O2D
11	b	1207	CLA	CAD-CBD-CGD-O2D
11	b	1210	CLA	CAD-CBD-CGD-O2D
11	b	1212	CLA	CAD-CBD-CGD-O2D
11	1	1125	CLA	CAD-CBD-CGD-O2D
11	1	1011	CLA	CAD-CBD-CGD-O2D
11	1	1012	CLA	CAD-CBD-CGD-O2D
11	2	1202	CLA	CAD-CBD-CGD-O2D
11	b	1229	CLA	C15-C16-C17-C18
11	1	1126	CLA	C13-C15-C16-C17
11	2	1204	CLA	O1A-CGA-O2A-C1
16	2	5002	LMG	C30-C31-C32-C33
15	1	5003	LHG	C24-C23-O8-C6
11	1	1102	CLA	C10-C11-C12-C13
11	A	1123	CLA	C16-C17-C18-C20
11	b	1224	CLA	C2C-C3C-CAC-CBC
11	A	1111	CLA	C2A-CAA-CBA-CGA
11	B	1023	CLA	C2A-CAA-CBA-CGA
11	b	1224	CLA	C2A-CAA-CBA-CGA
11	2	1224	CLA	C2A-CAA-CBA-CGA
11	1	1138	CLA	O1A-CGA-O2A-C1
11	l	1503	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	C11-C12-C13-C14
11	A	1111	CLA	CAD-CBD-CGD-O1D
11	A	1112	CLA	CHA-CBD-CGD-O1D
11	A	1112	CLA	CHA-CBD-CGD-O2D
11	A	1012	CLA	CAD-CBD-CGD-O1D
11	A	1129	CLA	CAD-CBD-CGD-O1D
11	A	1135	CLA	CAD-CBD-CGD-O1D
11	B	1201	CLA	CHA-CBD-CGD-O1D
11	B	1212	CLA	CAD-CBD-CGD-O1D
11	B	1227	CLA	CHA-CBD-CGD-O1D
11	B	1227	CLA	CHA-CBD-CGD-O2D
11	L	1502	CLA	CAD-CBD-CGD-O1D
11	a	1111	CLA	CAD-CBD-CGD-O1D
11	a	1118	CLA	CAD-CBD-CGD-O1D
11	a	1120	CLA	CAD-CBD-CGD-O1D
11	a	1129	CLA	CAD-CBD-CGD-O1D
11	b	1201	CLA	CHA-CBD-CGD-O1D
11	b	1201	CLA	CHA-CBD-CGD-O2D
11	b	1207	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	b	1210	CLA	CAD-CBD-CGD-O1D
11	b	1212	CLA	CAD-CBD-CGD-O1D
11	b	1227	CLA	CHA-CBD-CGD-O1D
11	b	1227	CLA	CHA-CBD-CGD-O2D
11	b	1236	CLA	CAD-CBD-CGD-O1D
11	1	1101	CLA	CHA-CBD-CGD-O1D
11	1	1101	CLA	CHA-CBD-CGD-O2D
11	1	1118	CLA	CHA-CBD-CGD-O1D
11	1	1118	CLA	CHA-CBD-CGD-O2D
11	1	1125	CLA	CAD-CBD-CGD-O1D
11	1	1011	CLA	CAD-CBD-CGD-O1D
11	1	1012	CLA	CAD-CBD-CGD-O1D
11	2	1202	CLA	CAD-CBD-CGD-O1D
11	2	1207	CLA	CAD-CBD-CGD-O1D
11	2	1223	CLA	CHA-CBD-CGD-O1D
11	2	1223	CLA	CHA-CBD-CGD-O2D
11	2	1226	CLA	CHA-CBD-CGD-O1D
11	2	1226	CLA	CHA-CBD-CGD-O2D
14	B	4011	BCR	C19-C20-C21-C22
14	L	4022	BCR	C19-C20-C21-C22
14	1	4001	BCR	C9-C10-C11-C12
15	A	5001	LHG	C4-O6-P-O3
15	a	5001	LHG	C4-O6-P-O4
15	2	5004	LHG	C3-O3-P-O5
11	a	1111	CLA	C3-C5-C6-C7
11	b	1221	CLA	C3-C5-C6-C7
11	B	1203	CLA	C4-C3-C5-C6
11	B	1229	CLA	C4-C3-C5-C6
11	B	1235	CLA	C4-C3-C5-C6
11	A	1022	CLA	C2B-C3B-CAB-CBB
11	A	1109	CLA	C2B-C3B-CAB-CBB
11	A	1116	CLA	C2B-C3B-CAB-CBB
11	A	1124	CLA	C2B-C3B-CAB-CBB
11	B	1013	CLA	C2B-C3B-CAB-CBB
11	B	1021	CLA	C2B-C3B-CAB-CBB
11	B	1204	CLA	C2B-C3B-CAB-CBB
11	B	1224	CLA	C2B-C3B-CAB-CBB
11	B	1232	CLA	C2B-C3B-CAB-CBB
11	B	1234	CLA	C2B-C3B-CAB-CBB
11	a	1101	CLA	C2B-C3B-CAB-CBB
11	a	1139	CLA	C2B-C3B-CAB-CBB
11	a	1120	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	a	1135	CLA	C2B-C3B-CAB-CBB
11	b	1202	CLA	C2B-C3B-CAB-CBB
11	b	1221	CLA	C2B-C3B-CAB-CBB
11	b	1224	CLA	C2B-C3B-CAB-CBB
11	b	1225	CLA	C2B-C3B-CAB-CBB
11	b	1227	CLA	C2B-C3B-CAB-CBB
11	b	1240	CLA	C2B-C3B-CAB-CBB
11	l	1502	CLA	C2B-C3B-CAB-CBB
11	1	1108	CLA	C2B-C3B-CAB-CBB
11	1	1127	CLA	C2B-C3B-CAB-CBB
11	1	1131	CLA	C2B-C3B-CAB-CBB
11	1	1138	CLA	C2B-C3B-CAB-CBB
11	1	1120	CLA	C2B-C3B-CAB-CBB
11	2	1220	CLA	C2B-C3B-CAB-CBB
11	2	1230	CLA	C2B-C3B-CAB-CBB
11	8	1502	CLA	C2B-C3B-CAB-CBB
14	B	4009	BCR	C23-C24-C25-C26
14	l	4022	BCR	C23-C24-C25-C30
11	1	1123	CLA	C2-C3-C5-C6
11	2	1204	CLA	C2-C3-C5-C6
11	B	1234	CLA	C8-C10-C11-C12
11	b	1229	CLA	C10-C11-C12-C13
14	A	4007	BCR	C7-C8-C9-C34
15	A	5001	LHG	C2-C3-O3-P
15	a	5001	LHG	C2-C3-O3-P
15	1	5003	LHG	C2-C3-O3-P
11	1	1114	CLA	C4C-C3C-CAC-CBC
11	2	1235	CLA	C5-C6-C7-C8
11	a	1123	CLA	C16-C17-C18-C20
11	l	1503	CLA	C2A-CAA-CBA-CGA
11	B	1239	CLA	C2C-C3C-CAC-CBC
11	a	1131	CLA	C2C-C3C-CAC-CBC
11	b	1209	CLA	C2C-C3C-CAC-CBC
11	B	1222	CLA	C11-C10-C8-C7
11	2	1221	CLA	C6-C7-C8-C9
16	2	5002	LMG	C9-C8-O7-C10
14	A	4007	BCR	C18-C19-C20-C21
14	A	4008	BCR	C18-C19-C20-C21
14	F	4013	BCR	C18-C19-C20-C21
14	L	4019	BCR	C18-C19-C20-C21
14	a	4007	BCR	C18-C19-C20-C21
14	a	4008	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
14	b	4010	BCR	C18-C19-C20-C21
14	f	4013	BCR	C18-C19-C20-C21
14	1	4007	BCR	C18-C19-C20-C21
14	1	4008	BCR	C18-C19-C20-C21
14	6	4013	BCR	C18-C19-C20-C21
11	2	1217	CLA	CAA-CBA-CGA-O2A
11	a	1140	CLA	C5-C6-C7-C8
11	b	1234	CLA	C2-C3-C5-C6
16	B	5002	LMG	C12-C13-C14-C15
14	a	4003	BCR	C19-C20-C21-C22
14	7	4021	BCR	C19-C20-C21-C22
11	1	1127	CLA	C16-C17-C18-C20
11	1	1012	CLA	C16-C17-C18-C19
11	a	1117	CLA	O1A-CGA-O2A-C1
11	A	1103	CLA	C11-C12-C13-C14
11	A	1123	CLA	C11-C10-C8-C9
11	B	1229	CLA	C11-C10-C8-C9
11	b	1222	CLA	C6-C7-C8-C9
11	b	1223	CLA	C11-C12-C13-C14
11	b	1223	CLA	C14-C13-C15-C16
11	b	1229	CLA	C6-C7-C8-C9
11	1	1103	CLA	C11-C10-C8-C9
11	1	1117	CLA	C6-C7-C8-C9
11	2	1021	CLA	C11-C10-C8-C9
11	2	1203	CLA	C11-C10-C8-C9
11	B	1210	CLA	C11-C10-C8-C7
11	B	1223	CLA	C6-C7-C8-C10
11	a	1128	CLA	C11-C10-C8-C7
11	b	1226	CLA	C11-C12-C13-C15
11	1	1106	CLA	C12-C13-C15-C16
11	8	1501	CLA	C12-C13-C15-C16
11	a	1131	CLA	C13-C15-C16-C17
14	b	4009	BCR	C16-C17-C18-C19
14	2	4005	BCR	C11-C10-C9-C8
11	B	1220	CLA	CBA-CGA-O2A-C1
11	A	1101	CLA	C16-C17-C18-C19
11	2	1202	CLA	C13-C15-C16-C17
11	1	1122	CLA	O1D-CGD-O2D-CED
11	A	1801	CLA	CAA-CBA-CGA-O2A
11	b	1229	CLA	CAA-CBA-CGA-O2A
11	b	1239	CLA	CAA-CBA-CGA-O2A
11	B	1223	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	1	1122	CLA	CBD-CGD-O2D-CED
15	1	5003	LHG	O10-C23-O8-C6
15	a	5003	LHG	C10-C11-C12-C13
11	2	1021	CLA	C2-C3-C5-C6
11	2	1213	CLA	C16-C17-C18-C19
11	a	1116	CLA	C2C-C3C-CAC-CBC
11	2	1224	CLA	C2C-C3C-CAC-CBC
15	A	5003	LHG	O7-C5-C6-O8
14	F	4020	BCR	C19-C20-C21-C22
11	1	1111	CLA	C11-C12-C13-C15
15	A	5001	LHG	C30-C31-C32-C33
11	B	1013	CLA	C2A-CAA-CBA-CGA
11	2	1013	CLA	C2A-CAA-CBA-CGA
11	1	1022	CLA	C10-C11-C12-C13
11	2	1217	CLA	C4C-C3C-CAC-CBC
12	1	2001	PQN	C13-C15-C16-C17
15	A	5001	LHG	C16-C17-C18-C19
11	a	1117	CLA	CBA-CGA-O2A-C1
11	1	1139	CLA	C2-C1-O2A-CGA
11	a	1237	CLA	C4-C3-C5-C6
11	b	1235	CLA	C4-C3-C5-C6
11	2	1219	CLA	C4-C3-C5-C6
11	1	1116	CLA	CAA-CBA-CGA-O2A
11	8	1503	CLA	CAA-CBA-CGA-O2A
16	b	5002	LMG	O7-C10-C11-C12
16	2	5002	LMG	C7-C8-C9-O8
11	a	1115	CLA	C2C-C3C-CAC-CBC
11	A	1140	CLA	C4C-C3C-CAC-CBC
11	A	1011	CLA	CAA-CBA-CGA-O2A
11	2	1215	CLA	CAA-CBA-CGA-O2A
11	a	1103	CLA	C5-C6-C7-C8
11	A	1132	CLA	C10-C11-C12-C13
15	A	5003	LHG	C17-C18-C19-C20
15	A	5001	LHG	C25-C26-C27-C28
11	2	1217	CLA	CBA-CGA-O2A-C1
11	A	1132	CLA	C2A-CAA-CBA-CGA
11	1	1127	CLA	C2A-CAA-CBA-CGA
11	1	1139	CLA	C2A-CAA-CBA-CGA
14	A	4007	BCR	C9-C10-C11-C12
14	B	4010	BCR	C19-C20-C21-C22
14	1	4007	BCR	C9-C10-C11-C12
14	2	4010	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	2	4014	BCR	C13-C14-C15-C16
14	7	4021	BCR	C9-C10-C11-C12
11	1	1140	CLA	C3-C5-C6-C7
11	B	1234	CLA	C4-C3-C5-C6
11	a	1114	CLA	O1A-CGA-O2A-C1
11	B	1223	CLA	O1D-CGD-O2D-CED
11	B	1240	CLA	C2C-C3C-CAC-CBC
11	A	1102	CLA	C11-C12-C13-C14
11	A	1111	CLA	C11-C10-C8-C9
11	L	1501	CLA	C14-C13-C15-C16
11	a	1119	CLA	C6-C7-C8-C9
11	a	1011	CLA	C6-C7-C8-C9
11	l	1503	CLA	C14-C13-C15-C16
11	1	1022	CLA	C11-C10-C8-C9
11	1	1126	CLA	C6-C7-C8-C9
11	2	1234	CLA	C6-C7-C8-C9
12	1	2001	PQN	C21-C22-C23-C24
11	A	1132	CLA	CBA-CGA-O2A-C1
11	2	1204	CLA	CBA-CGA-O2A-C1
11	A	1104	CLA	C4B-C3B-CAB-CBB
11	A	1133	CLA	C4B-C3B-CAB-CBB
11	L	1502	CLA	C4B-C3B-CAB-CBB
11	L	1503	CLA	C4B-C3B-CAB-CBB
11	b	1206	CLA	C4B-C3B-CAB-CBB
11	l	1502	CLA	C4B-C3B-CAB-CBB
11	1	1113	CLA	C4B-C3B-CAB-CBB
11	2	1209	CLA	C4B-C3B-CAB-CBB
11	A	1134	CLA	C2C-C3C-CAC-CBC
11	1	1134	CLA	C2C-C3C-CAC-CBC
11	a	1111	CLA	C11-C12-C13-C15
11	1	1124	CLA	C6-C7-C8-C10
15	A	5001	LHG	C29-C30-C31-C32
11	2	1235	CLA	CBA-CGA-O2A-C1
11	A	1125	CLA	C4-C3-C5-C6
11	b	1215	CLA	CAA-CBA-CGA-O2A
15	a	5003	LHG	C34-C35-C36-C37
11	A	1132	CLA	C2-C3-C5-C6
11	B	1203	CLA	C2-C3-C5-C6
11	B	1234	CLA	C2-C3-C5-C6
11	b	1235	CLA	C2-C3-C5-C6
11	2	1219	CLA	C2-C3-C5-C6
11	b	1209	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	2	1235	CLA	O1A-CGA-O2A-C1
14	b	4005	BCR	C13-C14-C15-C16
11	l	1503	CLA	C16-C17-C18-C19
11	A	1103	CLA	C11-C12-C13-C15
11	B	1214	CLA	C11-C10-C8-C7
11	a	1102	CLA	C11-C10-C8-C7
11	b	1222	CLA	C6-C7-C8-C10
11	1	1102	CLA	C6-C7-C8-C10
11	1	1119	CLA	C6-C7-C8-C10
11	1	1123	CLA	C6-C7-C8-C10
11	2	1214	CLA	C11-C10-C8-C7
11	2	1215	CLA	C6-C7-C8-C10
11	2	1238	CLA	C11-C10-C8-C7
11	2	1210	CLA	C15-C16-C17-C18
15	a	5001	LHG	C30-C31-C32-C33
11	2	1203	CLA	C5-C6-C7-C8
11	b	1210	CLA	O1A-CGA-O2A-C1
11	a	1237	CLA	C3A-C2A-CAA-CBA
11	b	1207	CLA	C4-C3-C5-C6
11	2	1209	CLA	C3A-C2A-CAA-CBA
11	2	1214	CLA	C3A-C2A-CAA-CBA
11	2	1216	CLA	C3A-C2A-CAA-CBA
11	A	1801	CLA	C2-C3-C5-C6
11	B	1229	CLA	C2-C3-C5-C6
11	b	1206	CLA	C2-C3-C5-C6
14	B	4006	BCR	C20-C21-C22-C37
14	F	4020	BCR	C20-C21-C22-C37
14	F	4013	BCR	C20-C21-C22-C37
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	4020	BCR	C20-C21-C22-C37
14	f	4013	BCR	C20-C21-C22-C37
14	1	4002	BCR	C16-C17-C18-C36
14	2	4006	BCR	C20-C21-C22-C37
14	2	4011	BCR	C16-C17-C18-C36
14	6	4020	BCR	C20-C21-C22-C37
14	6	4013	BCR	C20-C21-C22-C37
11	1	1132	CLA	C13-C15-C16-C17
11	B	1201	CLA	C2C-C3C-CAC-CBC
11	b	1220	CLA	CBA-CGA-O2A-C1
11	B	1234	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	1	4001	BCR	C19-C20-C21-C22
15	1	5003	LHG	C12-C13-C14-C15
11	A	1124	CLA	C6-C7-C8-C9
15	B	5004	LHG	C35-C36-C37-C38
11	B	1202	CLA	C15-C16-C17-C18
11	1	1119	CLA	C8-C10-C11-C12
11	A	1801	CLA	C4-C3-C5-C6
11	2	1202	CLA	C4-C3-C5-C6
11	B	1235	CLA	C2-C3-C5-C6
11	a	1132	CLA	C2-C3-C5-C6
15	2	5004	LHG	O10-C23-C24-C25
11	b	1209	CLA	CAA-CBA-CGA-O2A
16	b	5002	LMG	C30-C31-C32-C33
11	a	1130	CLA	C2C-C3C-CAC-CBC
11	A	1103	CLA	C11-C10-C8-C9
11	A	1104	CLA	C14-C13-C15-C16
11	B	1013	CLA	C6-C7-C8-C9
11	B	1202	CLA	C11-C12-C13-C14
11	B	1203	CLA	C11-C10-C8-C9
11	B	1210	CLA	C6-C7-C8-C9
11	B	1235	CLA	C6-C7-C8-C9
11	L	1503	CLA	C6-C7-C8-C9
11	a	1101	CLA	C14-C13-C15-C16
11	a	1103	CLA	C6-C7-C8-C9
11	a	1109	CLA	C6-C7-C8-C9
11	a	1118	CLA	C11-C10-C8-C9
11	a	1123	CLA	C11-C10-C8-C9
11	b	1213	CLA	C11-C10-C8-C9
11	b	1229	CLA	C11-C10-C8-C9
11	1	1109	CLA	C6-C7-C8-C9
11	1	1109	CLA	C11-C10-C8-C9
11	1	1131	CLA	C14-C13-C15-C16
11	2	1021	CLA	C14-C13-C15-C16
11	2	1216	CLA	C6-C7-C8-C9
11	8	1503	CLA	C6-C7-C8-C9
12	1	2001	PQN	C24-C23-C25-C26
16	2	5002	LMG	C37-C38-C39-C40
11	B	1229	CLA	C16-C17-C18-C19
11	1	1106	CLA	C13-C15-C16-C17
11	2	1210	CLA	C13-C15-C16-C17
16	2	5002	LMG	C7-C8-O7-C10
15	2	5004	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	1	5001	LHG	C27-C28-C29-C30
11	a	1106	CLA	C4-C3-C5-C6
11	1	1118	CLA	C4-C3-C5-C6
11	1	1119	CLA	C16-C17-C18-C20
11	1	1012	CLA	C16-C17-C18-C20
11	b	1203	CLA	C5-C6-C7-C8
11	B	1223	CLA	CBD-CGD-O2D-CED
11	1	1103	CLA	CAA-CBA-CGA-O2A
11	b	1207	CLA	C2-C3-C5-C6
15	B	5004	LHG	O1-C1-C2-O2
11	1	1113	CLA	CAA-CBA-CGA-O2A
11	2	1209	CLA	CAA-CBA-CGA-O1A
11	A	1012	CLA	C2A-CAA-CBA-CGA
11	B	1204	CLA	C13-C15-C16-C17
11	B	1021	CLA	C1A-C2A-CAA-CBA
11	B	1234	CLA	C1A-C2A-CAA-CBA
11	a	1137	CLA	C1A-C2A-CAA-CBA
11	b	1226	CLA	C1A-C2A-CAA-CBA
11	1	1123	CLA	C1A-C2A-CAA-CBA
11	1	1137	CLA	C1A-C2A-CAA-CBA
11	2	1209	CLA	C1A-C2A-CAA-CBA
11	2	1210	CLA	C1A-C2A-CAA-CBA
11	2	1214	CLA	C1A-C2A-CAA-CBA
14	B	4006	BCR	C20-C21-C22-C23
14	F	4020	BCR	C20-C21-C22-C23
14	F	4013	BCR	C20-C21-C22-C23
14	b	4006	BCR	C20-C21-C22-C23
14	b	4011	BCR	C16-C17-C18-C19
14	f	4020	BCR	C20-C21-C22-C23
14	f	4013	BCR	C20-C21-C22-C23
14	1	4002	BCR	C16-C17-C18-C19
14	2	4011	BCR	C16-C17-C18-C19
14	6	4020	BCR	C20-C21-C22-C23
14	6	4013	BCR	C20-C21-C22-C23
11	B	1222	CLA	C2C-C3C-CAC-CBC
11	a	1106	CLA	C16-C17-C18-C20
11	b	1209	CLA	CAA-CBA-CGA-O1A
11	1	1139	CLA	C2C-C3C-CAC-CBC
11	a	1118	CLA	C5-C6-C7-C8
11	2	1214	CLA	C8-C10-C11-C12
11	A	1102	CLA	C2B-C3B-CAB-CBB
11	A	1104	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	A	1127	CLA	C2B-C3B-CAB-CBB
11	A	1139	CLA	C2B-C3B-CAB-CBB
11	B	1207	CLA	C2B-C3B-CAB-CBB
11	B	1223	CLA	C2B-C3B-CAB-CBB
11	B	1225	CLA	C2B-C3B-CAB-CBB
11	B	1230	CLA	C2B-C3B-CAB-CBB
11	B	1235	CLA	C2B-C3B-CAB-CBB
11	B	1206	CLA	C2B-C3B-CAB-CBB
11	B	1239	CLA	C2B-C3B-CAB-CBB
11	L	1501	CLA	C2B-C3B-CAB-CBB
11	L	1502	CLA	C2B-C3B-CAB-CBB
11	L	1503	CLA	C2B-C3B-CAB-CBB
11	a	1124	CLA	C2B-C3B-CAB-CBB
11	a	1138	CLA	C2B-C3B-CAB-CBB
11	b	1205	CLA	C2B-C3B-CAB-CBB
11	b	1230	CLA	C2B-C3B-CAB-CBB
11	b	1231	CLA	C2B-C3B-CAB-CBB
11	b	1232	CLA	C2B-C3B-CAB-CBB
11	b	1236	CLA	C2B-C3B-CAB-CBB
11	l	1501	CLA	C2B-C3B-CAB-CBB
11	1	1801	CLA	C2B-C3B-CAB-CBB
11	1	1022	CLA	C2B-C3B-CAB-CBB
11	1	1113	CLA	C2B-C3B-CAB-CBB
11	1	1116	CLA	C2B-C3B-CAB-CBB
11	1	1129	CLA	C2B-C3B-CAB-CBB
11	2	1023	CLA	C2B-C3B-CAB-CBB
11	2	1201	CLA	C2B-C3B-CAB-CBB
11	2	1209	CLA	C2B-C3B-CAB-CBB
11	2	1218	CLA	C2B-C3B-CAB-CBB
11	2	1236	CLA	C2B-C3B-CAB-CBB
14	F	4020	BCR	C23-C24-C25-C30
14	L	4019	BCR	C5-C6-C7-C8
14	b	4004	BCR	C23-C24-C25-C30
14	b	4009	BCR	C23-C24-C25-C26
14	f	4020	BCR	C23-C24-C25-C26
14	l	4022	BCR	C23-C24-C25-C26
14	m	4021	BCR	C23-C24-C25-C30
14	2	4006	BCR	C5-C6-C7-C8
14	6	4020	BCR	C23-C24-C25-C26
14	6	4013	BCR	C23-C24-C25-C30
11	a	1113	CLA	CAA-CBA-CGA-O1A
11	a	1113	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	2	1240	CLA	CAA-CBA-CGA-O1A
11	A	1127	CLA	C4-C3-C5-C6
11	b	1021	CLA	C4-C3-C5-C6
11	b	1223	CLA	C4-C3-C5-C6
11	b	1229	CLA	C4-C3-C5-C6
11	1	1110	CLA	C4-C3-C5-C6
11	2	1234	CLA	C4-C3-C5-C6
11	2	1202	CLA	C2-C3-C5-C6
15	a	5003	LHG	C25-C26-C27-C28
11	A	1104	CLA	C11-C12-C13-C15
11	A	1104	CLA	C12-C13-C15-C16
11	a	1118	CLA	C11-C10-C8-C7
11	a	1123	CLA	C11-C10-C8-C7
11	a	1126	CLA	C12-C13-C15-C16
11	a	1011	CLA	C6-C7-C8-C10
11	b	1204	CLA	C11-C10-C8-C7
11	b	1229	CLA	C11-C10-C8-C7
11	b	1206	CLA	C11-C10-C8-C7
11	b	1206	CLA	C12-C13-C15-C16
11	1	1104	CLA	C11-C12-C13-C15
11	2	1206	CLA	C11-C10-C8-C7
11	2	1234	CLA	C6-C7-C8-C10
11	A	1124	CLA	C6-C7-C8-C10
11	B	1204	CLA	C2A-CAA-CBA-CGA
11	b	1225	CLA	C2A-CAA-CBA-CGA
11	2	1228	CLA	C2A-CAA-CBA-CGA
11	8	1501	CLA	O1D-CGD-O2D-CED
11	B	1218	CLA	CAA-CBA-CGA-O2A
11	b	1221	CLA	C6-C7-C8-C9
15	a	5001	LHG	C11-C10-C9-C8
16	B	5002	LMG	C15-C16-C17-C18
11	1	1124	CLA	CBD-CGD-O2D-CED
14	B	4004	BCR	C36-C18-C19-C20
14	a	4001	BCR	C36-C18-C19-C20
15	1	5001	LHG	C13-C14-C15-C16
11	2	1240	CLA	CAA-CBA-CGA-O2A
11	A	1106	CLA	C4-C3-C5-C6
11	A	1110	CLA	C4-C3-C5-C6
11	A	1111	CLA	C4-C3-C5-C6
11	A	1123	CLA	C4-C3-C5-C6
11	B	1204	CLA	C4-C3-C5-C6
11	B	1225	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	a	1127	CLA	C4-C3-C5-C6
11	1	1022	CLA	C4-C3-C5-C6
11	1	1127	CLA	C13-C15-C16-C17
11	A	1125	CLA	C2-C3-C5-C6
11	1	1110	CLA	C2-C3-C5-C6
11	1	1114	CLA	O1A-CGA-O2A-C1
11	A	1012	CLA	C5-C6-C7-C8
11	B	1207	CLA	C15-C16-C17-C18
11	B	1218	CLA	CAA-CBA-CGA-O1A
11	B	1201	CLA	C5-C6-C7-C8
16	B	5002	LMG	C16-C17-C18-C19
11	a	1106	CLA	C10-C11-C12-C13
11	1	1117	CLA	C15-C16-C17-C18
11	2	1223	CLA	CBA-CGA-O2A-C1
11	2	1209	CLA	CAA-CBA-CGA-O2A
11	A	1117	CLA	C11-C10-C8-C9
11	a	1107	CLA	C6-C7-C8-C9
11	b	1206	CLA	C14-C13-C15-C16
11	2	1207	CLA	C11-C10-C8-C9
14	a	4001	BCR	C9-C10-C11-C12
15	1	5001	LHG	C24-C25-C26-C27
11	1	1113	CLA	CAA-CBA-CGA-O1A
11	A	1132	CLA	O1A-CGA-O2A-C1
11	A	1119	CLA	C4-C3-C5-C6
11	B	1013	CLA	C4-C3-C5-C6
11	B	1210	CLA	C4-C3-C5-C6
11	a	1110	CLA	C4-C3-C5-C6
11	a	1137	CLA	C4-C3-C5-C6
11	b	1204	CLA	C4-C3-C5-C6
11	b	1205	CLA	C4-C3-C5-C6
11	b	1224	CLA	C4-C3-C5-C6
11	A	1110	CLA	C2-C3-C5-C6
11	b	1205	CLA	C2-C3-C5-C6
11	1	1022	CLA	C2-C3-C5-C6
16	2	5002	LMG	C20-C21-C22-C23
11	1	1111	CLA	C8-C10-C11-C12
11	2	1203	CLA	C8-C10-C11-C12
11	8	1503	CLA	C5-C6-C7-C8
12	1	2001	PQN	C15-C16-C17-C18
15	a	5001	LHG	C25-C26-C27-C28
11	b	1208	CLA	CAA-CBA-CGA-O2A
11	2	1232	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	A	1116	CLA	CAA-CBA-CGA-O1A
11	a	1011	CLA	CAA-CBA-CGA-O2A
11	B	1209	CLA	CAA-CBA-CGA-O2A
11	A	1124	CLA	C4C-C3C-CAC-CBC
11	a	1801	CLA	C2A-CAA-CBA-CGA
11	1	1136	CLA	C2A-CAA-CBA-CGA
11	2	1023	CLA	C2A-CAA-CBA-CGA
11	2	1240	CLA	C2A-CAA-CBA-CGA
15	b	5004	LHG	C35-C36-C37-C38
11	A	1113	CLA	CAA-CBA-CGA-O2A
15	1	5001	LHG	C19-C20-C21-C22
11	B	1206	CLA	C4-C3-C5-C6
11	1	1111	CLA	C4-C3-C5-C6
11	a	1110	CLA	C2-C3-C5-C6
11	A	1127	CLA	C4B-C3B-CAB-CBB
11	B	1230	CLA	C4B-C3B-CAB-CBB
11	B	1206	CLA	C4B-C3B-CAB-CBB
11	a	1140	CLA	C4B-C3B-CAB-CBB
11	b	1013	CLA	C4B-C3B-CAB-CBB
11	B	1213	CLA	C5-C6-C7-C8
11	B	1239	CLA	CAA-CBA-CGA-O1A
11	a	1132	CLA	C13-C15-C16-C17
14	b	4011	BCR	C11-C10-C9-C34
11	l	1501	CLA	C2C-C3C-CAC-CBC
11	B	1212	CLA	CAA-CBA-CGA-O2A
11	B	1021	CLA	CAA-CBA-CGA-O1A
15	A	5003	LHG	C12-C13-C14-C15
11	B	1210	CLA	C16-C17-C18-C19
11	a	1131	CLA	C4-C3-C5-C6
11	b	1213	CLA	C5-C6-C7-C8
11	A	1119	CLA	C2-C3-C5-C6
11	A	1123	CLA	C2-C3-C5-C6
11	B	1210	CLA	C2-C3-C5-C6
11	B	1225	CLA	C10-C11-C12-C13
15	B	5004	LHG	C2-C3-O3-P
15	1	5003	LHG	C9-C10-C11-C12
11	A	1122	CLA	C11-C10-C8-C7
11	a	1022	CLA	C6-C7-C8-C10
11	a	1102	CLA	C6-C7-C8-C10
11	1	1131	CLA	C12-C13-C15-C16
15	A	5003	LHG	C33-C34-C35-C36
11	B	1231	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	1	5003	LHG	C32-C33-C34-C35
11	a	1117	CLA	C10-C11-C12-C13
11	a	1012	CLA	C15-C16-C17-C18
11	B	1217	CLA	C2C-C3C-CAC-CBC
11	B	1219	CLA	C5-C6-C7-C8
11	A	1104	CLA	C2C-C3C-CAC-CBC
11	A	1112	CLA	CAA-CBA-CGA-O2A
11	2	1229	CLA	CAA-CBA-CGA-O1A
11	A	1106	CLA	C11-C12-C13-C14
11	B	1216	CLA	C6-C7-C8-C9
11	B	1225	CLA	C11-C10-C8-C9
11	a	1104	CLA	C11-C12-C13-C14
11	a	1117	CLA	C11-C12-C13-C14
11	b	1223	CLA	C11-C10-C8-C9
11	1	1126	CLA	C14-C13-C15-C16
11	0	1401	CLA	C14-C13-C15-C16
12	b	2002	PQN	C16-C17-C18-C19
11	2	1223	CLA	O1A-CGA-O2A-C1
11	a	1129	CLA	C2A-CAA-CBA-CGA
11	A	1801	CLA	C2-C1-O2A-CGA
11	a	1110	CLA	C2-C1-O2A-CGA
11	b	1213	CLA	C2-C1-O2A-CGA
11	1	1801	CLA	C2-C1-O2A-CGA
11	a	1116	CLA	C4C-C3C-CAC-CBC
11	1	1104	CLA	C13-C15-C16-C17
11	1	1124	CLA	O1D-CGD-O2D-CED
11	1	1133	CLA	C4C-C3C-CAC-CBC
11	B	1234	CLA	C3A-C2A-CAA-CBA
11	l	1501	CLA	C3A-C2A-CAA-CBA
11	1	1123	CLA	C3A-C2A-CAA-CBA
11	2	1223	CLA	C3A-C2A-CAA-CBA
11	K	1402	CLA	C3A-C2A-CAA-CBA
11	B	1232	CLA	CAA-CBA-CGA-O2A
11	1	1108	CLA	CAA-CBA-CGA-O2A
11	B	1204	CLA	C2-C3-C5-C6
11	a	1127	CLA	C2-C3-C5-C6
11	2	1234	CLA	C2-C3-C5-C6
11	1	1133	CLA	C2C-C3C-CAC-CBC
11	2	1232	CLA	CAA-CBA-CGA-O1A
15	A	5001	LHG	C13-C14-C15-C16
11	1	1237	CLA	O2A-C1-C2-C3
14	F	4013	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	B	1209	CLA	CAA-CBA-CGA-O1A
15	a	5001	LHG	C35-C36-C37-C38
11	a	1116	CLA	CAA-CBA-CGA-O2A
11	1	1011	CLA	CAA-CBA-CGA-O2A
11	A	1113	CLA	CAA-CBA-CGA-O1A
11	B	1232	CLA	CAA-CBA-CGA-O1A
11	1	1108	CLA	C2A-CAA-CBA-CGA
15	1	5001	LHG	C35-C36-C37-C38
11	2	1221	CLA	C4-C3-C5-C6
11	a	1108	CLA	CAA-CBA-CGA-O2A
11	a	1237	CLA	C2-C3-C5-C6
15	1	5003	LHG	C19-C20-C21-C22
11	a	1134	CLA	C2C-C3C-CAC-CBC
14	b	4011	BCR	C11-C10-C9-C8
14	2	4006	BCR	C20-C21-C22-C23
11	A	1112	CLA	CAA-CBA-CGA-O1A
11	b	1208	CLA	CAA-CBA-CGA-O1A
11	b	1210	CLA	CBA-CGA-O2A-C1
11	B	1203	CLA	O1A-CGA-O2A-C1
11	1	1137	CLA	C15-C16-C17-C18
11	a	1131	CLA	C4C-C3C-CAC-CBC
15	A	5001	LHG	C33-C34-C35-C36
11	1	1124	CLA	CAA-CBA-CGA-O2A
11	B	1231	CLA	CAA-CBA-CGA-O1A
11	1	1108	CLA	CAA-CBA-CGA-O1A
11	b	1021	CLA	C2-C3-C5-C6
14	b	4014	BCR	C13-C14-C15-C16
14	2	4009	BCR	C19-C20-C21-C22
11	2	1214	CLA	C11-C12-C13-C14
11	2	1227	CLA	C4C-C3C-CAC-CBC
11	a	1108	CLA	CAA-CBA-CGA-O1A
11	B	1235	CLA	CAA-CBA-CGA-O2A
11	a	1124	CLA	CAA-CBA-CGA-O2A
11	b	1021	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	C17-C18-C19-C20
11	a	1101	CLA	C15-C16-C17-C18
11	A	1022	CLA	C14-C13-C15-C16
11	A	1101	CLA	C11-C10-C8-C9
11	A	1128	CLA	C14-C13-C15-C16
11	B	1204	CLA	C6-C7-C8-C9
11	B	1210	CLA	C11-C10-C8-C9
11	B	1213	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	a	1103	CLA	C11-C12-C13-C14
11	b	1204	CLA	C14-C13-C15-C16
11	1	1012	CLA	C14-C13-C15-C16
11	2	1222	CLA	C6-C7-C8-C9
11	K	1401	CLA	C14-C13-C15-C16
11	k	1401	CLA	C14-C13-C15-C16
11	B	1201	CLA	C4C-C3C-CAC-CBC
11	A	1132	CLA	C16-C17-C18-C20
11	a	1111	CLA	C11-C12-C13-C14
11	1	1134	CLA	C4C-C3C-CAC-CBC
11	1	1110	CLA	CAA-CBA-CGA-O2A
11	b	1229	CLA	C2-C3-C5-C6
11	B	1212	CLA	CAA-CBA-CGA-O1A
11	B	1212	CLA	C2A-CAA-CBA-CGA
11	A	1117	CLA	C6-C7-C8-C10
11	A	1123	CLA	C11-C10-C8-C7
11	B	1210	CLA	C12-C13-C15-C16
11	B	1229	CLA	C11-C10-C8-C7
11	L	1501	CLA	C12-C13-C15-C16
11	a	1101	CLA	C12-C13-C15-C16
11	a	1102	CLA	C11-C12-C13-C15
11	a	1103	CLA	C11-C10-C8-C7
11	a	1104	CLA	C6-C7-C8-C10
11	a	1104	CLA	C11-C10-C8-C7
11	a	1106	CLA	C11-C10-C8-C7
11	b	1023	CLA	C11-C12-C13-C15
11	b	1210	CLA	C11-C10-C8-C7
11	1	1022	CLA	C11-C10-C8-C7
11	1	1107	CLA	C11-C10-C8-C7
11	1	1117	CLA	C11-C10-C8-C7
11	1	1012	CLA	C11-C10-C8-C7
11	2	1021	CLA	C11-C10-C8-C7
11	2	1207	CLA	C11-C10-C8-C7
11	2	1223	CLA	C12-C13-C15-C16
12	b	2002	PQN	C16-C17-C18-C20
11	B	1239	CLA	C4C-C3C-CAC-CBC
11	1	1139	CLA	C4C-C3C-CAC-CBC
11	A	1125	CLA	C2B-C3B-CAB-CBB
11	A	1133	CLA	C2B-C3B-CAB-CBB
11	b	1013	CLA	C2B-C3B-CAB-CBB
11	b	1219	CLA	C2B-C3B-CAB-CBB
11	b	1222	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	b	1206	CLA	C2B-C3B-CAB-CBB
11	1	1012	CLA	C2B-C3B-CAB-CBB
11	2	1013	CLA	C2B-C3B-CAB-CBB
14	A	4008	BCR	C1-C6-C7-C8
14	A	4008	BCR	C5-C6-C7-C8
14	F	4020	BCR	C23-C24-C25-C26
14	L	4019	BCR	C1-C6-C7-C8
14	b	4004	BCR	C23-C24-C25-C26
14	b	4006	BCR	C5-C6-C7-C8
14	m	4021	BCR	C23-C24-C25-C26
14	2	4009	BCR	C23-C24-C25-C26
11	2	1235	CLA	CAA-CBA-CGA-O2A
16	2	5002	LMG	O7-C10-C11-C12
11	A	1111	CLA	C2-C1-O2A-CGA
11	A	1011	CLA	C2-C1-O2A-CGA
11	B	1210	CLA	C2-C1-O2A-CGA
11	B	1214	CLA	C2-C1-O2A-CGA
11	B	1228	CLA	C2-C1-O2A-CGA
11	a	1116	CLA	C2-C1-O2A-CGA
11	a	1128	CLA	C2-C1-O2A-CGA
11	b	1214	CLA	C2-C1-O2A-CGA
11	b	1216	CLA	C2-C1-O2A-CGA
11	b	1225	CLA	C2-C1-O2A-CGA
11	1	1102	CLA	C2-C1-O2A-CGA
11	1	1109	CLA	C2-C1-O2A-CGA
11	1	1116	CLA	C2-C1-O2A-CGA
11	1	1127	CLA	C2-C1-O2A-CGA
11	2	1013	CLA	C16-C17-C18-C20
11	B	1202	CLA	CAA-CBA-CGA-O2A
11	B	1210	CLA	CAA-CBA-CGA-O2A
11	2	1216	CLA	CAA-CBA-CGA-O2A
15	a	5001	LHG	O8-C23-C24-C25
11	2	1215	CLA	C13-C15-C16-C17
11	8	1501	CLA	CBD-CGD-O2D-CED
11	a	1122	CLA	CAA-CBA-CGA-O2A
11	1	1801	CLA	CAA-CBA-CGA-O2A
11	2	1213	CLA	CAA-CBA-CGA-O2A
11	b	1204	CLA	C2-C3-C5-C6
15	A	5001	LHG	O9-C7-O7-C5
11	A	1127	CLA	C2A-CAA-CBA-CGA
11	a	1125	CLA	C2A-CAA-CBA-CGA
11	2	1217	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	B	1231	CLA	C2C-C3C-CAC-CBC
11	b	1226	CLA	C5-C6-C7-C8
11	2	1227	CLA	CAA-CBA-CGA-O2A
11	a	1135	CLA	C2C-C3C-CAC-CBC
11	B	1225	CLA	CAA-CBA-CGA-O2A
11	b	1206	CLA	CAA-CBA-CGA-O2A
15	a	5001	LHG	O7-C7-C8-C9
11	B	1229	CLA	C16-C17-C18-C20
11	1	1119	CLA	C16-C17-C18-C19
11	2	1216	CLA	C16-C17-C18-C20
11	b	1213	CLA	C2C-C3C-CAC-CBC
11	A	1101	CLA	C15-C16-C17-C18
11	2	1021	CLA	C10-C11-C12-C13
11	b	1219	CLA	CAA-CBA-CGA-O2A
11	1	1111	CLA	CAA-CBA-CGA-O2A
11	1	1131	CLA	CAA-CBA-CGA-O2A
16	b	5002	LMG	C12-C13-C14-C15
11	B	1201	CLA	O1A-CGA-O2A-C1
11	2	1222	CLA	C11-C10-C8-C7
15	b	5004	LHG	C32-C33-C34-C35
11	a	1106	CLA	C2-C3-C5-C6
11	B	1238	CLA	C15-C16-C17-C18
11	b	1202	CLA	C13-C15-C16-C17
15	A	5003	LHG	C9-C10-C11-C12
15	B	5004	LHG	C17-C18-C19-C20
15	A	5003	LHG	O7-C7-C8-C9
11	a	1126	CLA	C13-C15-C16-C17
11	A	1134	CLA	C4C-C3C-CAC-CBC
16	2	5002	LMG	C34-C35-C36-C37
11	b	1218	CLA	CAA-CBA-CGA-O2A
11	a	1130	CLA	C4C-C3C-CAC-CBC
11	1	1136	CLA	C4C-C3C-CAC-CBC
11	A	1104	CLA	C11-C12-C13-C14
11	a	1102	CLA	C11-C10-C8-C9
11	a	1107	CLA	C11-C10-C8-C9
11	1	1102	CLA	C11-C12-C13-C14
11	1	1104	CLA	C11-C12-C13-C14
11	1	1106	CLA	C6-C7-C8-C9
11	1	1106	CLA	C14-C13-C15-C16
11	1	1123	CLA	C11-C10-C8-C9
12	A	2001	PQN	C24-C23-C25-C26
11	1	1132	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	A	1101	CLA	CAA-CBA-CGA-O2A
11	2	1206	CLA	CAA-CBA-CGA-O2A
11	K	1401	CLA	CAA-CBA-CGA-O2A
11	k	1401	CLA	CAA-CBA-CGA-O2A
11	0	1401	CLA	CAA-CBA-CGA-O2A
15	B	5004	LHG	C15-C16-C17-C18
11	A	1111	CLA	C4B-C3B-CAB-CBB
11	A	1125	CLA	C4B-C3B-CAB-CBB
11	B	1203	CLA	C4B-C3B-CAB-CBB
11	B	1220	CLA	O1A-CGA-O2A-C1
11	a	1103	CLA	C1A-C2A-CAA-CBA
11	a	1012	CLA	C1A-C2A-CAA-CBA
11	b	1220	CLA	C1A-C2A-CAA-CBA
11	b	1222	CLA	C4B-C3B-CAB-CBB
11	b	1230	CLA	C1A-C2A-CAA-CBA
11	b	1238	CLA	C4B-C3B-CAB-CBB
11	1	1109	CLA	C4B-C3B-CAB-CBB
11	1	1119	CLA	C4B-C3B-CAB-CBB
11	1	1125	CLA	C4B-C3B-CAB-CBB
11	1	1135	CLA	C1A-C2A-CAA-CBA
11	2	1013	CLA	C4B-C3B-CAB-CBB
11	2	1021	CLA	C4B-C3B-CAB-CBB
11	2	1023	CLA	C4B-C3B-CAB-CBB
11	2	1201	CLA	C4B-C3B-CAB-CBB
11	2	1204	CLA	C4B-C3B-CAB-CBB
11	2	1223	CLA	C1A-C2A-CAA-CBA
11	2	1229	CLA	C4B-C3B-CAB-CBB
11	b	1240	CLA	CAA-CBA-CGA-O1A
11	B	1217	CLA	C2-C1-O2A-CGA
11	B	1213	CLA	C4-C3-C5-C6
11	A	1136	CLA	CAA-CBA-CGA-O2A
11	b	1204	CLA	CAA-CBA-CGA-O2A
11	b	1216	CLA	CAA-CBA-CGA-O2A
15	A	5001	LHG	O7-C7-C8-C9
15	a	5003	LHG	O7-C5-C6-O8
15	2	5004	LHG	O7-C5-C6-O8
14	A	4007	BCR	C7-C8-C9-C10
14	B	4004	BCR	C17-C18-C19-C20
14	B	4011	BCR	C17-C18-C19-C20
14	a	4001	BCR	C17-C18-C19-C20
14	l	4022	BCR	C19-C20-C21-C22
14	8	4022	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
11	B	1203	CLA	CBA-CGA-O2A-C1
11	b	1227	CLA	CAA-CBA-CGA-O2A
11	b	1240	CLA	CAA-CBA-CGA-O2A
11	A	1111	CLA	CAA-CBA-CGA-O2A
11	1	1136	CLA	CAA-CBA-CGA-O2A
11	2	1239	CLA	CAA-CBA-CGA-O2A
11	A	1131	CLA	C2A-CAA-CBA-CGA
15	1	5003	LHG	C24-C25-C26-C27
11	B	1240	CLA	CAA-CBA-CGA-O2A
11	b	1219	CLA	C6-C7-C8-C10
15	B	5004	LHG	O6-C4-C5-C6
11	b	1210	CLA	CAA-CBA-CGA-O2A
11	2	1202	CLA	CAA-CBA-CGA-O2A
11	L	1503	CLA	CAA-CBA-CGA-O1A
11	1	1118	CLA	CAA-CBA-CGA-O1A
11	A	1104	CLA	C10-C11-C12-C13
11	A	1135	CLA	C2-C3-C5-C6
11	B	1215	CLA	CAA-CBA-CGA-O1A
11	L	1502	CLA	C2C-C3C-CAC-CBC
11	A	1102	CLA	C2-C1-O2A-CGA
11	B	1201	CLA	C2-C1-O2A-CGA
11	a	1109	CLA	C2-C1-O2A-CGA
11	a	1111	CLA	C2-C1-O2A-CGA
11	b	1201	CLA	C2-C1-O2A-CGA
11	b	1210	CLA	C2-C1-O2A-CGA
11	b	1234	CLA	C2-C1-O2A-CGA
15	A	5003	LHG	O8-C23-C24-C25
11	A	1104	CLA	C11-C10-C8-C7
11	A	1012	CLA	C11-C10-C8-C7
11	B	1204	CLA	C11-C12-C13-C15
11	B	1216	CLA	C6-C7-C8-C10
11	B	1222	CLA	C6-C7-C8-C10
11	a	1117	CLA	C11-C12-C13-C15
11	a	1132	CLA	C11-C10-C8-C7
11	b	1021	CLA	C6-C7-C8-C10
11	1	1106	CLA	C11-C10-C8-C7
11	1	1123	CLA	C12-C13-C15-C16
11	1	1127	CLA	C11-C10-C8-C7
11	1	1128	CLA	C11-C12-C13-C15
11	1	1012	CLA	C12-C13-C15-C16
11	1	1132	CLA	C11-C10-C8-C7
11	2	1013	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	2	1210	CLA	C6-C7-C8-C10
11	a	1137	CLA	C2-C3-C5-C6
11	1	1126	CLA	C2C-C3C-CAC-CBC
11	b	1218	CLA	CAA-CBA-CGA-O1A
11	2	1013	CLA	O2A-C1-C2-C3
11	a	1110	CLA	C2C-C3C-CAC-CBC
11	B	1216	CLA	C15-C16-C17-C18
11	2	1235	CLA	C2C-C3C-CAC-CBC
11	B	1231	CLA	C4C-C3C-CAC-CBC
11	b	1234	CLA	C4C-C3C-CAC-CBC
11	b	1215	CLA	C8-C10-C11-C12
11	A	1107	CLA	C3A-C2A-CAA-CBA
11	a	1107	CLA	C3A-C2A-CAA-CBA
11	a	1012	CLA	C3A-C2A-CAA-CBA
11	K	1401	CLA	C4-C3-C5-C6
11	k	1401	CLA	C4-C3-C5-C6
11	0	1401	CLA	C4-C3-C5-C6
11	2	1235	CLA	CAA-CBA-CGA-O1A
11	B	1207	CLA	C10-C11-C12-C13
11	A	1137	CLA	CAA-CBA-CGA-O2A
11	1	1114	CLA	CAA-CBA-CGA-O2A
11	2	1227	CLA	CAA-CBA-CGA-O1A
11	L	1501	CLA	C5-C6-C7-C8
11	b	1021	CLA	CAA-CBA-CGA-O1A
11	b	1206	CLA	CAA-CBA-CGA-O1A
11	1	1801	CLA	CAA-CBA-CGA-O1A
11	2	1206	CLA	CAA-CBA-CGA-O1A
11	2	1023	CLA	C8-C10-C11-C12
11	a	1124	CLA	CAA-CBA-CGA-O1A
11	2	1216	CLA	CAA-CBA-CGA-O1A
15	A	5001	LHG	C8-C7-O7-C5
11	B	1234	CLA	C10-C11-C12-C13
11	1	1122	CLA	C5-C6-C7-C8
12	A	2001	PQN	C20-C21-C22-C23
11	B	1217	CLA	C2A-CAA-CBA-CGA
11	b	1213	CLA	C4C-C3C-CAC-CBC
11	a	1126	CLA	C14-C13-C15-C16
11	a	1127	CLA	C6-C7-C8-C9
11	a	1128	CLA	C11-C10-C8-C9
11	1	1128	CLA	C11-C12-C13-C14
16	b	5002	LMG	C23-C24-C25-C26
15	A	5003	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
12	B	2002	PQN	C25-C26-C27-C28
11	b	1210	CLA	C10-C11-C12-C13
11	1	1118	CLA	C5-C6-C7-C8
11	1	1111	CLA	CAA-CBA-CGA-O1A
11	2	1239	CLA	CAA-CBA-CGA-O1A
11	b	1214	CLA	CAA-CBA-CGA-O2A
11	1	1101	CLA	CAA-CBA-CGA-O2A
11	1	1127	CLA	CAA-CBA-CGA-O2A
11	1	1118	CLA	C2-C3-C5-C6
11	A	1126	CLA	C8-C10-C11-C12
11	b	1227	CLA	CAA-CBA-CGA-O1A
16	B	5002	LMG	C20-C21-C22-C23
11	B	1202	CLA	CAA-CBA-CGA-O1A
11	b	1219	CLA	CAA-CBA-CGA-O1A
11	1	1136	CLA	CAA-CBA-CGA-O1A
11	B	1203	CLA	C5-C6-C7-C8
11	2	1205	CLA	CBD-CGD-O2D-CED
14	A	4007	BCR	C11-C12-C13-C14
11	B	1210	CLA	CAA-CBA-CGA-O1A
11	B	1235	CLA	CAA-CBA-CGA-O1A
11	a	1122	CLA	CAA-CBA-CGA-O1A
11	1	1124	CLA	CAA-CBA-CGA-O1A
15	A	5003	LHG	O9-C7-C8-C9
11	2	1223	CLA	C10-C11-C12-C13
11	B	1225	CLA	CAA-CBA-CGA-O1A
15	A	5001	LHG	O9-C7-C8-C9
15	a	5001	LHG	O9-C7-C8-C9
11	A	1110	CLA	CAA-CBA-CGA-O2A
11	1	1122	CLA	CAA-CBA-CGA-O2A
11	2	1207	CLA	CAA-CBA-CGA-O2A
11	B	1221	CLA	C2A-CAA-CBA-CGA
11	B	1240	CLA	CAA-CBA-CGA-O1A
11	a	1126	CLA	C2C-C3C-CAC-CBC
11	1	1110	CLA	CAA-CBA-CGA-O1A
11	2	1202	CLA	CAA-CBA-CGA-O1A
11	A	1237	CLA	C4-C3-C5-C6
11	2	1226	CLA	C8-C10-C11-C12
11	B	1213	CLA	CAA-CBA-CGA-O2A
11	B	1229	CLA	CAA-CBA-CGA-O2A
11	a	1136	CLA	CAA-CBA-CGA-O2A
11	b	1235	CLA	CAA-CBA-CGA-O2A
11	b	1204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	A	1125	CLA	CAD-CBD-CGD-O2D
11	B	1225	CLA	CAD-CBD-CGD-O2D
11	B	1229	CLA	CAD-CBD-CGD-O2D
11	a	1125	CLA	CAD-CBD-CGD-O2D
11	b	1219	CLA	CAD-CBD-CGD-O2D
11	b	1236	CLA	CAD-CBD-CGD-O2D
11	2	1207	CLA	CAD-CBD-CGD-O2D
11	2	1219	CLA	CAD-CBD-CGD-O2D
11	a	1107	CLA	C15-C16-C17-C18
15	1	5001	LHG	O8-C23-C24-C25
11	b	1210	CLA	CAA-CBA-CGA-O1A
11	2	1213	CLA	CAA-CBA-CGA-O1A
11	A	1101	CLA	C8-C10-C11-C12
15	2	5004	LHG	C14-C15-C16-C17
11	A	1111	CLA	CAA-CBA-CGA-O1A
11	1	1131	CLA	CAA-CBA-CGA-O1A
11	A	1140	CLA	CAA-CBA-CGA-O2A
11	a	1012	CLA	CAA-CBA-CGA-O2A
11	a	1114	CLA	CAA-CBA-CGA-O2A
11	8	1502	CLA	CAA-CBA-CGA-O2A
11	B	1206	CLA	O1A-CGA-O2A-C1
11	A	1106	CLA	C16-C17-C18-C20
11	A	1101	CLA	CAA-CBA-CGA-O1A
11	A	1136	CLA	CAA-CBA-CGA-O1A
11	b	1216	CLA	CAA-CBA-CGA-O1A
11	1	1101	CLA	CAA-CBA-CGA-O1A
11	2	1215	CLA	C15-C16-C17-C18
11	A	1012	CLA	C11-C12-C13-C15
11	2	1210	CLA	C11-C10-C8-C7
11	A	1122	CLA	CAA-CBA-CGA-O2A
11	B	1205	CLA	CAA-CBA-CGA-O2A
11	B	1228	CLA	CAA-CBA-CGA-O2A
11	1	1140	CLA	CAA-CBA-CGA-O2A
11	1	1120	CLA	CAA-CBA-CGA-O2A
15	1	5003	LHG	O8-C23-C24-C25
11	a	1012	CLA	CAA-CBA-CGA-O1A
11	K	1401	CLA	CAA-CBA-CGA-O1A
11	A	1105	CLA	CAA-CBA-CGA-O2A
11	A	1124	CLA	CAA-CBA-CGA-O2A
11	a	1138	CLA	CAA-CBA-CGA-O2A
11	A	1110	CLA	CAA-CBA-CGA-O1A
11	1	1122	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	k	1401	CLA	CAA-CBA-CGA-O1A
11	0	1401	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

303 monomers are involved in 842 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	2	1214	CLA	3	0
14	B	4009	BCR	5	0
11	b	1214	CLA	2	0
14	A	4008	BCR	5	0
11	a	1801	CLA	7	0
11	B	1023	CLA	7	0
11	2	1211	CLA	1	0
11	B	1223	CLA	8	0
11	8	1501	CLA	6	0
14	b	4006	BCR	2	0
11	2	1239	CLA	4	0
11	1	1132	CLA	6	0
11	a	1135	CLA	4	0
14	A	4007	BCR	7	0
11	2	1023	CLA	4	0
11	2	1232	CLA	3	0
11	B	1226	CLA	2	0
11	2	1223	CLA	1	0
11	2	1212	CLA	3	0
15	2	5004	LHG	7	0
11	A	1123	CLA	9	0
11	B	1221	CLA	3	0
11	b	1219	CLA	3	0
15	b	5004	LHG	5	0
11	A	1103	CLA	2	0
11	2	1224	CLA	1	0
13	A	3001	SF4	3	0
11	2	1203	CLA	1	0
11	A	1129	CLA	5	0
11	A	1112	CLA	3	0
11	A	1122	CLA	2	0
11	1	1118	CLA	3	0
11	1	1121	CLA	1	0
12	a	2001	PQN	3	0
14	f	4018	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	b	1212	CLA	2	0
11	2	1235	CLA	3	0
11	b	1235	CLA	3	0
14	b	4010	BCR	10	0
11	A	1131	CLA	2	0
11	b	1201	CLA	3	0
11	A	1119	CLA	6	0
14	B	4017	BCR	8	0
11	2	1021	CLA	8	0
14	a	4003	BCR	4	0
14	2	4004	BCR	2	0
11	1	1104	CLA	1	0
13	c	3003	SF4	13	0
14	A	4001	BCR	3	0
14	A	4002	BCR	5	0
14	2	4009	BCR	5	0
11	2	1238	CLA	5	0
11	A	1117	CLA	1	0
11	a	1112	CLA	4	0
11	2	1207	CLA	4	0
14	8	4022	BCR	8	0
15	A	5001	LHG	5	0
11	B	1222	CLA	3	0
11	a	1126	CLA	4	0
11	b	1240	CLA	3	0
11	1	1112	CLA	3	0
11	a	1110	CLA	2	0
11	A	1126	CLA	9	0
11	b	1202	CLA	1	0
11	b	1225	CLA	2	0
11	1	1134	CLA	3	0
14	B	4006	BCR	3	0
11	B	1230	CLA	2	0
11	A	1135	CLA	2	0
11	B	1220	CLA	1	0
11	1	1122	CLA	1	0
11	B	1231	CLA	2	0
11	1	1127	CLA	1	0
11	b	1210	CLA	2	0
11	a	1138	CLA	3	0
11	b	1234	CLA	1	0
14	7	4021	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1133	CLA	3	0
14	B	4005	BCR	6	0
11	1	1140	CLA	2	0
11	a	1132	CLA	2	0
11	A	1136	CLA	3	0
11	B	1234	CLA	2	0
11	1	1137	CLA	4	0
11	1	1128	CLA	9	0
11	b	1211	CLA	3	0
11	A	1125	CLA	4	0
11	1	1131	CLA	2	0
11	1	1101	CLA	3	0
11	B	1215	CLA	1	0
11	a	1103	CLA	16	0
11	B	1206	CLA	3	0
11	a	1119	CLA	11	0
11	b	1227	CLA	3	0
14	f	4013	BCR	5	0
11	2	1229	CLA	4	0
11	a	1117	CLA	1	0
11	a	1121	CLA	4	0
11	A	1114	CLA	2	0
11	B	1214	CLA	1	0
15	B	5004	LHG	4	0
11	2	1205	CLA	4	0
14	a	4007	BCR	3	0
11	B	1202	CLA	2	0
14	L	4022	BCR	6	0
13	3	3002	SF4	8	0
11	a	1123	CLA	7	0
14	b	4011	BCR	7	0
11	a	1108	CLA	2	0
11	A	1022	CLA	5	0
14	8	4019	BCR	7	0
11	A	1012	CLA	2	0
11	1	1801	CLA	5	0
11	B	1239	CLA	1	0
11	2	1202	CLA	4	0
14	f	4020	BCR	4	0
11	A	1110	CLA	1	0
11	a	1107	CLA	1	0
11	B	1235	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1106	CLA	4	0
11	a	1104	CLA	1	0
11	2	1209	CLA	2	0
11	a	1011	CLA	1	0
11	1	1012	CLA	4	0
14	L	4019	BCR	8	0
14	F	4013	BCR	3	0
13	a	3001	SF4	2	0
11	a	1122	CLA	2	0
11	b	1204	CLA	3	0
11	b	1209	CLA	2	0
11	2	1201	CLA	3	0
15	1	5003	LHG	6	0
11	1	1105	CLA	1	0
14	A	4003	BCR	7	0
11	A	1118	CLA	3	0
14	a	4001	BCR	4	0
11	1	1111	CLA	1	0
11	B	1204	CLA	3	0
11	1	1109	CLA	2	0
11	a	1131	CLA	2	0
11	1	1022	CLA	5	0
13	C	3002	SF4	10	0
11	b	1021	CLA	5	0
14	m	4021	BCR	4	0
15	a	5003	LHG	9	0
11	1	1119	CLA	2	0
11	B	1238	CLA	4	0
11	a	1105	CLA	1	0
11	B	1210	CLA	2	0
14	B	4011	BCR	6	0
11	1	1106	CLA	8	0
11	A	1140	CLA	2	0
14	1	4003	BCR	2	0
11	A	1121	CLA	2	0
11	1	1115	CLA	5	0
11	0	1402	CLA	1	0
11	b	1222	CLA	4	0
11	b	1207	CLA	2	0
11	a	1129	CLA	1	0
11	B	1207	CLA	3	0
12	b	2002	PQN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1124	CLA	4	0
11	2	1231	CLA	7	0
11	2	1210	CLA	1	0
11	B	1228	CLA	2	0
11	2	1234	CLA	4	0
14	1	4001	BCR	8	0
14	B	4014	BCR	6	0
11	A	1107	CLA	2	0
11	B	1013	CLA	6	0
11	1	1129	CLA	2	0
14	2	4005	BCR	4	0
11	2	1240	CLA	2	0
14	b	4005	BCR	3	0
14	l	4022	BCR	4	0
14	a	4002	BCR	5	0
11	k	1402	CLA	1	0
11	a	1012	CLA	2	0
11	a	1137	CLA	1	0
11	A	1137	CLA	4	0
11	A	1128	CLA	3	0
11	a	1101	CLA	2	0
14	1	4002	BCR	5	0
11	A	1101	CLA	2	0
11	2	1206	CLA	7	0
11	A	1237	CLA	3	0
11	a	1118	CLA	4	0
11	a	1237	CLA	2	0
11	a	1111	CLA	3	0
11	1	1110	CLA	2	0
15	1	5001	LHG	10	0
11	a	1124	CLA	3	0
11	b	1230	CLA	1	0
11	a	1125	CLA	4	0
11	b	1206	CLA	3	0
11	1	1113	CLA	3	0
14	B	4004	BCR	3	0
11	2	1225	CLA	1	0
14	2	4017	BCR	10	0
11	2	1230	CLA	4	0
11	b	1023	CLA	8	0
14	a	4008	BCR	2	0
11	B	1227	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	b	1223	CLA	14	0
14	b	4017	BCR	5	0
11	B	1211	CLA	4	0
15	a	5001	LHG	2	0
11	b	1205	CLA	5	0
11	2	1227	CLA	3	0
11	A	1115	CLA	2	0
11	a	1113	CLA	2	0
11	A	1111	CLA	1	0
11	B	1205	CLA	4	0
16	B	5002	LMG	1	0
11	1	1103	CLA	2	0
13	3	3003	SF4	12	0
11	1	1125	CLA	3	0
14	l	4019	BCR	7	0
11	0	1401	CLA	3	0
11	B	1224	CLA	1	0
11	1	1237	CLA	4	0
11	b	1221	CLA	6	0
11	2	1208	CLA	1	0
11	A	1011	CLA	3	0
11	2	1013	CLA	8	0
11	a	1022	CLA	2	0
11	b	1208	CLA	2	0
16	2	5002	LMG	2	0
11	1	1107	CLA	3	0
11	b	1013	CLA	10	0
11	8	1503	CLA	2	0
11	1	1138	CLA	2	0
14	2	4006	BCR	1	0
11	1	1117	CLA	2	0
14	1	4008	BCR	4	0
11	B	1212	CLA	3	0
11	a	1106	CLA	1	0
13	1	3001	SF4	1	0
11	1	1102	CLA	1	0
11	2	1221	CLA	1	0
14	b	4014	BCR	4	0
11	b	1203	CLA	3	0
14	b	4004	BCR	3	0
11	B	1209	CLA	3	0
11	A	1102	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	l	1503	CLA	4	0
12	A	2001	PQN	2	0
11	A	1104	CLA	7	0
11	b	1236	CLA	2	0
11	2	1204	CLA	3	0
11	B	1219	CLA	1	0
11	B	1236	CLA	1	0
11	B	1201	CLA	3	0
11	2	1228	CLA	1	0
11	A	1133	CLA	1	0
12	B	2002	PQN	1	0
11	b	1231	CLA	1	0
11	2	1222	CLA	2	0
13	C	3003	SF4	3	0
11	a	1133	CLA	4	0
14	6	4013	BCR	7	0
11	1	1130	CLA	3	0
11	a	1134	CLA	1	0
12	2	2002	PQN	1	0
14	M	4021	BCR	5	0
11	A	1134	CLA	1	0
11	b	1229	CLA	3	0
11	b	1228	CLA	3	0
14	B	4010	BCR	7	0
13	c	3002	SF4	7	0
14	6	4020	BCR	4	0
14	2	4011	BCR	8	0
14	b	4009	BCR	4	0
11	b	1238	CLA	3	0
11	a	1116	CLA	3	0
11	l	1501	CLA	5	0
14	F	4020	BCR	4	0
11	B	1225	CLA	2	0
14	2	4010	BCR	6	0
11	1	1123	CLA	5	0
11	1	1011	CLA	1	0
11	L	1501	CLA	4	0
11	a	1128	CLA	2	0
11	a	1127	CLA	1	0
11	A	1132	CLA	2	0
11	1	1124	CLA	2	0
14	F	4018	BCR	9	0

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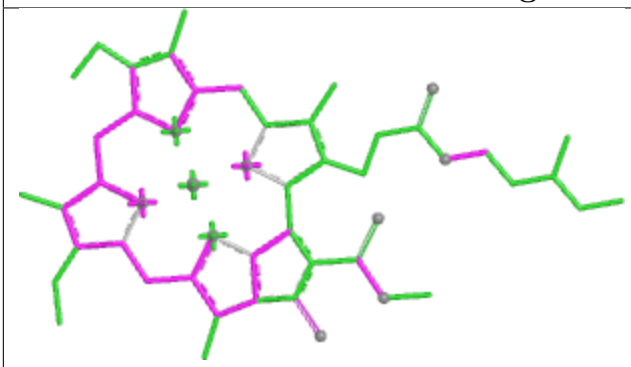
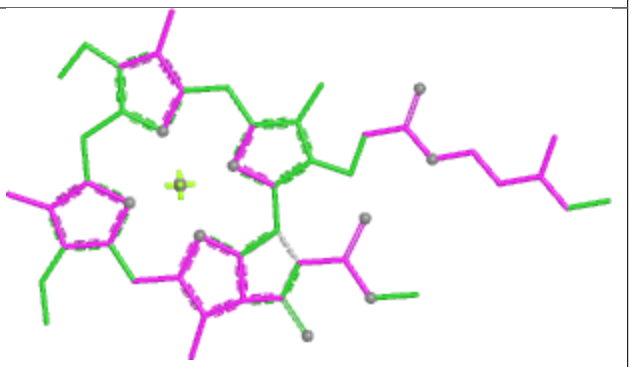
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	2	1217	CLA	1	0
14	2	4014	BCR	7	0
11	b	1217	CLA	2	0
11	K	1402	CLA	3	0
11	l	1502	CLA	1	0
11	2	1220	CLA	2	0
11	b	1220	CLA	6	0
11	A	1138	CLA	5	0
11	k	1401	CLA	4	0
14	6	4018	BCR	9	0
11	A	1801	CLA	3	0
15	A	5003	LHG	4	0
11	1	1126	CLA	5	0
11	B	1229	CLA	5	0
14	1	4007	BCR	7	0
11	B	1021	CLA	8	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.

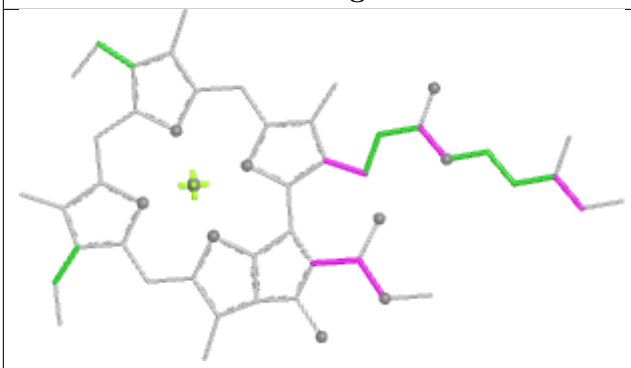
Ligand CLA 1 1135



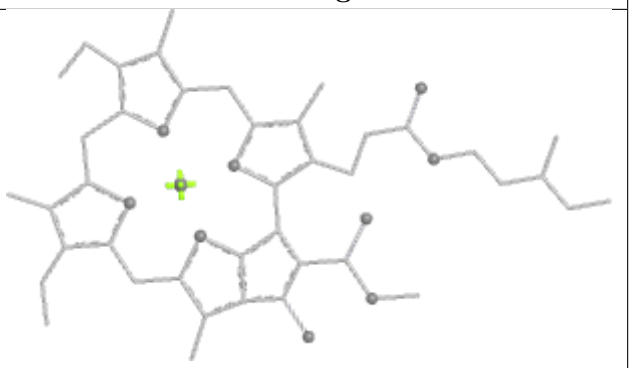
Bond lengths



Bond angles

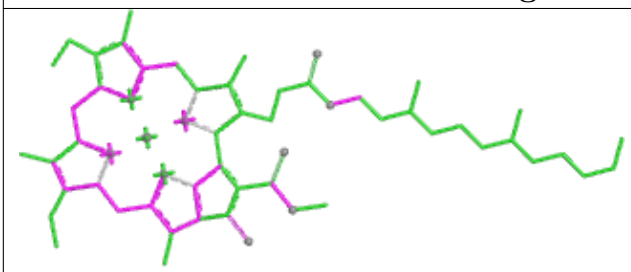


Torsions

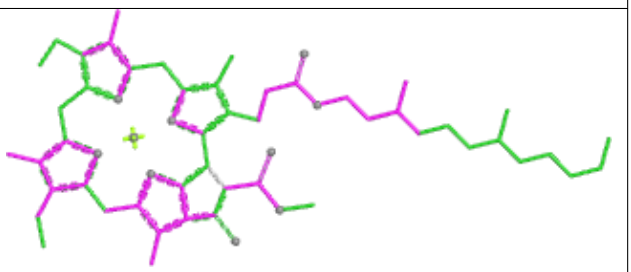


Rings

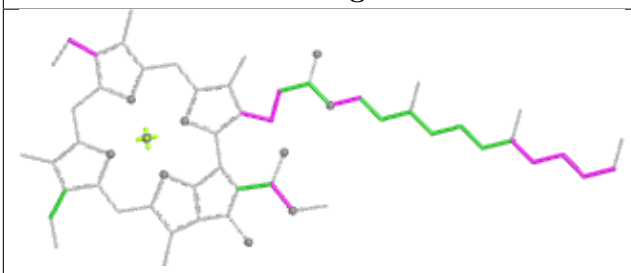
Ligand CLA 2 1214



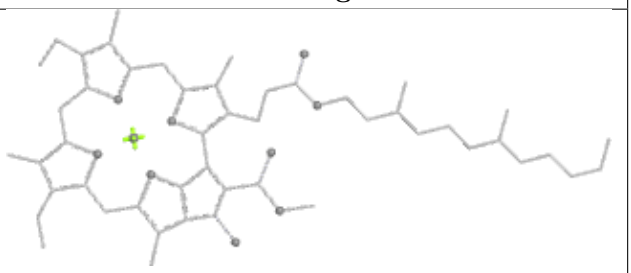
Bond lengths



Bond angles

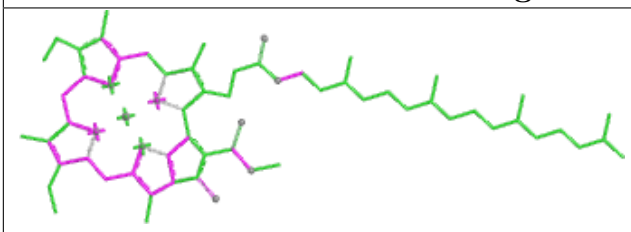


Torsions

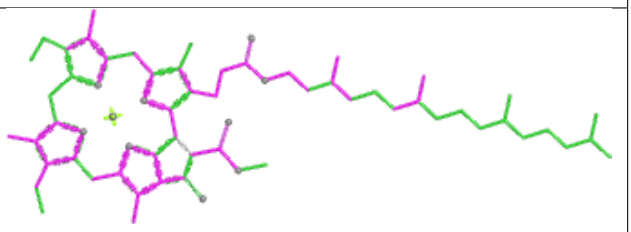


Rings

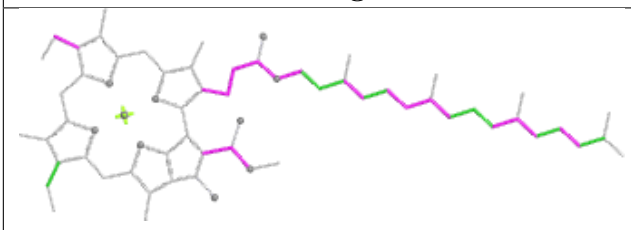
Ligand CLA K 1401



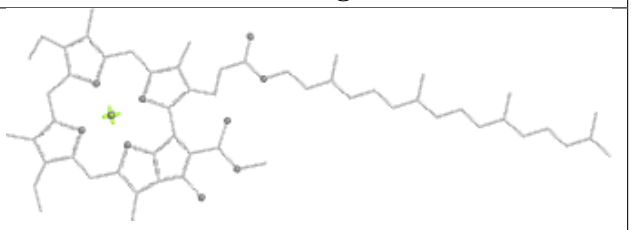
Bond lengths



Bond angles

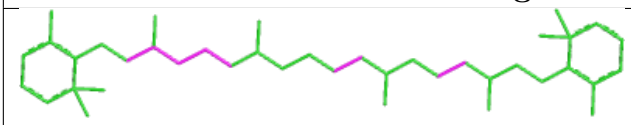


Torsions

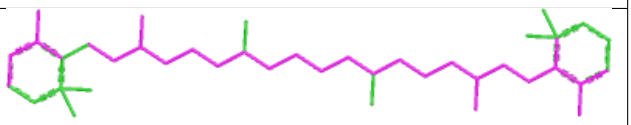


Rings

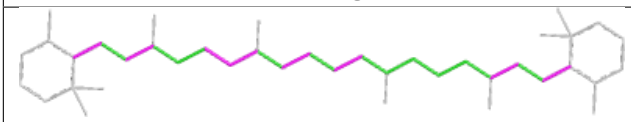
Ligand BCR B 4009



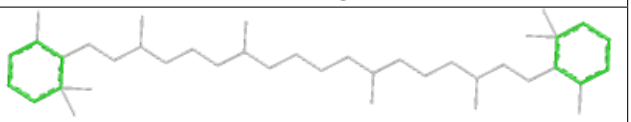
Bond lengths



Bond angles

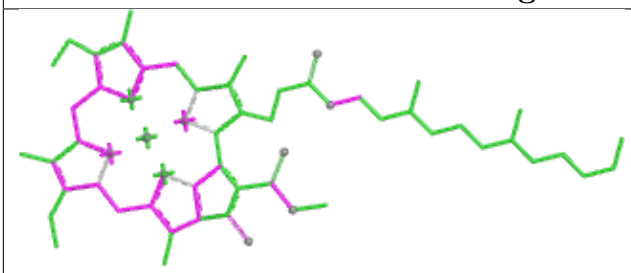


Torsions

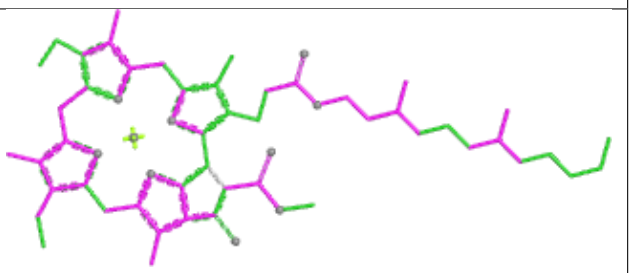


Rings

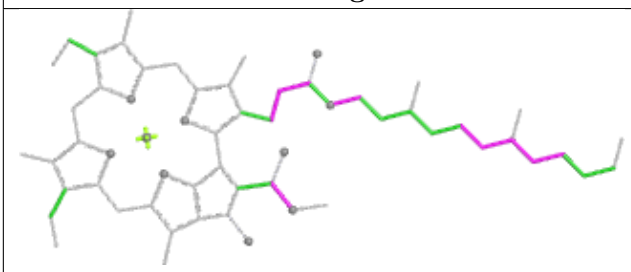
Ligand CLA b 1214



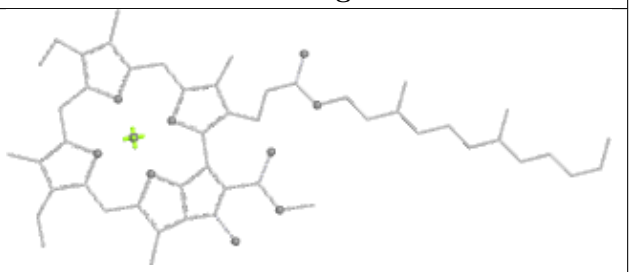
Bond lengths



Bond angles

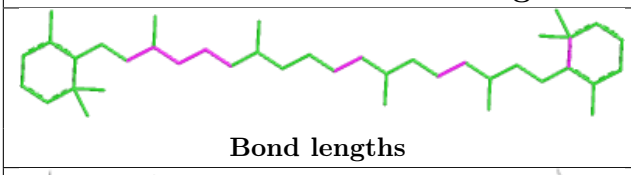


Torsions

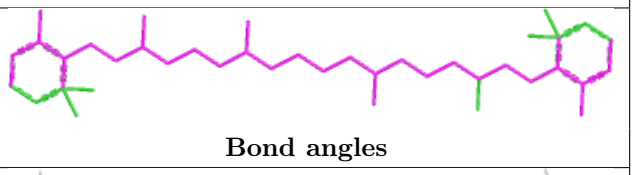


Rings

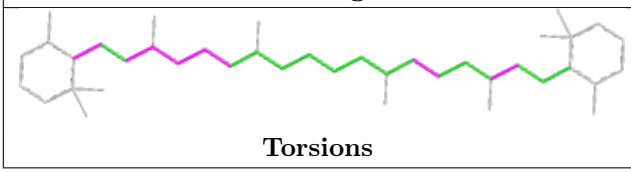
Ligand BCR A 4008



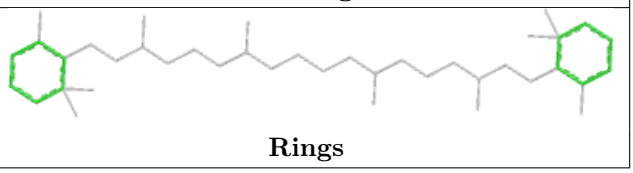
Bond lengths



Bond angles

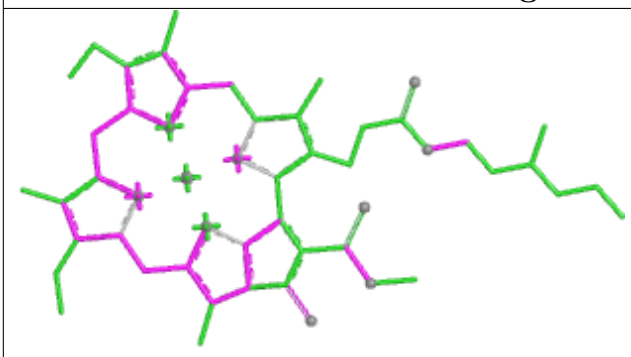


Torsions

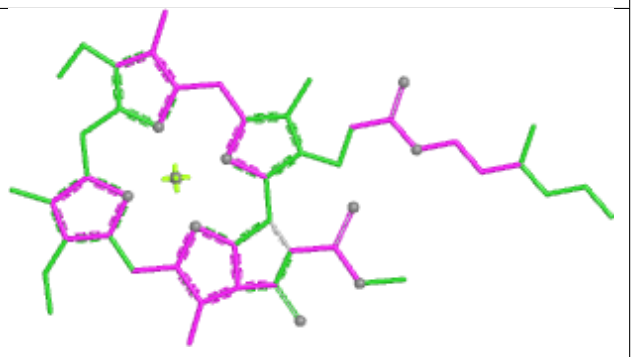


Rings

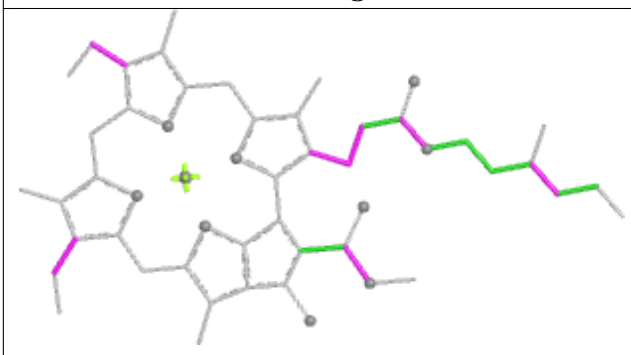
Ligand CLA a 1801



Bond lengths



Bond angles



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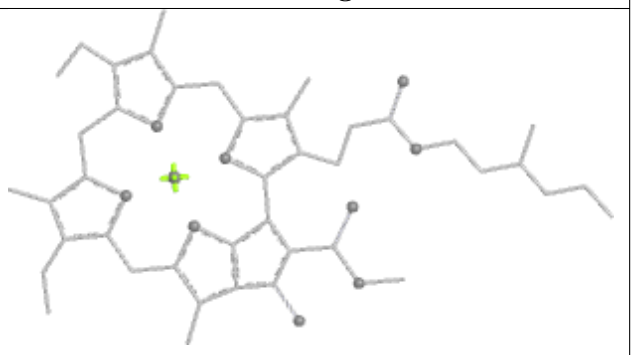
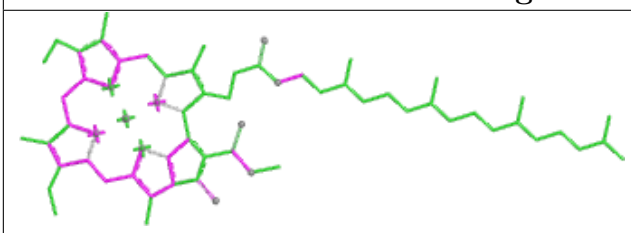


Rings

Ligand CLA B 1023



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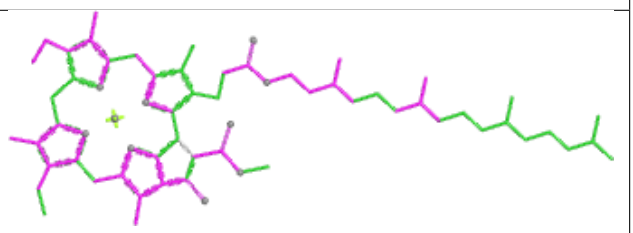

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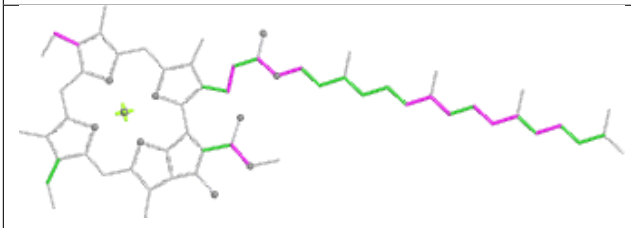

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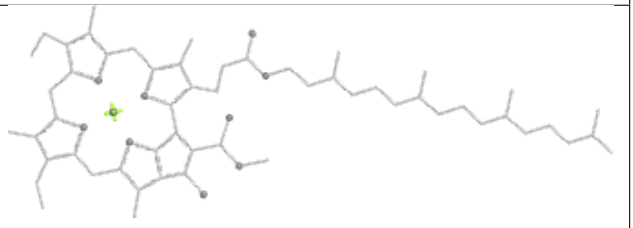
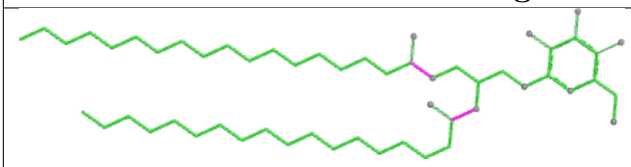


Rings

Ligand LMG b 5002



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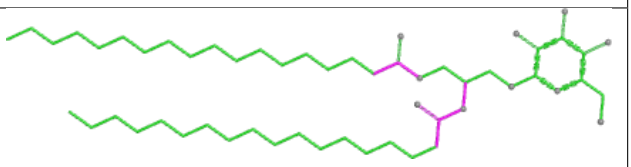
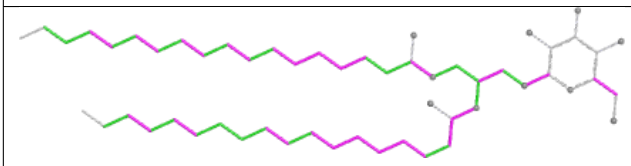


Bond angles



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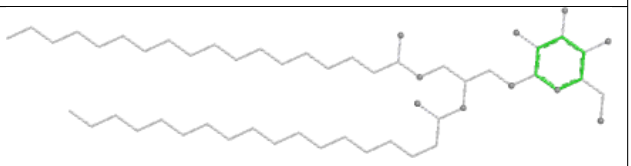
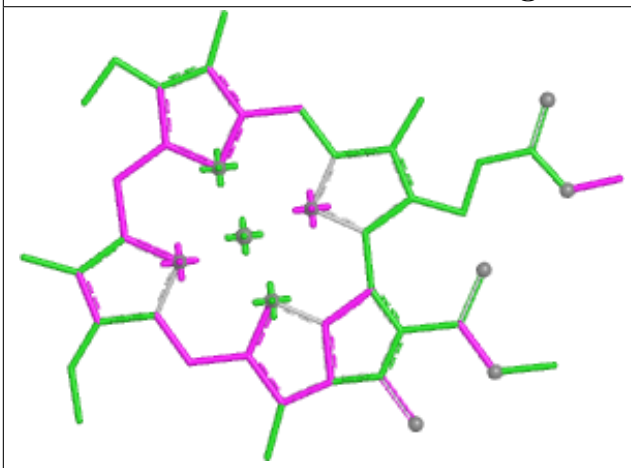


Rings

Ligand CLA 2 1211



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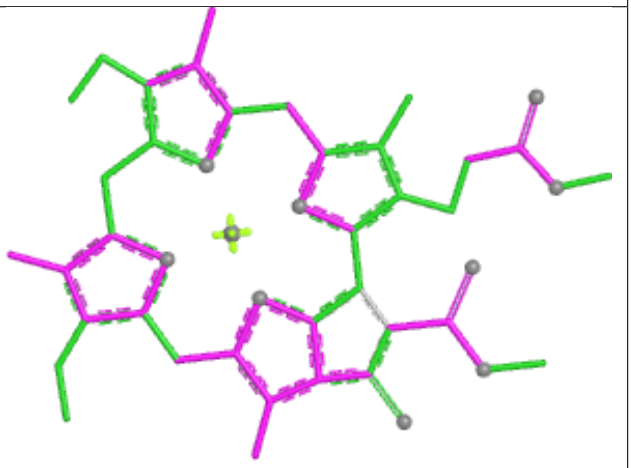
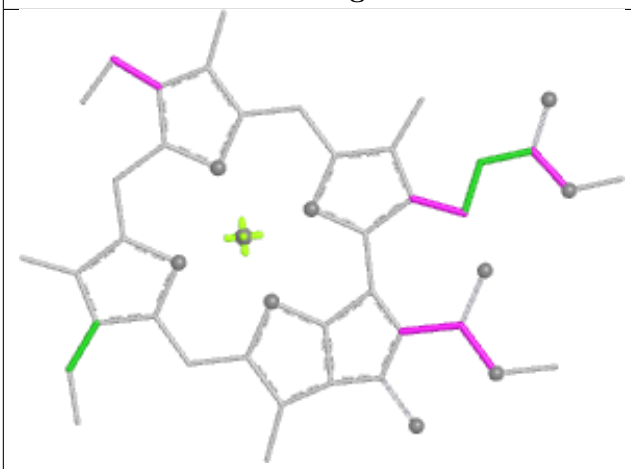


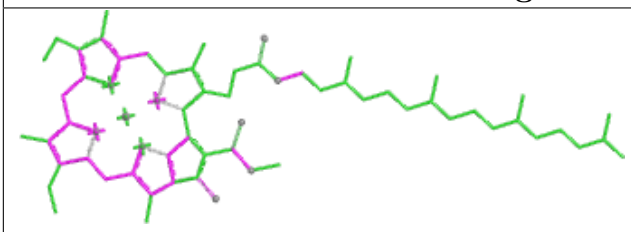
Bond angles



Torsions

Rings

Ligand CLA B 1223



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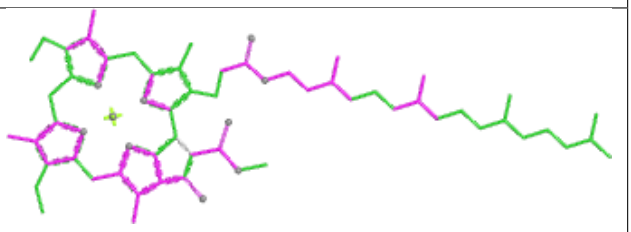

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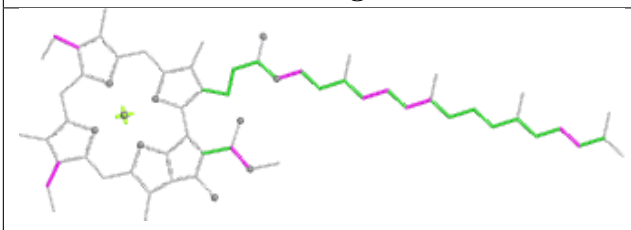

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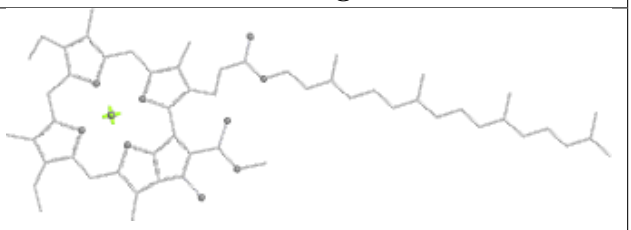
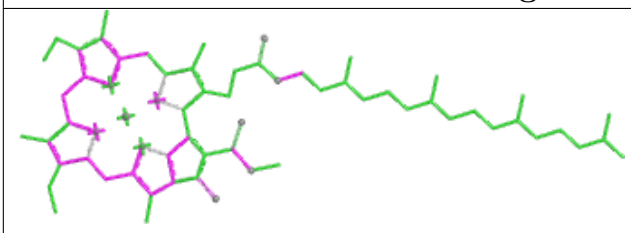


Rings

Ligand CLA 8 1501



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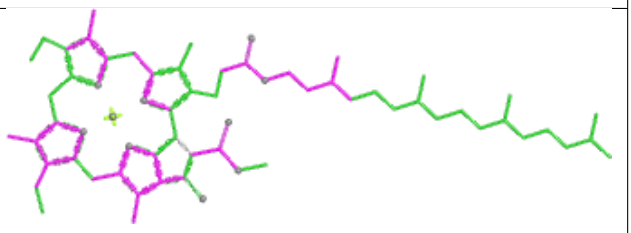

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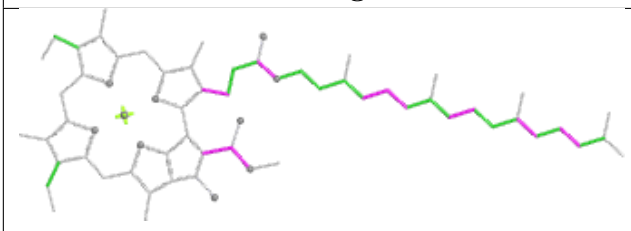

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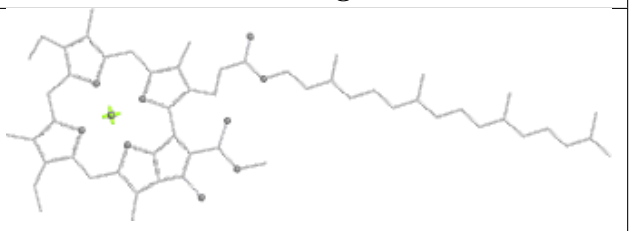
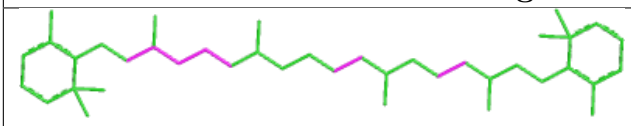


Rings

Ligand BCR b 4006



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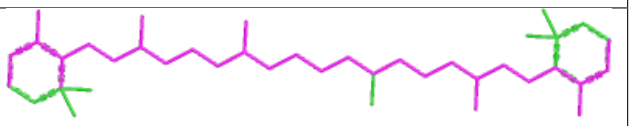

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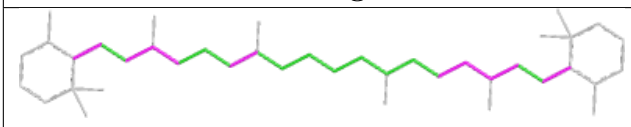

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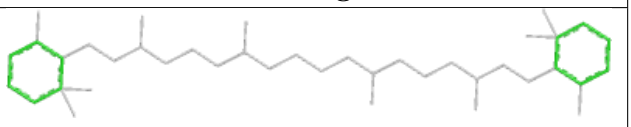
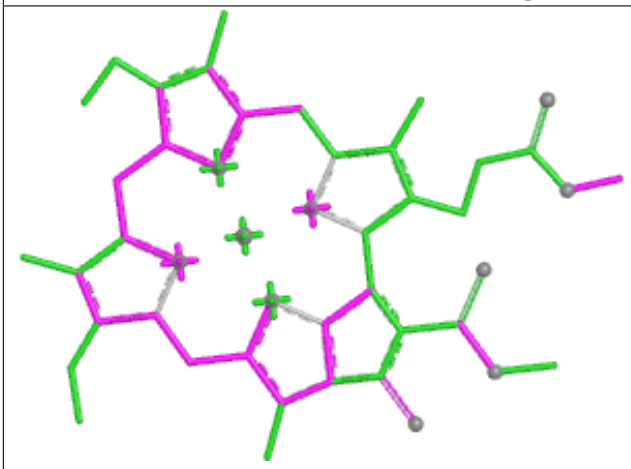


Rings

Ligand CLA 2 1239



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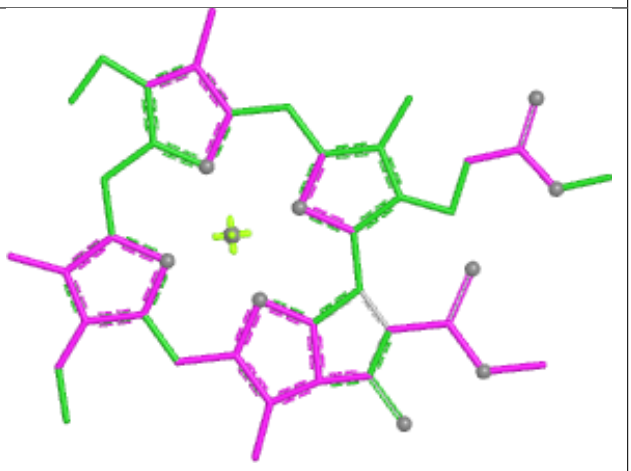
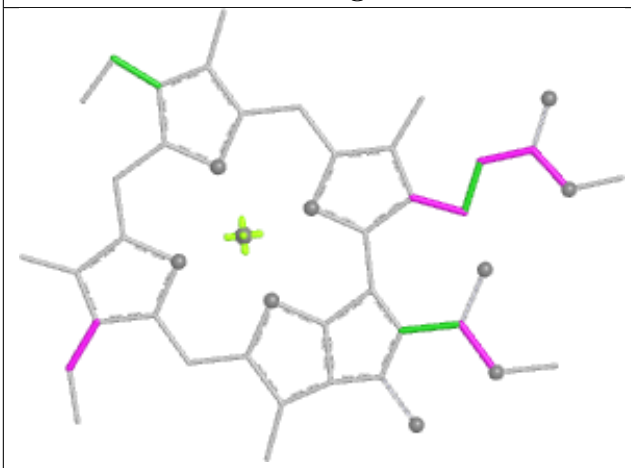


Bond angles



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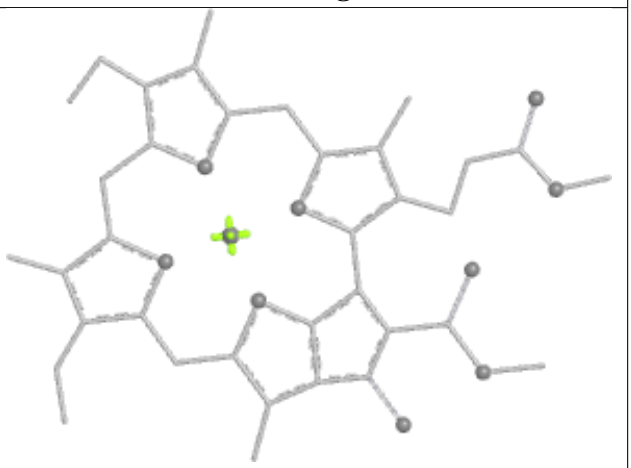
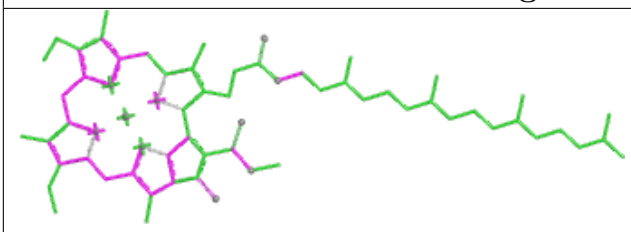


Rings

Ligand CLA 1 1132



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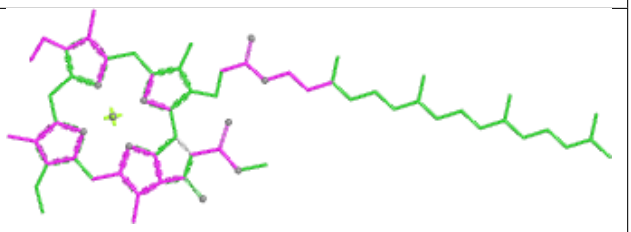
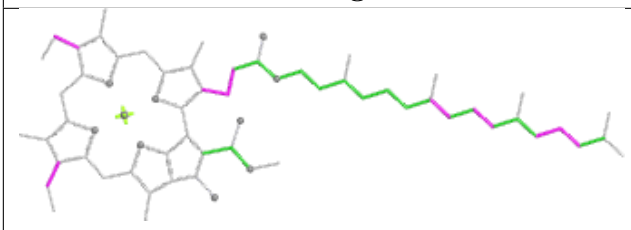


Bond angles



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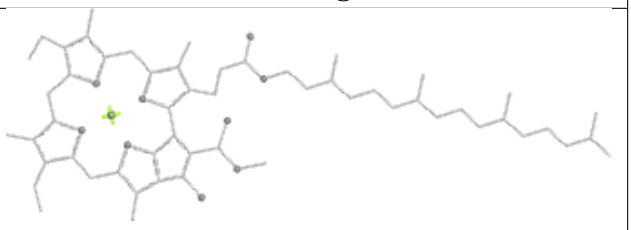
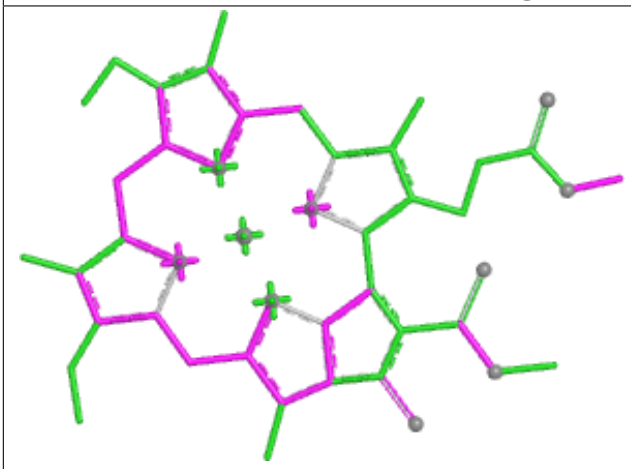


Rings

Ligand CLA b 1239



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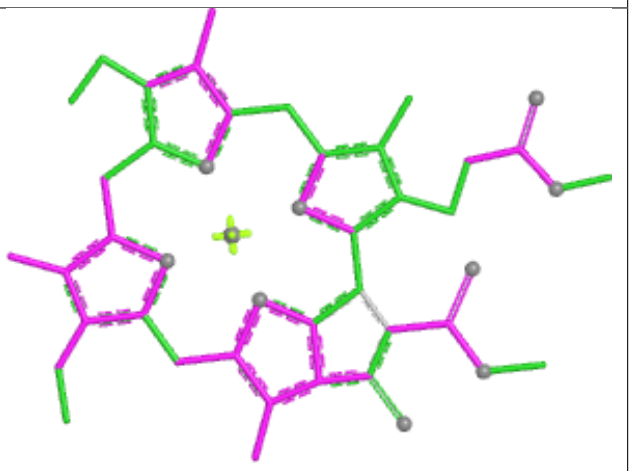

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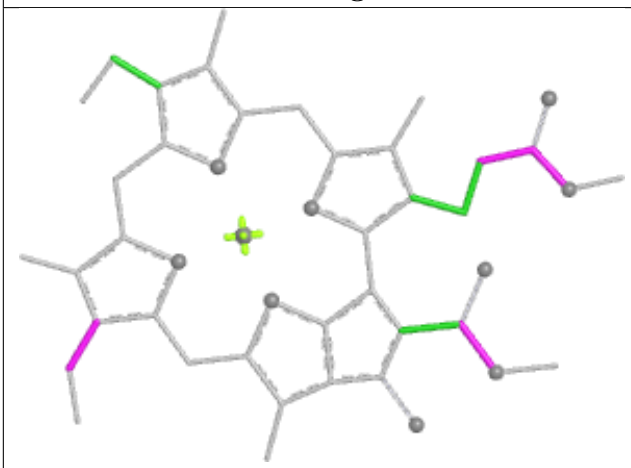

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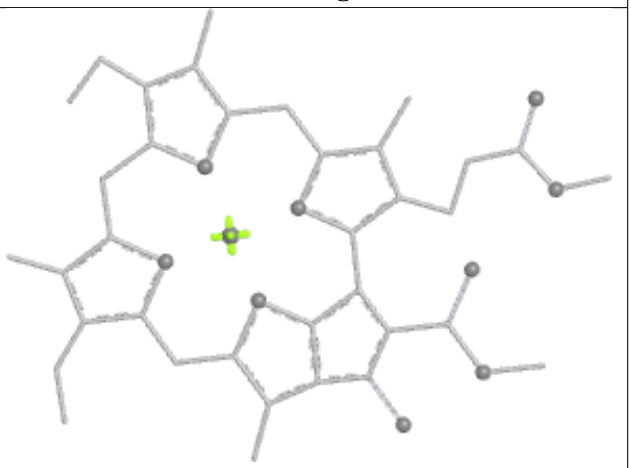
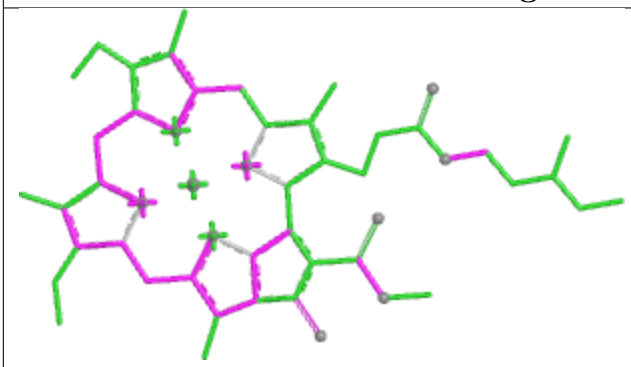


Rings

Ligand CLA a 1135



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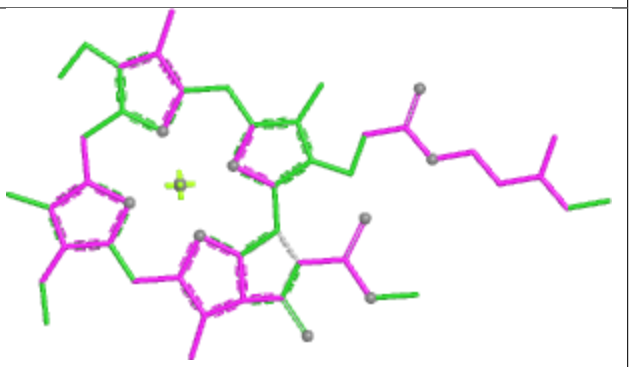
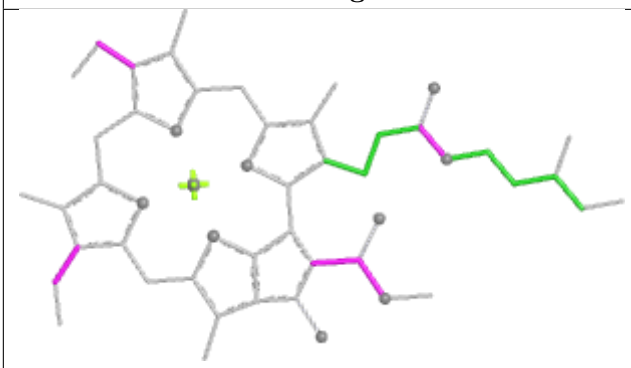


Bond angles



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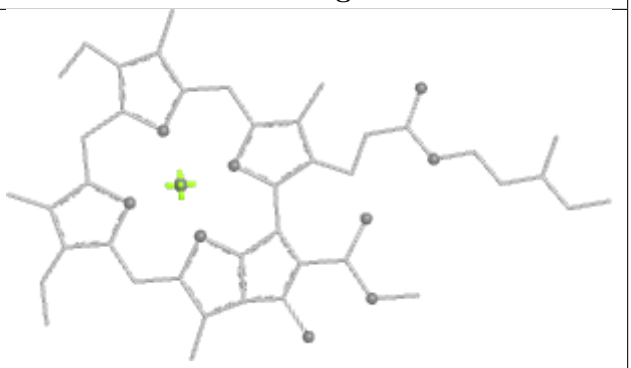
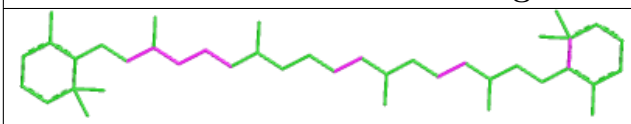


Rings

Ligand BCR A 4007



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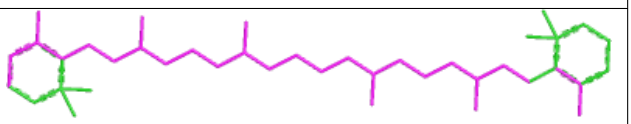
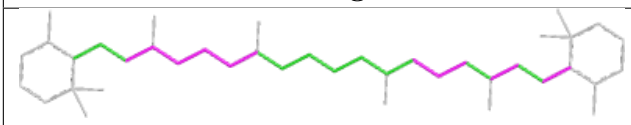
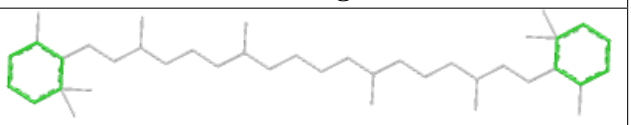


Bond angles

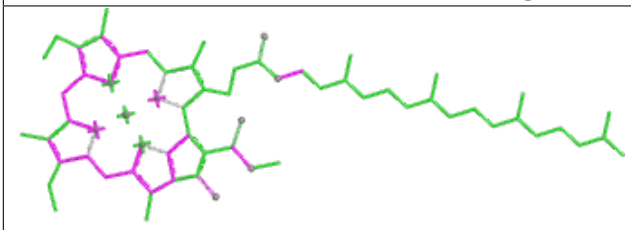


Torsions



Rings

Ligand CLA 2 1023



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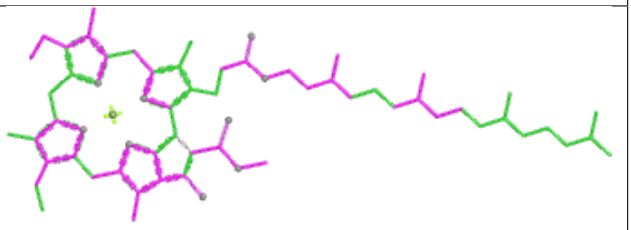
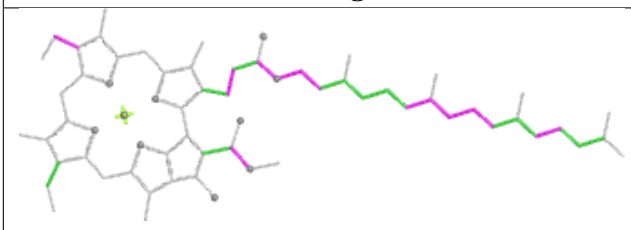
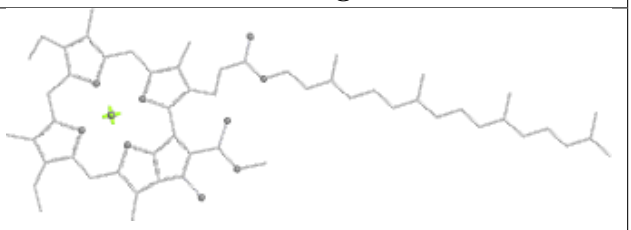


Bond angles

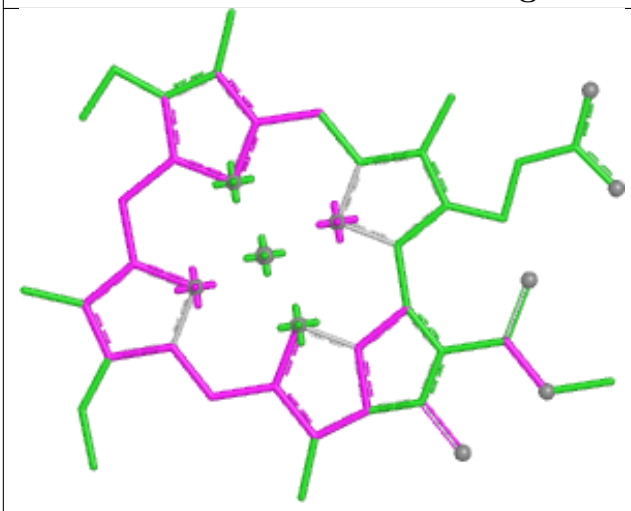


Torsions

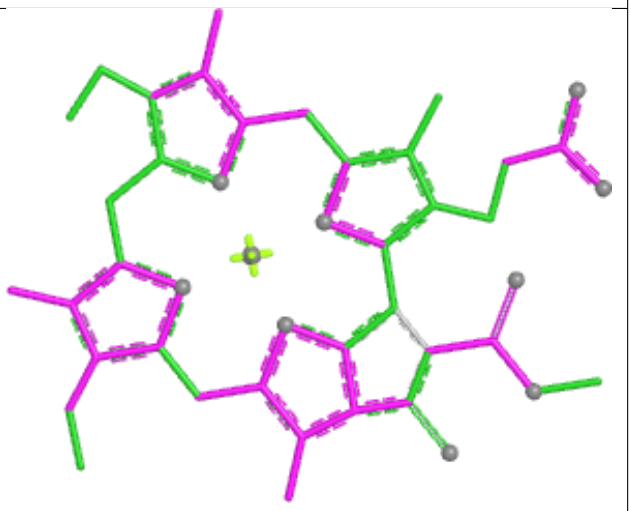


Rings

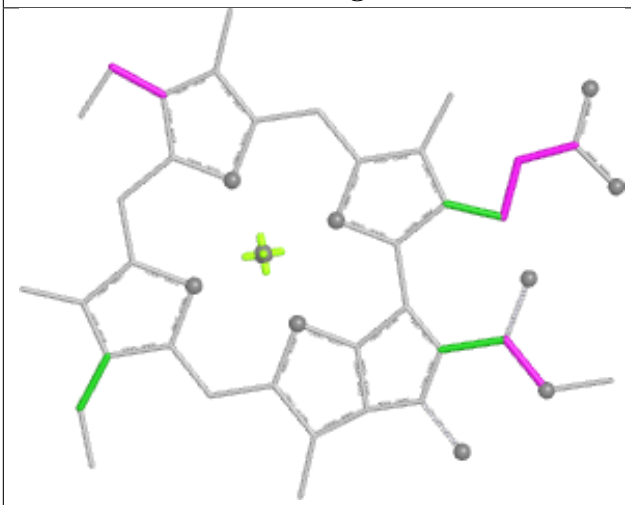
Ligand CLA 2 1232



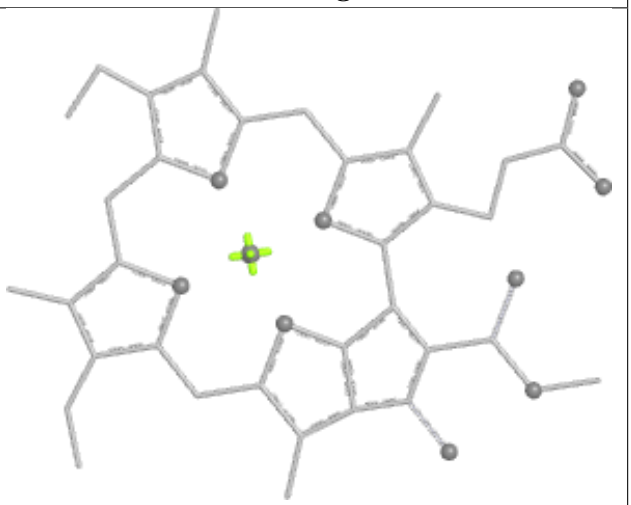
Bond lengths



Bond angles

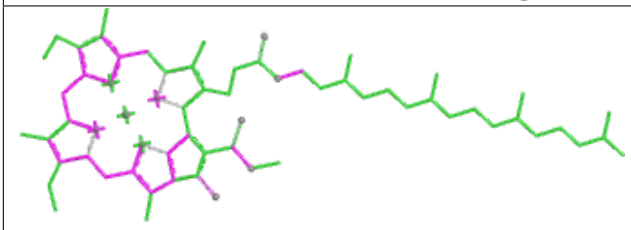


Torsions

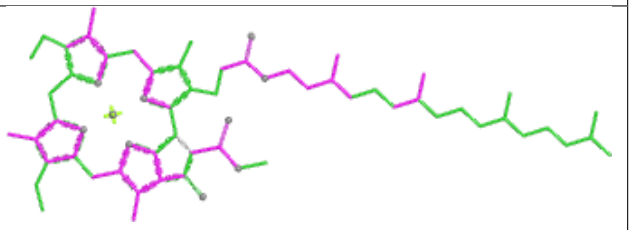


Rings

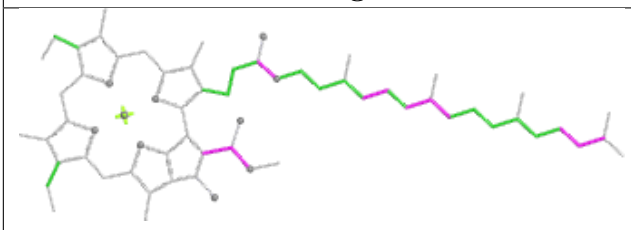
Ligand CLA B 1226



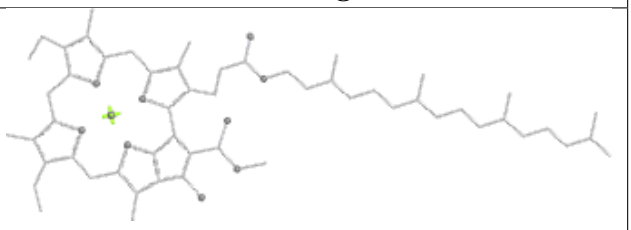
Bond lengths



Bond angles

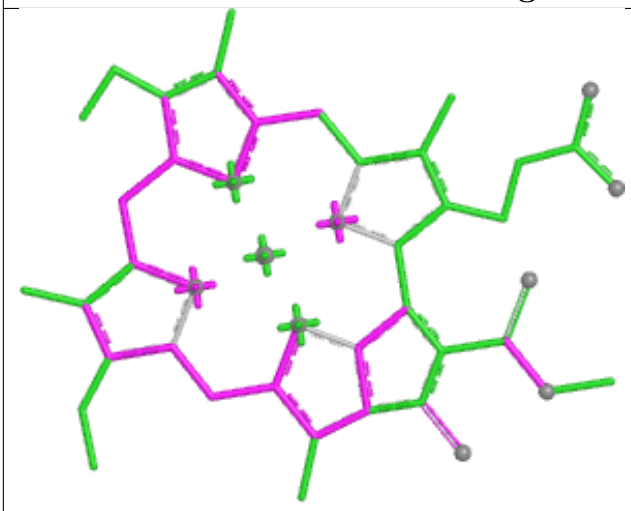


Torsions

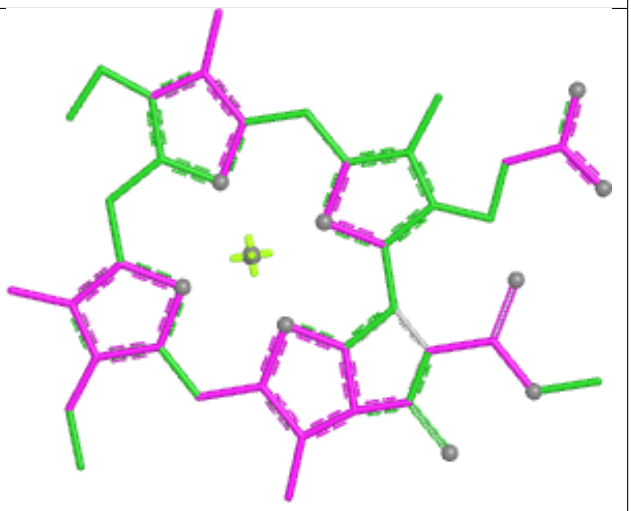


Rings

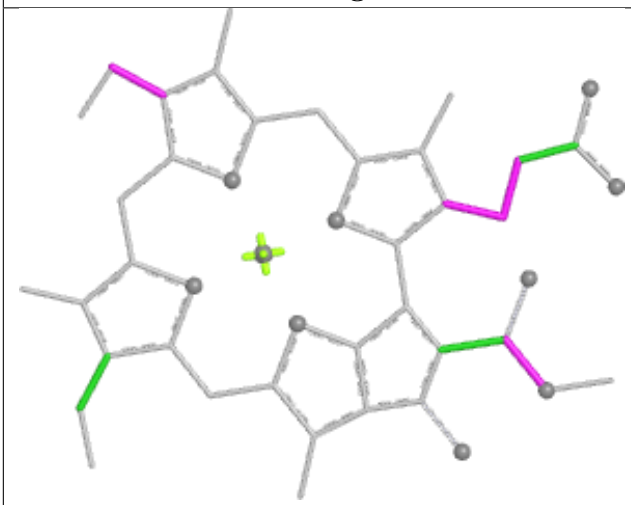
Ligand CLA b 1232



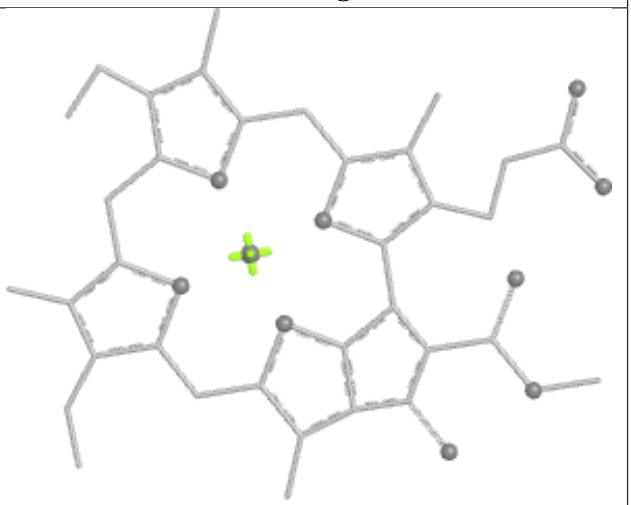
Bond lengths



Bond angles

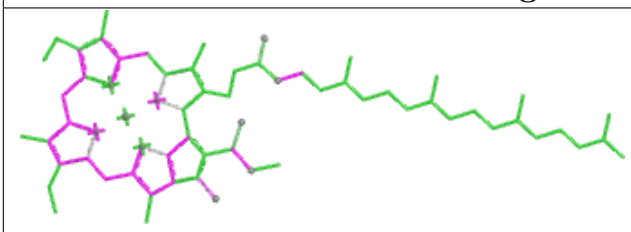


Torsions

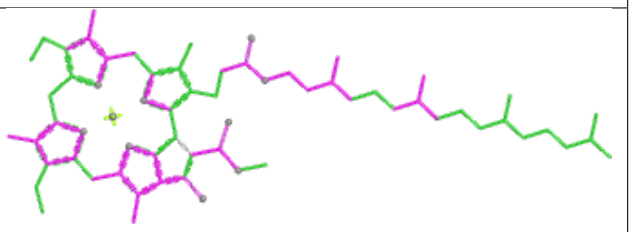


Rings

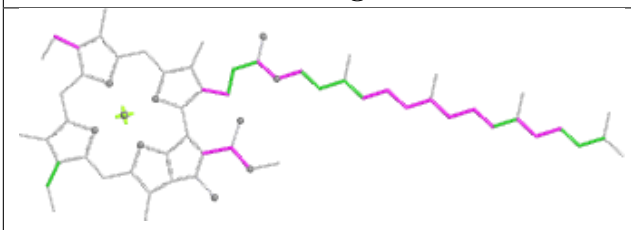
Ligand CLA 2 1223



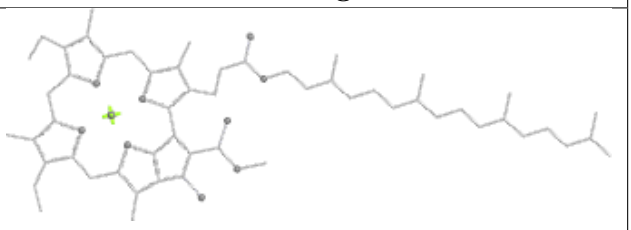
Bond lengths



Bond angles

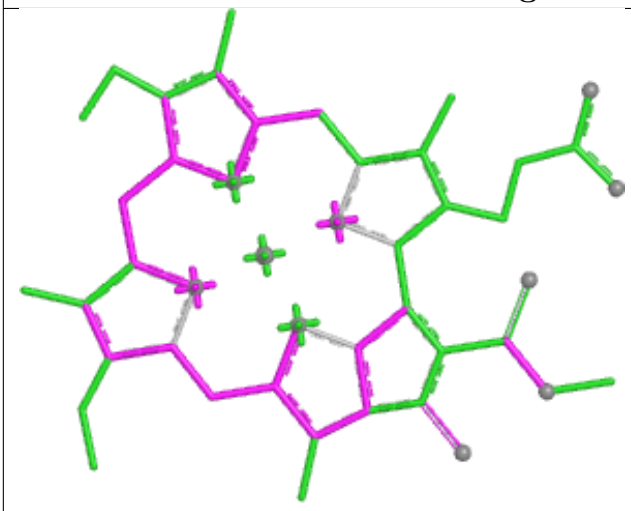


Torsions

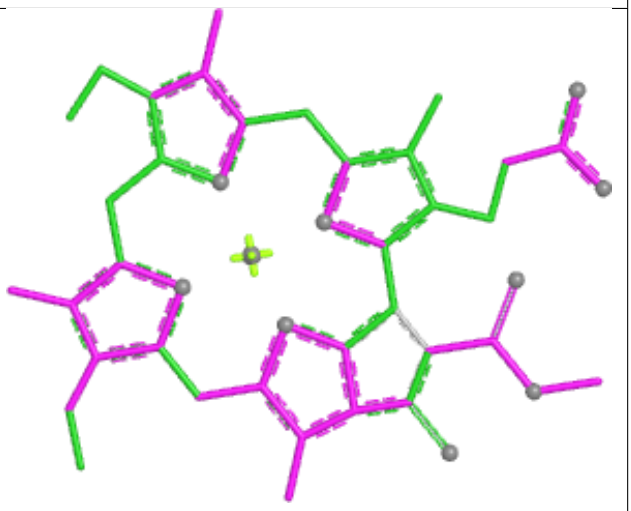


Rings

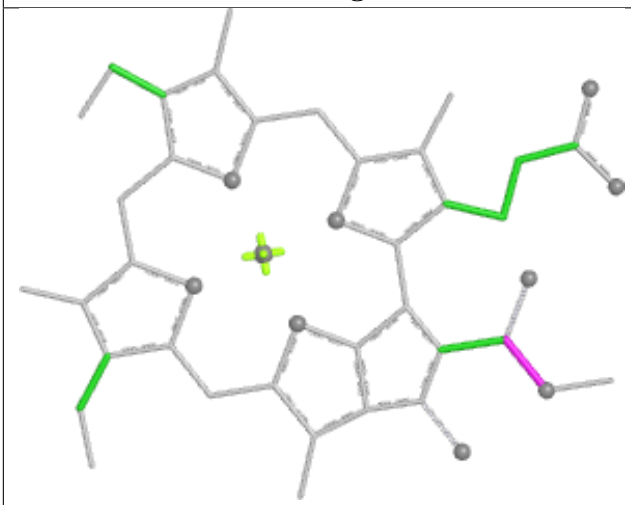
Ligand CLA 2 1212



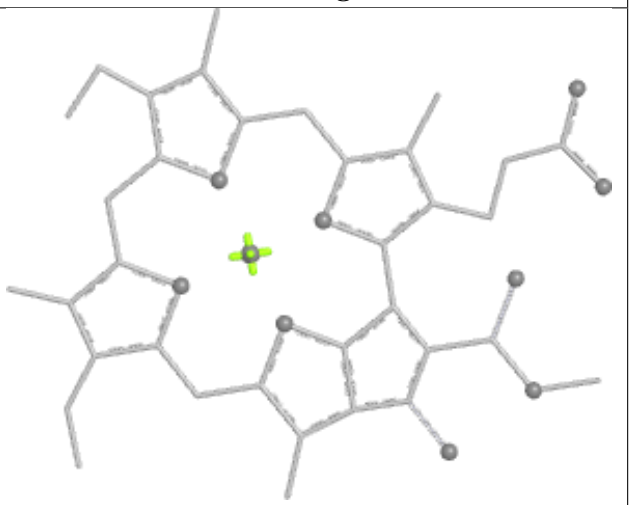
Bond lengths



Bond angles

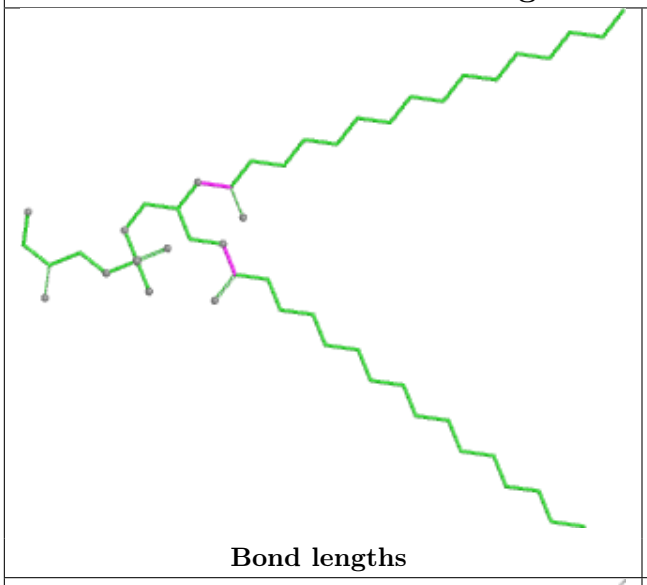


Torsions



Rings

Ligand LHG 2 5004



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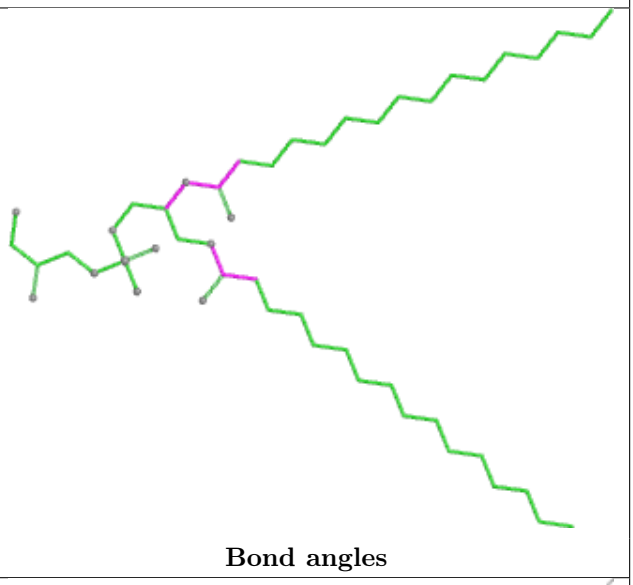
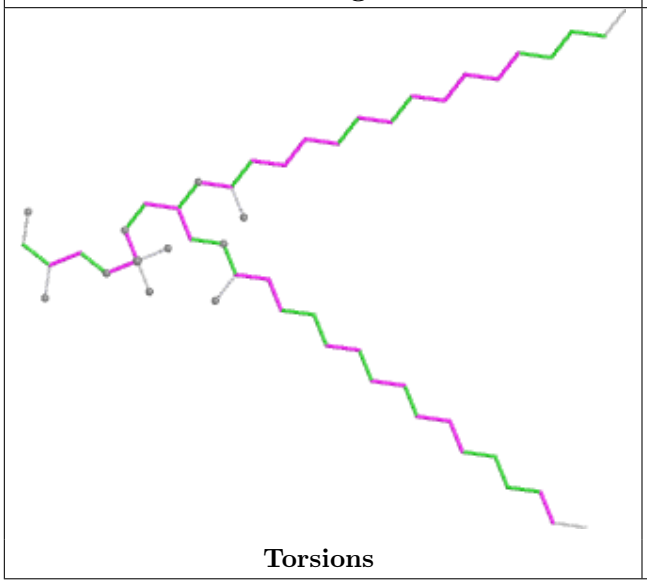


Bond angles



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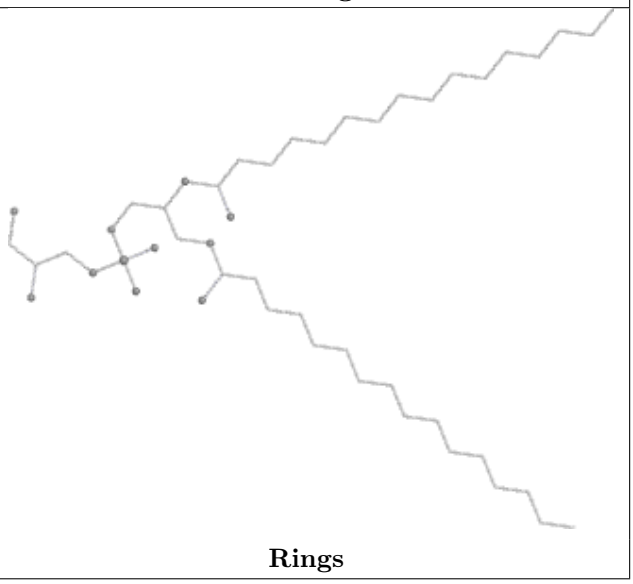
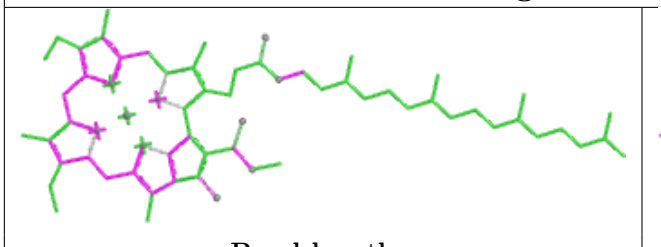
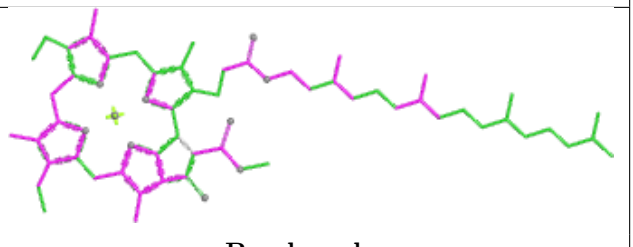


Rings

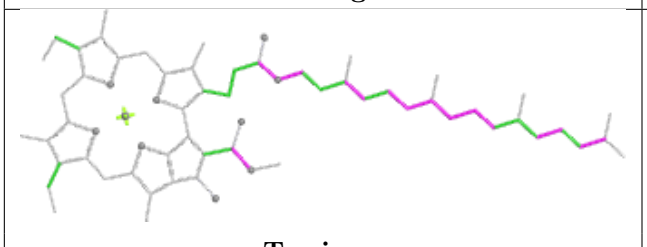
Ligand CLA A 1123



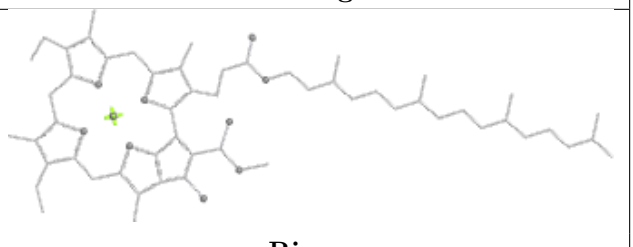
Bond lengths



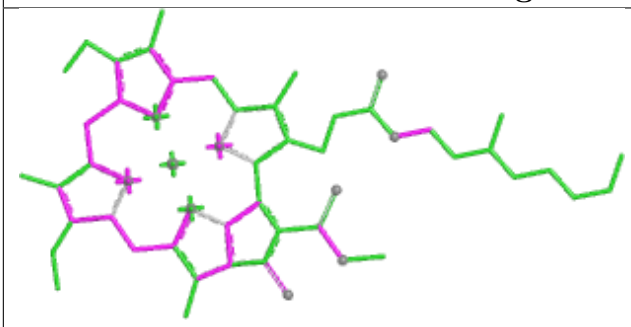
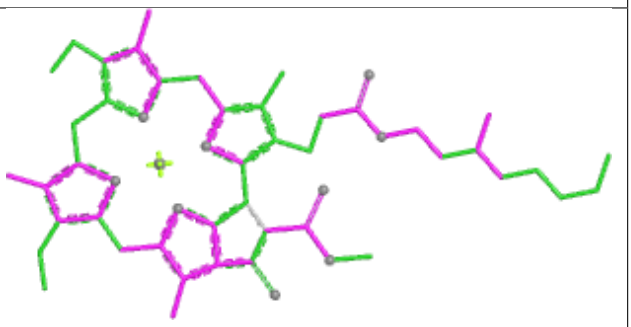
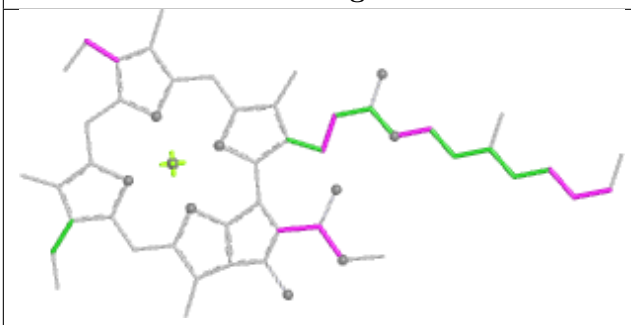
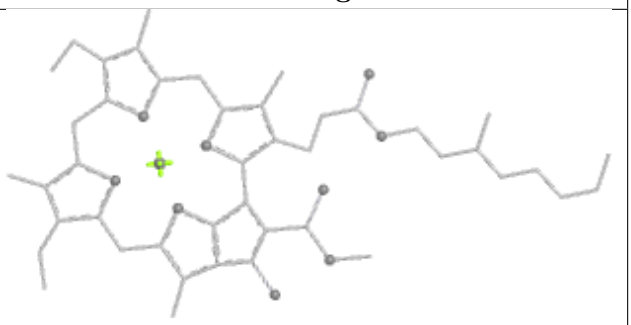
Bond angles

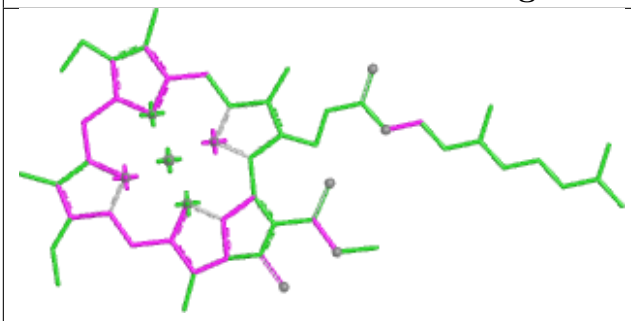
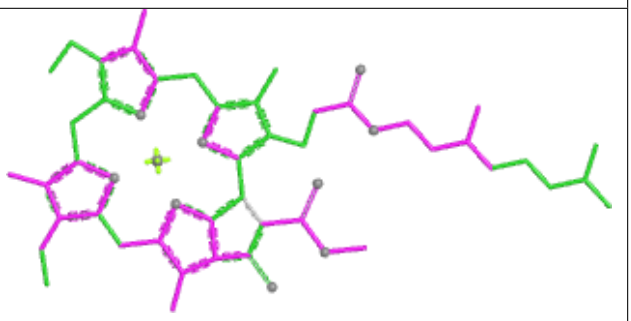
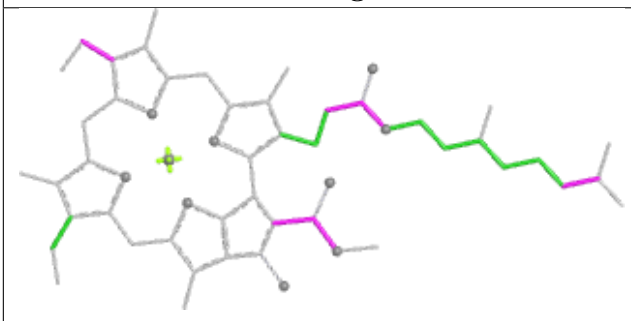
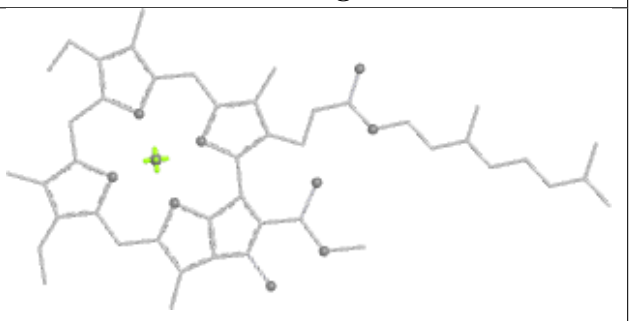


Torsions

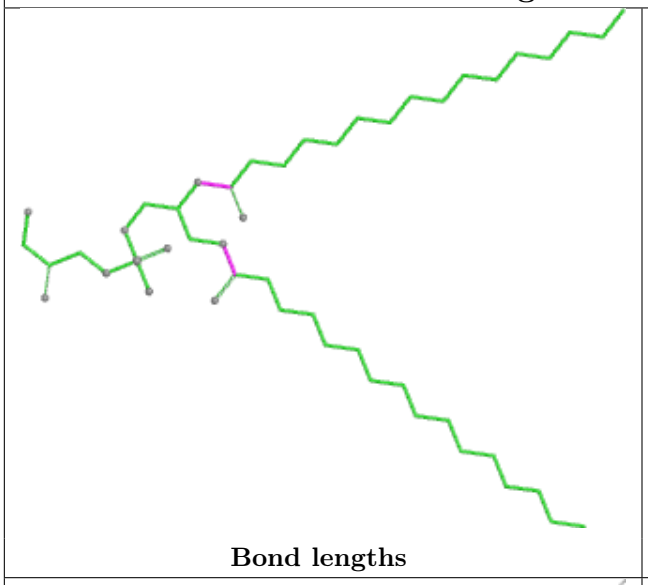


Rings

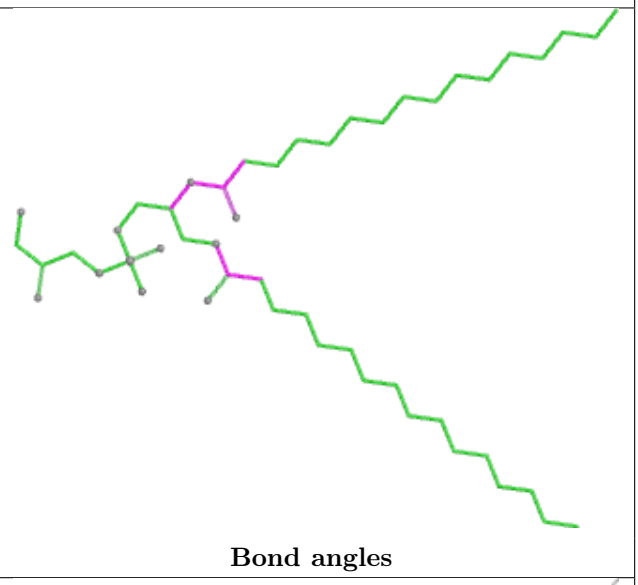
Ligand CLA B 1221	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1219	
	
Bond lengths	Bond angles
	
Torsions	Rings

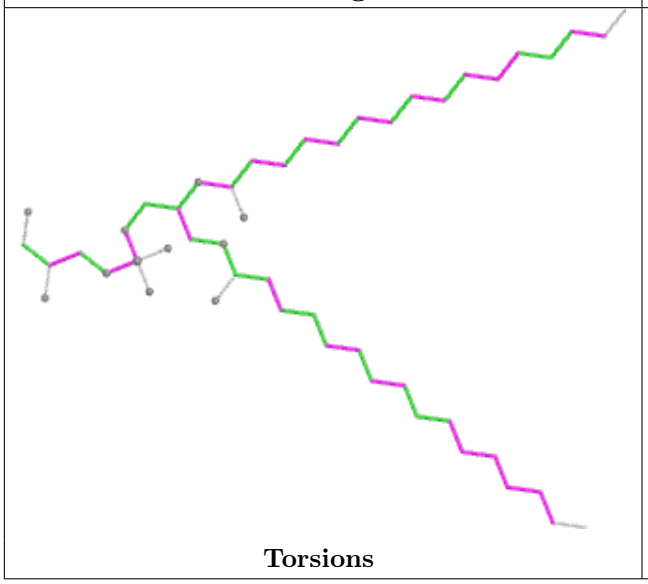
Ligand LHG b 5004



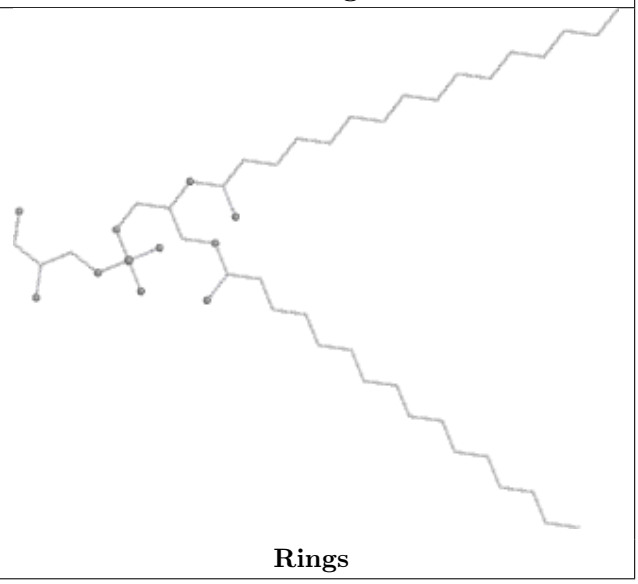
Bond lengths



Bond angles

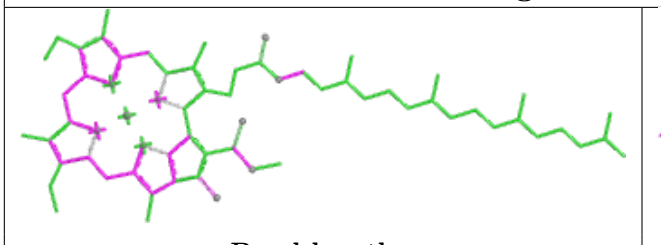


Torsions



Rings

Ligand CLA A 1103



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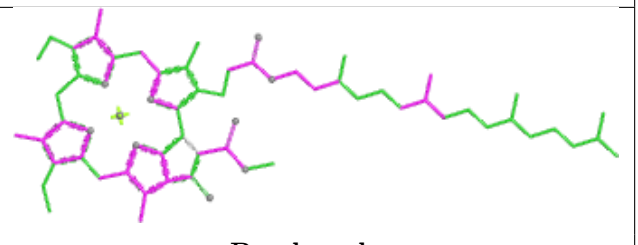
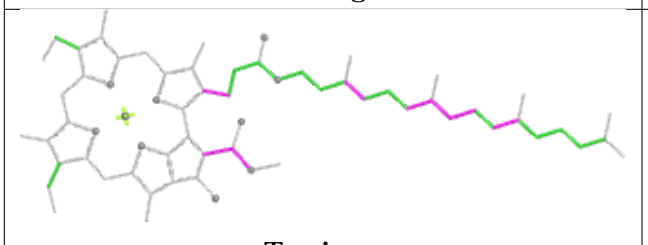
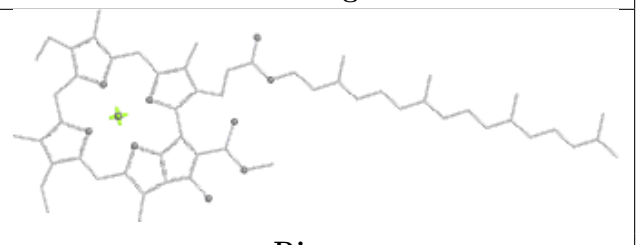


Bond angles

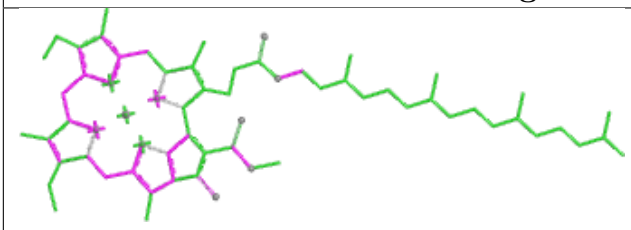


Torsions



Rings

Ligand CLA 2 1226



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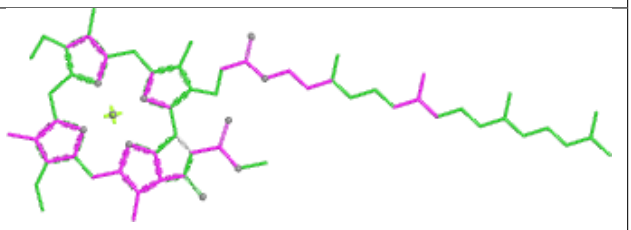
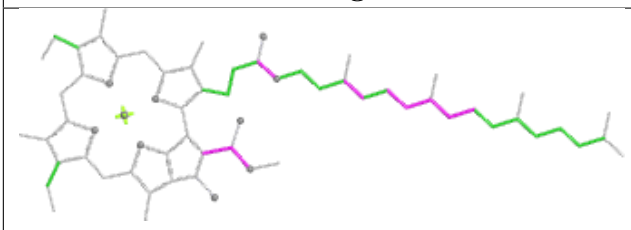
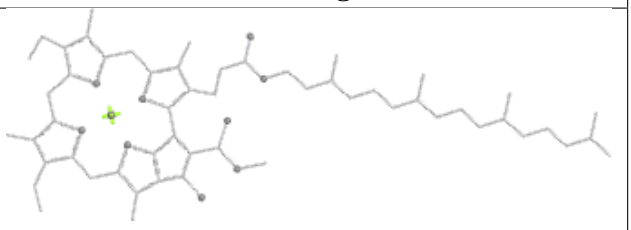


Bond angles

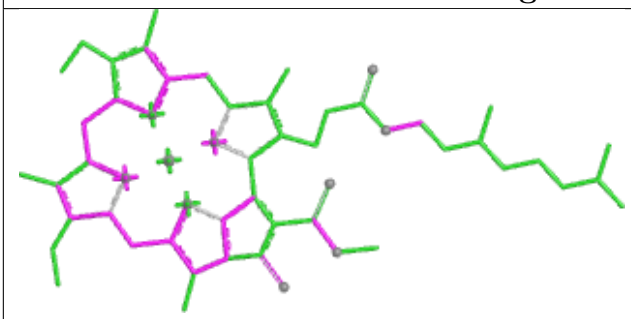


Torsions

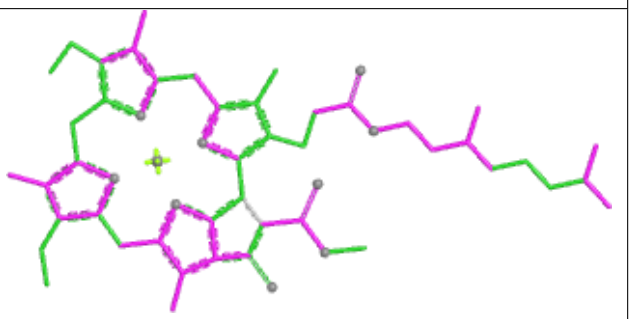


Rings

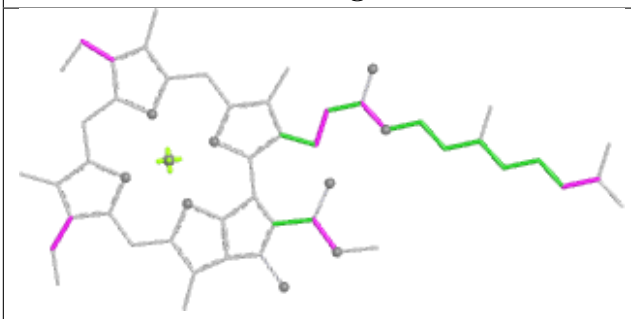
Ligand CLA 2 1224



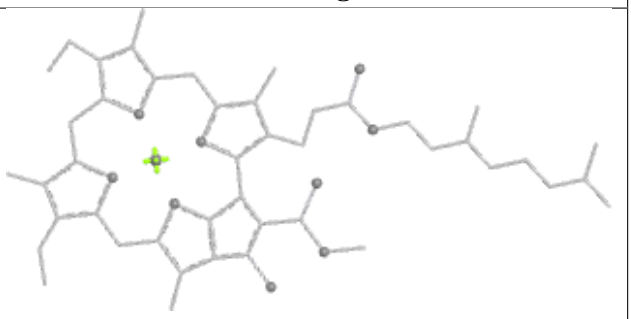
Bond lengths



Bond angles

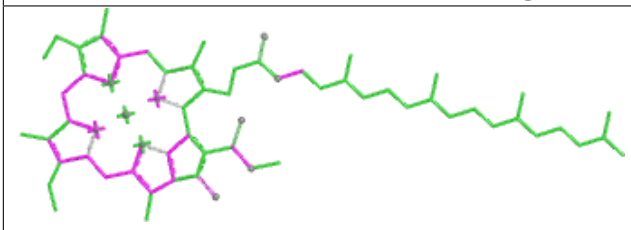


Torsions

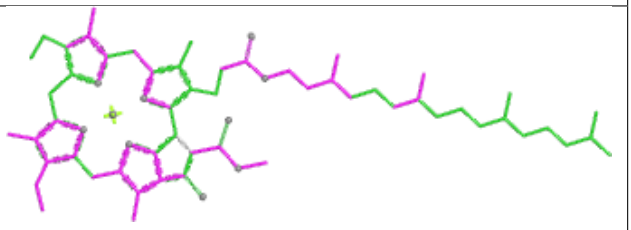


Rings

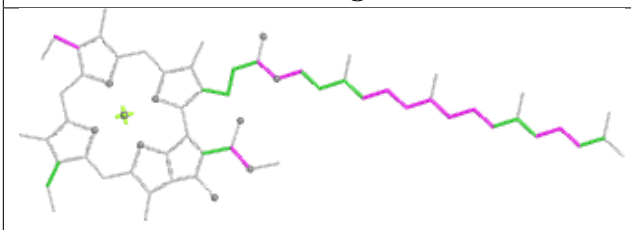
Ligand CLA 2 1203



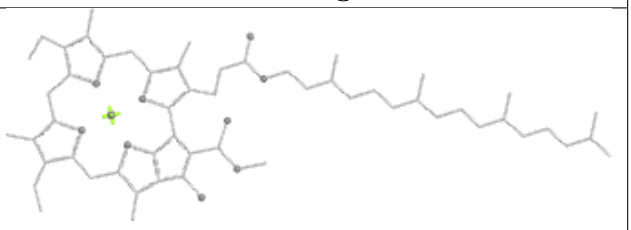
Bond lengths



Bond angles

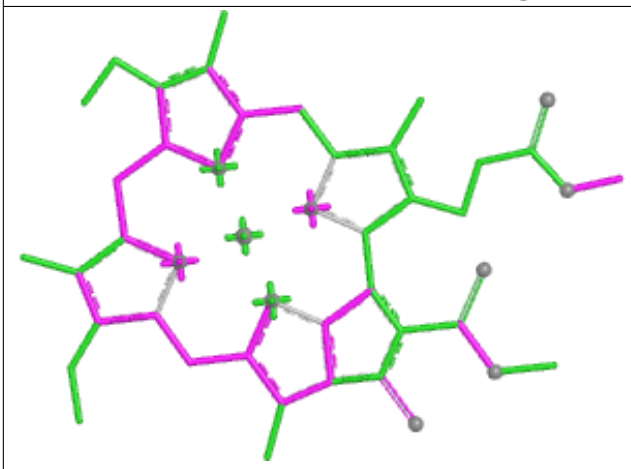


Torsions

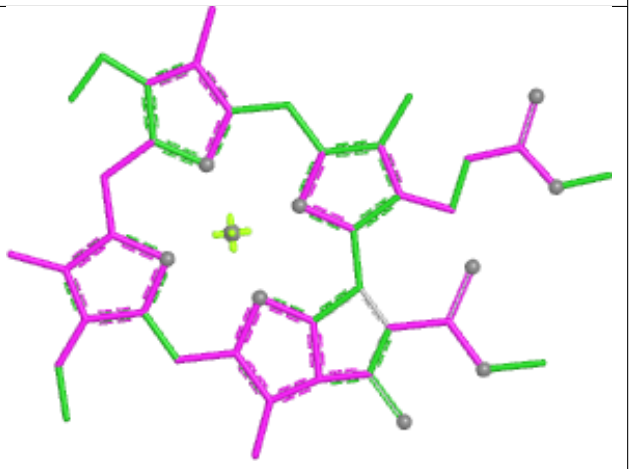


Rings

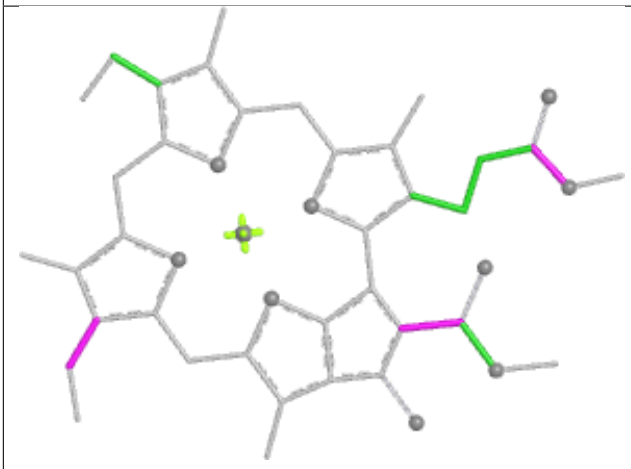
Ligand CLA A 1129



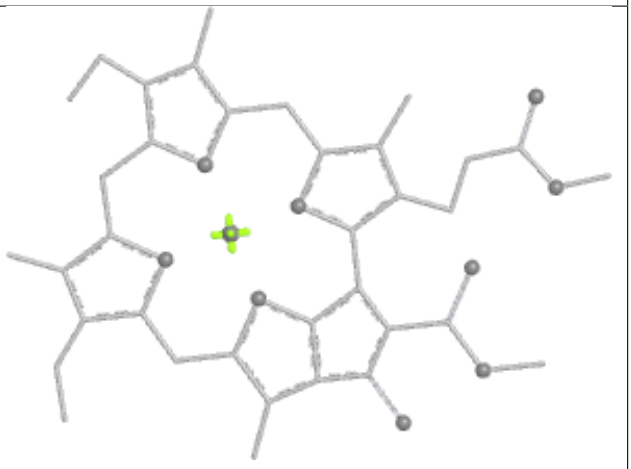
Bond lengths



Bond angles

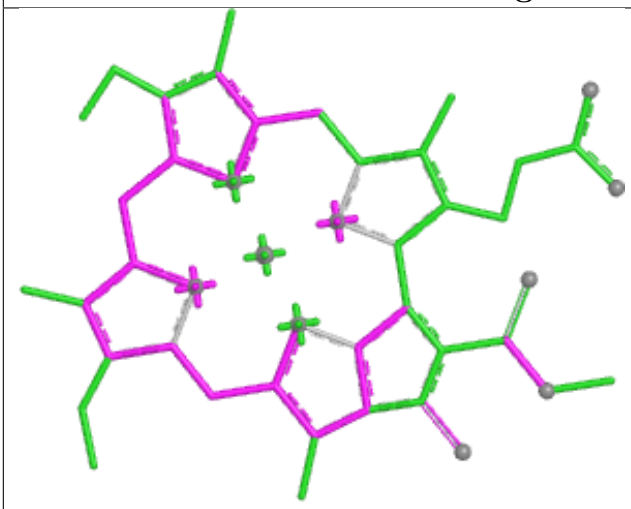


Torsions



Rings

Ligand CLA B 1208



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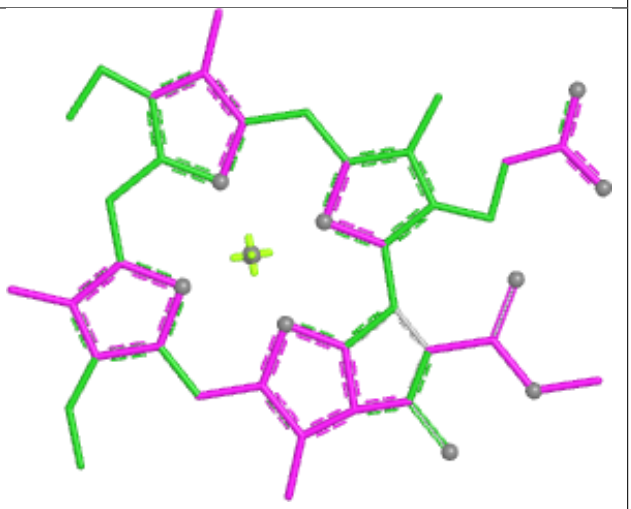
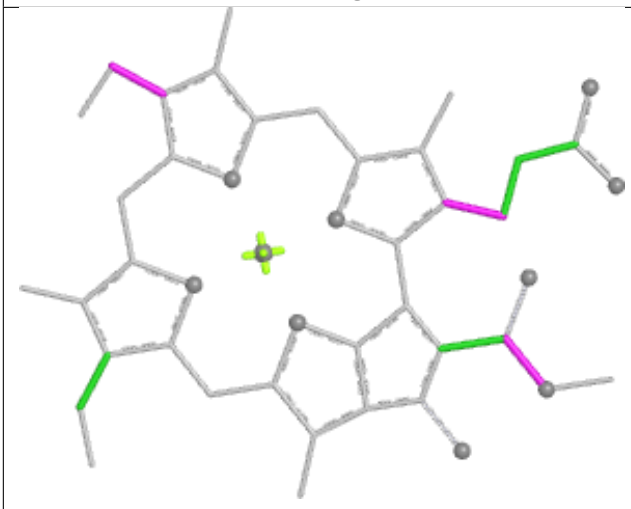


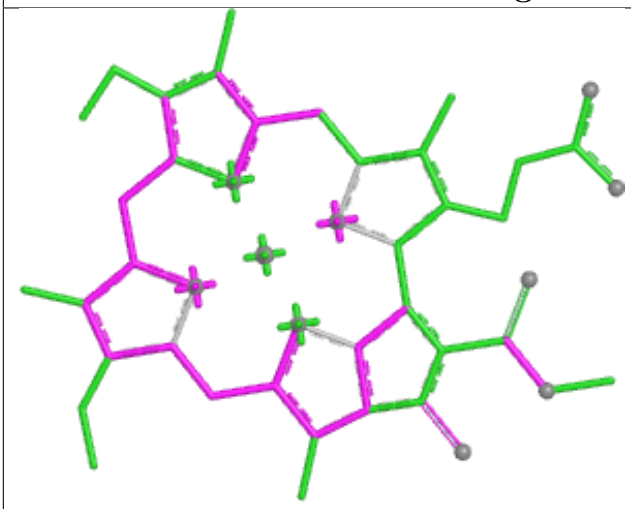
Bond angles



Torsions

Rings

Ligand CLA A 1112



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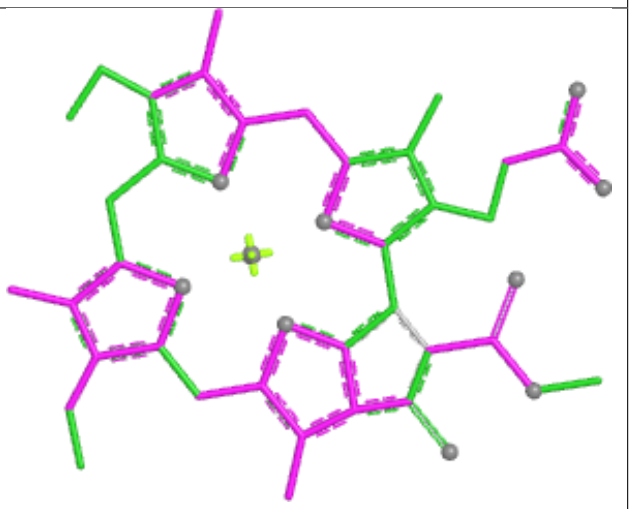
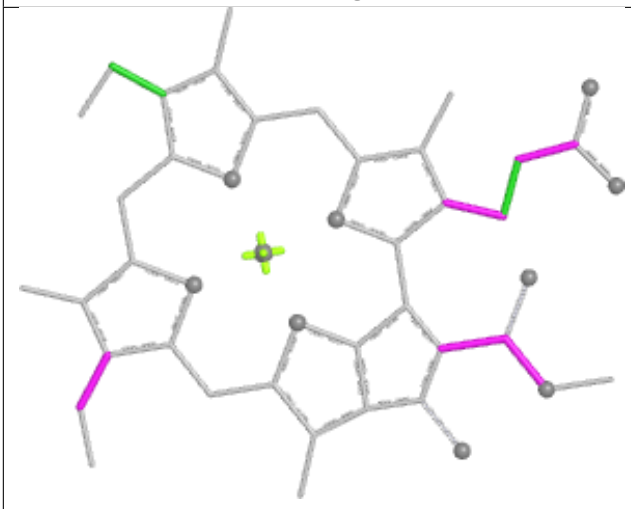


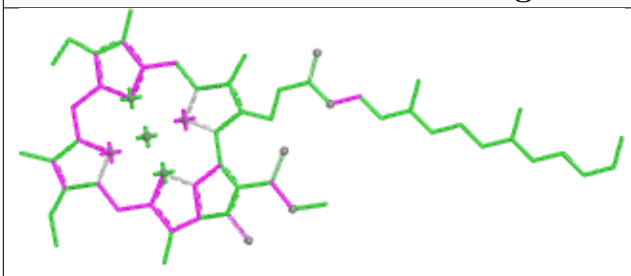
Bond angles



Torsions

Rings

Ligand CLA A 1122



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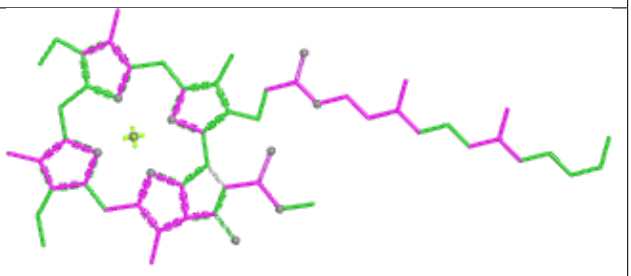
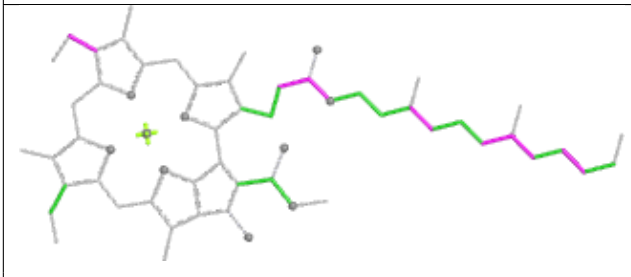
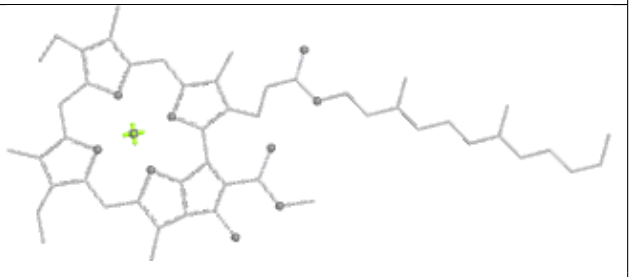


Bond angles

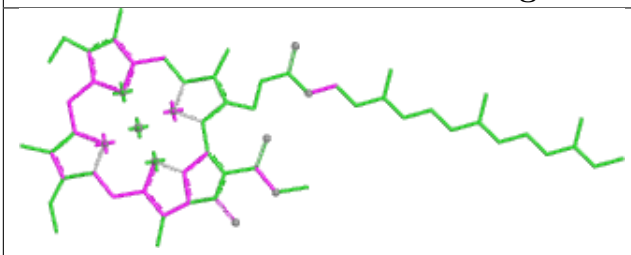


Torsions



Rings

Ligand CLA 1 1118



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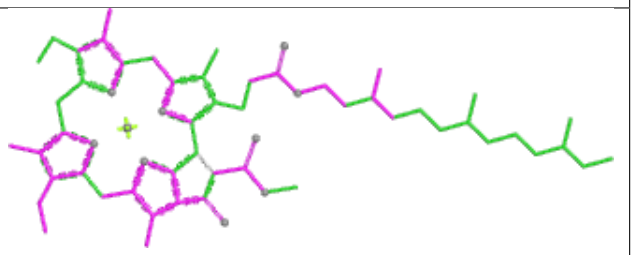
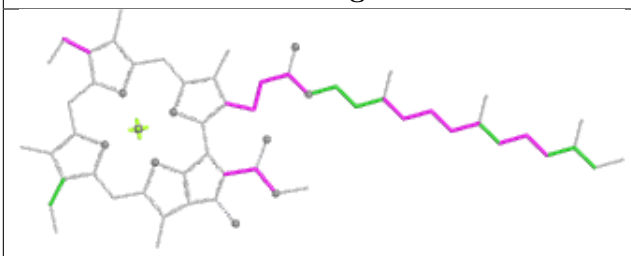
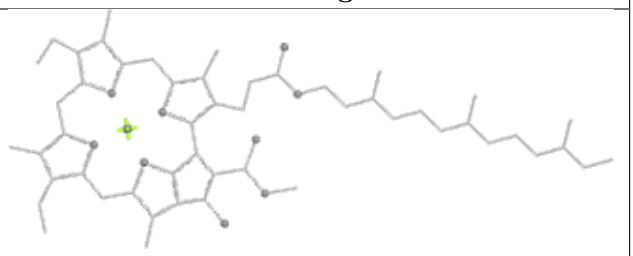


Bond angles

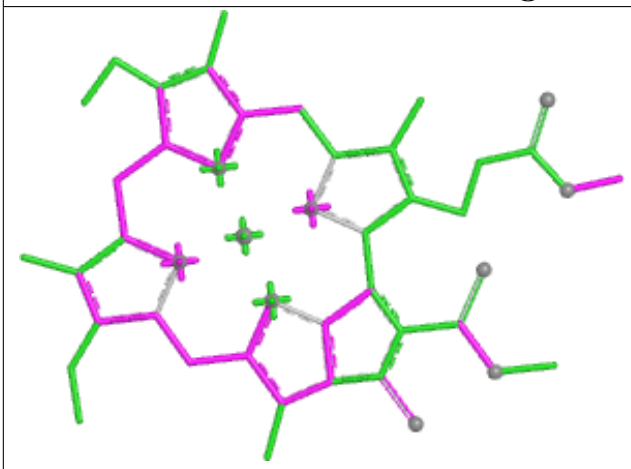


Torsions

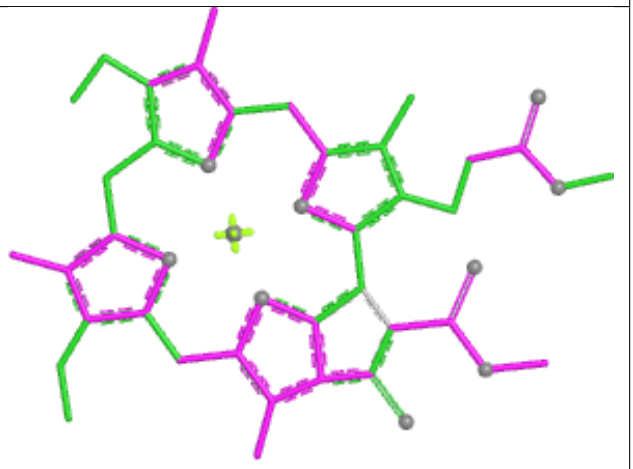


Rings

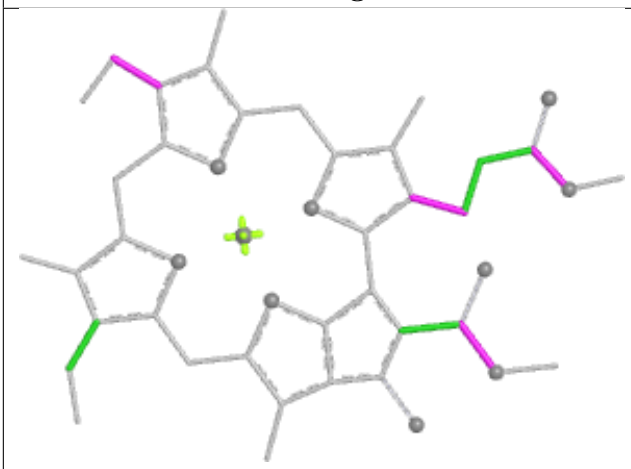
Ligand CLA 1 1121



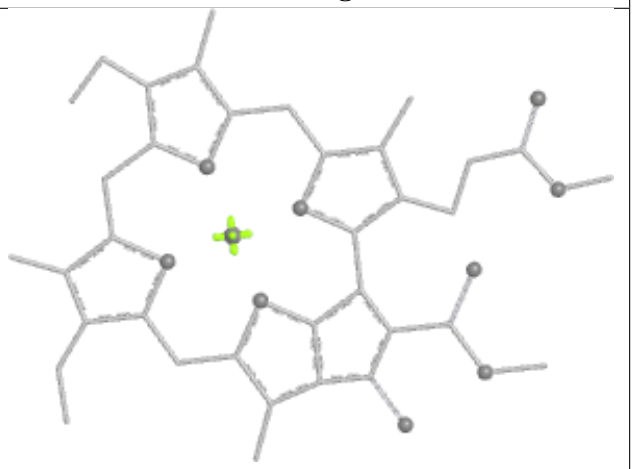
Bond lengths



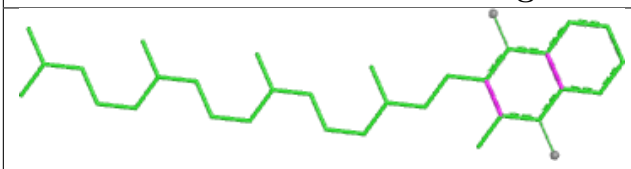
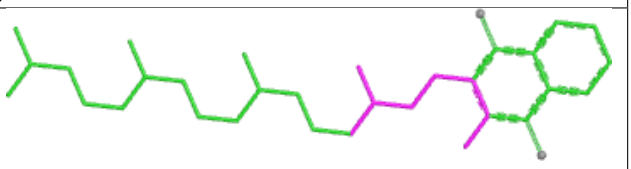
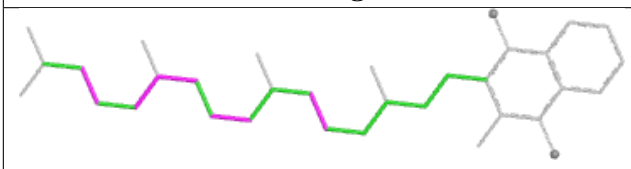
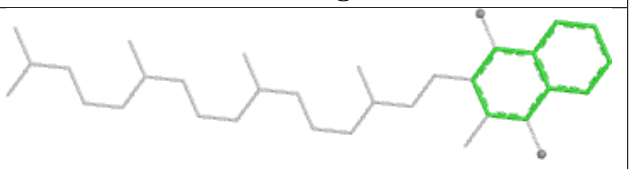
Bond angles

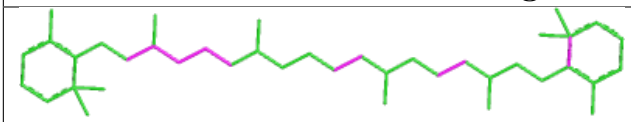
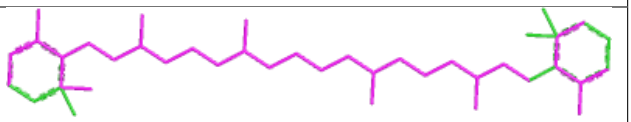
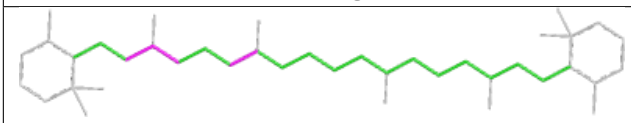
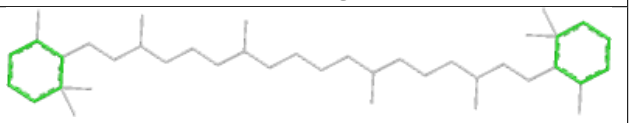


Torsions

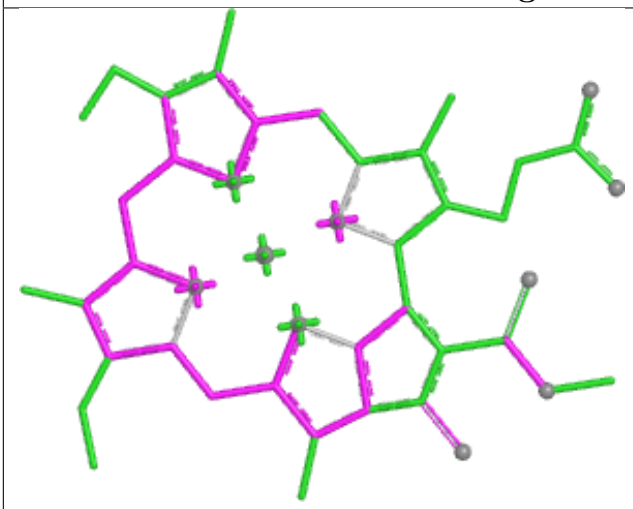


Rings

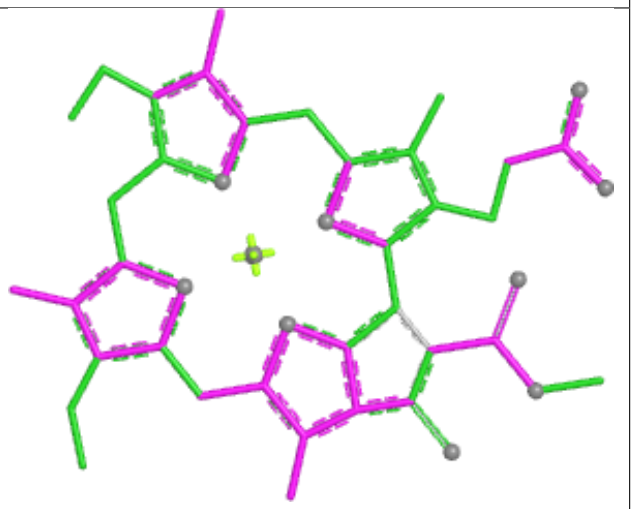
Ligand PQN a 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR f 4018	
 Bond lengths	 Bond angles
 Torsions	 Rings

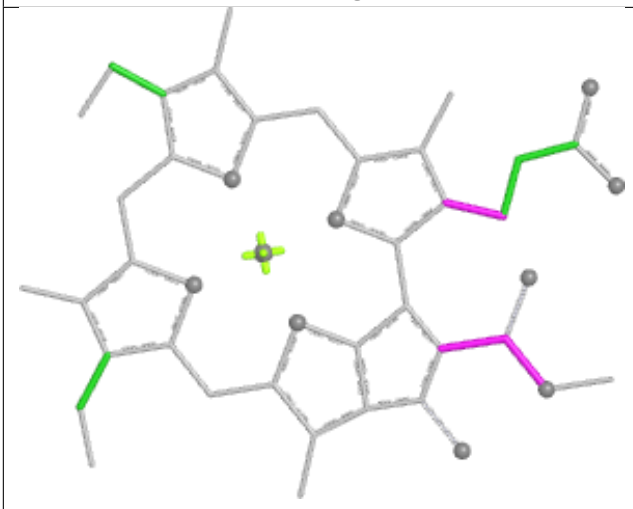
Ligand CLA b 1212



Bond lengths



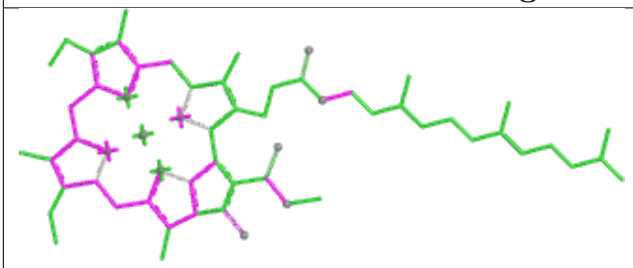
Bond angles



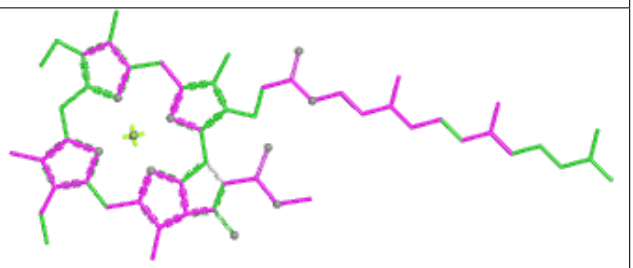
Torsions

Rings

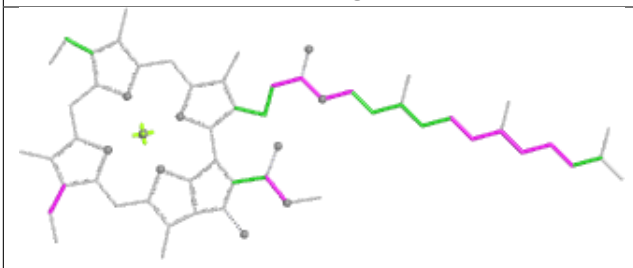
Ligand CLA 2 1235



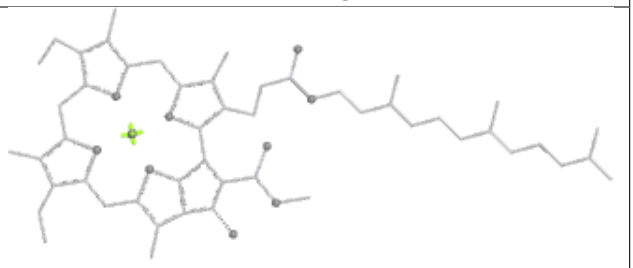
Bond lengths



Bond angles

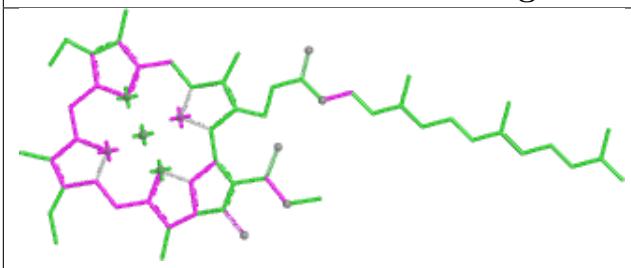


Torsions



Rings

Ligand CLA b 1235



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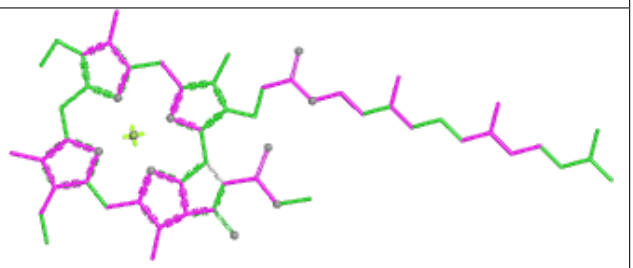

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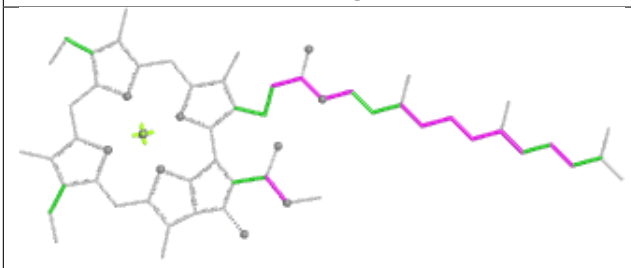
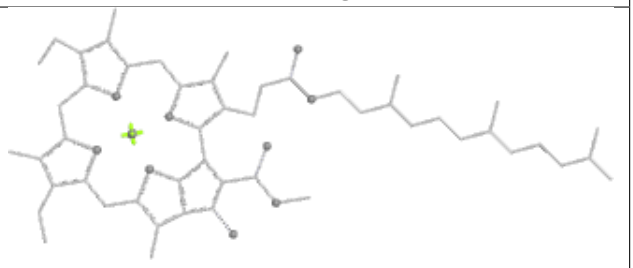
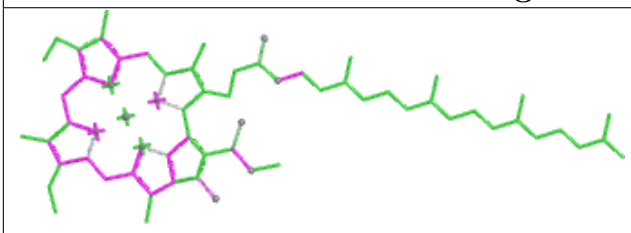


Torsions



Rings

Ligand CLA A 1109



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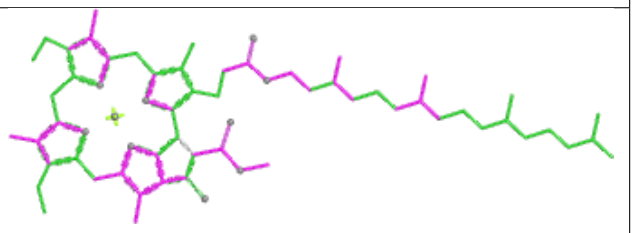
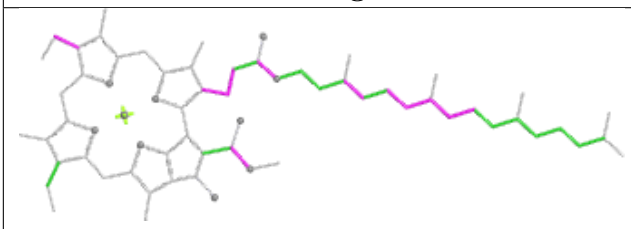
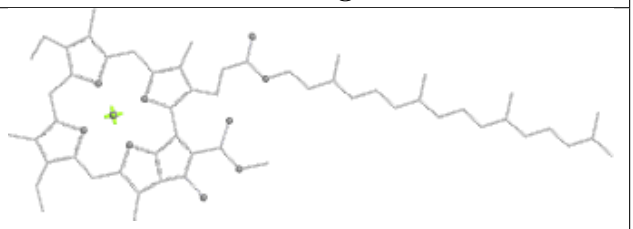


Bond angles

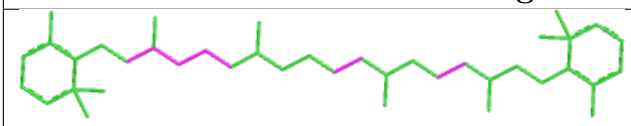


Torsions



Rings

Ligand BCR b 4010



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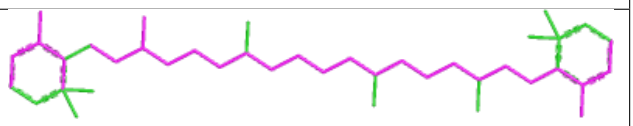
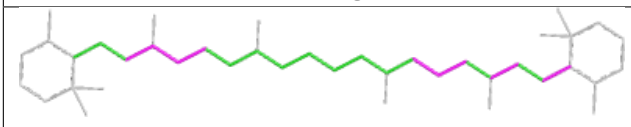
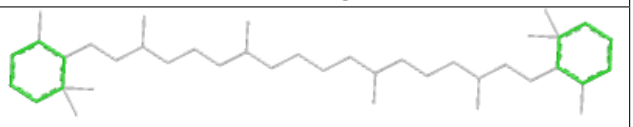


Bond angles

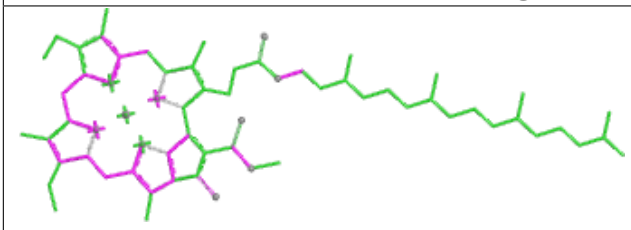


Torsions

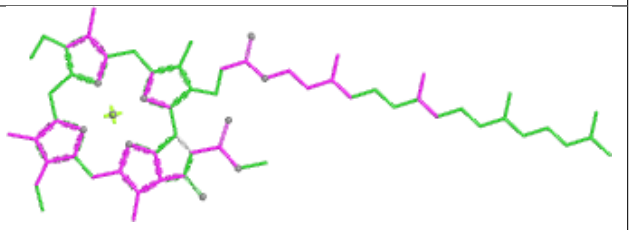


Rings

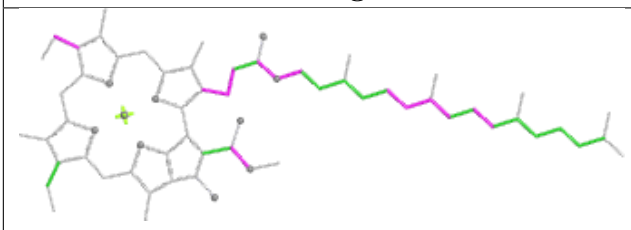
Ligand CLA A 1131



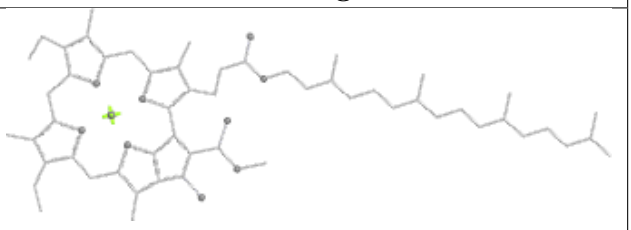
Bond lengths



Bond angles

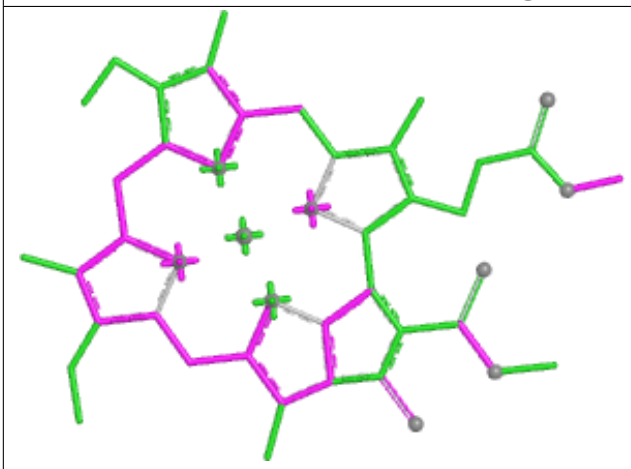


Torsions

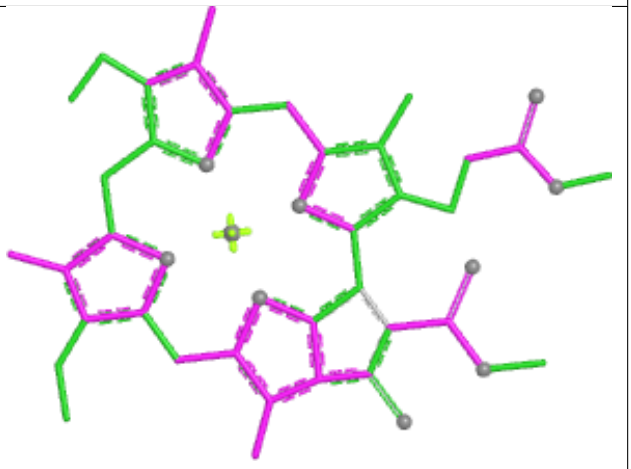


Rings

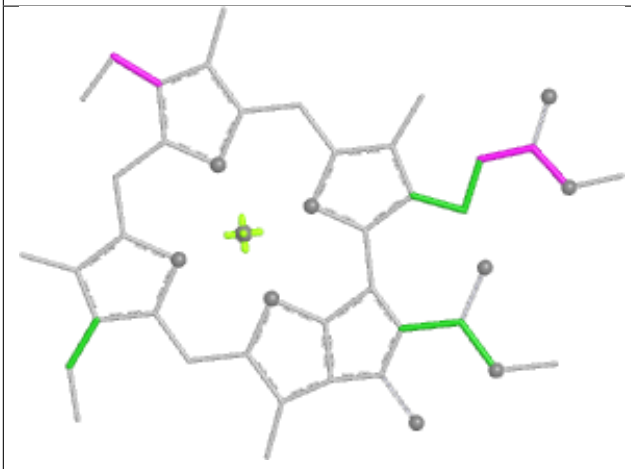
Ligand CLA 8 1502



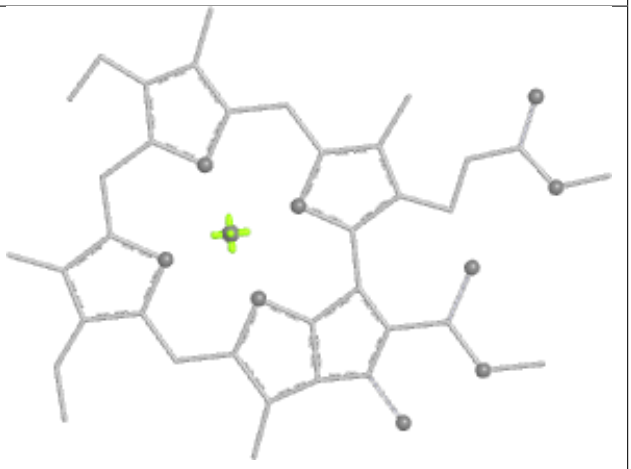
Bond lengths



Bond angles

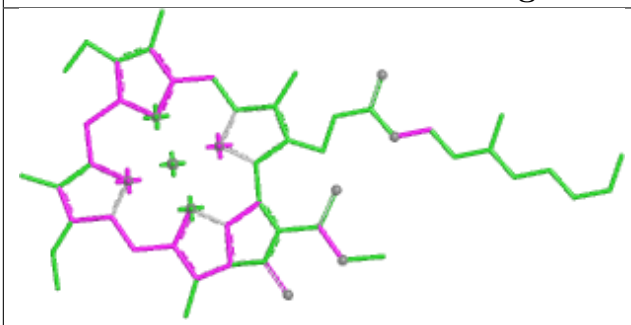


Torsions

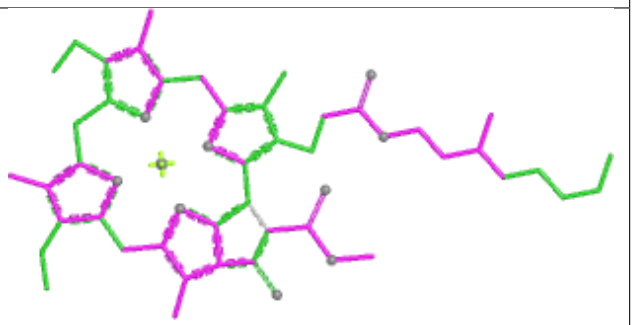


Rings

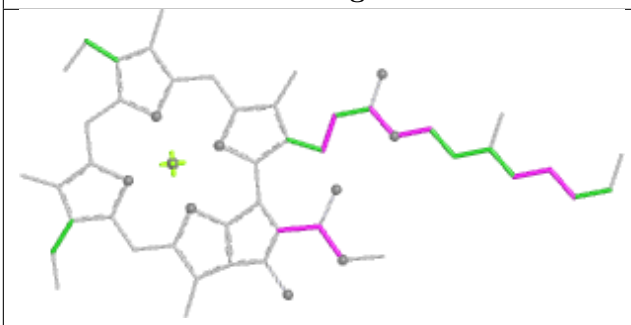
Ligand CLA b 1201



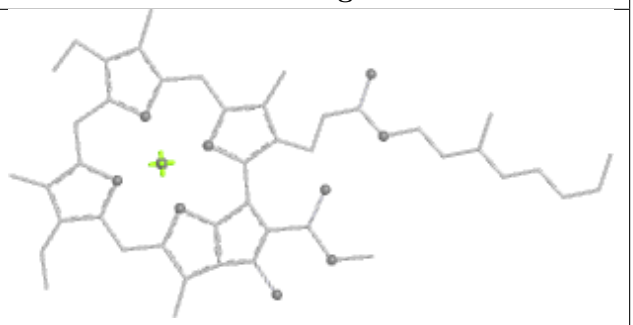
Bond lengths



Bond angles

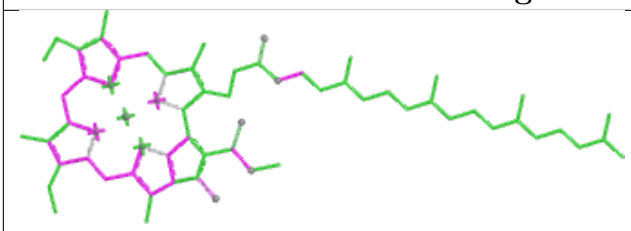


Torsions

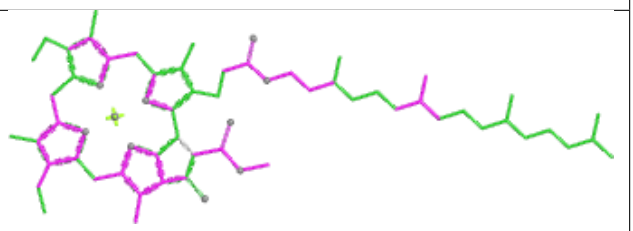


Rings

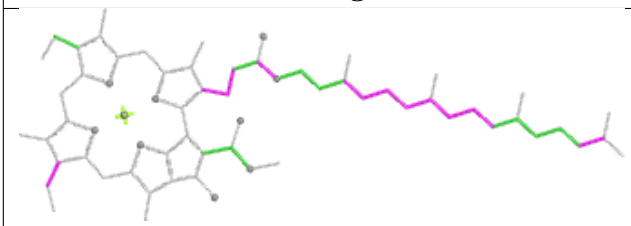
Ligand CLA A 1119



Bond lengths



Bond angles



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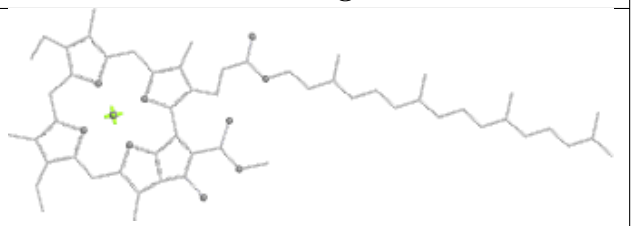
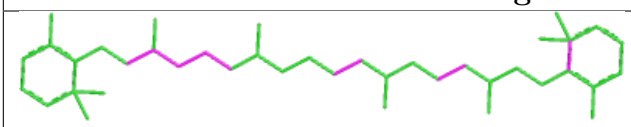
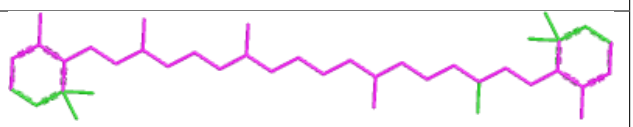


