Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2026 – 01:07 pm BST

PDB ID	:	6QPH / pdb_00006qph
Title	:	Dunaliella minimal PSI complex
Authors	:	Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on	:	2019-02-14
Resolution	:	3.40 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:

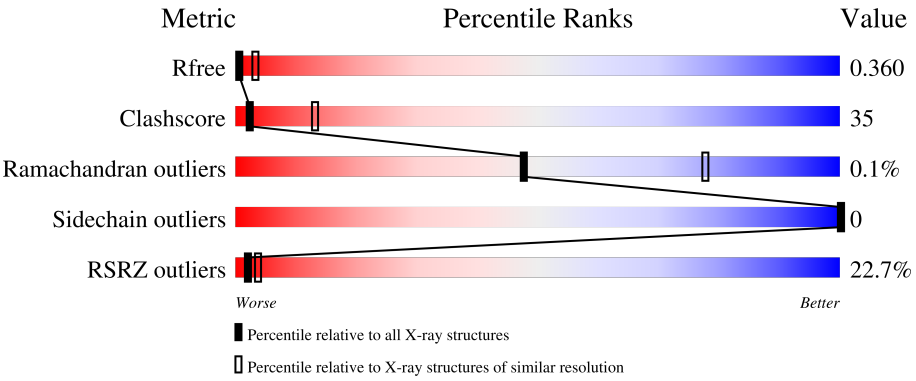
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	195	21% 57% 43%
2	2	211	23% 61% 39%
3	3	210	33% 51% 49%
4	4	211	24% 60% 40%
5	A	739	25% 48% 52%

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Mol	Chain	Length	Quality of chain
6	B	734	24% 52% 48%
7	C	80	19% 49% 50%
8	D	142	20% 49% 49%
9	E	64	3% 58% 42%
10	F	163	8% 56% 44%
11	J	41	12% 41% 56%

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	XAT	2	502	X	-	-	-
13	XAT	3	502	X	-	X	-
13	XAT	4	502	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	-	-	X	-
15	CLA	3	603	-	-	X	-
15	CLA	A	1012	-	-	X	-
15	CLA	A	1013	-	-	X	-
15	CLA	A	1111	-	-	X	-
15	CLA	B	1021	-	-	X	-
16	CHL	1	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	4	610	X	-	-	-
16	CHL	4	613	X	-	-	-
26	SF4	C	3003	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 30870 atoms, of which 32 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	195	Total	C	N	O	S	0	0	0
			1490	956	253	274	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Lhc2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	2	211	Total	C	H	N	O	S	0	0	0
			1663	1047	32	277	300	7			

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	210	Total	C	N	O	S	0	0	0
			1609	1050	263	291	5			

- Molecule 4 is a protein called Lhc4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	211	Total	C	N	O	S	0	0	0
			1637	1058	272	303	4			

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	739	Total	C	N	O	S	0	0	0
			5799	3789	991	1001	18			

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	734	Total	C	N	O	S	0	0	0
			5813	3818	975	1007	13			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	80	Total	C	N	O	S	0	0	0
			600	370	104	115	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	142	Total	C	N	O	S	0	0	0
			1123	718	195	204	6			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	64	Total	C	N	O	0	0	0
			515	327	89	99			

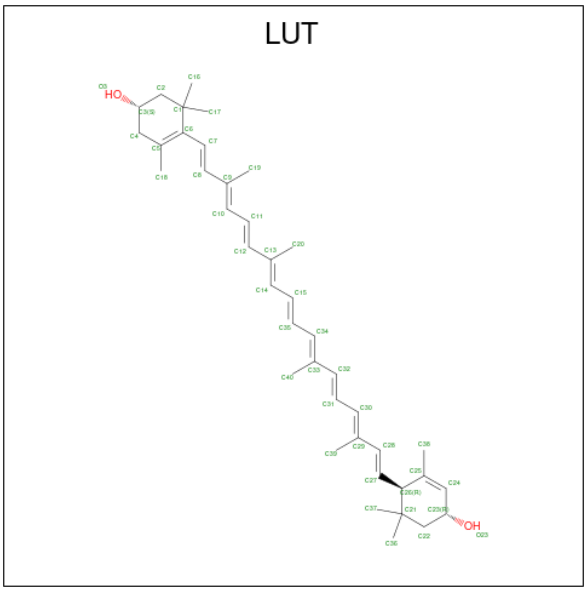
- Molecule 10 is a protein called PsaF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	163	Total	C	N	O	S	0	0	0
			1285	828	218	237	2			

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

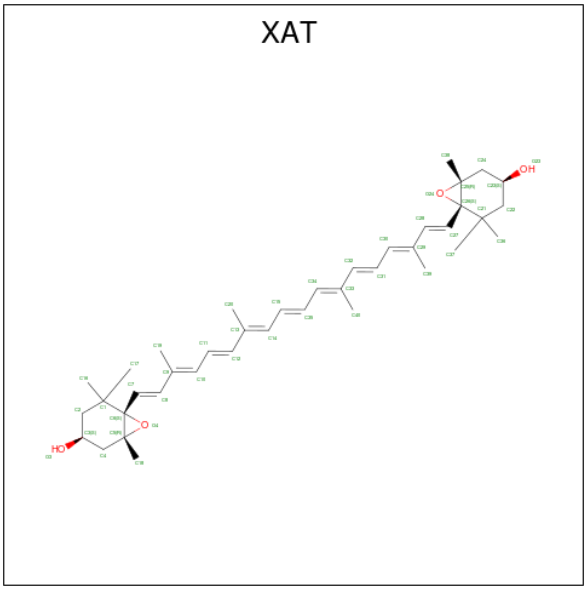
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	41	Total	C	N	O	S	0	0	0
			327	223	47	56	1			

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



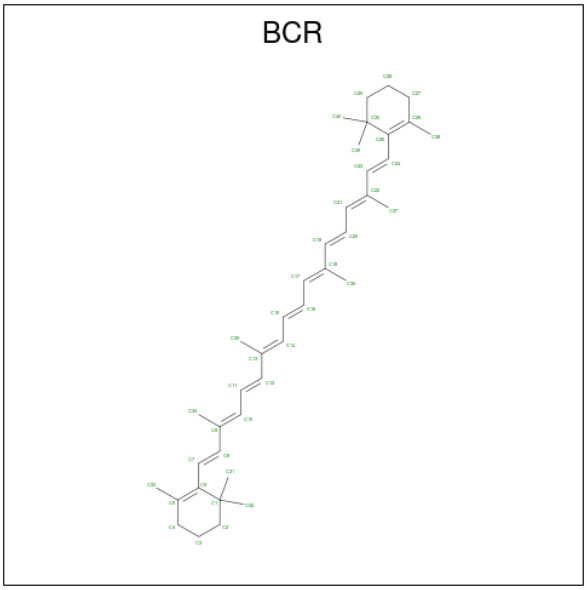
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	1	1	Total C O 42 40 2	0	0
12	2	1	Total C O 42 40 2	0	0
12	3	1	Total C O 42 40 2	0	0
12	4	1	Total C O 42 40 2	0	0

- Molecule 13 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	1	1	Total C O 44 40 4	0	0
13	2	1	Total C O 44 40 4	0	0
13	3	1	Total C O 44 40 4	0	0
13	4	1	Total C O 44 40 4	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	3	1	Total C 40 40	0	0
14	3	1	Total C 40 40	0	0
14	4	1	Total C 40 40	0	0
14	4	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0

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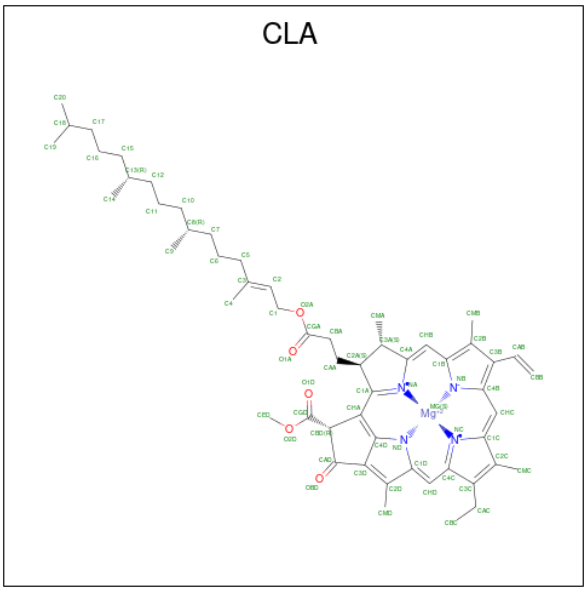
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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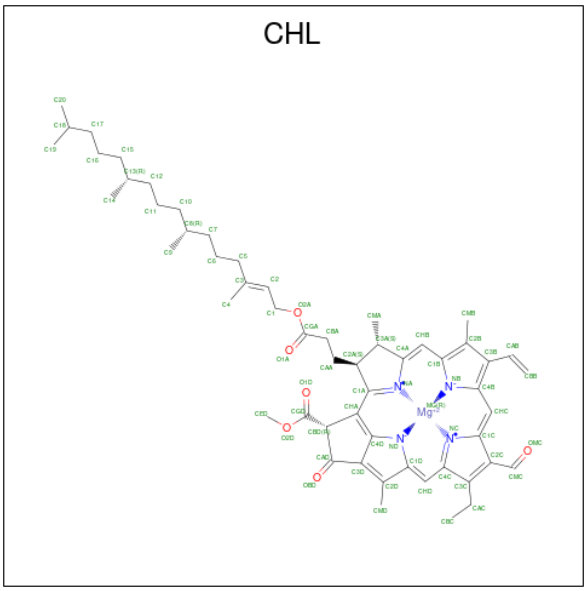
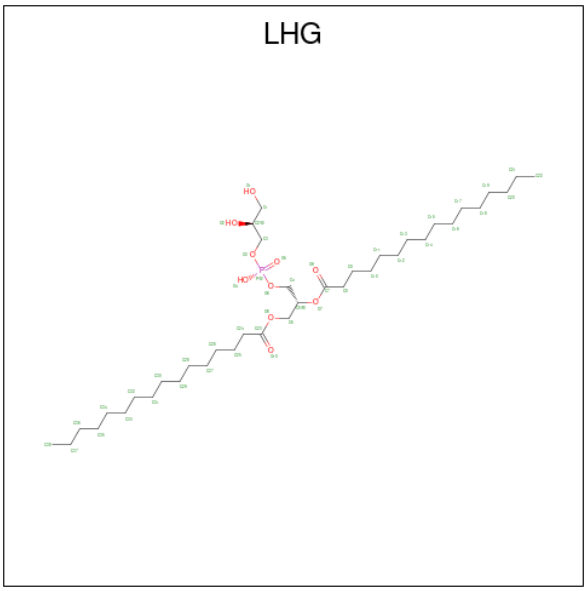
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



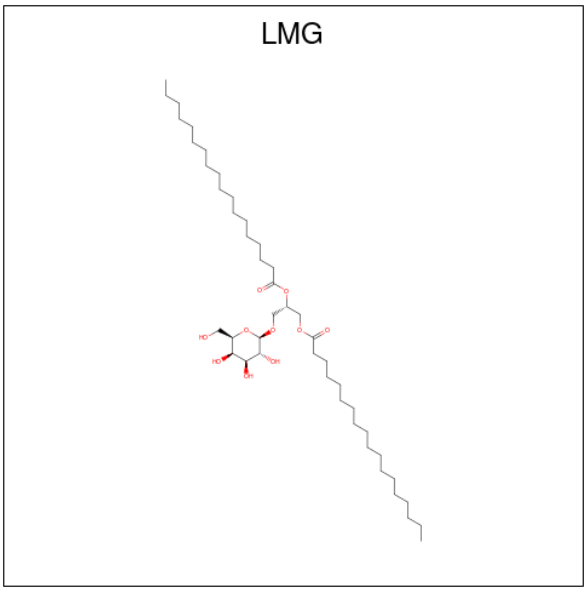
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	1	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
16	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



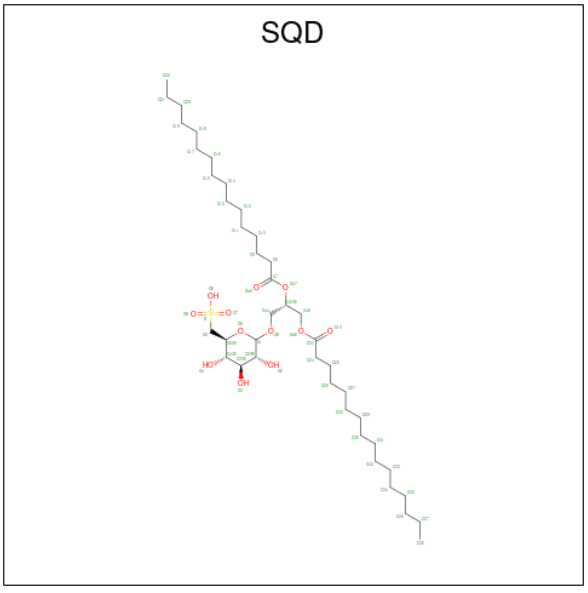
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	1	1	Total C O P 23 12 10 1	0	0
17	2	1	Total C O P 21 10 10 1	0	0
17	A	1	Total C O P 16 7 8 1	0	0
17	A	1	Total C O P 24 13 10 1	0	0
17	B	1	Total C O P 21 10 10 1	0	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



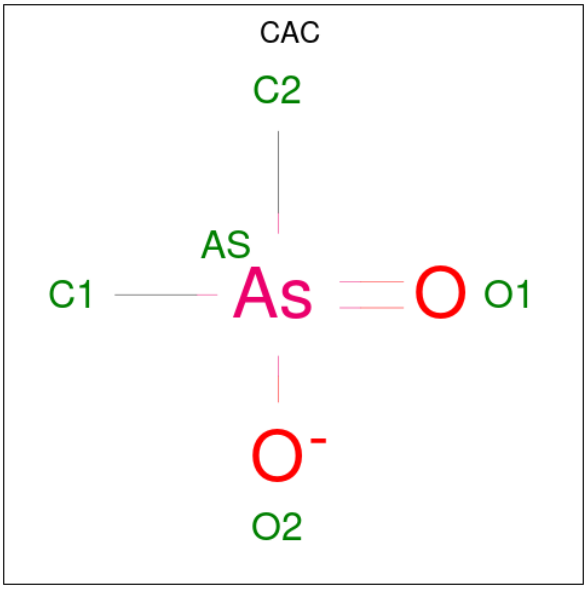
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C O 36 26 10	0	0
18	1	1	Total C O 23 13 10	0	0
18	2	1	Total C O 25 15 10	0	0
18	2	1	Total C O 16 9 7	0	0

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



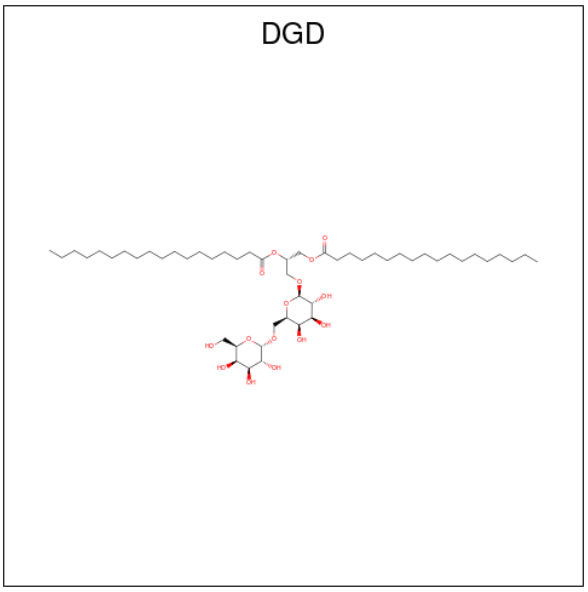
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	O	S	0	0
			40	27	12	1		

- Molecule 20 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



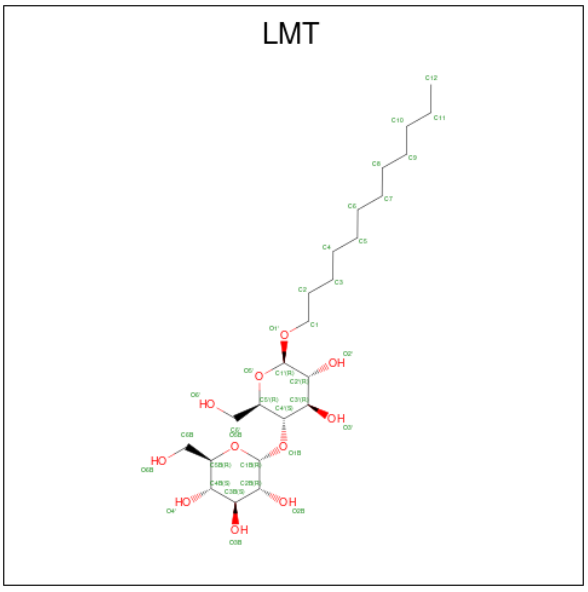
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



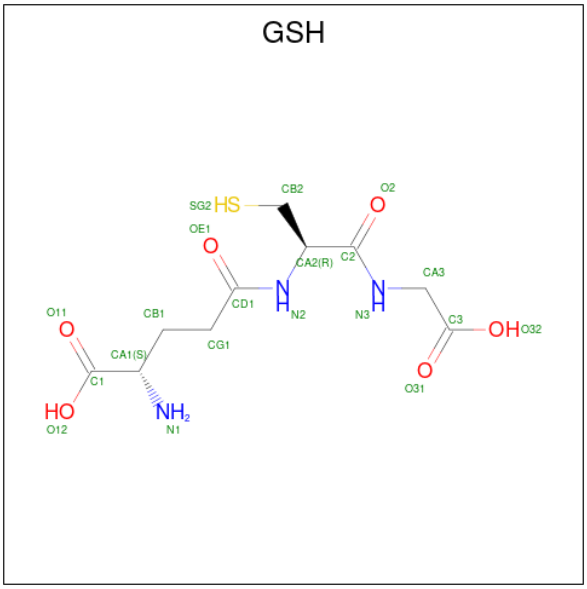
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	2	1	Total C O 47 32 15	0	0
21	4	1	Total C O 45 30 15	0	0
21	B	1	Total C O 38 23 15	0	0
21	J	1	Total C O 28 15 13	0	0

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



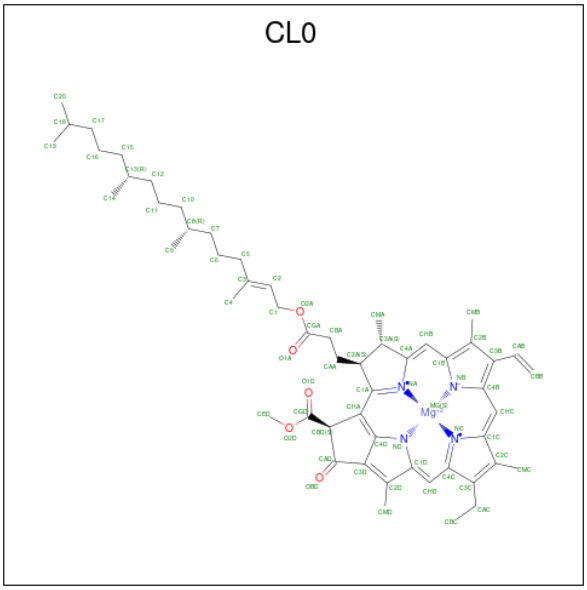
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	2	1	Total	C	O	0	0
			23	12	11		

- Molecule 23 is Glutathione (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



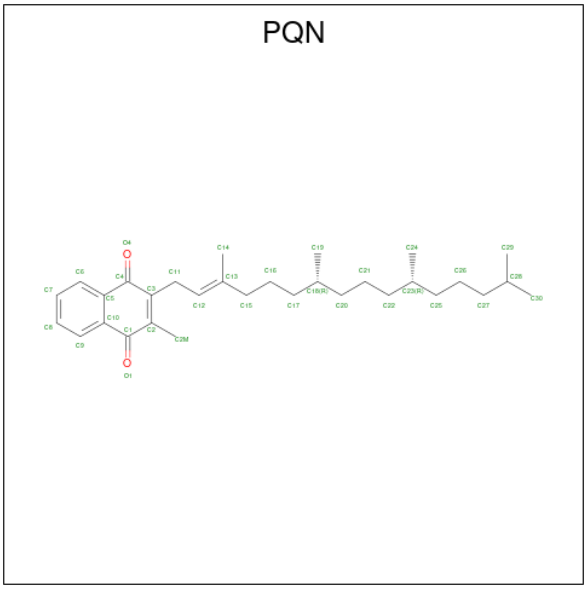
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	4	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
23	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



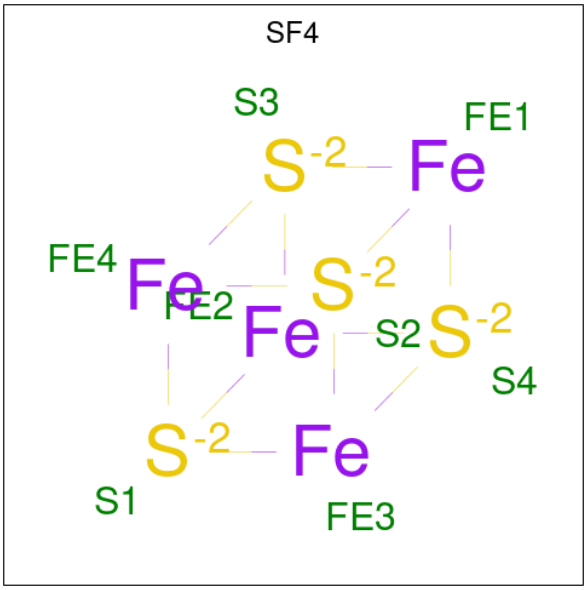
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total Ca 1 1	0	0

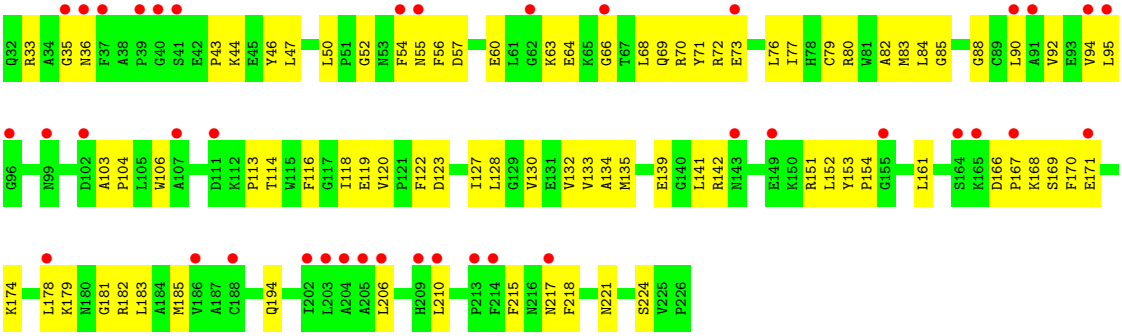
3 Residue-property plots (i)

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

• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

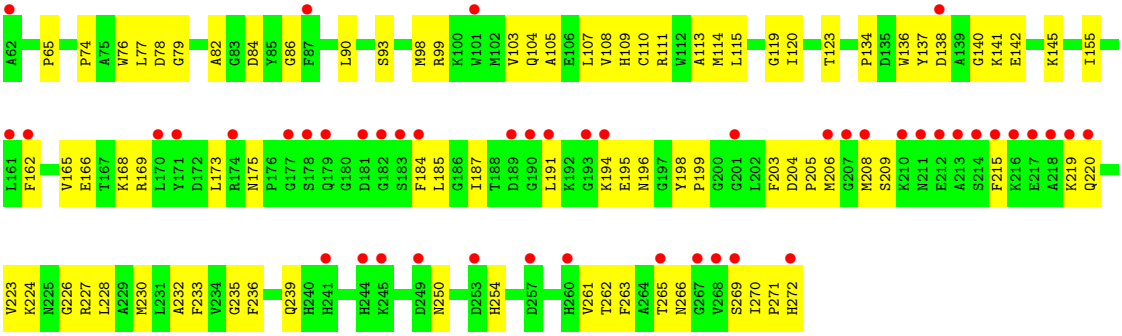




• Molecule 2: Lhc2

Chain 2:

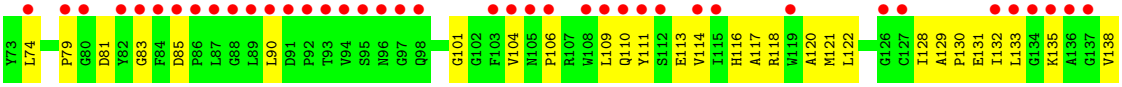


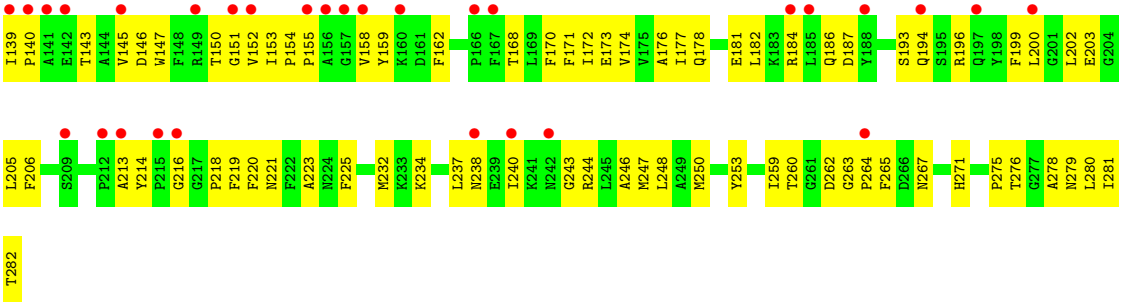


• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

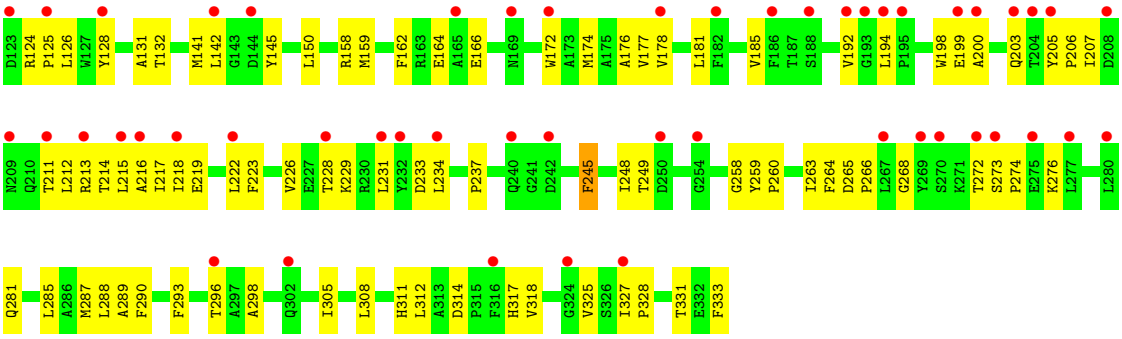






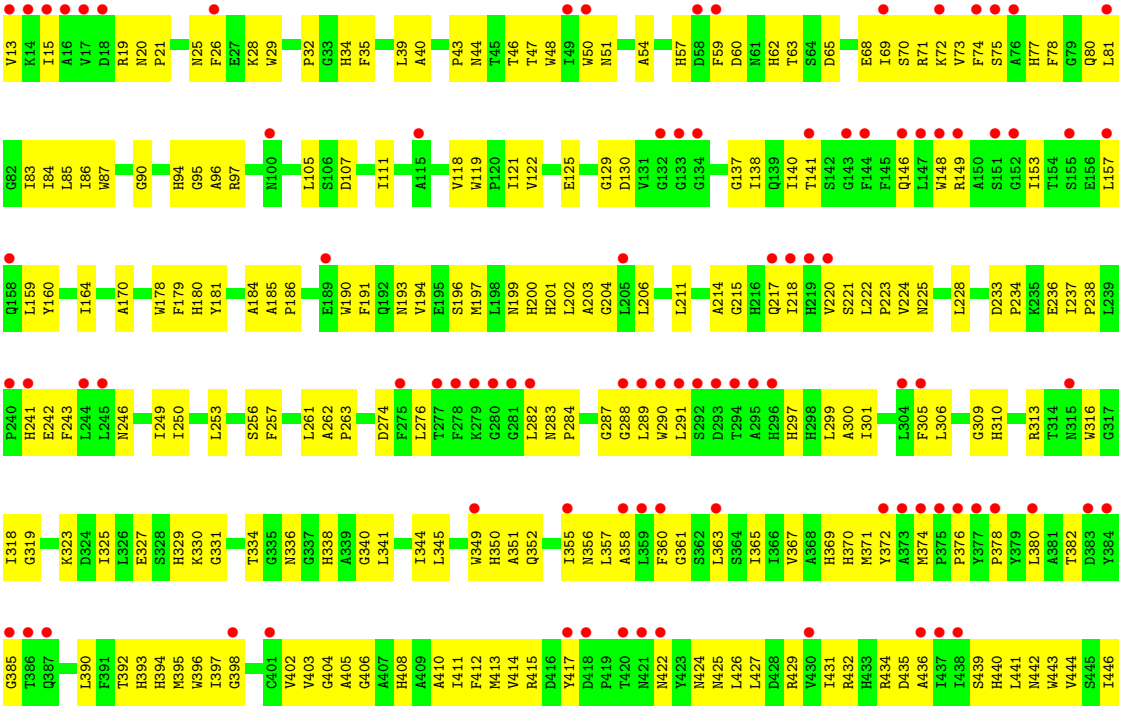
• Molecule 4: Lhc4

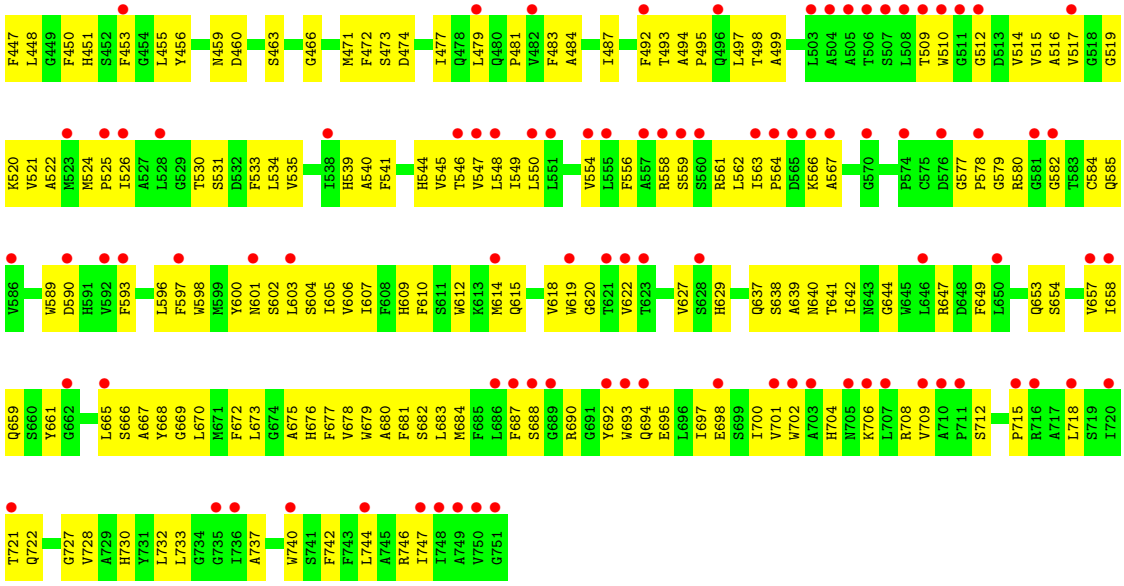




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



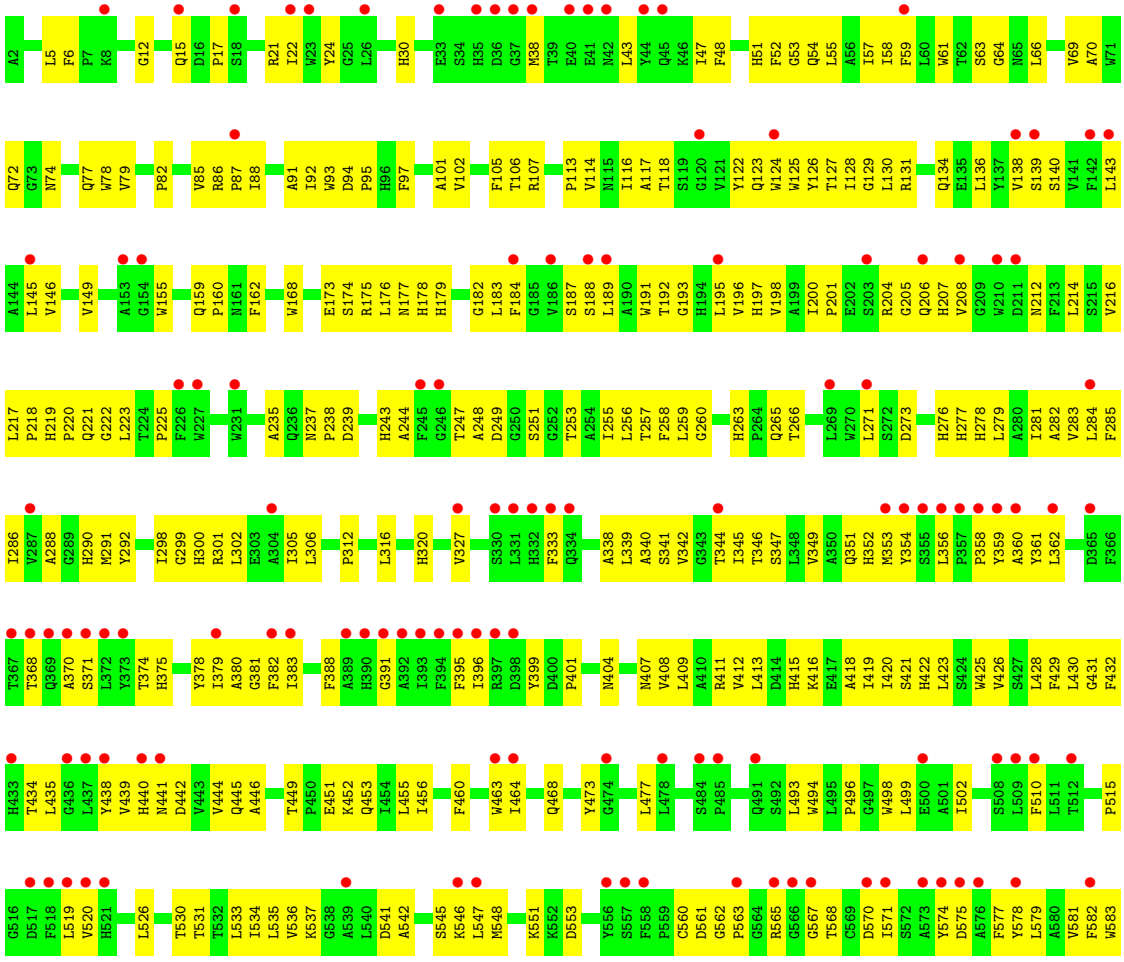


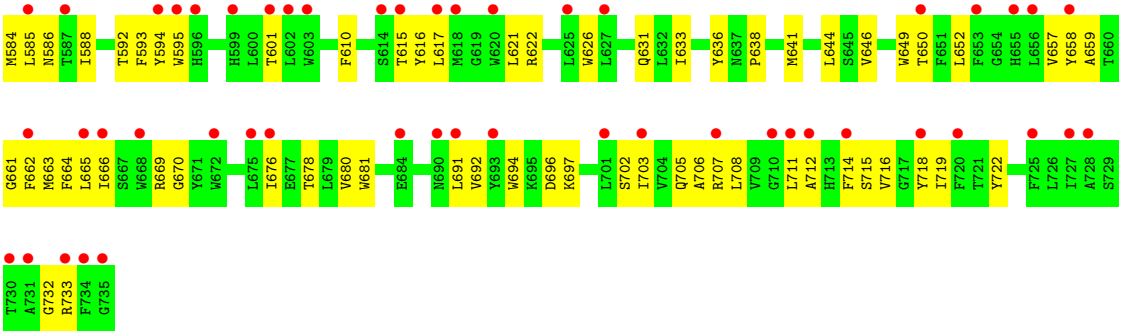


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

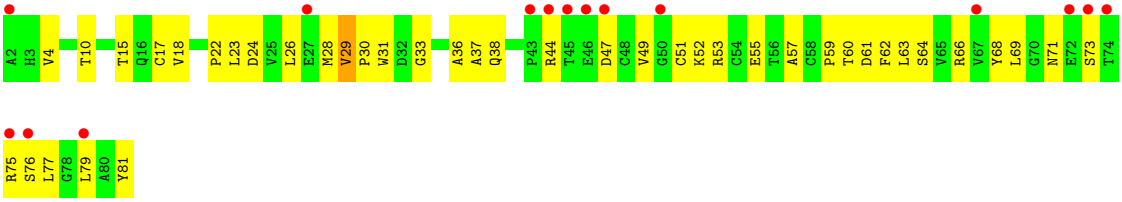






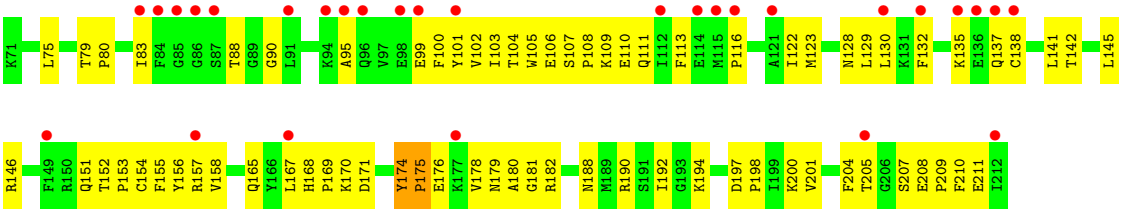
• Molecule 7: Photosystem I iron-sulfur center





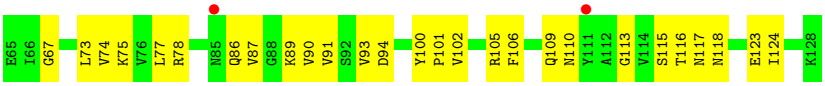
• Molecule 8: PsaD





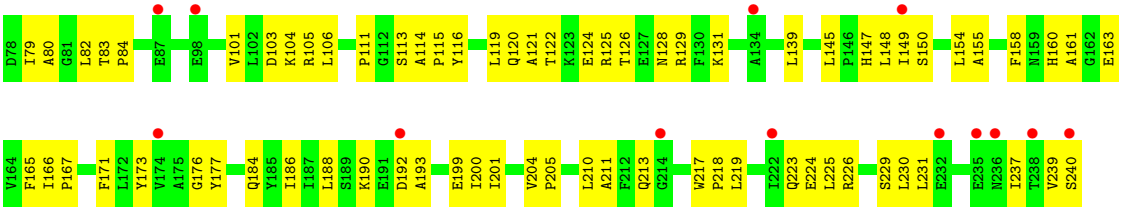
• Molecule 9: PsaE



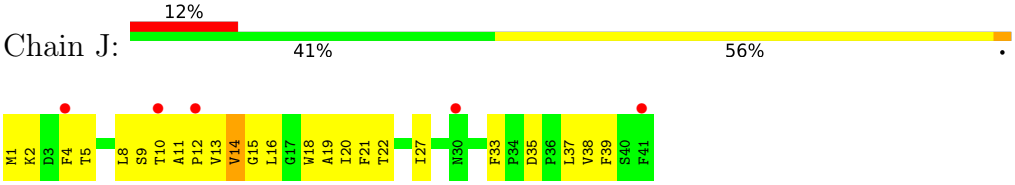


• Molecule 10: PsaF





• Molecule 11: Photosystem I reaction center subunit IX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	158.88Å 100.51Å 191.04Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	48.95 – 3.40 48.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-3.40) 89.4 (48.95-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.337 , 0.356 0.339 , 0.360	Depositor DCC
R_{free} test set	1593 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å^2)	79.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 17.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	30870	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LUT, CAC, CHL, BCR, LMT, LHG, PQN, CLA, CL0, SQD, SF4, CA, LMG, GSH, DGD

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	0.31	0/1529	0.34	0/2073
2	2	0.27	0/1680	0.34	0/2277
3	3	0.16	0/1657	0.36	0/2253
4	4	0.39	0/1687	0.41	0/2300
5	A	0.23	1/5995 (0.0%)	0.27	0/8179
6	B	0.26	0/6026	0.28	0/8237
7	C	0.24	0/610	0.30	0/828
8	D	0.21	0/1150	0.40	0/1551
9	E	0.34	0/525	0.31	0/712
10	F	0.40	0/1313	0.38	0/1776
11	J	0.38	0/338	0.45	0/461
All	All	0.28	1/22510 (0.0%)	0.32	0/30647

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
7	C	0	1
11	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	20	ASN	C-O	-5.06	1.21	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	245	PHE	Peptide
7	C	29	VAL	Peptide
11	J	14	VAL	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	1490	0	1457	108	1
2	2	1631	32	1575	112	0
3	3	1609	0	1567	138	0
4	4	1637	0	1579	139	0
5	A	5799	0	5629	446	0
6	B	5813	0	5565	403	0
7	C	600	0	582	52	0
8	D	1123	0	1134	83	0
9	E	515	0	508	21	0
10	F	1285	0	1304	91	0
11	J	327	0	328	46	0
12	1	42	0	55	10	0
12	2	42	0	55	13	0
12	3	42	0	55	11	0
12	4	42	0	55	18	0
13	1	44	0	56	11	0
13	2	44	0	56	13	0
13	3	44	0	56	21	0
13	4	44	0	56	5	0
14	1	80	0	105	15	0
14	2	40	0	53	8	0
14	3	80	0	105	25	0
14	4	80	0	105	12	0
14	A	240	0	318	39	0
14	B	240	0	316	34	0
14	F	40	0	52	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	120	0	159	27	0
15	1	593	0	468	105	0
15	2	501	0	402	58	0
15	3	525	0	391	96	0
15	4	542	0	423	82	0
15	A	2180	0	1773	276	0
15	B	2137	0	1760	230	0
15	F	96	0	72	7	0
15	J	49	0	38	9	0
16	1	97	0	66	26	0
16	2	194	0	134	25	0
16	3	47	0	30	15	0
16	4	147	0	102	22	0
17	1	23	0	16	2	0
17	2	21	0	12	2	0
17	A	40	0	30	5	0
17	B	21	0	12	2	0
18	1	59	0	58	1	0
18	2	41	0	34	1	0
19	1	40	0	46	4	0
20	1	10	0	0	0	0
20	3	10	0	0	1	0
20	4	10	0	0	1	0
21	2	47	0	52	2	0
21	4	45	0	48	7	0
21	B	38	0	34	5	0
21	J	28	0	26	0	0
22	2	23	0	21	0	0
23	4	20	0	15	0	1
23	B	20	0	15	2	0
24	A	50	0	39	19	0
25	A	33	0	46	9	0
25	B	33	0	46	8	0
26	A	8	0	0	0	0
26	C	16	0	0	2	0
27	B	1	0	0	0	0
All	All	30838	32	29094	2127	1

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 35.