Rings

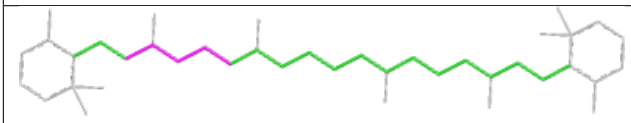
Ligand BCR B 4017



Bond lengths



Bond angles



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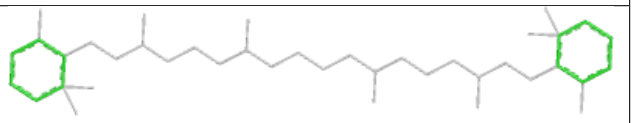
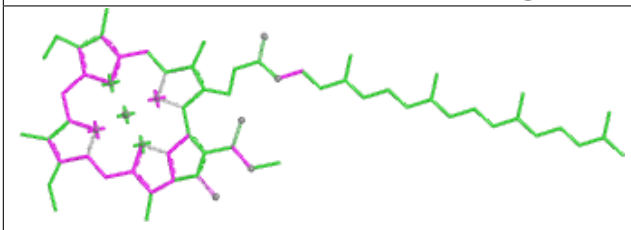
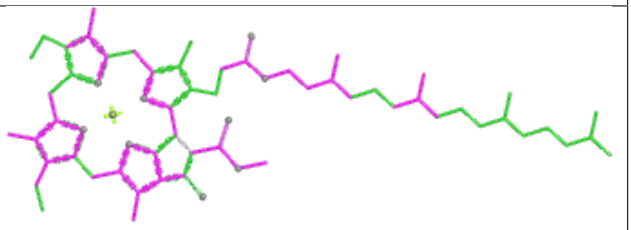


Rings

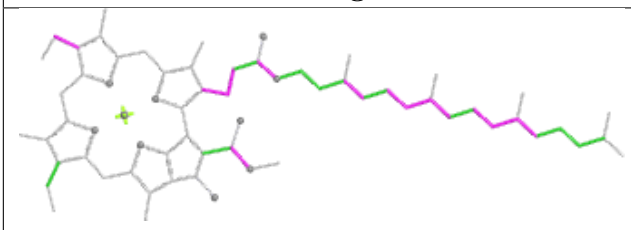
Ligand CLA 2 1021



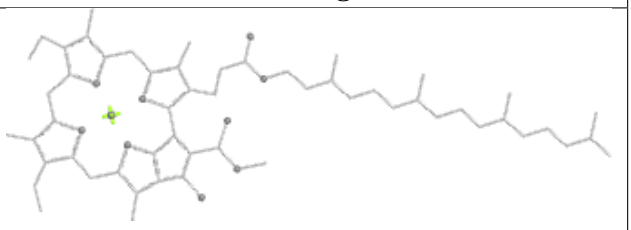
Bond lengths



Bond angles

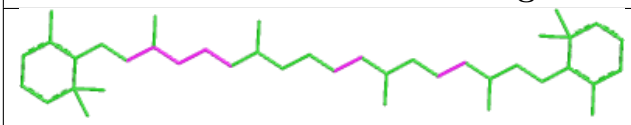


Torsions



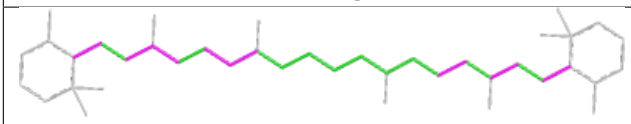
Rings

Ligand BCR a 4003



Bond lengths

Bond angles



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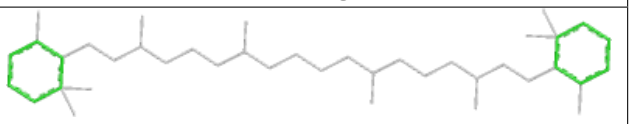
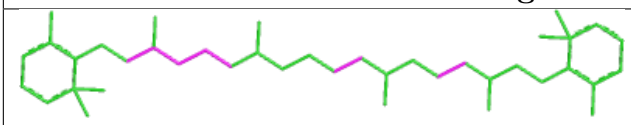
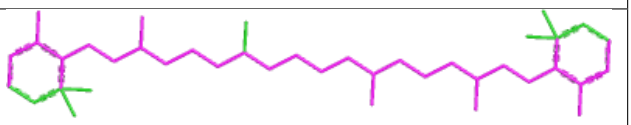


Rings

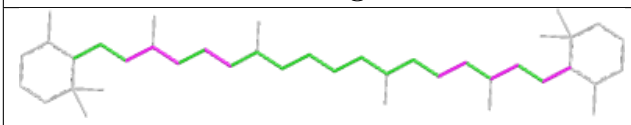
Ligand BCR 2 4004



Bond lengths



Bond angles



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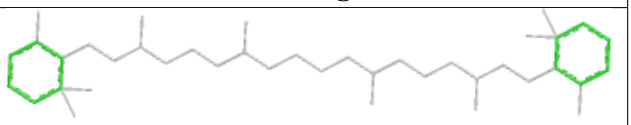
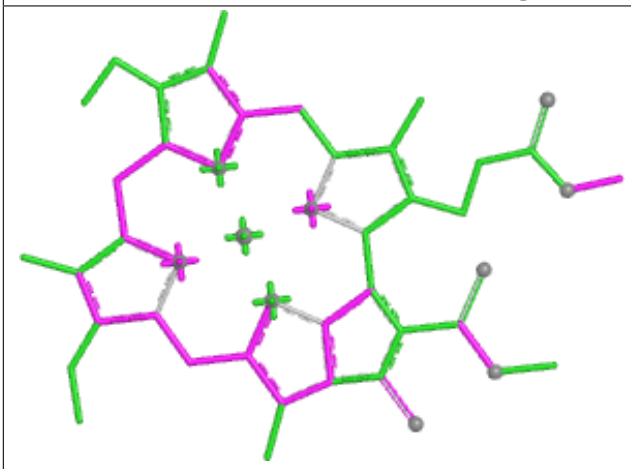


Rings

Ligand CLA A 1130



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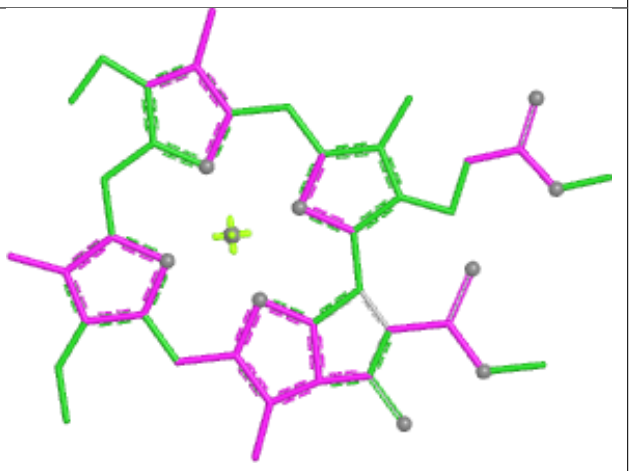
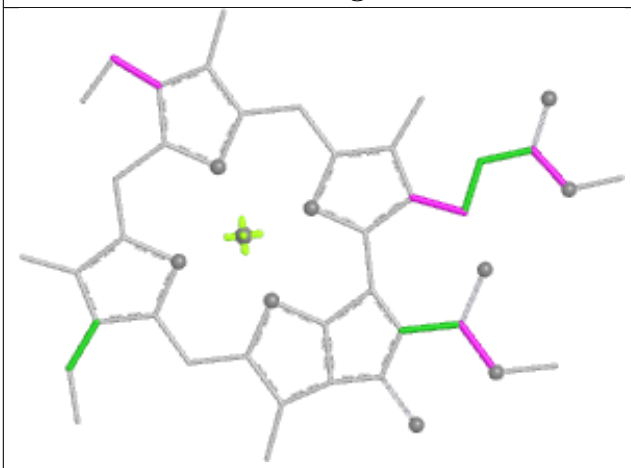


Bond angles



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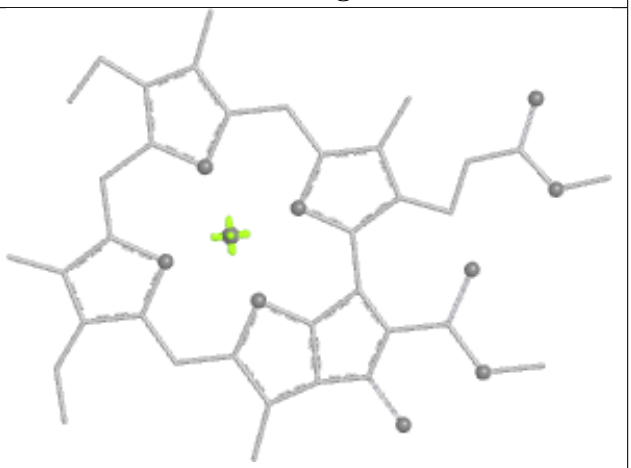
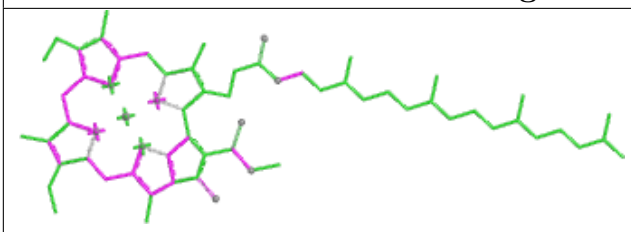
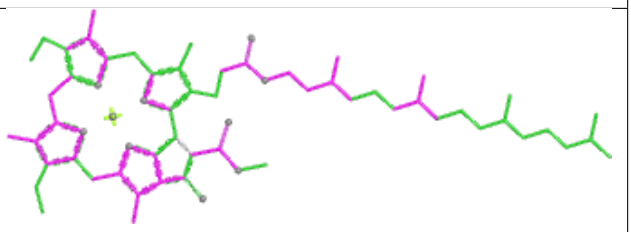


Rings

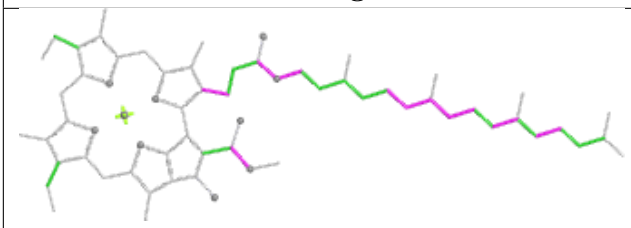
Ligand CLA 1 1104



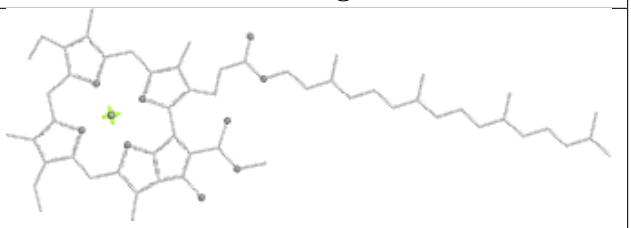
Bond lengths



Bond angles

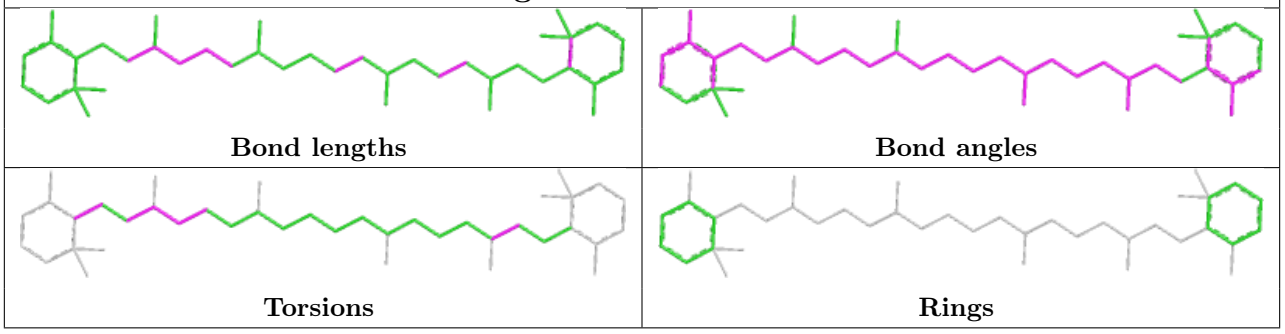


Torsions

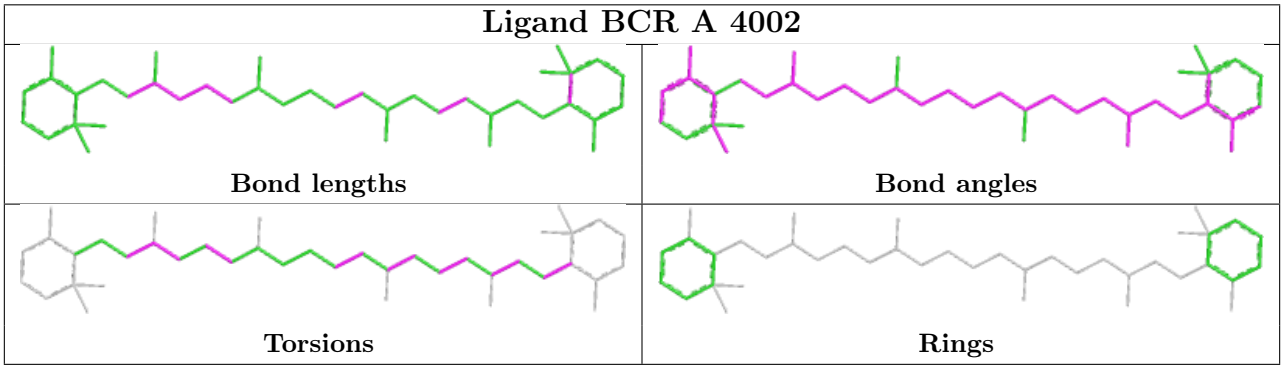


Rings

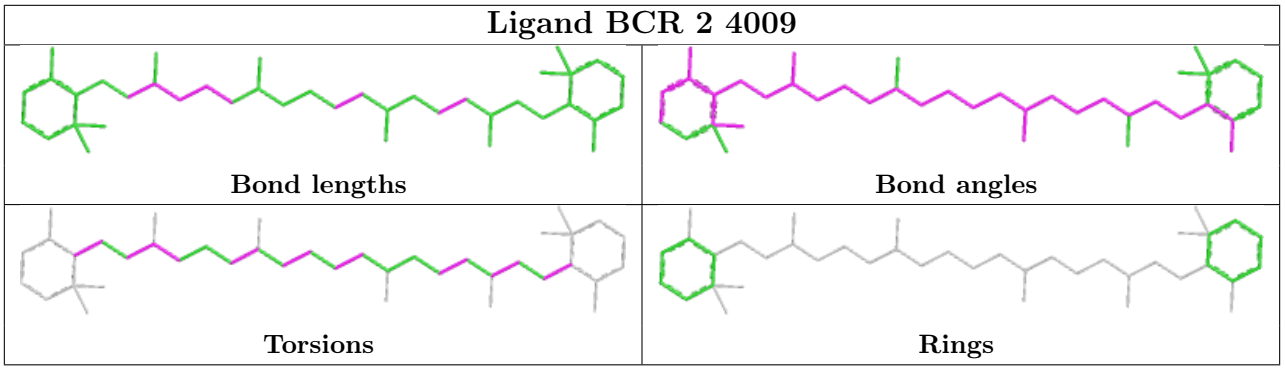
Ligand BCR A 4001



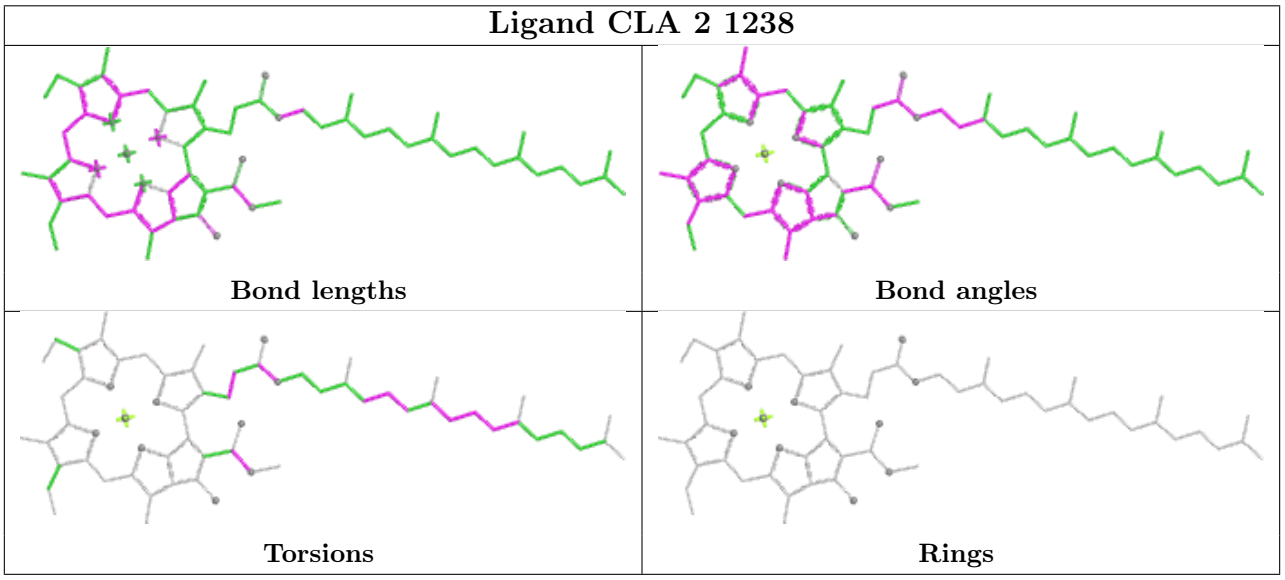
Ligand BCR A 4002



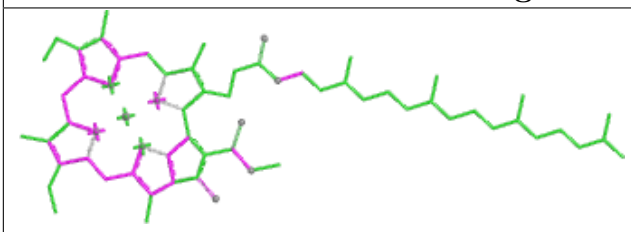
Ligand BCR 2 4009



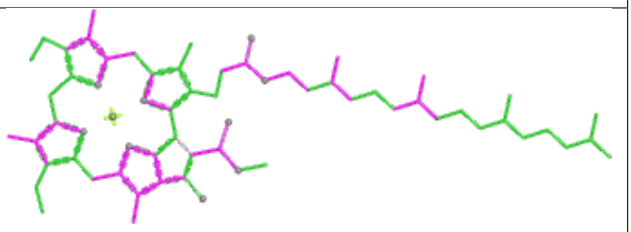
Ligand CLA 2 1238



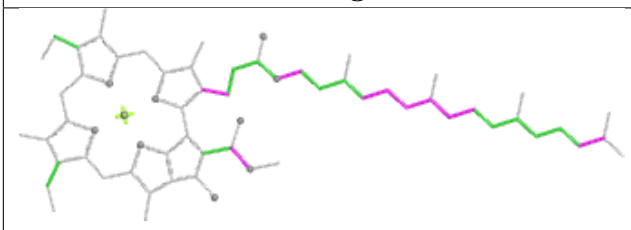
Ligand CLA A 1117



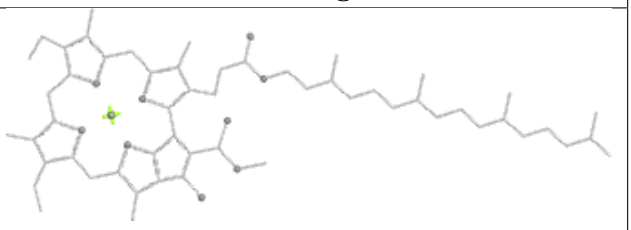
Bond lengths



Bond angles

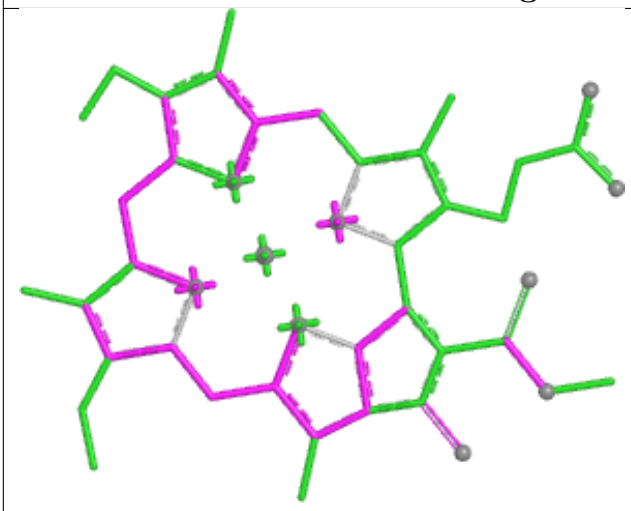


Torsions

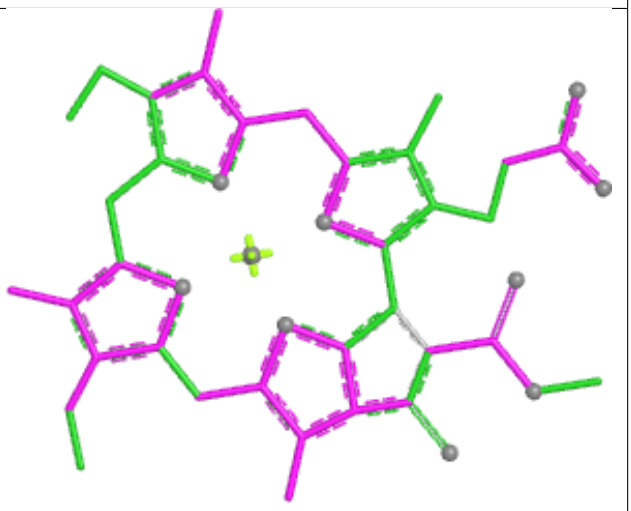


Rings

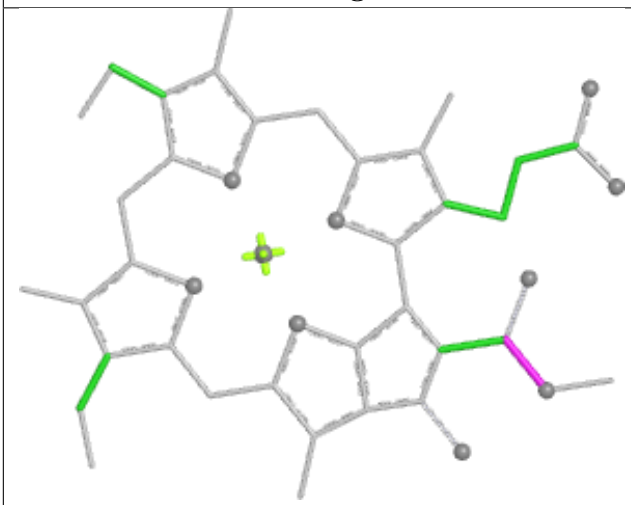
Ligand CLA a 1112



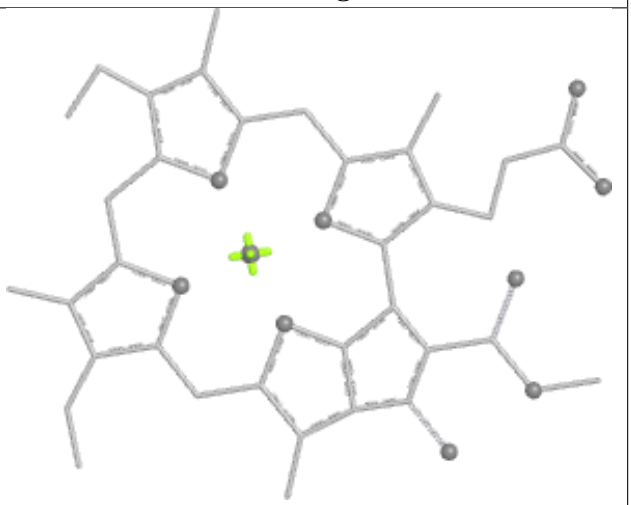
Bond lengths



Bond angles

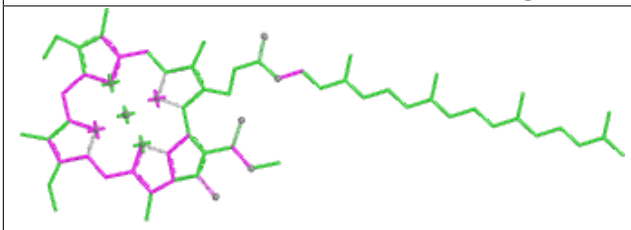


Torsions

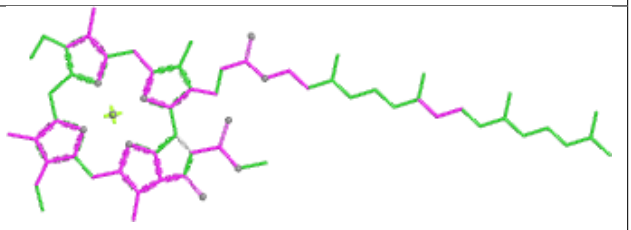


Rings

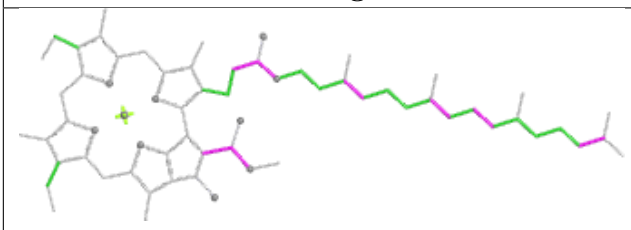
Ligand CLA 2 1207



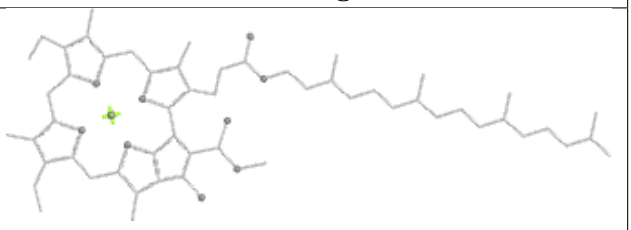
Bond lengths



Bond angles

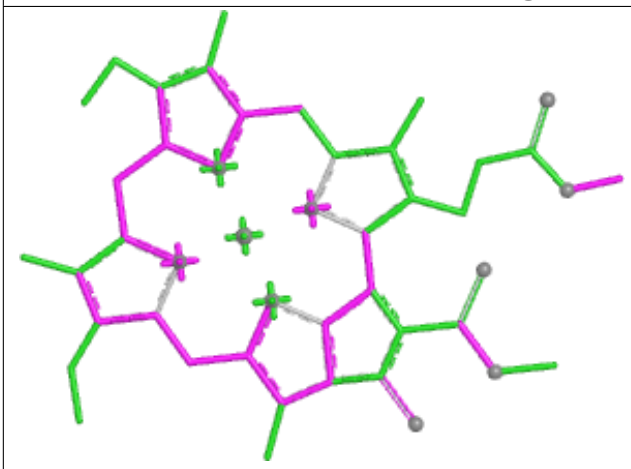


Torsions

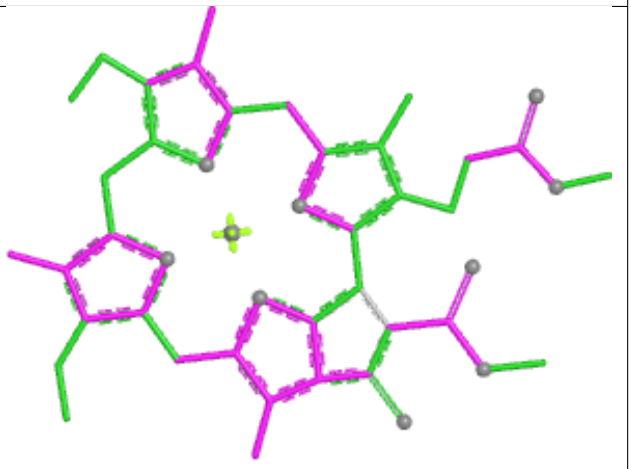


Rings

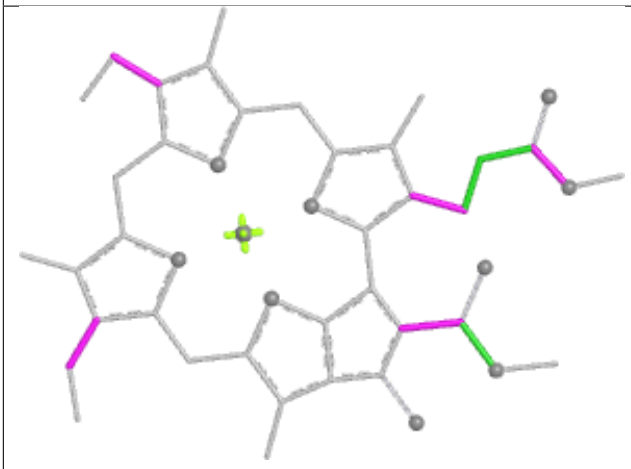
Ligand CLA a 1120



Bond lengths



Bond angles



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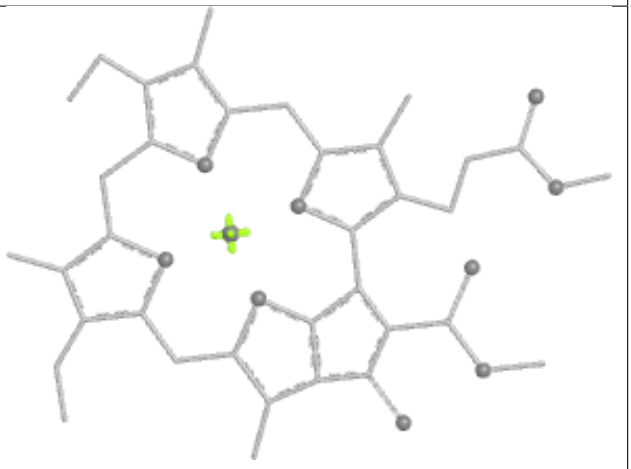
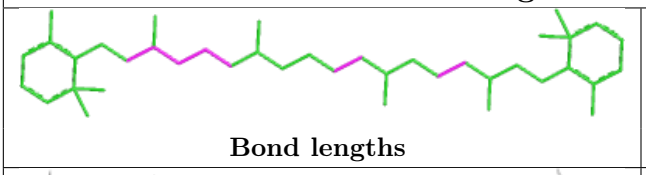
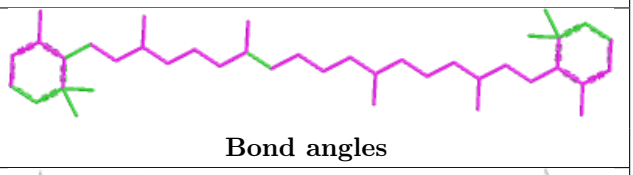


Rings

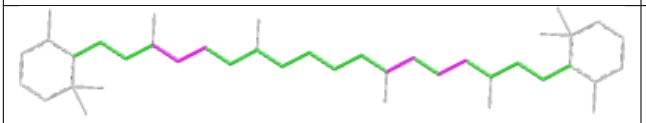
Ligand BCR 8 4022



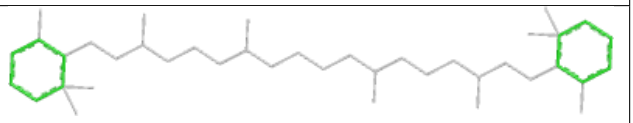
Bond lengths



Bond angles

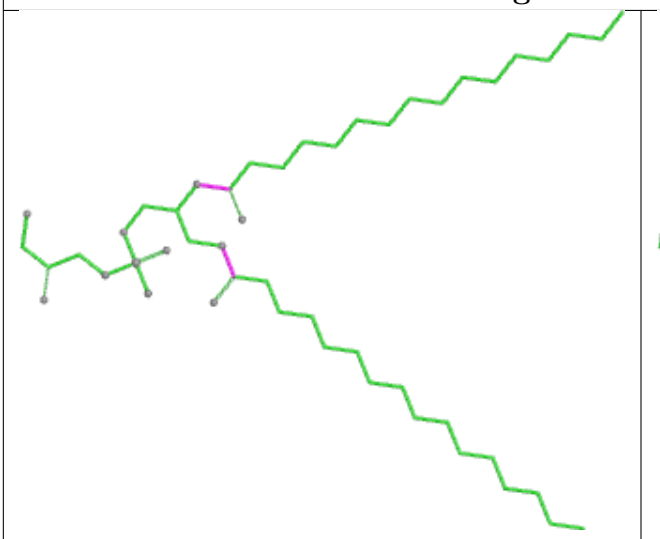


Torsions

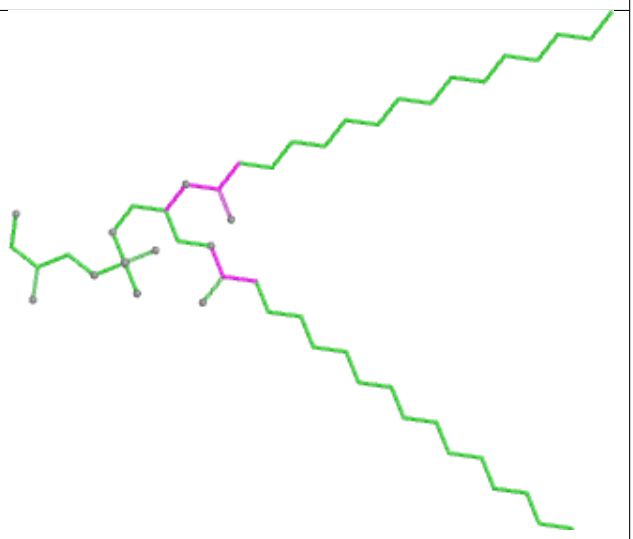


Rings

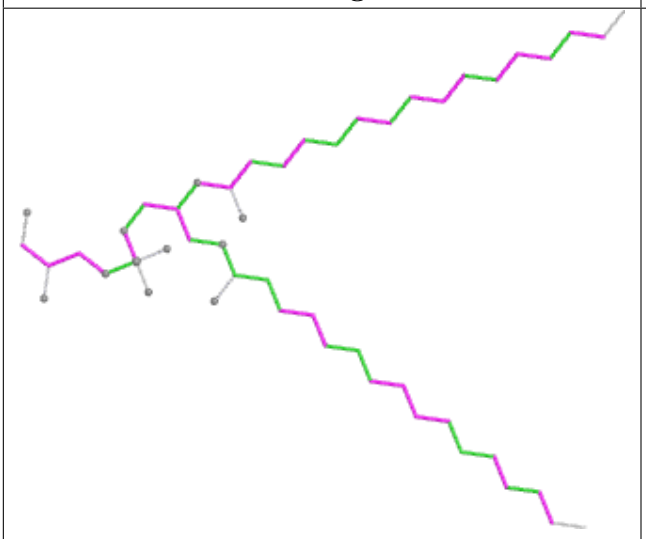
Ligand LHG A 5001



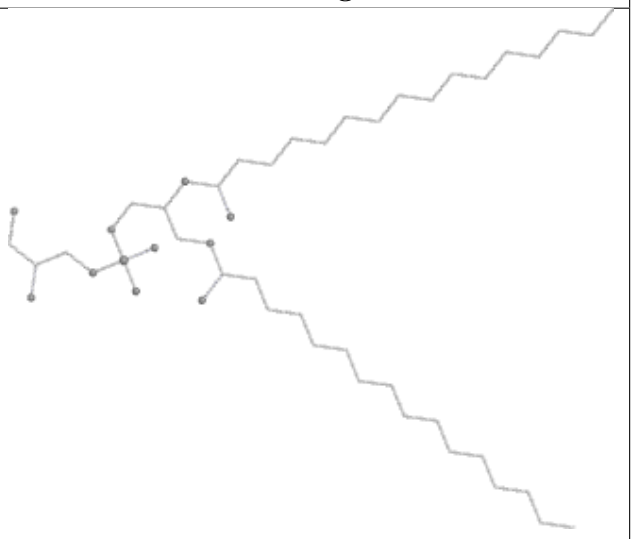
Bond lengths



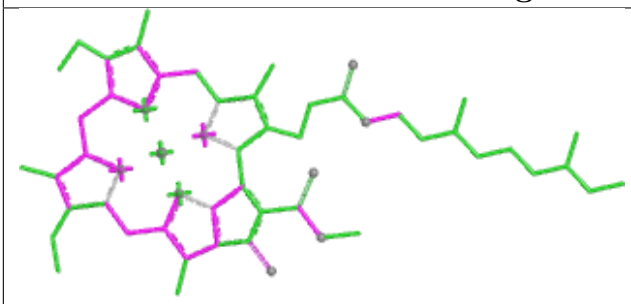
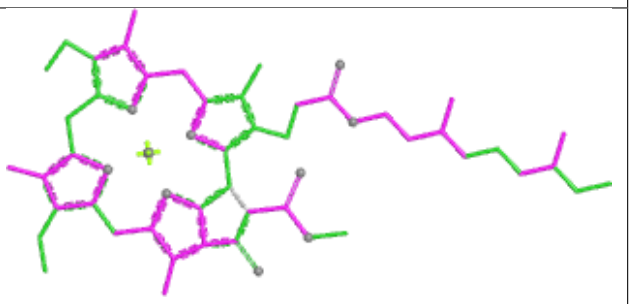
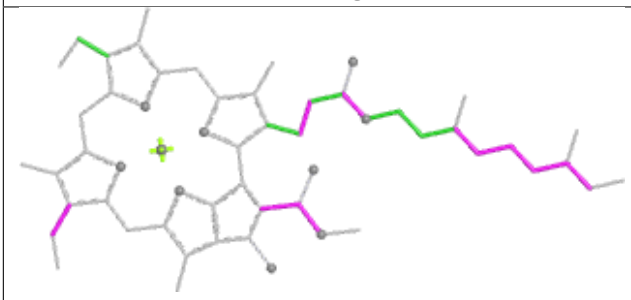
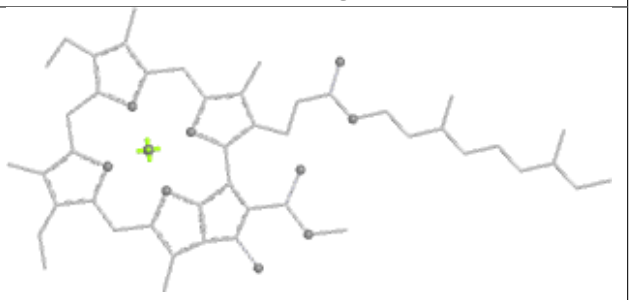
Bond angles

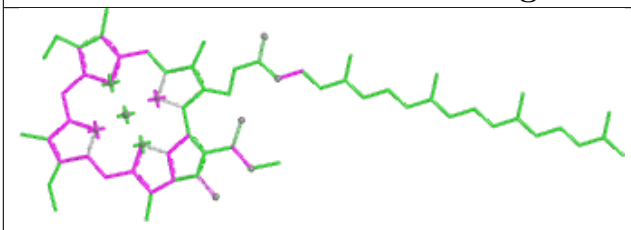
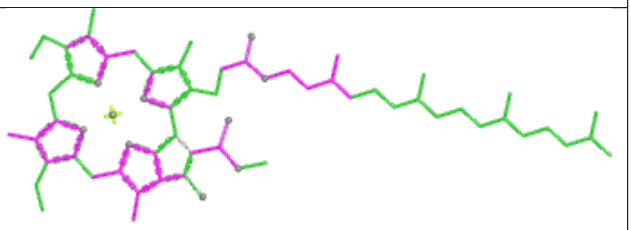
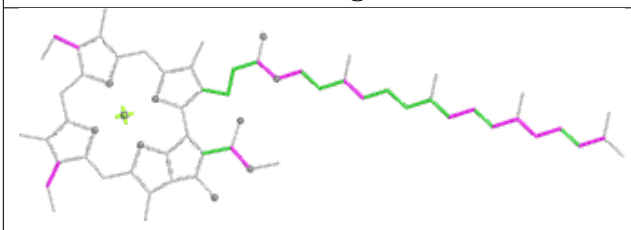
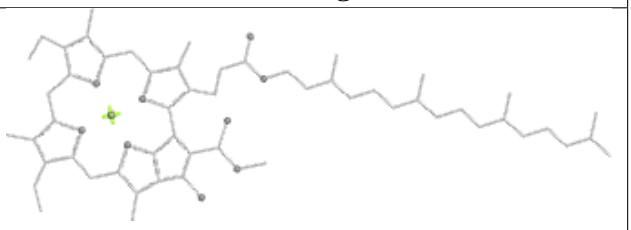


Torsions

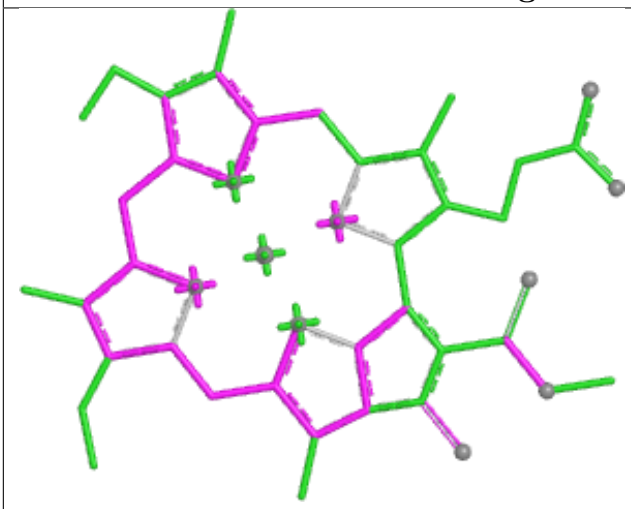


Rings

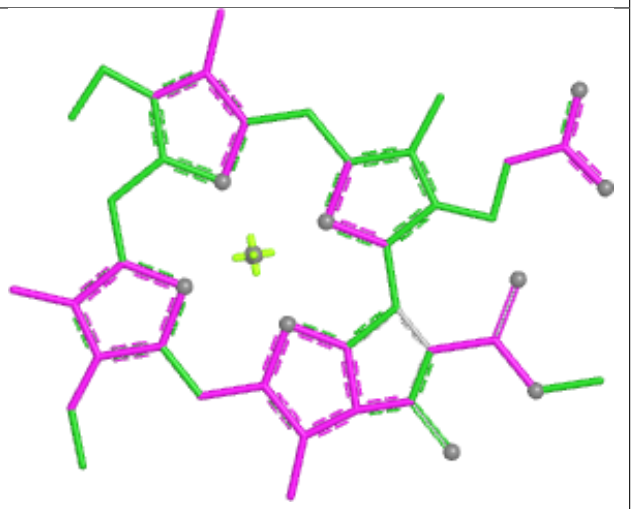
Ligand CLA B 1222	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1126	
	
Bond lengths	Bond angles
	
Torsions	Rings

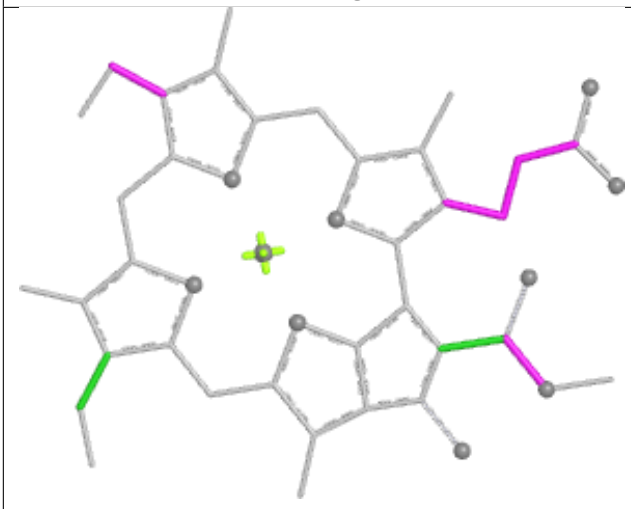
Ligand CLA b 1240



Bond lengths



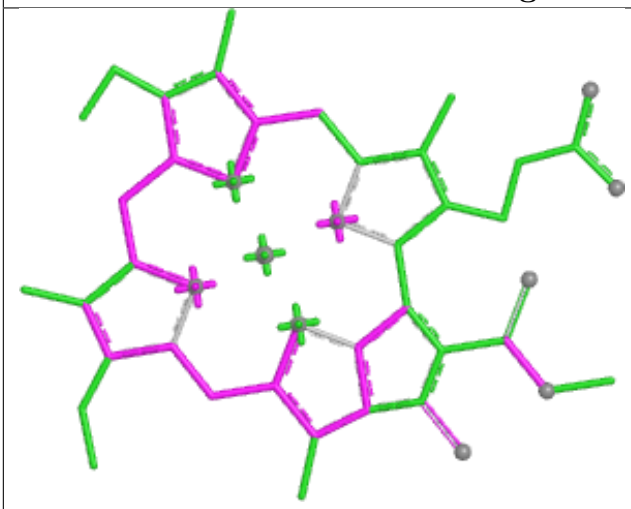
Bond angles



Torsions

Rings

Ligand CLA 1 1112



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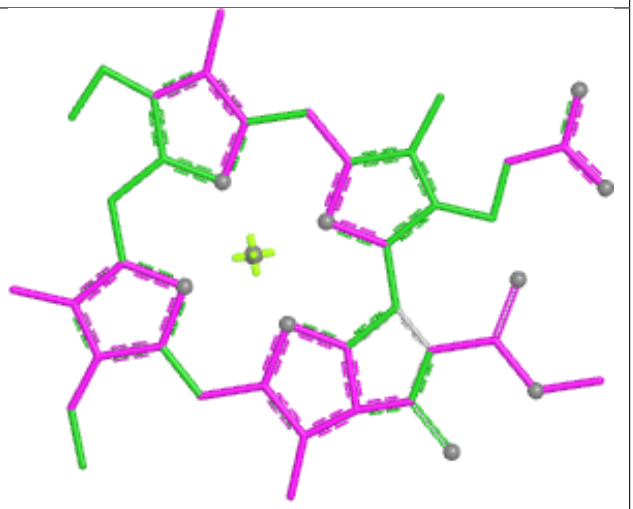
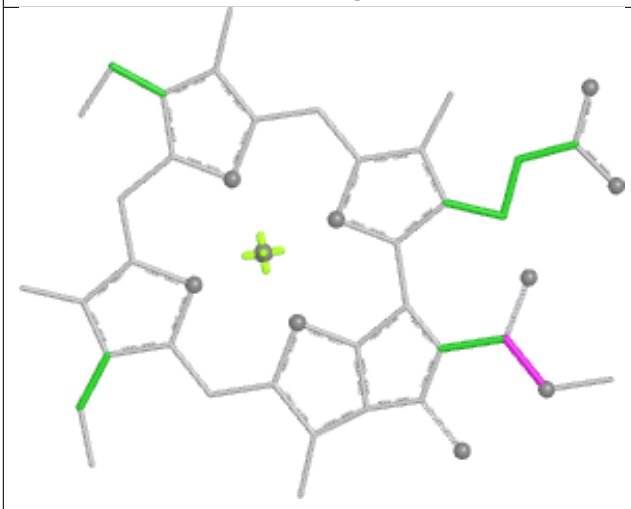


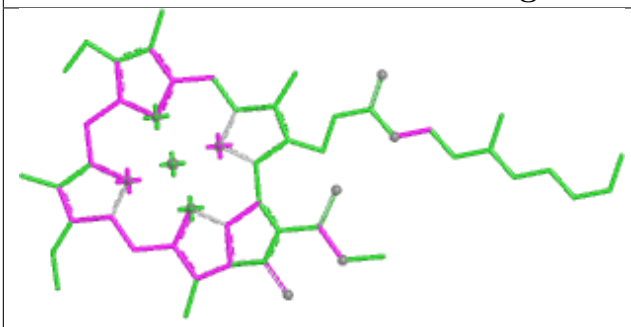
Bond angles



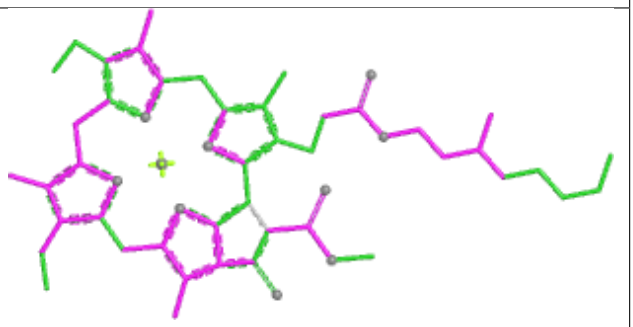
Torsions

Rings

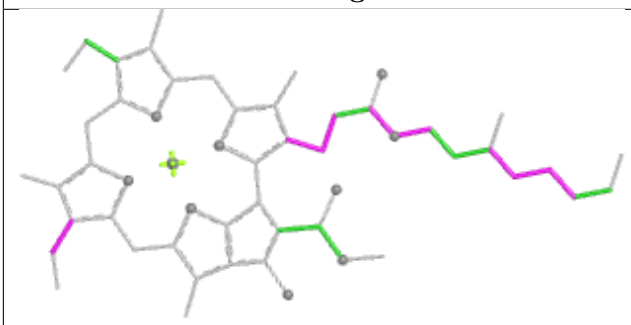
Ligand CLA a 1110



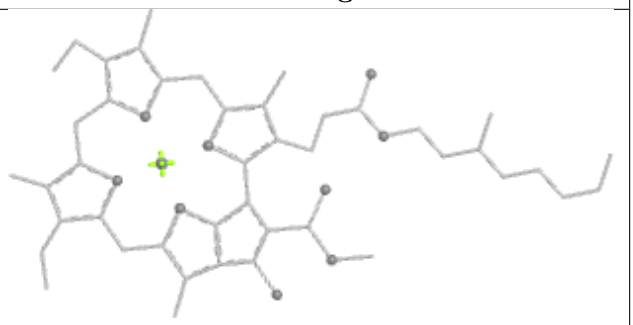
Bond lengths



Bond angles

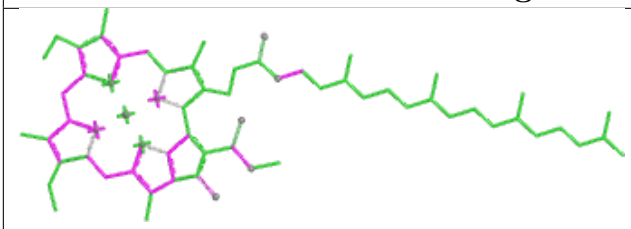


Torsions



Rings

Ligand CLA A 1126



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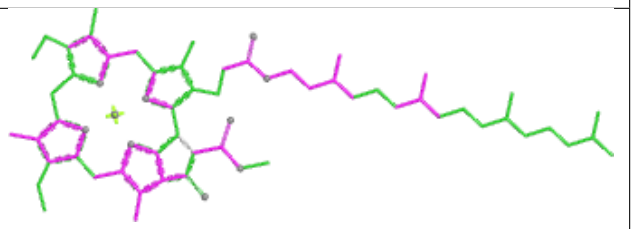
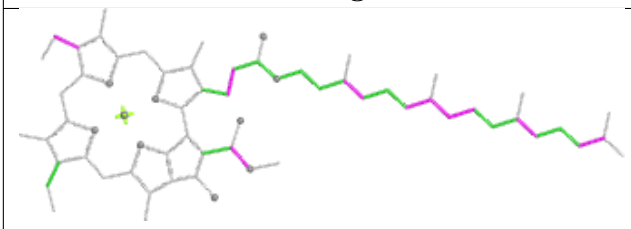
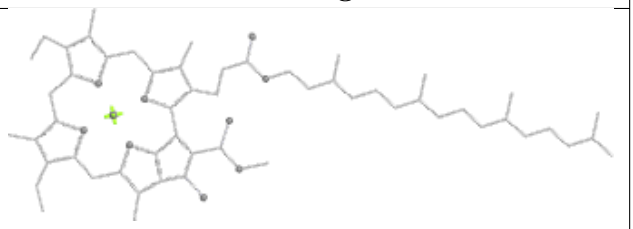


Bond angles

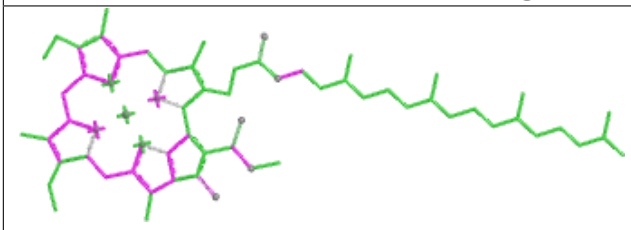


Torsions

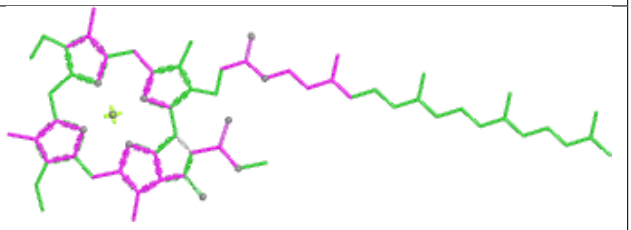


Rings

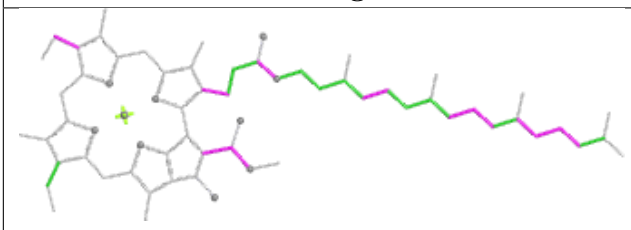
Ligand CLA b 1202



Bond lengths



Bond angles



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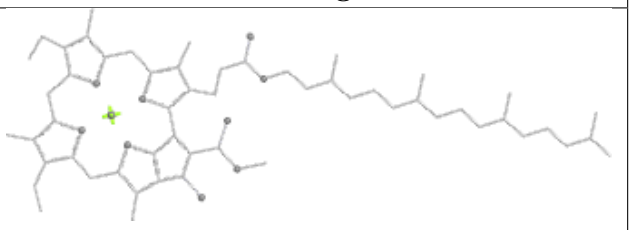
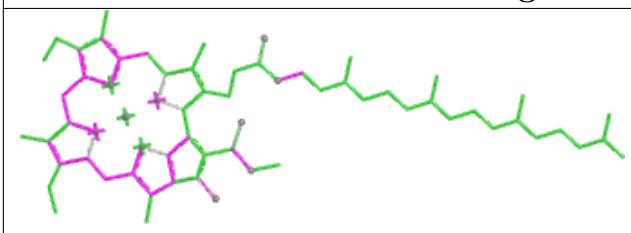
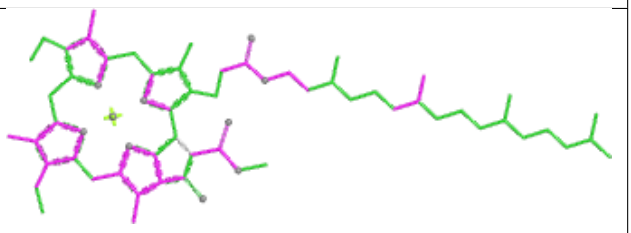


Rings

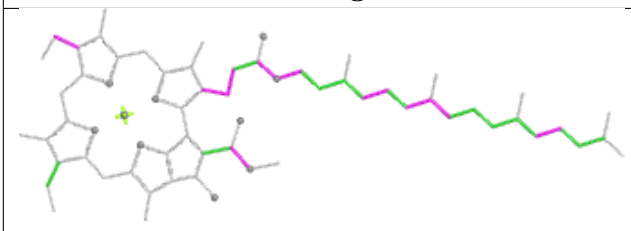
Ligand CLA b 1225



Bond lengths



Bond angles



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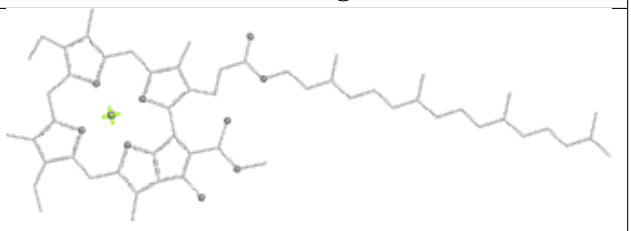
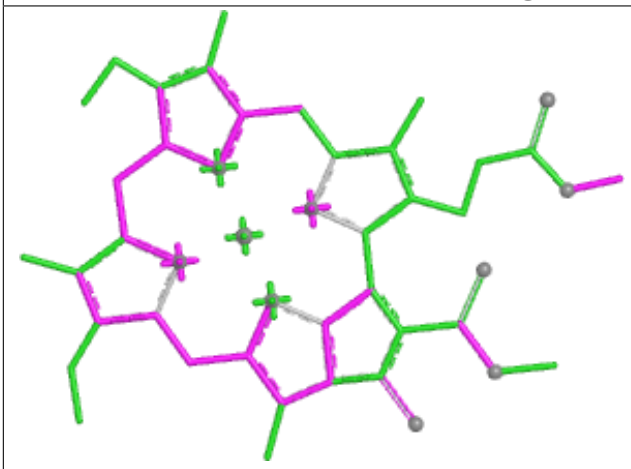
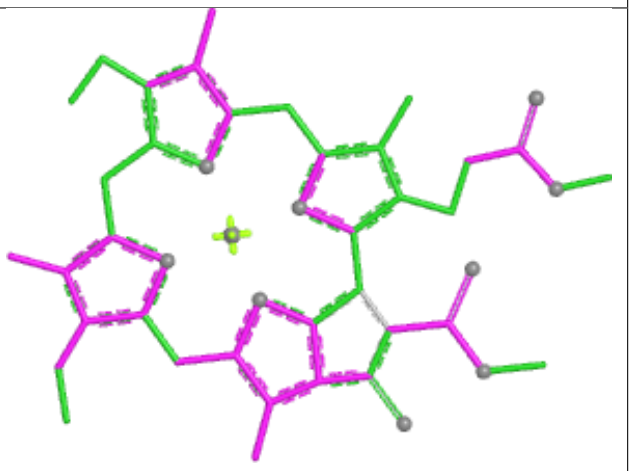


Rings

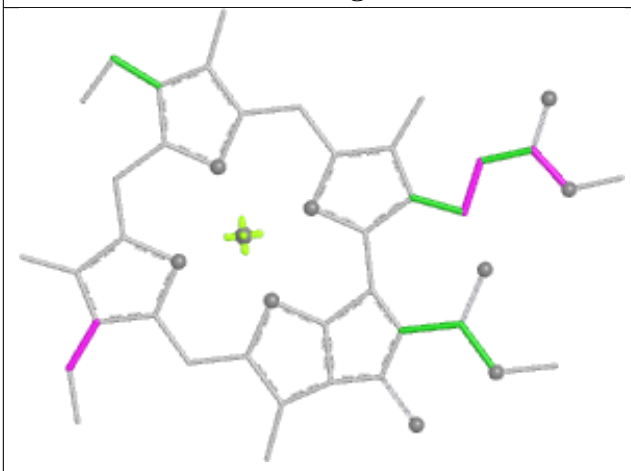
Ligand CLA 1 1134



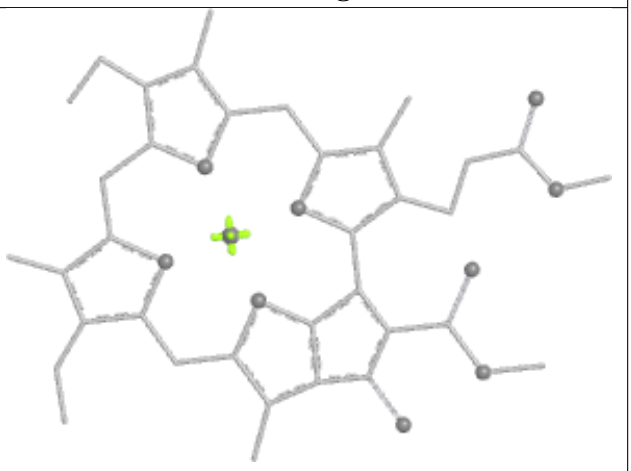
Bond lengths



Bond angles

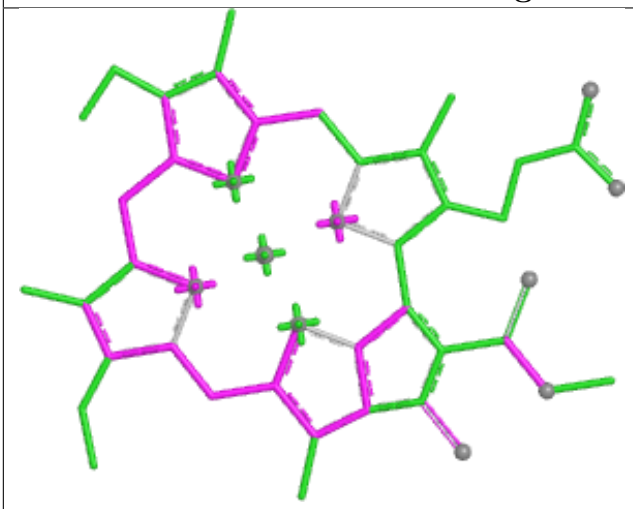


Torsions



Rings

Ligand CLA A 1108



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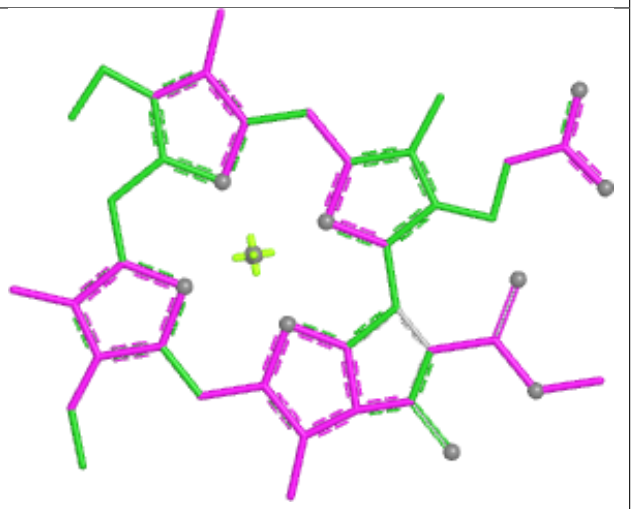
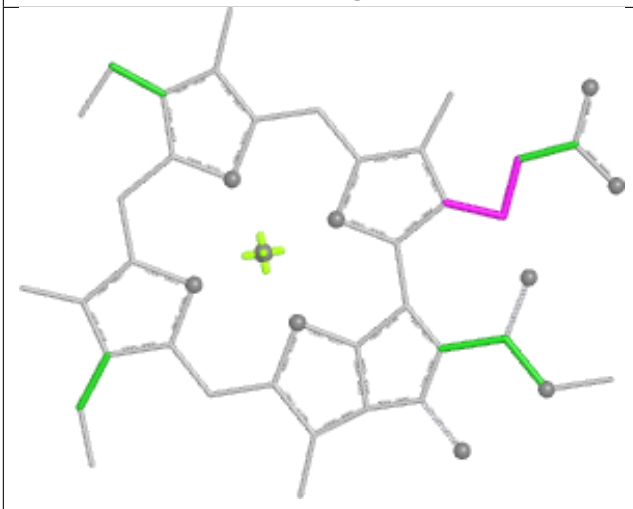


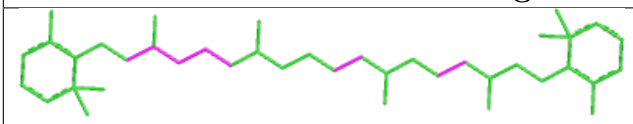
Bond angles



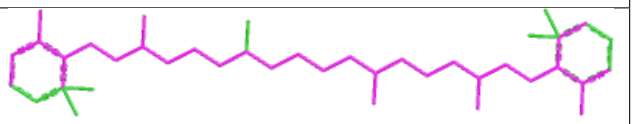
Torsions

Rings

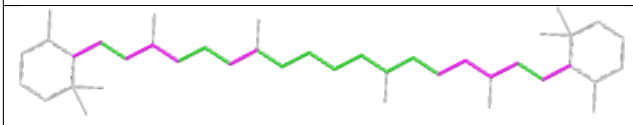
Ligand BCR B 4006



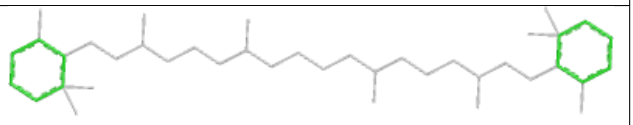
Bond lengths



Bond angles

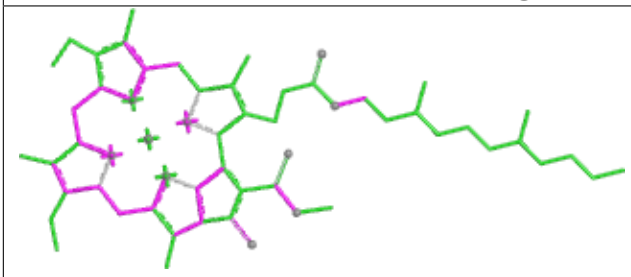


Torsions

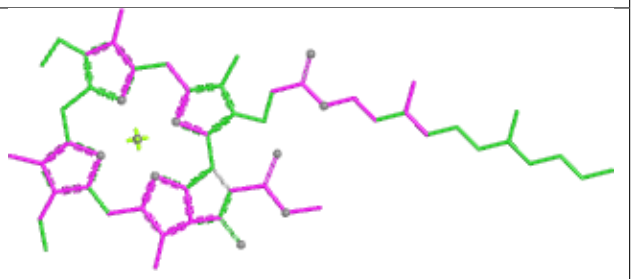


Rings

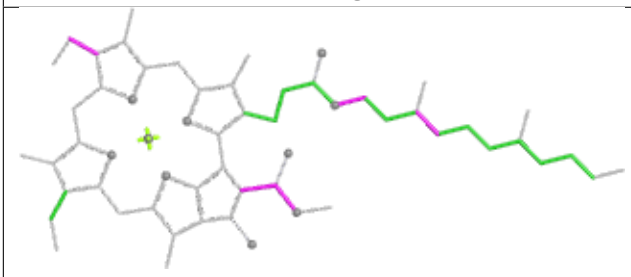
Ligand CLA B 1230



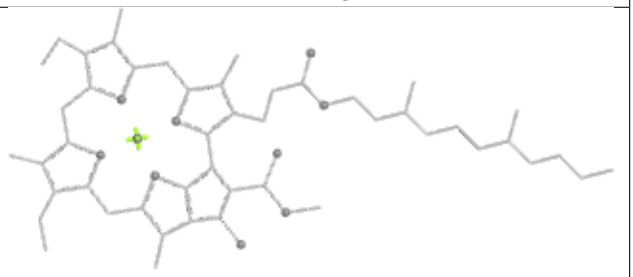
Bond lengths



Bond angles

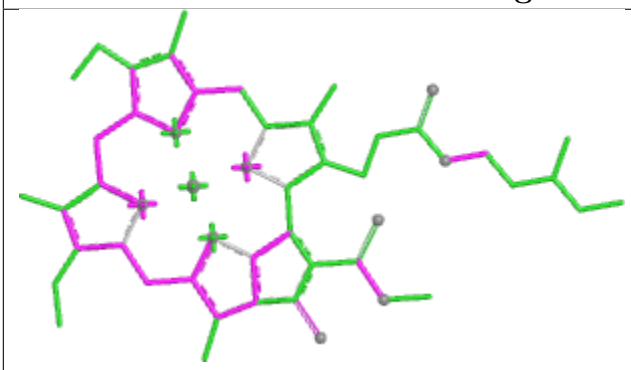


Torsions

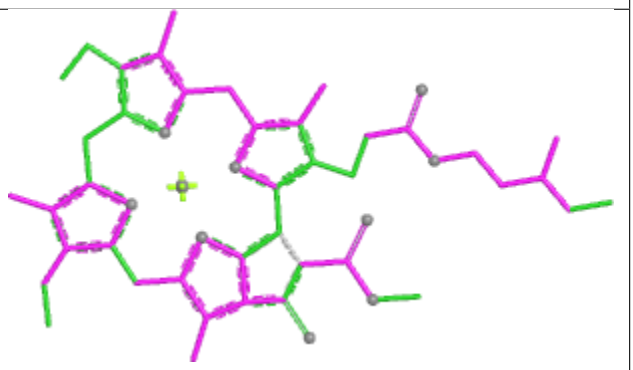


Rings

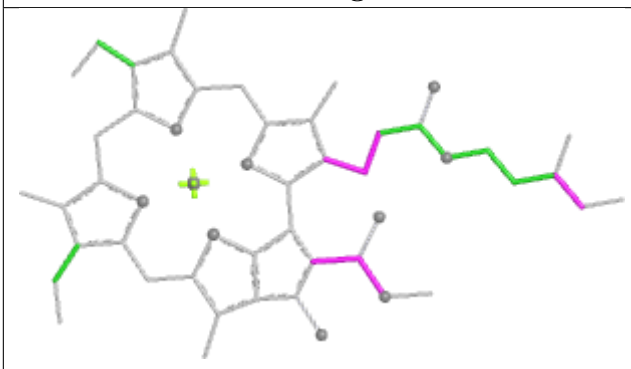
Ligand CLA A 1135



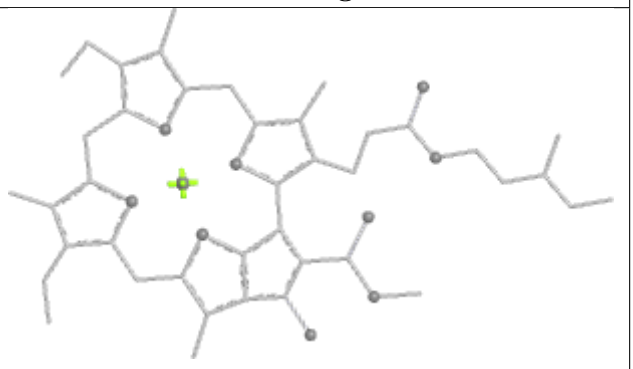
Bond lengths



Bond angles

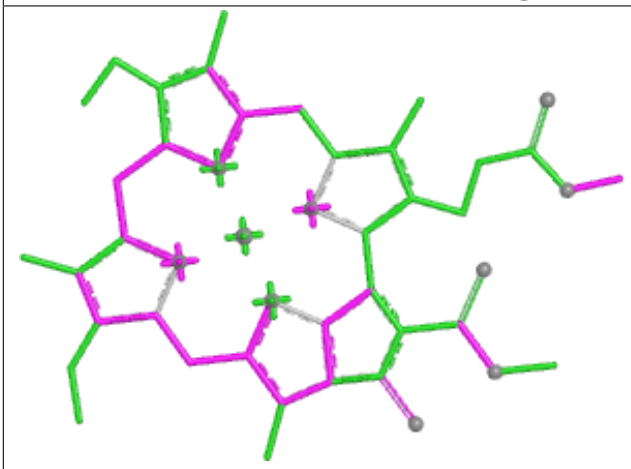


Torsions

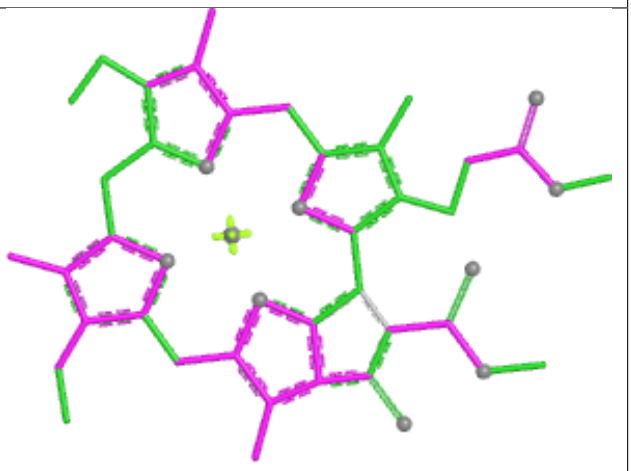


Rings

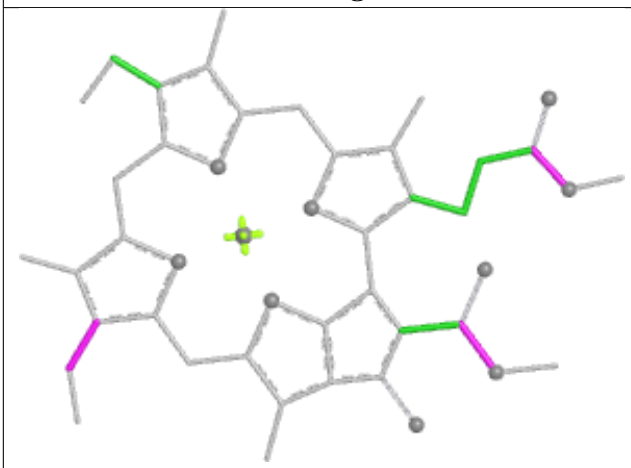
Ligand CLA B 1220



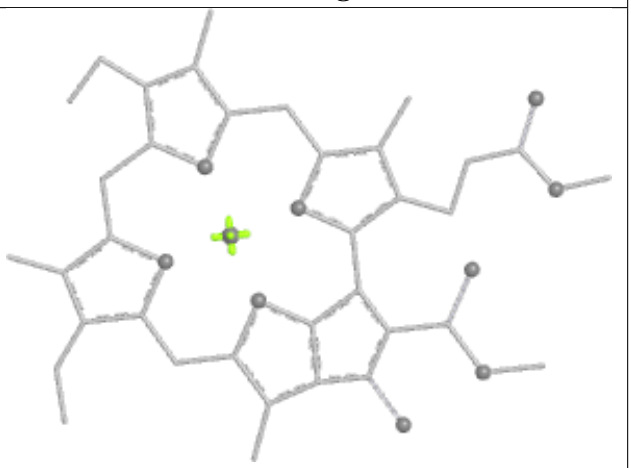
Bond lengths



Bond angles

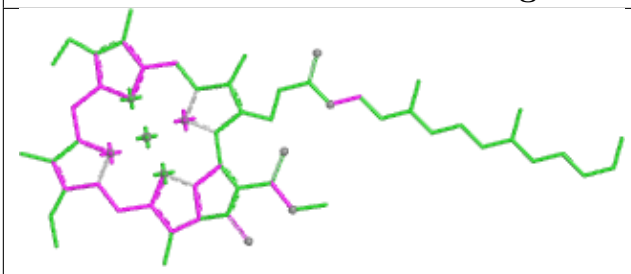


Torsions



Rings

Ligand CLA 1 1122



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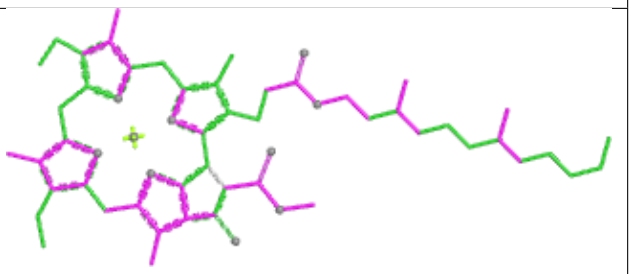
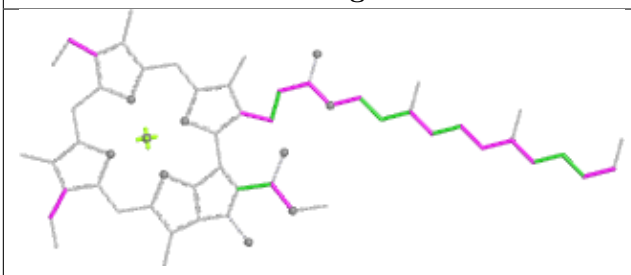
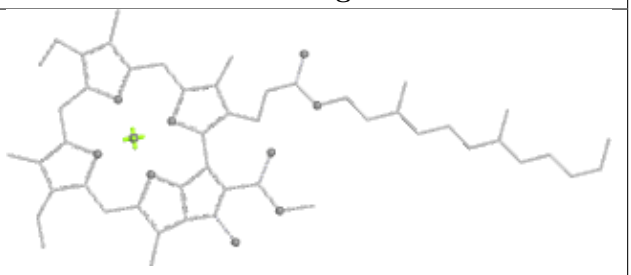


Bond angles

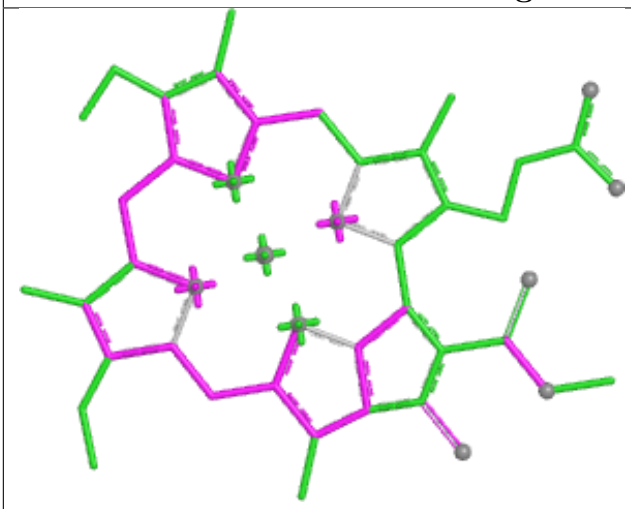


Torsions



Rings

Ligand CLA B 1231



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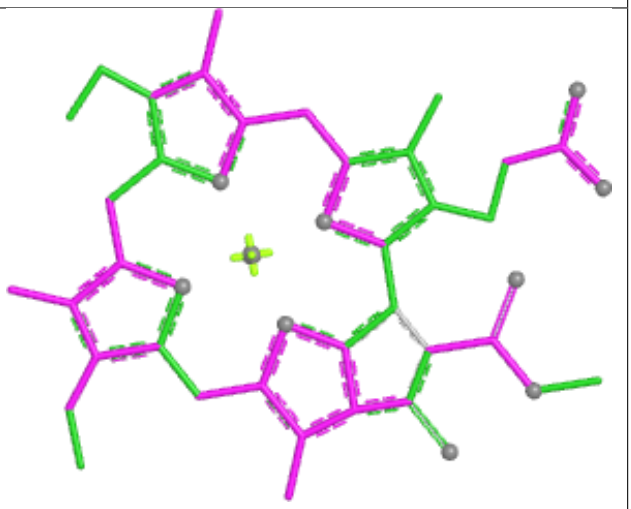
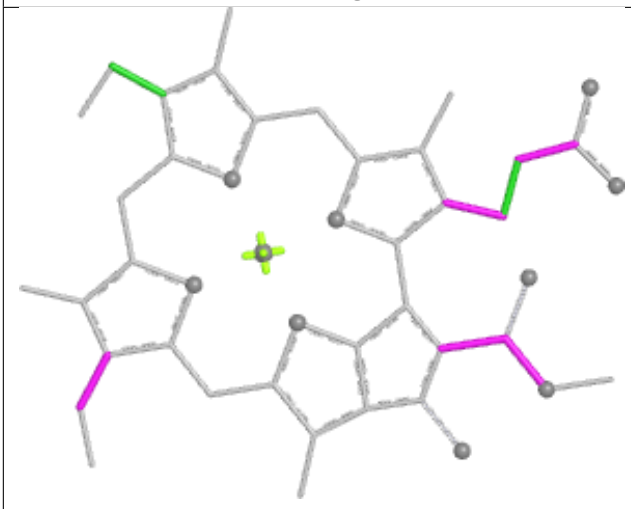


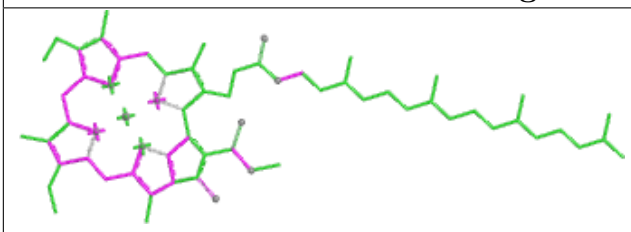
Bond angles



Torsions

Rings

Ligand CLA 1 1127



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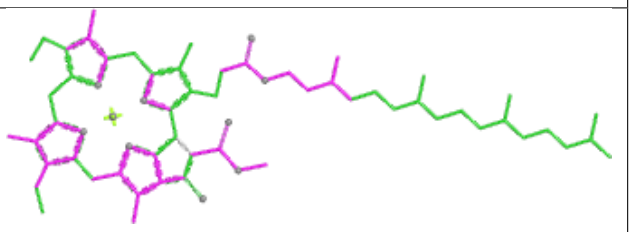
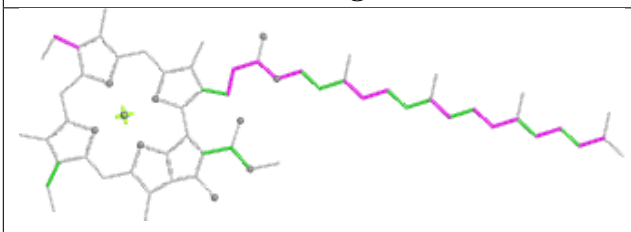


Bond angles



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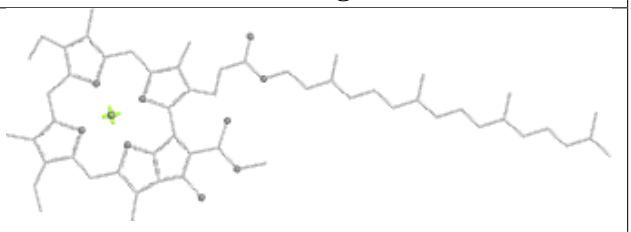
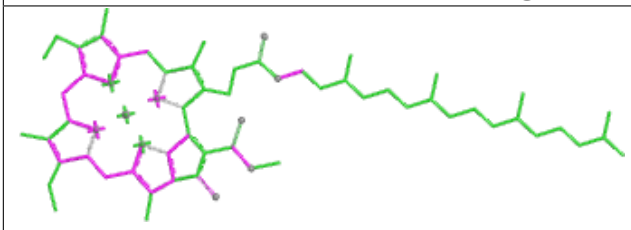


Rings

Ligand CLA b 1210



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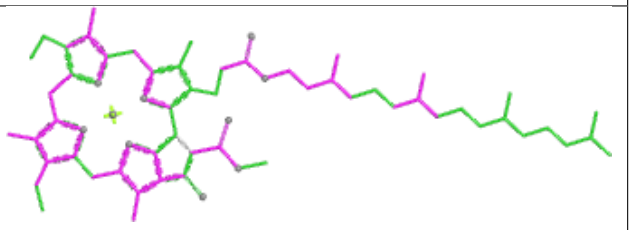
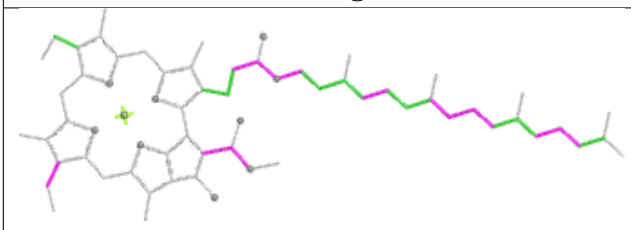


Bond angles



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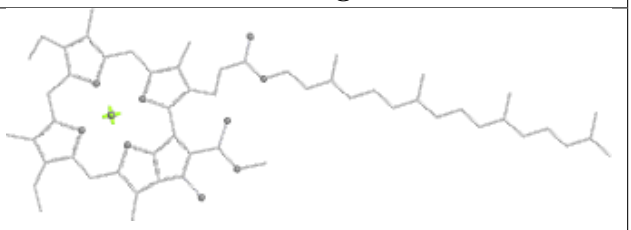
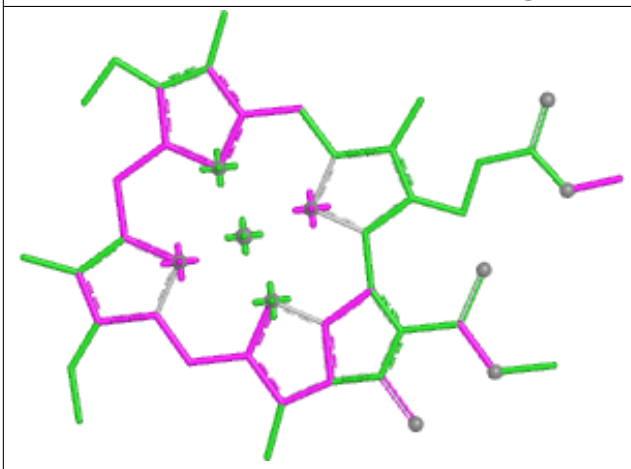


Rings

Ligand CLA a 1138



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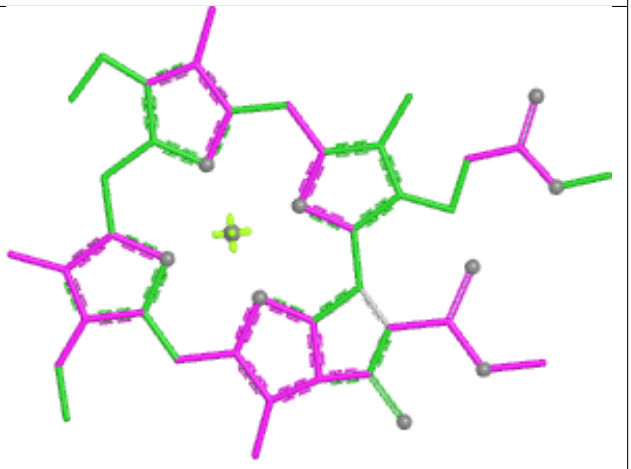
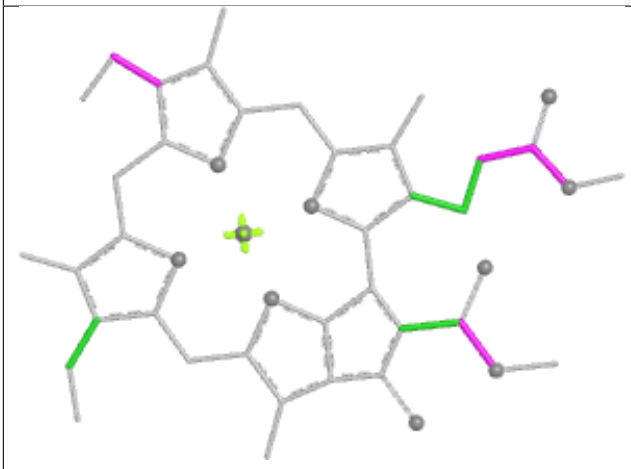


Bond angles



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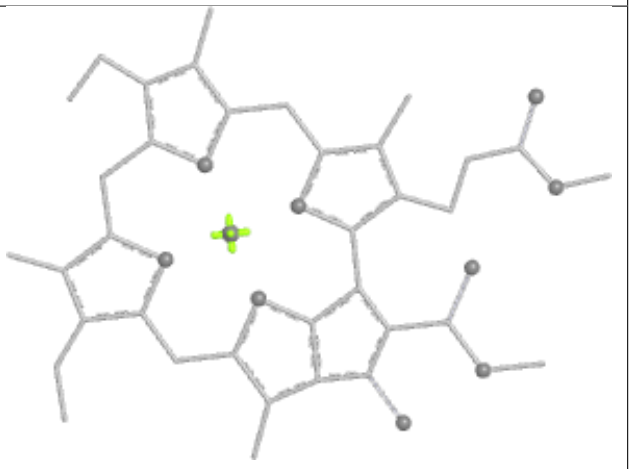
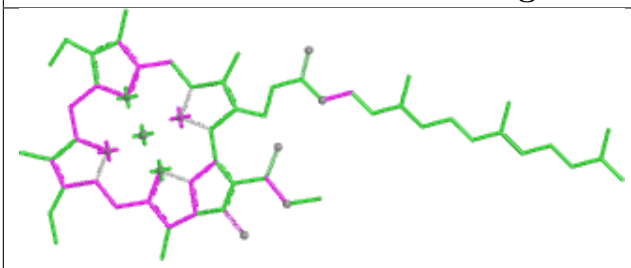


Rings

Ligand CLA b 1234



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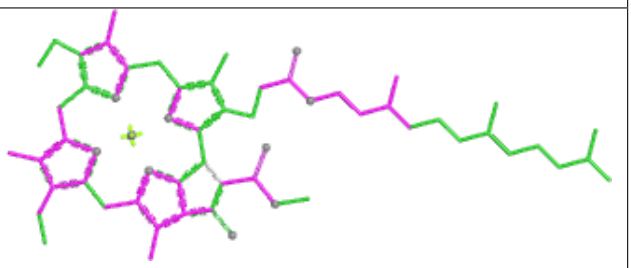
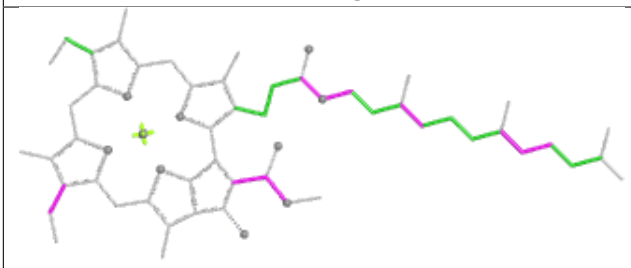


Bond angles



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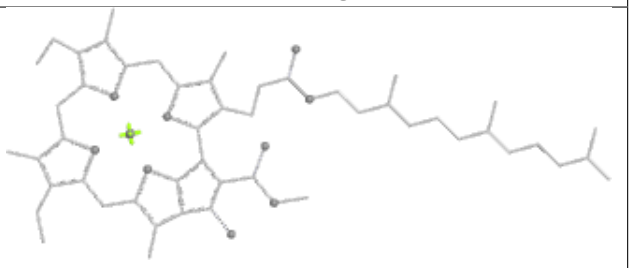
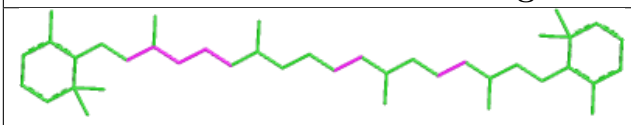


Rings

Ligand BCR 7 4021



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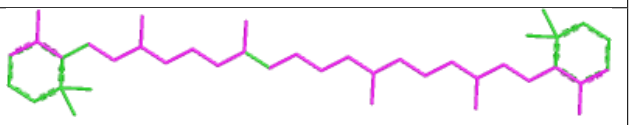
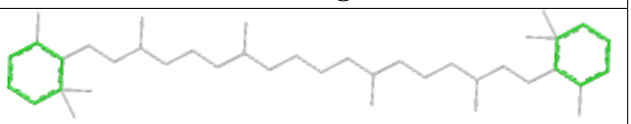


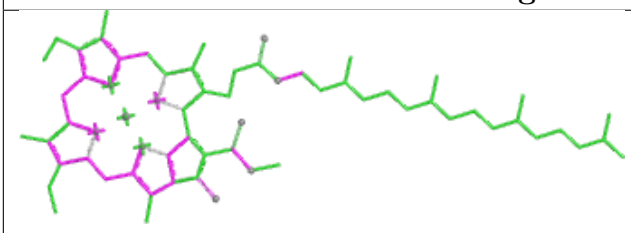
Bond angles

Torsions



Rings

Ligand CLA b 1216



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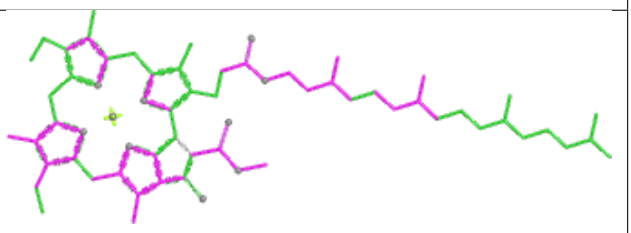
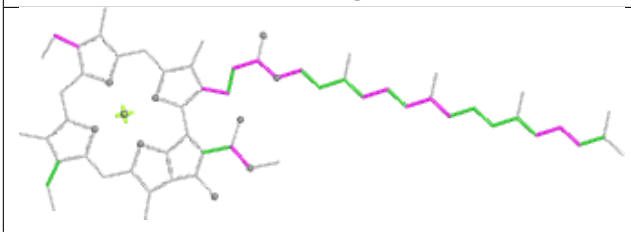
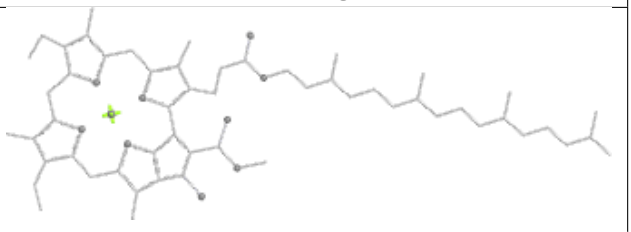


Bond angles

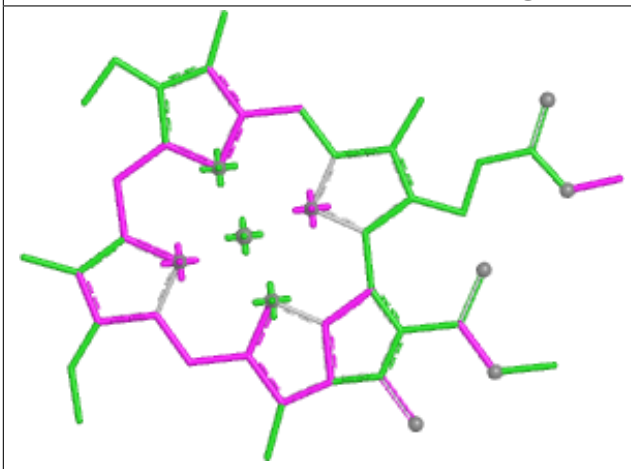


Torsions



Rings

Ligand CLA 1 1133



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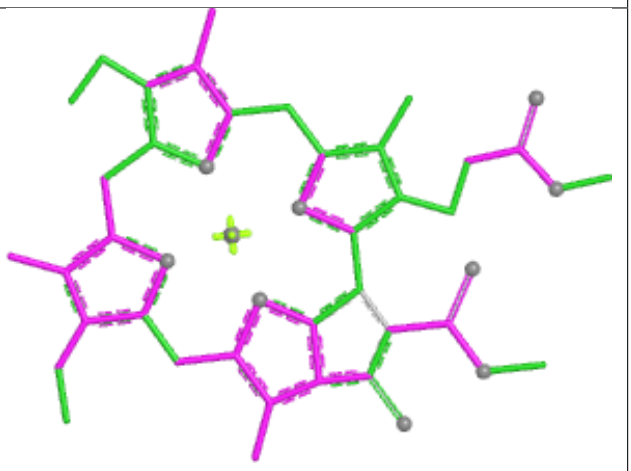
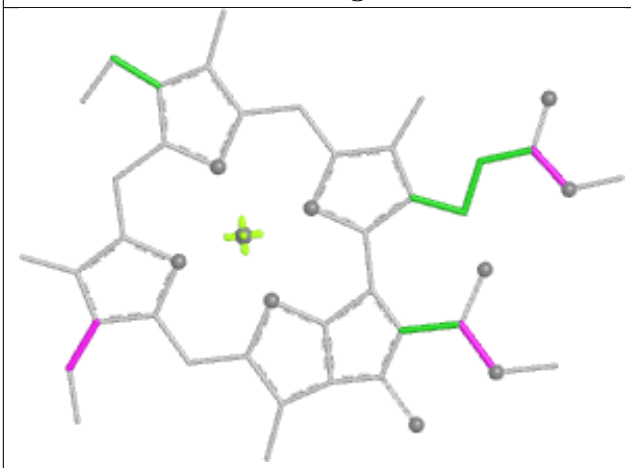
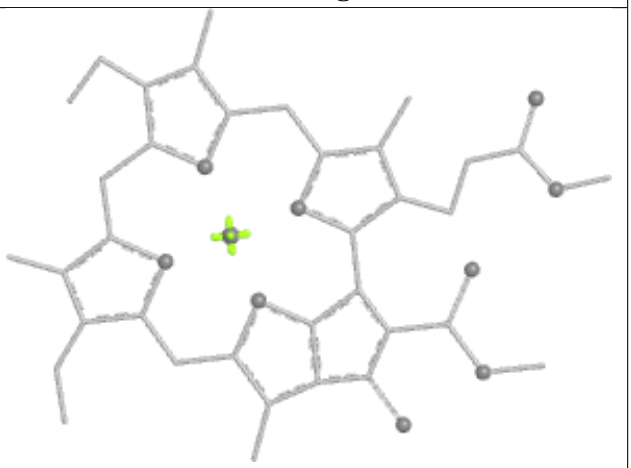


Bond angles

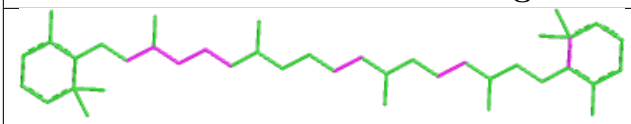


Torsions



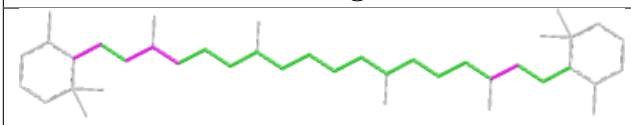
Rings

Ligand BCR B 4005



Bond lengths

Bond angles



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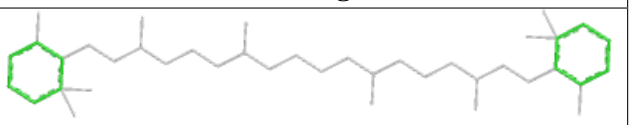
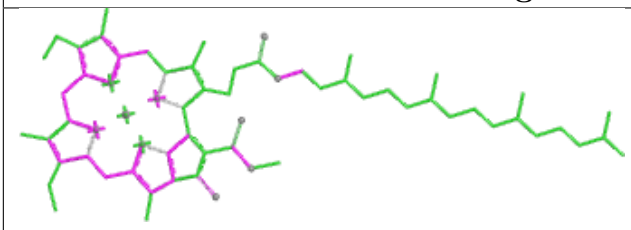
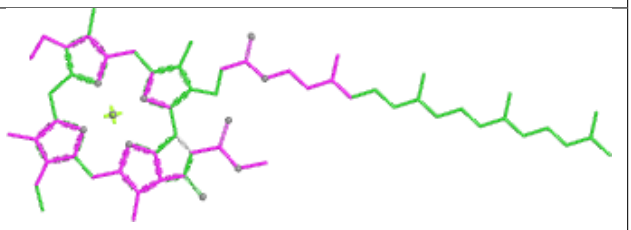


Rings

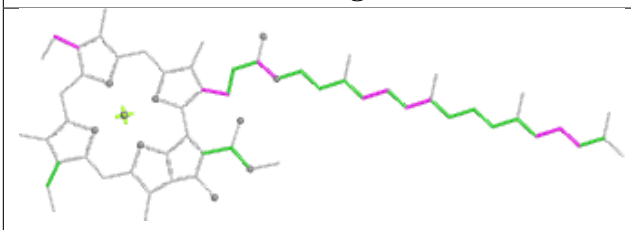
Ligand CLA B 1216



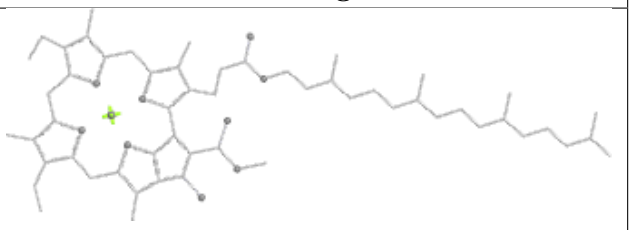
Bond lengths



Bond angles

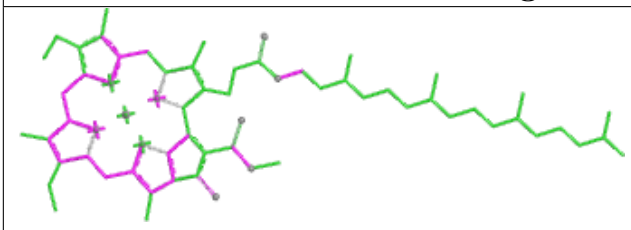


Torsions

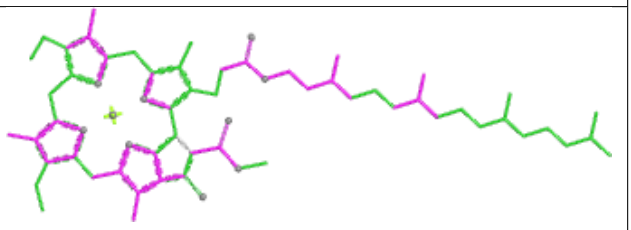


Rings

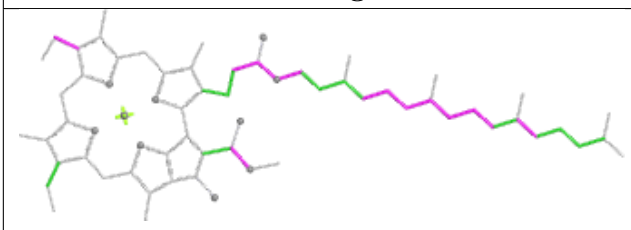
Ligand CLA 1 1140



Bond lengths



Bond angles



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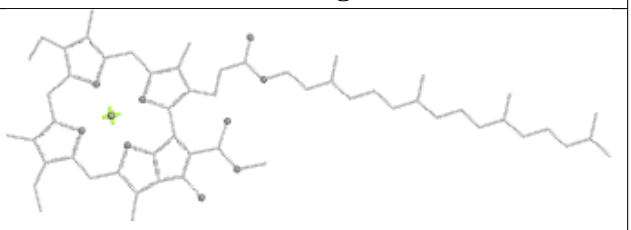
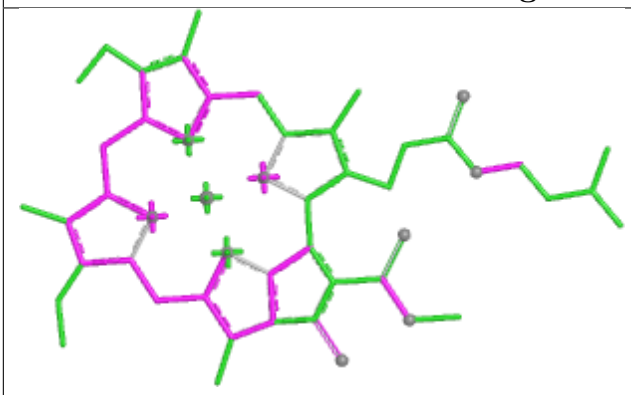


Rings

Ligand CLA 1 1139



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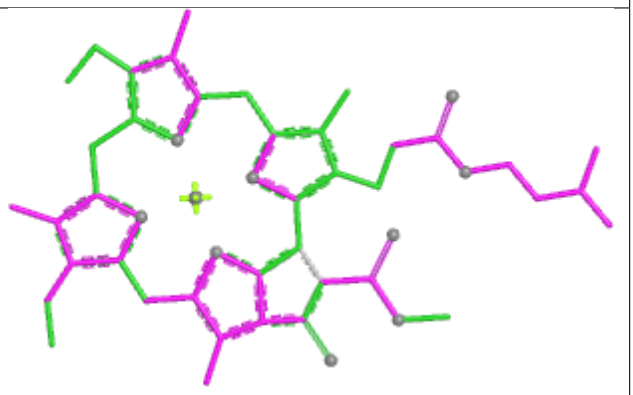
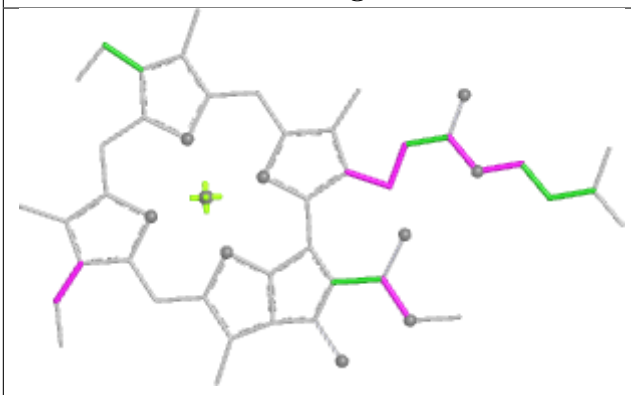
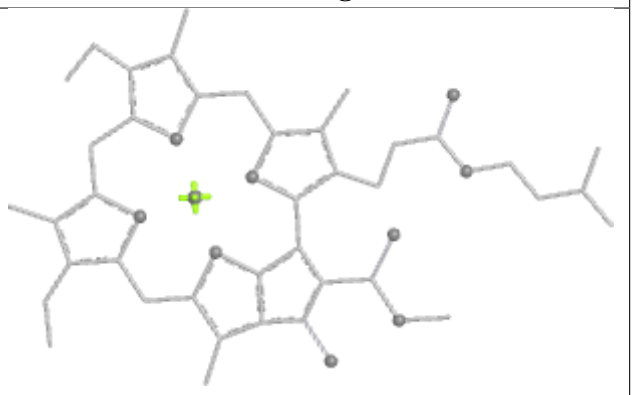


Bond angles

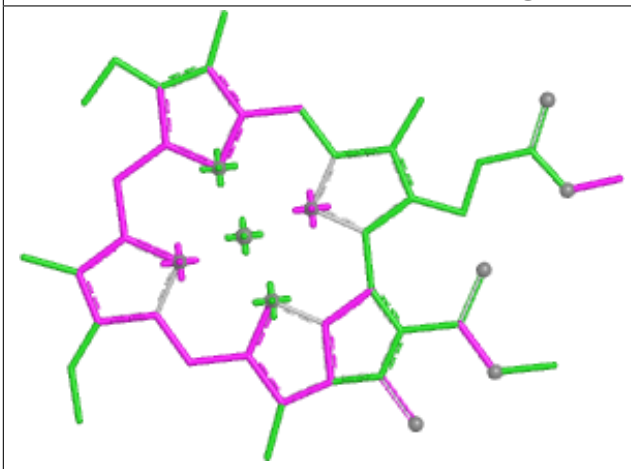


Torsions

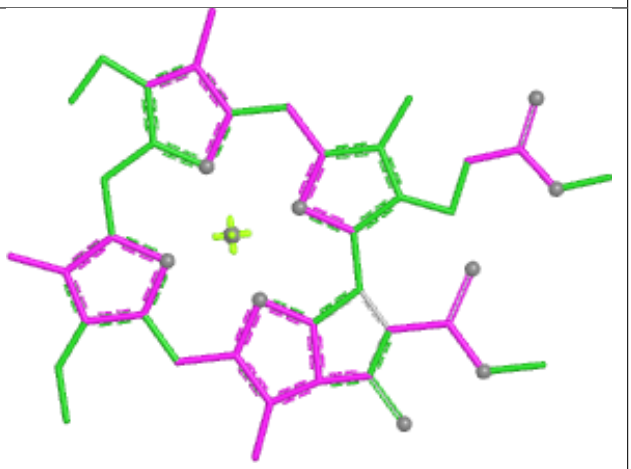


Rings

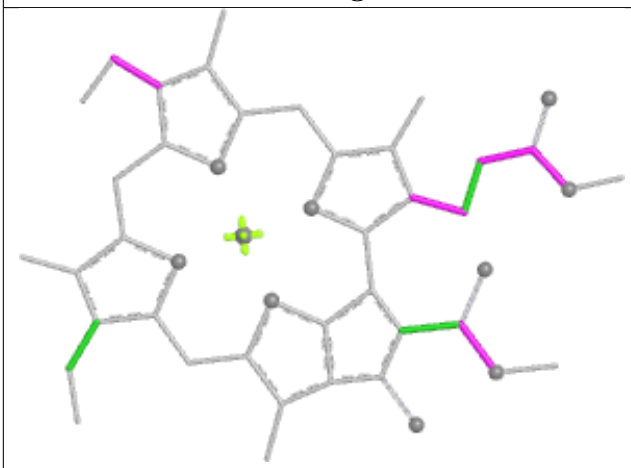
Ligand CLA 1 1120



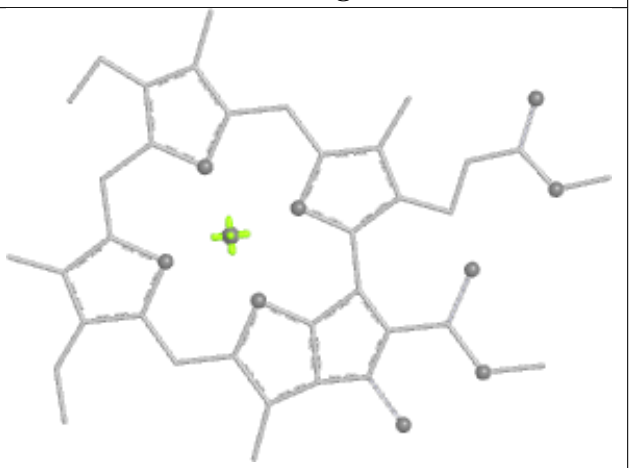
Bond lengths



Bond angles

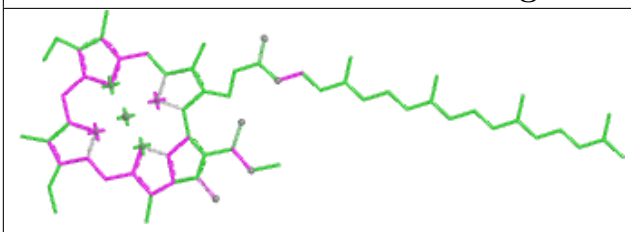


Torsions

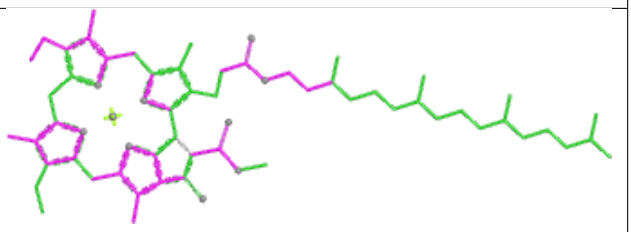


Rings

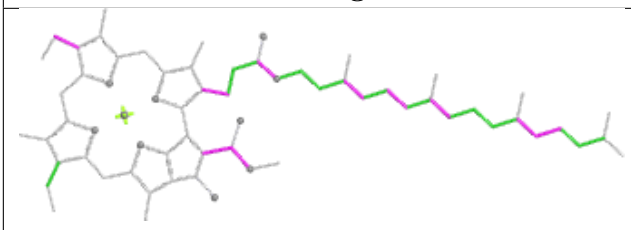
Ligand CLA a 1132



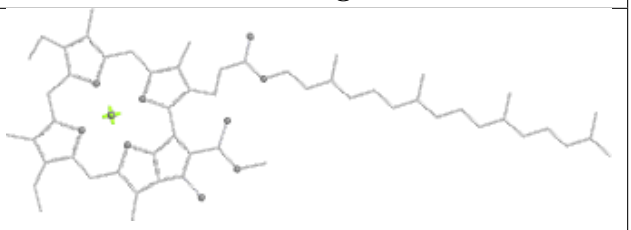
Bond lengths



Bond angles

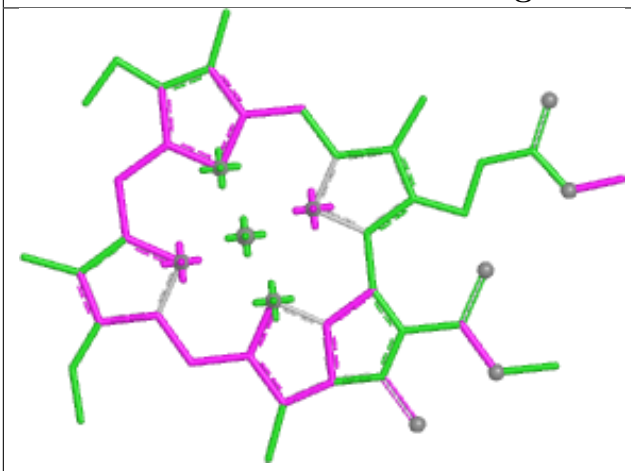


Torsions

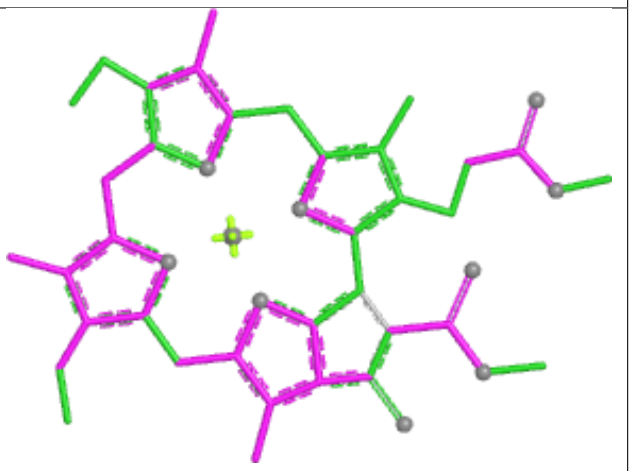


Rings

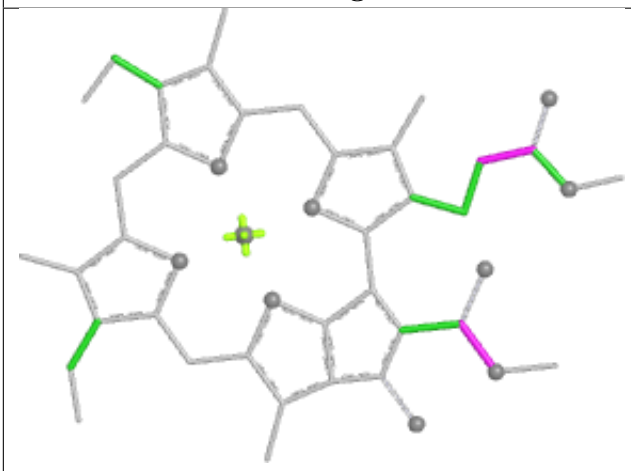
Ligand CLA A 1136



Bond lengths



Bond angles



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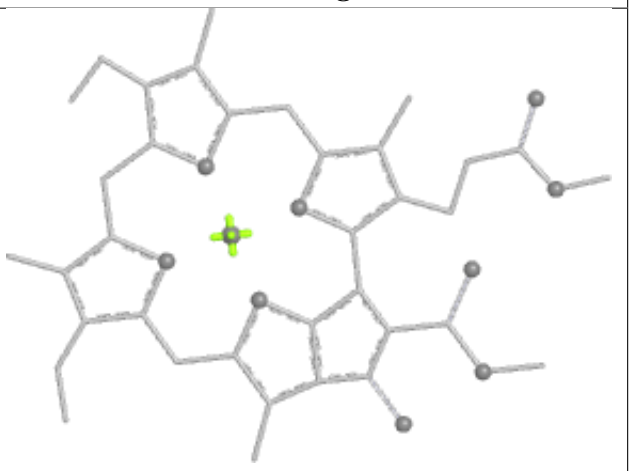
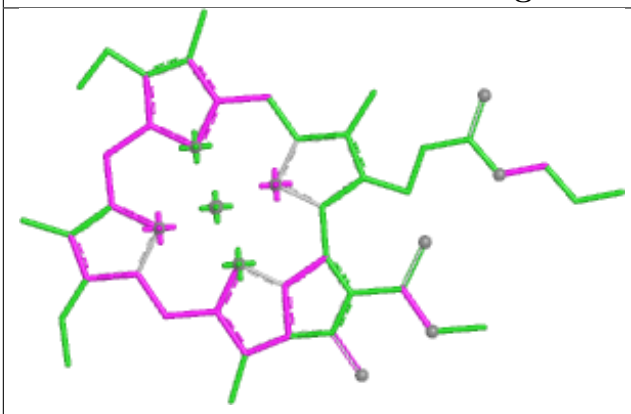
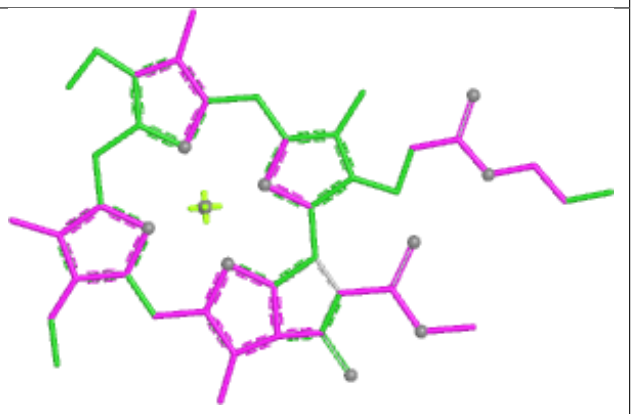


Rings

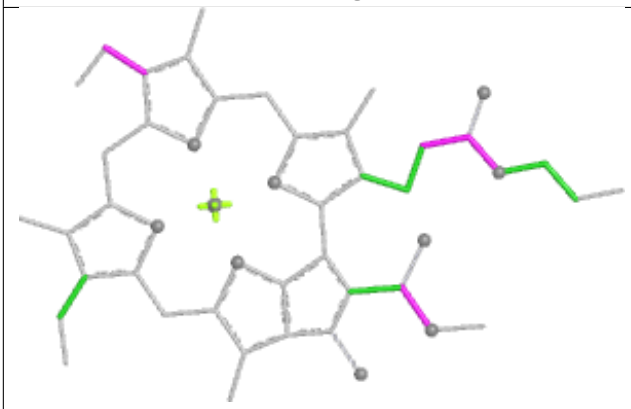
Ligand CLA A 1105



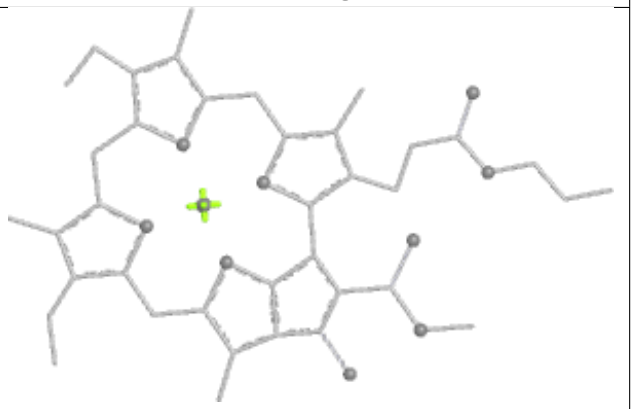
Bond lengths



Bond angles

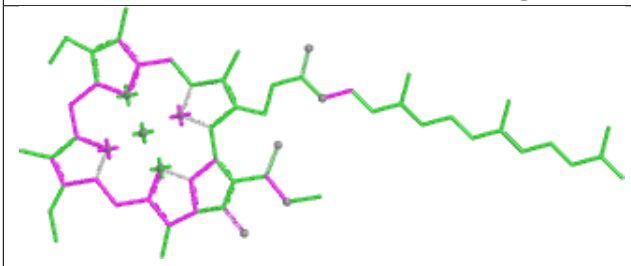


Torsions

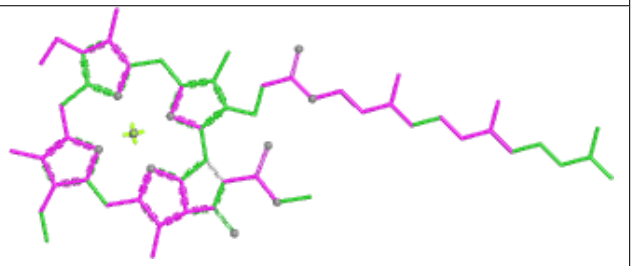


Rings

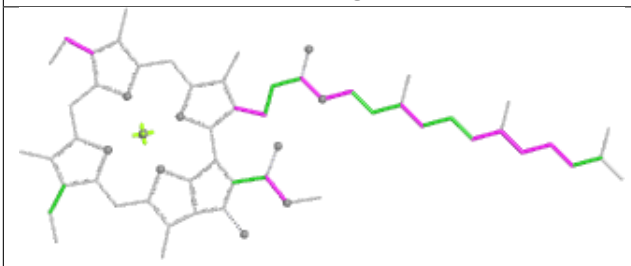
Ligand CLA B 1234



Bond lengths



Bond angles



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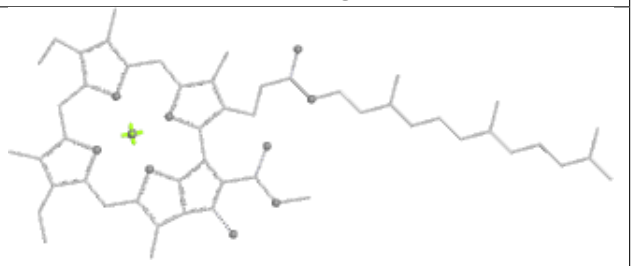
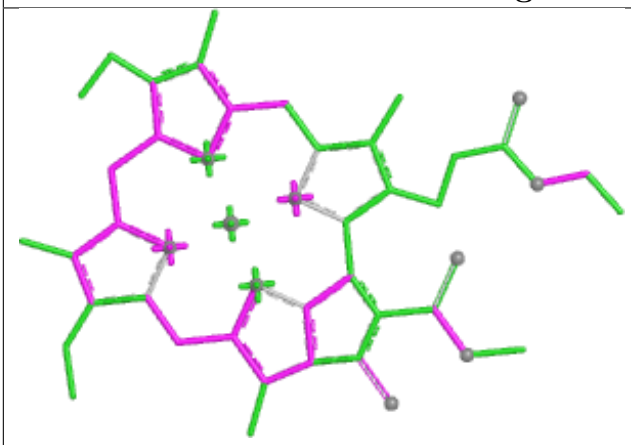
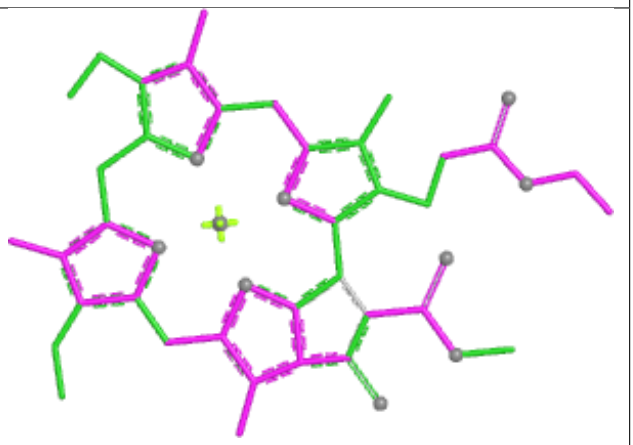


Rings

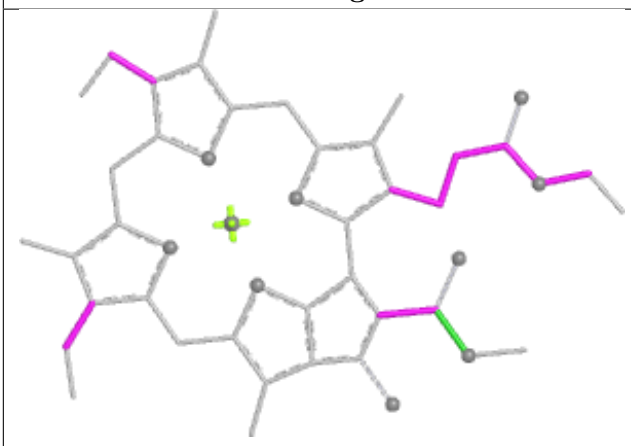
Ligand CLA B 1217



Bond lengths



Bond angles



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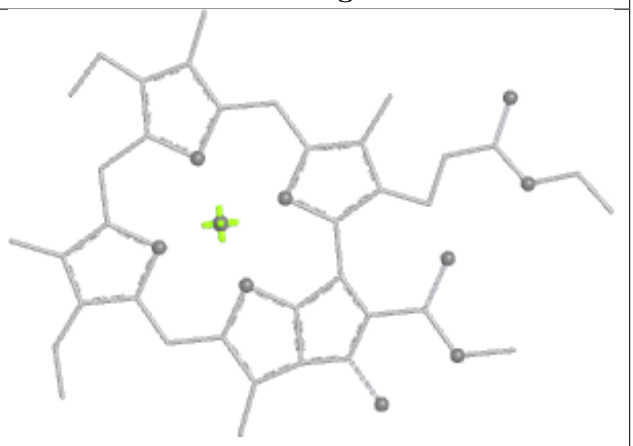
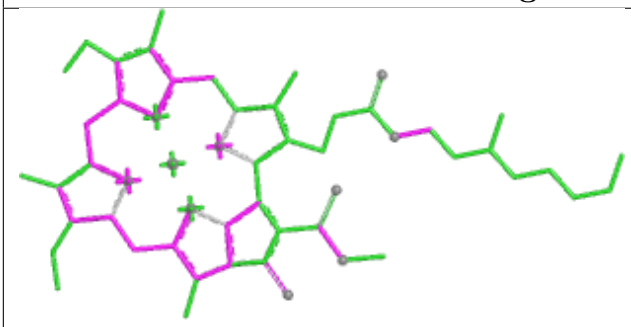


Rings

Ligand CLA 1 1116



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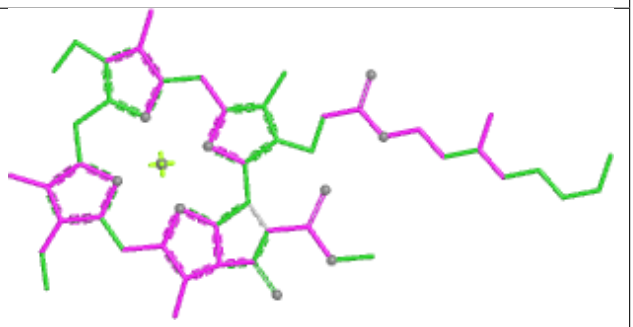
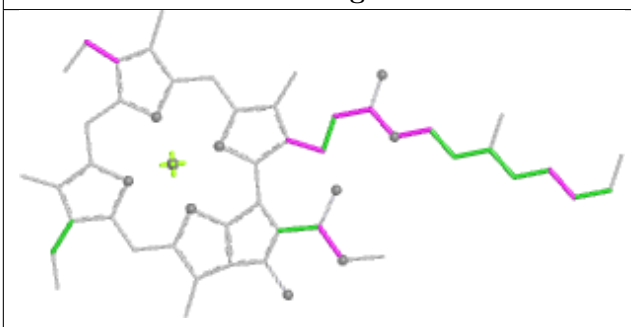


Bond angles



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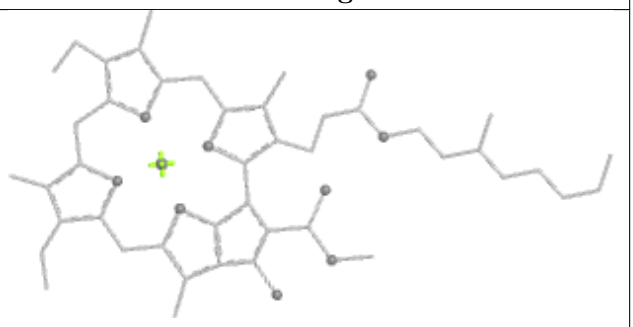
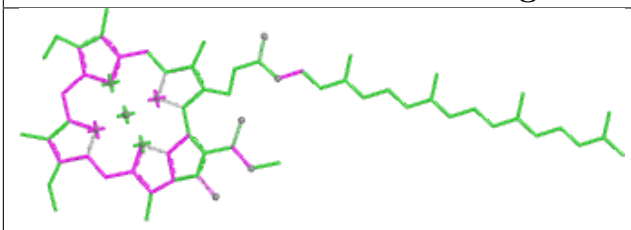
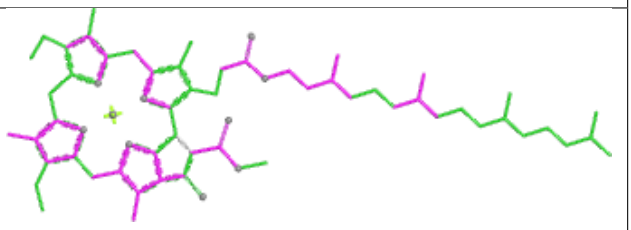


Rings

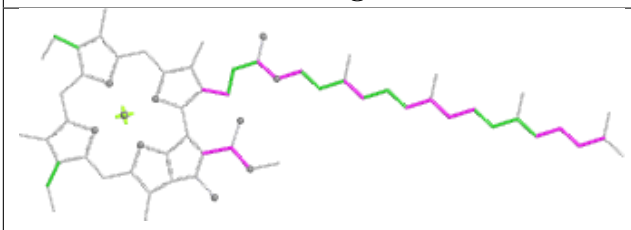
Ligand CLA 1 1137



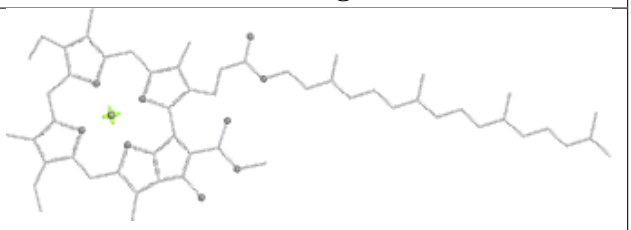
Bond lengths



Bond angles

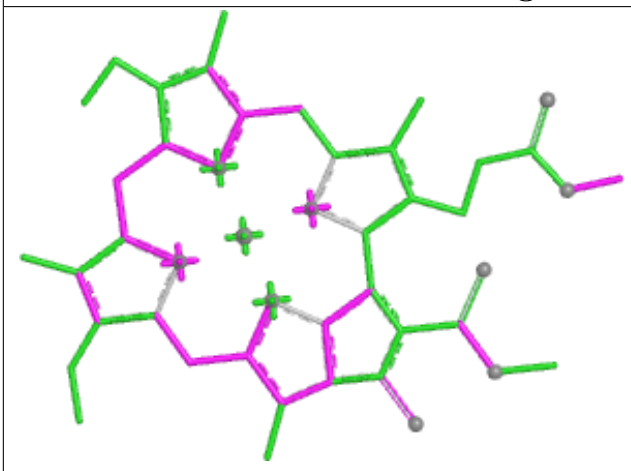


Torsions



Rings

Ligand CLA L 1502



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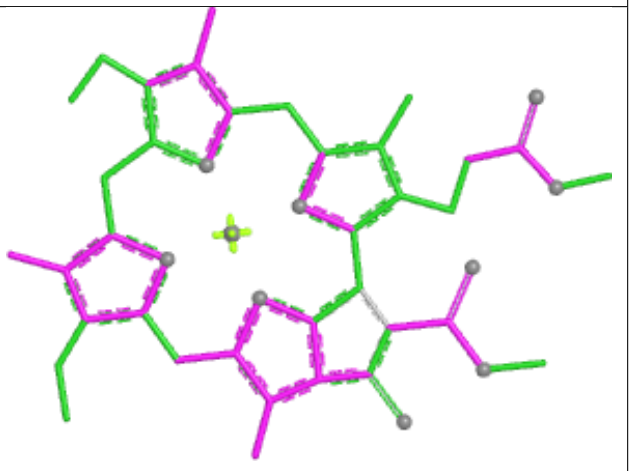
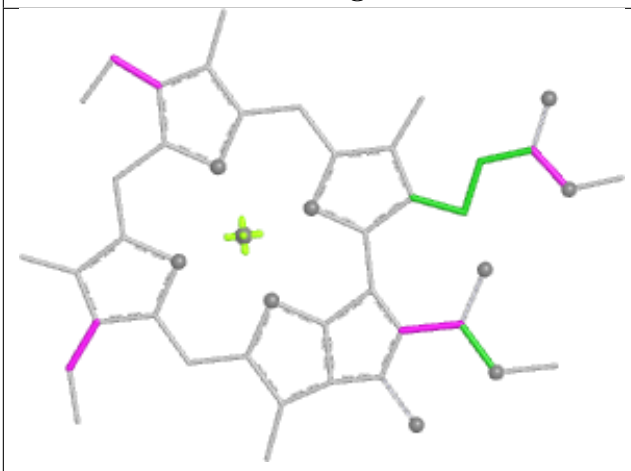


Bond angles



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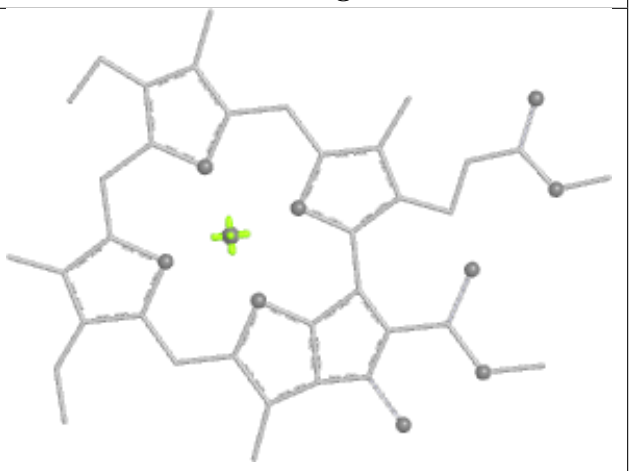
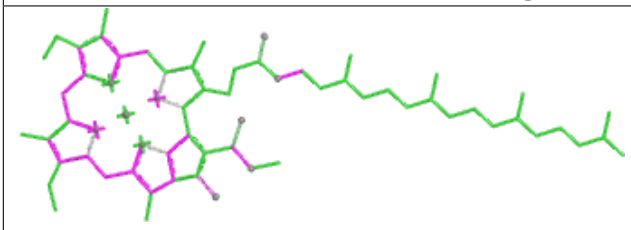


Rings

Ligand CLA 1 1128



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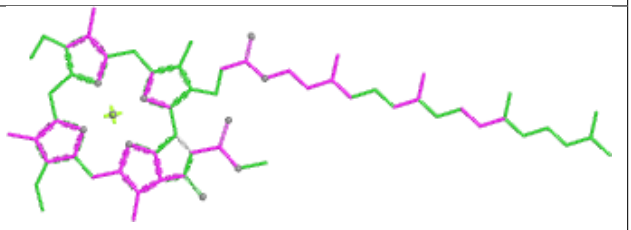
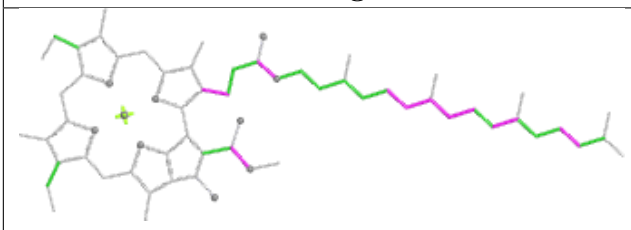


Bond angles



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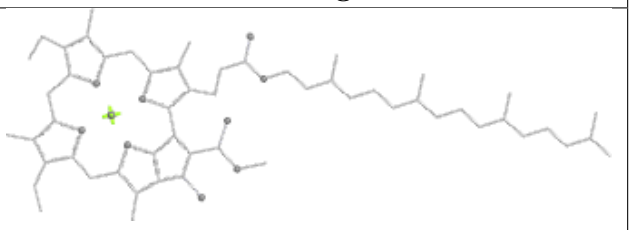
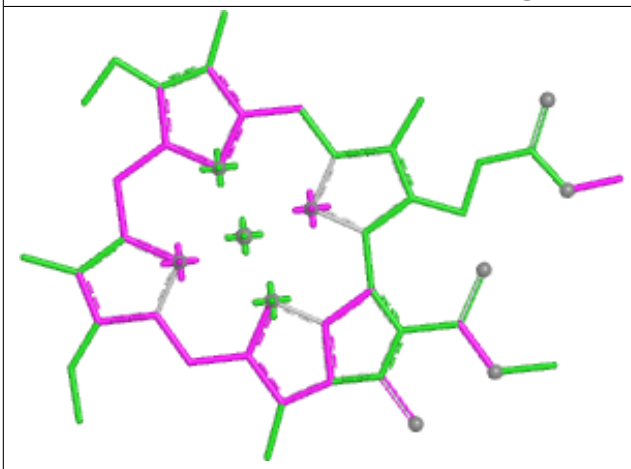


Rings

Ligand CLA b 1211



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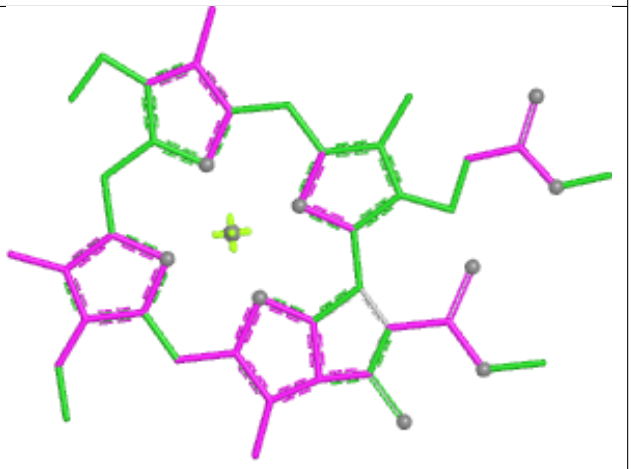
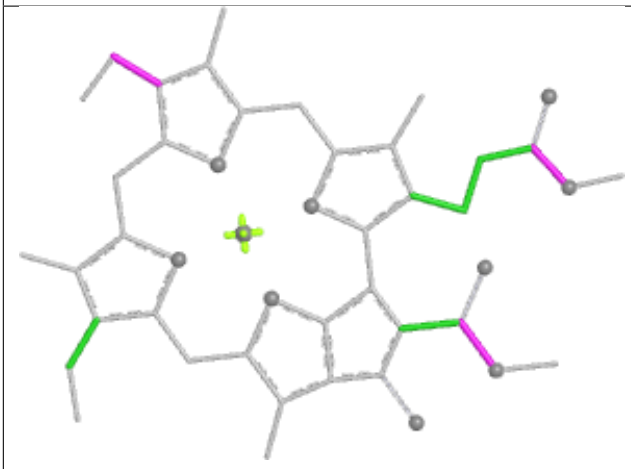
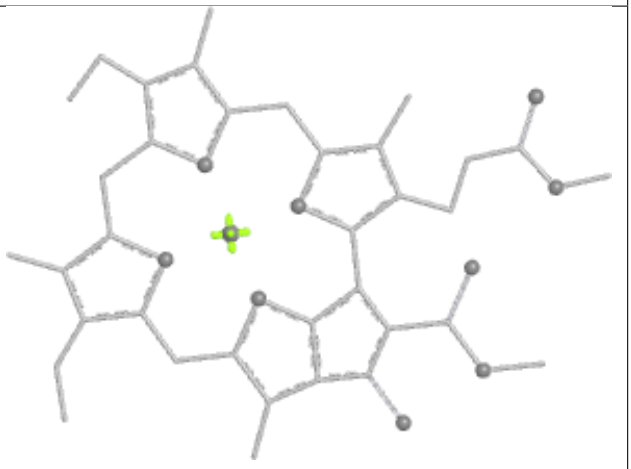


Bond angles

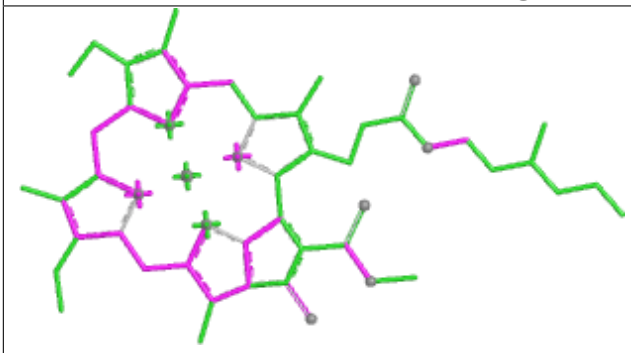


Torsions

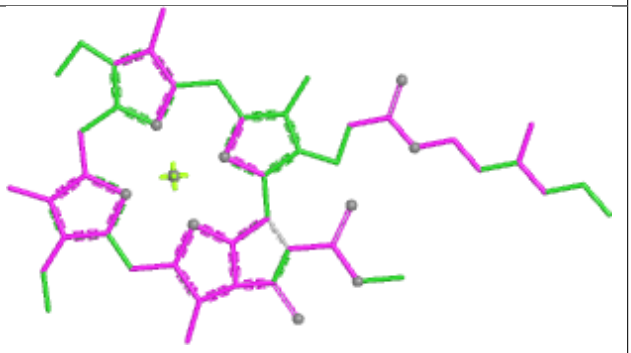


Rings

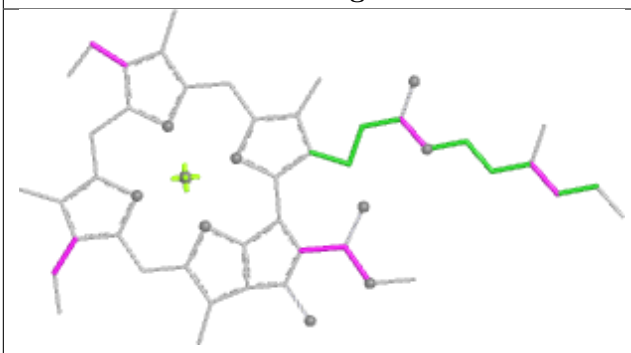
Ligand CLA A 1125



Bond lengths



Bond angles



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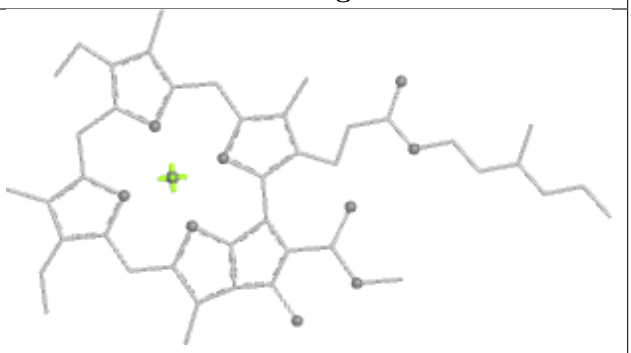
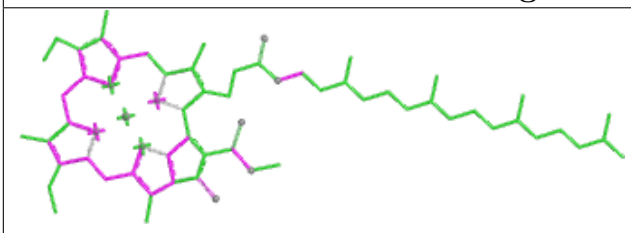
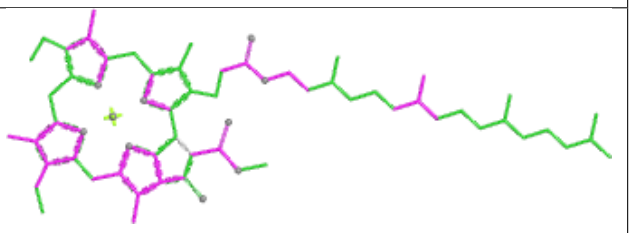


Rings

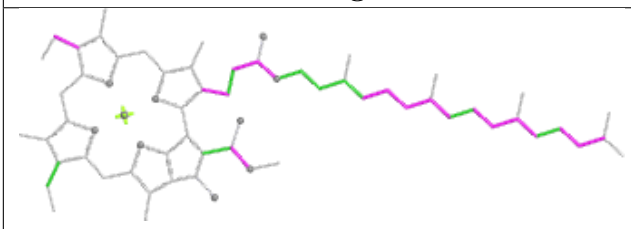
Ligand CLA 1 1131



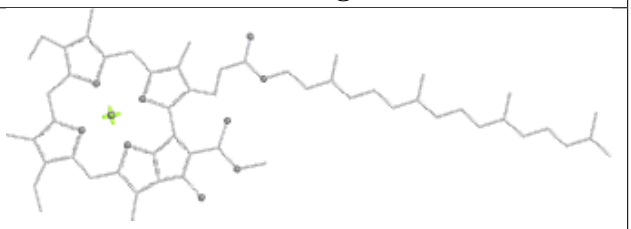
Bond lengths



Bond angles

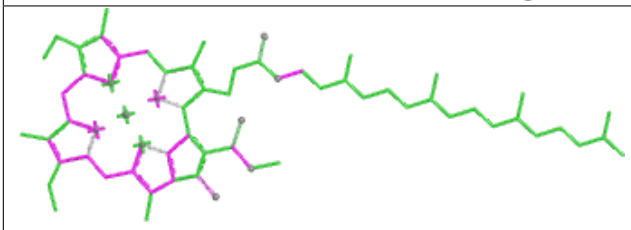


Torsions

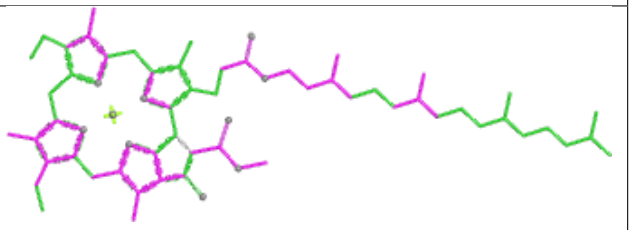


Rings

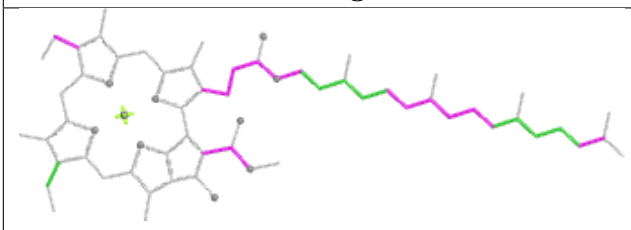
Ligand CLA 1 1101



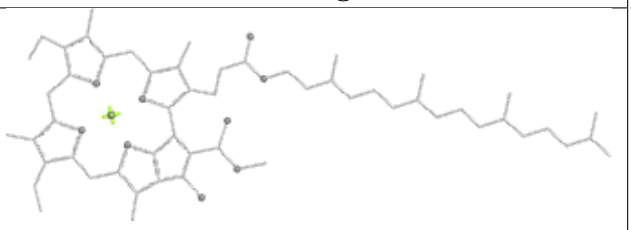
Bond lengths



Bond angles

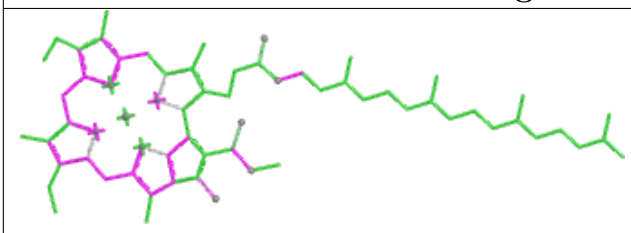


Torsions



Rings

Ligand CLA B 1215



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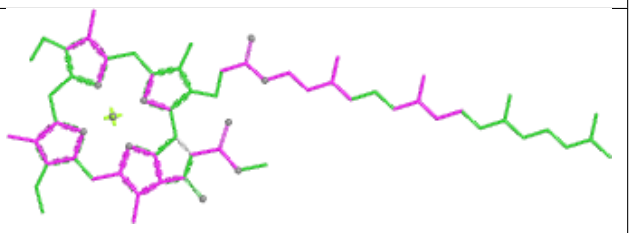
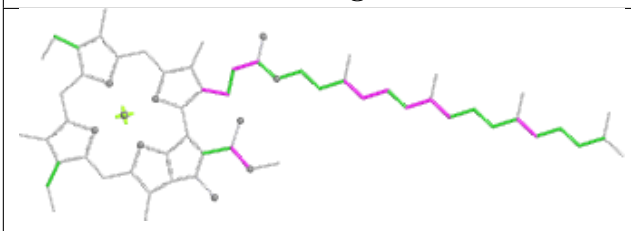


Bond angles



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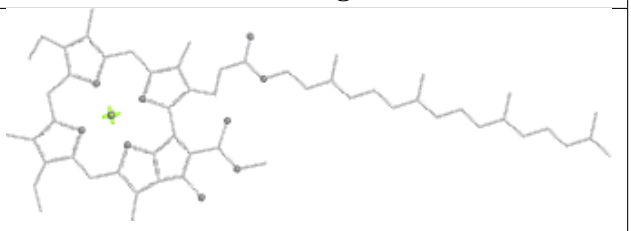
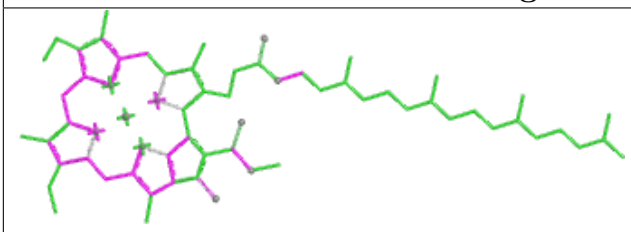


Rings

Ligand CLA a 1103



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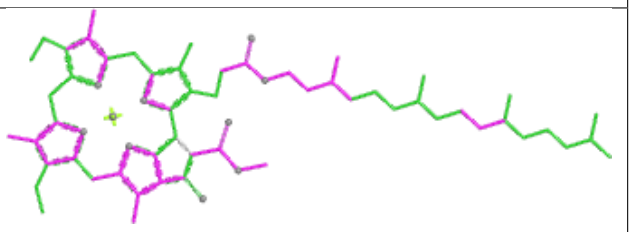
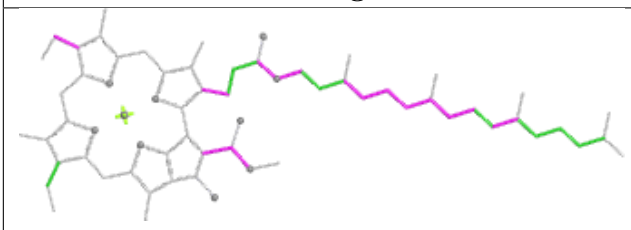
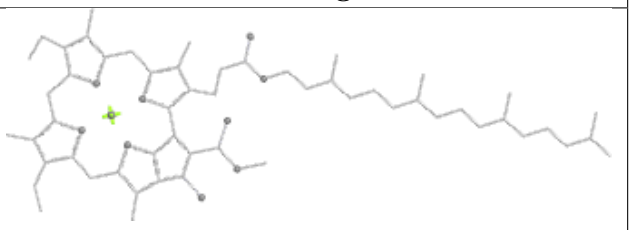


Bond angles

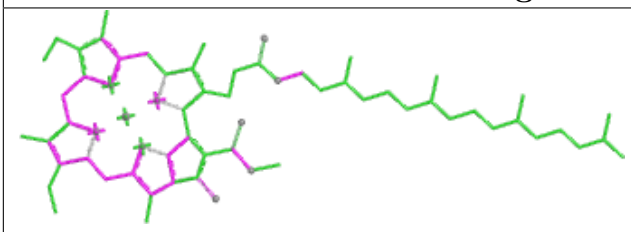


Torsions

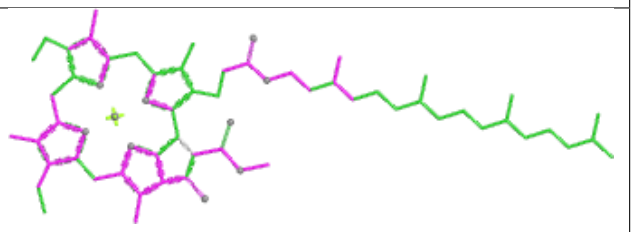


Rings

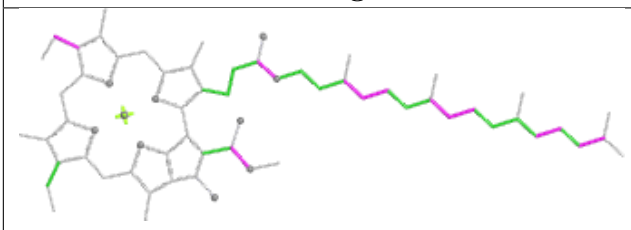
Ligand CLA B 1206



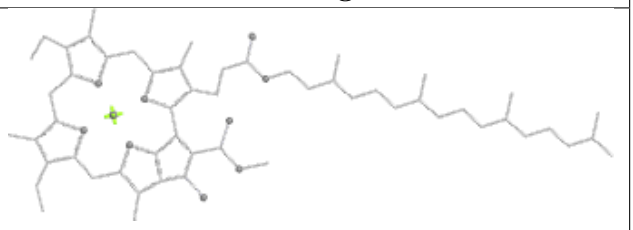
Bond lengths



Bond angles

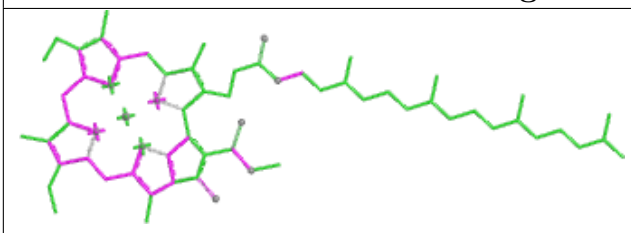


Torsions



Rings

Ligand CLA a 1119



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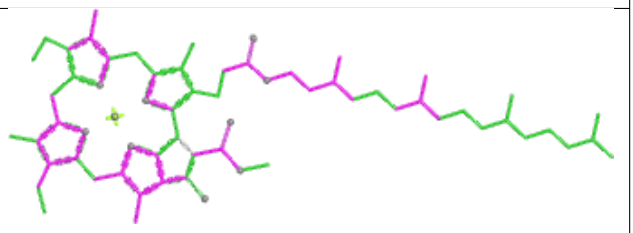
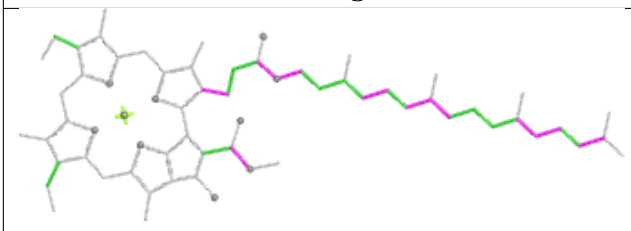
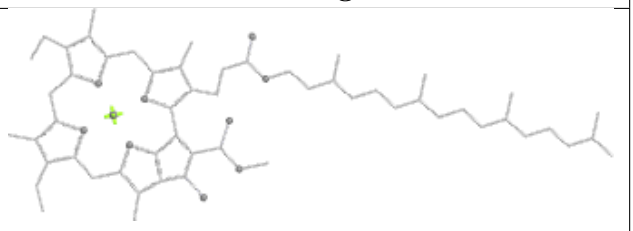


Bond angles

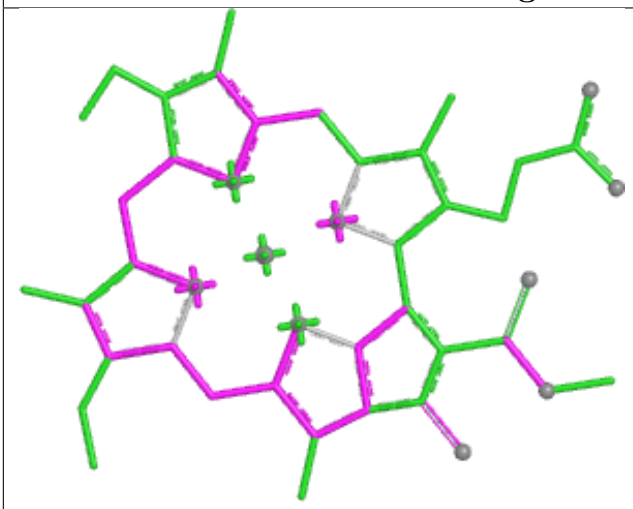


Torsions



Rings

Ligand CLA b 1227



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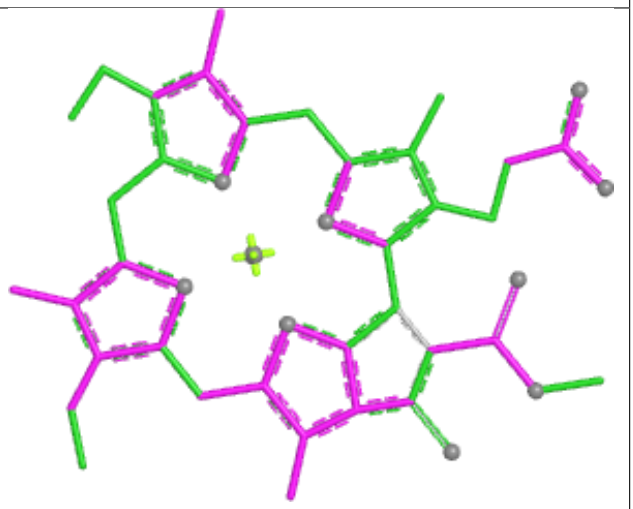
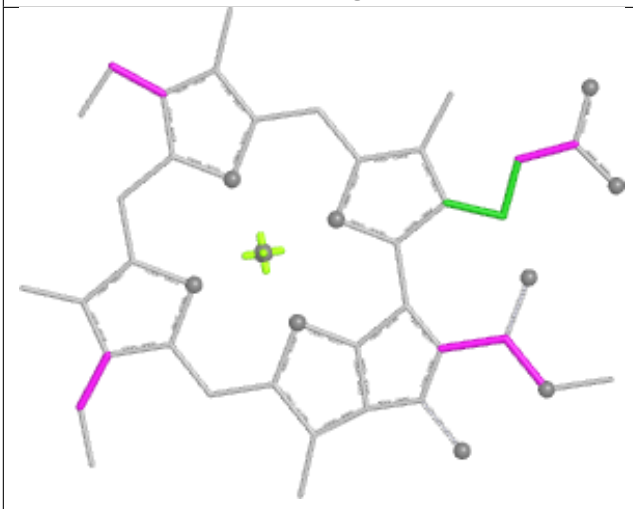


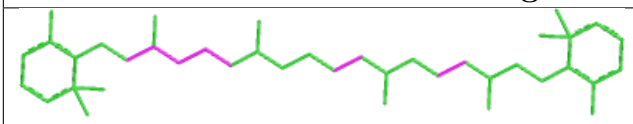
Bond angles



Torsions

Rings

Ligand BCR f 4013



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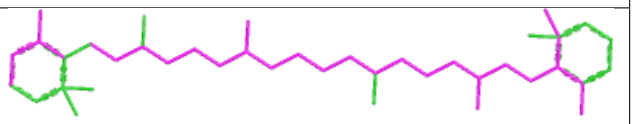
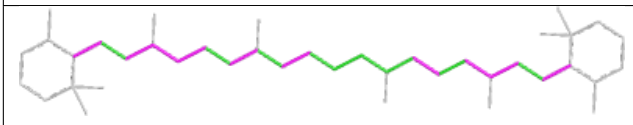
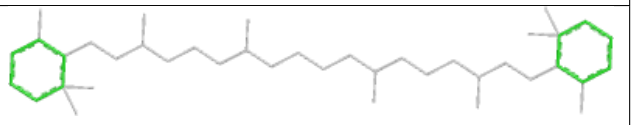


Bond angles

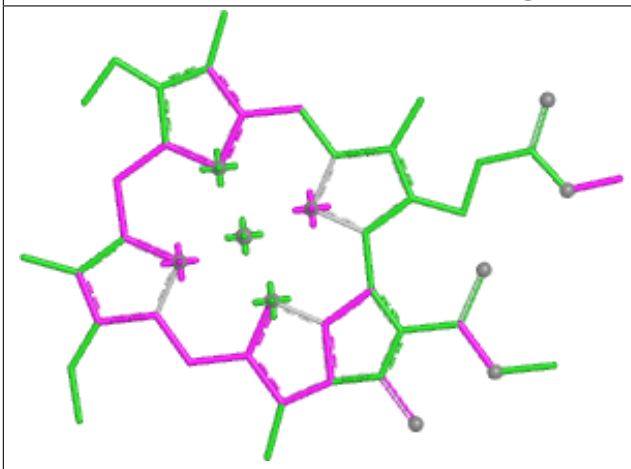


Torsions



Rings

Ligand CLA 1 1136



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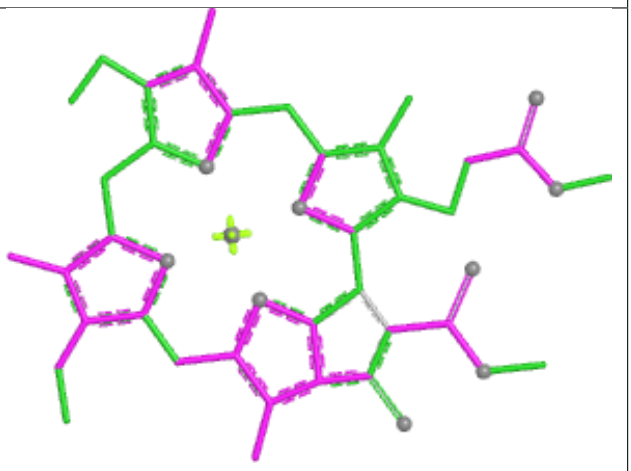
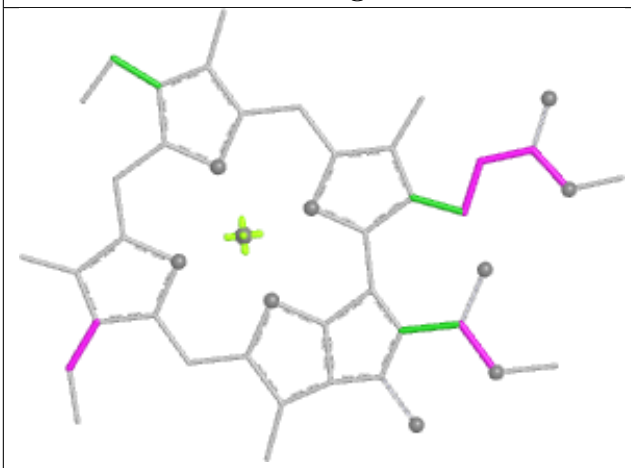


Bond angles



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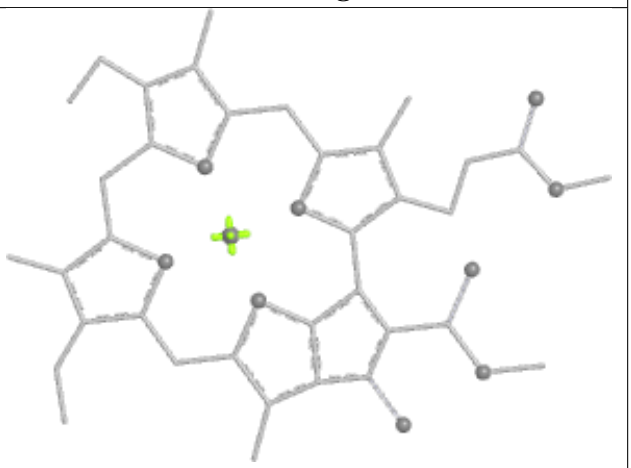
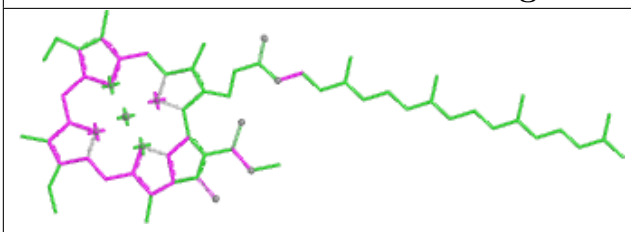


Rings

Ligand CLA 2 1229



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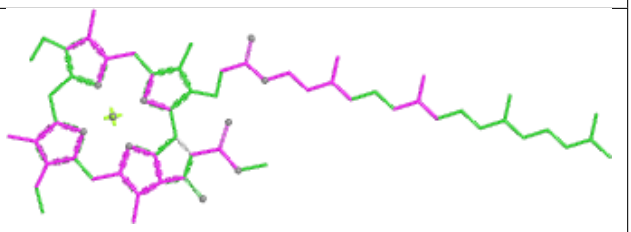
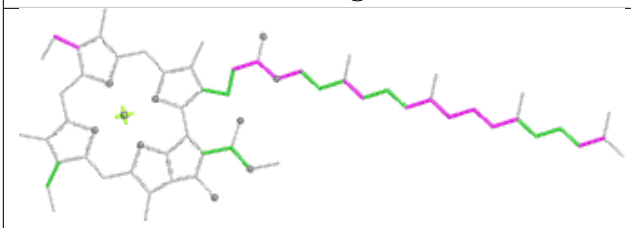
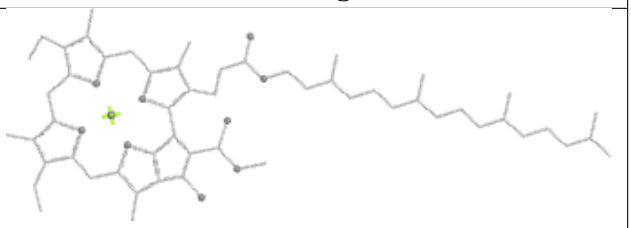


Bond angles

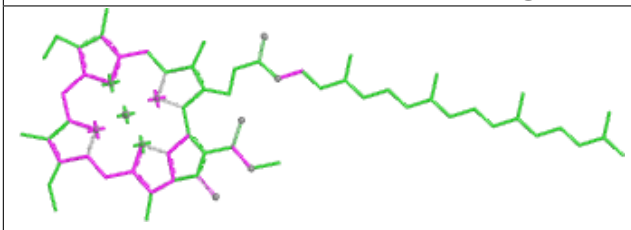


Torsions

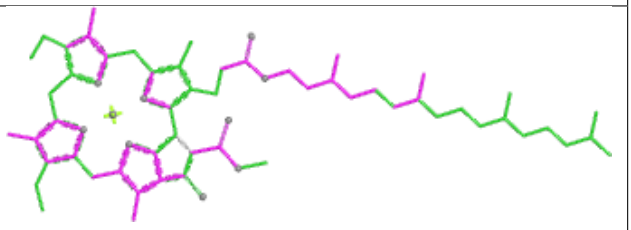


Rings

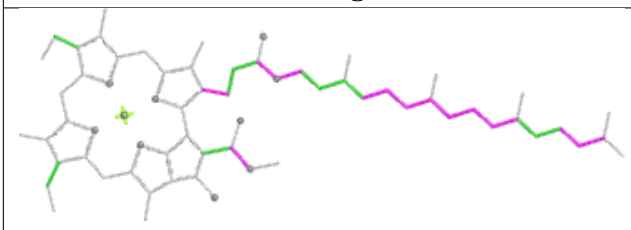
Ligand CLA a 1117



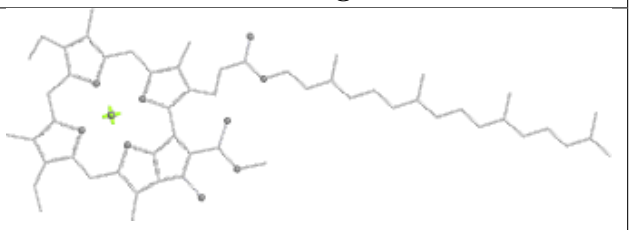
Bond lengths



Bond angles

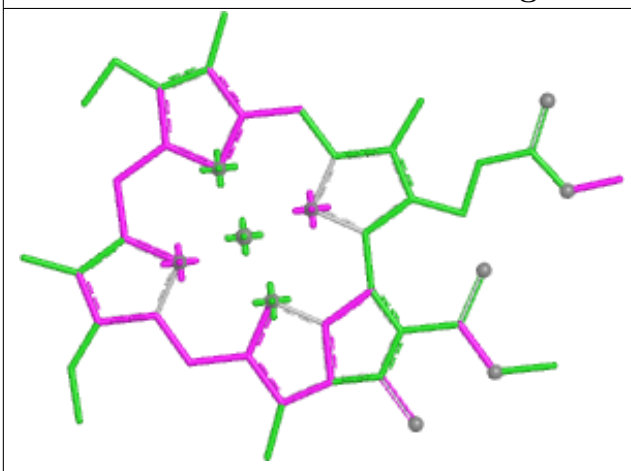


Torsions



Rings

Ligand CLA a 1121



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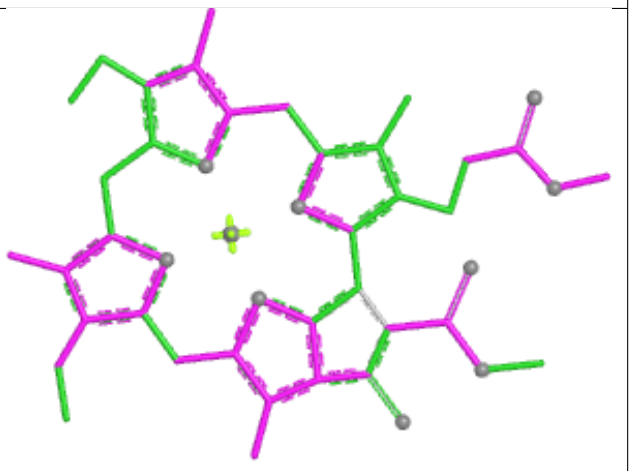
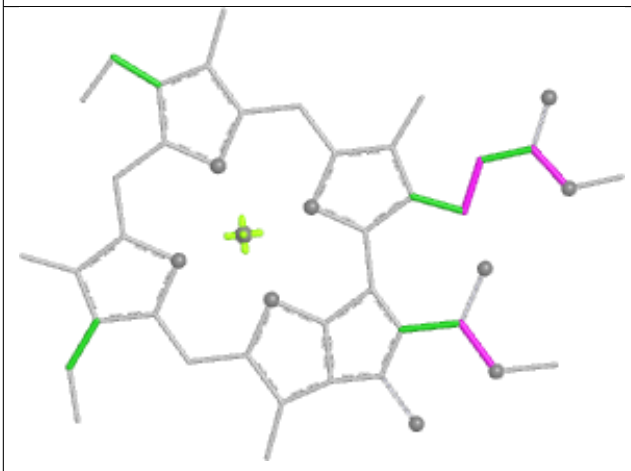
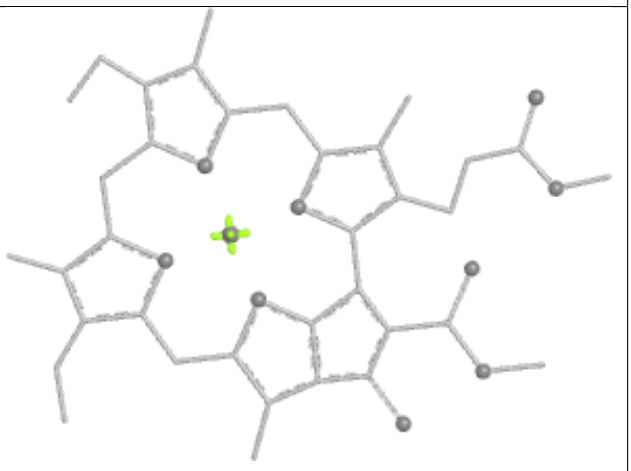


Bond angles

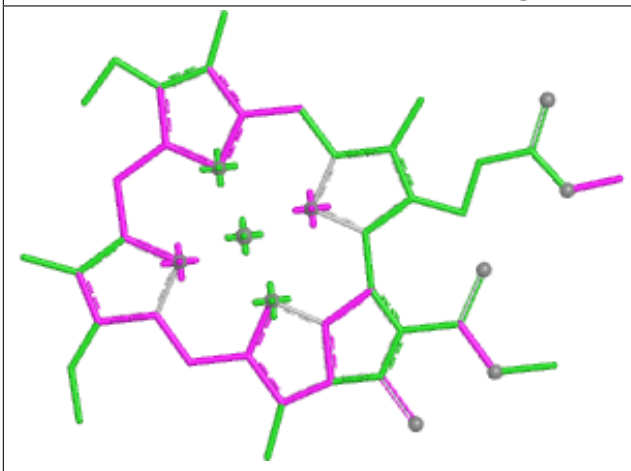


Torsions



Rings

Ligand CLA A 1114



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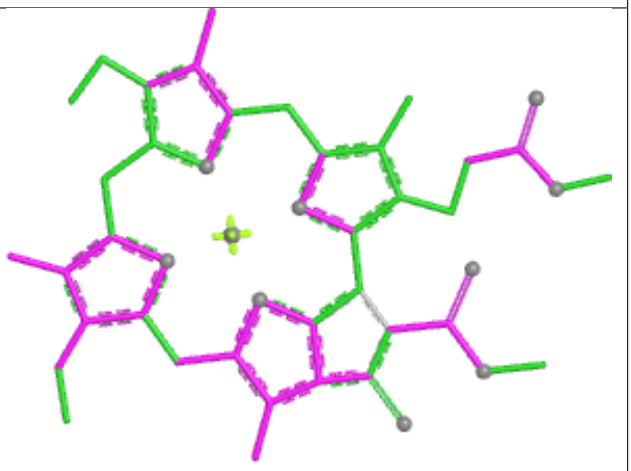
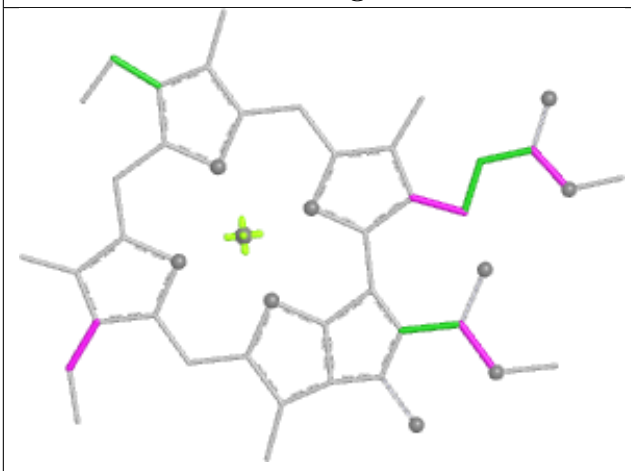
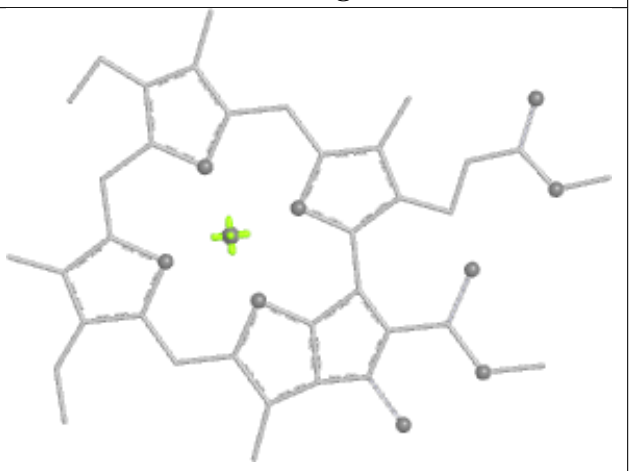


Bond angles

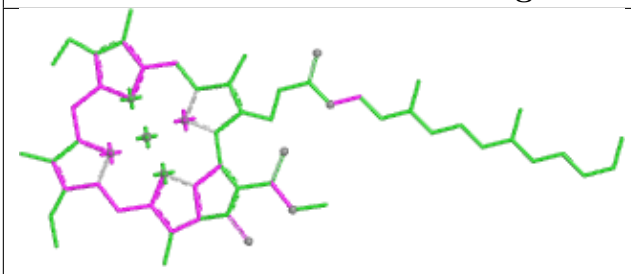


Torsions

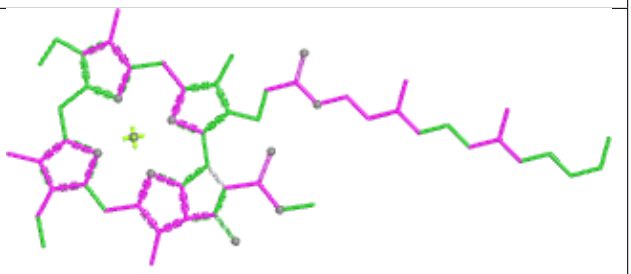


Rings

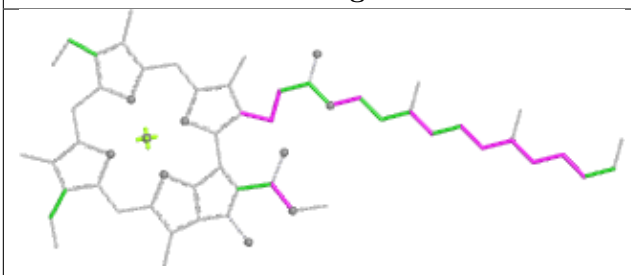
Ligand CLA B 1214



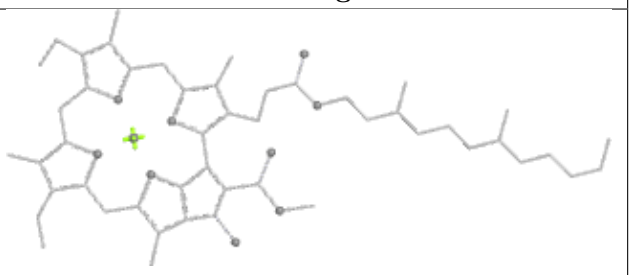
Bond lengths



Bond angles

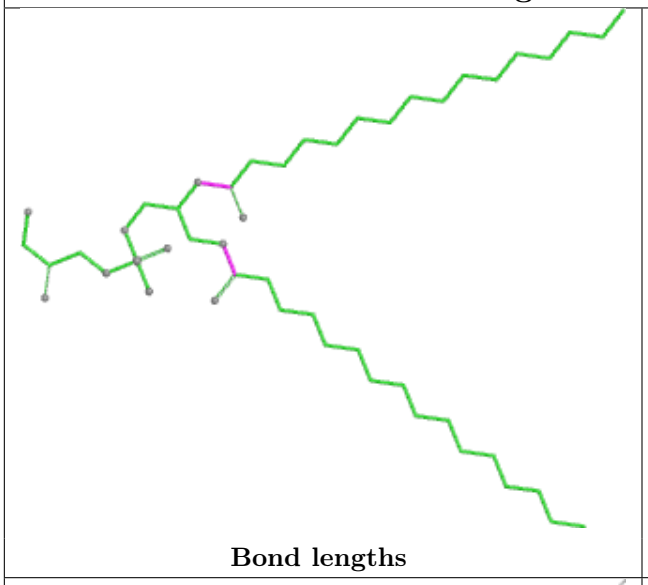


Torsions

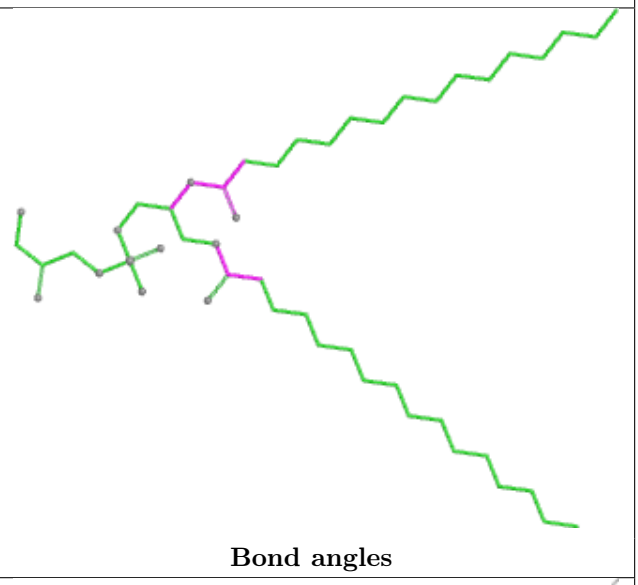


Rings

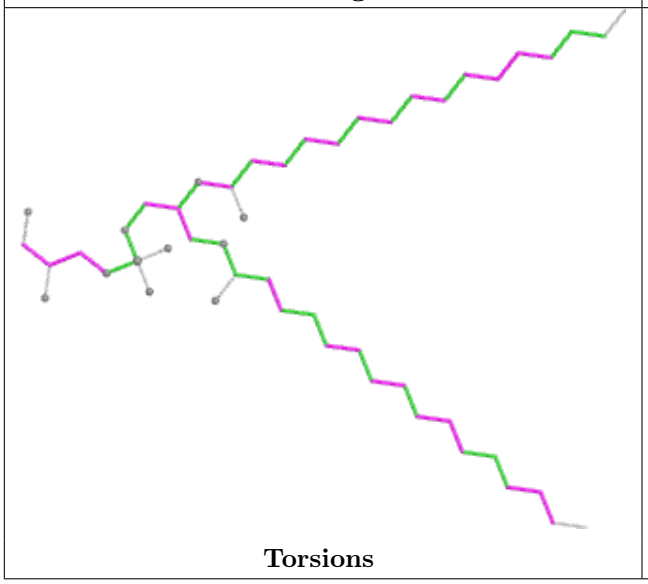
Ligand LHG B 5004



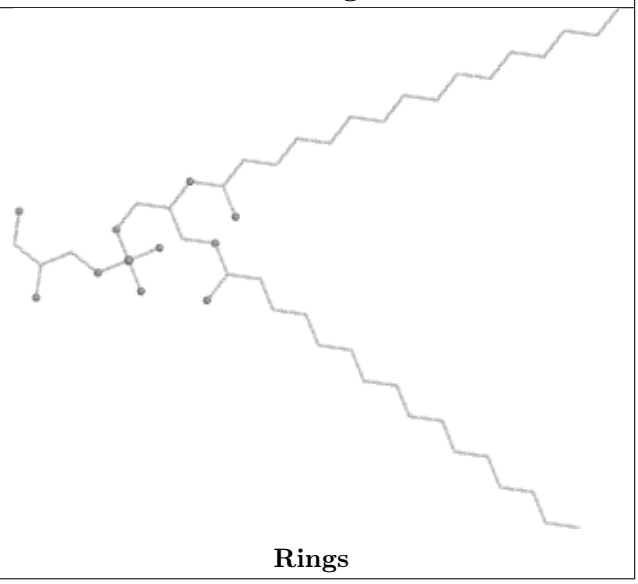
Bond lengths



Bond angles

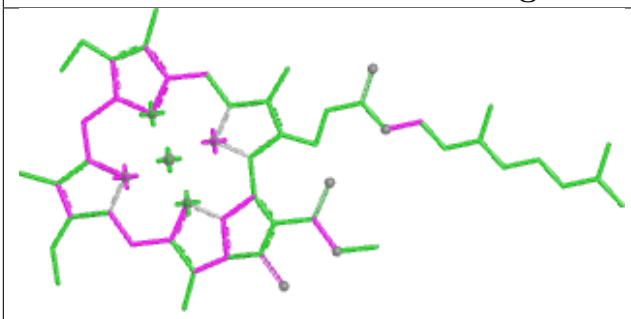


Torsions

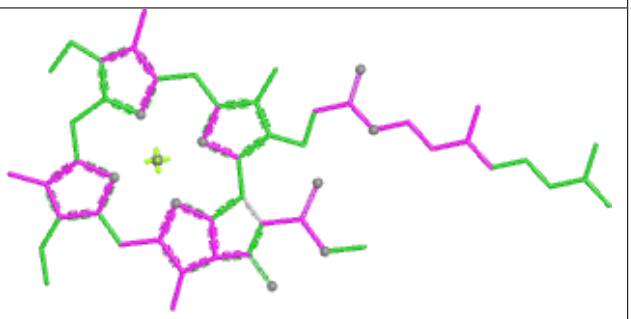


Rings

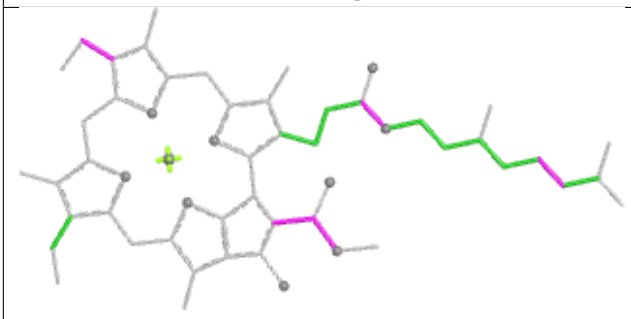
Ligand CLA 2 1205



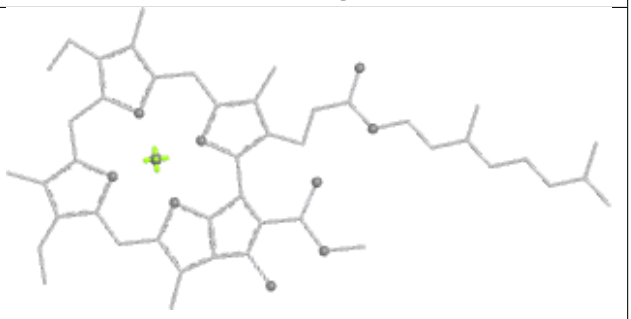
Bond lengths



Bond angles

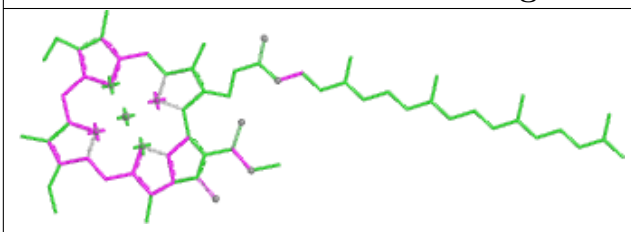


Torsions



Rings

Ligand CLA a 1102



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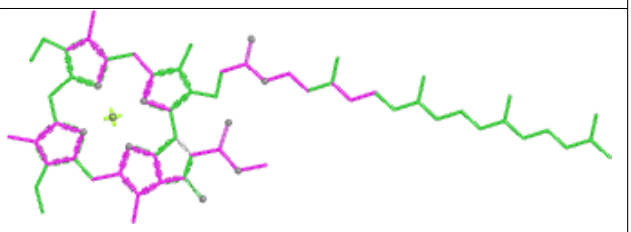

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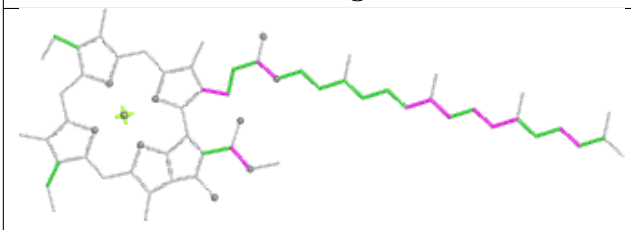

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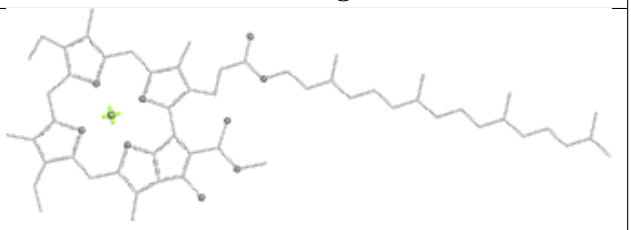
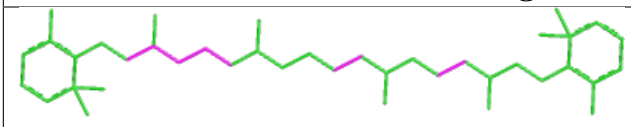


Rings

Ligand BCR a 4007



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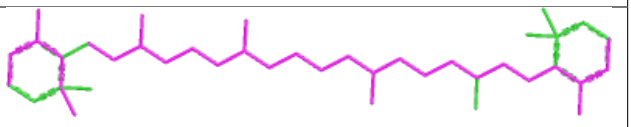

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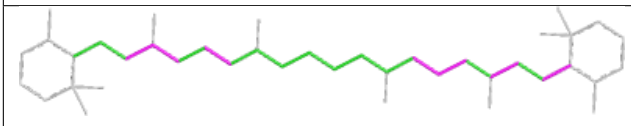

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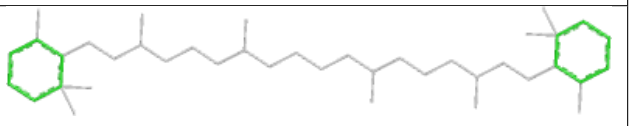
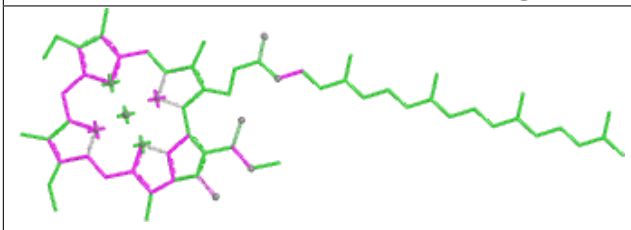


Rings

Ligand CLA B 1202



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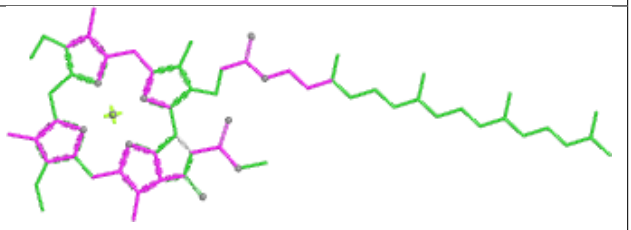

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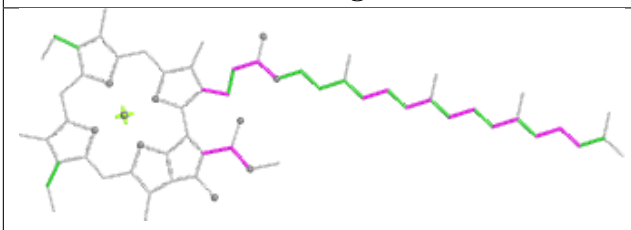

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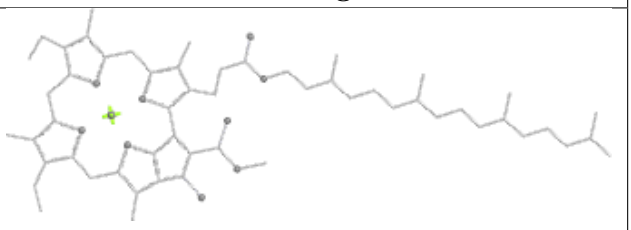
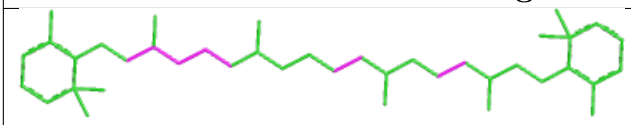


Rings

Ligand BCR L 4022



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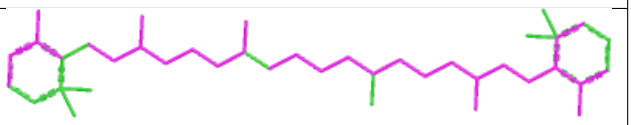

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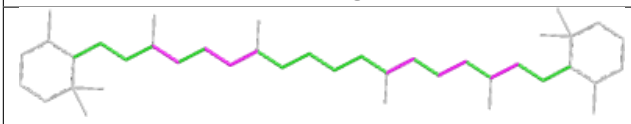

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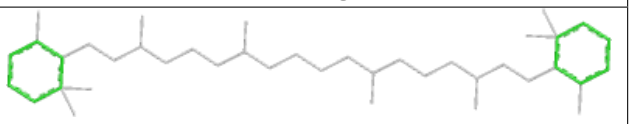
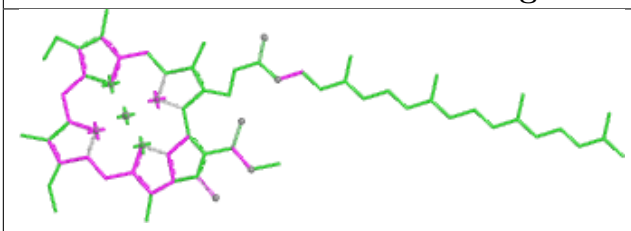


Rings

Ligand CLA a 1123



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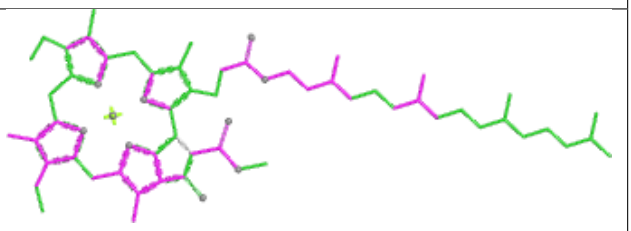

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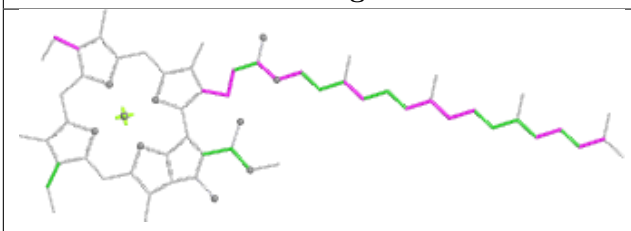

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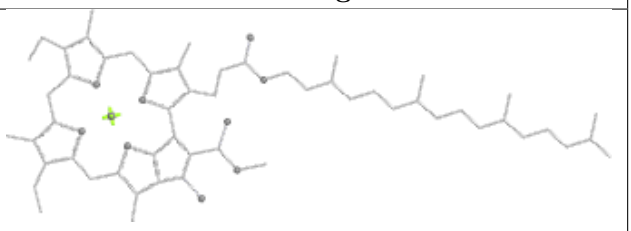
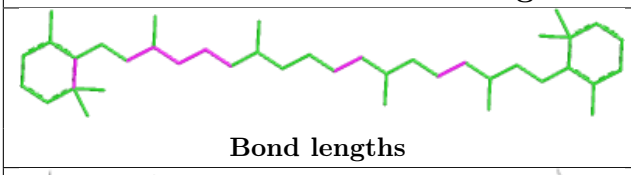


Rings

Ligand BCR b 4011



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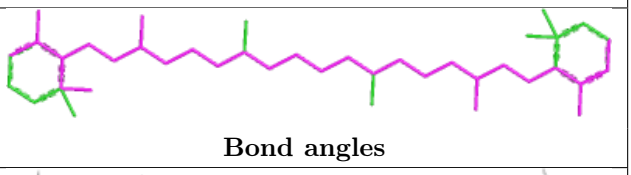

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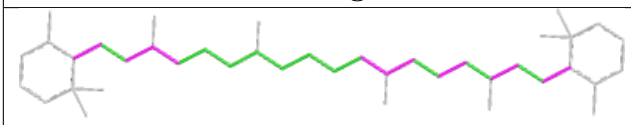

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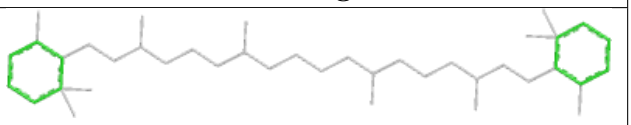
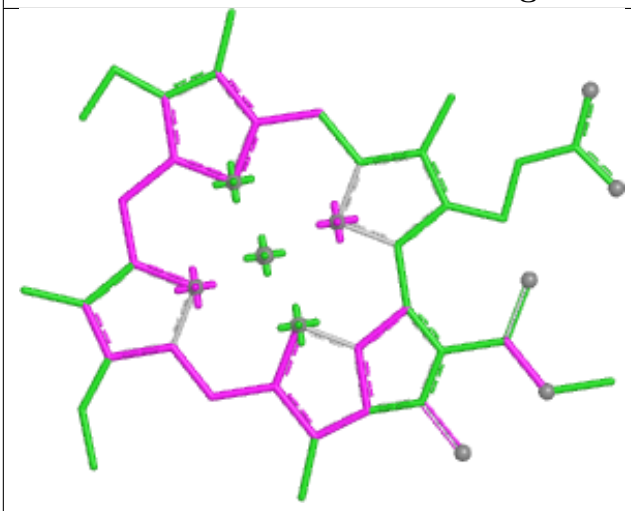


Rings

Ligand CLA a 1108



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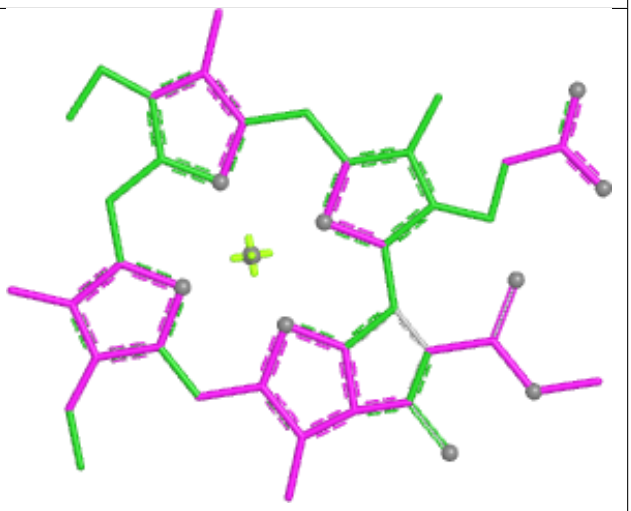

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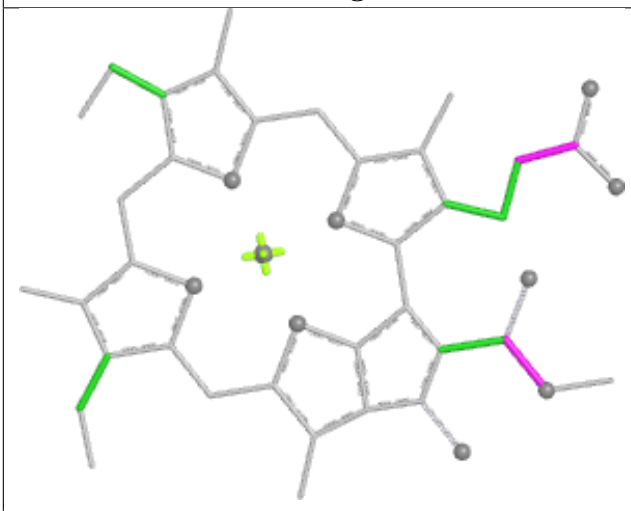
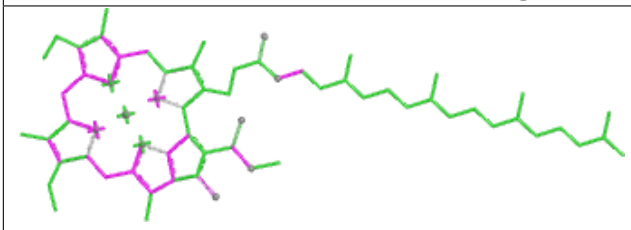


Torsions

Rings

Ligand CLA A 1022



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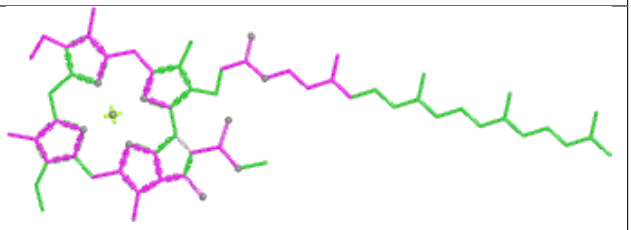

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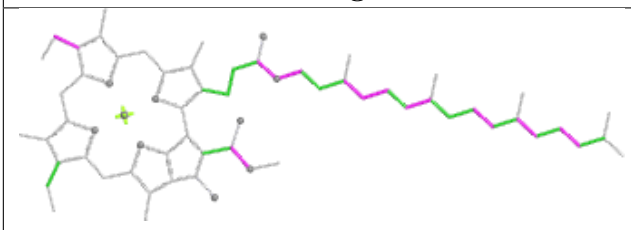

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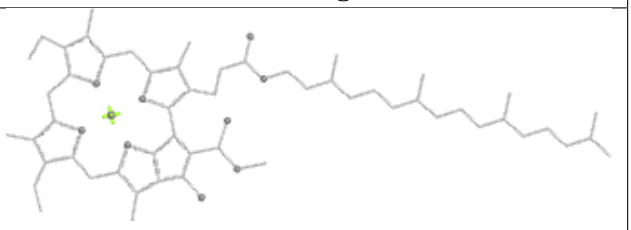
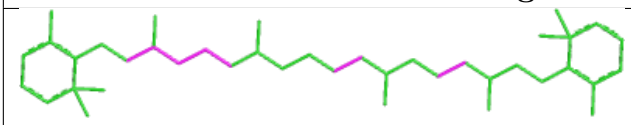


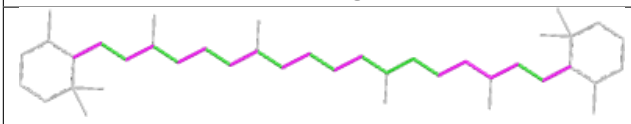
Rings

Ligand BCR 8 4019



Bond lengths

Bond angles



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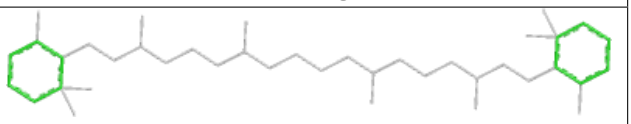
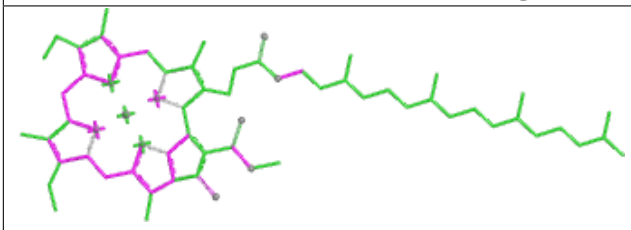


Rings

Ligand CLA A 1012



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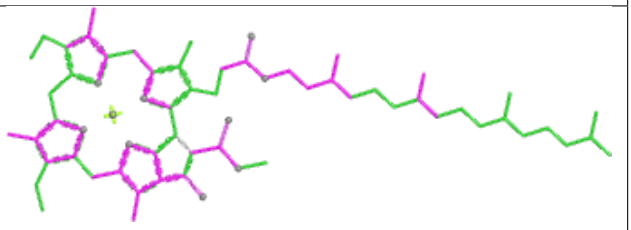
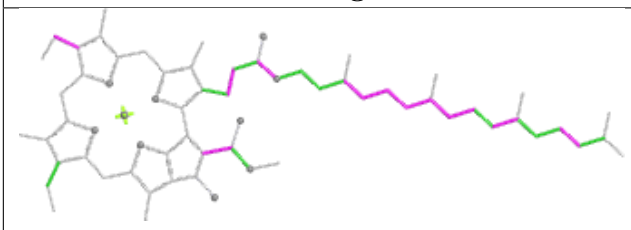


Bond angles



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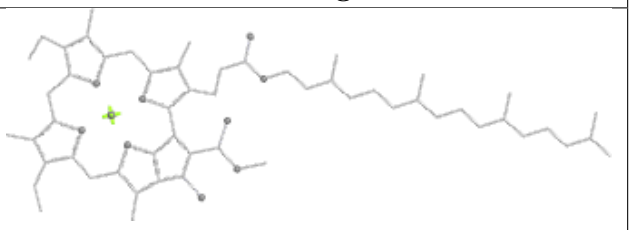
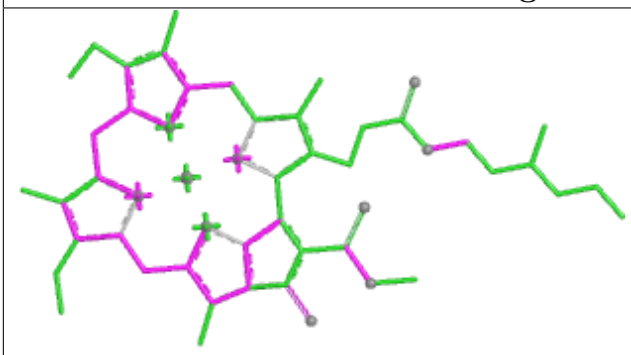


Rings

Ligand CLA 1 1801



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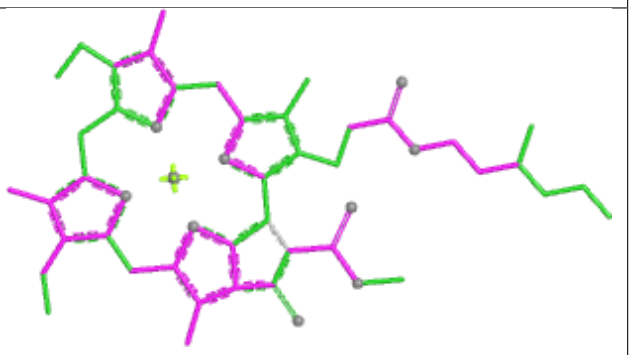
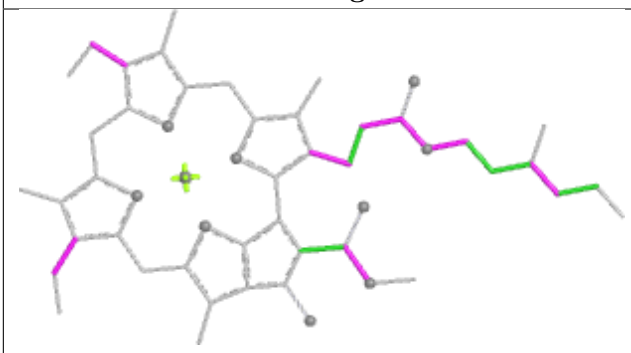


Bond angles



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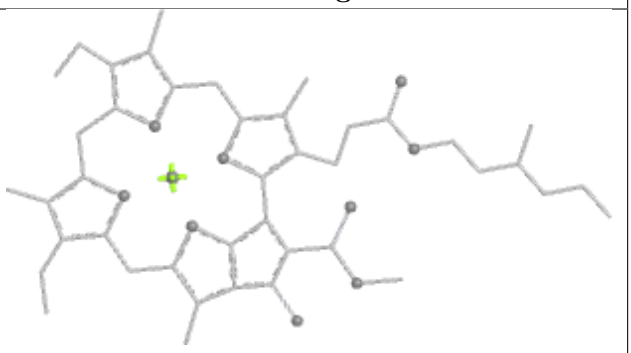
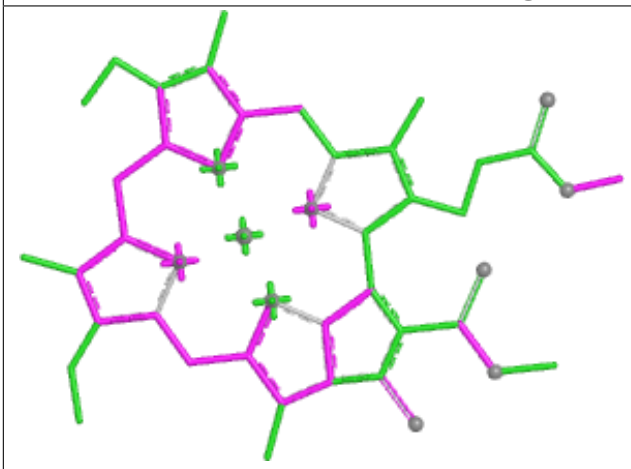


Rings

Ligand CLA a 1115



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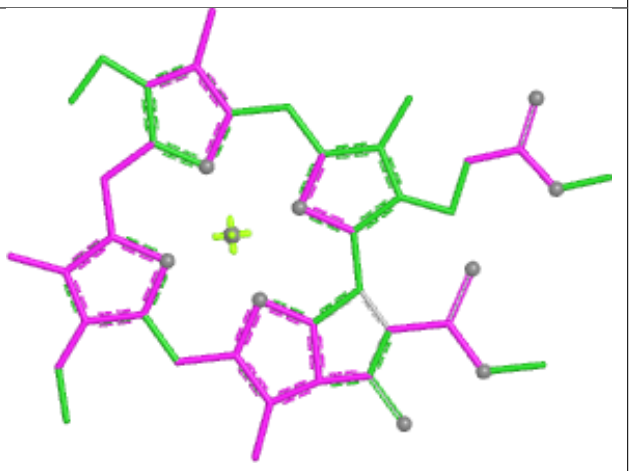
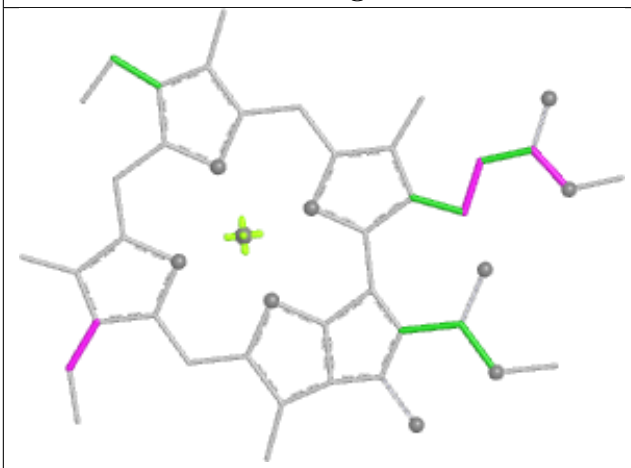


Bond angles



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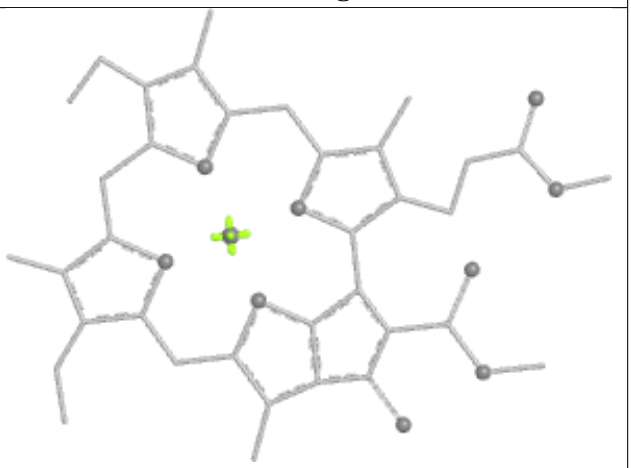
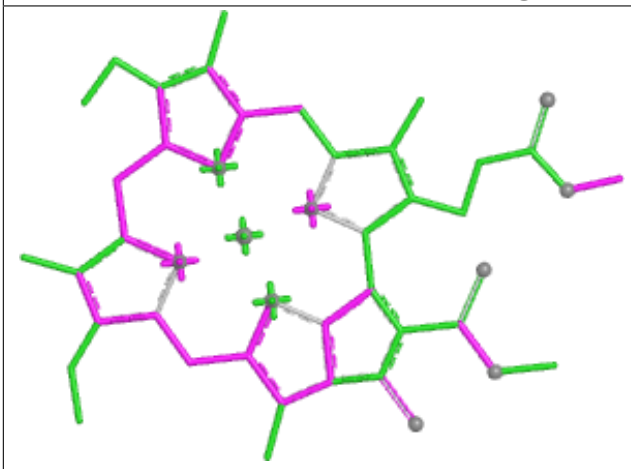


Rings

Ligand CLA B 1239



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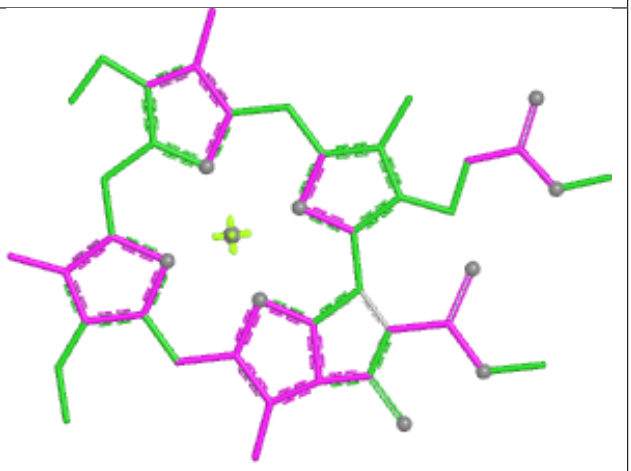
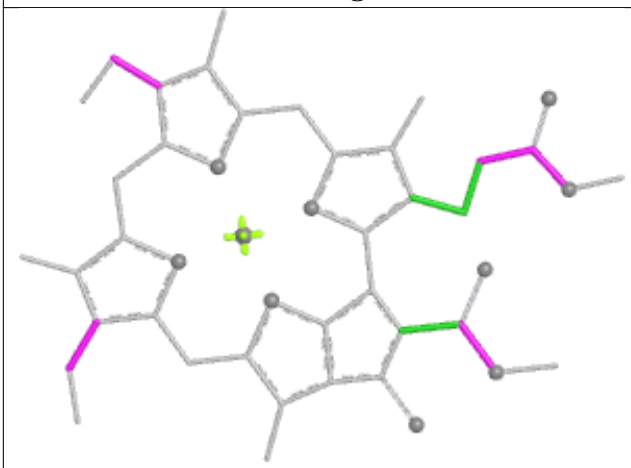
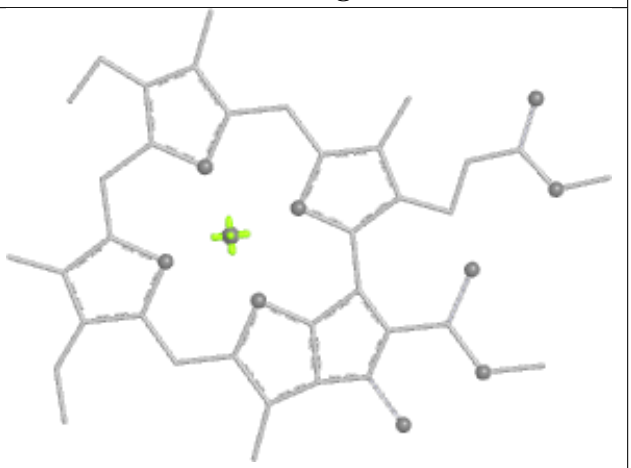


Bond angles

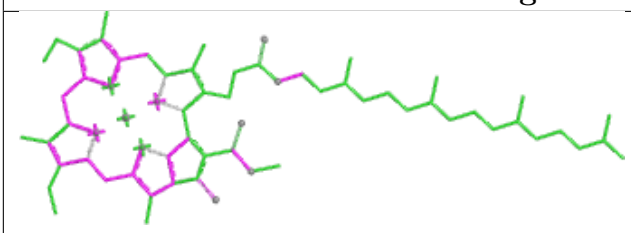


Torsions

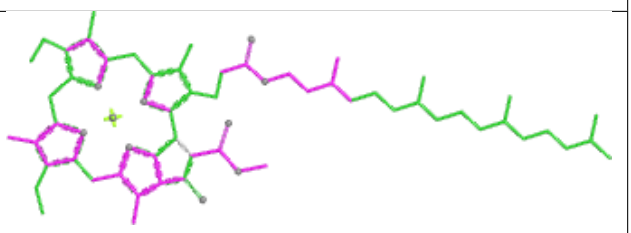


Rings

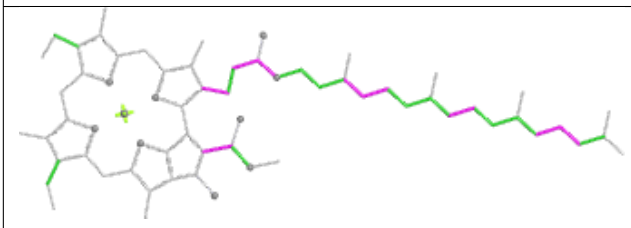
Ligand CLA 2 1202



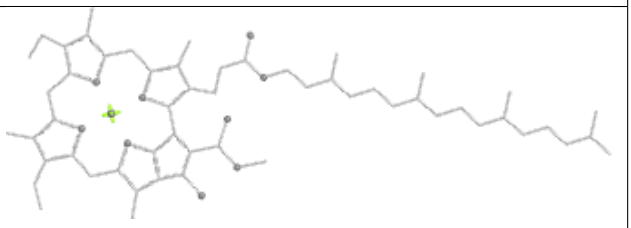
Bond lengths



Bond angles

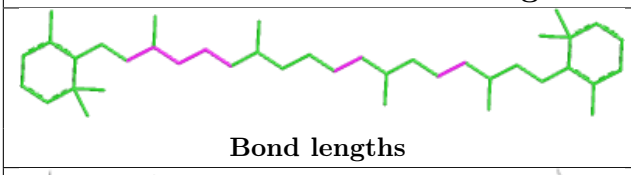


Torsions

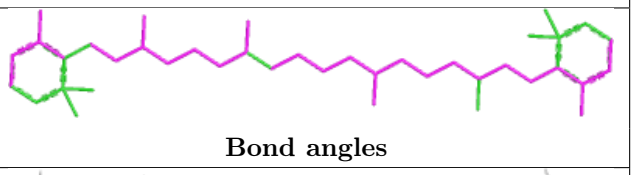


Rings

Ligand BCR f 4020



Bond lengths



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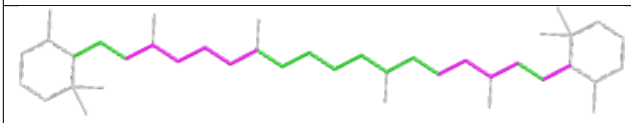

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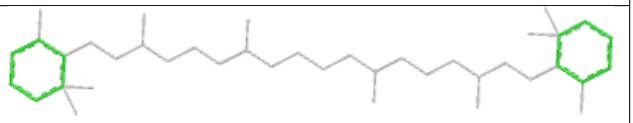
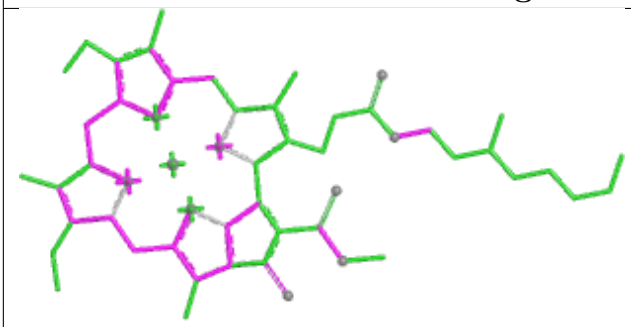
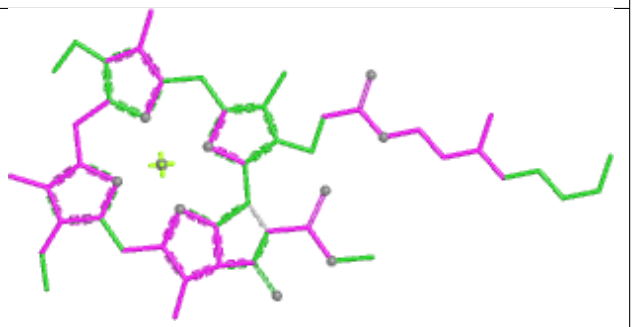


Rings

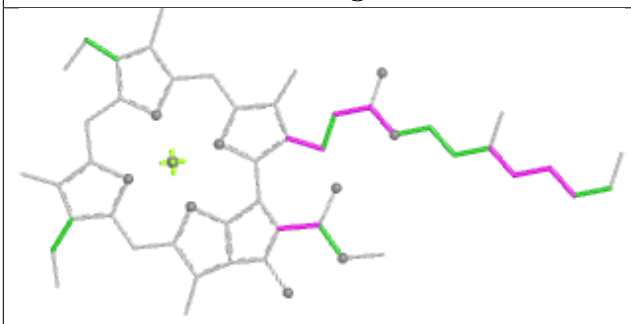
Ligand CLA A 1110



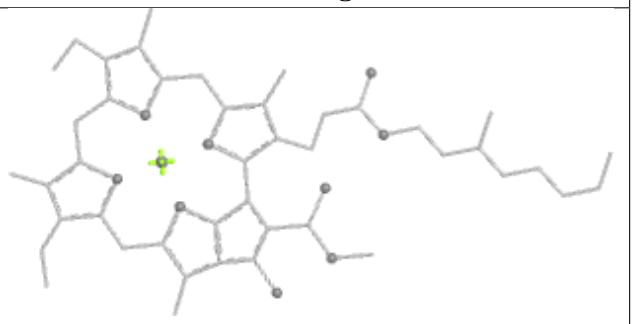
Bond lengths



Bond angles

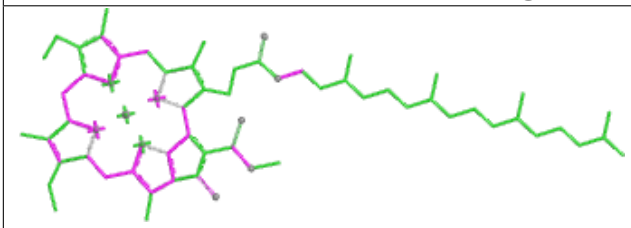


Torsions

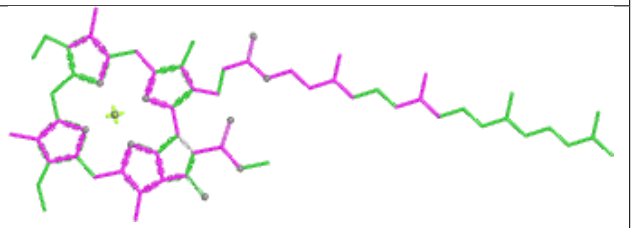


Rings

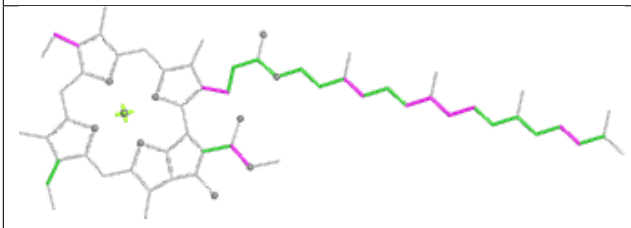
Ligand CLA a 1107



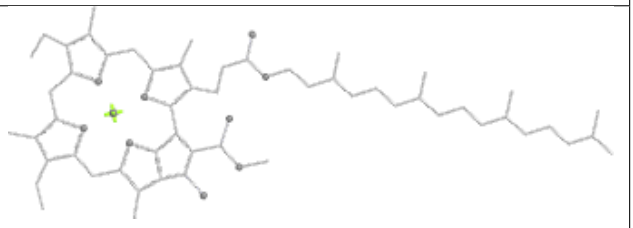
Bond lengths



Bond angles

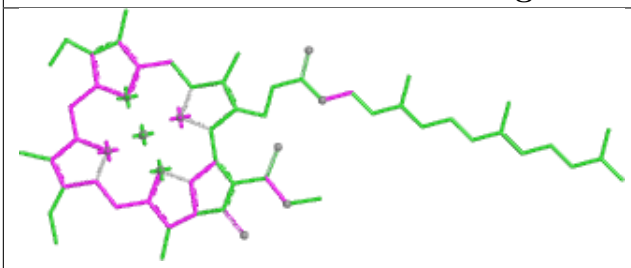


Torsions

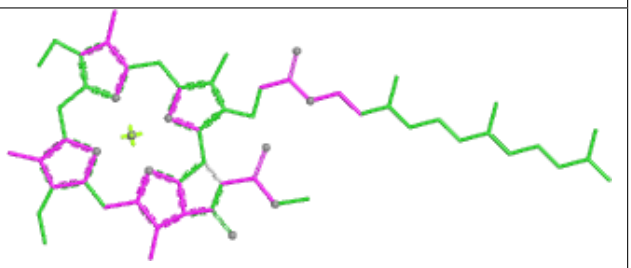


Rings

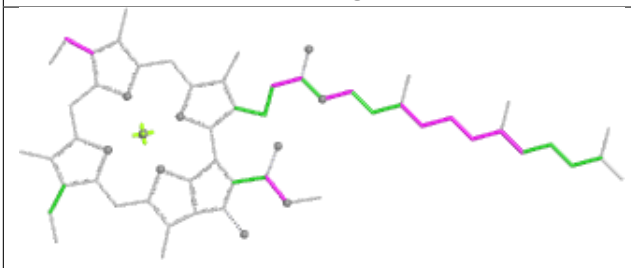
Ligand CLA B 1235



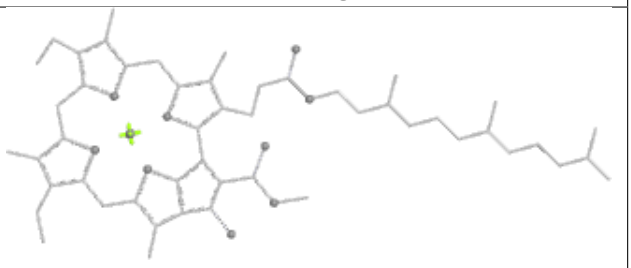
Bond lengths



Bond angles

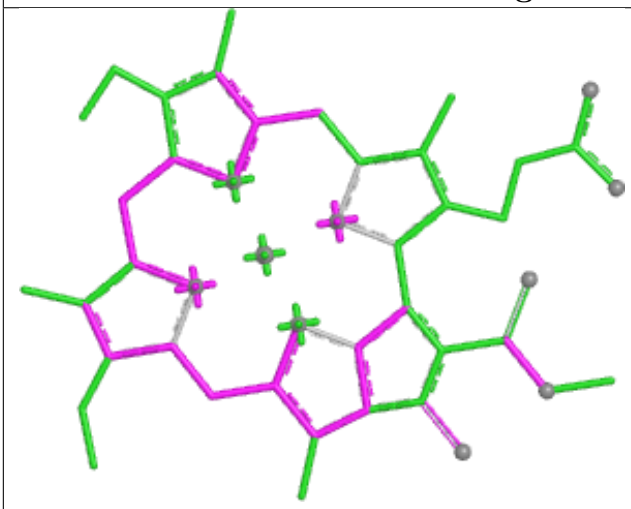


Torsions

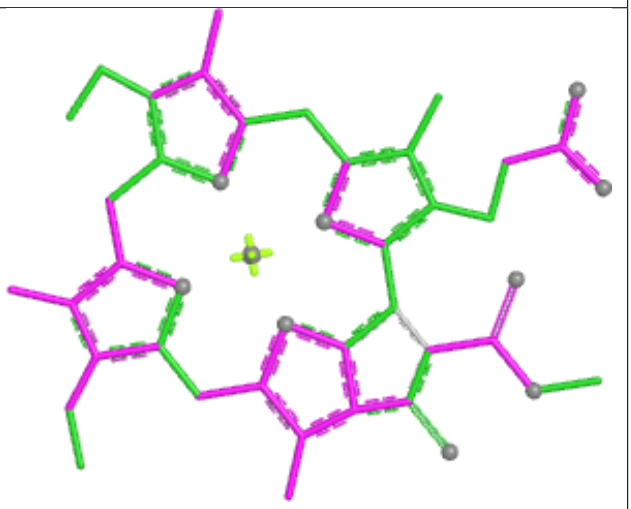


Rings

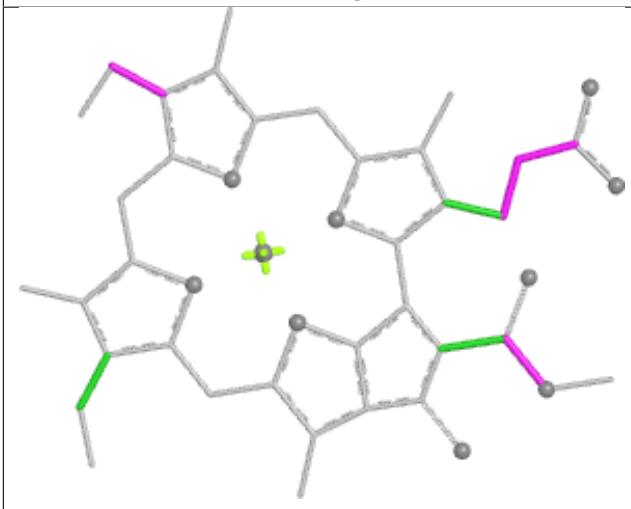
Ligand CLA B 1232



Bond lengths



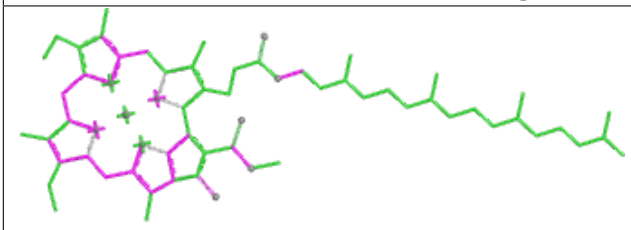
Bond angles



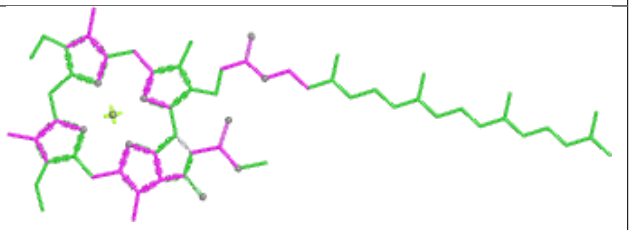
Torsions

Rings

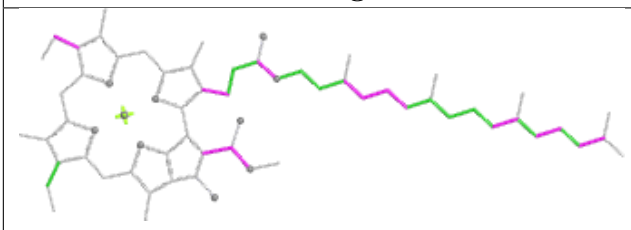
Ligand CLA A 1106



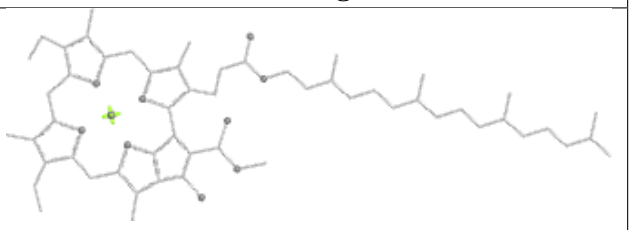
Bond lengths



Bond angles

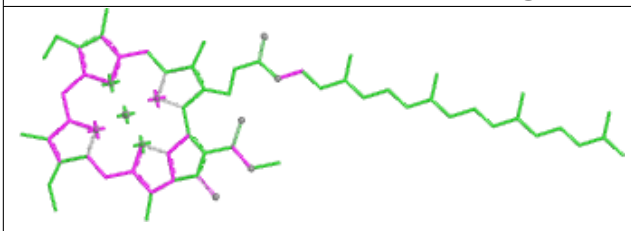


Torsions



Rings

Ligand CLA a 1104



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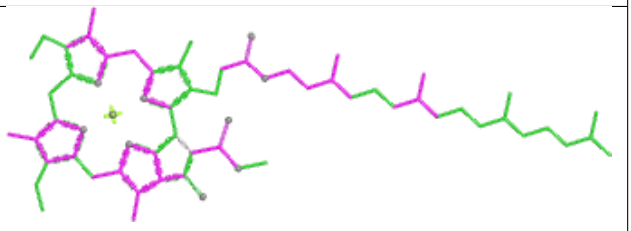
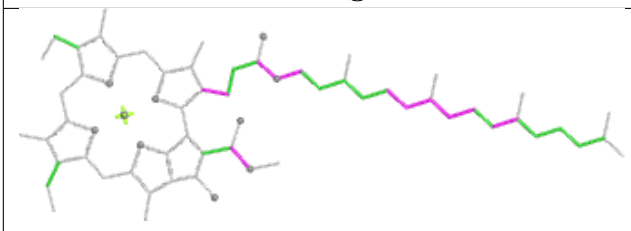
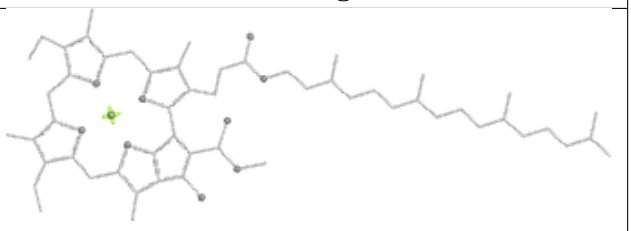


Bond angles

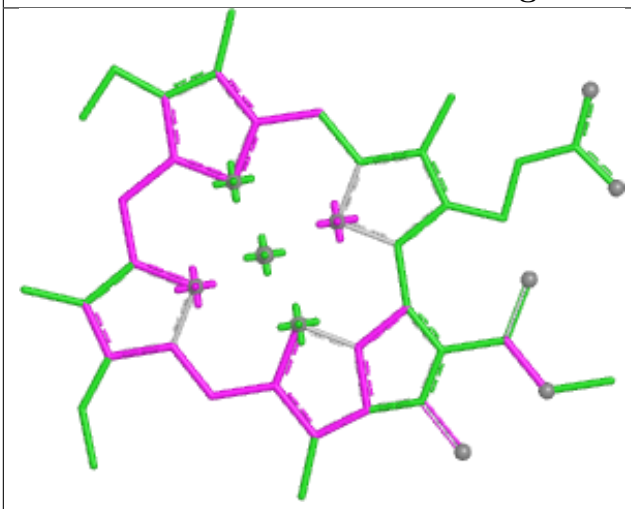


Torsions

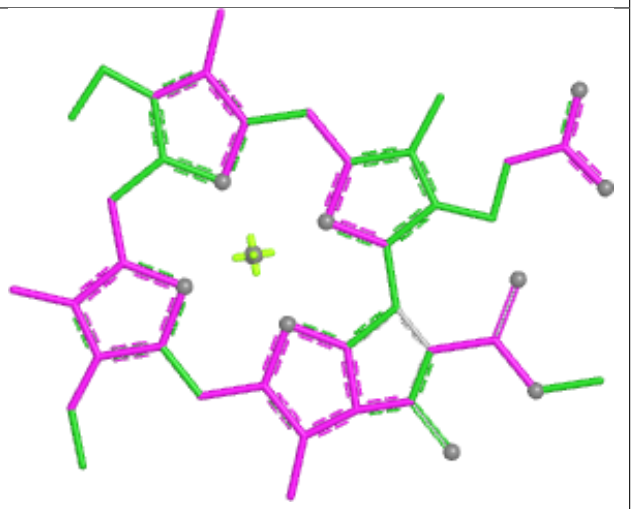


Rings

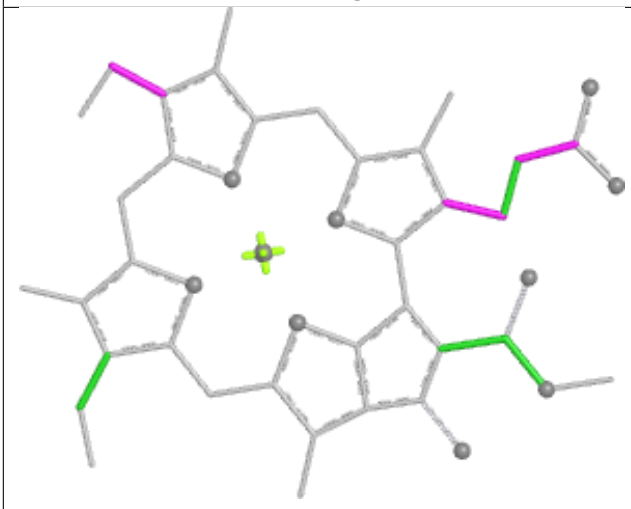
Ligand CLA 2 1209



Bond lengths



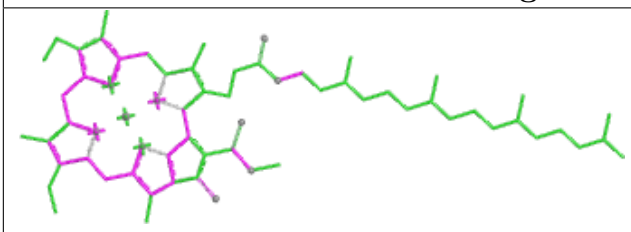
Bond angles



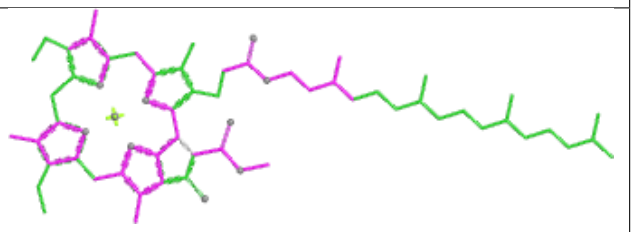
Torsions

Rings

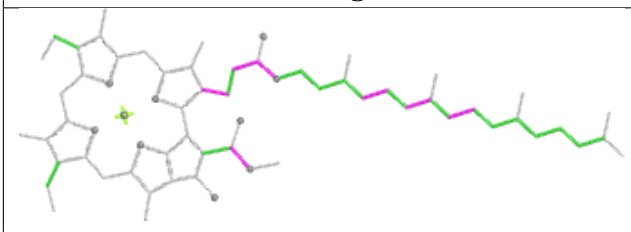
Ligand CLA a 1011



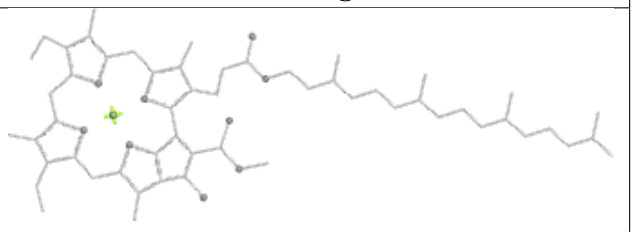
Bond lengths



Bond angles

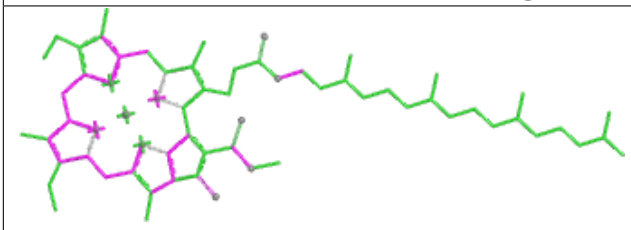


Torsions



Rings

Ligand CLA 1 1012



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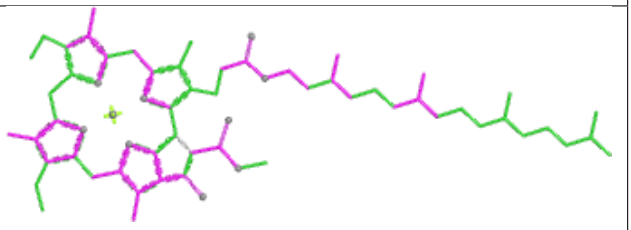
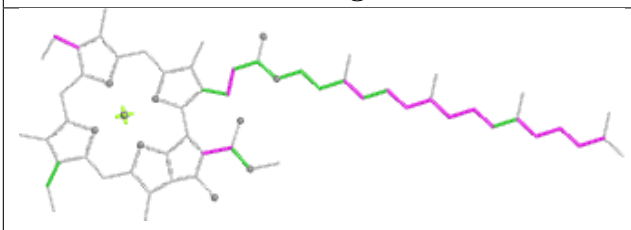
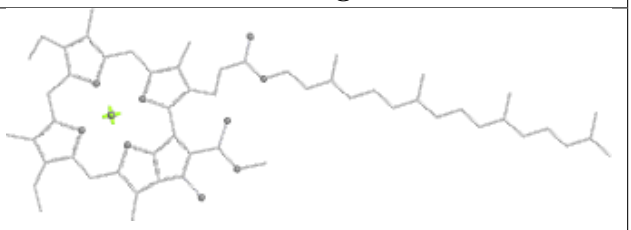


Bond angles

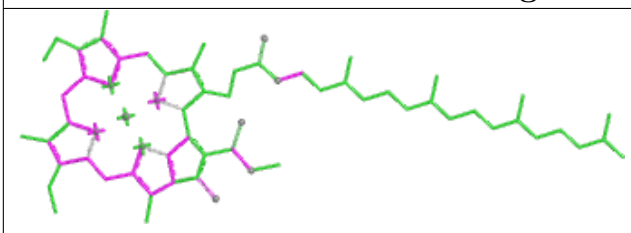


Torsions



Rings

Ligand CLA a 1109



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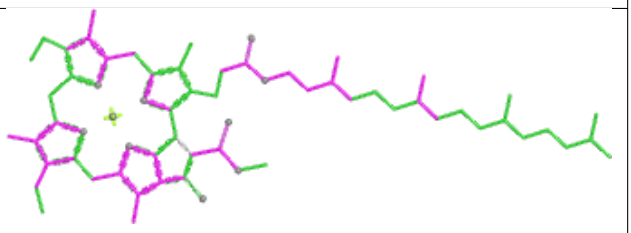
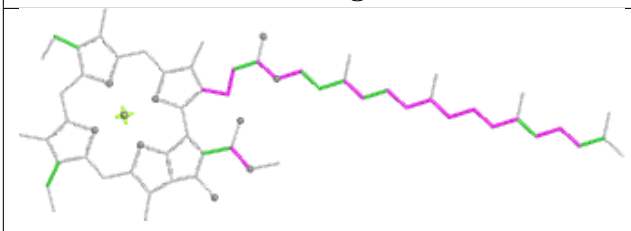


Bond angles



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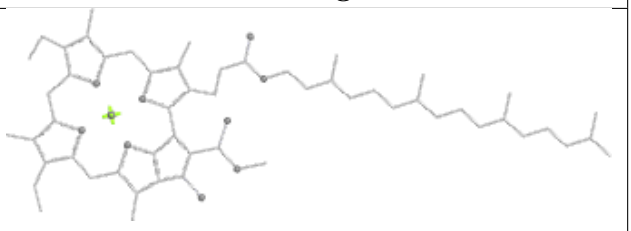
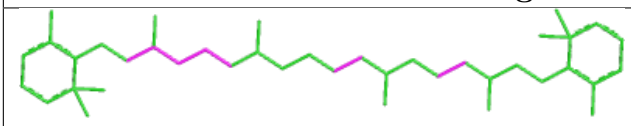
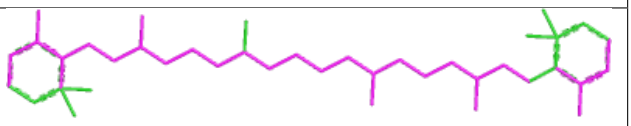


Rings

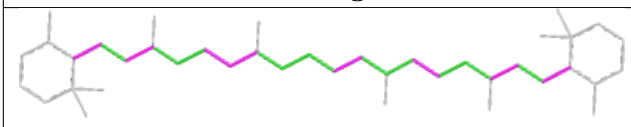
Ligand BCR L 4019



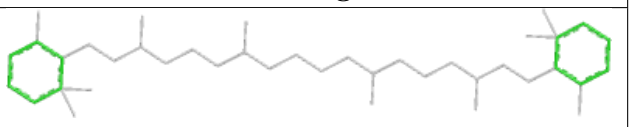
Bond lengths



Bond angles

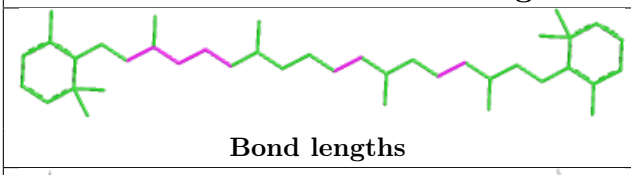


Torsions

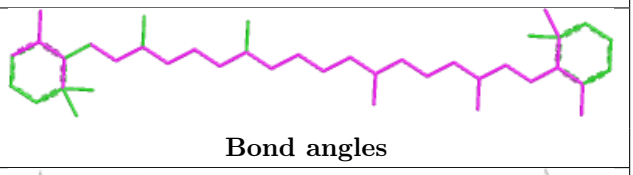


Rings

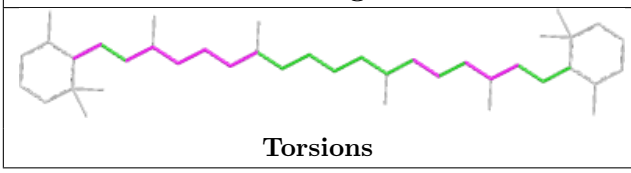
Ligand BCR F 4013



Bond lengths



Bond angles



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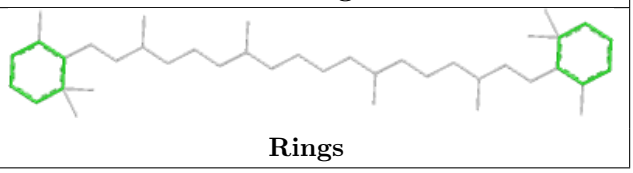
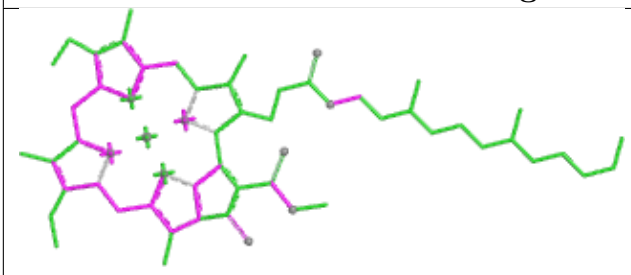
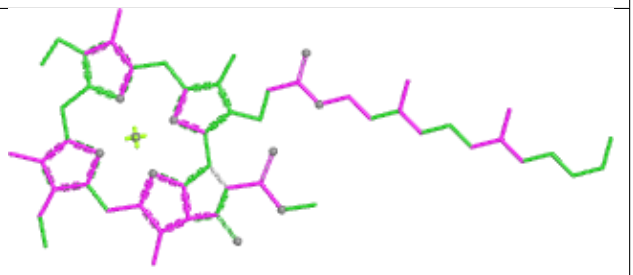


Rings

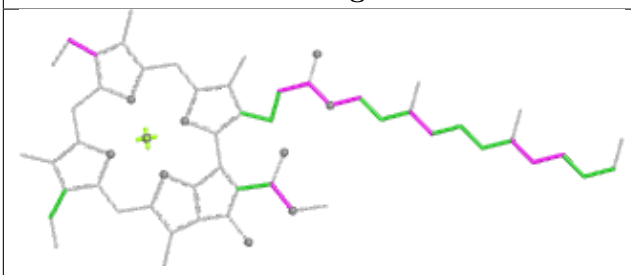
Ligand CLA a 1122



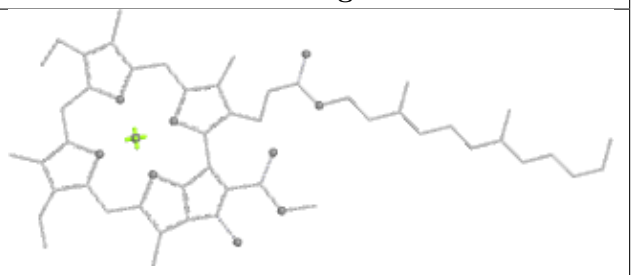
Bond lengths



Bond angles

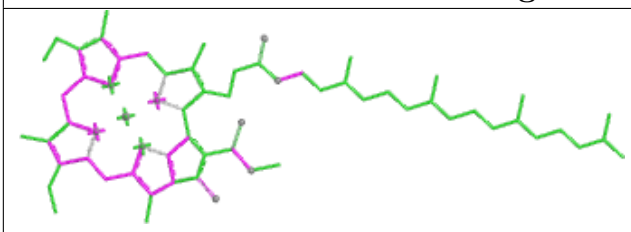


Torsions



Rings

Ligand CLA b 1204



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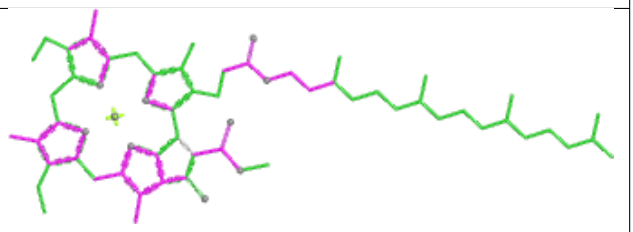
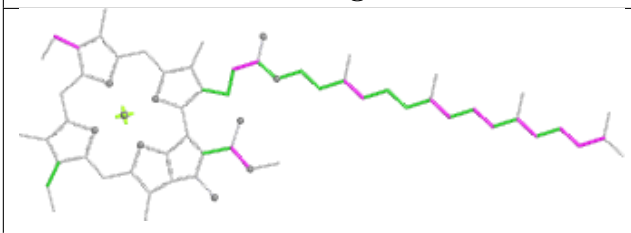


Bond angles



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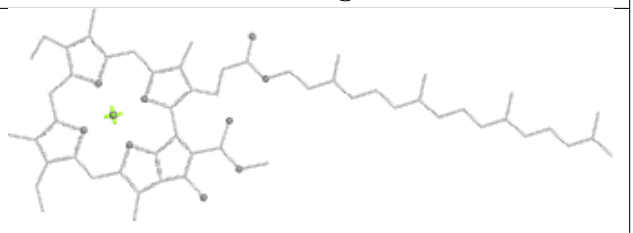
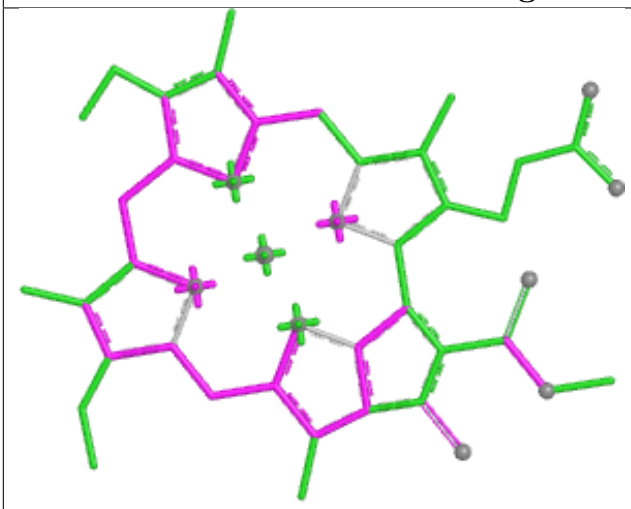


Rings

Ligand CLA b 1209



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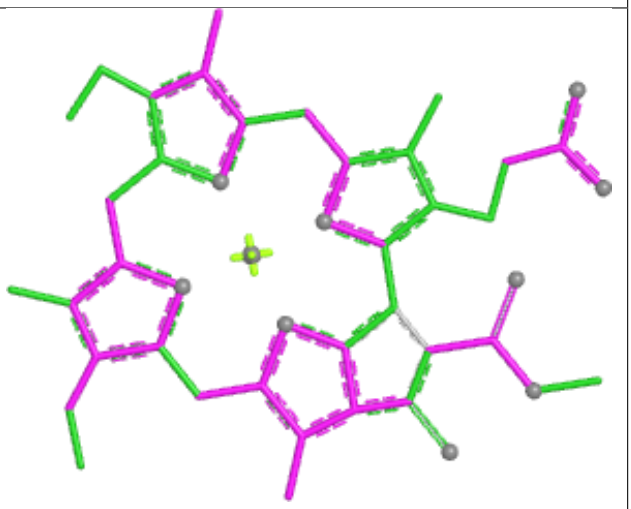
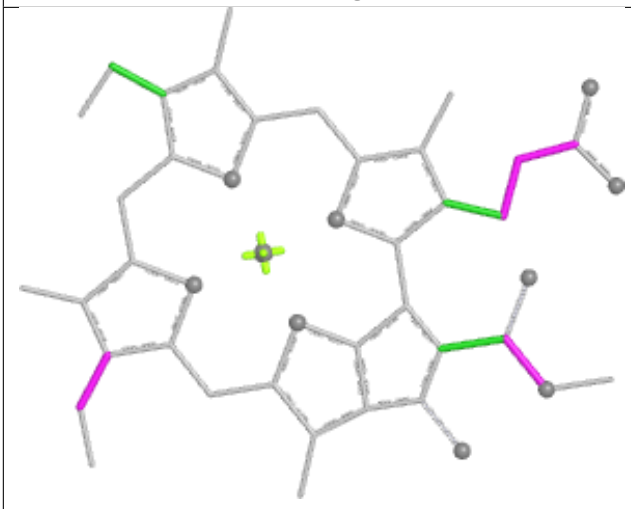


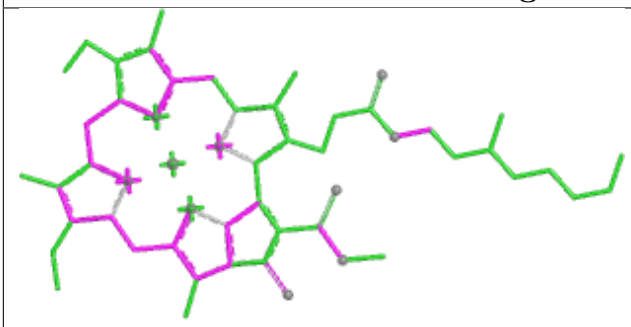
Bond angles



Torsions

Rings

Ligand CLA 2 1201



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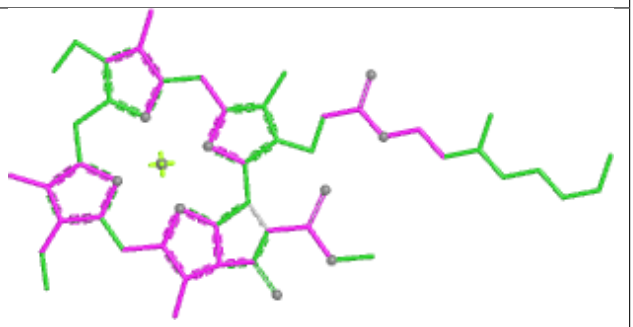
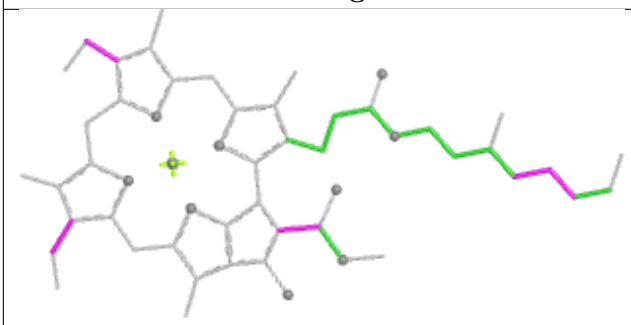
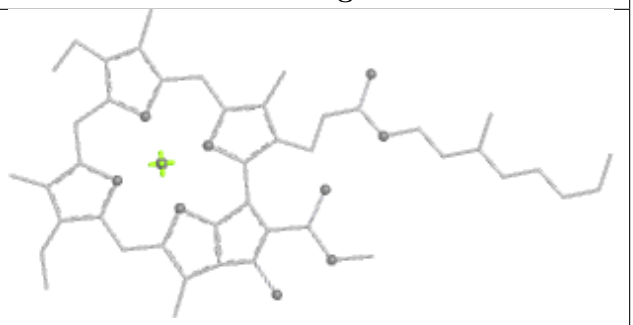


Bond angles

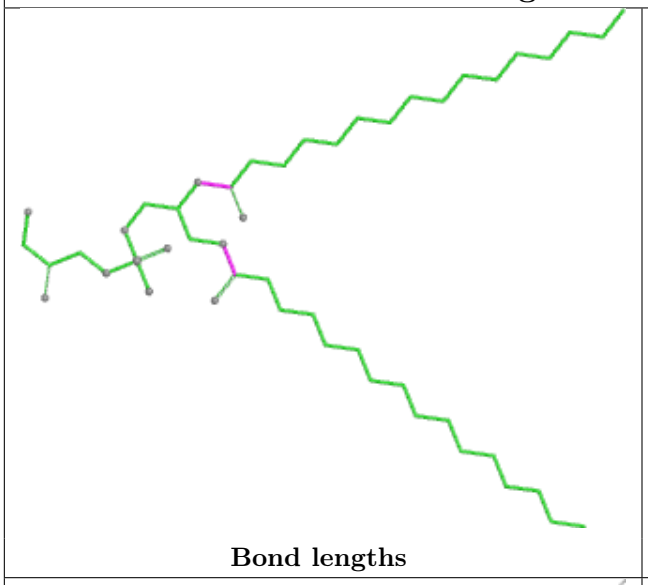


Torsions

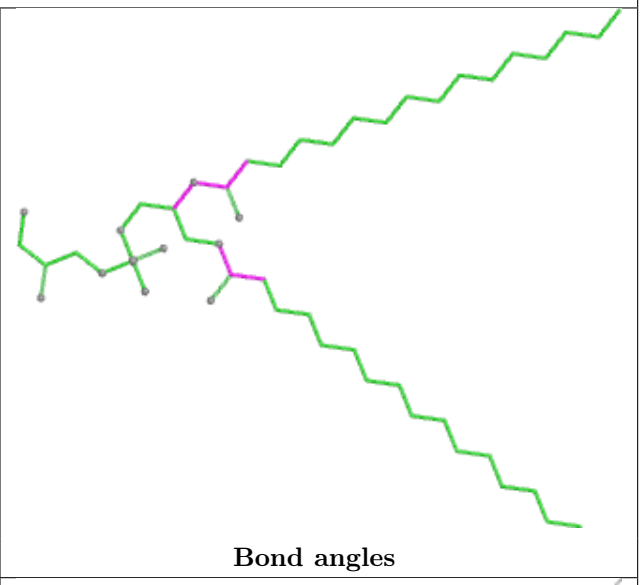


Rings

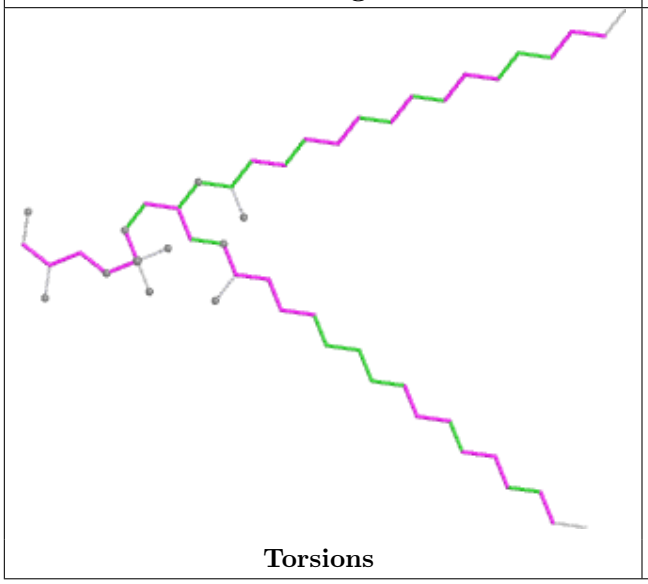
Ligand LHG 1 5003



Bond lengths



Bond angles



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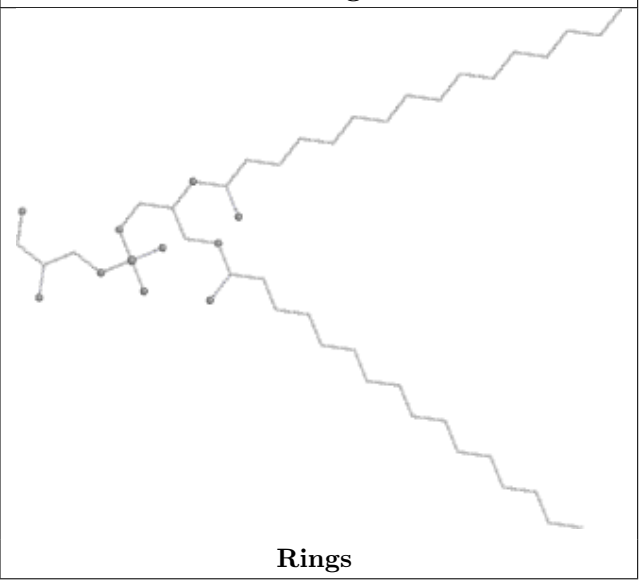
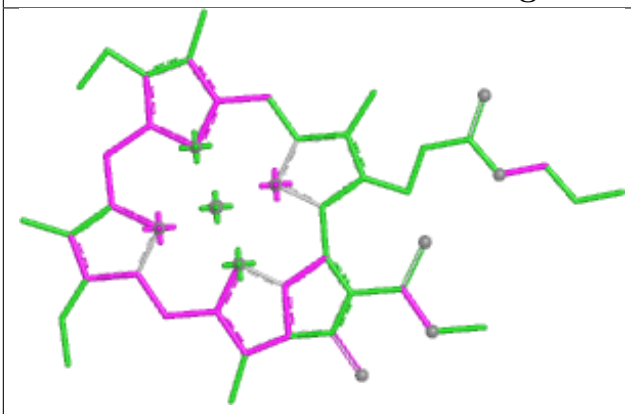


Rings

Ligand CLA 1 1105



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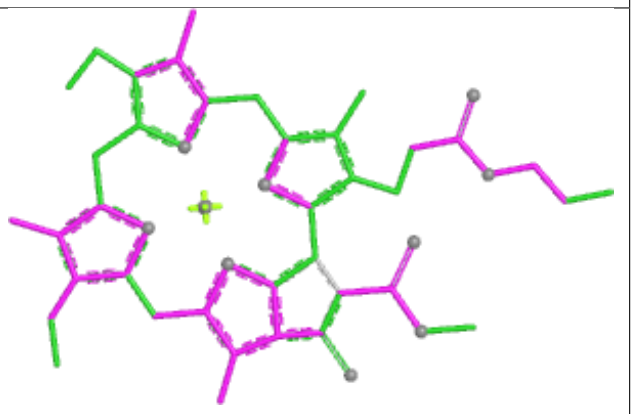
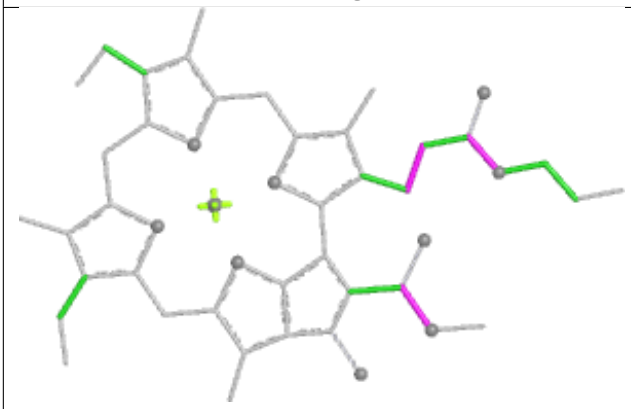


Bond angles



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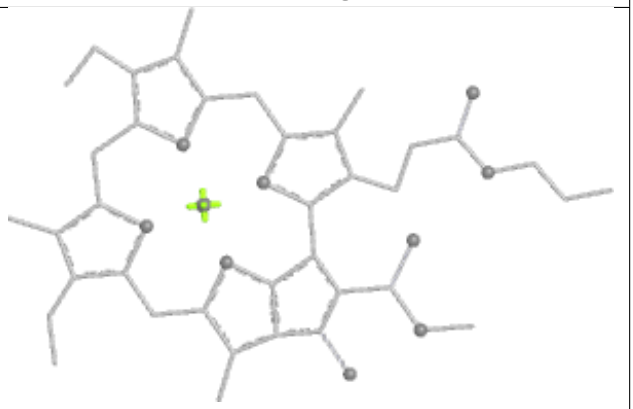
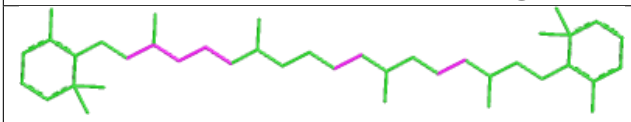
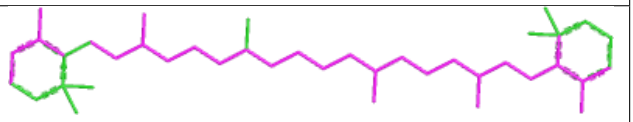


Rings

Ligand BCR A 4003

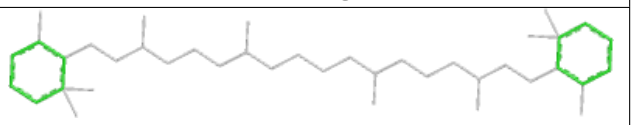


Bond lengths



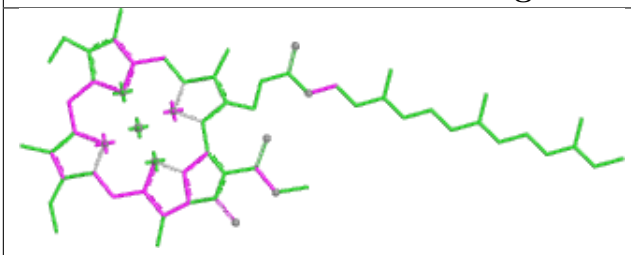
Bond angles

Torsions

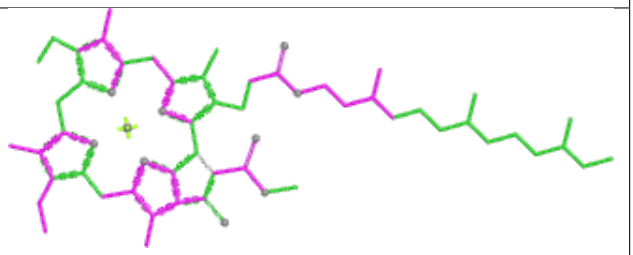


Rings

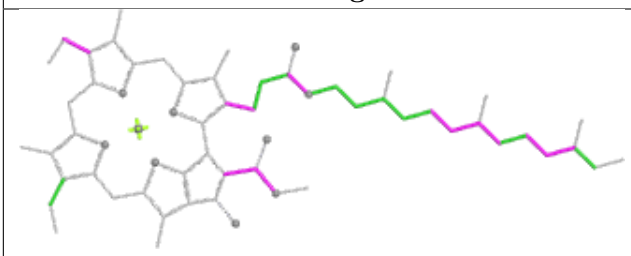
Ligand CLA A 1118



Bond lengths



Bond angles



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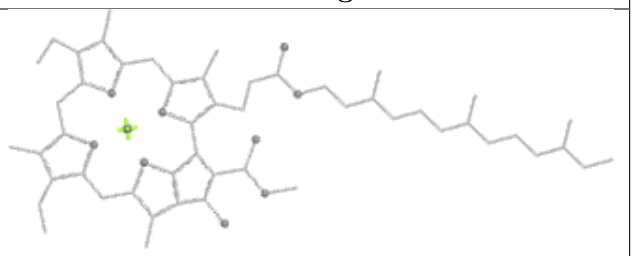
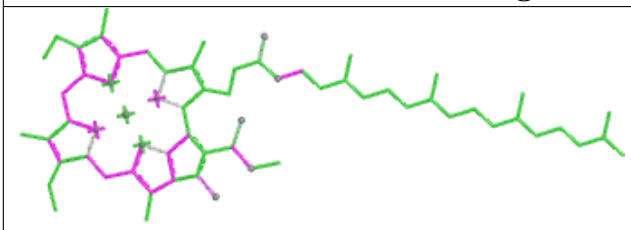


Rings

Ligand CLA B 1203



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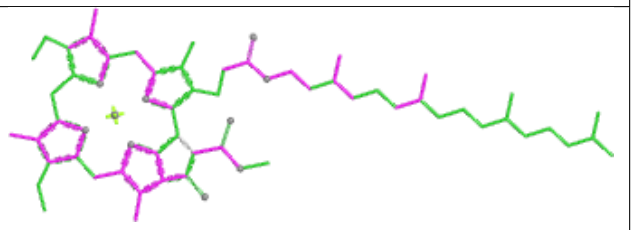
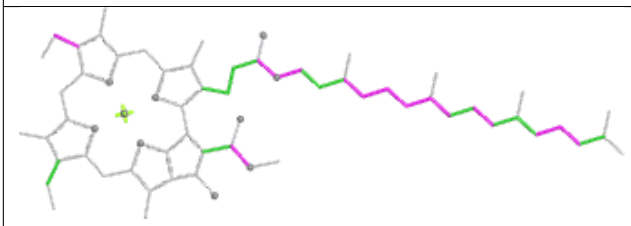


Bond angles



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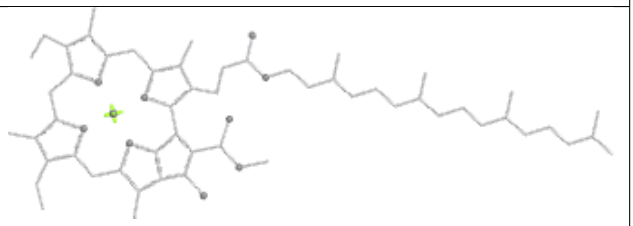
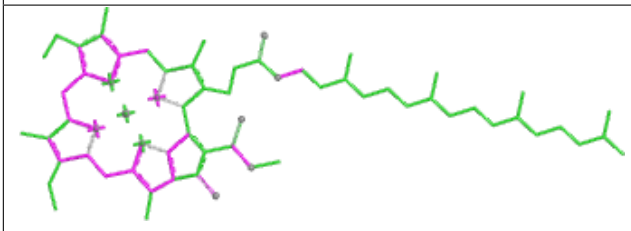
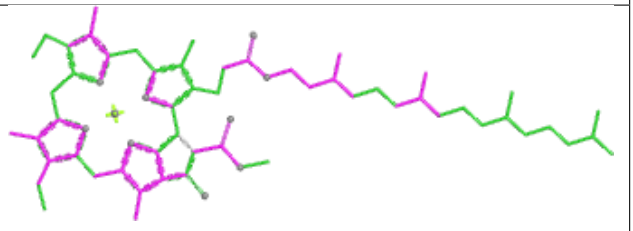


Rings

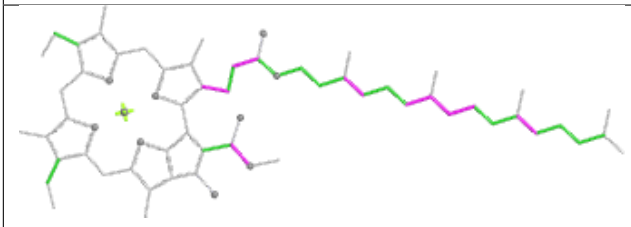
Ligand CLA b 1215



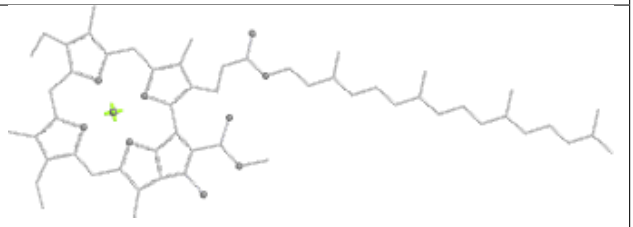
Bond lengths



Bond angles

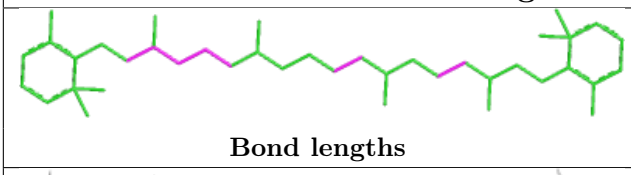


Torsions



Rings

Ligand BCR a 4001



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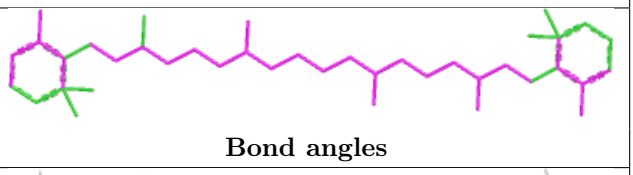
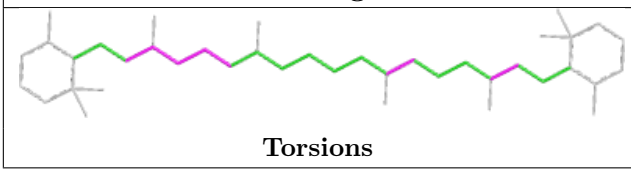


Bond angles



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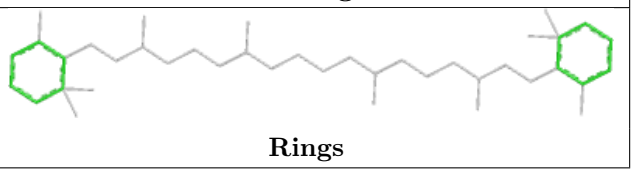
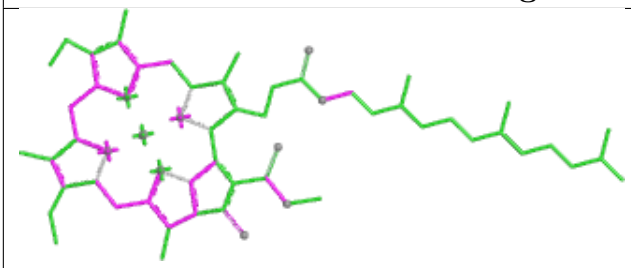


Rings

Ligand CLA 1 1111



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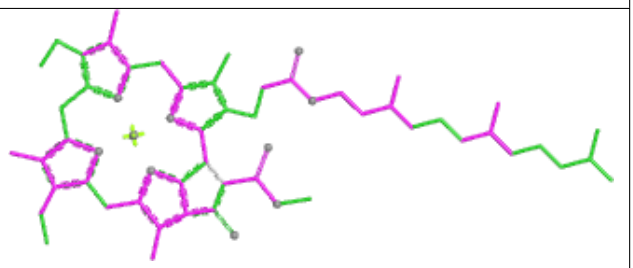
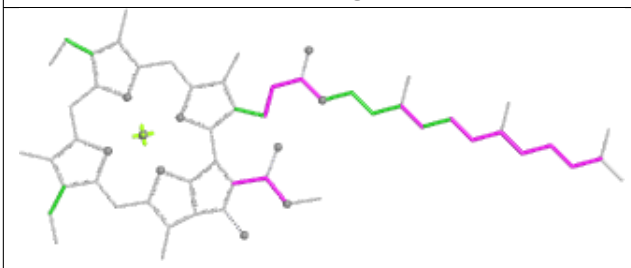
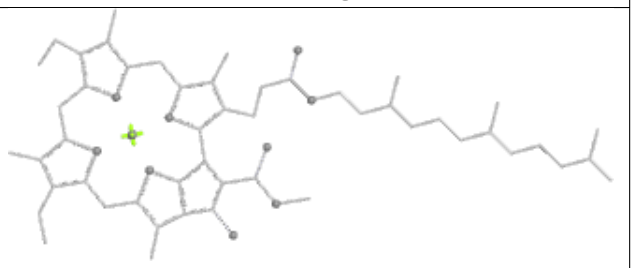


Bond angles

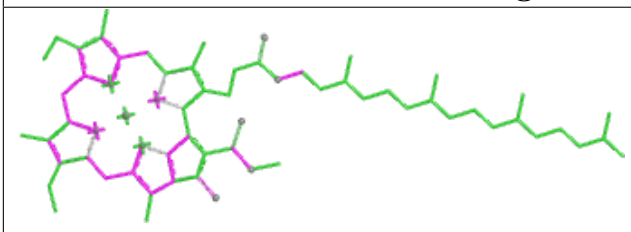


Torsions

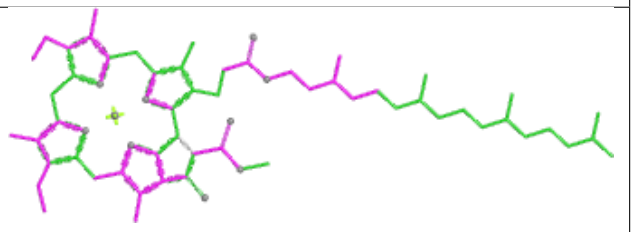


Rings

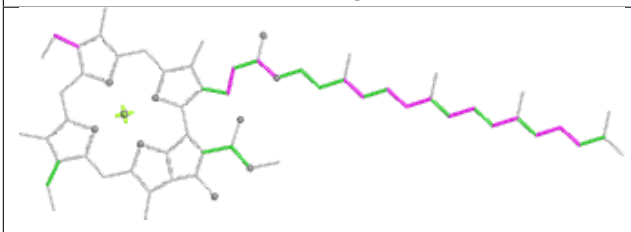
Ligand CLA B 1204



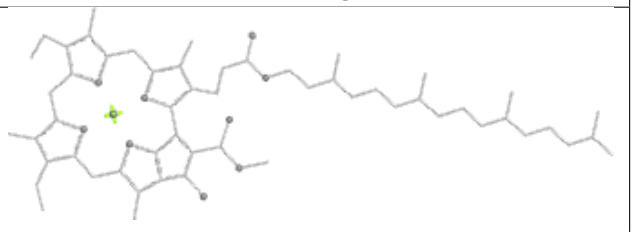
Bond lengths



Bond angles

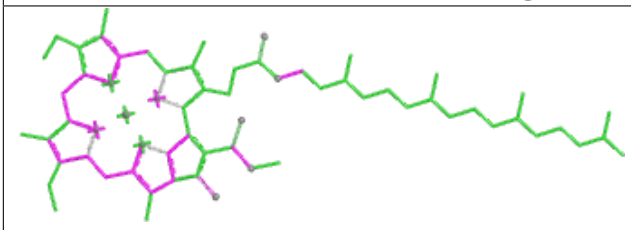


Torsions

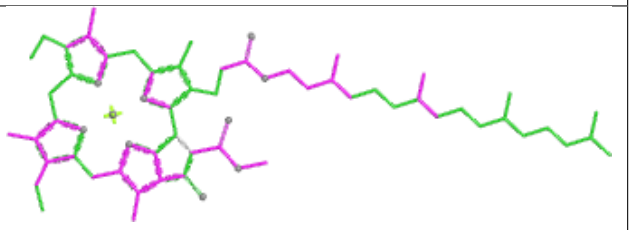


Rings

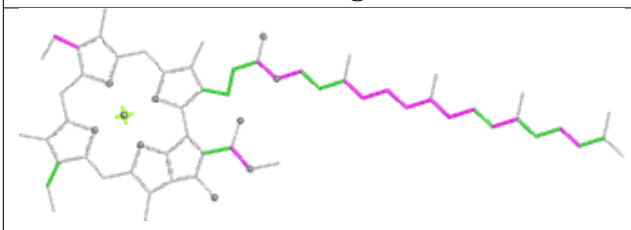
Ligand CLA 1 1109



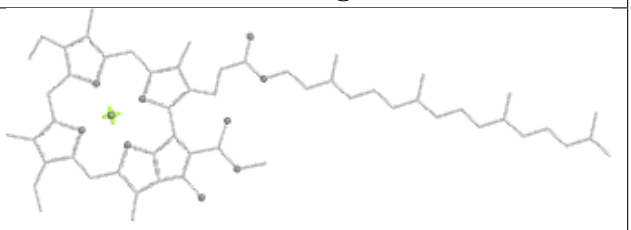
Bond lengths



Bond angles

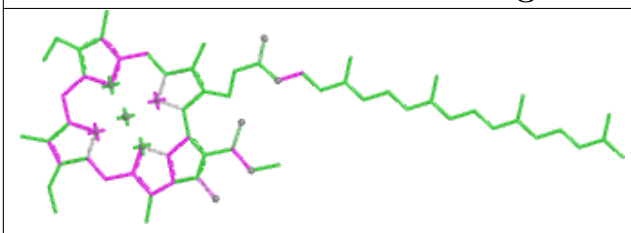


Torsions

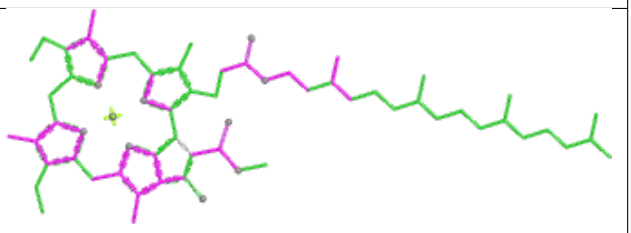


Rings

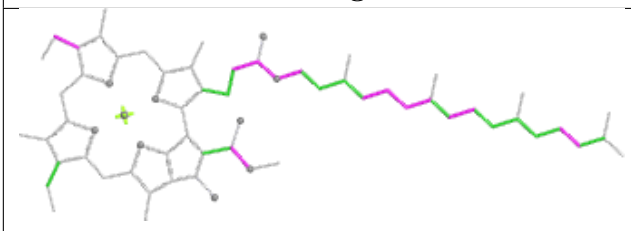
Ligand CLA L 1503



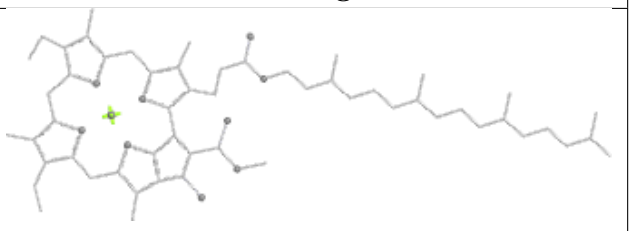
Bond lengths



Bond angles

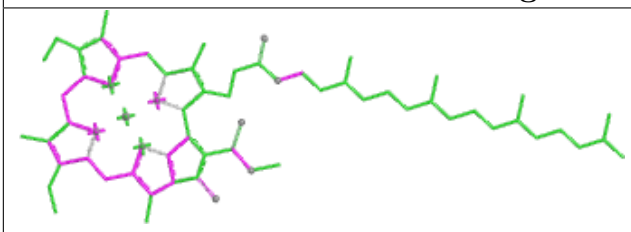


Torsions

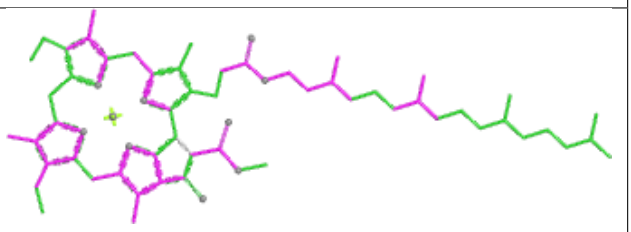


Rings

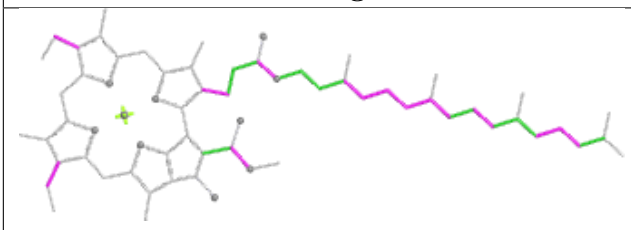
Ligand CLA a 1131



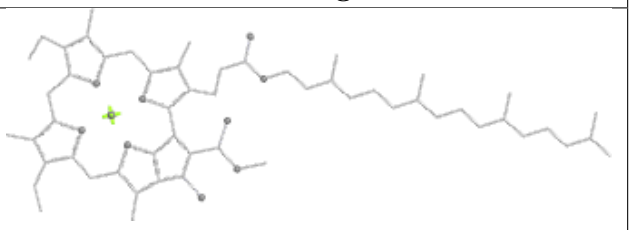
Bond lengths



Bond angles

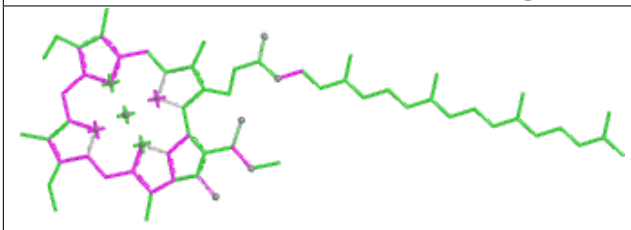


Torsions

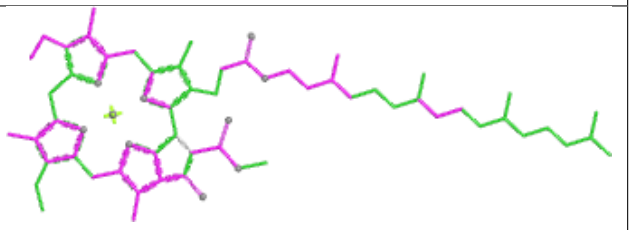


Rings

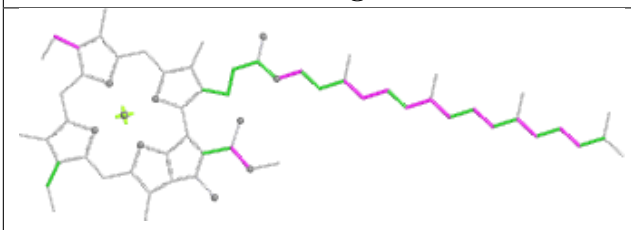
Ligand CLA 1 1022



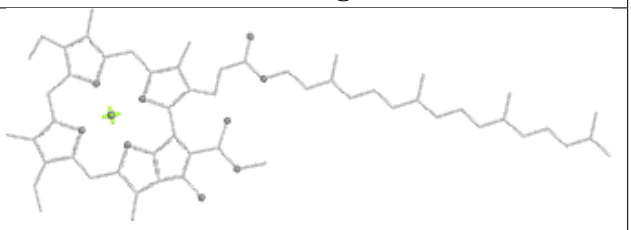
Bond lengths



Bond angles

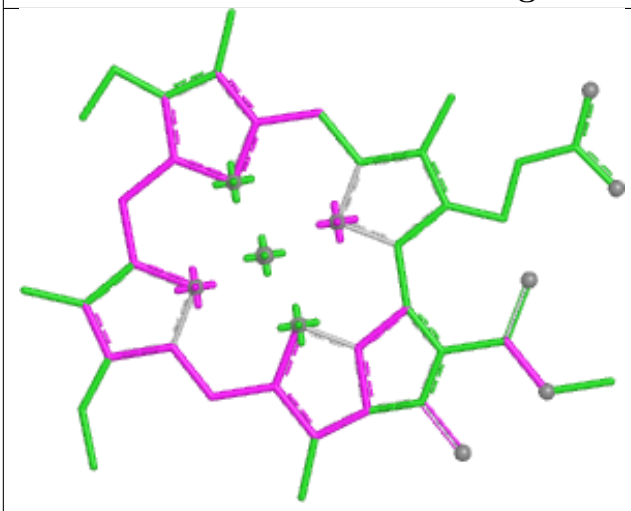


Torsions



Rings

Ligand CLA b 1218



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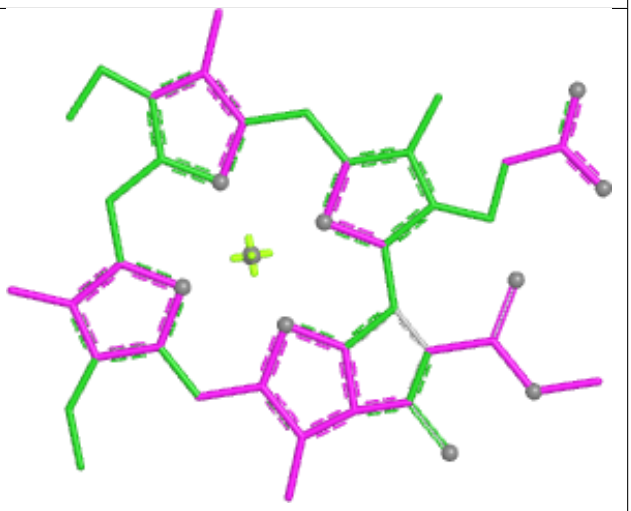
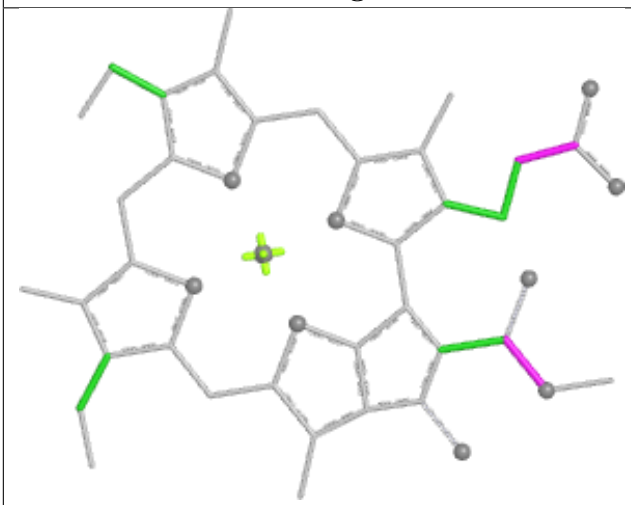


Bond angles



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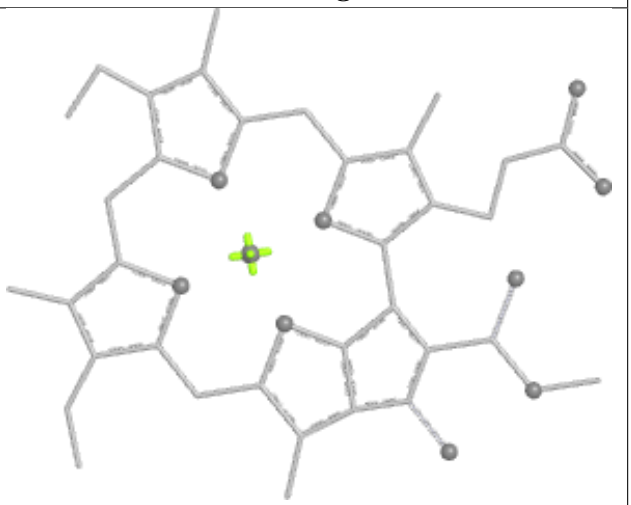
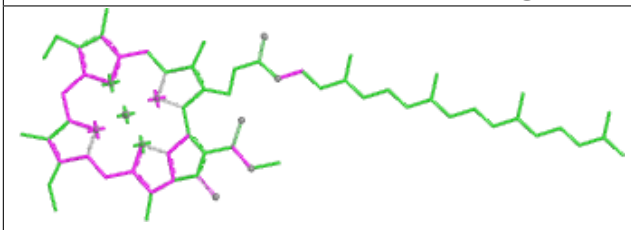
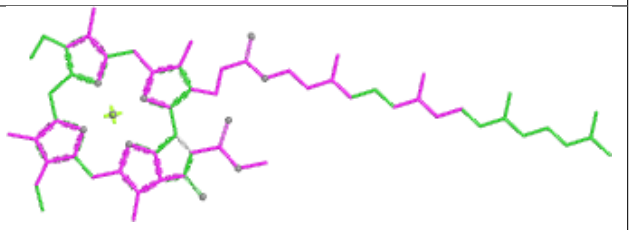


Rings

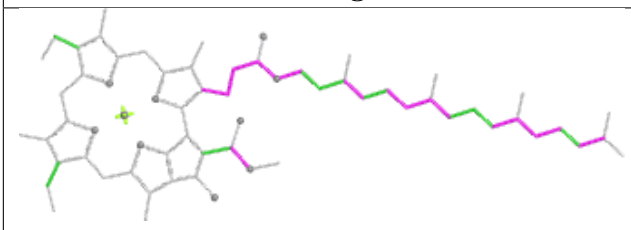
Ligand CLA b 1021



Bond lengths



Bond angles



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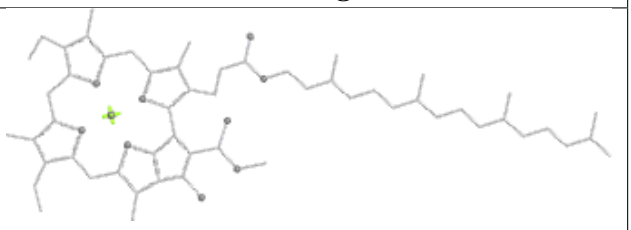
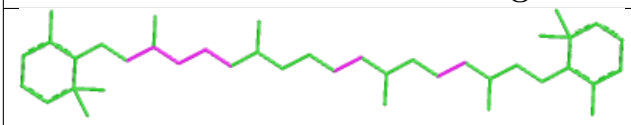


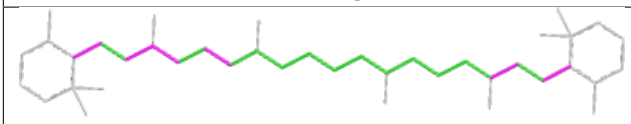
Rings

Ligand BCR m 4021



Bond lengths

Bond angles



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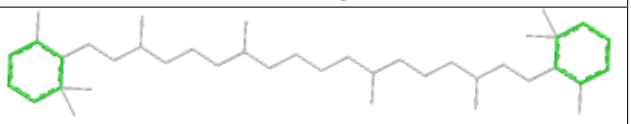
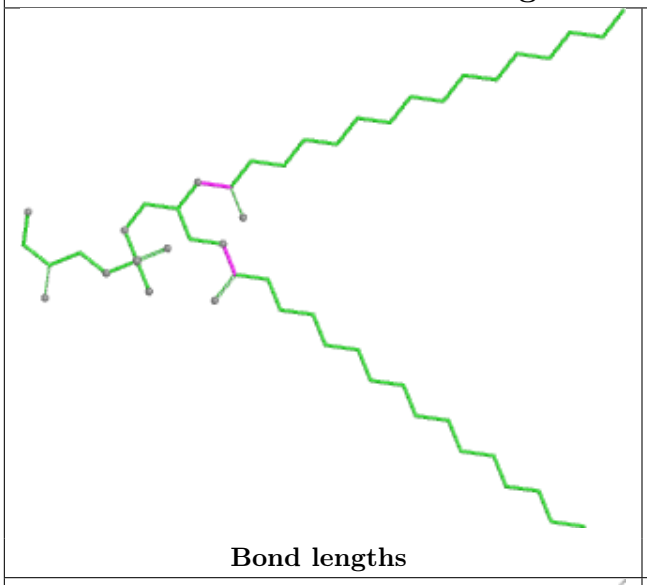
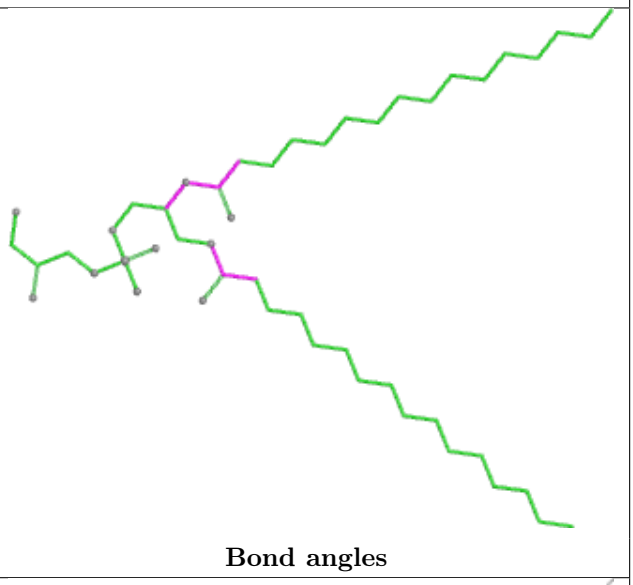


Rings

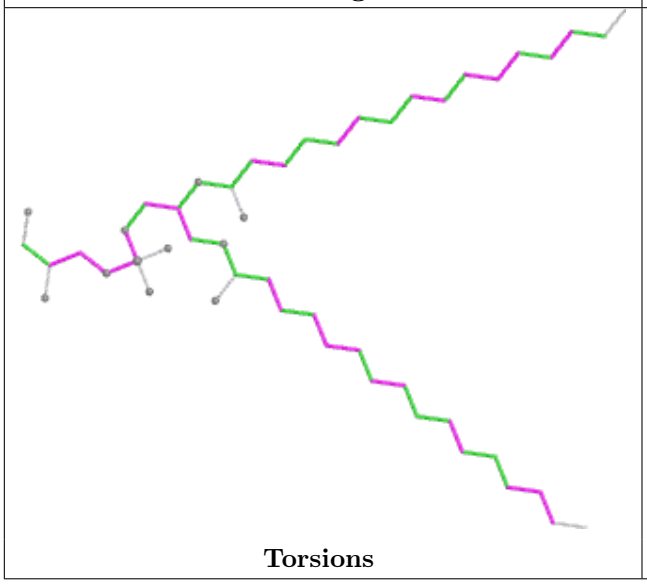
Ligand LHG a 5003



Bond lengths



Bond angles



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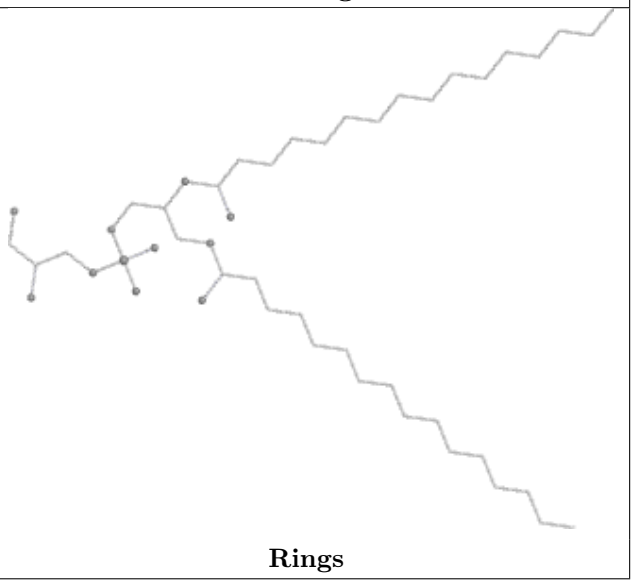
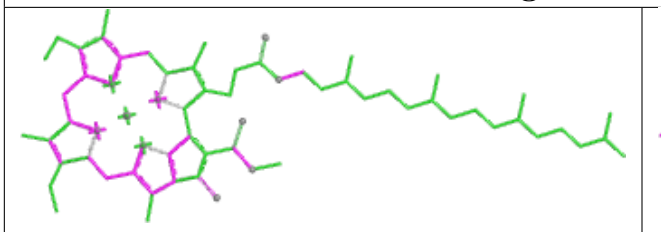


Rings

Ligand CLA 1 1119



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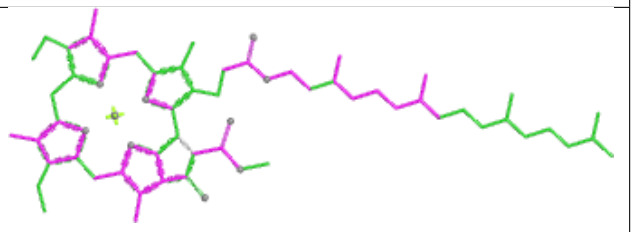
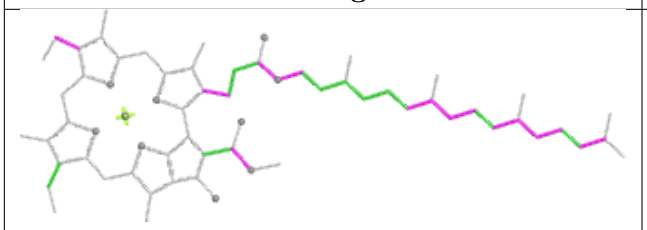


Bond angles



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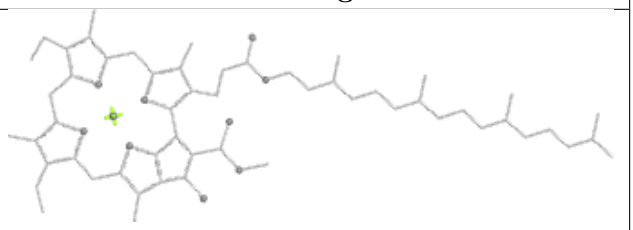
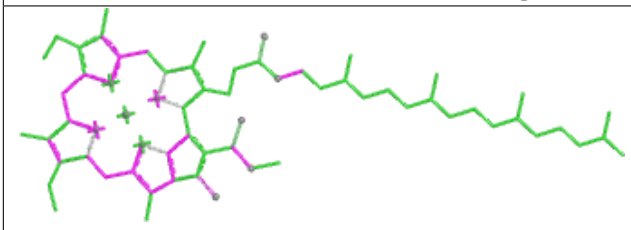
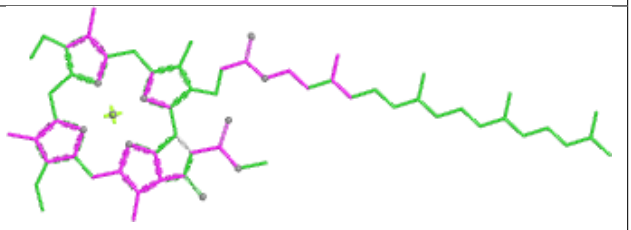


Rings

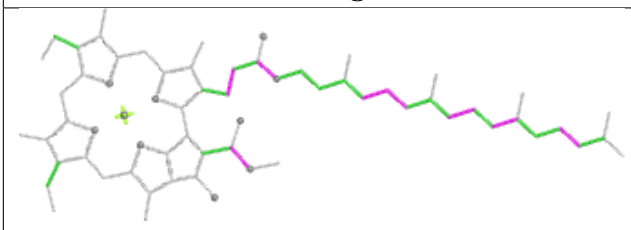
Ligand CLA B 1238



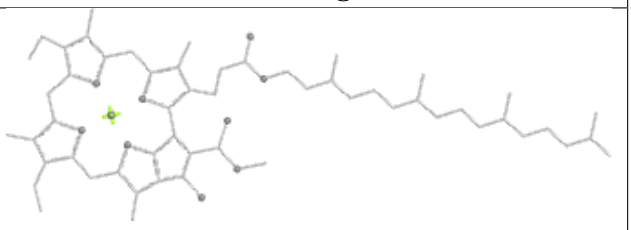
Bond lengths



Bond angles

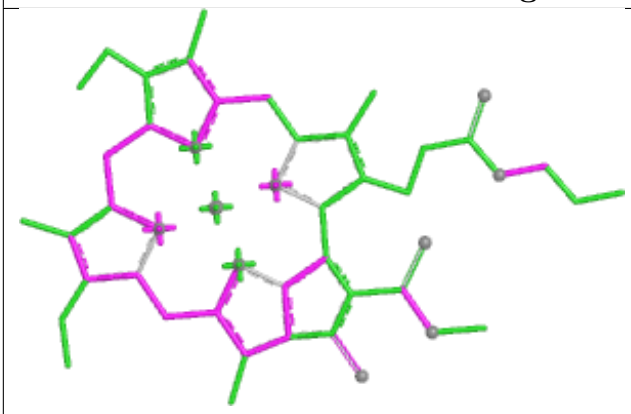


Torsions



Rings

Ligand CLA a 1105



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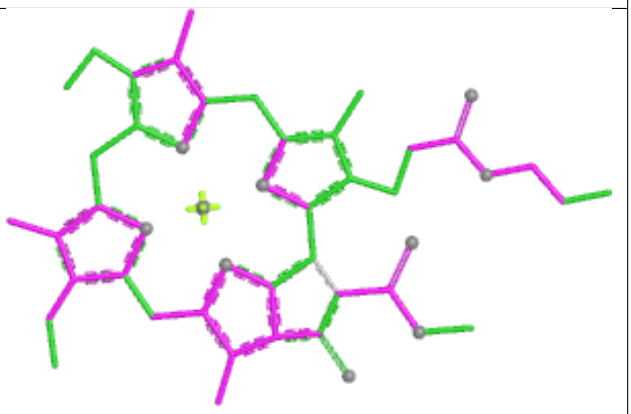
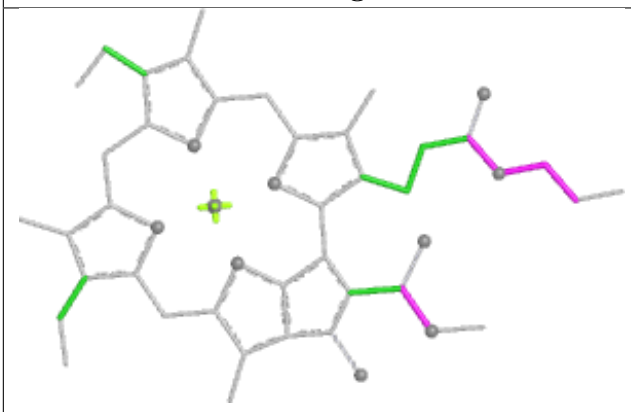


Bond angles



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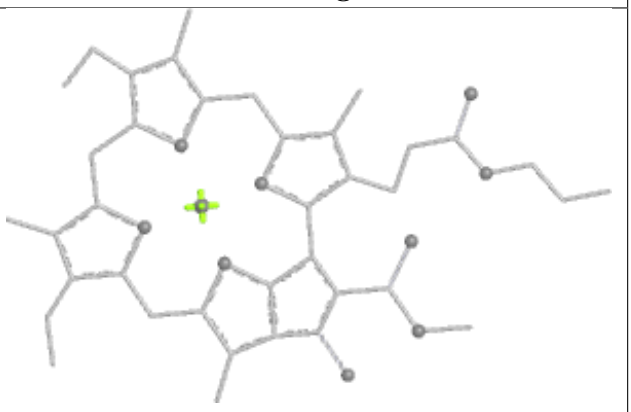
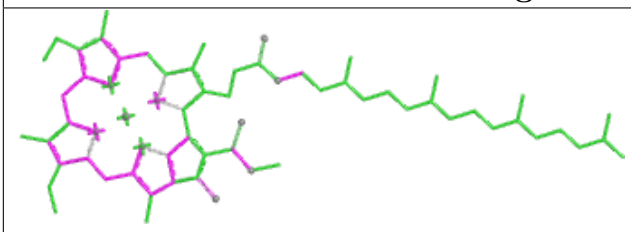
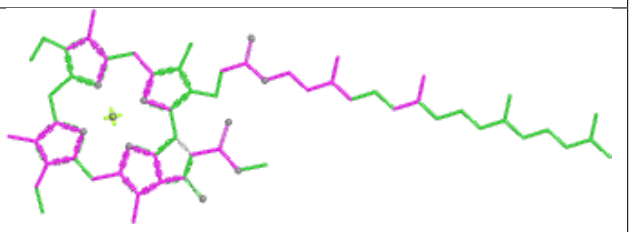


Rings

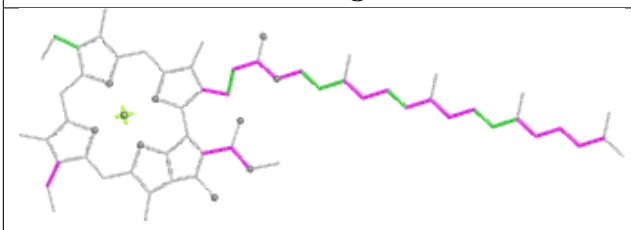
Ligand CLA B 1210



Bond lengths



Bond angles



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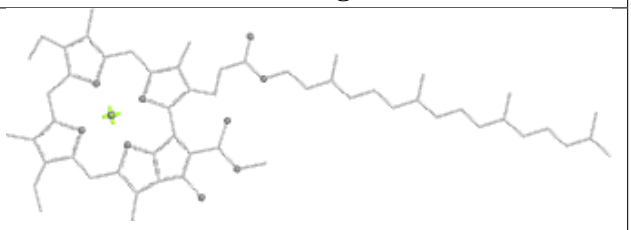
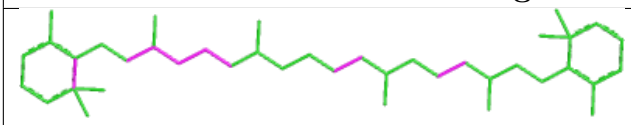


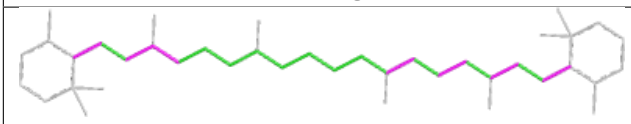
Rings

Ligand BCR B 4011



Bond lengths

Bond angles



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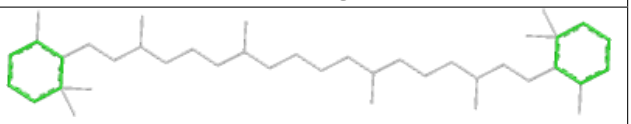
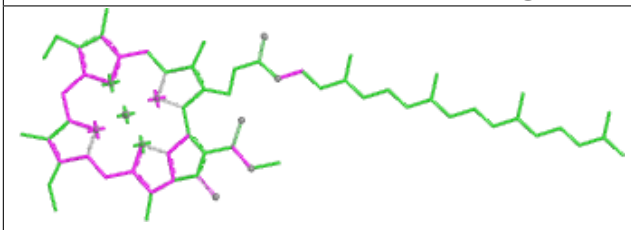
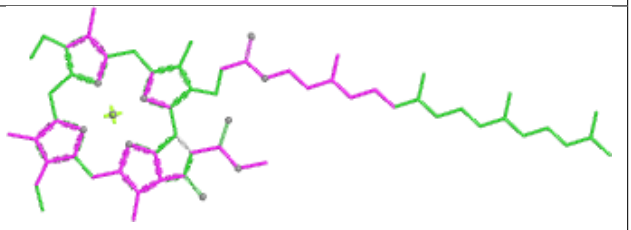


Rings

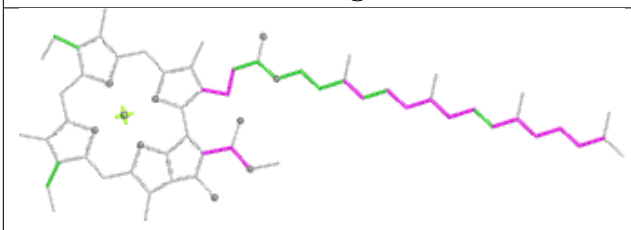
Ligand CLA 1 1106



Bond lengths



Bond angles



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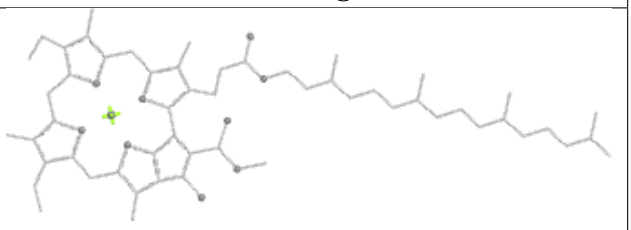
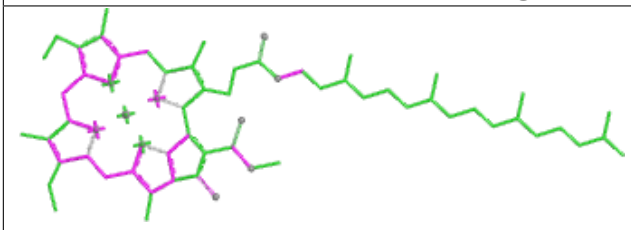
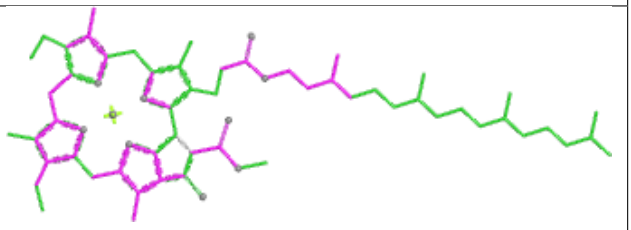


Rings

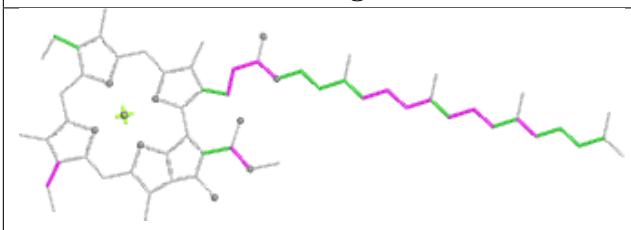
Ligand CLA A 1140



Bond lengths



Bond angles



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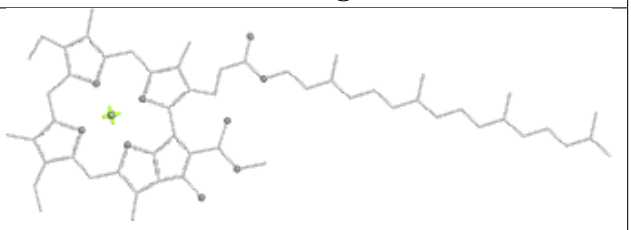
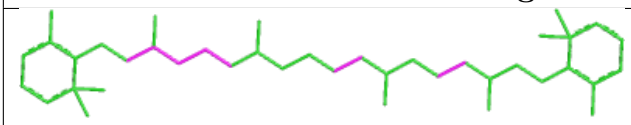


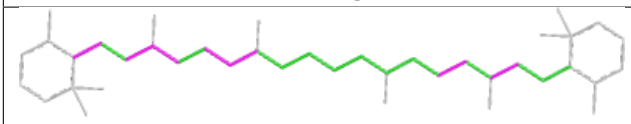
Rings

Ligand BCR 1 4003

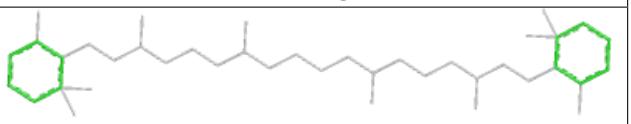


Bond lengths

Bond angles

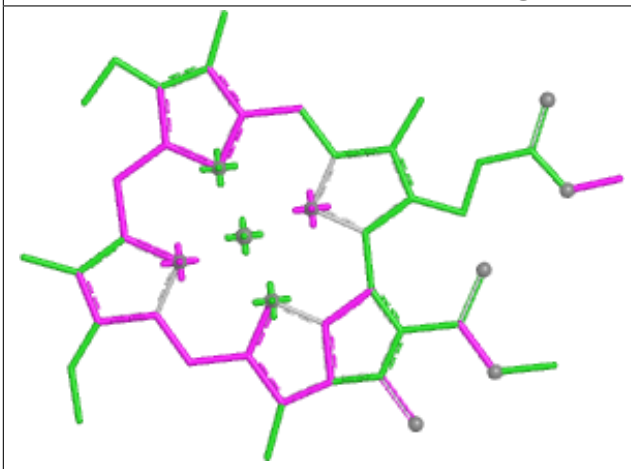


Torsions



Rings

Ligand CLA A 1121



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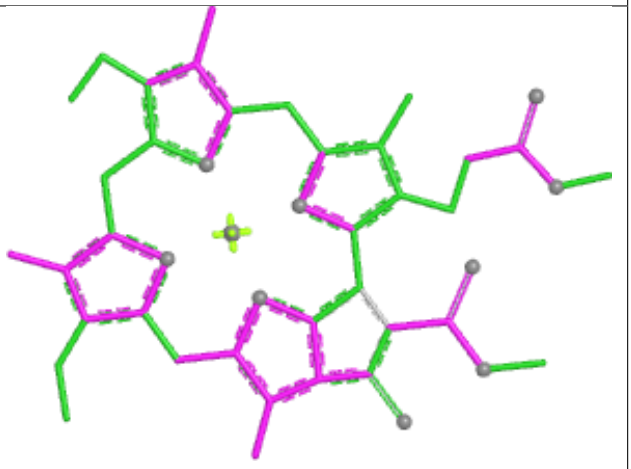
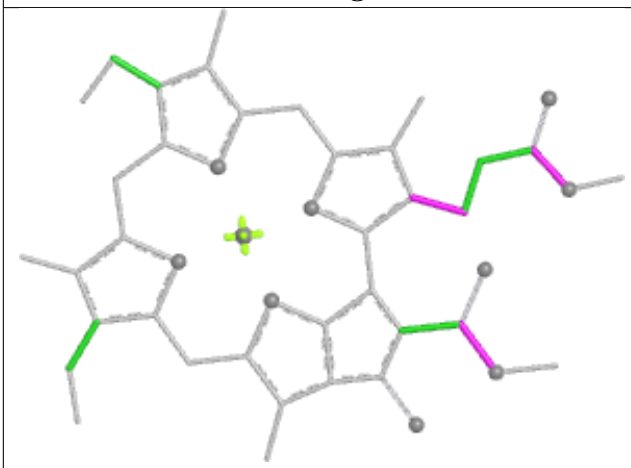
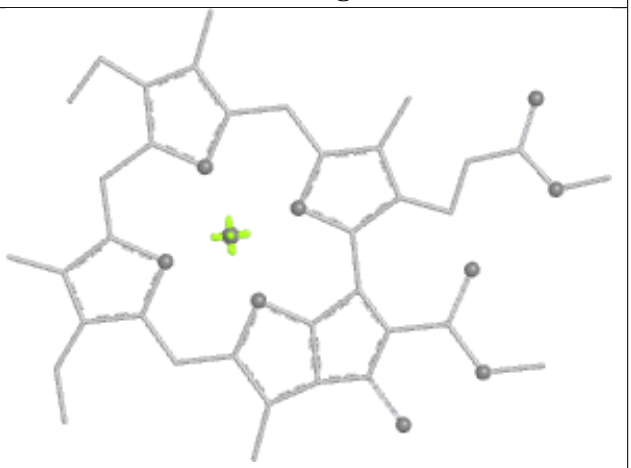


Bond angles

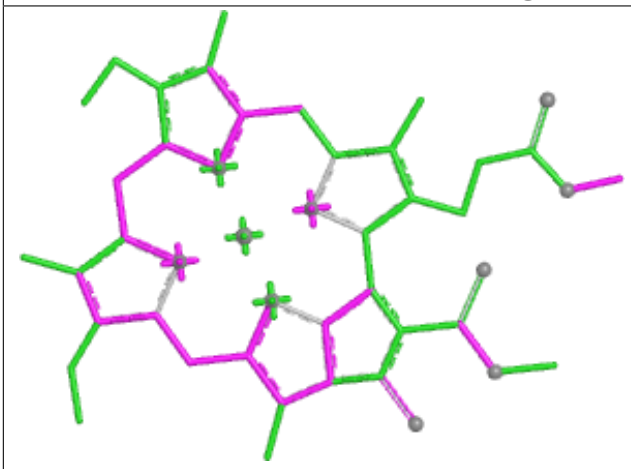


Torsions



Rings

Ligand CLA 1 1115



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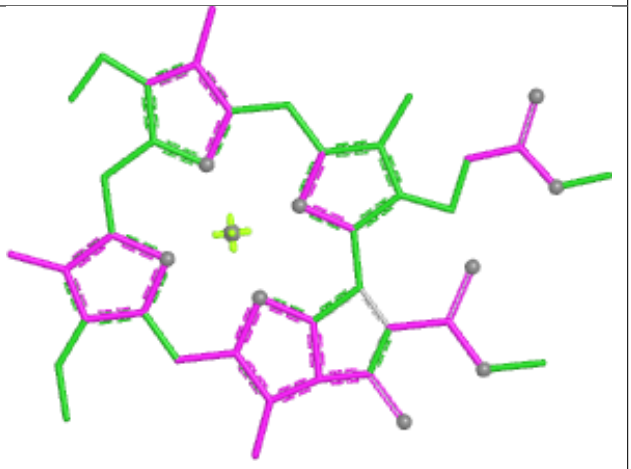
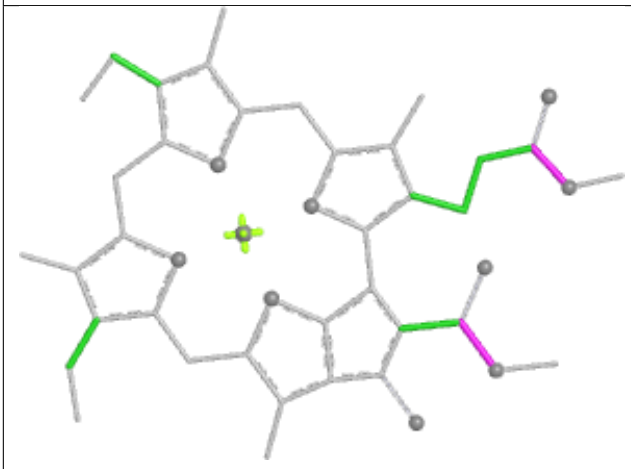


Bond angles



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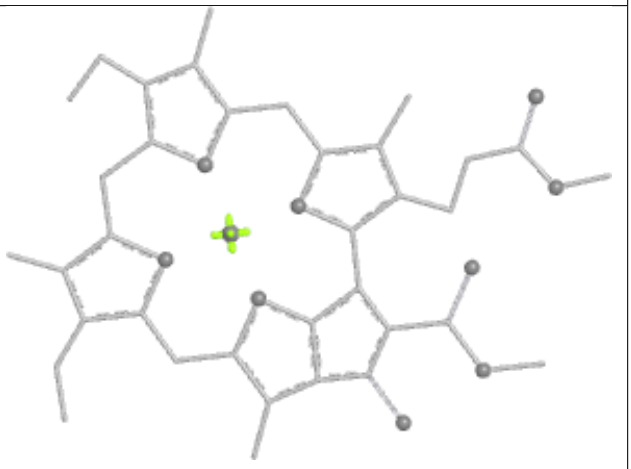
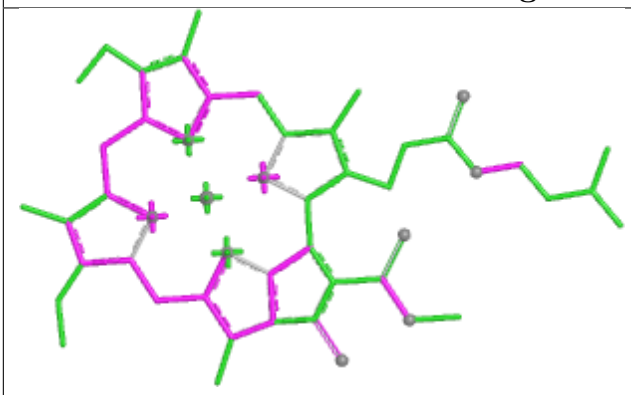


Rings

Ligand CLA 0 1402



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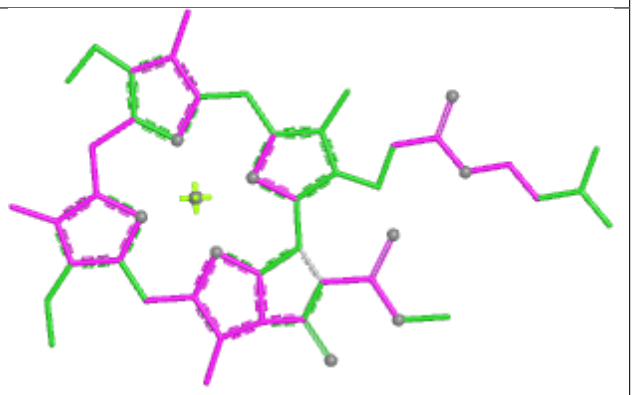
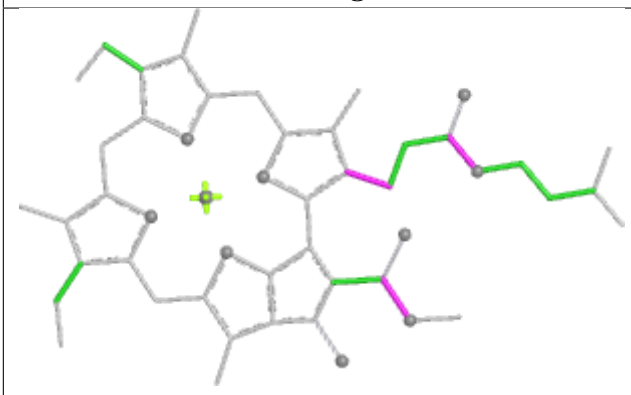


Bond angles



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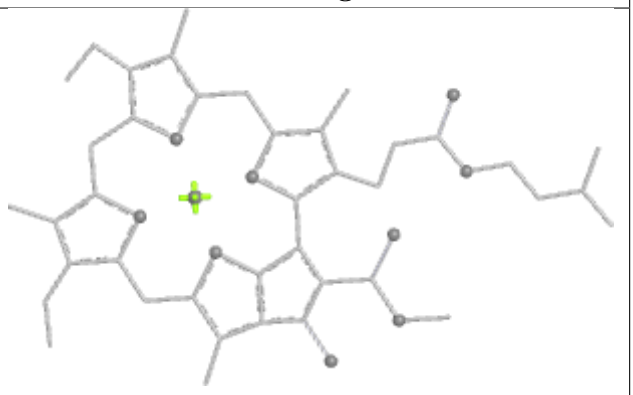
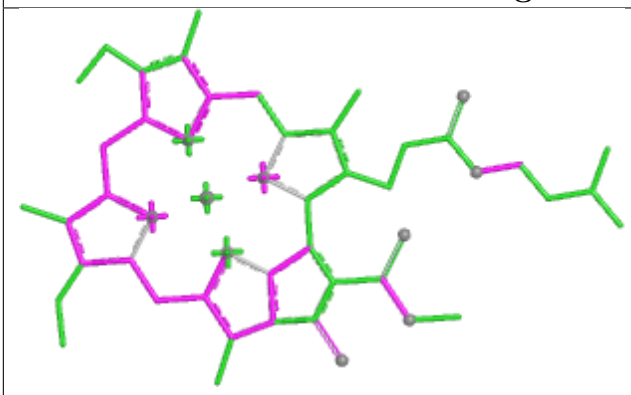


Rings

Ligand CLA A 1139



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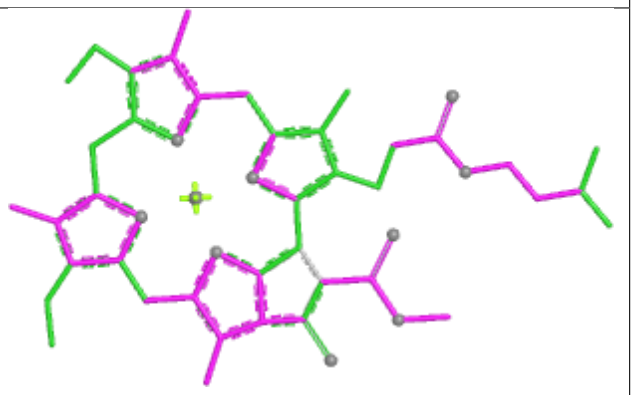
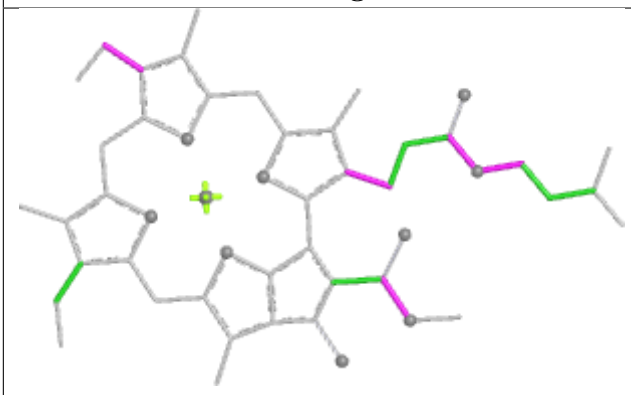


Bond angles



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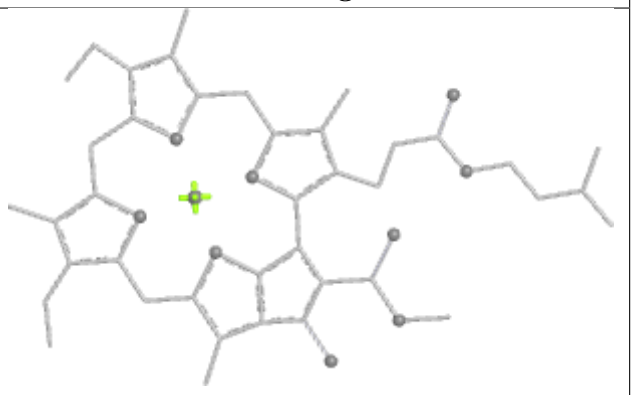
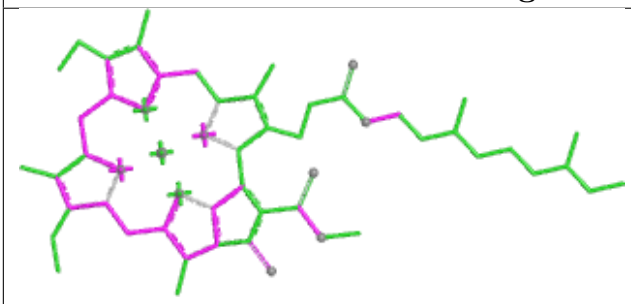


Rings

Ligand CLA b 1222



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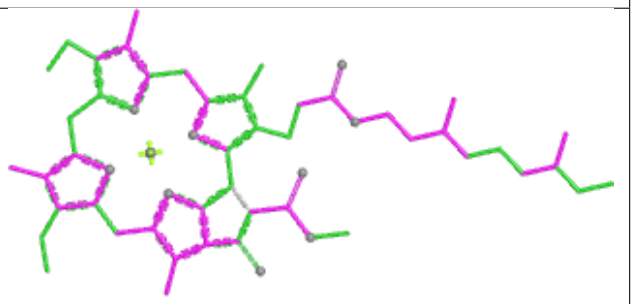

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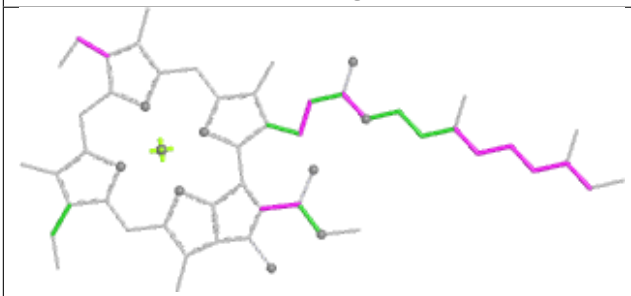

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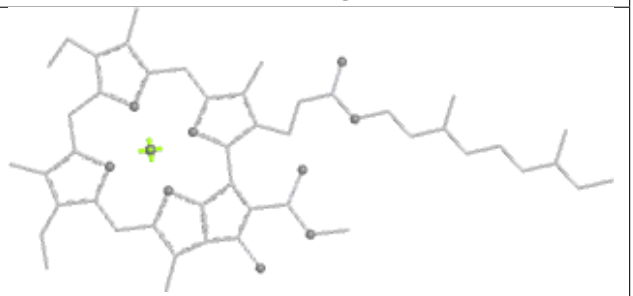
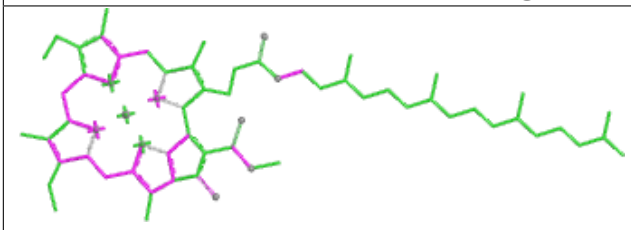


Rings

Ligand CLA b 1207



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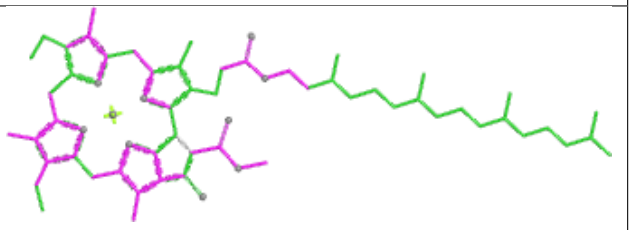
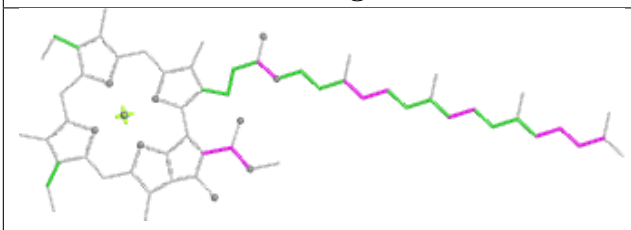


Bond angles



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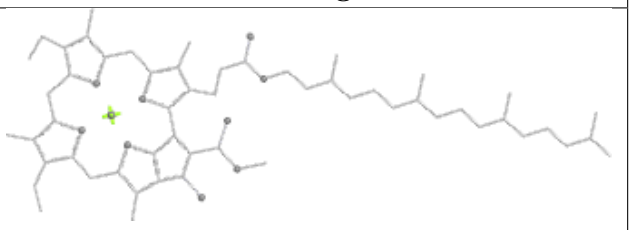
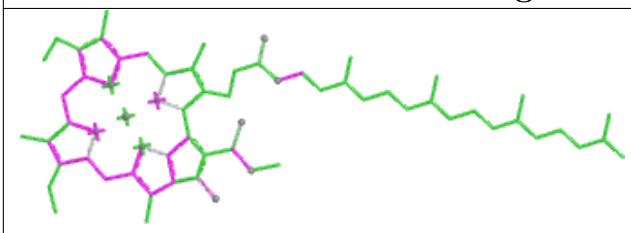


Rings

Ligand CLA B 1213



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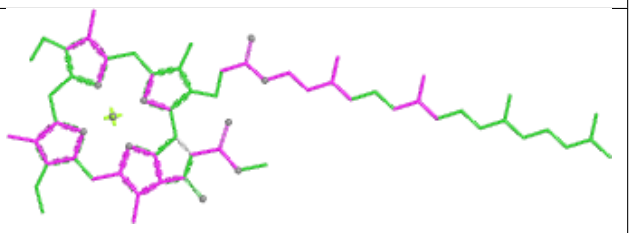
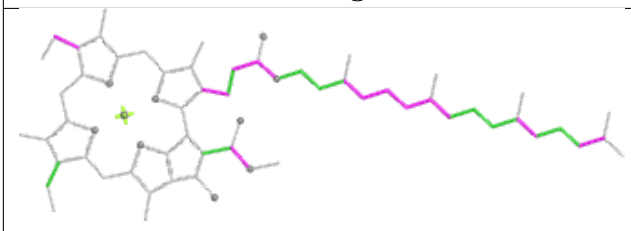


Bond angles



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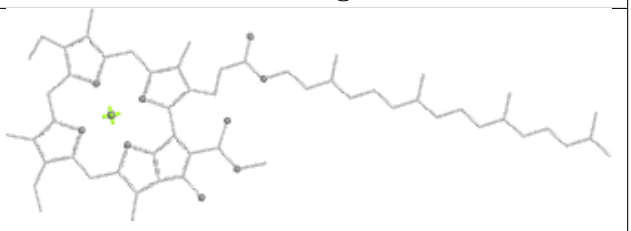
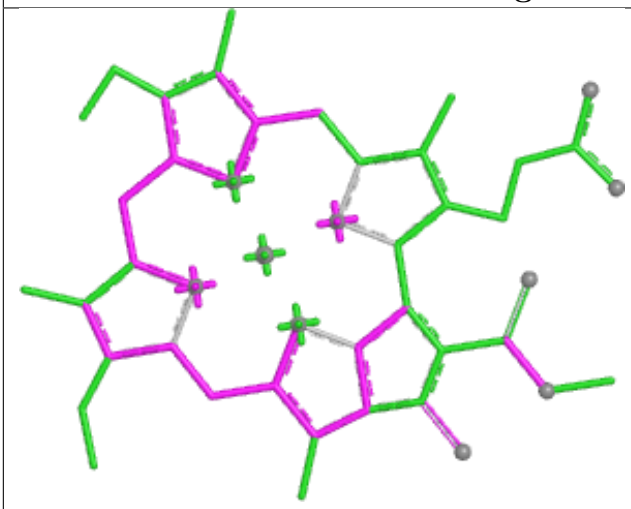


Rings

Ligand CLA A 1113



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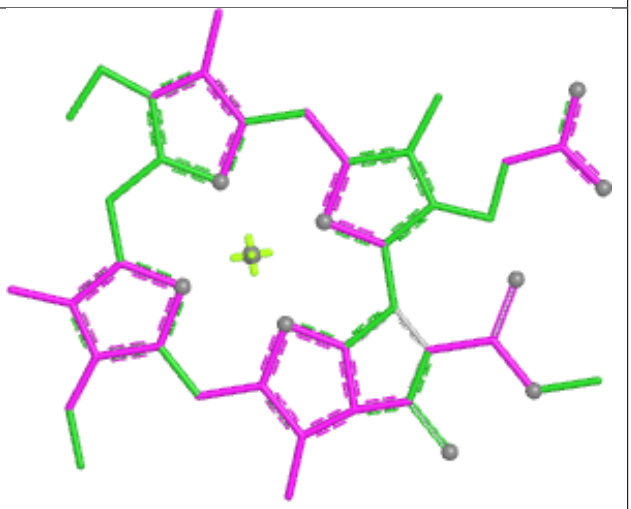
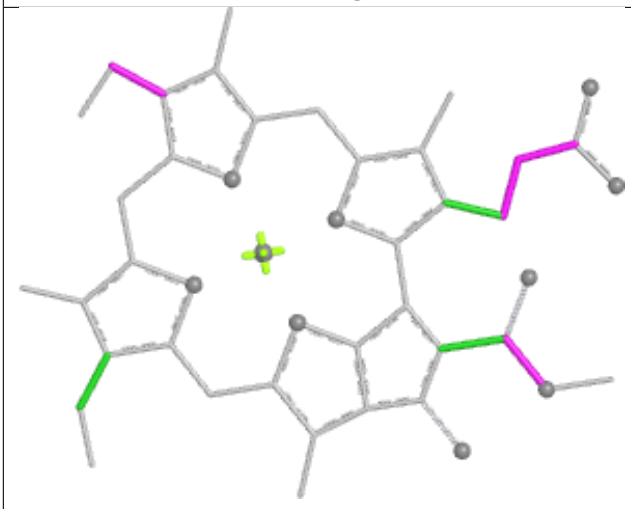


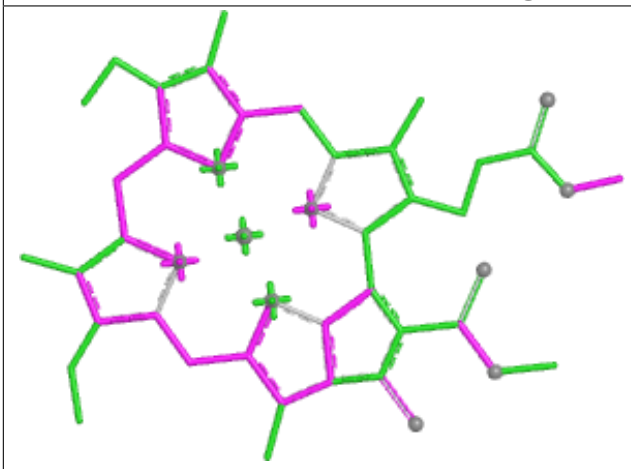
Bond angles



Torsions

Rings

Ligand CLA a 1129



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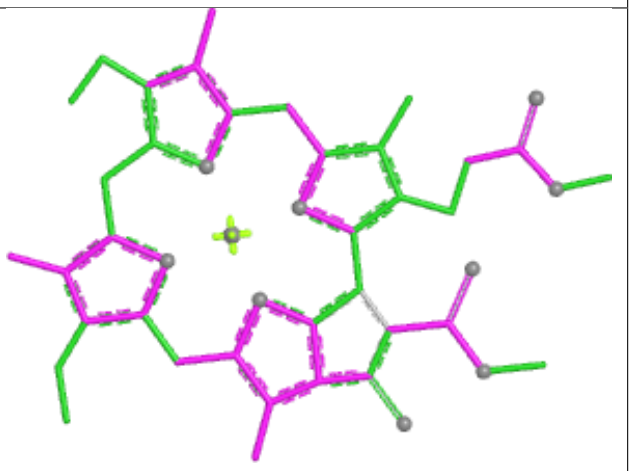

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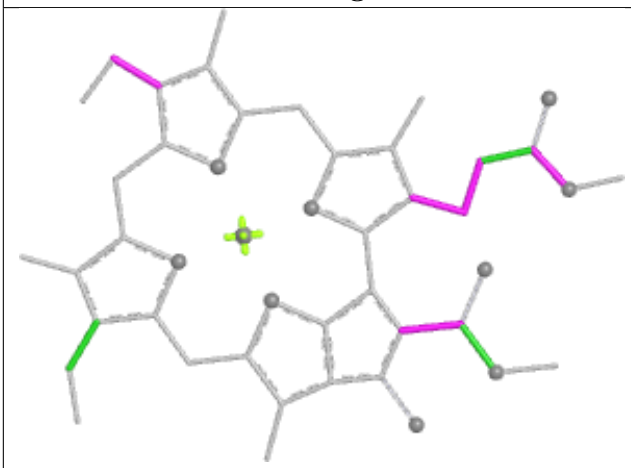

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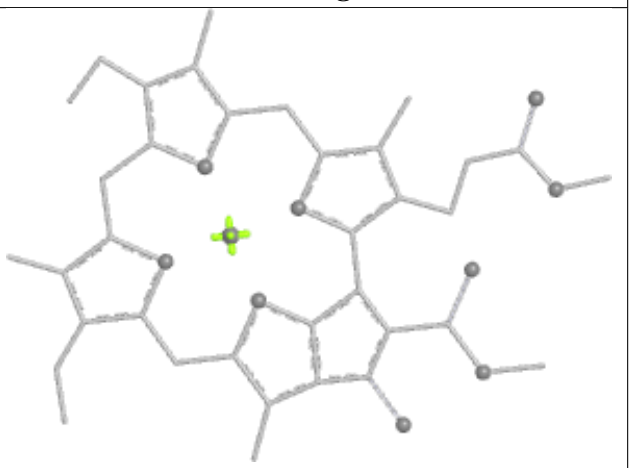
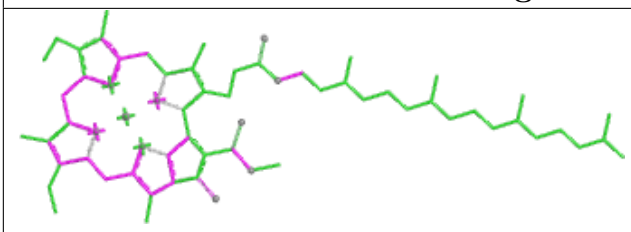


Rings

Ligand CLA A 1127



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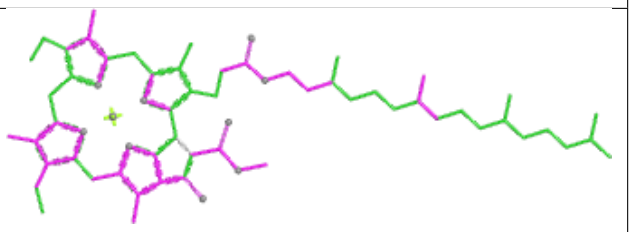
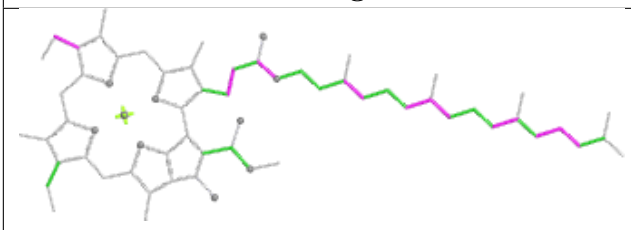


Bond angles



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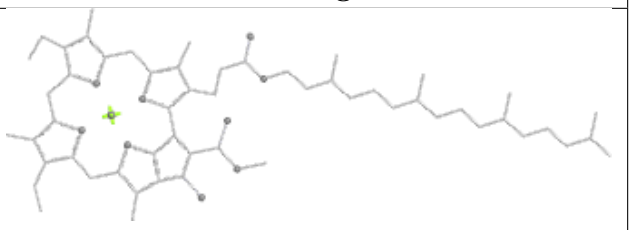
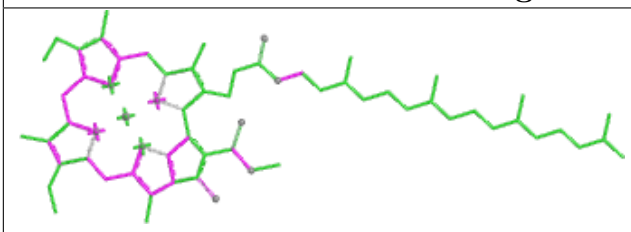


Rings

Ligand CLA B 1207



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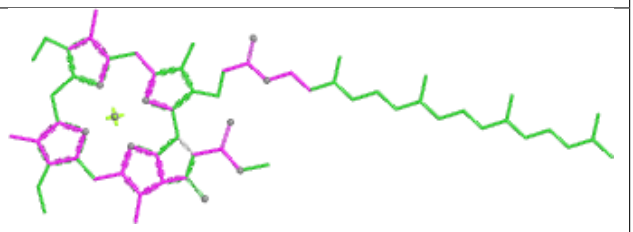
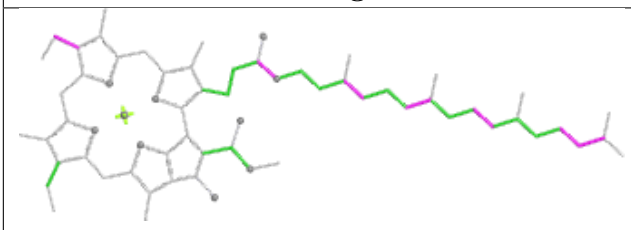
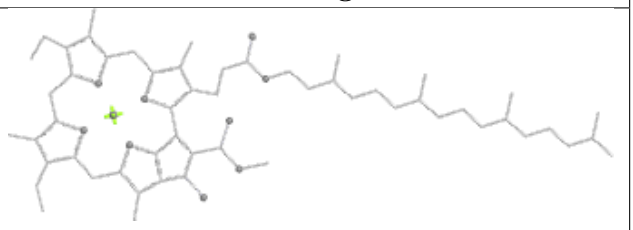


Bond angles

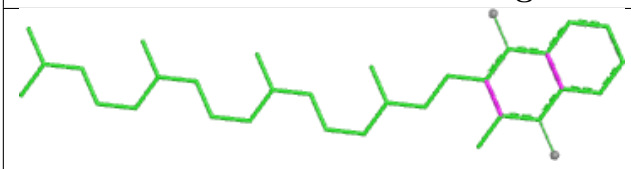


Torsions



Rings

Ligand PQN b 2002



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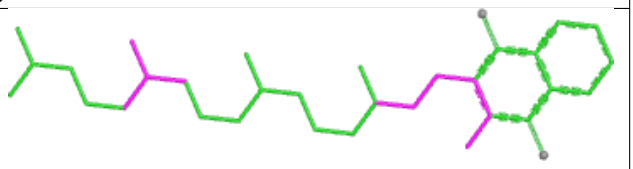
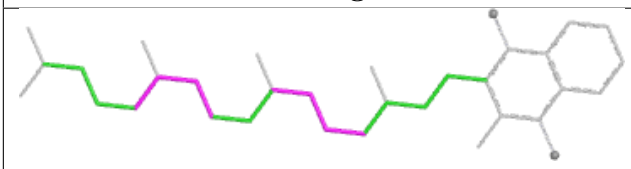
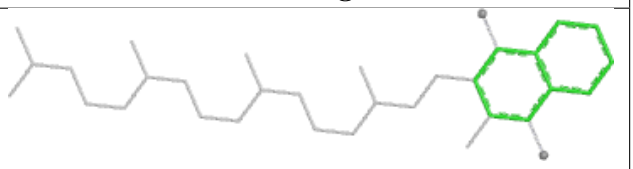


Bond angles

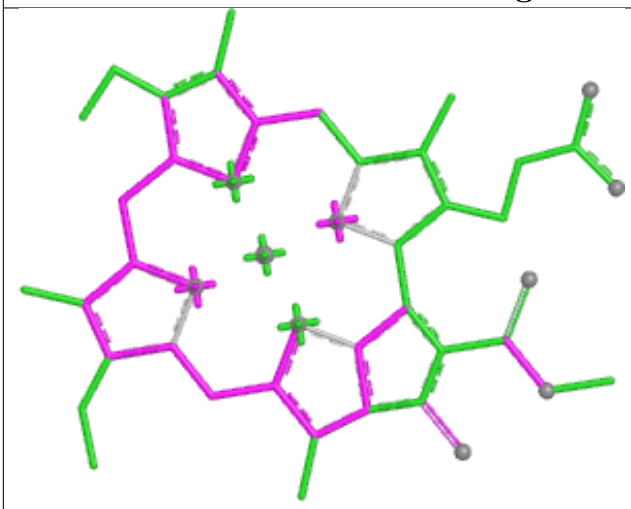


Torsions

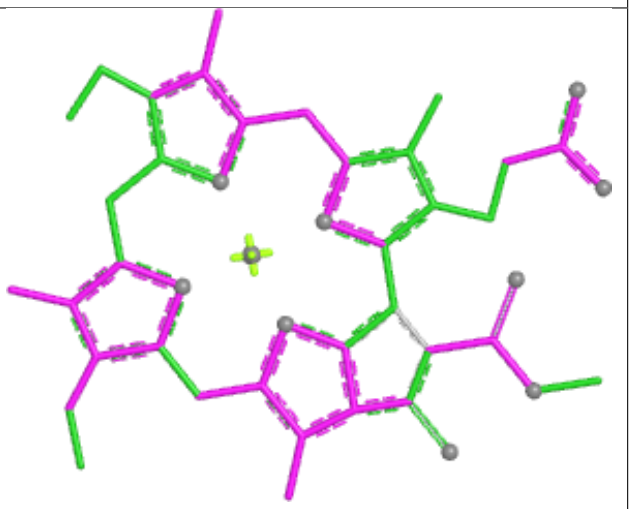


Rings

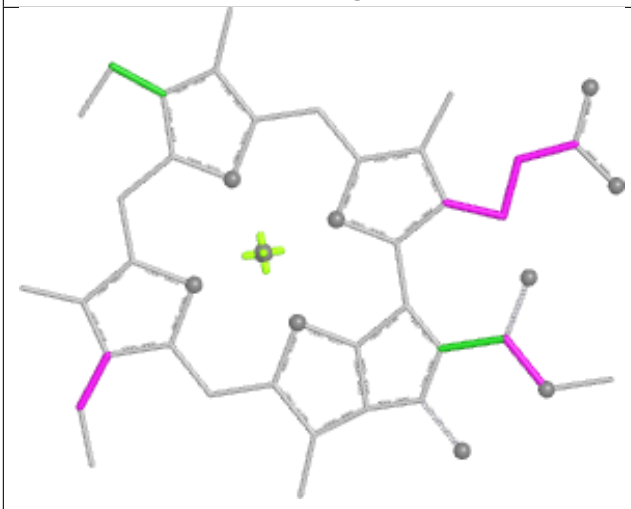
Ligand CLA B 1240



Bond lengths



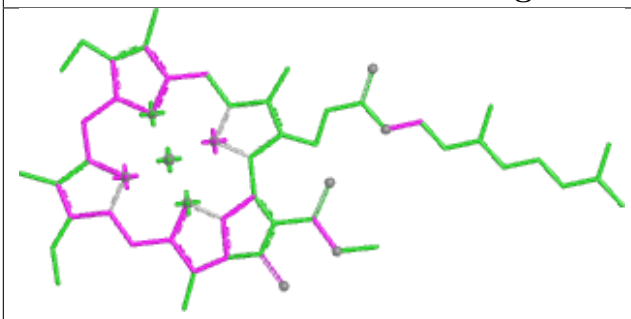
Bond angles



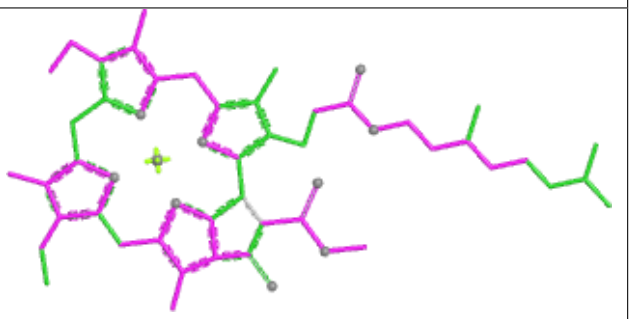
Torsions

Rings

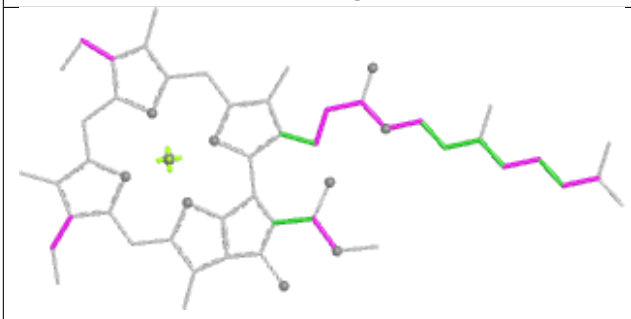
Ligand CLA A 1124



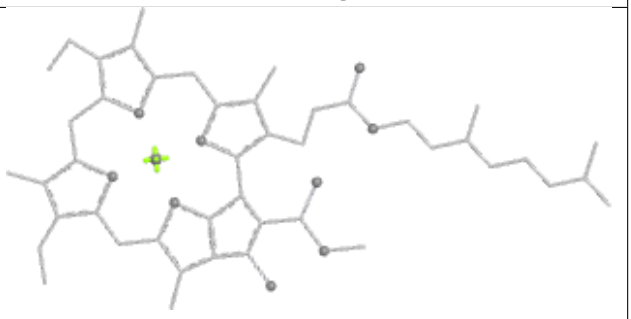
Bond lengths



Bond angles

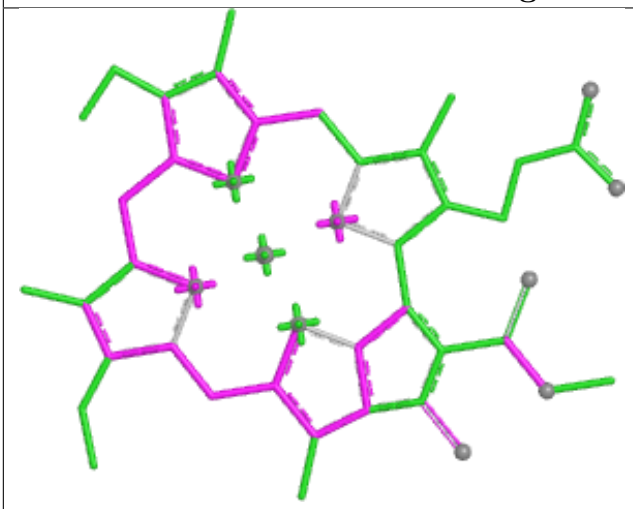


Torsions

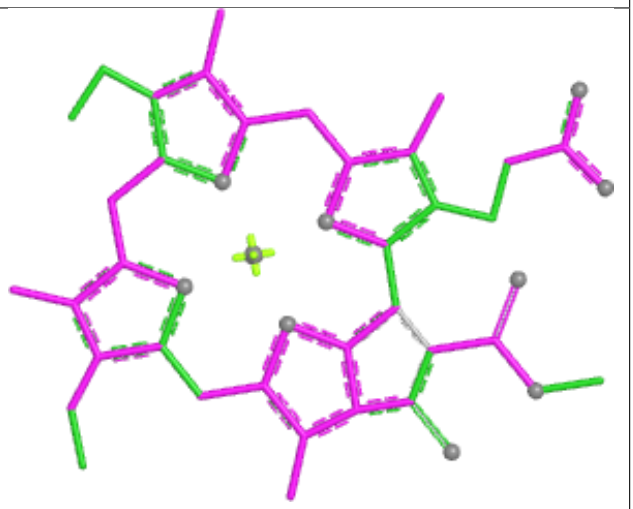


Rings

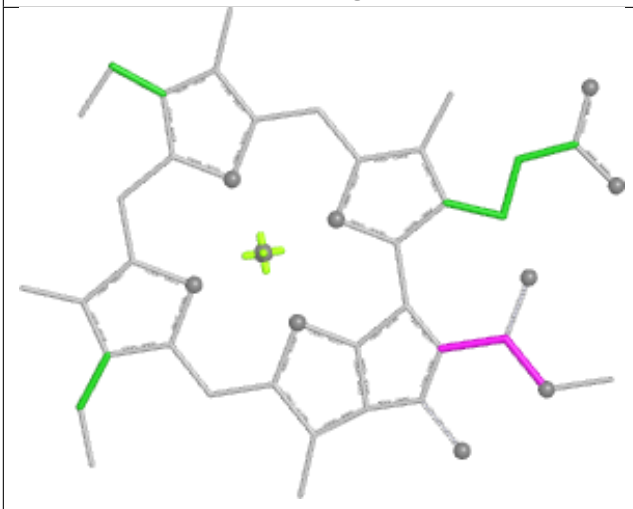
Ligand CLA 2 1231



Bond lengths



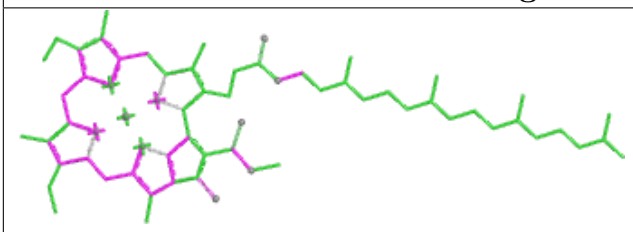
Bond angles



Torsions

Rings

Ligand CLA 2 1210



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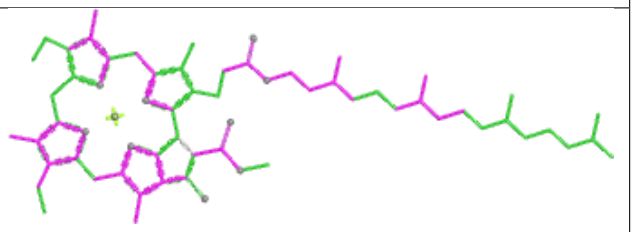
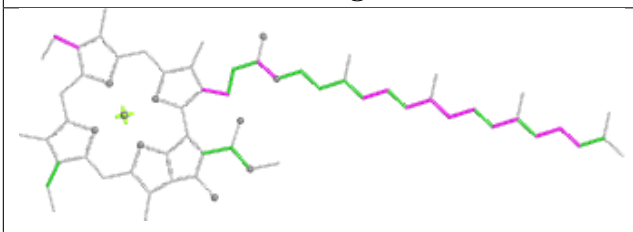
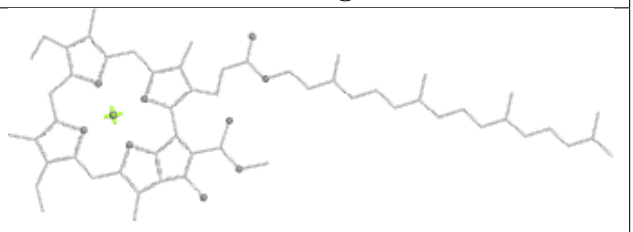


Bond angles

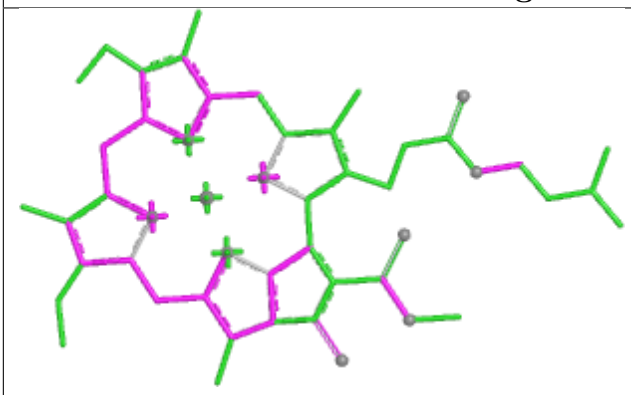


Torsions



Rings

Ligand CLA B 1228



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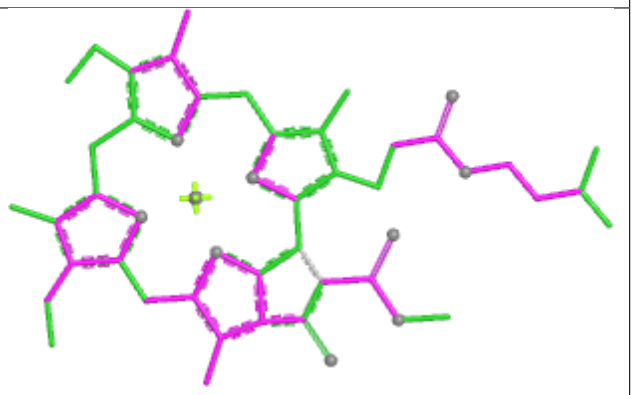
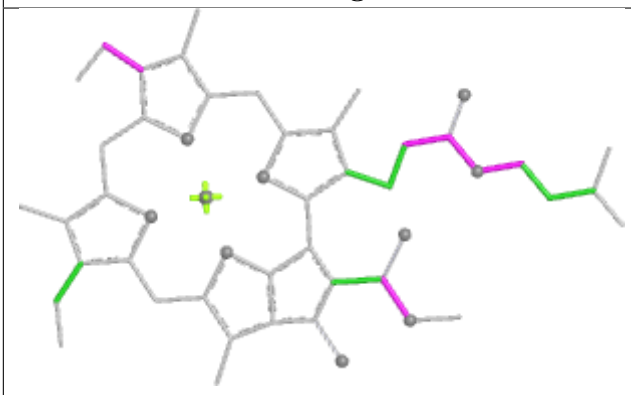
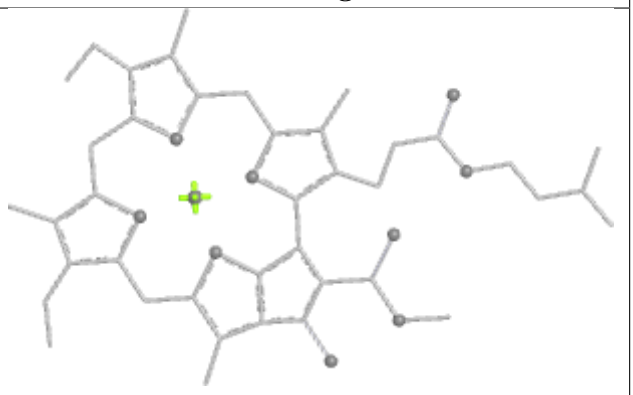


Bond angles

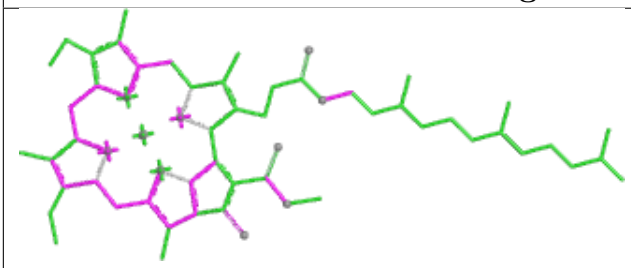


Torsions



Rings

Ligand CLA 2 1234



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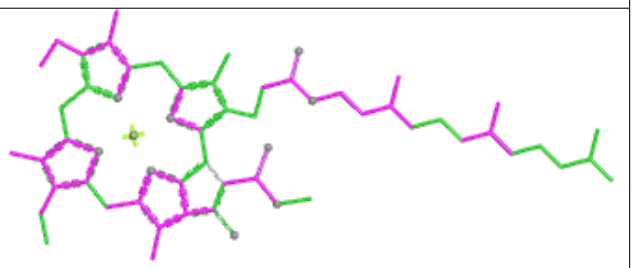
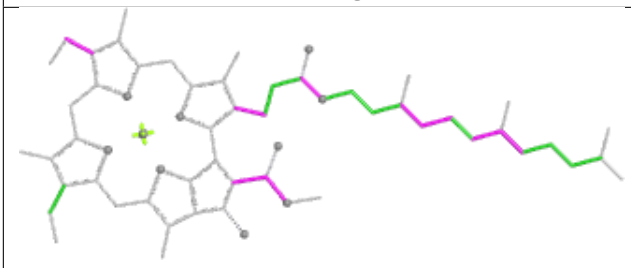
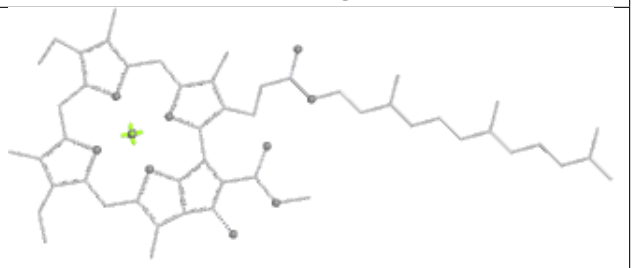


Bond angles

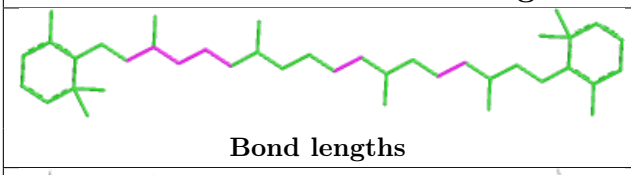


Torsions

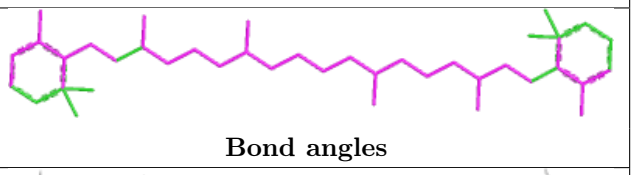


Rings

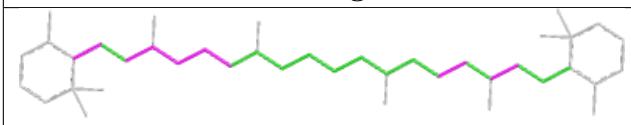
Ligand BCR 1 4001



Bond lengths



Bond angles



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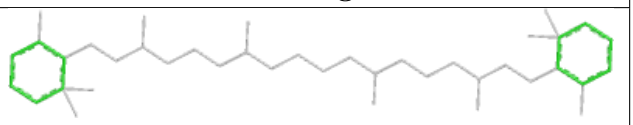
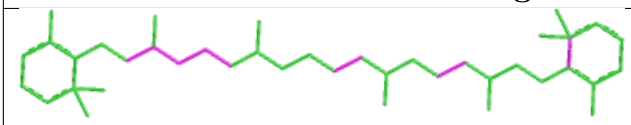


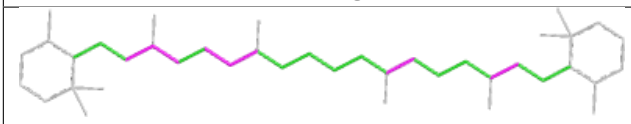
Rings

Ligand BCR B 4014

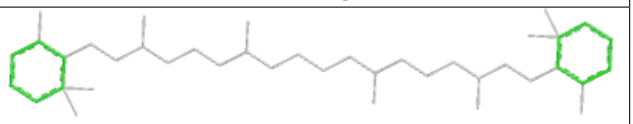


Bond lengths

Bond angles

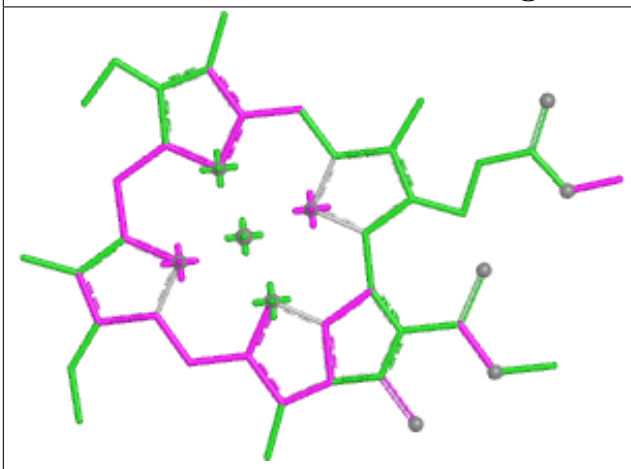


Torsions

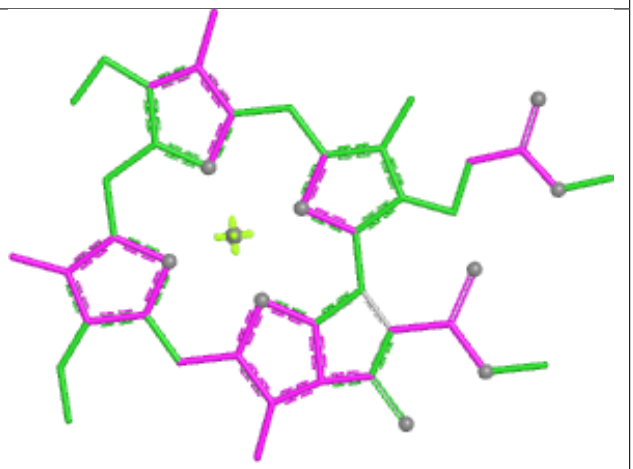


Rings

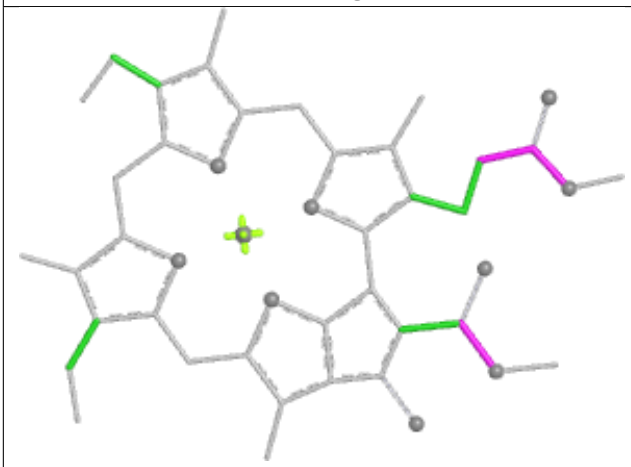
Ligand CLA a 1136



Bond lengths



Bond angles



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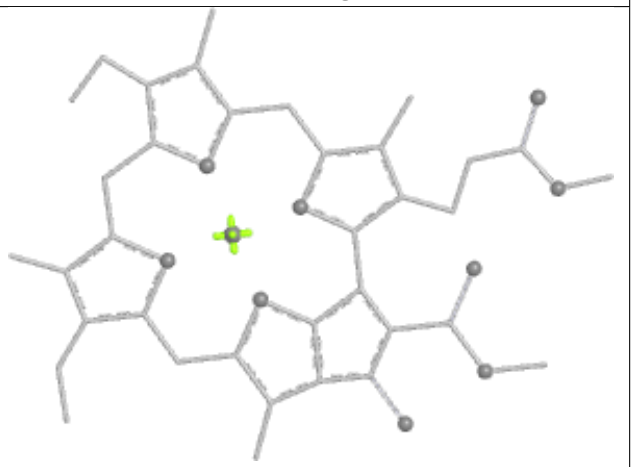
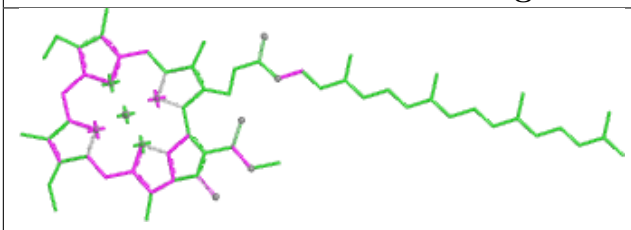


Rings

Ligand CLA A 1107



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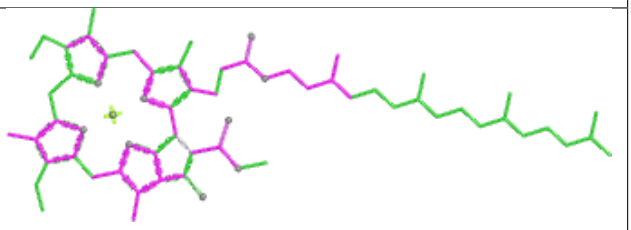
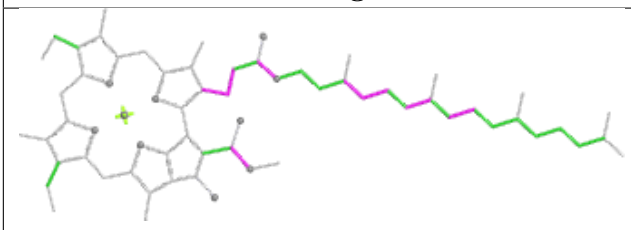


Bond angles



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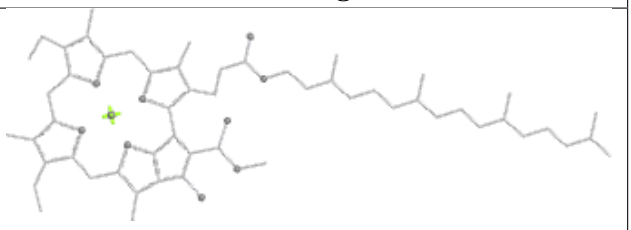
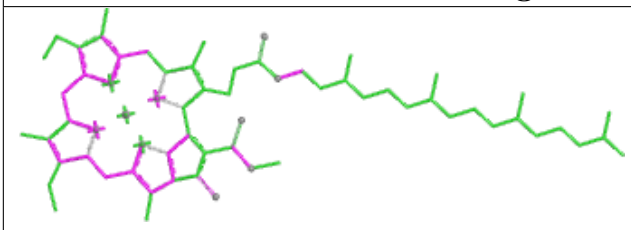
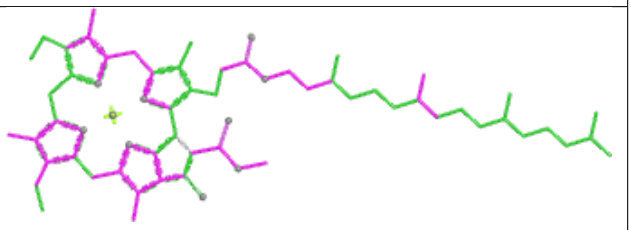


Rings

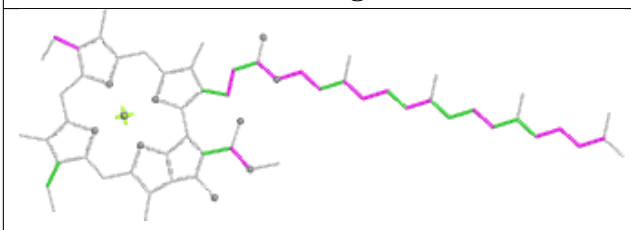
Ligand CLA B 1013



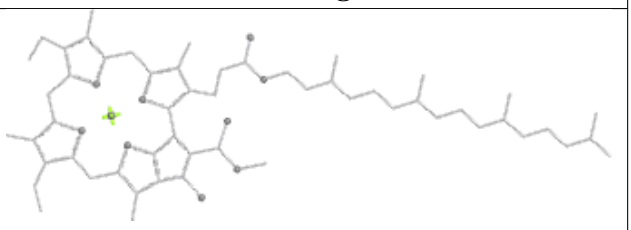
Bond lengths



Bond angles

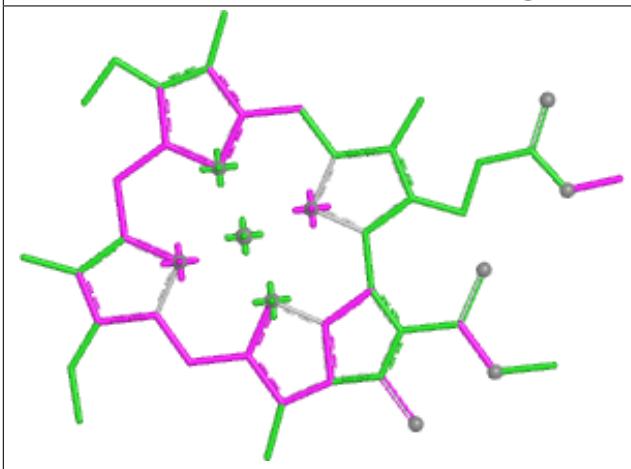


Torsions



Rings

Ligand CLA 1 1129



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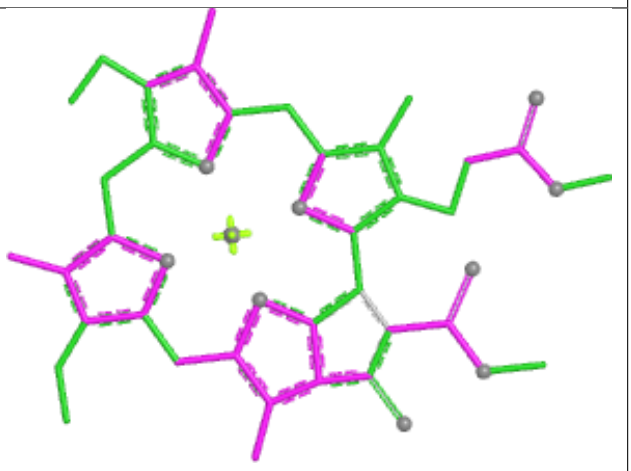
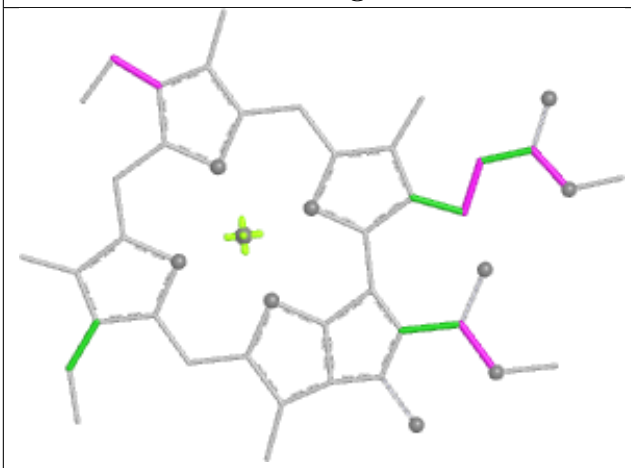


Bond angles



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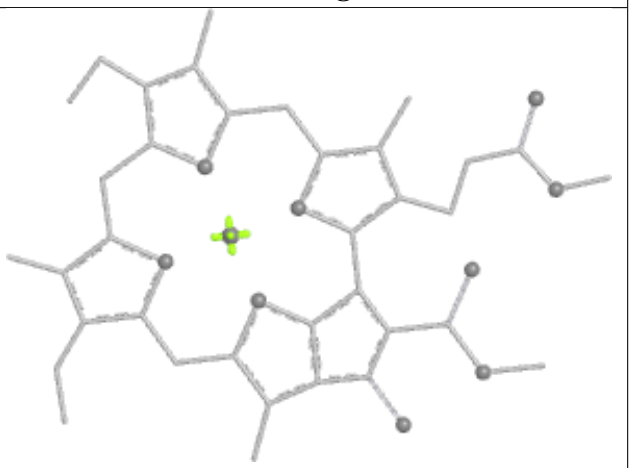
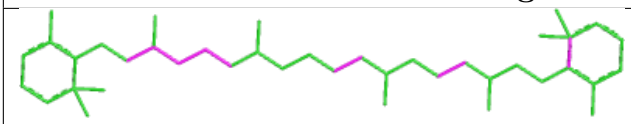


Rings

Ligand BCR 2 4005



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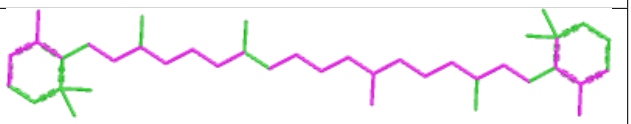
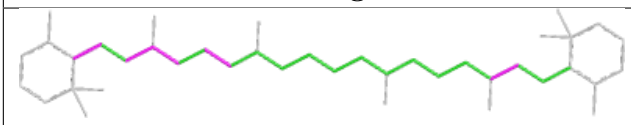
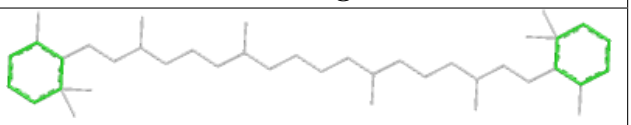


Bond angles

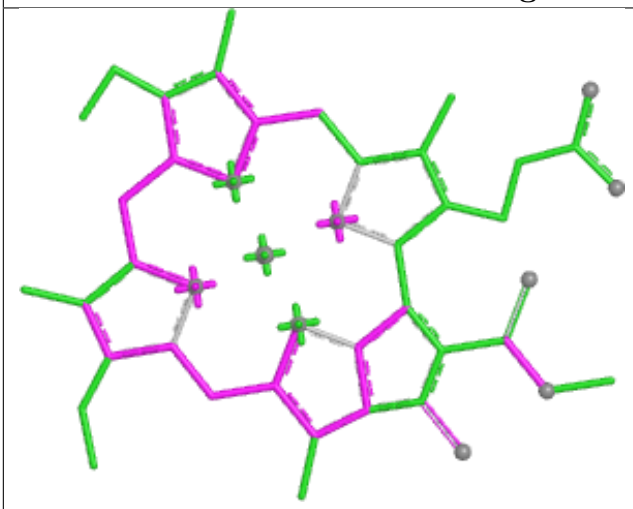


Torsions

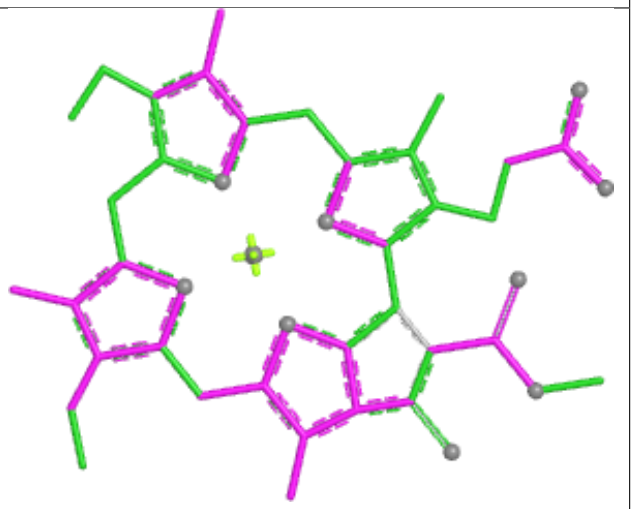


Rings

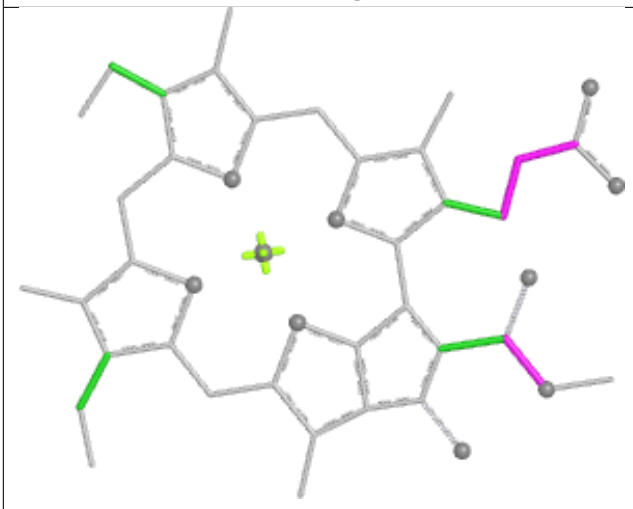
Ligand CLA 2 1240



Bond lengths



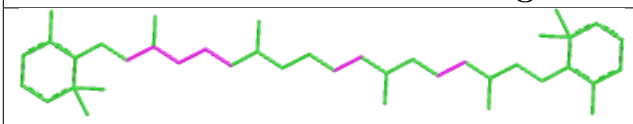
Bond angles



Torsions

Rings

Ligand BCR b 4005



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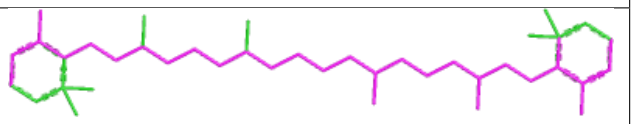
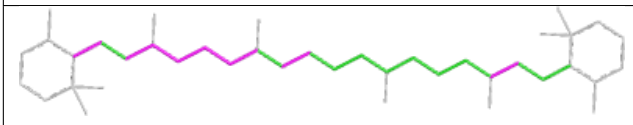
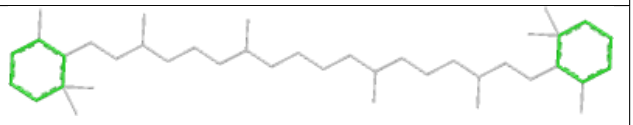


Bond angles

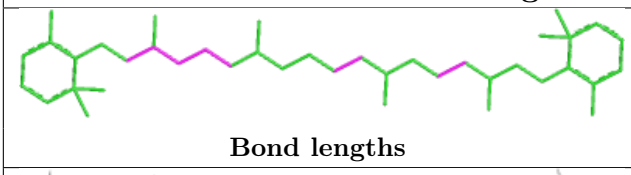


Torsions

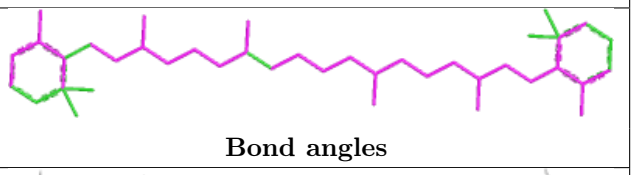


Rings

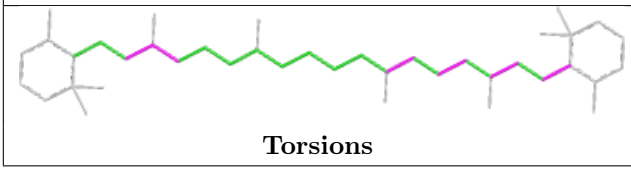
Ligand BCR l 4022



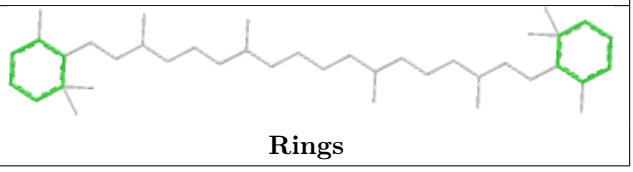
Bond lengths



Bond angles

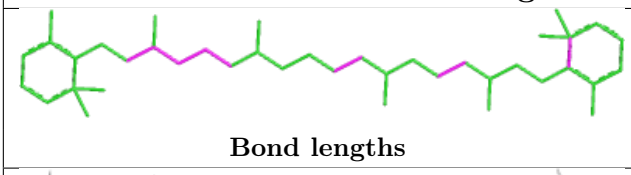


Torsions

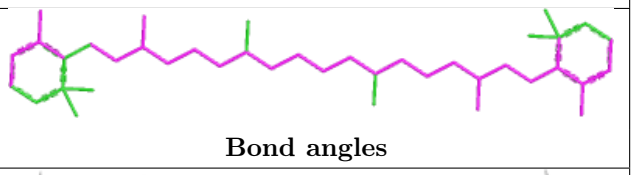


Rings

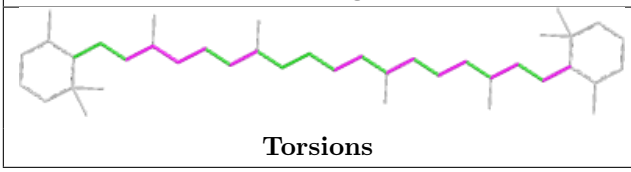
Ligand BCR a 4002



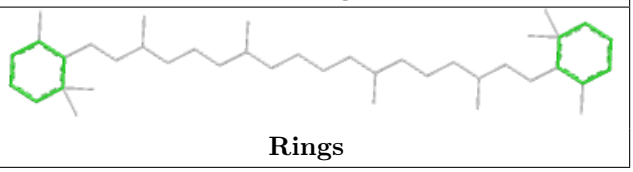
Bond lengths



Bond angles

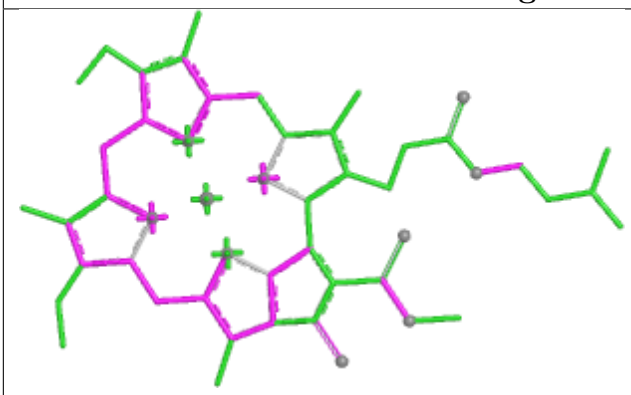


Torsions

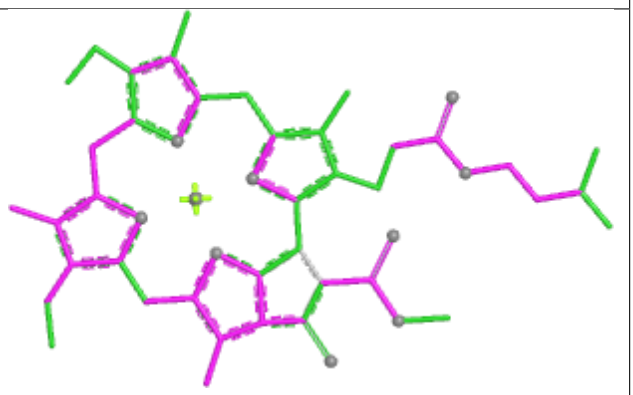


Rings

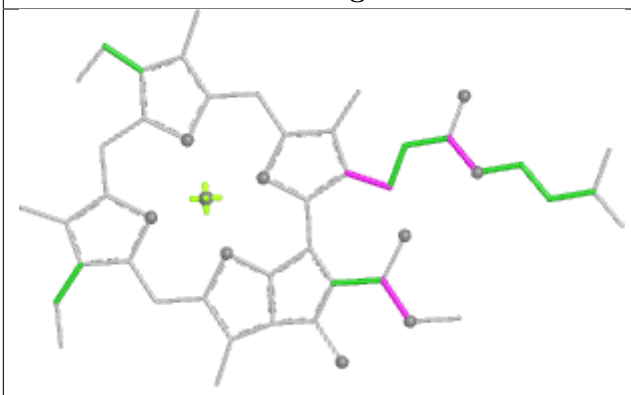
Ligand CLA k 1402



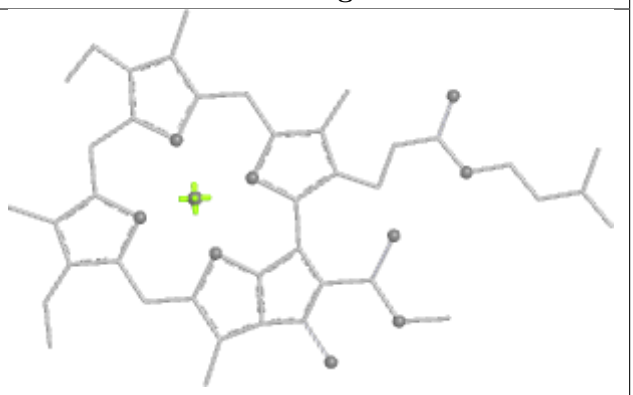
Bond lengths



Bond angles

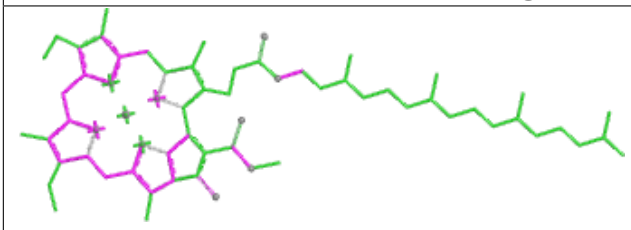


Torsions



Rings

Ligand CLA a 1012



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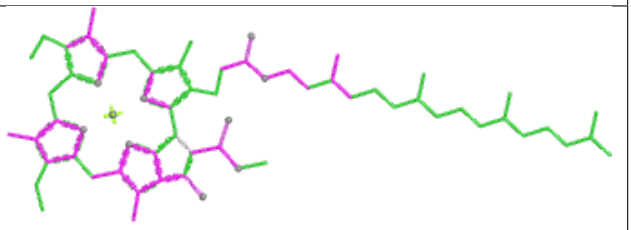
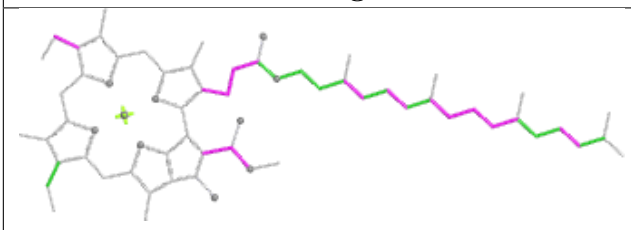