All (2127) 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)
14:A:4005:BCR:C11	14:A:4005:BCR:C12	1.83	1.49
14:A:4005:BCR:C11	14:A:4005:BCR:C10	1.92	1.45
7:C:29:VAL:HG12	7:C:30:PRO:HD3	1.20	1.17
8:D:105:TRP:HB3	8:D:153:PRO:HB3	1.40	1.02
6:B:5:LEU:HD13	6:B:6:PHE:H	1.24	1.02
15:A:1101:CLA:HBD	15:A:1101:CLA:HBA2	1.42	1.01
8:D:146:ARG:HH22	8:D:153:PRO:HD2	1.25	1.01
15:A:1012:CLA:H43	6:B:439:VAL:HG22	1.41	0.99
1:1:103:ALA:HA	15:1:606:CLA:HED1	1.45	0.98
15:2:605:CLA:HAC1	15:2:612:CLA:HAA1	1.44	0.97
1:1:217:ASN:HB3	15:1:608:CLA:HED1	1.43	0.97
14:A:4007:BCR:H363	15:B:1239:CLA:HBB1	1.47	0.96
2:2:187:ILE:HG21	2:2:191:LEU:HD13	1.47	0.96
15:B:1230:CLA:HED1	11:J:35:ASP:HA	1.48	0.96
4:4:265:ASP:HB2	4:4:266:PRO:HD3	1.44	0.95
7:C:29:VAL:HG12	7:C:30:PRO:CD	1.96	0.95
15:A:1110:CLA:HED1	15:A:1111:CLA:HHC	1.49	0.95
3:3:271:HIS:HD2	3:3:275:PRO:HA	1.31	0.95
3:3:250:MET:HG2	13:3:502:XAT:H12	1.47	0.95
5:A:584:CYS:H	6:B:670:GLY:HA3	1.31	0.95
4:4:158:ARG:NH2	20:4:902:CAC:O1	2.01	0.93
16:1:610:CHL:HMC	15:1:613:CLA:HAB	1.49	0.93
15:A:1013:CLA:H42	15:A:1013:CLA:HHB	1.50	0.93
1:1:50:LEU:HD11	1:1:68:LEU:HD21	1.47	0.93
15:A:1108:CLA:HBA1	15:A:1108:CLA:HBD	1.51	0.92
10:F:166:ILE:HG13	10:F:167:PRO:HD3	1.48	0.92
15:A:1124:CLA:HBB1	15:A:1124:CLA:HHC	1.51	0.92
15:1:608:CLA:HAA2	4:4:218:ILE:HG22	1.51	0.92
3:3:259:ILE:HD11	14:3:504:BCR:H281	1.51	0.92
15:1:605:CLA:HHC	15:1:605:CLA:HBB1	1.52	0.91
7:C:17:CYS:HB3	26:C:3003:SF4:S2	2.11	0.91
15:3:603:CLA:HBA2	15:3:603:CLA:HBD	1.53	0.91
5:A:15:ILE:HD11	15:A:1110:CLA:HBD	1.53	0.90
15:1:603:CLA:HBD	15:1:603:CLA:HBA1	1.54	0.90
13:3:502:XAT:H31	15:3:605:CLA:HMB3	1.55	0.89
3:3:271:HIS:CD2	3:3:275:PRO:HA	2.08	0.89
4:4:199:GLU:OE1	4:4:203:GLN:NE2	2.06	0.89
5:A:605:ILE:HD11	24:A:1011:CL0:H35	1.55	0.88
15:A:1127:CLA:HHC	15:A:1127:CLA:HBB1	1.53	0.88
5:A:481:PRO:HD3	5:A:533:PHE:HB2	1.55	0.88
6:B:575:ASP:OD1	6:B:707:ARG:NH1	2.07	0.88
4:4:265:ASP:HB2	4:4:266:PRO:CD	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:177:TYR:HE2	15:F:1301:CLA:HBD	1.37	0.87
6:B:585:LEU:HD21	6:B:715:SER:HA	1.56	0.87
16:3:604:CHL:HHD	16:3:604:CHL:HBC2	1.57	0.87
8:D:146:ARG:NH2	8:D:151:GLN:O	2.07	0.87
15:A:1013:CLA:HBA1	6:B:428:LEU:HD23	1.55	0.86
5:A:680:ALA:HB3	15:A:1013:CLA:HBB2	1.57	0.86
12:2:501:LUT:H28	12:2:501:LUT:H361	1.58	0.86
3:3:101:GLY:HA3	5:A:19:ARG:HD2	1.55	0.86
3:3:221:ASN:ND2	3:3:223:ALA:O	2.08	0.86
12:1:501:LUT:H371	12:1:501:LUT:H28	1.58	0.86
4:4:141:MET:HE1	4:4:159:MET:HE2	1.57	0.86
2:2:165:VAL:HG11	14:2:503:BCR:H16C	1.56	0.85
5:A:331:GLY:HA3	17:A:5001:LHG:HC32	1.58	0.85
15:A:1125:CLA:HBB1	15:A:1125:CLA:HHC	1.56	0.85
15:A:1107:CLA:HBB1	15:A:1107:CLA:HMB3	1.58	0.85
3:3:117:ALA:HB1	3:3:243:GLY:HA3	1.57	0.85
10:F:177:TYR:CE2	15:F:1301:CLA:HBD	2.12	0.85
3:3:151:GLY:HA3	15:3:613:CLA:HBC1	1.59	0.85
3:3:225:PHE:CD2	15:3:601:CLA:H12	2.12	0.85
6:B:64:GLY:HA3	15:B:1204:CLA:HBB1	1.59	0.85
15:1:615:CLA:HBB1	15:1:615:CLA:HMB1	1.59	0.85
4:4:128:TYR:HD2	4:4:132:THR:HG21	1.40	0.84
3:3:259:ILE:HG21	15:3:603:CLA:HBA1	1.59	0.84
6:B:388:PHE:HZ	15:B:1222:CLA:HAB	1.41	0.84
15:B:1227:CLA:HBB2	15:B:1236:CLA:HBB2	1.57	0.84
12:3:501:LUT:H221	15:3:601:CLA:H2	1.59	0.84
13:3:502:XAT:H22	15:3:606:CLA:HMB3	1.59	0.84
1:1:139:GLU:OE1	1:1:142:ARG:NH2	2.11	0.83
6:B:708:LEU:HD22	21:B:5002:DGD:HB22	1.60	0.83
5:A:345:LEU:HD11	5:A:355:ILE:HD12	1.60	0.83
15:B:1230:CLA:HBB1	15:B:1230:CLA:HMB3	1.60	0.83
6:B:659:ALA:HB3	15:B:1023:CLA:HBB2	1.60	0.83
5:A:43:PRO:HG3	10:F:200:ILE:HD13	1.61	0.83
5:A:87:TRP:HA	15:A:1105:CLA:HBB2	1.59	0.83
14:A:4005:BCR:C11	14:A:4005:BCR:C13	2.56	0.83
5:A:68:GLU:HG2	5:A:72:LYS:HE2	1.61	0.82
15:A:1012:CLA:HMB3	15:B:1021:CLA:H201	1.60	0.82
15:4:608:CLA:HMB1	15:4:608:CLA:HBB1	1.60	0.82
6:B:546:LYS:HE3	10:F:237:ILE:HG22	1.61	0.82
12:1:501:LUT:H162	15:1:608:CLA:HBC1	1.62	0.82
13:3:502:XAT:H381	13:3:502:XAT:H28	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:199:GLU:O	4:4:203:GLN:NE2	2.13	0.82
7:C:62:PHE:HB3	8:D:192:ILE:HG12	1.61	0.82
15:A:1133:CLA:H42	14:A:4005:BCR:HC7	1.61	0.81
5:A:679:TRP:CD2	24:A:1011:CL0:H6	2.14	0.81
3:3:205:LEU:HD23	3:3:218:PRO:HB2	1.63	0.80
15:B:1225:CLA:HHC	15:B:1225:CLA:HBB1	1.60	0.80
1:1:46:TYR:CE1	1:1:63:LYS:HG3	2.16	0.80
15:B:1239:CLA:HAC1	25:B:2002:PQN:H151	1.64	0.80
2:2:107:LEU:HB3	2:2:111:ARG:HH12	1.47	0.80
15:B:1022:CLA:HAC2	15:B:1023:CLA:HBC3	1.62	0.80
14:A:4005:BCR:C12	14:A:4005:BCR:C10	2.59	0.80
6:B:208:VAL:HA	6:B:212:ASN:HD21	1.46	0.80
2:2:109:HIS:HD2	15:2:612:CLA:HMD1	1.47	0.79
4:4:211:THR:HG23	4:4:215:LEU:HD21	1.63	0.79
15:B:1023:CLA:O2A	15:B:1023:CLA:H3A	1.82	0.79
10:F:177:TYR:OH	10:F:211:ALA:O	2.00	0.79
16:1:610:CHL:HHC	16:1:610:CHL:HBB1	1.65	0.79
4:4:145:TYR:HD2	15:4:609:CLA:HMC2	1.48	0.79
15:A:1131:CLA:HHC	15:A:1131:CLA:HBB1	1.63	0.79
12:3:501:LUT:H371	12:3:501:LUT:H28	1.65	0.79
5:A:463:SER:OG	5:A:471:MET:SD	2.41	0.79
5:A:75:SER:HB3	15:A:1109:CLA:HAC2	1.64	0.78
5:A:395:MET:HE1	5:A:606:VAL:HG11	1.66	0.78
1:1:141:LEU:O	15:1:611:CLA:HBC3	1.82	0.78
1:1:221:ASN:ND2	15:1:603:CLA:OBD	2.17	0.78
15:1:606:CLA:HHD	15:1:606:CLA:HBC2	1.64	0.78
3:3:122:LEU:HD11	14:3:503:BCR:C38	2.14	0.78
2:2:236:PHE:HE1	12:2:501:LUT:H363	1.49	0.77
5:A:687:PHE:HB2	15:A:1013:CLA:CBC	2.14	0.77
4:4:128:TYR:CD2	4:4:132:THR:HG21	2.20	0.77
14:4:505:BCR:H272	10:F:223:GLN:HE22	1.50	0.77
5:A:43:PRO:HB3	5:A:48:TRP:CE3	2.20	0.77
6:B:463:TRP:CD1	6:B:477:LEU:HD11	2.20	0.77
15:A:1102:CLA:HBA2	15:A:1109:CLA:H2	1.66	0.76
7:C:10:THR:O	7:C:64:SER:OG	2.03	0.76
3:3:246:ALA:HB2	12:3:501:LUT:H202	1.67	0.76
3:3:260:THR:HG21	3:3:267:ASN:HD21	1.49	0.76
15:A:1110:CLA:HED1	15:A:1111:CLA:HAB	1.68	0.76
15:B:1023:CLA:HBB1	15:B:1023:CLA:HMB3	1.65	0.76
3:3:122:LEU:HD11	14:3:503:BCR:H383	1.65	0.76
3:3:223:ALA:HB3	15:3:601:CLA:C3	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1102:CLA:HBB1	15:A:1102:CLA:HMB1	1.68	0.76
24:A:1011:CL0:H15	24:A:1011:CL0:H11	1.66	0.76
15:A:1128:CLA:HBB1	15:A:1128:CLA:HMB3	1.68	0.76
6:B:515:PRO:HG2	10:F:147:HIS:ND1	2.00	0.76
6:B:176:LEU:HD23	6:B:292:TYR:CE2	2.21	0.76
3:3:199:PHE:CZ	14:3:503:BCR:H10C	2.20	0.76
3:3:247:MET:HE1	16:3:604:CHL:HAB	1.68	0.76
5:A:73:VAL:HG21	15:A:1103:CLA:HBC2	1.68	0.76
15:1:606:CLA:HMA3	15:1:613:CLA:C2C	2.16	0.76
5:A:395:MET:HE1	5:A:606:VAL:CG1	2.16	0.76
11:J:9:SER:HA	11:J:13:VAL:HG21	1.65	0.76
15:1:608:CLA:HED2	15:1:608:CLA:H2A	1.68	0.75
6:B:69:VAL:HG13	6:B:122:TYR:HE1	1.51	0.75
6:B:722:TYR:HB2	15:B:1021:CLA:HED3	1.68	0.75
16:1:610:CHL:HBD	16:1:610:CHL:O2A	1.87	0.75
4:4:231:LEU:HD12	15:4:612:CLA:HMA1	1.68	0.75
5:A:84:ILE:HD13	15:A:1104:CLA:HBC3	1.69	0.75
5:A:406:GLY:HA2	14:A:4005:BCR:H292	1.66	0.75
6:B:594:TYR:CE2	15:B:1234:CLA:HBC3	2.22	0.75
5:A:682:SER:HB3	5:A:730:HIS:CB	2.16	0.75
11:J:10:THR:H	11:J:13:VAL:HG22	1.49	0.75
7:C:28:MET:O	8:D:178:VAL:HG22	1.86	0.75
12:2:501:LUT:H382	15:2:608:CLA:HBC1	1.69	0.75
6:B:221:GLN:HG2	6:B:225:PRO:HD3	1.67	0.74
5:A:47:THR:HG22	5:A:51:ASN:OD1	1.86	0.74
15:A:1136:CLA:HBB1	15:A:1136:CLA:HMB1	1.67	0.74
6:B:358:PRO:HG3	15:B:1215:CLA:HAA2	1.70	0.74
4:4:231:LEU:HD12	15:4:612:CLA:CMA	2.17	0.74
5:A:456:TYR:HB3	5:A:642:ILE:HG13	1.68	0.74
15:1:604:CLA:H3A	15:1:604:CLA:CGA	2.18	0.74
6:B:237:ASN:ND2	6:B:253:THR:OG1	2.20	0.74
1:1:33:ARG:NH1	1:1:36:ASN:OD1	2.21	0.74
3:3:276:THR:HA	3:3:279:ASN:ND2	2.03	0.74
5:A:370:HIS:ND1	15:A:1116:CLA:OBD	2.21	0.74
6:B:5:LEU:HD13	6:B:6:PHE:N	2.00	0.74
15:2:604:CLA:HED2	15:2:604:CLA:H2A	1.68	0.73
6:B:298:ILE:HG13	6:B:299:GLY:H	1.52	0.73
15:1:604:CLA:H3A	15:1:604:CLA:O1A	1.87	0.73
6:B:223:LEU:HD13	6:B:223:LEU:O	1.86	0.73
15:B:1211:CLA:HMA3	14:B:4003:BCR:H271	1.70	0.73
13:2:502:XAT:H383	15:2:606:CLA:C2B	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:605:CLA:OBD	15:4:612:CLA:HBA2	1.88	0.73
2:2:98:MET:HE1	11:J:1:MET:HE2	1.69	0.73
3:3:199:PHE:CZ	15:3:611:CLA:HBB2	2.22	0.73
3:3:205:LEU:CD2	3:3:218:PRO:HB2	2.18	0.73
2:2:77:LEU:HD12	2:2:77:LEU:O	1.89	0.73
15:A:1113:CLA:HAB	14:A:4002:BCR:H19C	1.71	0.73
15:2:607:CLA:HBB2	14:3:503:BCR:HC7	1.71	0.72
15:A:1138:CLA:HBB1	15:A:1138:CLA:HMB1	1.71	0.72
2:2:107:LEU:HB3	2:2:111:ARG:NH1	2.04	0.72
15:3:603:CLA:HBD	15:3:603:CLA:CBA	2.17	0.72
8:D:123:MET:SD	8:D:128:ASN:ND2	2.60	0.72
2:2:166:GLU:OE1	2:2:169:ARG:NH2	2.22	0.72
6:B:595:TRP:HD1	15:B:1234:CLA:HAC1	1.54	0.72
11:J:19:ALA:HA	11:J:22:THR:OG1	1.89	0.72
1:1:217:ASN:CB	15:1:608:CLA:HED1	2.18	0.72
6:B:423:LEU:HD13	6:B:533:LEU:HA	1.71	0.72
3:3:177:ILE:HD13	14:3:503:BCR:H361	1.72	0.72
16:3:604:CHL:HBB1	16:3:604:CHL:HMB3	1.71	0.72
4:4:260:PRO:CG	4:4:263:ILE:HD12	2.20	0.72
5:A:680:ALA:C	15:A:1013:CLA:HAB	2.15	0.72
6:B:548:MET:HE2	6:B:551:LYS:HA	1.70	0.72
6:B:578:TYR:OH	6:B:665:LEU:HD22	1.89	0.72
5:A:319:GLY:HA2	15:A:1121:CLA:HAC2	1.72	0.72
5:A:512:GLY:HA2	5:A:525:PRO:HG3	1.72	0.72
1:1:79:CYS:O	1:1:83:MET:HG3	1.90	0.72
15:1:603:CLA:HBA1	15:1:603:CLA:CBD	2.19	0.72
5:A:197:MET:CE	15:A:1111:CLA:HAC1	2.20	0.72
15:B:1227:CLA:HBB2	15:B:1236:CLA:CBB	2.18	0.72
6:B:429:PHE:CE2	15:B:1235:CLA:HAB	2.25	0.72
4:4:176:ALA:HA	15:4:606:CLA:HAB	1.71	0.71
15:2:601:CLA:HMB1	15:2:601:CLA:HBB1	1.70	0.71
10:F:121:ALA:O	10:F:125:ARG:HD3	1.90	0.71
15:B:1216:CLA:HMB3	15:B:1216:CLA:HBB1	1.72	0.71
3:3:205:LEU:HD22	3:3:219:PHE:H	1.55	0.71
3:3:250:MET:HE2	13:3:502:XAT:H10	1.71	0.71
2:2:195:GLU:HG2	2:2:196:ASN:H	1.54	0.71
15:A:1109:CLA:HBA1	15:A:1109:CLA:CHA	2.18	0.71
1:1:218:PHE:HA	1:1:221:ASN:ND2	2.06	0.71
1:1:170:PHE:CE2	1:1:174:LYS:HD2	2.25	0.71
6:B:66:LEU:HD13	6:B:139:SER:OG	1.90	0.71
6:B:577:PHE:HZ	15:B:1226:CLA:HBC3	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:612:CLA:HMC2	15:3:613:CLA:HMB1	1.73	0.71
15:4:602:CLA:HED1	15:4:602:CLA:H11	1.70	0.71
2:2:168:LYS:HA	15:4:609:CLA:HED1	1.73	0.71
16:1:609:CHL:HHC	16:1:609:CHL:HBB1	1.72	0.70
6:B:657:VAL:HG11	6:B:716:VAL:HG23	1.73	0.70
6:B:570:ASP:HA	6:B:575:ASP:OD2	1.91	0.70
3:3:199:PHE:HZ	15:3:611:CLA:HBB2	1.57	0.70
1:1:218:PHE:CZ	4:4:217:ILE:HG21	2.27	0.70
1:1:84:LEU:HG	15:1:601:CLA:HMC1	1.72	0.70
4:4:288:LEU:CD2	15:4:604:CLA:HAC1	2.22	0.70
15:4:601:CLA:HBB1	15:4:601:CLA:HMB1	1.73	0.70
5:A:585:GLN:HA	5:A:590:ASP:OD2	1.92	0.70
1:1:104:PRO:HB3	15:1:613:CLA:HMC1	1.74	0.70
3:3:152:VAL:HB	15:3:613:CLA:CMC	2.21	0.70
8:D:174:TYR:HB3	8:D:176:GLU:OE2	1.91	0.70
16:4:611:CHL:HHC	16:4:611:CHL:HBB1	1.73	0.70
8:D:145:LEU:HD12	8:D:153:PRO:HG3	1.73	0.70
9:E:67:GLY:HA3	9:E:93:VAL:HG11	1.72	0.70
3:3:109:LEU:HD13	16:3:604:CHL:C1	2.22	0.70
5:A:197:MET:HE2	15:A:1111:CLA:HHD	1.74	0.70
15:A:1110:CLA:HBD	15:A:1110:CLA:HBA1	1.72	0.70
15:B:1238:CLA:HAB	25:B:2002:PQN:H171	1.73	0.70
11:J:15:GLY:H	11:J:18:TRP:HB3	1.57	0.70
15:2:602:CLA:HAB	15:2:607:CLA:HBD	1.74	0.69
15:2:608:CLA:HED2	3:3:171:PHE:CD2	2.27	0.69
5:A:605:ILE:CD1	24:A:1011:CL0:H35	2.21	0.69
6:B:562:GLY:O	6:B:568:THR:OG1	2.09	0.69
10:F:166:ILE:CG1	10:F:167:PRO:HD3	2.22	0.69
4:4:245:PHE:O	4:4:249:THR:HG23	1.91	0.69
5:A:72:LYS:NZ	15:A:1109:CLA:OBD	2.25	0.69
16:1:610:CHL:CMC	15:1:613:CLA:HAB	2.20	0.69
6:B:176:LEU:HD23	6:B:292:TYR:HE2	1.56	0.69
6:B:439:VAL:HB	15:B:1230:CLA:HMC2	1.74	0.69
16:2:610:CHL:HBB1	16:2:610:CHL:HMB1	1.74	0.69
15:3:603:CLA:HBA2	15:3:603:CLA:CBD	2.22	0.69
4:4:198:TRP:O	16:4:610:CHL:HED2	1.92	0.69
13:3:502:XAT:H31	15:3:605:CLA:CMB	2.22	0.69
10:F:211:ALA:HB1	15:F:1301:CLA:HED2	1.73	0.69
21:4:811:DGD:HD3	11:J:33:PHE:HE1	1.58	0.69
5:A:15:ILE:HD11	15:A:1110:CLA:CBD	2.21	0.69
5:A:535:VAL:HG11	5:A:609:HIS:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1108:CLA:HBA1	15:A:1108:CLA:CBD	2.22	0.69
15:B:1239:CLA:HBC1	25:B:2002:PQN:H2M2	1.73	0.69
15:1:608:CLA:HAA2	4:4:218:ILE:CG2	2.22	0.69
2:2:115:LEU:HG	15:2:601:CLA:HMC3	1.74	0.69
15:A:1136:CLA:HMA2	15:A:1137:CLA:HED2	1.73	0.69
6:B:54:GLN:HE22	6:B:58:ILE:HD11	1.57	0.69
15:3:603:CLA:HHC	15:3:603:CLA:HBB1	1.74	0.69
8:D:105:TRP:CZ3	8:D:107:SER:HB3	2.27	0.69
15:1:605:CLA:H2	15:1:605:CLA:HBA1	1.74	0.69
2:2:120:ILE:HG23	2:2:136:TRP:HB3	1.75	0.68
4:4:200:ALA:HB1	15:4:606:CLA:HED3	1.75	0.68
4:4:260:PRO:HG2	4:4:263:ILE:HD12	1.76	0.68
16:4:610:CHL:HHC	16:4:610:CHL:HBB1	1.75	0.68
6:B:174:SER:O	6:B:178:HIS:ND1	2.25	0.68
6:B:382:PHE:O	15:B:1226:CLA:HBC2	1.93	0.68
15:B:1220:CLA:HBA2	14:B:4004:BCR:H14C	1.75	0.68
5:A:72:LYS:HA	15:A:1109:CLA:HMD2	1.74	0.68
2:2:198:TYR:HE2	2:2:219:LYS:HD2	1.57	0.68
1:1:194:GLN:HG2	15:1:603:CLA:O1D	1.93	0.68
15:B:1212:CLA:HED2	15:B:1212:CLA:H2A	1.75	0.68
3:3:276:THR:HA	3:3:279:ASN:HD22	1.57	0.68
15:B:1230:CLA:CED	11:J:35:ASP:HA	2.23	0.68
5:A:455:LEU:HD22	5:A:472:PHE:HE2	1.59	0.68
8:D:167:LEU:O	8:D:170:LYS:HG3	1.94	0.68
6:B:182:GLY:HA3	15:B:1210:CLA:HBB1	1.75	0.68
6:B:652:LEU:HB3	15:B:1022:CLA:H11	1.75	0.68
1:1:71:TYR:HB3	15:1:604:CLA:HMA1	1.75	0.68
15:1:613:CLA:HBD	15:1:613:CLA:HBA1	1.76	0.68
15:B:1201:CLA:HAB	15:B:1203:CLA:CAD	2.24	0.68
2:2:113:ALA:HB2	13:2:502:XAT:H402	1.75	0.68
5:A:516:ALA:HA	5:A:521:VAL:HA	1.75	0.68
5:A:589:TRP:HE1	15:A:1128:CLA:HMD3	1.59	0.68
15:A:1012:CLA:HAB	6:B:583:TRP:CH2	2.29	0.68
15:A:1138:CLA:H111	15:A:1138:CLA:HAB	1.76	0.68
13:2:502:XAT:H383	15:2:606:CLA:CMB	2.24	0.67
3:3:199:PHE:N	3:3:203:GLU:OE2	2.26	0.67
15:3:605:CLA:HED2	15:3:612:CLA:O1A	1.95	0.67
11:J:9:SER:O	11:J:10:THR:HG23	1.94	0.67
15:2:607:CLA:HED2	15:2:607:CLA:H2A	1.74	0.67
5:A:119:TRP:CH2	14:J:4002:BCR:H332	2.29	0.67
5:A:344:ILE:CD1	5:A:422:ASN:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:430:LEU:HD21	15:B:1235:CLA:HMB1	1.75	0.67
6:B:702:SER:O	6:B:706:ALA:N	2.25	0.67
9:E:110:ASN:OD1	9:E:113:GLY:N	2.28	0.67
15:1:605:CLA:HBA1	15:1:605:CLA:C2	2.23	0.67
16:4:611:CHL:HHD	16:4:611:CHL:HBC2	1.76	0.67
15:A:1012:CLA:H41	6:B:439:VAL:HG13	1.77	0.67
6:B:423:LEU:CB	6:B:533:LEU:HD13	2.24	0.67
6:B:520:VAL:HG11	6:B:594:TYR:CD1	2.30	0.67
15:3:603:CLA:HHD	15:3:603:CLA:CBC	2.24	0.67
16:2:609:CHL:HBB1	16:2:609:CHL:HHC	1.77	0.67
3:3:259:ILE:HG21	15:3:603:CLA:CBA	2.24	0.67
4:4:178:VAL:HG22	15:4:602:CLA:CBB	2.24	0.67
2:2:239:GLN:HG2	2:2:250:ASN:ND2	2.10	0.67
15:3:603:CLA:HBD	15:3:603:CLA:CGA	2.25	0.67
4:4:264:PHE:CE2	4:4:268:GLY:HA3	2.28	0.67
2:2:104:GLN:OE1	2:2:173:LEU:HD12	1.95	0.67
2:2:262:THR:HG23	2:2:263:PHE:CD2	2.30	0.67
6:B:284:LEU:CD1	15:B:1216:CLA:HMC3	2.25	0.67
6:B:452:LYS:HE3	15:B:1230:CLA:HED3	1.77	0.67
14:2:503:BCR:HC42	15:4:607:CLA:CAB	2.25	0.66
5:A:687:PHE:HB2	15:A:1013:CLA:HBC1	1.76	0.66
1:1:43:PRO:HA	1:1:55:ASN:ND2	2.10	0.66
15:1:606:CLA:HMB1	15:1:606:CLA:HBB1	1.78	0.66
14:3:503:BCR:H292	15:3:606:CLA:NC	2.11	0.66
15:B:1230:CLA:HED1	11:J:35:ASP:CA	2.23	0.66
8:D:171:ASP:O	8:D:179:ASN:ND2	2.27	0.66
5:A:367:VAL:HG22	15:A:1117:CLA:H42	1.77	0.66
15:F:1302:CLA:HAB	14:F:4002:BCR:H343	1.78	0.66
12:1:501:LUT:H371	12:1:501:LUT:C28	2.25	0.66
3:3:170:PHE:O	3:3:174:VAL:HG23	1.96	0.66
5:A:584:CYS:H	6:B:670:GLY:CA	2.05	0.66
10:F:184:GLN:HG3	10:F:210:LEU:HD13	1.76	0.66
16:2:611:CHL:HHC	16:2:611:CHL:HBB1	1.76	0.66
3:3:205:LEU:HD22	3:3:219:PHE:N	2.10	0.66
4:4:259:TYR:C	15:4:601:CLA:HED2	2.20	0.66
5:A:556:PHE:O	5:A:566:LYS:NZ	2.23	0.66
8:D:197:ASP:HB3	8:D:198:PRO:HD2	1.78	0.66
6:B:271:LEU:O	6:B:271:LEU:HD13	1.94	0.66
8:D:105:TRP:HB3	8:D:153:PRO:CB	2.21	0.66
1:1:113:PRO:HG2	1:1:120:VAL:HG13	1.76	0.66
15:4:605:CLA:HBA2	15:4:605:CLA:HBD	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:90:GLY:O	5:A:94:HIS:ND1	2.22	0.66
5:A:344:ILE:HD11	5:A:422:ASN:HB3	1.78	0.66
15:A:1124:CLA:H2	15:A:1125:CLA:HED3	1.77	0.66
6:B:298:ILE:HG13	6:B:299:GLY:N	2.10	0.66
5:A:323:LYS:NZ	5:A:327:GLU:OE2	2.29	0.66
5:A:325:ILE:O	5:A:329:HIS:ND1	2.27	0.66
2:2:198:TYR:HA	15:2:601:CLA:CED	2.25	0.66
5:A:658:ILE:HD12	6:B:622:ARG:HG3	1.78	0.66
4:4:141:MET:HE1	4:4:159:MET:CE	2.25	0.65
5:A:81:LEU:HD12	15:A:1111:CLA:HED1	1.77	0.65
15:A:1133:CLA:HBB2	15:A:1135:CLA:H2	1.78	0.65
16:1:609:CHL:HED1	4:4:229:LYS:HA	1.78	0.65
5:A:580:ARG:HH12	7:C:51:CYS:HB3	1.60	0.65
15:A:1013:CLA:H3A	15:A:1013:CLA:H2	1.79	0.65
2:2:90:LEU:HD12	13:2:502:XAT:H172	1.79	0.65
14:2:503:BCR:HC42	15:4:607:CLA:HAB	1.77	0.65
16:2:609:CHL:HBA2	3:3:182:LEU:HD12	1.78	0.65
5:A:700:ILE:HD13	15:A:1138:CLA:HMD2	1.79	0.65
6:B:423:LEU:HB2	6:B:533:LEU:HD13	1.76	0.65
7:C:15:THR:HG22	7:C:28:MET:HE1	1.77	0.65
7:C:75:ARG:HH22	8:D:99:GLU:HG2	1.61	0.65
13:3:502:XAT:H183	15:3:606:CLA:C3B	2.26	0.65
5:A:71:ARG:HD2	5:A:185:ALA:HB1	1.77	0.65
5:A:206:LEU:HD22	15:A:1117:CLA:HMC2	1.78	0.65
11:J:10:THR:H	11:J:13:VAL:CG2	2.10	0.65
5:A:197:MET:HE3	15:A:1111:CLA:HAC1	1.77	0.65
5:A:327:GLU:O	5:A:330:LYS:NZ	2.29	0.65
10:F:188:LEU:HD23	10:F:188:LEU:O	1.95	0.65
1:1:77:ILE:HD13	1:1:142:ARG:HH12	1.61	0.65
3:3:139:ILE:CG1	3:3:140:PRO:HD2	2.27	0.65
3:3:259:ILE:CG2	15:3:603:CLA:HBA1	2.27	0.65
5:A:178:TRP:CD1	15:A:1109:CLA:HBB1	2.31	0.65
5:A:215:GLY:HA3	15:A:1113:CLA:HBB1	1.77	0.65
15:A:1013:CLA:CBA	6:B:428:LEU:HD23	2.26	0.65
15:A:1128:CLA:HED2	15:A:1128:CLA:H2A	1.79	0.65
15:4:604:CLA:CHB	15:4:604:CLA:H2	2.27	0.65
15:A:1012:CLA:O1D	15:B:1021:CLA:H71	1.96	0.65
6:B:48:PHE:CE2	6:B:52:PHE:HE2	2.15	0.65
10:F:139:LEU:HD12	10:F:149:ILE:HD11	1.77	0.65
1:1:35:GLY:O	1:1:54:PHE:HA	1.97	0.65
15:3:610:CLA:HBB2	15:A:1114:CLA:NC	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:276:HIS:HB3	15:B:1214:CLA:HMB2	1.78	0.65
15:B:1230:CLA:H12	14:B:4006:BCR:H281	1.79	0.65
1:1:122:PHE:HE2	15:1:613:CLA:HED2	1.61	0.64
5:A:250:ILE:HD13	5:A:257:PHE:HB3	1.79	0.64
5:A:374:MET:HE1	15:A:1116:CLA:HAA2	1.79	0.64
4:4:312:LEU:HD21	15:4:608:CLA:HMC3	1.78	0.64
5:A:203:ALA:HB2	5:A:309:GLY:HA3	1.78	0.64
6:B:290:HIS:O	15:B:1218:CLA:HED3	1.97	0.64
5:A:57:HIS:HD1	15:A:1104:CLA:HBA1	1.63	0.64
5:A:718:LEU:HD22	5:A:722:GLN:NE2	2.12	0.64
8:D:146:ARG:NH2	8:D:153:PRO:HD2	2.05	0.64
5:A:374:MET:O	5:A:376:PRO:HD3	1.97	0.64
6:B:217:LEU:HD12	6:B:222:GLY:HA3	1.80	0.64
10:F:184:GLN:CD	10:F:210:LEU:HD22	2.23	0.64
14:1:505:BCR:HC21	10:F:226:ARG:HH12	1.63	0.64
6:B:705:GLN:HG3	21:B:5002:DGD:HA22	1.80	0.64
15:1:602:CLA:O1A	15:1:602:CLA:H2A	1.97	0.64
15:2:605:CLA:HBA2	15:2:605:CLA:CHA	2.28	0.64
14:4:503:BCR:H321	14:4:503:BCR:HC8	1.78	0.64
3:3:154:PRO:HG2	3:3:155:PRO:HD3	1.80	0.64
3:3:177:ILE:HD13	14:3:503:BCR:C36	2.27	0.64
5:A:429:ARG:O	5:A:432:ARG:HG3	1.97	0.64
4:4:141:MET:HE3	15:4:604:CLA:HED3	1.79	0.64
6:B:661:GLY:O	6:B:665:LEU:HG	1.98	0.64
5:A:305:PHE:HE1	15:A:1119:CLA:HAB	1.63	0.64
5:A:622:VAL:HA	5:A:627:VAL:HA	1.79	0.64
2:2:108:VAL:HG11	2:2:169:ARG:NH1	2.12	0.64
5:A:351:ALA:HB2	5:A:412:PHE:CD1	2.33	0.64
1:1:70:ARG:NH1	19:1:811:SQD:O49	2.32	0.63
4:4:174:MET:HB2	15:4:601:CLA:HMC2	1.80	0.63
6:B:128:ILE:HD12	15:B:1211:CLA:HMA2	1.80	0.63
3:3:116:HIS:HB3	3:3:247:MET:CE	2.28	0.63
14:4:505:BCR:H371	15:4:612:CLA:H12	1.80	0.63
7:C:29:VAL:CG1	7:C:30:PRO:HD3	2.14	0.63
15:3:603:CLA:HBD	15:3:603:CLA:O2A	1.98	0.63
15:4:605:CLA:HAC1	16:4:610:CHL:HBB2	1.79	0.63
15:B:1218:CLA:HBA1	15:B:1218:CLA:CHA	2.27	0.63
16:1:609:CHL:HAA1	4:4:228:THR:HG21	1.79	0.63
3:3:116:HIS:HB3	3:3:247:MET:HE3	1.81	0.63
15:3:605:CLA:HMB3	15:3:605:CLA:HBB1	1.80	0.63
15:4:612:CLA:HED2	15:4:612:CLA:H2A	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:410:ALA:O	5:A:414:VAL:HG23	1.98	0.63
15:B:1202:CLA:HED1	15:B:1202:CLA:C3	2.29	0.63
15:J:1302:CLA:HMB1	15:J:1302:CLA:HBB1	1.79	0.63
3:3:280:LEU:HD22	15:3:603:CLA:NB	2.14	0.63
4:4:205:TYR:CG	4:4:206:PRO:HD3	2.32	0.63
6:B:537:LYS:NZ	6:B:541:ASP:OD2	2.32	0.63
15:A:1013:CLA:H101	15:A:1140:CLA:CMC	2.28	0.63
2:2:162:PHE:HZ	14:2:503:BCR:H373	1.62	0.63
16:2:613:CHL:HHC	16:2:613:CHL:HBB1	1.80	0.63
4:4:199:GLU:HA	16:4:610:CHL:HED1	1.80	0.63
3:3:247:MET:HB3	13:3:502:XAT:H402	1.79	0.63
3:3:139:ILE:HG13	3:3:140:PRO:HD2	1.80	0.63
15:B:1222:CLA:HAA2	15:B:1223:CLA:OBD	1.98	0.62
8:D:103:ILE:HD12	8:D:155:PHE:HE1	1.63	0.62
1:1:52:GLY:HA3	1:1:178:LEU:HD23	1.81	0.62
1:1:80:ARG:HB3	15:1:601:CLA:CBC	2.29	0.62
1:1:103:ALA:CA	15:1:606:CLA:HED1	2.27	0.62
3:3:193:SER:HA	3:3:196:ARG:HD3	1.80	0.62
5:A:75:SER:OG	5:A:181:TYR:HB2	1.99	0.62
5:A:647:ARG:HA	6:B:633:ILE:CG2	2.29	0.62
15:1:605:CLA:HHC	15:1:605:CLA:CBB	2.28	0.62
5:A:718:LEU:HD22	5:A:722:GLN:CD	2.24	0.62
6:B:79:VAL:HG13	6:B:126:TYR:CE1	2.34	0.62
3:3:260:THR:HG21	3:3:267:ASN:ND2	2.13	0.62
13:3:502:XAT:H192	15:3:606:CLA:HBB2	1.81	0.62
4:4:288:LEU:HD23	15:4:604:CLA:HAC1	1.81	0.62
6:B:78:TRP:HA	6:B:85:VAL:HG11	1.81	0.62
15:B:1225:CLA:HHC	15:B:1225:CLA:CBB	2.30	0.62
14:1:503:BCR:H24C	15:1:613:CLA:CGA	2.29	0.62
2:2:265:THR:HG23	2:2:266:ASN:H	1.63	0.62
14:3:503:BCR:H392	15:3:613:CLA:O2A	2.00	0.62
15:4:605:CLA:H11	10:F:219:LEU:HG	1.80	0.62
15:A:1125:CLA:HHC	15:A:1125:CLA:CBB	2.29	0.62
15:B:1231:CLA:H42	15:B:1232:CLA:HBA1	1.80	0.62
10:F:192:ASP:OD1	10:F:193:ALA:N	2.33	0.62
6:B:412:VAL:HA	6:B:415:HIS:CE1	2.35	0.62
8:D:102:VAL:HG13	8:D:129:LEU:HD21	1.80	0.62
10:F:155:ALA:HA	10:F:160:HIS:HB2	1.81	0.62
4:4:314:ASP:OD2	4:4:317:HIS:ND1	2.28	0.62
5:A:682:SER:HB3	5:A:730:HIS:HB2	1.82	0.62
15:B:1227:CLA:HBC1	14:B:4004:BCR:H23C	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:PHE:HZ	4:4:217:ILE:HG21	1.65	0.62
12:1:501:LUT:H402	15:1:601:CLA:HMC2	1.81	0.62
5:A:284:PRO:HA	5:A:515:VAL:HG13	1.82	0.62
15:A:1012:CLA:HAB	6:B:583:TRP:HH2	1.64	0.62
6:B:238:PRO:HG3	6:B:259:LEU:HD11	1.82	0.62
6:B:255:ILE:HD12	15:B:1212:CLA:HAC2	1.81	0.62
15:A:1101:CLA:HBA2	15:A:1101:CLA:CBD	2.25	0.62
14:A:4007:BCR:C36	15:B:1239:CLA:HBB1	2.26	0.62
15:B:1216:CLA:HMB2	15:B:1221:CLA:HED1	1.81	0.62
7:C:61:ASP:HB3	9:E:117:ASN:ND2	2.15	0.62
1:1:77:ILE:HD13	1:1:142:ARG:NH1	2.15	0.62
5:A:119:TRP:CZ3	14:J:4002:BCR:H332	2.34	0.62
5:A:222:LEU:HB2	5:A:223:PRO:HD3	1.80	0.61
15:A:1129:CLA:HBB1	15:A:1129:CLA:HMB3	1.80	0.61
6:B:92:ILE:HG23	15:B:1206:CLA:O1D	2.00	0.61
6:B:441:ASN:OD1	6:B:453:GLN:HB2	2.00	0.61
4:4:124:ARG:HB3	4:4:125:PRO:CD	2.30	0.61
6:B:658:TYR:CE2	15:B:1021:CLA:HMA3	2.35	0.61
10:F:111:PRO:HA	10:F:116:TYR:CD2	2.35	0.61
13:1:502:XAT:H383	15:1:606:CLA:C3B	2.30	0.61
15:A:1013:CLA:H101	15:A:1140:CLA:HMC2	1.82	0.61
15:A:1124:CLA:HHC	15:A:1124:CLA:CBB	2.28	0.61
6:B:123:GLN:HG2	6:B:362:LEU:HA	1.81	0.61
15:3:606:CLA:HMB1	15:3:606:CLA:HBB1	1.81	0.61
4:4:327:ILE:HD12	15:4:615:CLA:O1D	2.01	0.61
5:A:221:SER:OG	5:A:225:ASN:OD1	2.16	0.61
5:A:345:LEU:HB2	15:A:1123:CLA:HBC3	1.81	0.61
5:A:396:TRP:CD1	15:A:1126:CLA:HAB	2.36	0.61
16:4:613:CHL:HHC	16:4:613:CHL:HBB1	1.82	0.61
5:A:191:PHE:HA	15:A:1111:CLA:HBC1	1.82	0.61
6:B:204:ARG:NH1	6:B:239:ASP:OD1	2.25	0.61
15:B:1231:CLA:HBA2	15:B:1232:CLA:HMB3	1.81	0.61
14:A:4007:BCR:H271	25:B:2002:PQN:H142	1.82	0.61
15:B:1235:CLA:HAC2	14:F:4002:BCR:HC22	1.82	0.61
15:3:601:CLA:HAC2	15:3:611:CLA:HED2	1.82	0.61
5:A:434:ARG:NH1	5:A:559:SER:OG	2.33	0.61
15:A:1127:CLA:HHC	15:A:1127:CLA:CBB	2.30	0.61
15:3:611:CLA:HBB1	15:3:611:CLA:HMB3	1.81	0.61
5:A:358:ALA:O	14:A:4005:BCR:H372	2.00	0.61
21:2:811:DGD:HG32	21:2:811:DGD:O2D	1.99	0.60
5:A:708:ARG:NH2	10:F:229:SER:O	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1101:CLA:CAB	14:J:4002:BCR:H271	2.31	0.60
1:1:183:LEU:HD21	15:1:607:CLA:HHD	1.84	0.60
15:A:1013:CLA:O2A	6:B:428:LEU:HA	2.00	0.60
6:B:575:ASP:O	6:B:578:TYR:HB3	2.01	0.60
4:4:145:TYR:OH	4:4:281:GLN:NE2	2.34	0.60
5:A:334:THR:HG23	5:A:429:ARG:HD2	1.83	0.60
6:B:300:HIS:ND1	6:B:305:ILE:HD11	2.16	0.60
10:F:184:GLN:NE2	10:F:210:LEU:HD22	2.16	0.60
14:1:505:BCR:H372	15:4:612:CLA:H42	1.82	0.60
3:3:133:LEU:O	3:3:139:ILE:HG22	2.02	0.60
5:A:580:ARG:HA	7:C:76:SER:O	2.01	0.60
5:A:666:SER:HB2	6:B:446:ALA:HB1	1.84	0.60
16:1:610:CHL:HBA2	16:1:610:CHL:CHA	2.31	0.60
4:4:181:LEU:O	4:4:185:VAL:HG23	2.01	0.60
15:B:1231:CLA:H61	15:B:1232:CLA:H12	1.83	0.60
13:3:502:XAT:H162	15:3:606:CLA:CMB	2.32	0.60
4:4:172:TRP:HE1	13:4:502:XAT:H191	1.67	0.60
8:D:174:TYR:O	8:D:176:GLU:N	2.35	0.60
16:1:610:CHL:CBC	15:1:613:CLA:HBC2	2.31	0.60
3:3:247:MET:HB3	13:3:502:XAT:C40	2.32	0.60
5:A:620:GLY:HA3	5:A:629:HIS:HA	1.84	0.60
4:4:142:LEU:HD11	4:4:276:LYS:HD2	1.84	0.60
4:4:245:PHE:H	4:4:249:THR:CG2	2.15	0.60
5:A:647:ARG:HA	6:B:633:ILE:HG23	1.84	0.60
6:B:378:TYR:CD2	15:B:1224:CLA:HAB	2.36	0.60
7:C:22:PRO:HD3	7:C:53:ARG:HD2	1.84	0.60
9:E:75:LYS:O	9:E:124:ILE:HG23	2.02	0.60
2:2:233:PHE:CE1	13:2:502:XAT:H30	2.36	0.60
5:A:194:VAL:HG13	15:A:1123:CLA:HMD3	1.83	0.60
6:B:143:LEU:HD21	14:B:4003:BCR:C40	2.32	0.60
6:B:536:VAL:HG22	14:B:4004:BCR:H291	1.84	0.60
12:3:501:LUT:H382	15:3:601:CLA:C1D	2.32	0.60
5:A:80:GLN:HG2	15:A:1103:CLA:HMA1	1.83	0.60
5:A:561:ARG:NH2	8:D:88:THR:O	2.35	0.60
15:A:1132:CLA:HHD	15:B:1206:CLA:HBB2	1.83	0.60
6:B:493:LEU:O	6:B:496:PRO:HD2	2.02	0.60
7:C:29:VAL:HG11	8:D:182:ARG:HB2	1.84	0.60
2:2:99:ARG:O	2:2:103:VAL:HG23	2.02	0.59
15:4:615:CLA:HBC3	21:4:811:DGD:HB31	1.82	0.59
5:A:605:ILE:HD11	24:A:1011:CL0:C4	2.31	0.59
5:A:612:TRP:HB2	5:A:649:PHE:CE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:80:ARG:HB3	15:1:601:CLA:HBC2	1.85	0.59
14:1:503:BCR:H24C	15:1:613:CLA:O1A	2.02	0.59
7:C:26:LEU:HD23	7:C:26:LEU:H	1.67	0.59
13:3:502:XAT:H402	16:3:604:CHL:OMC	2.03	0.59
5:A:316:TRP:O	5:A:318:ILE:HG13	2.01	0.59
6:B:341:SER:O	6:B:345:ILE:HG12	2.02	0.59
6:B:577:PHE:CZ	15:B:1226:CLA:HBC3	2.35	0.59
8:D:100:PHE:CE1	8:D:158:VAL:HG11	2.37	0.59
2:2:187:ILE:CG2	2:2:191:LEU:HD13	2.28	0.59
2:2:198:TYR:CE2	2:2:219:LYS:HD2	2.37	0.59
12:2:501:LUT:H12	15:2:601:CLA:HAB	1.84	0.59
3:3:247:MET:HE1	16:3:604:CHL:CAB	2.33	0.59
12:4:501:LUT:H371	12:4:501:LUT:H28	1.83	0.59
5:A:369:HIS:HA	5:A:372:TYR:CD1	2.37	0.59
6:B:646:VAL:HG11	15:B:1205:CLA:HBC1	1.83	0.59
16:1:609:CHL:CAA	4:4:228:THR:HG21	2.32	0.59
2:2:220:GLN:HE22	2:2:224:LYS:HE3	1.67	0.59
5:A:77:HIS:HB3	15:A:1111:CLA:HED2	1.84	0.59
5:A:514:VAL:HG22	5:A:524:MET:HG3	1.84	0.59
5:A:524:MET:HG3	5:A:525:PRO:HD2	1.83	0.59
5:A:579:GLY:C	5:A:580:ARG:HD2	2.28	0.59
15:A:1138:CLA:HED3	6:B:421:SER:HB2	1.83	0.59
6:B:388:PHE:CD2	6:B:535:LEU:HD13	2.38	0.59
15:1:603:CLA:HBA1	15:1:603:CLA:CHA	2.33	0.59
9:E:106:PHE:O	9:E:115:SER:OG	2.18	0.59
5:A:589:TRP:NE1	15:A:1128:CLA:HMD3	2.18	0.59
15:A:1013:CLA:HMD3	6:B:534:ILE:HG12	1.83	0.59
6:B:244:ALA:HA	6:B:265:GLN:OE1	2.03	0.59
6:B:292:TYR:CZ	6:B:302:LEU:HD21	2.37	0.59
8:D:106:GLU:HG3	8:D:108:PRO:HD3	1.85	0.59
5:A:157:LEU:HD23	5:A:157:LEU:O	2.02	0.59
5:A:194:VAL:HG11	15:A:1123:CLA:HAC2	1.85	0.59
6:B:359:TYR:HB2	6:B:362:LEU:HD22	1.85	0.59
10:F:101:VAL:HG13	10:F:104:LYS:HE3	1.83	0.59