Bond angles



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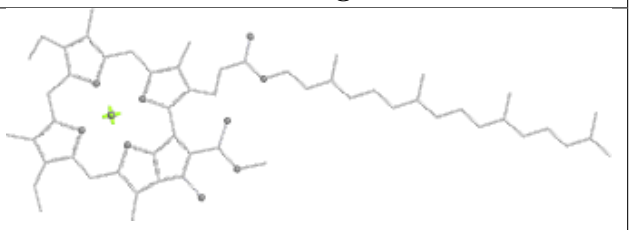
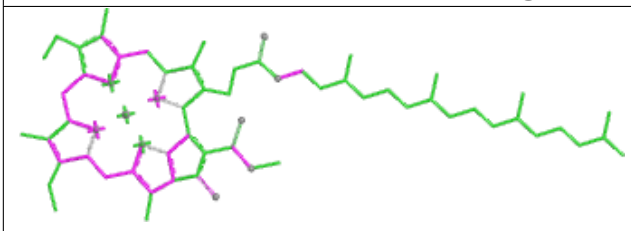


Rings

Ligand CLA a 1137



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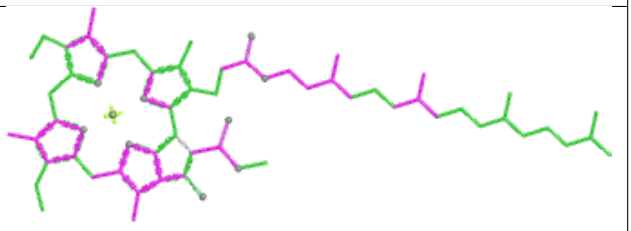
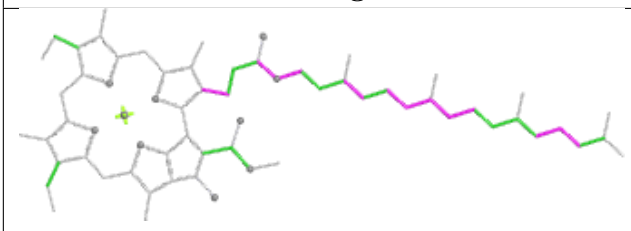


Bond angles



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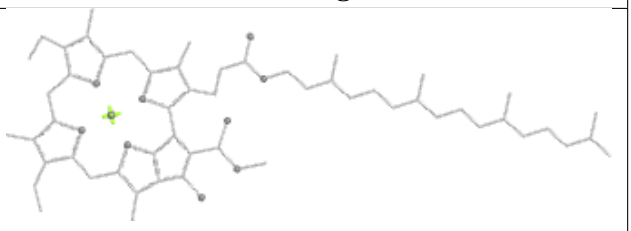
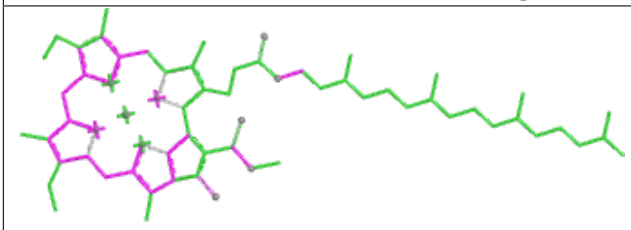


Rings

Ligand CLA A 1137



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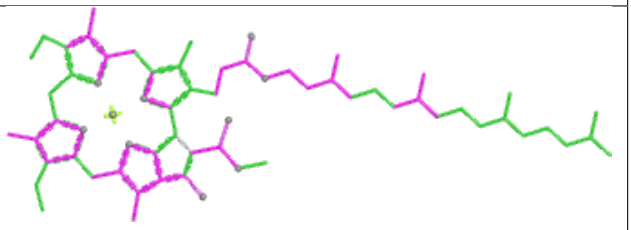

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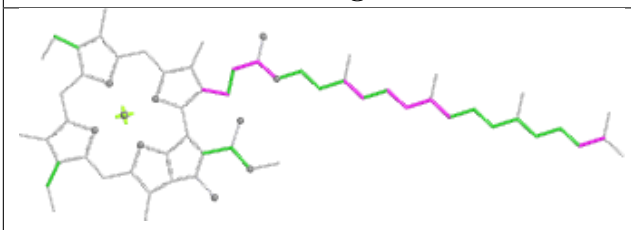

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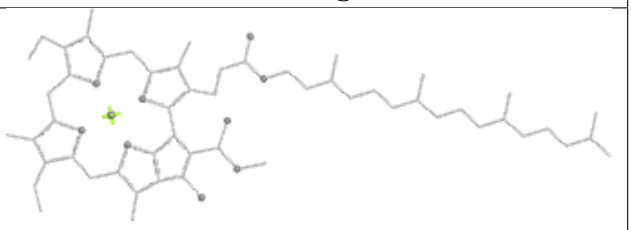
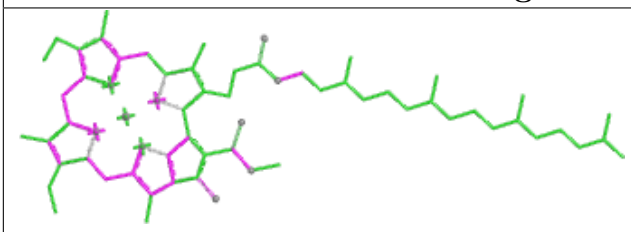


Rings

Ligand CLA A 1128



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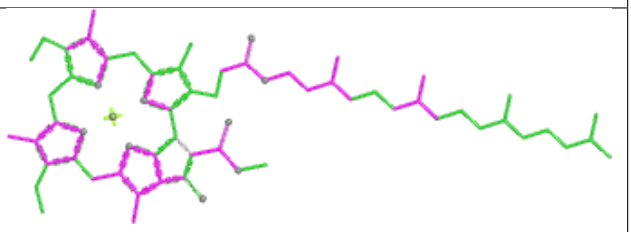

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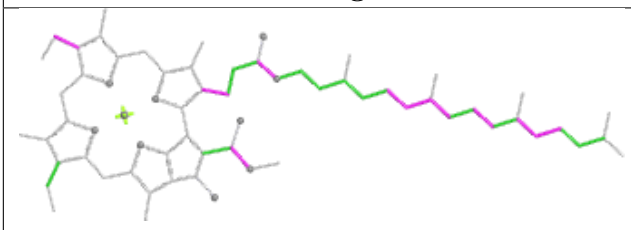

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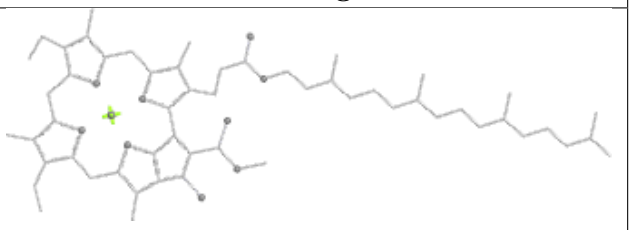
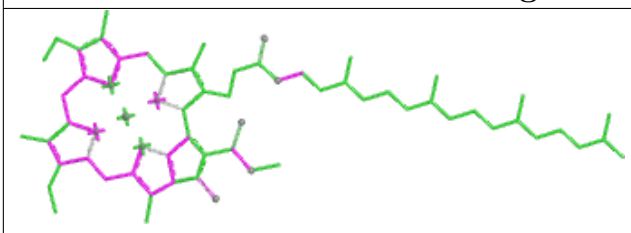


Rings

Ligand CLA a 1101



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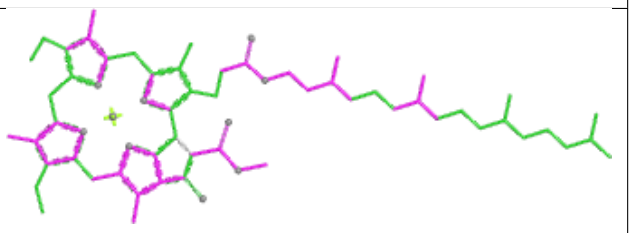
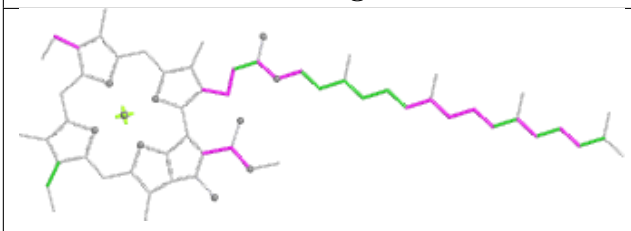


Bond angles



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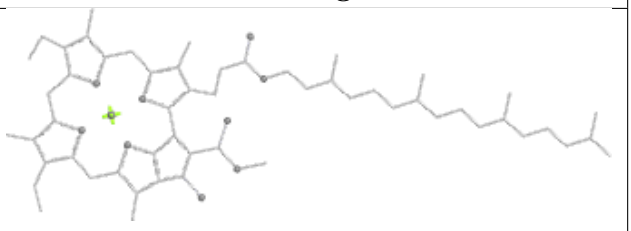
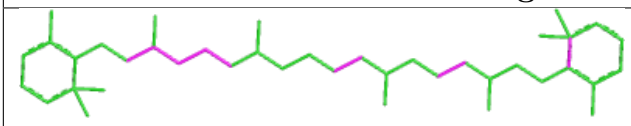
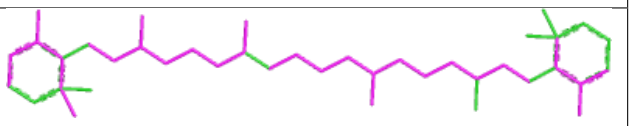


Rings

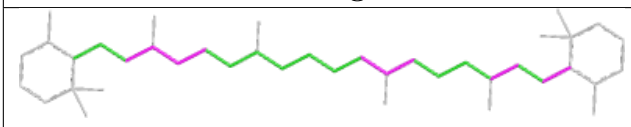
Ligand BCR 1 4002



Bond lengths



Bond angles



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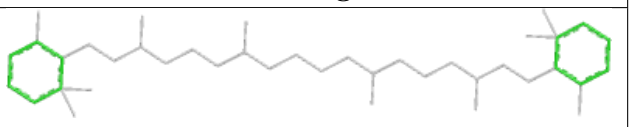
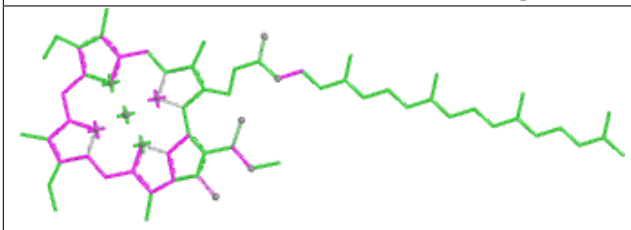


Rings

Ligand CLA A 1101



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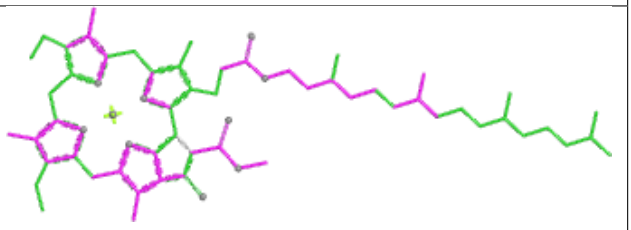
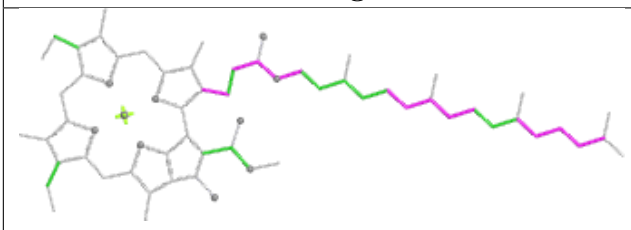


Bond angles



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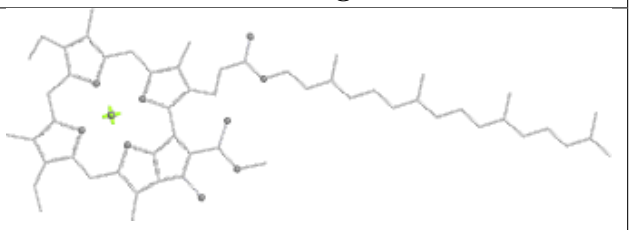
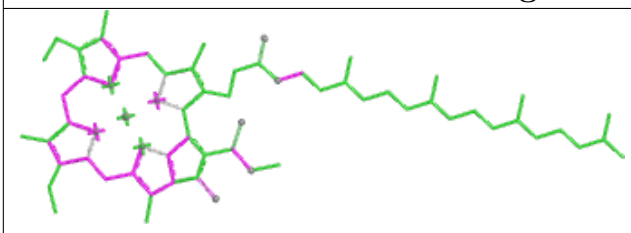


Rings

Ligand CLA 2 1206



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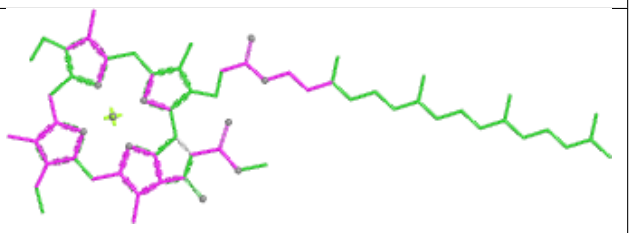
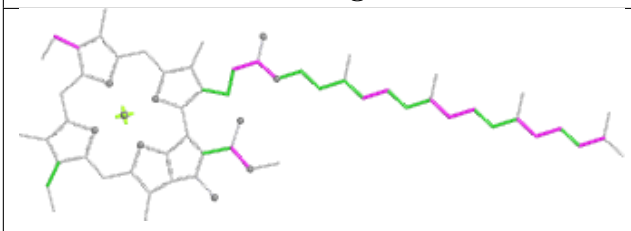


Bond angles



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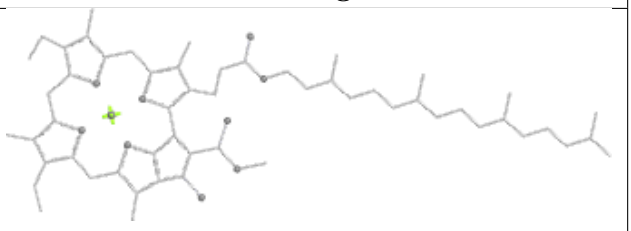
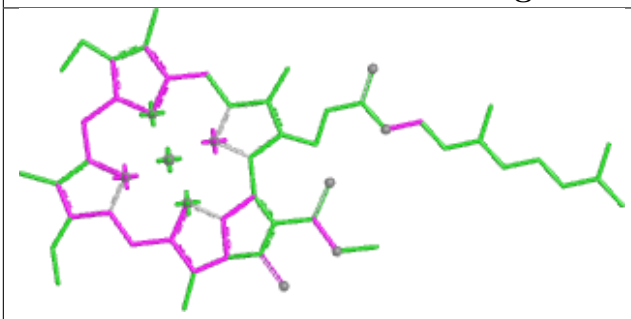
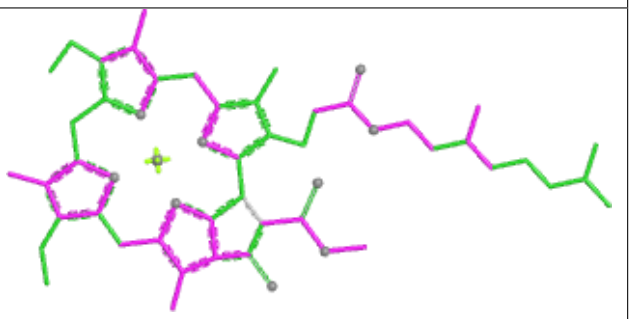
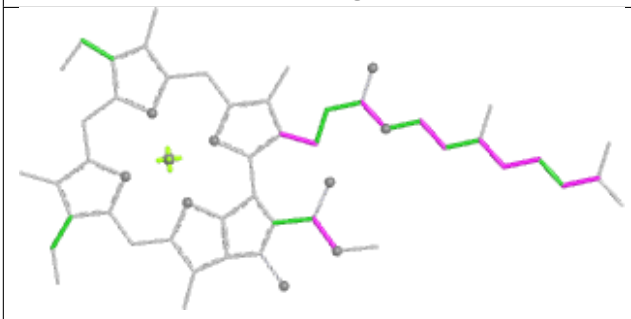
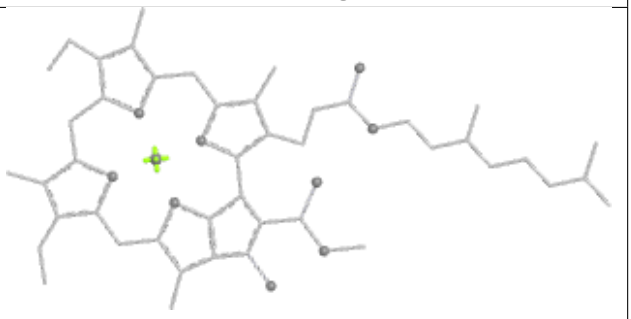
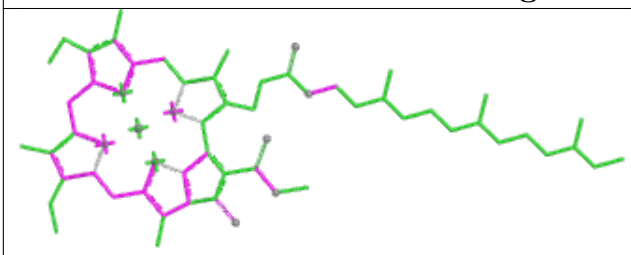
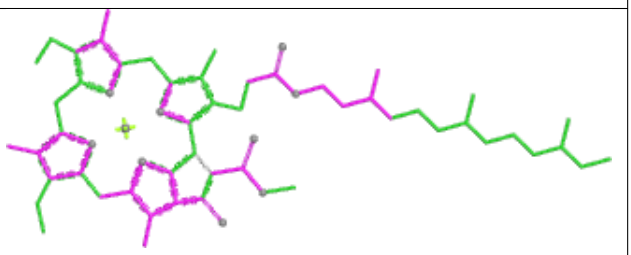
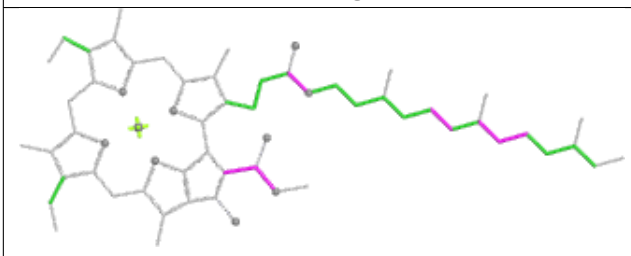
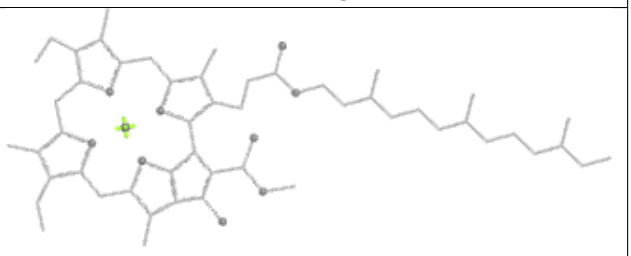
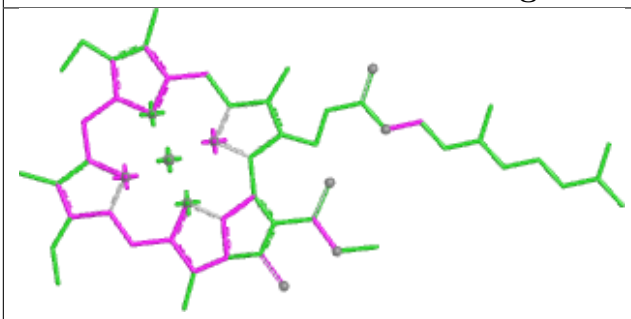
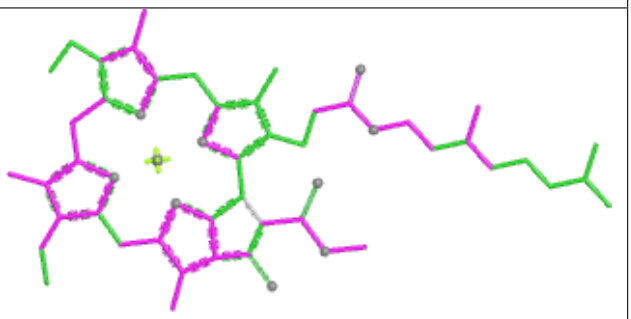
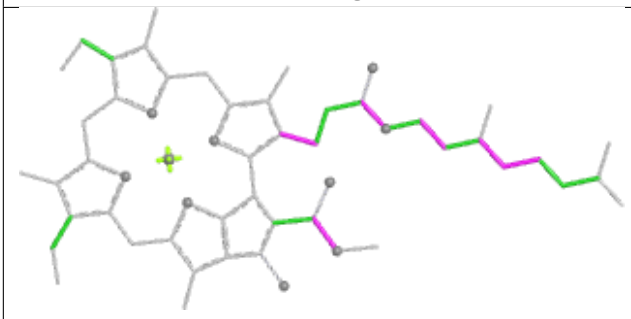
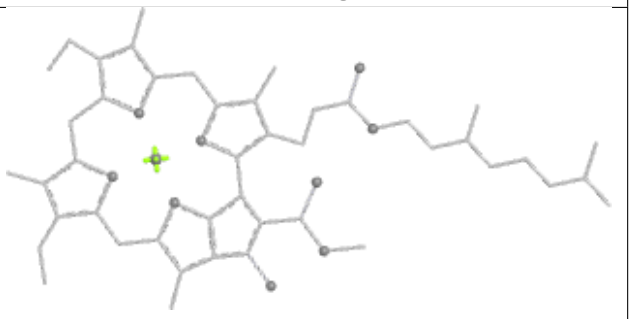
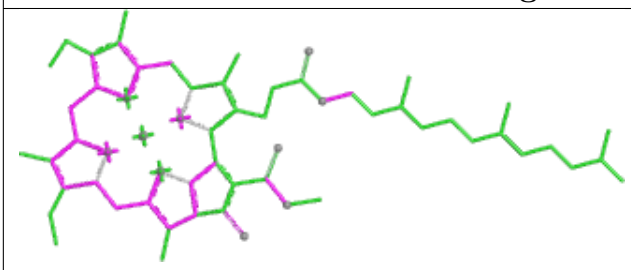
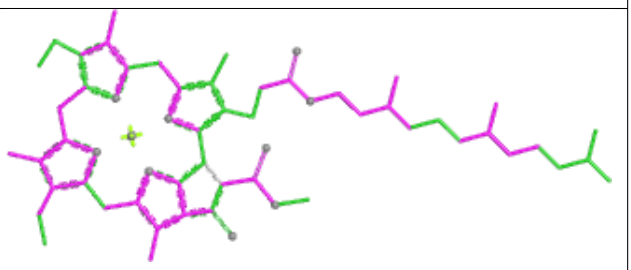
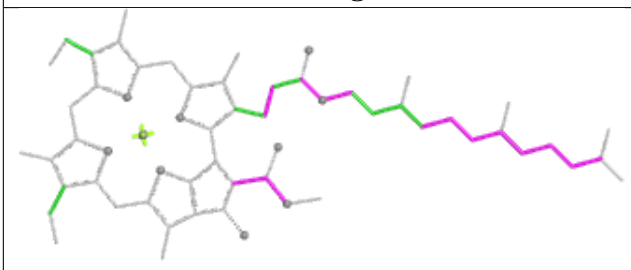
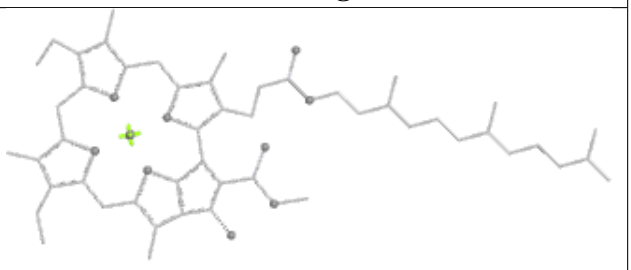


Rings

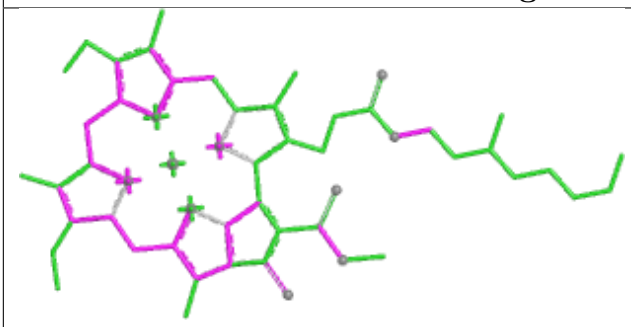
Ligand CLA A 1237	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1118	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1237	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1111	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1110



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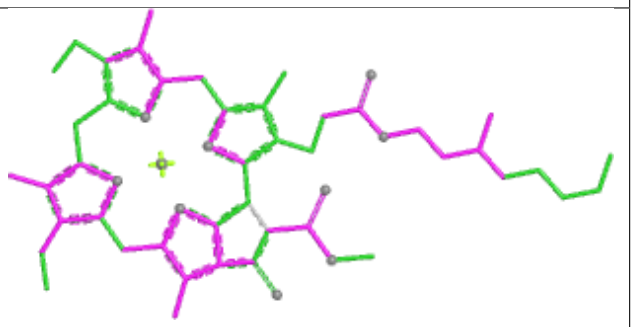
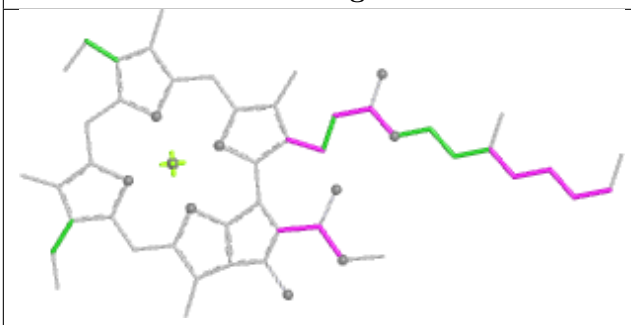


Bond angles



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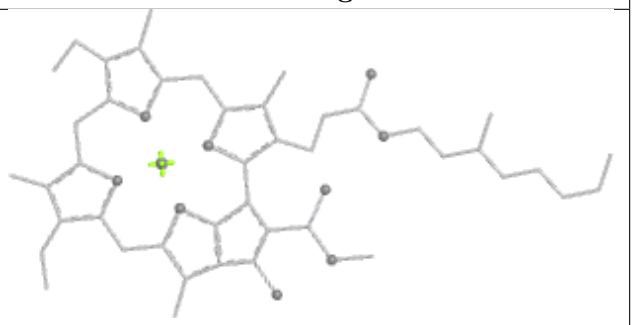
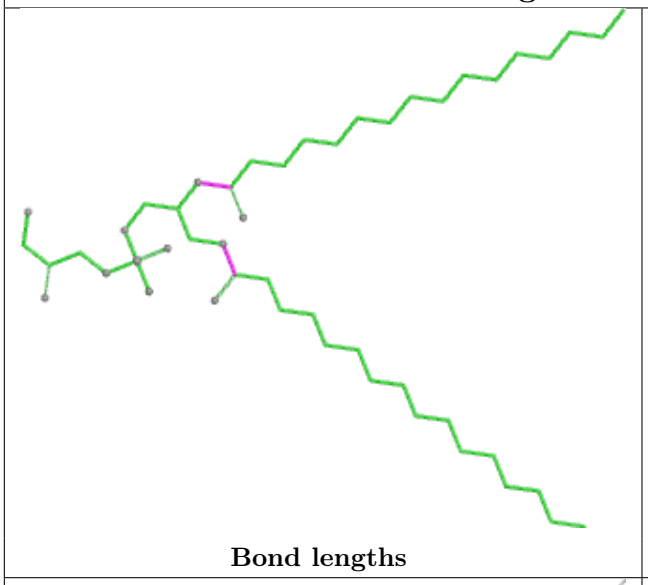


Rings

Ligand LHG 1 5001



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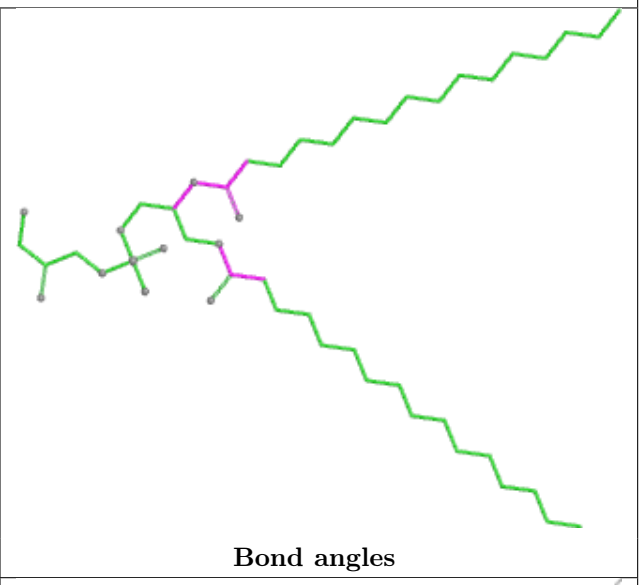

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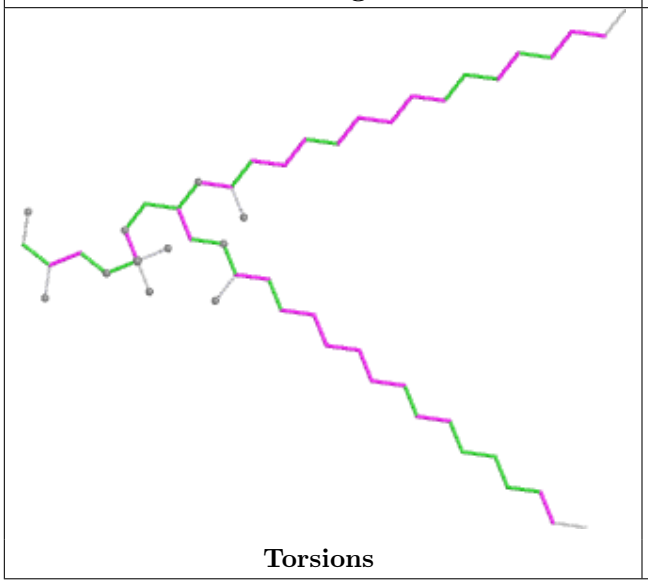

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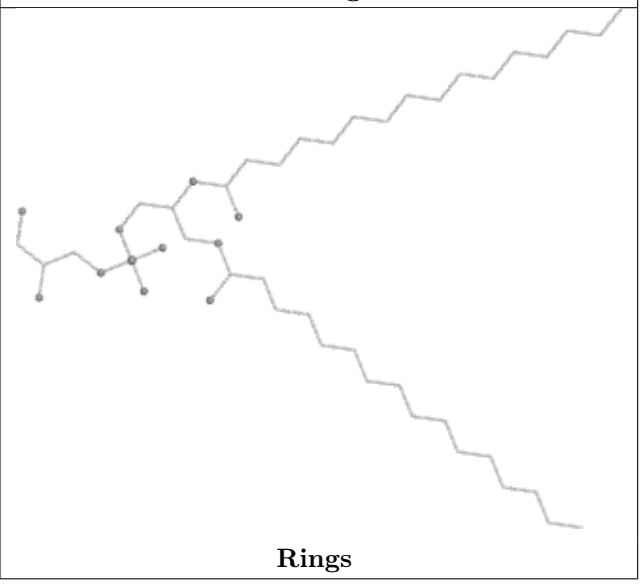
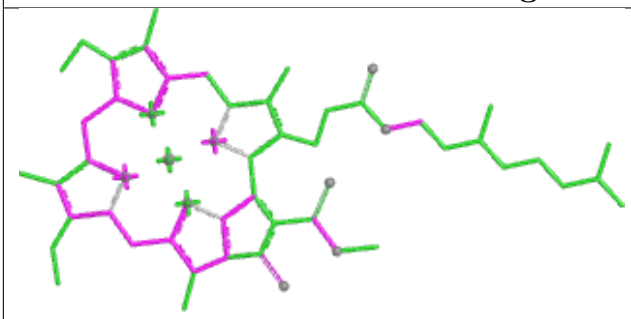


Rings

Ligand CLA a 1124



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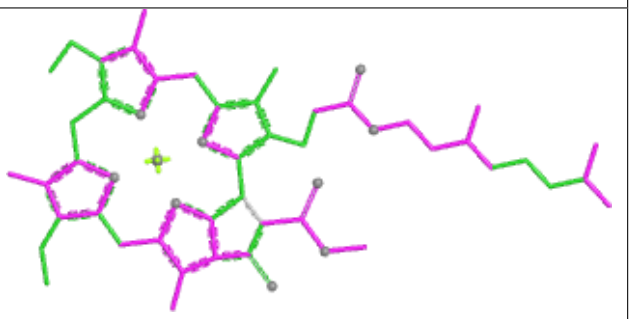

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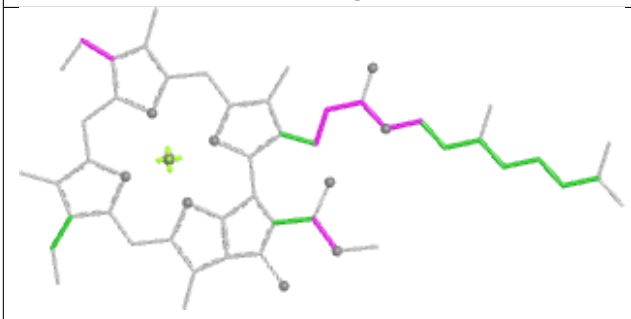

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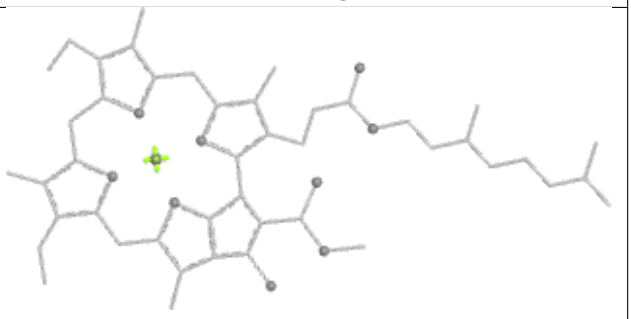
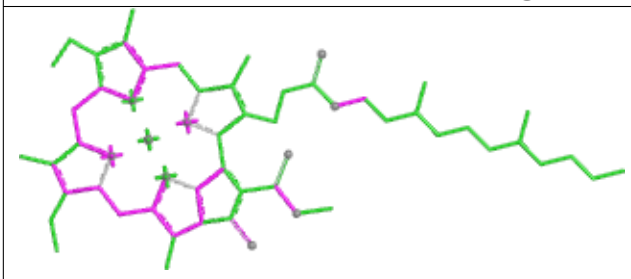


Rings

Ligand CLA b 1230



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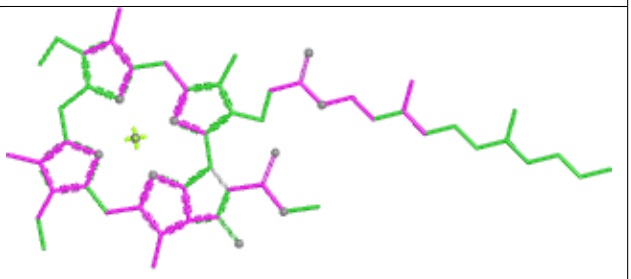

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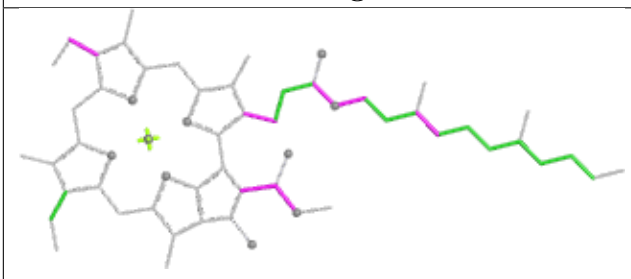

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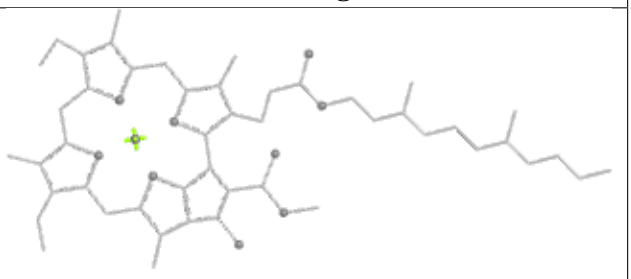

Rings

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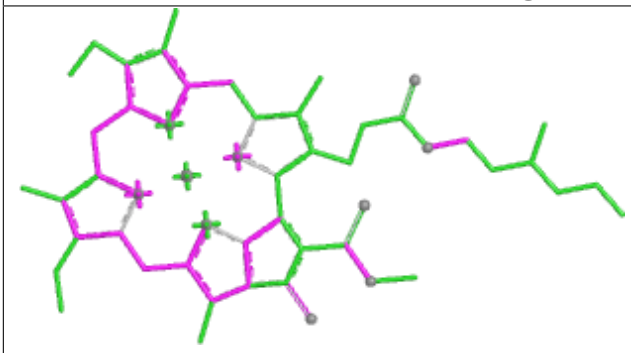
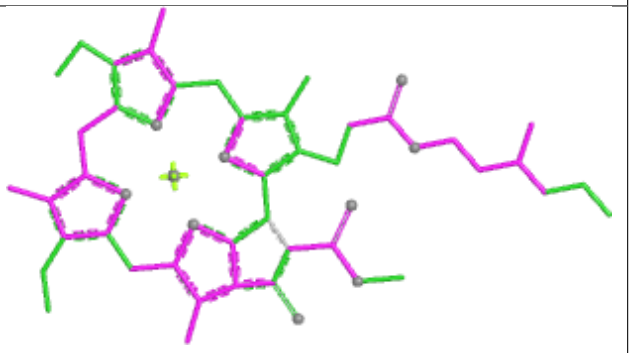
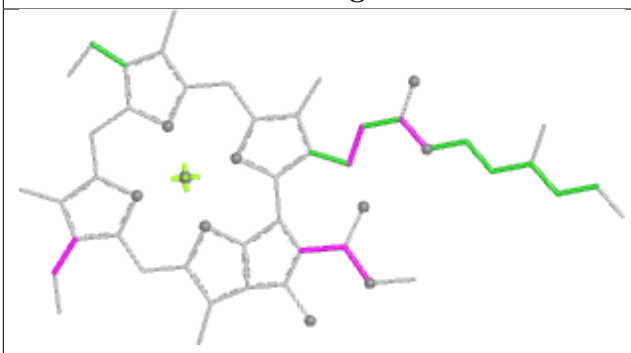
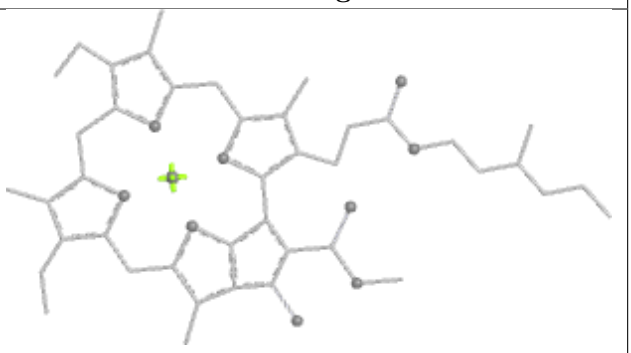
	
Bond lengths	Bond angles
	
Torsions	Rings

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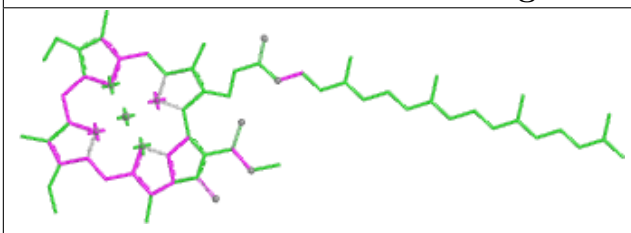	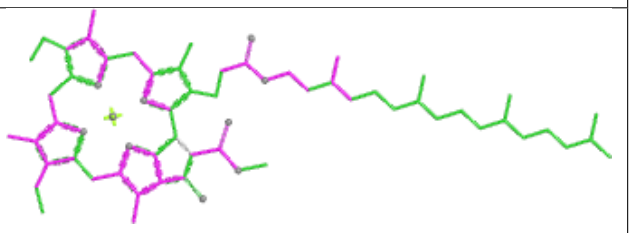
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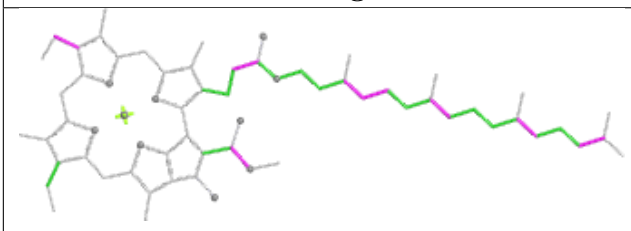
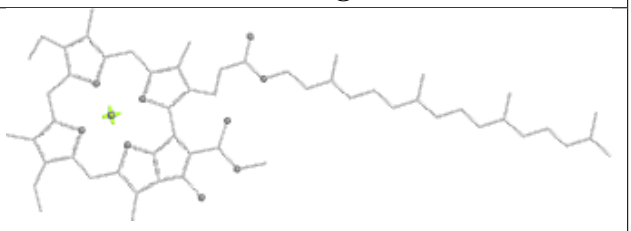
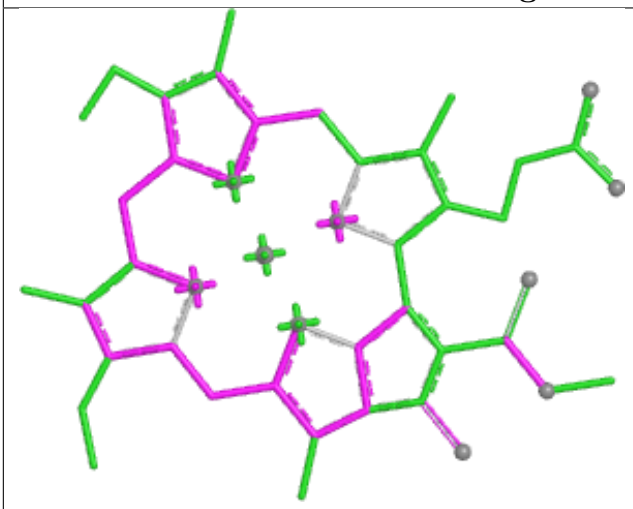
	
Torsions	Rings

Ligand CLA 1 1113



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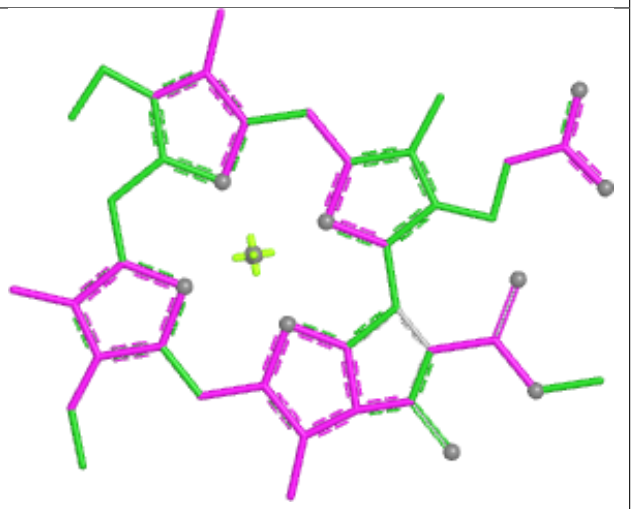
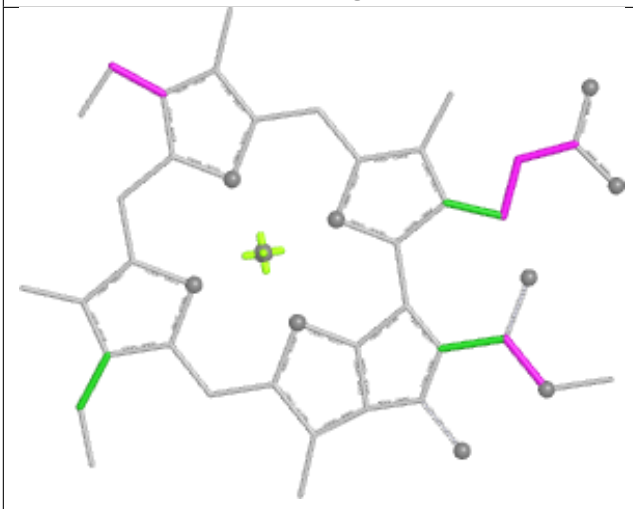


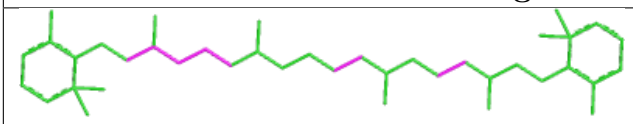
Bond angles



Torsions

Rings

Ligand BCR B 4004



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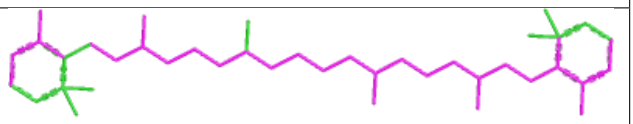

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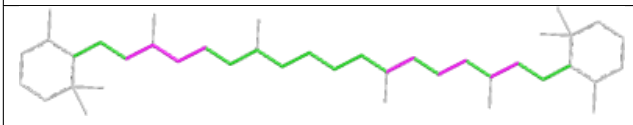

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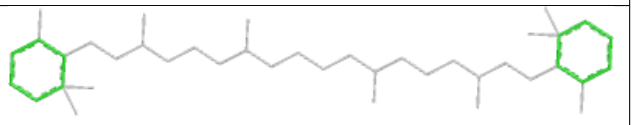
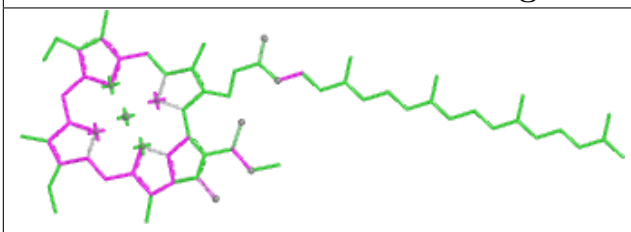


Rings

Ligand CLA 2 1213



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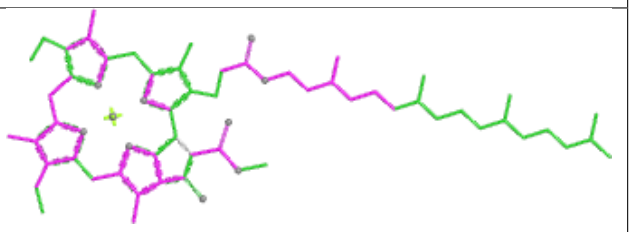
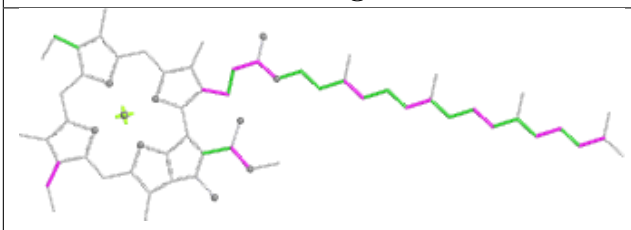


Bond angles



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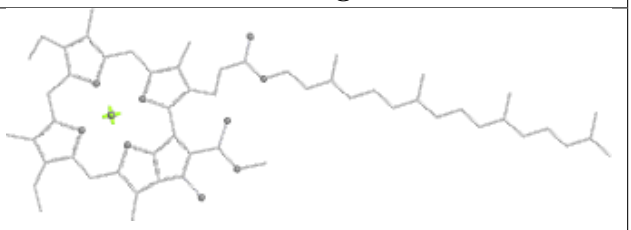

Rings

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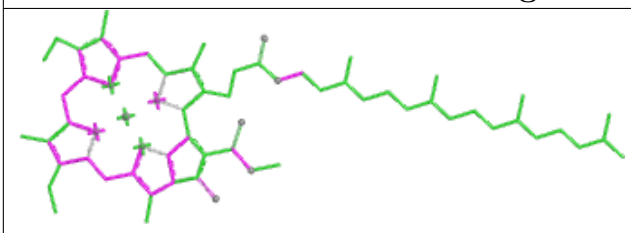

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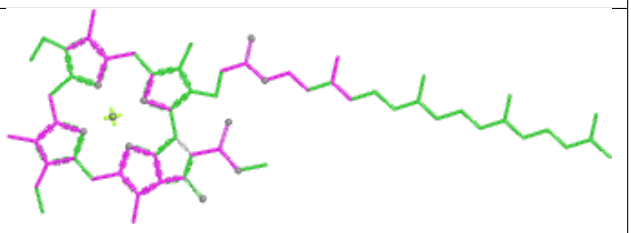
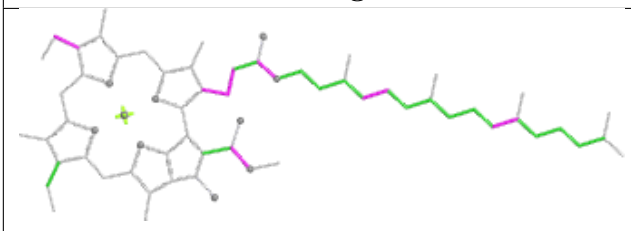


Bond angles



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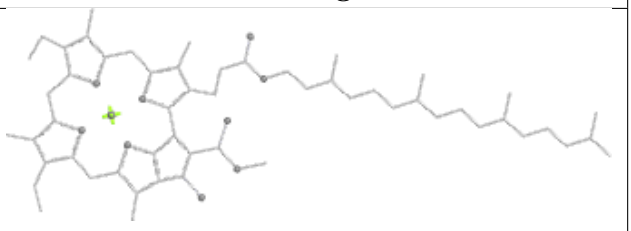
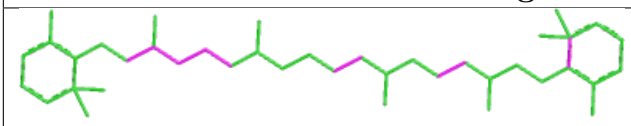


Rings

Ligand BCR 2 4017



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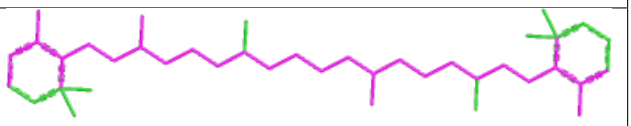

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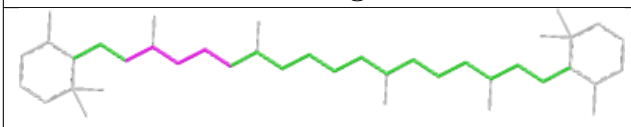

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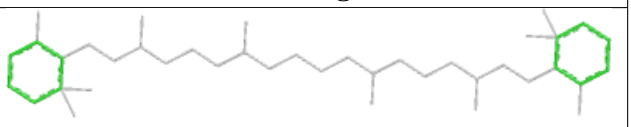
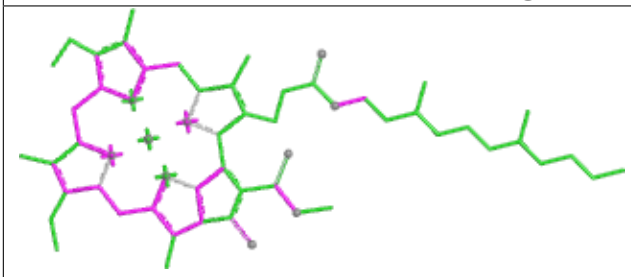
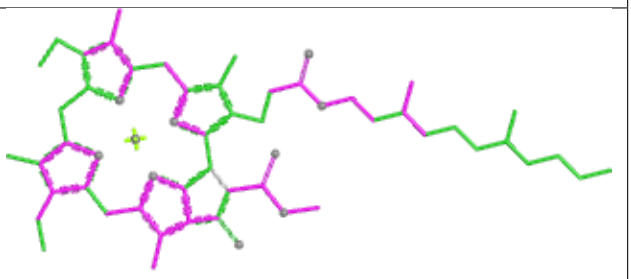
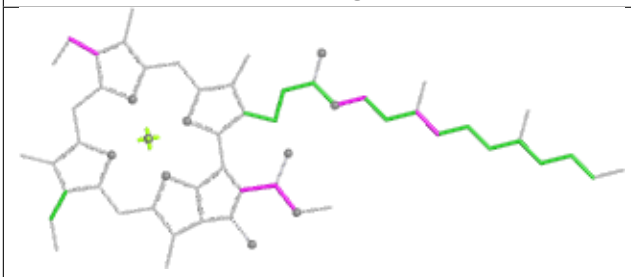
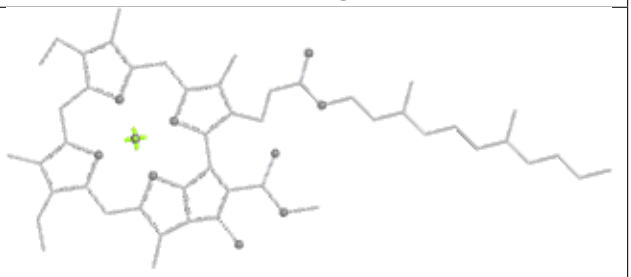
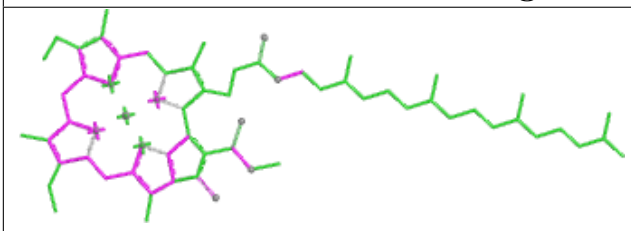
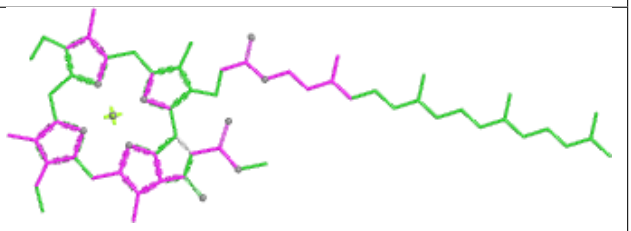
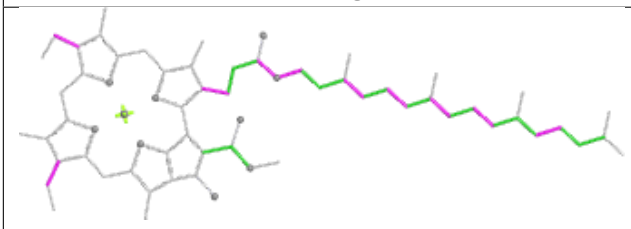
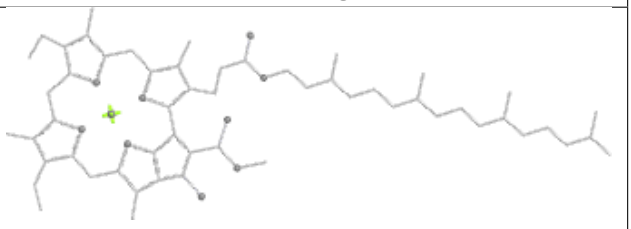
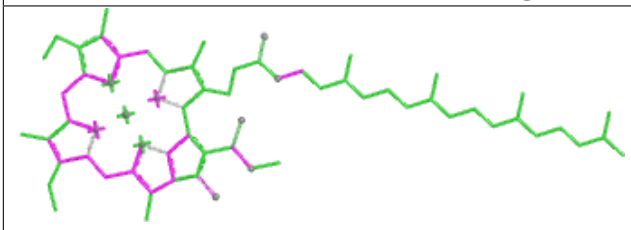


Rings

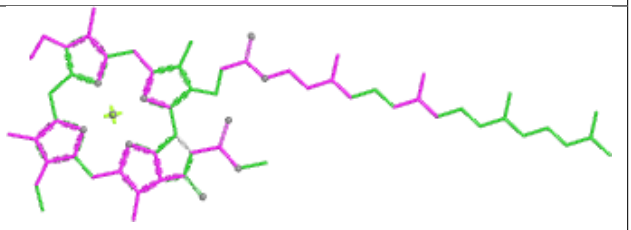
Ligand CLA 2 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 1213	
 Bond lengths	 Bond angles
 Torsions	 Rings

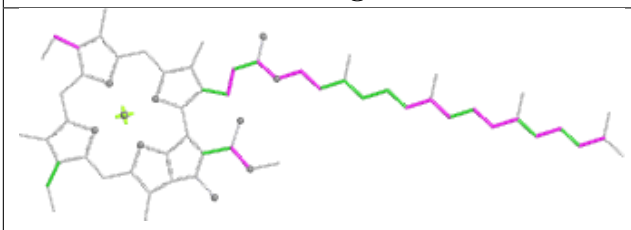
Ligand CLA b 1023



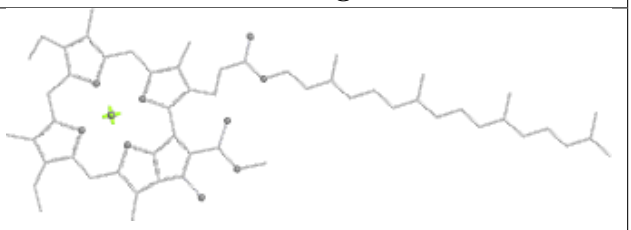
Bond lengths



Bond angles

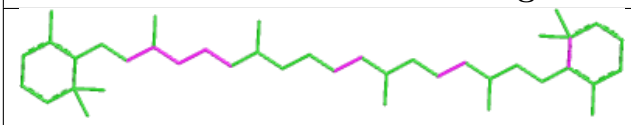


Torsions



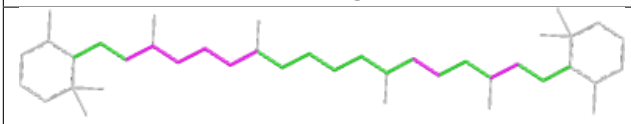
Rings

Ligand BCR a 4008

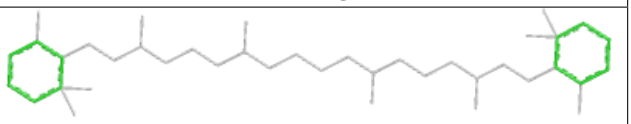


Bond lengths

Bond angles

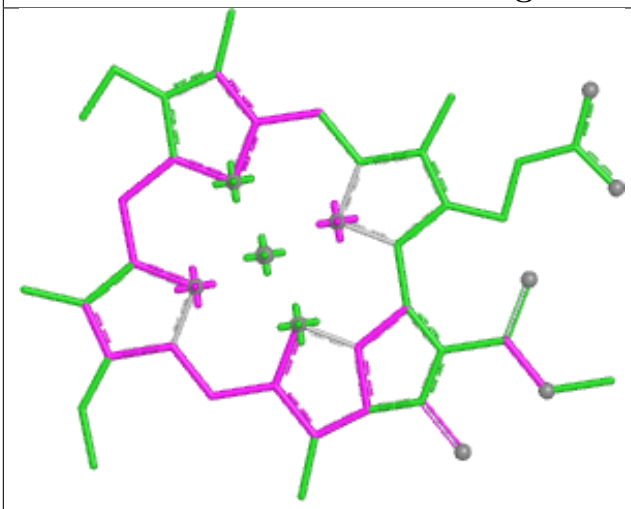


Torsions

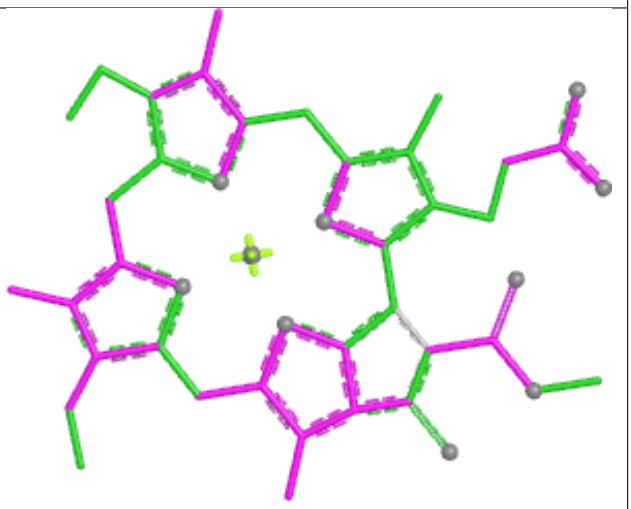


Rings

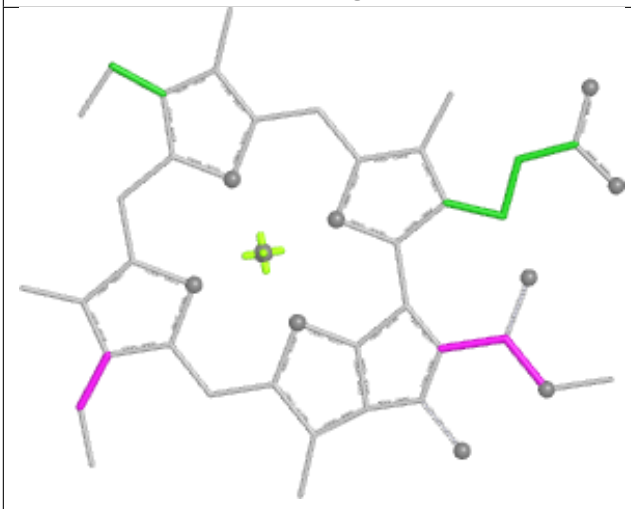
Ligand CLA B 1227



Bond lengths



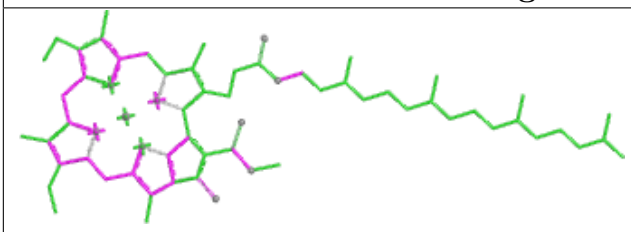
Bond angles



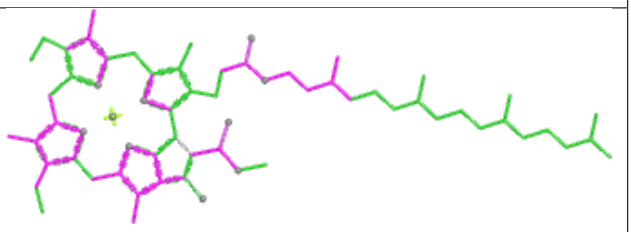
Torsions

Rings

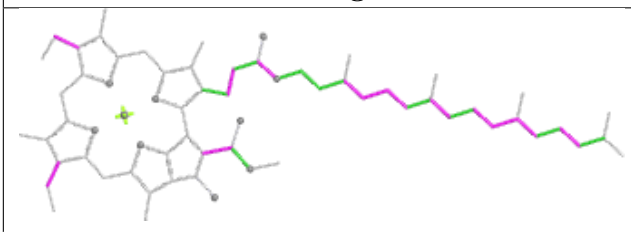
Ligand CLA b 1223



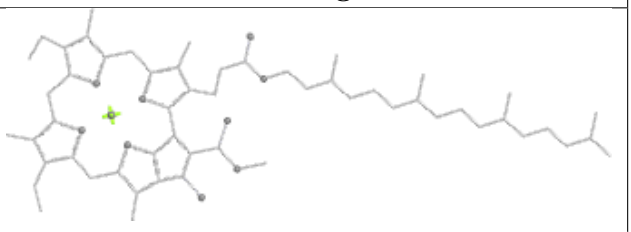
Bond lengths



Bond angles

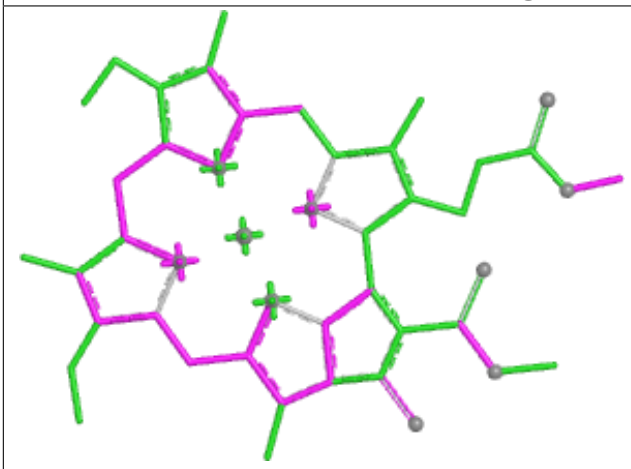


Torsions

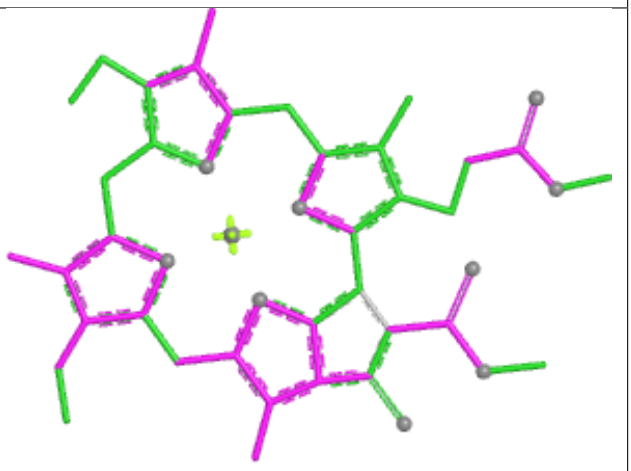


Rings

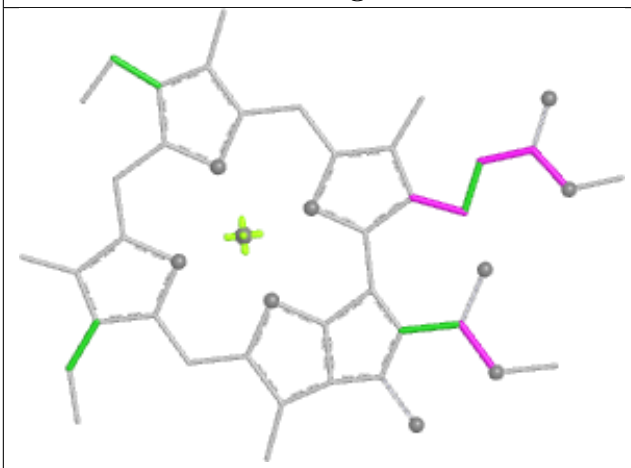
Ligand CLA a 1114



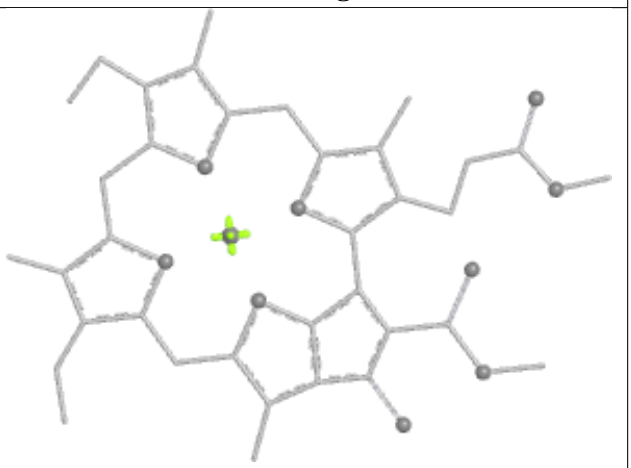
Bond lengths



Bond angles

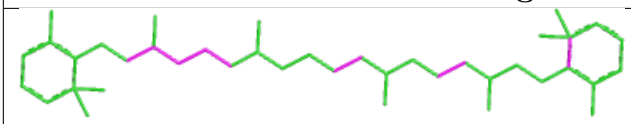


Torsions



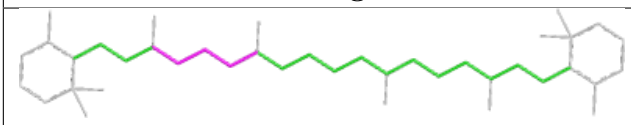
Rings

Ligand BCR b 4017

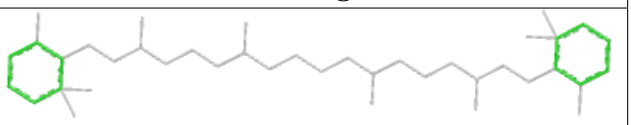


Bond lengths

Bond angles

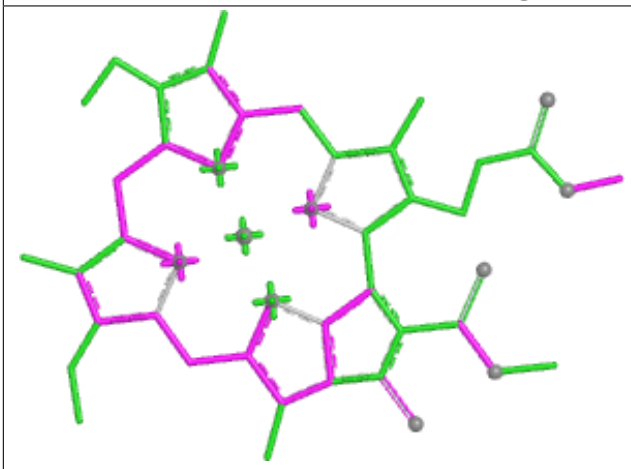


Torsions

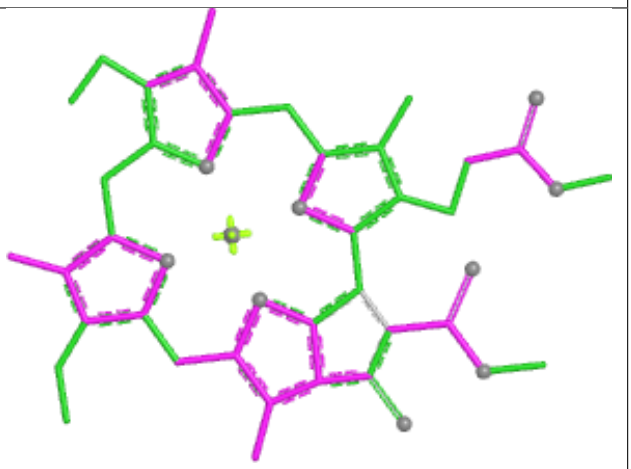


Rings

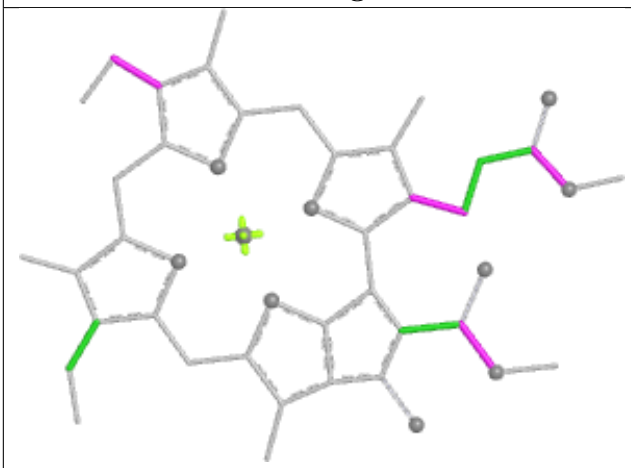
Ligand CLA B 1211



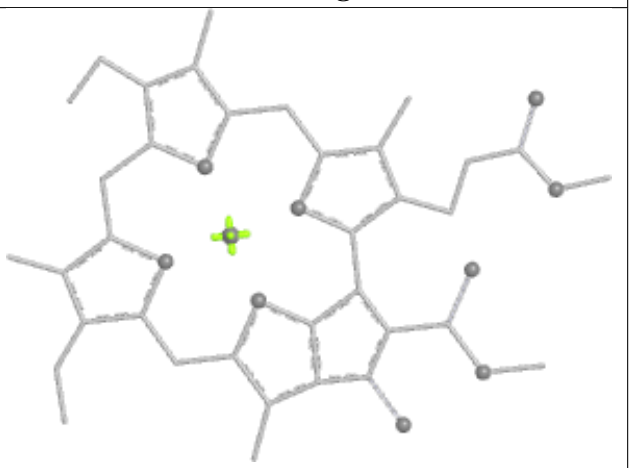
Bond lengths



Bond angles

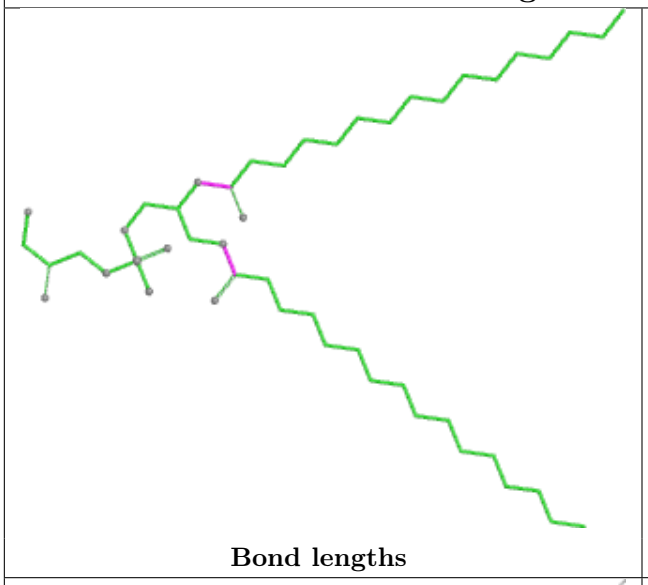


Torsions



Rings

Ligand LHG a 5001



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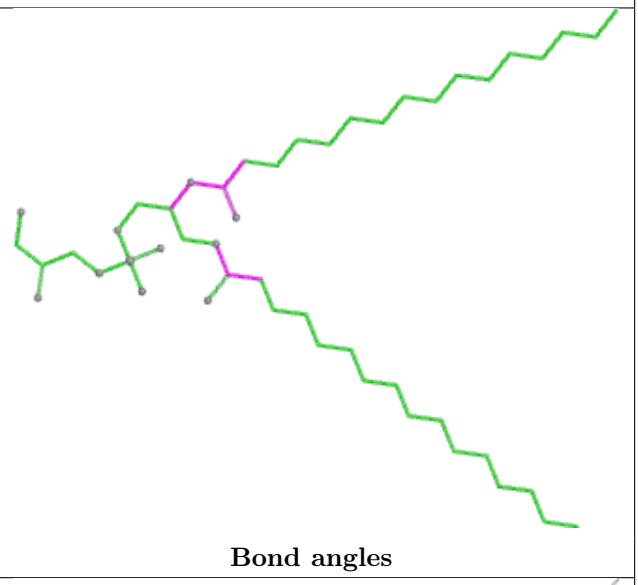
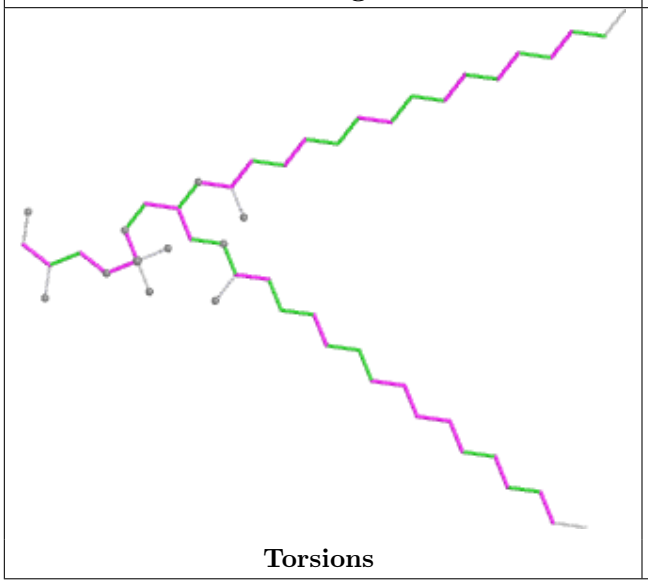


Bond angles



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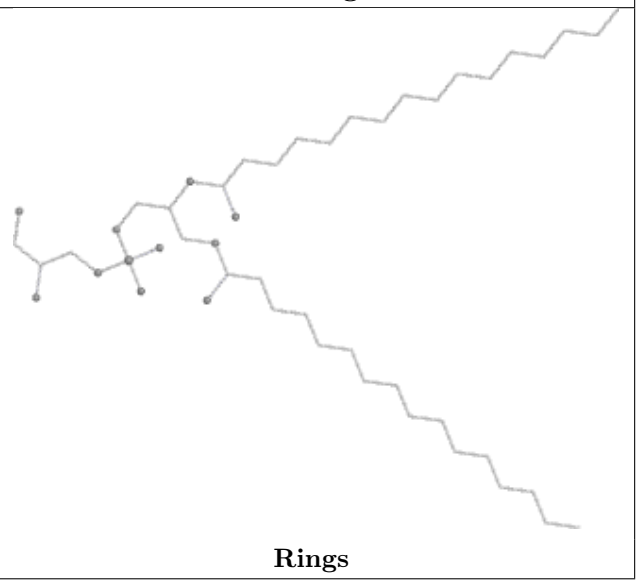
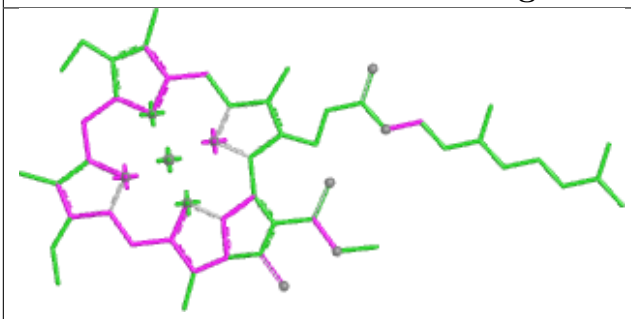
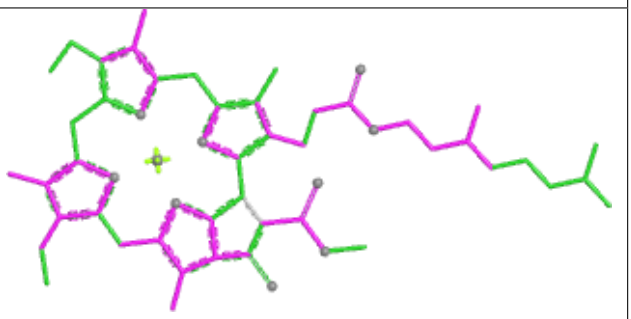


Rings

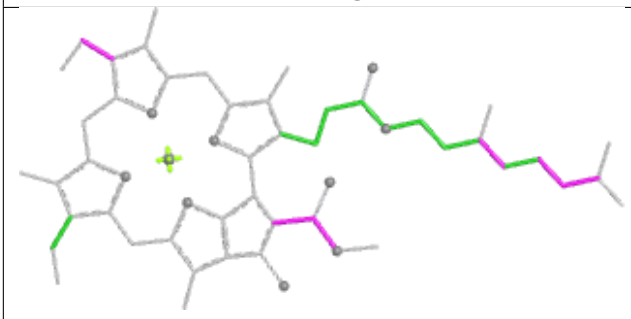
Ligand CLA b 1205



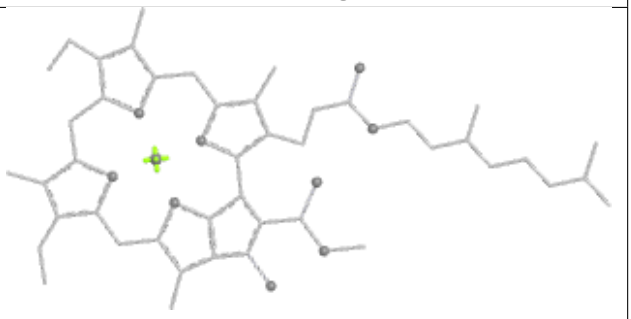
Bond lengths



Bond angles

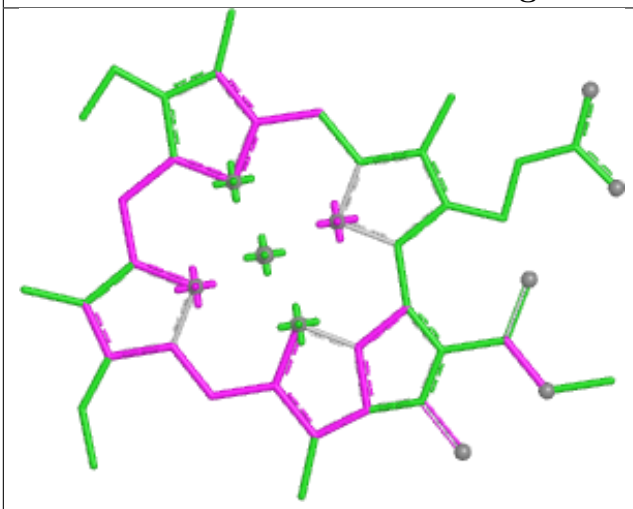


Torsions



Rings

Ligand CLA 2 1227



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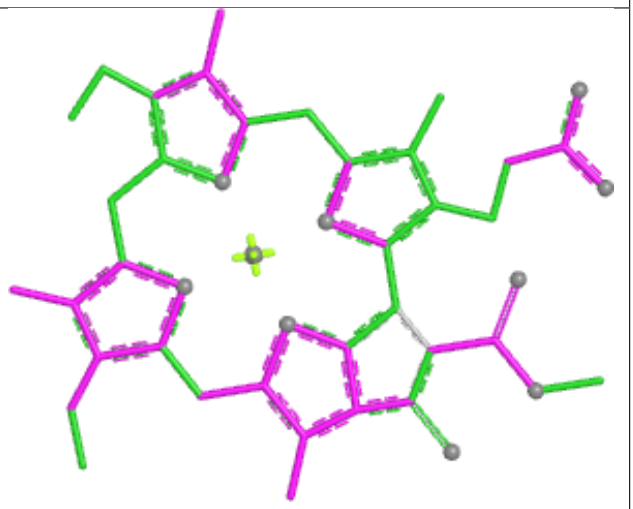
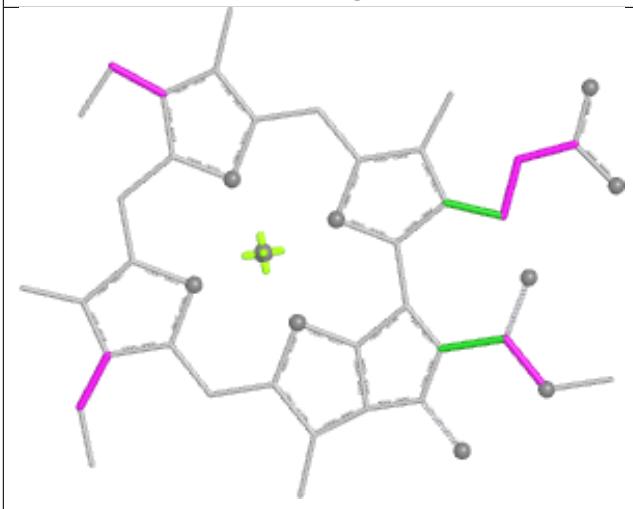


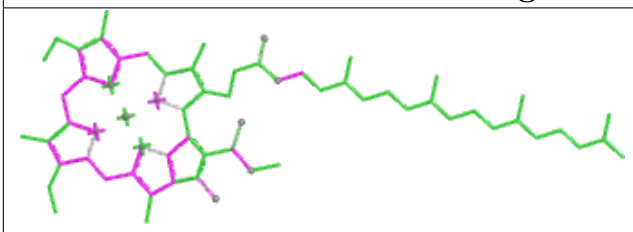
Bond angles



Torsions

Rings

Ligand CLA b 1226



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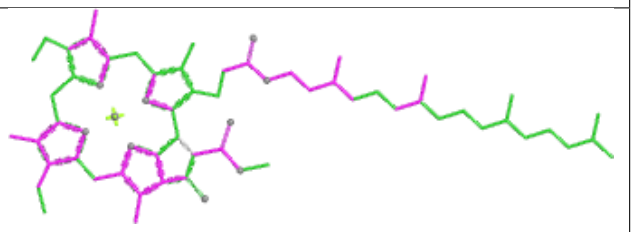
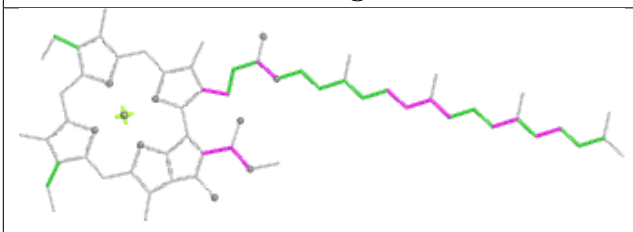
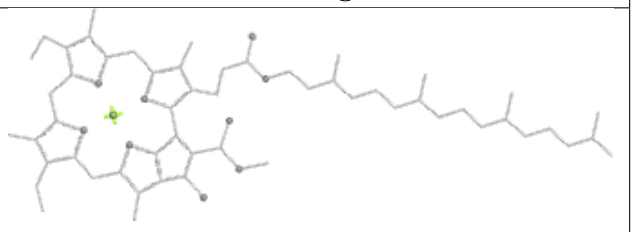


Bond angles

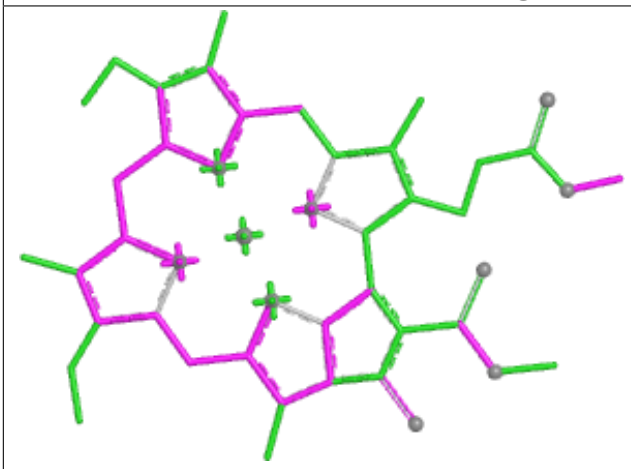


Torsions



Rings

Ligand CLA A 1115



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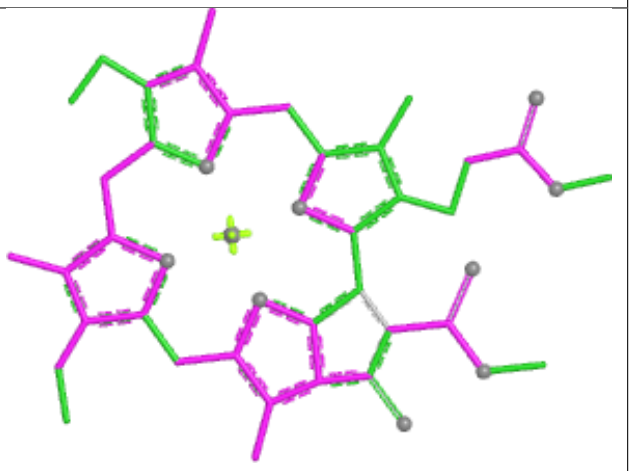
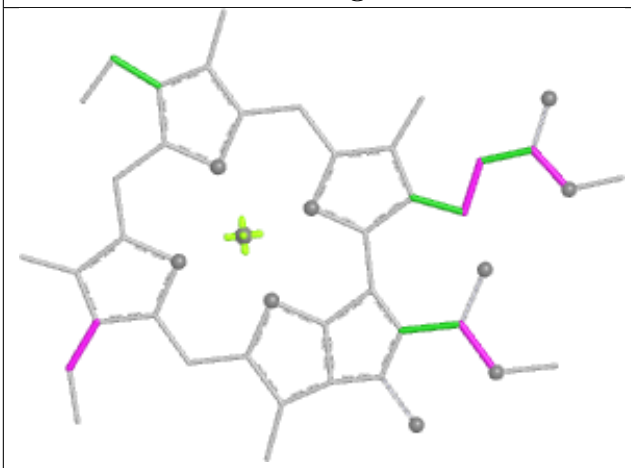
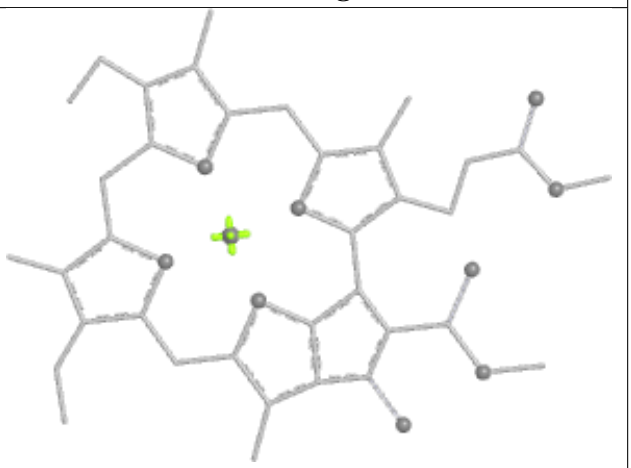


Bond angles

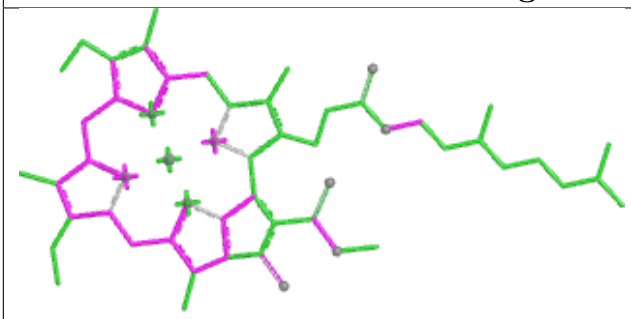


Torsions



Rings

Ligand CLA b 1224



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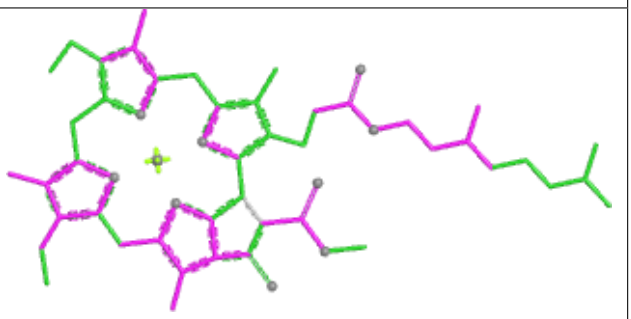
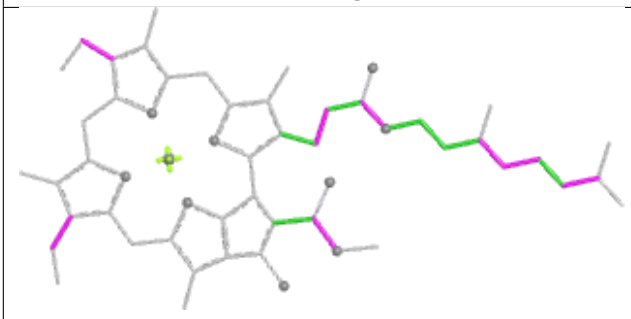
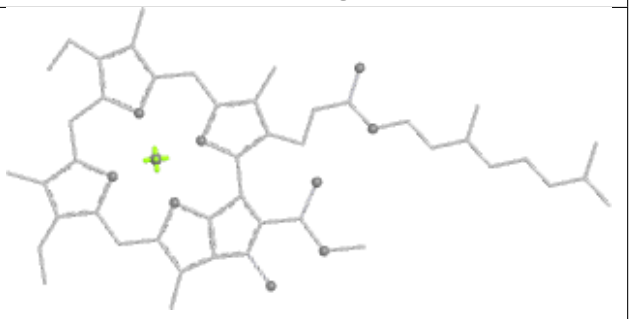


Bond angles

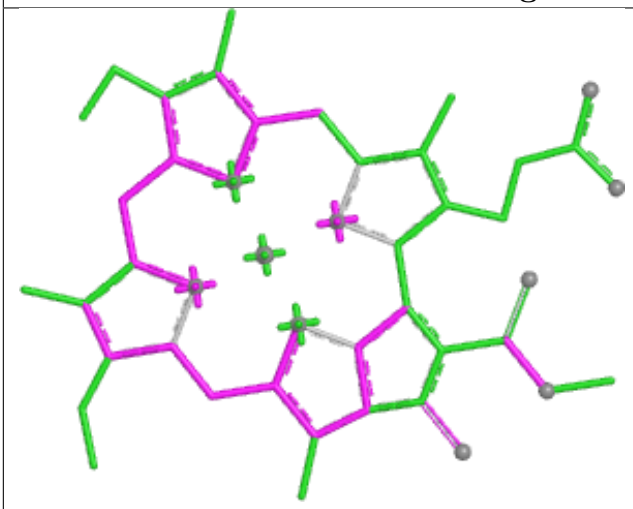


Torsions

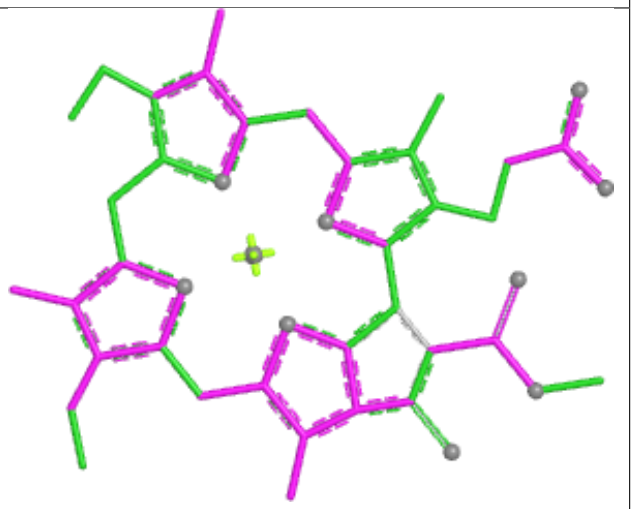


Rings

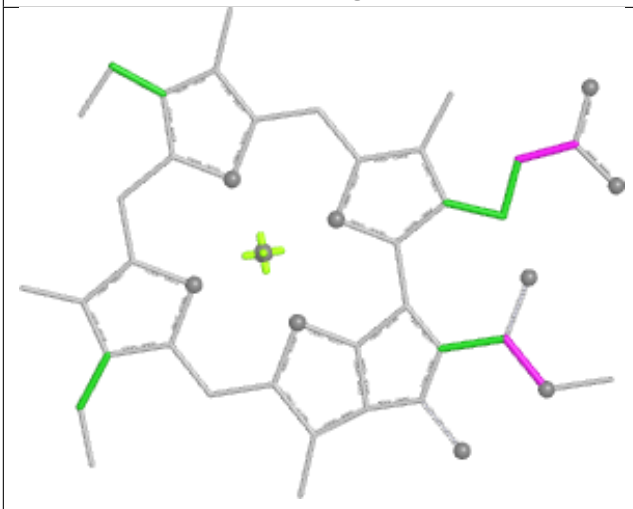
Ligand CLA a 1113



Bond lengths



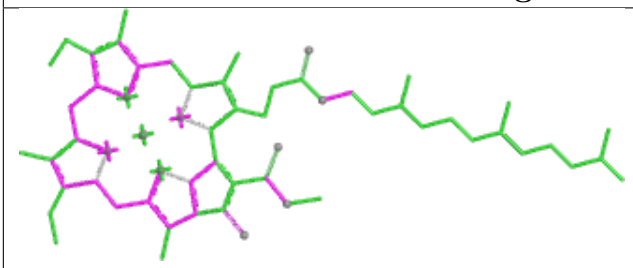
Bond angles



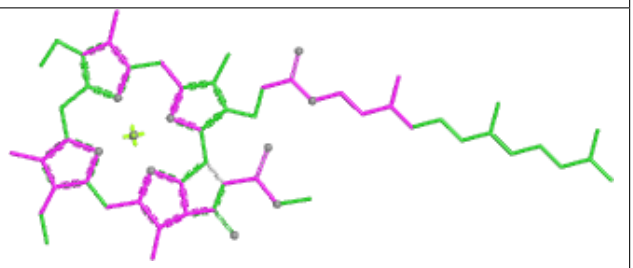
Torsions

Rings

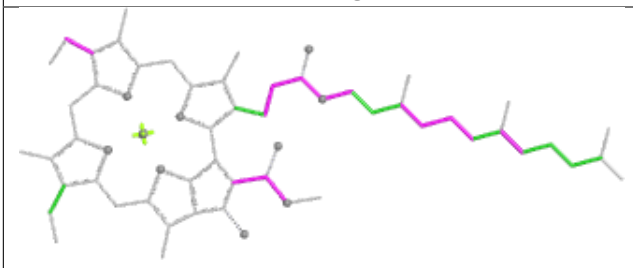
Ligand CLA A 1111



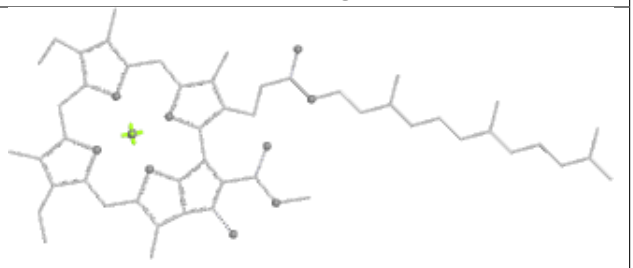
Bond lengths



Bond angles

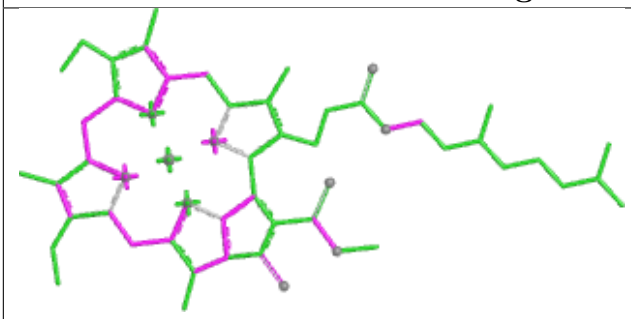


Torsions

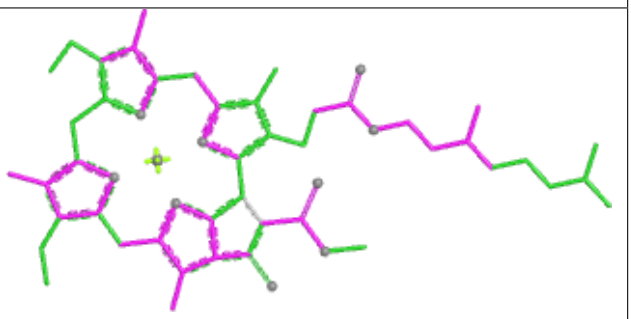


Rings

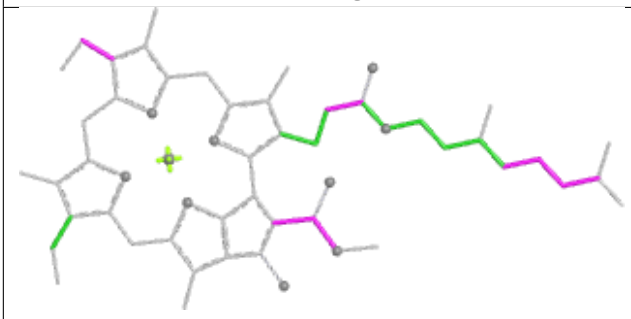
Ligand CLA B 1205



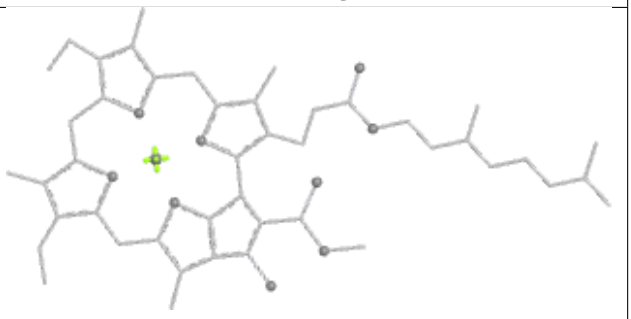
Bond lengths



Bond angles

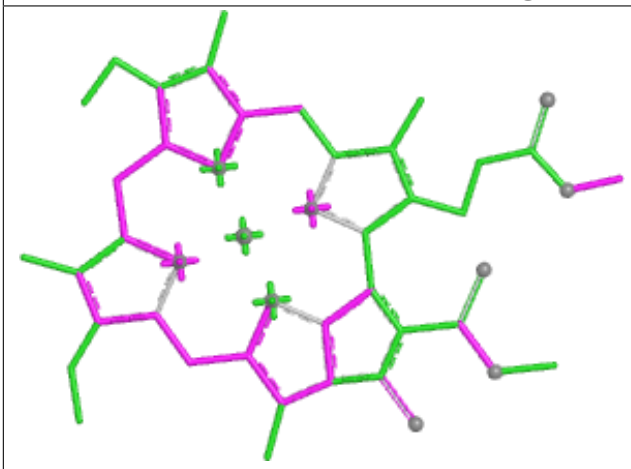


Torsions



Rings

Ligand CLA 1 1114



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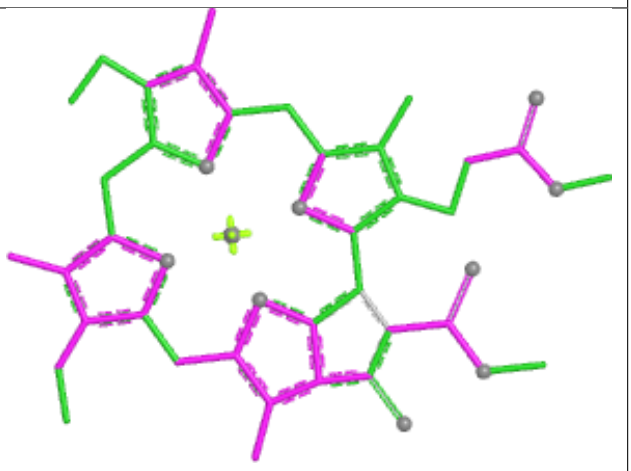
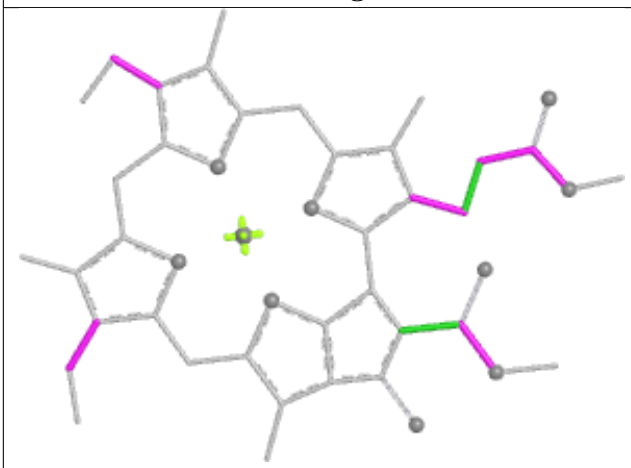


Bond angles



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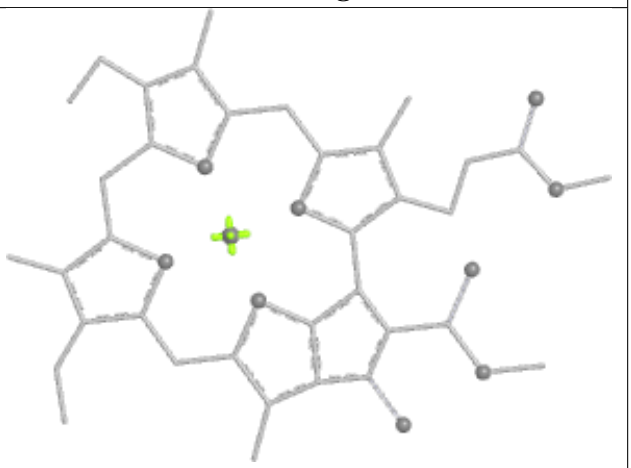
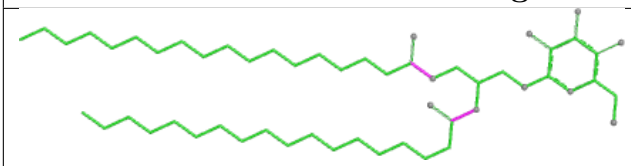


Rings

Ligand LMG B 5002



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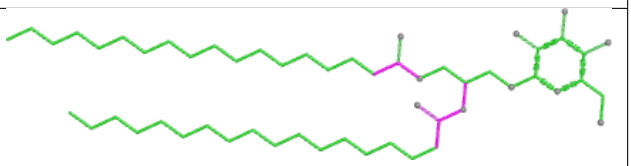
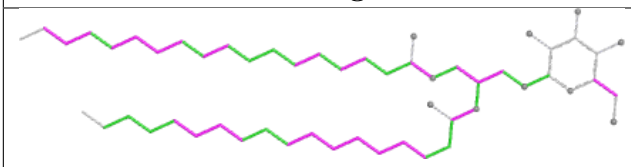


Bond angles



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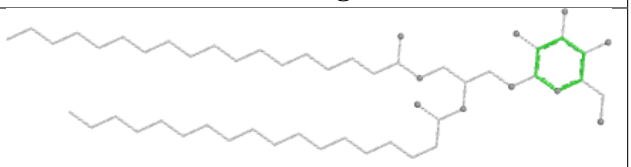
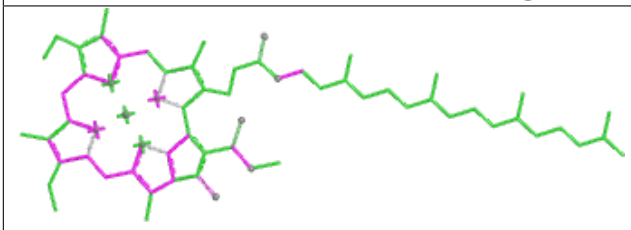
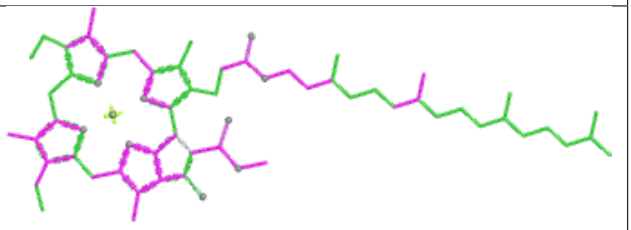


Rings

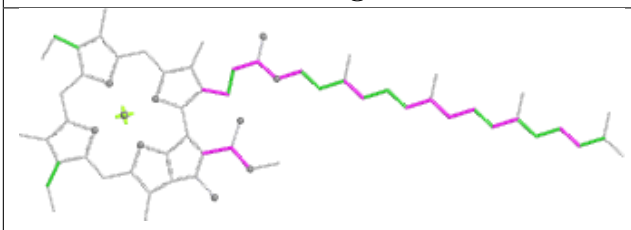
Ligand CLA 1 1103



Bond lengths



Bond angles



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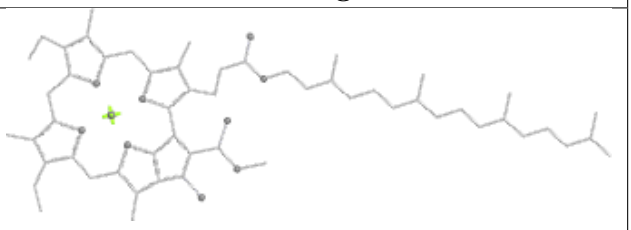
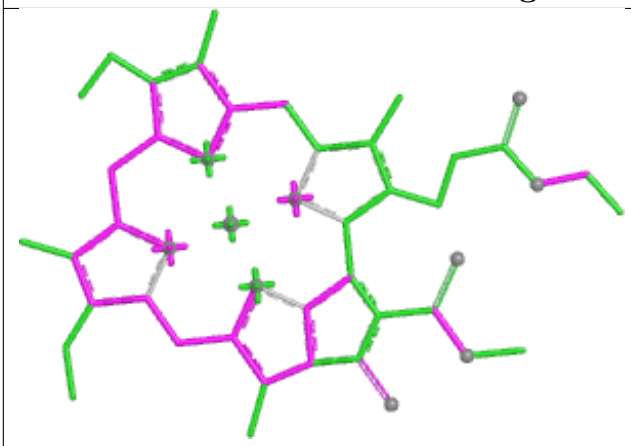


Rings

Ligand CLA 2 1236



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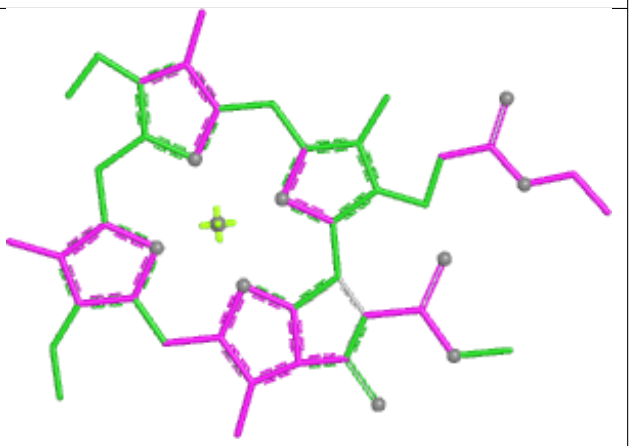
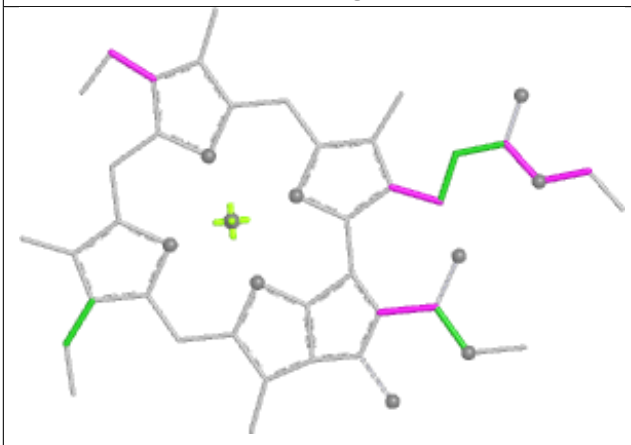


Bond angles



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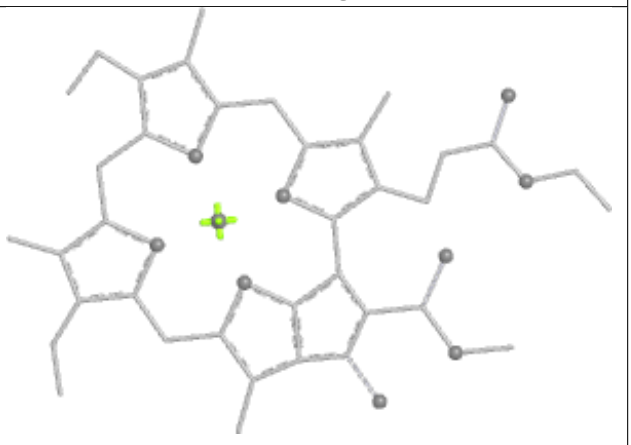
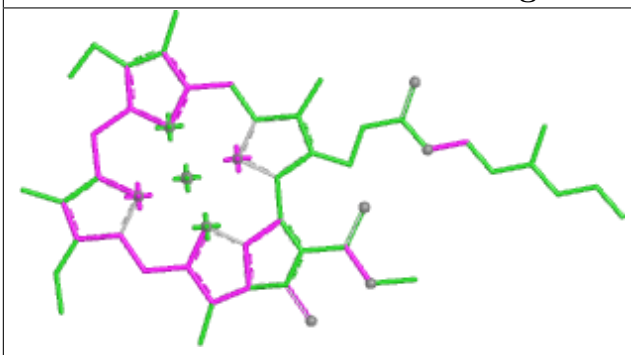
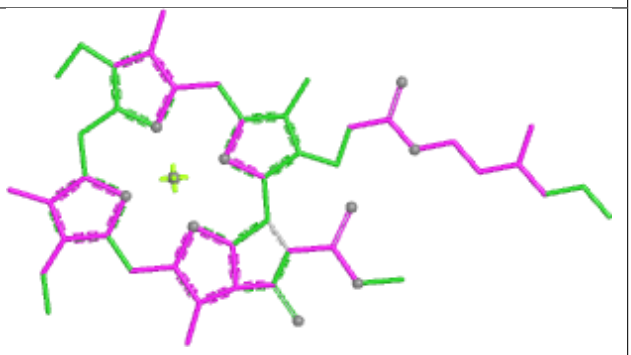


Rings

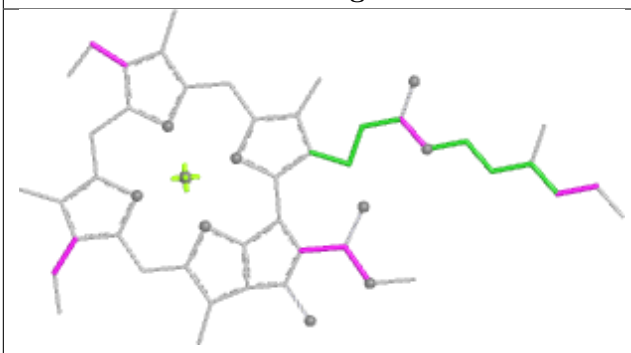
Ligand CLA 1 1125



Bond lengths



Bond angles



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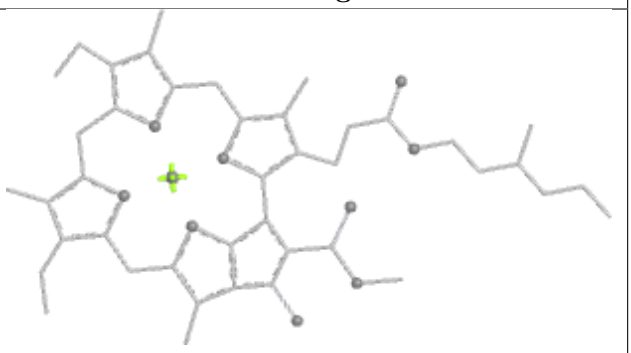
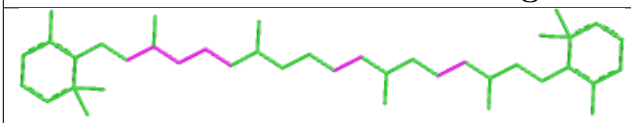
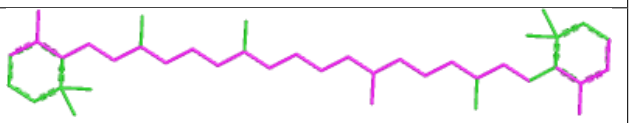


Rings

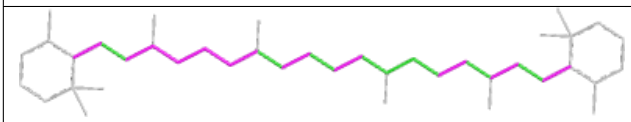
Ligand BCR l 4019



Bond lengths



Bond angles



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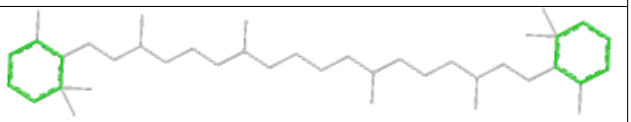
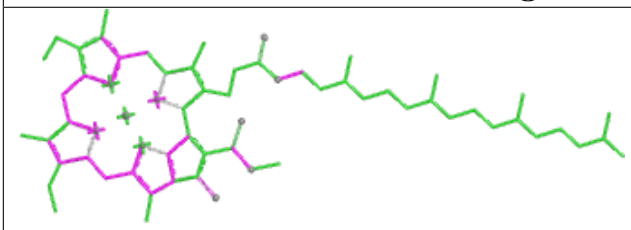


Rings

Ligand CLA 0 1401



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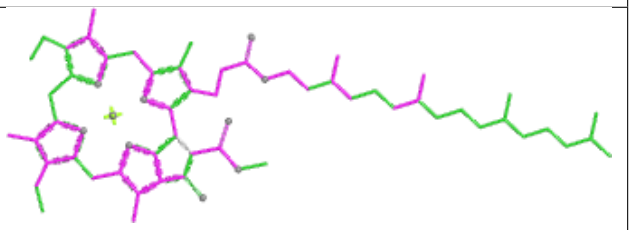
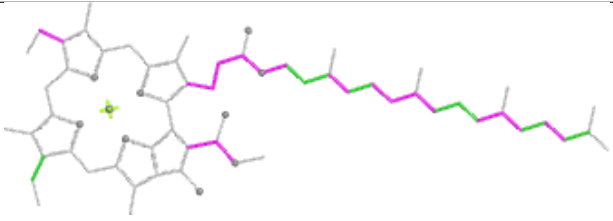


Bond angles



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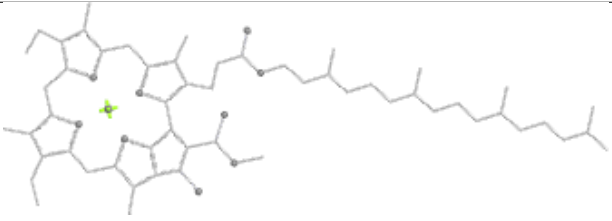
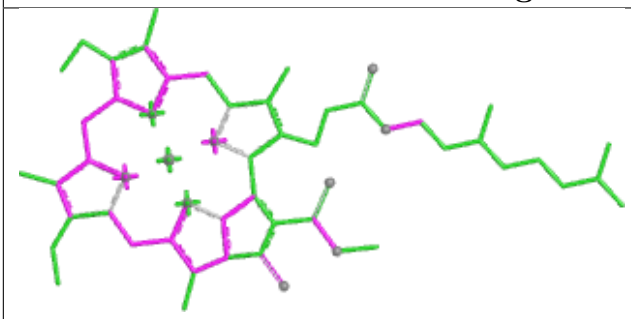


Rings

Ligand CLA B 1224



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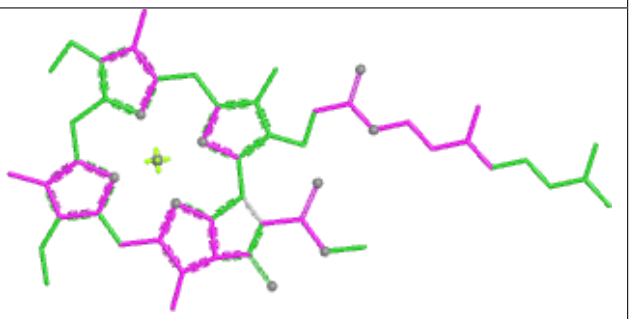
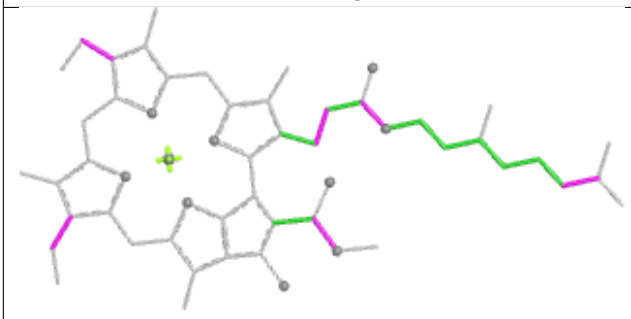
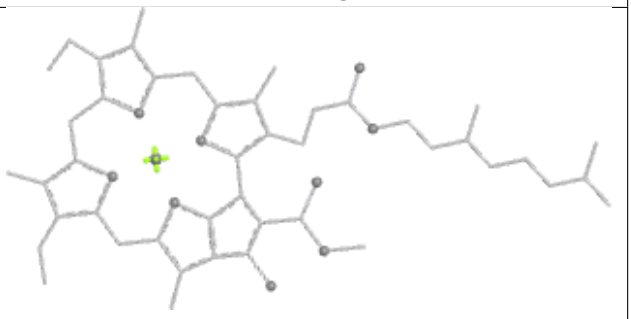


Bond angles

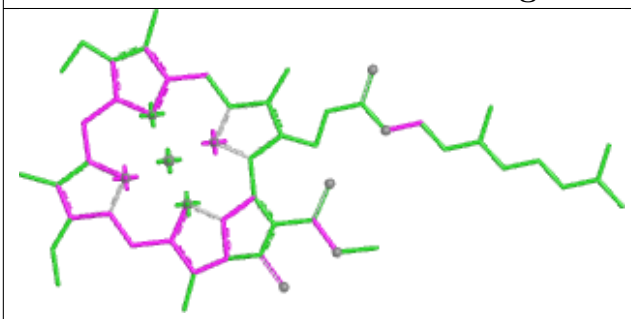


Torsions



Rings

Ligand CLA 1 1237



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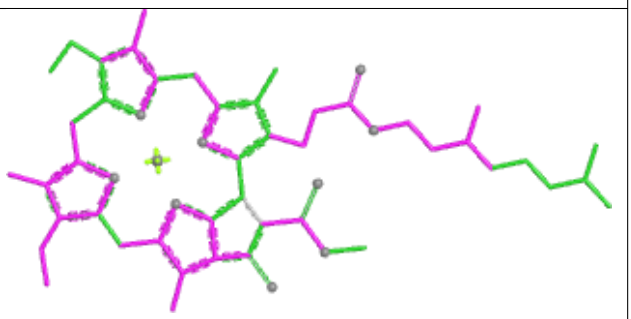
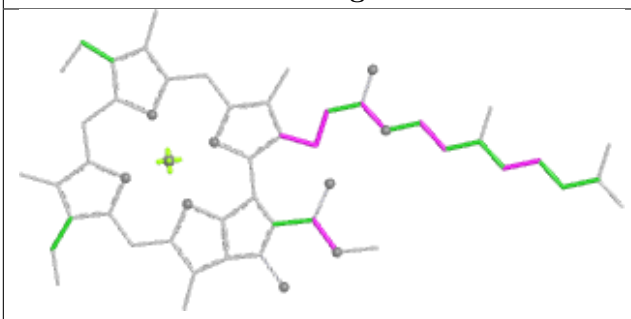


Bond angles



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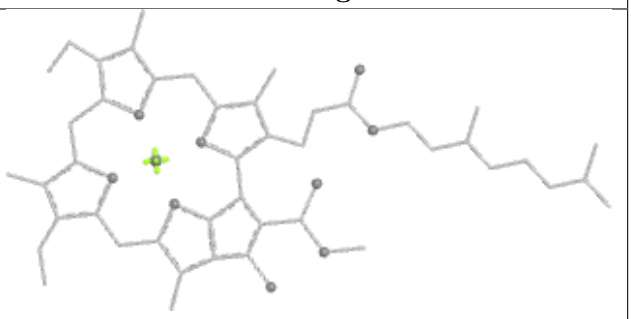
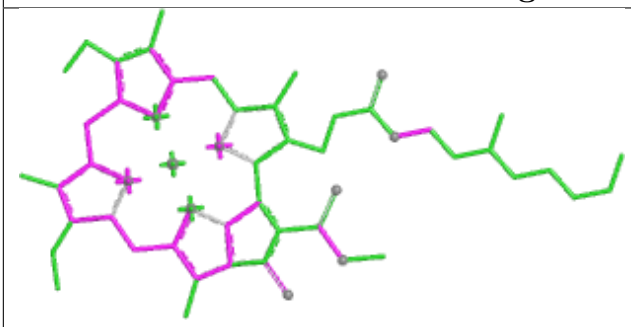


Rings

Ligand CLA b 1221



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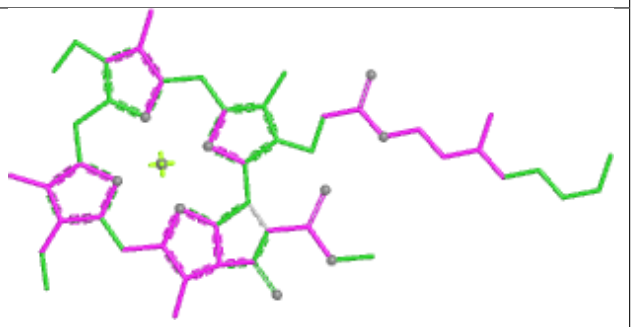
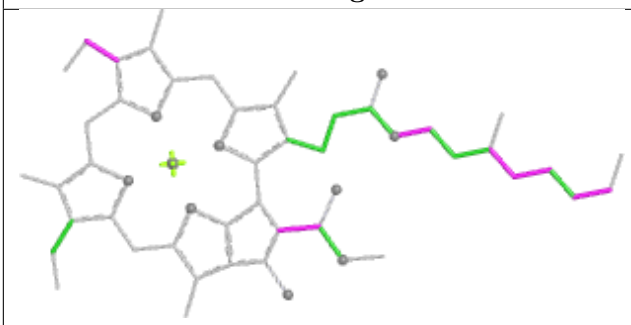


Bond angles



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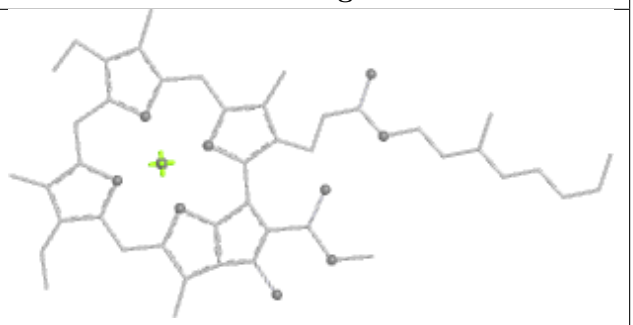
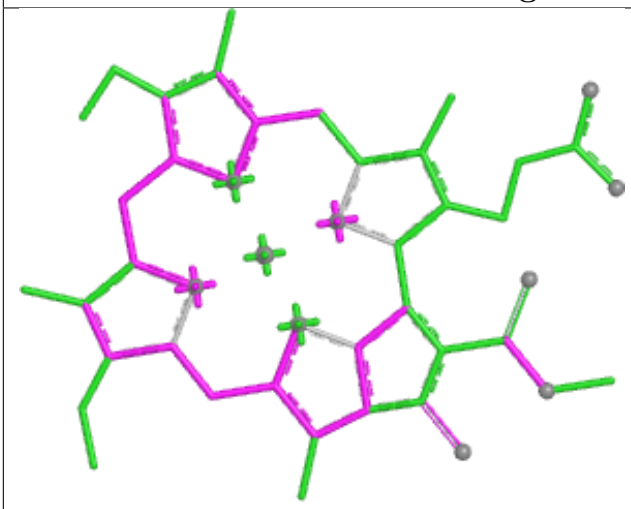


Rings

Ligand CLA 2 1208



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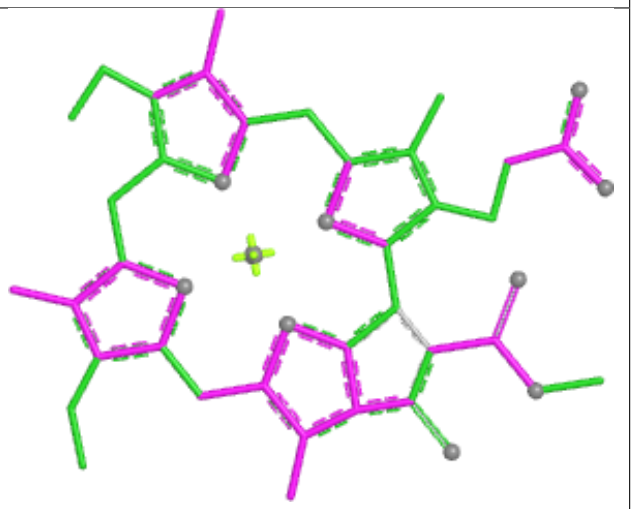
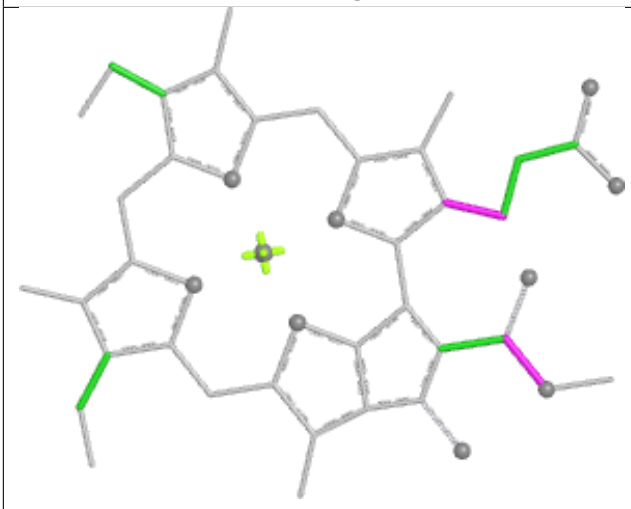


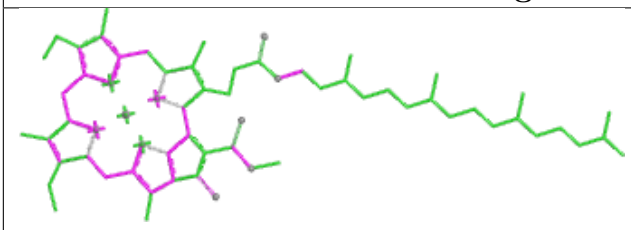
Bond angles



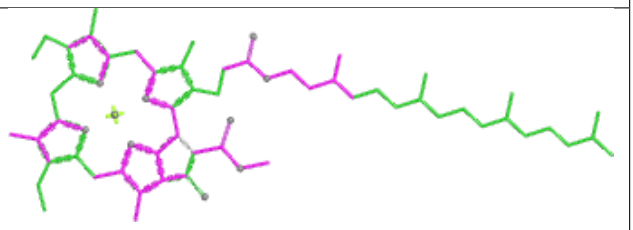
Torsions

Rings

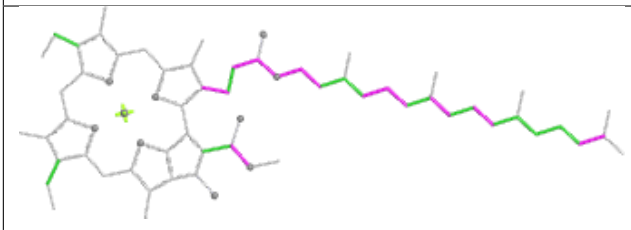
Ligand CLA A 1011



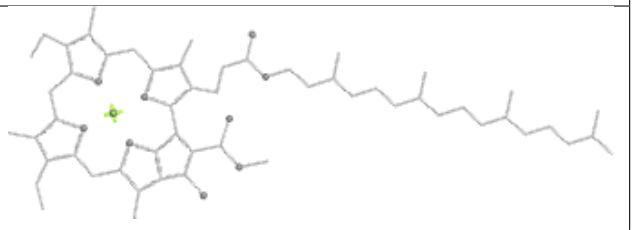
Bond lengths



Bond angles

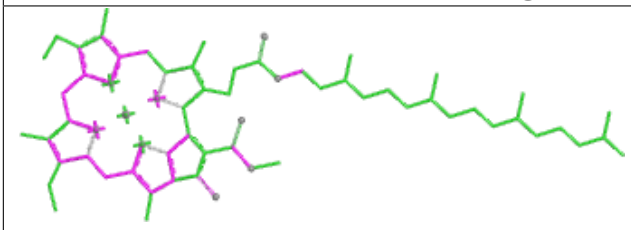


Torsions



Rings

Ligand CLA 2 1013



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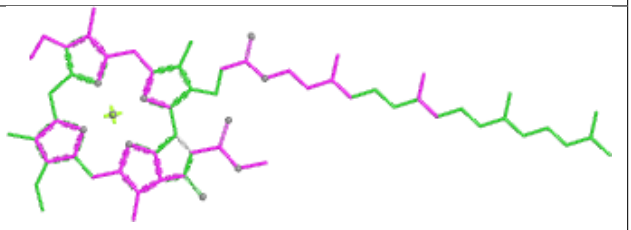
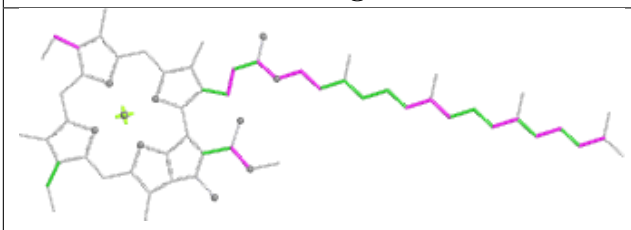
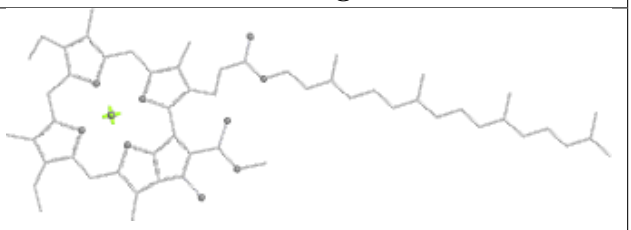


Bond angles

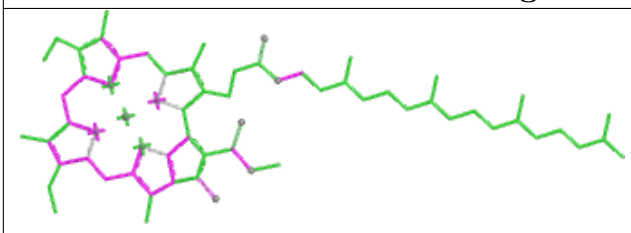


Torsions

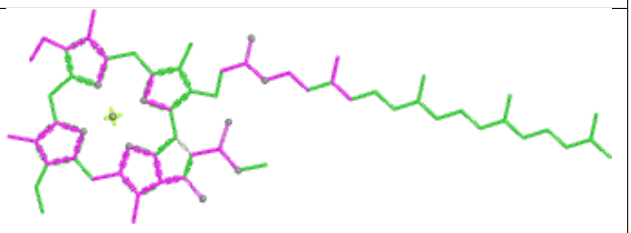


Rings

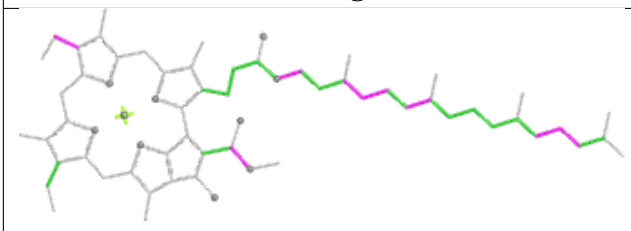
Ligand CLA a 1022



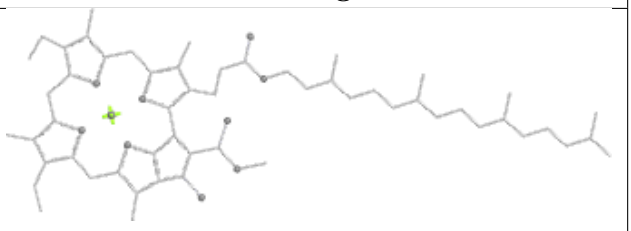
Bond lengths



Bond angles

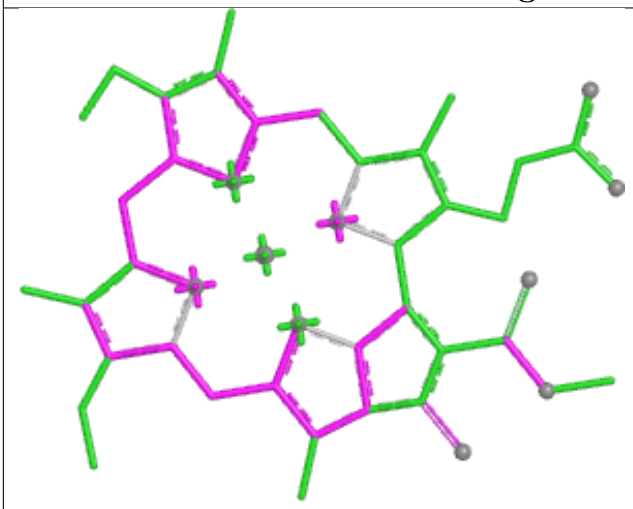


Torsions



Rings

Ligand CLA b 1208



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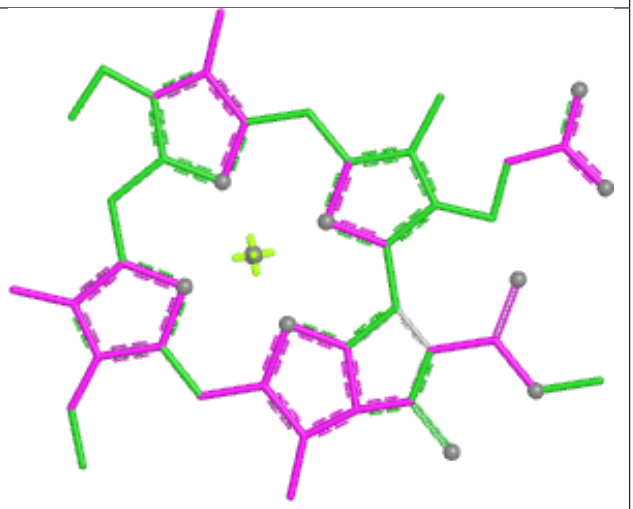

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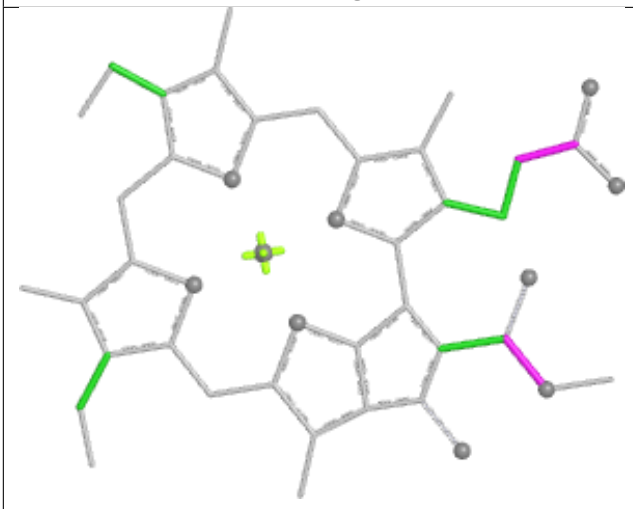
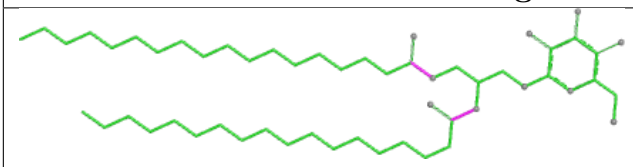


Torsions

Rings

Ligand LMG 2 5002



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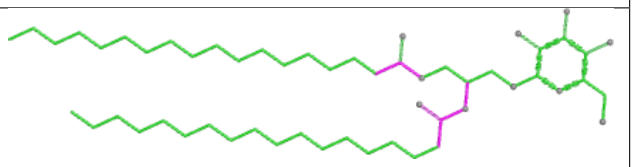

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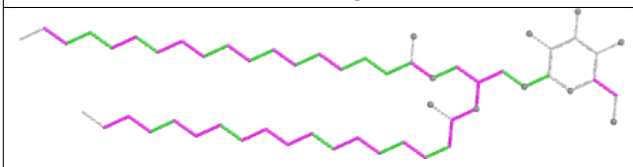

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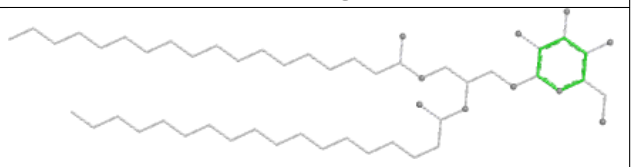
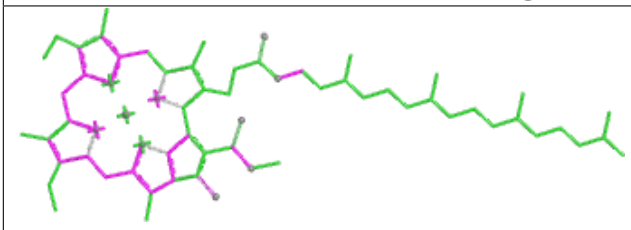


Rings

Ligand CLA 1 1107



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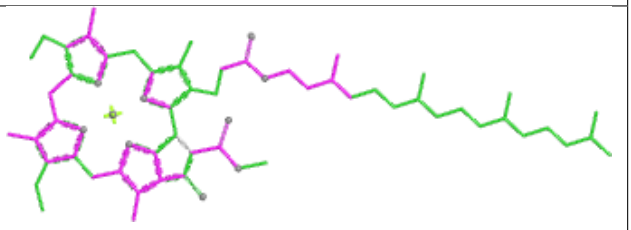

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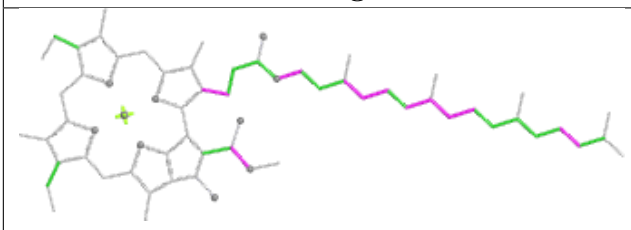

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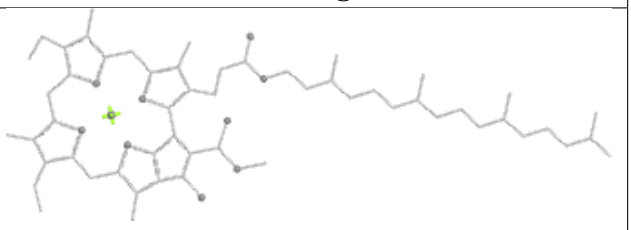
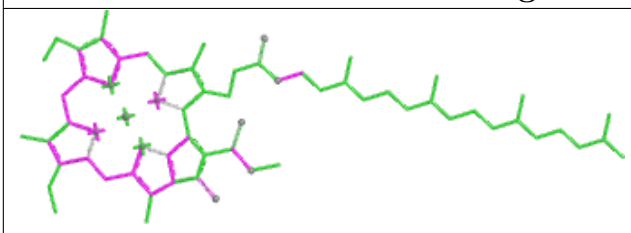


Rings

Ligand CLA b 1013



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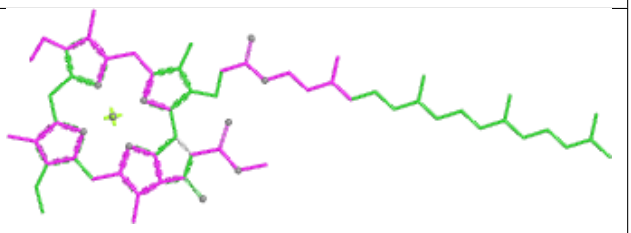

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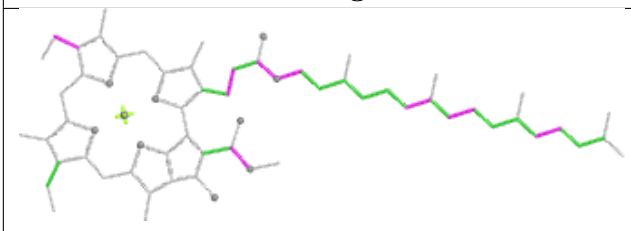

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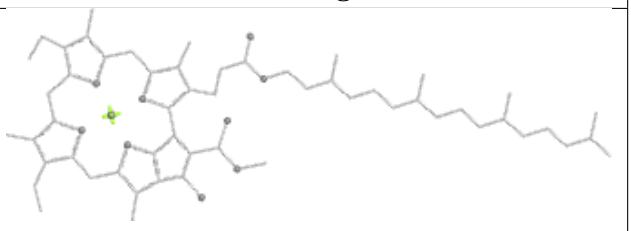
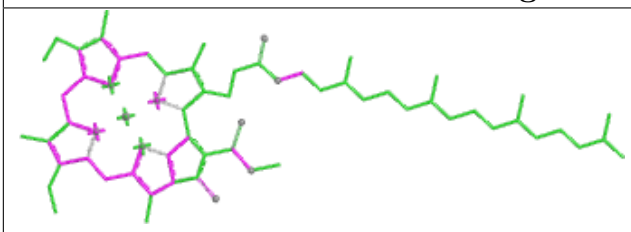


Rings

Ligand CLA 8 1503



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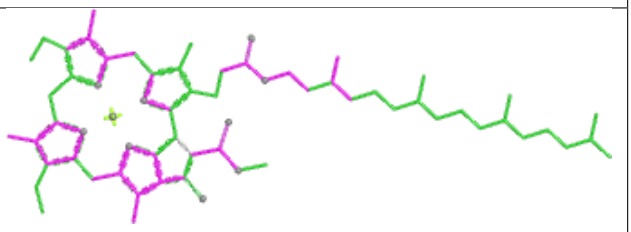

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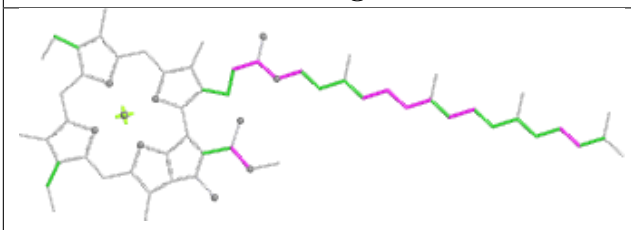

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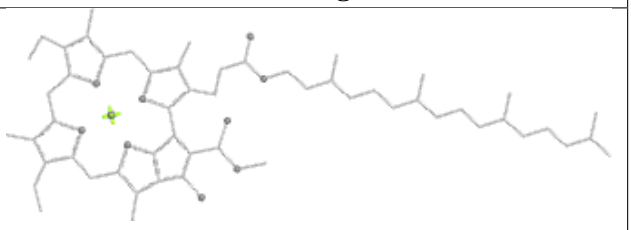
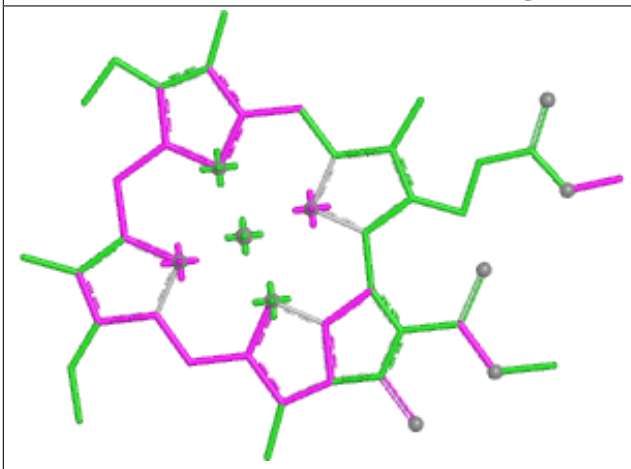


Rings

Ligand CLA 1 1138



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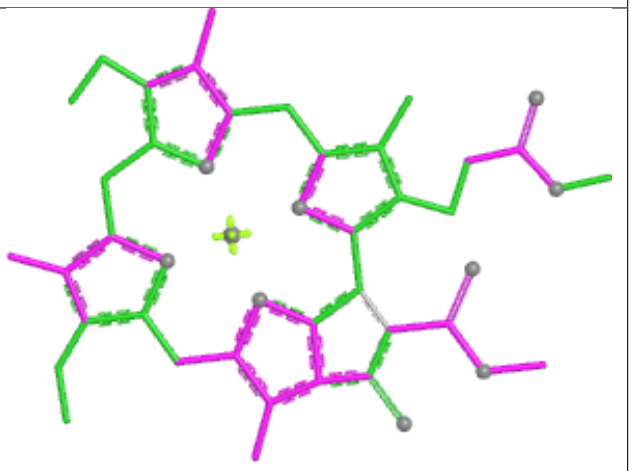

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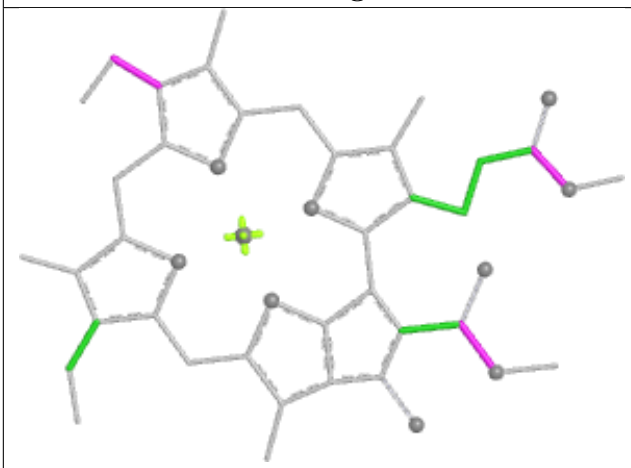

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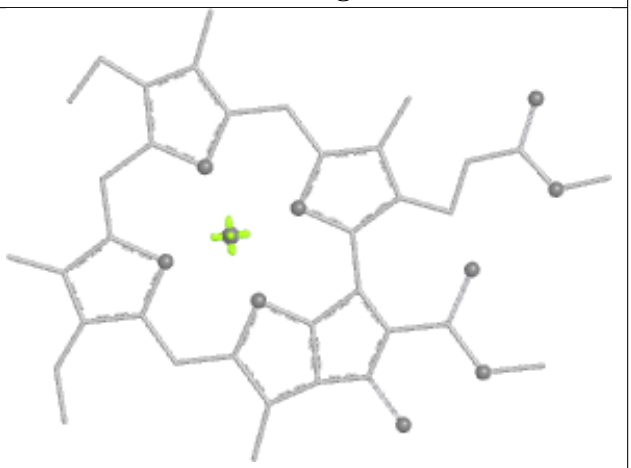
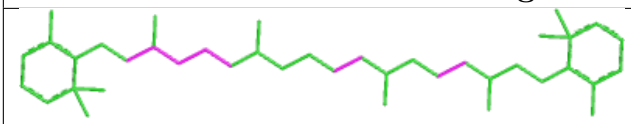


Rings

Ligand BCR 2 4006



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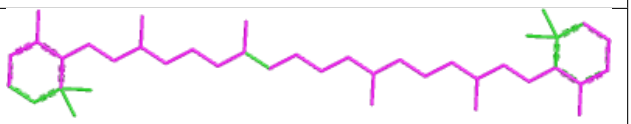

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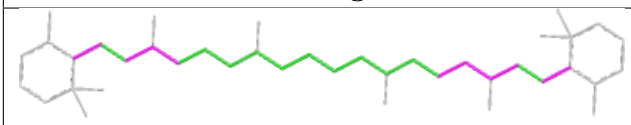

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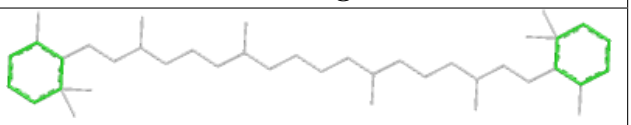
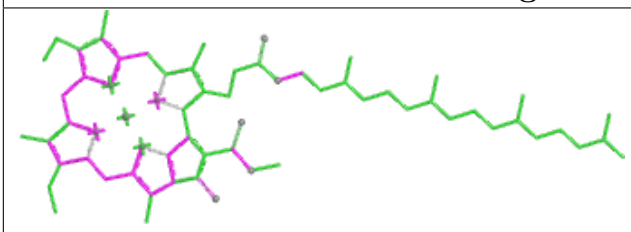


Rings

Ligand CLA 1 1117



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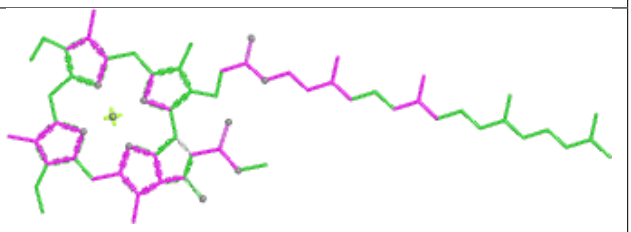
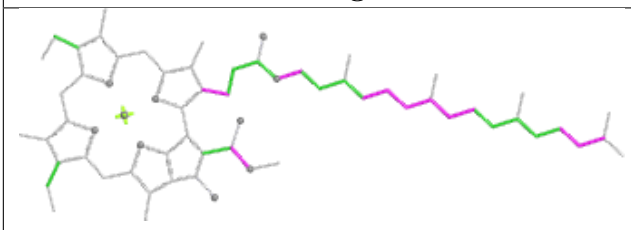


Bond angles



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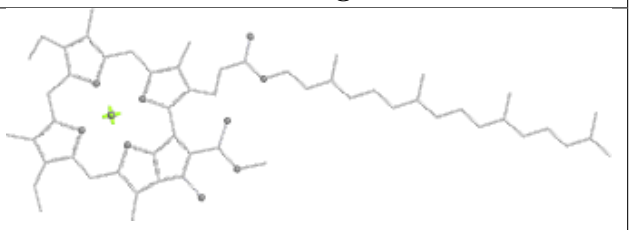
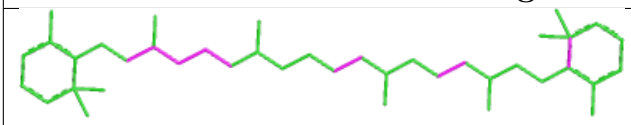


Rings

Ligand BCR 1 4008



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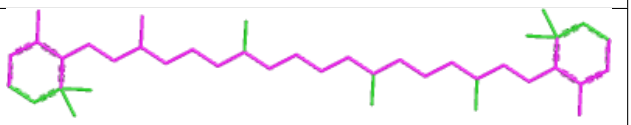
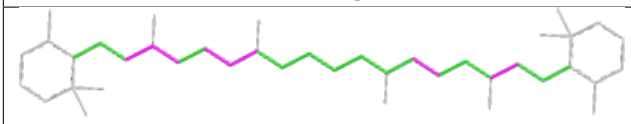


Bond angles



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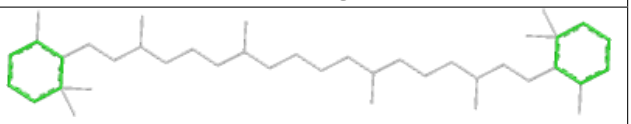
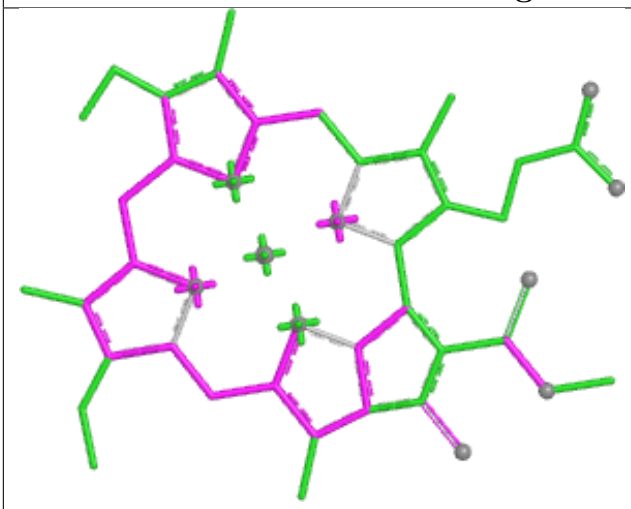


Rings

Ligand CLA B 1212



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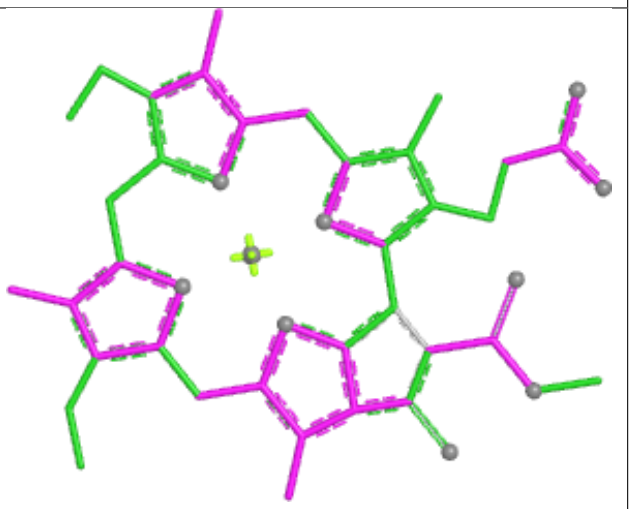
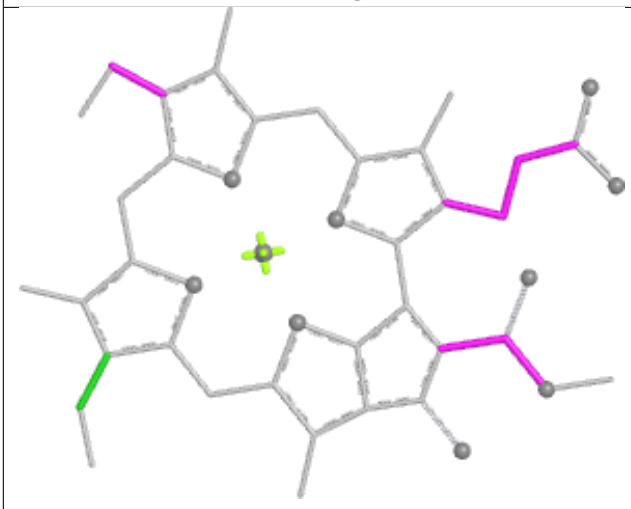


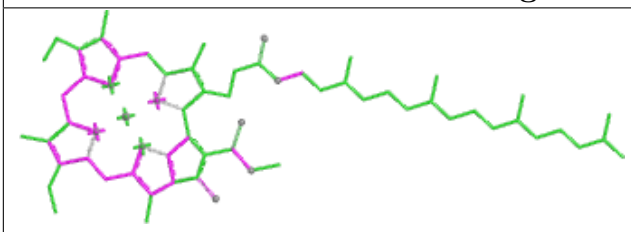
Bond angles



Torsions

Rings

Ligand CLA a 1106



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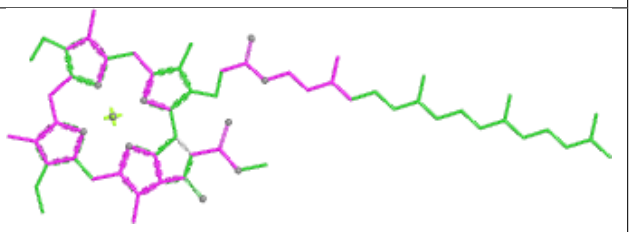
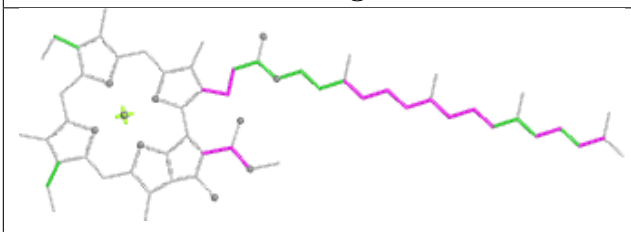
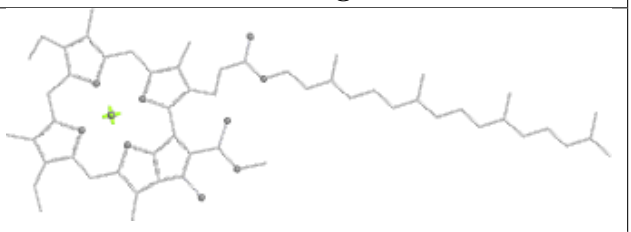


Bond angles

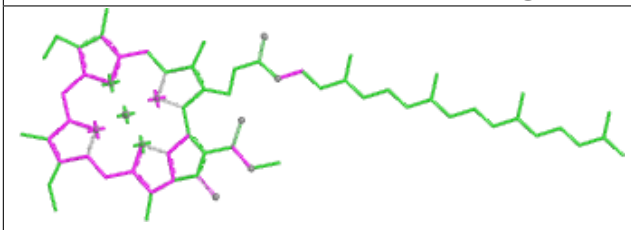


Torsions



Rings

Ligand CLA 1 1102



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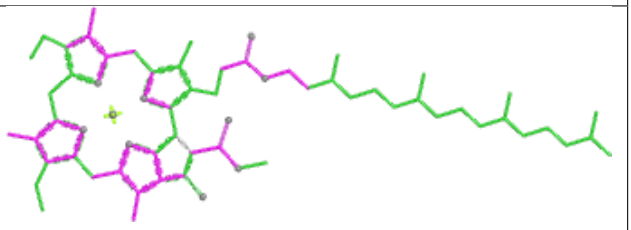
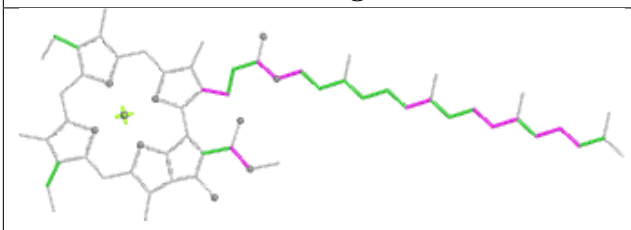
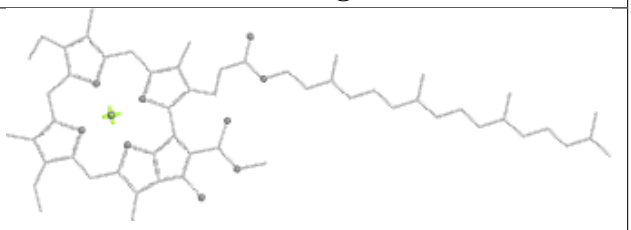


Bond angles

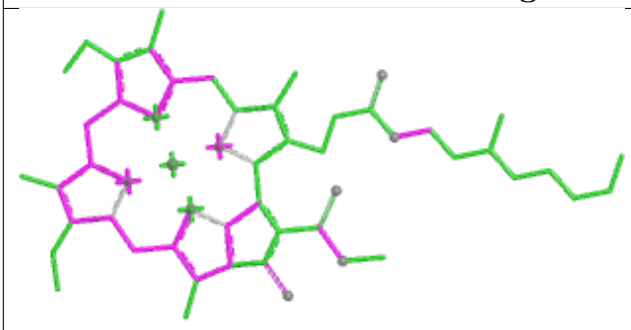


Torsions



Rings

Ligand CLA 2 1221



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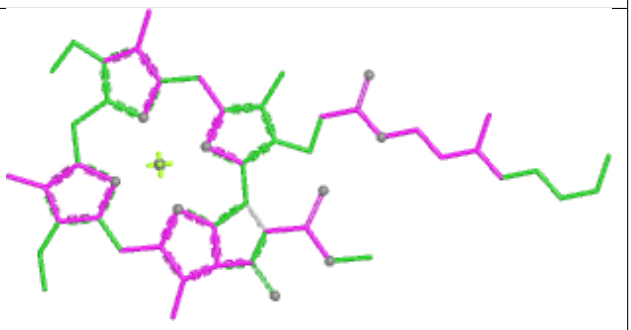
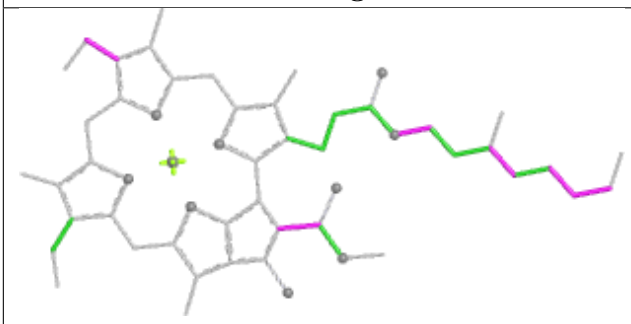
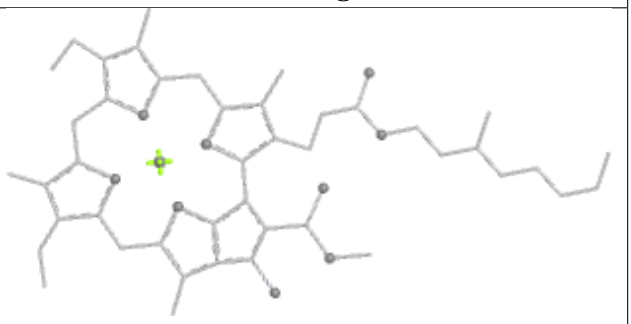


Bond angles

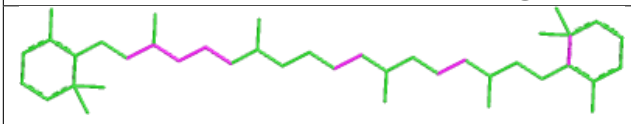


Torsions

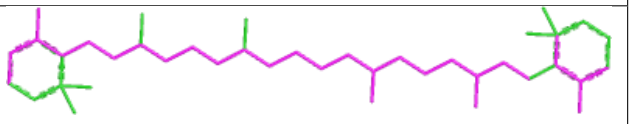


Rings

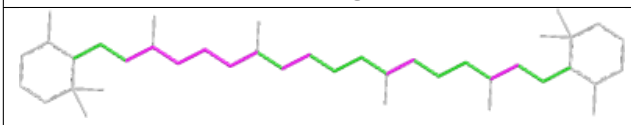
Ligand BCR b 4014



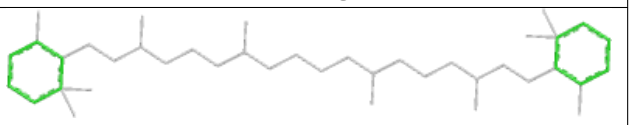
Bond lengths



Bond angles

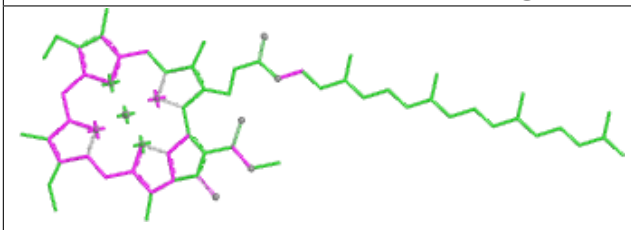


Torsions



Rings

Ligand CLA b 1203



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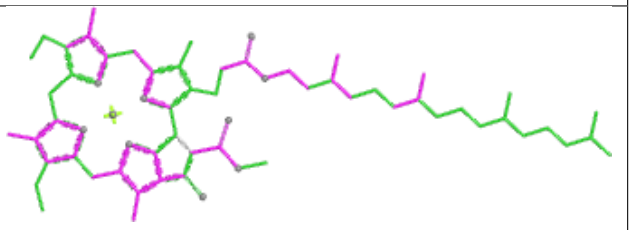
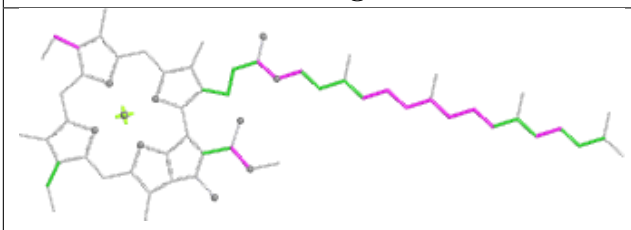


Bond angles



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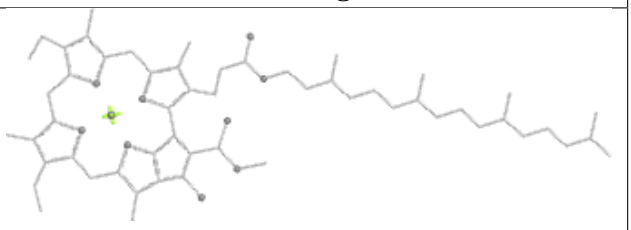
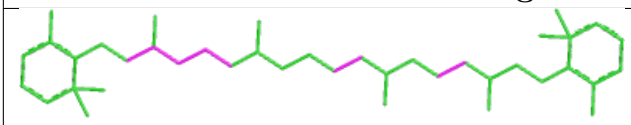


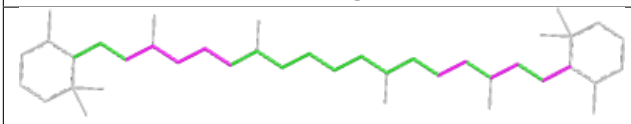
Rings

Ligand BCR b 4004

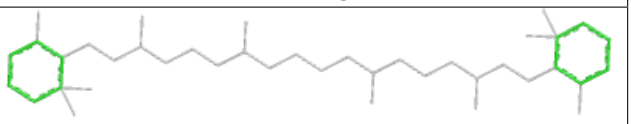


Bond lengths

Bond angles

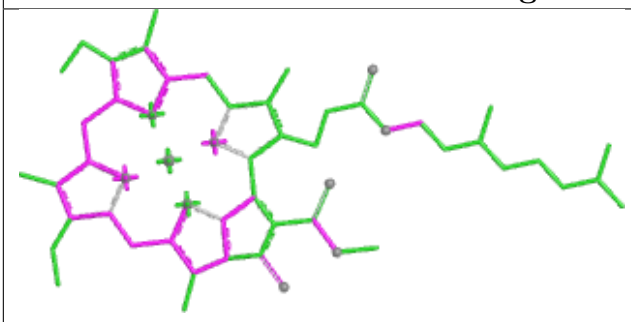


Torsions



Rings

Ligand CLA 2 1219



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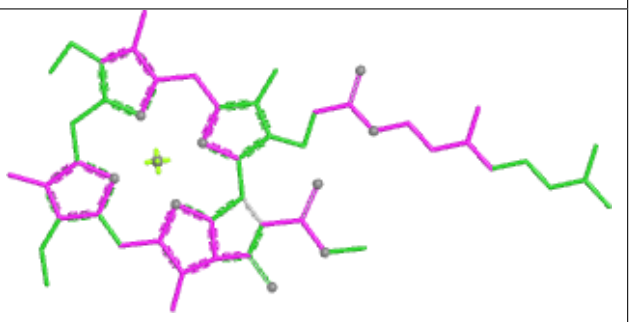
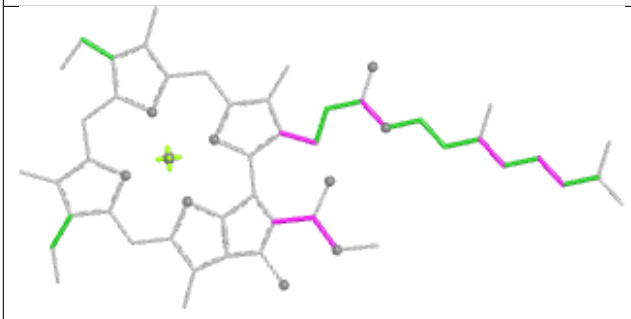
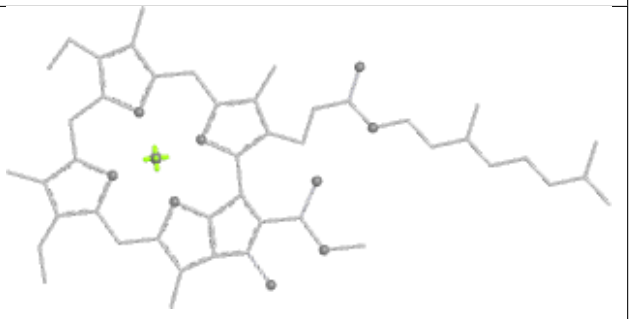


Bond angles

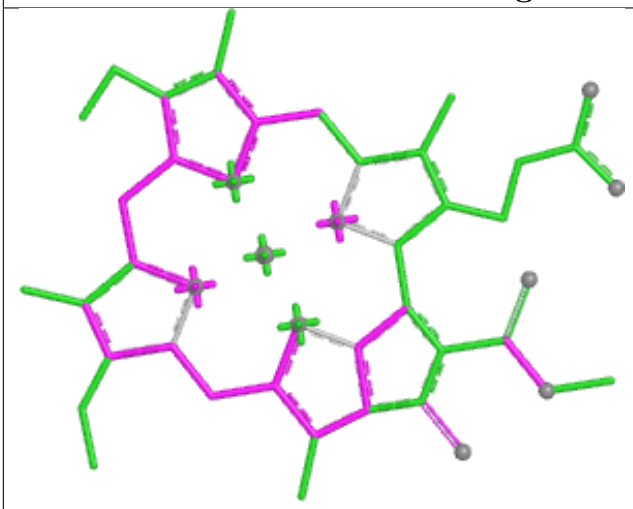


Torsions



Rings

Ligand CLA B 1209



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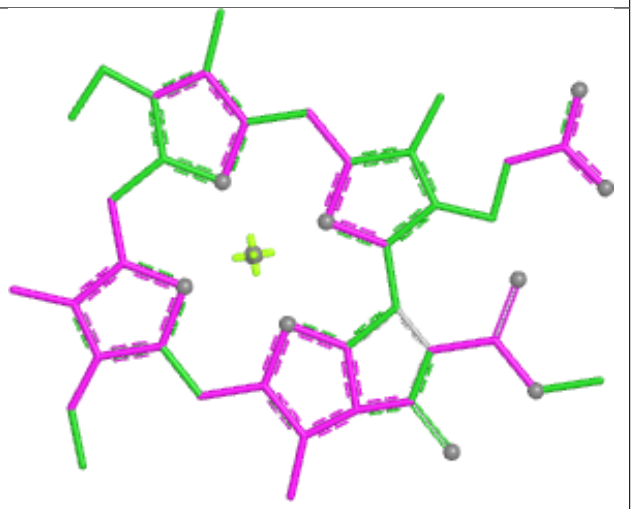
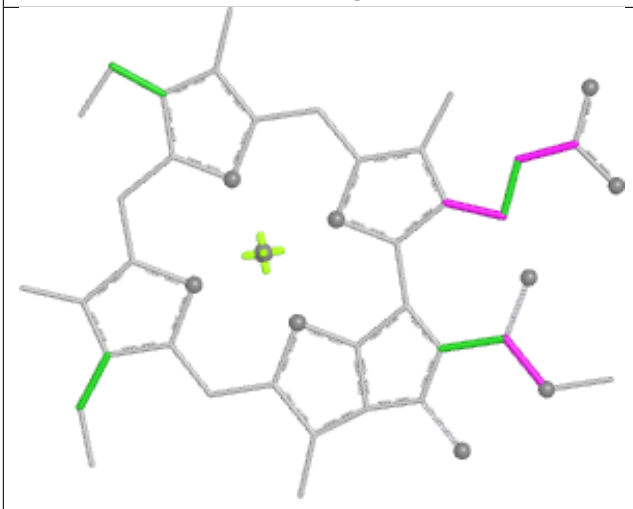


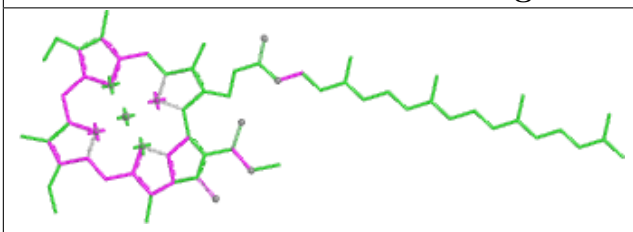
Bond angles



Torsions

Rings

Ligand CLA A 1102



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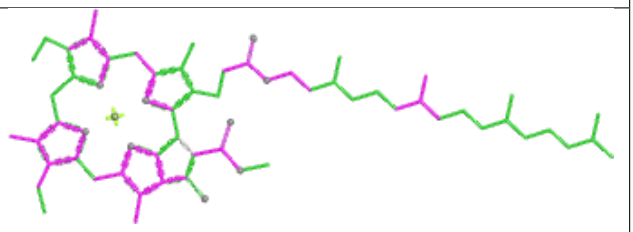
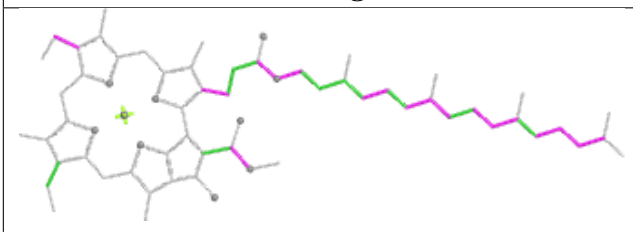


Bond angles



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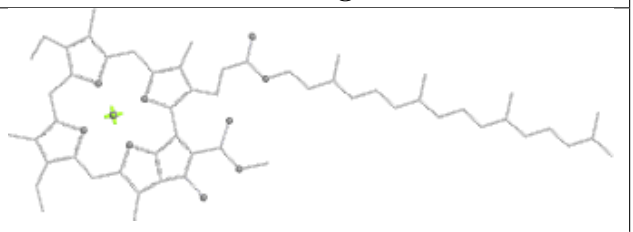
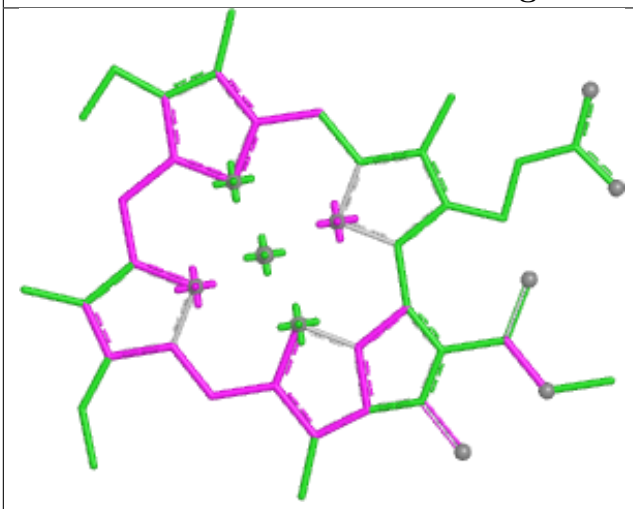


Rings

Ligand CLA 1 1108



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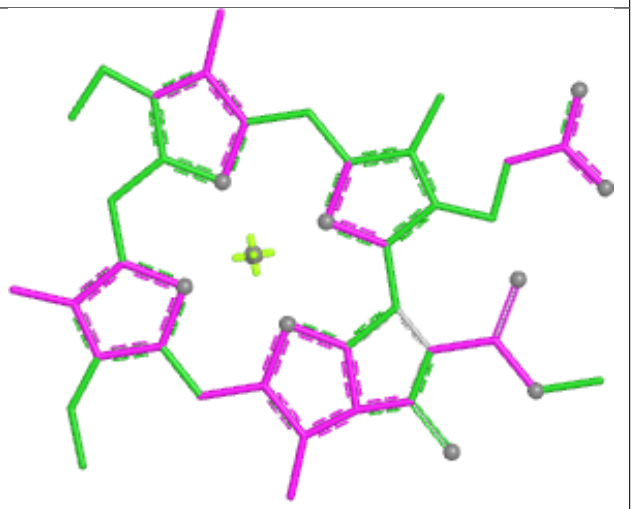
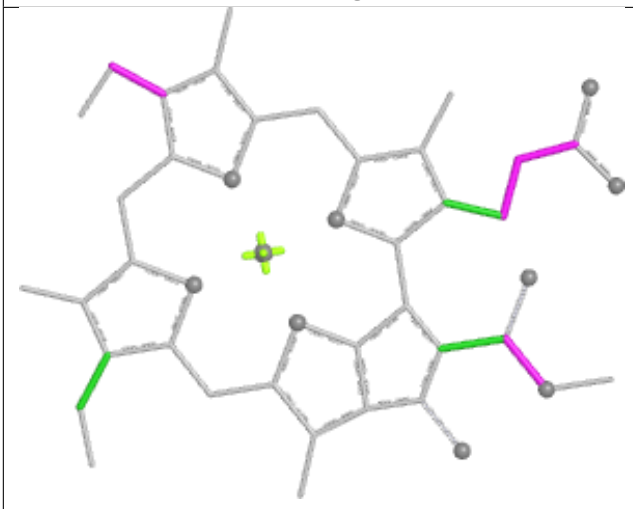


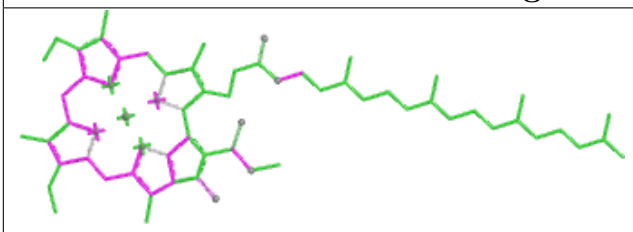
Bond angles



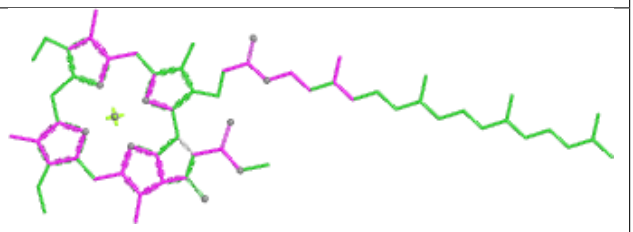
Torsions

Rings

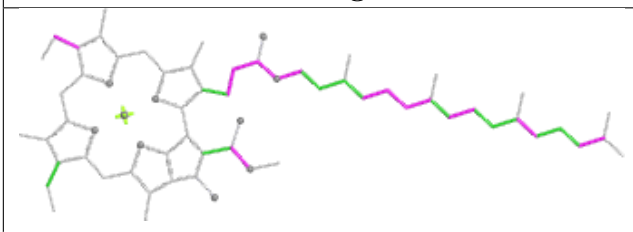
Ligand CLA l 1503



Bond lengths



Bond angles



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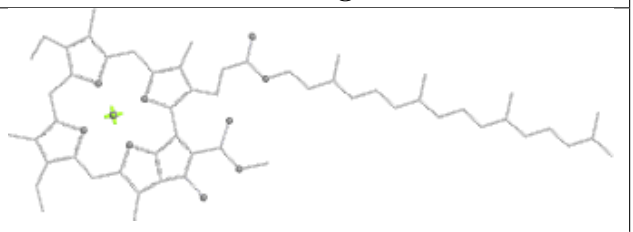
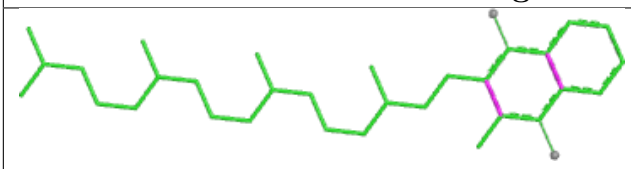
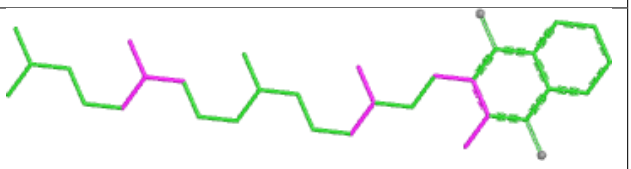
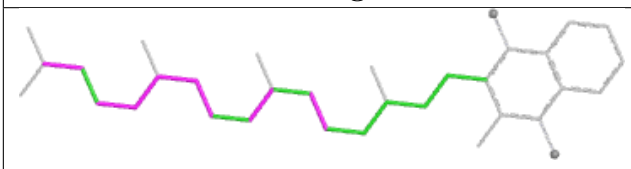
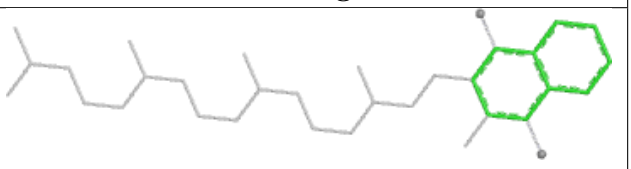
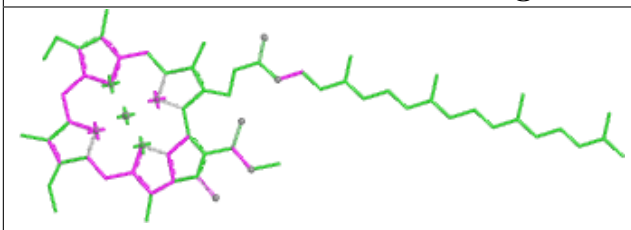
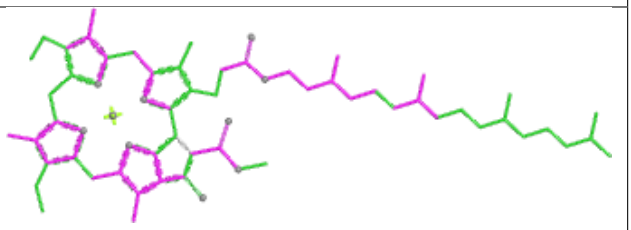
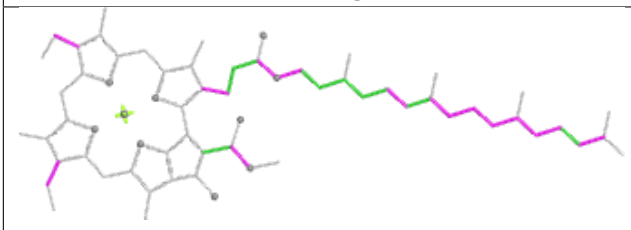
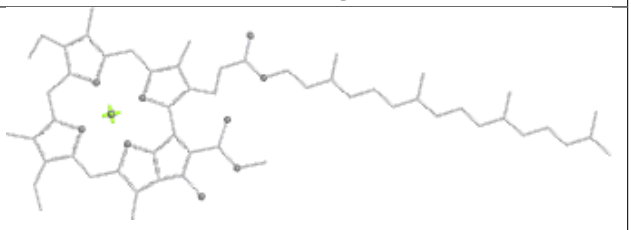
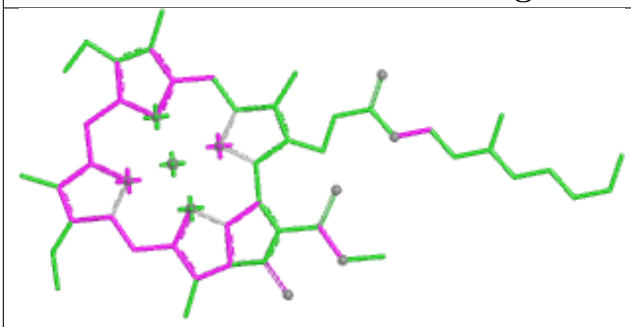


Rings

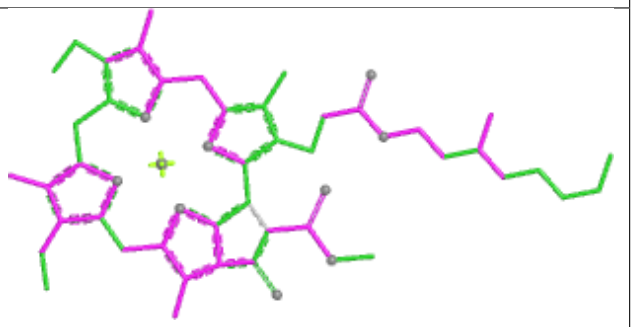
Ligand PQN A 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

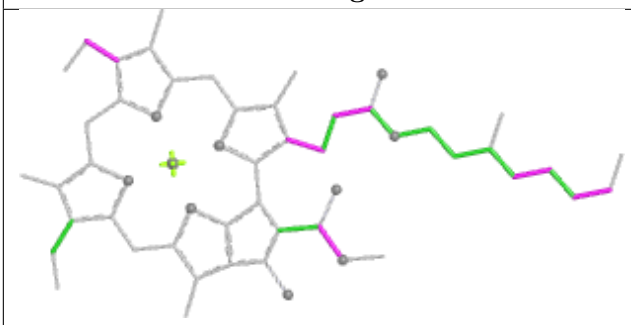
Ligand CLA A 1116



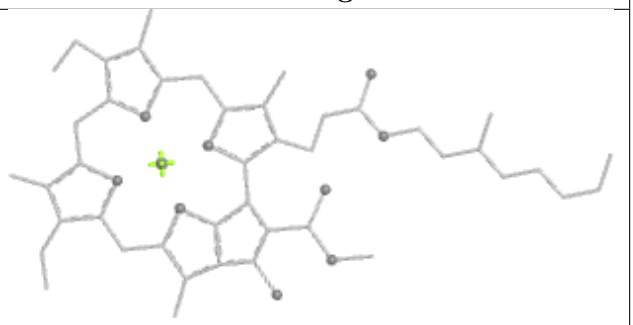
Bond lengths



Bond angles

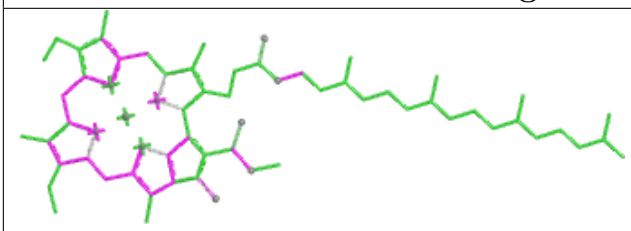


Torsions



Rings

Ligand CLA 2 1215



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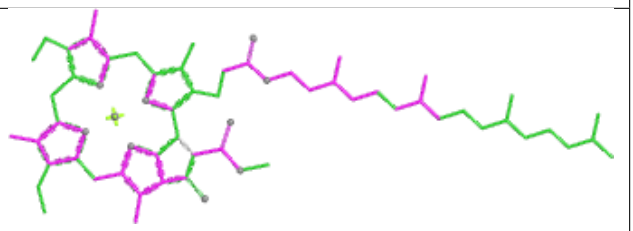
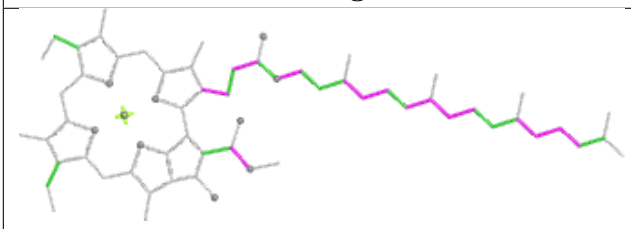


Bond angles



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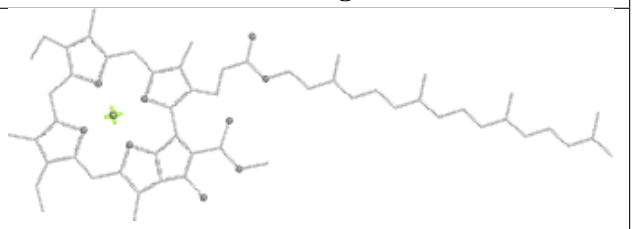
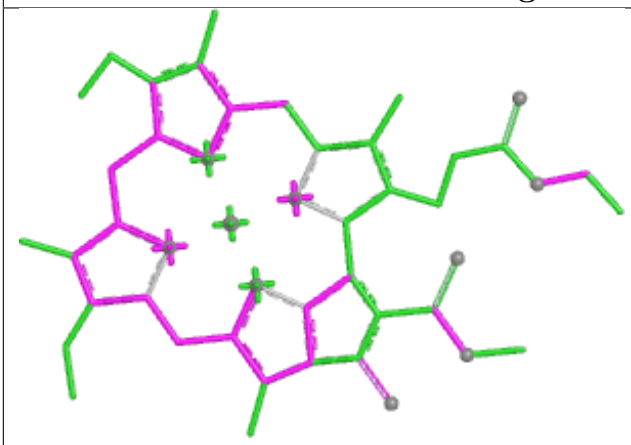


Rings

Ligand CLA b 1236



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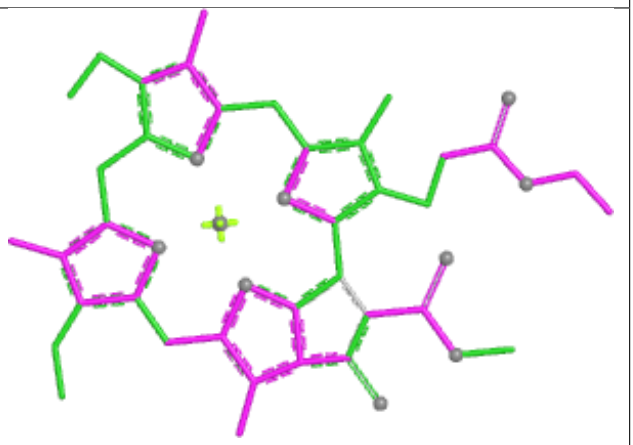
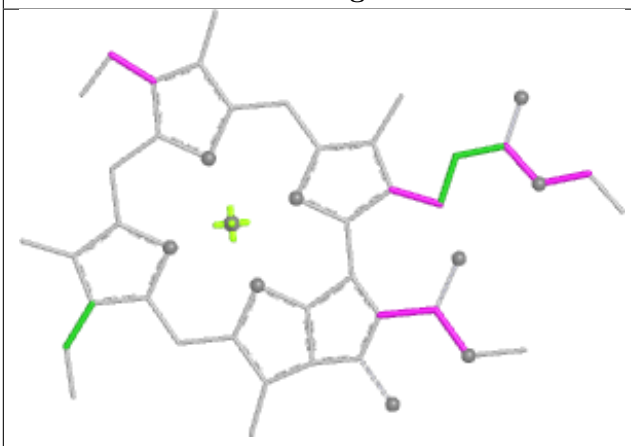
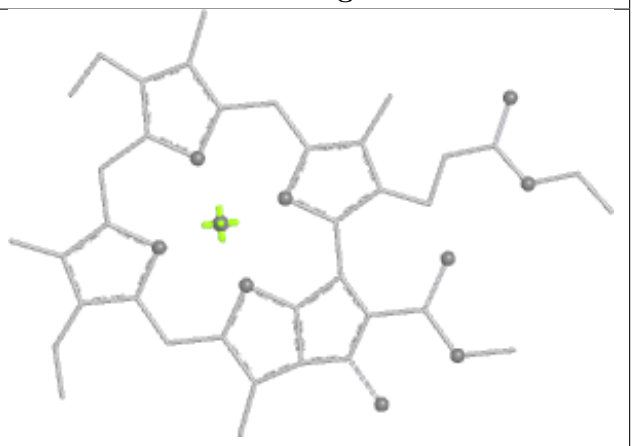