14:1:505:BCR:HC41	10:F:226:ARG:NH1	2.18	0.59
3:3:111:TYR:O	3:3:114:VAL:HG22	2.03	0.59
5:A:334:THR:HG21	5:A:426:LEU:HD23	1.84	0.59
5:A:682:SER:HB3	5:A:730:HIS:HB3	1.84	0.59
15:A:1141:CLA:HHC	15:A:1141:CLA:HBB1	1.85	0.59
6:B:439:VAL:HG12	15:B:1230:CLA:HAC1	1.84	0.59
2:2:110:CYS:HB3	2:2:226:GLY:HA3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:107:ARG:HH11	6:B:116:ILE:HG12	1.67	0.58
6:B:631:GLN:HB3	6:B:644:LEU:HD13	1.85	0.58
2:2:239:GLN:HE21	2:2:250:ASN:HB2	1.68	0.58
3:3:155:PRO:HG3	15:A:1114:CLA:HMD2	1.85	0.58
14:3:504:BCR:H341	15:3:610:CLA:HBC2	1.84	0.58
5:A:75:SER:O	15:A:1109:CLA:HBC1	2.02	0.58
6:B:188:SER:O	6:B:192:THR:HG23	2.03	0.58
10:F:225:LEU:HA	10:F:230:LEU:HD21	1.84	0.58
4:4:142:LEU:HD13	4:4:276:LYS:HB3	1.86	0.58
4:4:172:TRP:HH2	14:4:503:BCR:H371	1.67	0.58
5:A:160:TYR:O	5:A:164:ILE:HG12	2.03	0.58
5:A:194:VAL:HG13	15:A:1123:CLA:HHD	1.84	0.58
5:A:301:ILE:HG23	5:A:305:PHE:CE2	2.38	0.58
5:A:596:LEU:HD21	15:A:1128:CLA:HBC1	1.85	0.58
15:A:1012:CLA:HMA1	6:B:617:LEU:HD13	1.86	0.58
6:B:143:LEU:HA	6:B:146:VAL:HG22	1.85	0.58
15:B:1023:CLA:HBB1	15:B:1023:CLA:CMB	2.33	0.58
7:C:44:ARG:NE	8:D:167:LEU:HD11	2.19	0.58
10:F:128:ASN:HA	10:F:131:LYS:HG2	1.84	0.58
5:A:582:GLY:O	6:B:669:ARG:NH1	2.35	0.58
8:D:201:VAL:O	8:D:201:VAL:HG12	2.02	0.58
15:1:606:CLA:HMA3	15:1:613:CLA:C3C	2.33	0.58
4:4:290:PHE:CE1	13:4:502:XAT:H8	2.39	0.58
5:A:460:ASP:OD1	5:A:641:THR:HB	2.03	0.58
5:A:697:ILE:O	5:A:701:VAL:HG23	2.04	0.58
6:B:388:PHE:CZ	15:B:1222:CLA:HAB	2.32	0.58
5:A:450:PHE:CE1	15:B:1023:CLA:H71	2.38	0.58
14:A:4007:BCR:H383	15:B:1237:CLA:HMD3	1.85	0.58
5:A:396:TRP:CZ3	5:A:600:TYR:HA	2.38	0.58
6:B:284:LEU:HD12	15:B:1216:CLA:HMC3	1.84	0.58
3:3:150:THR:HG21	13:3:502:XAT:O3	2.03	0.58
3:3:282:THR:HB	15:3:603:CLA:HED2	1.84	0.58
6:B:82:PRO:HG2	6:B:361:TYR:CE2	2.38	0.58
6:B:179:HIS:HD2	6:B:183:LEU:HD22	1.68	0.58
6:B:375:HIS:O	6:B:379:ILE:HG12	2.03	0.58
8:D:108:PRO:HD2	8:D:151:GLN:NE2	2.19	0.58
6:B:196:VAL:HA	6:B:200:ILE:HD12	1.86	0.58
12:3:501:LUT:C22	15:3:601:CLA:H2	2.32	0.58
5:A:125:GLU:OE2	10:F:125:ARG:NH2	2.32	0.58
15:A:1110:CLA:CED	15:A:1111:CLA:HAB	2.34	0.58
6:B:438:TYR:HE2	15:B:1021:CLA:H171	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:124:ARG:HB3	4:4:125:PRO:HD2	1.84	0.57
4:4:233:ASP:OD2	16:4:611:CHL:HBC1	2.03	0.57
5:A:121:ILE:HG23	5:A:122:VAL:HG22	1.85	0.57
5:A:186:PRO:HB2	5:A:191:PHE:CE2	2.38	0.57
5:A:690:ARG:NE	5:A:718:LEU:O	2.36	0.57
15:A:1101:CLA:O2A	25:A:2001:PQN:H222	2.04	0.57
1:1:52:GLY:C	15:1:604:CLA:HED1	2.29	0.57
3:3:74:LEU:HD22	3:3:83:GLY:HA2	1.86	0.57
3:3:214:TYR:HB3	15:3:601:CLA:HED3	1.85	0.57
4:4:211:THR:HG23	4:4:211:THR:O	2.04	0.57
5:A:105:LEU:HD12	5:A:149:ARG:NH1	2.20	0.57
5:A:288:GLY:HA3	5:A:378:PRO:HA	1.84	0.57
6:B:101:ALA:HA	6:B:641:MET:HE1	1.86	0.57
15:B:1212:CLA:CHA	15:B:1212:CLA:HBA1	2.33	0.57
15:B:1222:CLA:HED2	15:B:1222:CLA:H2A	1.86	0.57
10:F:217:TRP:CG	10:F:218:PRO:HD3	2.38	0.57
3:3:176:ALA:HB1	14:3:503:BCR:C16	2.34	0.57
5:A:396:TRP:HZ3	5:A:600:TYR:HA	1.68	0.57
5:A:524:MET:CG	5:A:525:PRO:HD2	2.34	0.57
6:B:155:TRP:NE1	6:B:159:GLN:HE22	2.02	0.57
6:B:574:TYR:OH	6:B:708:LEU:HD13	2.05	0.57
16:2:609:CHL:H2A	16:2:609:CHL:O2D	2.05	0.57
5:A:679:TRP:CZ3	5:A:683:LEU:HD11	2.39	0.57
6:B:464:ILE:HG12	15:B:1231:CLA:HMC2	1.85	0.57
1:1:95:LEU:HD13	1:1:116:PHE:HZ	1.70	0.57
16:1:609:CHL:CED	4:4:229:LYS:HA	2.34	0.57
2:2:220:GLN:NE2	2:2:224:LYS:HE3	2.19	0.57
6:B:102:VAL:O	6:B:106:THR:OG1	2.22	0.57
6:B:291:MET:O	6:B:292:TYR:CG	2.57	0.57
2:2:113:ALA:HB2	13:2:502:XAT:C40	2.35	0.57
15:3:612:CLA:HAC1	15:3:613:CLA:CBB	2.34	0.57
6:B:200:ILE:HB	6:B:201:PRO:HD3	1.87	0.57
2:2:162:PHE:HD2	15:2:612:CLA:HMC3	1.70	0.57
12:2:501:LUT:H12	15:2:601:CLA:CAB	2.34	0.57
5:A:363:LEU:O	5:A:367:VAL:HG23	2.05	0.57
5:A:441:LEU:HD23	5:A:548:LEU:HD13	1.87	0.57
5:A:677:PHE:CD2	14:A:4006:BCR:H363	2.40	0.57
15:A:1105:CLA:C1	15:A:1107:CLA:H42	2.34	0.57
6:B:351:GLN:HA	6:B:354:TYR:HE1	1.70	0.57
6:B:419:ILE:HA	15:B:1227:CLA:HBB1	1.85	0.57
2:2:145:LYS:HG2	4:4:333:PHE:HD1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:248:ILE:O	4:4:248:ILE:HG22	2.03	0.57
5:A:694:GLN:O	5:A:698:GLU:HG3	2.05	0.57
15:A:1115:CLA:HBB1	15:A:1115:CLA:HMB1	1.86	0.57
15:A:1122:CLA:HBC2	14:A:4004:BCR:HC8	1.87	0.57
6:B:442:ASP:OD1	6:B:616:TYR:HB2	2.05	0.57
7:C:4:VAL:HG21	8:D:207:SER:HB2	1.86	0.57
1:1:43:PRO:HA	1:1:55:ASN:HD21	1.69	0.57
15:3:603:CLA:HHC	15:3:603:CLA:CBB	2.34	0.57
13:4:502:XAT:H183	15:4:606:CLA:C2B	2.35	0.57
5:A:678:VAL:HG21	5:A:733:LEU:HD12	1.86	0.57
6:B:66:LEU:HD23	6:B:125:TRP:CH2	2.39	0.57
6:B:82:PRO:HG2	6:B:361:TYR:CD2	2.40	0.57
6:B:581:VAL:HB	6:B:711:LEU:HD21	1.87	0.57
2:2:265:THR:HG23	2:2:266:ASN:N	2.20	0.56
5:A:217:GLN:HA	5:A:220:VAL:HG12	1.87	0.56
15:A:1131:CLA:HHC	15:A:1131:CLA:CBB	2.33	0.56
6:B:12:GLY:HA3	7:C:71:ASN:ND2	2.20	0.56
6:B:197:HIS:O	6:B:201:PRO:HG2	2.05	0.56
6:B:453:GLN:HE21	6:B:455:LEU:HD11	1.70	0.56
6:B:561:ASP:OD2	6:B:565:ARG:NH2	2.29	0.56
7:C:17:CYS:CB	26:C:3003:SF4:S2	2.83	0.56
10:F:201:ILE:HA	11:J:9:SER:O	2.04	0.56
3:3:128:ILE:HG12	3:3:132:ILE:CD1	2.35	0.56
5:A:29:TRP:CD1	15:A:1109:CLA:H12	2.40	0.56
6:B:260:GLY:HA3	6:B:494:TRP:HB2	1.87	0.56
6:B:663:MET:HB2	15:B:1023:CLA:CHC	2.35	0.56
1:1:135:MET:CE	14:1:503:BCR:H362	2.35	0.56
2:2:224:LYS:HZ2	15:2:607:CLA:CED	2.19	0.56
5:A:68:GLU:HA	5:A:71:ARG:HE	1.69	0.56
5:A:77:HIS:C	15:A:1111:CLA:HED2	2.30	0.56
5:A:80:GLN:O	5:A:84:ILE:HG12	2.05	0.56
5:A:345:LEU:HD12	5:A:352:GLN:OE1	2.05	0.56
5:A:563:ILE:HG13	5:A:563:ILE:O	2.04	0.56
15:A:1013:CLA:H3A	15:A:1013:CLA:C2	2.36	0.56
6:B:282:ALA:O	6:B:286:ILE:HG12	2.05	0.56
6:B:520:VAL:HG11	6:B:594:TYR:HB2	1.87	0.56
1:1:181:GLY:O	1:1:185:MET:HG3	2.05	0.56
15:2:607:CLA:H2A	15:2:607:CLA:CED	2.34	0.56
5:A:28:LYS:HE3	5:A:34:HIS:CE1	2.40	0.56
5:A:70:SER:OG	5:A:349:TRP:NE1	2.23	0.56
5:A:121:ILE:HG23	5:A:122:VAL:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:692:TYR:CE1	6:B:537:LYS:HD2	2.40	0.56
6:B:257:THR:O	6:B:273:ASP:HA	2.06	0.56
6:B:266:THR:HG22	6:B:361:TYR:CE1	2.41	0.56
15:B:1228:CLA:H2	14:F:4002:BCR:H373	1.87	0.56
15:4:615:CLA:HBB1	15:4:615:CLA:HHC	1.88	0.56
5:A:360:PHE:O	5:A:363:LEU:HG	2.06	0.56
15:A:1012:CLA:CBB	6:B:526:LEU:HD21	2.35	0.56
15:A:1110:CLA:HBA1	15:A:1110:CLA:CBD	2.35	0.56
15:A:1127:CLA:HBA2	15:A:1127:CLA:CHA	2.35	0.56
6:B:473:TYR:HB3	10:F:80:ALA:HA	1.88	0.56
8:D:103:ILE:HG13	8:D:154:CYS:O	2.05	0.56
15:J:1302:CLA:CMC	14:J:4002:BCR:H10C	2.35	0.56
4:4:200:ALA:CB	15:4:606:CLA:HED3	2.36	0.56
15:A:1127:CLA:HBA2	15:A:1127:CLA:H2	1.87	0.56
15:A:1137:CLA:HBB1	15:A:1137:CLA:HHC	1.88	0.56
6:B:145:LEU:O	6:B:149:VAL:HG23	2.06	0.56
2:2:162:PHE:HE2	16:2:613:CHL:HMB2	1.70	0.56
15:3:603:CLA:HBA2	15:3:603:CLA:CHA	2.34	0.56
4:4:259:TYR:HB3	15:4:601:CLA:CED	2.35	0.56
5:A:197:MET:HE2	15:A:1111:CLA:HAC1	1.87	0.56
6:B:340:ALA:HB2	14:B:4005:BCR:H372	1.88	0.56
6:B:644:LEU:HD11	6:B:732:GLY:HA3	1.86	0.56
2:2:105:ALA:HB2	15:2:612:CLA:HED2	1.88	0.56
5:A:80:GLN:HG2	15:A:1103:CLA:CMA	2.36	0.56
5:A:121:ILE:HG13	5:A:122:VAL:HG13	1.87	0.56
6:B:63:SER:HB2	6:B:143:LEU:HB2	1.88	0.56
6:B:712:ALA:O	6:B:716:VAL:HG22	2.05	0.56
1:1:135:MET:HE2	14:1:503:BCR:H362	1.88	0.56
5:A:59:PHE:HE1	15:A:1102:CLA:HED1	1.71	0.56
5:A:204:GLY:HA2	15:A:1118:CLA:HBC1	1.87	0.56
6:B:59:PHE:HD1	6:B:143:LEU:HD22	1.71	0.56
15:B:1220:CLA:CHB	15:B:1240:CLA:HED1	2.36	0.56
7:C:73:SER:H	7:C:76:SER:HB2	1.71	0.56
8:D:155:PHE:CD2	8:D:168:HIS:HB3	2.41	0.56
1:1:71:TYR:HB3	15:1:604:CLA:CMA	2.36	0.56
5:A:369:HIS:NE2	15:A:1124:CLA:OBD	2.39	0.56
5:A:385:GLY:HA2	5:A:747:ILE:HG12	1.88	0.56
5:A:540:ALA:HB2	15:A:1136:CLA:HMA1	1.87	0.56
15:A:1124:CLA:HBA1	15:A:1124:CLA:CHA	2.36	0.56
15:A:1127:CLA:NC	14:A:4003:BCR:H271	2.20	0.56
6:B:520:VAL:HG11	6:B:594:TYR:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:584:MET:HE2	6:B:588:ILE:HG13	1.88	0.56
8:D:113:PHE:CE1	8:D:123:MET:HE2	2.41	0.56
5:A:390:LEU:HD12	5:A:394:HIS:HE1	1.70	0.55
16:3:604:CHL:HHD	16:3:604:CHL:CBC	2.34	0.55
4:4:222:LEU:HG	14:4:503:BCR:C17	2.36	0.55
5:A:59:PHE:CD2	15:A:1103:CLA:HMC2	2.41	0.55
5:A:224:VAL:HA	5:A:228:LEU:HD12	1.89	0.55
5:A:233:ASP:CG	5:A:234:PRO:HD2	2.32	0.55
15:A:1106:CLA:H2A	15:A:1106:CLA:HED2	1.87	0.55
15:A:1124:CLA:C4	15:A:1125:CLA:HED3	2.36	0.55
15:A:1124:CLA:H42	15:A:1125:CLA:HED3	1.88	0.55
6:B:212:ASN:O	6:B:216:VAL:HG23	2.06	0.55
6:B:423:LEU:HD21	15:B:1236:CLA:HMB2	1.88	0.55
9:E:105:ARG:HG3	9:E:116:THR:HG22	1.89	0.55
3:3:205:LEU:HD13	3:3:219:PHE:HB2	1.88	0.55
5:A:456:TYR:HE1	5:A:534:LEU:HD13	1.70	0.55
5:A:597:PHE:CE1	5:A:728:VAL:HG23	2.41	0.55
6:B:72:GLN:HE22	15:B:1204:CLA:HED1	1.71	0.55
6:B:452:LYS:HD2	10:F:129:ARG:HE	1.71	0.55
6:B:455:LEU:O	10:F:148:LEU:N	2.35	0.55
7:C:62:PHE:HE2	7:C:66:ARG:HH11	1.55	0.55
3:3:132:ILE:HG12	3:3:265:PHE:CD1	2.41	0.55
4:4:312:LEU:HD21	15:4:608:CLA:CMC	2.37	0.55
5:A:211:LEU:HD23	15:A:1113:CLA:HBB2	1.88	0.55
6:B:258:PHE:HD1	15:B:1214:CLA:HMB1	1.72	0.55
10:F:176:GLY:HA3	10:F:217:TRP:CZ2	2.40	0.55
1:1:90:LEU:O	1:1:94:VAL:HG23	2.04	0.55
16:1:610:CHL:HBC2	15:1:613:CLA:HBC2	1.87	0.55
15:1:613:CLA:HBA1	15:1:613:CLA:CBD	2.36	0.55
14:A:4006:BCR:H331	14:A:4006:BCR:C8	2.36	0.55
6:B:204:ARG:O	6:B:248:ALA:HB2	2.06	0.55
15:1:601:CLA:HMD3	15:1:611:CLA:HBA2	1.89	0.55
4:4:142:LEU:CD1	4:4:276:LYS:HD2	2.36	0.55
5:A:68:GLU:O	5:A:72:LYS:HG3	2.07	0.55
10:F:225:LEU:HA	10:F:230:LEU:CD2	2.36	0.55
3:3:150:THR:HG23	15:3:613:CLA:HAC2	1.89	0.55
8:D:200:LYS:O	8:D:200:LYS:HG2	2.06	0.55
6:B:431:GLY:HA2	6:B:526:LEU:HD22	1.89	0.55
7:C:31:TRP:O	7:C:37:ALA:HB1	2.07	0.55
15:3:605:CLA:OBD	15:3:612:CLA:HBA2	2.07	0.55
4:4:260:PRO:HG3	4:4:263:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:606:CLA:HMA3	16:4:613:CHL:C2C	2.37	0.55
5:A:34:HIS:CE1	15:A:1109:CLA:HAA1	2.41	0.55
5:A:140:ILE:HD12	5:A:140:ILE:O	2.06	0.55
5:A:413:MET:O	5:A:558:ARG:NH2	2.40	0.54
15:A:1012:CLA:CMA	6:B:617:LEU:HD13	2.38	0.54
15:A:1013:CLA:H51	6:B:432:PHE:CD1	2.43	0.54
15:A:1136:CLA:HBA1	15:A:1137:CLA:OBD	2.08	0.54
6:B:127:THR:OG1	6:B:360:ALA:N	2.39	0.54
6:B:358:PRO:CG	15:B:1215:CLA:HAA2	2.37	0.54
4:4:308:LEU:O	4:4:312:LEU:HD23	2.08	0.54
16:4:613:CHL:HAA1	16:4:613:CHL:O1D	2.08	0.54
5:A:178:TRP:HB2	15:A:1109:CLA:HMC3	1.88	0.54
5:A:336:ASN:HB3	5:A:425:ASN:ND2	2.22	0.54
15:A:1108:CLA:HAB	15:A:1111:CLA:NA	2.21	0.54
14:A:4007:BCR:C27	25:B:2002:PQN:H142	2.38	0.54
6:B:277:HIS:HD2	15:B:1214:CLA:NA	2.05	0.54
2:2:82:ALA:HB1	2:2:220:GLN:HA	1.88	0.54
21:4:811:DGD:O3D	21:4:811:DGD:HG32	2.07	0.54
5:A:580:ARG:H	7:C:49:VAL:HG22	1.73	0.54
15:A:1013:CLA:CGA	6:B:428:LEU:HA	2.37	0.54
6:B:530:THR:HG21	6:B:583:TRP:CE2	2.42	0.54
15:B:1023:CLA:C2	15:B:1023:CLA:HMA2	2.37	0.54
10:F:122:THR:HA	10:F:125:ARG:HE	1.73	0.54
5:A:305:PHE:CE1	15:A:1119:CLA:HAB	2.43	0.54
5:A:510:TRP:HZ3	15:A:1125:CLA:HBC2	1.72	0.54
15:A:1013:CLA:C2	15:A:1013:CLA:HMA2	2.38	0.54
8:D:101:TYR:CE2	8:D:135:LYS:HB2	2.42	0.54
3:3:90:LEU:HB2	16:3:604:CHL:HBA1	1.90	0.54
4:4:164:GLU:HG3	4:4:234:LEU:HD12	1.89	0.54
14:A:4007:BCR:H383	15:B:1237:CLA:HHD	1.89	0.54
10:F:105:ARG:HD2	10:F:119:LEU:HD21	1.88	0.54
2:2:109:HIS:HD2	15:2:612:CLA:CMD	2.17	0.54
5:A:673:LEU:O	15:A:1012:CLA:HBA1	2.08	0.54
15:A:1139:CLA:H52	11:J:14:VAL:CG2	2.37	0.54
7:C:28:MET:HE2	7:C:38:GLN:HB3	1.90	0.54
8:D:205:THR:HG22	8:D:205:THR:O	2.07	0.54
5:A:680:ALA:CB	15:A:1013:CLA:HBB2	2.34	0.54
15:A:1012:CLA:H143	14:J:4001:BCR:H14C	1.88	0.54
6:B:431:GLY:N	6:B:526:LEU:HD13	2.23	0.54
6:B:659:ALA:HB3	15:B:1023:CLA:CBB	2.36	0.54
6:B:694:TRP:CH2	6:B:697:LYS:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:187:ASP:OD2	15:3:611:CLA:HBC1	2.08	0.54
5:A:688:SER:OG	5:A:693:TRP:NE1	2.36	0.54
15:A:1125:CLA:C4B	15:A:1133:CLA:HMA3	2.38	0.54
15:A:1140:CLA:H91	11:J:16:LEU:HD22	1.88	0.54
5:A:28:LYS:HB2	15:A:1109:CLA:HMA2	1.89	0.54
5:A:677:PHE:HB2	15:A:1012:CLA:O1A	2.08	0.54
6:B:279:LEU:HD21	15:B:1213:CLA:HMB1	1.88	0.54
6:B:434:THR:HG21	15:B:1021:CLA:H192	1.90	0.54
15:B:1021:CLA:C2	15:B:1021:CLA:HBA2	2.37	0.54
8:D:141:LEU:O	8:D:145:LEU:HG	2.07	0.54
2:2:77:LEU:HD11	2:2:86:GLY:HA2	1.89	0.54
2:2:199:PRO:HD2	15:2:601:CLA:HED1	1.90	0.54
15:2:608:CLA:HED2	3:3:171:PHE:HD2	1.73	0.54
5:A:59:PHE:CE1	15:A:1102:CLA:HED1	2.43	0.54
6:B:173:GLU:HA	6:B:292:TYR:CD2	2.43	0.54
8:D:110:GLU:HA	8:D:123:MET:O	2.07	0.54
15:2:601:CLA:HMB2	15:2:602:CLA:HBC3	1.89	0.53
4:4:285:LEU:HD21	15:4:602:CLA:HAC1	1.90	0.53
15:4:601:CLA:HBB1	15:4:601:CLA:CMB	2.38	0.53
5:A:200:HIS:HB3	15:A:1111:CLA:CAB	2.36	0.53
5:A:403:VAL:HG11	5:A:596:LEU:HD23	1.89	0.53
5:A:545:VAL:O	5:A:549:ILE:HG12	2.07	0.53
6:B:266:THR:HB	6:B:361:TYR:H	1.72	0.53
15:B:1224:CLA:HED3	15:B:1225:CLA:HMA2	1.90	0.53
7:C:36:ALA:HB1	7:C:38:GLN:OE1	2.08	0.53
1:1:103:ALA:HB3	1:1:104:PRO:HD3	1.90	0.53
1:1:183:LEU:CD1	17:1:801:LHG:HC82	2.37	0.53
16:2:613:CHL:HAA2	16:2:613:CHL:HBD	1.90	0.53
5:A:146:GLN:HG2	5:A:380:LEU:HB3	1.89	0.53
5:A:547:VAL:HG22	15:A:1124:CLA:HBB1	1.89	0.53
8:D:104:THR:O	8:D:153:PRO:HA	2.08	0.53
15:1:606:CLA:HBB1	15:1:606:CLA:CMB	2.38	0.53
16:1:609:CHL:CHA	16:1:609:CHL:HBA1	2.38	0.53
3:3:129:ALA:HB3	3:3:130:PRO:HD3	1.90	0.53
5:A:44:ASN:O	5:A:44:ASN:ND2	2.40	0.53
5:A:679:TRP:CE3	24:A:1011:CL0:H6	2.42	0.53
6:B:105:PHE:HA	6:B:107:ARG:NH2	2.22	0.53
6:B:184:PHE:HB3	6:B:285:PHE:CD2	2.42	0.53
6:B:371:SER:HB2	15:B:1224:CLA:HMA1	1.90	0.53
15:J:1302:CLA:HBB1	15:J:1302:CLA:CMB	2.39	0.53
15:1:613:CLA:HBA1	15:1:613:CLA:CHA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:208:MET:HE2	15:2:601:CLA:C3	2.39	0.53
4:4:177:VAL:HG13	4:4:293:PHE:CE2	2.43	0.53
4:4:199:GLU:HA	16:4:610:CHL:CED	2.39	0.53
4:4:288:LEU:HD21	15:4:604:CLA:HAC1	1.89	0.53
21:4:811:DGD:HD3	11:J:33:PHE:CE1	2.42	0.53
15:B:1212:CLA:HMB1	15:B:1212:CLA:HBB1	1.91	0.53
15:B:1212:CLA:NC	14:B:4001:BCR:H332	2.24	0.53
8:D:174:TYR:HB3	8:D:176:GLU:CD	2.33	0.53
11:J:14:VAL:HA	11:J:18:TRP:H	1.72	0.53
1:1:123:ASP:O	1:1:127:ILE:HG12	2.09	0.53
3:3:79:PRO:HB2	3:3:240:ILE:HD12	1.90	0.53
5:A:197:MET:HE2	15:A:1111:CLA:CHD	2.39	0.53
5:A:441:LEU:HD23	5:A:548:LEU:CD1	2.39	0.53
5:A:450:PHE:HE1	15:B:1023:CLA:H71	1.72	0.53
6:B:66:LEU:HD12	6:B:143:LEU:HD12	1.91	0.53
6:B:106:THR:O	6:B:106:THR:HG22	2.08	0.53
8:D:181:GLY:C	8:D:182:ARG:HD2	2.32	0.53
8:D:204:PHE:HA	8:D:208:GLU:OE2	2.08	0.53
10:F:122:THR:HA	10:F:125:ARG:NE	2.24	0.53
10:F:225:LEU:HD12	10:F:230:LEU:HD21	1.90	0.53
11:J:10:THR:OG1	11:J:12:PRO:HD2	2.09	0.53
15:J:1302:CLA:HMC2	14:J:4002:BCR:H10C	1.91	0.53
5:A:39:LEU:O	5:A:48:TRP:NE1	2.41	0.53
15:A:1113:CLA:HBA1	15:A:1113:CLA:CHA	2.38	0.53
6:B:223:LEU:H	15:B:1212:CLA:HMD2	1.73	0.53
2:2:77:LEU:HD13	2:2:84:ASP:OD1	2.09	0.53
12:4:501:LUT:H371	12:4:501:LUT:C28	2.39	0.53
9:E:73:LEU:HB3	9:E:87:VAL:CG1	2.39	0.53
3:3:90:LEU:HB2	16:3:604:CHL:CBA	2.38	0.53
3:3:155:PRO:HG3	15:A:1114:CLA:CMD	2.39	0.53
15:3:611:CLA:HBB1	15:3:611:CLA:CMB	2.39	0.53
5:A:742:PHE:CG	24:A:1011:CL0:H25	2.44	0.53
15:A:1115:CLA:HAC2	15:A:1116:CLA:CBB	2.39	0.53
6:B:192:THR:HG22	6:B:278:HIS:HB2	1.91	0.53
2:2:198:TYR:HD2	2:2:215:PHE:HZ	1.57	0.53
15:3:612:CLA:CMC	15:3:613:CLA:HMB1	2.39	0.53
4:4:177:VAL:HG13	4:4:293:PHE:HE2	1.72	0.53
6:B:582:PHE:CE2	6:B:711:LEU:HD13	2.44	0.53
3:3:262:ASP:OD1	3:3:263:GLY:N	2.42	0.53
4:4:211:THR:CG2	4:4:215:LEU:HD21	2.37	0.53
6:B:216:VAL:O	6:B:218:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:493:LEU:HB3	6:B:494:TRP:CE3	2.44	0.53
15:B:1226:CLA:CAD	21:B:5002:DGD:HB32	2.39	0.53
2:2:162:PHE:CZ	14:2:503:BCR:H373	2.43	0.52
15:3:603:CLA:HHD	15:3:603:CLA:HBC2	1.90	0.52
6:B:128:ILE:HD12	15:B:1211:CLA:CMA	2.39	0.52
7:C:28:MET:HE2	7:C:38:GLN:CB	2.39	0.52
9:E:78:ARG:HE	9:E:123:GLU:CD	2.17	0.52
15:3:605:CLA:CMB	15:3:605:CLA:HBB1	2.39	0.52
5:A:550:LEU:O	5:A:554:VAL:HG23	2.09	0.52
5:A:590:ASP:O	5:A:593:PHE:HB3	2.10	0.52
15:A:1110:CLA:HED3	15:A:1111:CLA:HMC1	1.91	0.52
15:A:1114:CLA:HED2	15:A:1114:CLA:H2A	1.91	0.52
15:A:1115:CLA:HAC2	15:A:1116:CLA:HBB2	1.91	0.52
3:3:151:GLY:HA3	15:3:613:CLA:CBC	2.37	0.52
4:4:233:ASP:O	4:4:237:PRO:HA	2.08	0.52
15:B:1229:CLA:O2A	14:B:4006:BCR:H362	2.09	0.52
13:1:502:XAT:H381	13:1:502:XAT:C28	2.38	0.52
16:1:610:CHL:HBC2	15:1:613:CLA:C2C	2.40	0.52
5:A:484:ALA:HA	15:A:1135:CLA:HBA1	1.90	0.52
15:A:1013:CLA:C1D	6:B:583:TRP:HE1	2.21	0.52
15:A:1110:CLA:HBC2	15:A:1110:CLA:HHD	1.91	0.52
15:A:1128:CLA:HBB1	15:A:1128:CLA:CMB	2.37	0.52
6:B:338:ALA:O	6:B:342:VAL:HG23	2.09	0.52
6:B:494:TRP:HE1	15:B:1231:CLA:CED	2.22	0.52
6:B:553:ASP:HB3	7:C:68:TYR:HE1	1.75	0.52
11:J:18:TRP:CE3	11:J:19:ALA:HB2	2.45	0.52
5:A:197:MET:HG2	15:A:1123:CLA:OBD	2.10	0.52
5:A:668:TYR:CE1	15:A:1106:CLA:HAC1	2.44	0.52
6:B:301:ARG:H	6:B:301:ARG:HD2	1.75	0.52
6:B:351:GLN:HA	6:B:354:TYR:CE1	2.45	0.52
7:C:15:THR:CG2	7:C:28:MET:HE1	2.39	0.52
13:1:502:XAT:H202	15:1:604:CLA:CMC	2.40	0.52
3:3:133:LEU:CD1	3:3:138:VAL:HG21	2.39	0.52
3:3:282:THR:N	15:3:603:CLA:HED2	2.23	0.52
6:B:396:ILE:HD11	6:B:542:ALA:HB1	1.90	0.52
15:B:1211:CLA:CMA	14:B:4003:BCR:H271	2.37	0.52
8:D:194:LYS:HG3	8:D:194:LYS:O	2.10	0.52
15:1:604:CLA:H2A	15:1:604:CLA:O1D	2.10	0.52
15:2:604:CLA:H12	15:2:604:CLA:C3A	2.38	0.52
3:3:271:HIS:HA	3:3:278:ALA:HB3	1.91	0.52
5:A:493:THR:O	5:A:497:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:700:ILE:HG22	5:A:704:HIS:CE1	2.45	0.52
14:A:4007:BCR:H362	15:B:1023:CLA:H72	1.92	0.52
6:B:187:SER:OG	15:B:1215:CLA:HAC1	2.10	0.52
6:B:391:GLY:HA2	14:B:4005:BCR:H393	1.92	0.52
6:B:561:ASP:OD1	7:C:66:ARG:NH2	2.42	0.52
1:1:73:GLU:OE2	1:1:151:ARG:NE	2.36	0.52
2:2:194:LYS:NZ	2:2:209:SER:O	2.43	0.52
13:2:502:XAT:C8	13:2:502:XAT:H181	2.39	0.52
15:2:607:CLA:HBB1	15:2:607:CLA:HMB1	1.91	0.52
15:4:615:CLA:HHC	15:4:615:CLA:CBB	2.39	0.52
5:A:95:GLY:HA3	5:A:148:TRP:CH2	2.45	0.52
6:B:256:LEU:HD11	15:B:1212:CLA:HBC1	1.92	0.52
15:B:1218:CLA:HAB	15:B:1219:CLA:CGA	2.40	0.52
23:B:5031:GSH:O11	23:B:5031:GSH:N2	2.43	0.52
8:D:75:LEU:CD1	8:D:102:VAL:HG11	2.40	0.52
2:2:199:PRO:HB3	16:2:611:CHL:HBC2	1.92	0.52
5:A:201:HIS:HB3	15:A:1123:CLA:HED3	1.92	0.52
5:A:370:HIS:O	5:A:374:MET:HB2	2.10	0.52
5:A:519:GLY:O	5:A:622:VAL:HG12	2.10	0.52
5:A:612:TRP:CZ3	5:A:639:ALA:HB2	2.44	0.52
6:B:340:ALA:CB	14:B:4005:BCR:H372	2.40	0.52
15:B:1216:CLA:HMD2	15:B:1219:CLA:HAC1	1.92	0.52
14:B:4006:BCR:H372	10:F:171:PHE:CD1	2.45	0.52
7:C:24:ASP:O	7:C:44:ARG:NH2	2.43	0.52
7:C:29:VAL:CG1	7:C:30:PRO:CD	2.80	0.52
10:F:83:THR:HG23	10:F:84:PRO:HD2	1.92	0.52
15:2:603:CLA:HHC	15:2:603:CLA:HBB1	1.91	0.52
3:3:259:ILE:HD13	15:3:603:CLA:HAA2	1.92	0.52
15:4:609:CLA:HMB1	15:4:609:CLA:HBB1	1.91	0.52
5:A:443:TRP:CD2	15:A:1130:CLA:HAB	2.45	0.52
15:A:1137:CLA:HHC	15:A:1137:CLA:CBB	2.40	0.52
15:A:1141:CLA:HHC	15:A:1141:CLA:CBB	2.39	0.52
6:B:664:PHE:CE1	15:B:1239:CLA:HBC3	2.45	0.52
8:D:102:VAL:HB	8:D:156:TYR:HB2	1.91	0.52
1:1:44:LYS:HB3	1:1:46:TYR:CD2	2.45	0.51
13:1:502:XAT:H12	15:1:605:CLA:HMB3	1.92	0.51
2:2:103:VAL:O	2:2:107:LEU:HG	2.10	0.51
3:3:216:GLY:N	15:3:601:CLA:HED2	2.24	0.51
4:4:223:PHE:CZ	15:4:612:CLA:HBC2	2.45	0.51
5:A:60:ASP:OD2	5:A:350:HIS:NE2	2.43	0.51
5:A:612:TRP:HZ3	5:A:639:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:143:LEU:HD11	14:B:4003:BCR:H401	1.91	0.51
2:2:175:ASN:HB3	4:4:131:ALA:HB2	1.91	0.51
5:A:238:PRO:HB2	5:A:243:PHE:CE1	2.45	0.51
6:B:15:GLN:O	6:B:17:PRO:HD3	2.09	0.51
15:B:1223:CLA:C4B	15:B:1231:CLA:HMA3	2.40	0.51
5:A:330:LYS:HE3	5:A:336:ASN:HA	1.92	0.51
5:A:336:ASN:HB3	5:A:425:ASN:HD22	1.76	0.51
5:A:439:SER:HB3	6:B:678:THR:HG22	1.91	0.51
5:A:545:VAL:HG11	5:A:598:TRP:CH2	2.45	0.51
15:A:1111:CLA:HMB1	15:A:1111:CLA:HBB1	1.93	0.51
6:B:198:VAL:C	6:B:201:PRO:HD2	2.35	0.51
6:B:396:ILE:CD1	6:B:542:ALA:HB1	2.41	0.51
6:B:588:ILE:O	6:B:592:THR:HG23	2.10	0.51
8:D:110:GLU:HG3	8:D:123:MET:O	2.10	0.51
2:2:109:HIS:CD2	15:2:612:CLA:HMD1	2.35	0.51
3:3:232:MET:HE1	15:3:601:CLA:HMA3	1.92	0.51
4:4:259:TYR:HB3	15:4:601:CLA:HED3	1.92	0.51
5:A:107:ASP:HB3	5:A:111:ILE:HD12	1.91	0.51
5:A:345:LEU:HD11	5:A:355:ILE:CD1	2.38	0.51
6:B:47:ILE:HG22	6:B:51:HIS:CE1	2.45	0.51
6:B:105:PHE:HA	6:B:107:ARG:HH21	1.75	0.51
6:B:204:ARG:HG3	6:B:251:SER:HB2	1.92	0.51
6:B:259:LEU:O	6:B:494:TRP:HA	2.11	0.51
15:B:1202:CLA:HED2	15:B:1221:CLA:HBA1	1.91	0.51
8:D:101:TYR:HE2	8:D:135:LYS:HB2	1.74	0.51
8:D:190:ARG:HH22	8:D:210:PHE:HB2	1.76	0.51
1:1:161:LEU:HD12	12:1:501:LUT:H222	1.92	0.51
2:2:114:MET:HB3	12:2:501:LUT:C15	2.41	0.51
13:2:502:XAT:H41	15:2:604:CLA:O1A	2.10	0.51
5:A:709:VAL:HG22	5:A:709:VAL:O	2.11	0.51
15:A:1110:CLA:CED	15:A:1111:CLA:HMC1	2.41	0.51
6:B:438:TYR:CE1	6:B:519:LEU:HD13	2.45	0.51
6:B:676:ILE:O	6:B:680:VAL:HG23	2.11	0.51
15:B:1216:CLA:HBB1	15:B:1216:CLA:CMB	2.38	0.51
7:C:57:ALA:O	7:C:59:PRO:HD3	2.11	0.51
8:D:111:GLN:O	8:D:122:ILE:HD12	2.11	0.51
14:J:4001:BCR:H311	14:J:4001:BCR:HC8	1.91	0.51
15:1:607:CLA:CBB	14:4:503:BCR:H333	2.41	0.51
5:A:395:MET:HB3	5:A:603:LEU:HD12	1.93	0.51
15:A:1138:CLA:HMD1	14:B:4006:BCR:HC41	1.93	0.51
10:F:114:ALA:HB3	10:F:115:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:606:CLA:HBC2	15:1:606:CLA:CHD	2.38	0.51
2:2:168:LYS:CA	15:4:609:CLA:HED1	2.39	0.51
2:2:239:GLN:HG2	2:2:250:ASN:HD22	1.74	0.51
5:A:83:ILE:O	5:A:86:ILE:HG22	2.10	0.51
5:A:220:VAL:HG22	5:A:220:VAL:O	2.10	0.51
5:A:369:HIS:HA	5:A:372:TYR:HD1	1.74	0.51
5:A:509:THR:O	5:A:526:ILE:N	2.37	0.51
6:B:72:GLN:HE22	15:B:1204:CLA:CED	2.24	0.51
1:1:88:GLY:O	1:1:92:VAL:HG23	2.11	0.51
1:1:106:TRP:CE2	1:1:113:PRO:HB3	2.45	0.51
15:4:606:CLA:HMA3	16:4:613:CHL:CMC	2.41	0.51
6:B:177:ASN:OD1	6:B:292:TYR:HB2	2.10	0.51
16:2:609:CHL:H11	3:3:178:GLN:HE21	1.75	0.51
16:2:609:CHL:HBC2	16:2:609:CHL:HHD	1.92	0.51
3:3:118:ARG:HH12	15:3:601:CLA:C1D	2.22	0.51
5:A:85:LEU:HB2	5:A:170:ALA:HB2	1.92	0.51
6:B:356:LEU:HD13	15:B:1214:CLA:HAA1	1.93	0.51
11:J:9:SER:CA	11:J:13:VAL:HG21	2.37	0.51
1:1:120:VAL:HG11	15:1:613:CLA:HMD3	1.93	0.51
3:3:121:MET:HE3	15:3:601:CLA:HMC3	1.91	0.51
4:4:192:VAL:CG1	4:4:194:LEU:HG	2.41	0.51
15:A:1116:CLA:O1D	15:A:1117:CLA:HHB	2.11	0.51
6:B:703:ILE:HG22	6:B:707:ARG:HH21	1.76	0.51
9:E:86:GLN:NE2	10:F:237:ILE:HD11	2.25	0.51
11:J:13:VAL:O	11:J:14:VAL:C	2.53	0.51
15:1:604:CLA:HMB2	15:1:604:CLA:H42	1.92	0.50
14:2:503:BCR:H271	15:2:606:CLA:C1B	2.40	0.50
15:2:605:CLA:OBD	15:2:605:CLA:H8	2.10	0.50
5:A:29:TRP:NE1	15:A:1109:CLA:O1A	2.43	0.50
5:A:601:ASN:OD1	24:A:1011:CL0:H36	2.11	0.50
6:B:595:TRP:CD1	15:B:1234:CLA:HAC1	2.42	0.50
7:C:75:ARG:HH12	8:D:99:GLU:HG2	1.76	0.50
5:A:477:ILE:HG23	5:A:477:ILE:O	2.11	0.50
6:B:425:TRP:CH2	15:B:1228:CLA:HAB	2.45	0.50
15:B:1220:CLA:HMA1	15:B:1240:CLA:HED3	1.93	0.50
3:3:154:PRO:N	3:3:155:PRO:CD	2.74	0.50
14:3:504:BCR:H312	15:3:605:CLA:HMD2	1.94	0.50
6:B:430:LEU:HB3	6:B:526:LEU:HB2	1.92	0.50
6:B:468:GLN:HG3	6:B:510:PHE:CE2	2.46	0.50
7:C:18:VAL:HG22	7:C:26:LEU:HG	1.93	0.50
1:1:183:LEU:HD12	17:1:801:LHG:HC82	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:505:BCR:H23C	15:4:605:CLA:HMD2	1.94	0.50
2:2:228:LEU:HD23	15:2:602:CLA:HAA1	1.93	0.50
3:3:159:TYR:HB3	3:3:162:PHE:CE2	2.47	0.50
5:A:206:LEU:HD22	15:A:1117:CLA:CMC	2.41	0.50
15:A:1013:CLA:H51	6:B:432:PHE:CE1	2.46	0.50
15:B:1220:CLA:O2D	15:B:1220:CLA:H2A	2.12	0.50
8:D:188:ASN:HD21	8:D:211:GLU:HB3	1.76	0.50
1:1:95:LEU:HD13	1:1:116:PHE:CZ	2.47	0.50
15:2:602:CLA:O1D	15:2:602:CLA:H2	2.10	0.50
13:3:502:XAT:H21	15:3:613:CLA:HMC2	1.94	0.50
15:3:601:CLA:HHD	15:3:601:CLA:HBC2	1.94	0.50
5:A:83:ILE:HA	5:A:86:ILE:HG22	1.92	0.50
5:A:499:ALA:HB1	15:A:1134:CLA:HED1	1.94	0.50
5:A:712:SER:N	10:F:199:GLU:OE2	2.31	0.50
15:A:1108:CLA:H2A	15:A:1108:CLA:CED	2.41	0.50
6:B:290:HIS:CE1	14:B:4001:BCR:H363	2.47	0.50
6:B:382:PHE:N	6:B:584:MET:HE3	2.26	0.50
1:1:54:PHE:HZ	1:1:179:LYS:HE2	1.77	0.50
15:1:606:CLA:HMA3	15:1:613:CLA:CMC	2.42	0.50
3:3:101:GLY:HA3	5:A:19:ARG:NH1	2.27	0.50
3:3:106:PRO:O	3:3:110:GLN:HG2	2.12	0.50
5:A:96:ALA:HB2	5:A:159:LEU:HB3	1.92	0.50
5:A:340:GLY:N	5:A:424:ASN:OD1	2.30	0.50
6:B:63:SER:OG	6:B:140:SER:O	2.27	0.50
6:B:92:ILE:HG21	6:B:97:PHE:CE2	2.47	0.50
6:B:530:THR:HG21	6:B:583:TRP:CZ2	2.46	0.50
11:J:27:ILE:HG21	14:J:4002:BCR:H343	1.94	0.50
3:3:170:PHE:O	3:3:173:GLU:HG2	2.11	0.50
4:4:158:ARG:HE	10:F:223:GLN:HG3	1.77	0.50
5:A:340:GLY:O	5:A:344:ILE:HG12	2.12	0.50
25:A:2001:PQN:H161	14:B:4006:BCR:H333	1.92	0.50
6:B:441:ASN:HB3	6:B:616:TYR:HB3	1.93	0.50
8:D:181:GLY:O	8:D:182:ARG:HD2	2.12	0.50
10:F:161:ALA:O	10:F:165:PHE:HB3	2.11	0.50
14:J:4001:BCR:C8	14:J:4001:BCR:H321	2.41	0.50
1:1:218:PHE:HE1	15:1:608:CLA:O1D	1.93	0.50
2:2:261:VAL:HG22	2:2:262:THR:N	2.26	0.50
15:3:603:CLA:HHD	15:3:603:CLA:HBC3	1.92	0.50
4:4:259:TYR:CA	15:4:601:CLA:HED2	2.42	0.50
5:A:141:THR:HG21	5:A:744:LEU:HD11	1.93	0.50
5:A:287:GLY:HA2	5:A:517:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1012:CLA:HMB1	15:B:1021:CLA:H191	1.94	0.50
6:B:658:TYR:CZ	15:B:1021:CLA:HMA3	2.46	0.50
7:C:79:LEU:HD22	7:C:81:TYR:CZ	2.47	0.50
11:J:16:LEU:O	11:J:20:ILE:HG12	2.11	0.50
5:A:564:PRO:HB3	8:D:116:PRO:HB2	1.94	0.50
5:A:647:ARG:NH1	6:B:638:PRO:HD3	2.27	0.50
6:B:381:GLY:HA3	6:B:584:MET:CE	2.41	0.50
6:B:464:ILE:O	6:B:468:GLN:HG2	2.12	0.50
10:F:106:LEU:HD13	10:F:119:LEU:HB3	1.93	0.50
13:1:502:XAT:H202	15:1:604:CLA:HMC1	1.94	0.49
15:2:603:CLA:HHC	15:2:603:CLA:CBB	2.42	0.49
21:2:811:DGD:O2G	21:2:811:DGD:HA32	2.12	0.49
4:4:287:MET:SD	15:4:604:CLA:HBB1	2.52	0.49
4:4:289:ALA:HB2	12:4:501:LUT:C10	2.42	0.49
5:A:202:LEU:HA	5:A:206:LEU:HD12	1.94	0.49
15:A:1136:CLA:HBB1	15:A:1136:CLA:CMB	2.38	0.49
6:B:425:TRP:CZ2	15:B:1228:CLA:HAB	2.47	0.49
7:C:15:THR:HG22	7:C:28:MET:CE	2.41	0.49
10:F:166:ILE:HD11	11:J:39:PHE:HB2	1.92	0.49
1:1:127:ILE:HD12	15:1:613:CLA:C3D	2.41	0.49
2:2:138:ASP:HA	16:2:610:CHL:O1D	2.11	0.49
3:3:181:GLU:OE1	3:3:184:ARG:NH1	2.45	0.49
15:3:606:CLA:HBB1	15:3:606:CLA:CMB	2.41	0.49
4:4:264:PHE:CB	12:4:501:LUT:H24	2.42	0.49
5:A:440:HIS:O	5:A:444:VAL:HG23	2.12	0.49
6:B:205:GLY:HA3	6:B:247:THR:HA	1.94	0.49
6:B:438:TYR:HE1	6:B:519:LEU:HD13	1.77	0.49
2:2:263:PHE:CE1	15:2:615:CLA:HAC2	2.47	0.49
4:4:162:PHE:HB3	15:4:604:CLA:CMA	2.41	0.49
4:4:203:GLN:O	4:4:207:ILE:HG13	2.11	0.49
4:4:296:THR:C	4:4:298:ALA:H	2.20	0.49
15:4:605:CLA:HBA2	15:4:605:CLA:CBD	2.42	0.49
5:A:382:THR:HB	5:A:520:LYS:HZ2	1.76	0.49
5:A:561:ARG:CZ	8:D:90:GLY:H	2.26	0.49
5:A:564:PRO:HG2	8:D:137:GLN:HA	1.93	0.49
15:A:1102:CLA:HMB1	15:A:1102:CLA:CBB	2.41	0.49
15:A:1106:CLA:HMB3	15:A:1107:CLA:H11	1.93	0.49