Bond angles

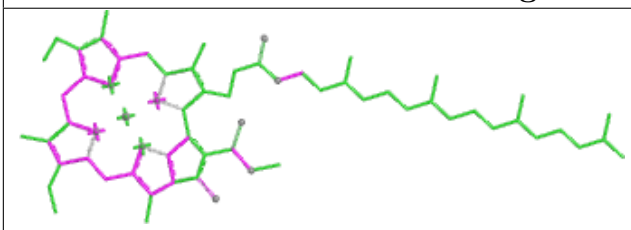


Torsions

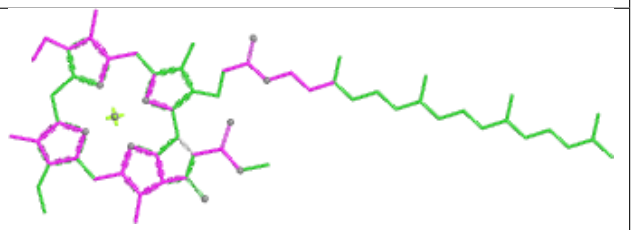


Rings

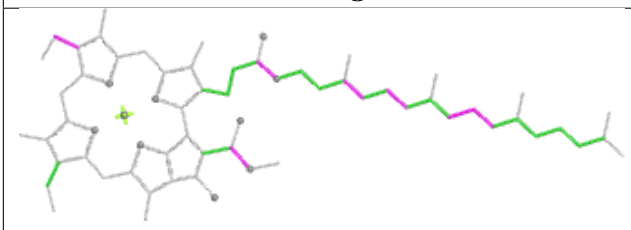
Ligand CLA 2 1204



Bond lengths



Bond angles



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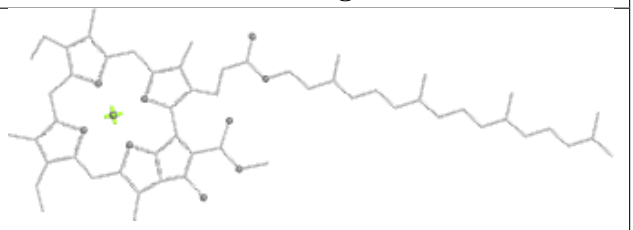
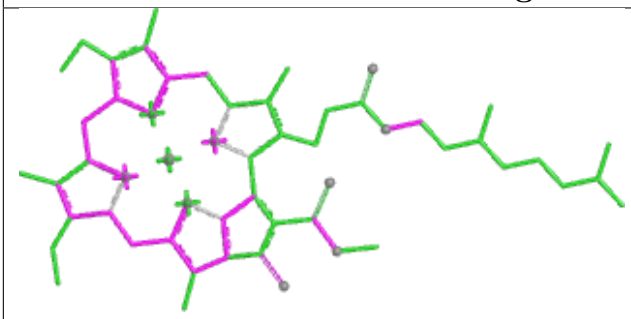


Rings

Ligand CLA B 1219



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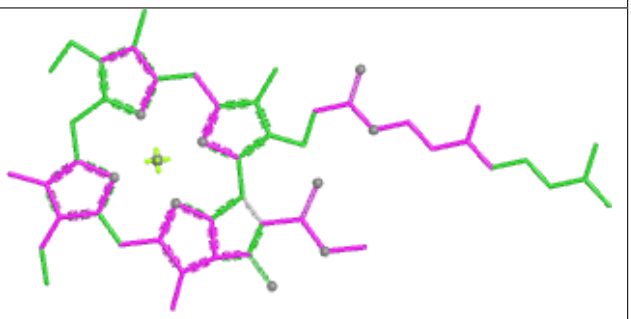
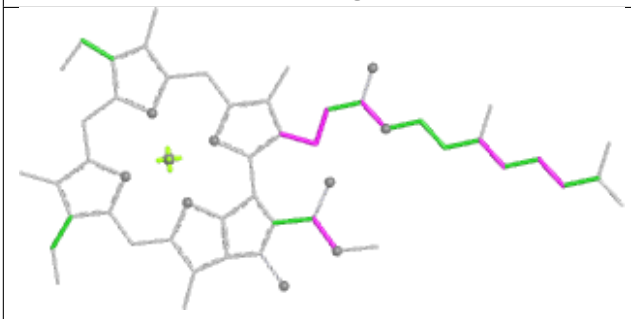
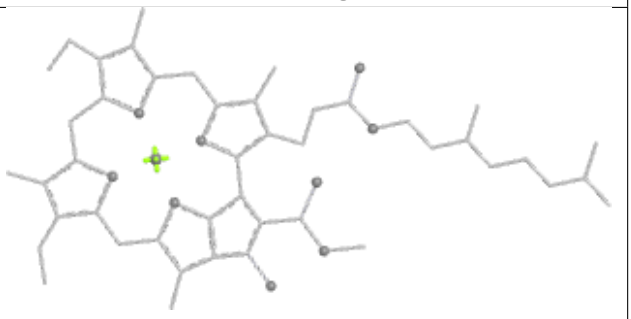


Bond angles

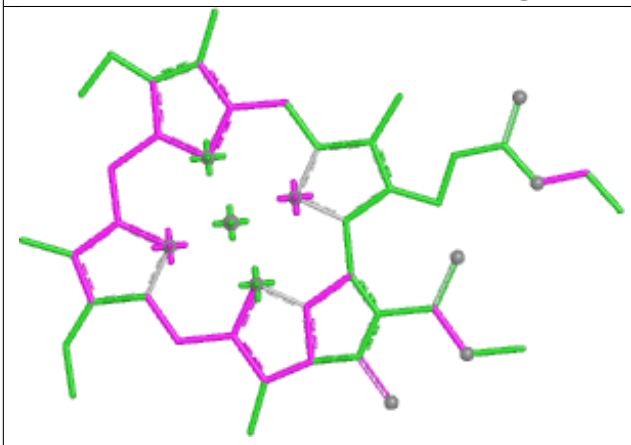


Torsions

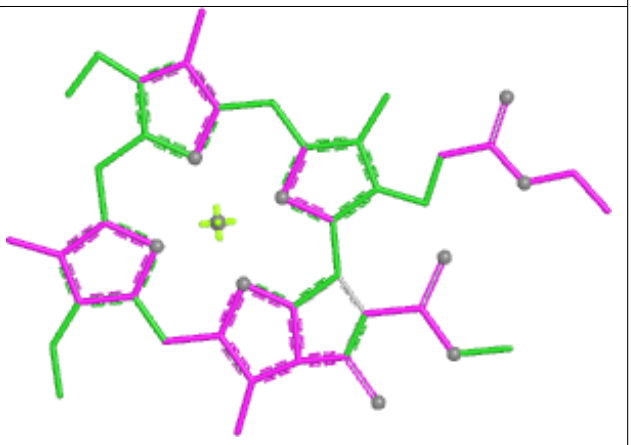


Rings

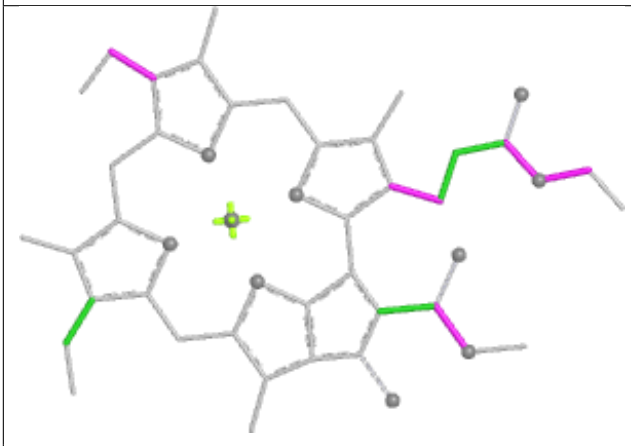
Ligand CLA B 1236



Bond lengths



Bond angles



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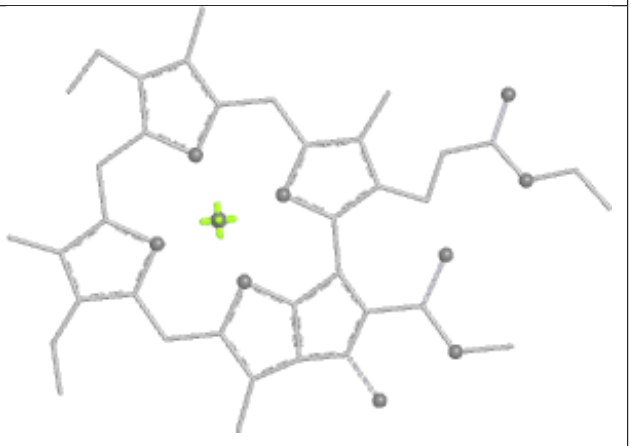
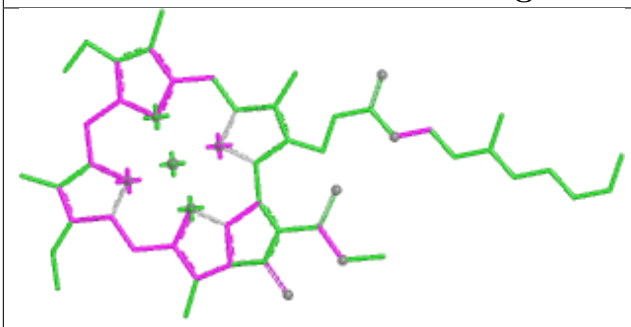


Rings

Ligand CLA B 1201



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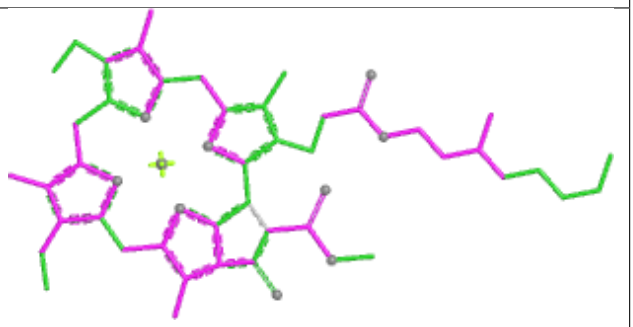
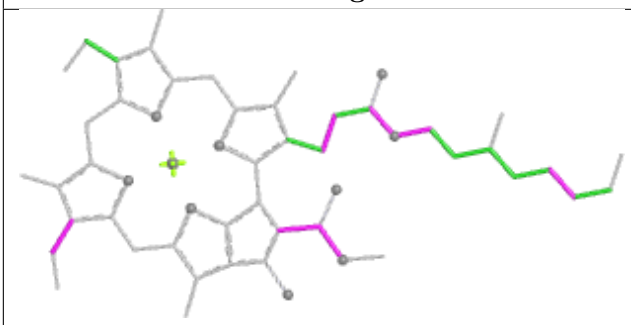


Bond angles



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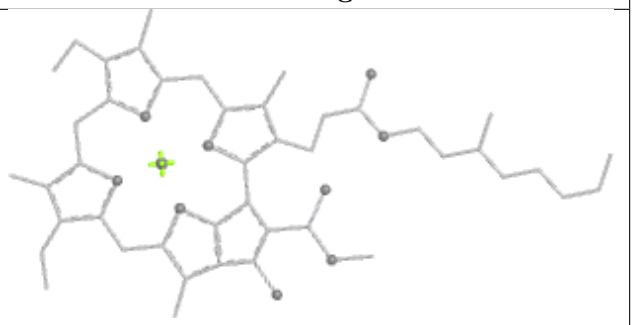
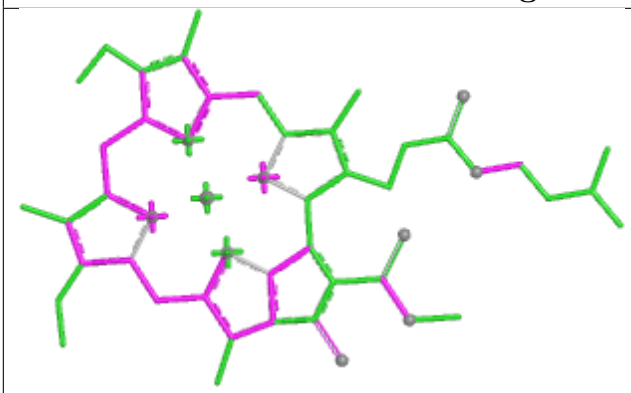


Rings

Ligand CLA 2 1228



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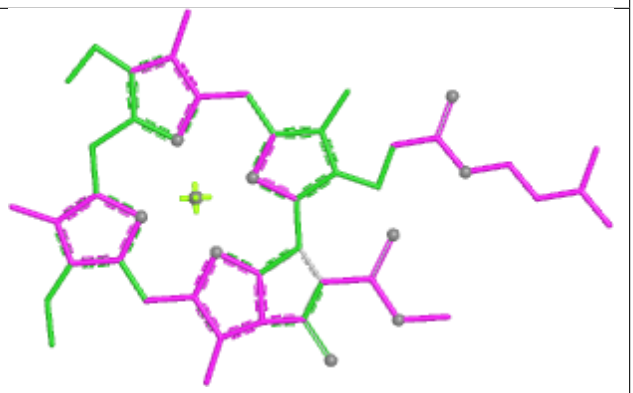
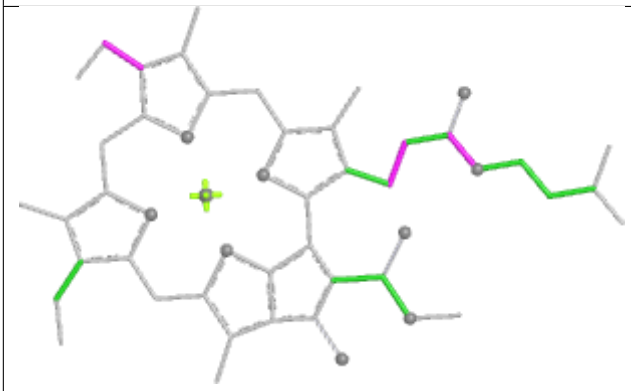


Bond angles



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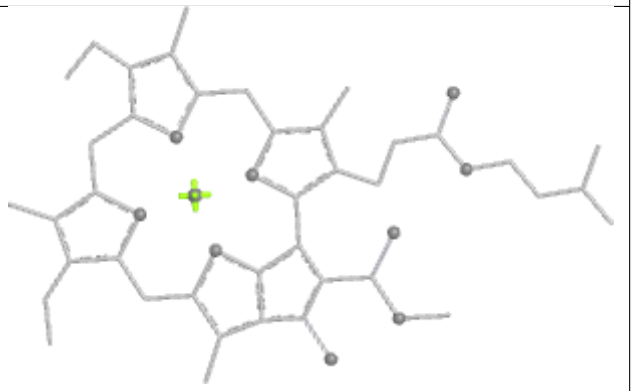
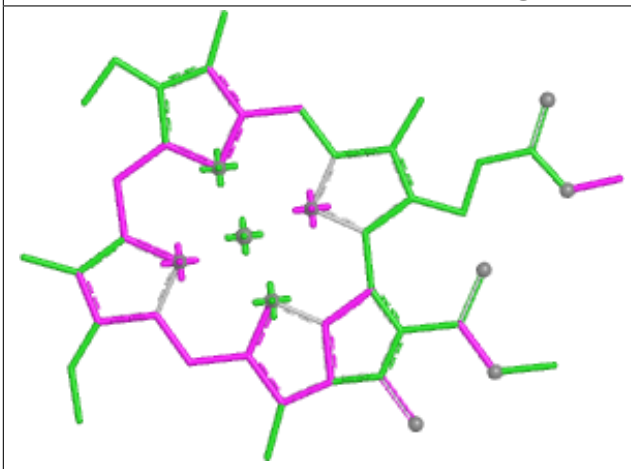


Rings

Ligand CLA A 1133



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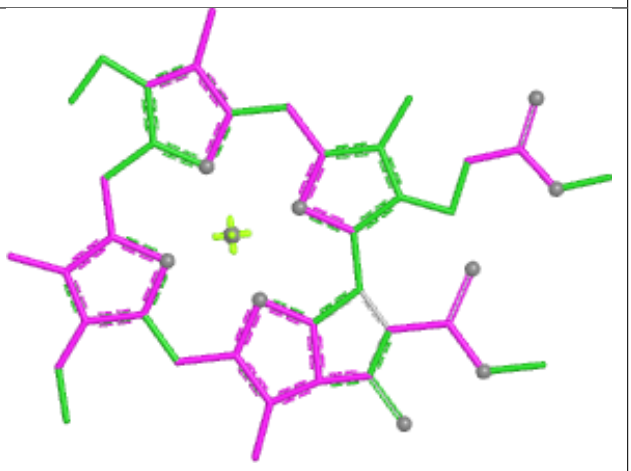
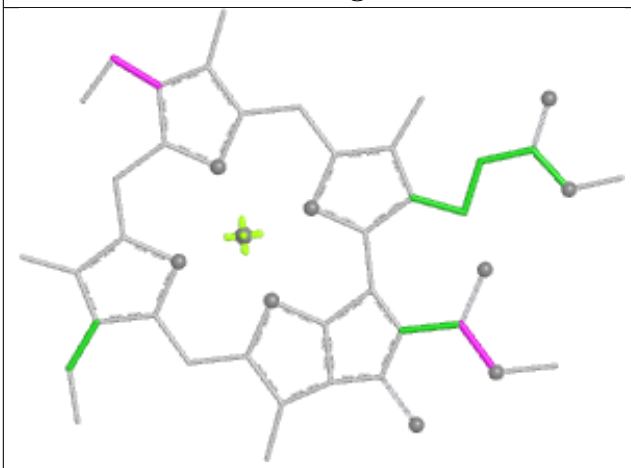


Bond angles



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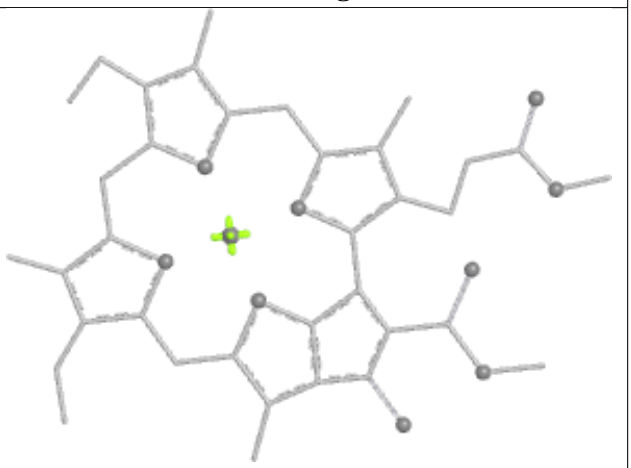
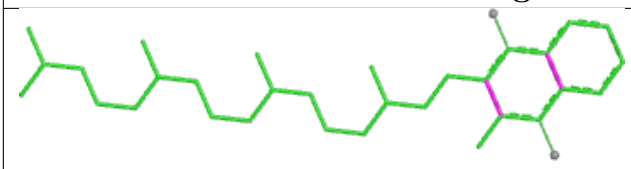


Rings

Ligand PQN B 2002



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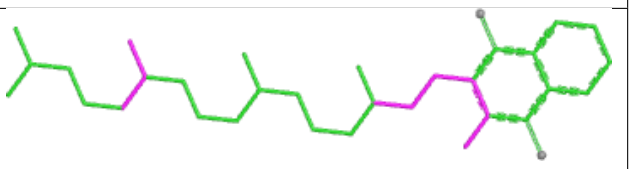
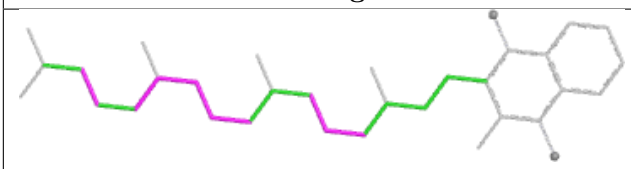


Bond angles



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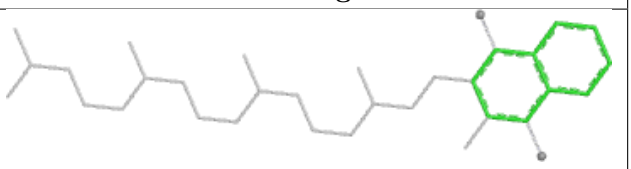
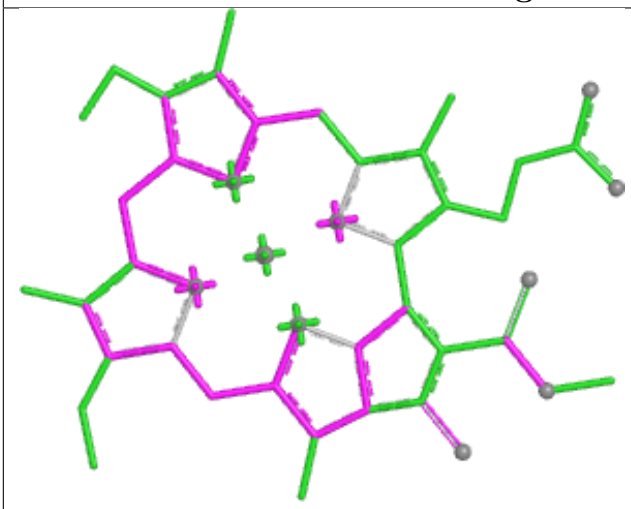


Rings

Ligand CLA B 1218



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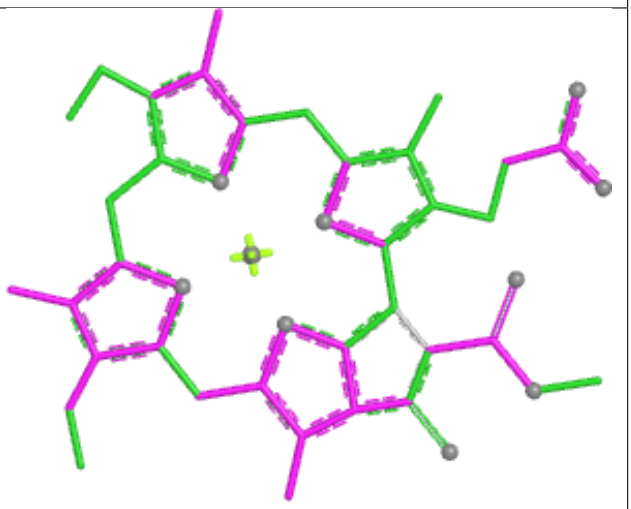
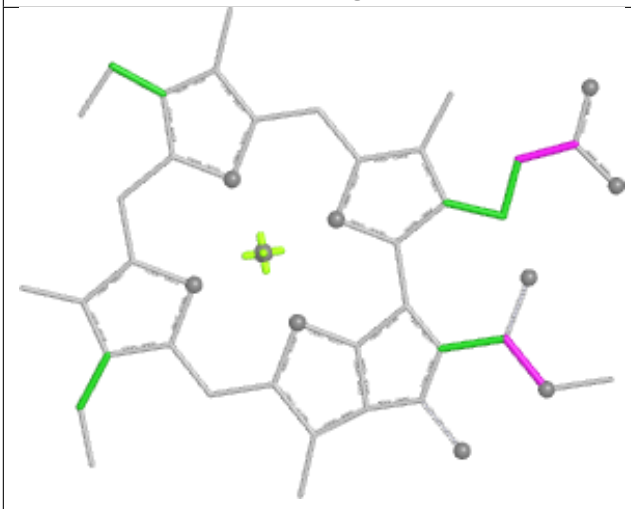


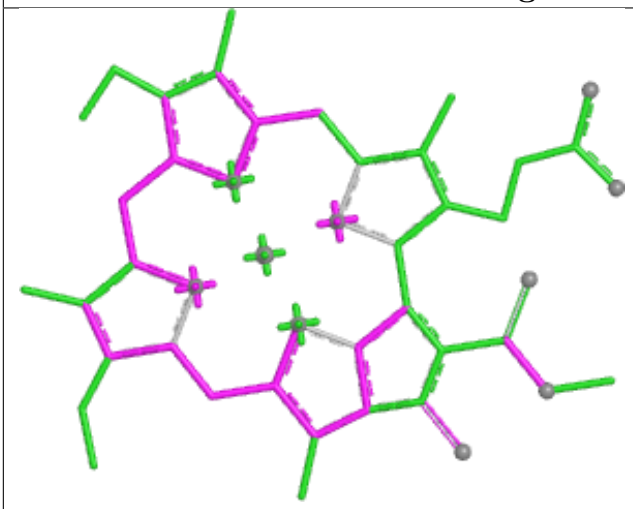
Bond angles



Torsions

Rings

Ligand CLA b 1231



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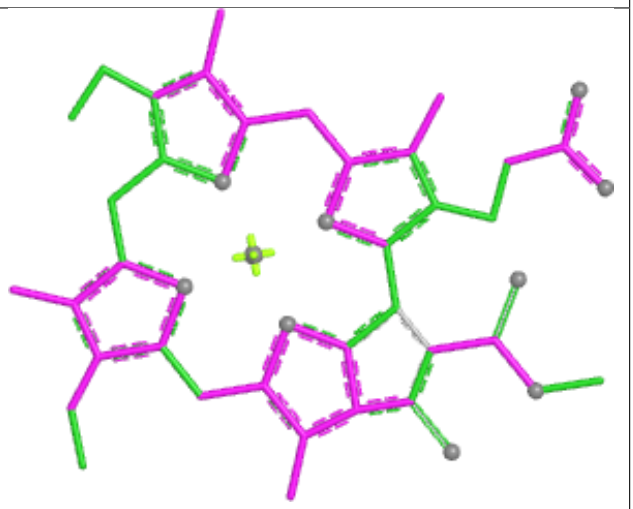
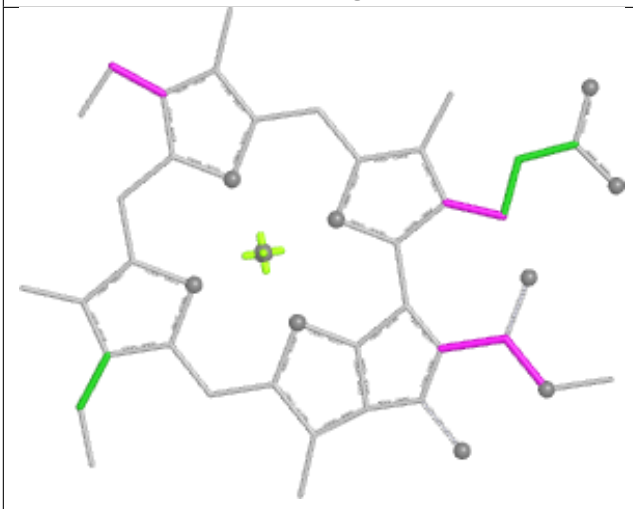


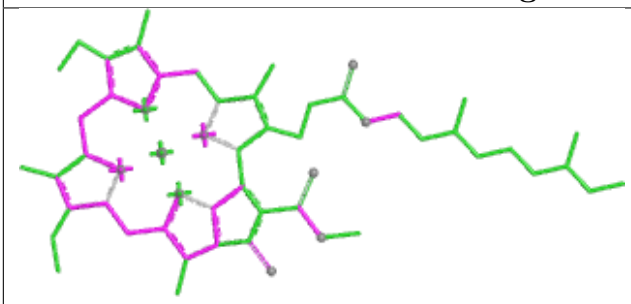
Bond angles



Torsions

Rings

Ligand CLA 2 1222



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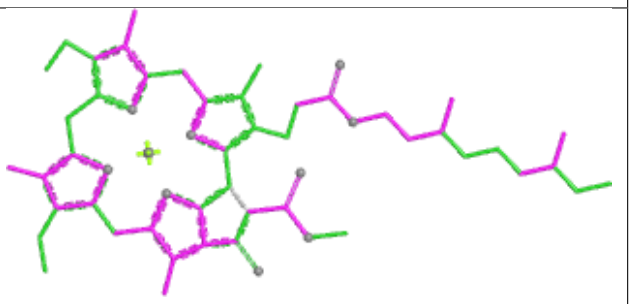
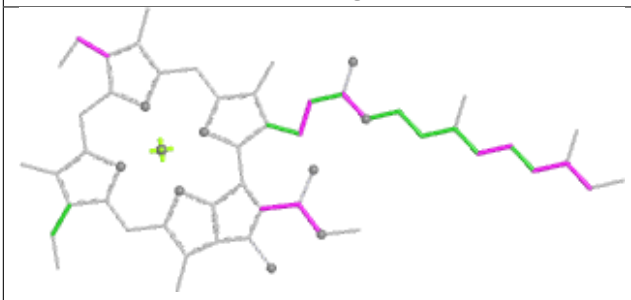
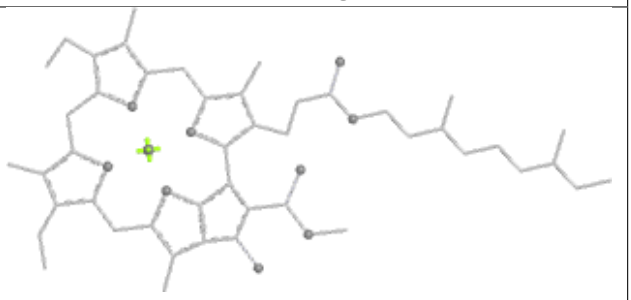


Bond angles

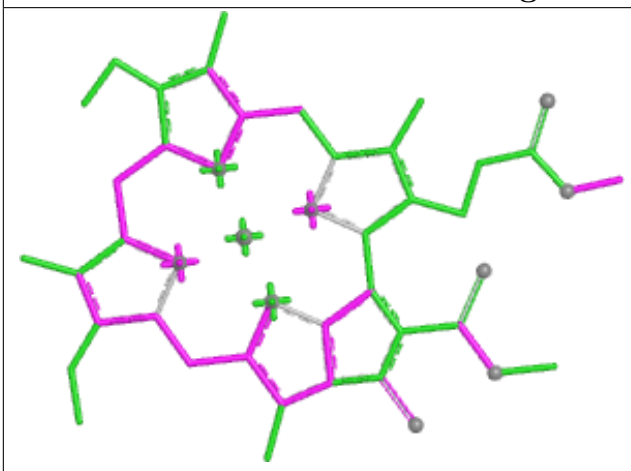


Torsions

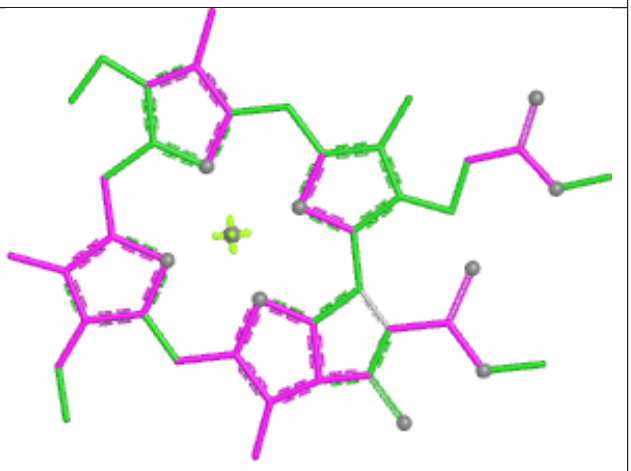


Rings

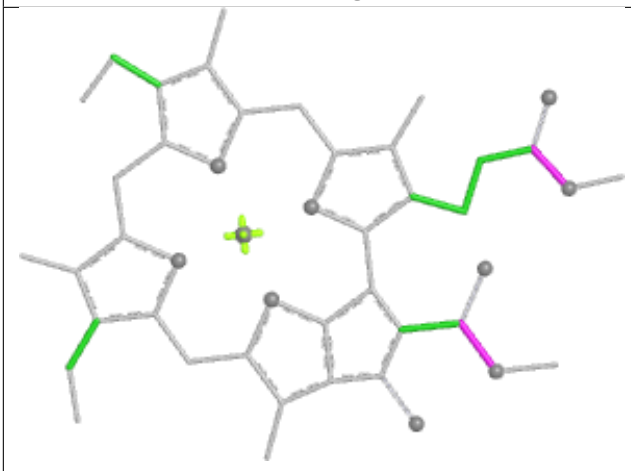
Ligand CLA a 1133



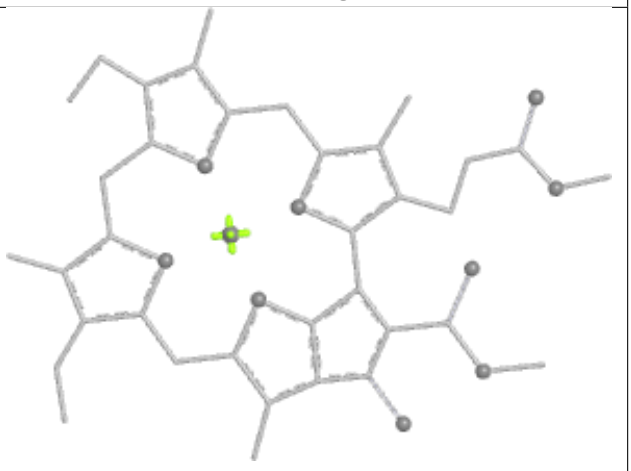
Bond lengths



Bond angles

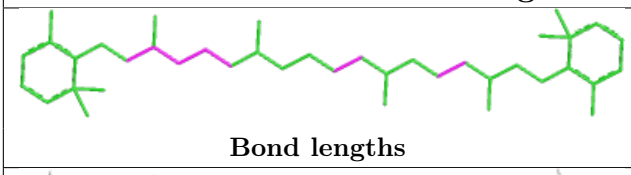


Torsions



Rings

Ligand BCR 6 4013



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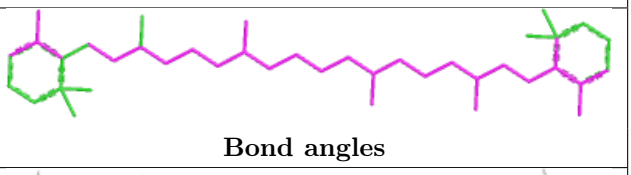
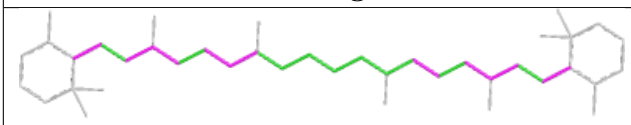


Bond angles



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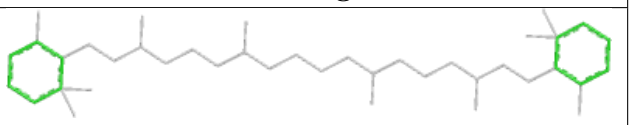
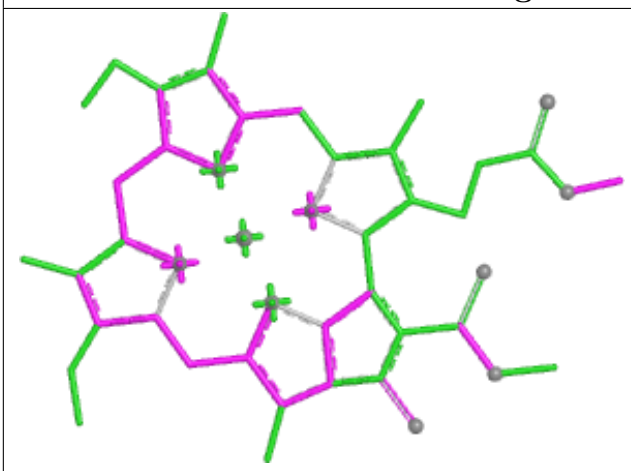


Rings

Ligand CLA A 1120



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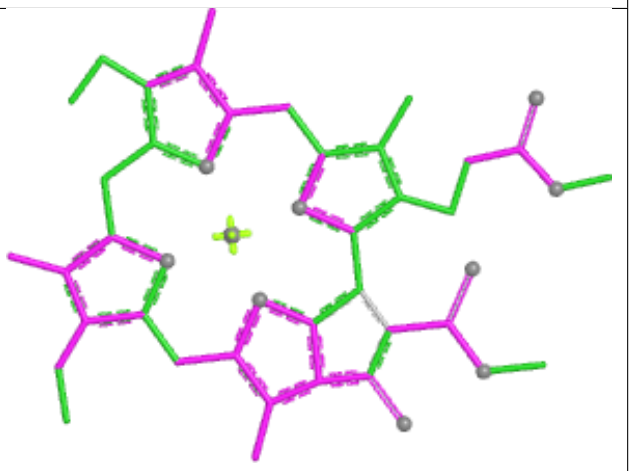
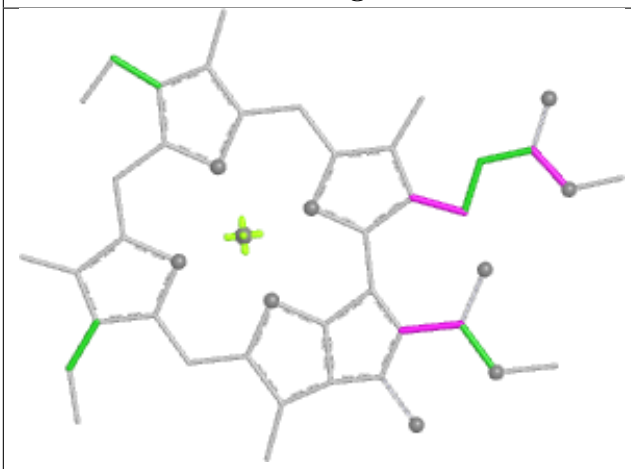


Bond angles



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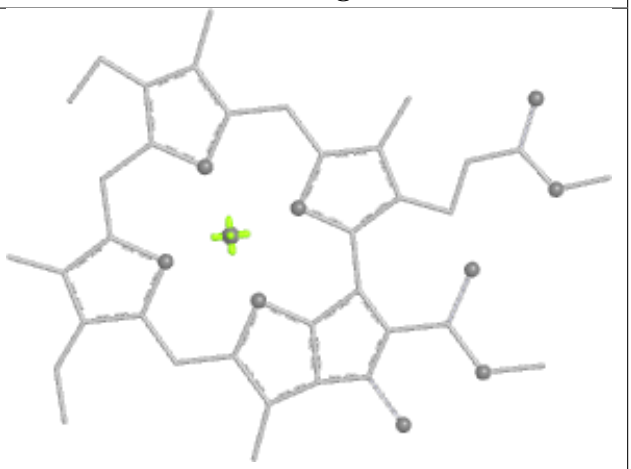
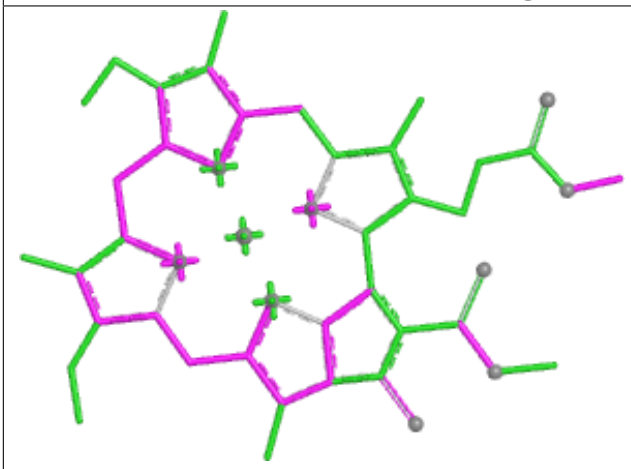


Rings

Ligand CLA 1 1130



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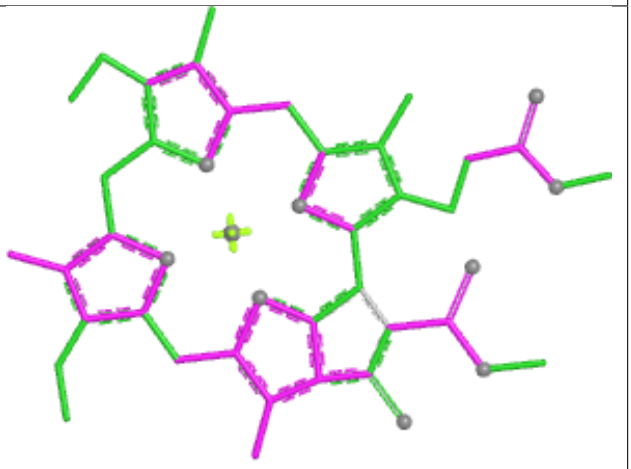
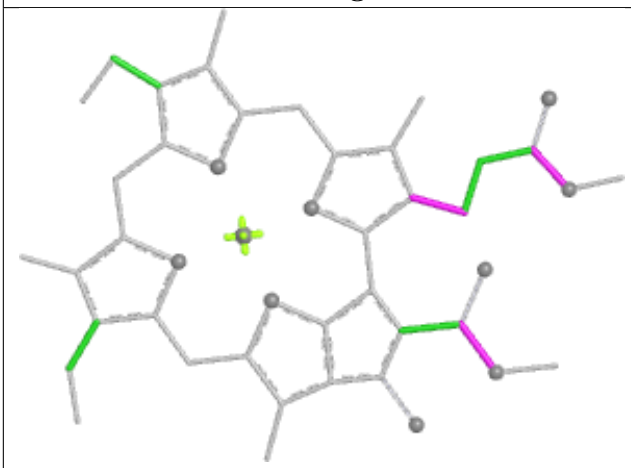


Bond angles



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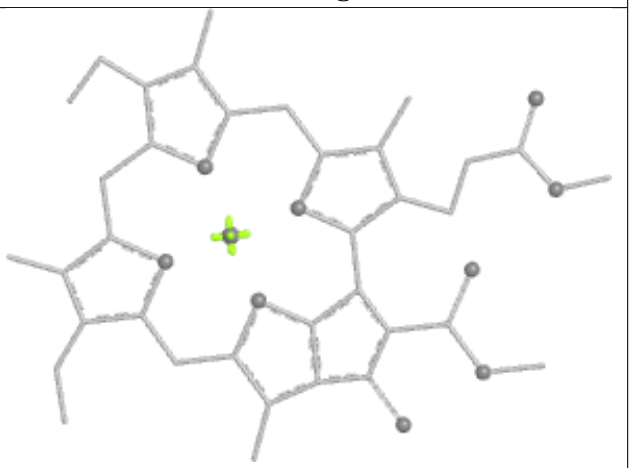
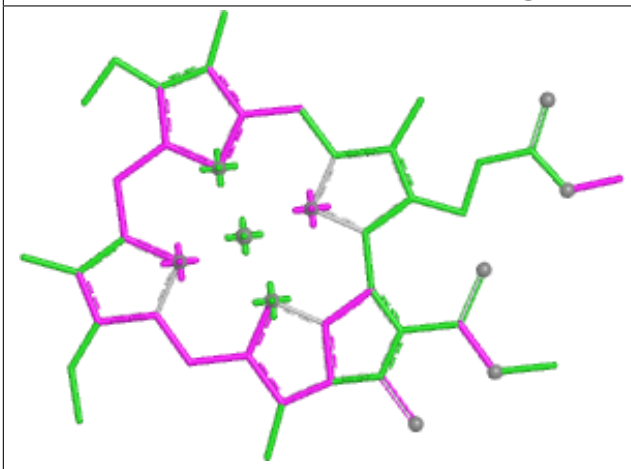


Rings

Ligand CLA a 1134



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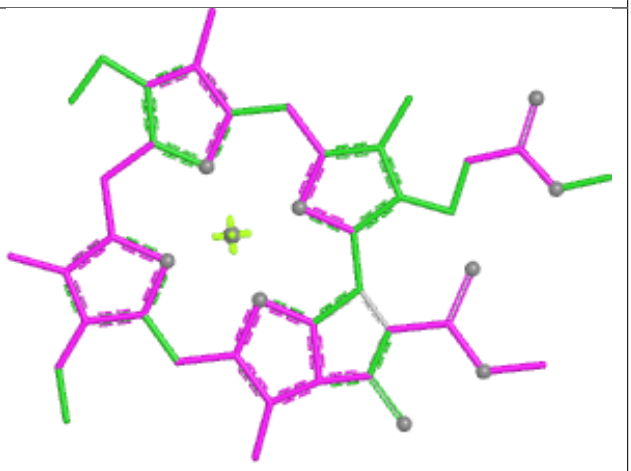
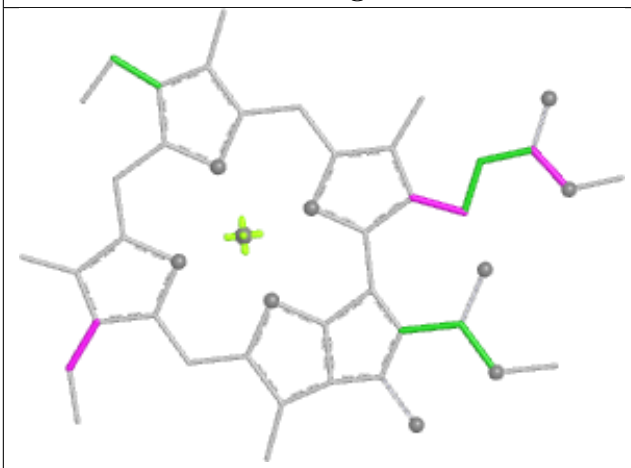
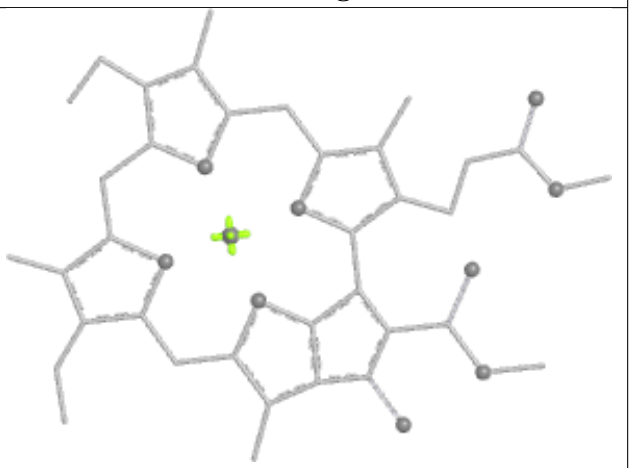


Bond angles

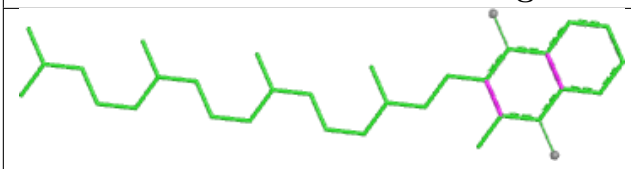


Torsions



Rings

Ligand PQN 2 2002



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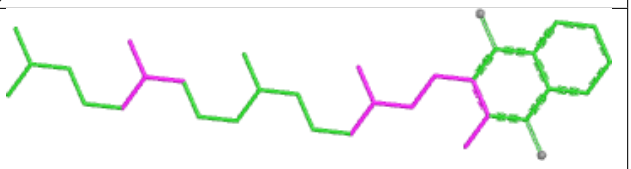
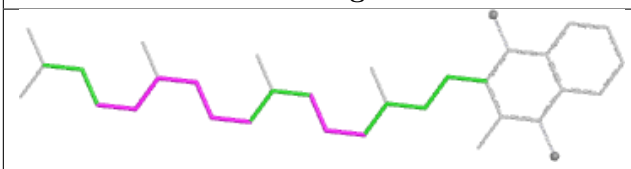
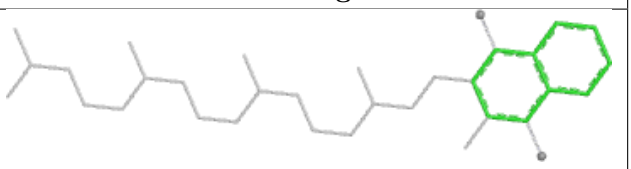


Bond angles

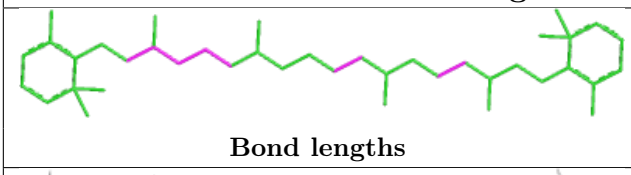


Torsions

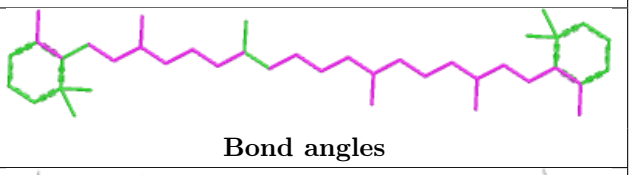


Rings

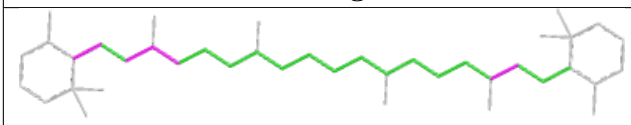
Ligand BCR M 4021



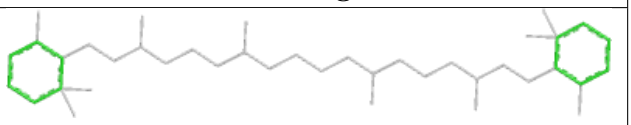
Bond lengths



Bond angles

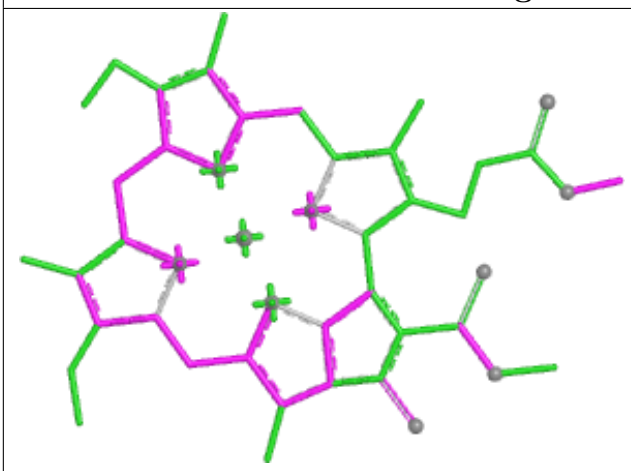


Torsions



Rings

Ligand CLA A 1134



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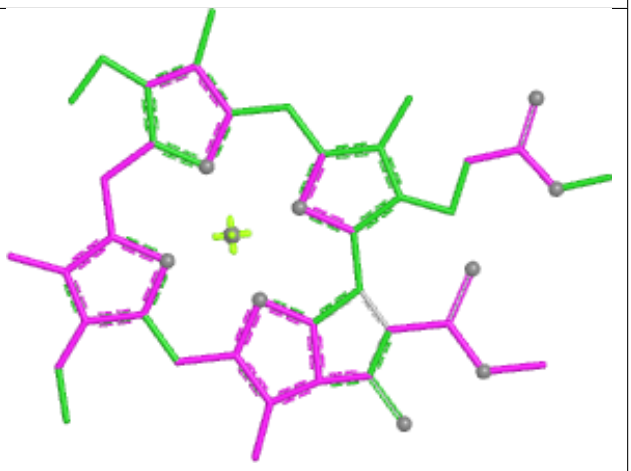
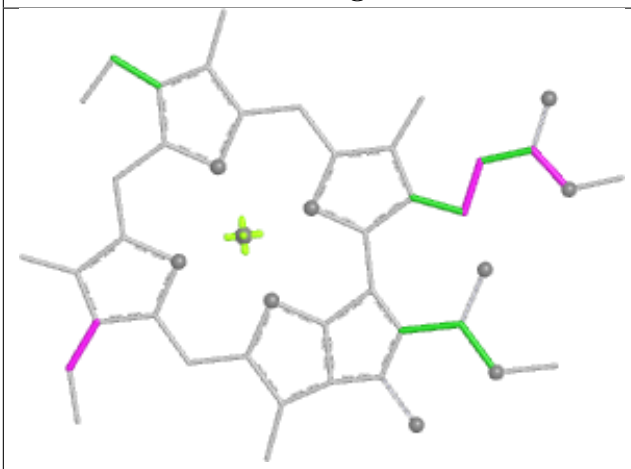
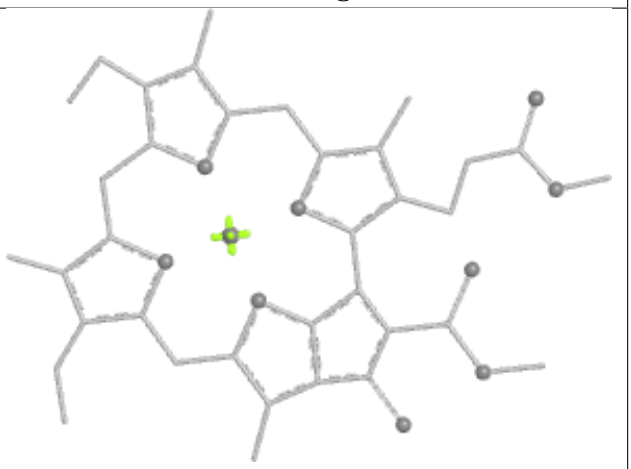


Bond angles

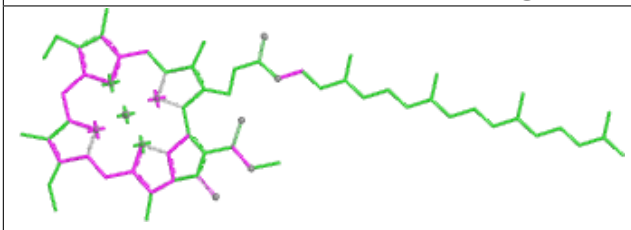


Torsions



Rings

Ligand CLA b 1229



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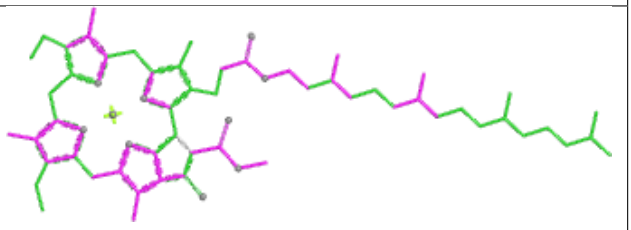
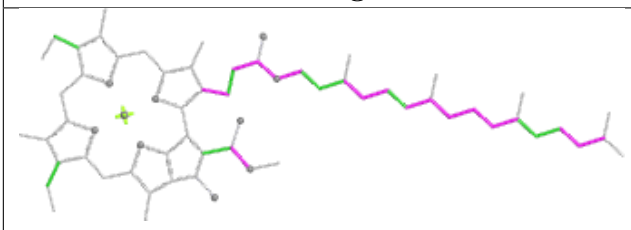


Bond angles



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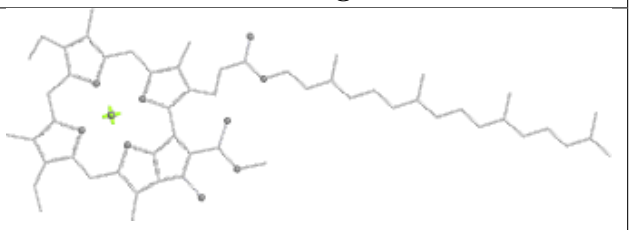
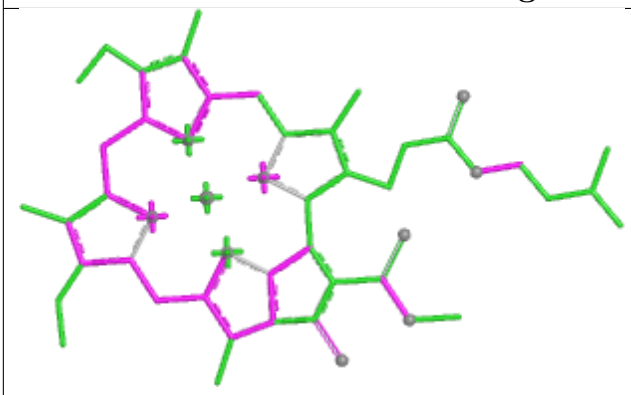


Rings

Ligand CLA b 1228



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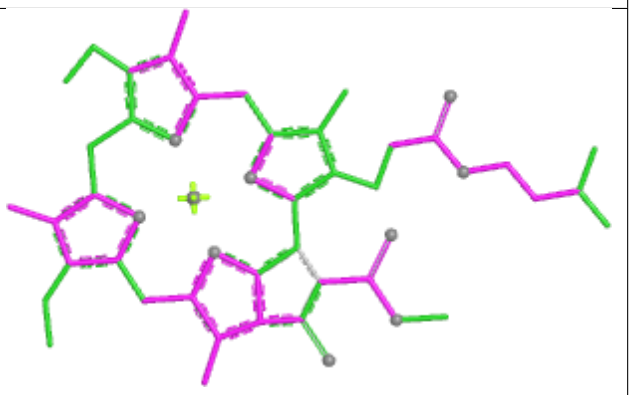
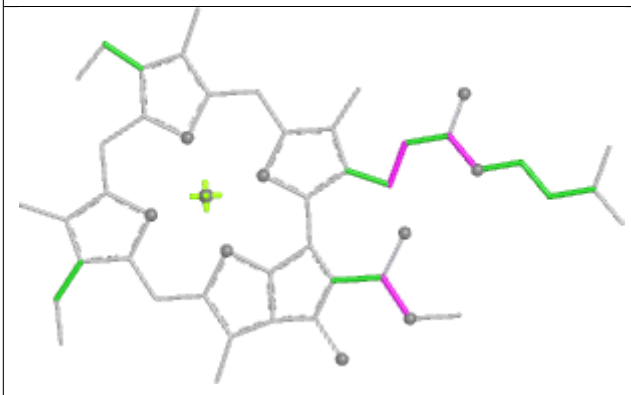


Bond angles



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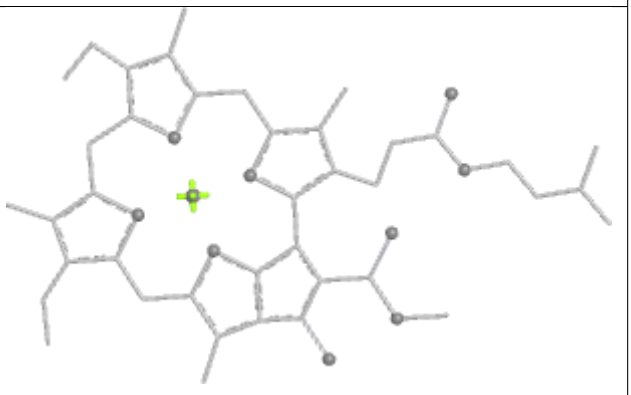
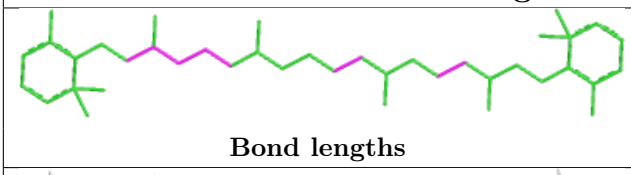


Rings

Ligand BCR B 4010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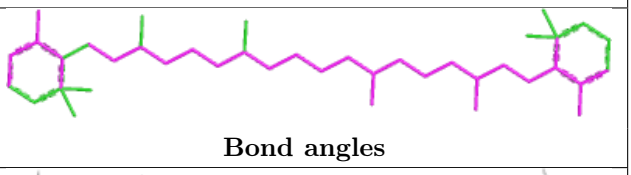
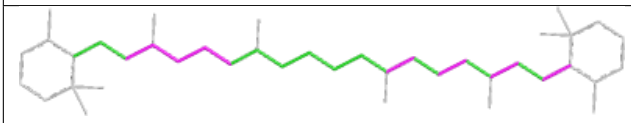

Bond angles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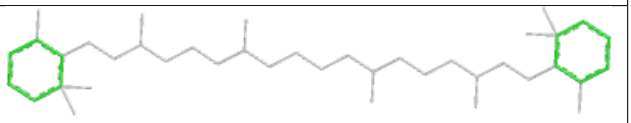
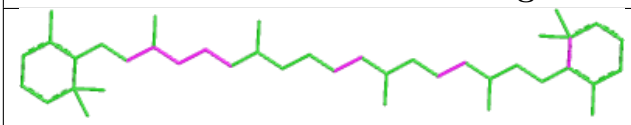
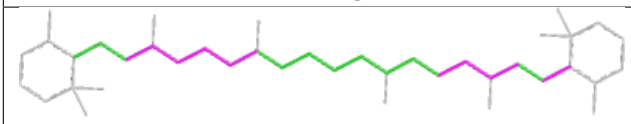

Rings

Ligand BCR 6 4020


Bond lengths

Bond angles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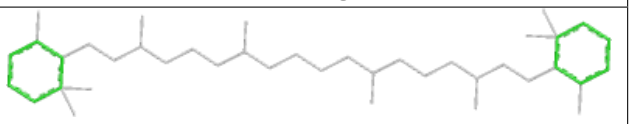
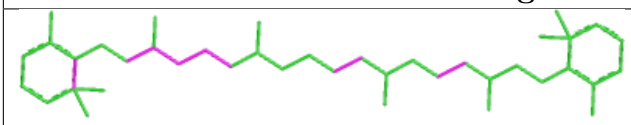

Rings

Ligand BCR 2 4011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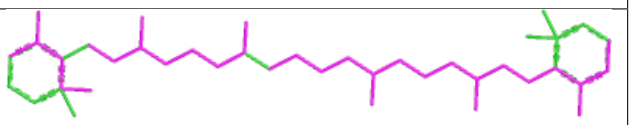
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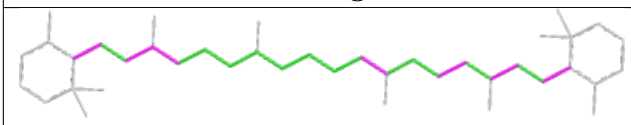
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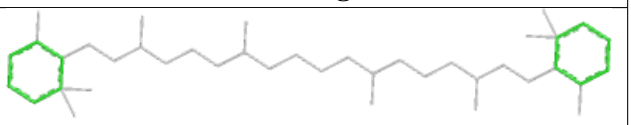
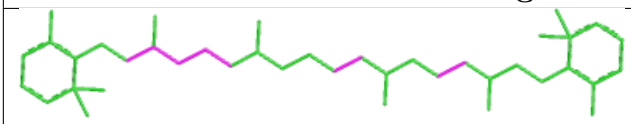
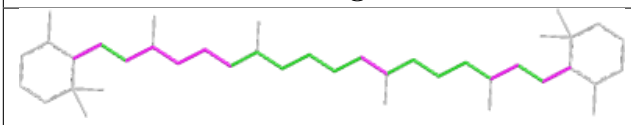

Rings

Ligand BCR b 4009


Bond lengths

Bond angles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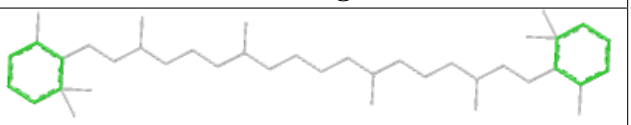
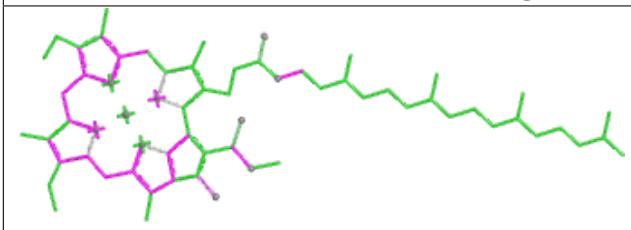
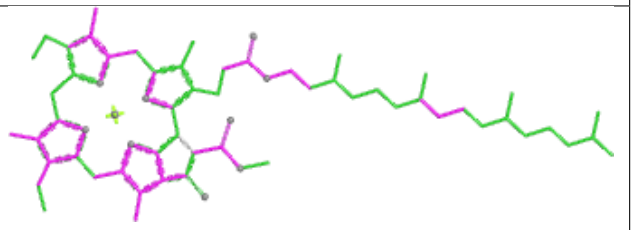

Rings

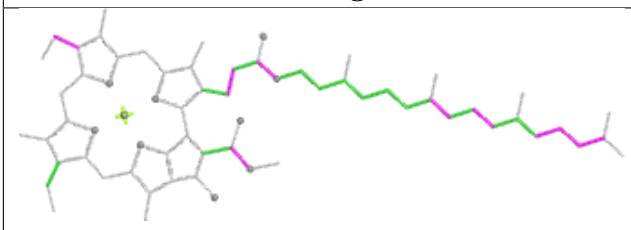
Ligand CLA b 1238



Bond lengths



Bond angles



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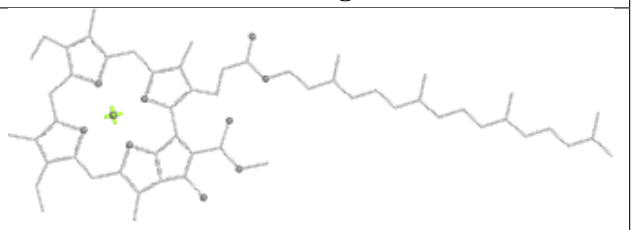
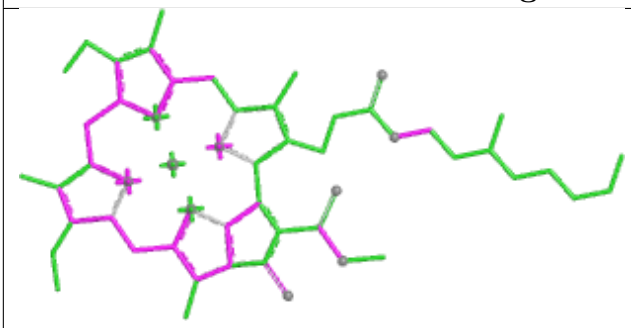


Rings

Ligand CLA a 1116



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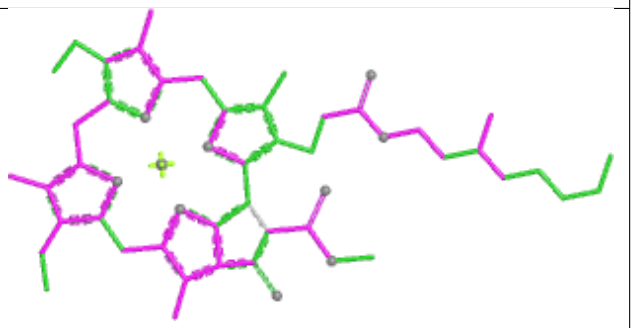
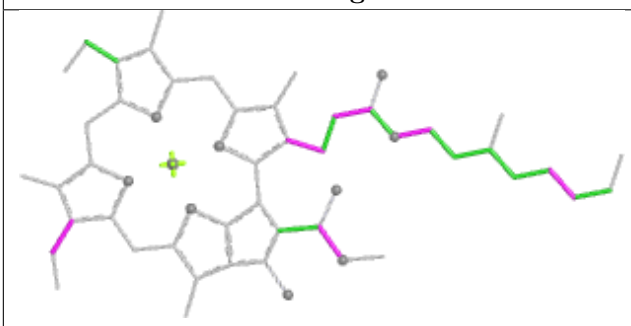


Bond angles



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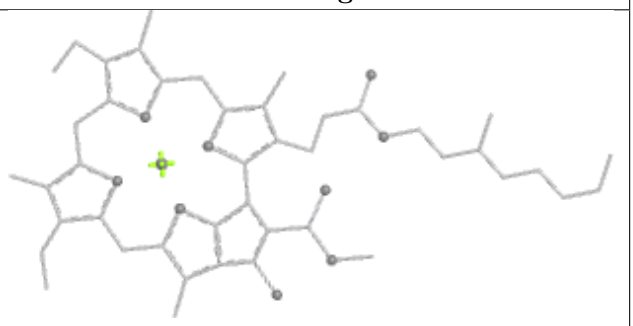
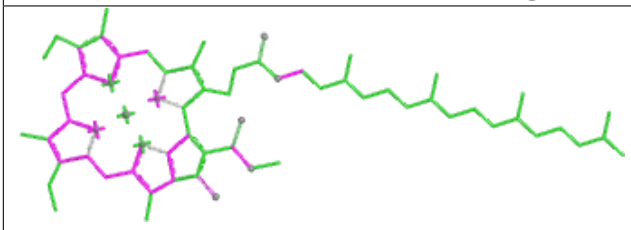
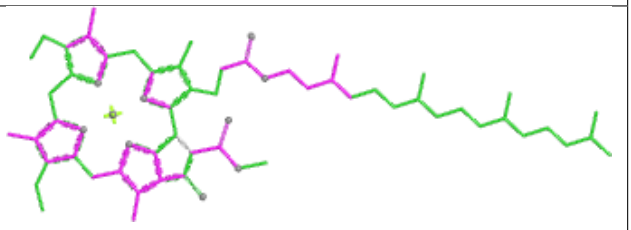


Rings

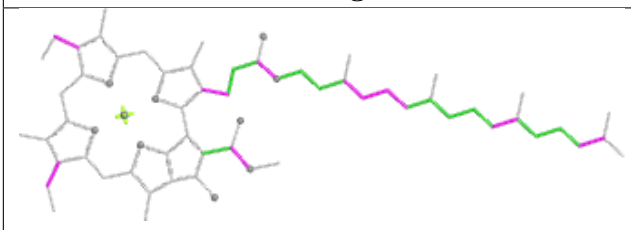
Ligand CLA l 1501



Bond lengths



Bond angles



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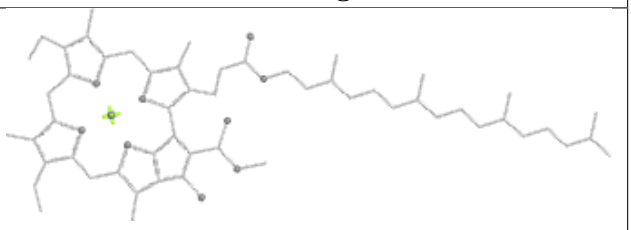
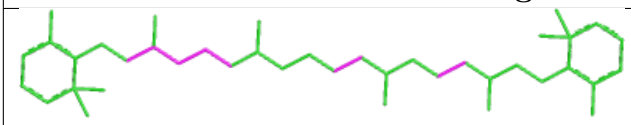


Rings

Ligand BCR F 4020



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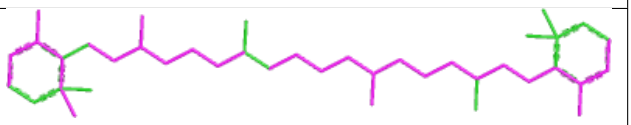
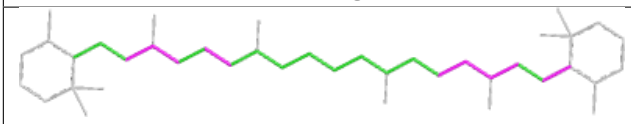


Bond angles



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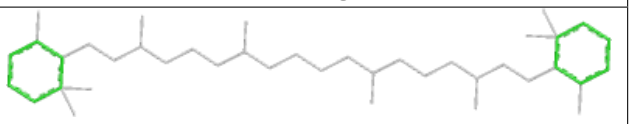
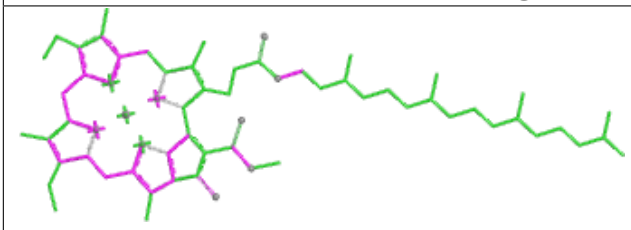


Rings

Ligand CLA B 1225



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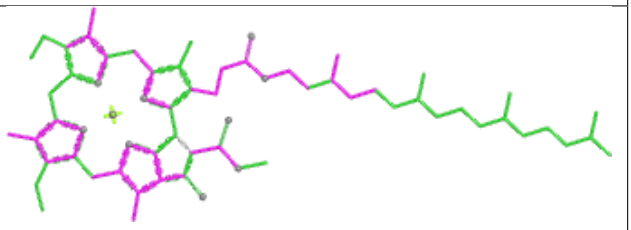
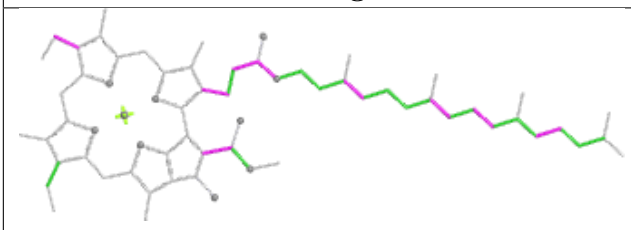
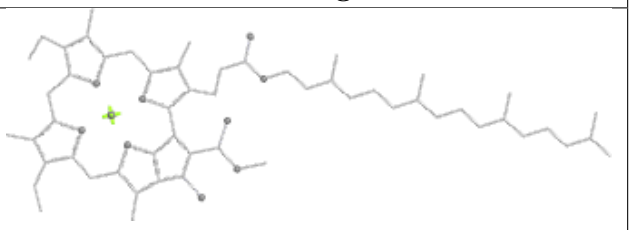


Bond angles

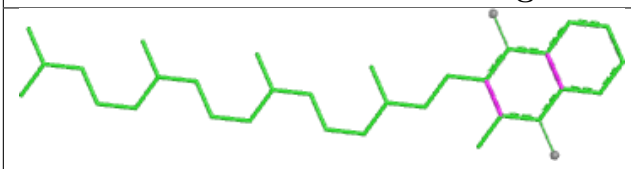


Torsions

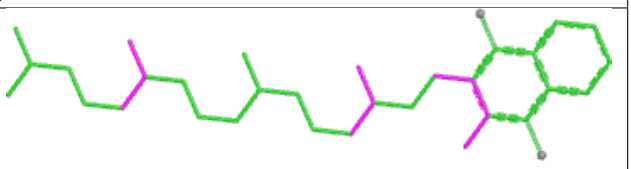


Rings

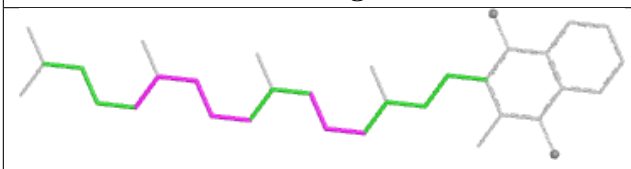
Ligand PQN 1 2001



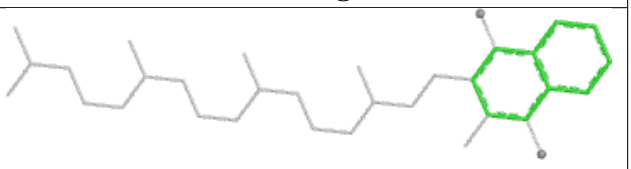
Bond lengths



Bond angles

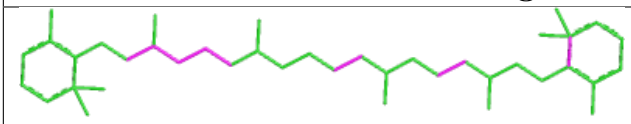


Torsions

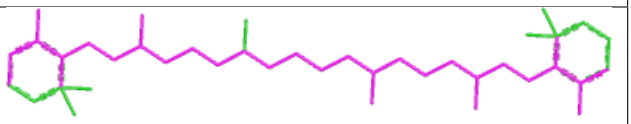


Rings

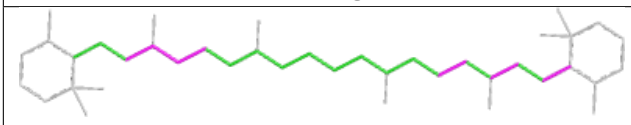
Ligand BCR 2 4010



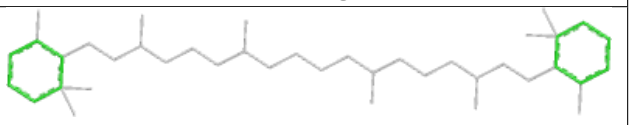
Bond lengths



Bond angles

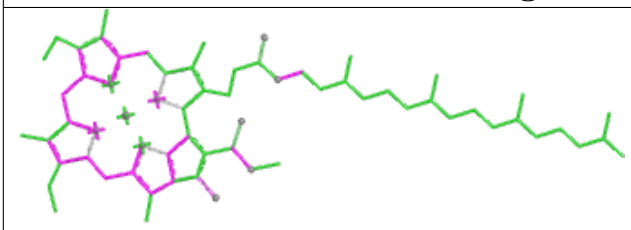


Torsions

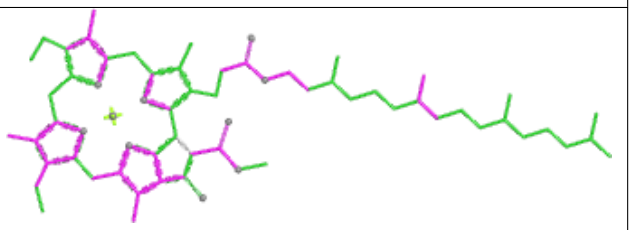


Rings

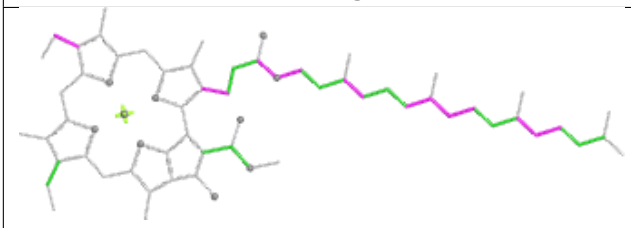
Ligand CLA 1 1123



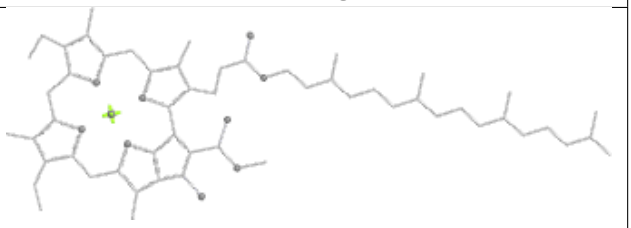
Bond lengths



Bond angles

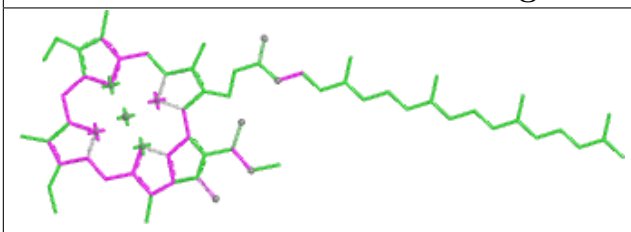


Torsions

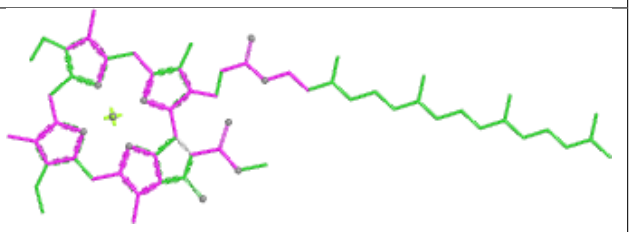


Rings

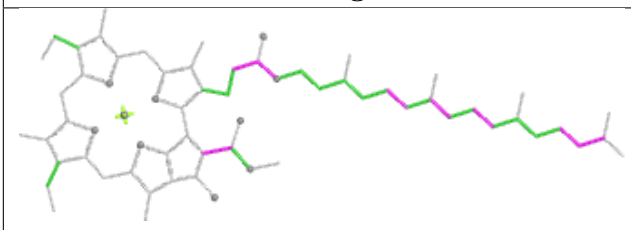
Ligand CLA 1 1011



Bond lengths



Bond angles



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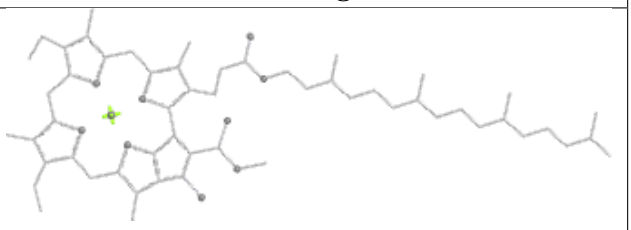
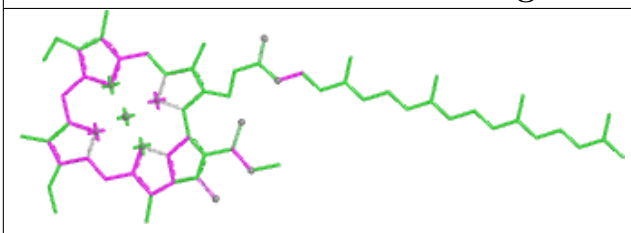
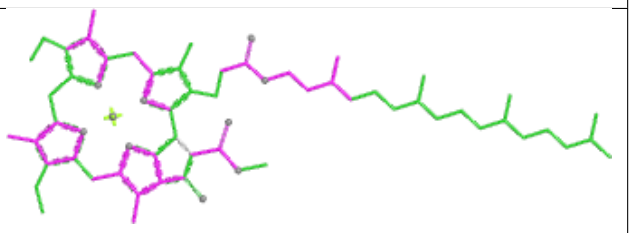


Rings

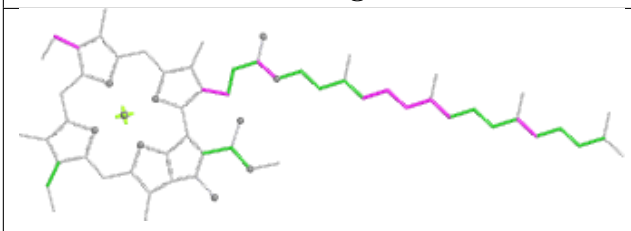
Ligand CLA L 1501



Bond lengths



Bond angles



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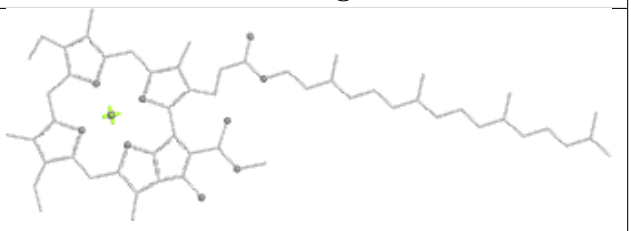
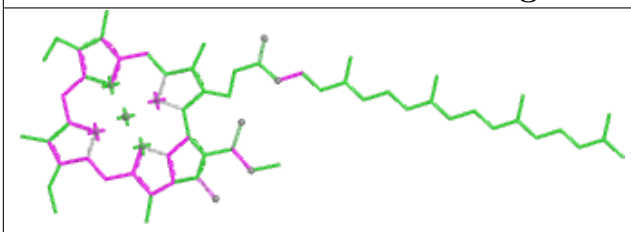


Rings

Ligand CLA a 1128



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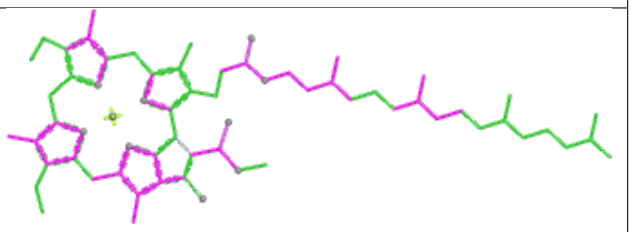
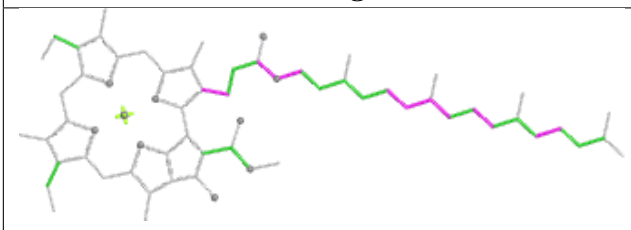


Bond angles



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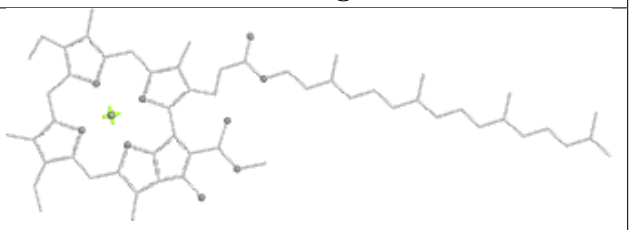
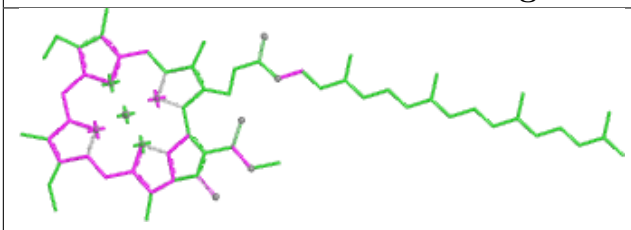
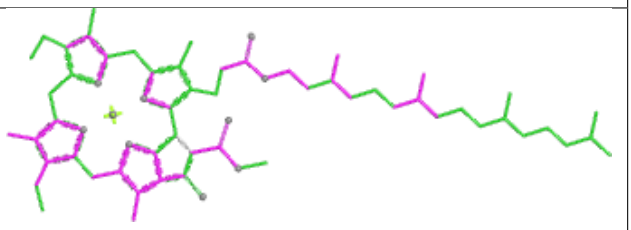


Rings

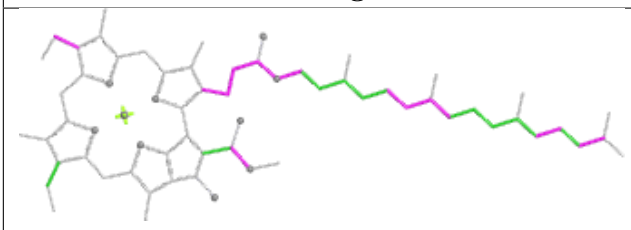
Ligand CLA 2 1216



Bond lengths



Bond angles



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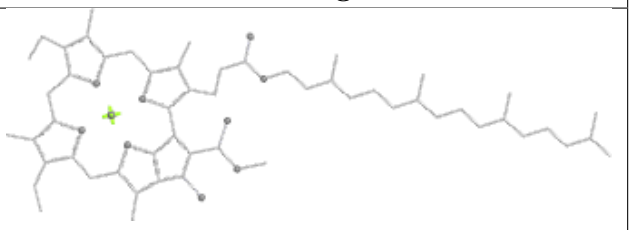
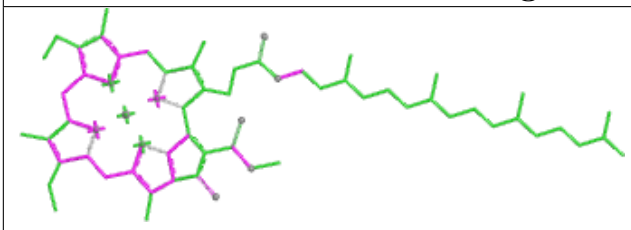
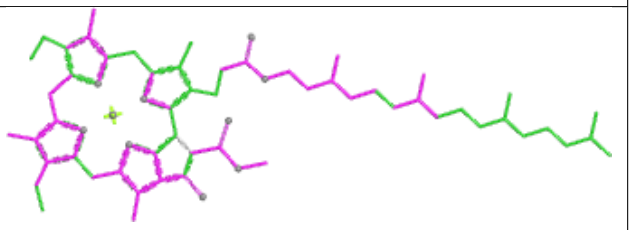


Rings

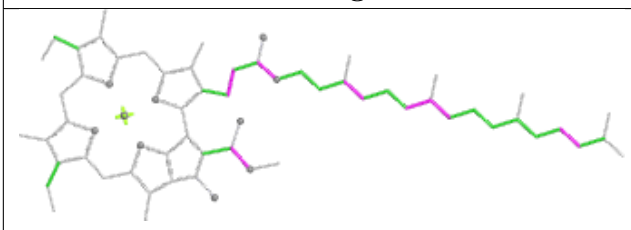
Ligand CLA a 1127



Bond lengths



Bond angles



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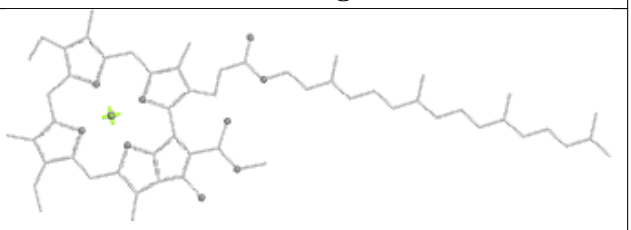
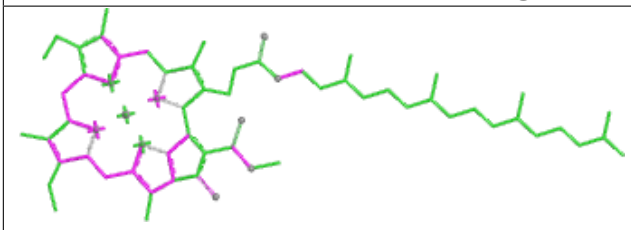
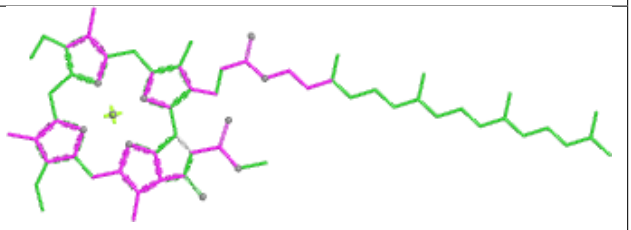


Rings

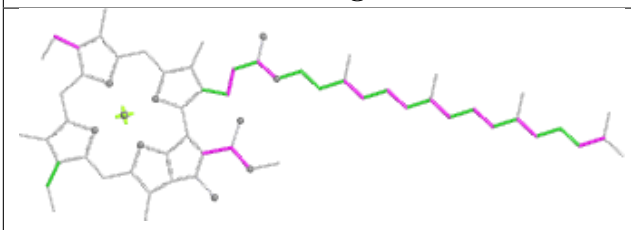
Ligand CLA A 1132



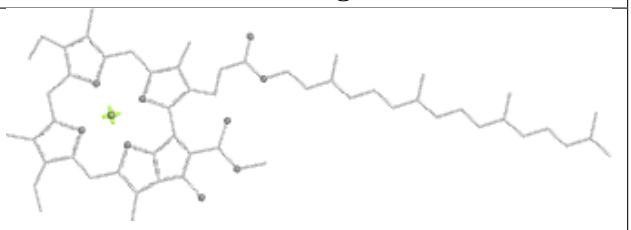
Bond lengths



Bond angles

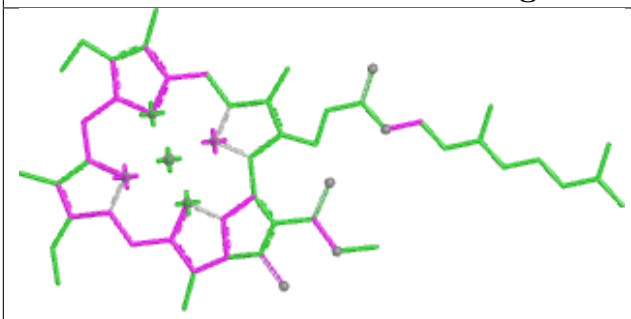


Torsions



Rings

Ligand CLA 1 1124



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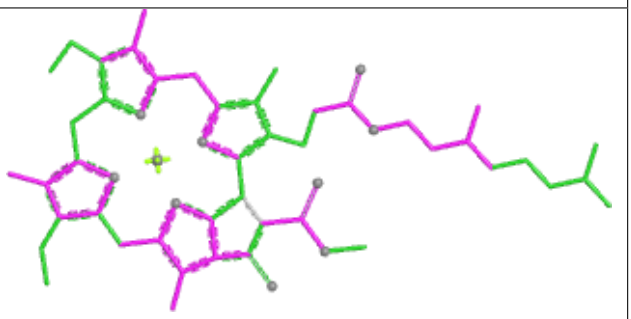
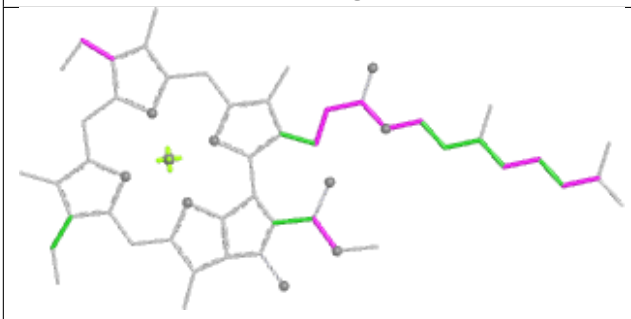


Bond angles



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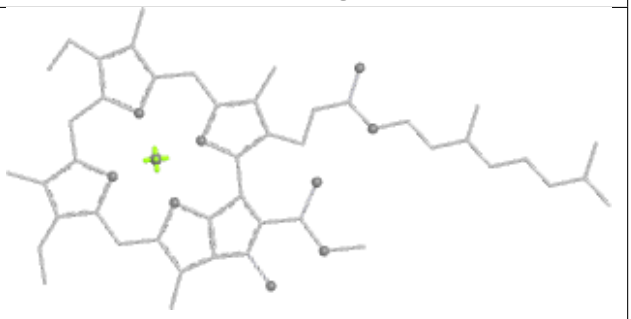
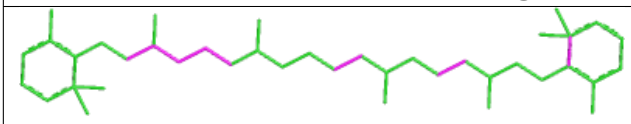
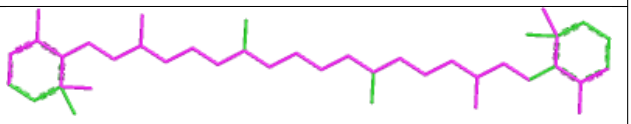


Rings

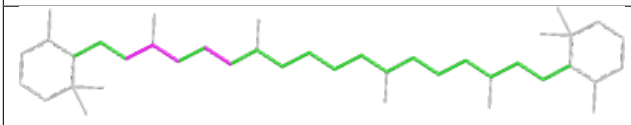
Ligand BCR F 4018



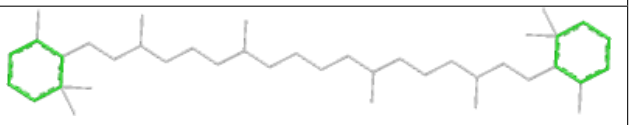
Bond lengths



Bond angles

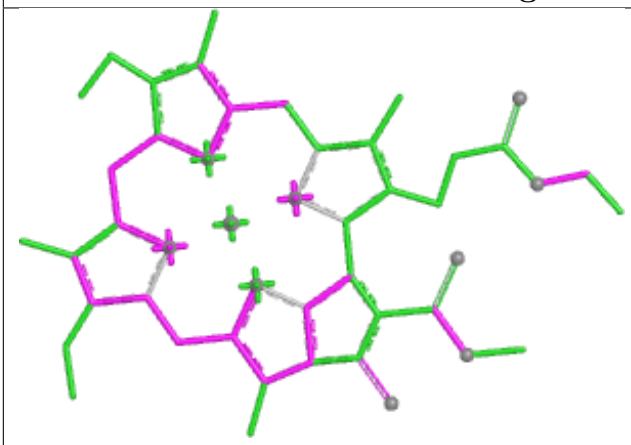


Torsions

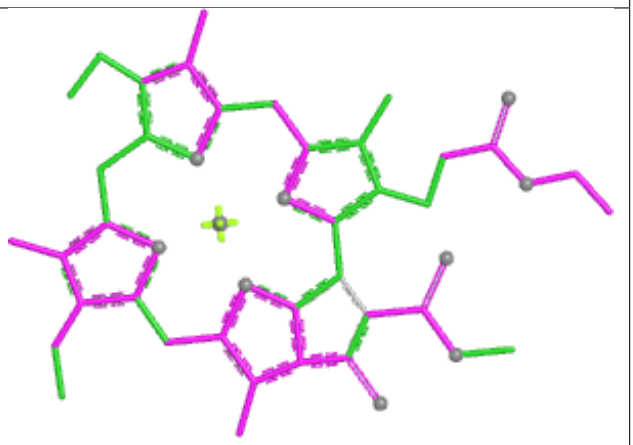


Rings

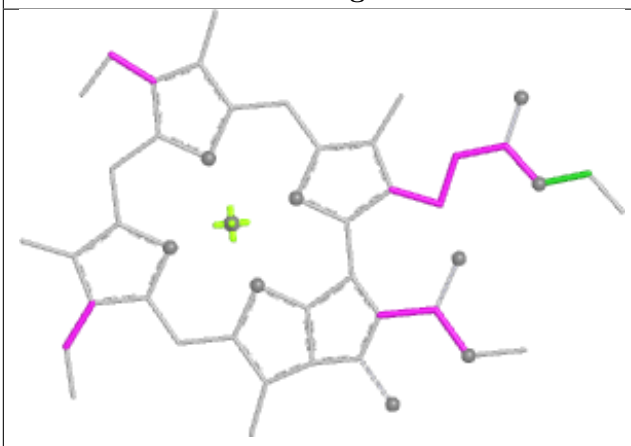
Ligand CLA 2 1217



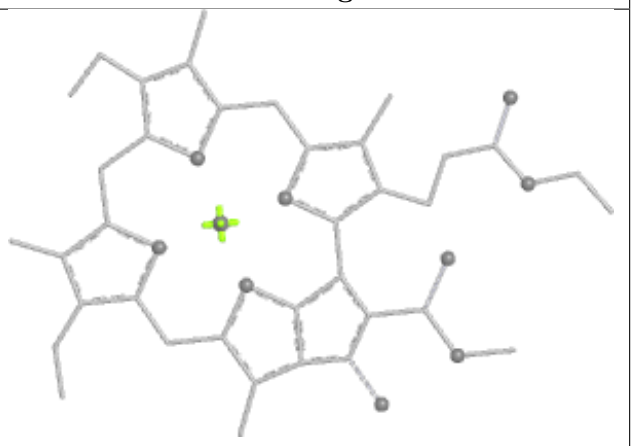
Bond lengths



Bond angles

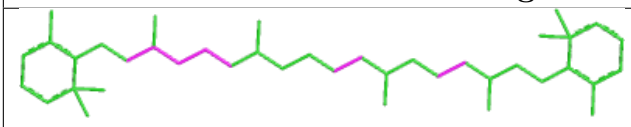


Torsions

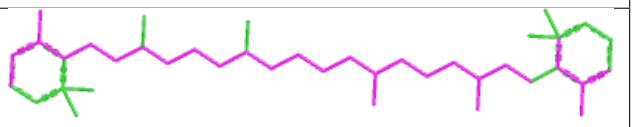


Rings

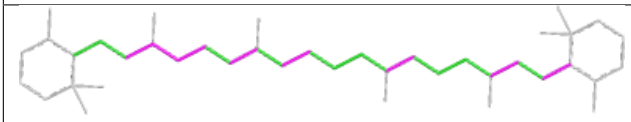
Ligand BCR 2 4014



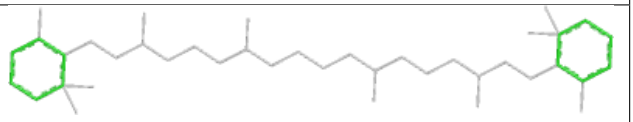
Bond lengths



Bond angles

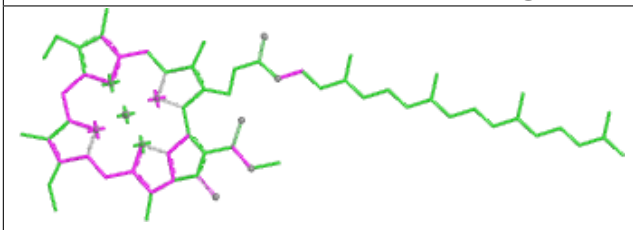


Torsions

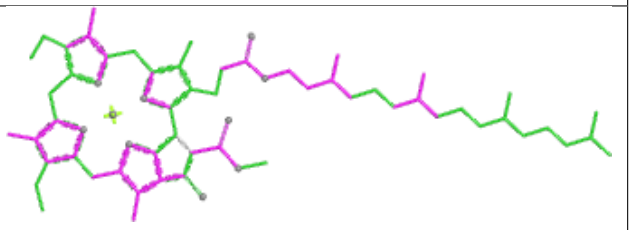


Rings

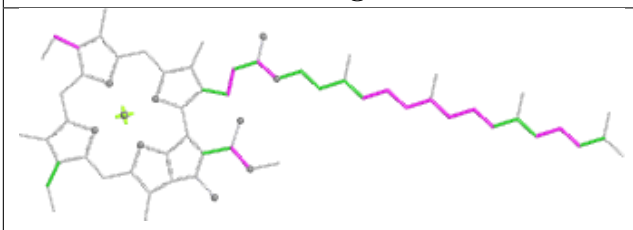
Ligand CLA a 1140



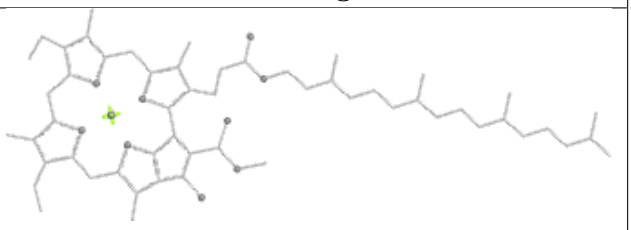
Bond lengths



Bond angles

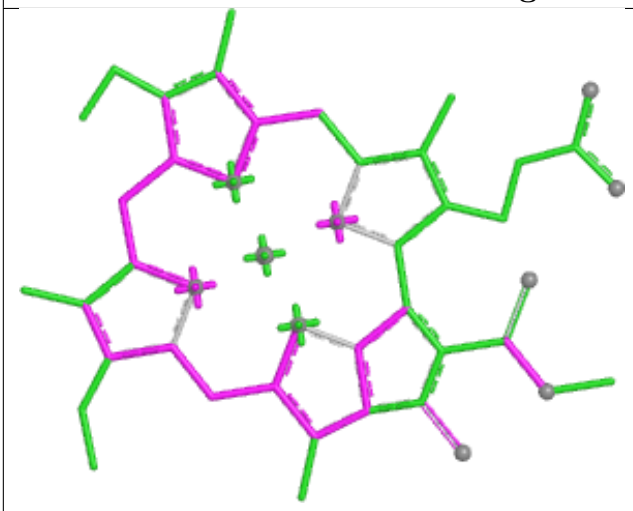


Torsions

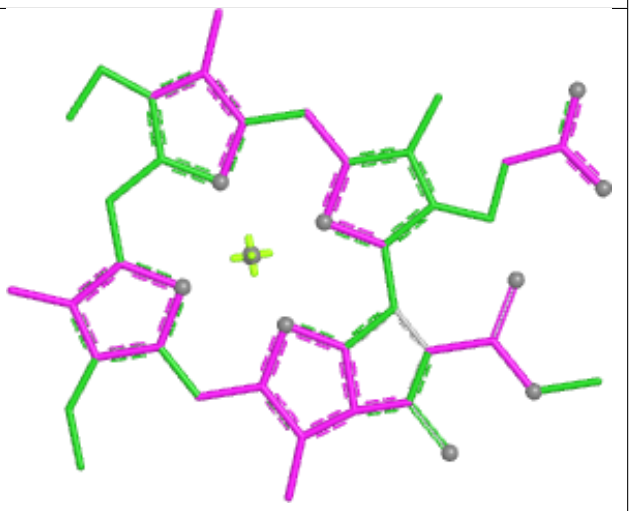


Rings

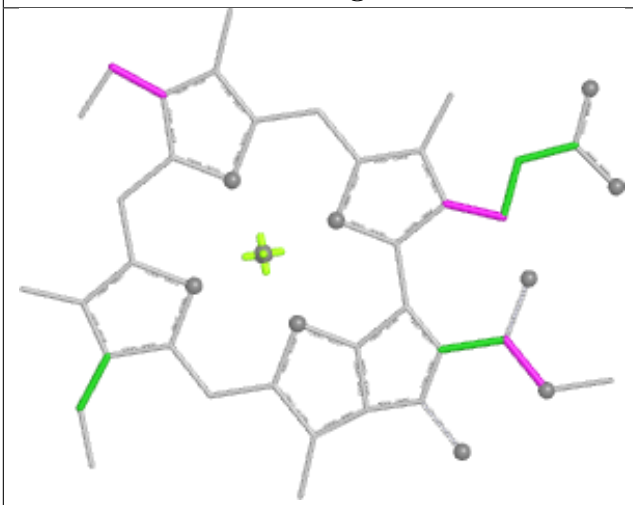
Ligand CLA 2 1218



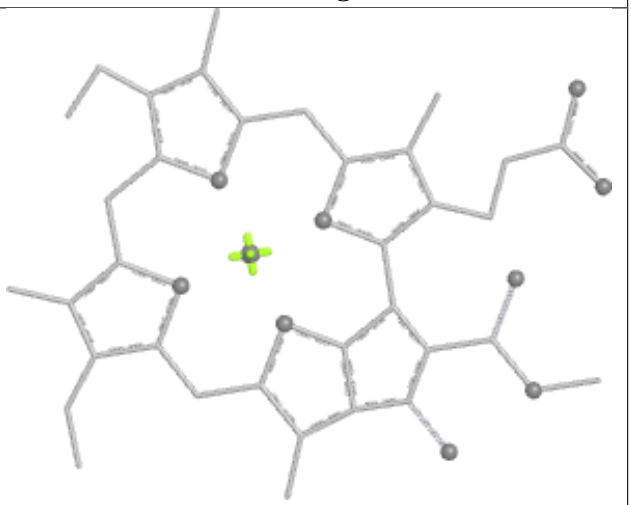
Bond lengths



Bond angles

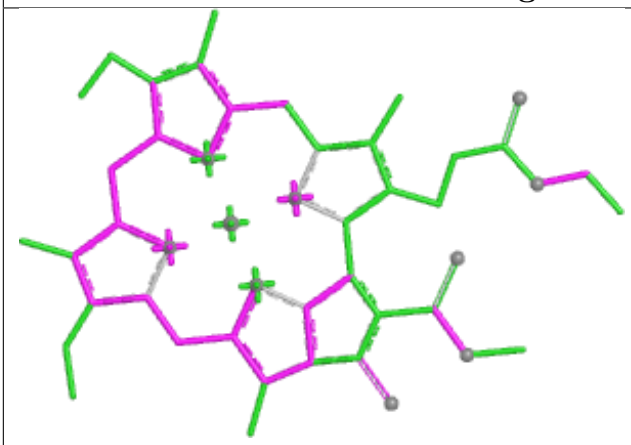


Torsions

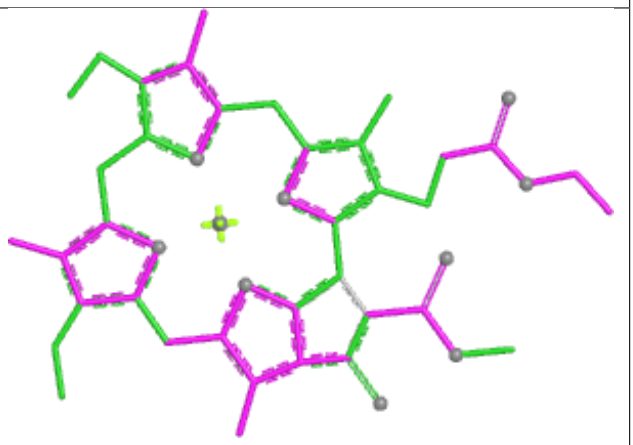


Rings

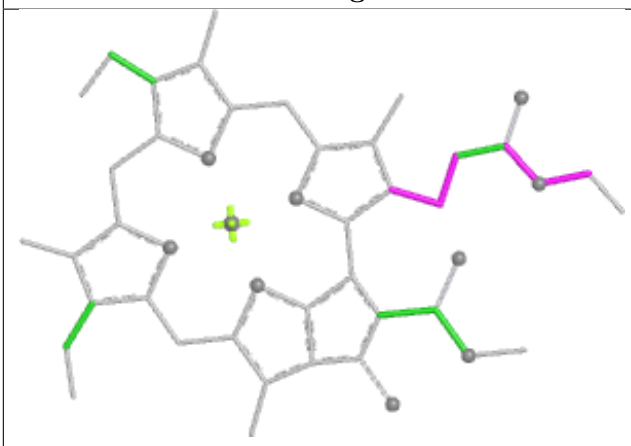
Ligand CLA b 1217



Bond lengths



Bond angles



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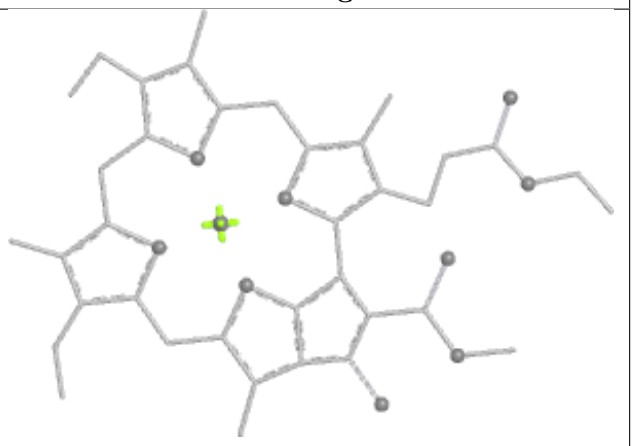
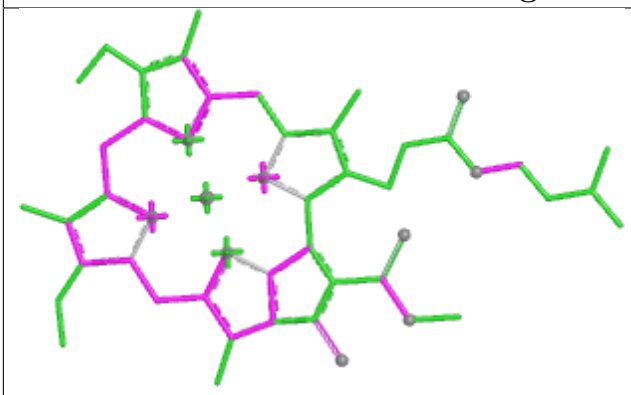


Rings

Ligand CLA a 1139



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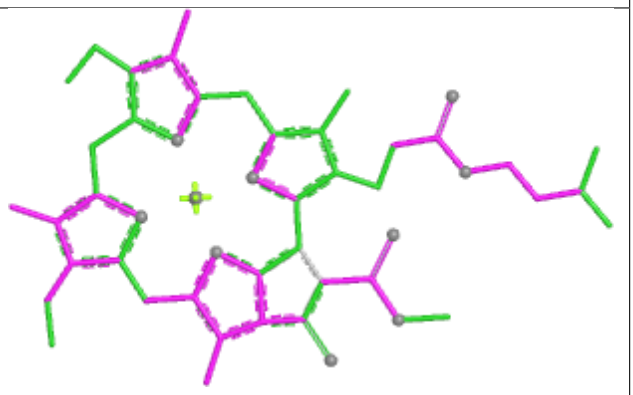
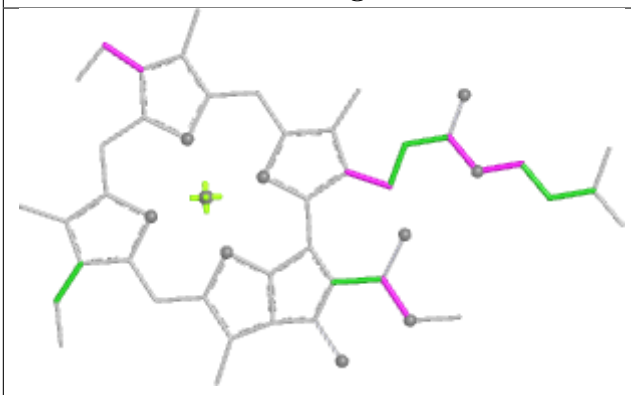
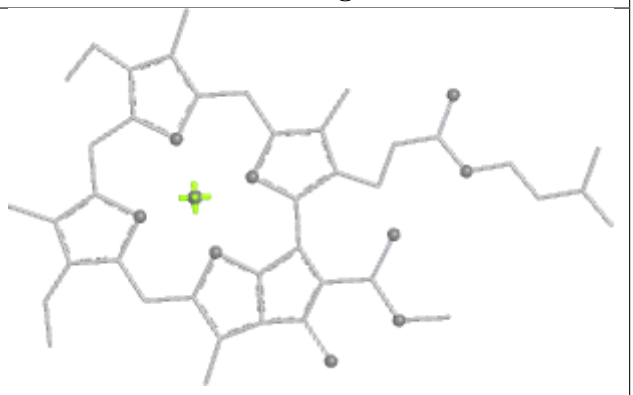


Bond angles

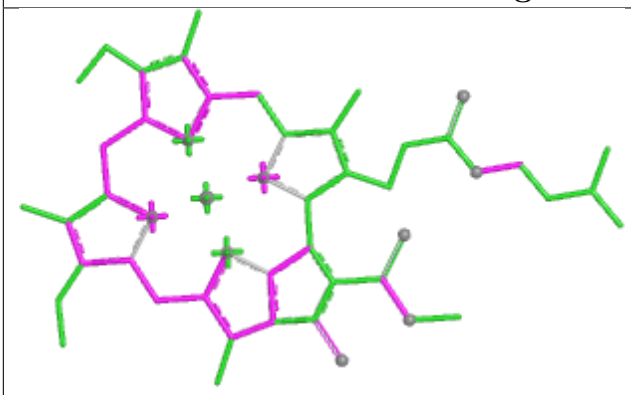


Torsions

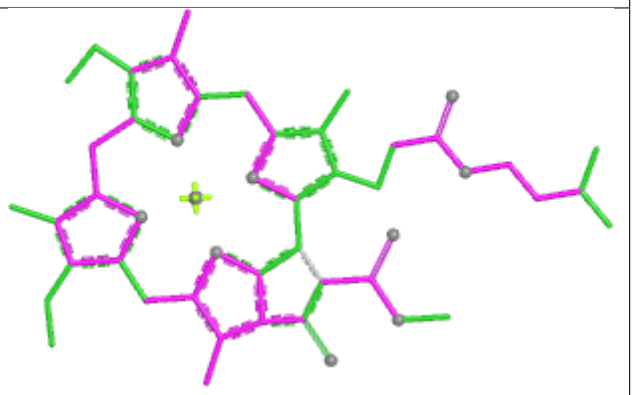


Rings

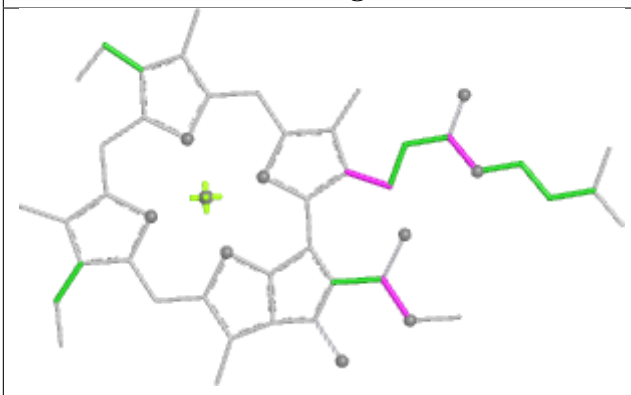
Ligand CLA K 1402



Bond lengths



Bond angles



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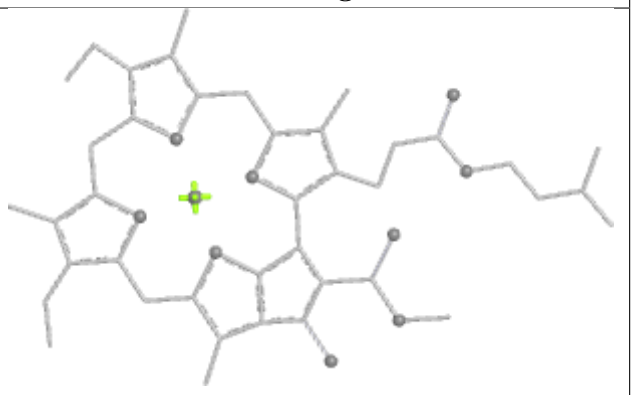
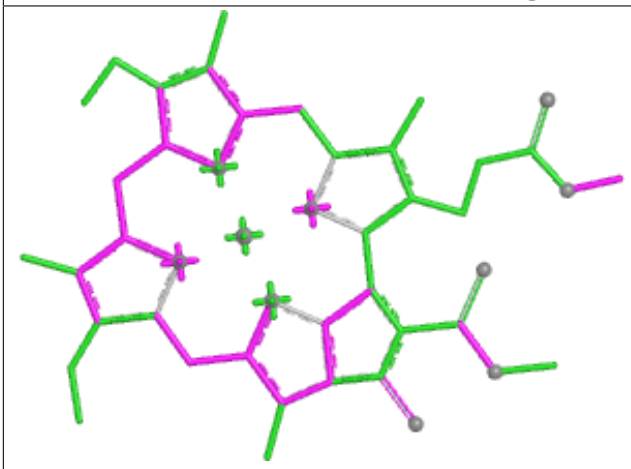


Rings

Ligand CLA l 1502



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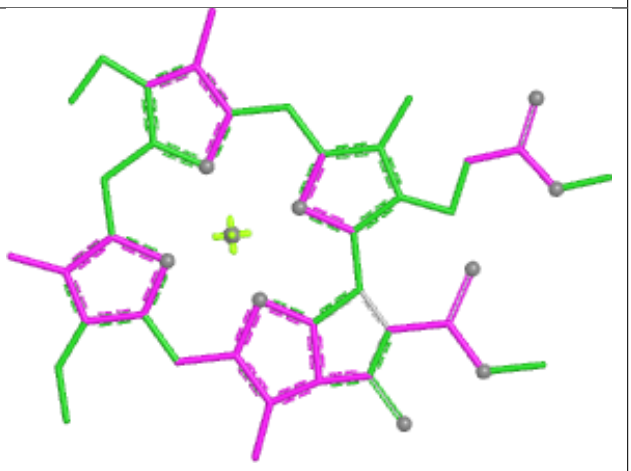
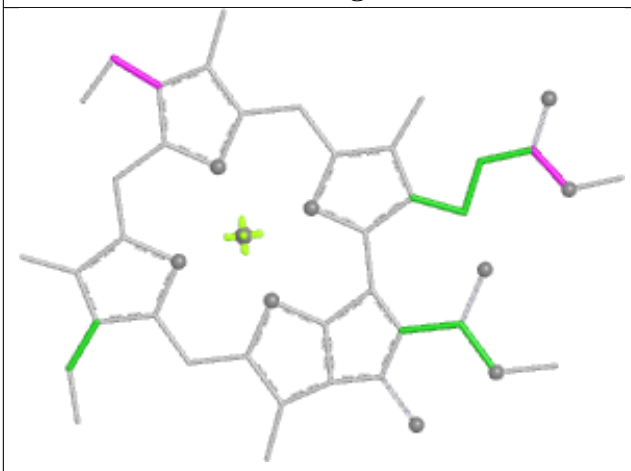


Bond angles



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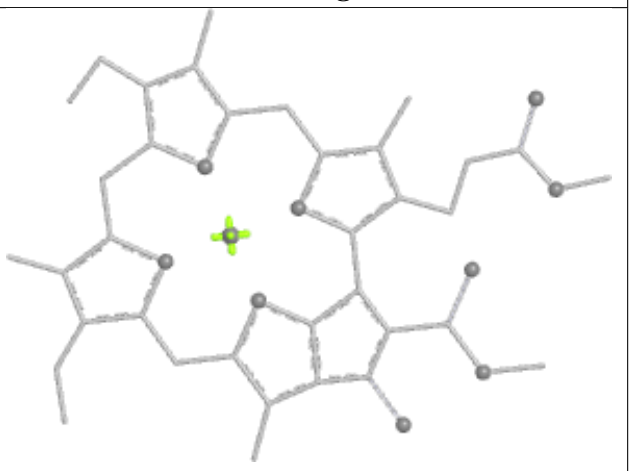
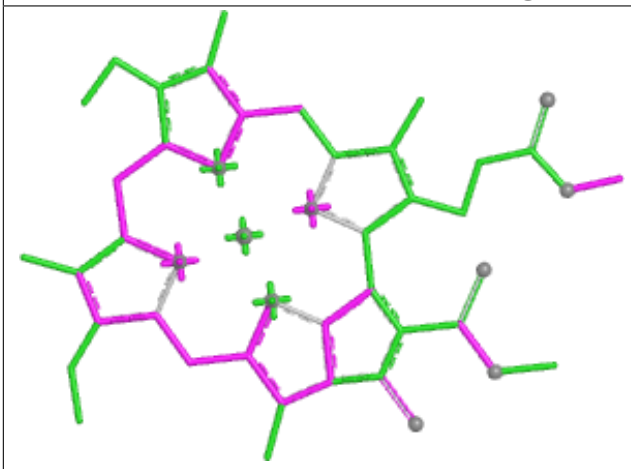


Rings

Ligand CLA 2 1220



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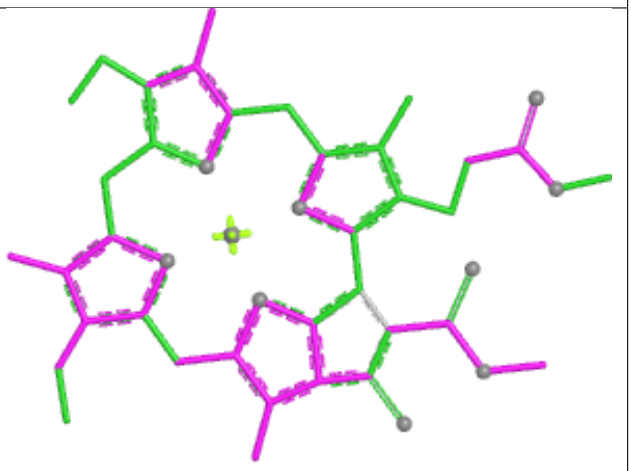

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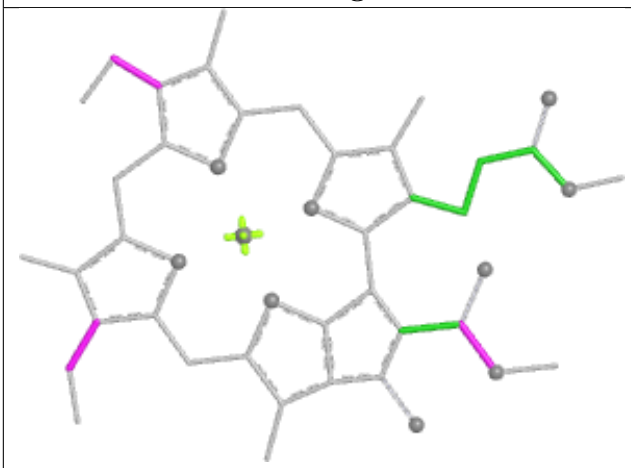

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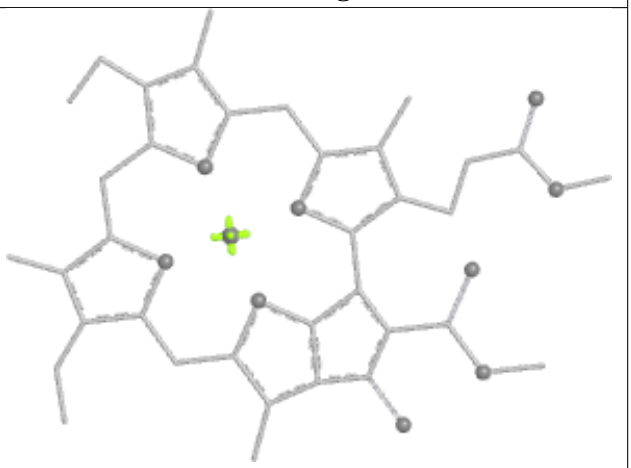
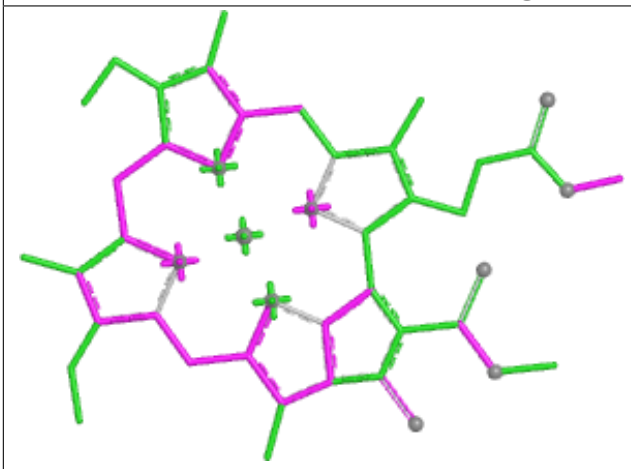


Rings

Ligand CLA b 1220



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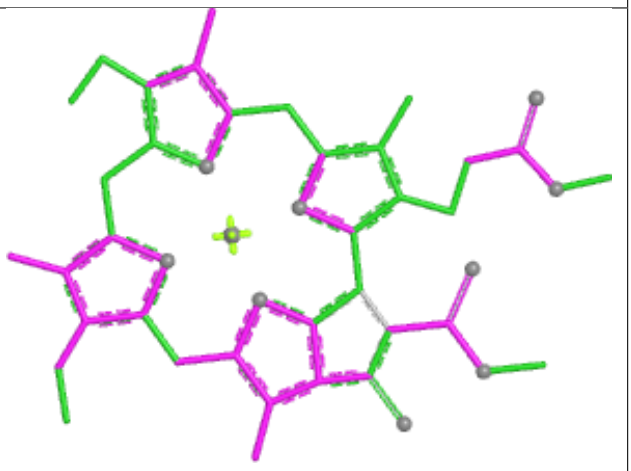
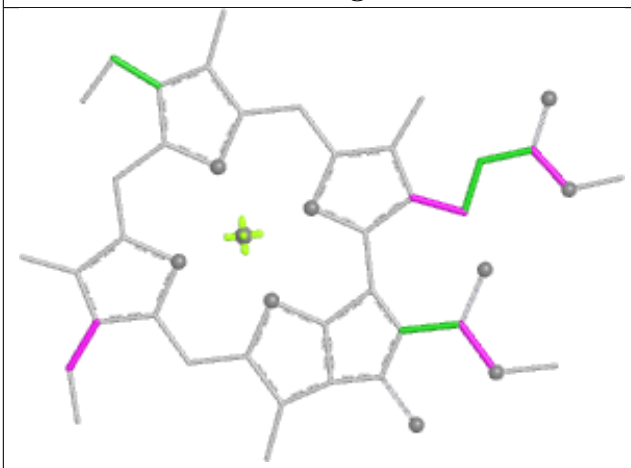


Bond angles



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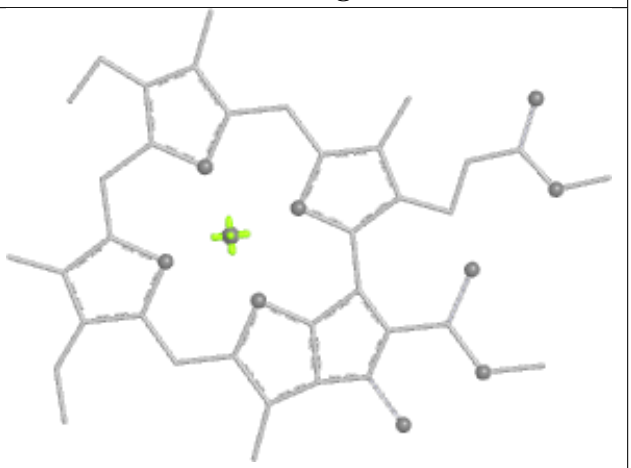
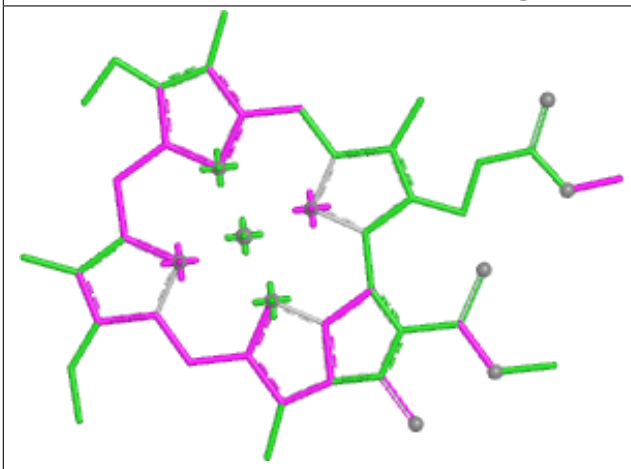


Rings

Ligand CLA A 1138



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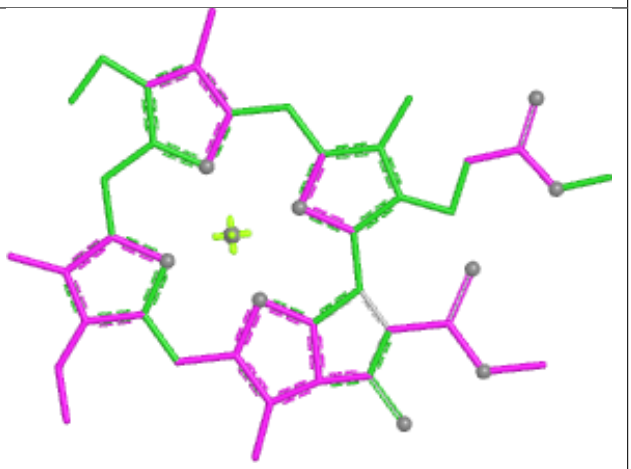
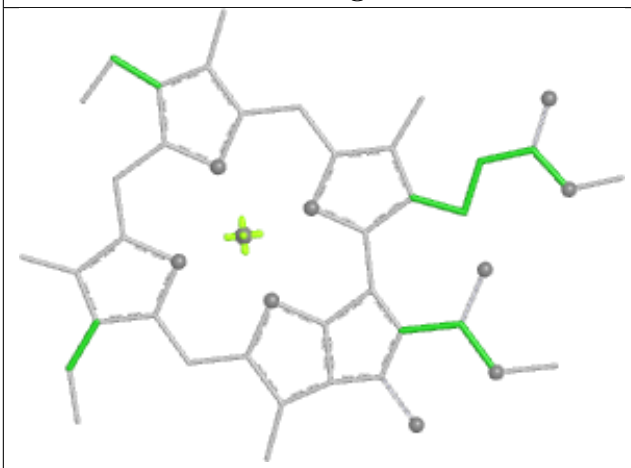


Bond angles



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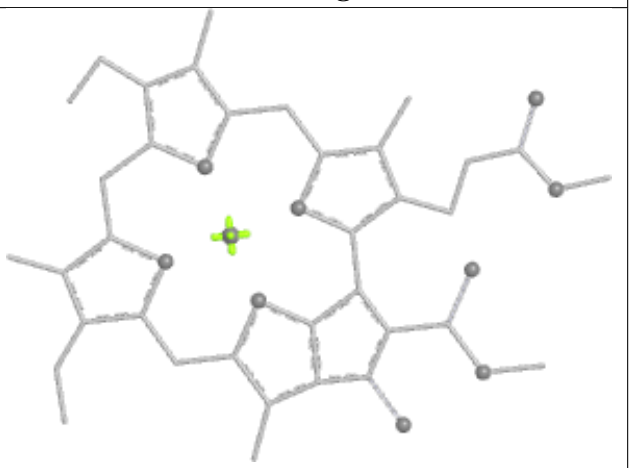
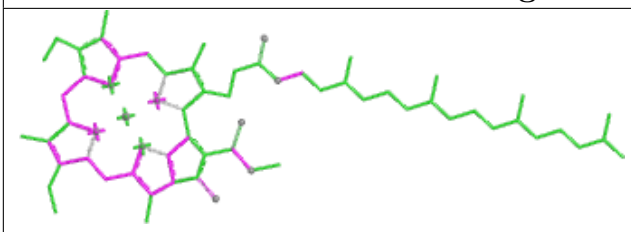


Rings

Ligand CLA k 1401



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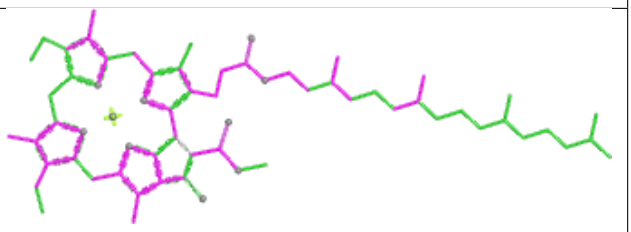
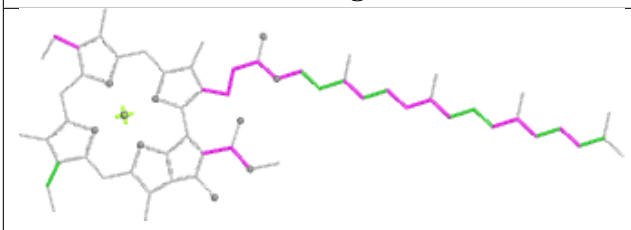
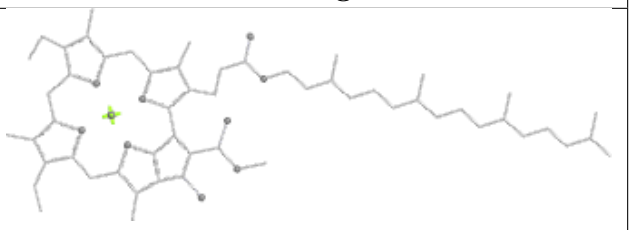


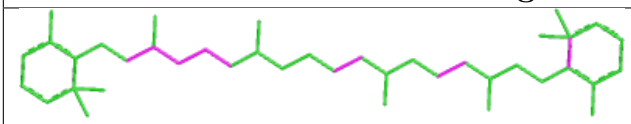
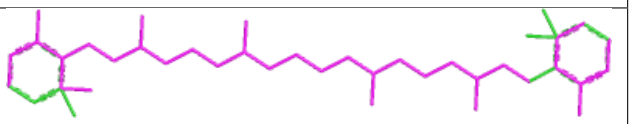
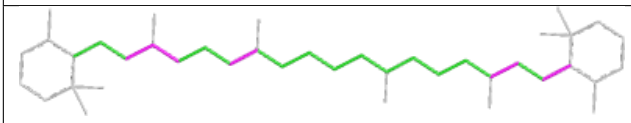
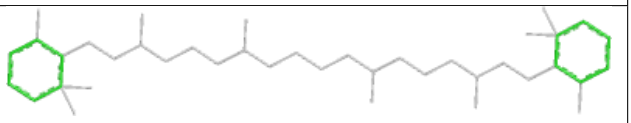
Bond angles

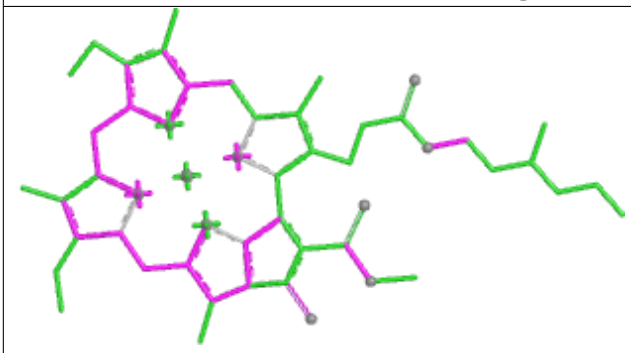
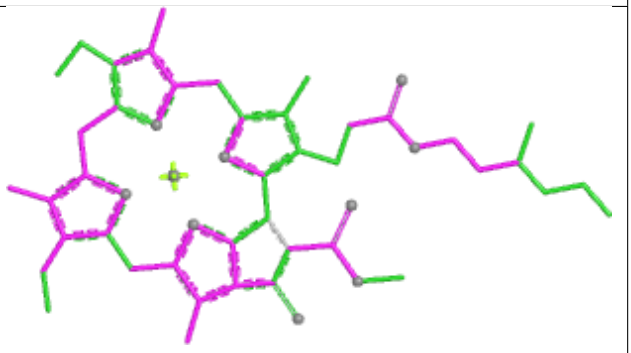
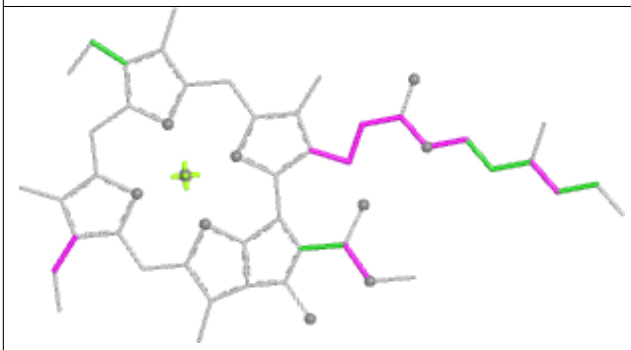
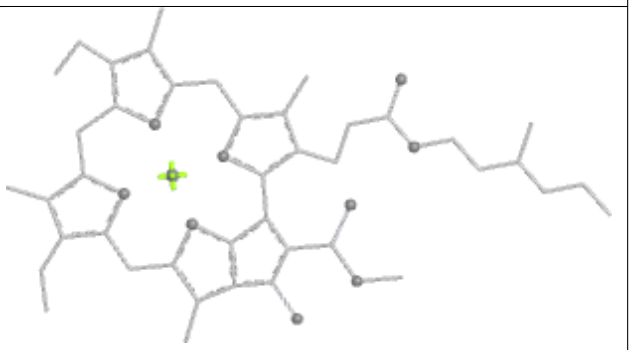


Torsions

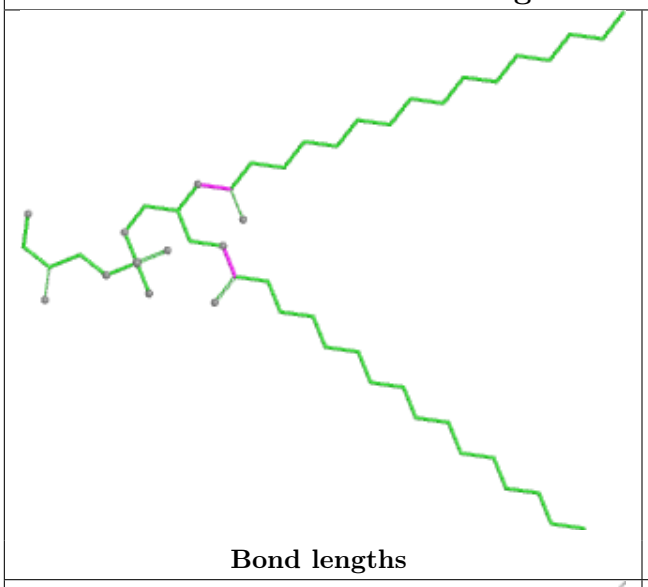


Rings

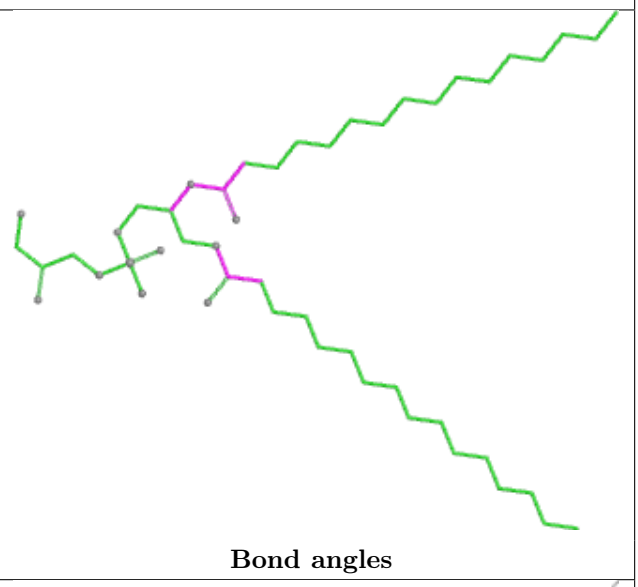
Ligand BCR 6 4018	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

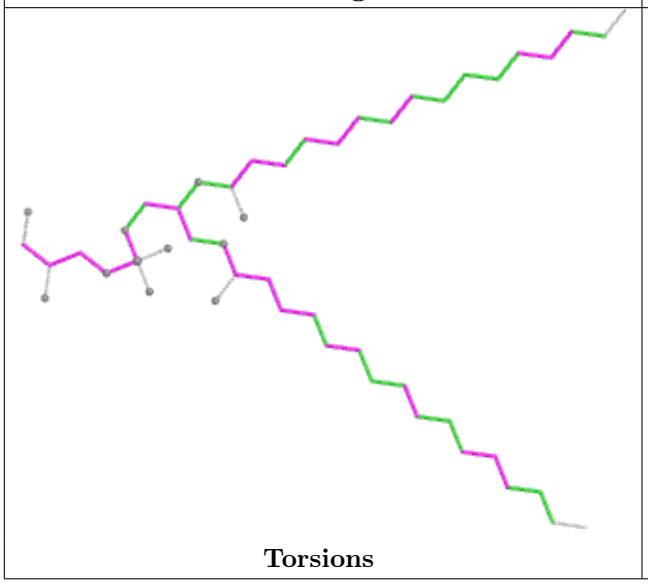
Ligand LHG A 5003



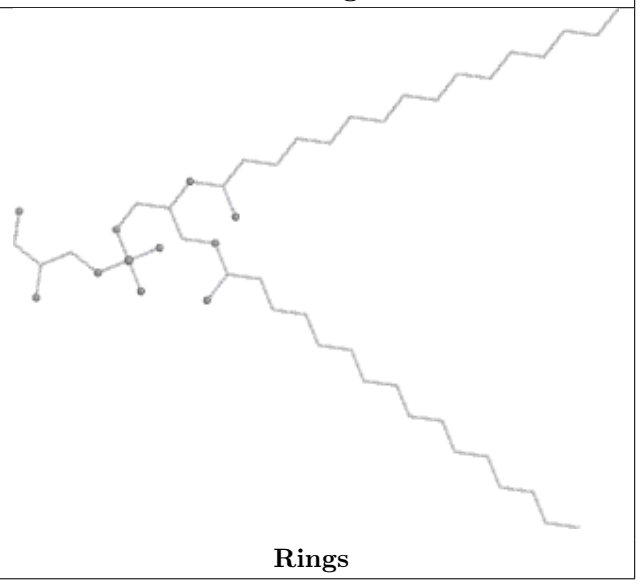
Bond lengths



Bond angles

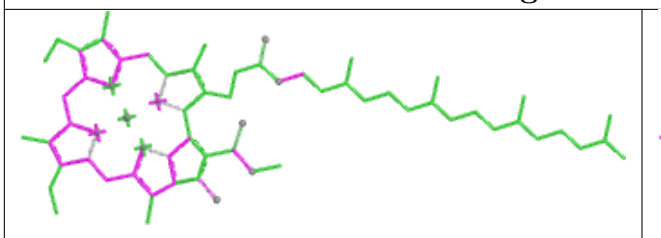


Torsions



Rings

Ligand CLA 1 1126



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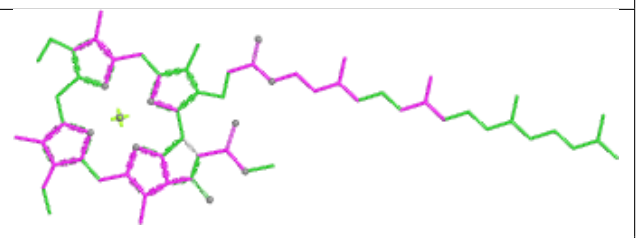
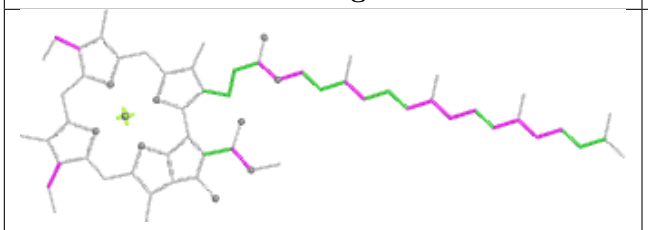
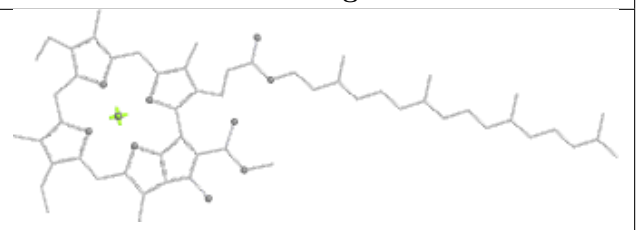


Bond angles

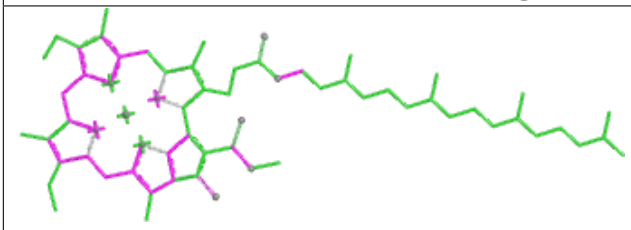


Torsions

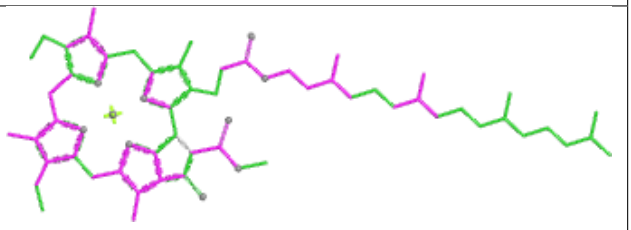


Rings

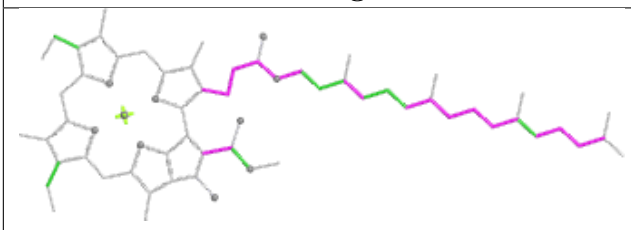
Ligand CLA B 1229



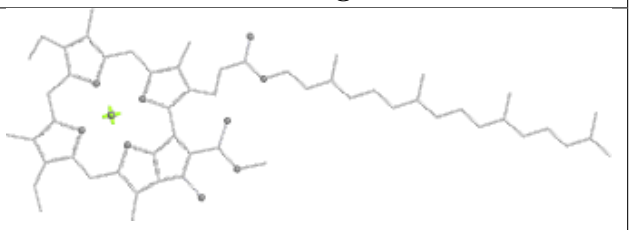
Bond lengths



Bond angles

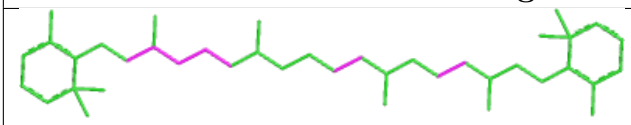


Torsions



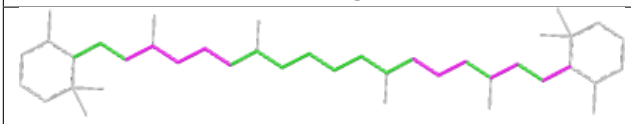
Rings

Ligand BCR 1 4007

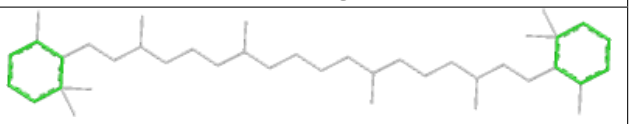


Bond lengths

Bond angles

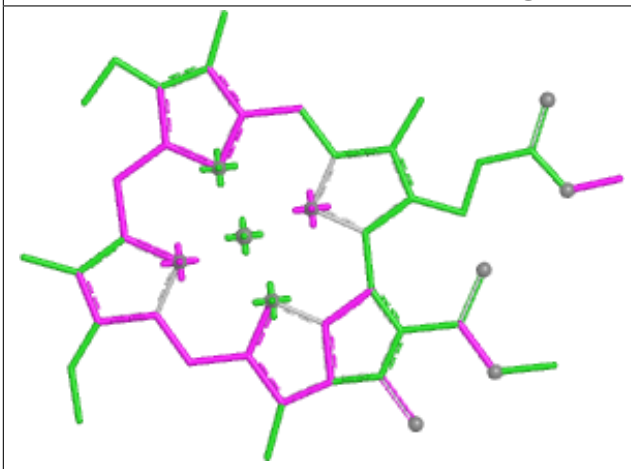


Torsions

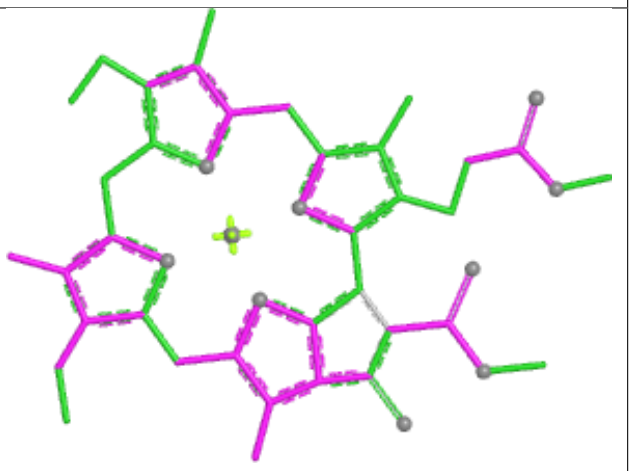


Rings

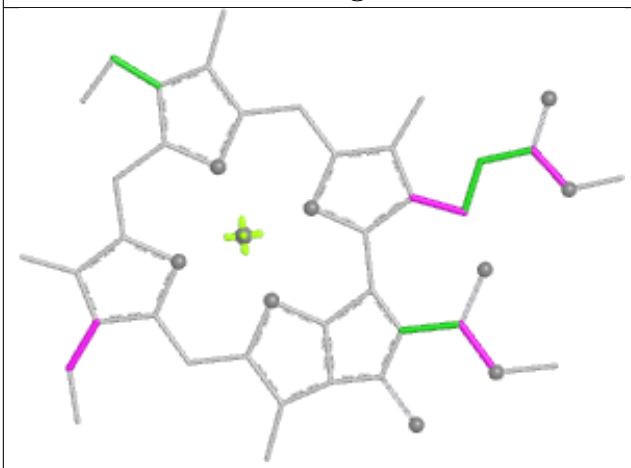
Ligand CLA a 1130



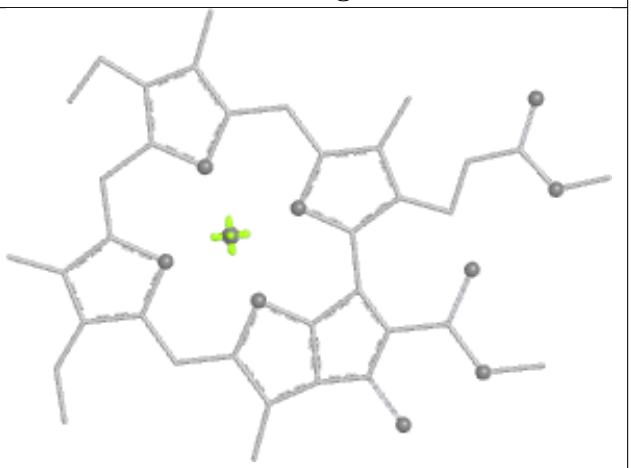
Bond lengths



Bond angles

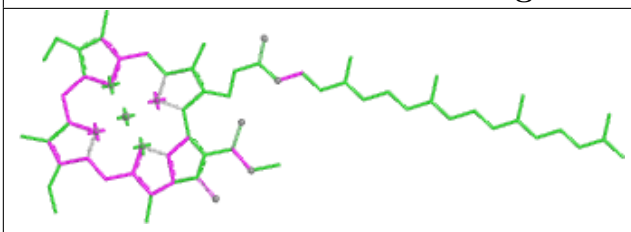


Torsions

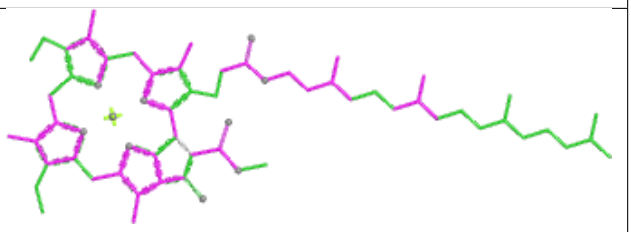


Rings

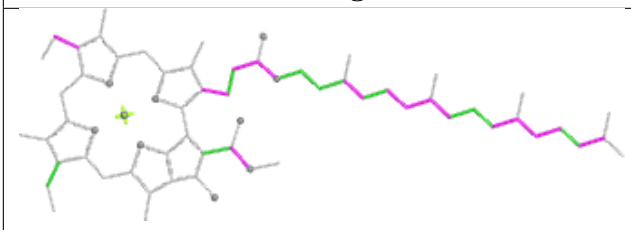
Ligand CLA B 1021



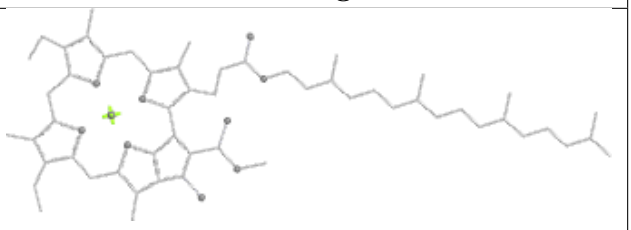
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	1	739/751 (98%)	-0.45	2 (0%)	90	78	100, 203, 296, 388	0
1	A	739/751 (98%)	-0.41	1 (0%)	92	87	80, 112, 176, 250	0
1	a	739/751 (98%)	-0.45	3 (0%)	88	74	125, 205, 289, 372	0
2	2	728/731 (99%)	-0.46	1 (0%)	92	87	91, 133, 197, 293	0
2	B	728/731 (99%)	-0.43	3 (0%)	88	74	81, 133, 213, 297	0
2	b	728/731 (99%)	-0.51	2 (0%)	90	78	112, 221, 302, 414	0
3	3	80/81 (98%)	-0.13	3 (3%)	44	31	143, 185, 231, 268	0
3	C	80/81 (98%)	-0.19	0	100	100	100, 116, 140, 196	0
3	c	80/81 (98%)	-0.20	0	100	100	149, 205, 255, 292	0
4	4	138/141 (97%)	-0.50	0	100	100	93, 195, 240, 290	0
4	D	138/141 (97%)	-0.41	0	100	100	88, 119, 165, 202	0
4	d	138/141 (97%)	-0.51	1 (0%)	84	65	83, 185, 253, 282	0
5	5	68/74 (91%)	-0.61	0	100	100	175, 220, 285, 372	0
5	E	68/74 (91%)	-0.43	0	100	100	111, 151, 185, 210	0
5	e	68/74 (91%)	-0.51	0	100	100	198, 253, 319, 365	0
6	6	125/125 (100%)	-0.48	0	100	100	188, 307, 389, 486	0
6	F	125/125 (100%)	-0.52	0	100	100	154, 241, 336, 388	0
6	f	125/125 (100%)	-0.38	0	100	100	245, 333, 408, 478	0
7	8	151/157 (96%)	-0.46	0	100	100	97, 125, 211, 294	0
7	L	151/157 (96%)	-0.38	1 (0%)	84	65	88, 109, 163, 229	0
7	l	151/157 (96%)	-0.44	0	100	100	107, 122, 165, 258	0
8	7	31/31 (100%)	-0.70	0	100	100	89, 95, 139, 147	0
8	M	31/31 (100%)	-0.57	0	100	100	108, 124, 158, 172	0
8	m	31/31 (100%)	-0.48	0	100	100	150, 174, 211, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
9	9	38/40 (95%)	-0.53	0	100	100	89, 97, 152, 208	0
9	I	38/40 (95%)	-0.65	0	100	100	92, 112, 198, 208	0
9	i	38/40 (95%)	-0.62	0	100	100	125, 151, 224, 233	0
10	0	80/128 (62%)	-0.41	0	100	100	220, 289, 383, 449	0
10	K	80/128 (62%)	-0.30	0	100	100	118, 160, 246, 314	0
10	k	80/128 (62%)	-0.29	0	100	100	189, 227, 344, 404	0
All	All	6534/6777 (96%)	-0.45	17 (0%)	90	78	80, 168, 303, 486	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	593	LEU	5.1
1	a	321	MET	3.9
1	1	387	LEU	3.9
1	a	348	TRP	3.6
2	b	617	PHE	3.6
2	b	506	PHE	2.8
3	3	67	VAL	2.7
1	a	102	GLY	2.6
7	L	25	SER	2.6
2	2	718	TYR	2.5
3	3	81	TYR	2.4
1	A	478	LEU	2.4
2	B	563	GLY	2.3
2	B	474	VAL	2.3
4	d	65	CYS	2.3
2	B	542	LYS	2.1
3	3	65	ILE	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
11	CLA	2	1240	45/65	0.59	0.09	224,246,269,289	0
11	CLA	b	1240	45/65	0.62	0.09	286,304,319,324	0
11	CLA	1	1110	54/65	0.64	0.11	258,268,295,299	0
11	CLA	B	1240	45/65	0.65	0.09	211,230,239,242	0
14	BCR	6	4013	40/40	0.65	0.10	254,275,285,291	0
11	CLA	a	1114	46/65	0.68	0.10	248,267,279,284	0
14	BCR	f	4013	40/40	0.70	0.10	275,292,321,326	0
14	BCR	1	4002	40/40	0.72	0.15	220,241,266,270	0
11	CLA	b	1218	45/65	0.73	0.09	273,286,303,305	0
11	CLA	b	1227	45/65	0.73	0.08	277,302,310,314	0
11	CLA	1	1113	45/65	0.73	0.11	235,255,277,284	0
11	CLA	1	1121	46/65	0.73	0.10	195,211,221,226	0
14	BCR	2	4011	40/40	0.74	0.12	187,207,215,220	0
11	CLA	B	1213	65/65	0.74	0.17	190,205,222,228	0
14	BCR	b	4011	40/40	0.75	0.14	204,219,248,251	0
11	CLA	1	1118	61/65	0.75	0.13	279,308,317,321	0
11	CLA	b	1209	45/65	0.75	0.10	226,238,250,254	0
11	CLA	1	1108	45/65	0.75	0.09	247,270,284,289	0
14	BCR	a	4002	40/40	0.75	0.16	214,227,233,235	0
11	CLA	0	1402	50/65	0.76	0.09	282,304,319,325	0
11	CLA	b	1208	45/65	0.76	0.11	227,240,247,250	0
14	BCR	m	4021	40/40	0.76	0.16	175,183,191,194	0
14	BCR	1	4003	40/40	0.77	0.18	193,227,269,270	0
14	BCR	F	4013	40/40	0.77	0.10	163,191,214,225	0
11	CLA	B	1227	45/65	0.77	0.09	168,175,199,212	0
15	LHG	B	5004	49/49	0.77	0.12	158,169,178,183	0
12	PQN	a	2001	33/33	0.78	0.13	181,201,225,229	0
11	CLA	b	1230	58/65	0.79	0.10	250,275,310,317	0
11	CLA	b	1234	60/65	0.79	0.11	220,242,268,270	0
11	CLA	b	1228	50/65	0.79	0.10	262,267,290,297	0
11	CLA	b	1219	55/65	0.80	0.09	267,284,296,299	0
15	LHG	b	5004	49/49	0.80	0.10	270,283,301,308	0
11	CLA	1	1114	46/65	0.81	0.08	262,279,288,293	0
11	CLA	b	1213	65/65	0.81	0.13	261,273,288,291	0
11	CLA	A	1114	46/65	0.82	0.10	150,165,173,175	0
11	CLA	1	1105	48/65	0.82	0.10	208,225,238,242	0
14	BCR	a	4003	40/40	0.83	0.14	192,210,235,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CLA	a	1109	65/65	0.83	0.12	224,238,254,259	0
11	CLA	b	1232	45/65	0.83	0.06	249,265,277,284	0
11	CLA	b	1216	65/65	0.83	0.10	221,239,260,264	0
11	CLA	b	1201	54/65	0.83	0.10	150,157,164,166	0
11	CLA	a	1105	48/65	0.84	0.08	249,270,280,285	0
11	CLA	2	1219	55/65	0.84	0.09	177,196,211,233	0
14	BCR	b	4005	40/40	0.84	0.10	193,207,227,230	0
14	BCR	L	4022	40/40	0.85	0.15	110,121,132,133	0
14	BCR	M	4021	40/40	0.85	0.10	103,111,125,126	0
11	CLA	k	1401	65/65	0.85	0.11	196,201,206,207	0
11	CLA	k	1402	50/65	0.85	0.09	225,232,238,242	0
11	CLA	a	1126	65/65	0.85	0.12	210,232,258,266	0
15	LHG	A	5003	49/49	0.85	0.09	92,97,104,115	0
11	CLA	b	1229	65/65	0.85	0.10	249,269,282,289	0
11	CLA	a	1110	54/65	0.85	0.09	211,224,241,244	0
15	LHG	2	5004	49/49	0.85	0.10	183,200,224,236	0
14	BCR	2	4004	40/40	0.86	0.14	123,137,161,163	0
14	BCR	B	4004	40/40	0.86	0.12	168,175,187,190	0
11	CLA	2	1229	65/65	0.86	0.11	177,187,202,209	0
11	CLA	1	1107	65/65	0.86	0.09	207,232,269,282	0
12	PQN	B	2002	33/33	0.86	0.12	86,88,98,133	0
11	CLA	b	1211	46/65	0.86	0.10	210,224,234,240	0
15	LHG	1	5003	49/49	0.86	0.12	154,173,196,198	0
14	BCR	A	4008	40/40	0.86	0.10	82,86,94,95	0
16	LMG	2	5002	55/55	0.86	0.13	122,136,148,155	0
14	BCR	b	4014	40/40	0.87	0.14	230,259,294,299	0
14	BCR	f	4018	40/40	0.87	0.11	132,138,152,154	0
11	CLA	B	1234	60/65	0.87	0.12	124,143,166,172	0
11	CLA	b	1221	54/65	0.87	0.12	241,253,261,266	0
11	CLA	b	1210	65/65	0.87	0.11	207,221,229,232	0
11	CLA	1	1102	65/65	0.87	0.10	199,219,239,246	0
11	CLA	2	1209	45/65	0.87	0.09	124,135,140,143	0
14	BCR	2	4005	40/40	0.87	0.11	102,108,118,120	0
14	BCR	2	4010	40/40	0.87	0.13	132,140,147,150	0
14	BCR	B	4005	40/40	0.87	0.10	118,135,161,162	0
11	CLA	a	1121	46/65	0.87	0.10	162,173,180,183	0
14	BCR	7	4021	40/40	0.87	0.12	106,110,121,131	0
11	CLA	a	1118	61/65	0.87	0.10	202,218,238,243	0
11	CLA	2	1230	58/65	0.87	0.09	222,240,273,278	0
11	CLA	b	1217	47/65	0.87	0.08	240,259,267,270	0
11	CLA	A	1801	52/65	0.87	0.10	89,95,98,103	0
11	CLA	1	1111	60/65	0.87	0.10	229,246,266,273	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CLA	0	1401	65/65	0.87	0.10	251,268,277,306	0
14	BCR	1	4001	40/40	0.88	0.14	241,254,269,271	0
11	CLA	a	1117	65/65	0.88	0.11	167,191,206,211	0
14	BCR	F	4018	40/40	0.88	0.10	94,101,113,114	0
14	BCR	1	4008	40/40	0.88	0.09	169,180,189,192	0
11	CLA	K	1401	65/65	0.88	0.12	141,148,155,157	0
11	CLA	K	1402	50/65	0.88	0.12	169,178,200,223	0
11	CLA	B	1218	45/65	0.88	0.09	168,176,189,196	0
11	CLA	a	1102	65/65	0.88	0.12	213,223,246,250	0
11	CLA	1	1109	65/65	0.88	0.12	239,261,278,283	0
14	BCR	a	4007	40/40	0.88	0.12	144,153,167,170	0
11	CLA	2	1218	45/65	0.88	0.08	164,178,189,194	0
11	CLA	A	1107	65/65	0.88	0.09	122,130,137,141	0
15	LHG	a	5003	49/49	0.88	0.10	144,147,154,158	0
11	CLA	2	1227	45/65	0.88	0.09	197,210,223,231	0
14	BCR	A	4001	40/40	0.88	0.20	110,115,129,130	0
11	CLA	B	1230	58/65	0.88	0.09	159,178,203,214	0
11	CLA	A	1118	61/65	0.88	0.11	130,138,152,163	0
14	BCR	b	4006	40/40	0.89	0.11	193,210,237,241	0
14	BCR	b	4010	40/40	0.89	0.10	230,257,283,284	0
11	CLA	1	1115	46/65	0.89	0.10	236,256,261,267	0
11	CLA	a	1139	50/65	0.89	0.10	210,233,255,263	0
11	CLA	a	1107	65/65	0.89	0.08	235,255,266,271	0
11	CLA	1	1120	46/65	0.89	0.08	227,248,258,262	0
11	CLA	l	1501	65/65	0.89	0.10	137,139,157,168	0
11	CLA	1	1801	52/65	0.89	0.08	199,212,225,231	0
12	PQN	b	2002	33/33	0.89	0.09	140,146,156,158	0
11	CLA	B	1228	50/65	0.89	0.09	181,188,206,208	0
11	CLA	b	1013	65/65	0.89	0.13	201,226,239,244	0
11	CLA	B	1229	65/65	0.89	0.10	151,164,176,181	0
11	CLA	2	1228	50/65	0.89	0.08	191,205,224,232	0
14	BCR	B	4010	40/40	0.89	0.14	128,141,167,171	0
14	BCR	B	4011	40/40	0.89	0.12	108,121,138,141	0
14	BCR	2	4014	40/40	0.89	0.12	184,206,223,228	0
11	CLA	a	1113	45/65	0.89	0.09	233,253,273,278	0
11	CLA	L	1503	65/65	0.89	0.13	106,116,134,148	0
11	CLA	2	1232	45/65	0.89	0.08	148,157,170,176	0
11	CLA	2	1234	60/65	0.89	0.11	151,164,196,206	0
11	CLA	2	1235	60/65	0.89	0.11	154,169,185,191	0
11	CLA	B	1209	45/65	0.89	0.07	149,160,170,173	0
11	CLA	a	1125	52/65	0.89	0.10	157,167,173,177	0
14	BCR	a	4008	40/40	0.89	0.10	150,152,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	LMG	b	5002	55/55	0.89	0.10	149,160,167,167	0
11	CLA	B	1232	45/65	0.89	0.08	168,184,196,202	0
14	BCR	b	4004	40/40	0.90	0.10	242,256,279,281	0
11	CLA	A	1106	65/65	0.90	0.12	123,134,140,152	0
11	CLA	L	1501	65/65	0.90	0.10	116,126,140,160	0
14	BCR	b	4009	40/40	0.90	0.12	254,280,313,316	0
11	CLA	A	1105	48/65	0.90	0.08	118,132,139,142	0
11	CLA	1	1122	59/65	0.90	0.09	168,189,205,209	0
11	CLA	1	1125	52/65	0.90	0.11	168,181,193,200	0
11	CLA	1	1131	65/65	0.90	0.12	108,119,126,130	0
11	CLA	a	1801	52/65	0.90	0.11	156,164,182,184	0
11	CLA	a	1101	65/65	0.90	0.10	236,245,257,265	0
11	CLA	B	1216	65/65	0.90	0.12	151,164,179,185	0
12	PQN	1	2001	33/33	0.90	0.11	184,204,226,230	0
11	CLA	1	1132	65/65	0.90	0.10	99,105,118,123	0
14	BCR	A	4002	40/40	0.90	0.11	118,122,130,131	0
11	CLA	2	1203	65/65	0.90	0.10	97,104,108,110	0
11	CLA	a	1103	65/65	0.90	0.12	199,214,239,246	0
11	CLA	2	1213	65/65	0.90	0.12	142,149,160,181	0
14	BCR	B	4009	40/40	0.90	0.13	169,203,225,226	0
11	CLA	a	1140	65/65	0.90	0.08	203,218,260,267	0
11	CLA	1	1101	65/65	0.90	0.08	214,232,245,253	0
14	BCR	8	4022	40/40	0.90	0.11	123,131,145,146	0
14	BCR	B	4014	40/40	0.90	0.12	138,157,191,200	0
15	LHG	A	5001	49/49	0.90	0.12	94,99,108,110	0
11	CLA	B	1208	45/65	0.90	0.07	128,136,143,147	0
11	CLA	1	1104	65/65	0.90	0.11	205,230,242,264	0
11	CLA	a	1120	46/65	0.90	0.10	190,204,214,230	0
11	CLA	b	1223	65/65	0.90	0.09	218,233,240,242	0
15	LHG	1	5001	49/49	0.90	0.11	182,196,208,213	0
11	CLA	b	1224	55/65	0.90	0.10	163,171,178,179	0
11	CLA	b	1225	65/65	0.90	0.10	183,198,210,214	0
16	LMG	B	5002	55/55	0.90	0.12	110,116,120,125	0
11	CLA	B	1219	55/65	0.90	0.07	158,173,186,192	0
11	CLA	B	1222	56/65	0.90	0.11	121,136,161,169	0
14	BCR	l	4022	40/40	0.91	0.15	121,122,124,124	0
14	BCR	B	4006	40/40	0.91	0.10	128,148,172,176	0
11	CLA	A	1131	65/65	0.91	0.11	81,84,88,109	0
11	CLA	2	1236	47/65	0.91	0.10	149,159,173,177	0
11	CLA	b	1214	59/65	0.91	0.10	229,247,262,266	0
11	CLA	2	1238	65/65	0.91	0.09	93,106,113,116	0
11	CLA	8	1503	65/65	0.91	0.12	137,142,156,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CLA	2	1201	54/65	0.91	0.12	91,100,104,107	0
14	BCR	L	4019	40/40	0.91	0.11	87,90,93,93	0
11	CLA	a	1112	45/65	0.91	0.10	233,251,261,266	0
11	CLA	A	1116	54/65	0.91	0.11	96,102,108,123	0
14	BCR	6	4018	40/40	0.91	0.09	93,97,107,113	0
14	BCR	6	4020	40/40	0.91	0.10	93,104,116,117	0
11	CLA	b	1235	60/65	0.91	0.08	235,252,263,268	0
11	CLA	B	1238	65/65	0.91	0.12	82,86,90,93	0
11	CLA	a	1134	46/65	0.91	0.08	160,175,184,187	0
12	PQN	A	2001	33/33	0.91	0.11	104,115,128,137	0
11	CLA	2	1221	54/65	0.91	0.12	120,128,140,143	0
11	CLA	2	1222	56/65	0.91	0.11	141,153,179,185	0
11	CLA	2	1223	65/65	0.91	0.11	131,134,148,153	0
11	CLA	A	1120	46/65	0.91	0.11	99,107,111,112	0
11	CLA	a	1124	55/65	0.91	0.10	156,166,174,176	0
11	CLA	b	1207	65/65	0.91	0.11	120,127,132,133	0
11	CLA	A	1101	65/65	0.91	0.10	143,151,160,175	0
11	CLA	a	1108	45/65	0.91	0.08	215,233,245,250	0
14	BCR	f	4020	40/40	0.91	0.10	113,119,125,126	0
11	CLA	A	1126	65/65	0.91	0.12	95,105,125,130	0
11	CLA	2	1204	65/65	0.92	0.12	88,90,94,99	0
11	CLA	2	1207	65/65	0.92	0.12	99,103,107,121	0
14	BCR	b	4017	40/40	0.92	0.12	143,150,160,162	0
11	CLA	2	1208	45/65	0.92	0.09	102,111,118,120	0
11	CLA	1	1103	65/65	0.92	0.09	218,234,261,272	0
11	CLA	B	1206	65/65	0.92	0.11	94,99,104,106	0
14	BCR	l	4019	40/40	0.92	0.12	122,133,149,151	0
11	CLA	a	1132	65/65	0.92	0.10	113,128,133,136	0
11	CLA	1	1106	65/65	0.92	0.10	187,201,212,222	0
14	BCR	A	4007	40/40	0.92	0.10	91,93,99,109	0
11	CLA	A	1119	65/65	0.92	0.11	82,95,99,109	0
11	CLA	B	1221	54/65	0.92	0.12	126,134,140,146	0
11	CLA	A	1122	59/65	0.92	0.11	83,88,92,94	0
11	CLA	2	1226	65/65	0.92	0.10	99,113,120,122	0
11	CLA	b	1202	65/65	0.92	0.12	169,187,198,202	0
14	BCR	2	4009	40/40	0.92	0.14	189,224,256,263	0
11	CLA	A	1121	46/65	0.92	0.09	97,103,120,155	0
11	CLA	A	1134	46/65	0.92	0.07	98,106,111,113	0
11	CLA	A	1125	52/65	0.92	0.09	95,99,105,127	0
14	BCR	B	4017	40/40	0.92	0.13	80,85,96,96	0
11	CLA	A	1102	65/65	0.92	0.10	123,130,142,144	0
11	CLA	a	1137	65/65	0.92	0.11	153,164,174,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	BCR	8	4019	40/40	0.92	0.12	125,129,144,154	0
11	CLA	A	1113	45/65	0.92	0.10	121,133,146,148	0
11	CLA	b	1206	65/65	0.92	0.10	135,142,149,151	0
11	CLA	1	1137	65/65	0.92	0.10	155,167,185,189	0
14	BCR	a	4001	40/40	0.92	0.12	173,199,227,229	0
11	CLA	2	1211	46/65	0.92	0.11	98,104,109,112	0
11	CLA	1	1139	50/65	0.92	0.08	181,204,222,225	0
11	CLA	b	1215	65/65	0.92	0.10	226,238,256,265	0
11	CLA	A	1139	50/65	0.92	0.11	112,126,138,142	0
11	CLA	a	1012	65/65	0.92	0.13	185,204,226,230	0
11	CLA	1	1237	55/65	0.92	0.10	113,120,130,133	0
11	CLA	1	1134	46/65	0.92	0.07	212,228,242,244	0
11	CLA	B	1235	60/65	0.92	0.08	141,154,163,166	0
11	CLA	A	1140	65/65	0.92	0.09	124,136,172,178	0
11	CLA	l	1503	65/65	0.93	0.11	125,130,137,187	0
11	CLA	A	1137	65/65	0.93	0.08	81,83,91,110	0
11	CLA	a	1111	60/65	0.93	0.10	198,205,225,229	0
11	CLA	2	1023	65/65	0.93	0.11	117,135,145,149	0
11	CLA	B	1231	45/65	0.93	0.08	154,169,180,185	0
11	CLA	a	1237	55/65	0.93	0.10	116,121,126,128	0
11	CLA	b	1222	56/65	0.93	0.09	230,254,284,293	0
11	CLA	a	1022	65/65	0.93	0.14	142,156,166,168	0
11	CLA	B	1204	65/65	0.93	0.10	100,109,115,117	0
11	CLA	a	1122	59/65	0.93	0.09	134,144,153,156	0
12	PQN	2	2002	33/33	0.93	0.09	106,118,130,131	0
11	CLA	2	1210	65/65	0.93	0.14	104,112,120,123	0
11	CLA	b	1226	65/65	0.93	0.10	165,186,192,194	0
14	BCR	A	4003	40/40	0.93	0.10	100,112,129,132	0
14	BCR	1	4007	40/40	0.93	0.09	202,218,231,231	0
11	CLA	2	1216	65/65	0.93	0.09	141,156,169,176	0
11	CLA	2	1217	47/65	0.93	0.08	127,139,146,149	0
11	CLA	B	1220	46/65	0.93	0.08	133,148,155,158	0
14	BCR	2	4006	40/40	0.93	0.10	98,105,120,122	0
11	CLA	b	1203	65/65	0.93	0.09	169,178,189,193	0
11	CLA	b	1204	65/65	0.93	0.10	163,169,175,177	0
11	CLA	A	1104	65/65	0.93	0.10	93,99,105,107	0
11	CLA	1	1112	45/65	0.93	0.07	263,286,301,303	0
14	BCR	2	4017	40/40	0.93	0.10	96,102,117,117	0
11	CLA	b	1231	45/65	0.93	0.07	275,294,305,311	0
11	CLA	A	1129	46/65	0.93	0.12	82,85,88,89	0
11	CLA	a	1131	65/65	0.93	0.10	121,124,131,134	0
11	CLA	a	1106	65/65	0.93	0.08	212,222,232,234	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	BCR	F	4020	40/40	0.93	0.10	84,87,94,94	0
11	CLA	1	1124	55/65	0.93	0.09	176,181,188,196	0
11	CLA	2	1231	45/65	0.93	0.09	139,147,159,168	0
11	CLA	b	1236	47/65	0.93	0.07	239,254,268,270	0
11	CLA	1	1126	65/65	0.93	0.08	179,200,211,215	0
15	LHG	a	5001	49/49	0.93	0.08	181,190,210,212	0
11	CLA	1	1127	65/65	0.93	0.10	214,223,233,237	0
11	CLA	a	1138	46/65	0.93	0.08	226,242,255,260	0
11	CLA	B	1212	45/65	0.93	0.10	160,174,184,187	0
11	CLA	A	1132	65/65	0.93	0.12	90,92,97,100	0
11	CLA	1	1140	65/65	0.93	0.08	180,188,218,225	0
11	CLA	8	1501	65/65	0.93	0.12	131,138,145,158	0
11	CLA	b	1238	65/65	0.93	0.10	121,126,133,135	0
11	CLA	A	1133	46/65	0.93	0.08	89,96,101,103	0
11	CLA	a	1136	46/65	0.94	0.08	140,148,157,173	0
11	CLA	B	1225	65/65	0.94	0.09	110,123,143,148	0
11	CLA	1	1012	65/65	0.94	0.11	147,161,195,201	0
11	CLA	B	1226	65/65	0.94	0.11	104,114,121,124	0
11	CLA	A	1130	46/65	0.94	0.10	88,90,93,107	0
11	CLA	a	1123	65/65	0.94	0.10	159,181,191,193	0
11	CLA	B	1210	65/65	0.94	0.10	126,135,144,149	0
11	CLA	1	1133	46/65	0.94	0.09	179,192,203,206	0
11	CLA	b	1205	55/65	0.94	0.09	146,156,165,167	0
11	CLA	A	1103	65/65	0.94	0.12	93,100,116,120	0
11	CLA	A	1124	55/65	0.94	0.11	85,89,93,93	0
11	CLA	B	1214	59/65	0.94	0.10	143,159,171,177	0
11	CLA	A	1138	46/65	0.94	0.09	121,131,139,143	0
11	CLA	2	1206	65/65	0.94	0.08	91,95,98,100	0
11	CLA	B	1217	47/65	0.94	0.08	159,172,182,186	0
11	CLA	A	1110	54/65	0.94	0.07	113,119,131,135	0
11	CLA	1	1117	65/65	0.94	0.10	185,202,216,219	0
11	CLA	A	1237	55/65	0.94	0.12	80,83,86,87	0
11	CLA	a	1011	65/65	0.94	0.14	161,188,194,198	0
11	CLA	A	1136	46/65	0.94	0.09	82,86,88,89	0
11	CLA	B	1211	46/65	0.94	0.08	137,146,156,161	0
11	CLA	A	1012	65/65	0.94	0.12	105,116,126,129	0
11	CLA	B	1239	46/65	0.94	0.08	87,91,94,95	0
11	CLA	2	1220	46/65	0.94	0.09	145,153,163,167	0
11	CLA	1	1128	65/65	0.94	0.11	197,213,223,224	0
13	SF4	C	3002	8/8	0.94	0.07	60,88,151,152	0
13	SF4	c	3002	8/8	0.94	0.09	60,88,151,152	0
11	CLA	1	1130	46/65	0.94	0.09	131,140,148,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CLA	A	1128	65/65	0.94	0.13	102,108,118,128	0
11	CLA	2	1225	65/65	0.94	0.11	100,105,110,112	0
11	CLA	a	1115	46/65	0.94	0.08	188,200,211,232	0
11	CLA	1	1138	46/65	0.94	0.08	175,188,205,208	0
11	CLA	B	1207	65/65	0.95	0.11	99,106,116,180	0
11	CLA	b	1021	65/65	0.95	0.12	185,193,223,226	0
11	CLA	2	1202	65/65	0.95	0.13	114,123,128,130	0
11	CLA	b	1023	65/65	0.95	0.12	135,142,156,159	0
11	CLA	B	1236	47/65	0.95	0.09	136,145,152,153	0
11	CLA	2	1205	55/65	0.95	0.09	92,96,98,99	0
11	CLA	A	1108	45/65	0.95	0.07	111,120,127,130	0
11	CLA	a	1127	65/65	0.95	0.11	186,200,211,220	0
11	CLA	a	1128	65/65	0.95	0.08	185,196,213,224	0
11	CLA	1	1116	54/65	0.95	0.10	201,212,225,236	0
11	CLA	a	1130	46/65	0.95	0.09	117,123,125,128	0
11	CLA	A	1111	60/65	0.95	0.09	106,111,121,124	0
11	CLA	2	1214	59/65	0.95	0.09	120,130,139,145	0
13	SF4	c	3003	8/8	0.95	0.12	60,67,100,115	0
13	SF4	3	3002	8/8	0.95	0.06	60,88,151,152	0
11	CLA	1	1119	65/65	0.95	0.11	197,237,248,254	0
11	CLA	B	1223	65/65	0.95	0.12	154,166,176,183	0
11	CLA	1	1123	65/65	0.95	0.09	208,227,237,242	0
11	CLA	A	1109	65/65	0.95	0.10	111,119,129,132	0
11	CLA	A	1135	51/65	0.95	0.11	90,94,97,99	0
11	CLA	b	1212	45/65	0.95	0.08	248,260,269,270	0
11	CLA	A	1115	46/65	0.95	0.07	111,121,126,126	0
11	CLA	b	1239	46/65	0.95	0.08	155,159,164,171	0
11	CLA	2	1224	55/65	0.95	0.11	103,107,124,141	0
11	CLA	L	1502	46/65	0.95	0.10	86,91,96,114	0
11	CLA	l	1502	46/65	0.95	0.08	111,114,119,120	0
11	CLA	B	1023	65/65	0.95	0.10	80,82,87,88	0
11	CLA	B	1215	65/65	0.95	0.15	135,141,147,154	0
11	CLA	B	1201	54/65	0.95	0.08	99,107,110,111	0
11	CLA	1	1022	65/65	0.95	0.11	101,124,132,137	0
11	CLA	1	1011	65/65	0.95	0.12	124,133,140,142	0
11	CLA	B	1203	65/65	0.95	0.09	104,109,117,121	0
11	CLA	a	1129	46/65	0.95	0.11	141,147,154,156	0
11	CLA	a	1119	65/65	0.95	0.10	143,162,172,177	0
11	CLA	a	1133	46/65	0.95	0.07	158,171,178,183	0
11	CLA	1	1129	46/65	0.95	0.10	166,179,190,191	0
11	CLA	A	1123	65/65	0.95	0.12	89,95,99,100	0
11	CLA	a	1135	51/65	0.95	0.10	140,155,162,167	0

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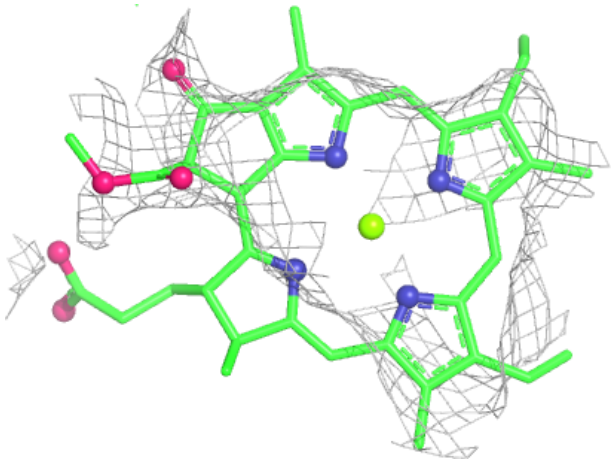
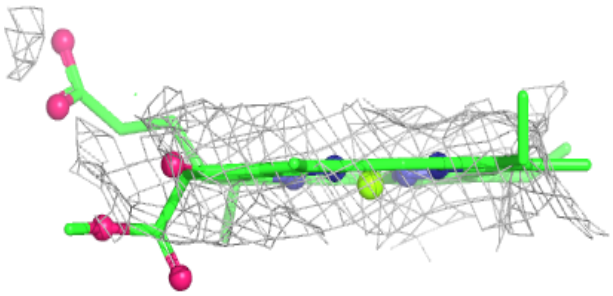
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CLA	2	1239	46/65	0.95	0.08	103,112,115,119	0
11	CLA	B	1205	55/65	0.95	0.08	97,104,114,127	0
11	CLA	1	1135	51/65	0.95	0.09	174,178,184,187	0
11	CLA	2	1013	65/65	0.95	0.10	153,169,194,196	0
11	CLA	a	1104	65/65	0.96	0.10	189,200,213,217	0
11	CLA	A	1011	65/65	0.96	0.13	85,97,106,141	0
11	CLA	A	1117	65/65	0.96	0.09	92,103,111,114	0
11	CLA	a	1116	54/65	0.96	0.08	170,177,186,189	0
11	CLA	1	1136	46/65	0.96	0.08	154,164,170,176	0
11	CLA	B	1224	55/65	0.96	0.12	116,122,128,136	0
11	CLA	2	1212	45/65	0.96	0.08	114,120,125,126	0
11	CLA	8	1502	46/65	0.96	0.10	153,164,178,197	0
11	CLA	2	1021	65/65	0.96	0.13	122,129,148,156	0
11	CLA	A	1112	45/65	0.96	0.09	132,143,149,153	0
13	SF4	3	3003	8/8	0.96	0.13	60,67,100,115	0
11	CLA	2	1215	65/65	0.96	0.11	107,116,134,140	0
11	CLA	b	1220	46/65	0.96	0.07	254,281,294,297	0
11	CLA	B	1013	65/65	0.96	0.09	99,112,120,139	0
11	CLA	B	1021	65/65	0.96	0.13	110,119,135,150	0
11	CLA	A	1022	65/65	0.96	0.10	82,88,92,93	0
13	SF4	1	3001	8/8	0.97	0.07	50,62,210,290	0
11	CLA	B	1202	65/65	0.97	0.10	107,117,127,130	0
13	SF4	C	3003	8/8	0.97	0.04	60,67,100,115	0
13	SF4	a	3001	8/8	0.97	0.06	50,62,210,290	0
11	CLA	A	1127	65/65	0.97	0.08	94,101,108,110	0
13	SF4	A	3001	8/8	0.97	0.07	50,62,210,290	0

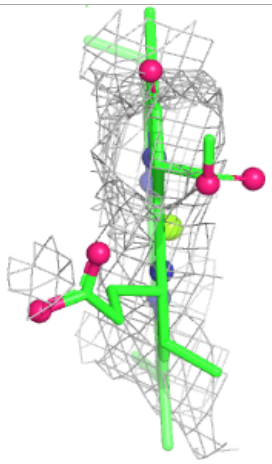
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA 2 1240:

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

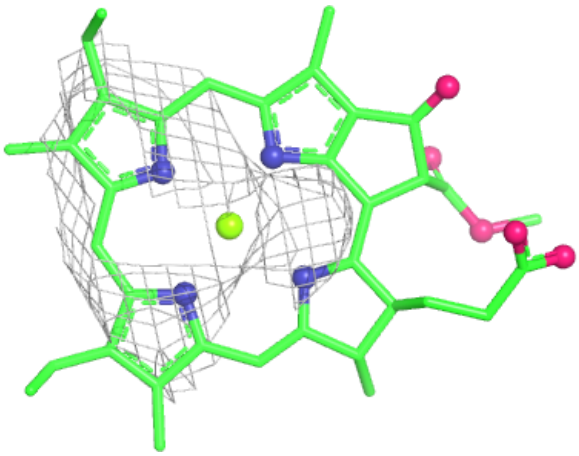


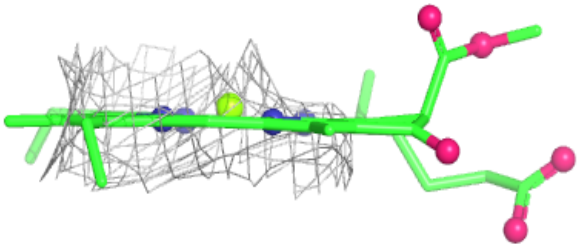


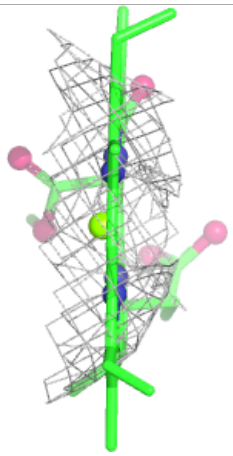


Electron density around CLA b 1240:

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

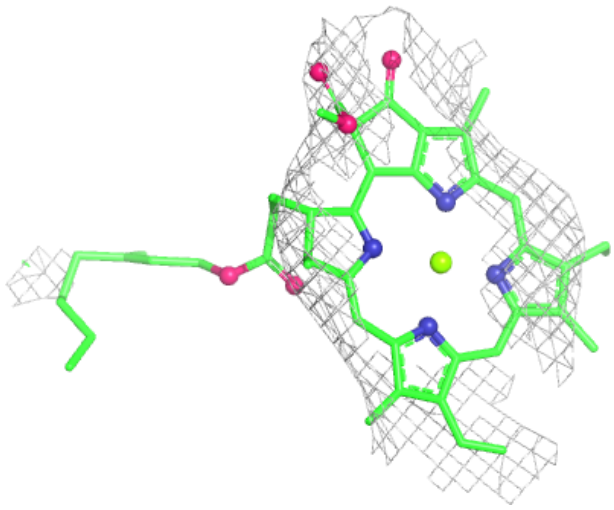


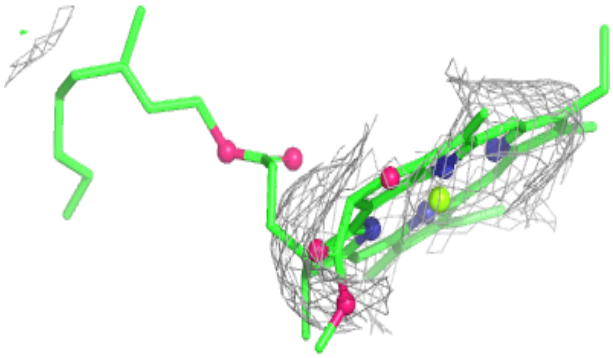


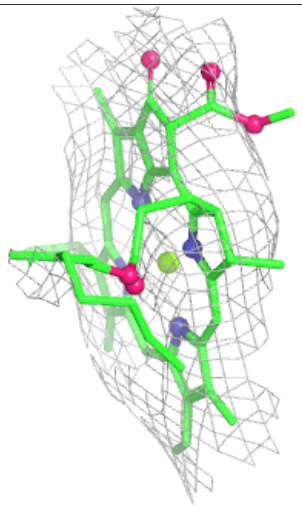


Electron density around CLA 1 1110:

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

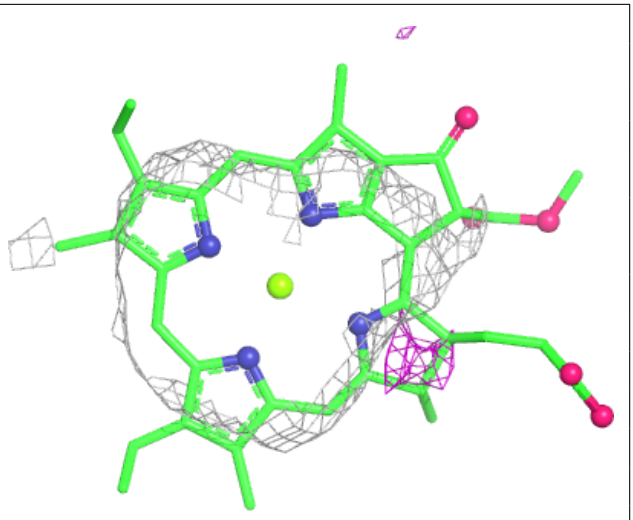


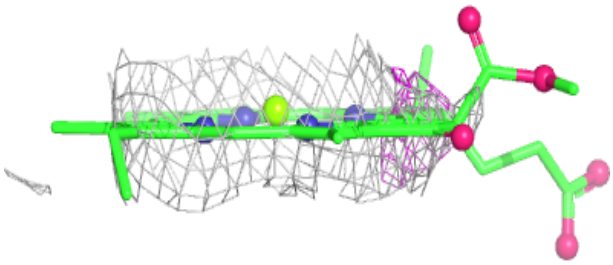


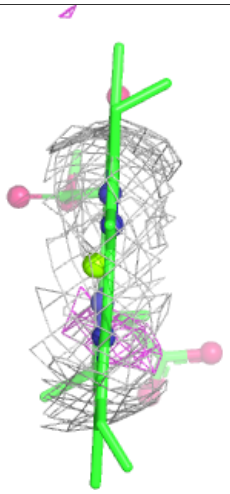


Electron density around CLA B 1240:

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

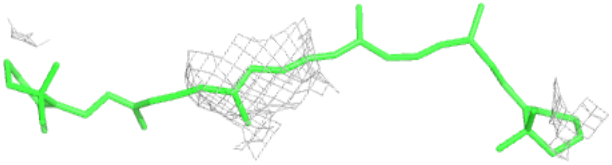


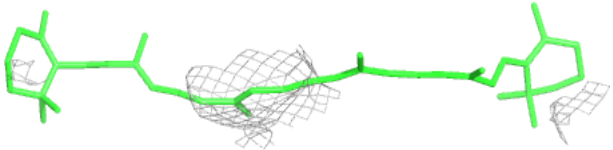


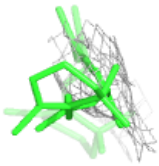


Electron density around BCR 6 4013:

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

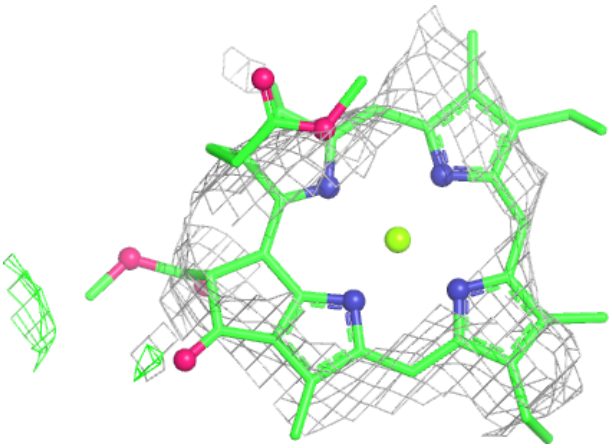


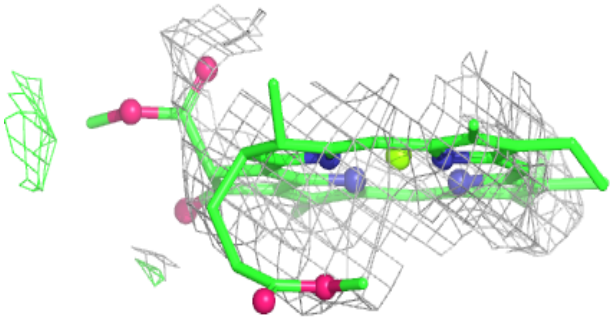


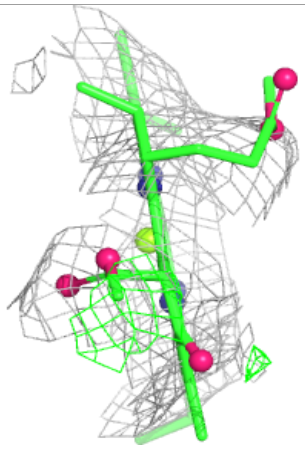


Electron density around CLA a 1114:

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

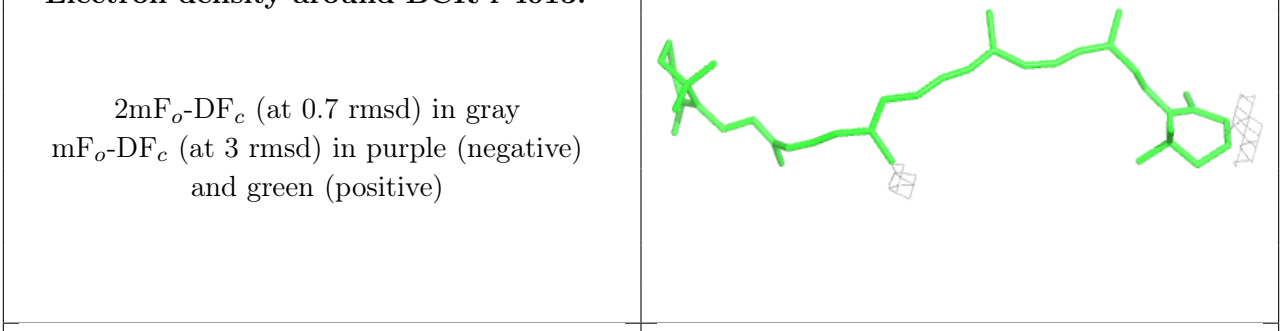


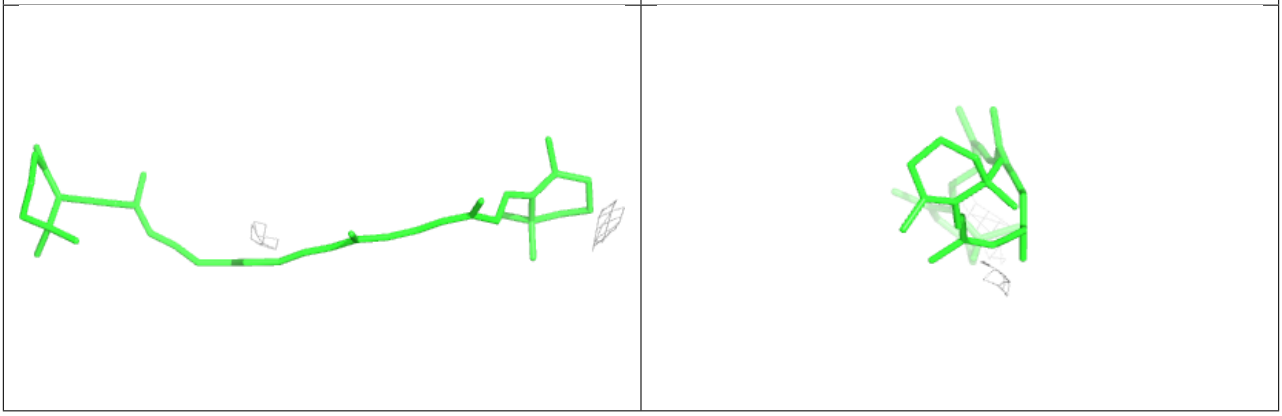




Electron density around BCR f 4013:

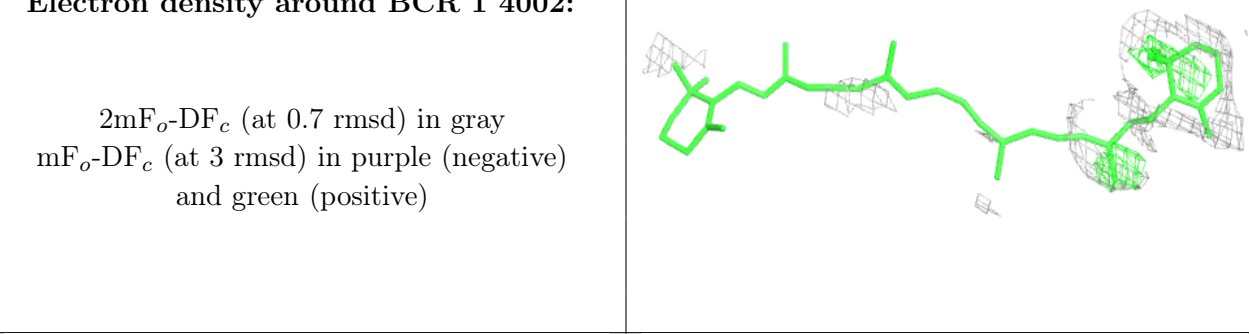
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

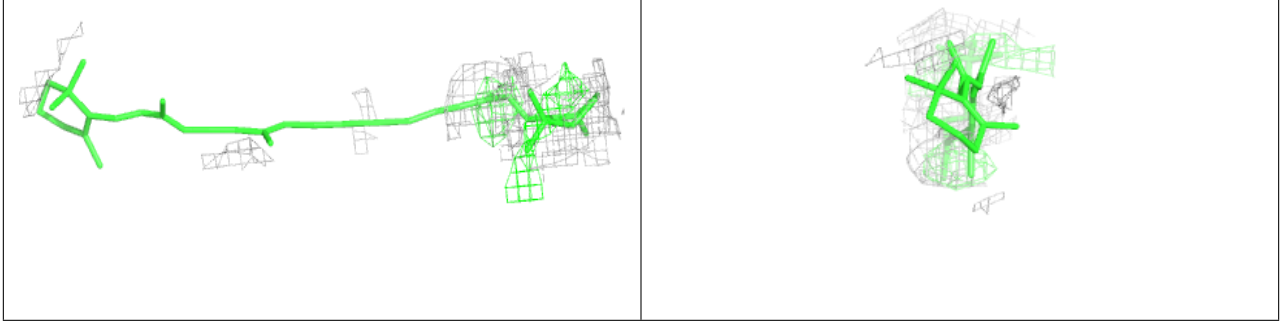




Electron density around BCR 1 4002:

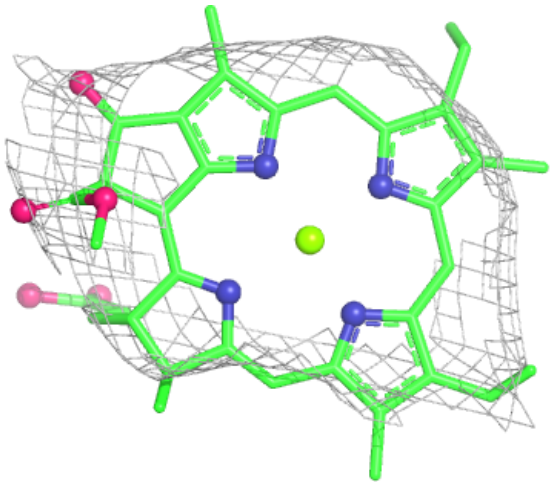
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

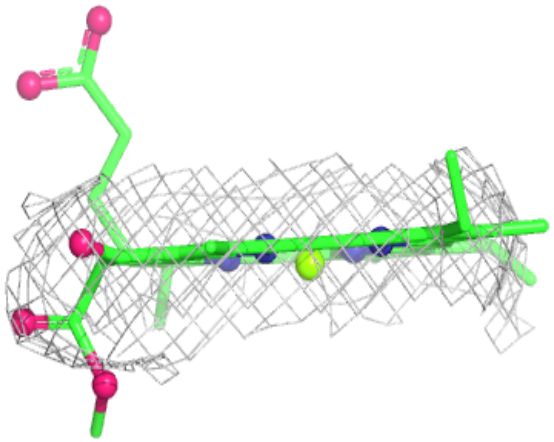


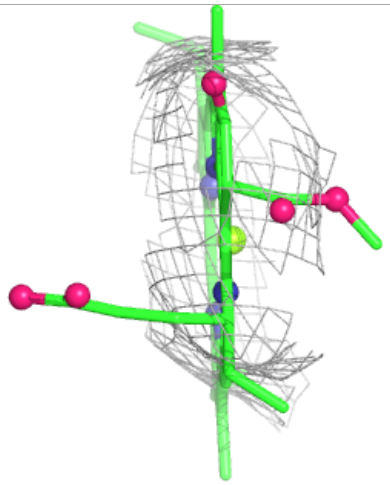


Electron density around CLA b 1218:

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

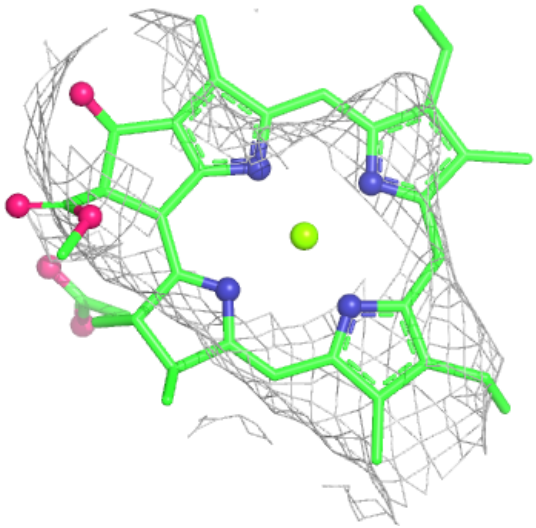


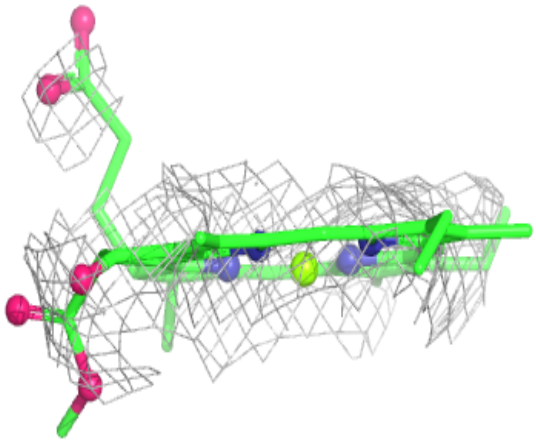


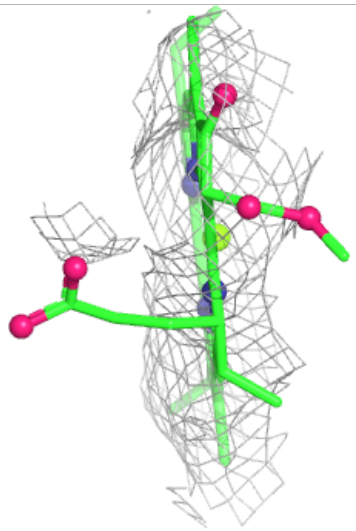


Electron density around CLA b 1227:

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

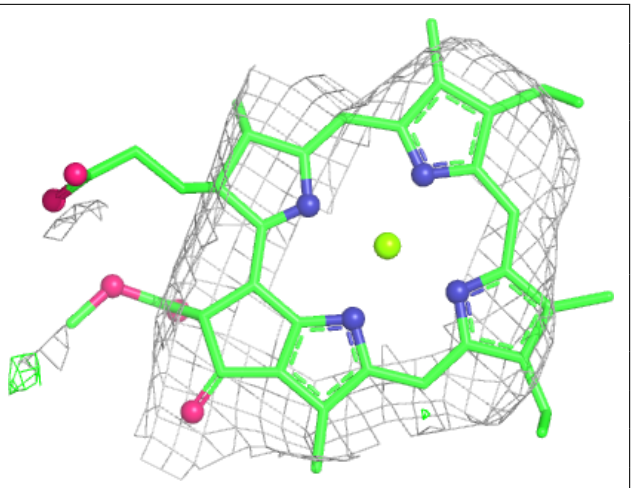


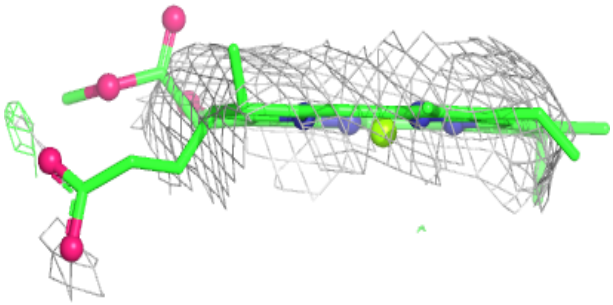




Electron density around CLA 1 1113:

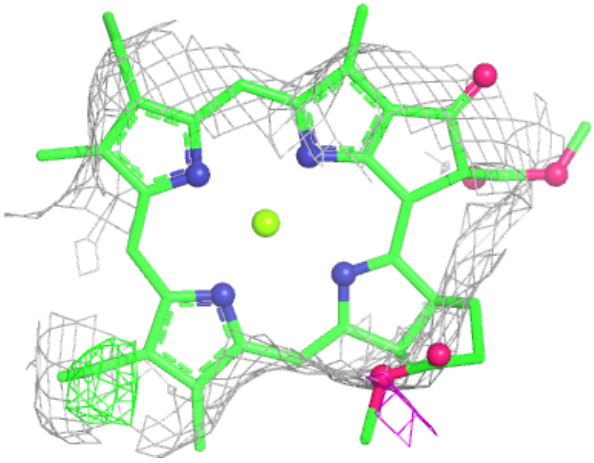
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

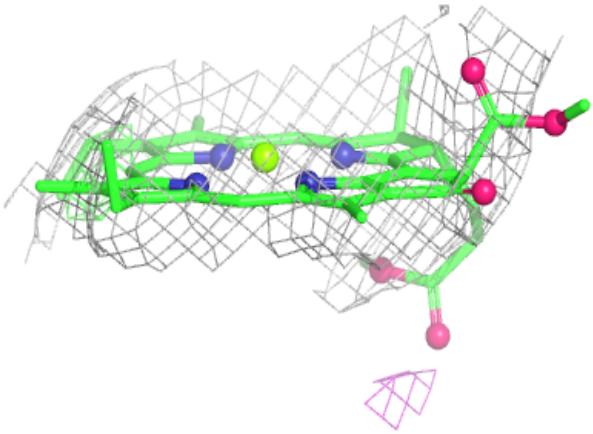


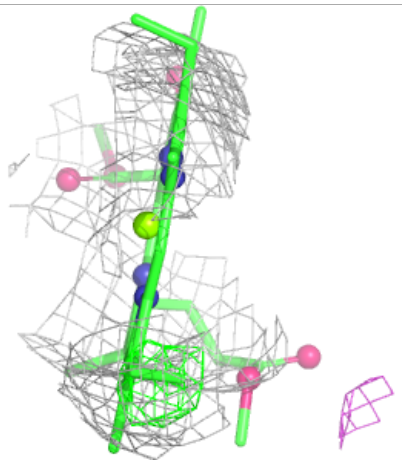


Electron density around CLA 1 1121:

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

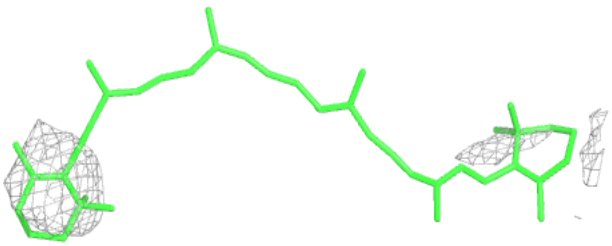


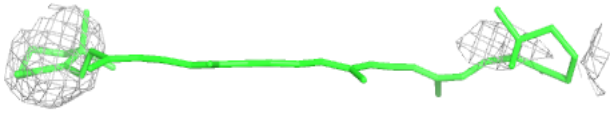


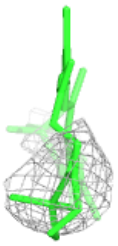


Electron density around BCR 2 4011:

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

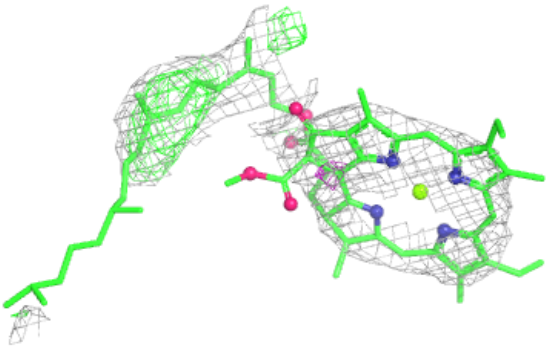


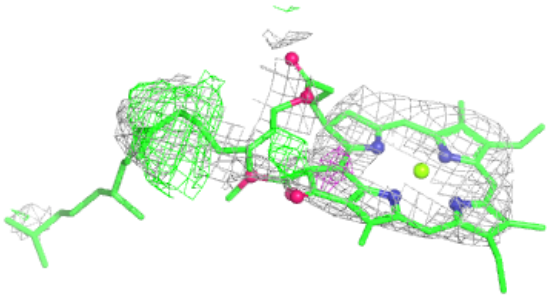




Electron density around CLA B 1213:

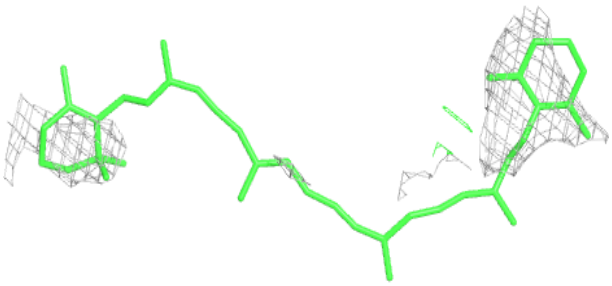
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

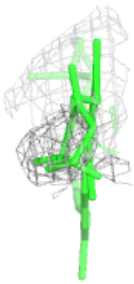




Electron density around BCR b 4011:

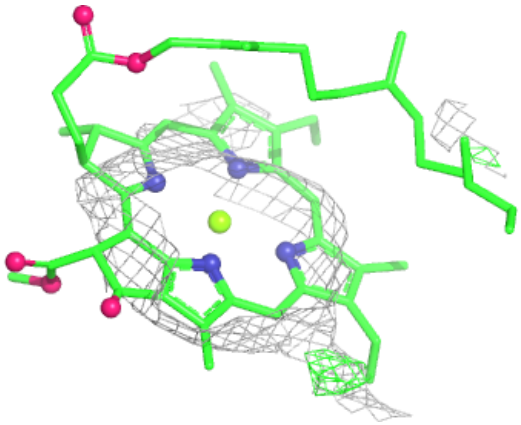
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

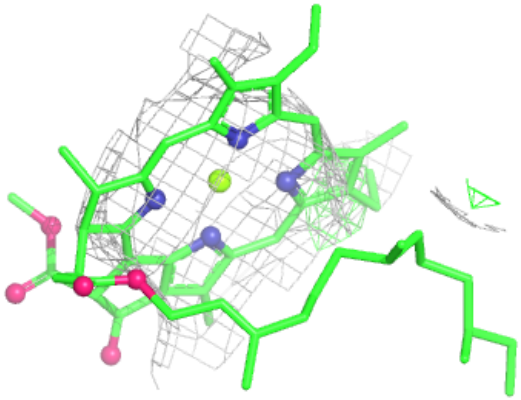


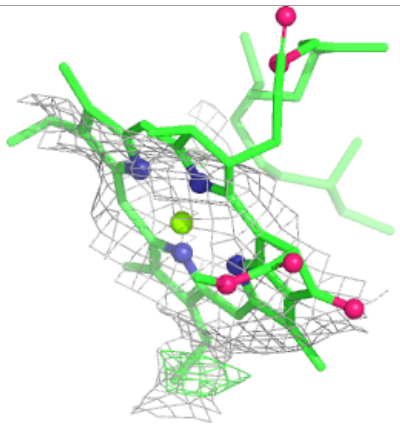


Electron density around CLA 1 1118:

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

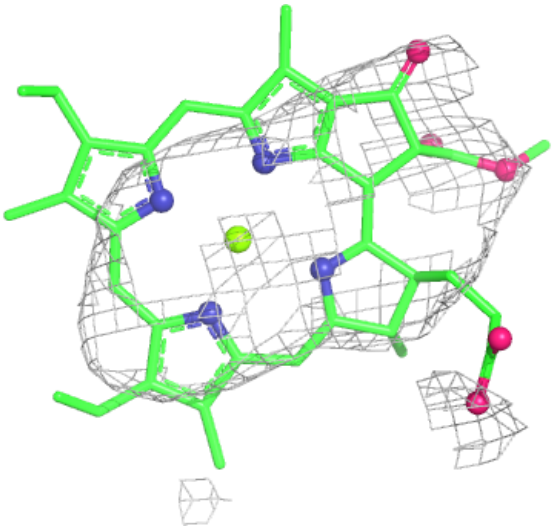


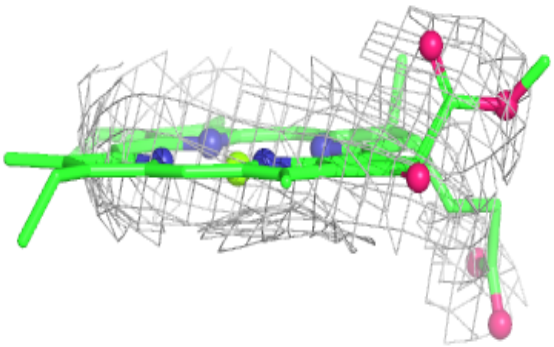


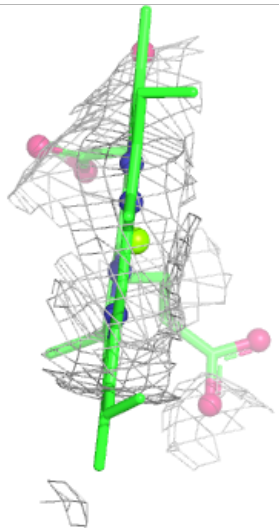


Electron density around CLA b 1209:

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

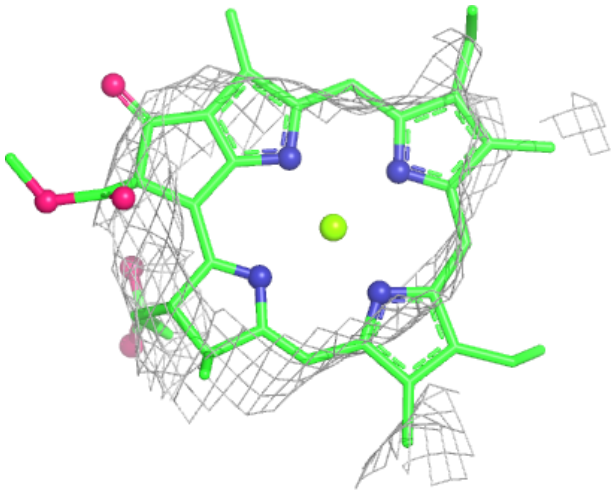


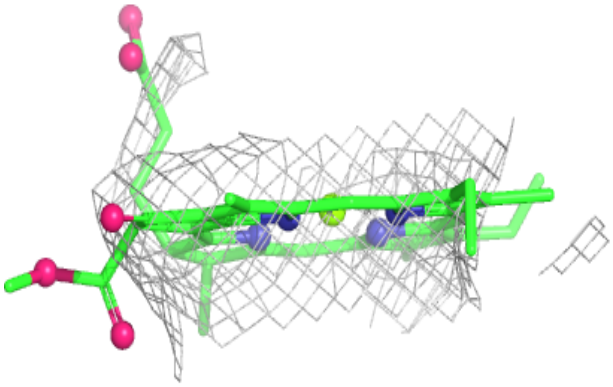




Electron density around CLA 1 1108:

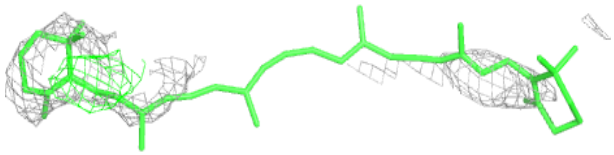
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

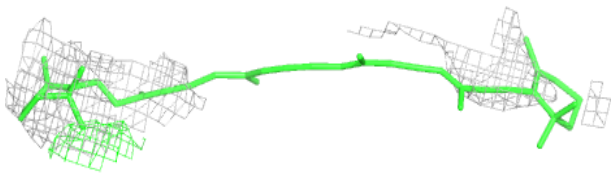


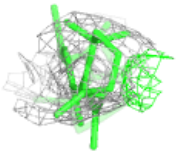


Electron density around BCR a 4002:

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

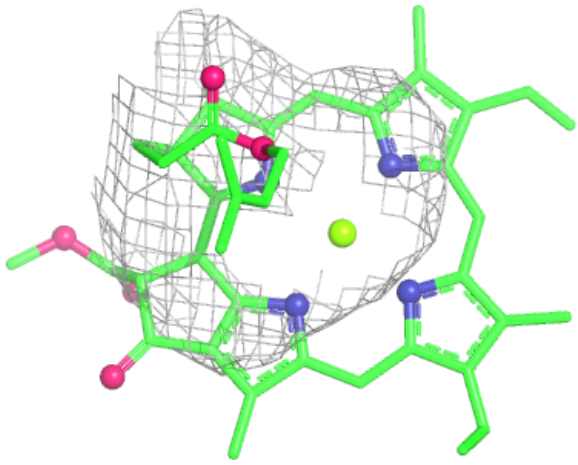


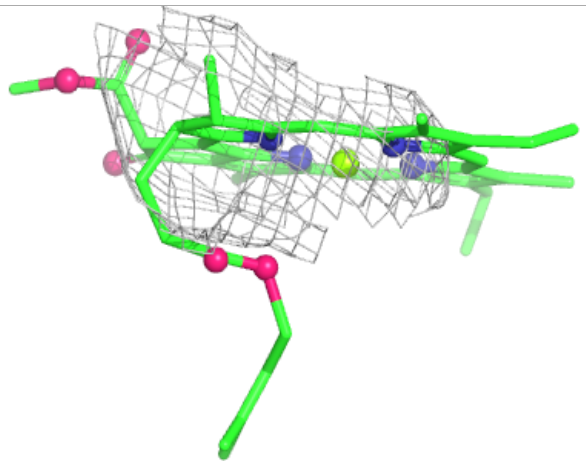


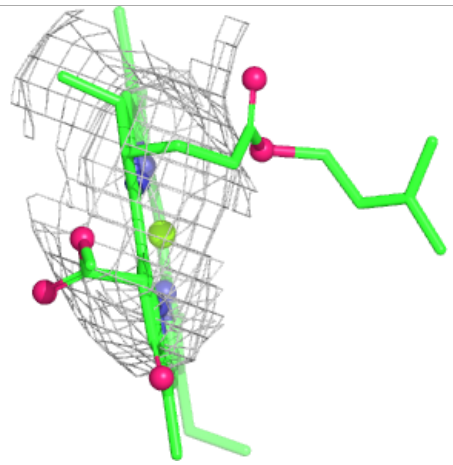


Electron density around CLA 0 1402:

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

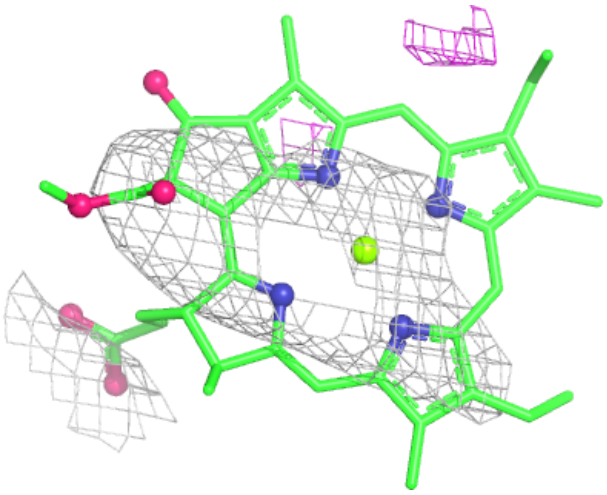


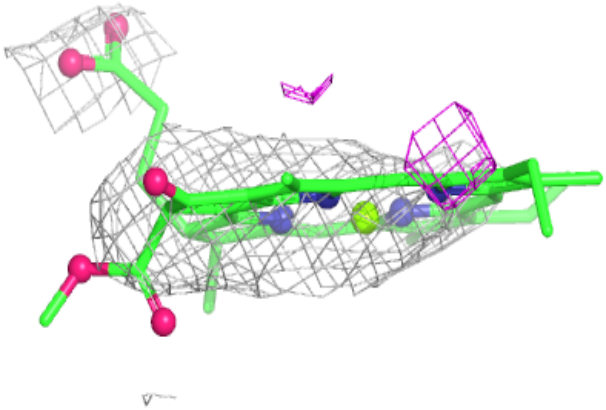




Electron density around CLA b 1208:

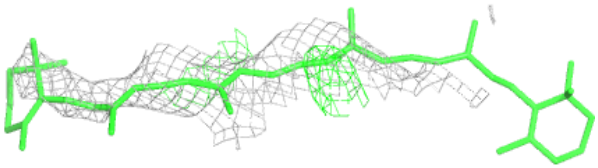
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

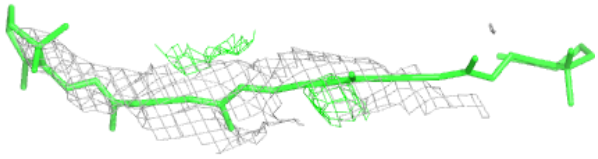


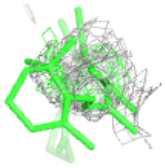


Electron density around BCR m 4021:

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

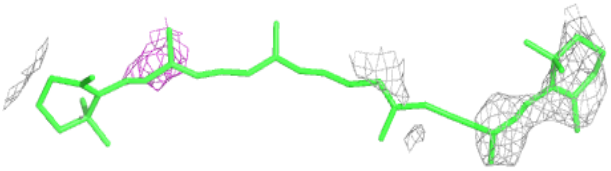


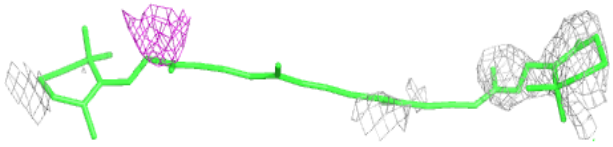


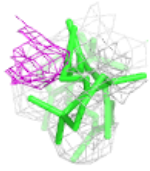


Electron density around BCR 1 4003:

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

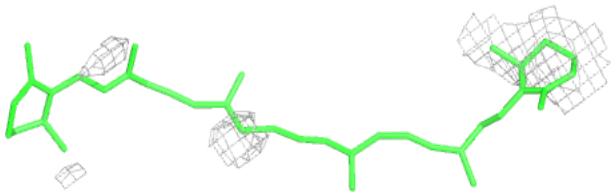


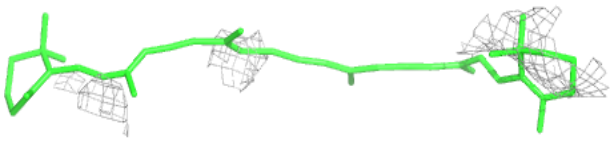




Electron density around BCR F 4013:

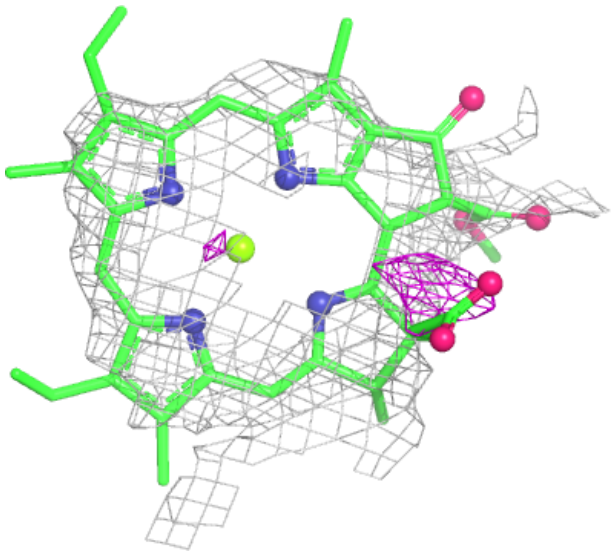
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

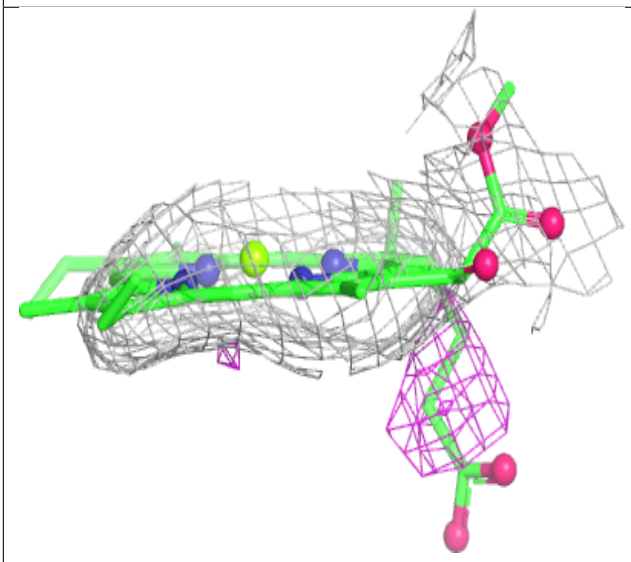


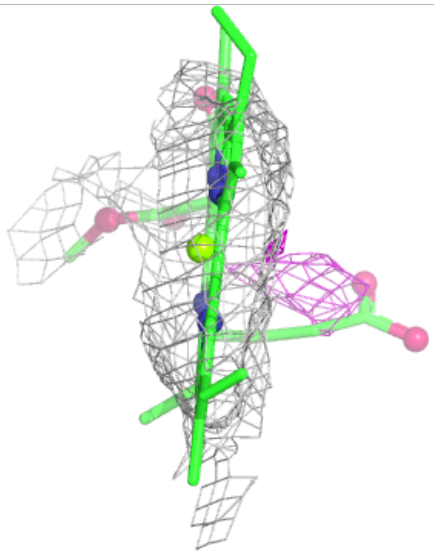


Electron density around CLA B 1227:

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

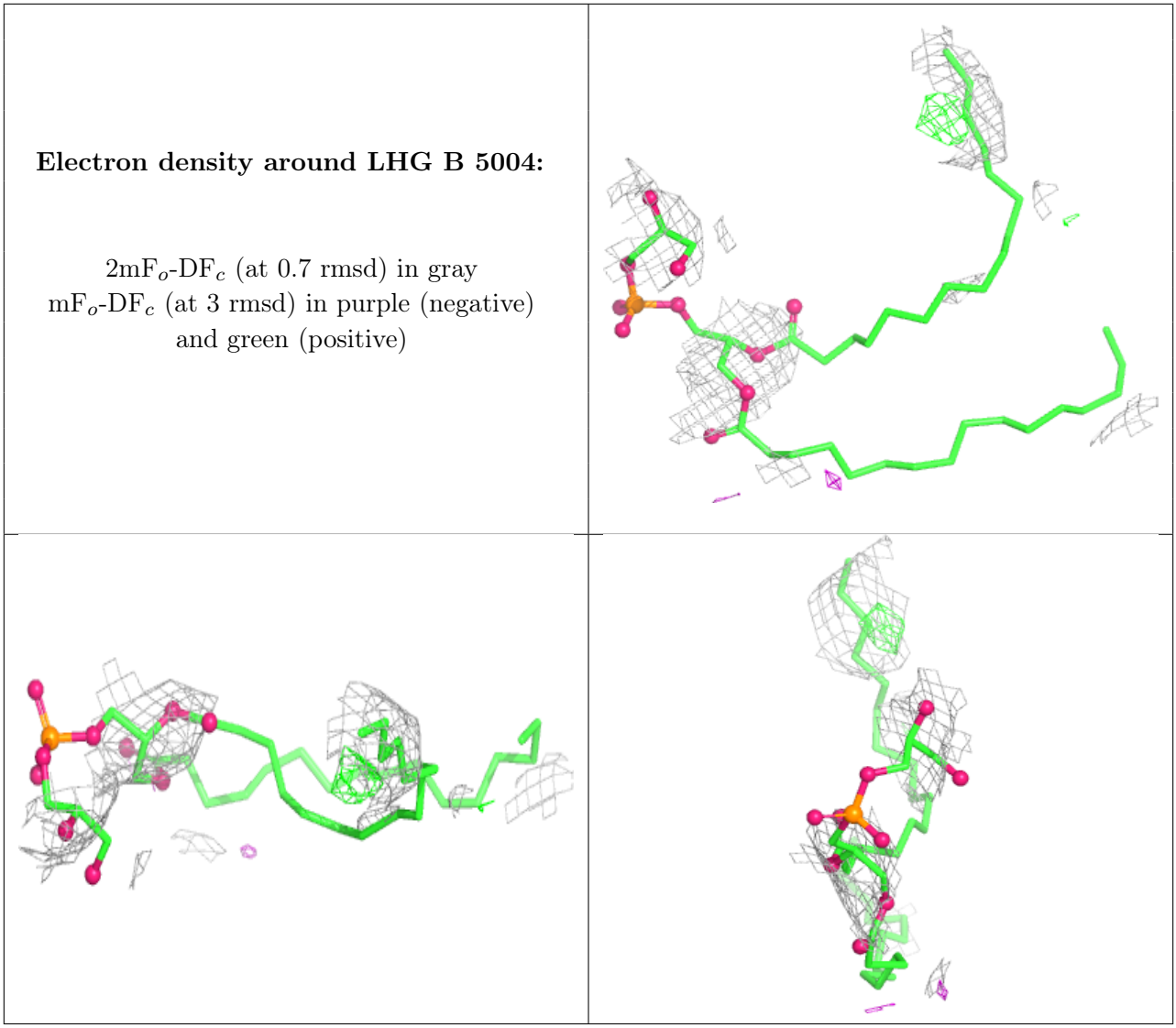






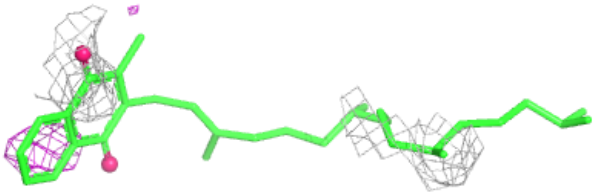
Electron density around LHG B 5004:

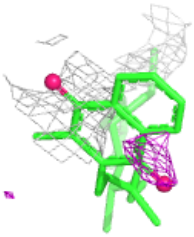
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PQN a 2001:

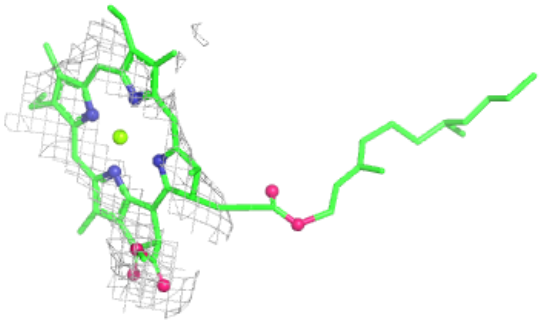
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

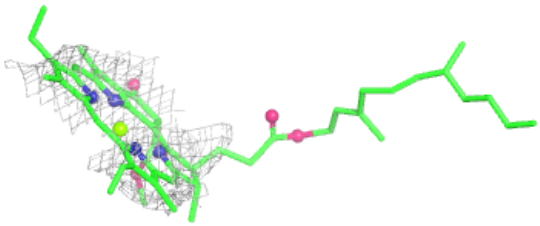


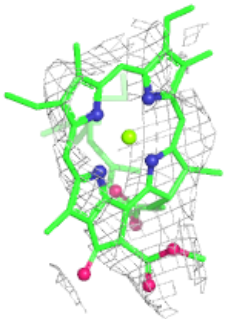


Electron density around CLA b 1230:

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

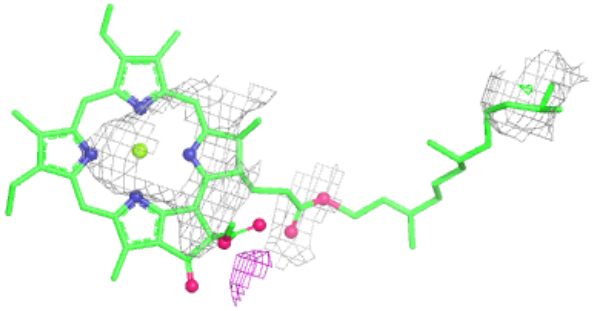


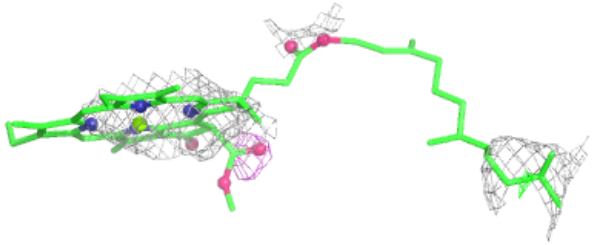


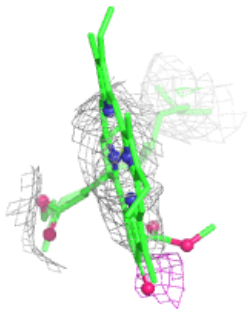


Electron density around CLA b 1234:

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

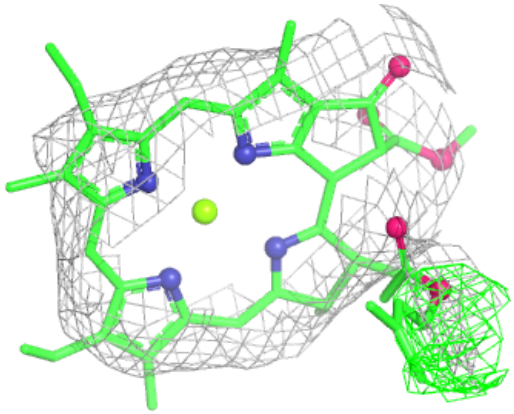


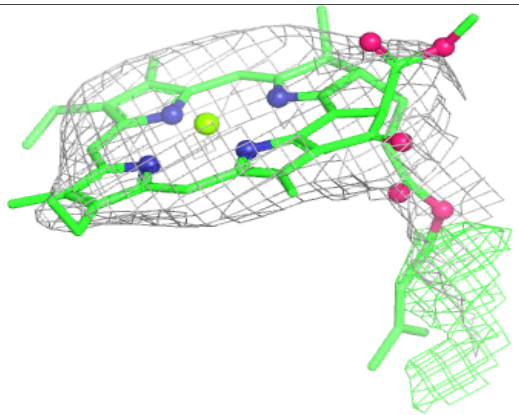


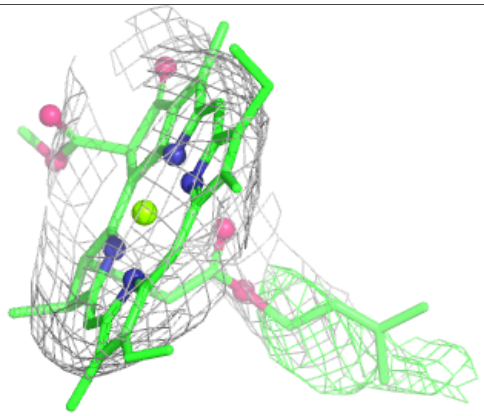


Electron density around CLA b 1228:

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

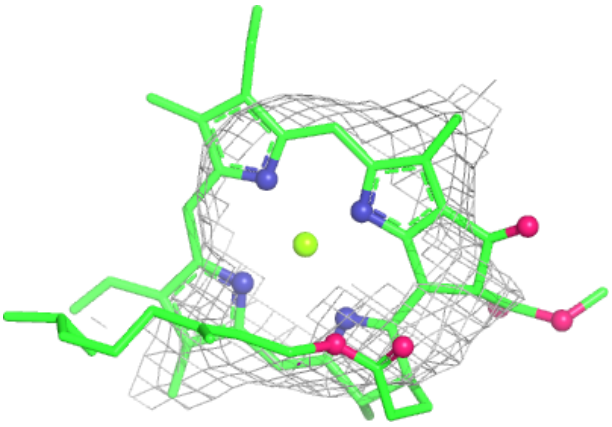


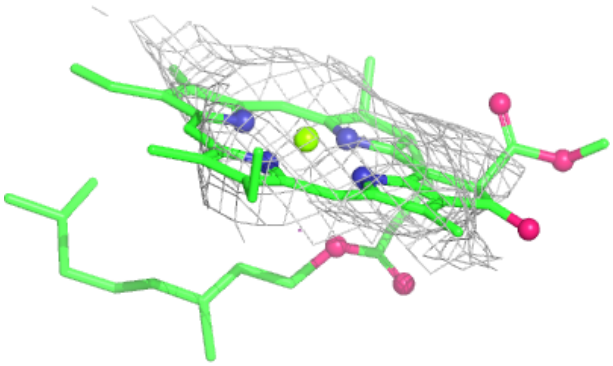


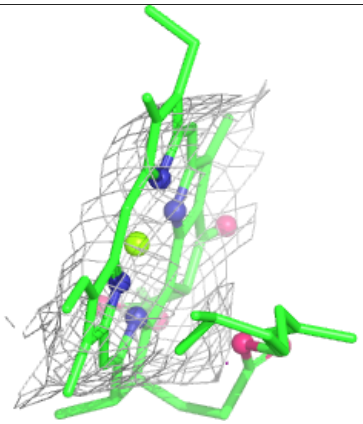


Electron density around CLA b 1219:

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

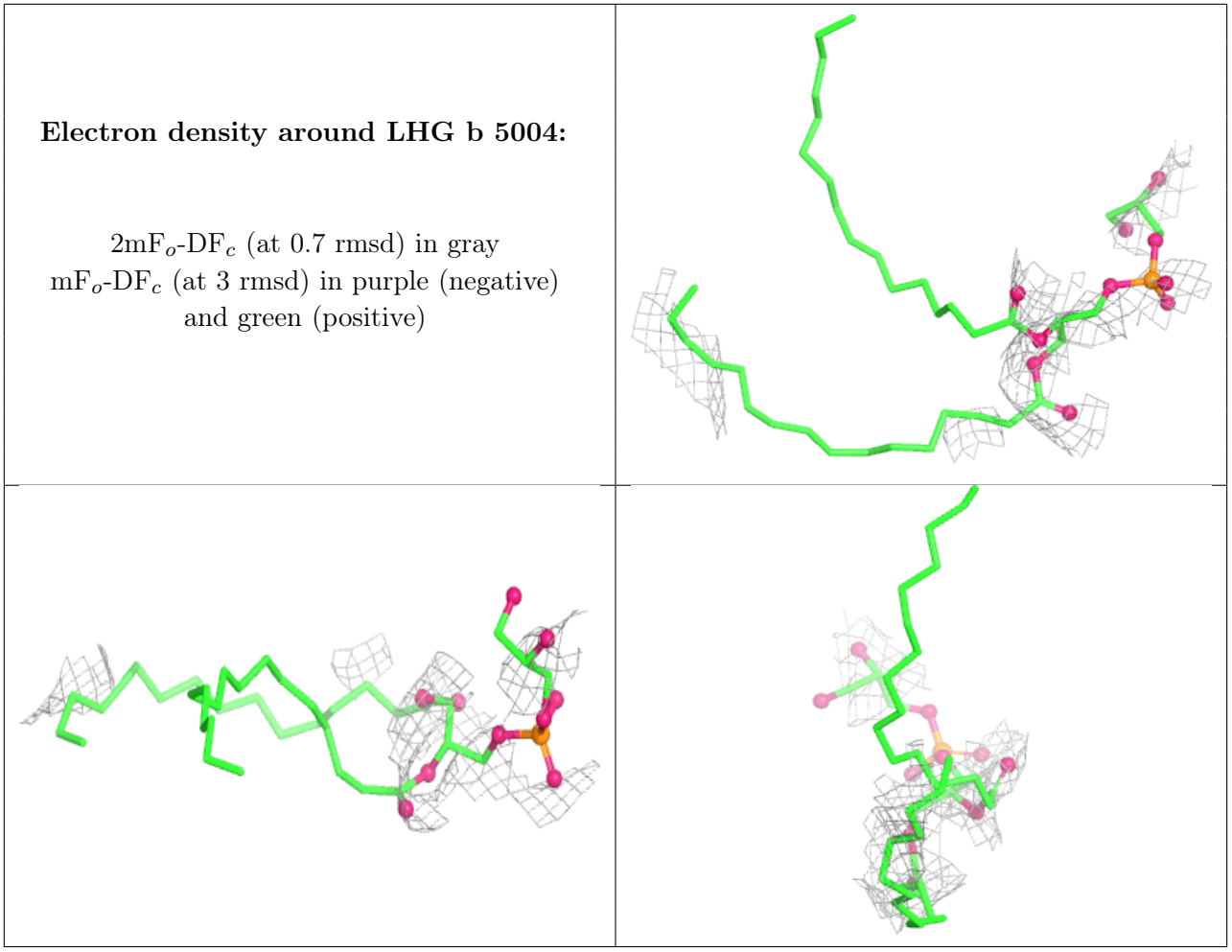






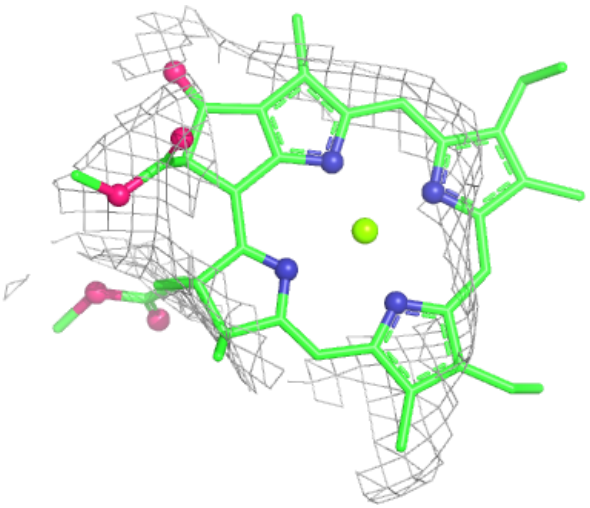
Electron density around LHG b 5004:

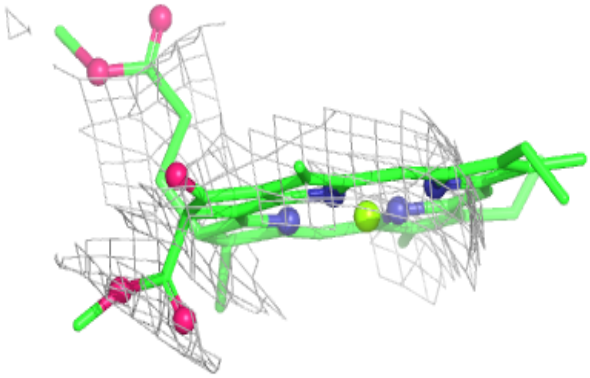
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

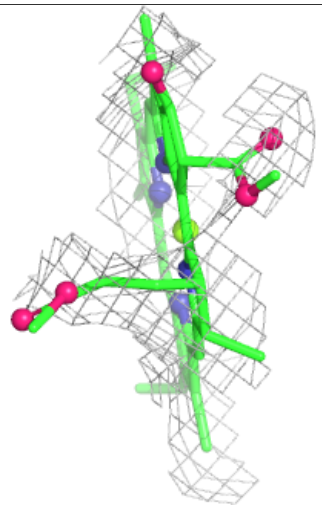


Electron density around CLA 1 1114:

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

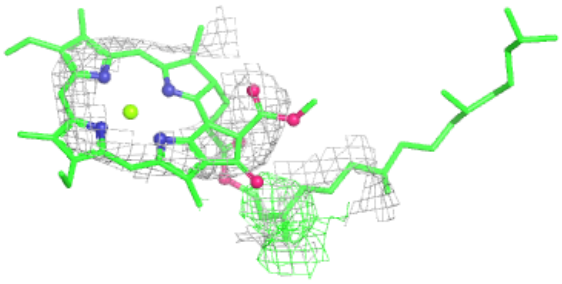


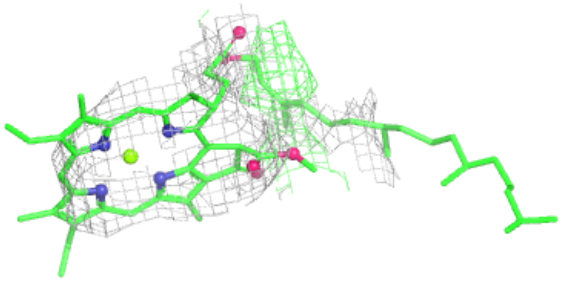


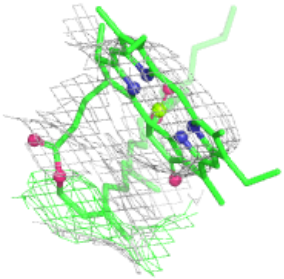


Electron density around CLA b 1213:

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

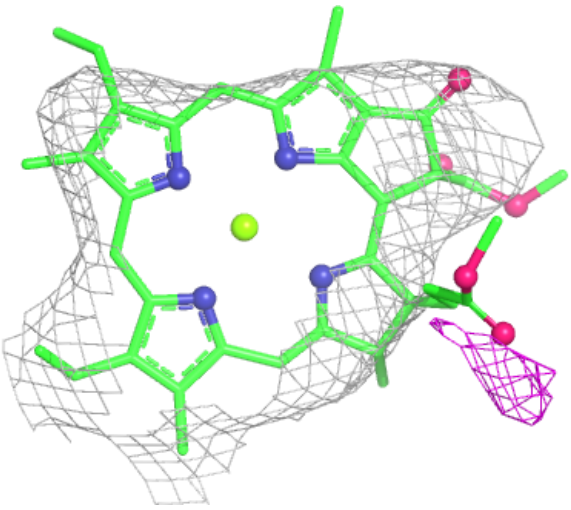


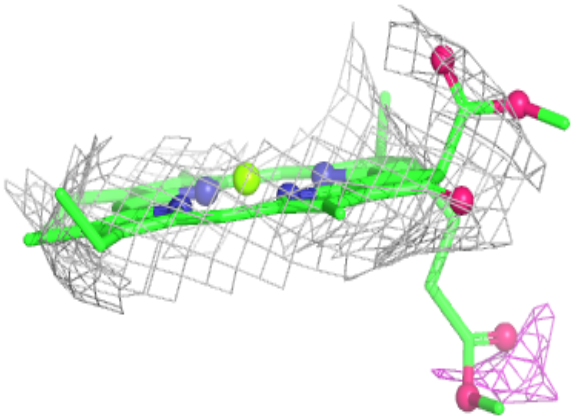


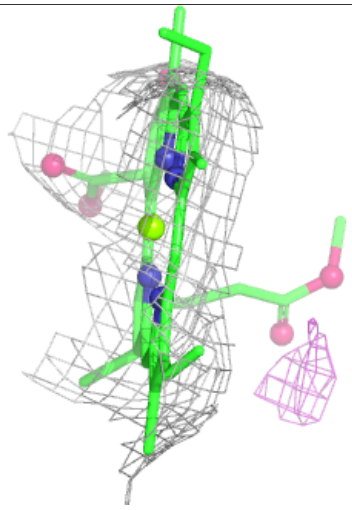


Electron density around CLA A 1114:

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

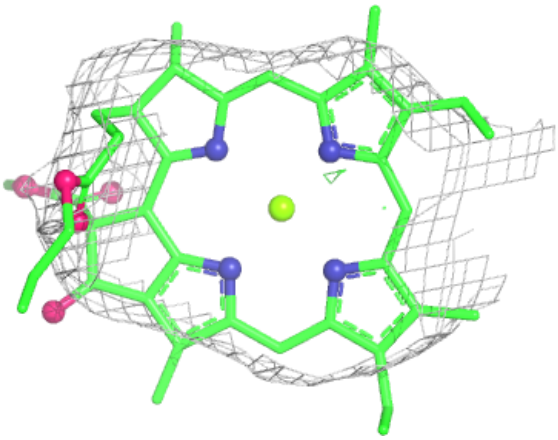


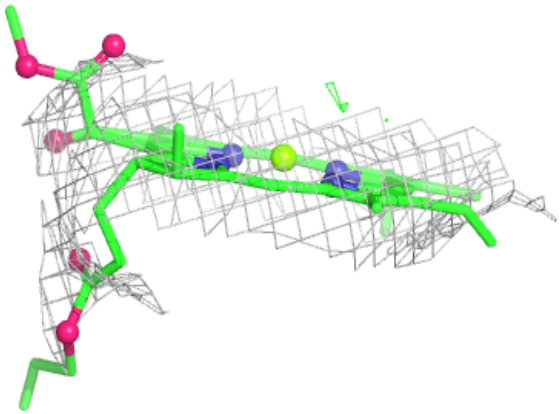


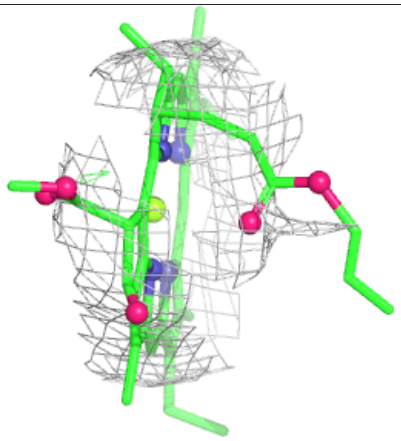


Electron density around CLA 1 1105:

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

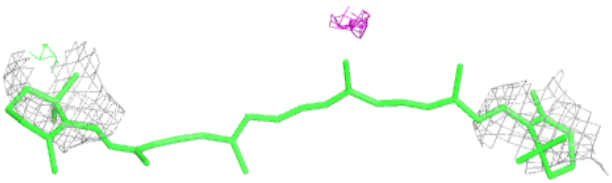


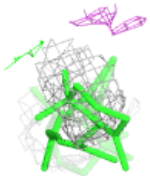




Electron density around BCR a 4003:

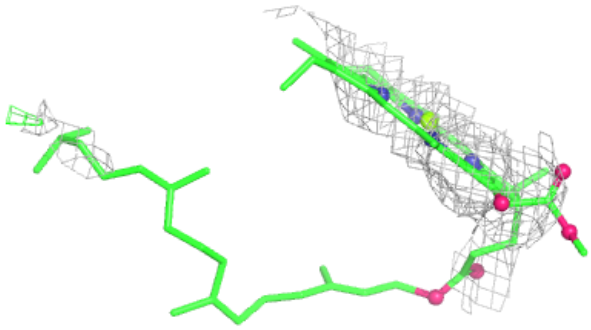
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

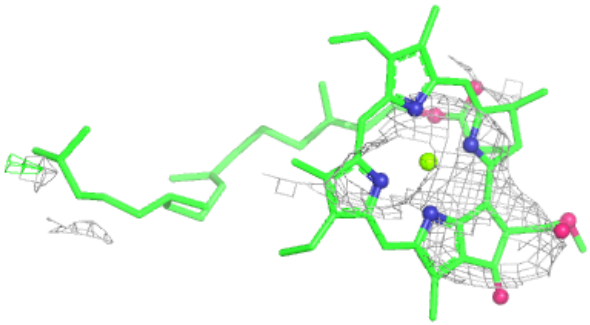


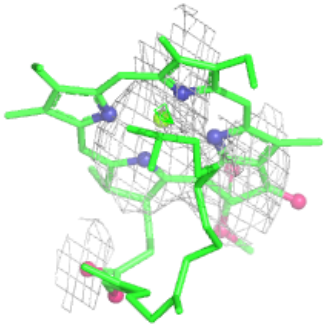


Electron density around CLA a 1109:

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

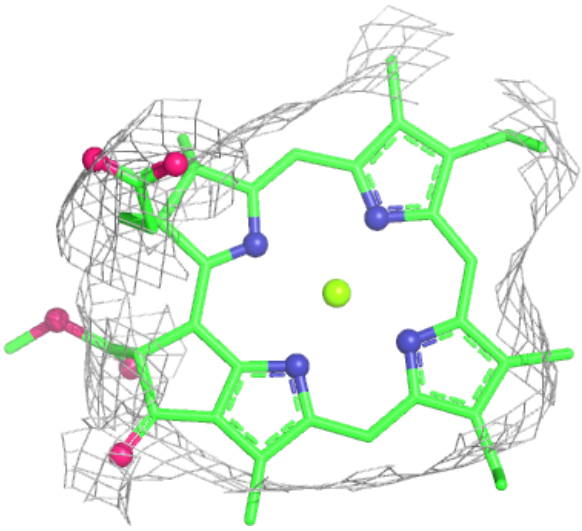


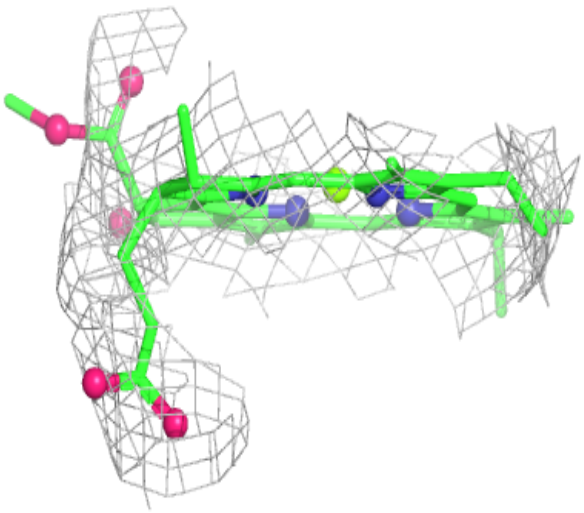


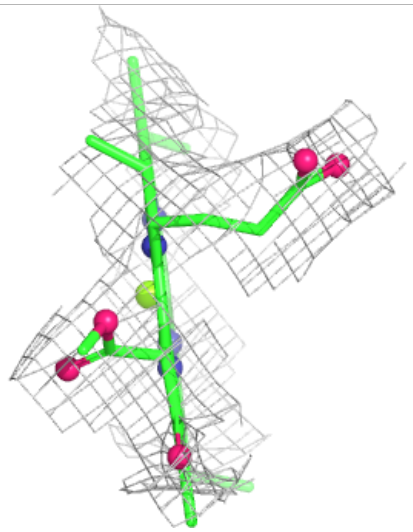


Electron density around CLA b 1232:

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

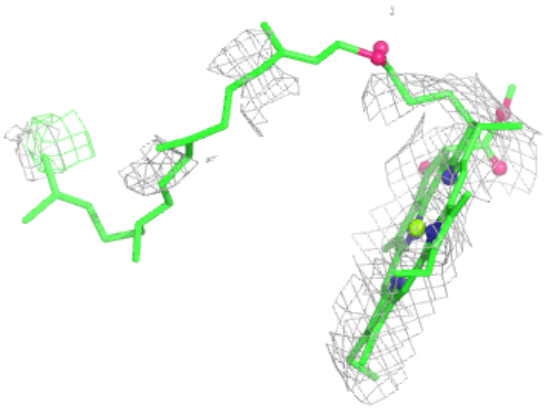


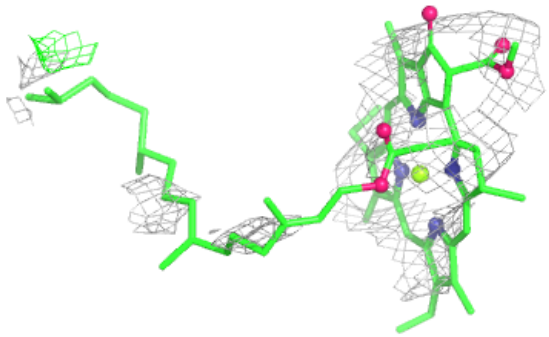


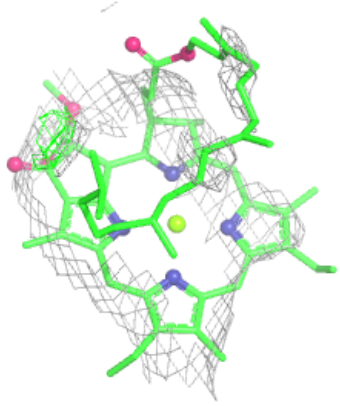


Electron density around CLA b 1216:

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

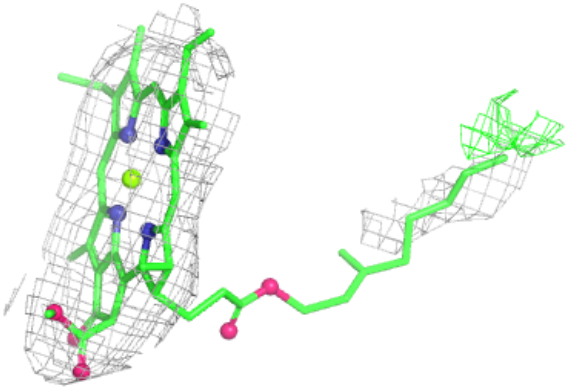


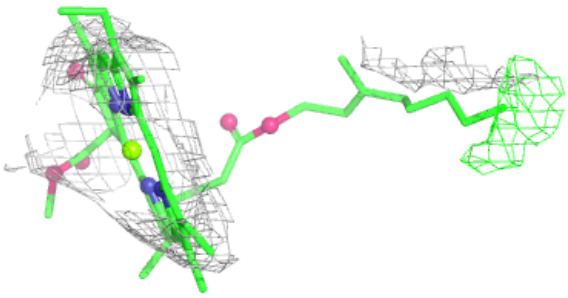


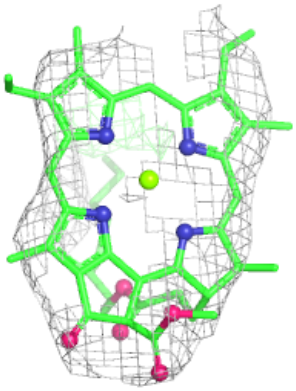


Electron density around CLA b 1201:

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

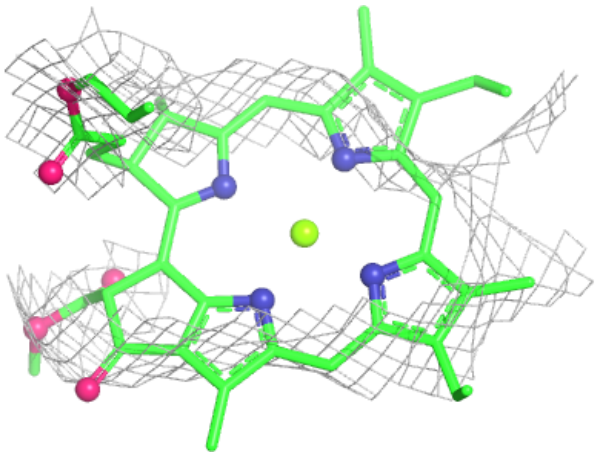


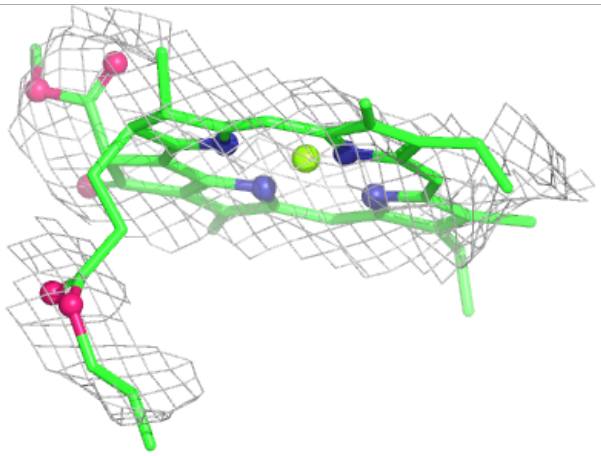


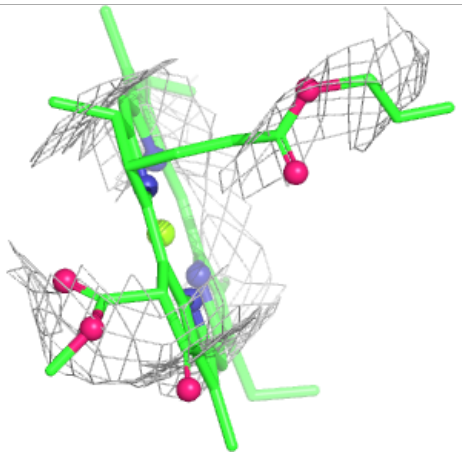


Electron density around CLA a 1105:

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

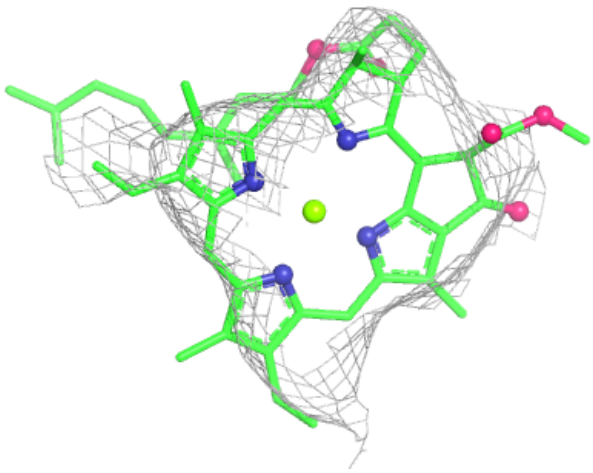


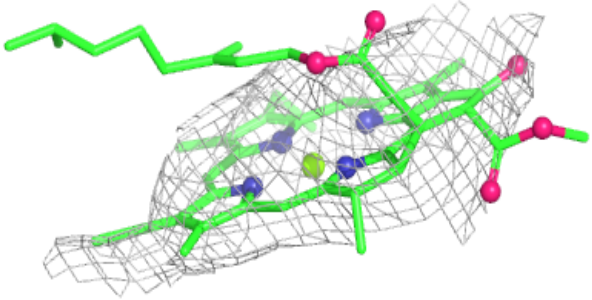


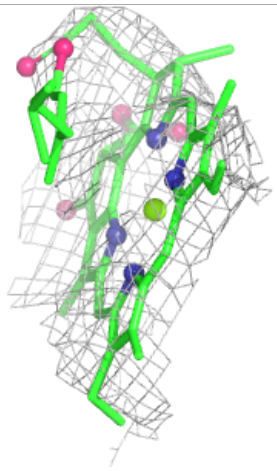


Electron density around CLA 2 1219:

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

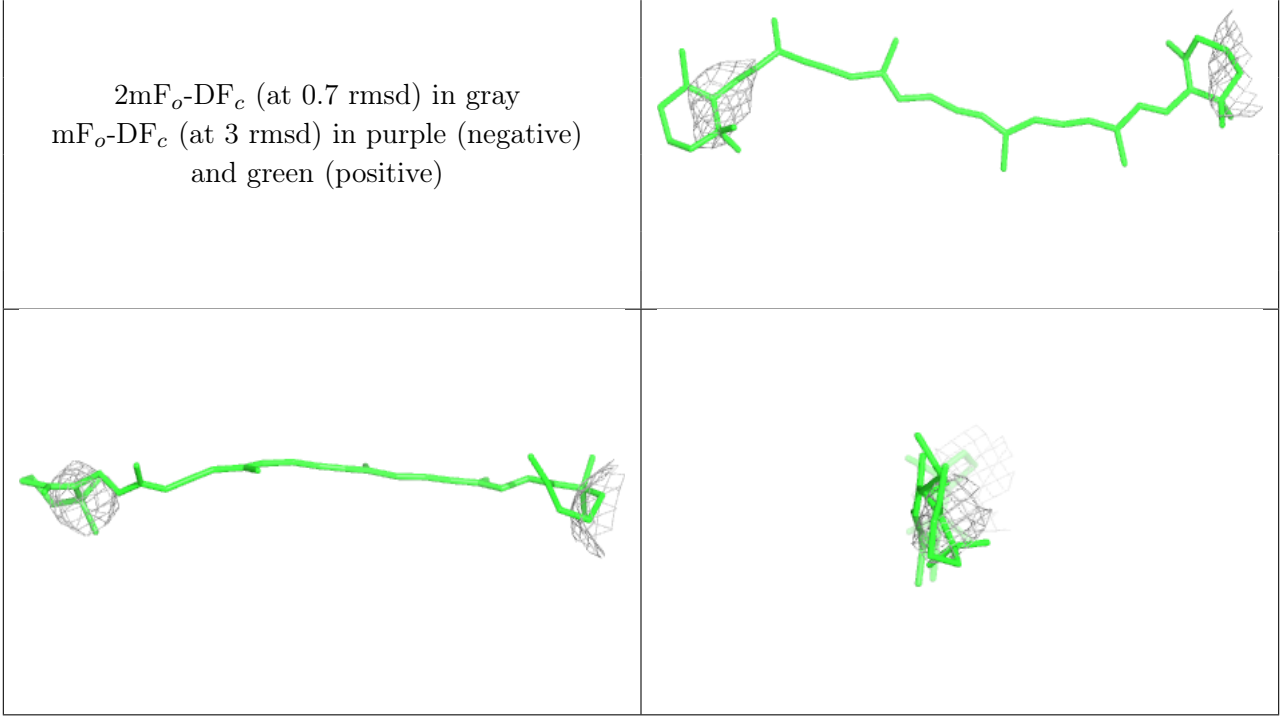






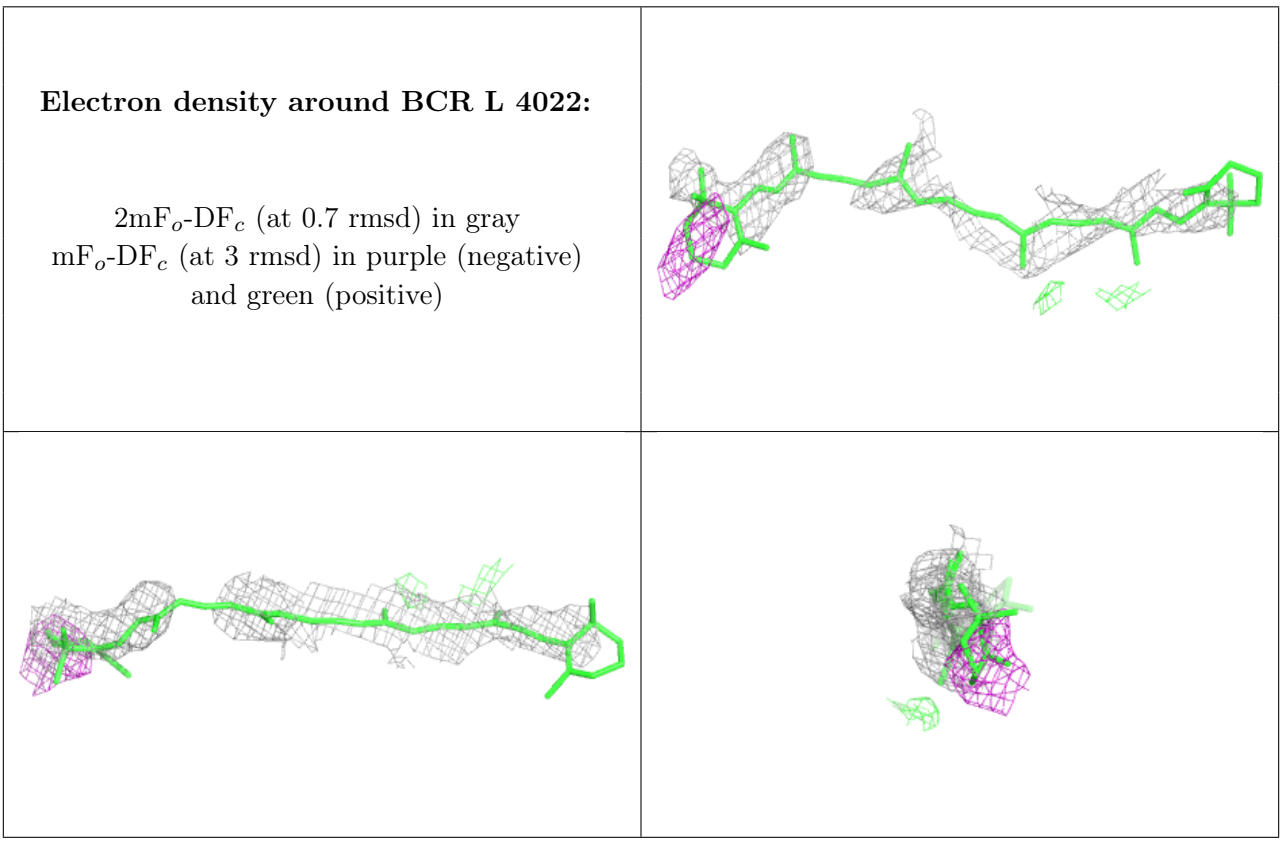
Electron density around BCR b 4005:

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



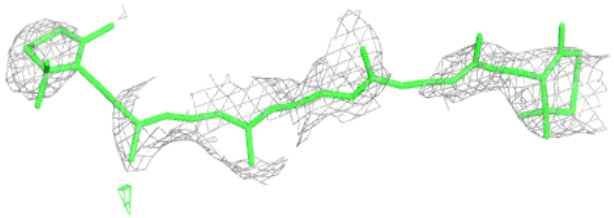
Electron density around BCR L 4022:

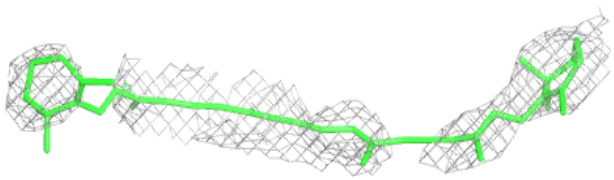
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

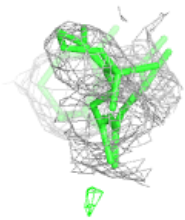


Electron density around BCR M 4021:

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

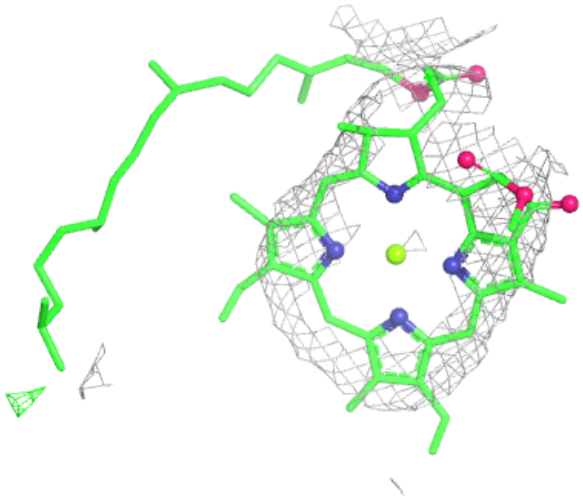


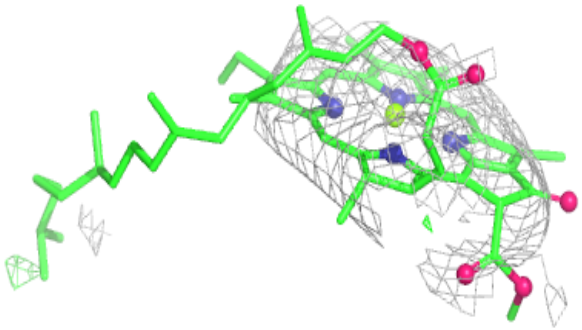


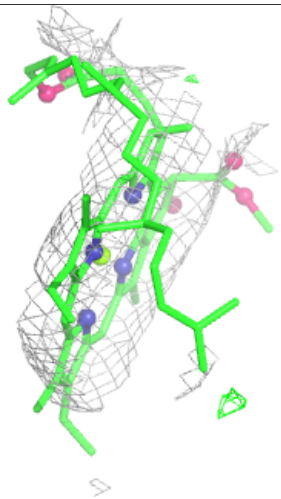


Electron density around CLA k 1401:

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

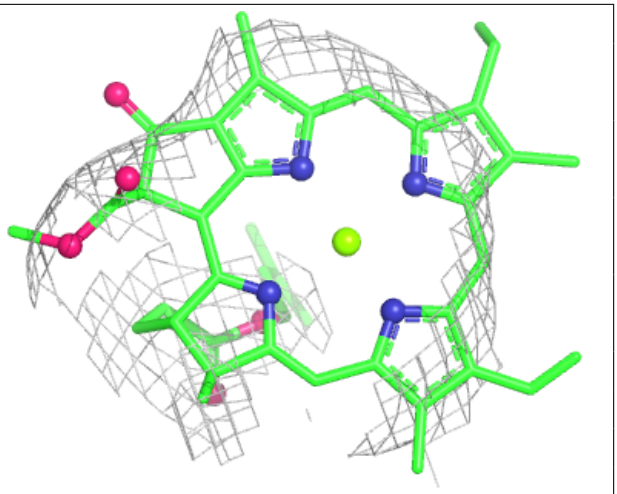


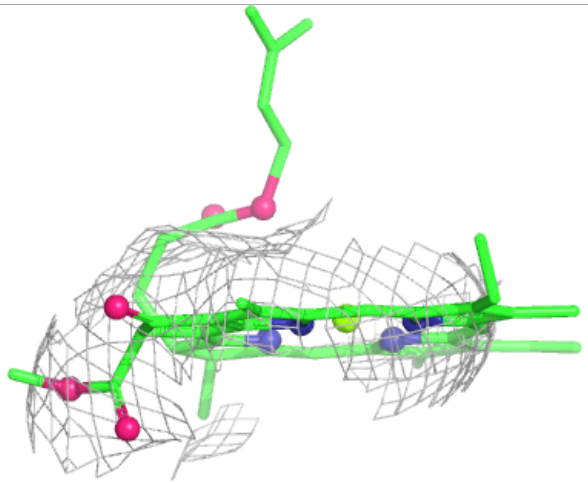


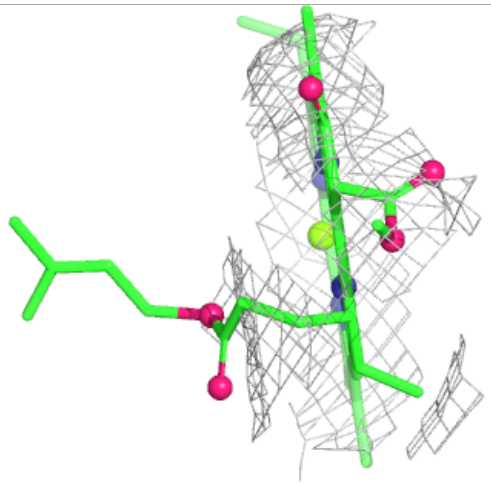


Electron density around CLA k 1402:

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

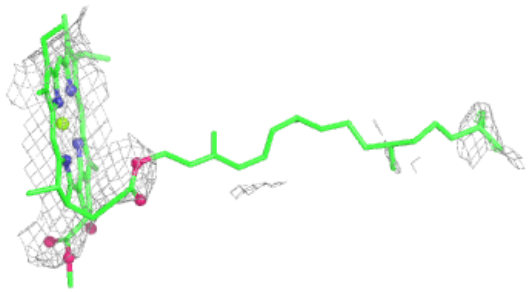


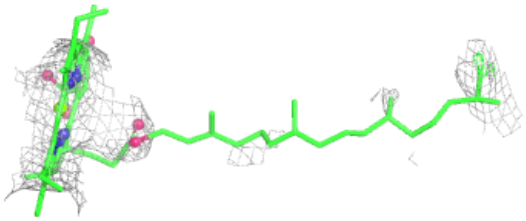


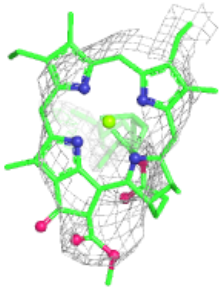


Electron density around CLA a 1126:

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

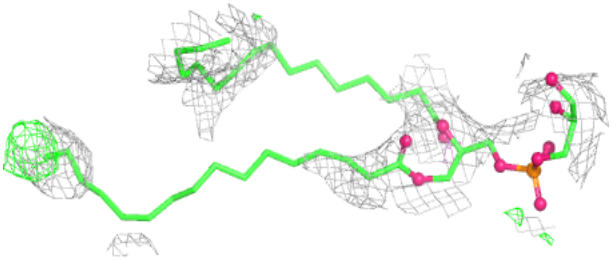


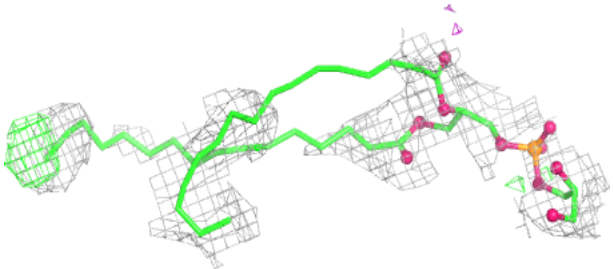


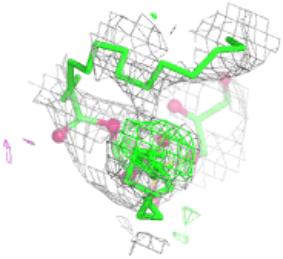


Electron density around LHG A 5003:

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

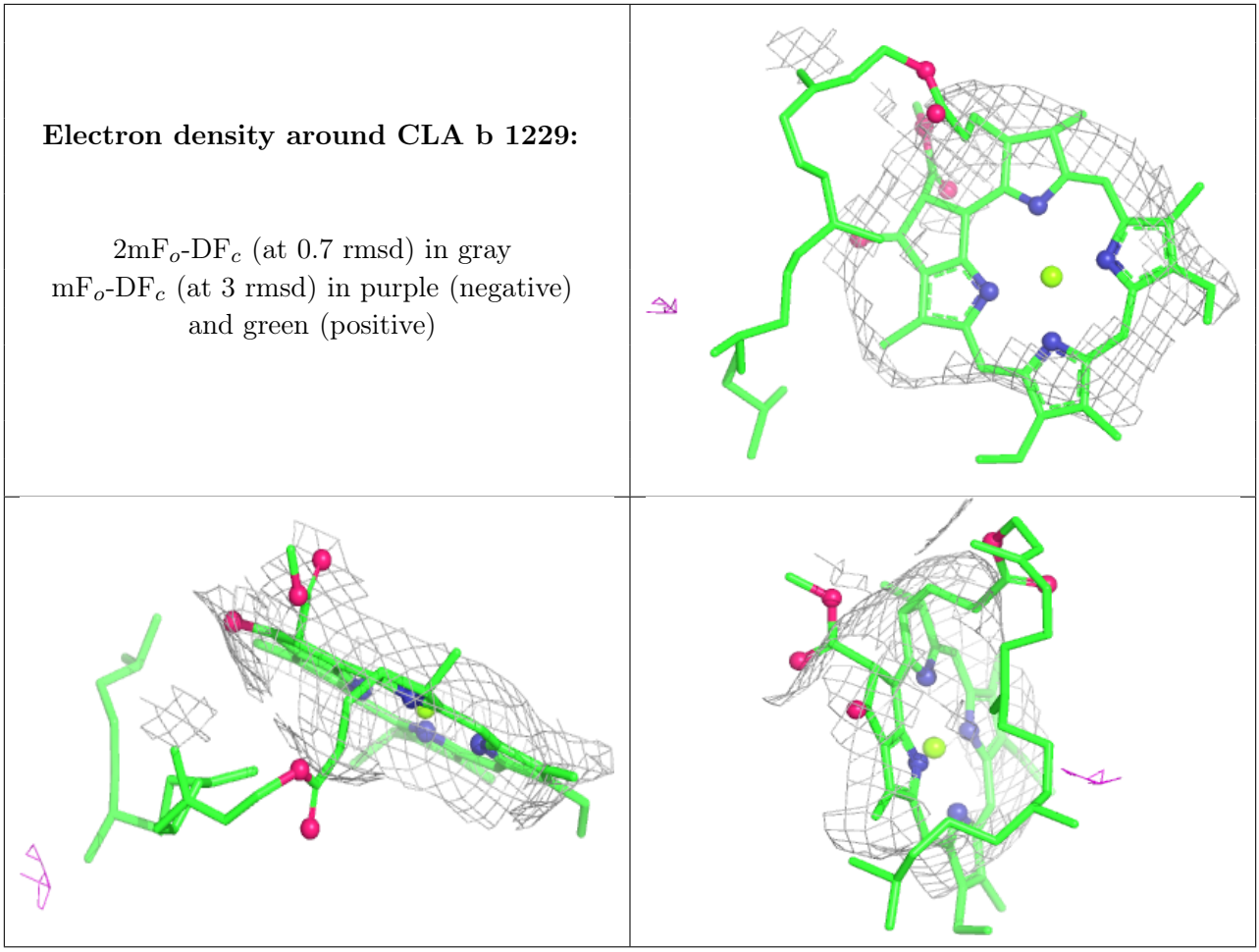






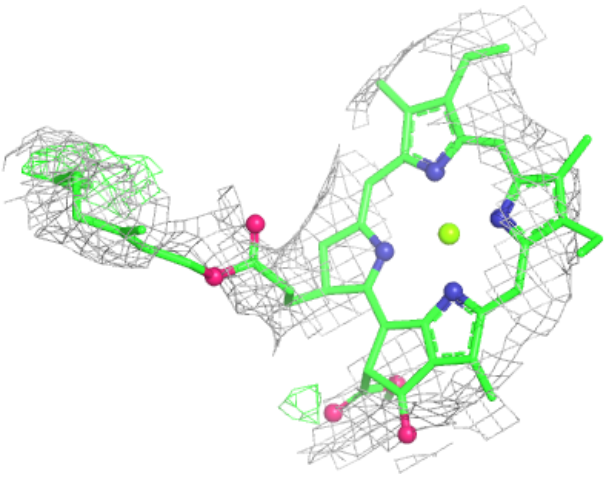
Electron density around CLA b 1229:

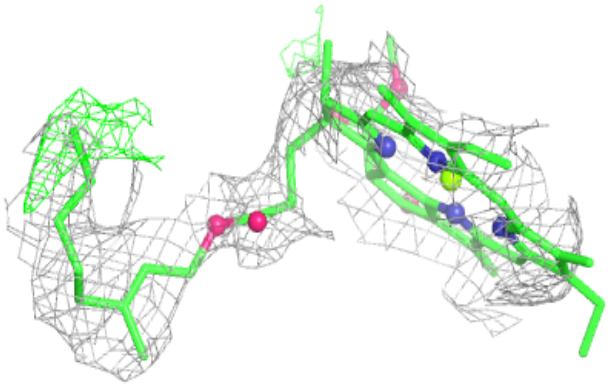
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 1110:

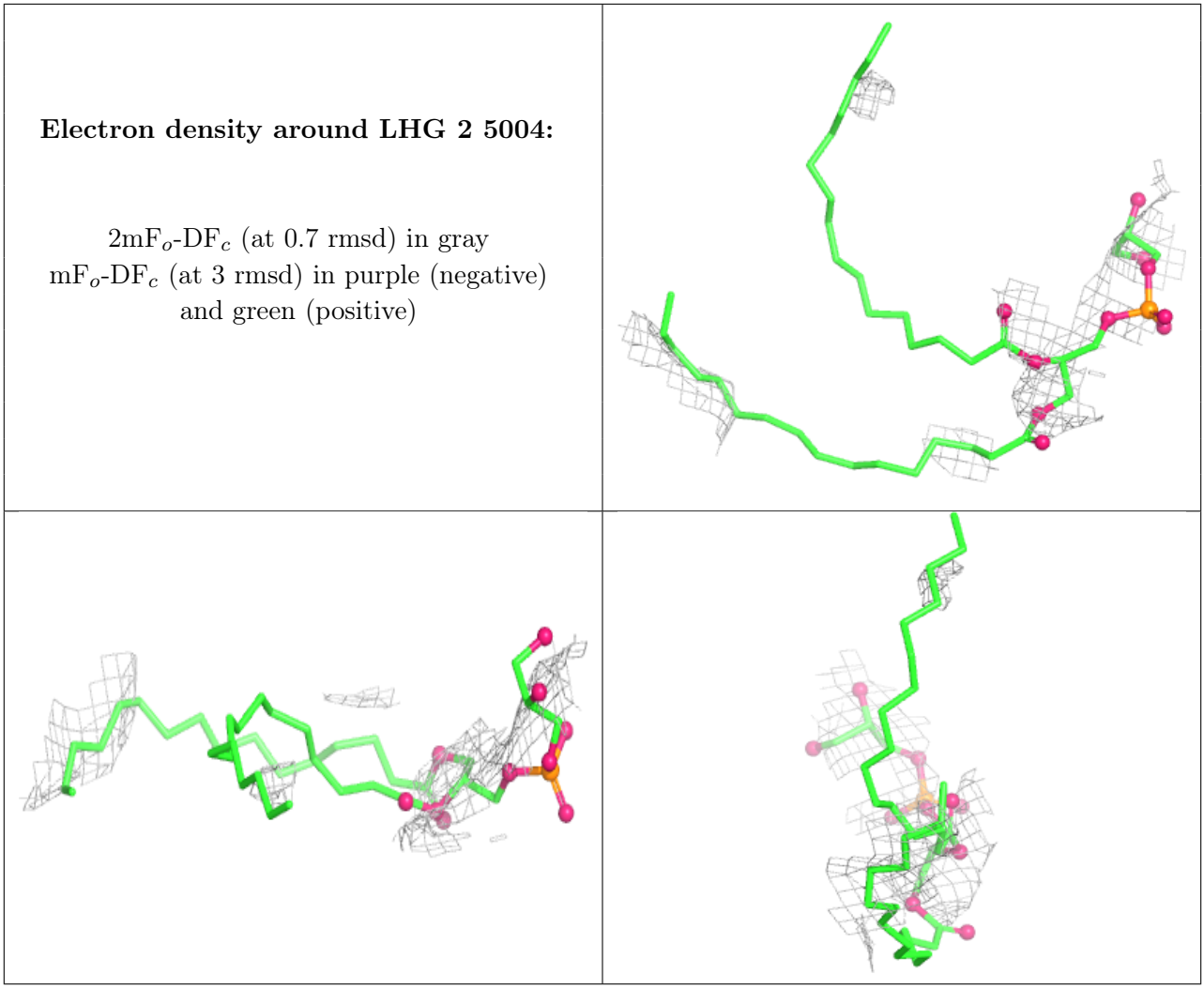
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





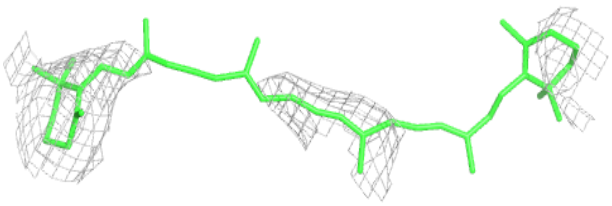
Electron density around LHG 2 5004:

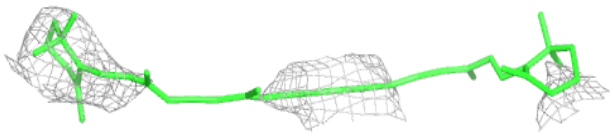
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

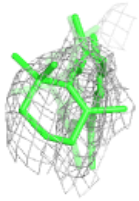


Electron density around BCR 2 4004:

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

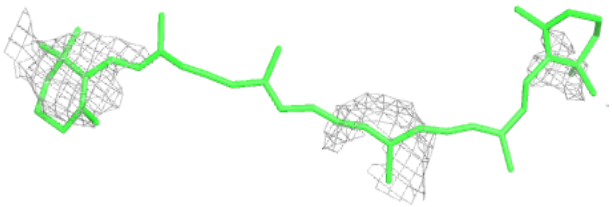


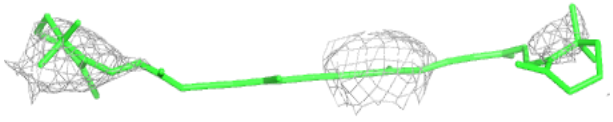


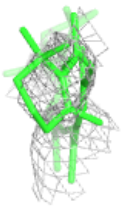


Electron density around BCR B 4004:

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

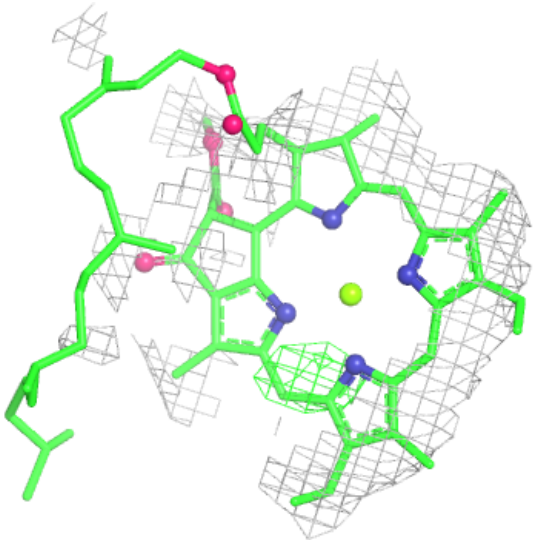


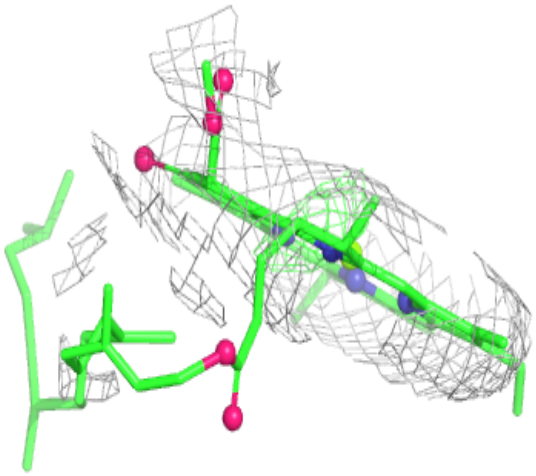




Electron density around CLA 2 1229:

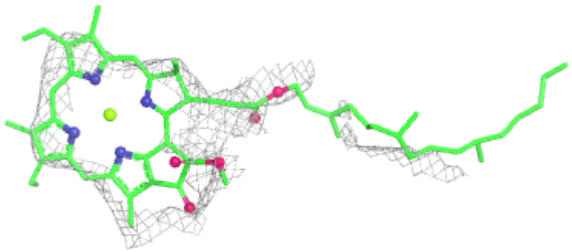
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

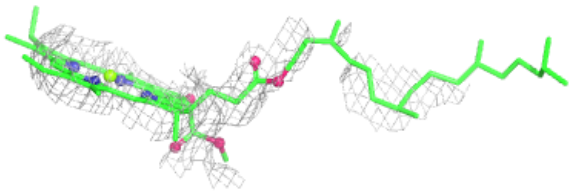


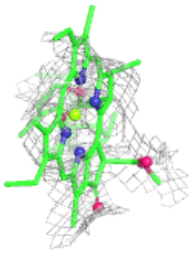


Electron density around CLA 1 1107:

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

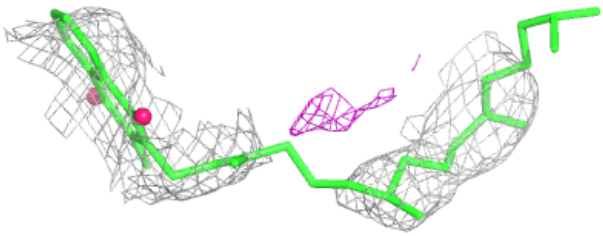


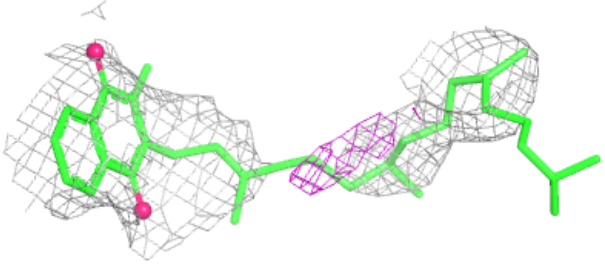


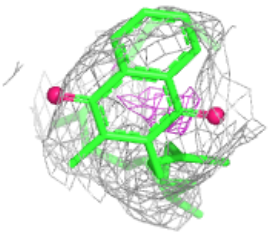


Electron density around PQN B 2002:

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

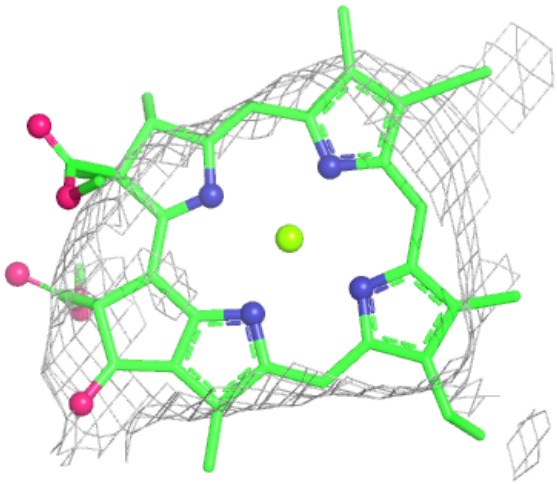


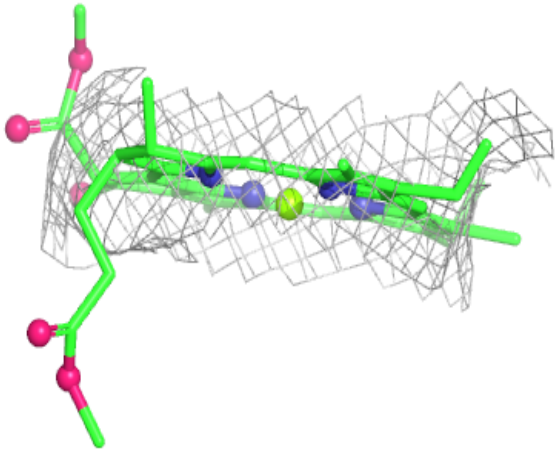


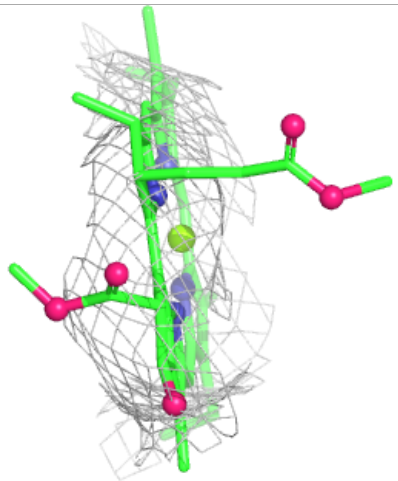


Electron density around CLA b 1211:

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

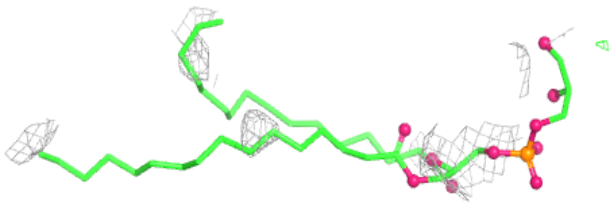






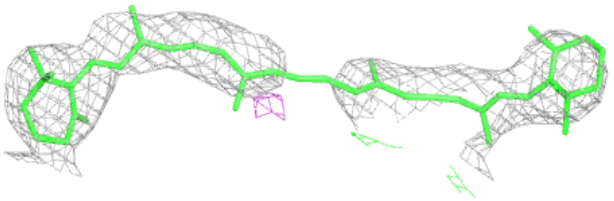
Electron density around LHG 1 5003:

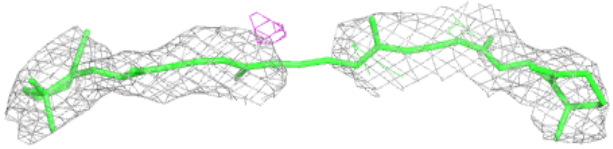
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

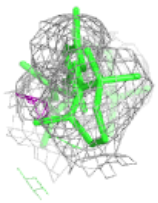


Electron density around BCR A 4008:

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

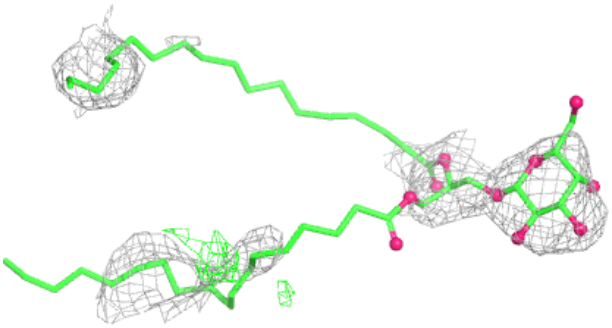


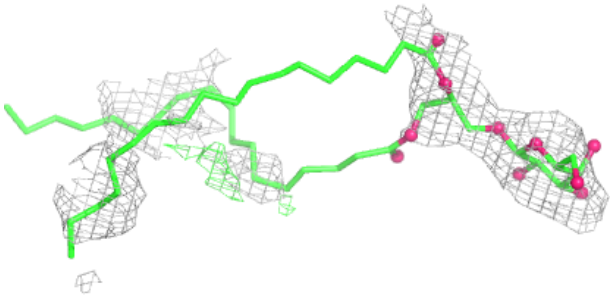


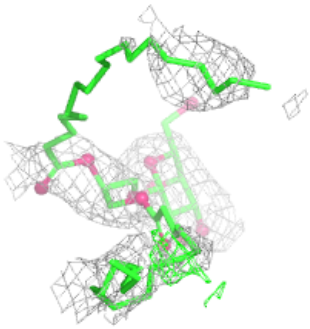


Electron density around LMG 2 5002:

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

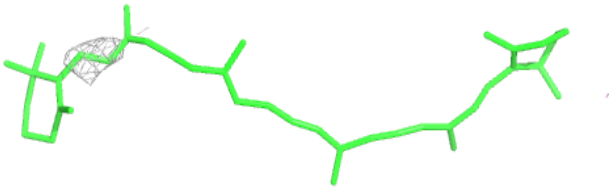


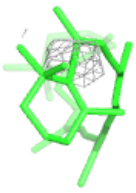




Electron density around BCR b 4014:

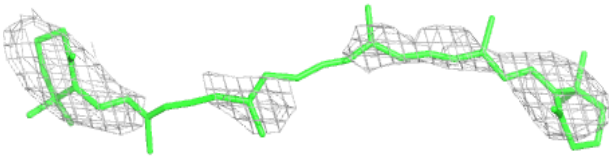
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

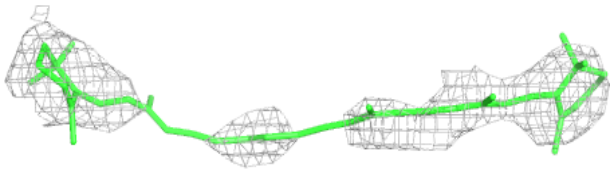


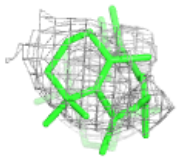


Electron density around BCR f 4018:

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

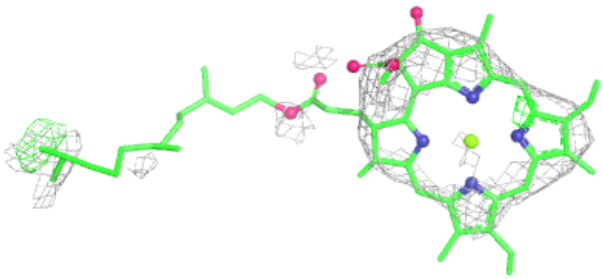


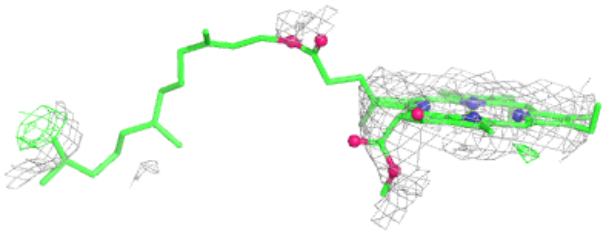


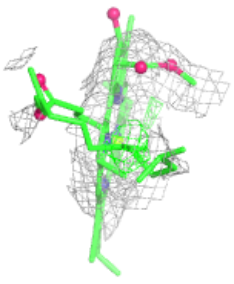


Electron density around CLA B 1234:

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

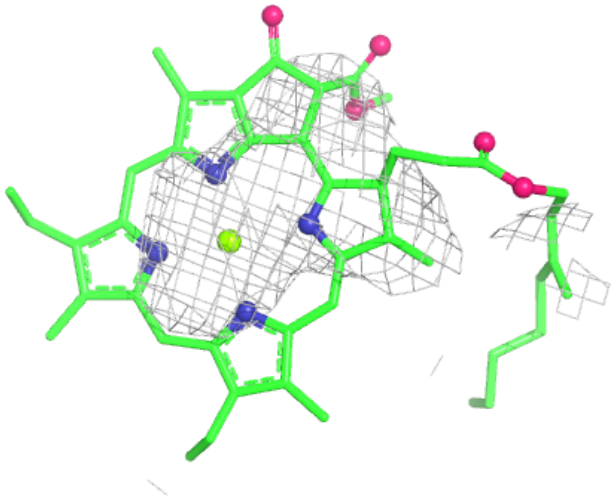


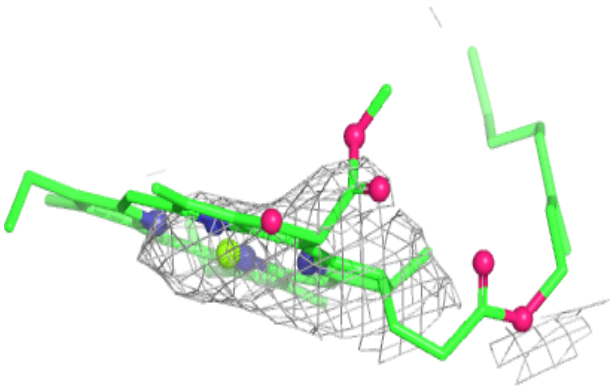




Electron density around CLA b 1221:

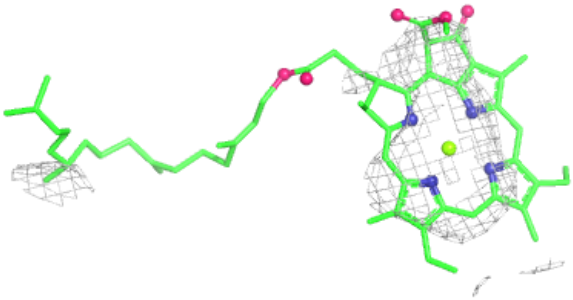
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

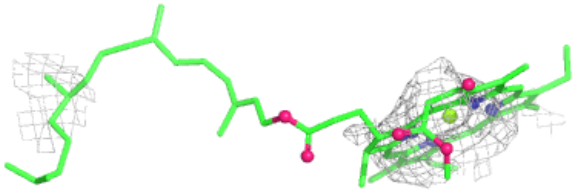




Electron density around CLA b 1210:

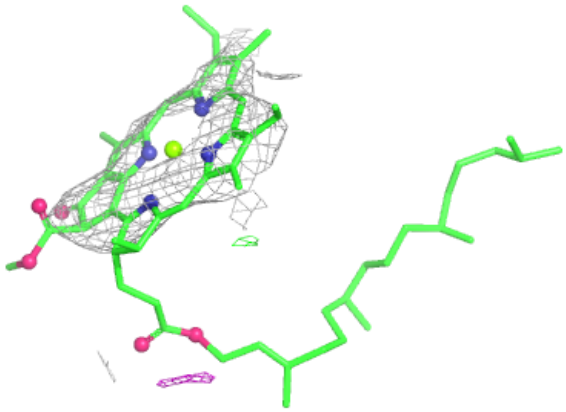
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

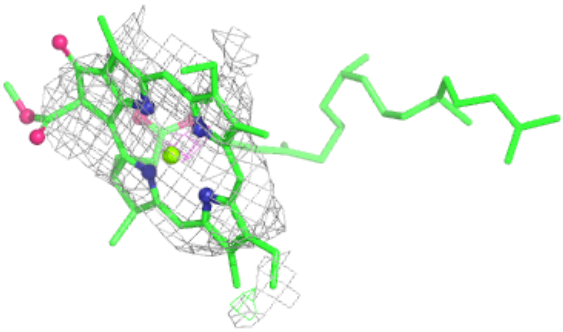


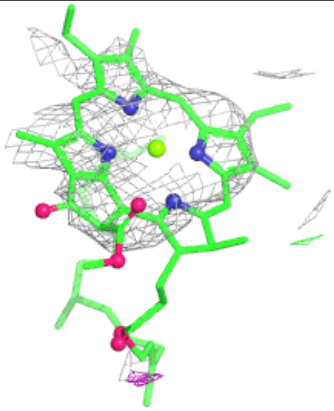


Electron density around CLA 1 1102:

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

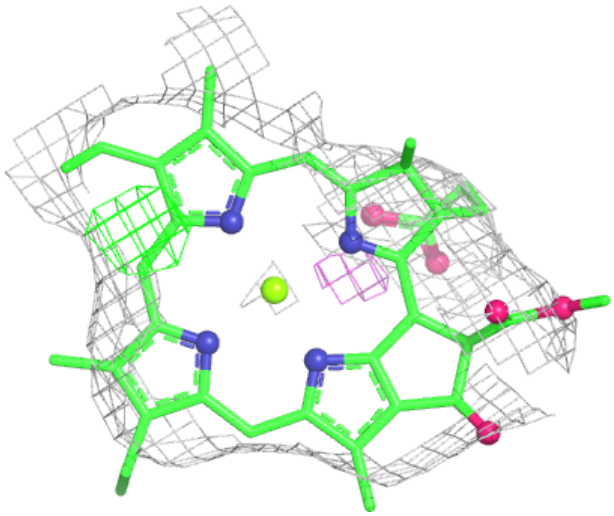


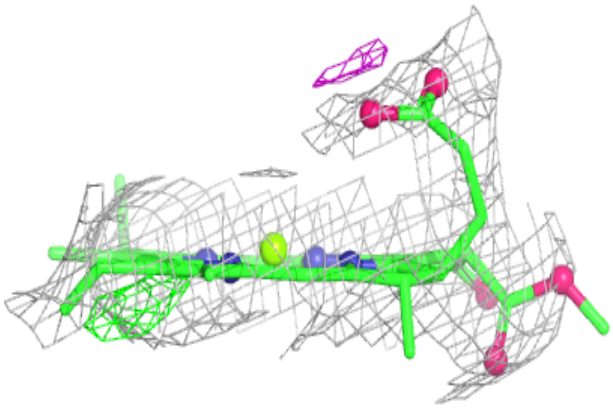


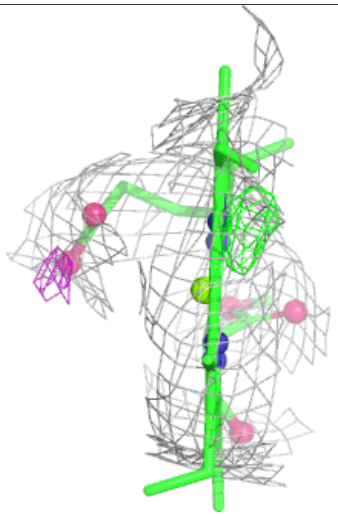


Electron density around CLA 2 1209:

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

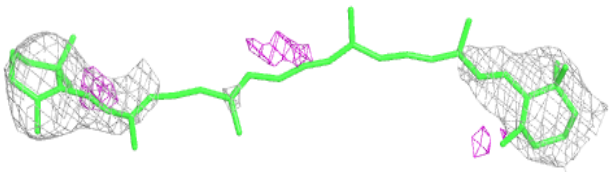


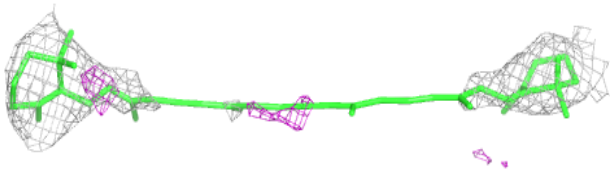


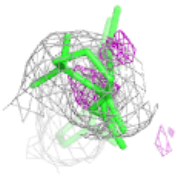


Electron density around BCR 2 4005:

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

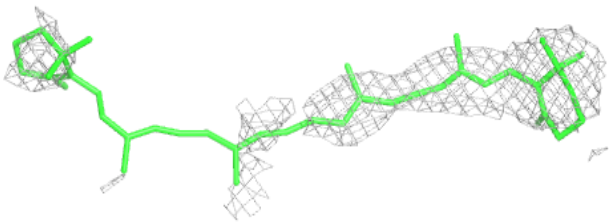


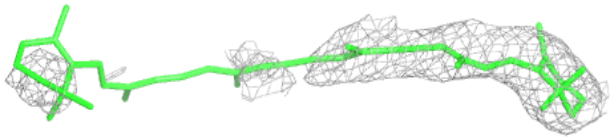


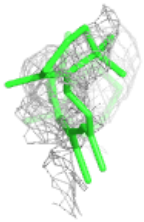


Electron density around BCR 2 4010:

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

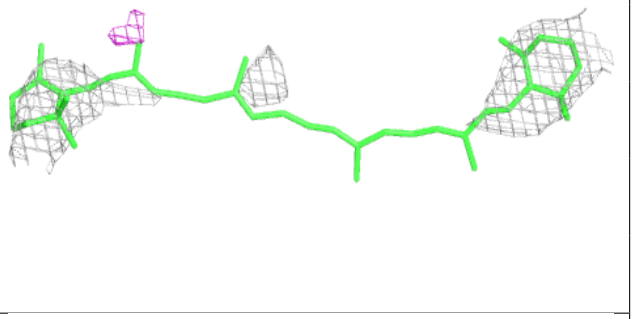


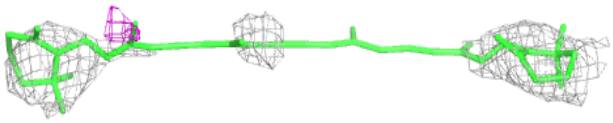


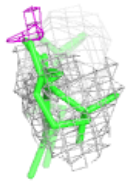


Electron density around BCR B 4005:

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

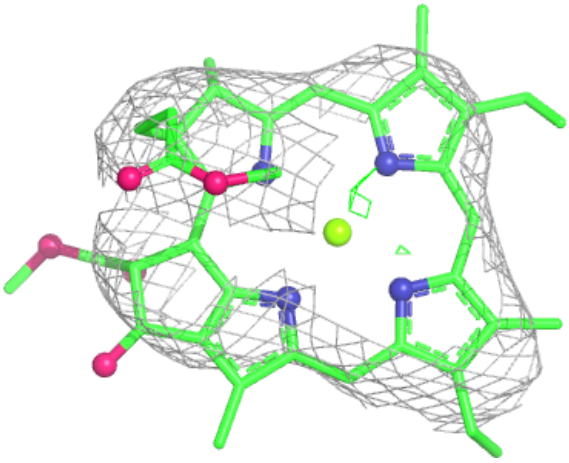


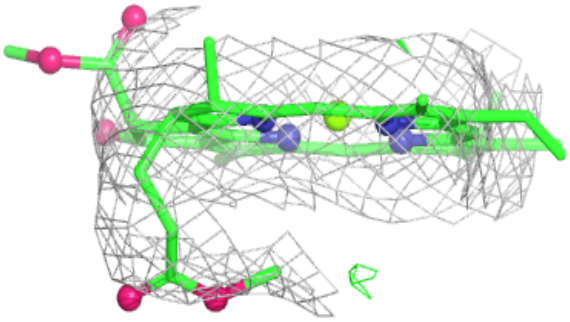


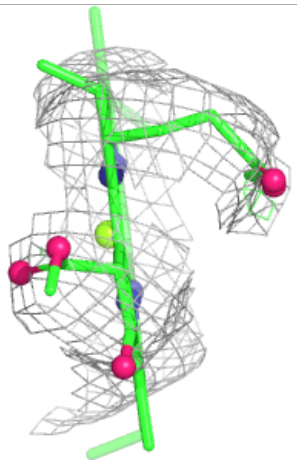


Electron density around CLA a 1121:

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

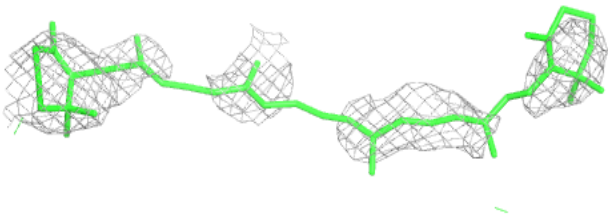


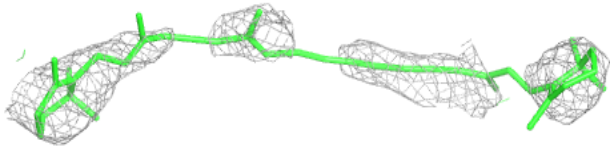


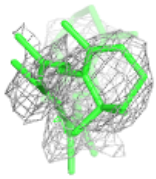


Electron density around BCR 7 4021:

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

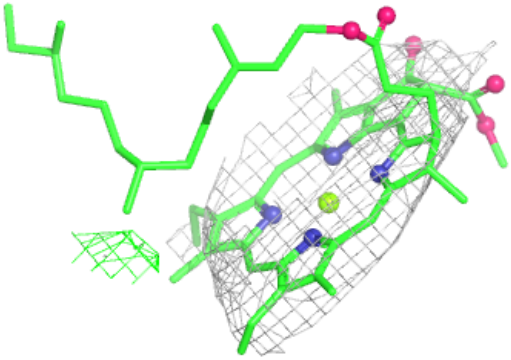


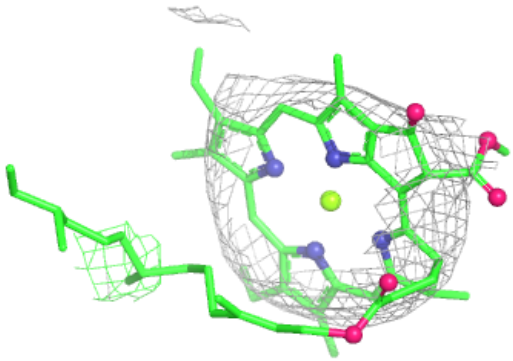


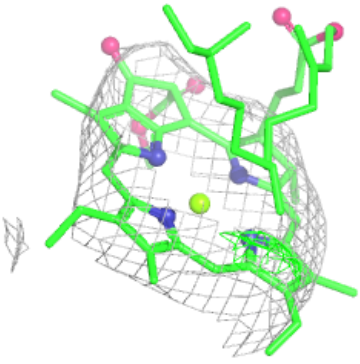


Electron density around CLA a 1118:

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

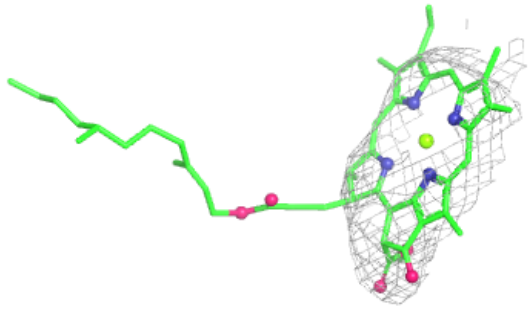


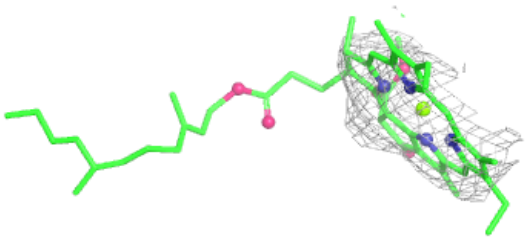


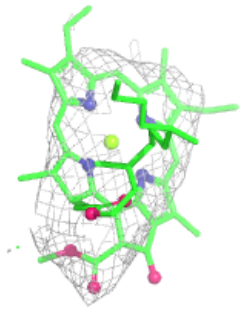


Electron density around CLA 2 1230:

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

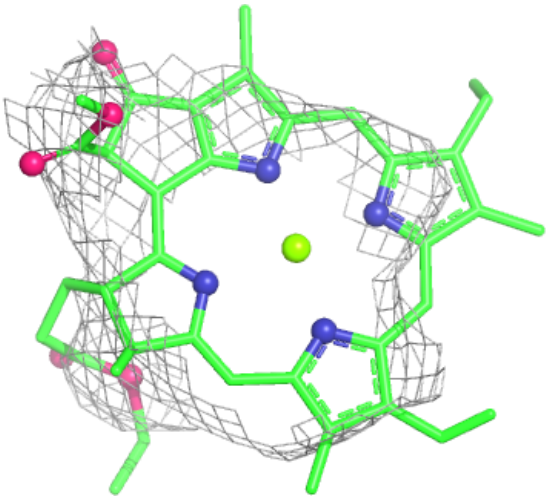


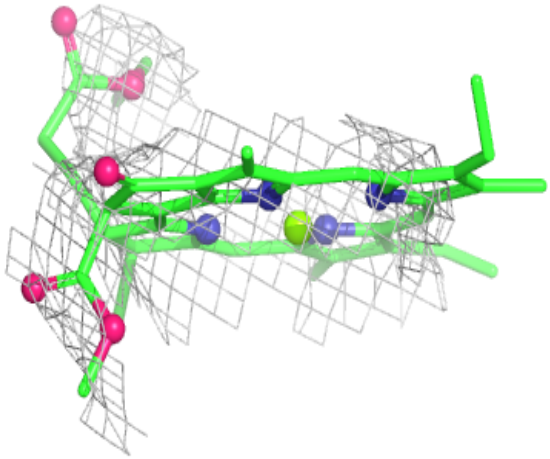


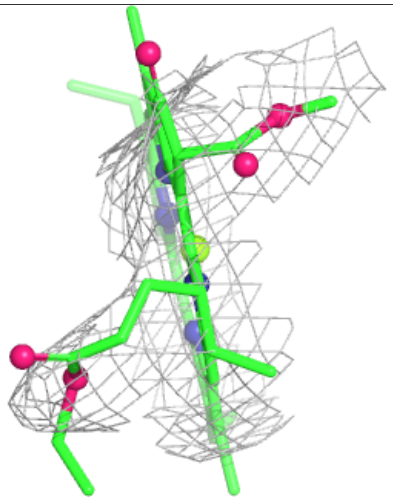


Electron density around CLA b 1217:

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

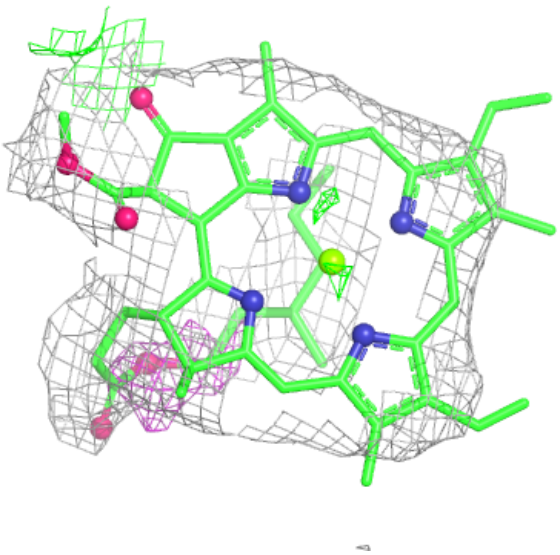


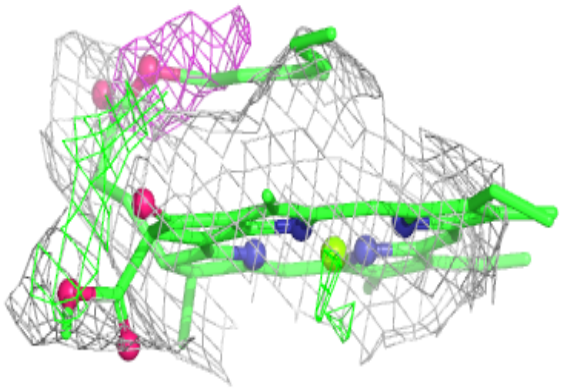


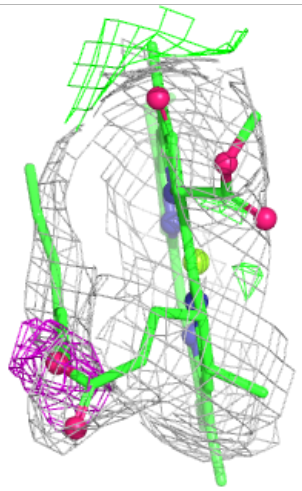


Electron density around CLA A 1801:

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

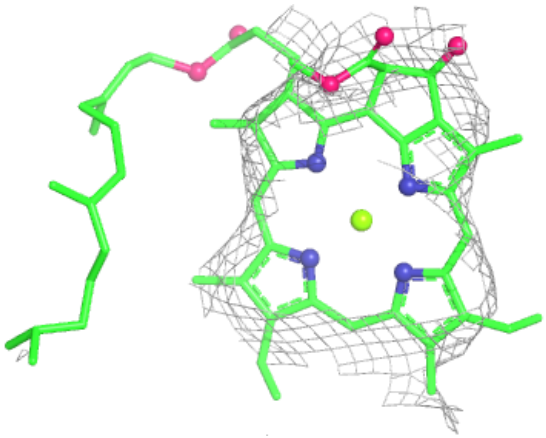


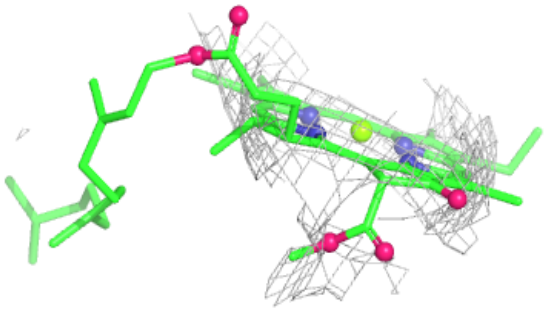




Electron density around CLA 1 1111:

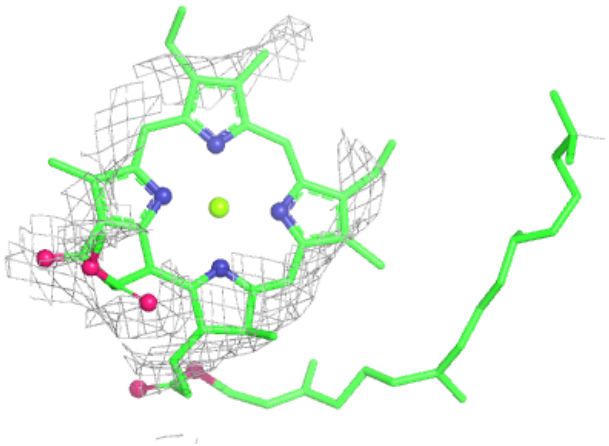
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

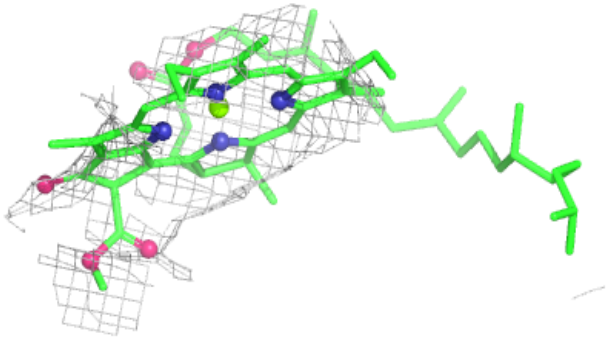


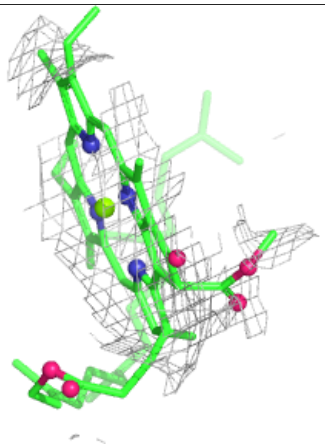


Electron density around CLA 0 1401:

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

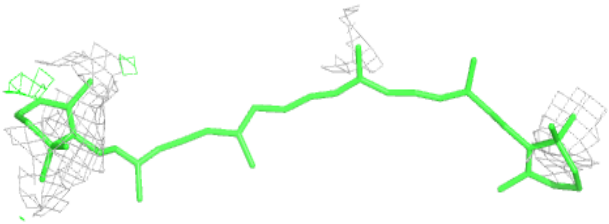


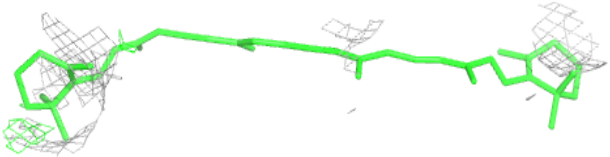


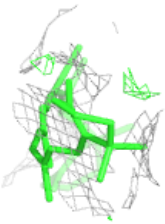


Electron density around BCR 1 4001:

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

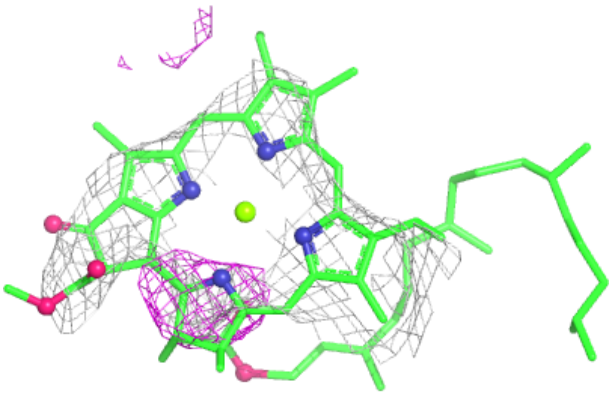


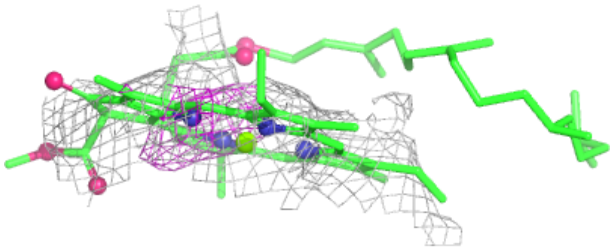


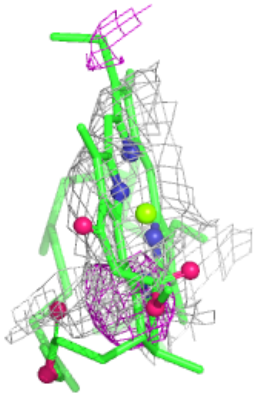


Electron density around CLA a 1117:

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

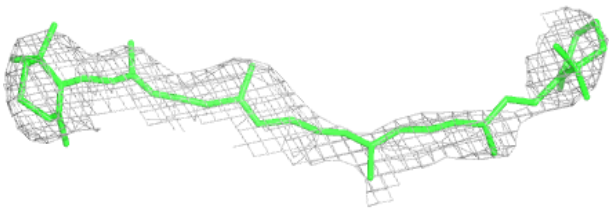


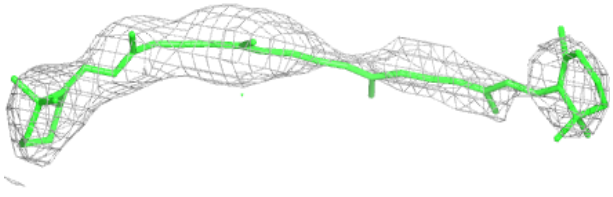


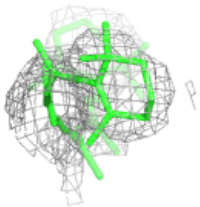


Electron density around BCR F 4018:

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

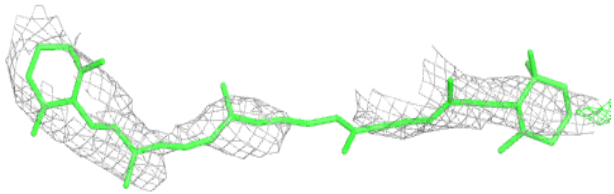


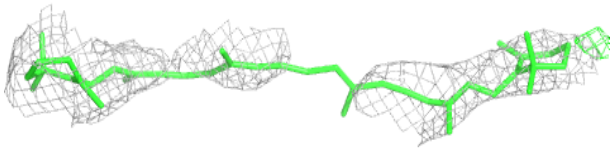


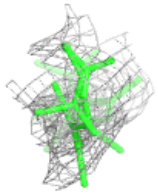


Electron density around BCR 1 4008:

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

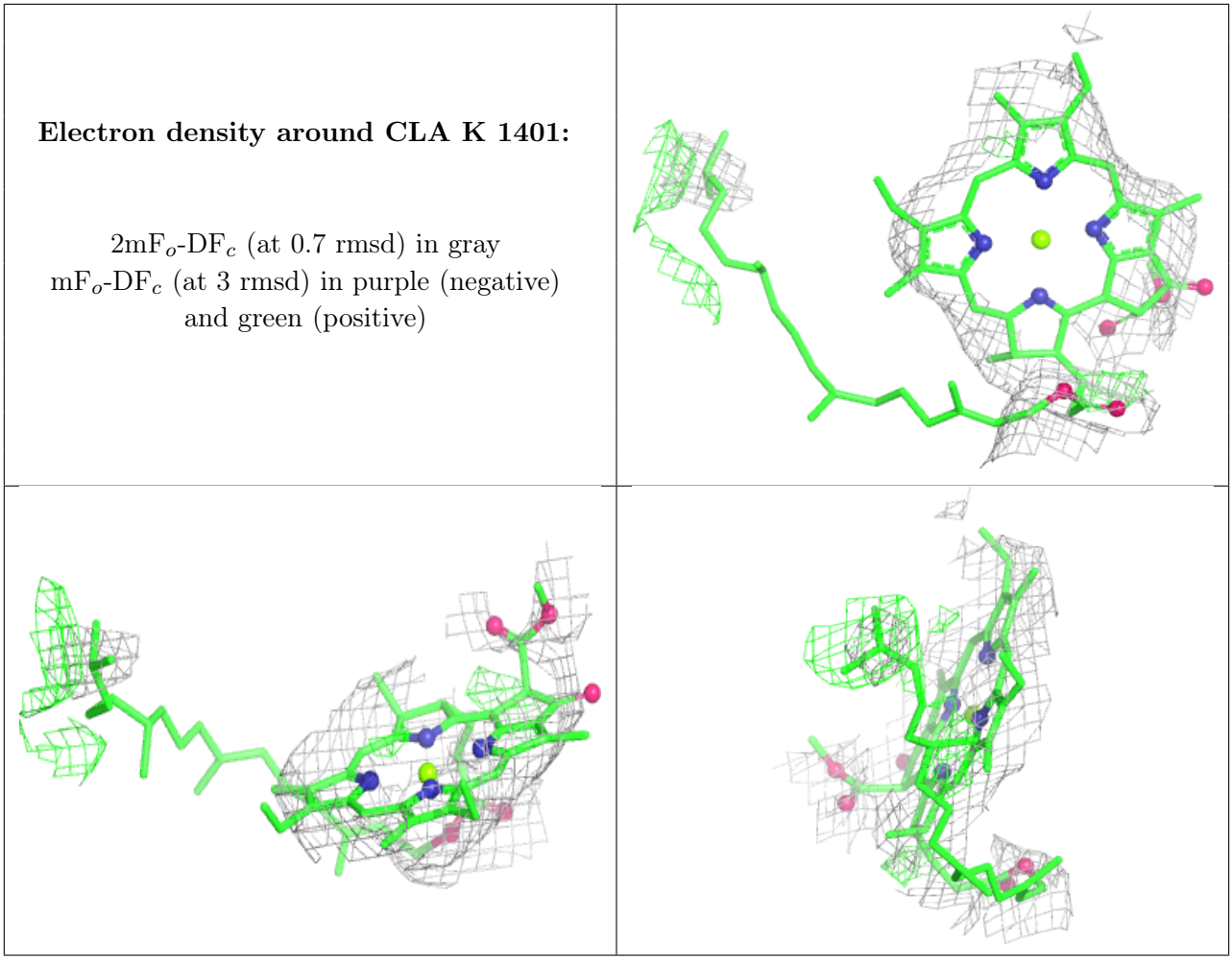






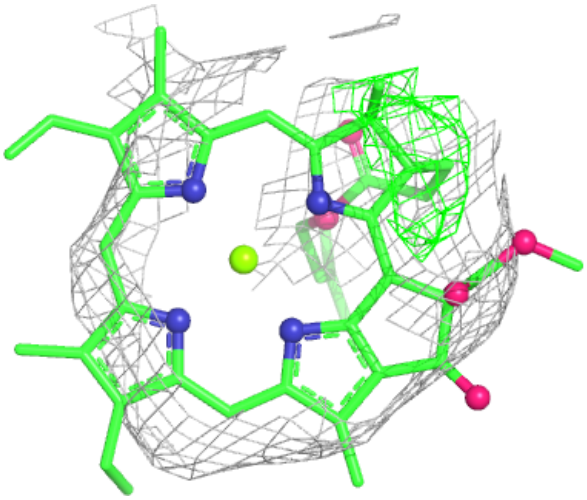
Electron density around CLA K 1401:

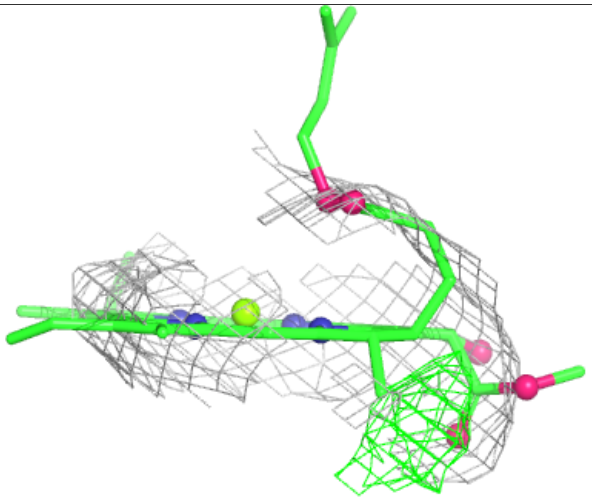
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

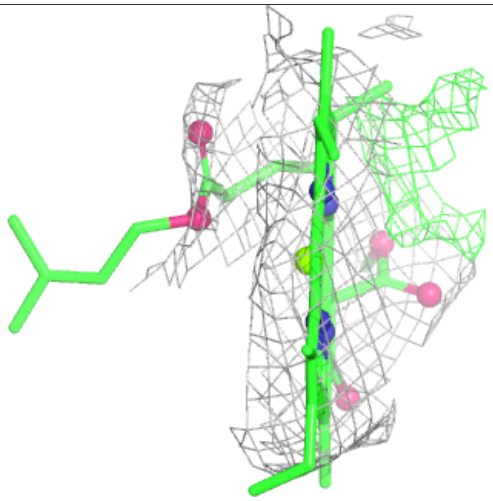


Electron density around CLA K 1402:

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

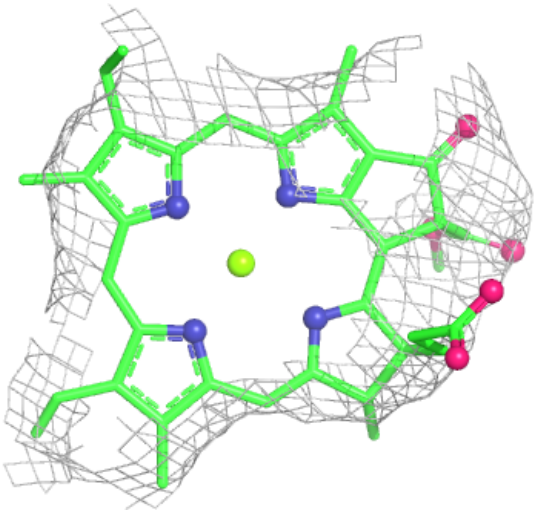


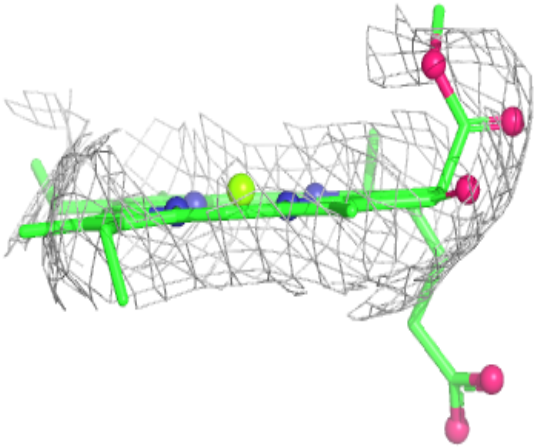


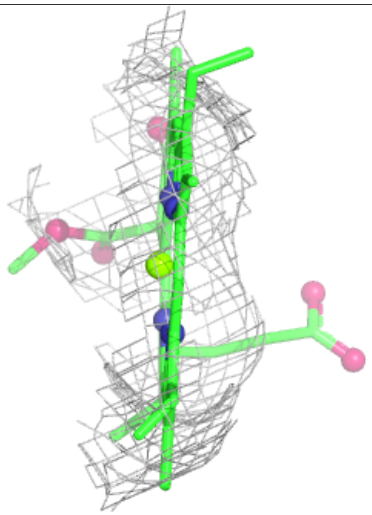


Electron density around CLA B 1218:

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

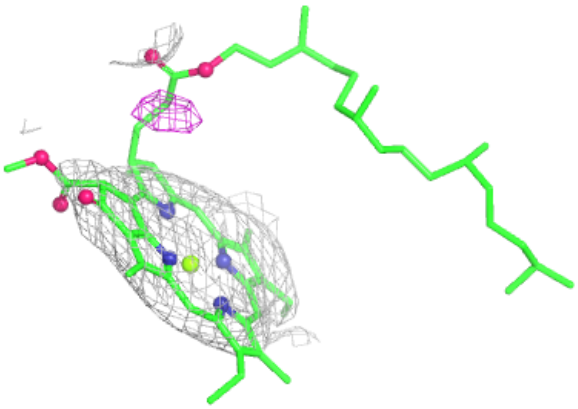


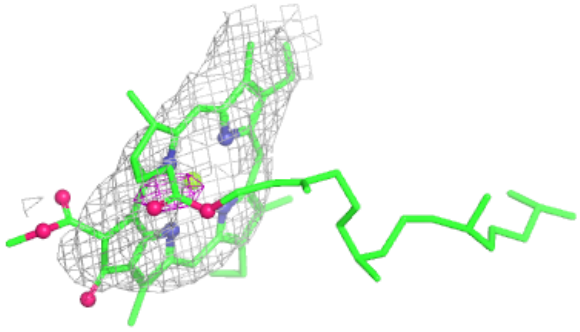




Electron density around CLA a 1102:

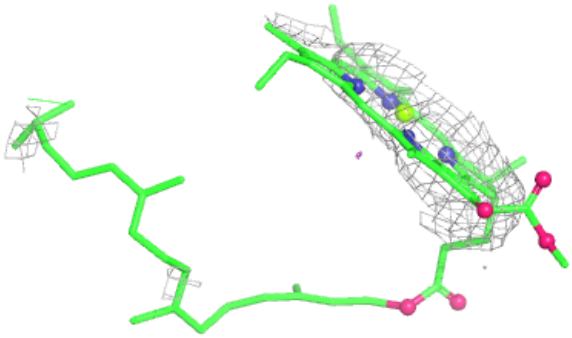
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

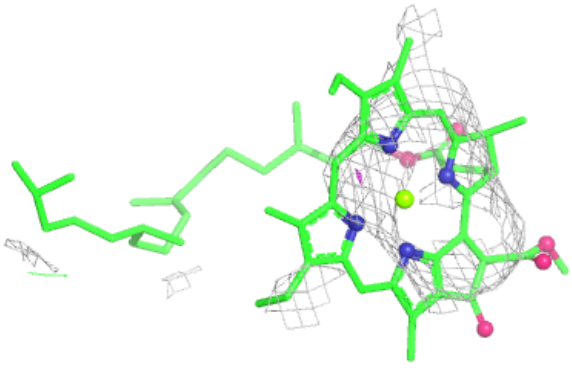


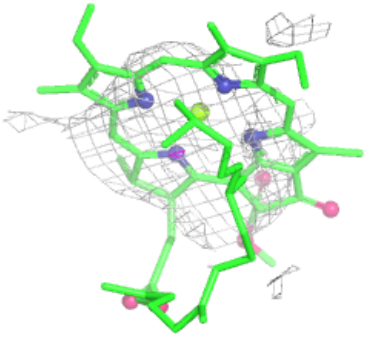


Electron density around CLA 1 1109:

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

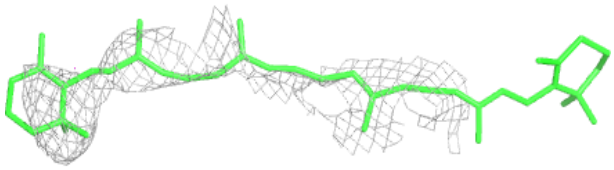


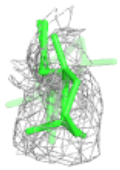




Electron density around BCR a 4007:

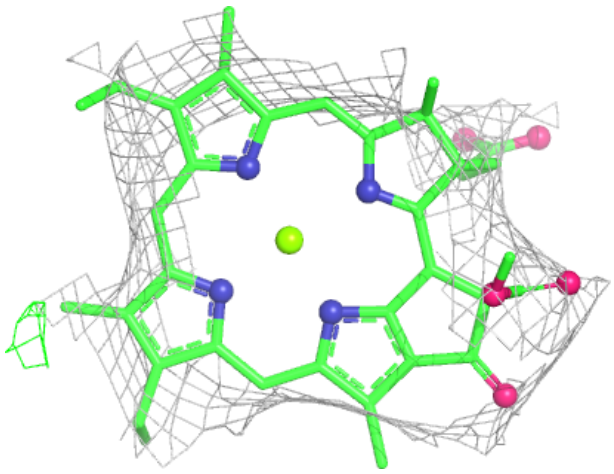
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

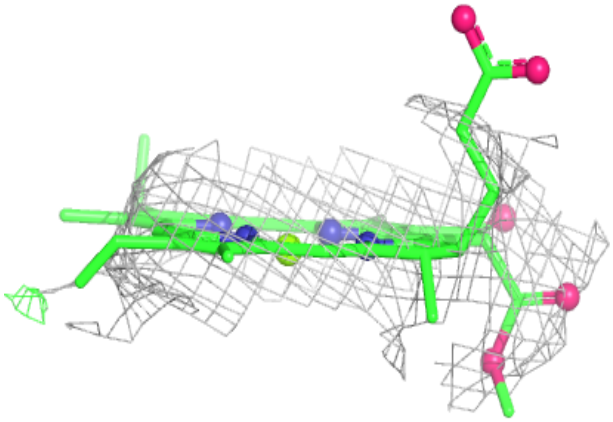




Electron density around CLA 2 1218:

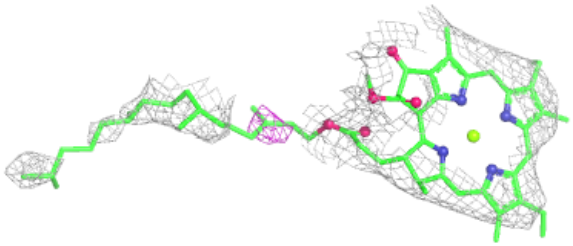
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

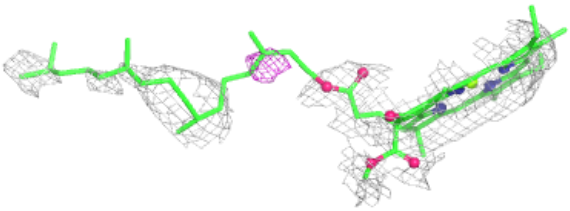




Electron density around CLA A 1107:

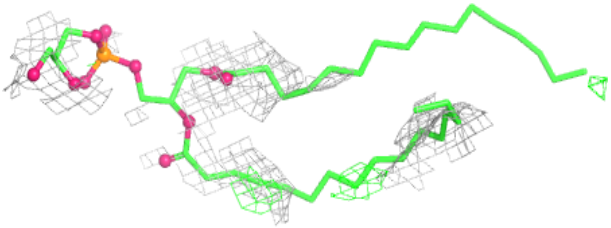
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

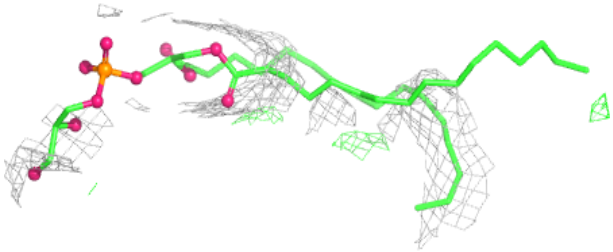


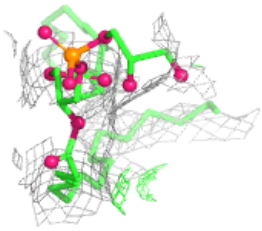


Electron density around LHG a 5003:

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

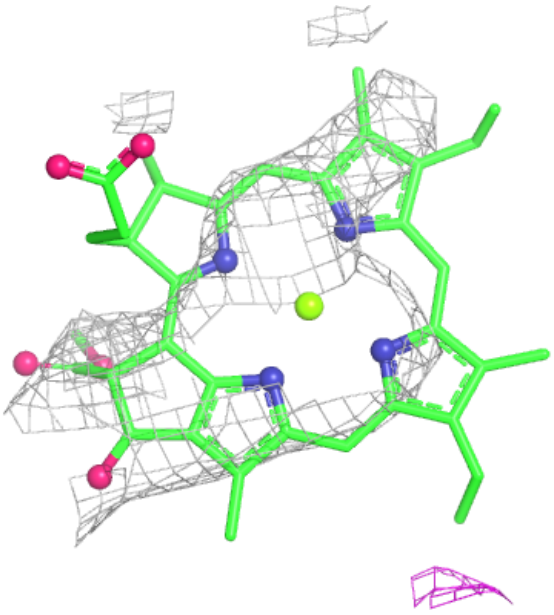


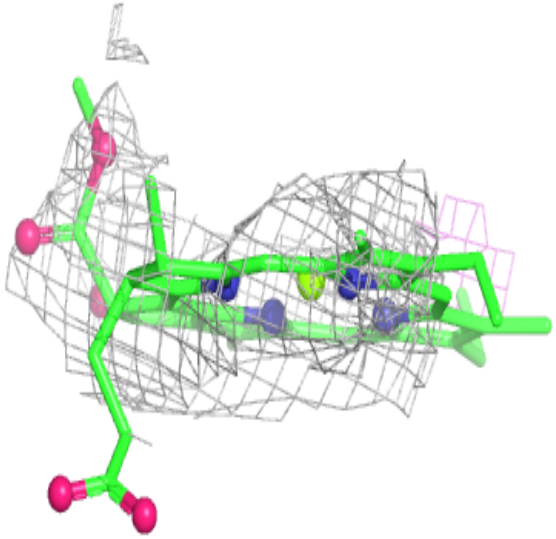


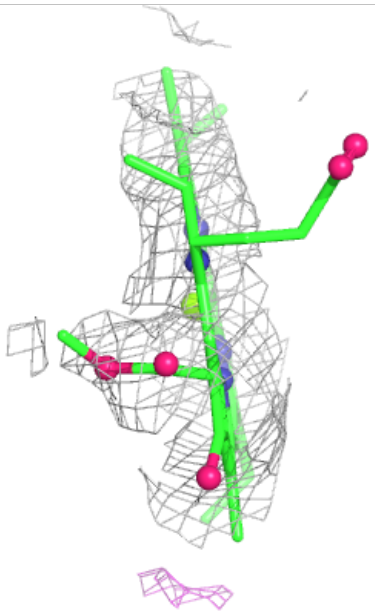


Electron density around CLA 2 1227:

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

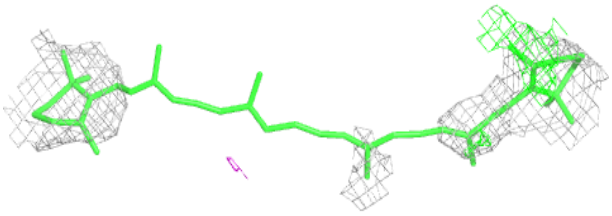


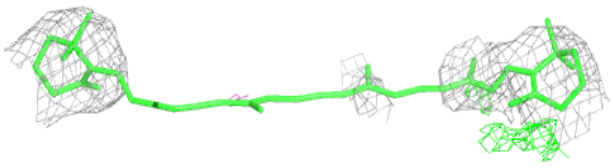


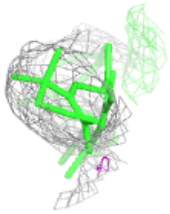


Electron density around BCR A 4001:

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

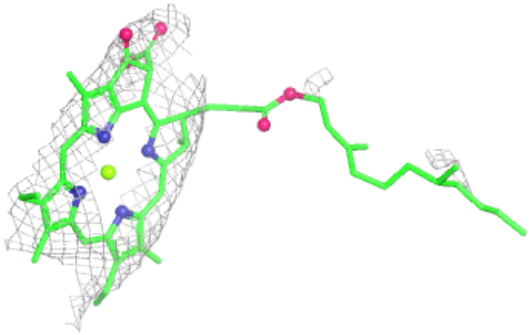


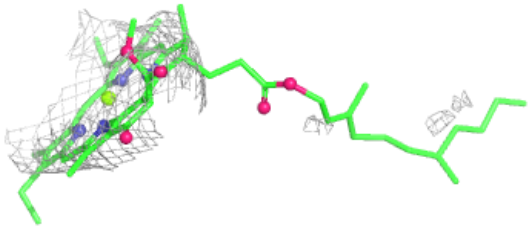


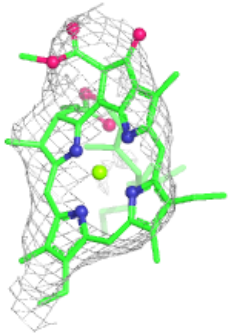


Electron density around CLA B 1230:

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

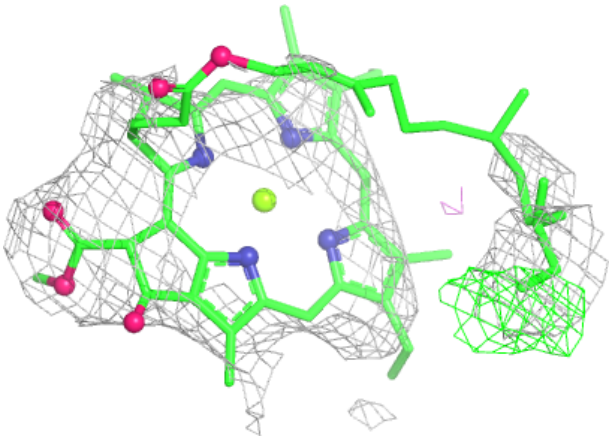


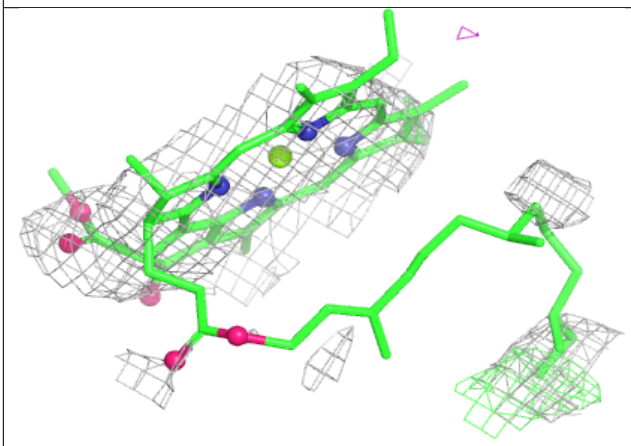


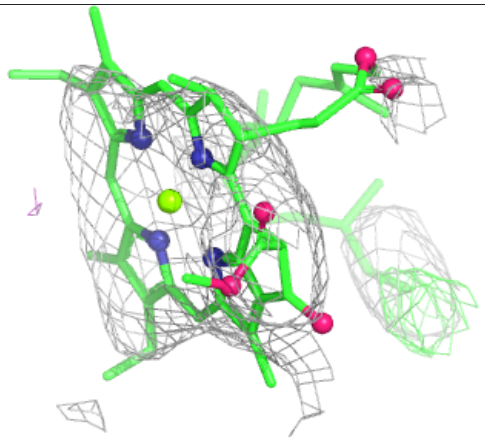


Electron density around CLA A 1118:

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

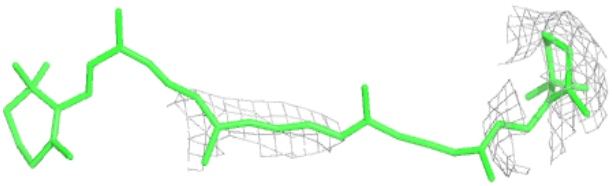


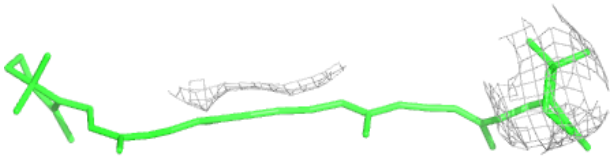


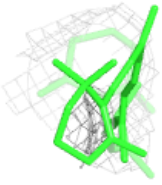


Electron density around BCR b 4006:

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

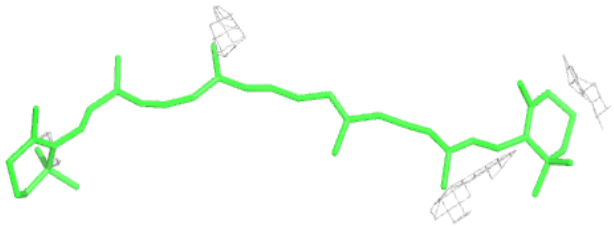


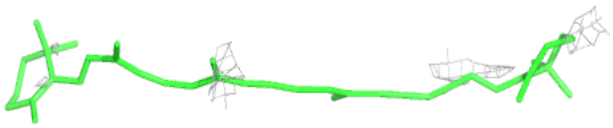


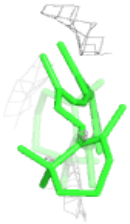


Electron density around BCR b 4010:

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

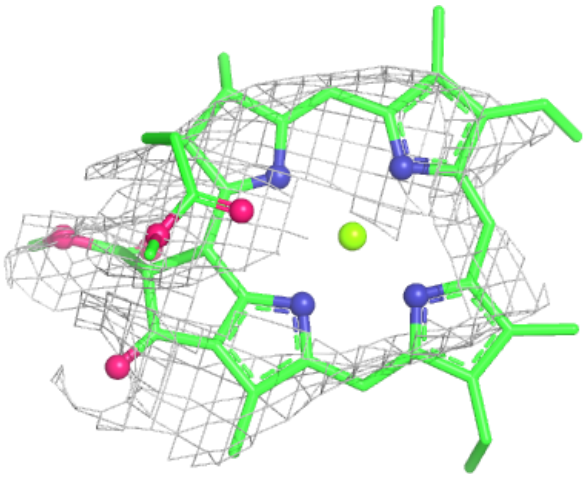


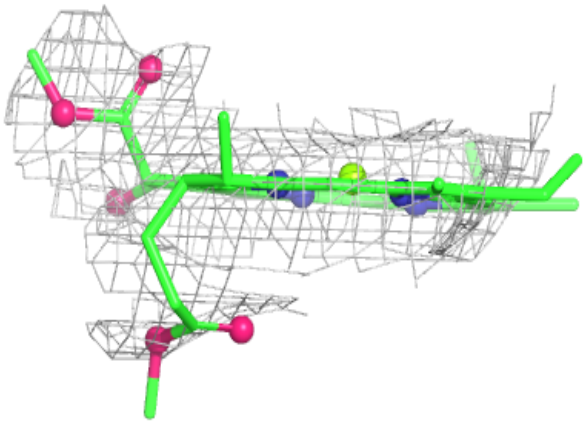


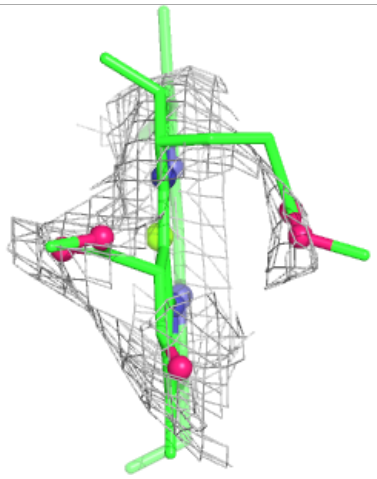


Electron density around CLA 1 1115:

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

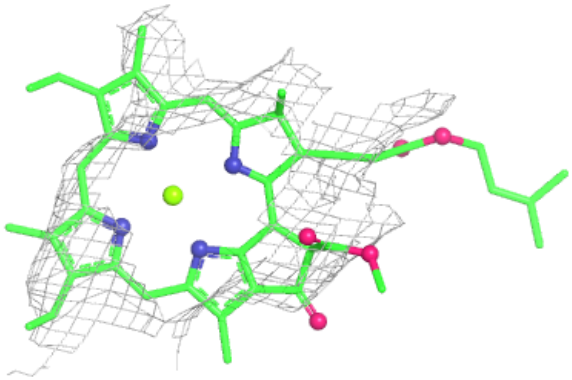


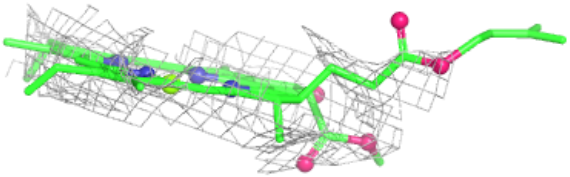


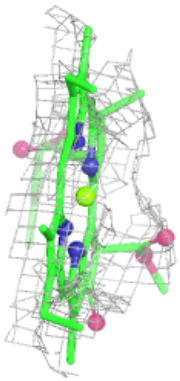


Electron density around CLA a 1139:

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

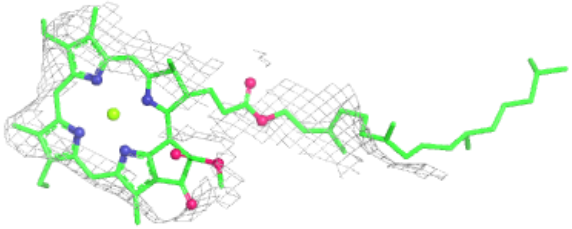


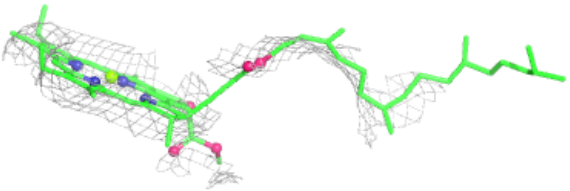


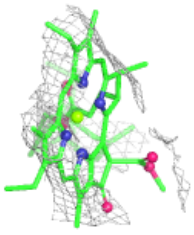


Electron density around CLA a 1107:

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

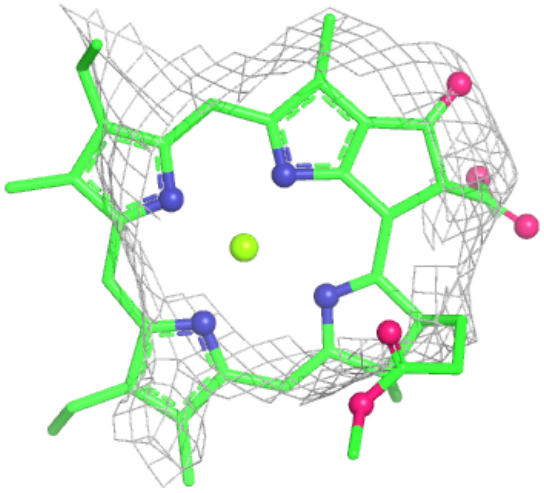


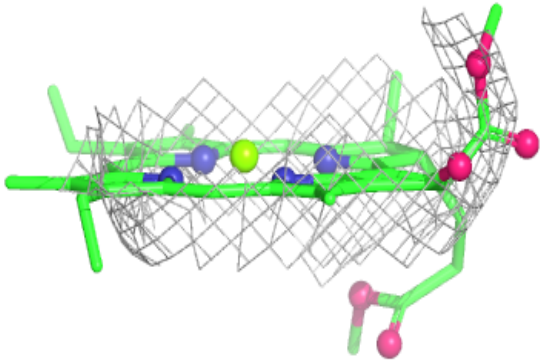


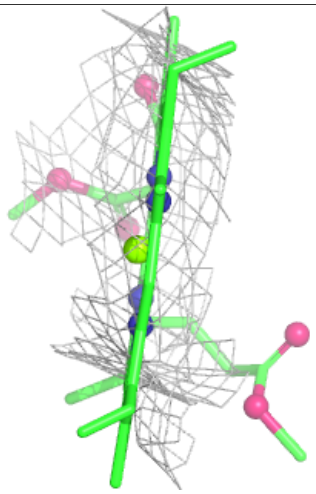


Electron density around CLA 1 1120:

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

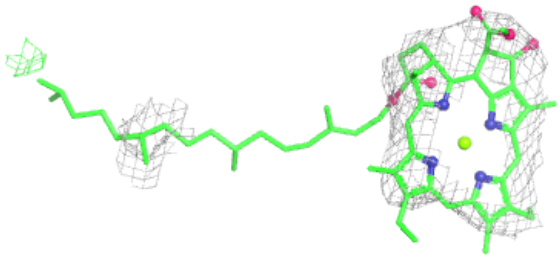


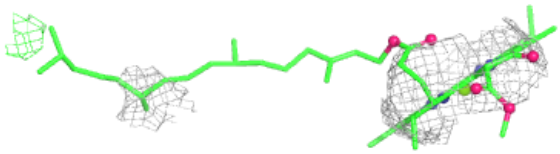


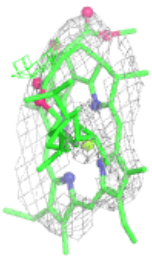


Electron density around CLA l 1501:

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

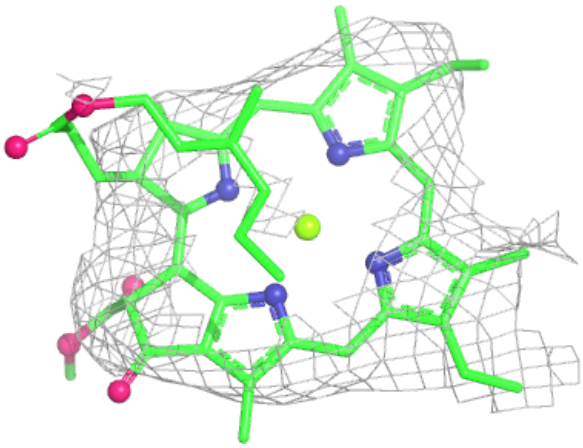


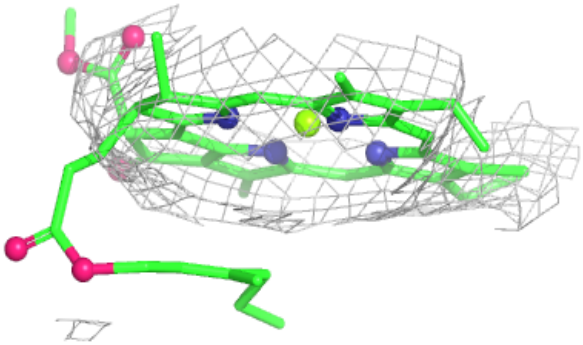




Electron density around CLA 1 1801:

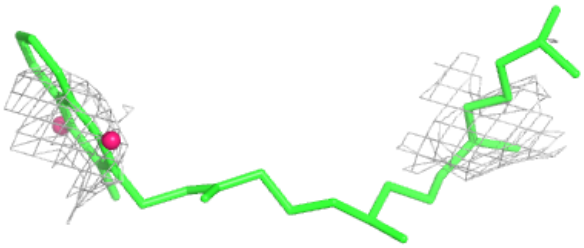
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

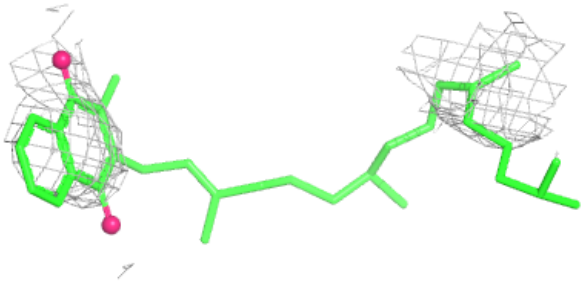




Electron density around PQN b 2002:

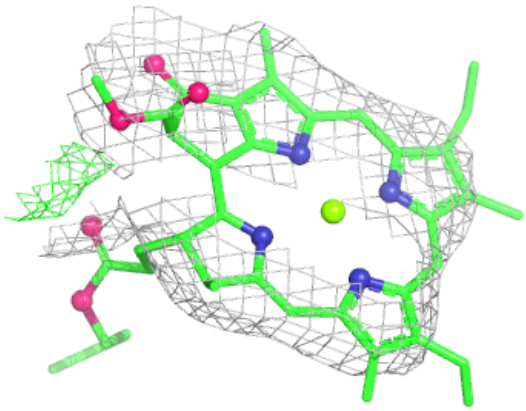
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

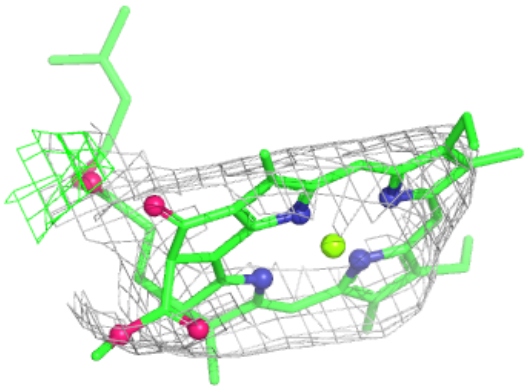


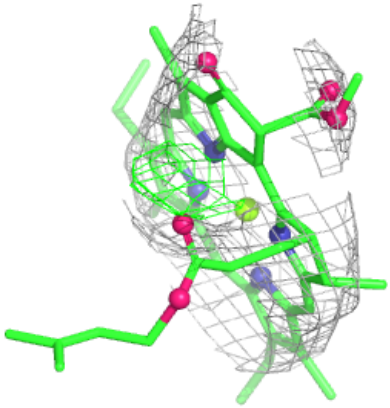


Electron density around CLA B 1228:

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

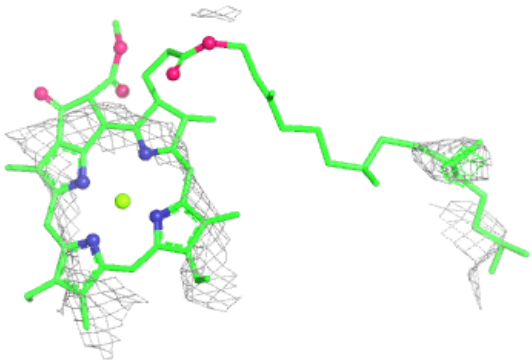


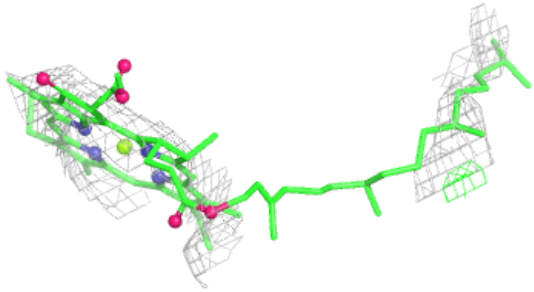


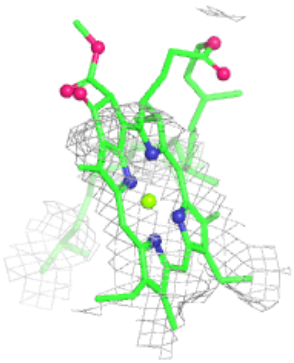


Electron density around CLA b 1013:

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

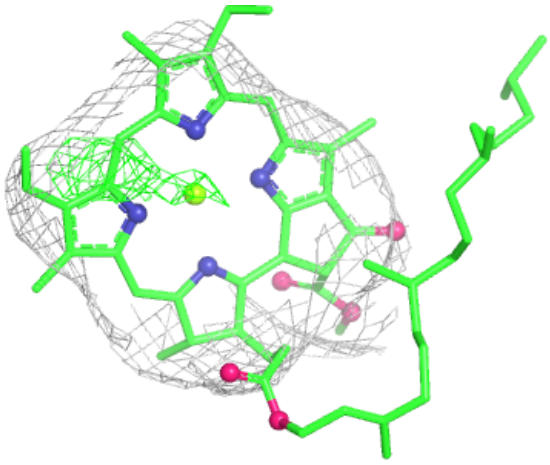


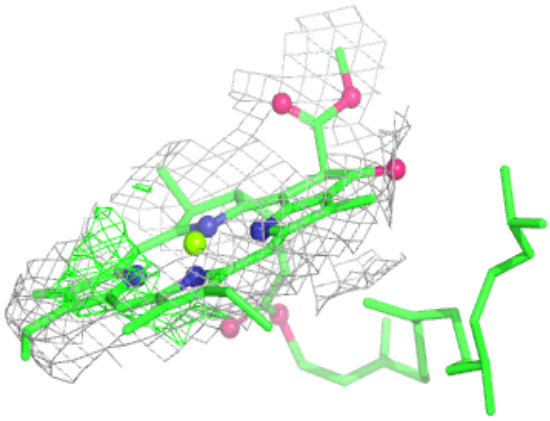


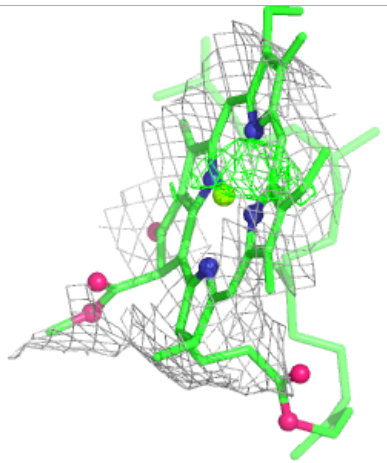


Electron density around CLA B 1229:

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

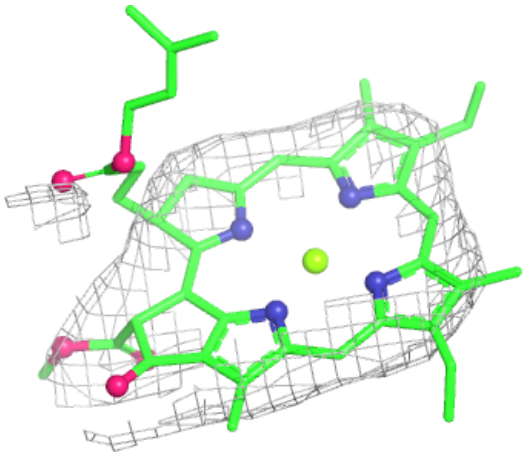


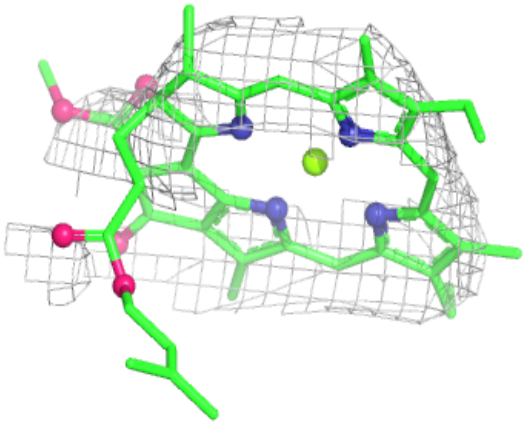


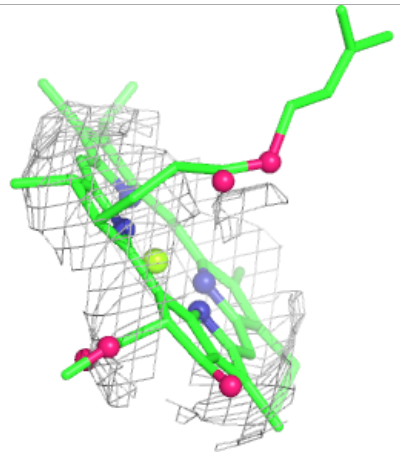


Electron density around CLA 2 1228:

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

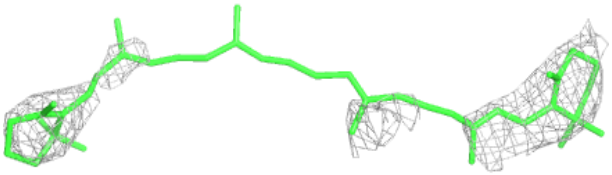


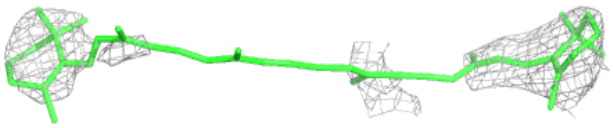


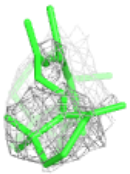


Electron density around BCR B 4010:

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

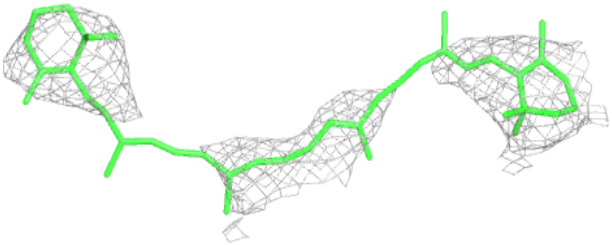


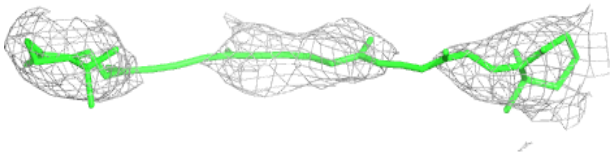


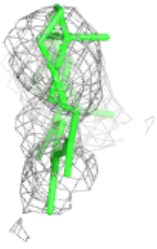


Electron density around BCR B 4011:

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

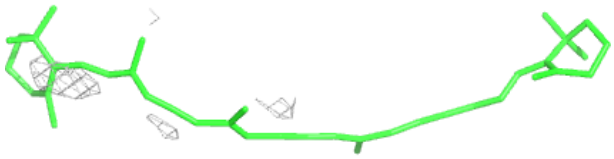


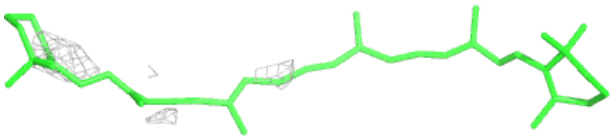


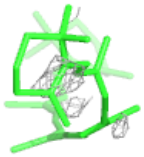


Electron density around BCR 2 4014:

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

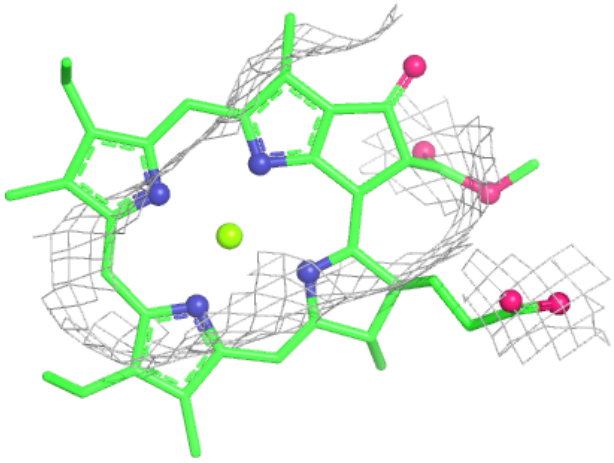


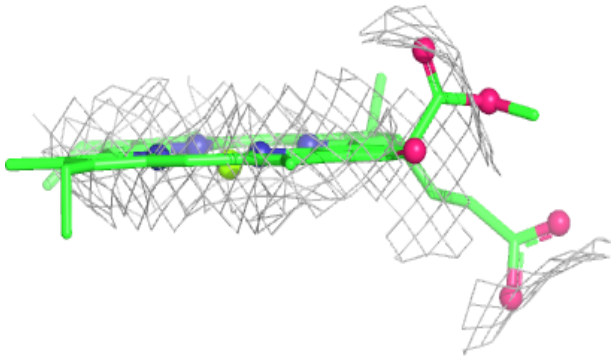


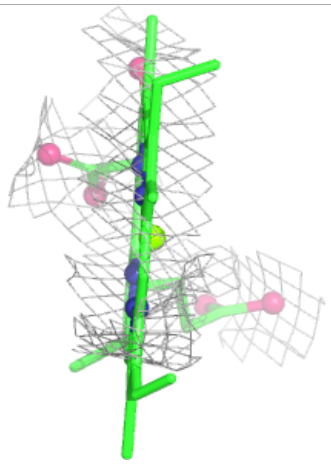


Electron density around CLA a 1113:

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

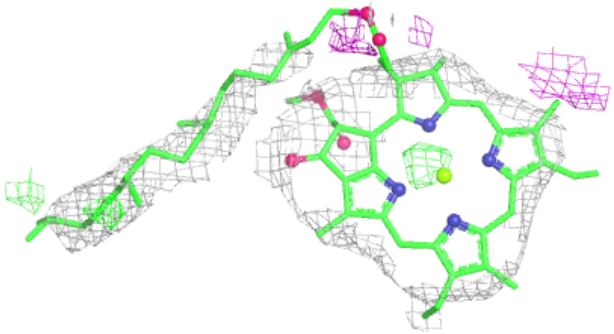


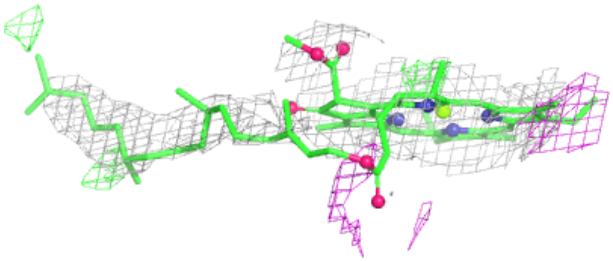




Electron density around CLA L 1503:

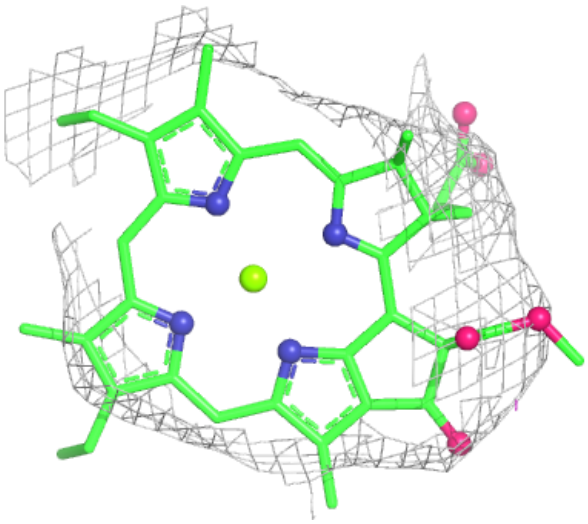
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

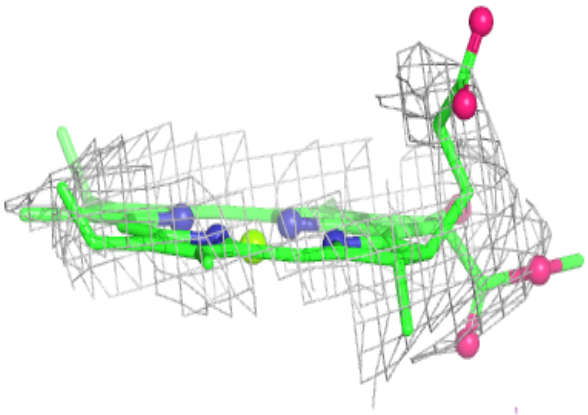


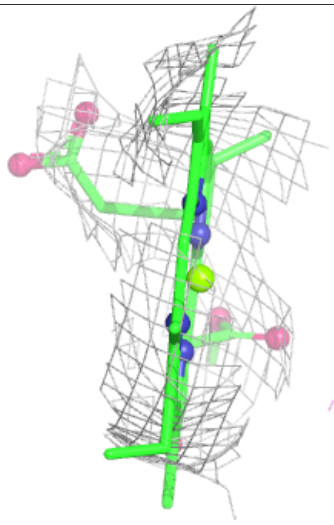


Electron density around CLA 2 1232:

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

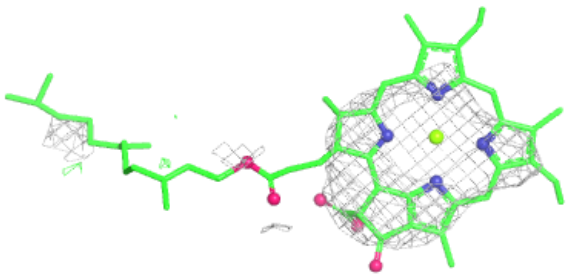


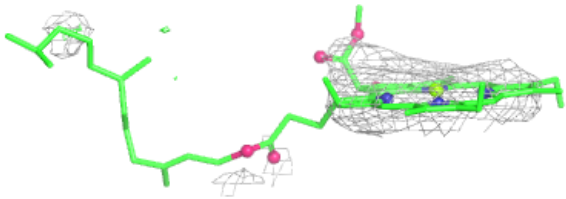


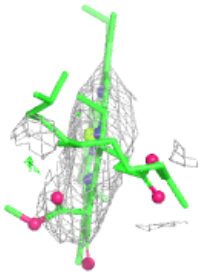


Electron density around CLA 2 1234:

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

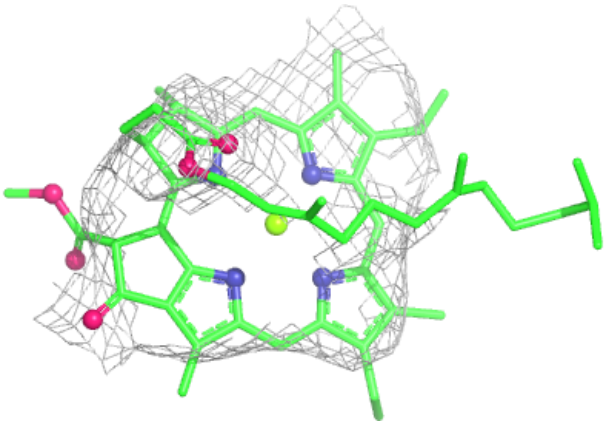


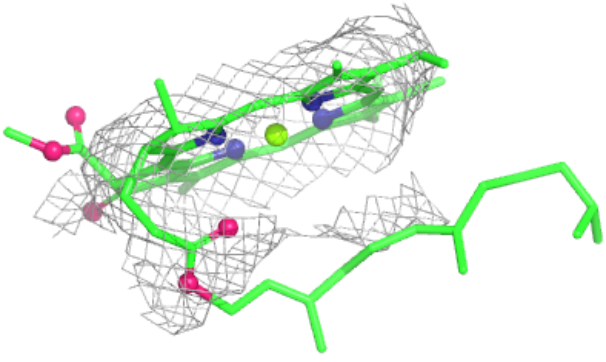


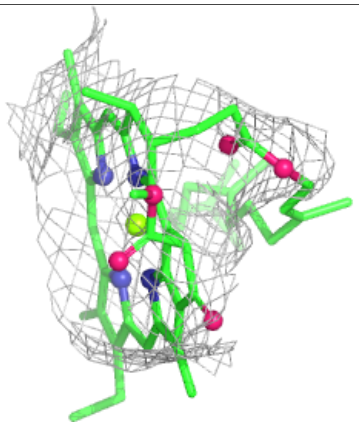


Electron density around CLA 2 1235:

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

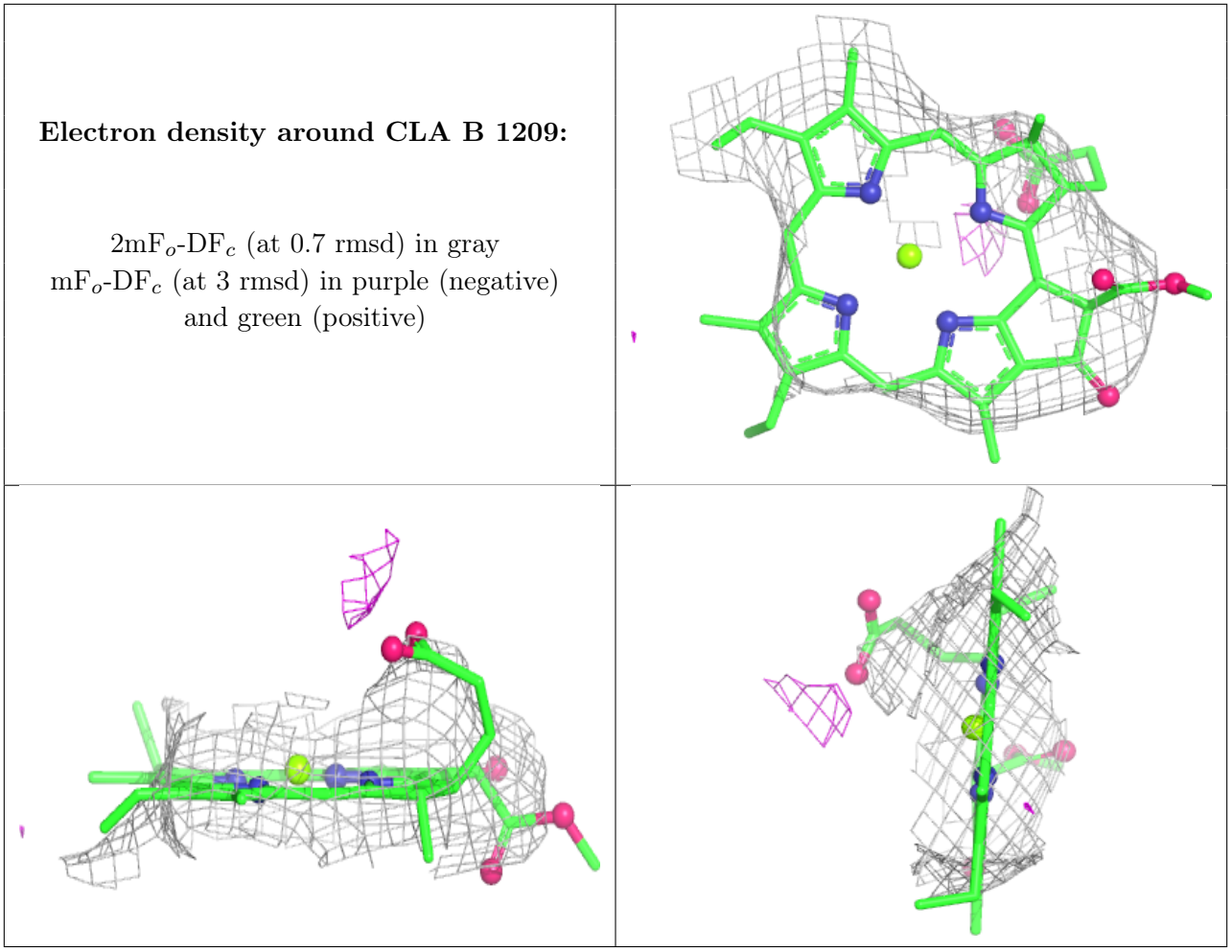






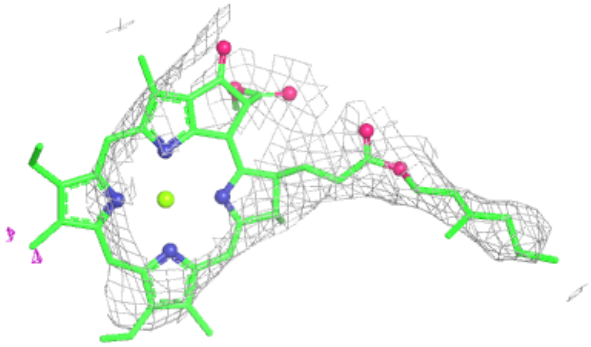
Electron density around CLA B 1209:

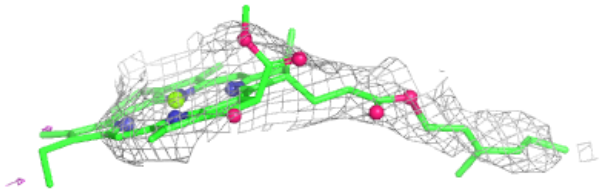
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

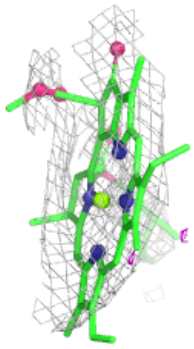


Electron density around CLA a 1125:

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

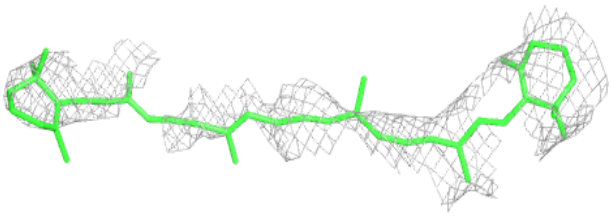


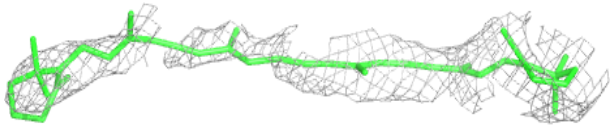


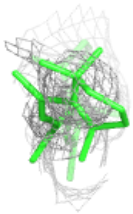


Electron density around BCR a 4008:

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

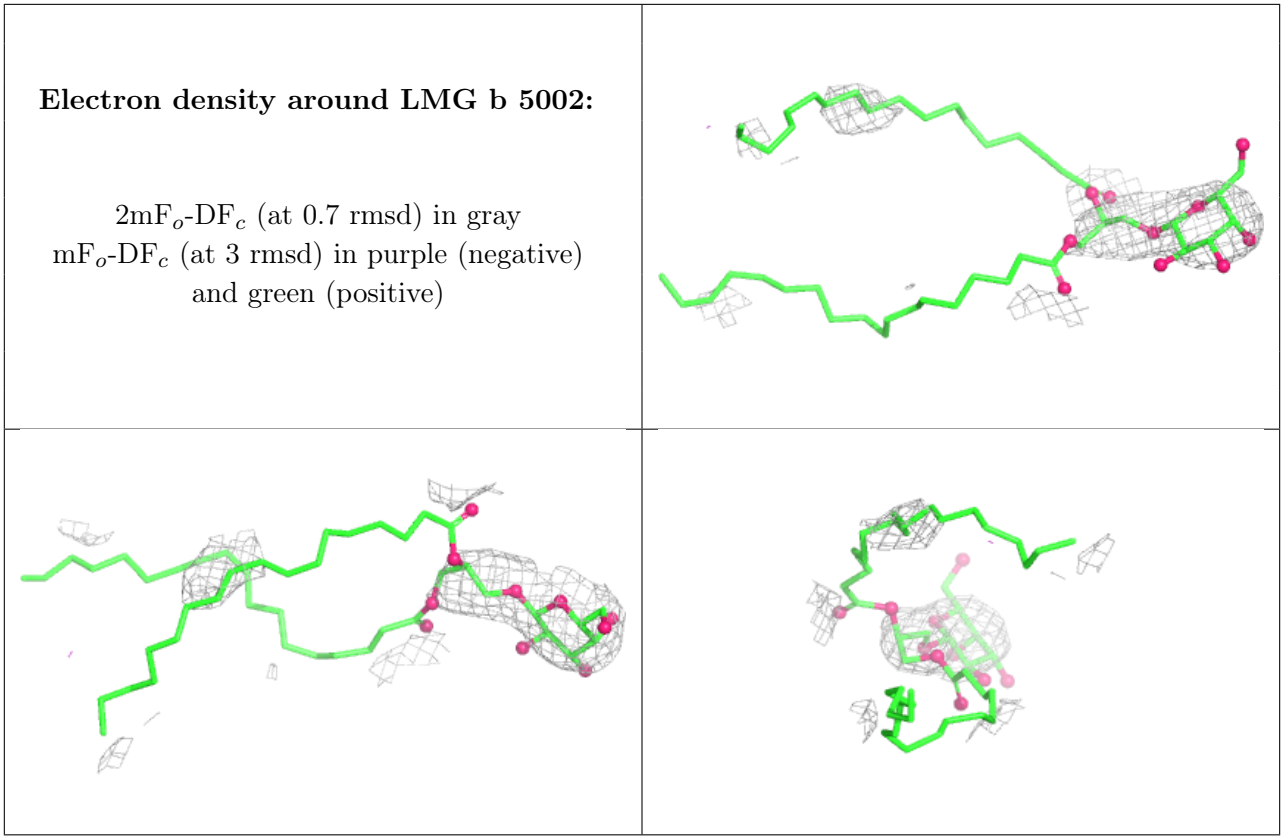






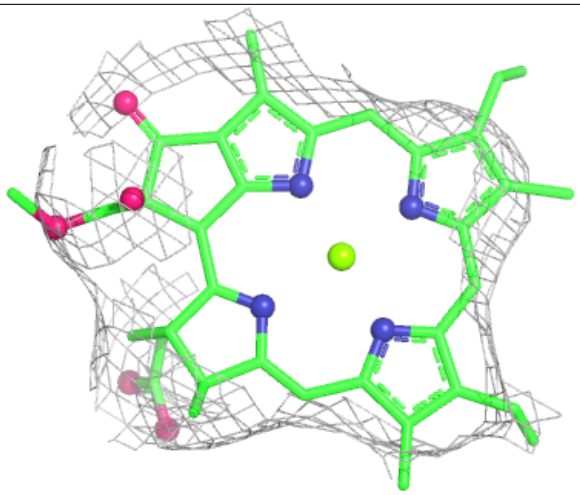
Electron density around LMG b 5002:

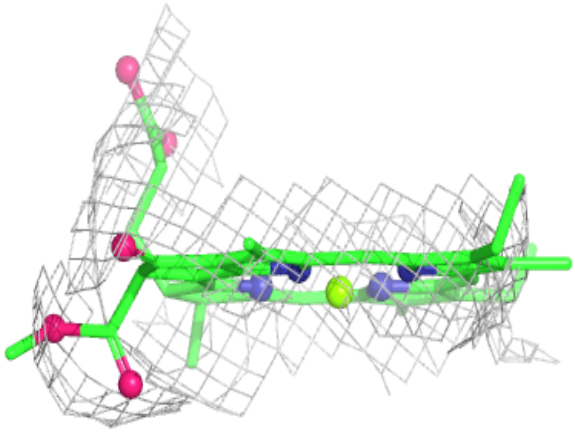
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

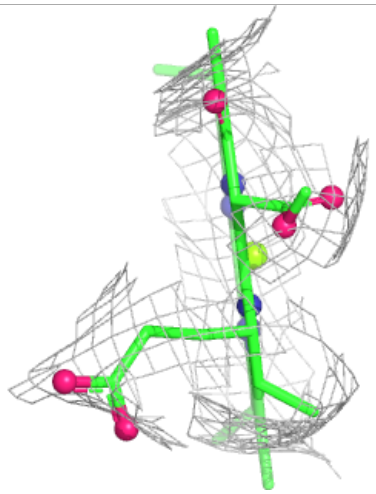


Electron density around CLA B 1232:

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

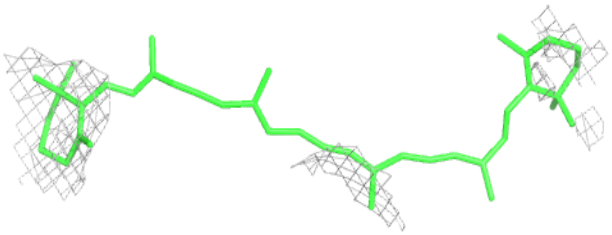


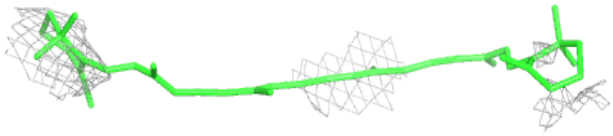


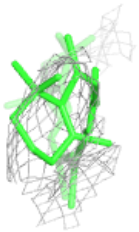


Electron density around BCR b 4004:

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

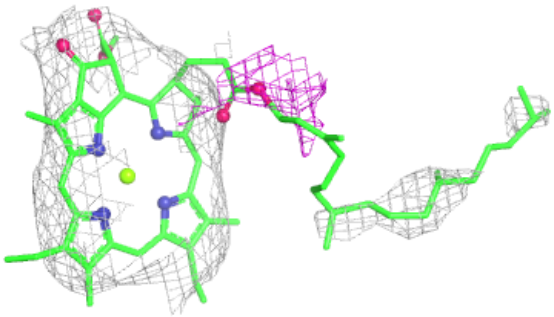


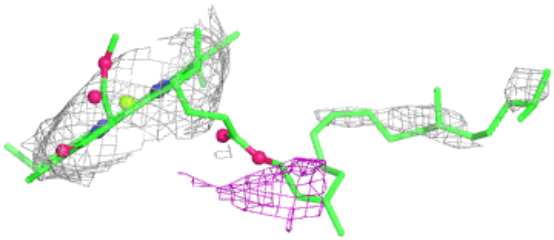


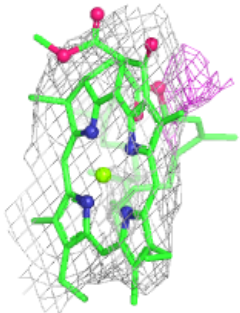


Electron density around CLA A 1106:

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

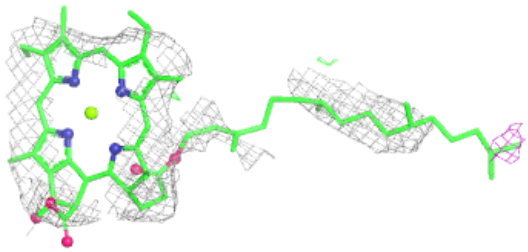


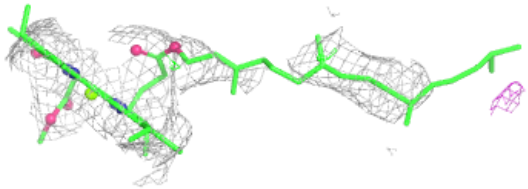


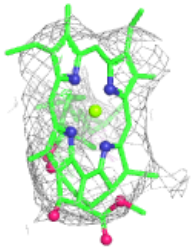


Electron density around CLA L 1501:

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

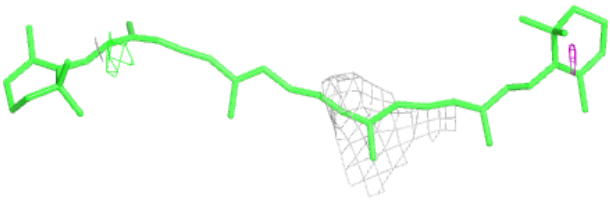


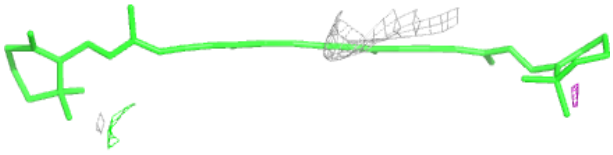


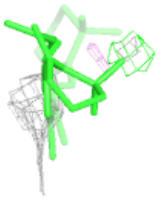


Electron density around BCR b 4009:

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

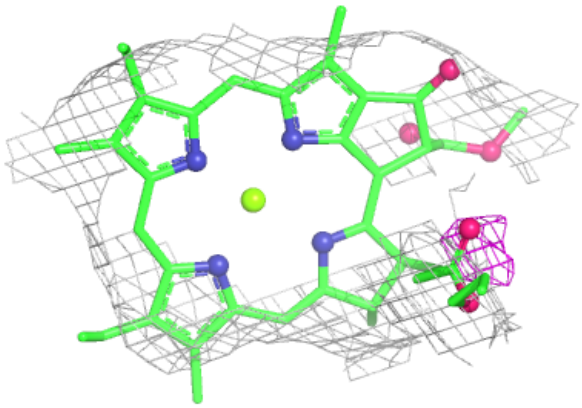


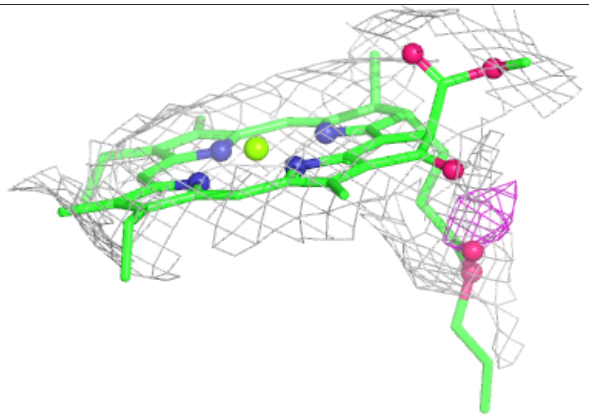


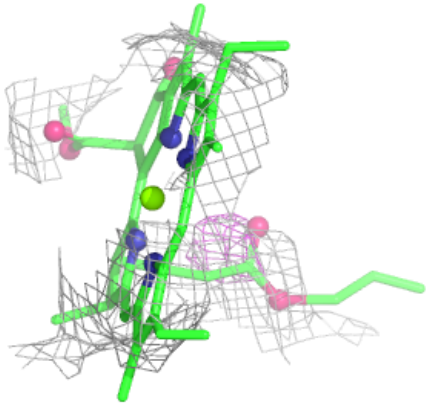


Electron density around CLA A 1105:

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

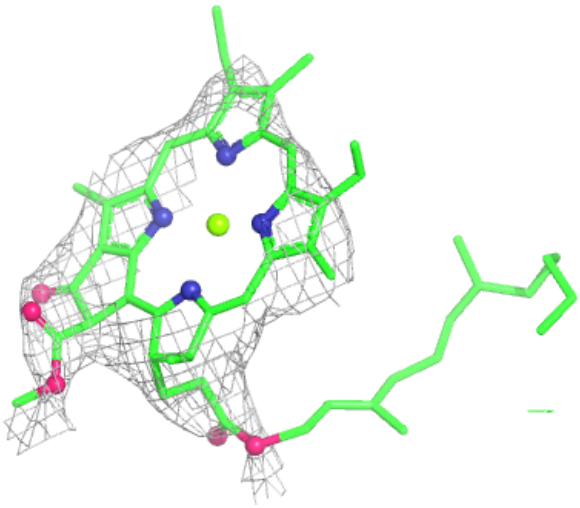


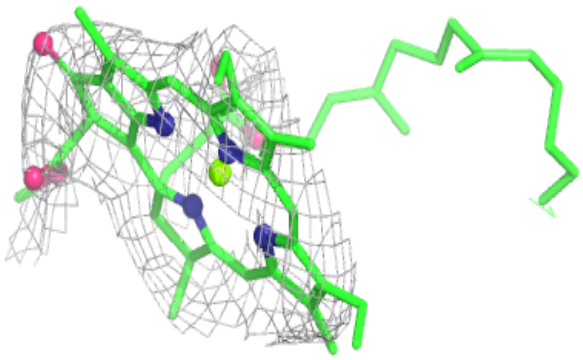


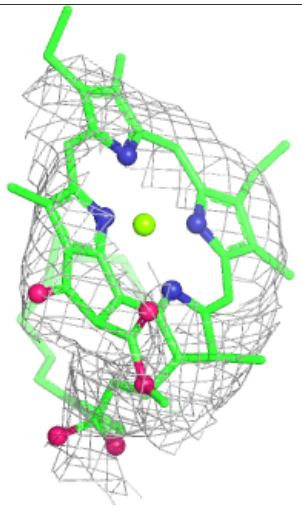


Electron density around CLA 1 1122:

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

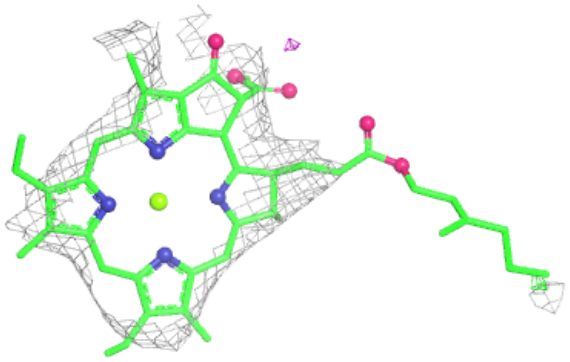


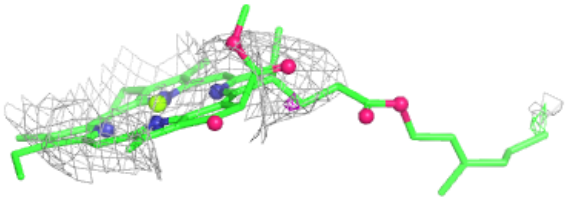




Electron density around CLA 1 1125:

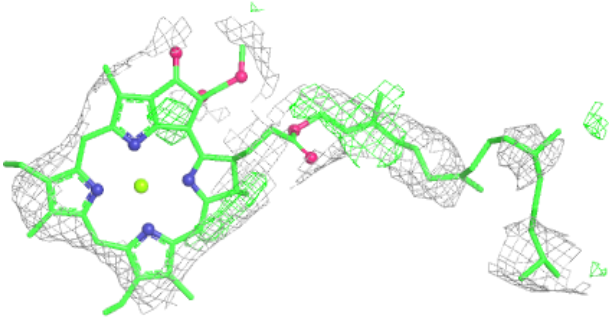
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

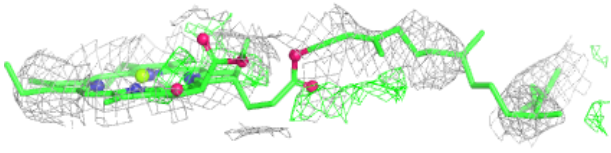


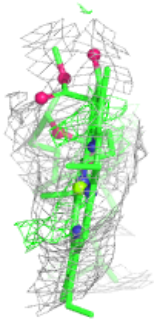


Electron density around CLA 1 1131:

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

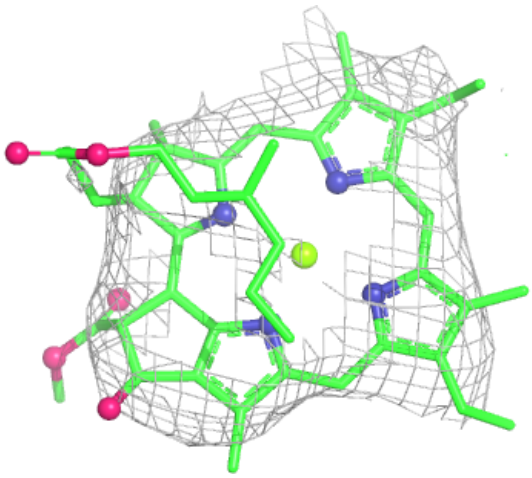


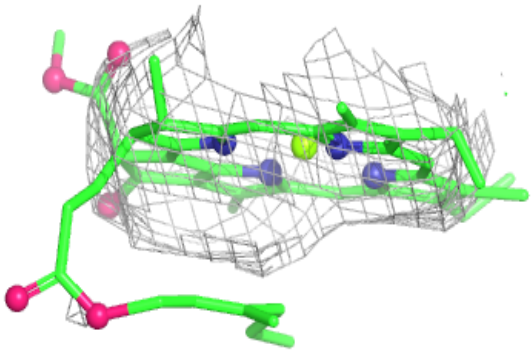


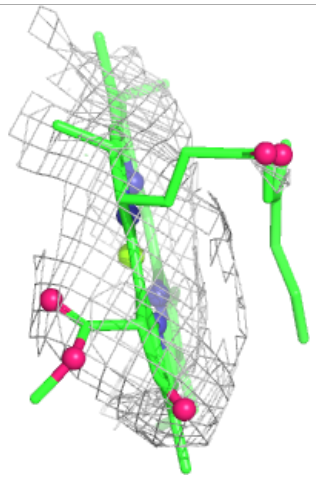


Electron density around CLA a 1801:

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

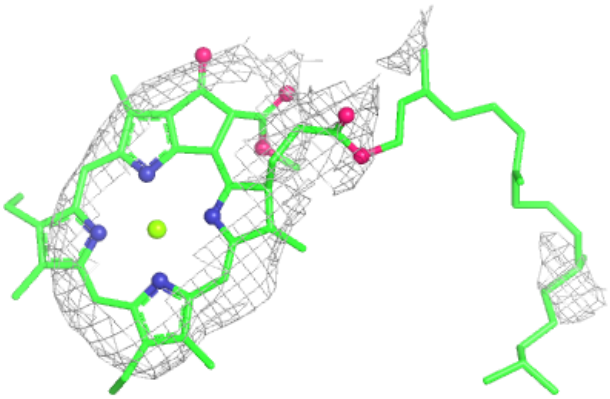


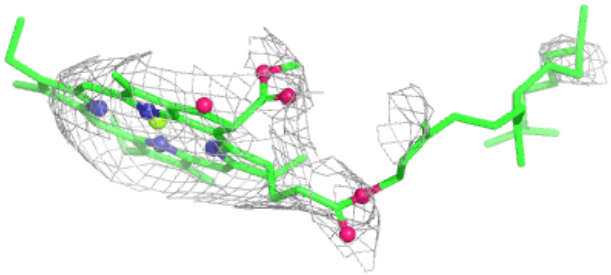


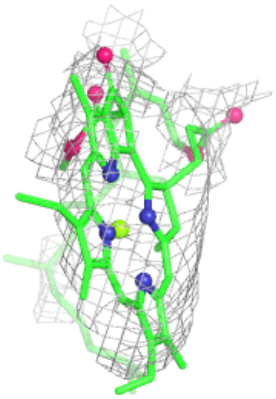


Electron density around CLA a 1101:

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

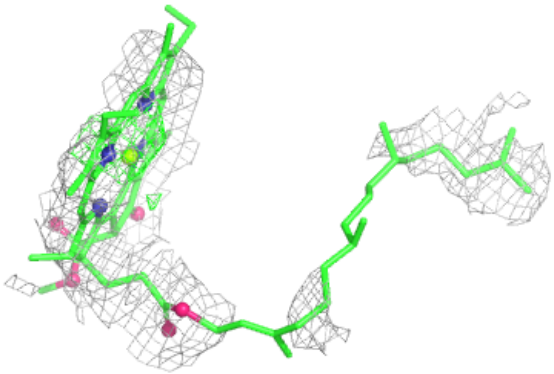


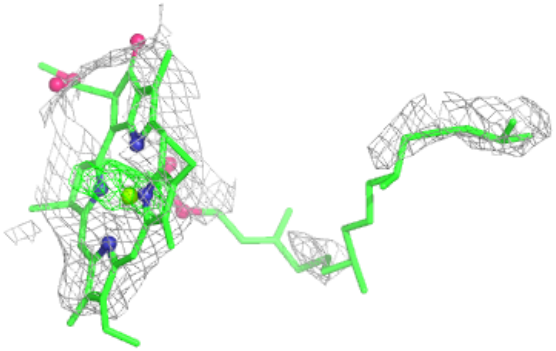


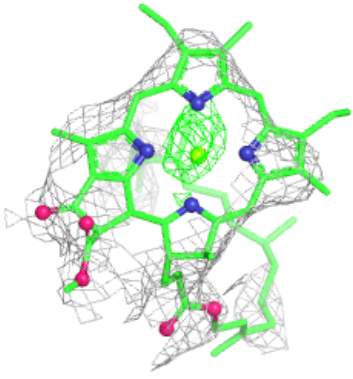


Electron density around CLA B 1216:

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

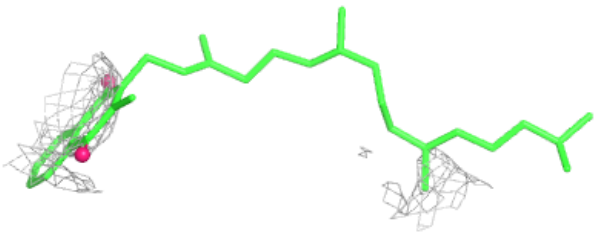


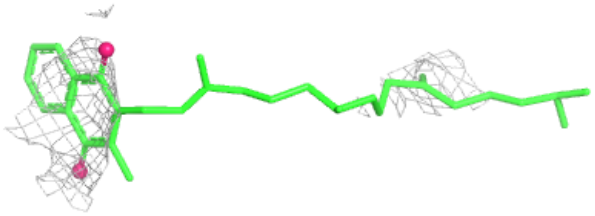


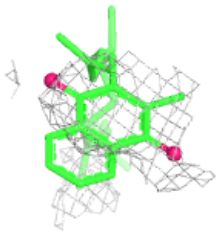


Electron density around PQN 1 2001:

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

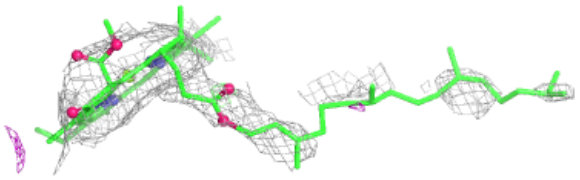


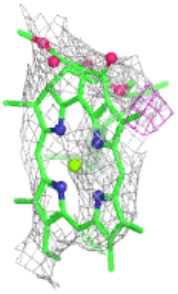




Electron density around CLA 1 1132:

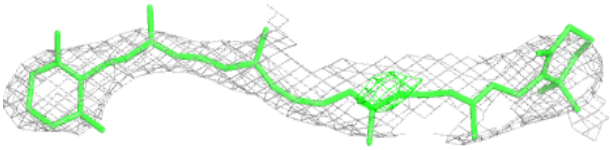
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

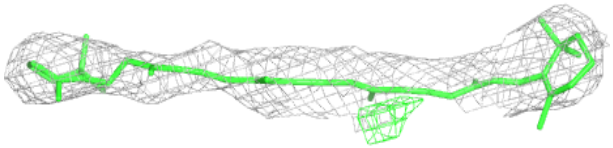


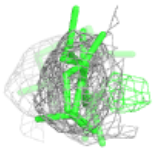


Electron density around BCR A 4002:

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

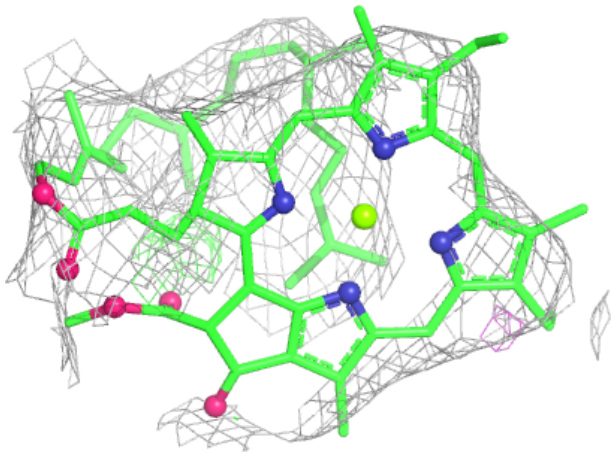


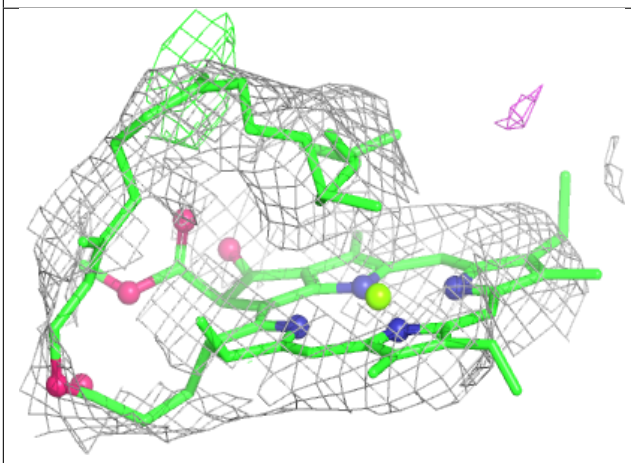


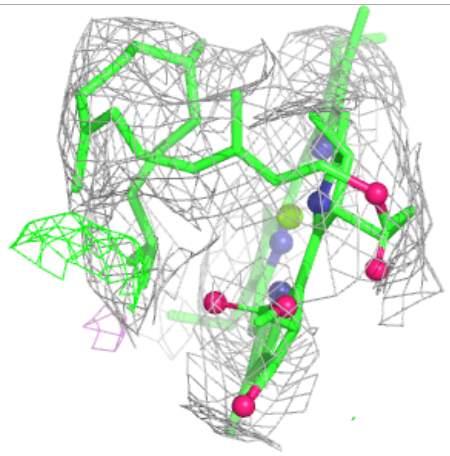


Electron density around CLA 2 1203:

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

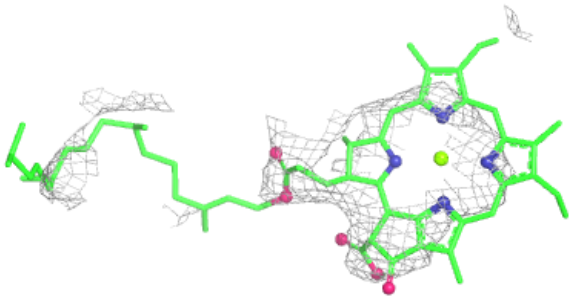


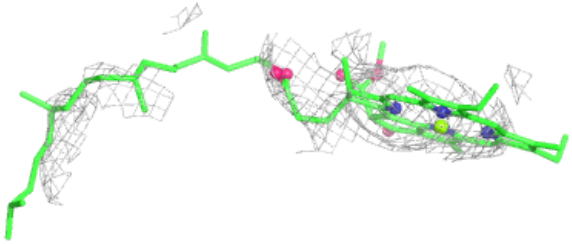


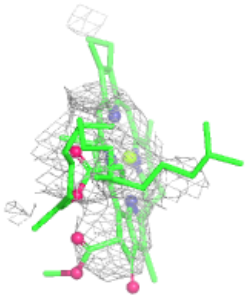


Electron density around CLA a 1103:

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

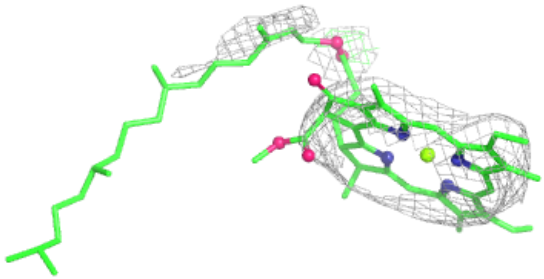


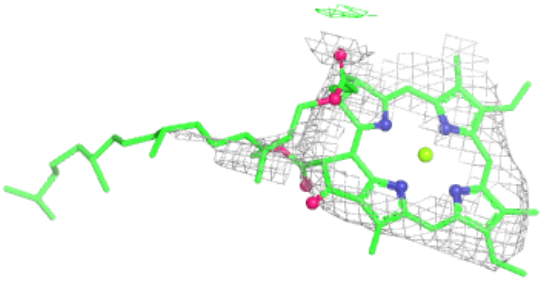


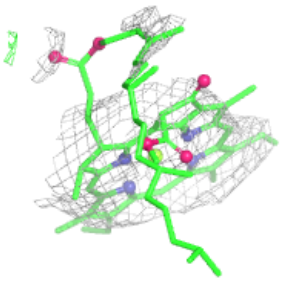


Electron density around CLA 2 1213:

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

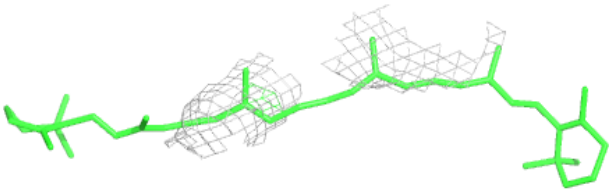


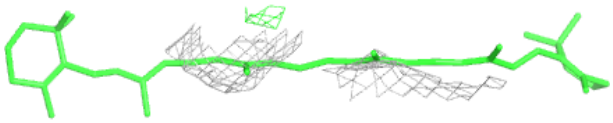


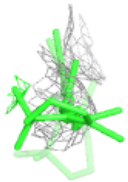


Electron density around BCR B 4009:

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

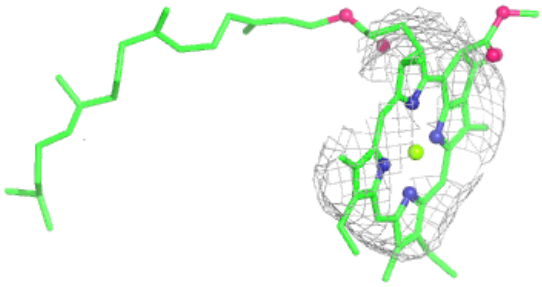


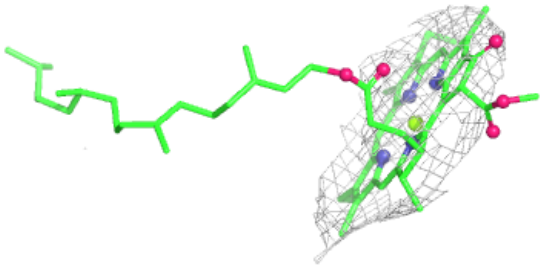


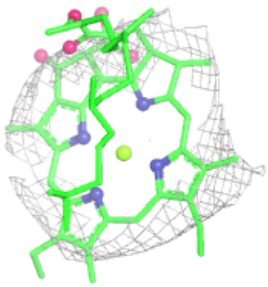


Electron density around CLA a 1140:

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

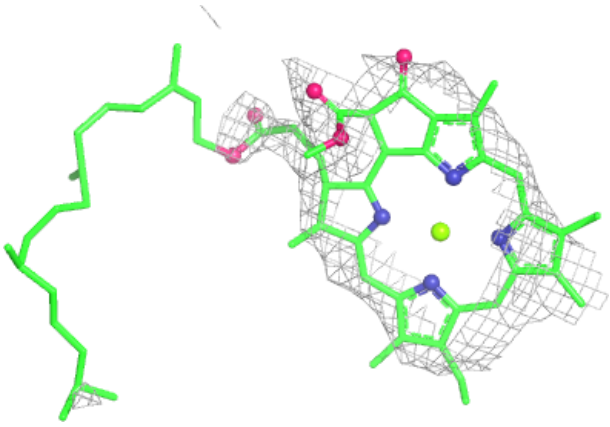


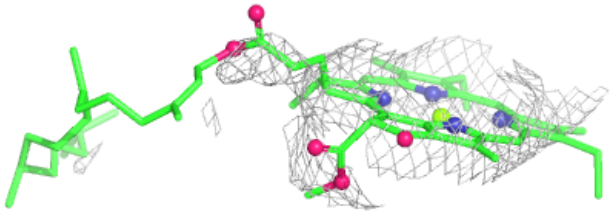




Electron density around CLA 1 1101:

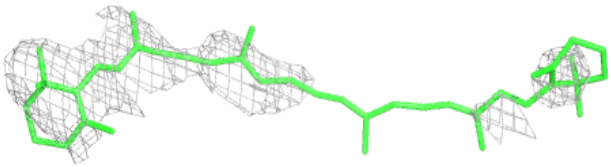
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

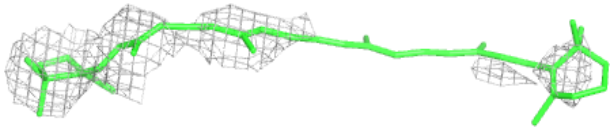


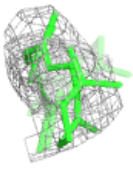


Electron density around BCR 8 4022:

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

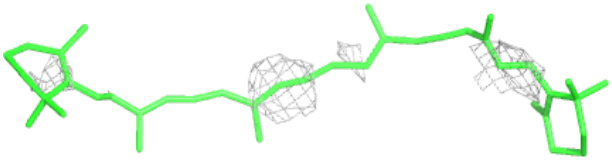


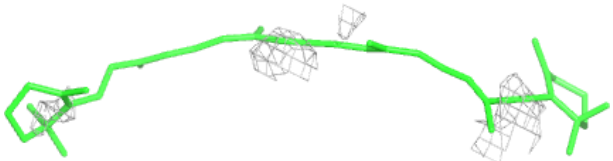


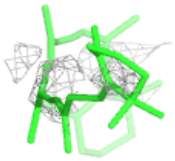


Electron density around BCR B 4014:

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

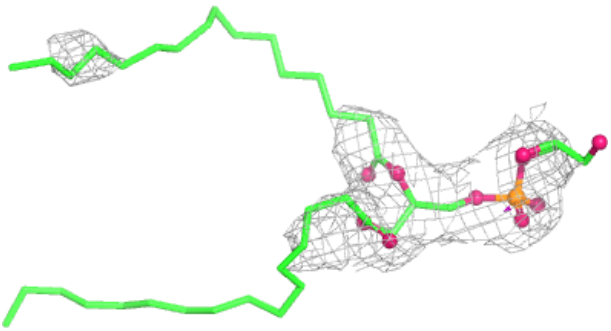


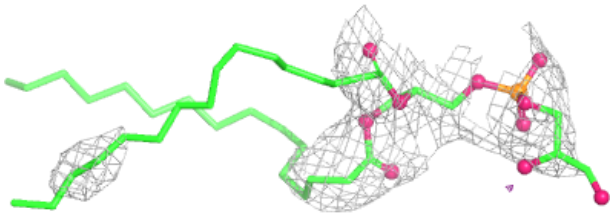


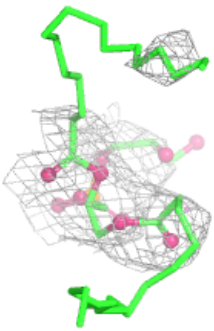


Electron density around LHG A 5001:

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

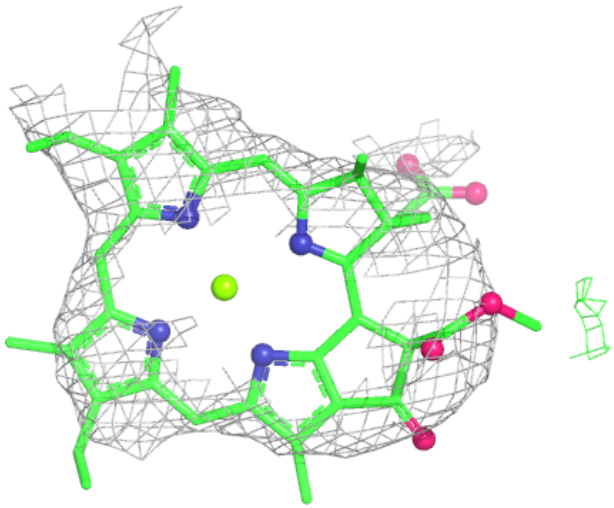


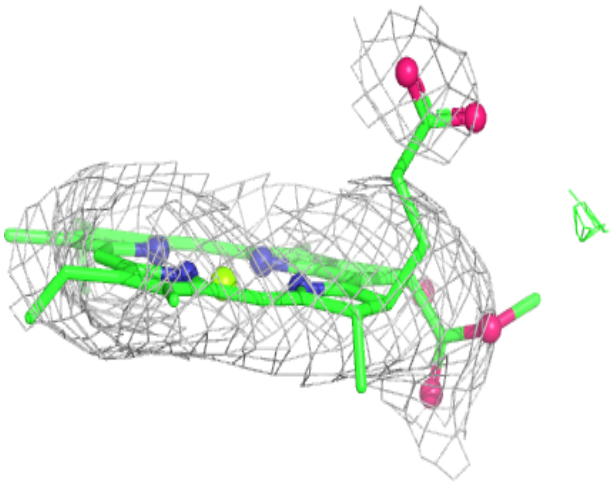


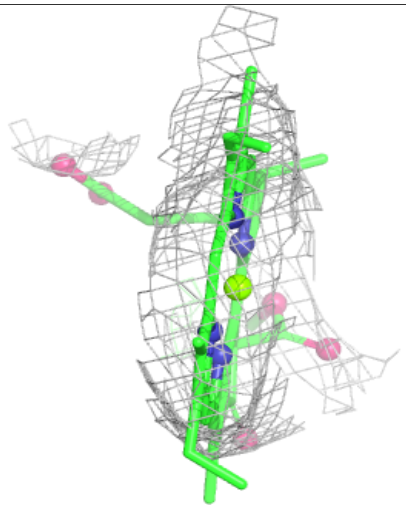


Electron density around CLA B 1208:

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

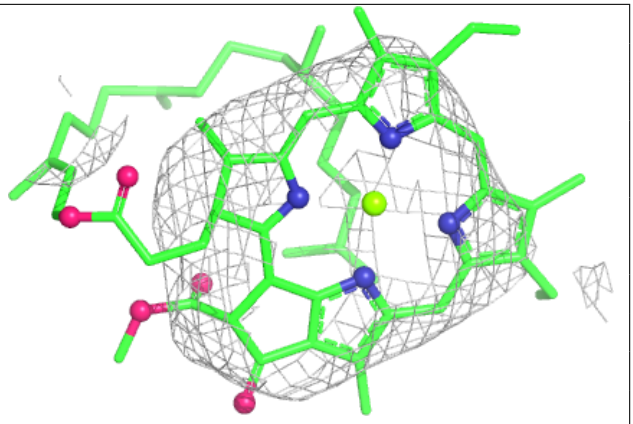


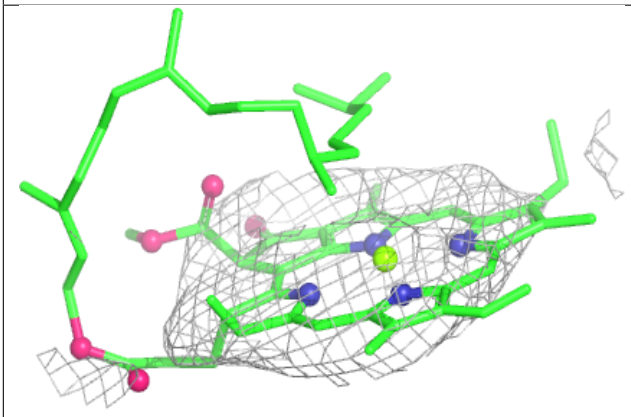


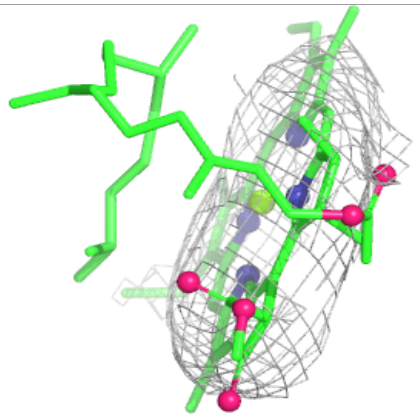


Electron density around CLA 1 1104:

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

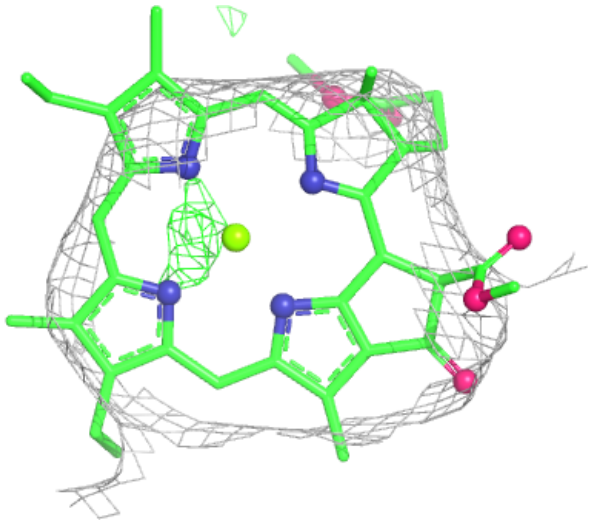


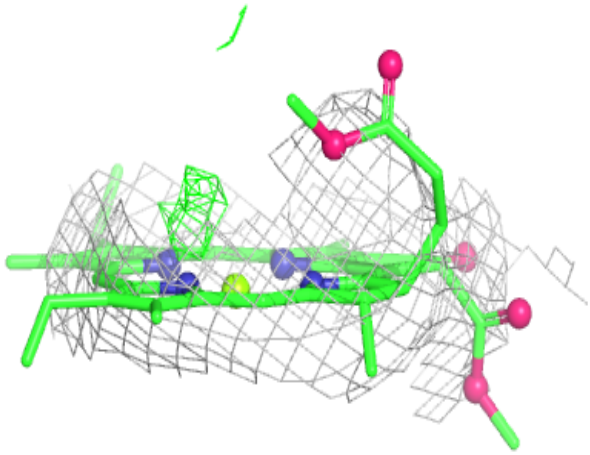


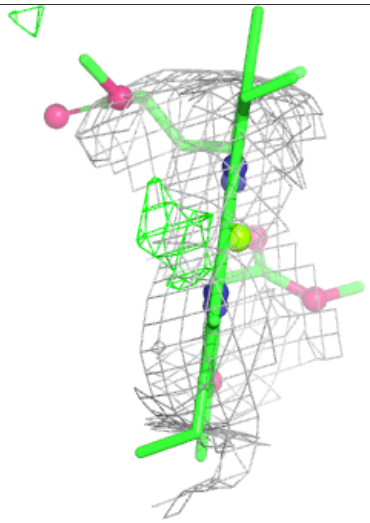


Electron density around CLA a 1120:

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

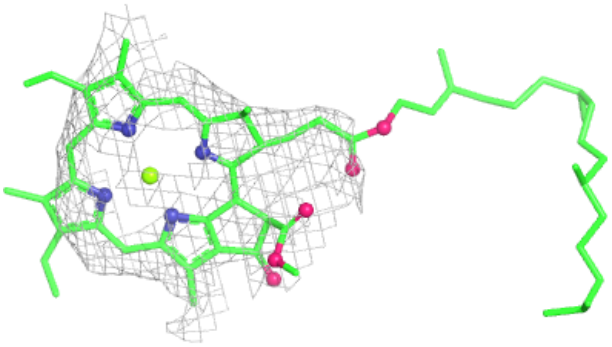


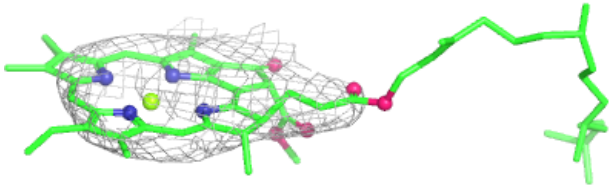


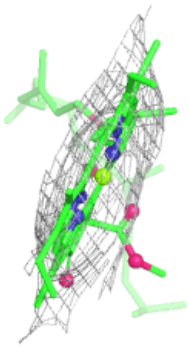


Electron density around CLA b 1223:

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

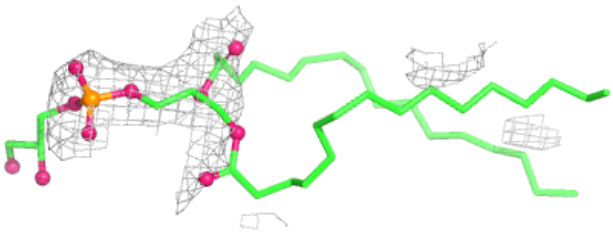


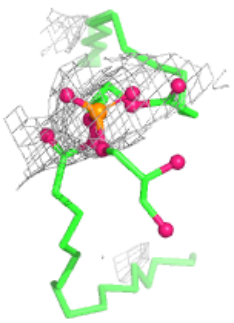




Electron density around LHG 1 5001:

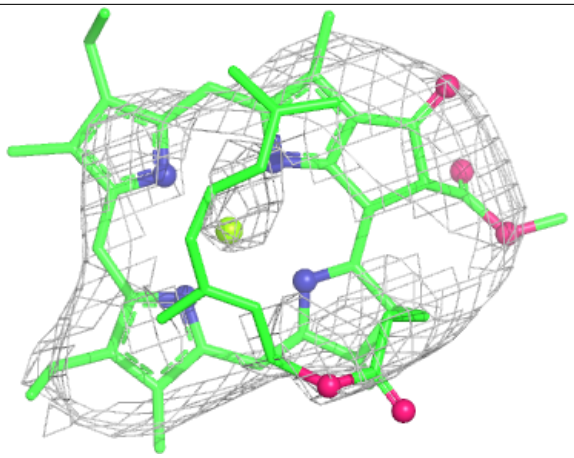
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

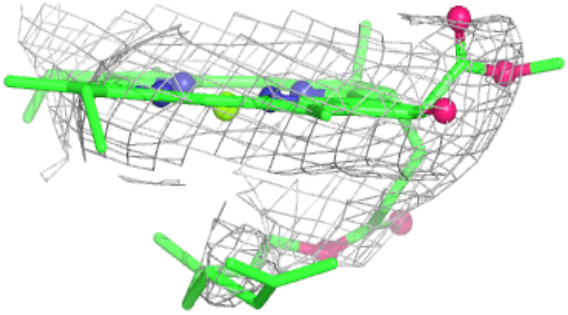


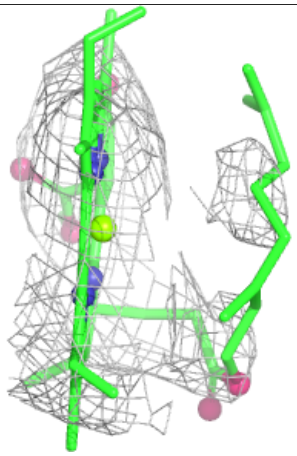


Electron density around CLA b 1224:

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

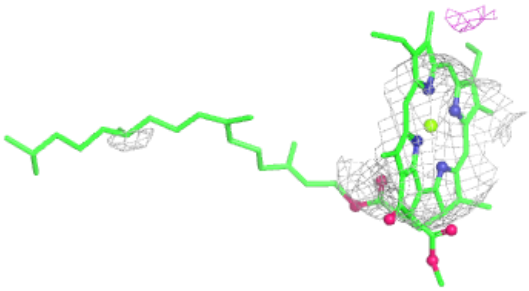


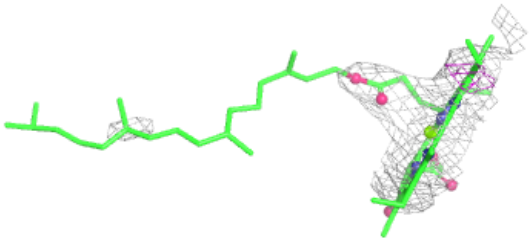


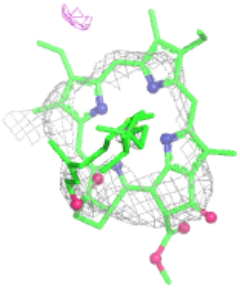


Electron density around CLA b 1225:

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

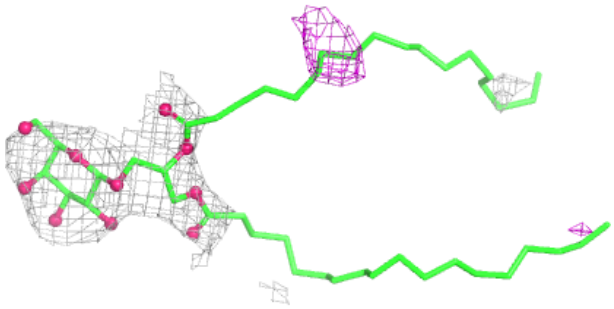


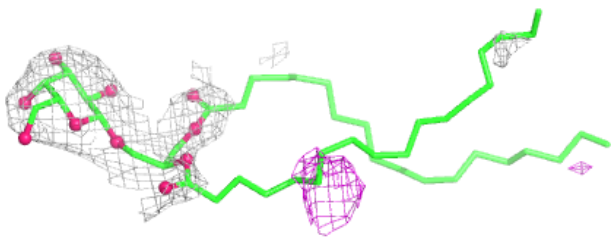


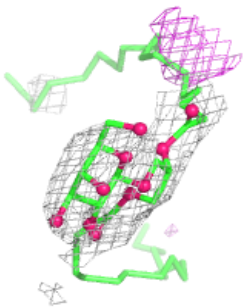


Electron density around LMG B 5002:

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

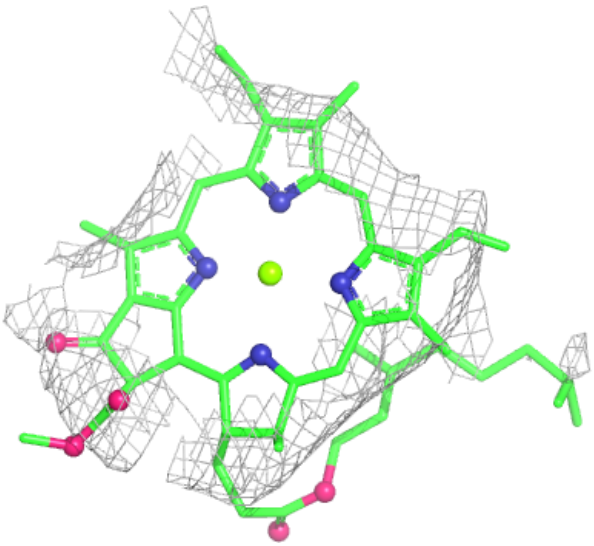


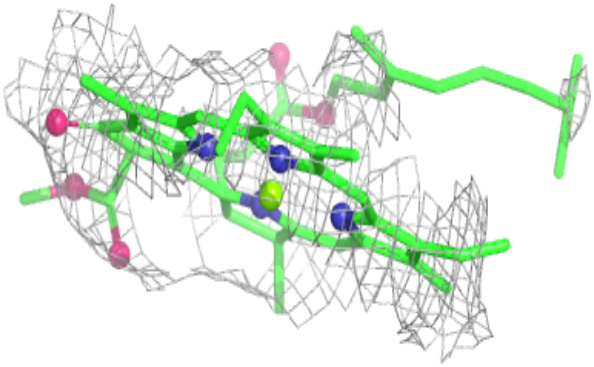


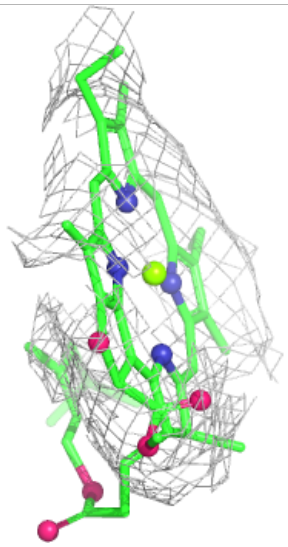


Electron density around CLA B 1219:

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

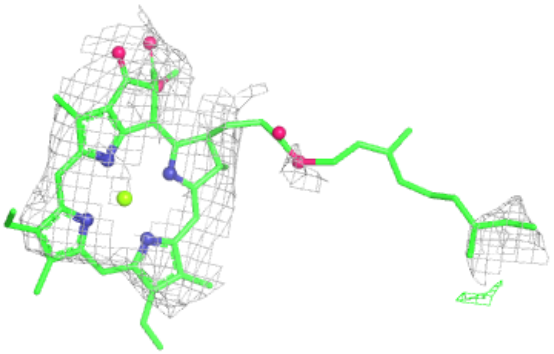


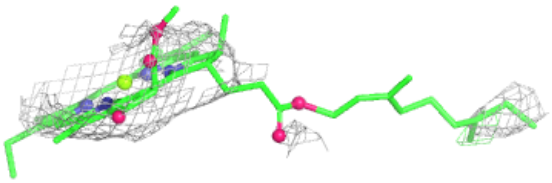




Electron density around CLA B 1222:

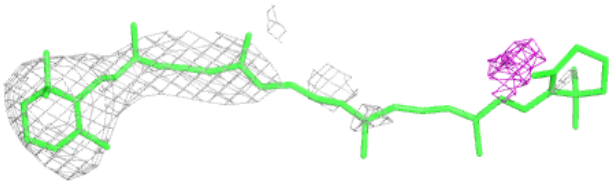
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

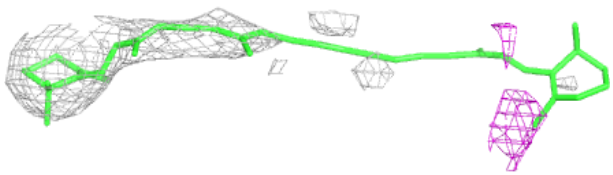


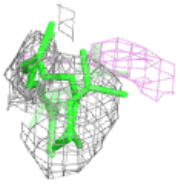


Electron density around BCR l 4022:

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

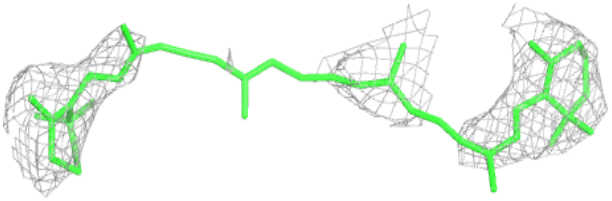


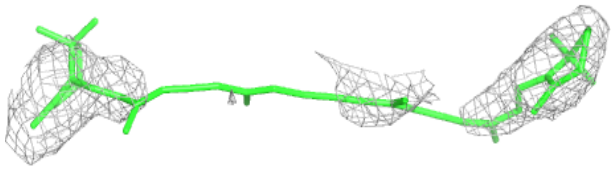


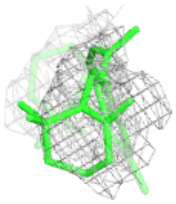


Electron density around BCR B 4006:

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

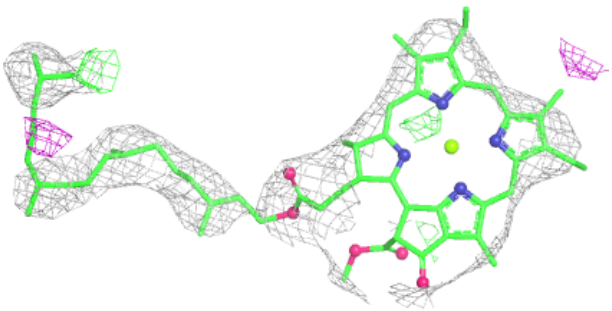


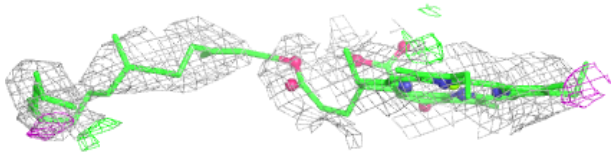




Electron density around CLA A 1131:

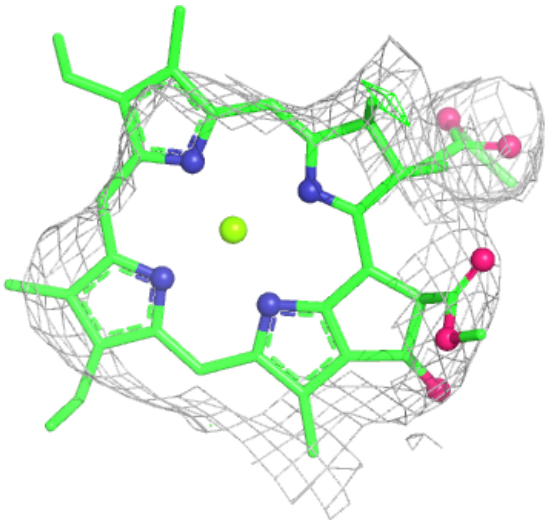
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

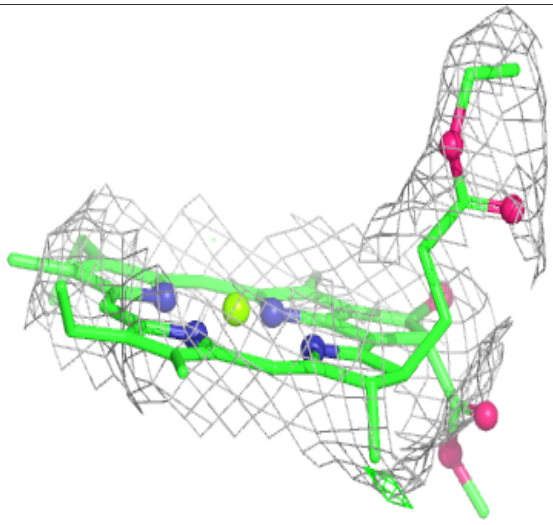


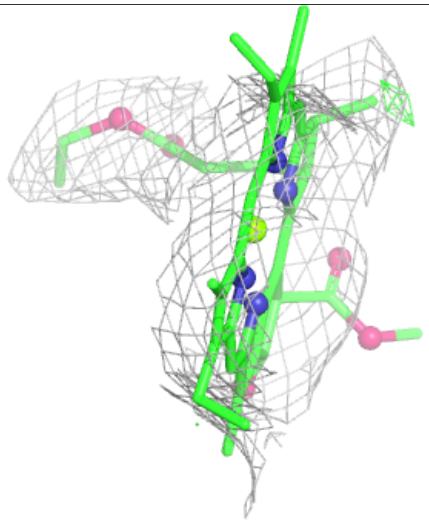


Electron density around CLA 2 1236:

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

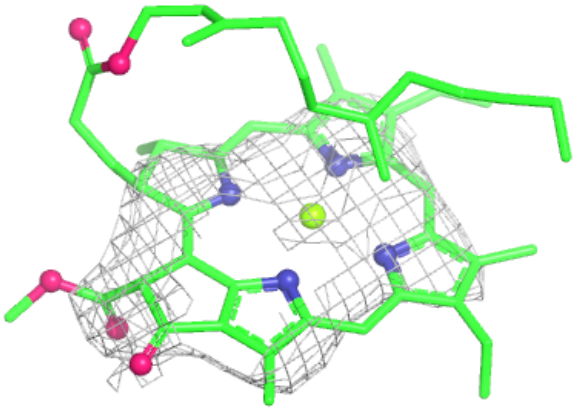


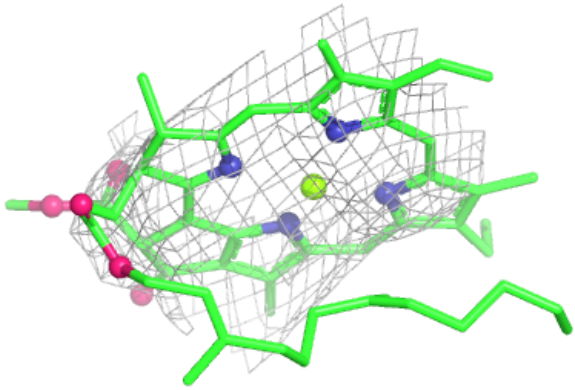


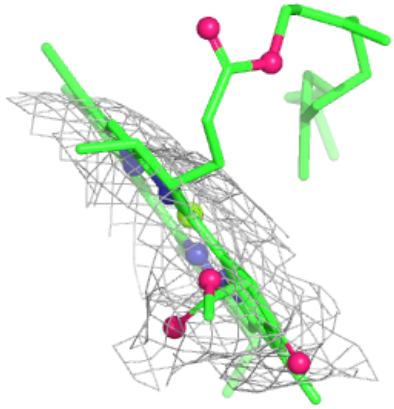


Electron density around CLA b 1214:

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

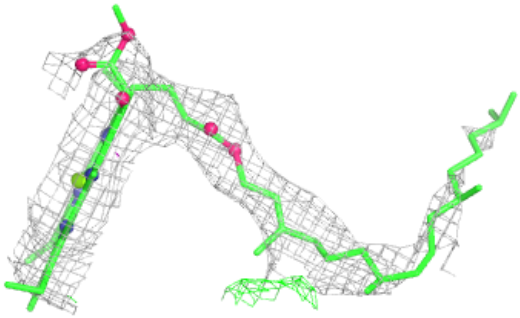


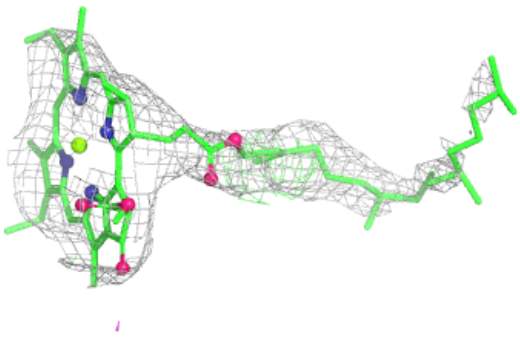


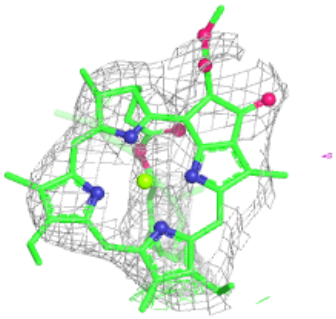


Electron density around CLA 2 1238:

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

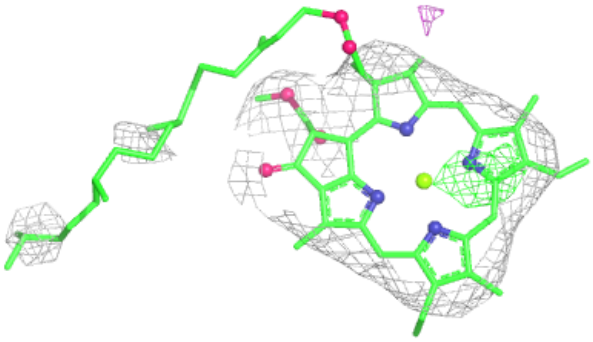


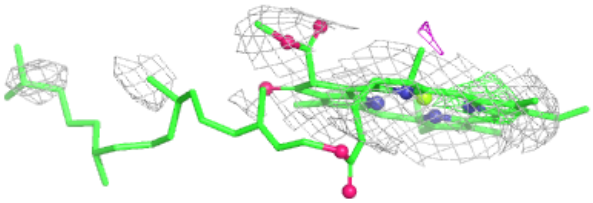


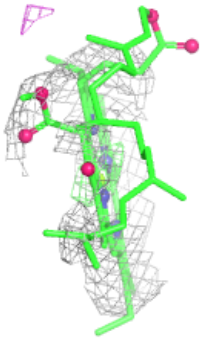


Electron density around CLA 8 1503:

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

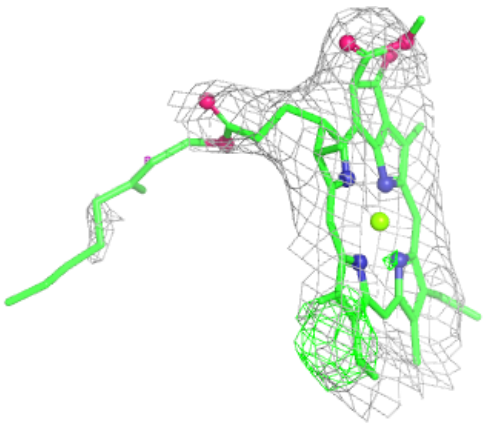


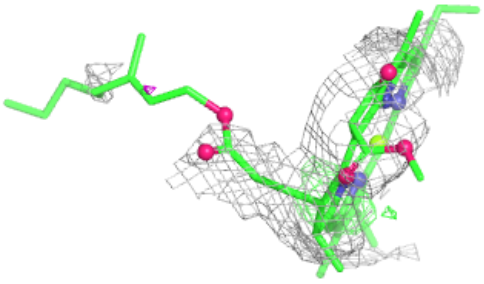


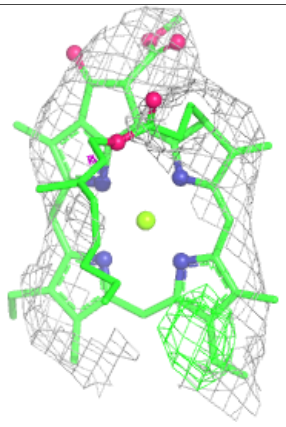


Electron density around CLA 2 1201:

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

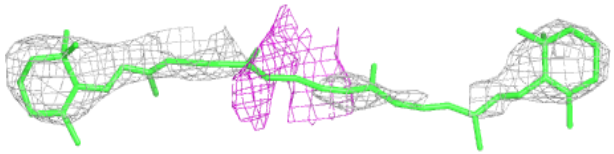


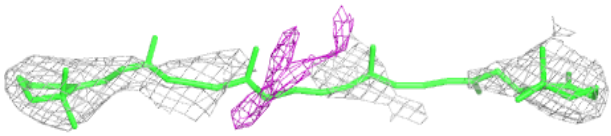


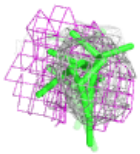


Electron density around BCR L 4019:

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

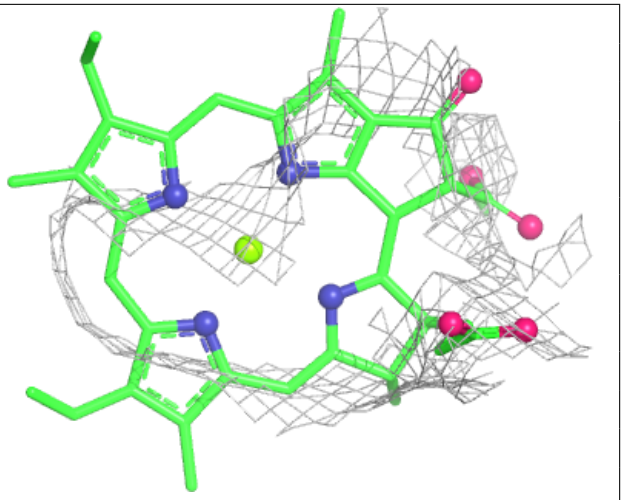


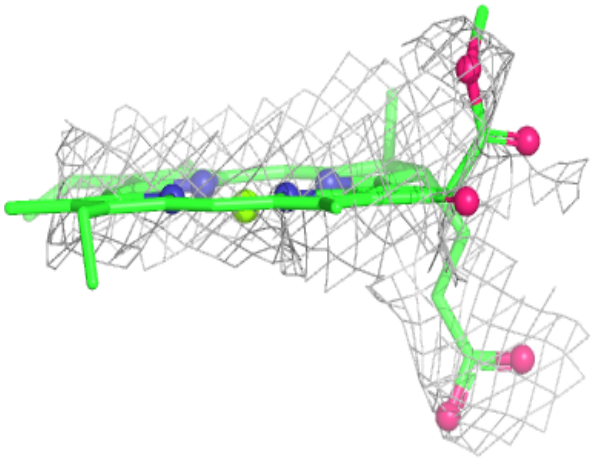


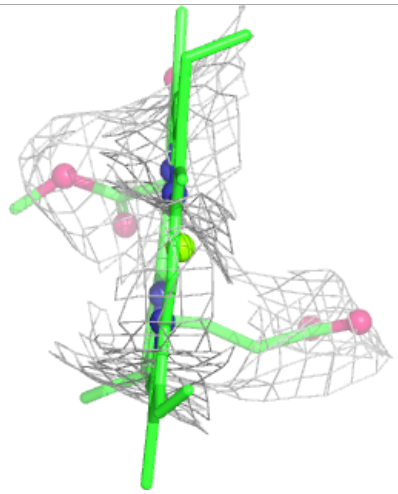


Electron density around CLA a 1112:

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

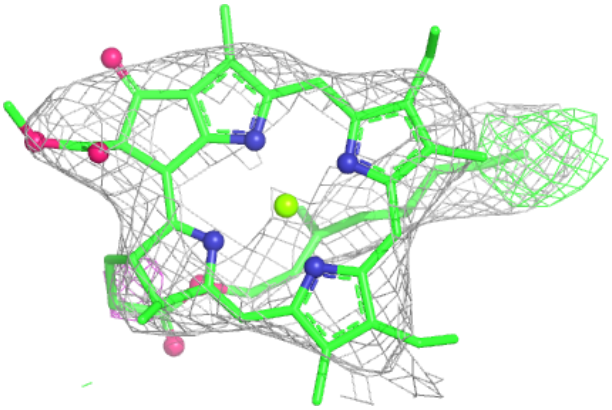


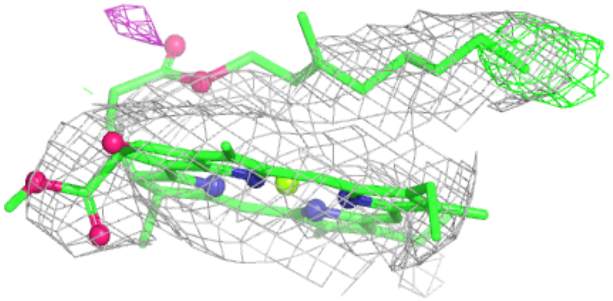


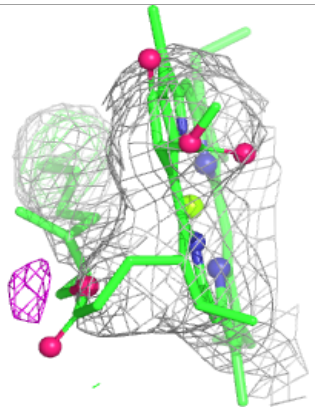


Electron density around CLA A 1116:

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

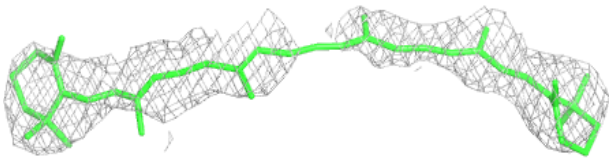


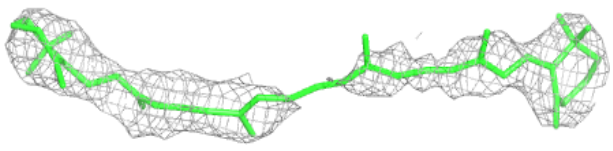


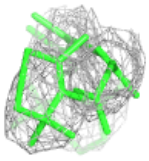


Electron density around BCR 6 4018:

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

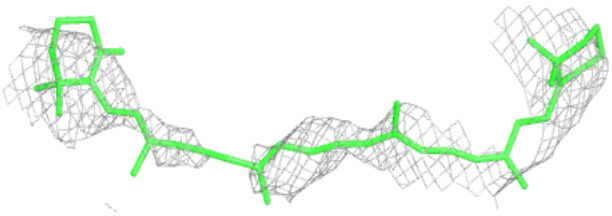


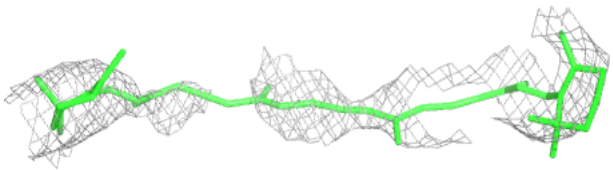


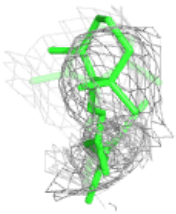


Electron density around BCR 6 4020:

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

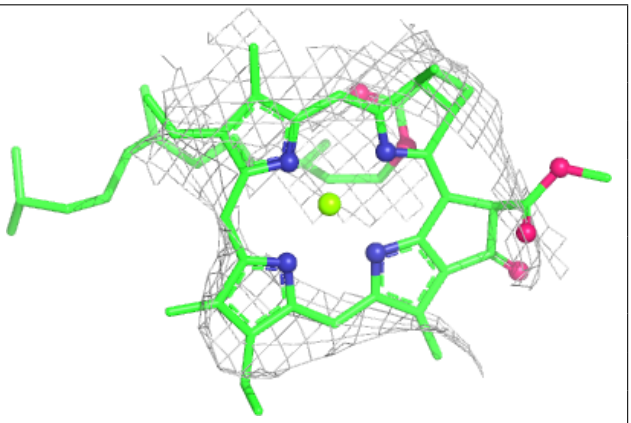






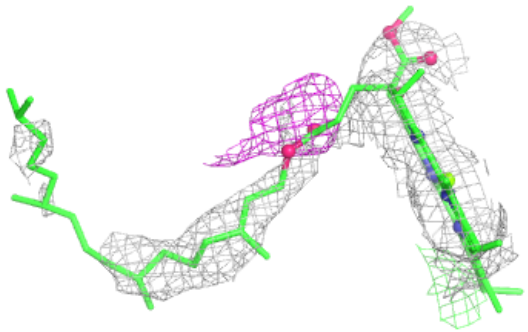
Electron density around CLA b 1235:

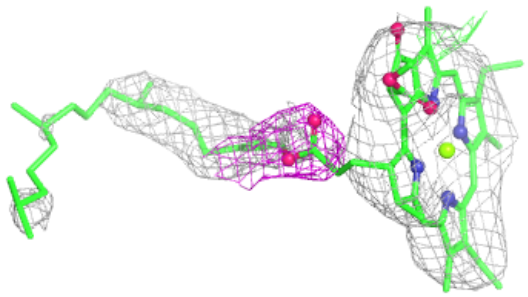
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

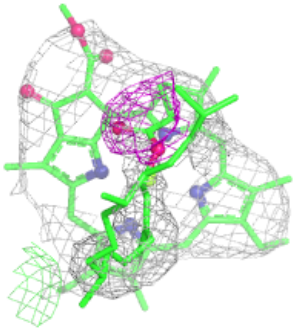


Electron density around CLA B 1238:

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

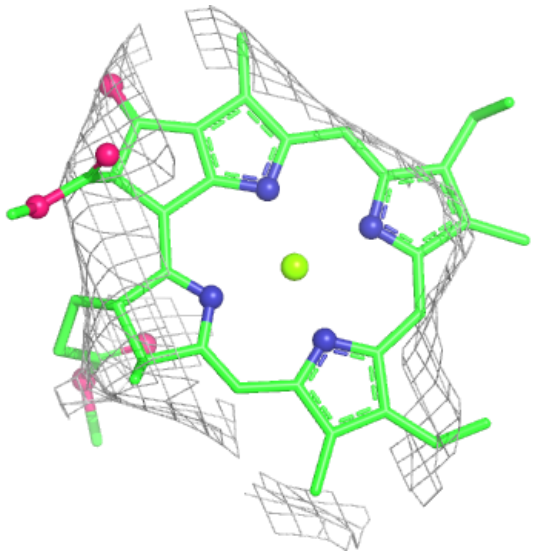


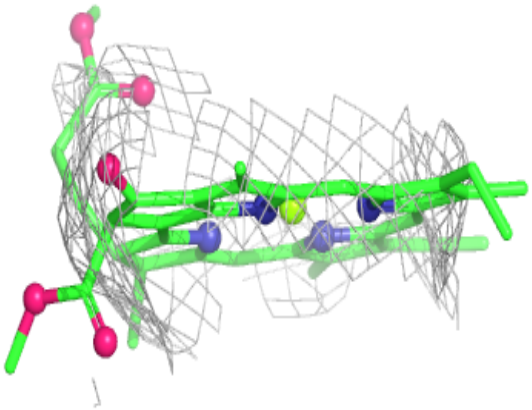


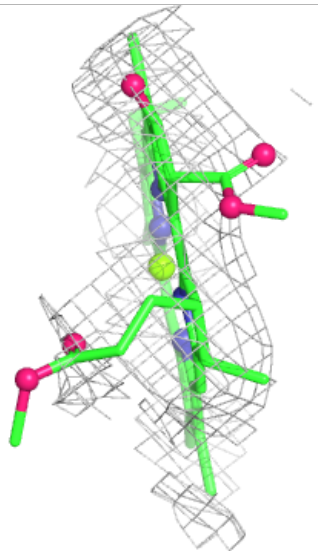


Electron density around CLA a 1134:

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

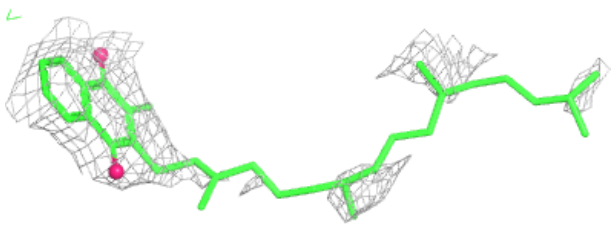


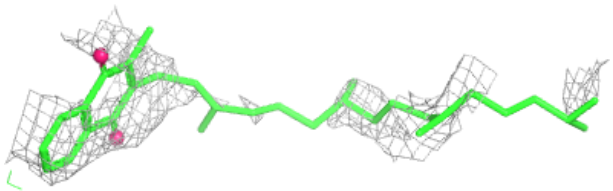


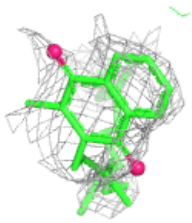


Electron density around PQN A 2001:

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

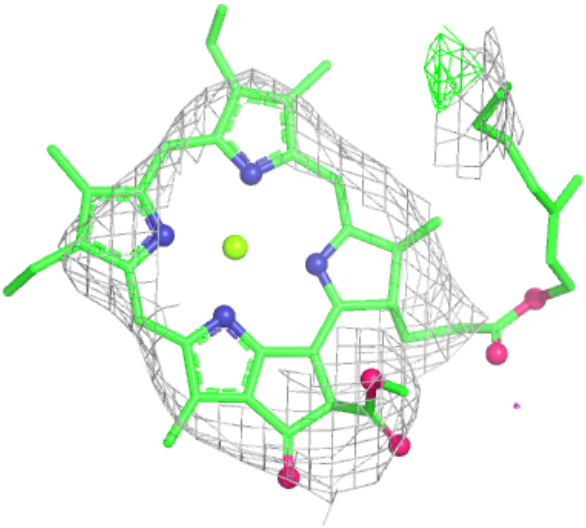


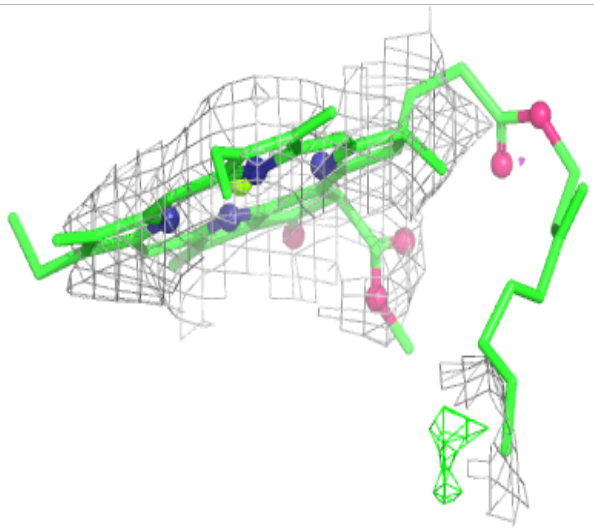




Electron density around CLA 2 1221:

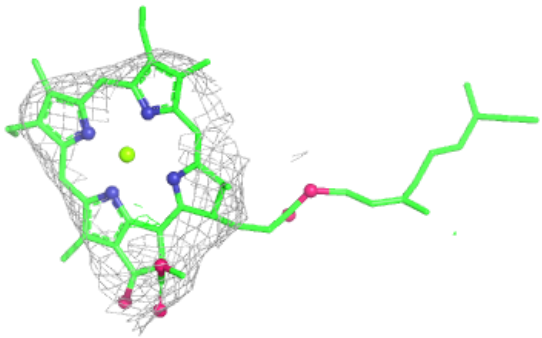
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

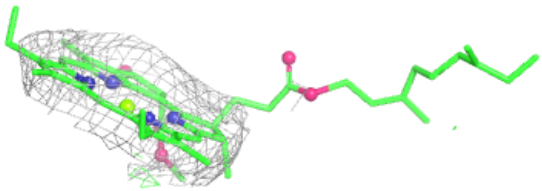


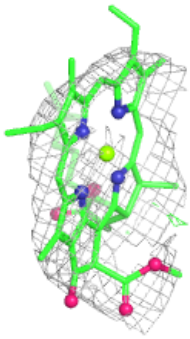


Electron density around CLA 2 1222:

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

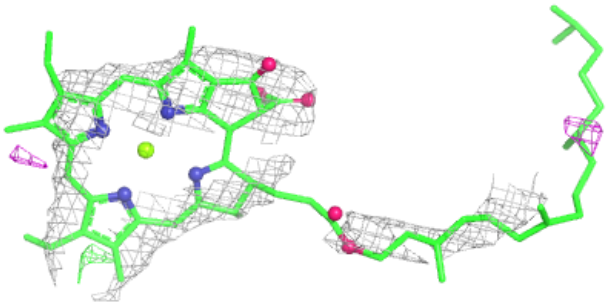


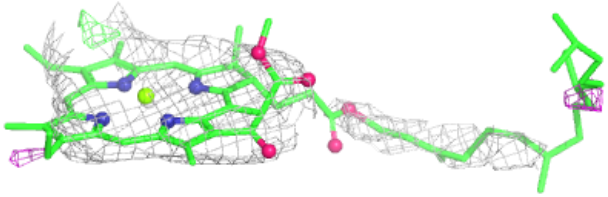


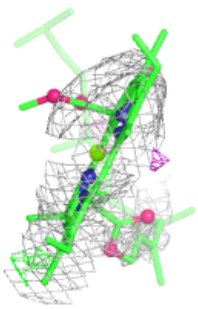


Electron density around CLA 2 1223:

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

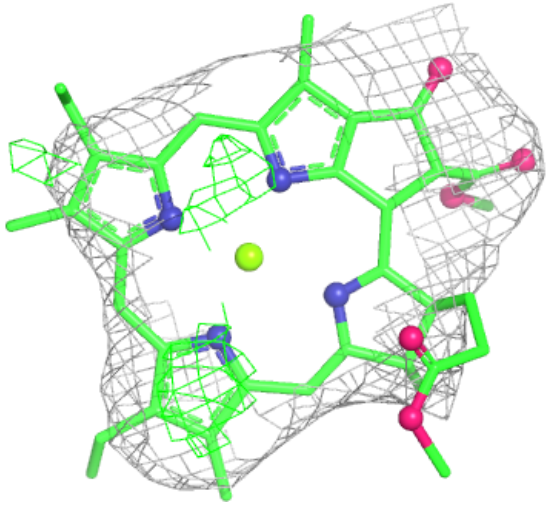


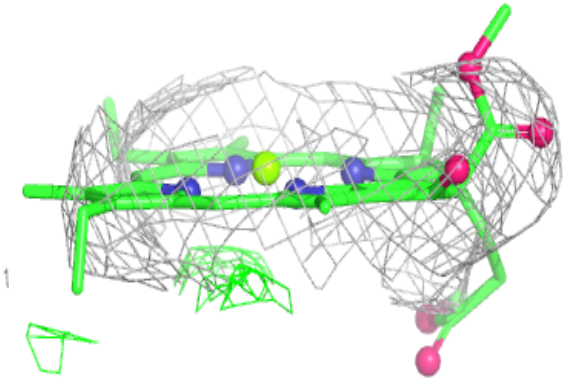


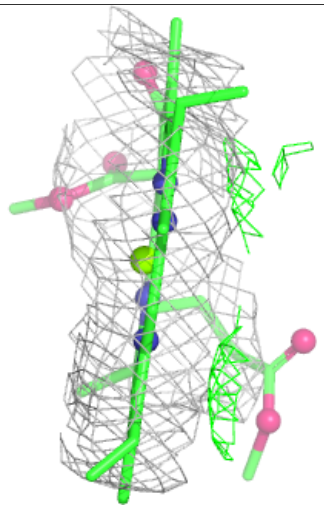


Electron density around CLA A 1120:

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

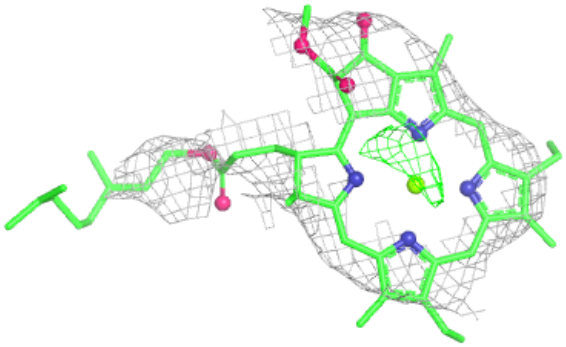


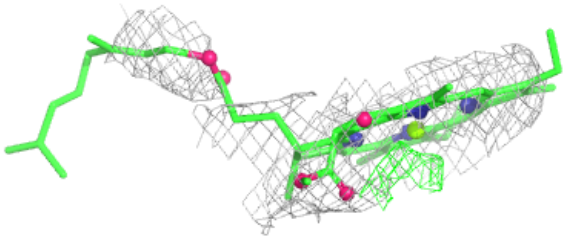


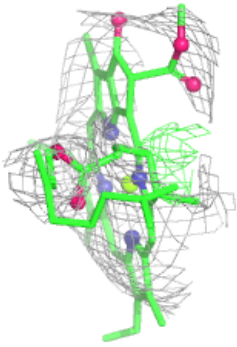


Electron density around CLA a 1124:

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

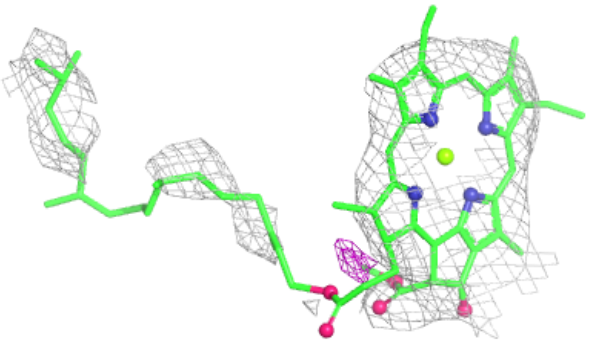


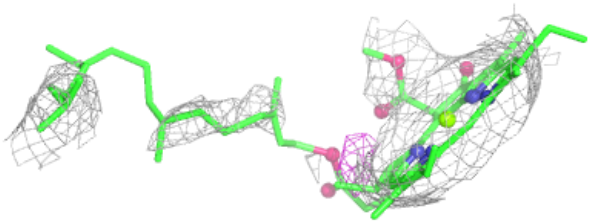


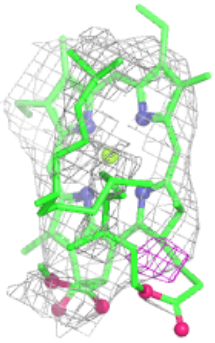


Electron density around CLA b 1207:

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

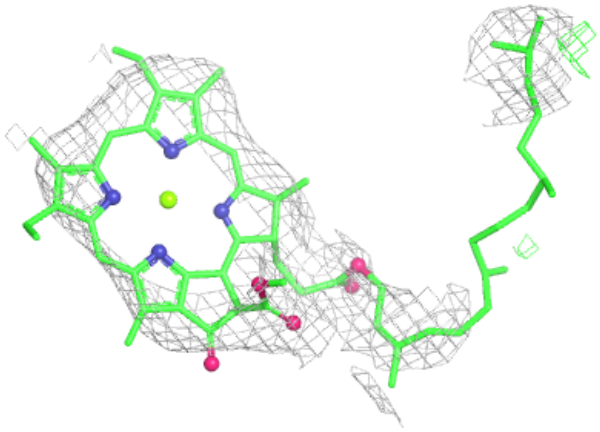


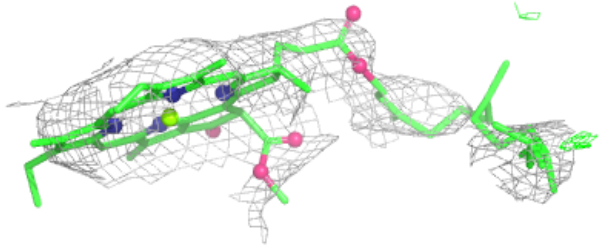


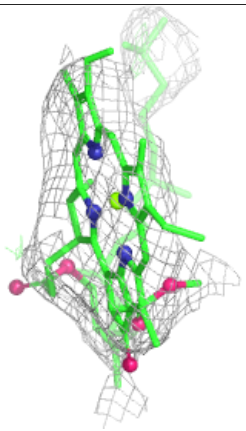


Electron density around CLA A 1101:

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

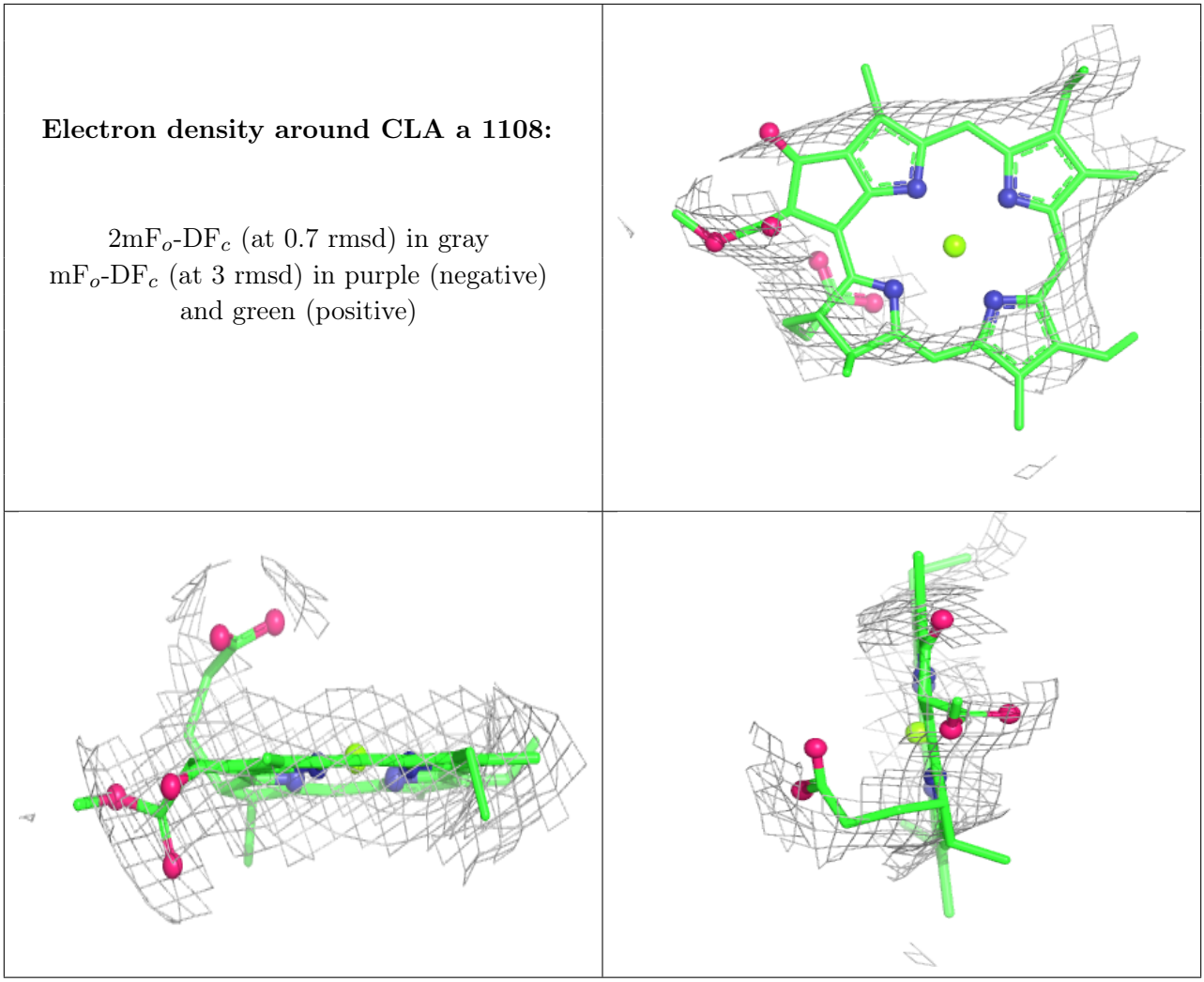






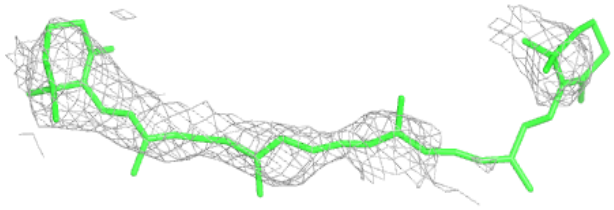
Electron density around CLA a 1108:

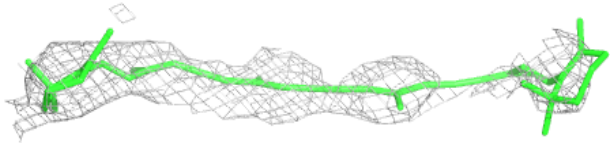
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

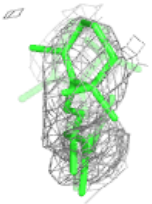


Electron density around BCR f 4020:

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

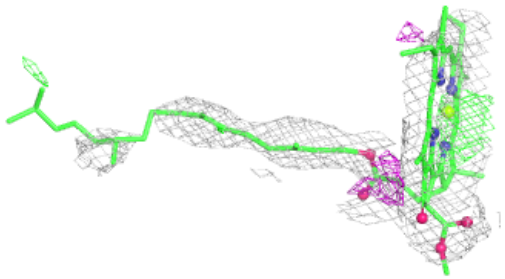


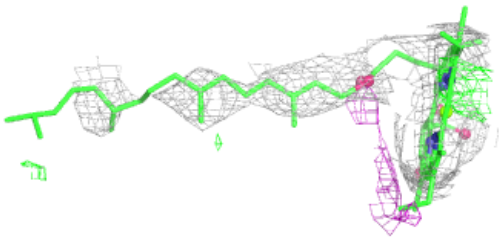


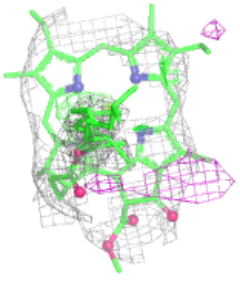


Electron density around CLA A 1126:

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

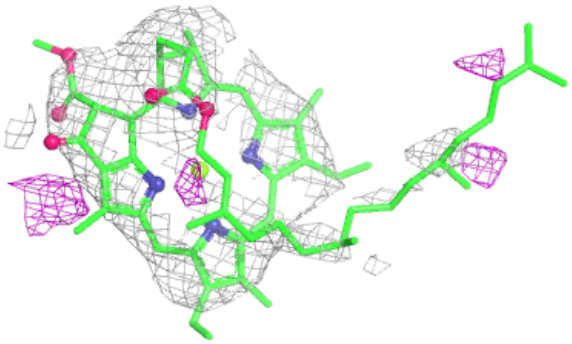


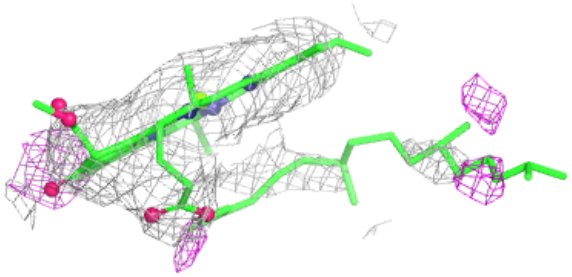


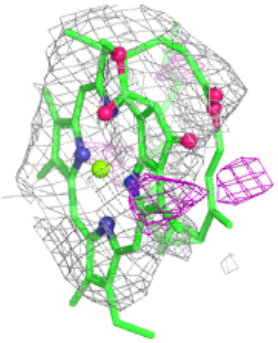


Electron density around CLA 2 1204:

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

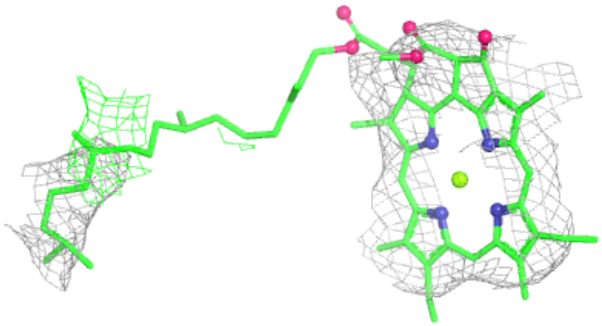


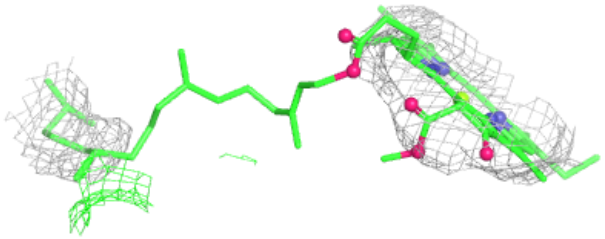


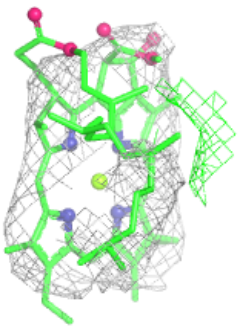


Electron density around CLA 2 1207:

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

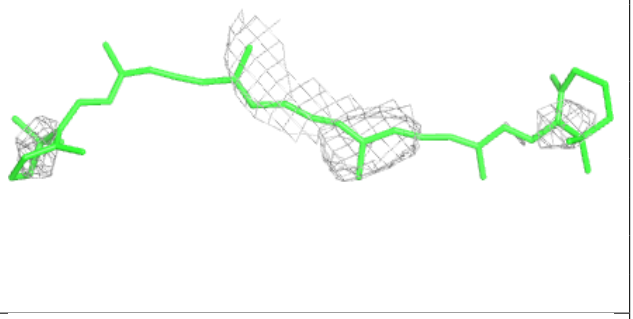


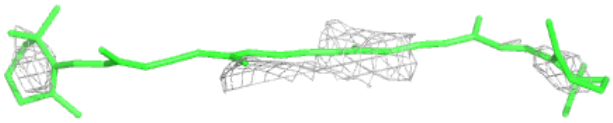


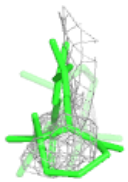


Electron density around BCR b 4017:

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

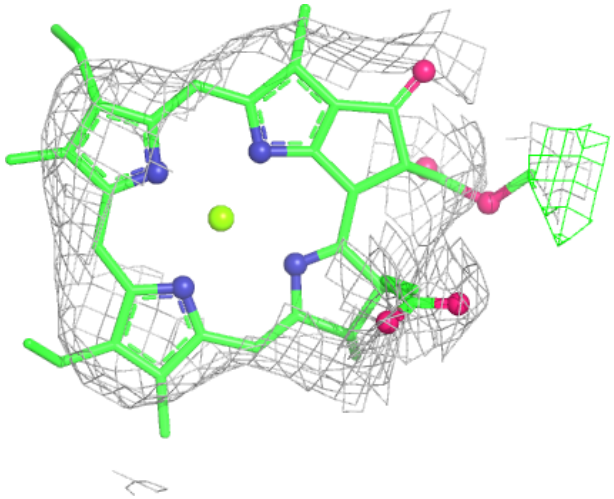


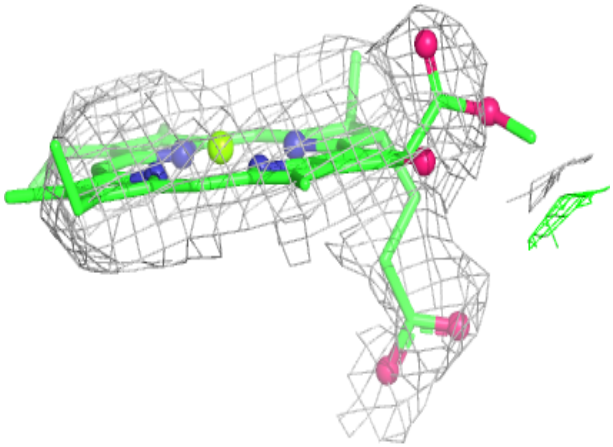


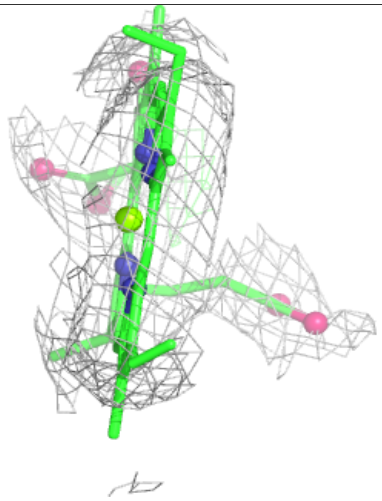


Electron density around CLA 2 1208:

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

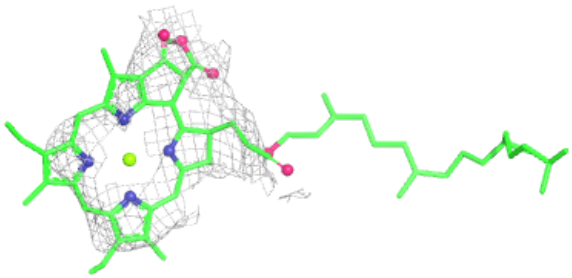


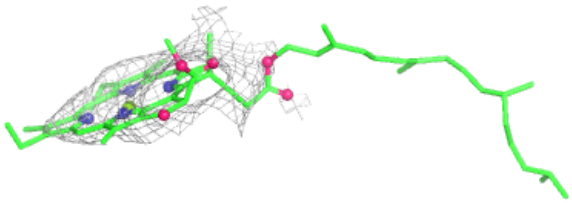


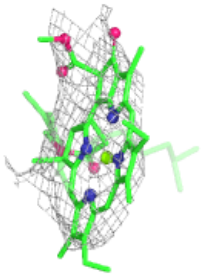


Electron density around CLA 1 1103:

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

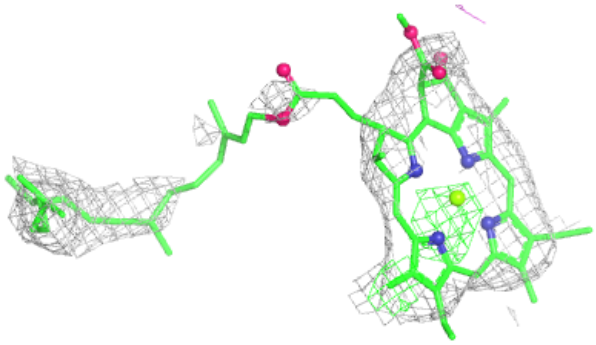


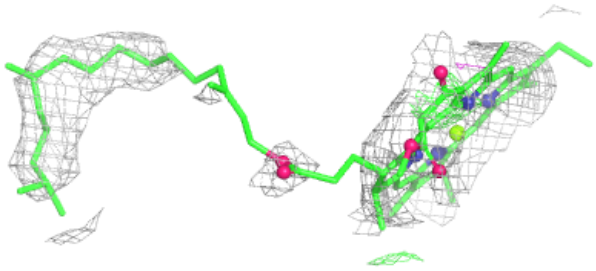


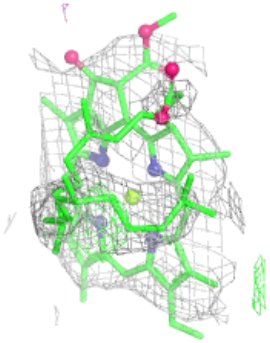


Electron density around CLA B 1206:

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

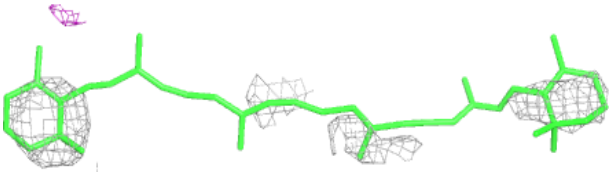


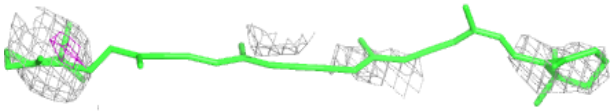


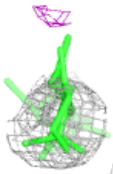


Electron density around BCR l 4019:

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

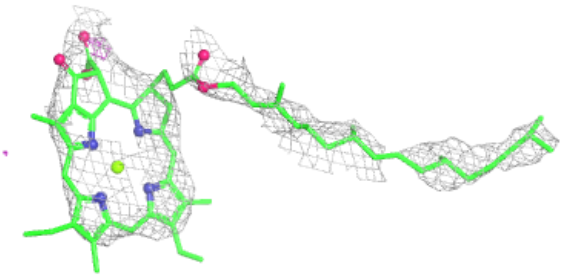


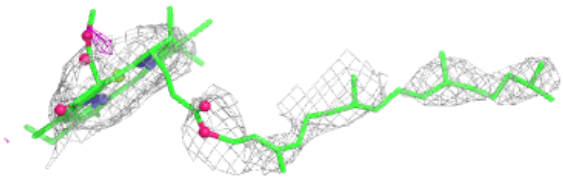




Electron density around CLA a 1132:

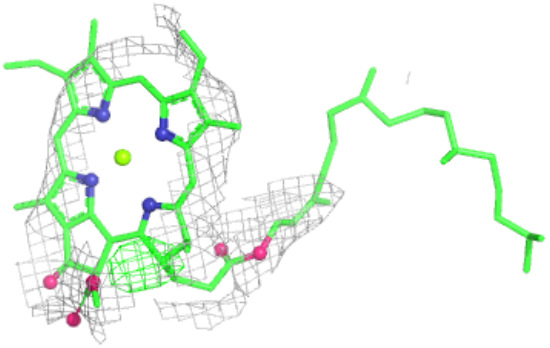
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

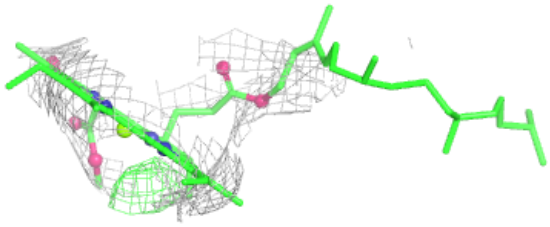


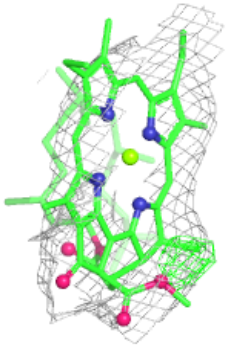


Electron density around CLA 1 1106:

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

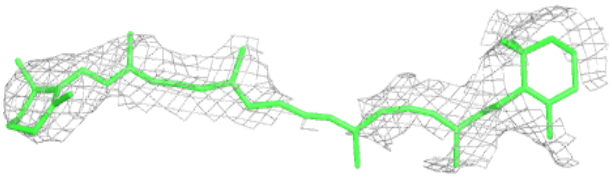


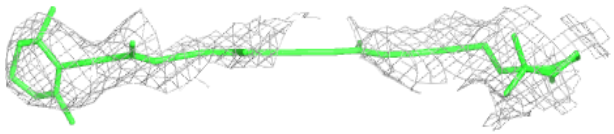


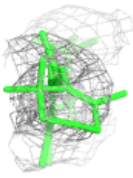


Electron density around BCR A 4007:

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

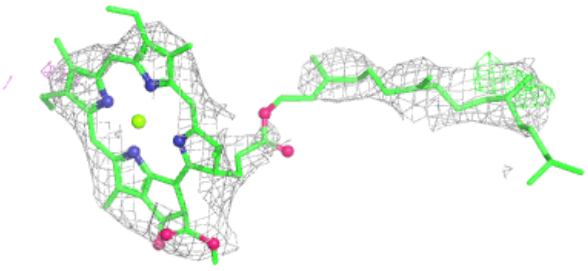


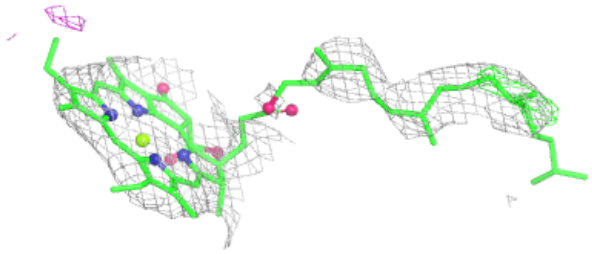


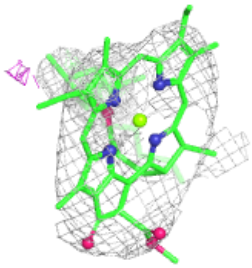


Electron density around CLA A 1119:

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

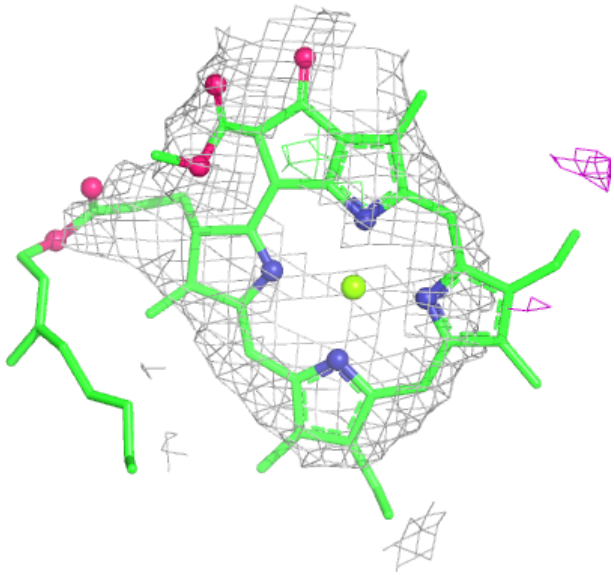


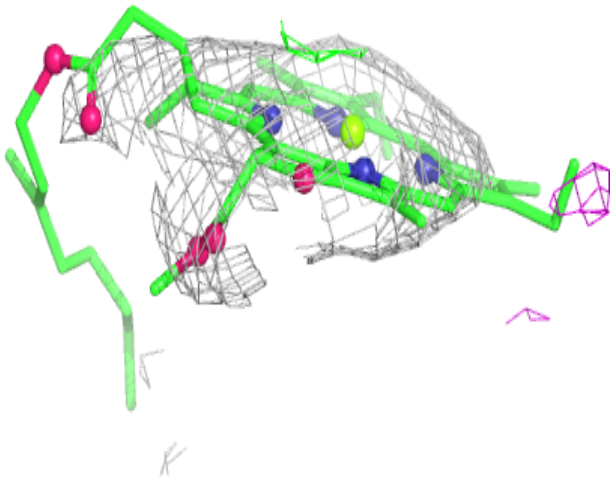




Electron density around CLA B 1221:

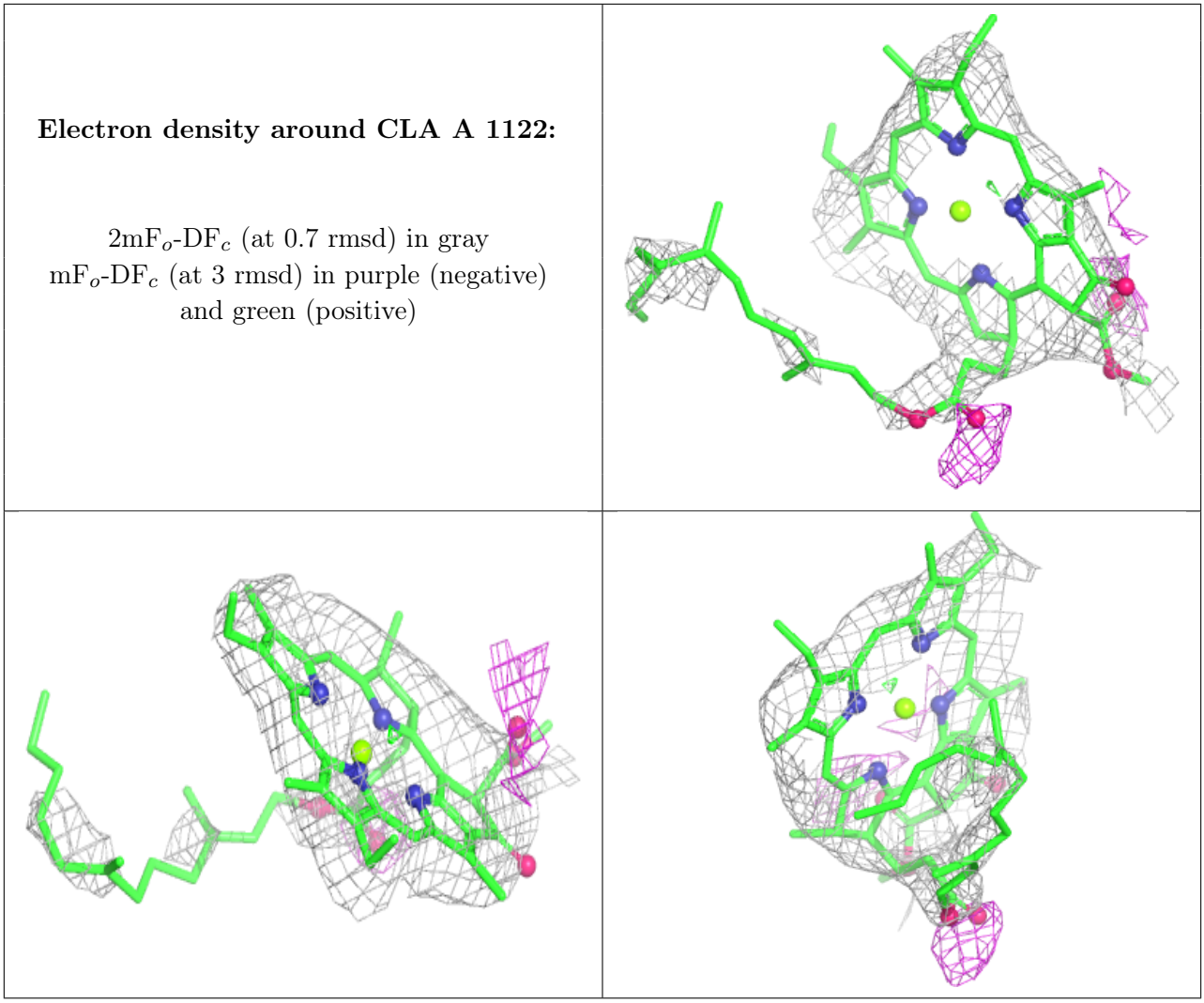
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





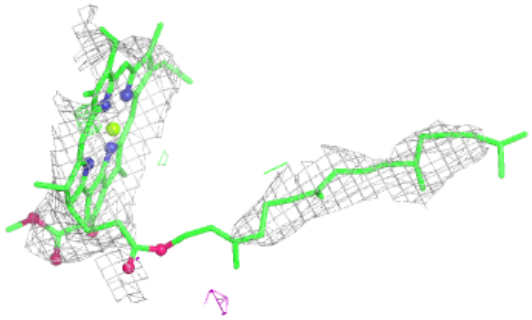
Electron density around CLA A 1122:

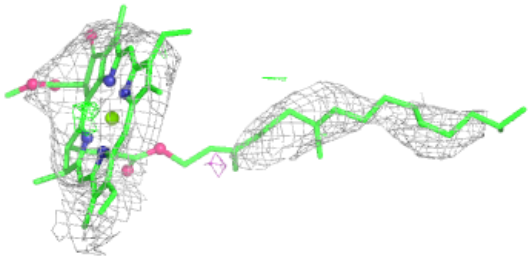
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

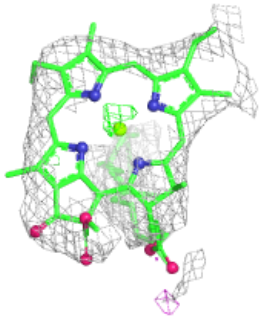


Electron density around CLA 2 1226:

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

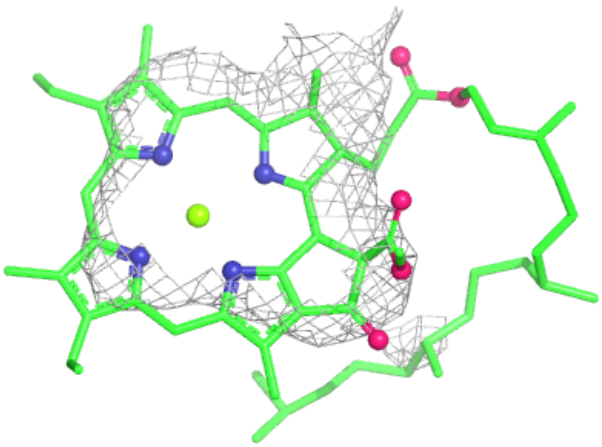


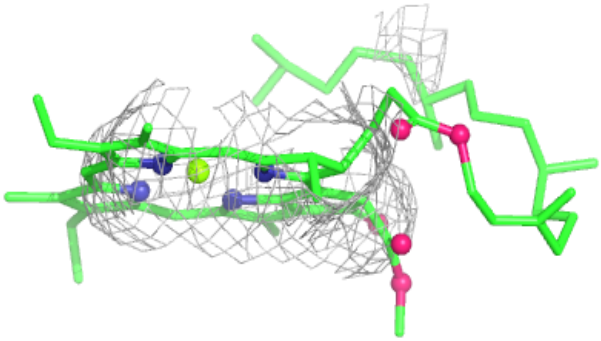


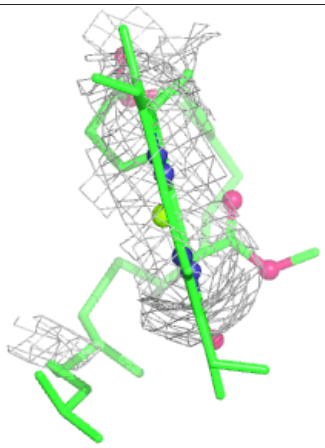


Electron density around CLA b 1202:

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

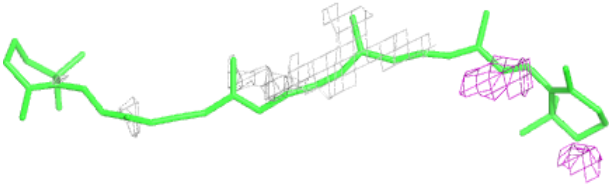


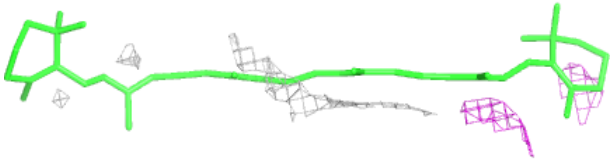


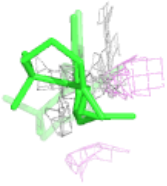


Electron density around BCR 2 4009:

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

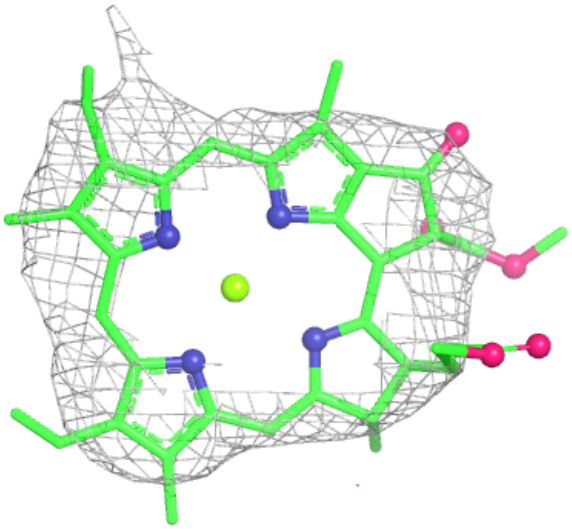


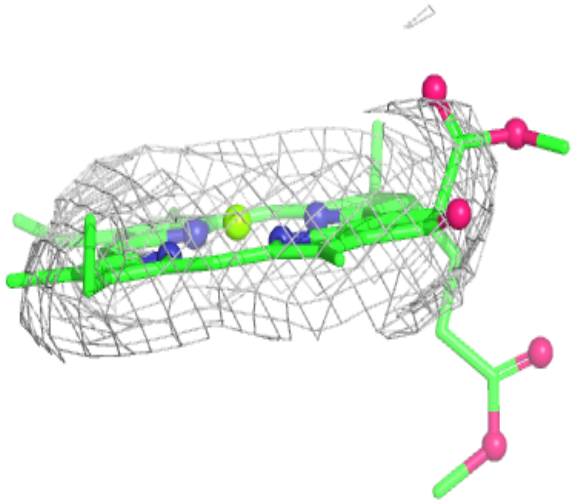


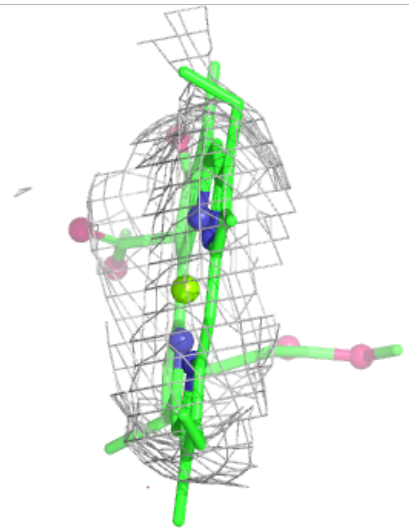


Electron density around CLA A 1121:

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

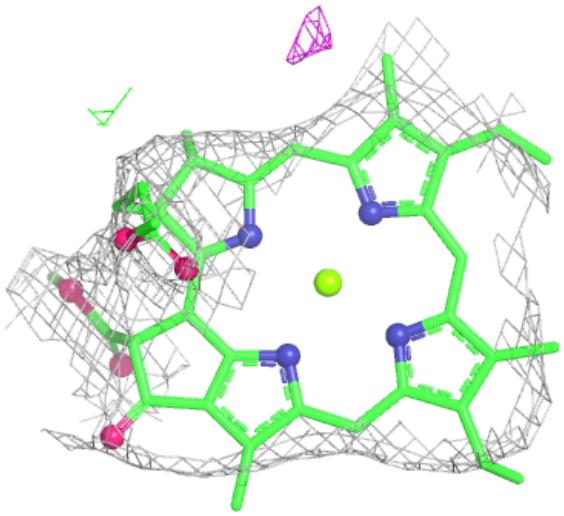


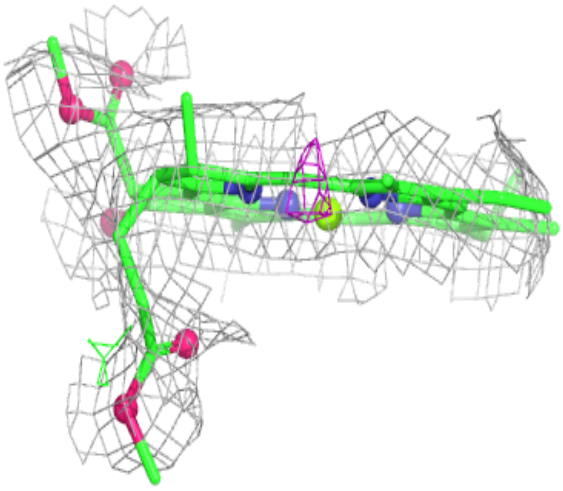


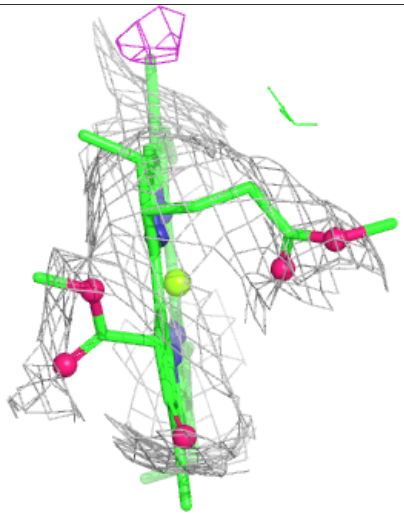


Electron density around CLA A 1134:

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

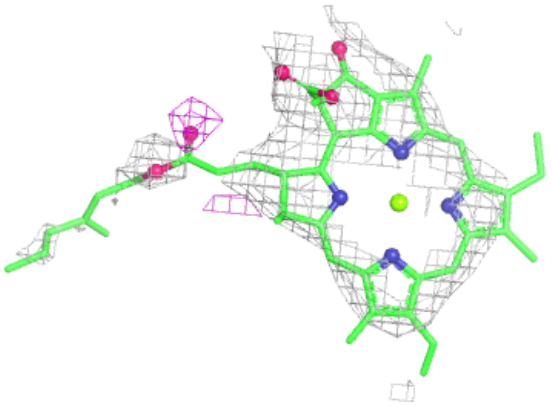


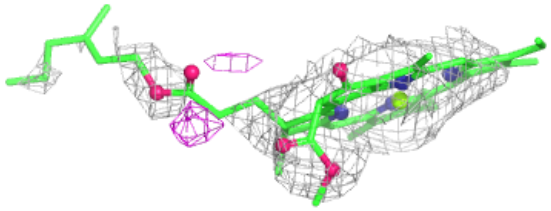


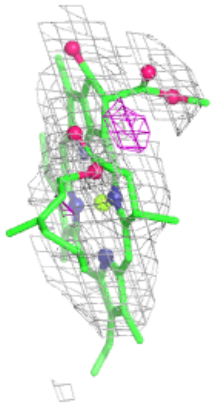


Electron density around CLA A 1125:

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

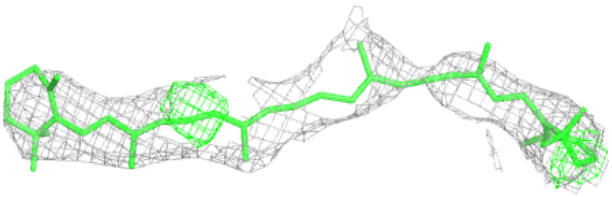


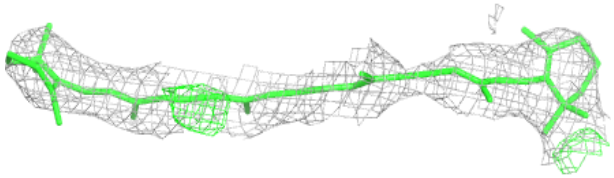


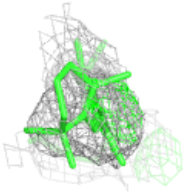


Electron density around BCR B 4017:

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

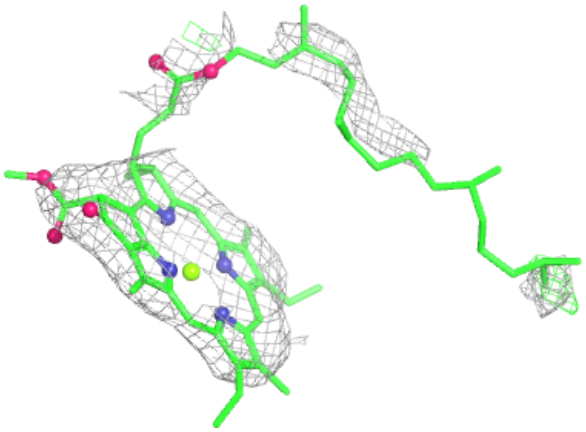


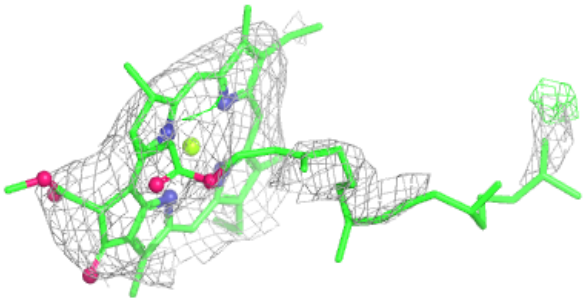


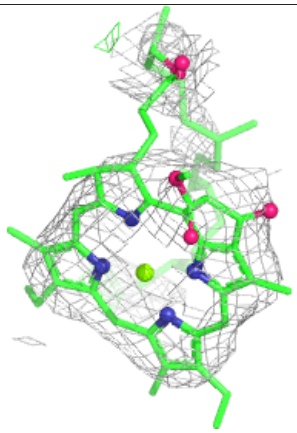


Electron density around CLA A 1102:

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

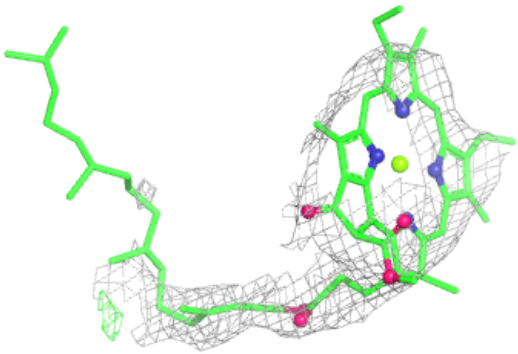


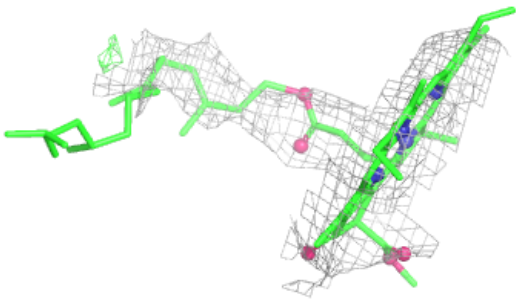




Electron density around CLA a 1137:

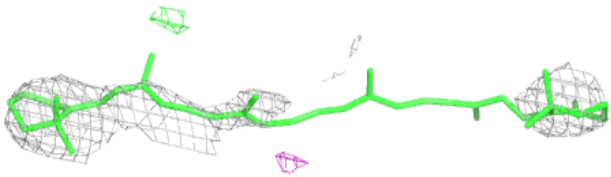
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

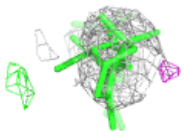




Electron density around BCR 8 4019:

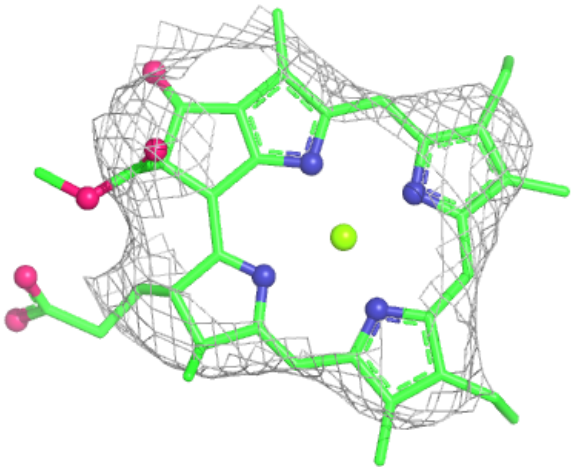
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

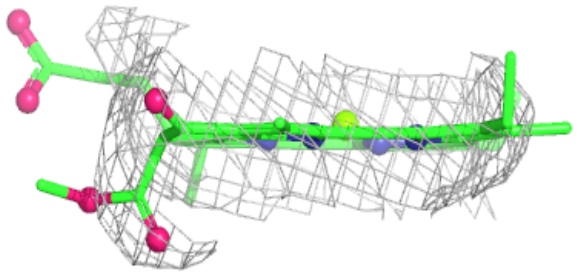


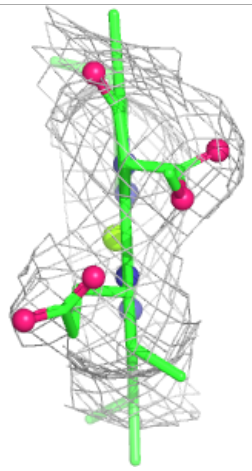


Electron density around CLA A 1113:

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

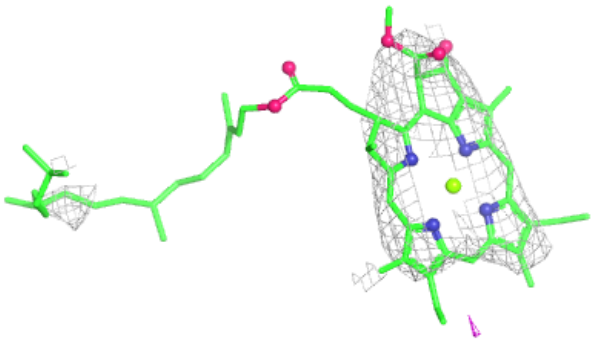


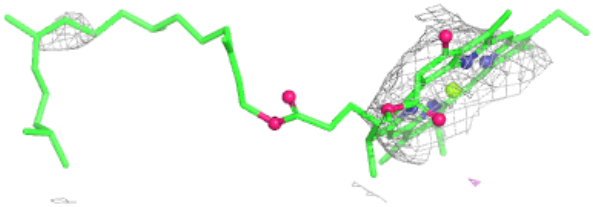


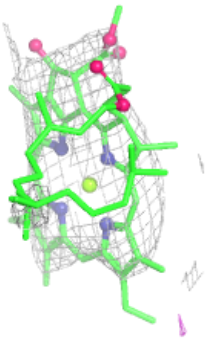


Electron density around CLA b 1206:

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

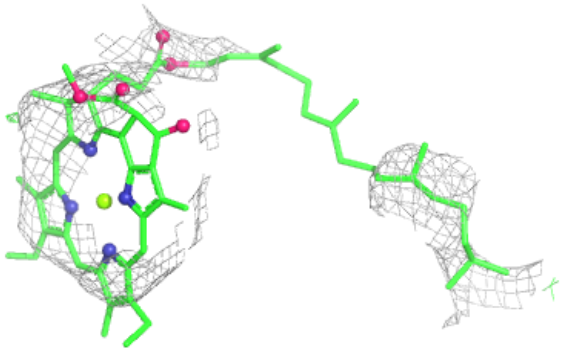


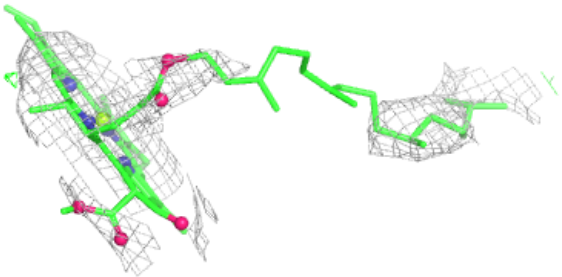


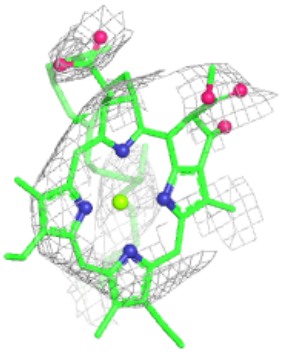


Electron density around CLA 1 1137:

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

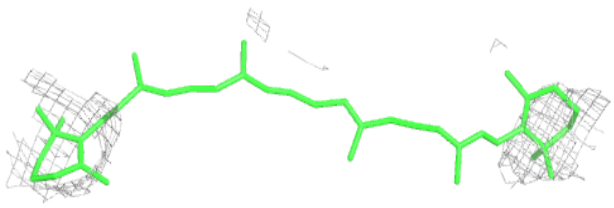


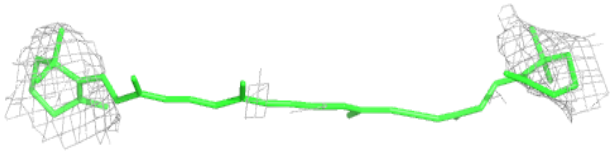


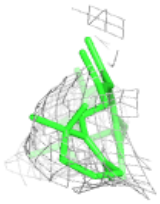


Electron density around BCR a 4001:

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

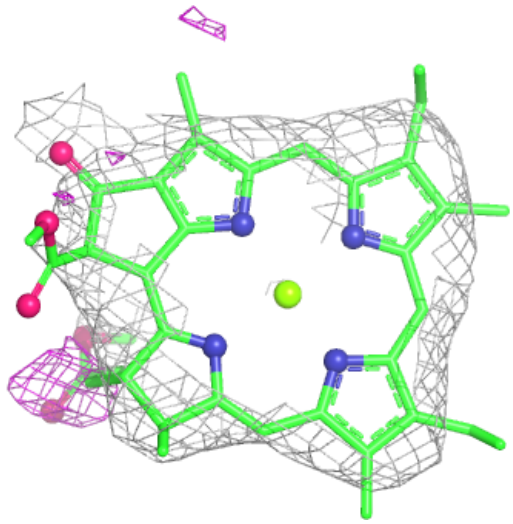


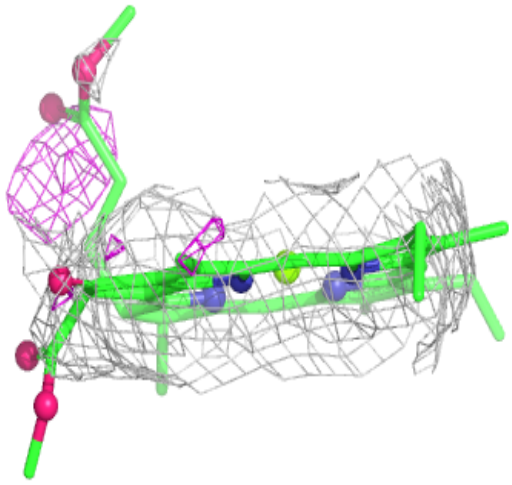


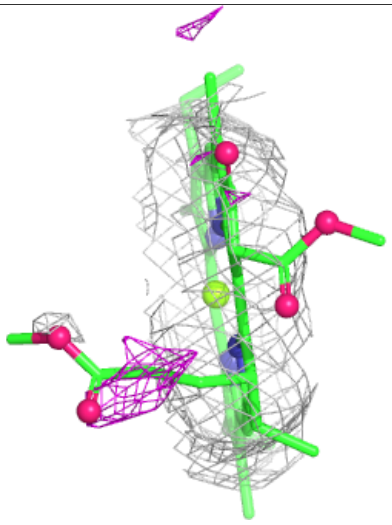


Electron density around CLA 2 1211:

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

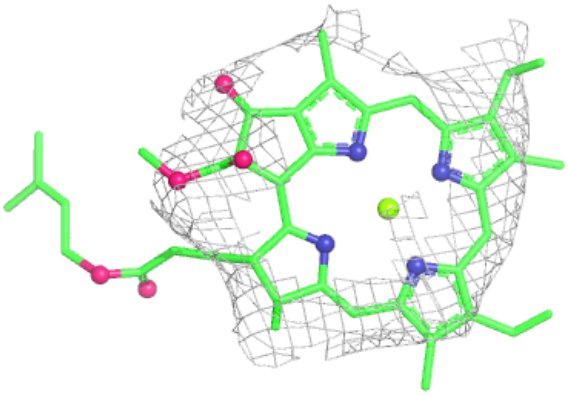


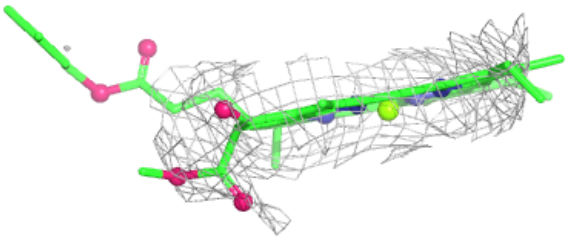


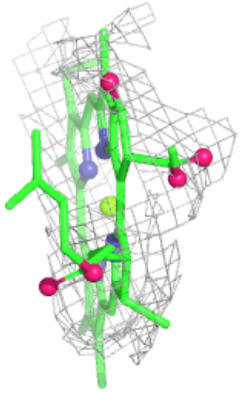


Electron density around CLA 1 1139:

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

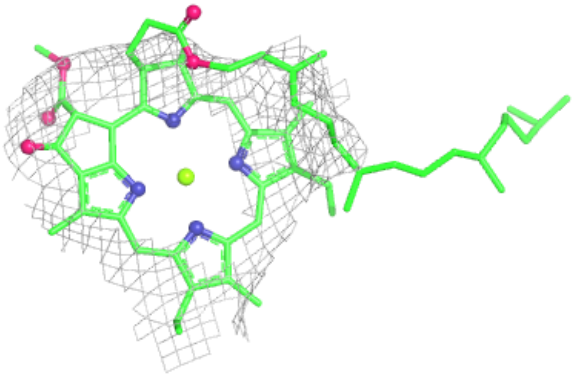


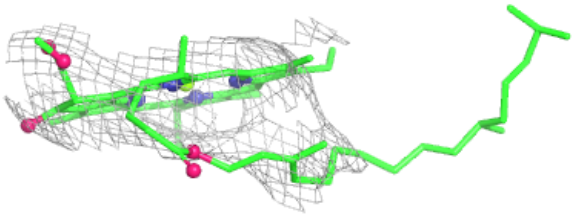


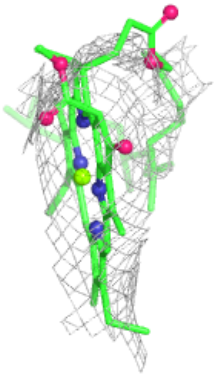


Electron density around CLA b 1215:

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

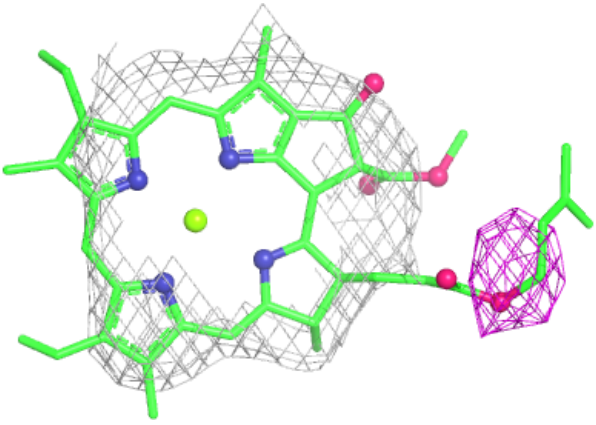


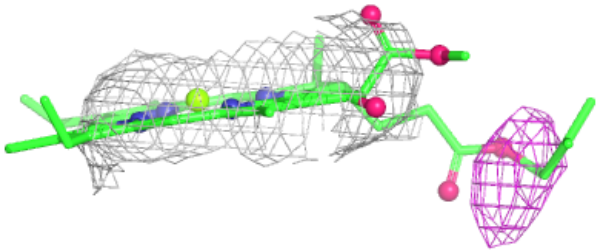


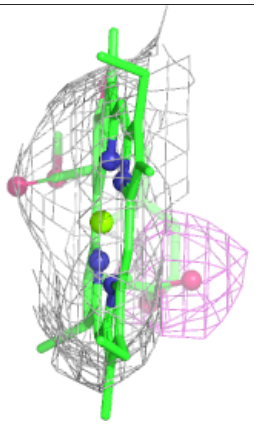


Electron density around CLA A 1139:

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

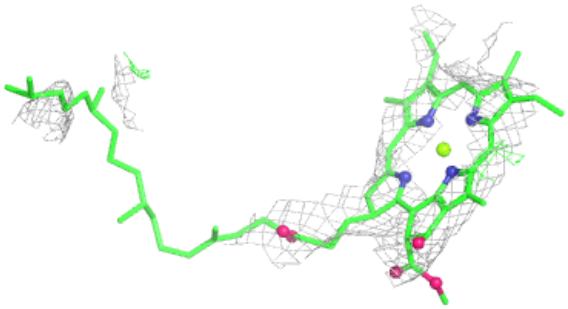


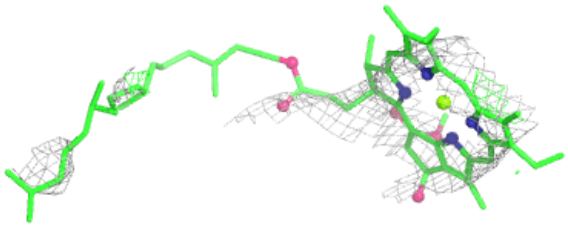


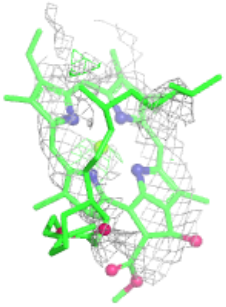


Electron density around CLA a 1012:

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

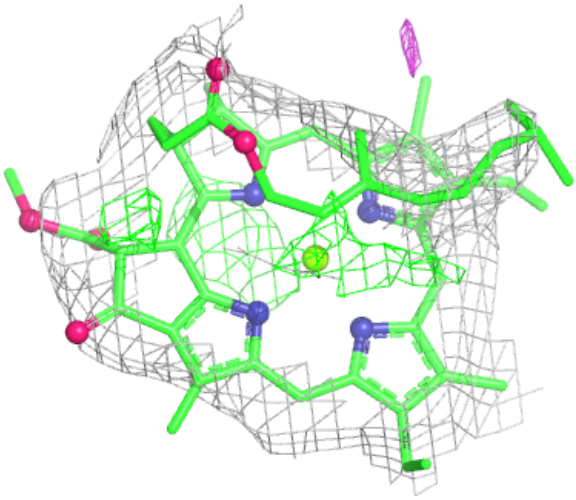


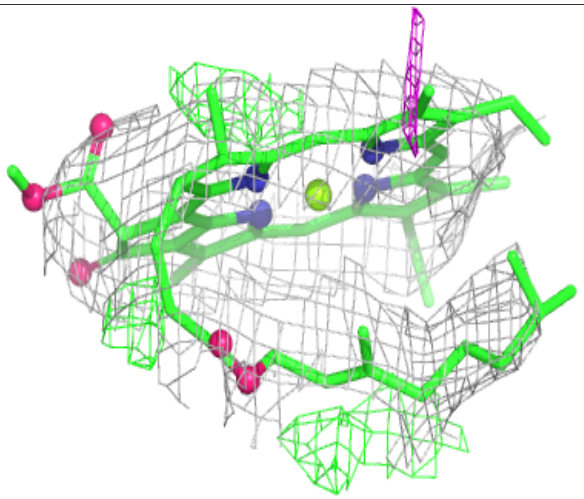


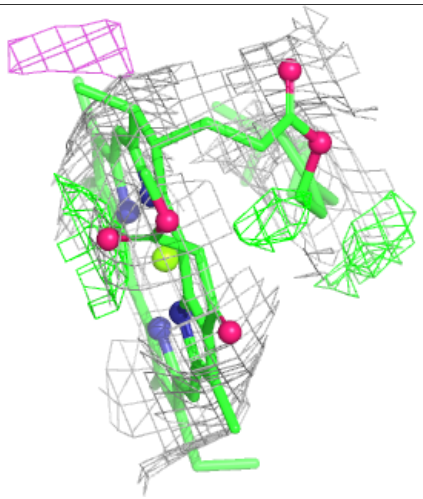


Electron density around CLA 1 1237:

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

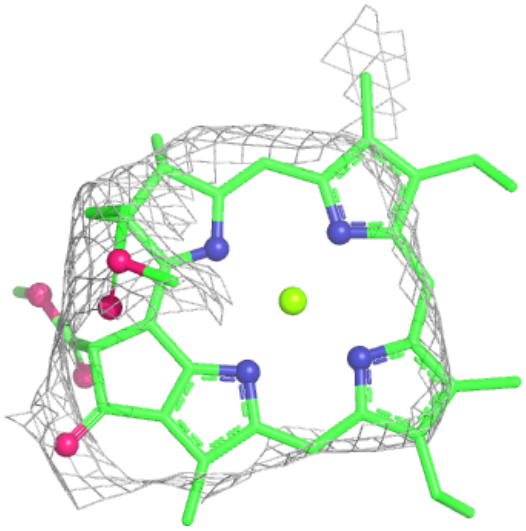


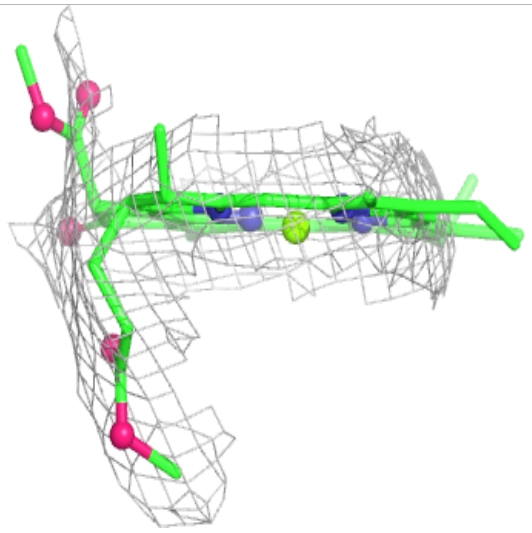


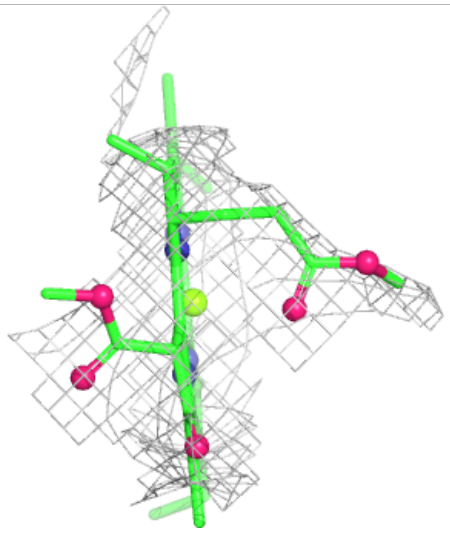


Electron density around CLA 1 1134:

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

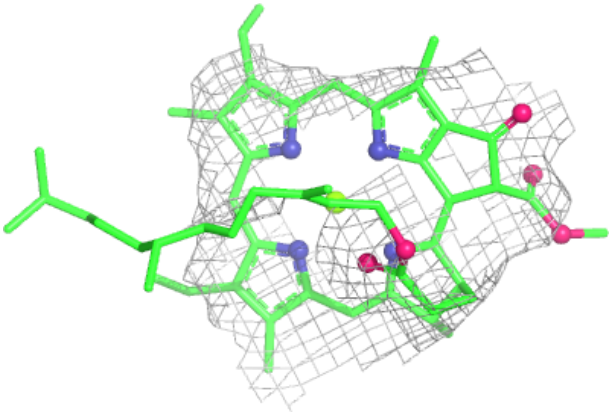


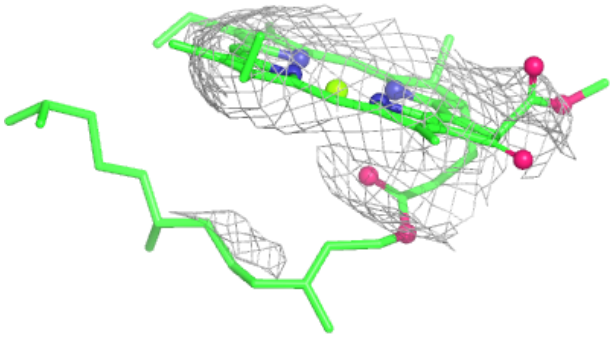


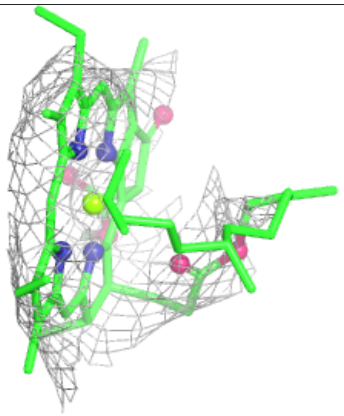


Electron density around CLA B 1235:

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

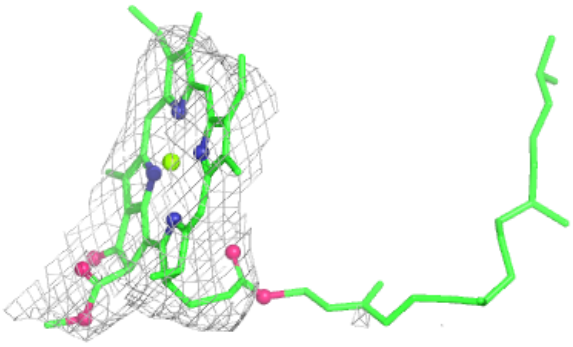


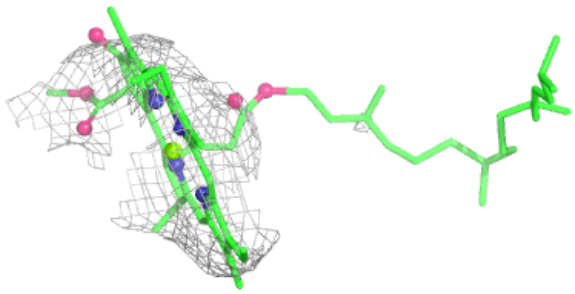


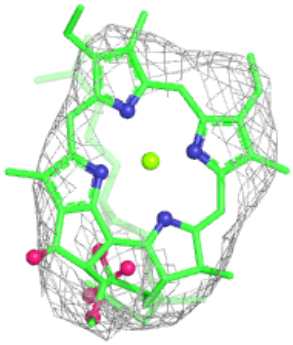


Electron density around CLA A 1140:

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

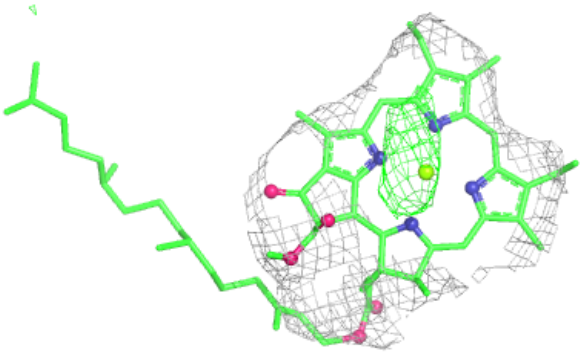


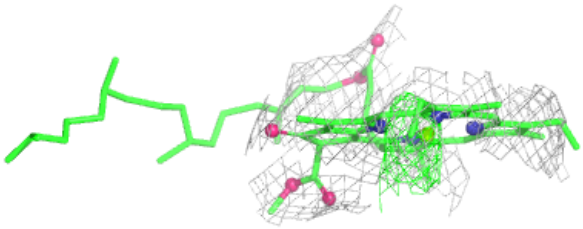




Electron density around CLA l 1503:

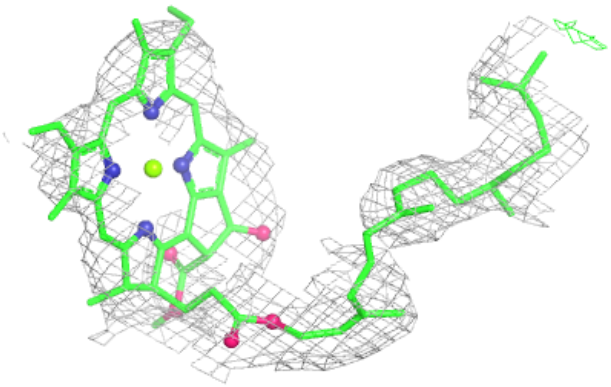
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

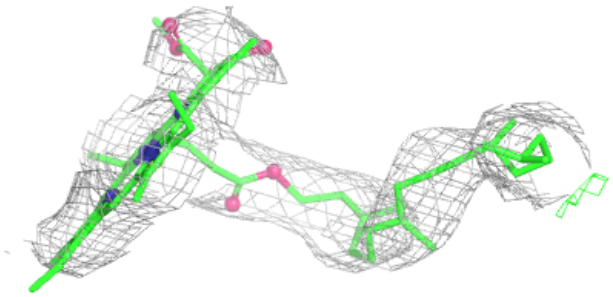


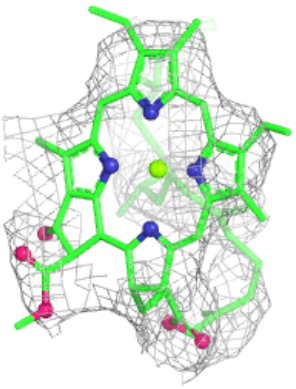


Electron density around CLA A 1137:

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

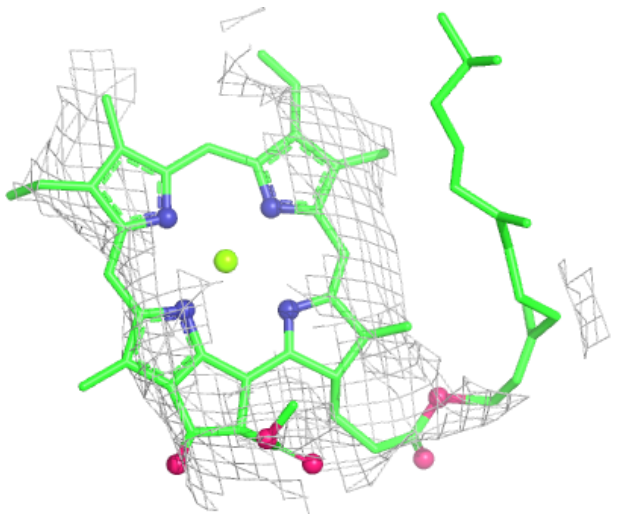


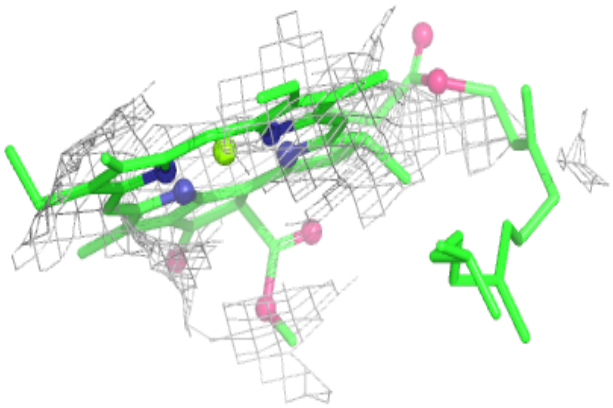




Electron density around CLA a 1111:

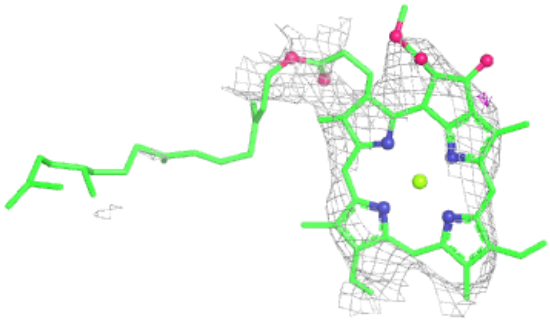
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

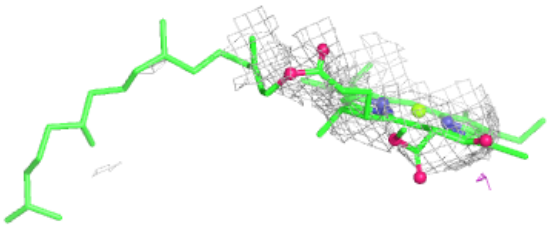


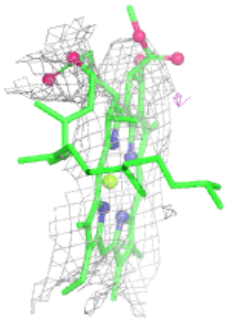


Electron density around CLA 2 1023:

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

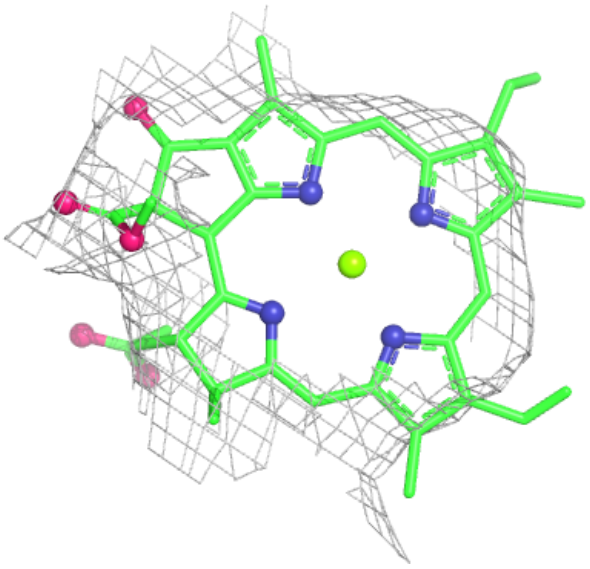


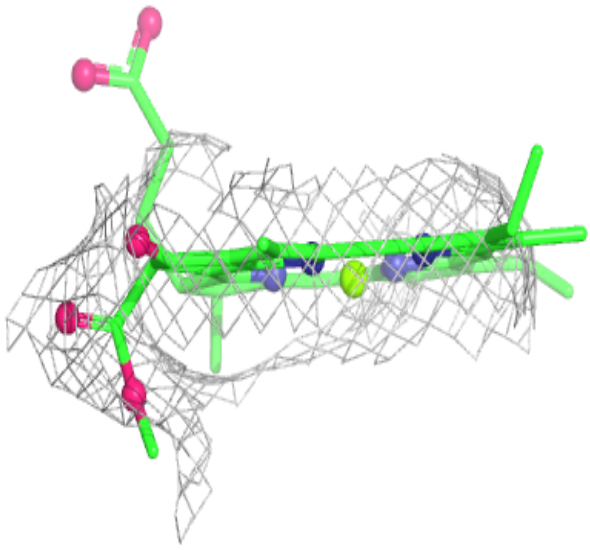




Electron density around CLA B 1231:

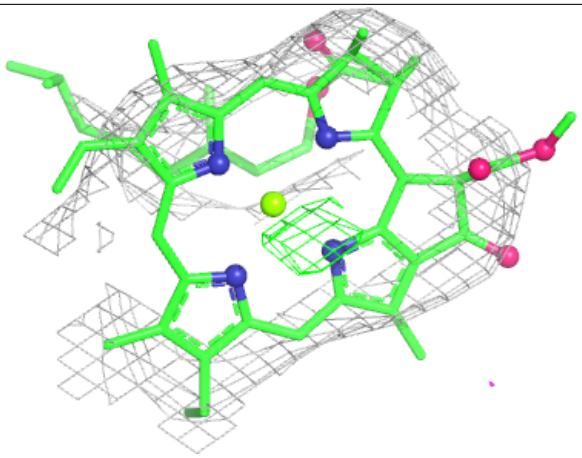
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

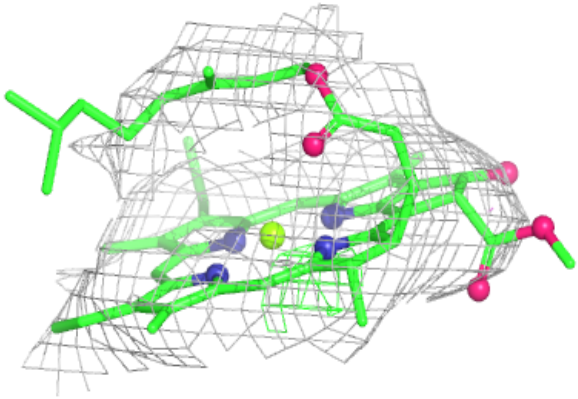


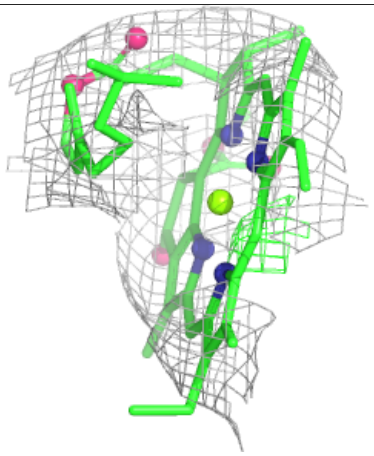


Electron density around CLA a 1237:

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

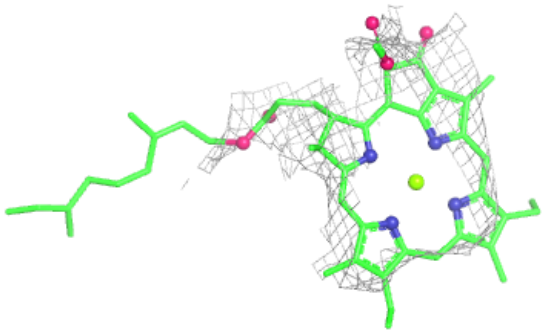


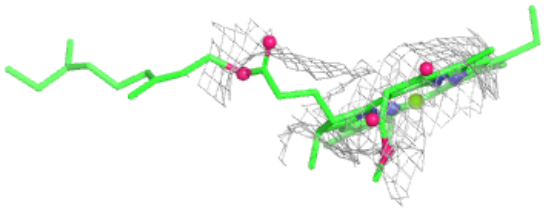


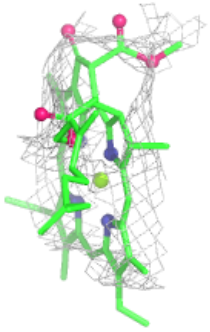


Electron density around CLA b 1222:

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

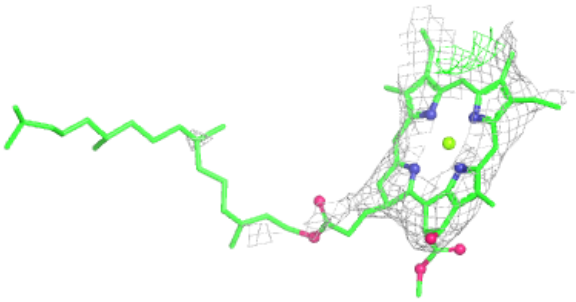


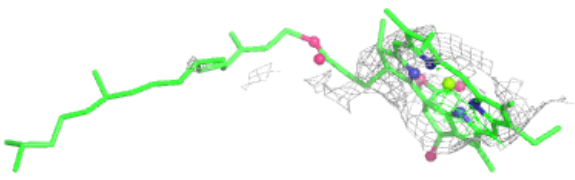




Electron density around CLA a 1022:

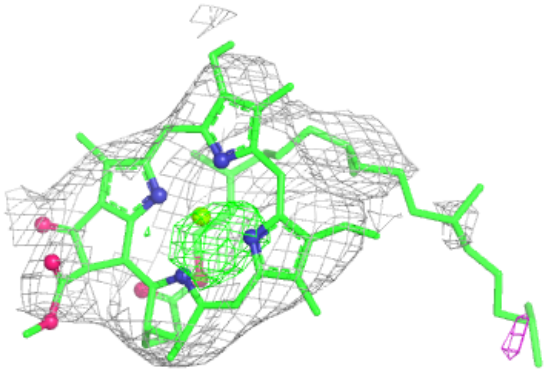
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

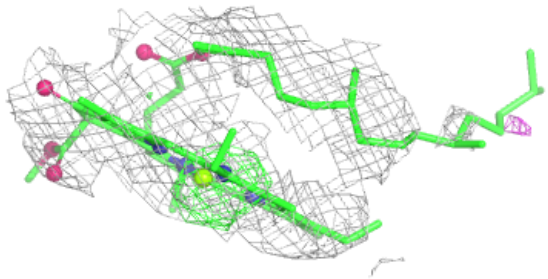


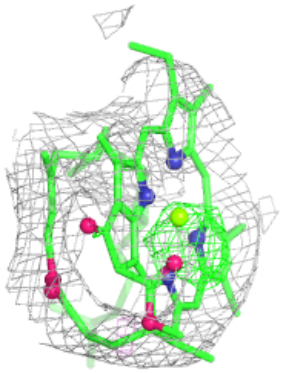


Electron density around CLA B 1204:

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

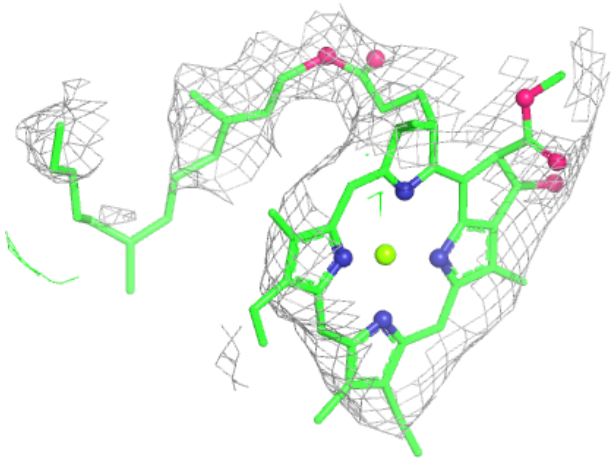


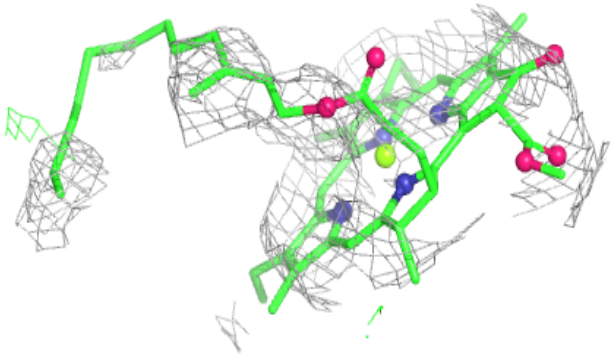


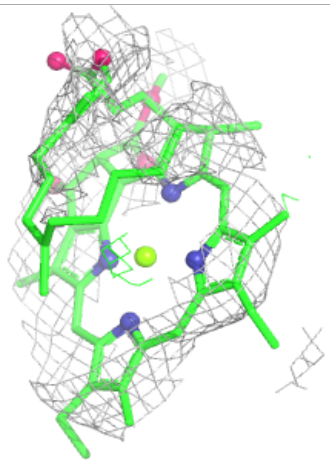


Electron density around CLA a 1122:

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

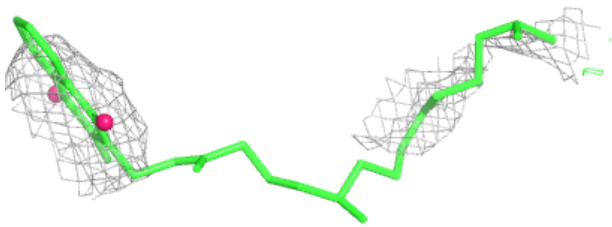


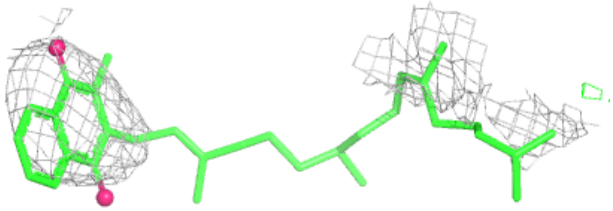


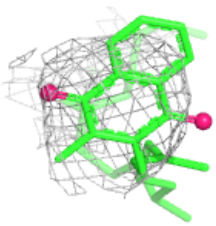


Electron density around PQN 2 2002:

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

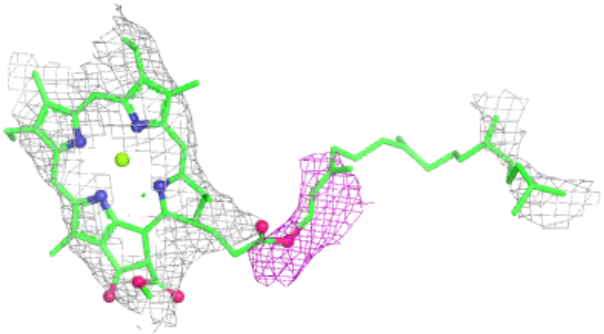


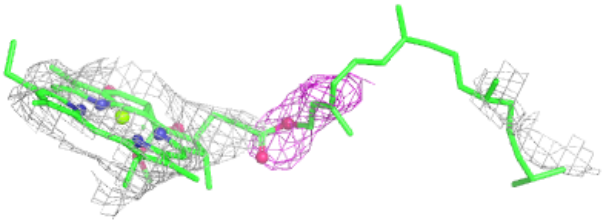


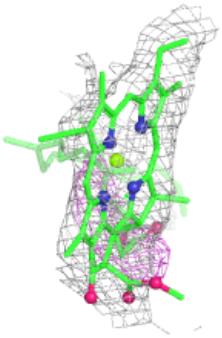


Electron density around CLA 2 1210:

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

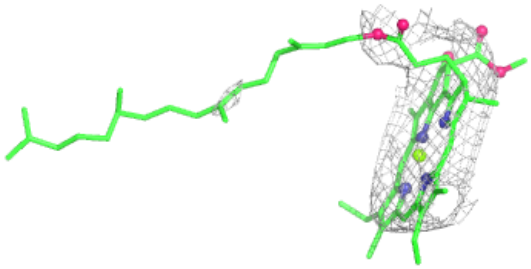


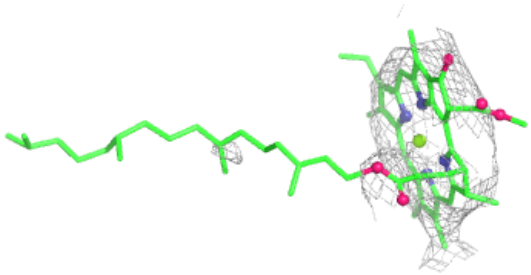


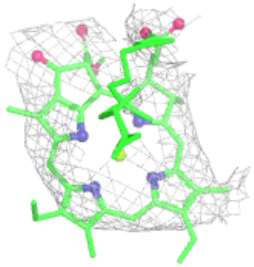


Electron density around CLA b 1226:

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

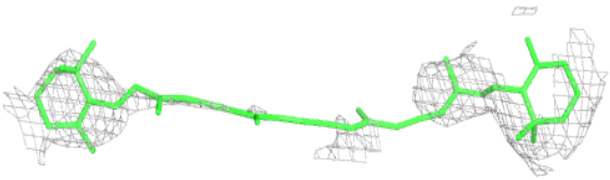


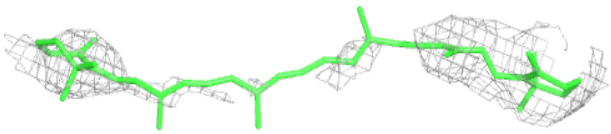


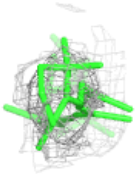


Electron density around BCR A 4003:

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

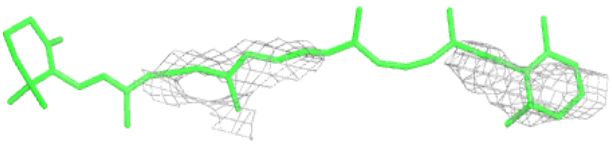


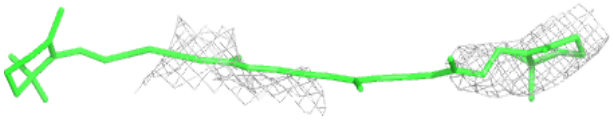


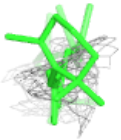


Electron density around BCR 1 4007:

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

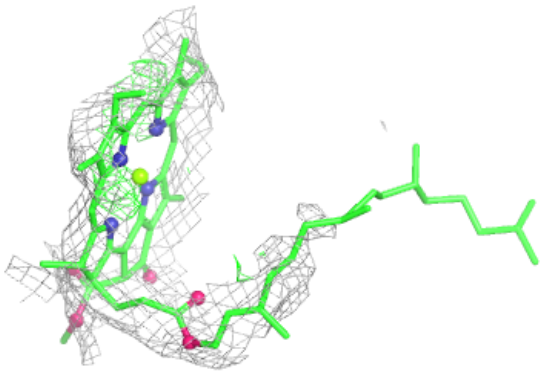


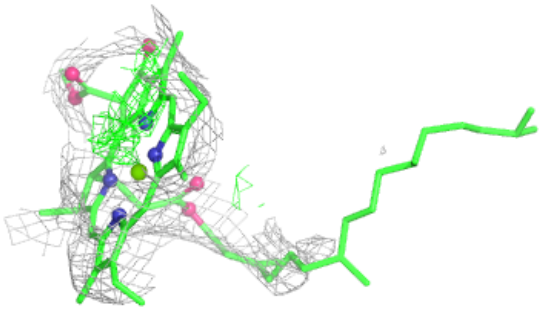


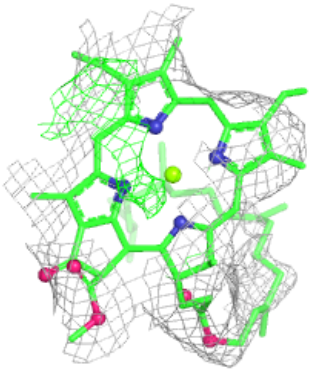


Electron density around CLA 2 1216:

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

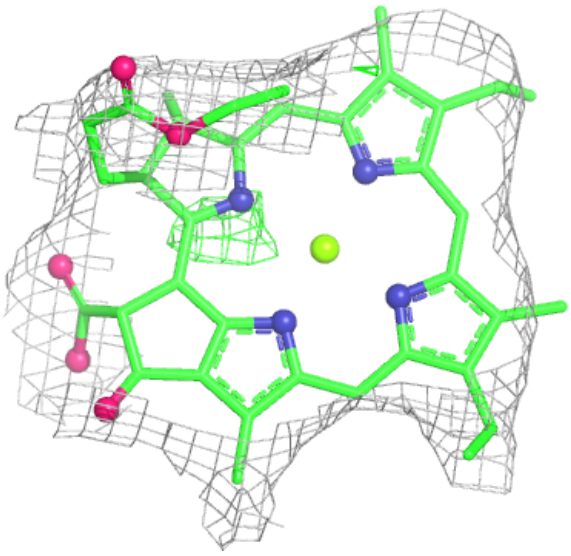


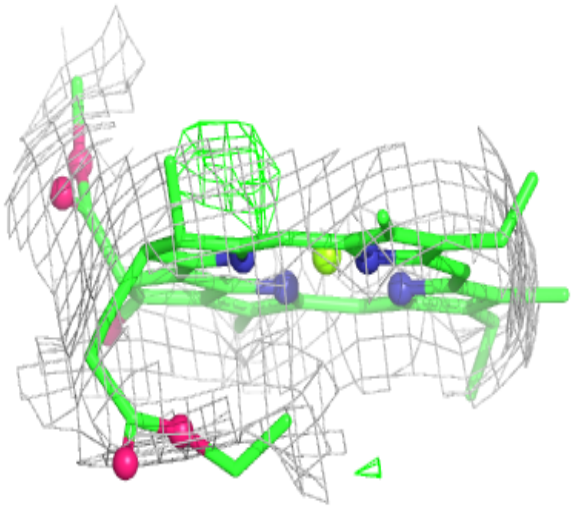


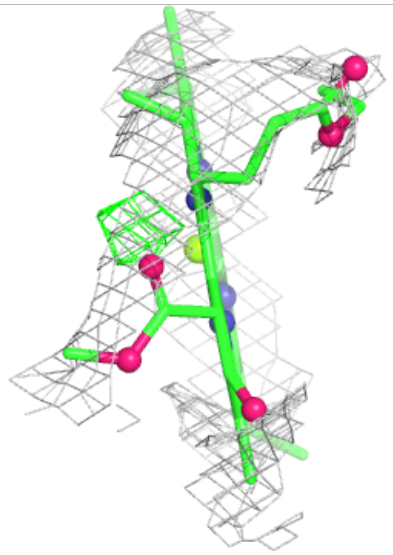


Electron density around CLA 2 1217:

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

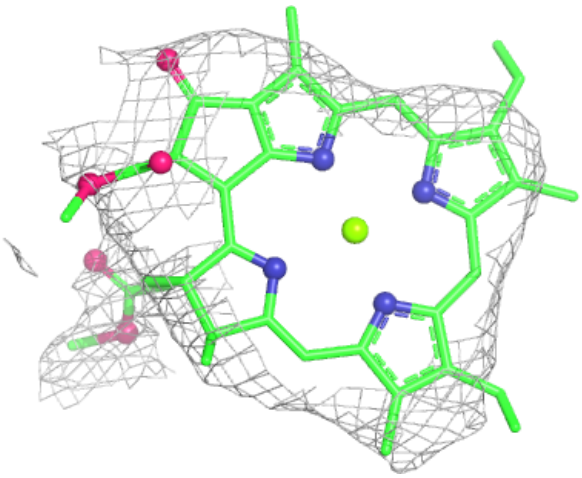


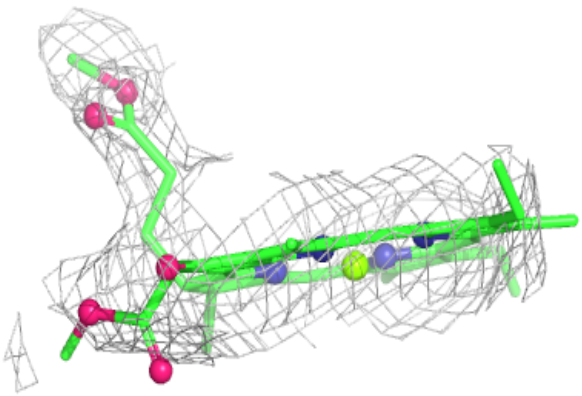




Electron density around CLA B 1220:

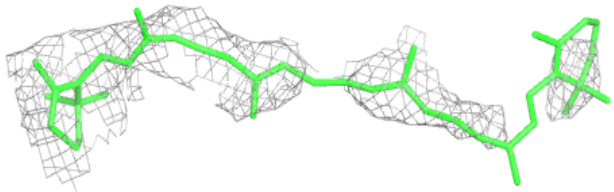
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

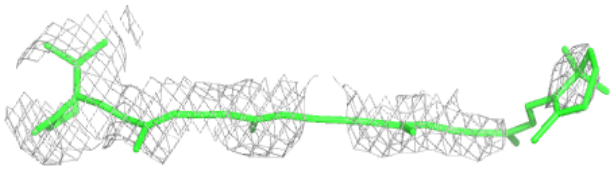


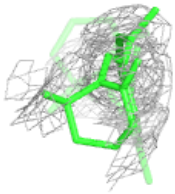


Electron density around BCR 2 4006:

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

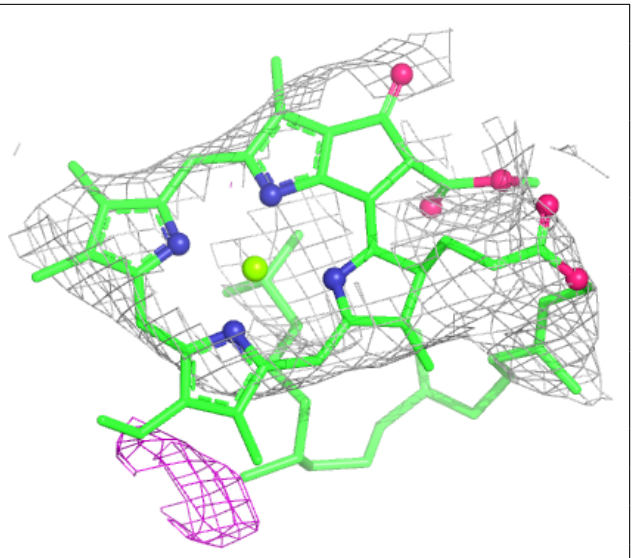


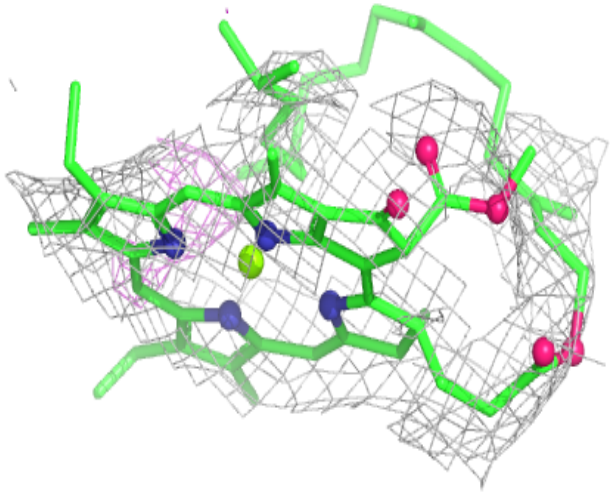


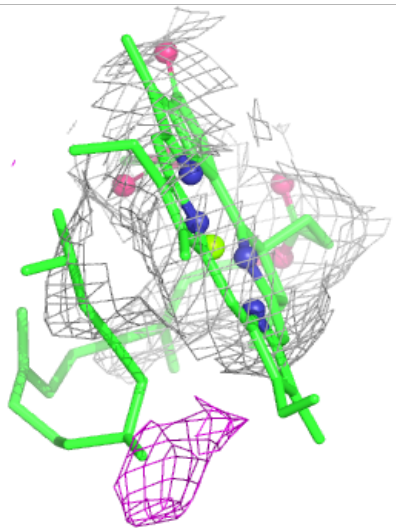


Electron density around CLA b 1203:

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

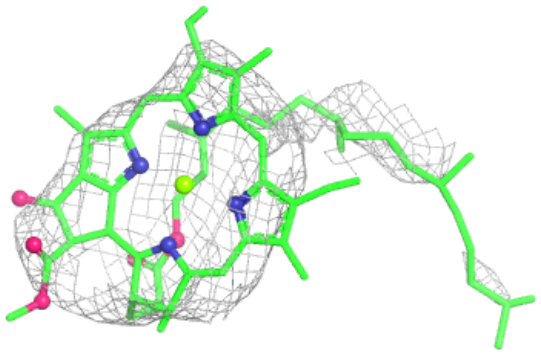


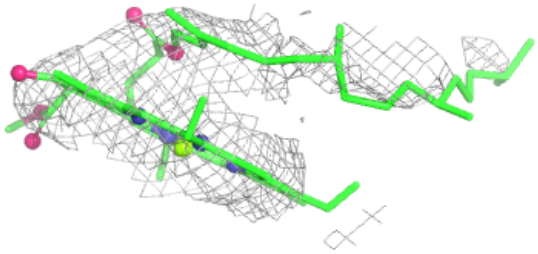


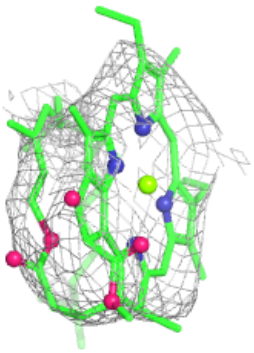


Electron density around CLA b 1204:

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

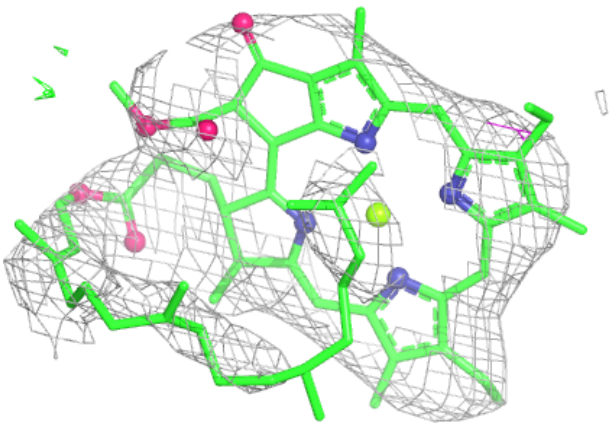


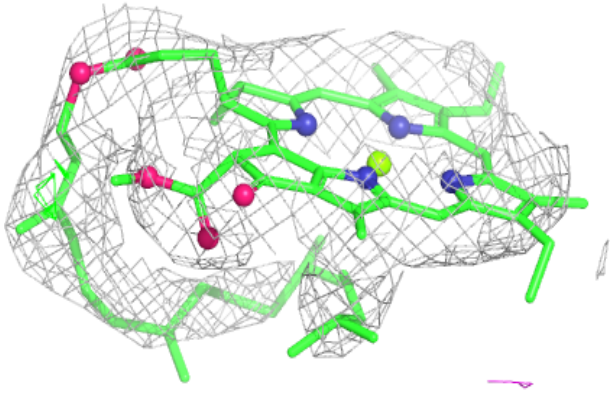


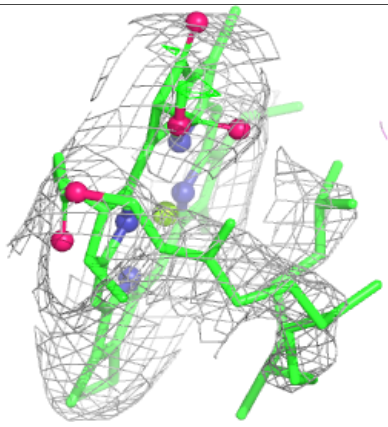


Electron density around CLA A 1104:

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

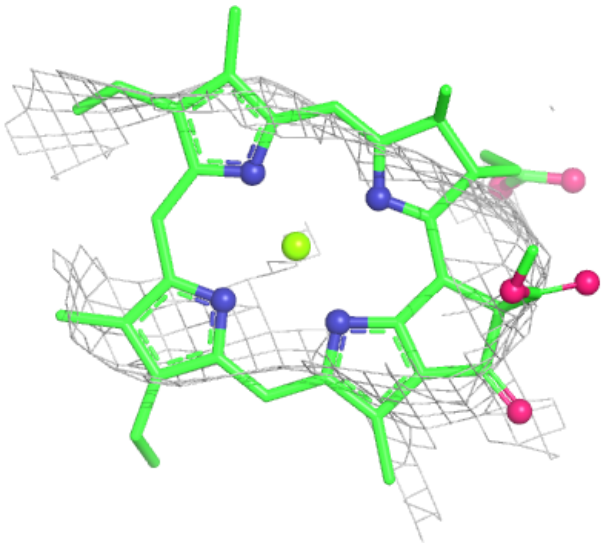


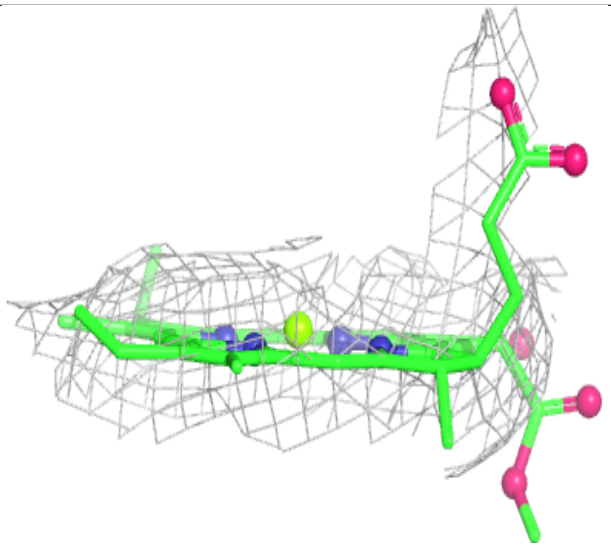


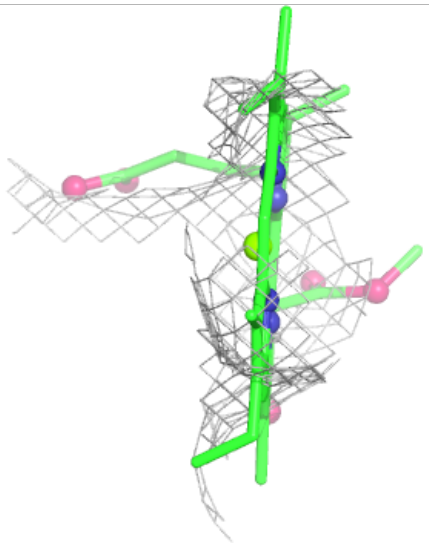


Electron density around CLA 1 1112:

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

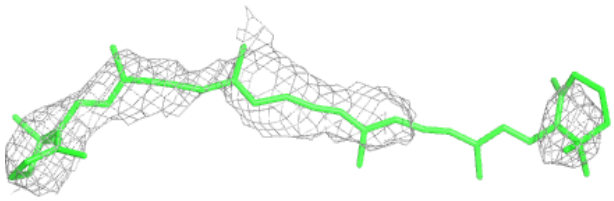


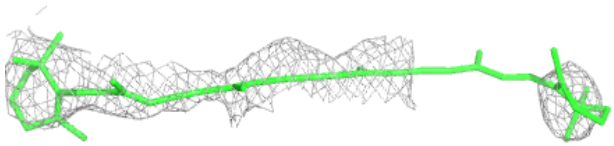


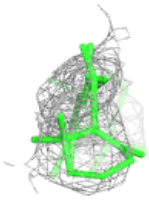


Electron density around BCR 2 4017:

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

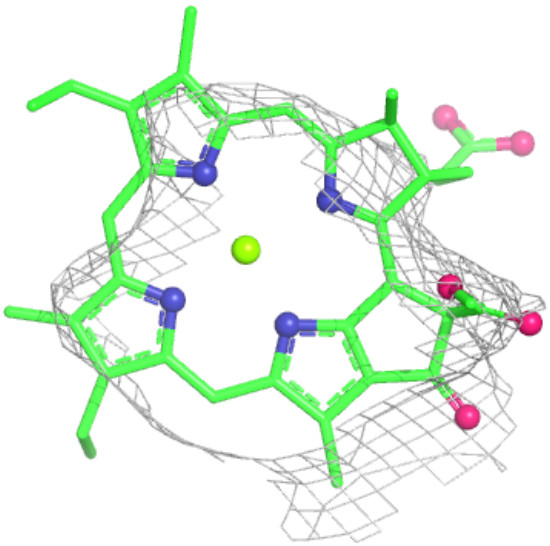


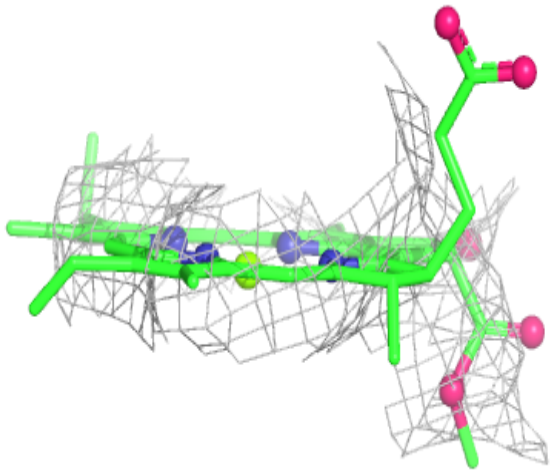


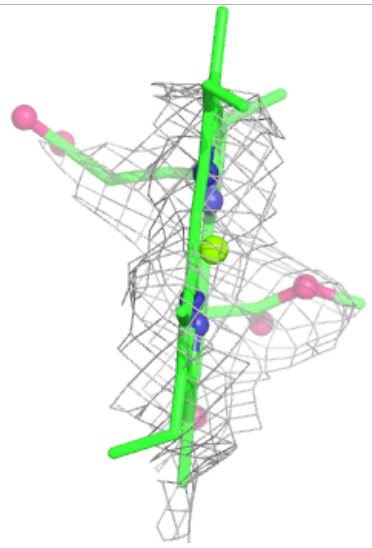


Electron density around CLA b 1231:

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

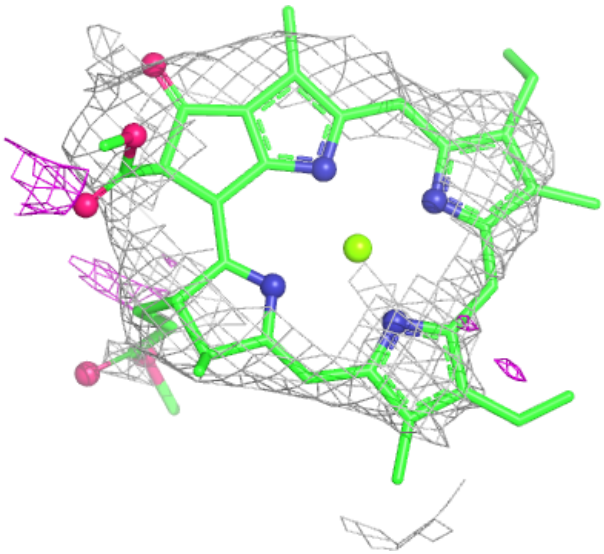


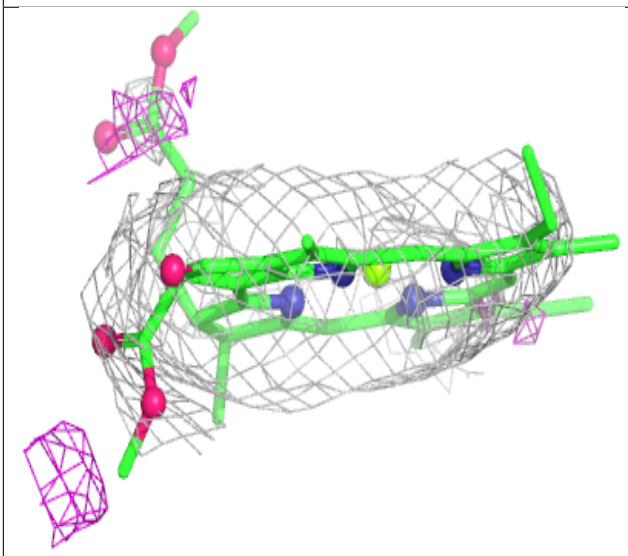




Electron density around CLA A 1129:

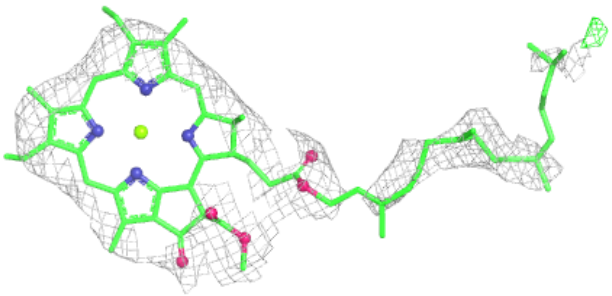
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

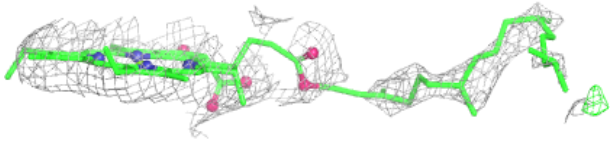


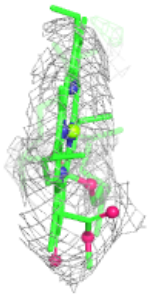


Electron density around CLA a 1131:

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

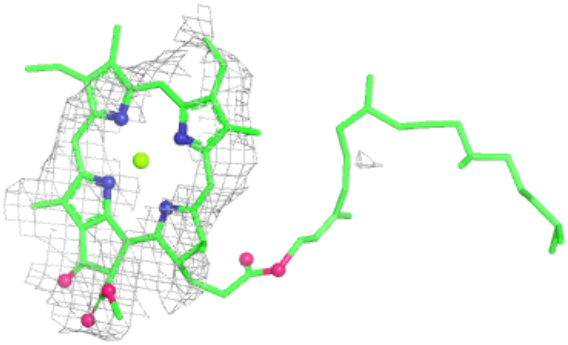


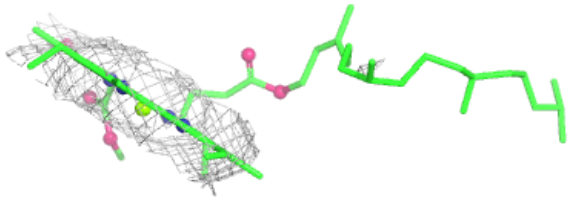


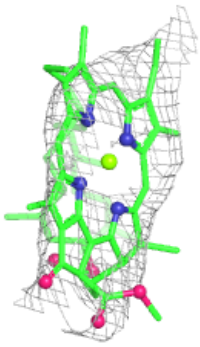


Electron density around CLA a 1106:

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

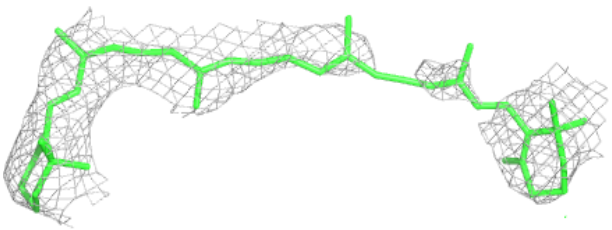


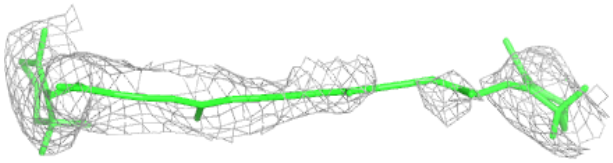


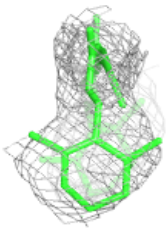


Electron density around BCR F 4020:

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

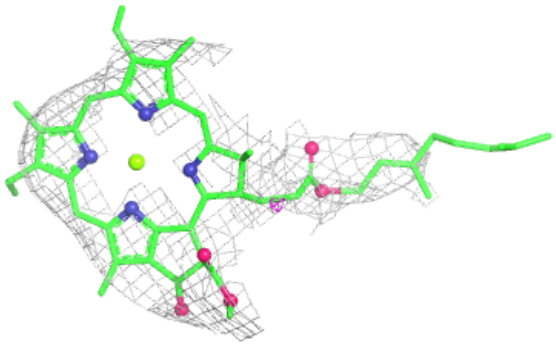


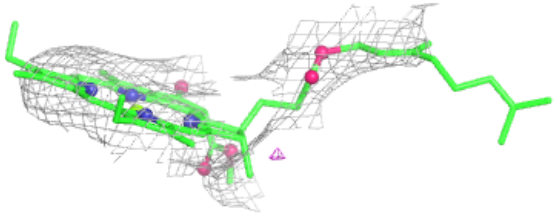


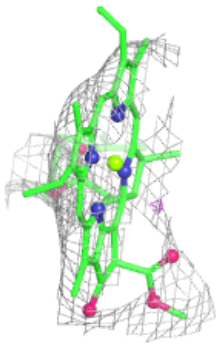


Electron density around CLA 1 1124:

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

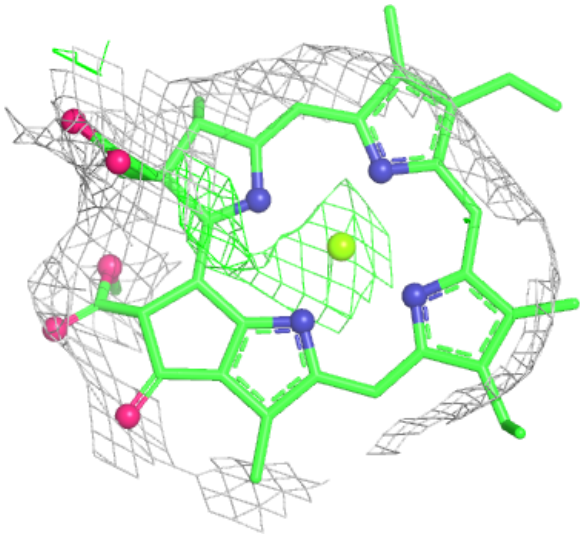






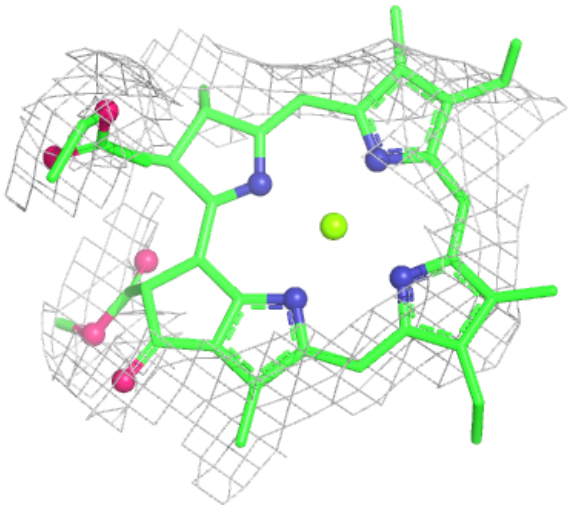
Electron density around CLA 2 1231:

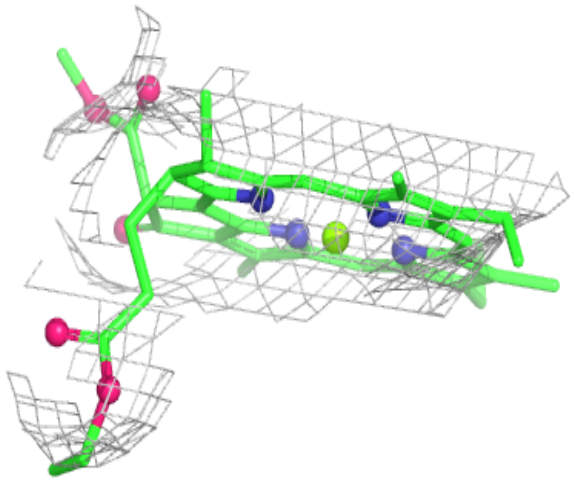
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

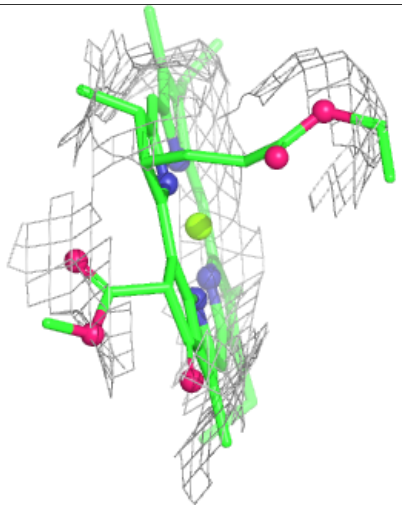


Electron density around CLA b 1236:

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

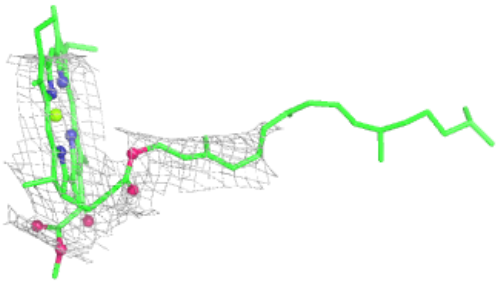


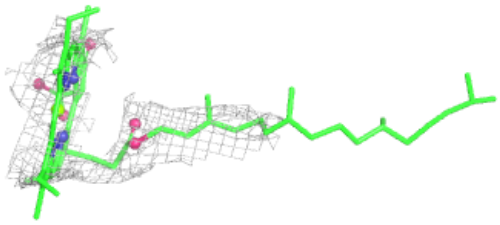


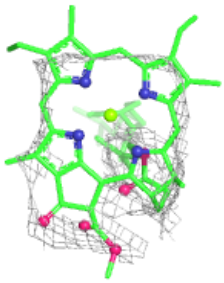


Electron density around CLA 1 1126:

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

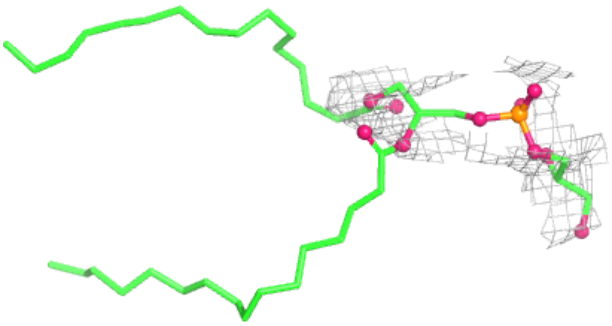


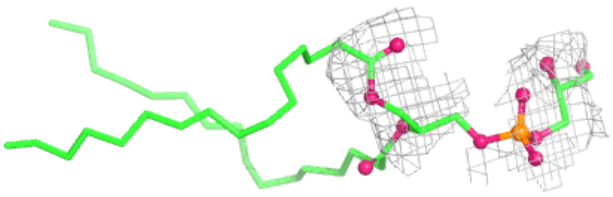




Electron density around LHG a 5001:

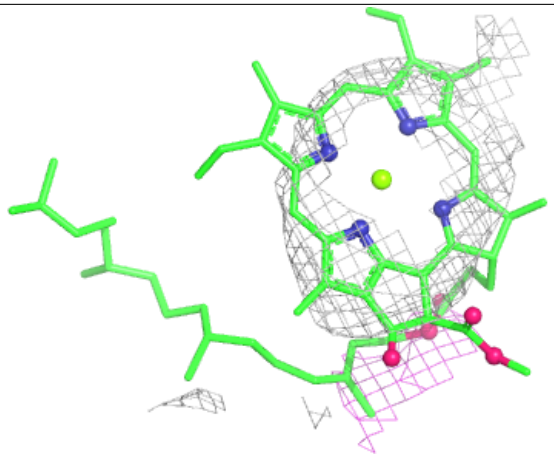
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

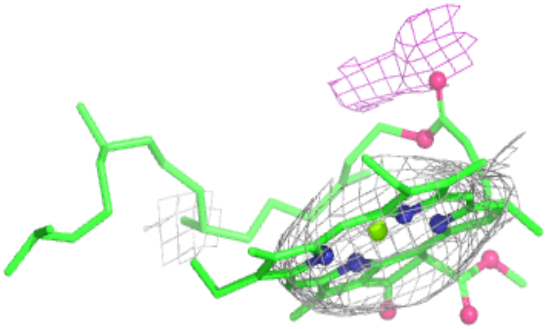


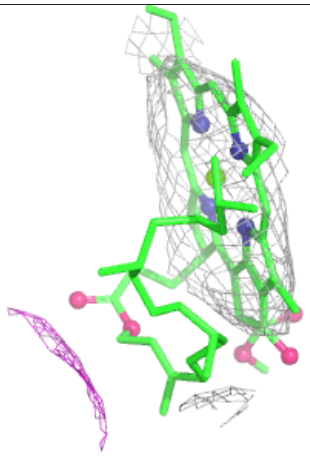


Electron density around CLA 1 1127:

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

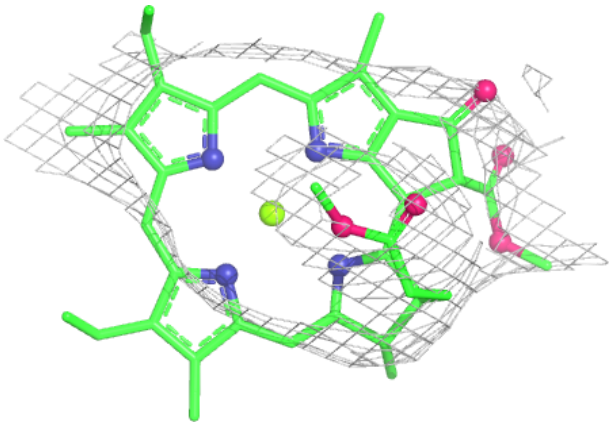


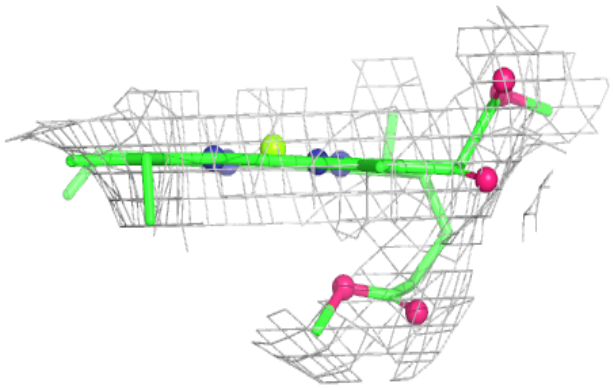


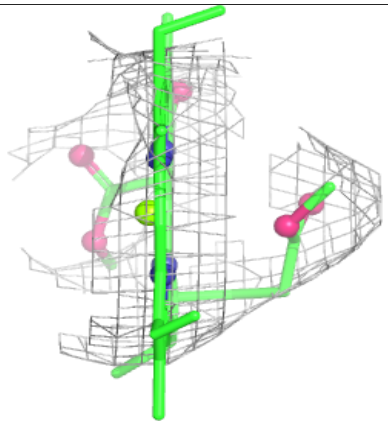


Electron density around CLA a 1138:

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

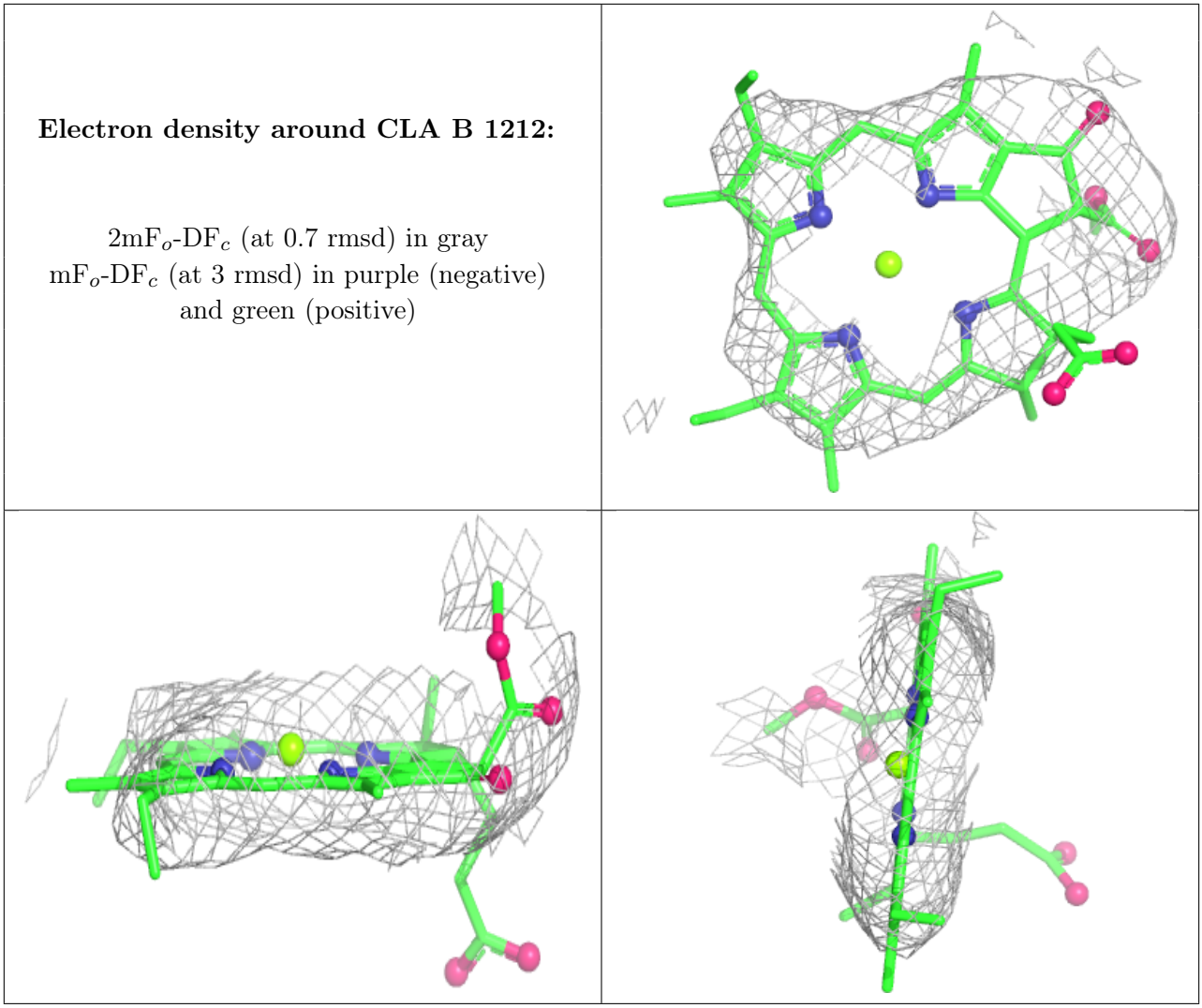






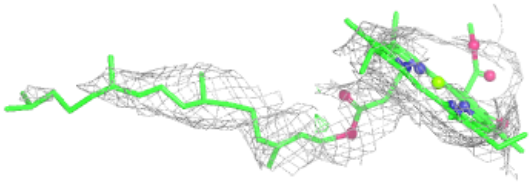
Electron density around CLA B 1212:

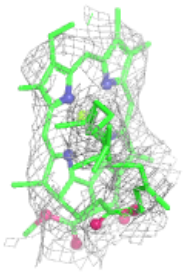
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 1132:

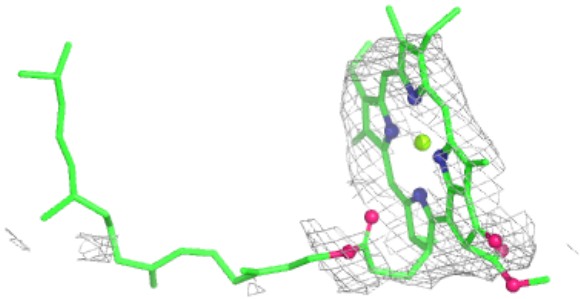
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

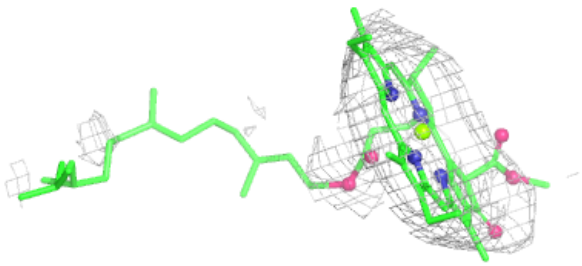


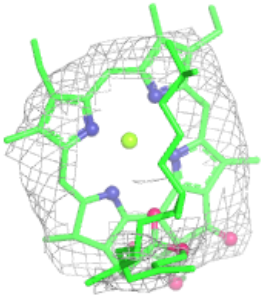


Electron density around CLA 1 1140:

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

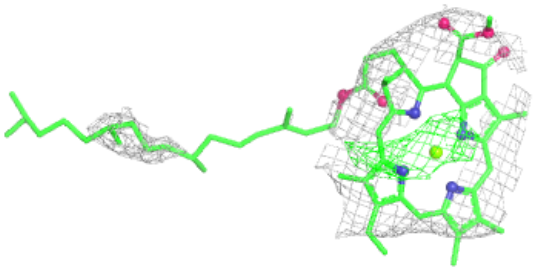


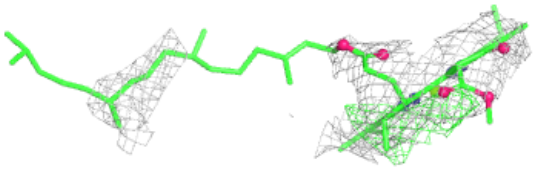




Electron density around CLA 8 1501:

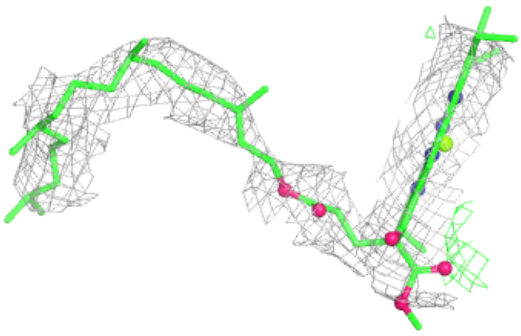
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

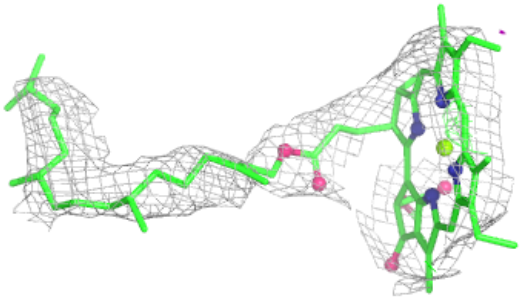


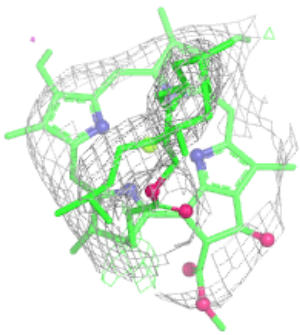


Electron density around CLA b 1238:

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

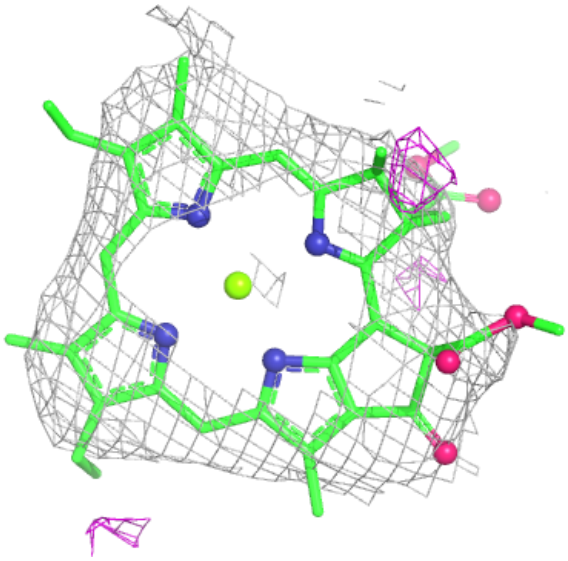


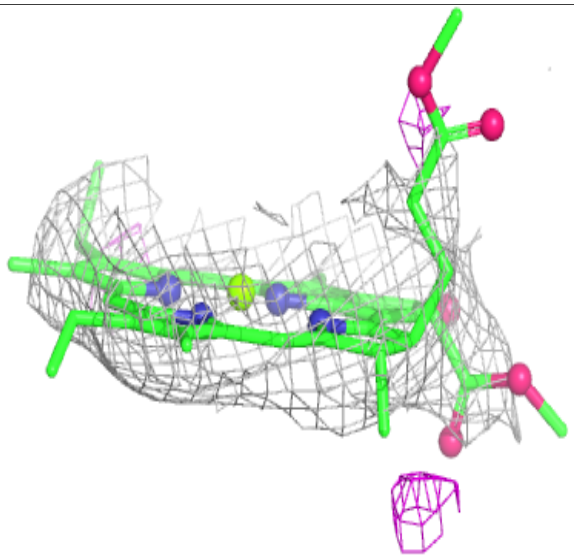


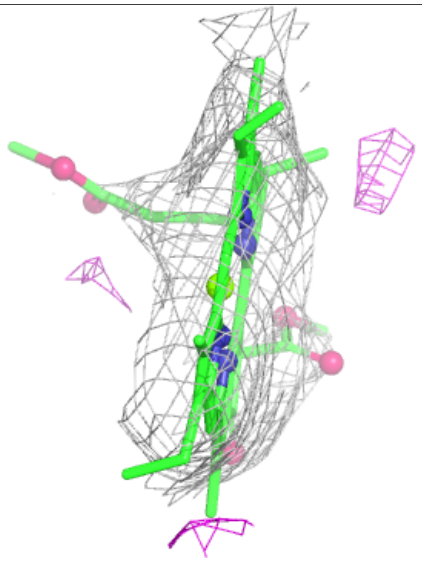


Electron density around CLA A 1133:

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

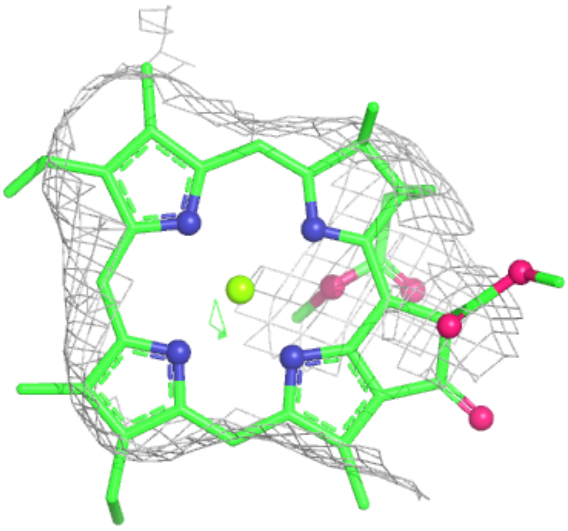


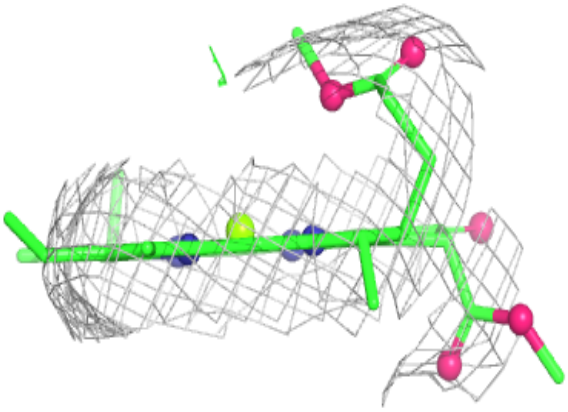


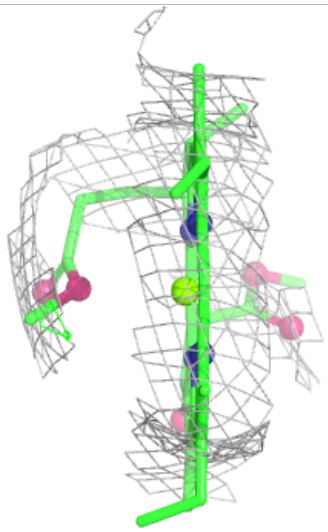


Electron density around CLA a 1136:

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

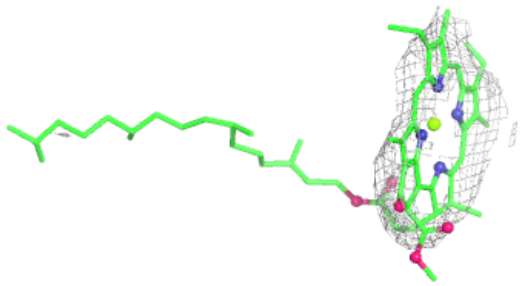


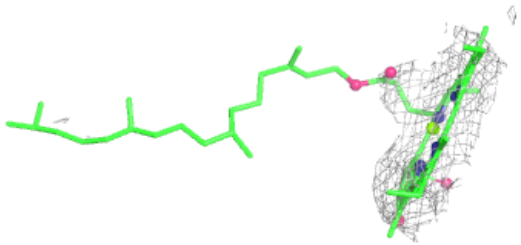


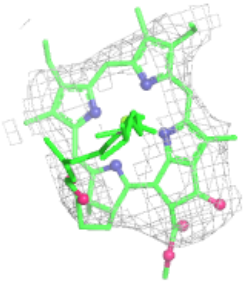


Electron density around CLA B 1225:

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

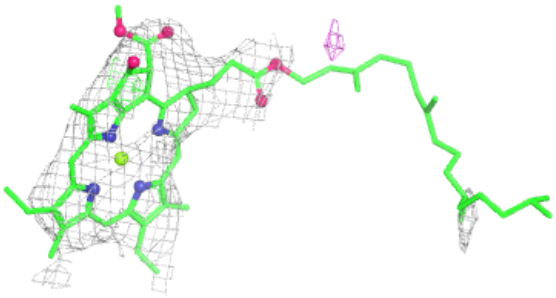


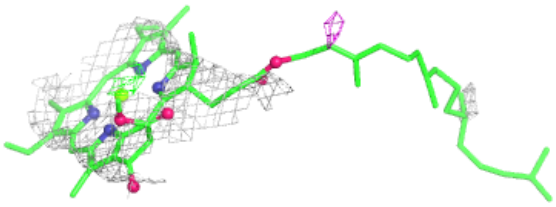


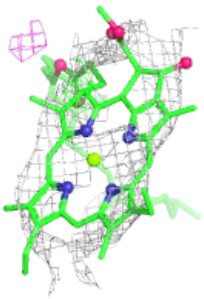


Electron density around CLA 1 1012:

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

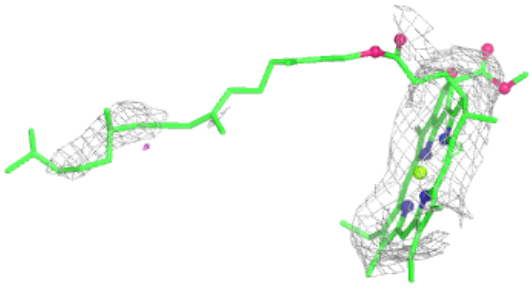


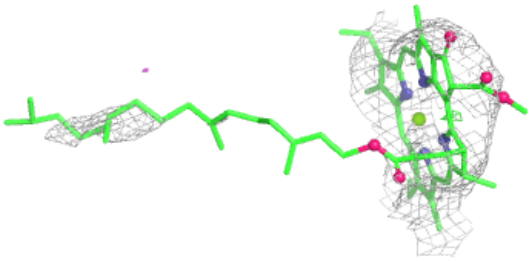


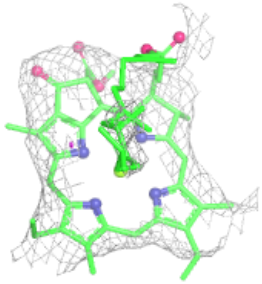


Electron density around CLA B 1226:

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

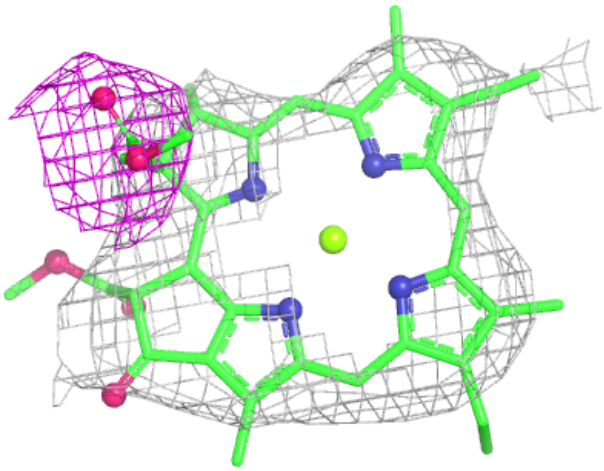


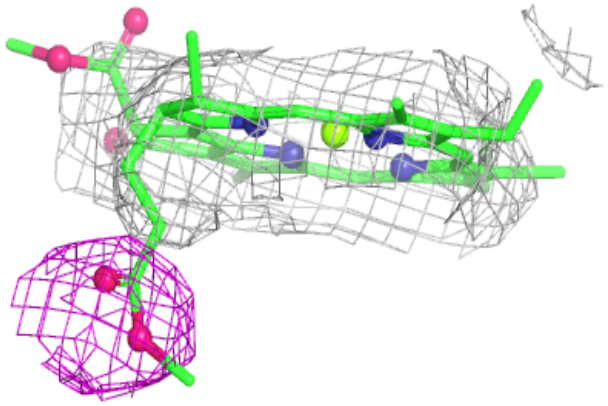


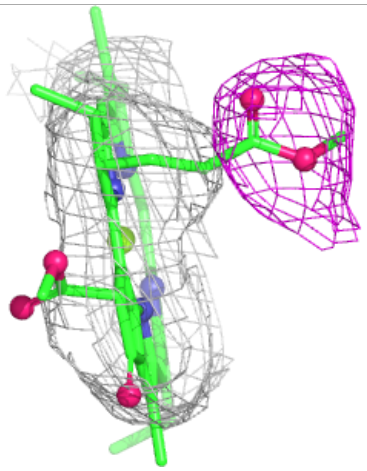


Electron density around CLA A 1130:

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

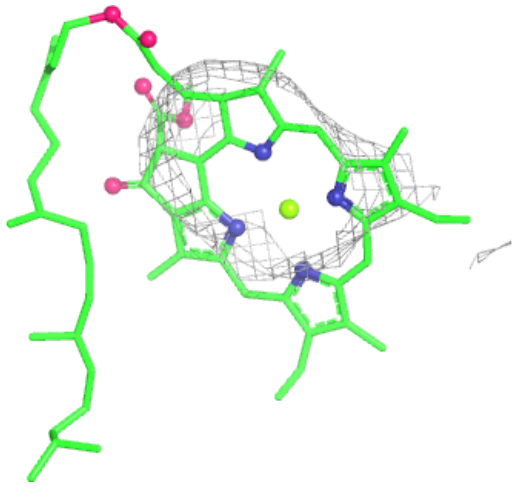


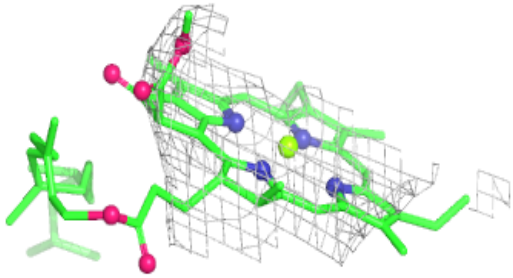


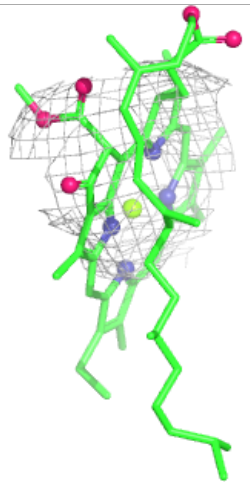


Electron density around CLA a 1123:

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

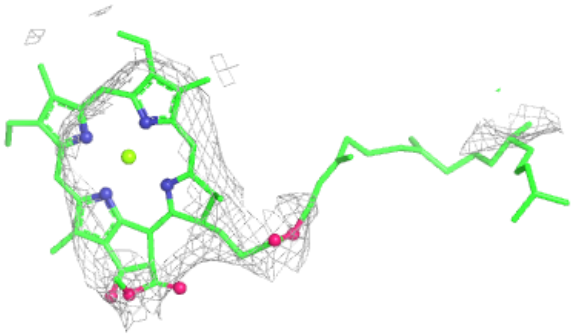


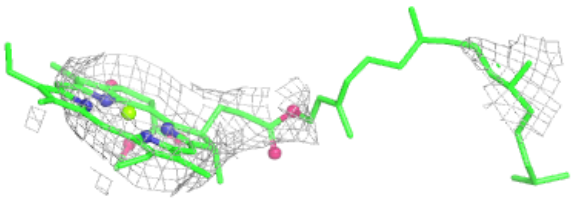


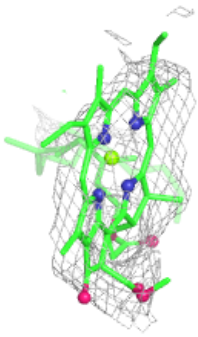


Electron density around CLA B 1210:

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

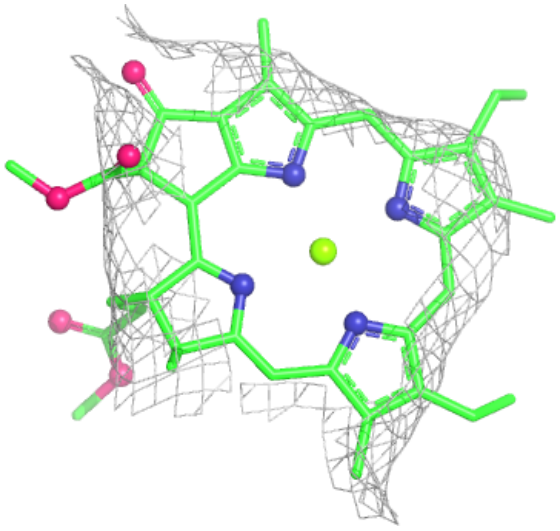


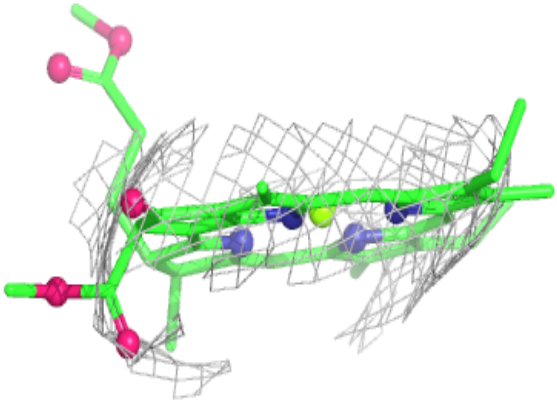


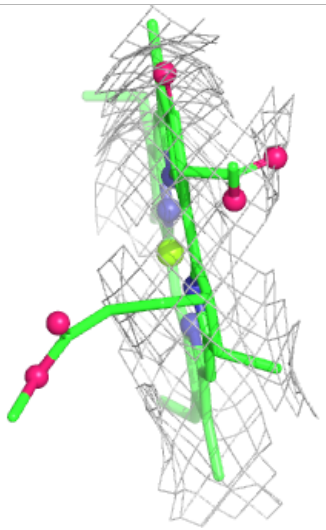


Electron density around CLA 1 1133:

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

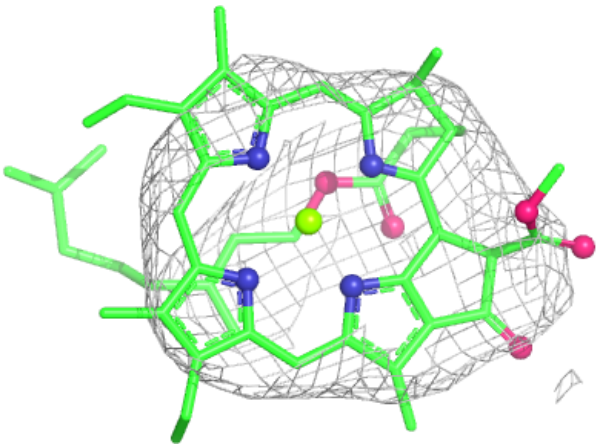


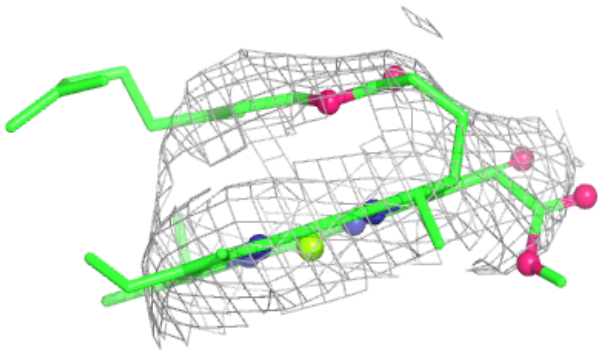


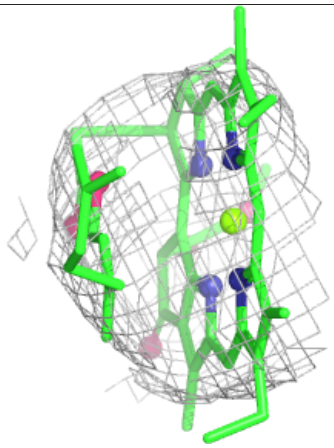


Electron density around CLA b 1205:

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

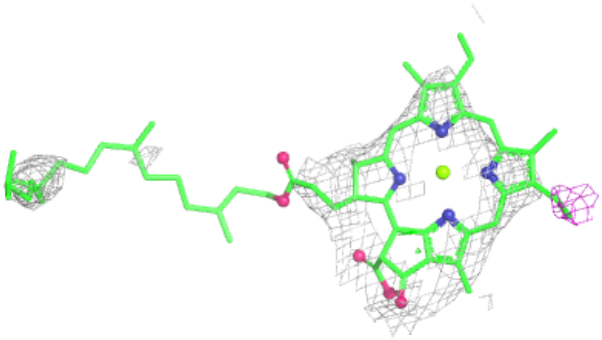


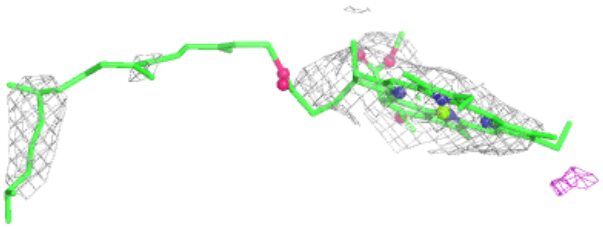




Electron density around CLA A 1103:

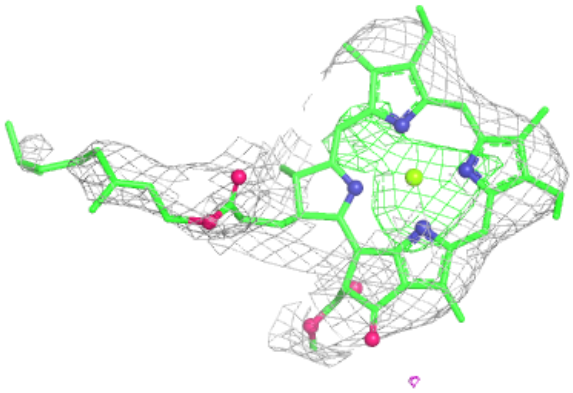
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

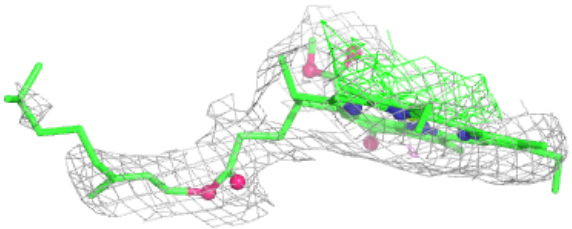


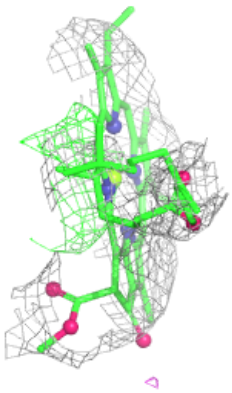


Electron density around CLA A 1124:

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

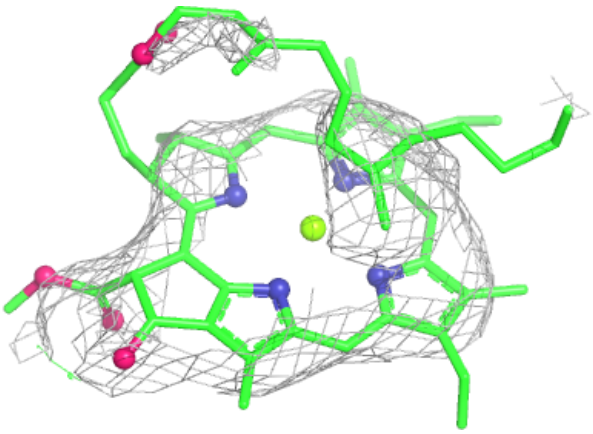


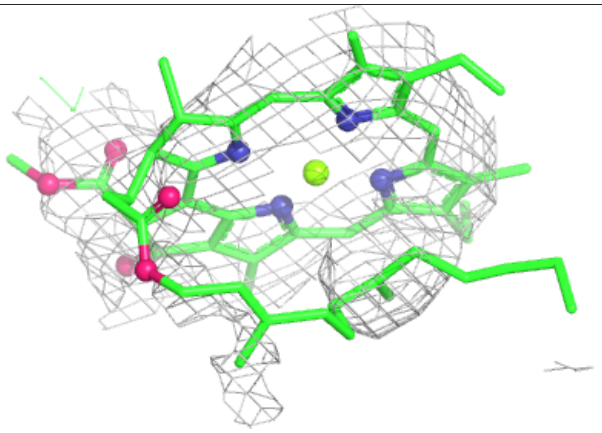


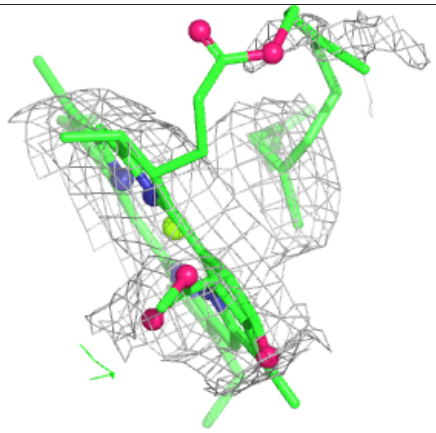


Electron density around CLA B 1214:

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

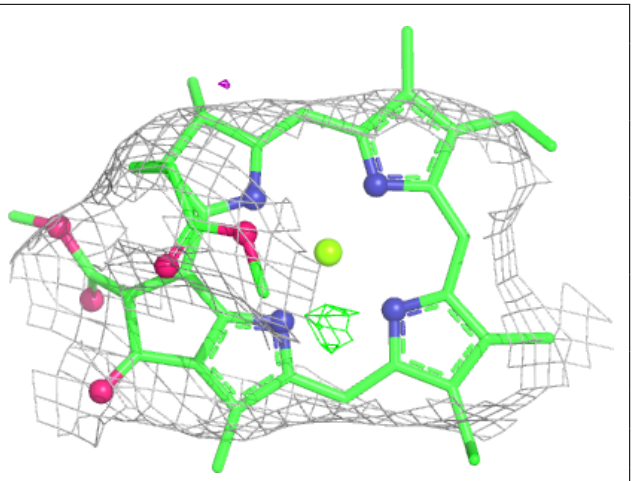


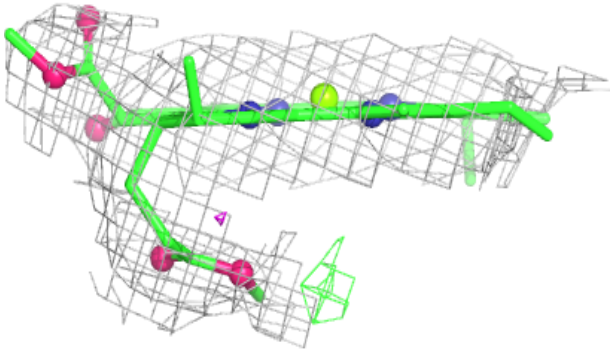


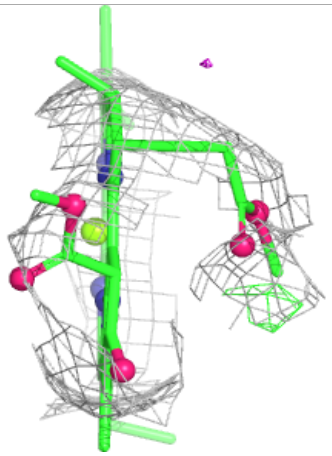


Electron density around CLA A 1138:

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

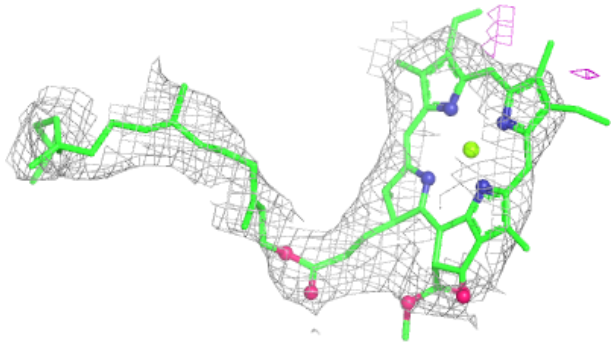


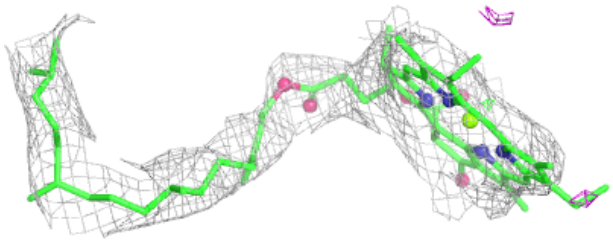


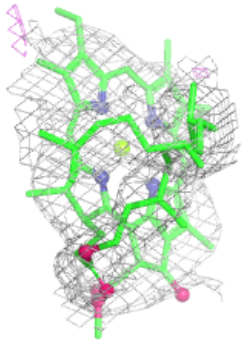


Electron density around CLA 2 1206:

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

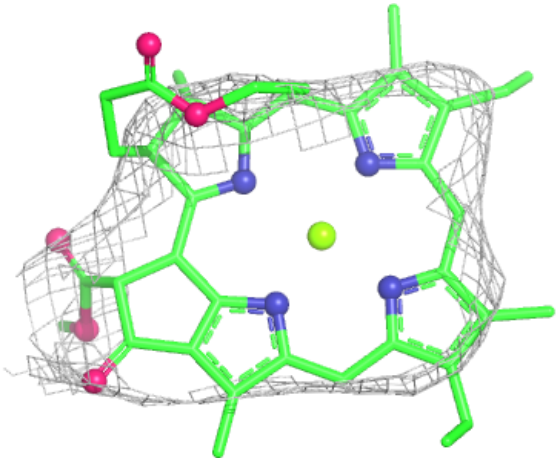


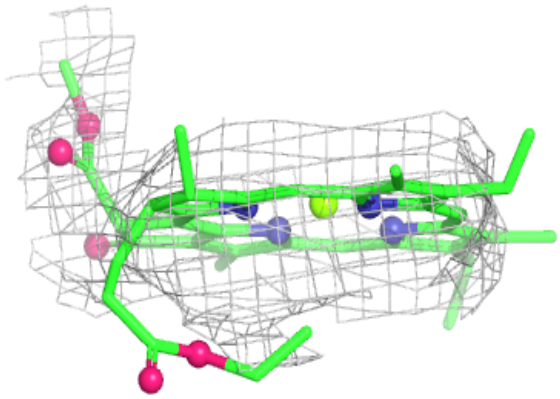


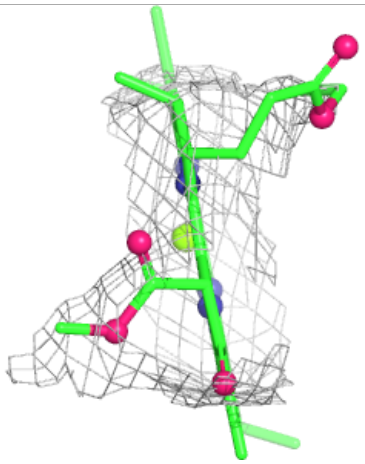


Electron density around CLA B 1217:

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

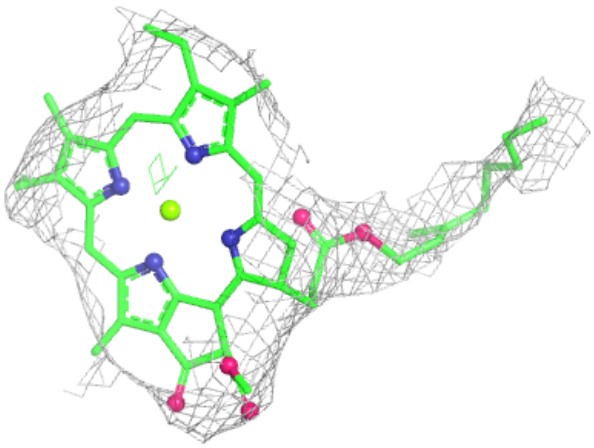


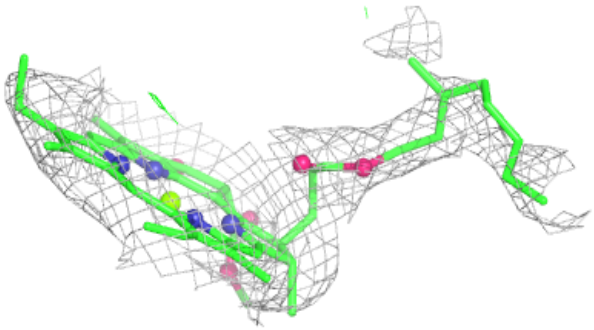


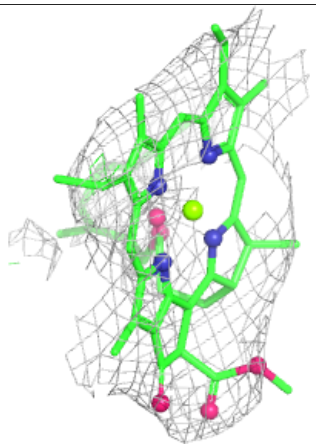


Electron density around CLA A 1110:

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

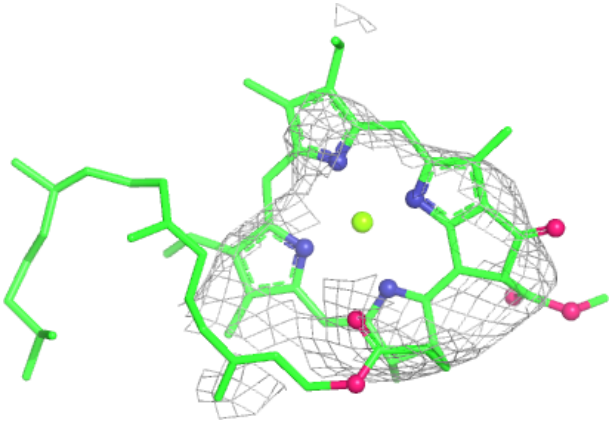


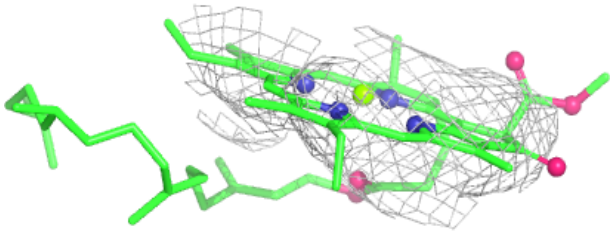




Electron density around CLA 1 1117:

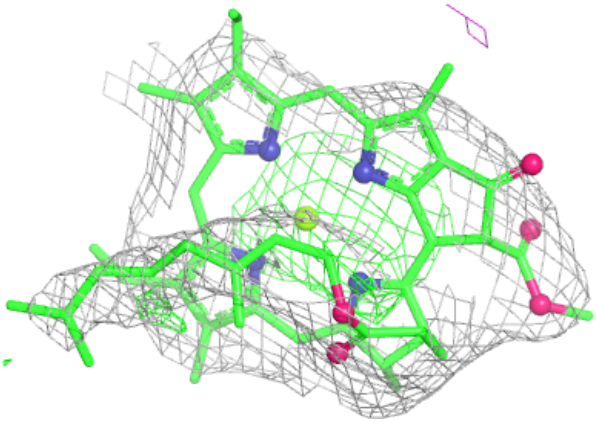
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

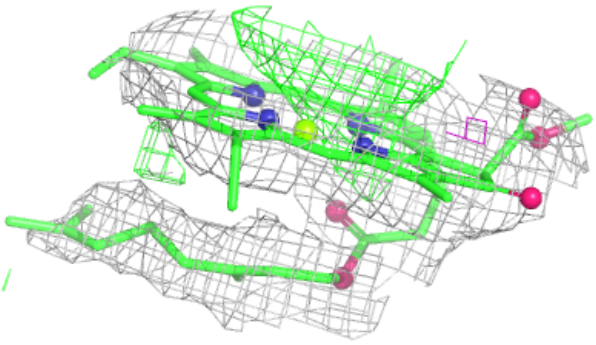


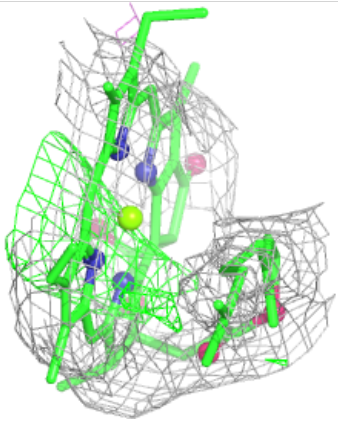


Electron density around CLA A 1237:

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

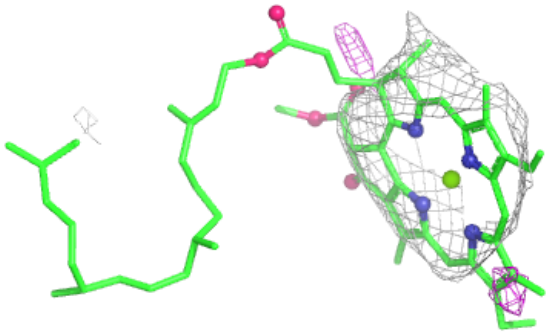


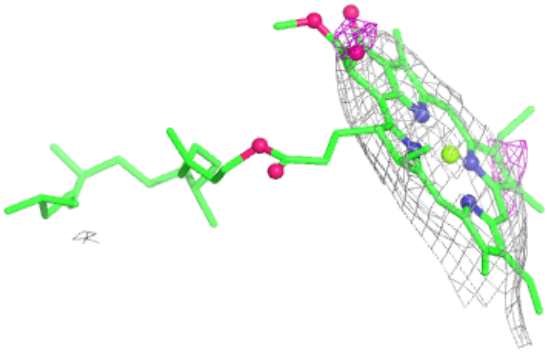


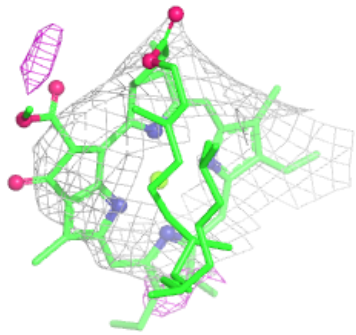


Electron density around CLA a 1011:

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

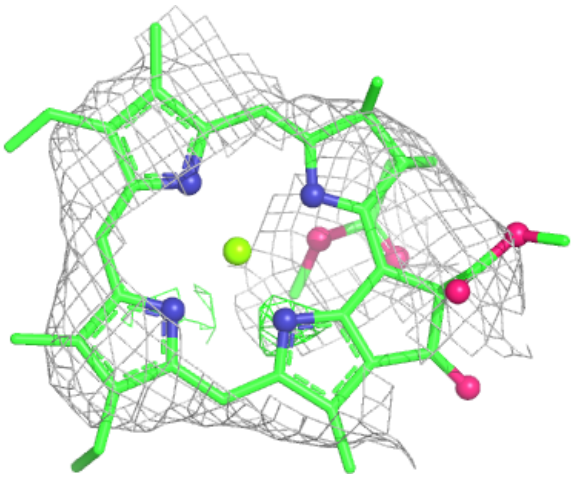


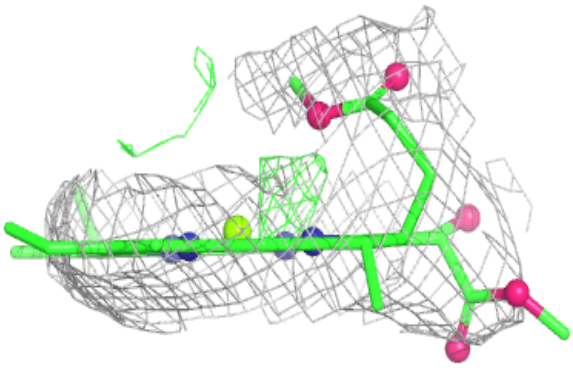


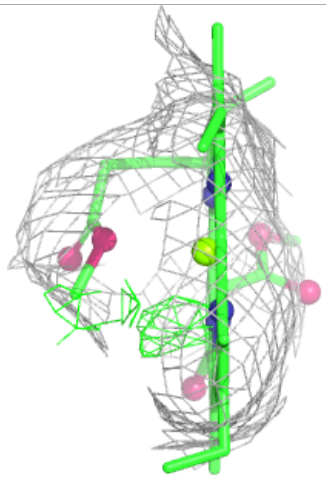


Electron density around CLA A 1136:

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

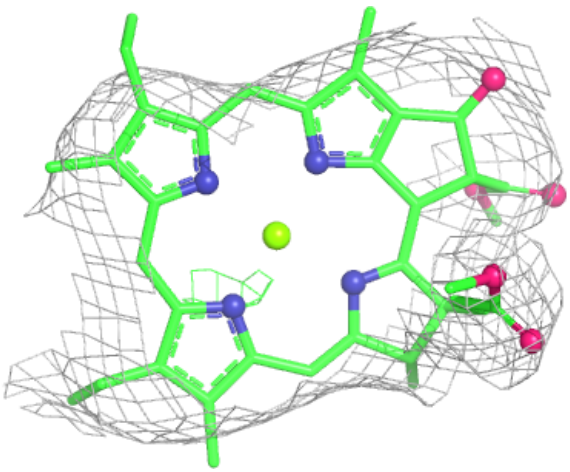


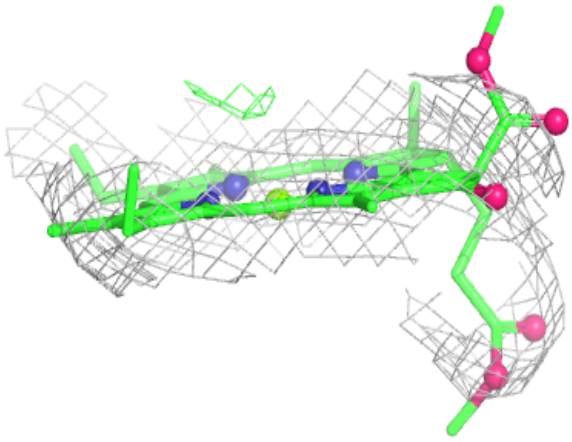


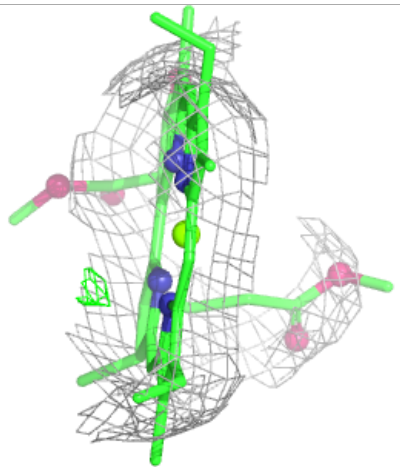


Electron density around CLA B 1211:

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

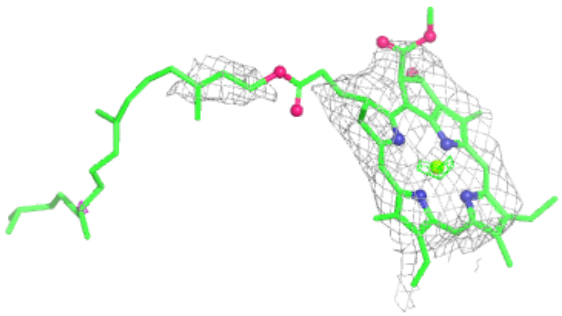


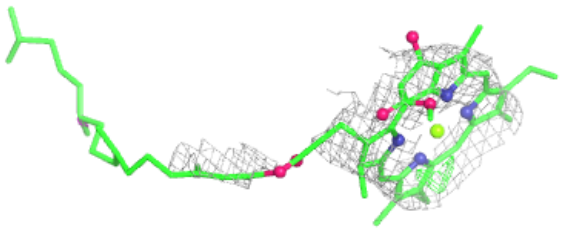


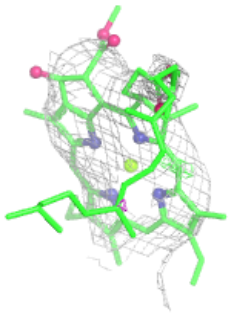


Electron density around CLA A 1012:

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

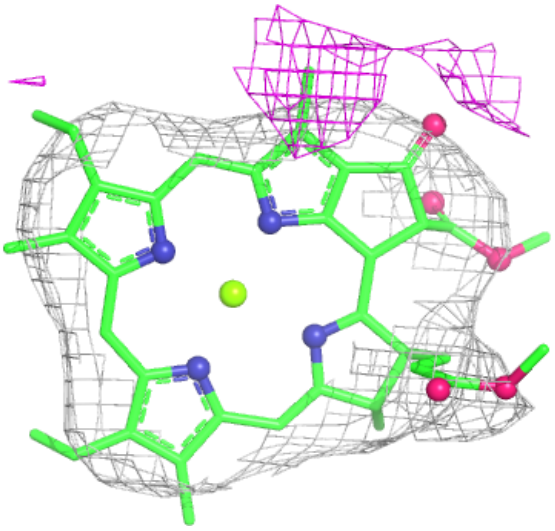


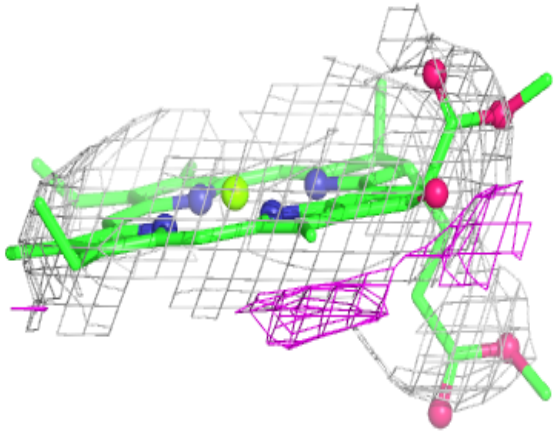




Electron density around CLA B 1239:

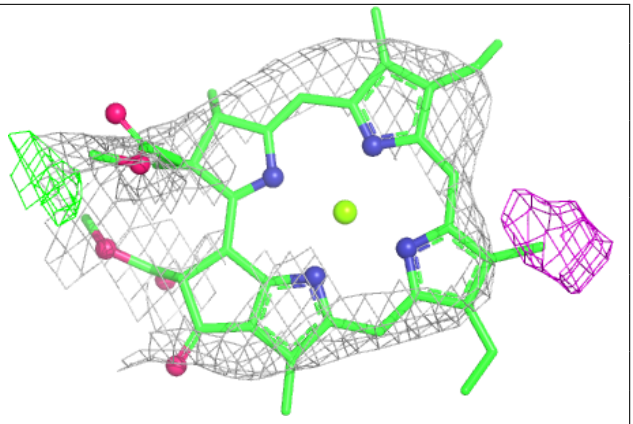
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

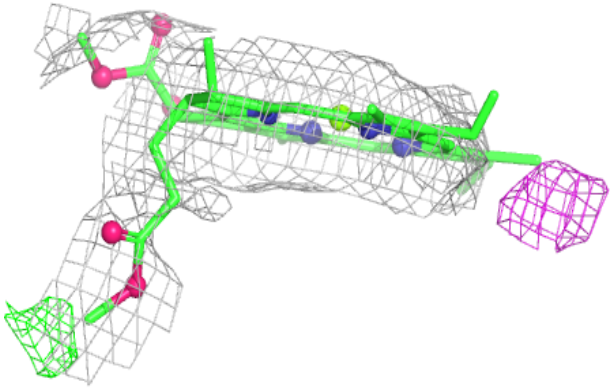


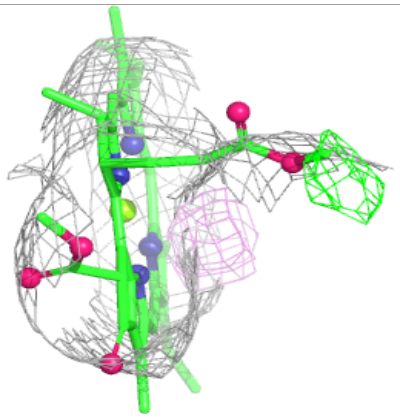


Electron density around CLA 2 1220:

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

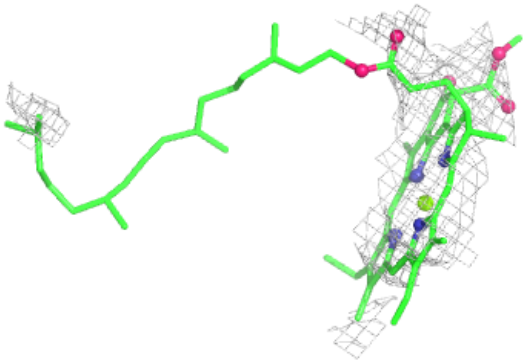


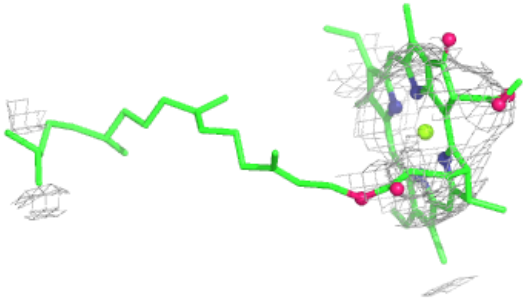


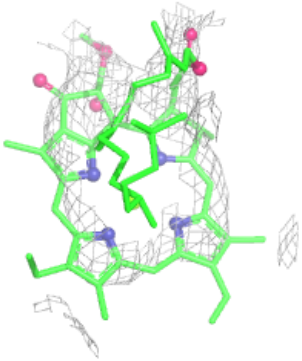


Electron density around CLA 1 1128:

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

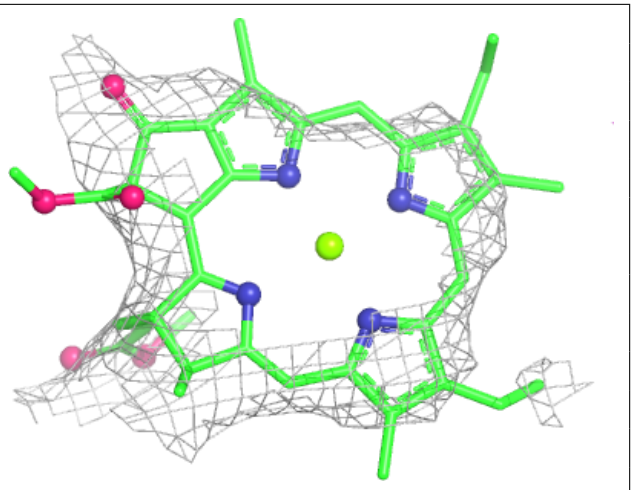


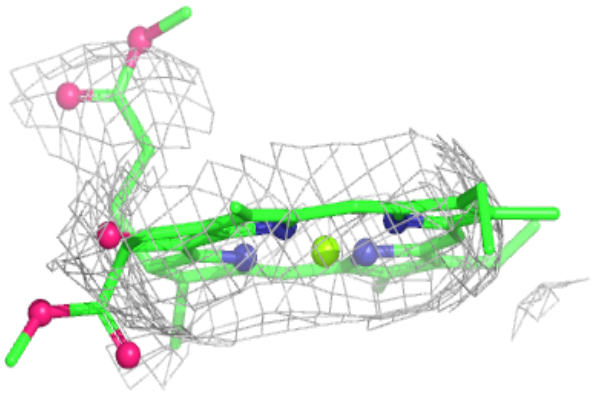


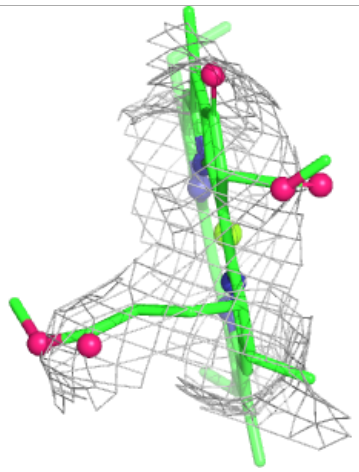


Electron density around CLA 1 1130:

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

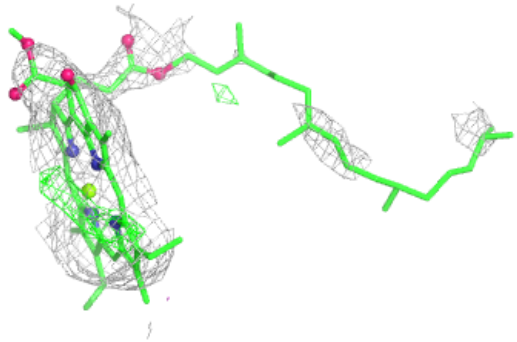


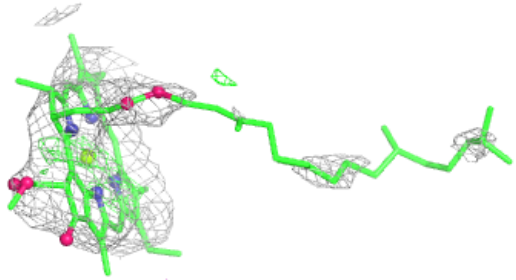


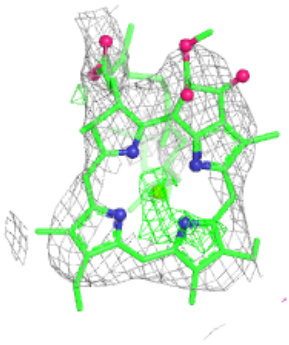


Electron density around CLA A 1128:

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

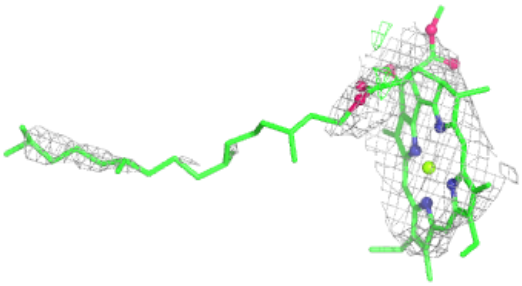


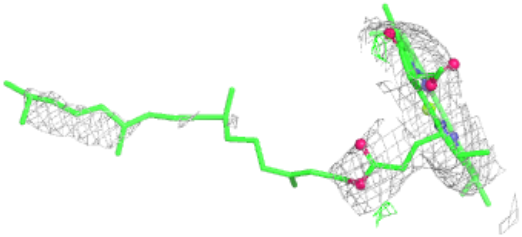


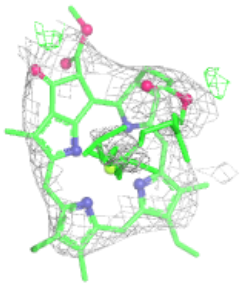


Electron density around CLA 2 1225:

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

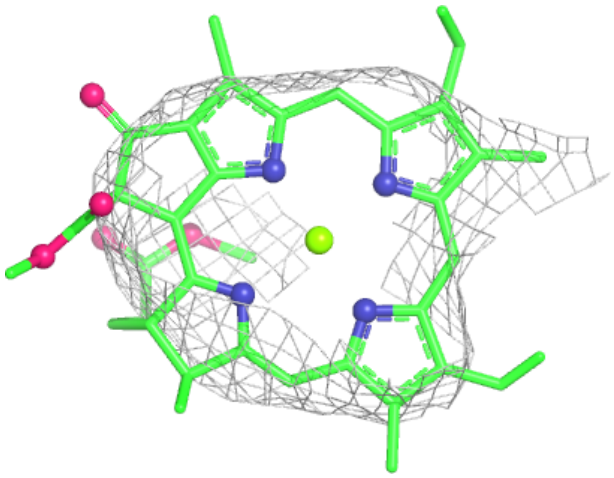


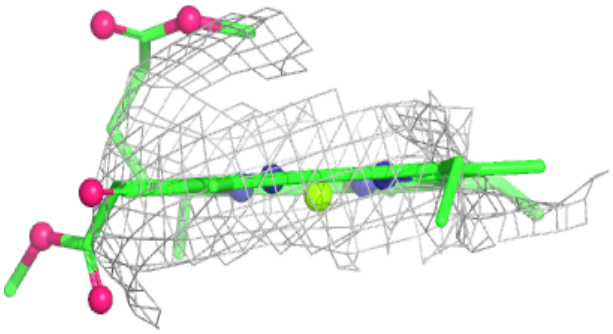


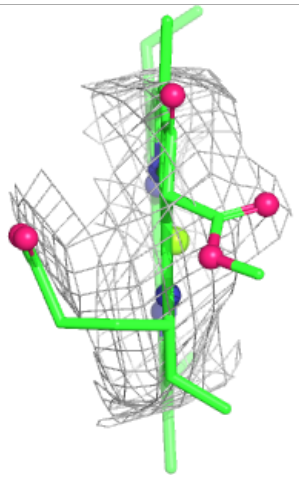


Electron density around CLA a 1115:

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

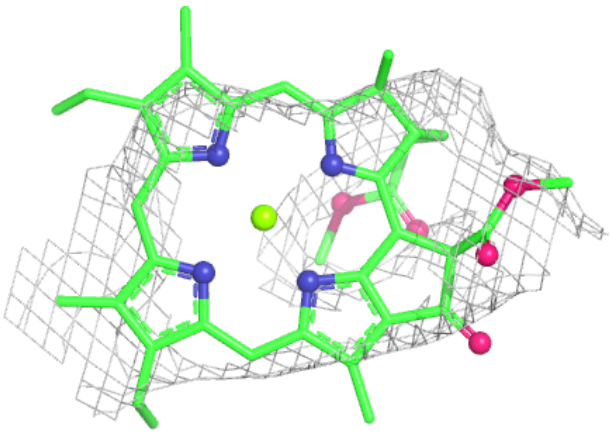


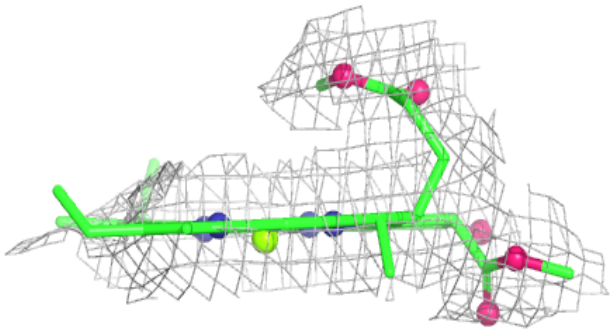


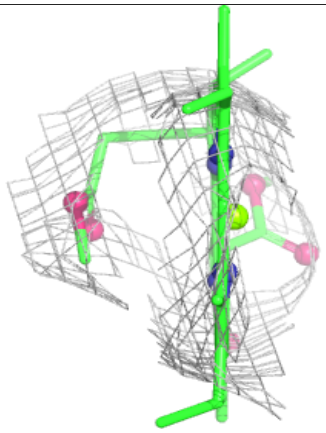


Electron density around CLA 1 1138:

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

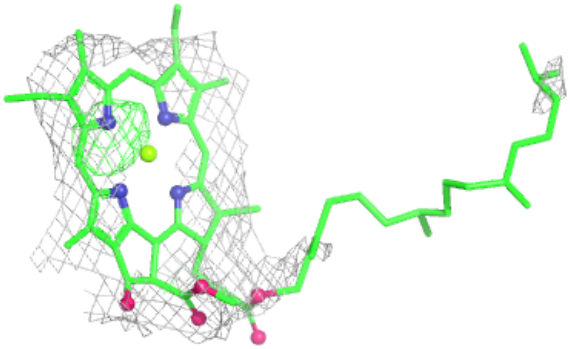


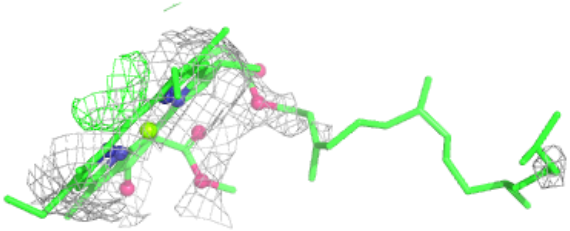


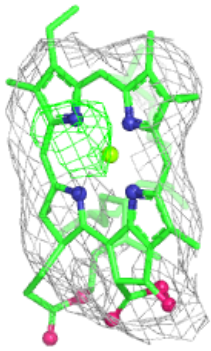


Electron density around CLA B 1207:

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

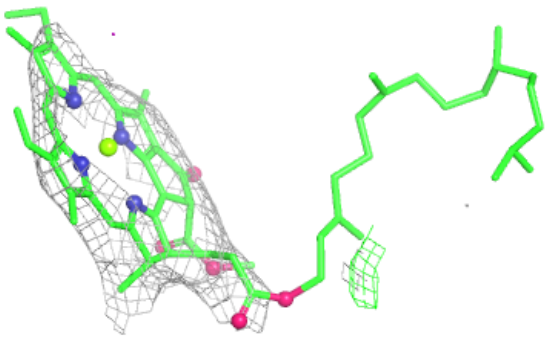


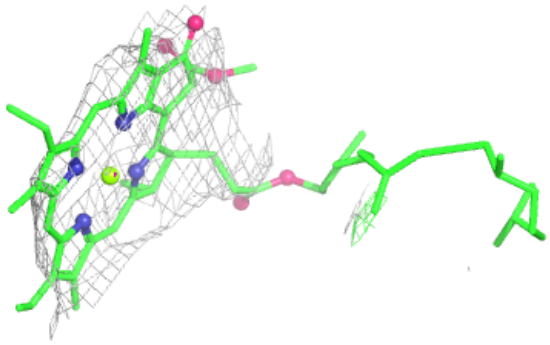


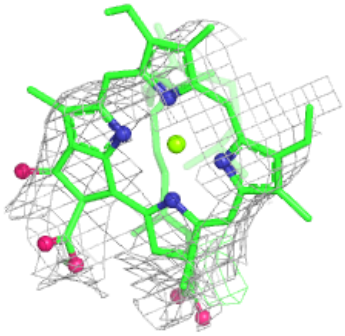


Electron density around CLA b 1021:

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

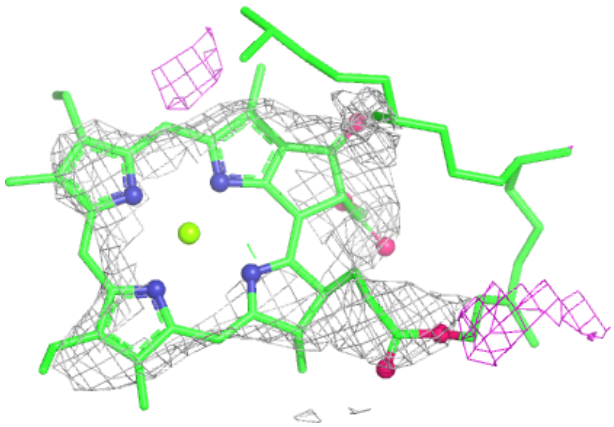


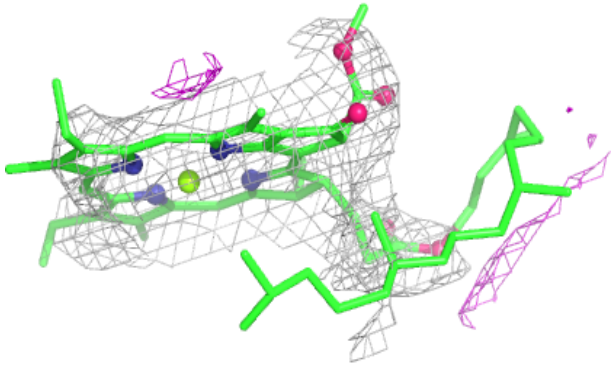


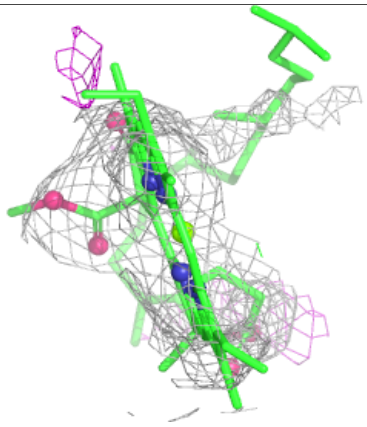


Electron density around CLA 2 1202:

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

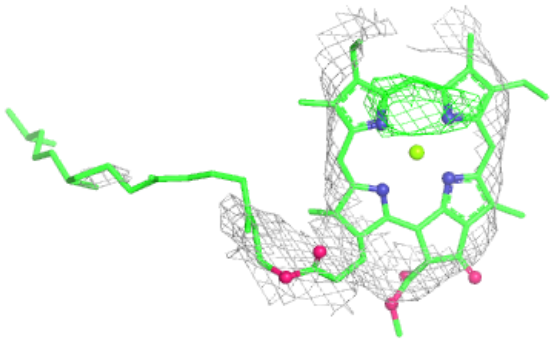


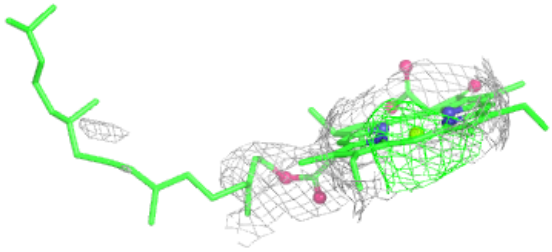


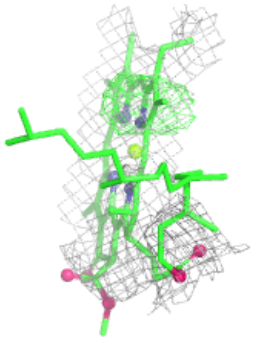


Electron density around CLA b 1023:

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

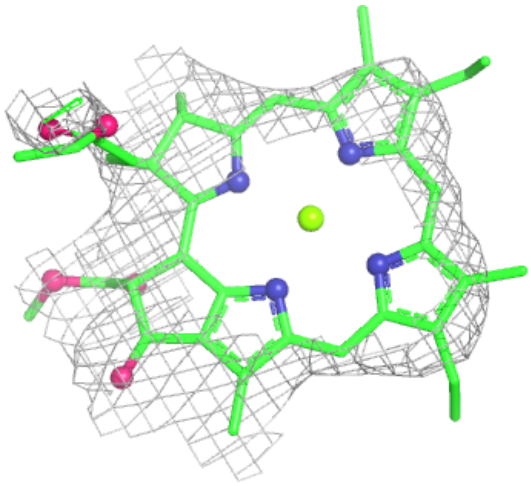


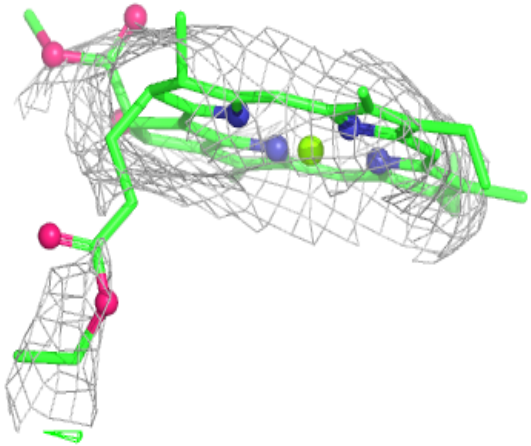


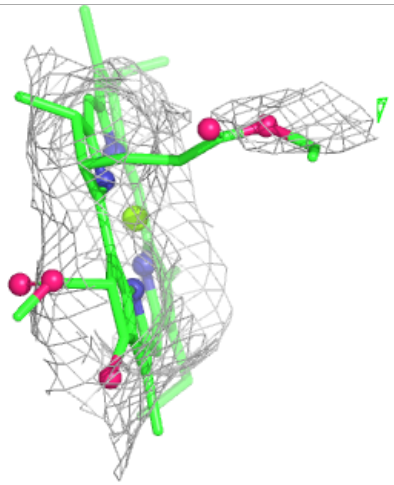


Electron density around CLA B 1236:

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

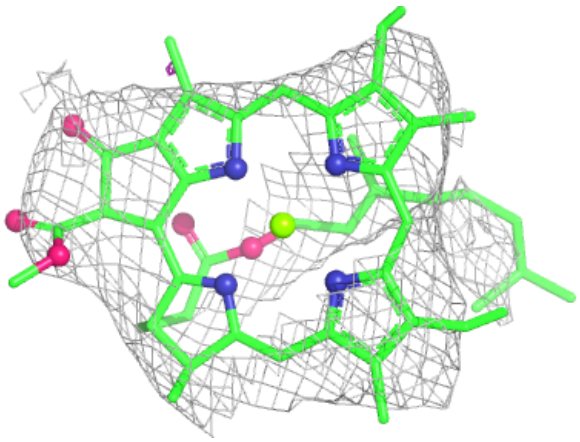


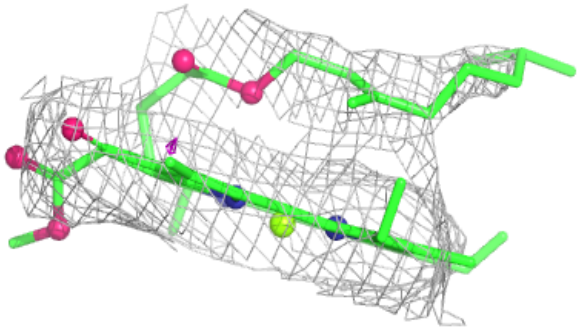


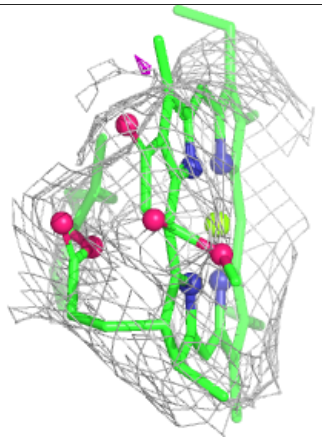


Electron density around CLA 2 1205:

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

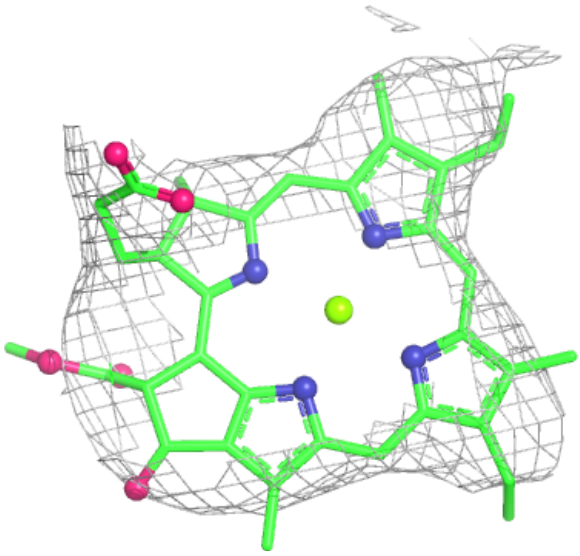


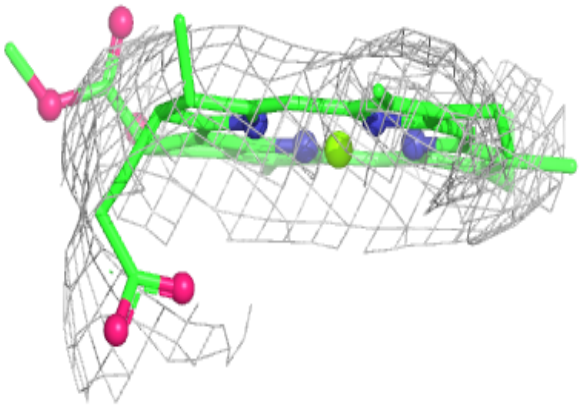


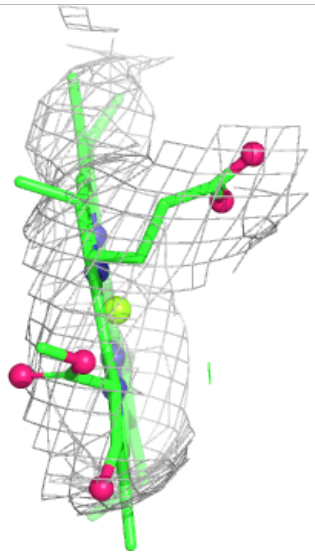


Electron density around CLA A 1108:

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

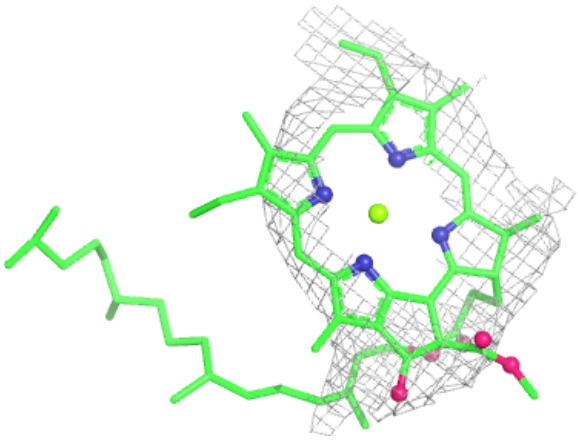


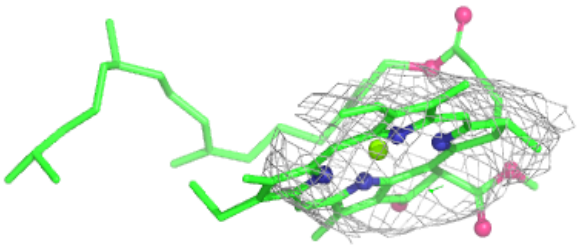


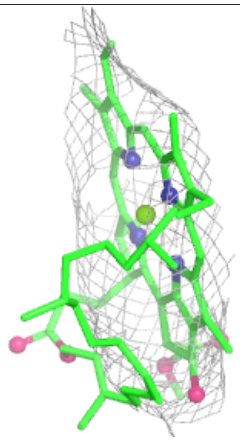


Electron density around CLA a 1127:

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

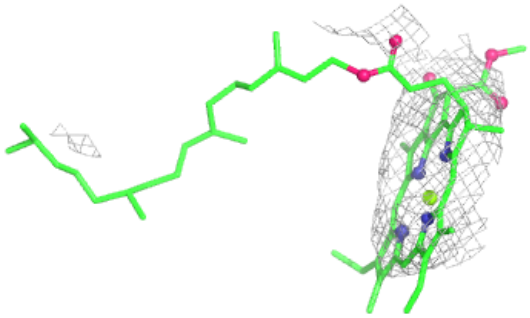


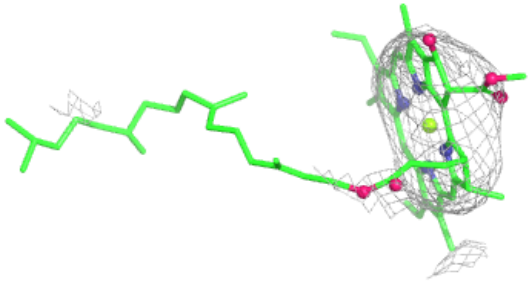


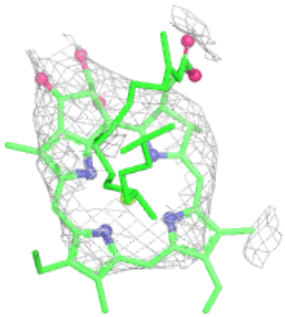


Electron density around CLA a 1128:

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

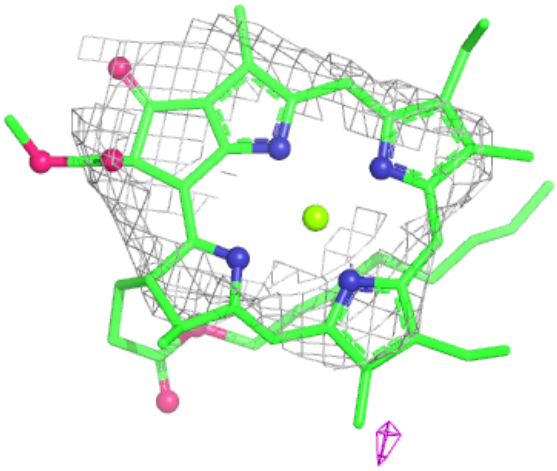


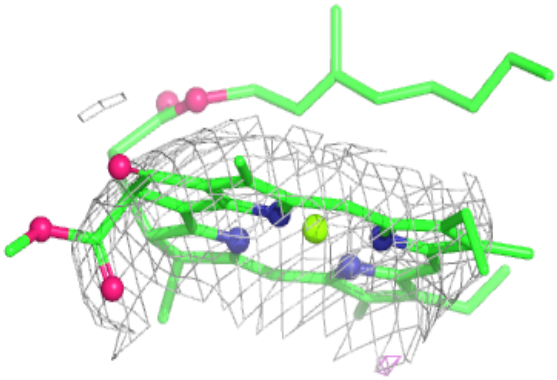


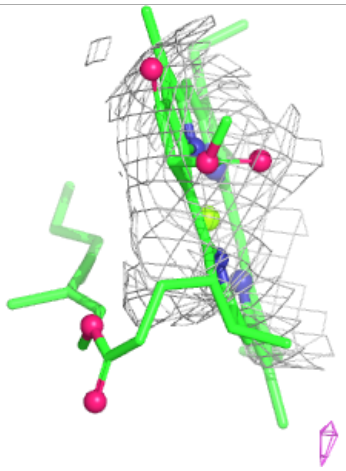


Electron density around CLA 1 1116:

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

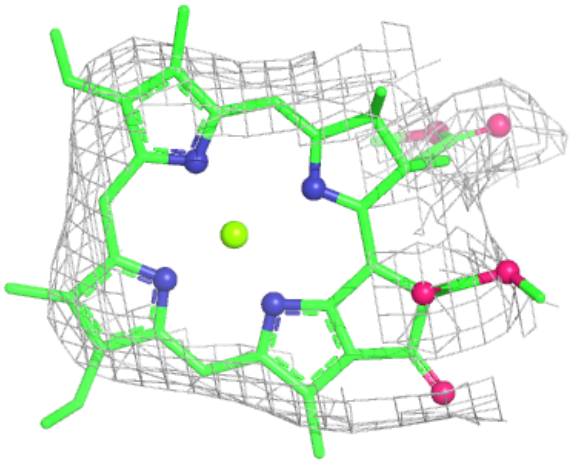


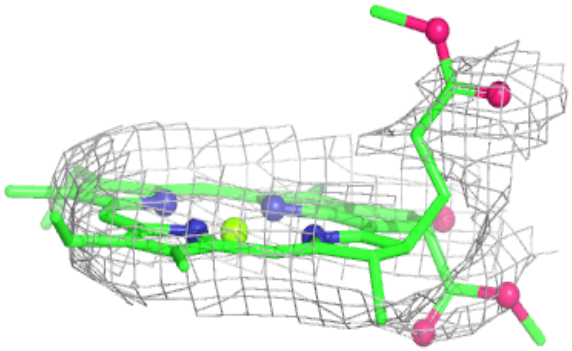


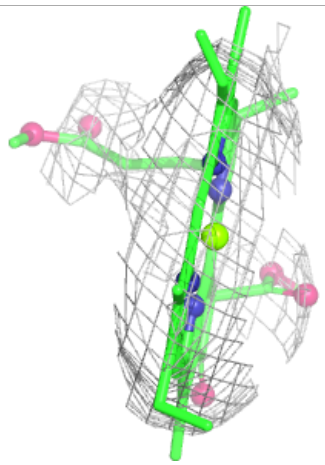


Electron density around CLA a 1130:

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

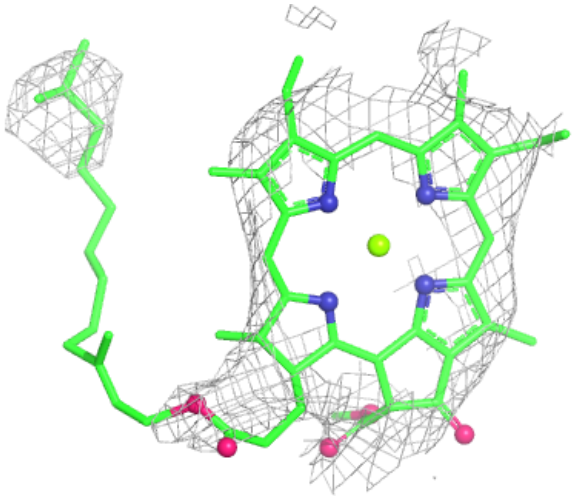


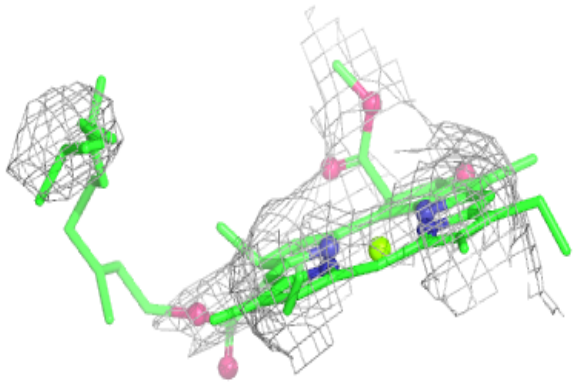


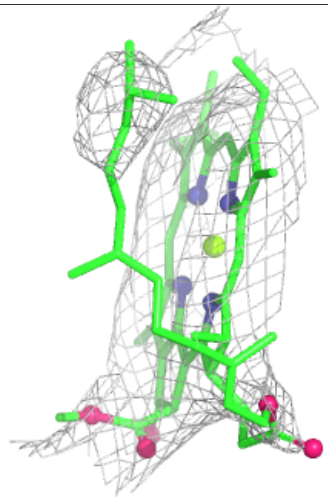


Electron density around CLA A 1111:

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

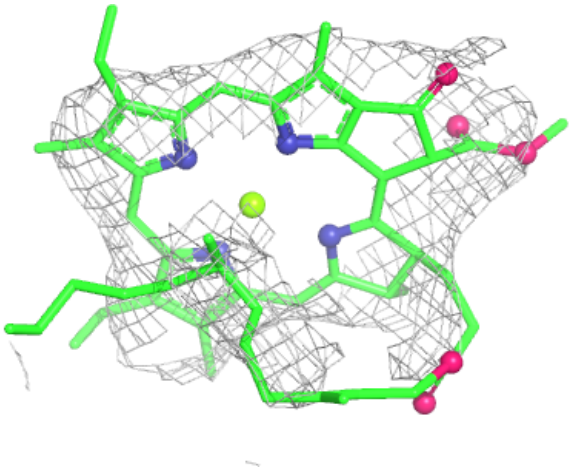


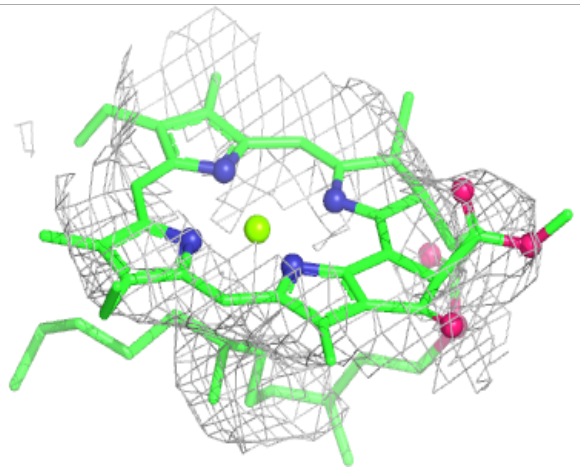


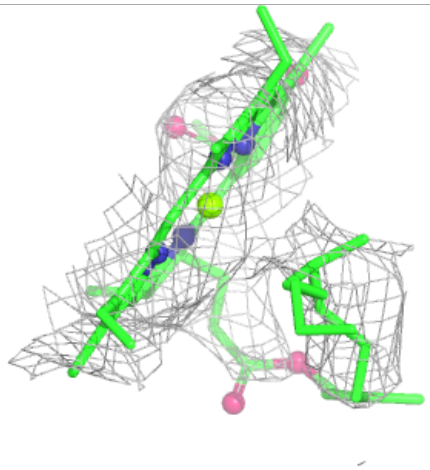


Electron density around CLA 2 1214:

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

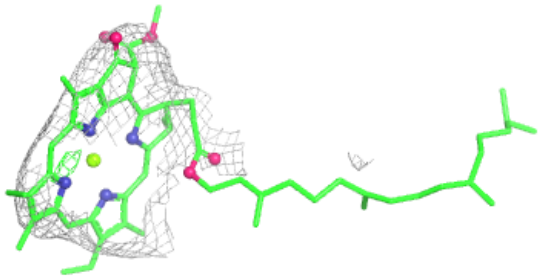


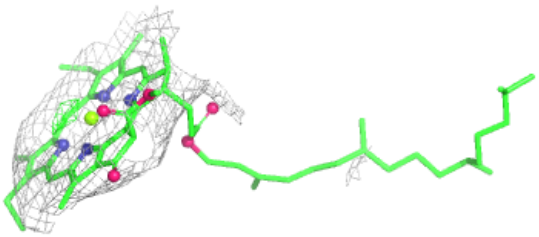


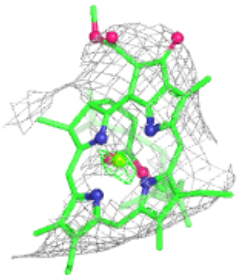


Electron density around CLA 1 1119:

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

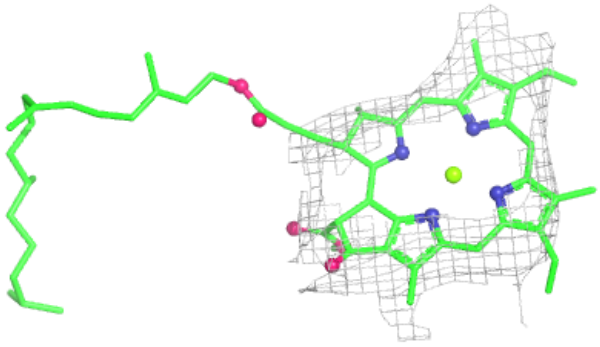


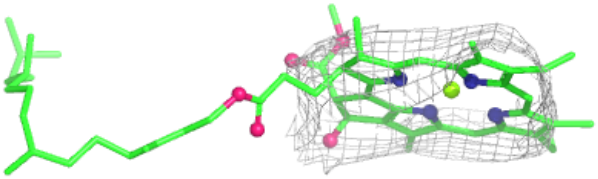


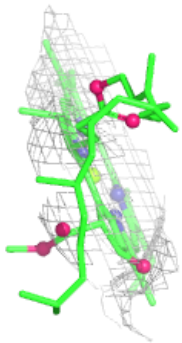


Electron density around CLA B 1223:

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

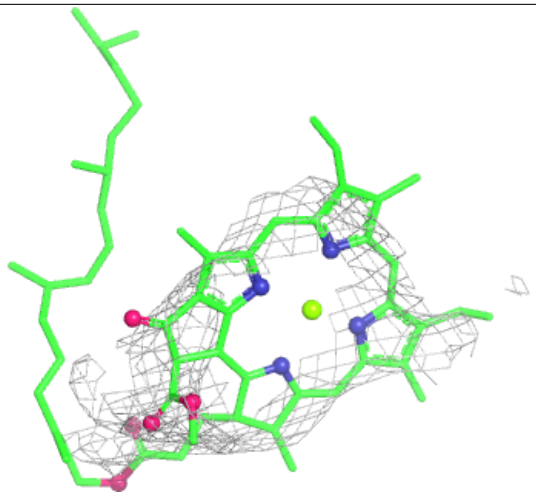


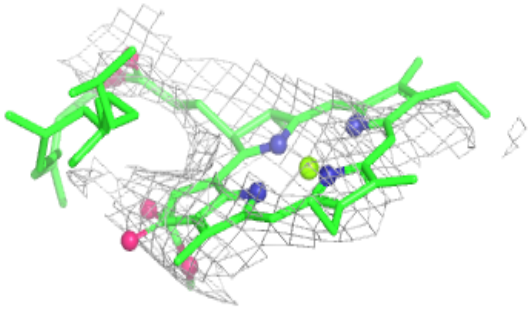


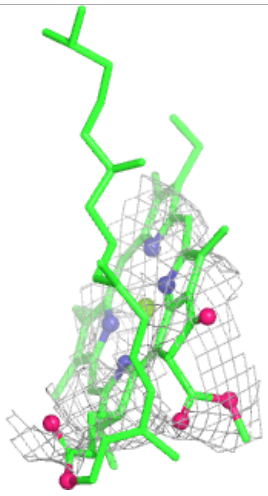


Electron density around CLA 1 1123:

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

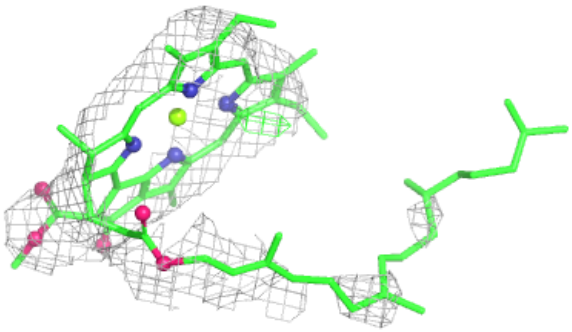


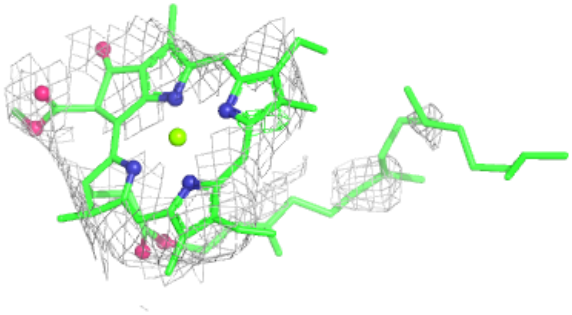


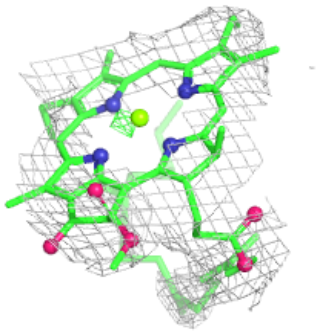


Electron density around CLA A 1109:

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

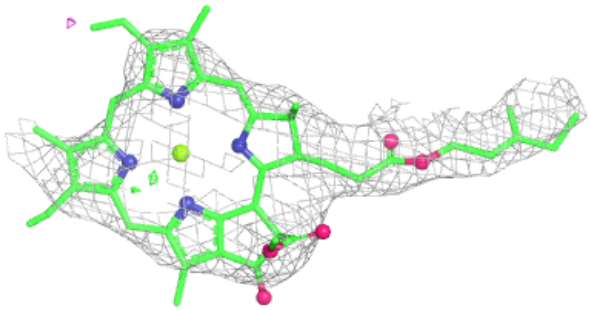


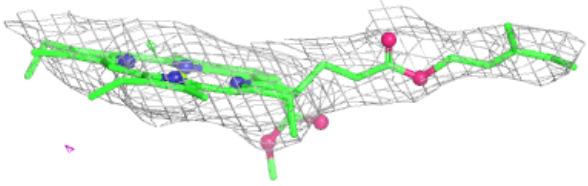


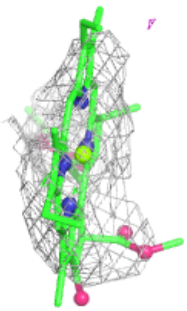


Electron density around CLA A 1135:

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

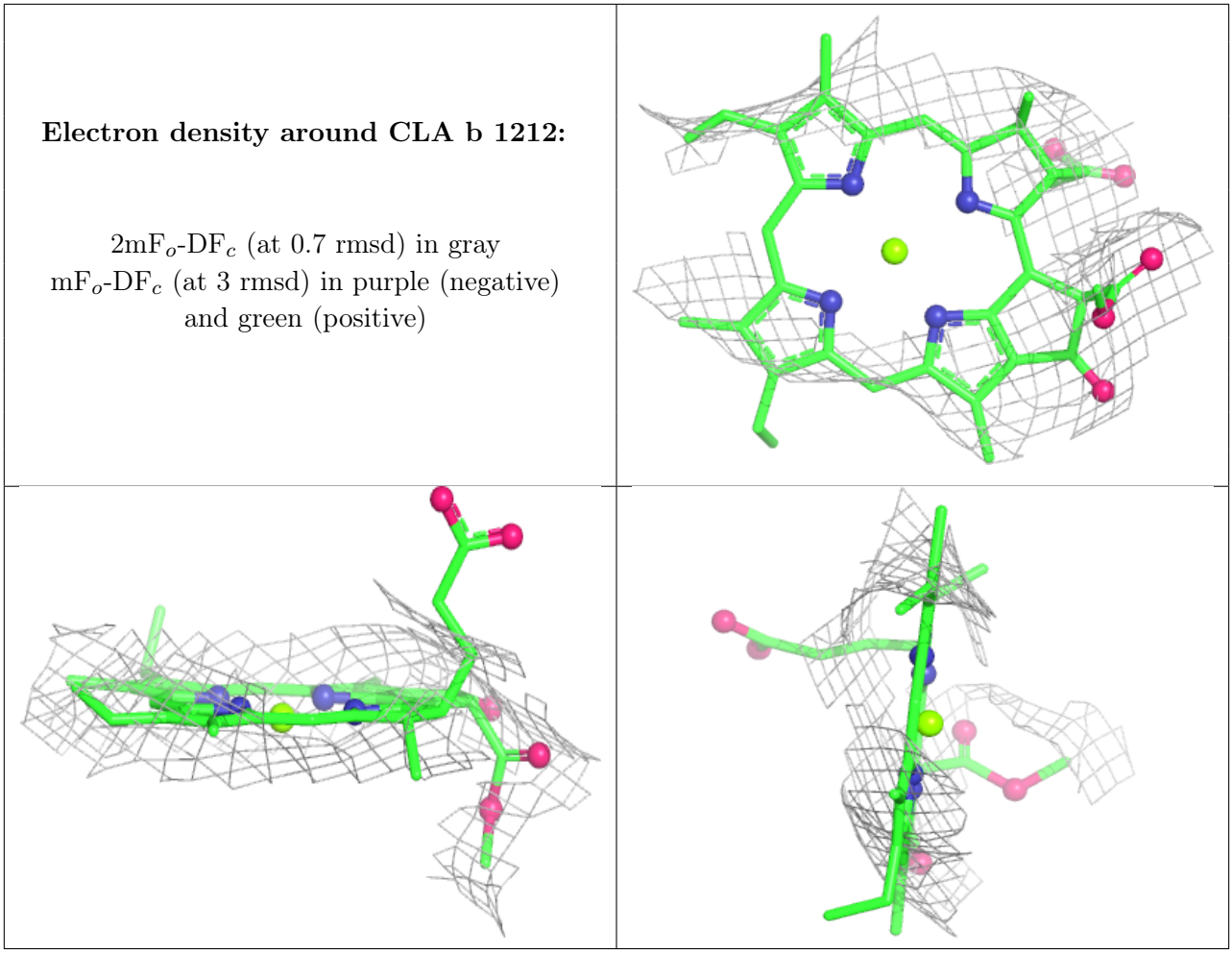






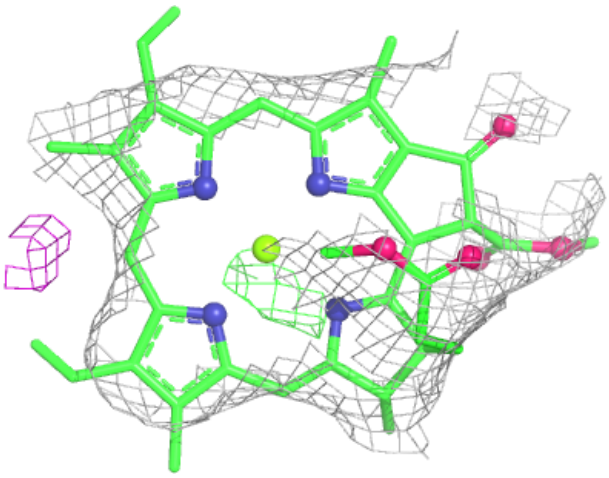
Electron density around CLA b 1212:

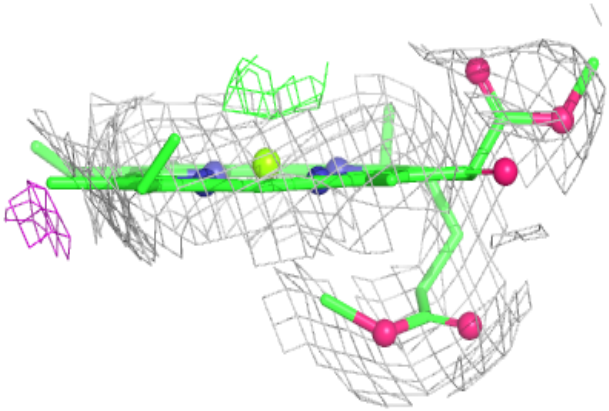
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

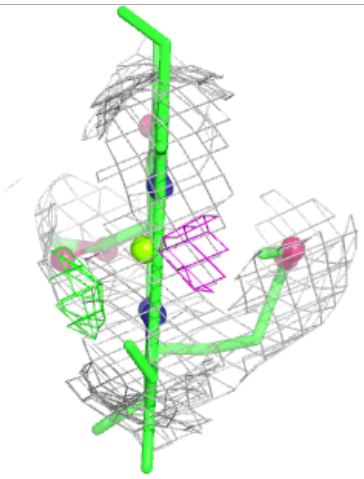


Electron density around CLA A 1115:

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

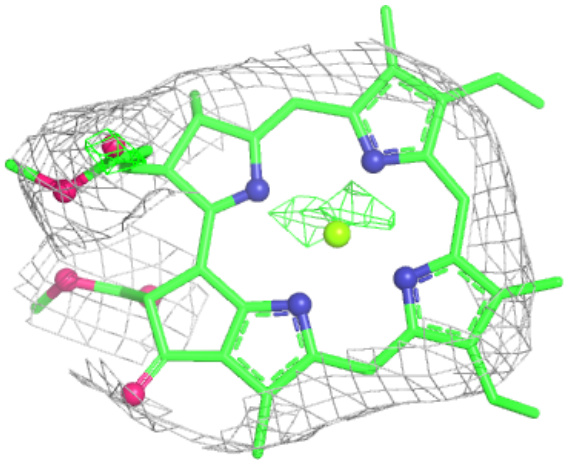


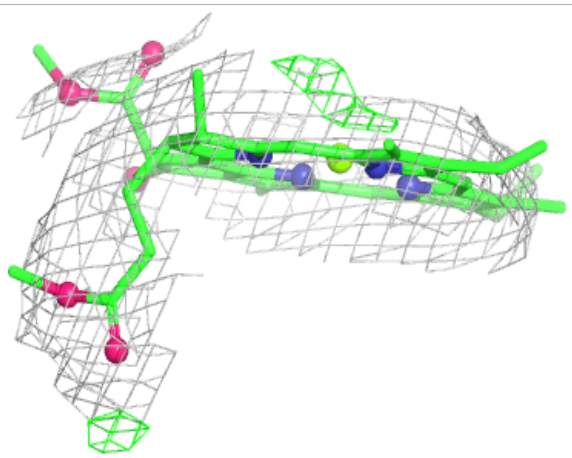


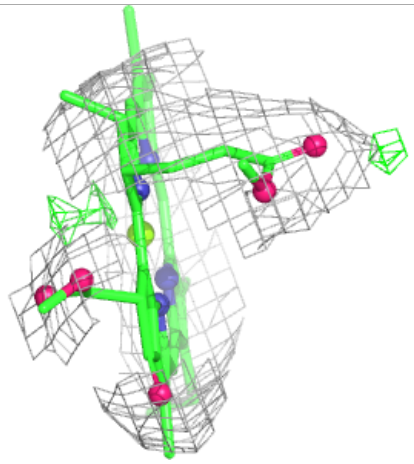


Electron density around CLA b 1239:

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

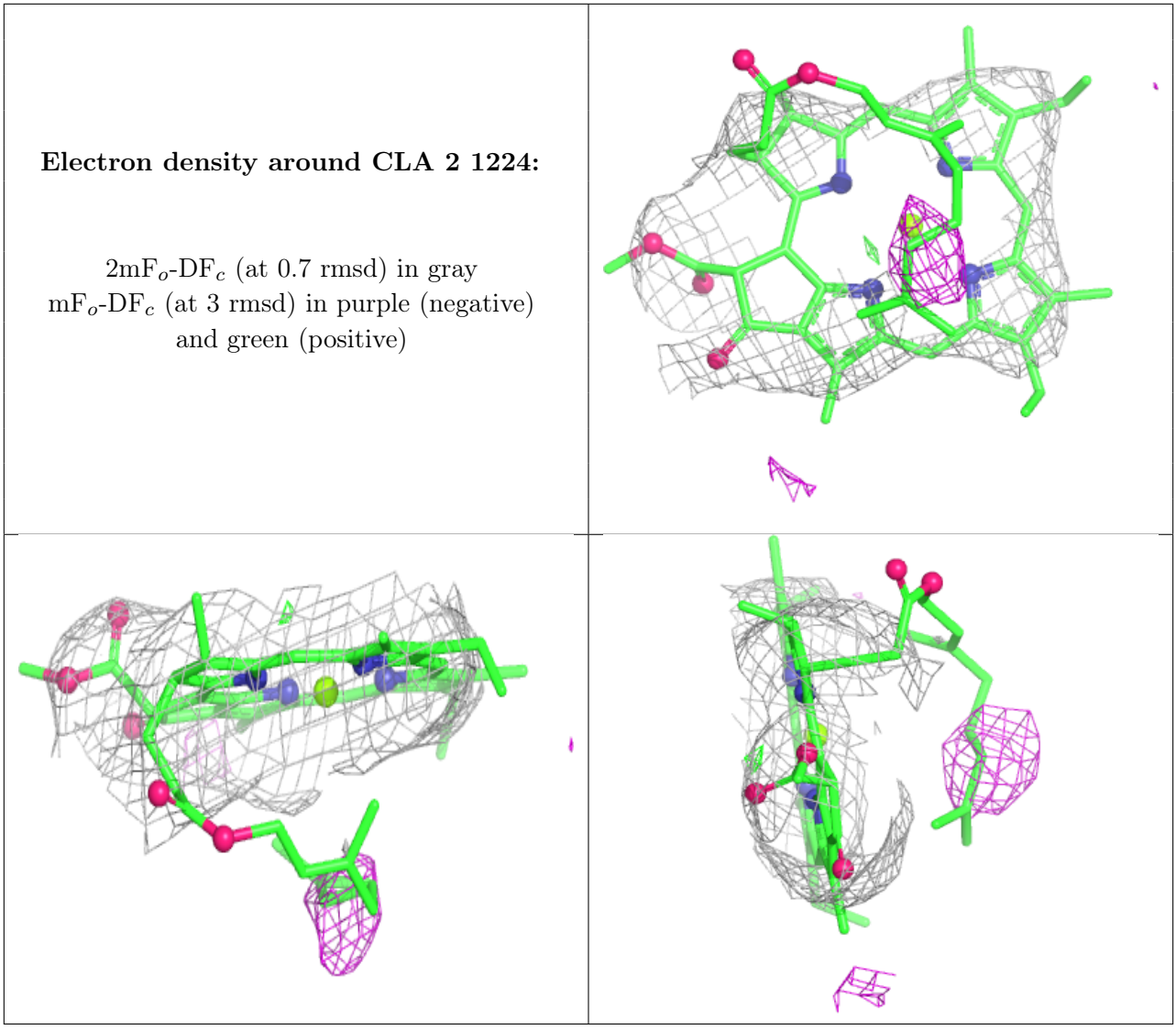






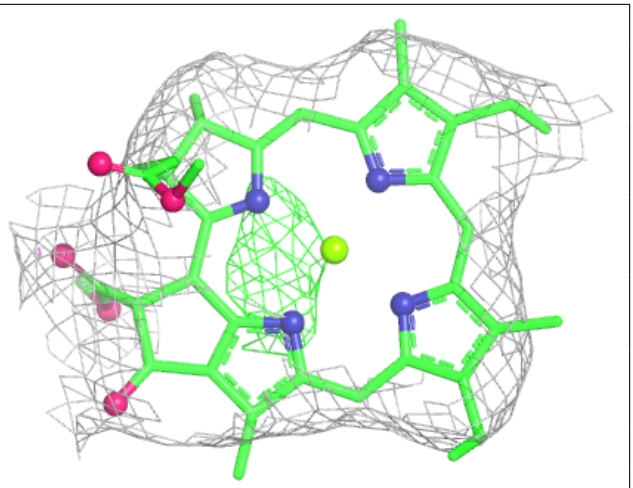
Electron density around CLA 2 1224:

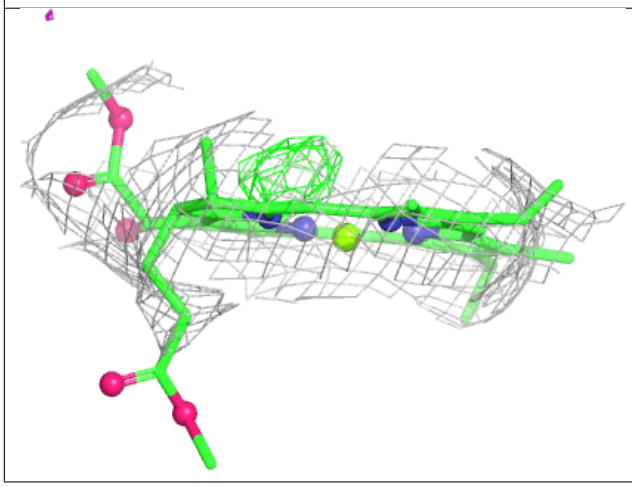
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

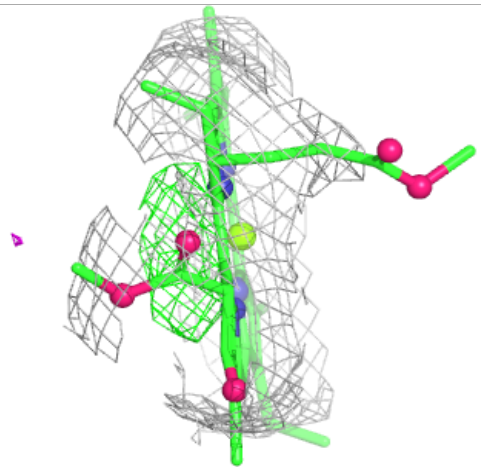


Electron density around CLA L 1502:

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

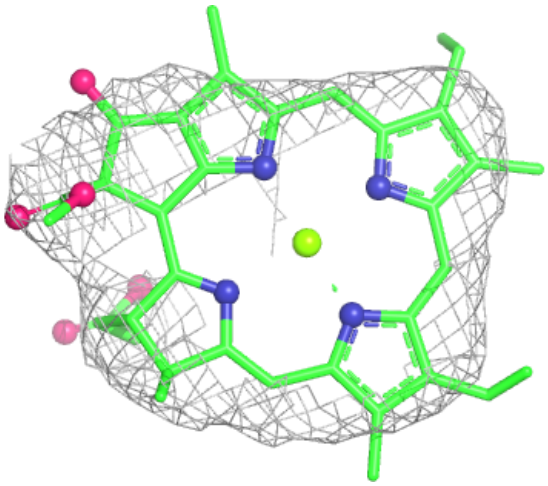


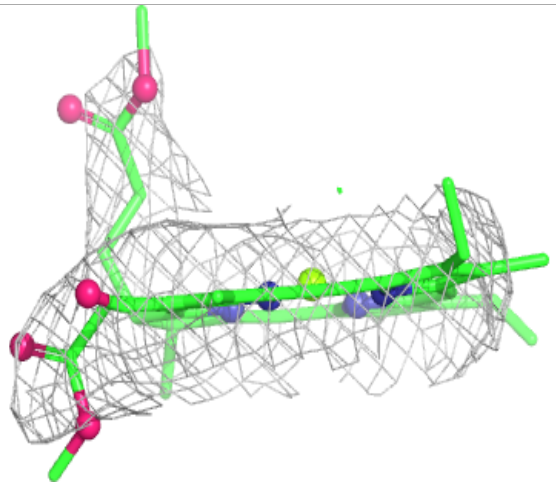


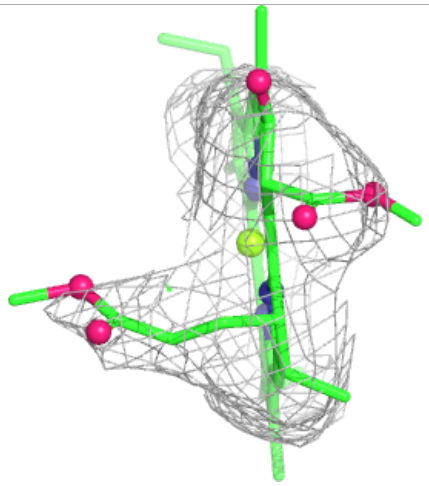


Electron density around CLA l 1502:

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

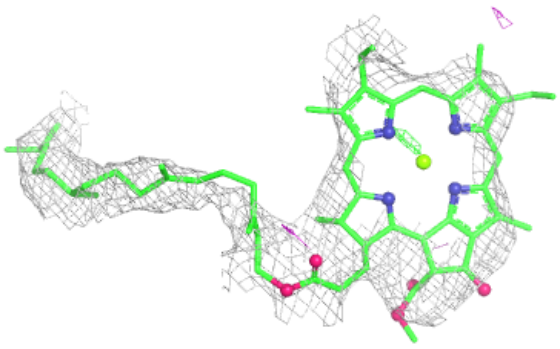


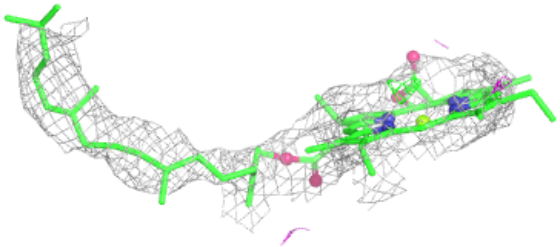


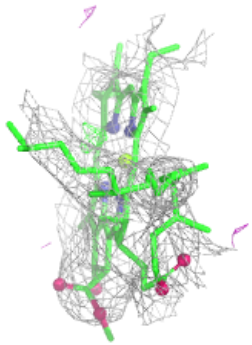


Electron density around CLA B 1023:

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

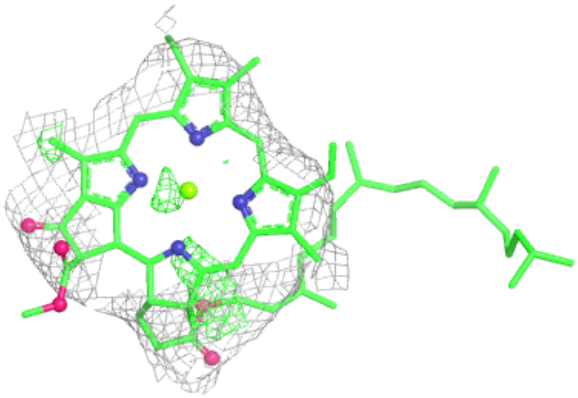


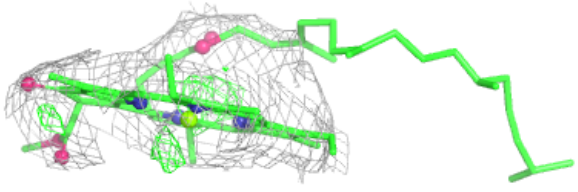


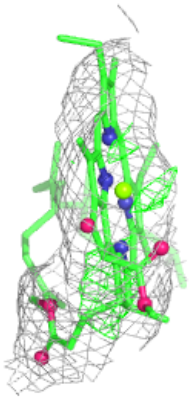


Electron density around CLA B 1215:

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

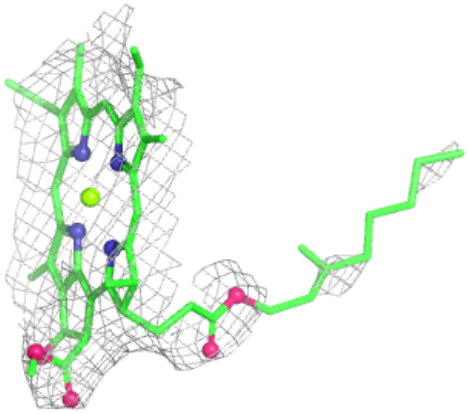


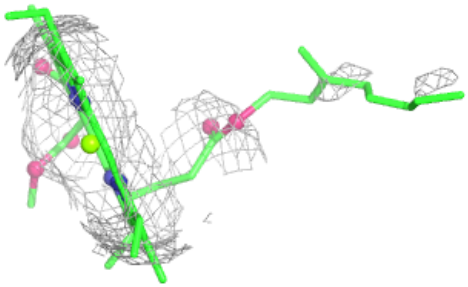


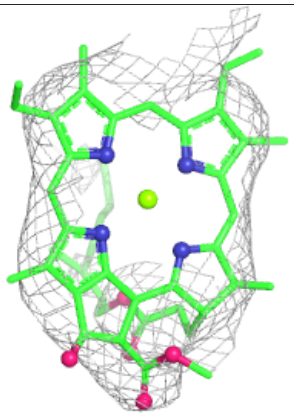


Electron density around CLA B 1201:

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

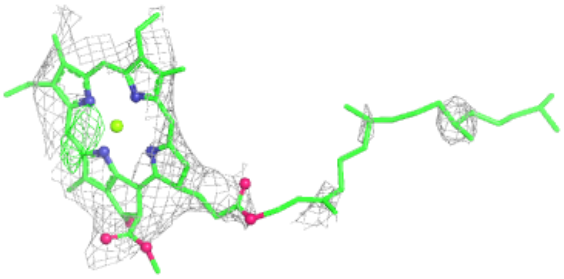


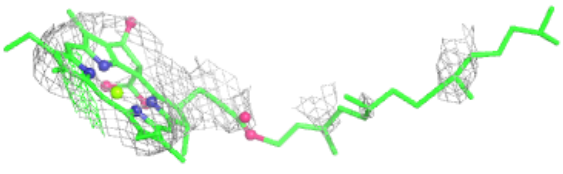


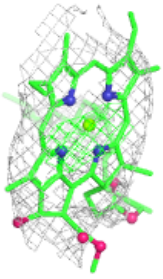


Electron density around CLA 1 1022:

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

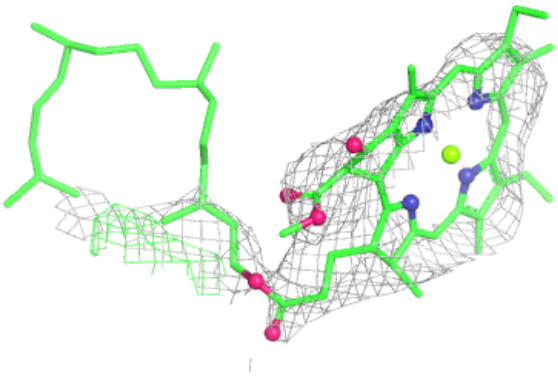


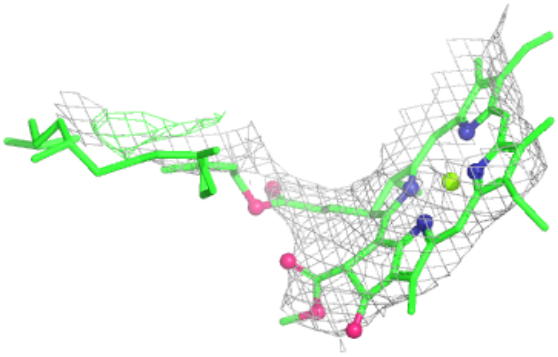


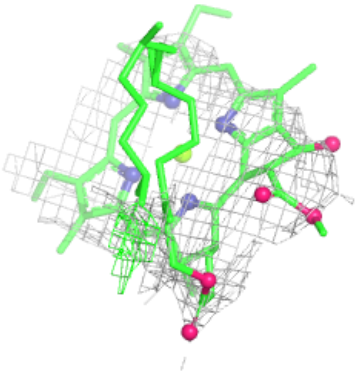


Electron density around CLA 1 1011:

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

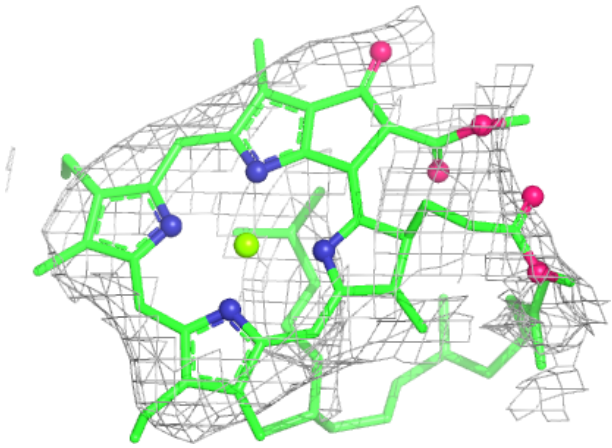


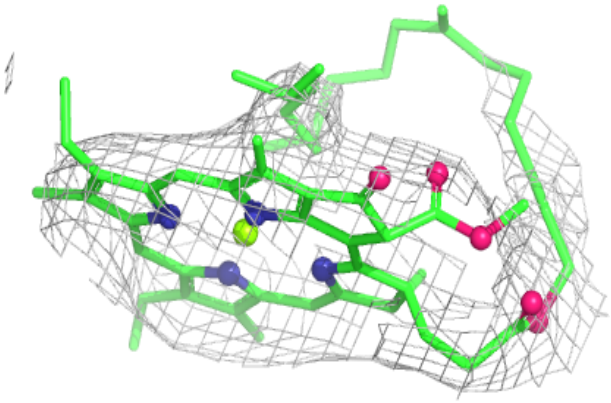




Electron density around CLA B 1203:

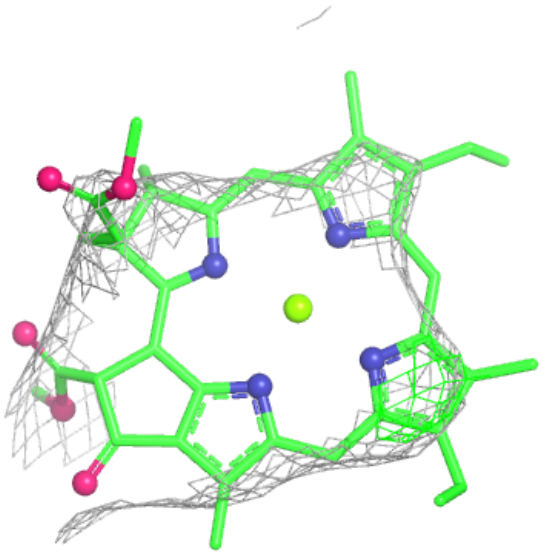
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

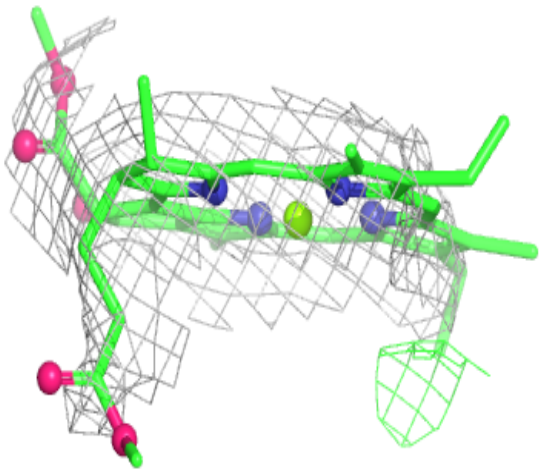


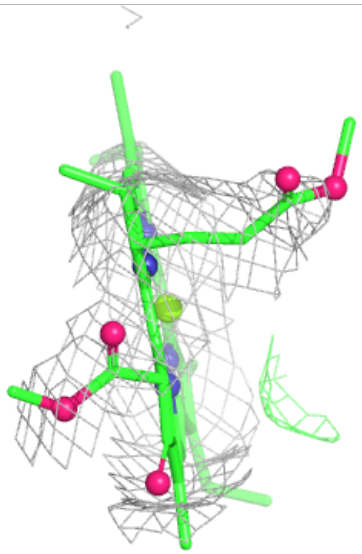


Electron density around CLA a 1129:

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

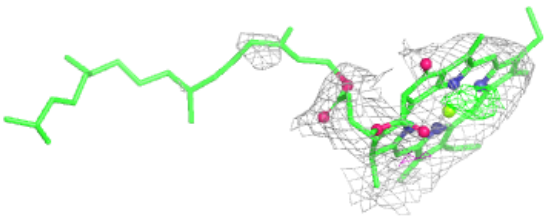


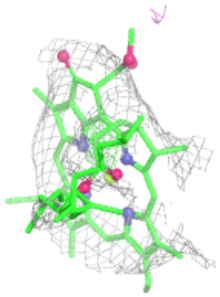




Electron density around CLA a 1119:

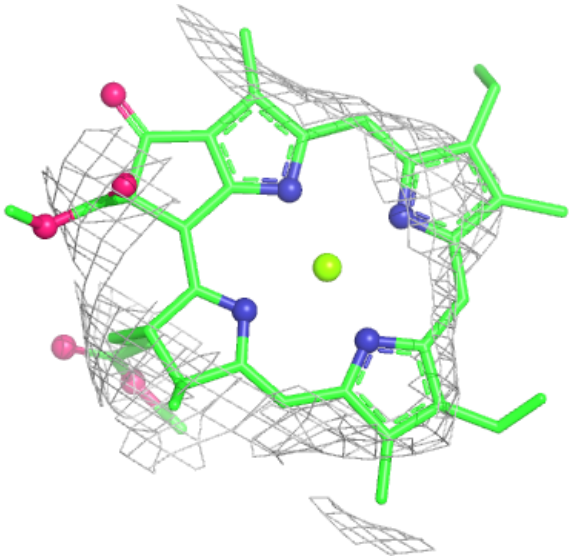
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

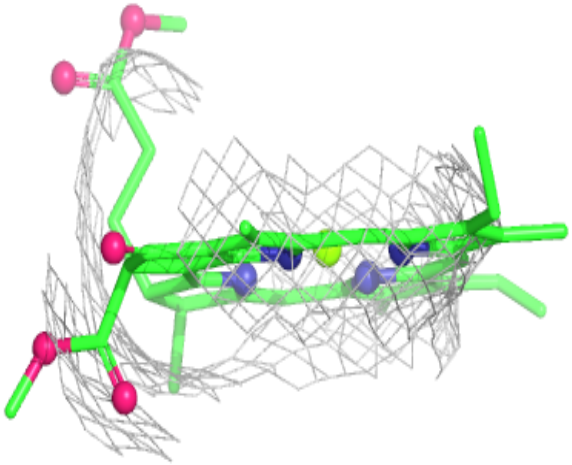


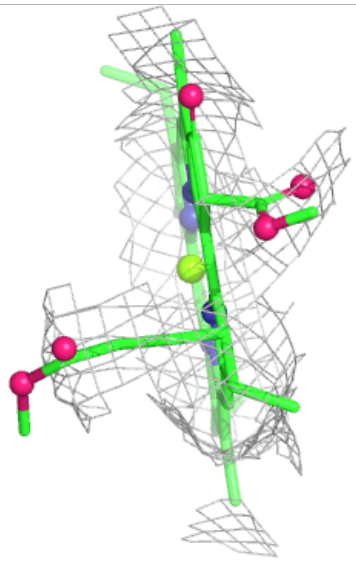


Electron density around CLA a 1133:

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

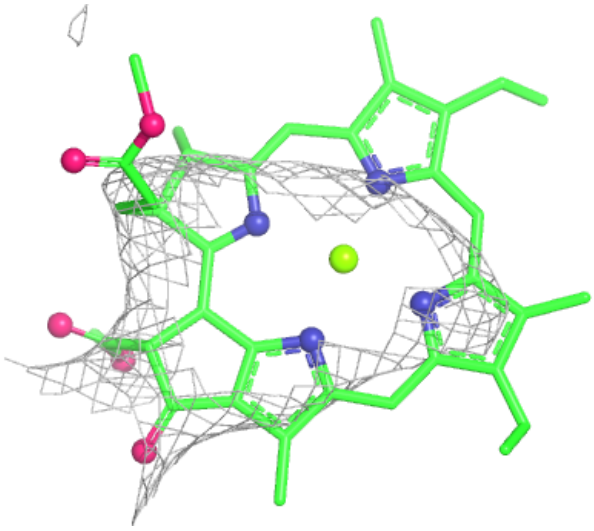


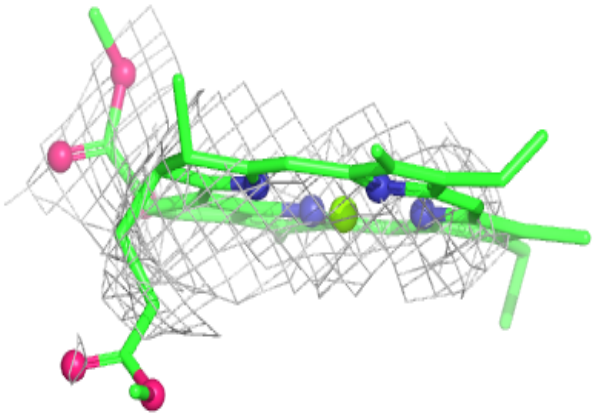


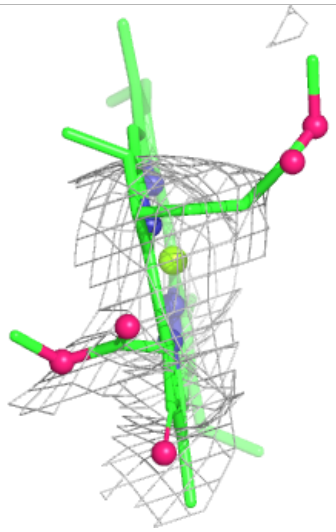


Electron density around CLA 1 1129:

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

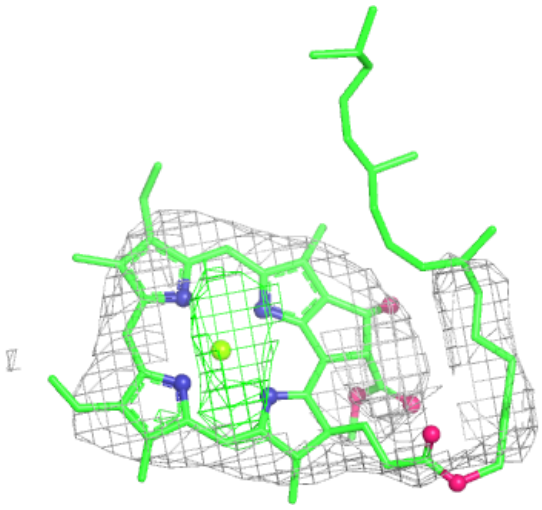


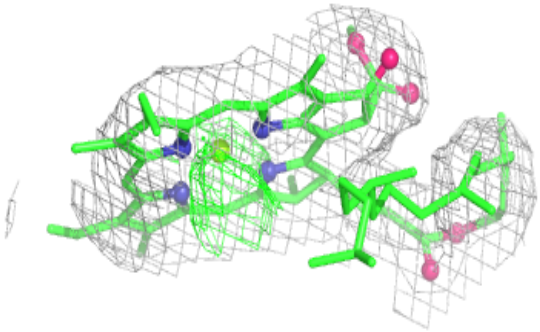


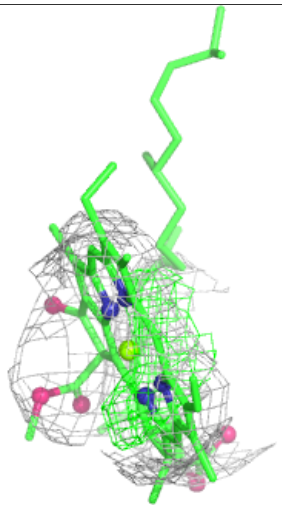


Electron density around CLA A 1123:

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

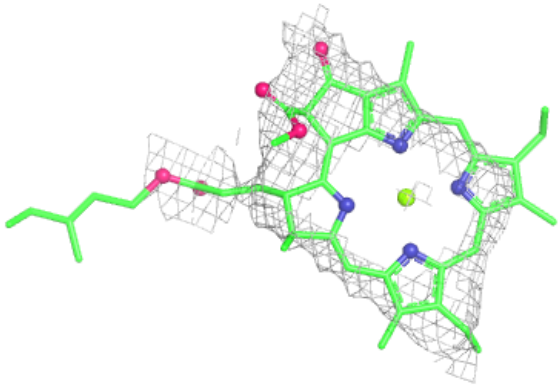


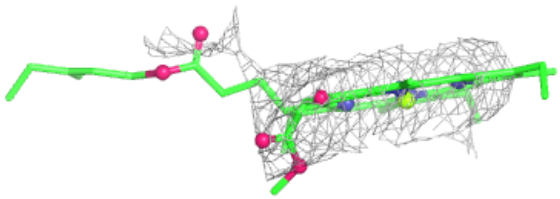


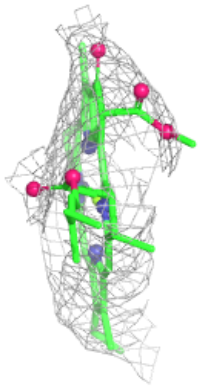


Electron density around CLA a 1135:

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

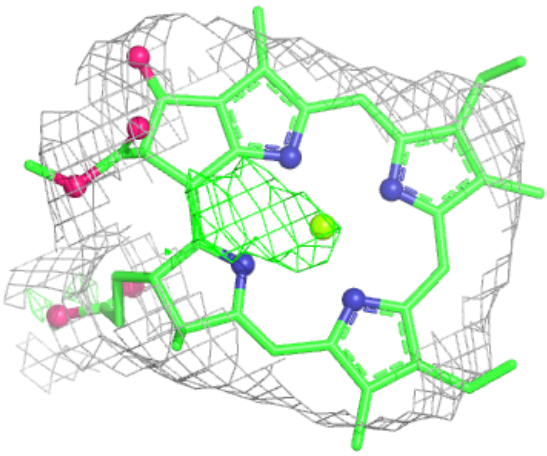


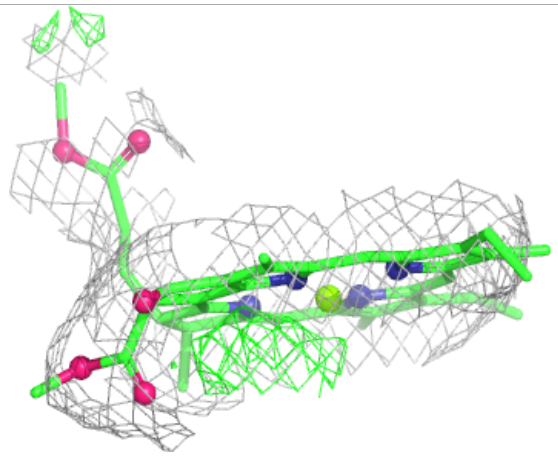


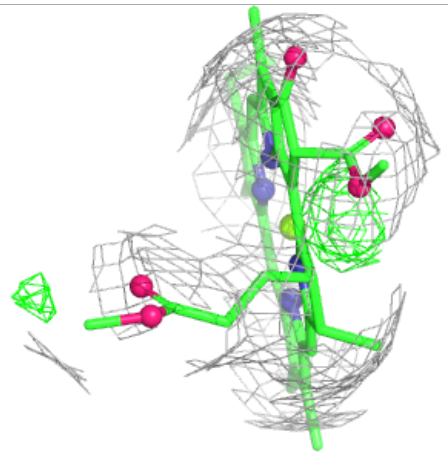


Electron density around CLA 2 1239:

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

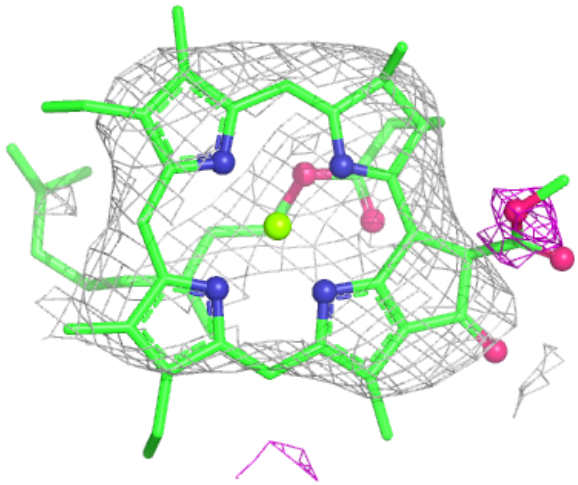


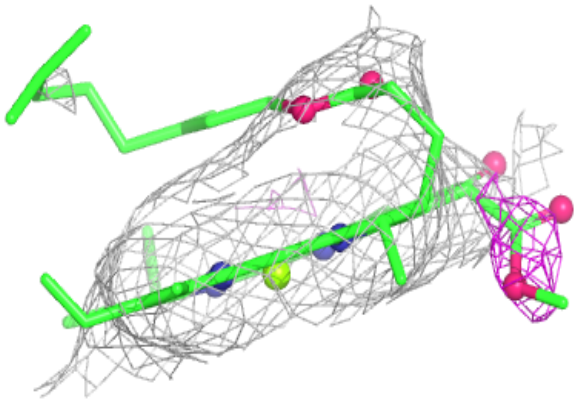


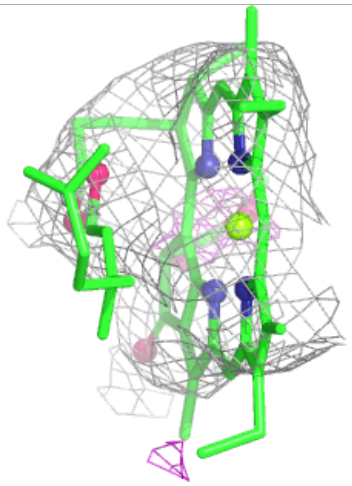


Electron density around CLA B 1205:

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

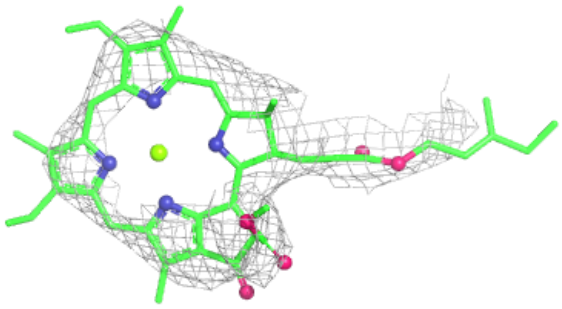


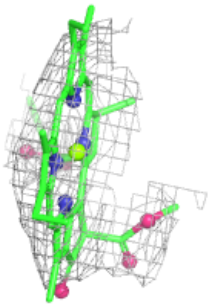




Electron density around CLA 1 1135:

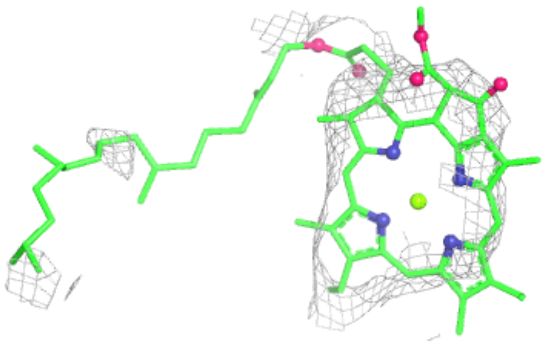
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

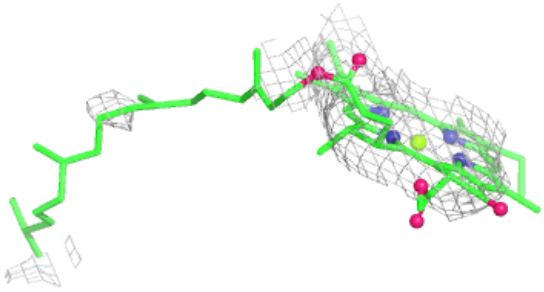


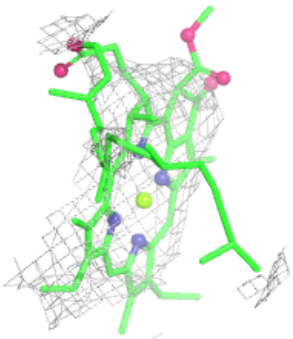


Electron density around CLA 2 1013:

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

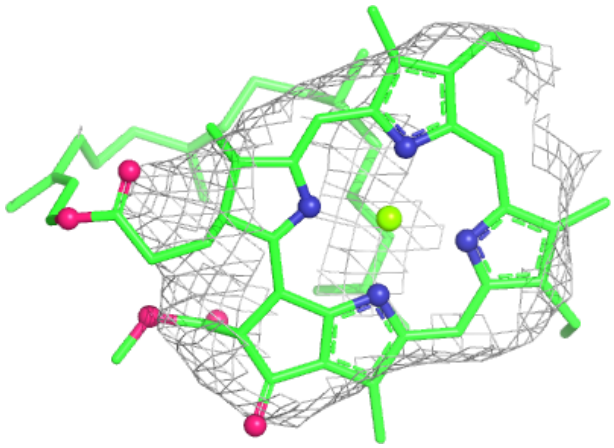


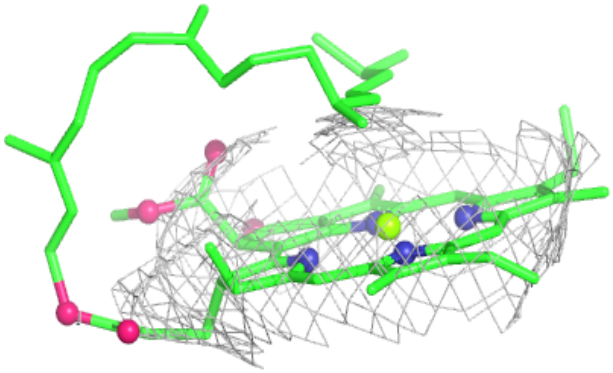


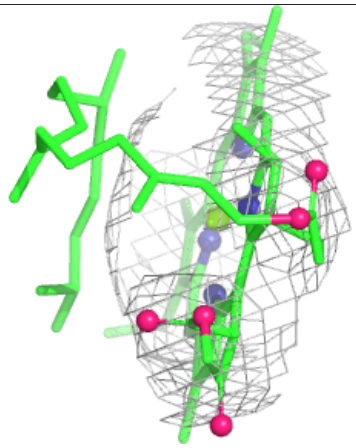


Electron density around CLA a 1104:

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

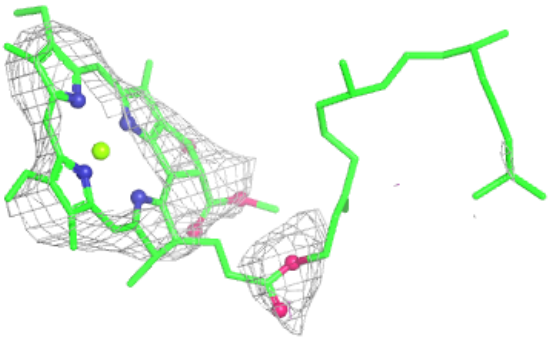


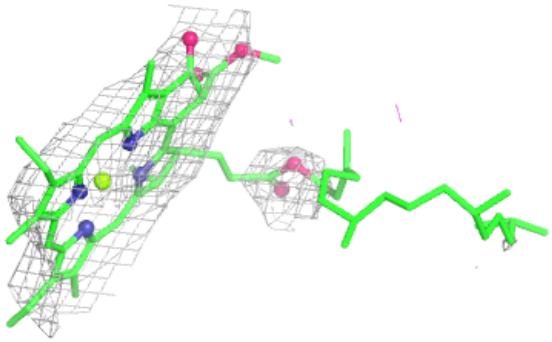


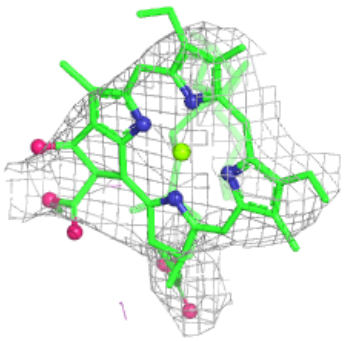


Electron density around CLA A 1011:

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

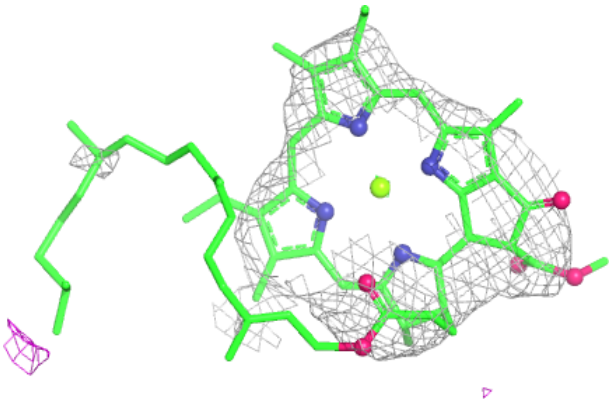


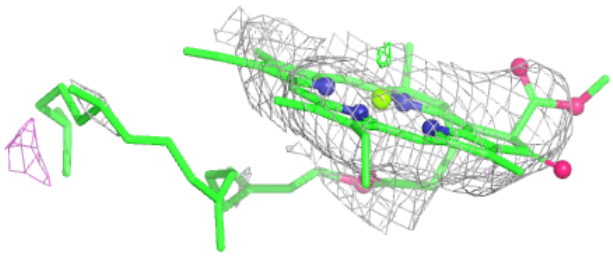


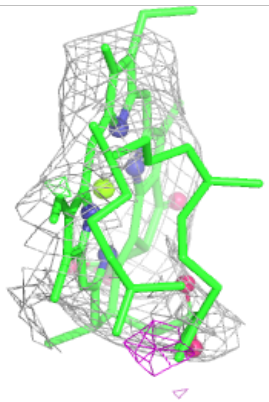


Electron density around CLA A 1117:

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

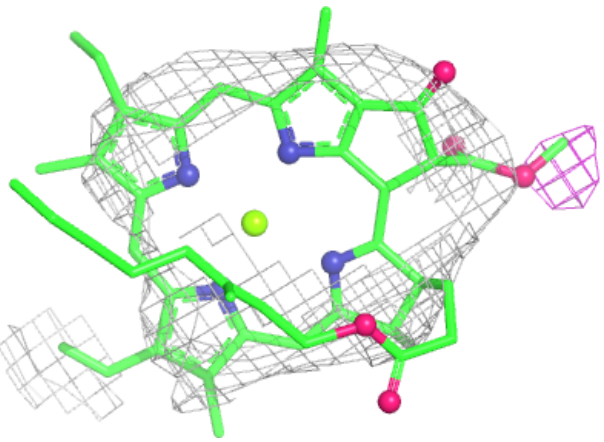


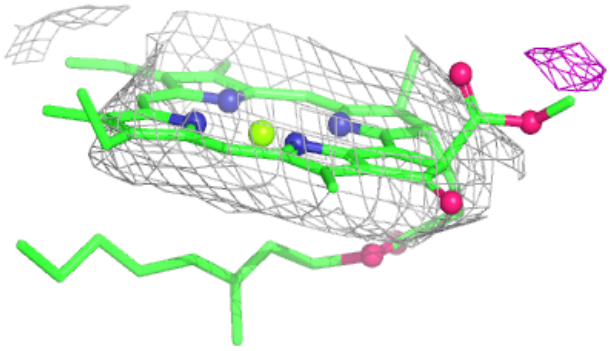


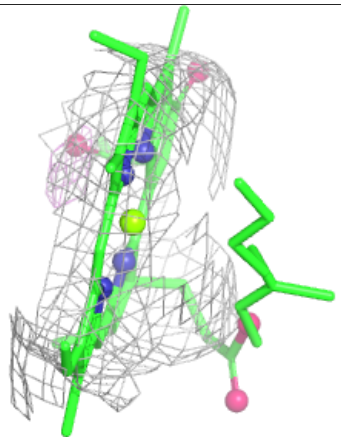


Electron density around CLA a 1116:

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

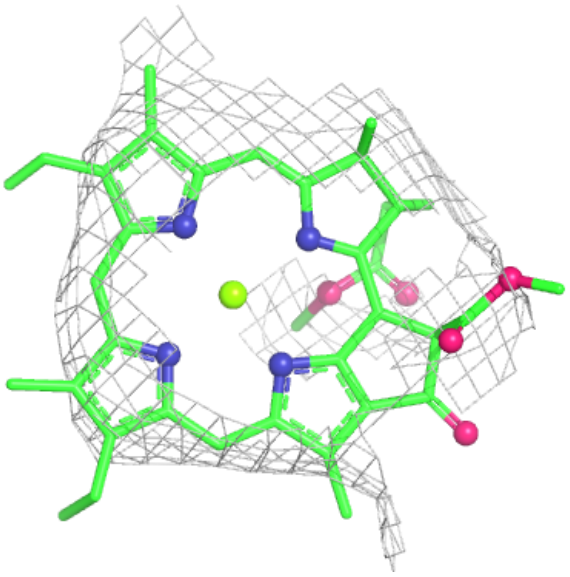


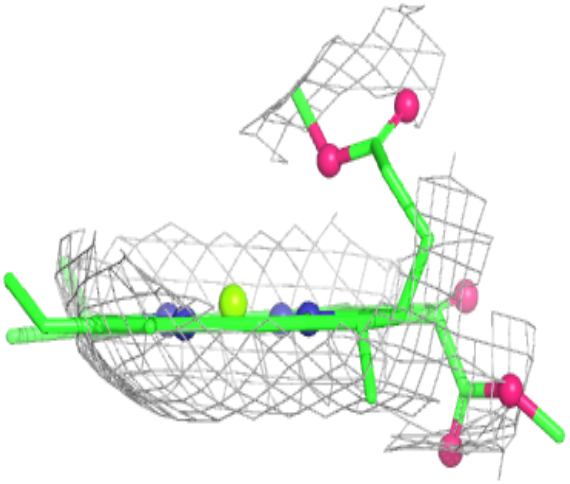


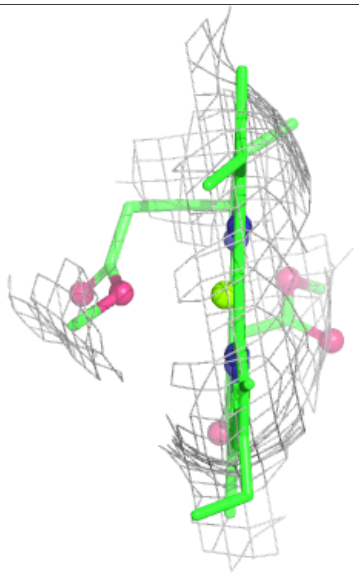


Electron density around CLA 1 1136:

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

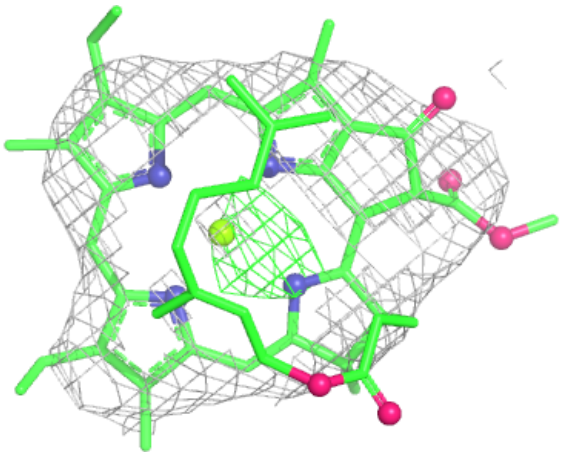


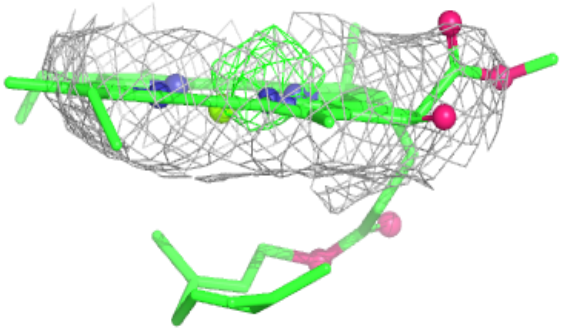


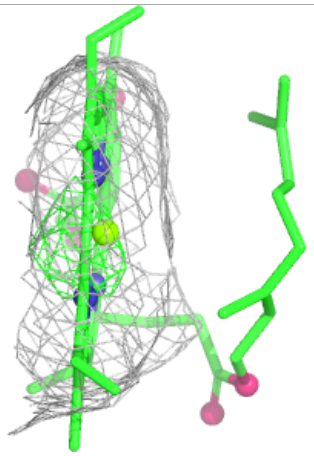


Electron density around CLA B 1224:

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

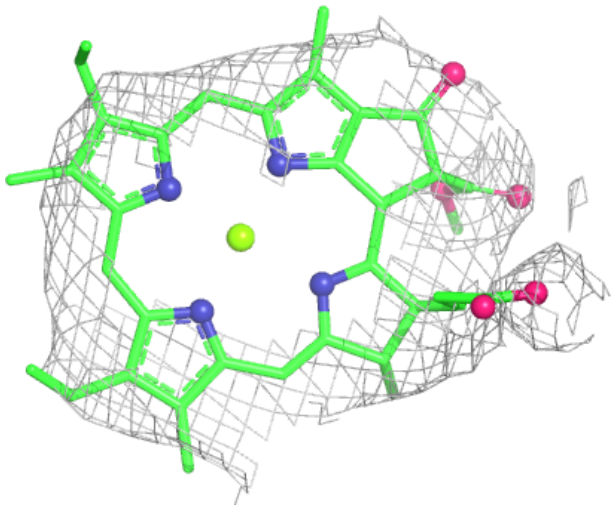


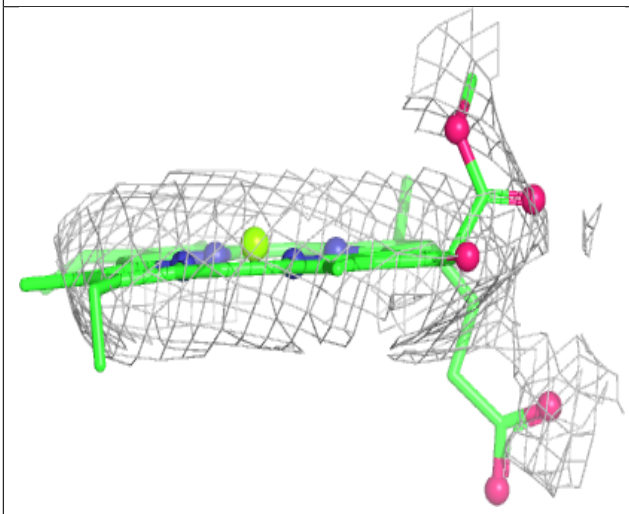


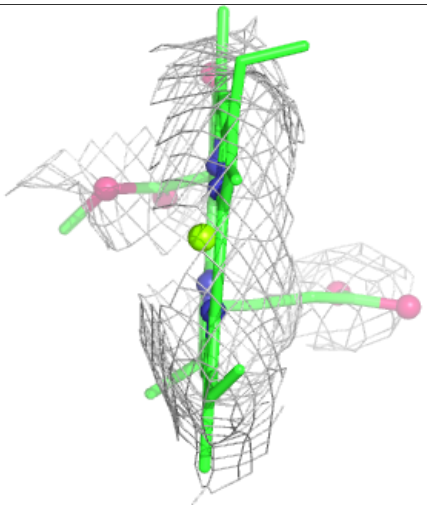


Electron density around CLA 2 1212:

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

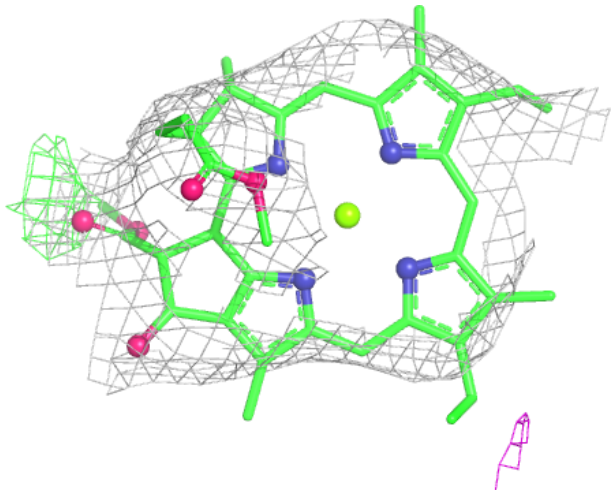


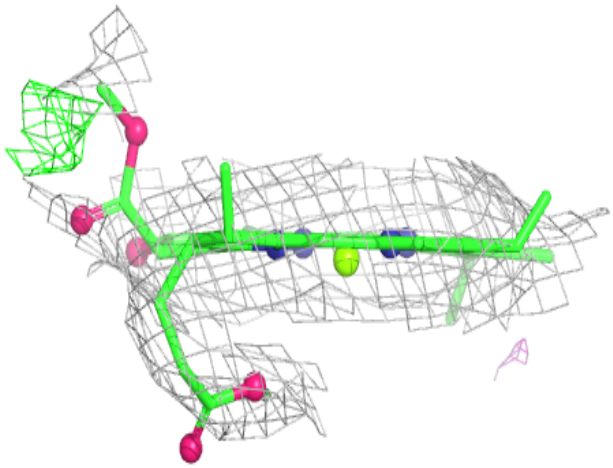


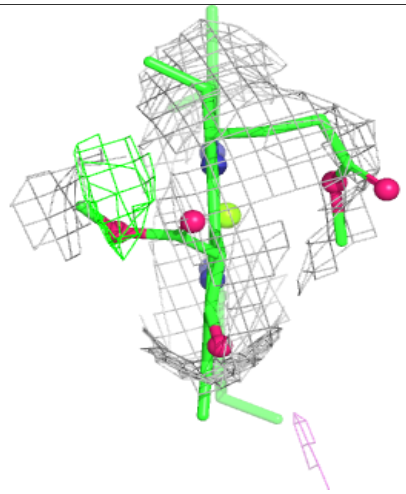


Electron density around CLA 8 1502:

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

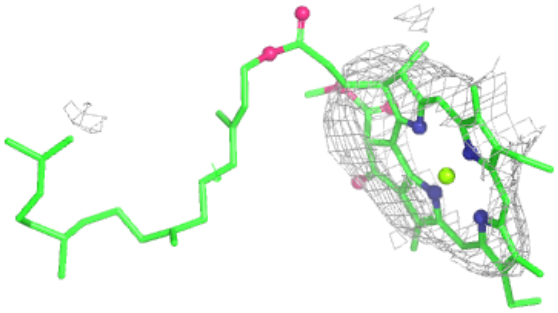


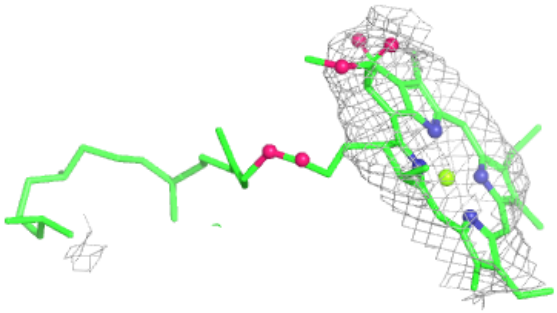


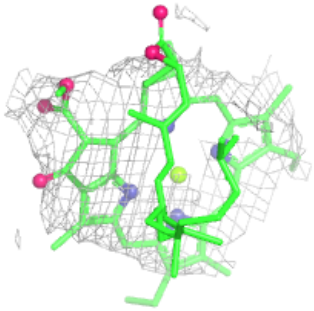


Electron density around CLA 2 1021:

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

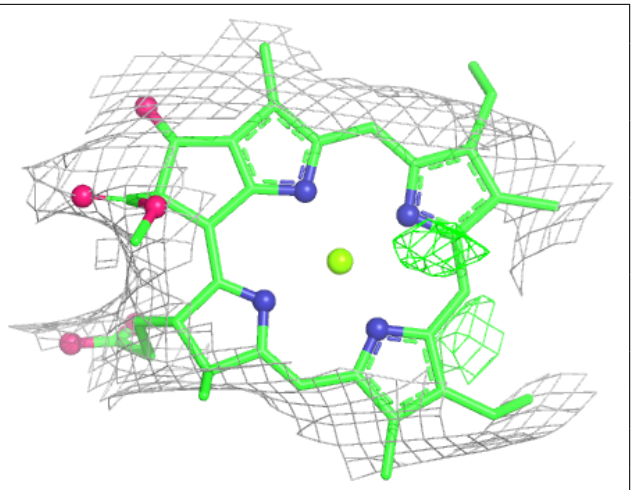


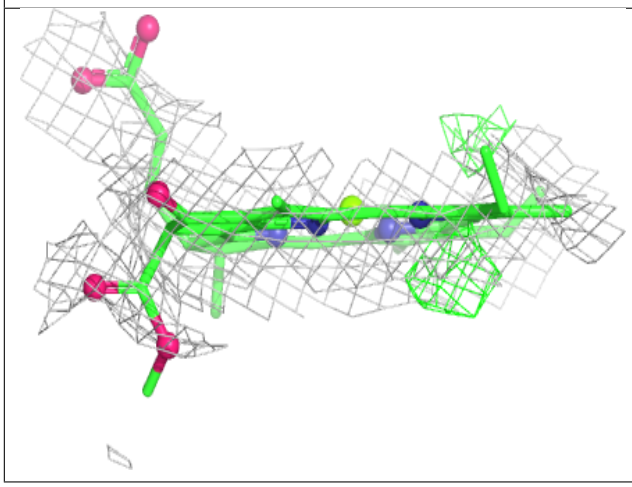


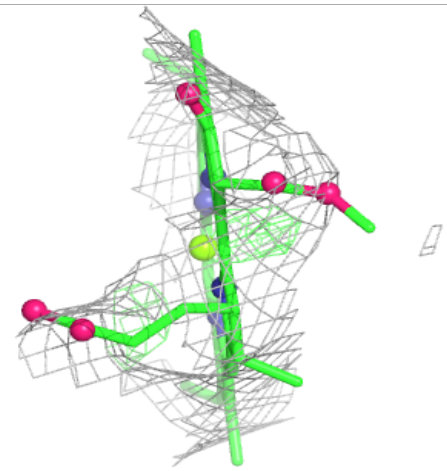


Electron density around CLA A 1112:

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

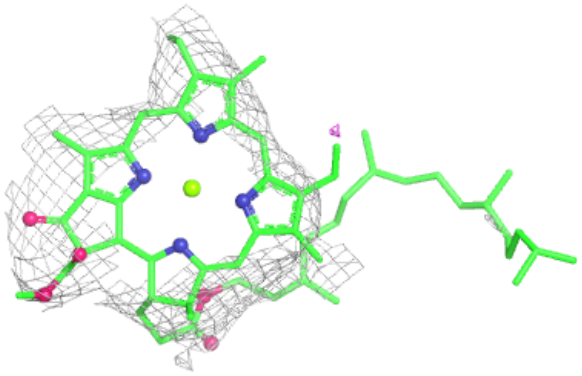


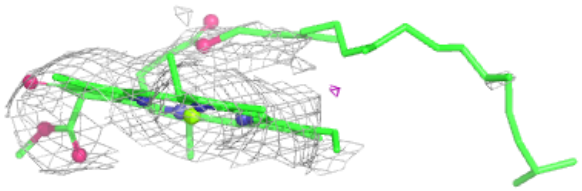


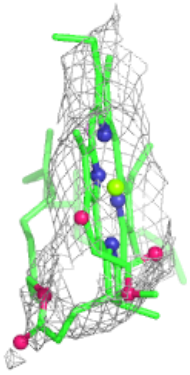


Electron density around CLA 2 1215:

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

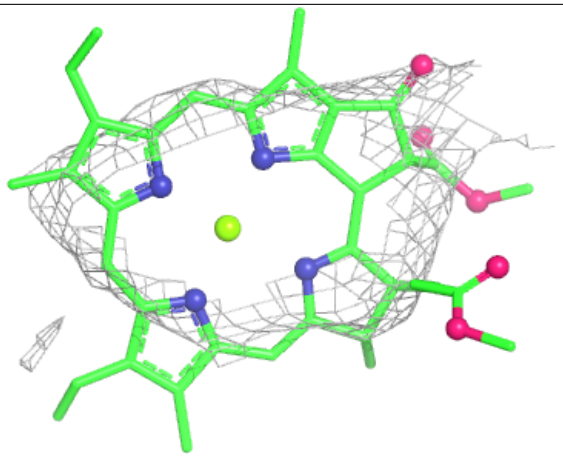


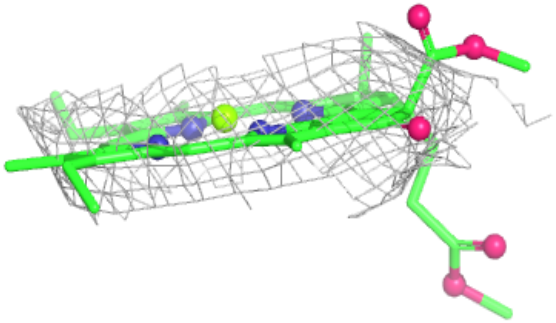


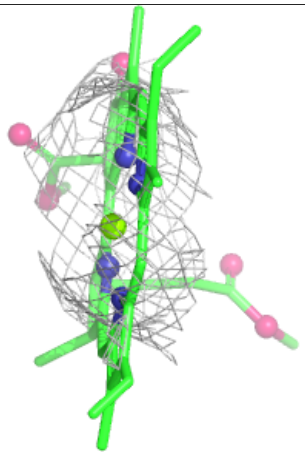


Electron density around CLA b 1220:

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

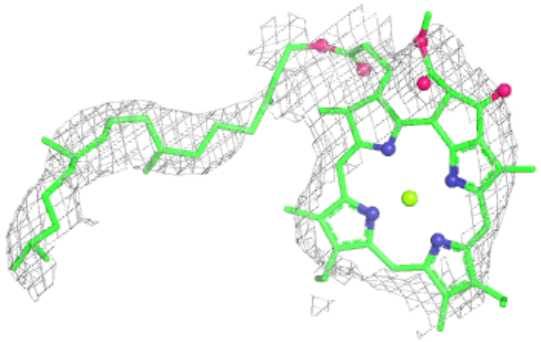


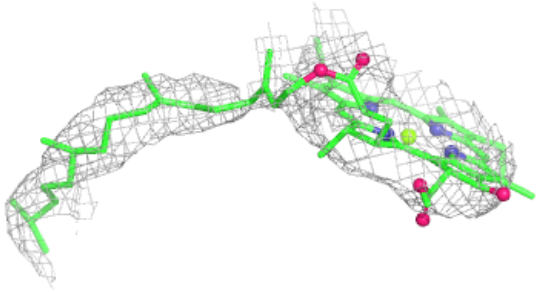


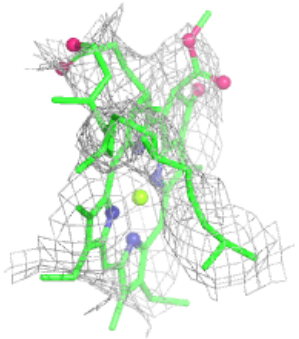


Electron density around CLA B 1013:

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

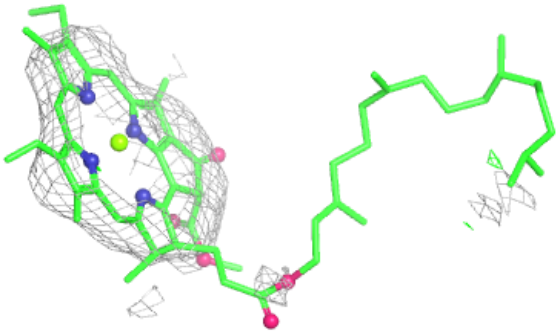


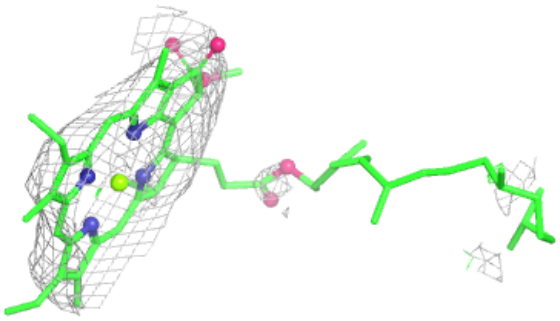


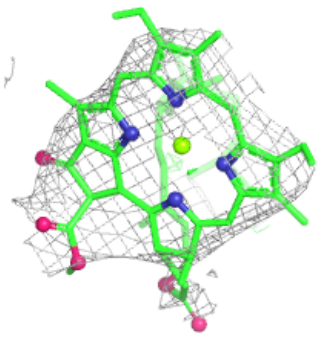


Electron density around CLA B 1021:

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

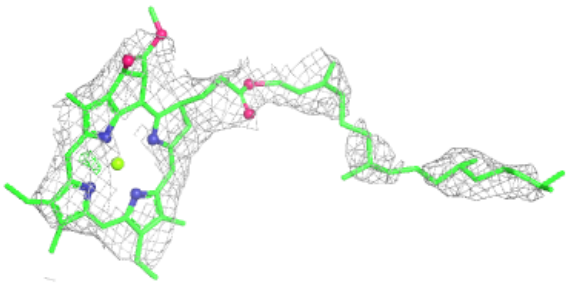


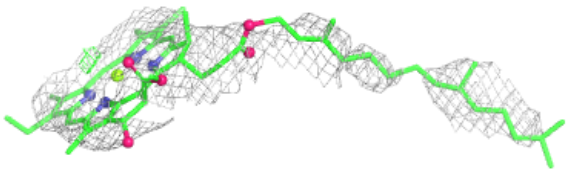


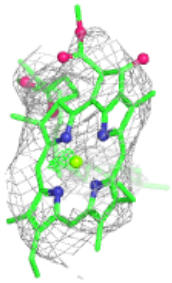


Electron density around CLA A 1022:

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

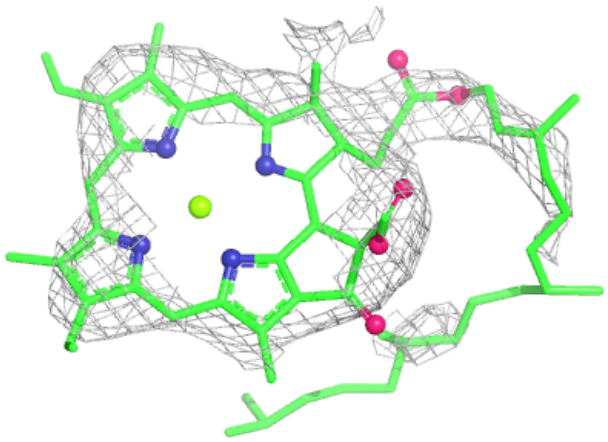


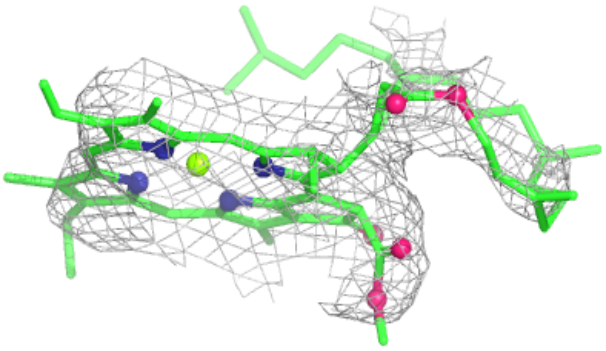


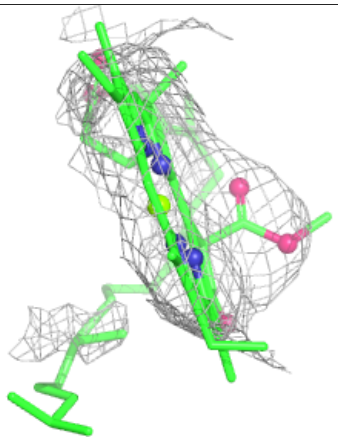


Electron density around CLA B 1202:

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

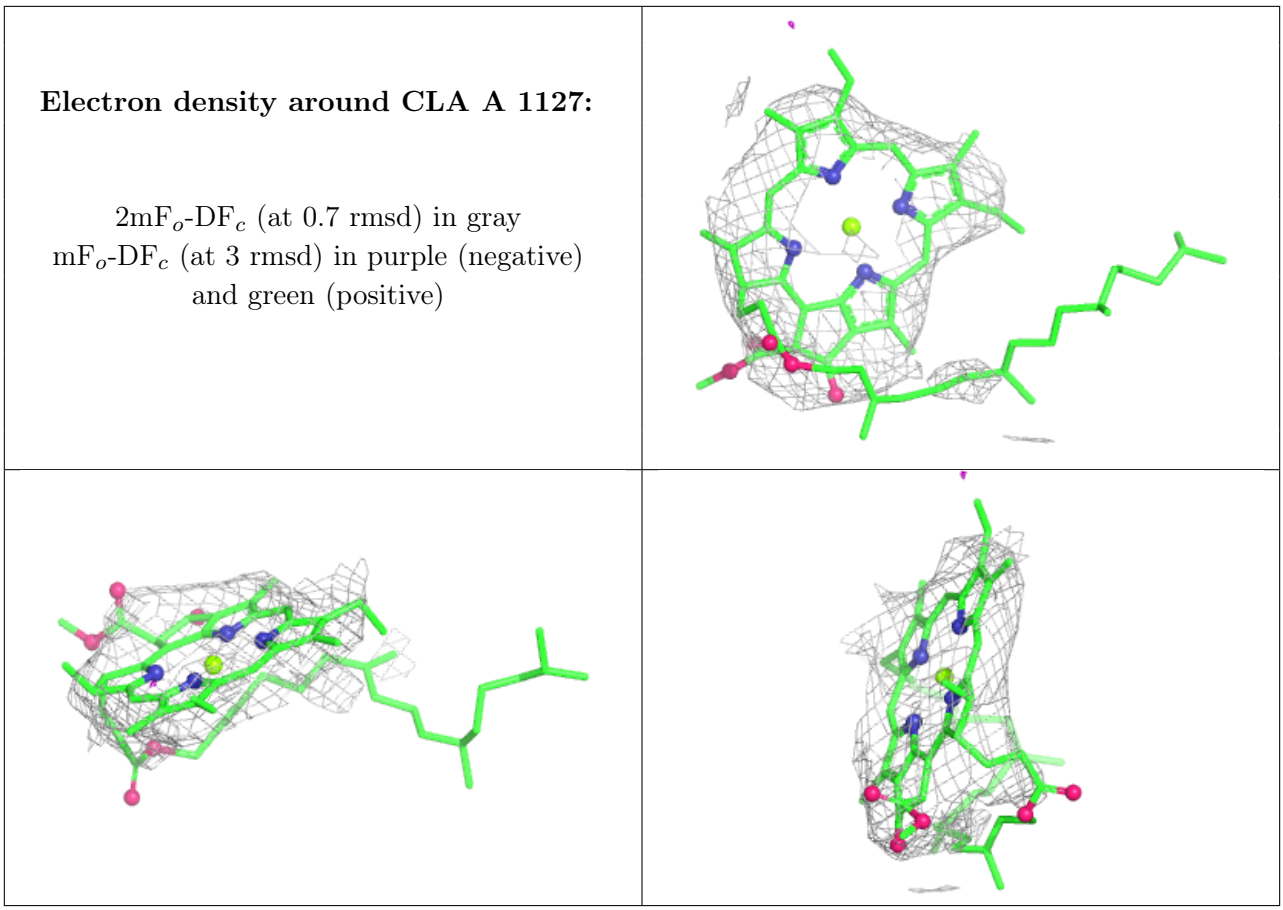






Electron density around CLA A 1127:

$2mF_o$-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

There are no such residues in this entry.