15:A:1139:CLA:H52	11:J:14:VAL:HG23	1.93	0.49
15:B:1204:CLA:HED2	15:B:1204:CLA:H2A	1.94	0.49
15:B:1230:CLA:HMB3	15:B:1230:CLA:CBB	2.38	0.49
8:D:83:ILE:HB	8:D:122:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:57:ASP:OD2	1:1:60:GLU:HA	2.12	0.49
16:1:610:CHL:HBC3	16:1:610:CHL:HHD	1.94	0.49
5:A:540:ALA:O	5:A:544:HIS:ND1	2.29	0.49
15:A:1119:CLA:HBA1	15:A:1123:CLA:HBB1	1.94	0.49
15:A:1124:CLA:H12	15:A:1135:CLA:HMA1	1.95	0.49
6:B:54:GLN:NE2	6:B:58:ILE:HD11	2.26	0.49
6:B:143:LEU:HD21	14:B:4003:BCR:H401	1.93	0.49
6:B:191:TRP:O	6:B:195:LEU:HD13	2.12	0.49
1:1:127:ILE:HD12	15:1:613:CLA:C2D	2.43	0.49
3:3:101:GLY:HA3	5:A:19:ARG:CD	2.35	0.49
3:3:205:LEU:HA	3:3:218:PRO:HD2	1.94	0.49
15:4:605:CLA:HED2	15:4:612:CLA:C1	2.43	0.49
16:4:611:CHL:HAA1	16:4:611:CHL:HBD	1.93	0.49
15:A:1141:CLA:C1B	14:A:4004:BCR:H402	2.43	0.49
6:B:395:PHE:CE2	6:B:413:LEU:HD21	2.47	0.49
15:2:604:CLA:HHD	16:2:609:CHL:HBB2	1.95	0.49
3:3:168:THR:O	3:3:172:ILE:HG12	2.12	0.49
3:3:176:ALA:O	14:3:503:BCR:H16C	2.12	0.49
5:A:558:ARG:HD3	5:A:567:ALA:HB2	1.94	0.49
6:B:434:THR:CG2	15:B:1021:CLA:H192	2.43	0.49
7:C:23:LEU:HD13	7:C:47:ASP:O	2.13	0.49
1:1:83:MET:CE	15:1:601:CLA:HAB	2.43	0.49
16:1:610:CHL:C2C	15:1:613:CLA:HMC3	2.42	0.49
2:2:239:GLN:HE21	2:2:250:ASN:CB	2.26	0.49
5:A:679:TRP:CD2	24:A:1011:CL0:CMA	2.93	0.49
15:A:1115:CLA:HBB1	15:A:1115:CLA:CMB	2.42	0.49
25:A:2001:PQN:H141	14:B:4006:BCR:H333	1.95	0.49
6:B:38:MET:HE2	6:B:43:LEU:HD13	1.94	0.49
2:2:113:ALA:CB	13:2:502:XAT:H402	2.42	0.49
2:2:145:LYS:HG2	4:4:333:PHE:CD1	2.48	0.49
4:4:325:VAL:HG13	4:4:328:PRO:CG	2.43	0.49
5:A:398:GLY:O	5:A:402:VAL:HG23	2.12	0.49
15:A:1104:CLA:H143	15:A:1127:CLA:HBB2	1.94	0.49
15:A:1134:CLA:HBA1	15:A:1134:CLA:CHA	2.41	0.49
6:B:288:ALA:HB2	15:B:1216:CLA:HBC2	1.95	0.49
10:F:106:LEU:HD21	10:F:120:GLN:OE1	2.13	0.49
16:1:610:CHL:HHC	16:1:610:CHL:CBB	2.40	0.49
2:2:169:ARG:HD2	2:2:169:ARG:O	2.12	0.49
6:B:87:PRO:HB3	6:B:122:TYR:CE2	2.47	0.49
15:B:1234:CLA:H12	15:B:1235:CLA:O1A	2.13	0.49
15:F:1301:CLA:HBC2	11:J:18:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:212:LEU:O	4:4:214:THR:N	2.46	0.49
5:A:492:PHE:O	5:A:495:PRO:HD2	2.12	0.49
6:B:53:GLY:O	6:B:57:ILE:HG12	2.12	0.49
6:B:441:ASN:O	6:B:445:GLN:HG2	2.12	0.49
10:F:125:ARG:O	10:F:129:ARG:HG3	2.13	0.49
11:J:19:ALA:HA	11:J:22:THR:HG1	1.78	0.49
1:1:171:GLU:HA	1:1:174:LYS:HD3	1.95	0.48
1:1:206:LEU:O	1:1:210:LEU:HD13	2.13	0.48
15:1:601:CLA:CMD	15:1:611:CLA:HBA2	2.42	0.48
2:2:184:PHE:CE1	2:2:185:LEU:HD13	2.46	0.48
15:2:607:CLA:HBB1	15:2:607:CLA:CMB	2.42	0.48
13:3:502:XAT:H183	15:3:606:CLA:CAB	2.43	0.48
14:3:504:BCR:H383	14:A:4002:BCR:H381	1.94	0.48
5:A:221:SER:HA	5:A:291:LEU:HD12	1.94	0.48
5:A:446:ILE:HA	15:B:1023:CLA:O1A	2.13	0.48
1:1:85:GLY:HA2	13:1:502:XAT:H382	1.95	0.48
2:2:269:SER:C	2:2:271:PRO:HD3	2.38	0.48
14:3:503:BCR:C21	15:3:613:CLA:HBA1	2.44	0.48
4:4:145:TYR:CD2	15:4:609:CLA:HMC2	2.38	0.48
4:4:172:TRP:HE1	13:4:502:XAT:C19	2.26	0.48
5:A:96:ALA:HB2	5:A:159:LEU:CB	2.42	0.48
5:A:297:HIS:O	5:A:301:ILE:HG12	2.13	0.48
5:A:301:ILE:HG23	5:A:305:PHE:CD2	2.47	0.48
10:F:120:GLN:O	10:F:124:GLU:HG3	2.13	0.48
11:J:8:LEU:CA	11:J:13:VAL:HG11	2.43	0.48
3:3:133:LEU:HD11	3:3:138:VAL:HG21	1.94	0.48
3:3:170:PHE:CD1	15:3:610:CLA:HBD	2.49	0.48
5:A:415:ARG:HH12	15:A:1128:CLA:HED3	1.78	0.48
15:A:1111:CLA:HBB1	15:A:1111:CLA:CMB	2.43	0.48
2:2:137:TYR:O	2:2:138:ASP:OD1	2.32	0.48
13:3:502:XAT:H162	15:3:606:CLA:HMB1	1.94	0.48
15:3:611:CLA:C4A	15:3:611:CLA:HBA2	2.43	0.48
15:4:605:CLA:C1	10:F:219:LEU:HG	2.44	0.48
5:A:299:LEU:HD21	15:A:1113:CLA:CMC	2.42	0.48
5:A:443:TRP:CE3	15:A:1130:CLA:HAB	2.48	0.48
5:A:702:TRP:CZ3	6:B:418:ALA:HB2	2.49	0.48
7:C:60:THR:HG22	7:C:62:PHE:O	2.13	0.48
2:2:98:MET:CE	11:J:1:MET:HE2	2.41	0.48
5:A:521:VAL:HG11	5:A:627:VAL:HG21	1.95	0.48
6:B:69:VAL:HG21	6:B:125:TRP:CZ3	2.48	0.48
6:B:182:GLY:HA3	15:B:1210:CLA:CBB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:191:TRP:CE2	6:B:195:LEU:HD11	2.48	0.48
11:J:37:LEU:HG	11:J:37:LEU:O	2.13	0.48
15:J:1302:CLA:C2C	14:J:4002:BCR:H10C	2.43	0.48
1:1:85:GLY:HA2	13:1:502:XAT:C38	2.44	0.48
1:1:221:ASN:HD21	15:1:603:CLA:CAD	2.26	0.48
2:2:115:LEU:HD11	15:2:601:CLA:CBC	2.43	0.48
15:2:601:CLA:HBB1	15:2:601:CLA:CMB	2.40	0.48
5:A:77:HIS:CB	15:A:1111:CLA:HED2	2.42	0.48
6:B:24:TYR:CD1	21:B:5002:DGD:HG32	2.48	0.48
11:J:27:ILE:CG2	14:J:4002:BCR:H343	2.43	0.48
1:1:44:LYS:HB3	1:1:46:TYR:CE2	2.49	0.48
1:1:46:TYR:OH	1:1:60:GLU:HG3	2.12	0.48
1:1:166:ASP:HB3	1:1:169:SER:OG	2.14	0.48
1:1:170:PHE:O	1:1:174:LYS:HG3	2.14	0.48
15:4:604:CLA:H43	10:F:219:LEU:CD2	2.43	0.48
6:B:69:VAL:HG13	6:B:122:TYR:CE1	2.41	0.48
6:B:237:ASN:HD21	6:B:253:THR:HG1	1.56	0.48
15:B:1218:CLA:HAB	15:B:1219:CLA:H2	1.95	0.48
10:F:115:PRO:O	10:F:119:LEU:HD13	2.14	0.48
15:1:606:CLA:CHA	15:1:606:CLA:HBA2	2.39	0.48
4:4:178:VAL:HG21	12:4:501:LUT:H401	1.95	0.48
5:A:81:LEU:HD12	15:A:1111:CLA:CED	2.43	0.48
5:A:153:ILE:HD13	5:A:159:LEU:HD21	1.96	0.48
6:B:168:TRP:CZ2	15:B:1210:CLA:HAC2	2.48	0.48
1:1:64:GLU:HG2	1:1:66:GLY:H	1.79	0.48
2:2:199:PRO:HD2	15:2:601:CLA:CED	2.44	0.48
13:2:502:XAT:H31	13:2:502:XAT:H391	1.75	0.48
5:A:403:VAL:HG11	5:A:596:LEU:CD2	2.44	0.48
5:A:408:HIS:HA	5:A:411:ILE:HD12	1.95	0.48
5:A:451:HIS:HA	15:A:1132:CLA:HBB2	1.96	0.48
5:A:677:PHE:CG	14:A:4006:BCR:H363	2.48	0.48
5:A:690:ARG:NH1	6:B:567:GLY:O	2.46	0.48
6:B:92:ILE:HG22	6:B:94:ASP:H	1.77	0.48
6:B:440:HIS:O	6:B:444:VAL:HG23	2.14	0.48
8:D:157:ARG:HH21	8:D:165:GLN:HB3	1.79	0.48
10:F:173:TYR:HA	10:F:217:TRP:HZ2	1.77	0.48
1:1:56:PHE:O	1:1:57:ASP:C	2.57	0.48
1:1:134:ALA:HB1	14:1:503:BCR:H363	1.96	0.48
2:2:203:PHE:C	2:2:205:PRO:HD3	2.39	0.48
2:2:261:VAL:HG22	2:2:262:THR:H	1.79	0.48
5:A:44:ASN:OD1	9:E:109:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:57:HIS:ND1	15:A:1104:CLA:HBA1	2.27	0.48
5:A:638:SER:O	5:A:644:GLY:HA3	2.14	0.48
5:A:740:TRP:HD1	15:A:1126:CLA:HMB2	1.79	0.48
6:B:74:ASN:HB2	6:B:77:GLN:HB2	1.96	0.48
6:B:214:LEU:HD23	6:B:214:LEU:H	1.78	0.48
6:B:346:THR:HB	6:B:380:ALA:HB2	1.94	0.48
1:1:218:PHE:HA	1:1:221:ASN:HD21	1.79	0.47
5:A:687:PHE:HB2	15:A:1013:CLA:HBC2	1.93	0.47
15:A:1116:CLA:H43	15:A:1133:CLA:HAA2	1.96	0.47
15:A:1126:CLA:C1C	14:A:4006:BCR:HC22	2.44	0.47
6:B:124:TRP:HB2	6:B:359:TYR:CE2	2.49	0.47
6:B:358:PRO:HG3	15:B:1215:CLA:CAA	2.43	0.47
6:B:441:ASN:ND2	6:B:615:THR:O	2.47	0.47
14:B:4006:BCR:C21	15:F:1301:CLA:HAB	2.44	0.47
14:J:4002:BCR:H392	14:J:4002:BCR:H23C	1.96	0.47
4:4:174:MET:HB3	12:4:501:LUT:C34	2.45	0.47
5:A:118:VAL:HG13	5:A:138:ILE:HD11	1.96	0.47
6:B:316:LEU:HD22	6:B:408:VAL:HG12	1.96	0.47
6:B:408:VAL:O	6:B:412:VAL:HG23	2.13	0.47
6:B:423:LEU:HB3	6:B:533:LEU:HD13	1.95	0.47
6:B:435:LEU:O	6:B:439:VAL:HG23	2.14	0.47
11:J:9:SER:HA	11:J:13:VAL:CG2	2.41	0.47
15:1:611:CLA:CMC	15:1:611:CLA:HBC2	2.44	0.47
5:A:667:ALA:HB3	15:A:1106:CLA:CBC	2.44	0.47
15:A:1012:CLA:CMB	15:B:1021:CLA:H191	2.45	0.47
15:B:1212:CLA:HBB1	15:B:1212:CLA:CMB	2.43	0.47
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.65	0.47
7:C:10:THR:HA	9:E:100:TYR:HE2	1.79	0.47
12:1:501:LUT:H31	12:1:501:LUT:H391	1.54	0.47
15:1:608:CLA:HHC	15:1:608:CLA:HBB1	1.96	0.47
2:2:270:ILE:N	2:2:271:PRO:HD3	2.29	0.47
3:3:85:ASP:OD2	16:3:604:CHL:HBA1	2.14	0.47
3:3:104:VAL:HG23	3:3:104:VAL:O	2.15	0.47
5:A:223:PRO:HG3	5:A:243:PHE:HE2	1.80	0.47
5:A:593:PHE:CE1	5:A:728:VAL:HB	2.49	0.47
6:B:125:TRP:HB3	6:B:130:LEU:HD12	1.96	0.47
6:B:189:LEU:O	6:B:192:THR:OG1	2.24	0.47
6:B:347:SER:O	6:B:351:GLN:HG2	2.14	0.47
7:C:24:ASP:OD1	8:D:175:PRO:HG2	2.15	0.47
10:F:176:GLY:O	10:F:177:TYR:C	2.57	0.47
1:1:206:LEU:HD23	1:1:210:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:605:CLA:CAC	15:2:612:CLA:HAA1	2.31	0.47
4:4:178:VAL:CG2	12:4:501:LUT:H401	2.45	0.47
4:4:258:GLY:HA2	16:4:611:CHL:CMD	2.45	0.47
4:4:311:HIS:HA	4:4:318:VAL:CG2	2.45	0.47
4:4:318:VAL:HB	15:4:603:CLA:HED1	1.95	0.47
21:4:811:DGD:HA51	15:B:1230:CLA:H12	1.97	0.47
5:A:97:ARG:HA	5:A:160:TYR:OH	2.13	0.47
5:A:105:LEU:HD12	5:A:149:ARG:HH11	1.79	0.47
14:A:4002:BCR:C6	14:A:4002:BCR:H342	2.45	0.47
15:B:1225:CLA:ND	14:B:4002:BCR:H282	2.30	0.47
7:C:63:LEU:O	8:D:192:ILE:HD13	2.14	0.47
10:F:166:ILE:HD12	10:F:167:PRO:N	2.29	0.47
16:1:610:CHL:HAC2	16:1:610:CHL:OMC	2.13	0.47
3:3:281:ILE:N	15:3:603:CLA:HED1	2.30	0.47
12:3:501:LUT:H222	15:3:601:CLA:C4	2.45	0.47
15:3:606:CLA:HMA2	15:3:613:CLA:C4C	2.45	0.47
15:A:1122:CLA:CBC	14:A:4004:BCR:HC8	2.44	0.47
6:B:173:GLU:HB3	6:B:292:TYR:HB3	1.97	0.47
6:B:266:THR:HG21	6:B:360:ALA:HB1	1.95	0.47
6:B:452:LYS:HD2	10:F:129:ARG:NE	2.30	0.47
8:D:152:THR:HA	8:D:174:TYR:OH	2.15	0.47
10:F:126:THR:OG1	10:F:129:ARG:NH1	2.48	0.47
1:1:84:LEU:O	15:1:606:CLA:HMC3	2.15	0.47
2:2:74:PRO:HB3	2:2:76:TRP:CZ2	2.50	0.47
4:4:218:ILE:CD1	16:4:613:CHL:HED2	2.44	0.47
5:A:26:PHE:HE1	15:A:1109:CLA:HMB2	1.80	0.47
5:A:344:ILE:HD13	5:A:422:ASN:HB3	1.95	0.47
5:A:435:ASP:CG	6:B:678:THR:HG23	2.39	0.47
5:A:448:LEU:HB2	5:A:541:PHE:HD1	1.79	0.47
24:A:1011:CL0:H13	15:A:1012:CLA:OBD	2.14	0.47
6:B:57:ILE:HG13	15:B:1201:CLA:HBB1	1.95	0.47
6:B:188:SER:HB3	6:B:282:ALA:HB2	1.96	0.47
6:B:381:GLY:HA3	6:B:584:MET:HE3	1.96	0.47
15:B:1226:CLA:HMD3	21:B:5002:DGD:HB41	1.97	0.47
15:B:1229:CLA:HBB1	15:B:1229:CLA:HMB1	1.97	0.47
7:C:61:ASP:HA	7:C:62:PHE:HA	1.66	0.47
10:F:224:GLU:OE2	10:F:230:LEU:HB3	2.14	0.47
2:2:65:PRO:HG2	17:2:801:LHG:O2	2.14	0.47
2:2:162:PHE:CD2	15:2:612:CLA:HMC3	2.49	0.47
2:2:168:LYS:HE3	16:2:611:CHL:OMC	2.14	0.47
2:2:254:HIS:CD2	15:2:603:CLA:HAA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:607:CLA:CAB	14:3:503:BCR:HC31	2.45	0.47
3:3:81:ASP:HA	16:3:604:CHL:HED2	1.96	0.47
3:3:131:GLU:OE1	3:3:264:PRO:HD2	2.14	0.47
5:A:68:GLU:HB2	5:A:71:ARG:HH21	1.80	0.47
5:A:306:LEU:O	5:A:310:HIS:ND1	2.44	0.47
5:A:404:GLY:HA3	15:A:1128:CLA:HMC2	1.97	0.47
25:A:2001:PQN:H161	25:A:2001:PQN:H141	1.43	0.47
6:B:718:TYR:HE1	15:B:1021:CLA:O2A	1.97	0.47
8:D:109:LYS:O	8:D:110:GLU:C	2.57	0.47
11:J:21:PHE:CE1	14:J:4003:BCR:HC21	2.50	0.47
14:1:503:BCR:H24C	15:1:613:CLA:O2A	2.15	0.47
2:2:198:TYR:HD2	2:2:215:PHE:CZ	2.32	0.47
3:3:152:VAL:HB	15:3:613:CLA:HMC1	1.94	0.47
4:4:162:PHE:HB3	15:4:604:CLA:HMA1	1.96	0.47
5:A:57:HIS:HB2	15:A:1128:CLA:O1A	2.15	0.47
15:A:1103:CLA:H72	15:A:1111:CLA:O2A	2.15	0.47
10:F:106:LEU:HD13	10:F:119:LEU:CB	2.45	0.47
1:1:182:ARG:HH22	15:1:604:CLA:HED2	1.79	0.47
1:1:215:PHE:CD1	4:4:212:LEU:HD22	2.50	0.47
15:1:604:CLA:HBC2	16:1:609:CHL:HBB2	1.96	0.47
12:4:501:LUT:H32	15:4:601:CLA:CAB	2.45	0.47
5:A:442:ASN:C	5:A:442:ASN:HD22	2.21	0.47
15:A:1112:CLA:HHB	14:A:4002:BCR:H331	1.96	0.47
15:A:1124:CLA:HBB2	14:A:4005:BCR:H392	1.96	0.47
6:B:411:ARG:HD3	15:B:1227:CLA:OBD	2.15	0.47
6:B:494:TRP:HE1	15:B:1231:CLA:HED2	1.80	0.47
6:B:657:VAL:HG22	15:B:1239:CLA:HMB3	1.96	0.47
15:B:1228:CLA:H102	15:B:1229:CLA:H162	1.95	0.47
15:B:1235:CLA:H41	14:F:4002:BCR:H321	1.96	0.47
10:F:166:ILE:N	10:F:167:PRO:CD	2.78	0.47
13:3:502:XAT:H192	15:3:606:CLA:CBB	2.43	0.46
5:A:484:ALA:HB2	15:A:1136:CLA:HED2	1.97	0.46
6:B:85:VAL:HG22	6:B:86:ARG:N	2.30	0.46
6:B:243:HIS:ND1	6:B:251:SER:HA	2.30	0.46
6:B:244:ALA:HB2	6:B:249:ASP:HB2	1.97	0.46
8:D:75:LEU:HD13	8:D:102:VAL:HG11	1.96	0.46
9:E:77:LEU:HB2	9:E:123:GLU:O	2.16	0.46
9:E:117:ASN:OD1	9:E:118:ASN:N	2.48	0.46
14:1:503:BCR:H393	15:1:606:CLA:C1C	2.45	0.46
2:2:270:ILE:HG22	2:2:270:ILE:O	2.15	0.46
4:4:128:TYR:OH	15:4:609:CLA:HMA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:222:LEU:HG	14:4:503:BCR:C16	2.46	0.46
5:A:54:ALA:HB2	17:A:5002:LHG:O9	2.15	0.46
5:A:119:TRP:CZ2	14:J:4002:BCR:H332	2.50	0.46
5:A:453:PHE:HE1	15:B:1022:CLA:HMA1	1.81	0.46
5:A:546:THR:OG1	5:A:598:TRP:HB3	2.16	0.46
5:A:615:GLN:OE1	5:A:653:GLN:NE2	2.48	0.46
5:A:672:PHE:HE2	6:B:621:LEU:HD21	1.80	0.46
14:A:4004:BCR:H351	14:A:4004:BCR:H15C	1.64	0.46
6:B:131:ARG:HH11	6:B:207:HIS:CE1	2.33	0.46
2:2:168:LYS:HG2	15:4:609:CLA:CED	2.45	0.46
3:3:101:GLY:CA	5:A:19:ARG:HD2	2.34	0.46
4:4:318:VAL:HG23	4:4:318:VAL:O	2.15	0.46
5:A:659:GLN:HG2	5:A:659:GLN:O	2.16	0.46
15:A:1012:CLA:HMB3	15:B:1021:CLA:C20	2.40	0.46
7:C:29:VAL:HA	8:D:178:VAL:HG13	1.98	0.46
10:F:201:ILE:HG23	11:J:9:SER:HB2	1.96	0.46
11:J:12:PRO:HB3	14:J:4002:BCR:H291	1.97	0.46
15:J:1302:CLA:HMC2	14:J:4002:BCR:C10	2.45	0.46
1:1:71:TYR:OH	15:B:1240:CLA:HAB	2.16	0.46
3:3:121:MET:HG3	3:3:243:GLY:HA2	1.96	0.46
3:3:206:PHE:HD1	3:3:220:PHE:HE2	1.63	0.46
3:3:248:LEU:HG	16:3:604:CHL:HAC1	1.97	0.46
5:A:57:HIS:NE2	15:A:1103:CLA:HBB2	2.30	0.46
5:A:119:TRP:CG	14:J:4002:BCR:HC41	2.50	0.46
5:A:190:TRP:HA	5:A:193:ASN:OD1	2.15	0.46
5:A:392:THR:HG22	15:A:1126:CLA:CAB	2.45	0.46
15:A:1013:CLA:H101	15:A:1140:CLA:HMC3	1.97	0.46
6:B:346:THR:OG1	15:B:1225:CLA:HAC1	2.16	0.46
6:B:468:GLN:HE21	6:B:510:PHE:HE2	1.62	0.46
6:B:631:GLN:HE22	6:B:733:ARG:HE	1.62	0.46
15:B:1235:CLA:H142	15:B:1235:CLA:H111	1.69	0.46
10:F:103:ASP:HA	10:F:106:LEU:HB3	1.96	0.46
10:F:217:TRP:CD1	10:F:218:PRO:HD3	2.50	0.46
15:1:608:CLA:HHC	15:1:608:CLA:CBB	2.46	0.46
2:2:155:ILE:HG12	16:2:610:CHL:HBC3	1.97	0.46
16:2:609:CHL:HED1	3:3:182:LEU:HB3	1.97	0.46
4:4:159:MET:HE1	15:4:604:CLA:HAA2	1.96	0.46
5:A:612:TRP:HB2	5:A:649:PHE:CD1	2.49	0.46
6:B:283:VAL:HG21	15:B:1213:CLA:HAB	1.97	0.46
6:B:349:VAL:O	6:B:353:MET:HG3	2.16	0.46
6:B:460:PHE:HB3	15:B:1234:CLA:H2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:113:SER:OG	10:F:115:PRO:HD2	2.16	0.46
2:2:235:GLY:O	2:2:239:GLN:HB3	2.15	0.46
4:4:285:LEU:HD21	15:4:602:CLA:CAC	2.45	0.46
15:4:609:CLA:HBB1	15:4:609:CLA:CMB	2.46	0.46
6:B:198:VAL:HG11	15:B:1211:CLA:O1D	2.15	0.46
6:B:438:TYR:CD2	6:B:617:LEU:HD21	2.51	0.46
12:1:501:LUT:C24	12:1:501:LUT:H363	2.46	0.46
13:1:502:XAT:H12	15:1:605:CLA:CMB	2.45	0.46
2:2:236:PHE:CE1	12:2:501:LUT:H363	2.39	0.46
3:3:135:LYS:HE2	3:3:135:LYS:HA	1.98	0.46
15:3:605:CLA:HBC2	15:3:605:CLA:CMC	2.46	0.46
4:4:289:ALA:HB2	12:4:501:LUT:C9	2.46	0.46
5:A:180:HIS:O	5:A:185:ALA:HA	2.15	0.46
5:A:345:LEU:CB	15:A:1123:CLA:HBC3	2.44	0.46
5:A:372:TYR:CD2	5:A:610:PHE:HE1	2.34	0.46
5:A:737:ALA:HA	14:A:4006:BCR:HC42	1.98	0.46
15:A:1110:CLA:CGA	15:A:1110:CLA:C1A	2.94	0.46
15:A:1138:CLA:HMB1	15:A:1138:CLA:CBB	2.43	0.46
6:B:370:ALA:HA	6:B:595:TRP:CZ3	2.51	0.46
6:B:416:LYS:O	6:B:420:ILE:HG12	2.15	0.46
15:B:1228:CLA:H52	14:F:4002:BCR:H372	1.97	0.46
15:B:1231:CLA:H92	15:B:1231:CLA:H62	1.82	0.46
11:J:11:ALA:O	11:J:16:LEU:HD23	2.16	0.46
1:1:128:LEU:O	1:1:132:VAL:HG23	2.15	0.46
2:2:113:ALA:CA	13:2:502:XAT:H402	2.46	0.46
2:2:198:TYR:CE2	2:2:219:LYS:HB2	2.50	0.46
2:2:272:HIS:HB2	15:A:1114:CLA:OBD	2.16	0.46
5:A:246:ASN:ND2	5:A:249:ILE:HG12	2.30	0.46
5:A:494:ALA:HA	5:A:498:THR:OG1	2.16	0.46
6:B:22:ILE:HD11	6:B:696:ASP:OD2	2.16	0.46
6:B:339:LEU:O	6:B:383:ILE:HG22	2.16	0.46
6:B:460:PHE:HB2	15:B:1235:CLA:CAD	2.46	0.46
7:C:22:PRO:HB3	7:C:53:ARG:NH1	2.31	0.46
1:1:46:TYR:CD1	1:1:63:LYS:HG3	2.50	0.46
1:1:217:ASN:CG	15:1:608:CLA:HED1	2.41	0.46
14:1:503:BCR:H271	15:1:606:CLA:NC	2.31	0.46
16:3:604:CHL:HMB3	16:3:604:CHL:CBB	2.45	0.46
15:4:607:CLA:CMB	15:4:607:CLA:HBB1	2.46	0.46
5:A:647:ARG:NH2	6:B:636:TYR:O	2.49	0.46
5:A:668:TYR:HE1	15:A:1106:CLA:HAC1	1.81	0.46
5:A:682:SER:HB2	5:A:727:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1011:CL0:H16	15:B:1021:CLA:HAA1	1.96	0.46
15:A:1121:CLA:CBB	15:A:1121:CLA:HHC	2.46	0.46
7:C:33:GLY:H	7:C:37:ALA:CB	2.29	0.46
7:C:52:LYS:HE2	7:C:69:LEU:HD21	1.98	0.46
2:2:114:MET:HB3	12:2:501:LUT:C14	2.46	0.46
5:A:43:PRO:HB3	5:A:48:TRP:CD2	2.50	0.46
5:A:199:ASN:O	5:A:203:ALA:HB3	2.16	0.46
5:A:580:ARG:HA	7:C:77:LEU:HA	1.97	0.46
5:A:675:ALA:HA	5:A:678:VAL:HG22	1.98	0.46
1:1:69:GLN:OE1	1:1:152:LEU:HD11	2.16	0.45
16:1:610:CHL:HBD	16:1:610:CHL:CGA	2.46	0.45
3:3:250:MET:CE	13:3:502:XAT:H10	2.42	0.45
5:A:46:THR:CG2	5:A:715:PRO:HA	2.46	0.45
5:A:344:ILE:HG23	5:A:412:PHE:CZ	2.51	0.45
5:A:580:ARG:NH1	7:C:51:CYS:HB3	2.29	0.45
15:A:1110:CLA:HMB1	15:A:1118:CLA:C4D	2.46	0.45
6:B:715:SER:O	6:B:719:ILE:HG12	2.16	0.45
5:A:21:PRO:HG3	5:A:185:ALA:CB	2.46	0.45
5:A:21:PRO:HG3	5:A:185:ALA:HB3	1.97	0.45
5:A:179:PHE:O	5:A:184:ALA:N	2.49	0.45
15:A:1012:CLA:C4	6:B:439:VAL:HG13	2.46	0.45
6:B:69:VAL:HG21	6:B:125:TRP:HZ3	1.81	0.45
6:B:258:PHE:CD1	15:B:1214:CLA:HMB1	2.51	0.45
15:B:1220:CLA:H61	15:B:1220:CLA:H93	1.73	0.45
2:2:93:SER:HB2	2:2:99:ARG:HA	1.97	0.45
16:2:609:CHL:HBC3	17:2:801:LHG:HC42	1.98	0.45
3:3:253:TYR:OH	12:3:501:LUT:H8	2.16	0.45
4:4:263:ILE:CG2	16:4:611:CHL:H11	2.46	0.45
5:A:13:VAL:HG11	5:A:196:SER:HB2	1.98	0.45
5:A:32:PRO:HB2	5:A:48:TRP:CH2	2.50	0.45
5:A:233:ASP:OD1	5:A:234:PRO:HD2	2.15	0.45
5:A:351:ALA:HB2	5:A:412:PHE:CE1	2.51	0.45
5:A:417:TYR:HD2	5:A:558:ARG:HH21	1.64	0.45
5:A:721:THR:HB	17:A:5002:LHG:HC41	1.97	0.45
6:B:327:VAL:HG13	6:B:333:PHE:HD2	1.82	0.45
1:1:72:ARG:O	1:1:76:LEU:HD13	2.17	0.45
1:1:83:MET:HE1	15:1:601:CLA:CAB	2.46	0.45
18:1:802:LMG:HC2	18:1:802:LMG:HC71	1.55	0.45
2:2:78:ASP:OD1	2:2:79:GLY:N	2.48	0.45
2:2:141:LYS:O	2:2:145:LYS:HG3	2.16	0.45
3:3:199:PHE:HZ	14:3:503:BCR:H10C	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:50:TRP:HE1	15:A:1139:CLA:CBB	2.29	0.45
5:A:121:ILE:HG23	5:A:122:VAL:H	1.81	0.45
5:A:584:CYS:N	6:B:670:GLY:HA3	2.14	0.45
5:A:721:THR:CG2	17:A:5002:LHG:HC41	2.46	0.45
15:B:1209:CLA:CMB	15:B:1209:CLA:HBB1	2.46	0.45
15:B:1217:CLA:HHC	15:B:1217:CLA:CBB	2.46	0.45
4:4:124:ARG:HB2	4:4:145:TYR:CE1	2.51	0.45
4:4:314:ASP:O	4:4:318:VAL:HG22	2.17	0.45
4:4:325:VAL:HG13	4:4:328:PRO:CD	2.46	0.45
12:4:501:LUT:C11	15:4:602:CLA:HMC1	2.46	0.45
5:A:382:THR:HB	5:A:520:LYS:NZ	2.31	0.45
5:A:618:VAL:HG12	5:A:619:TRP:CD1	2.52	0.45
15:B:1226:CLA:HBB1	15:B:1226:CLA:CMB	2.46	0.45
7:C:4:VAL:CG2	8:D:207:SER:HB2	2.45	0.45
10:F:79:ILE:HD11	10:F:158:PHE:CZ	2.51	0.45
11:J:11:ALA:N	11:J:12:PRO:HD2	2.31	0.45
15:1:606:CLA:HMA3	15:1:613:CLA:HMC2	1.98	0.45
3:3:153:ILE:C	3:3:155:PRO:HD2	2.41	0.45
5:A:494:ALA:O	5:A:499:ALA:N	2.49	0.45
5:A:564:PRO:HG3	8:D:137:GLN:HG2	1.98	0.45
5:A:706:LYS:HE2	15:B:1228:CLA:HED1	1.98	0.45
24:A:1011:CL0:H10	24:A:1011:CL0:H72	1.31	0.45
15:A:1102:CLA:HED2	15:A:1102:CLA:H2A	1.99	0.45
15:A:1140:CLA:H61	15:A:1140:CLA:H41	1.47	0.45
6:B:87:PRO:HB2	6:B:117:ALA:HB3	1.98	0.45
6:B:306:LEU:O	6:B:320:HIS:HB2	2.17	0.45
15:B:1023:CLA:H3A	15:B:1023:CLA:CGA	2.46	0.45
10:F:83:THR:CG2	10:F:84:PRO:HD2	2.47	0.45
16:2:609:CHL:HBD	16:2:609:CHL:HAA2	1.99	0.45
3:3:246:ALA:HB2	12:3:501:LUT:C20	2.40	0.45
15:3:605:CLA:HAC1	15:3:612:CLA:HBC2	1.98	0.45
12:4:501:LUT:H15	12:4:501:LUT:H201	1.79	0.45
5:A:283:ASN:OD1	5:A:284:PRO:HD2	2.17	0.45
5:A:300:ALA:HA	15:A:1115:CLA:HMC1	1.98	0.45
6:B:105:PHE:O	6:B:113:PRO:HA	2.17	0.45
15:B:1021:CLA:H3A	15:B:1021:CLA:HBA1	1.30	0.45
15:B:1211:CLA:HMA3	14:B:4003:BCR:C27	2.44	0.45
9:E:74:VAL:HG21	9:E:124:ILE:HG21	1.98	0.45
11:J:18:TRP:O	11:J:19:ALA:HB3	2.17	0.45
15:1:605:CLA:H2A	15:1:605:CLA:O1D	2.17	0.45
15:1:615:CLA:HMB1	15:1:615:CLA:CBB	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:502:XAT:H203	15:2:605:CLA:HMA1	1.98	0.45
15:3:606:CLA:HMA2	15:3:613:CLA:CHD	2.46	0.45
4:4:176:ALA:HA	15:4:606:CLA:CAB	2.43	0.45
5:A:57:HIS:CD2	15:A:1103:CLA:HBB2	2.51	0.45
5:A:256:SER:OG	5:A:274:ASP:HB2	2.17	0.45
5:A:443:TRP:CE2	15:A:1130:CLA:HAB	2.52	0.45
5:A:654:SER:O	5:A:658:ILE:HG12	2.17	0.45
15:A:1129:CLA:HMB3	15:A:1129:CLA:CBB	2.47	0.45
6:B:498:TRP:CD1	15:B:1231:CLA:HED3	2.51	0.45
6:B:510:PHE:CE1	15:B:1223:CLA:HBC2	2.52	0.45
9:E:93:VAL:HG22	9:E:102:VAL:HG22	1.99	0.45
3:3:139:ILE:HG12	3:3:140:PRO:HD2	1.98	0.45
5:A:217:GLN:NE2	15:A:1117:CLA:O1D	2.50	0.45
5:A:357:LEU:C	5:A:405:ALA:HB2	2.42	0.45
24:A:1011:CL0:CBC	6:B:626:TRP:HB2	2.47	0.45
6:B:381:GLY:C	6:B:584:MET:HE3	2.42	0.45
13:3:502:XAT:H42	15:3:606:CLA:C1B	2.47	0.45
4:4:331:THR:HG23	4:4:331:THR:O	2.16	0.45
5:A:681:PHE:O	5:A:684:MET:HB3	2.16	0.45
15:A:1106:CLA:HMC2	15:A:1107:CLA:HHD	1.99	0.45
15:B:1214:CLA:HBA2	15:B:1223:CLA:HBB2	1.98	0.45
25:B:2002:PQN:H261	25:B:2002:PQN:H222	1.62	0.45
8:D:208:GLU:HB2	8:D:210:PHE:CE1	2.52	0.45
10:F:186:ILE:HG13	10:F:190:LYS:NZ	2.31	0.45
1:1:77:ILE:HG23	15:1:611:CLA:HED3	1.99	0.44
2:2:233:PHE:CZ	13:2:502:XAT:H30	2.52	0.44
3:3:117:ALA:HB1	3:3:243:GLY:CA	2.36	0.44
3:3:200:LEU:HG	3:3:200:LEU:O	2.17	0.44
3:3:202:LEU:HD22	3:3:205:LEU:HD12	1.99	0.44
4:4:172:TRP:CH2	14:4:503:BCR:H371	2.50	0.44
4:4:234:LEU:HD23	4:4:234:LEU:C	2.42	0.44
4:4:325:VAL:HG13	4:4:328:PRO:HD2	1.98	0.44
5:A:684:MET:HB2	15:A:1013:CLA:CHC	2.47	0.44
15:A:1013:CLA:HMA2	15:A:1013:CLA:HBA2	1.99	0.44
15:A:1013:CLA:CMA	15:A:1013:CLA:HBA2	2.46	0.44
15:A:1106:CLA:CAB	14:J:4001:BCR:H363	2.47	0.44
6:B:175:ARG:HB2	15:B:1210:CLA:HBC3	1.99	0.44
15:B:1209:CLA:HBB1	15:B:1209:CLA:HMB3	1.98	0.44
9:E:91:VAL:CG2	9:E:105:ARG:HB2	2.47	0.44
10:F:101:VAL:O	10:F:104:LYS:HG2	2.16	0.44
15:1:611:CLA:HBC2	15:1:611:CLA:HMC3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:503:BCR:H271	15:2:606:CLA:NB	2.32	0.44
4:4:216:ALA:O	4:4:219:GLU:HB3	2.16	0.44
14:A:4005:BCR:C11	14:A:4005:BCR:C35	2.96	0.44
6:B:219:HIS:ND1	6:B:220:PRO:O	2.49	0.44
6:B:277:HIS:O	6:B:281:ILE:HG12	2.17	0.44
6:B:438:TYR:HB3	6:B:617:LEU:HG	1.98	0.44
6:B:663:MET:HA	15:B:1023:CLA:C2C	2.47	0.44
15:B:1240:CLA:HBA1	17:B:5001:LHG:HC41	1.99	0.44
8:D:128:ASN:OD1	8:D:129:LEU:N	2.51	0.44
8:D:132:PHE:HB3	8:D:137:GLN:OE1	2.17	0.44
8:D:157:ARG:NE	8:D:167:LEU:HB2	2.31	0.44
1:1:71:TYR:CB	15:1:604:CLA:HMA1	2.45	0.44
15:3:606:CLA:HBC2	15:3:606:CLA:HHD	1.99	0.44
5:A:704:HIS:CE1	15:A:1139:CLA:HAC1	2.52	0.44
15:A:1013:CLA:HMD1	6:B:579:LEU:HB3	1.99	0.44
6:B:593:PHE:HE2	15:B:1021:CLA:H61	1.82	0.44
6:B:646:VAL:O	6:B:650:THR:HG23	2.18	0.44
15:B:1219:CLA:HBC2	15:B:1220:CLA:CGA	2.48	0.44
8:D:141:LEU:HD13	8:D:141:LEU:C	2.43	0.44
10:F:186:ILE:HG13	10:F:190:LYS:HZ3	1.82	0.44
1:1:33:ARG:HH11	1:1:55:ASN:HB2	1.82	0.44
15:3:608:CLA:CBB	15:3:608:CLA:HHC	2.47	0.44
5:A:282:LEU:HB3	5:A:289:LEU:HD23	1.99	0.44
5:A:282:LEU:HD11	5:A:515:VAL:HG11	1.98	0.44
5:A:604:SER:HA	5:A:607:ILE:HG12	1.98	0.44
15:A:1013:CLA:H42	15:A:1013:CLA:HMA1	1.99	0.44
15:A:1128:CLA:HMB3	15:A:1128:CLA:CBB	2.45	0.44
15:A:1139:CLA:CMB	15:A:1139:CLA:HBB1	2.48	0.44
6:B:292:TYR:CE1	6:B:302:LEU:HD21	2.53	0.44
1:1:83:MET:O	12:1:501:LUT:H15	2.17	0.44
2:2:162:PHE:CE2	16:2:613:CHL:HMB2	2.52	0.44
2:2:235:GLY:O	2:2:239:GLN:CB	2.66	0.44
3:3:145:VAL:HG22	3:3:146:ASP:N	2.33	0.44
4:4:258:GLY:HA2	16:4:611:CHL:HMD2	1.99	0.44
5:A:695:GLU:HB3	6:B:537:LYS:NZ	2.32	0.44
23:B:5031:GSH:HN2	23:B:5031:GSH:C1	2.30	0.44
10:F:79:ILE:HG21	10:F:154:LEU:HD12	2.00	0.44
10:F:82:LEU:HB3	10:F:139:LEU:HB3	1.99	0.44
14:2:503:BCR:C8	14:2:503:BCR:H321	2.48	0.44
15:2:612:CLA:H12	18:2:802:LMG:HC72	2.00	0.44
12:3:501:LUT:H35	12:3:501:LUT:H401	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:392:THR:HG22	5:A:396:TRP:CD1	2.52	0.44
5:A:515:VAL:O	5:A:522:ALA:N	2.51	0.44
5:A:661:TYR:HA	5:A:666:SER:HB3	1.98	0.44
5:A:694:GLN:HG2	6:B:547:LEU:HD12	1.99	0.44
24:A:1011:CL0:CGD	24:A:1011:CL0:H8	2.47	0.44
6:B:30:HIS:HD2	15:B:1202:CLA:HBB2	1.82	0.44
15:B:1235:CLA:C4A	15:B:1235:CLA:HBA2	2.45	0.44
16:1:609:CHL:HAA1	4:4:228:THR:CG2	2.46	0.44
12:4:501:LUT:H32	15:4:601:CLA:HAB	1.99	0.44
14:4:503:BCR:C23	14:4:503:BCR:H403	2.48	0.44
5:A:32:PRO:HB2	5:A:48:TRP:HH2	1.83	0.44
5:A:34:HIS:HA	5:A:40:ALA:HB2	2.00	0.44
5:A:262:ALA:HB3	5:A:263:PRO:HD3	1.99	0.44
5:A:276:LEU:HD21	5:A:299:LEU:HD12	1.99	0.44
25:A:2001:PQN:H111	25:A:2001:PQN:H2M1	1.82	0.44
6:B:395:PHE:CZ	6:B:409:LEU:HD11	2.52	0.44
9:E:73:LEU:HA	9:E:89:LYS:HA	1.99	0.44
10:F:155:ALA:HB1	10:F:161:ALA:HA	1.98	0.44
14:J:4001:BCR:H351	14:J:4001:BCR:H15C	1.80	0.44
1:1:166:ASP:OD1	1:1:167:PRO:HD2	2.18	0.44
12:1:501:LUT:H31	12:1:501:LUT:H403	1.79	0.44
3:3:223:ALA:C	15:3:601:CLA:H11	2.43	0.44
4:4:128:TYR:CE1	15:4:609:CLA:HMA2	2.53	0.44
5:A:261:LEU:HG	5:A:261:LEU:O	2.18	0.44
5:A:313:ARG:HB2	5:A:319:GLY:C	2.43	0.44
6:B:439:VAL:CG1	15:B:1230:CLA:HAC1	2.48	0.44
9:E:91:VAL:HG23	9:E:105:ARG:HB2	2.00	0.44
3:3:121:MET:CG	3:3:243:GLY:HA2	2.48	0.44
15:3:607:CLA:HBA1	15:3:607:CLA:O2D	2.18	0.44
5:A:214:ALA:O	5:A:218:ILE:HG13	2.18	0.44
5:A:580:ARG:HB2	7:C:77:LEU:C	2.43	0.44
5:A:682:SER:CB	5:A:730:HIS:HB2	2.47	0.44
6:B:456:ILE:HG23	10:F:150:SER:OG	2.18	0.44
15:B:1023:CLA:H3A	15:B:1023:CLA:C1	2.47	0.44
1:1:113:PRO:HG2	1:1:120:VAL:CG1	2.47	0.43
4:4:150:LEU:CD2	10:F:213:GLN:HA	2.47	0.43
4:4:214:THR:O	4:4:218:ILE:HG23	2.18	0.43
15:4:615:CLA:H11	15:4:615:CLA:H51	1.79	0.43
6:B:69:VAL:HG11	6:B:125:TRP:HZ3	1.82	0.43
6:B:134:GLN:O	6:B:138:VAL:HG23	2.18	0.43
6:B:463:TRP:CG	15:F:1302:CLA:HMA1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:499:LEU:HA	6:B:502:ILE:HG22	1.99	0.43
6:B:585:LEU:HD22	6:B:714:PHE:CD2	2.53	0.43
15:B:1226:CLA:HBB1	15:B:1226:CLA:HMB1	1.99	0.43
8:D:100:PHE:CZ	8:D:158:VAL:HG21	2.53	0.43
8:D:105:TRP:CZ2	8:D:123:MET:HE3	2.53	0.43
8:D:190:ARG:HH22	8:D:210:PHE:CB	2.31	0.43
1:1:153:TYR:CE2	1:1:174:LYS:HE3	2.53	0.43
16:1:609:CHL:H2A	16:1:609:CHL:O1D	2.17	0.43
16:2:609:CHL:HMD1	14:3:503:BCR:HC42	1.99	0.43
4:4:192:VAL:HG12	4:4:194:LEU:HG	2.00	0.43
4:4:205:TYR:CD2	4:4:206:PRO:HD3	2.53	0.43
4:4:264:PHE:CZ	4:4:268:GLY:HA3	2.52	0.43
15:A:1110:CLA:HBA1	15:A:1110:CLA:CHA	2.48	0.43
6:B:88:ILE:HG23	6:B:114:VAL:HB	2.00	0.43
6:B:438:TYR:HD2	15:B:1021:CLA:H203	1.83	0.43
6:B:449:THR:HB	6:B:451:GLU:OE2	2.18	0.43
15:B:1235:CLA:H52	15:B:1235:CLA:H8	1.85	0.43
15:B:1239:CLA:CBC	25:B:2002:PQN:H2M2	2.46	0.43
1:1:154:PRO:HG3	15:1:611:CLA:HMD1	1.99	0.43
15:1:604:CLA:CMB	15:1:604:CLA:HBB1	2.48	0.43
2:2:108:VAL:HG11	2:2:169:ARG:HH12	1.80	0.43
12:3:501:LUT:C28	12:3:501:LUT:H361	2.48	0.43
15:3:605:CLA:HMD3	15:3:612:CLA:C4D	2.49	0.43
5:A:197:MET:HB3	15:A:1123:CLA:HMD1	1.99	0.43
5:A:728:VAL:HG22	5:A:732:LEU:HD13	2.00	0.43
15:A:1012:CLA:C4	6:B:439:VAL:HA	2.48	0.43
15:A:1124:CLA:HAA1	15:A:1125:CLA:CAD	2.47	0.43
15:A:1126:CLA:O1D	15:A:1127:CLA:HMA1	2.18	0.43
6:B:691:LEU:O	6:B:692:VAL:C	2.62	0.43
15:B:1210:CLA:O1A	14:B:4002:BCR:H372	2.17	0.43
8:D:105:TRP:CE3	8:D:107:SER:HB3	2.53	0.43
8:D:138:CYS:O	8:D:142:THR:HG23	2.18	0.43
16:1:609:CHL:HED3	4:4:228:THR:O	2.19	0.43
15:3:605:CLA:HMD1	15:3:612:CLA:C1D	2.49	0.43
5:A:71:ARG:CD	5:A:185:ALA:HB1	2.46	0.43
5:A:352:GLN:HG3	5:A:356:ASN:HD21	1.82	0.43
5:A:531:SER:HB3	5:A:639:ALA:HB3	1.99	0.43
5:A:698:GLU:CD	6:B:546:LYS:HB3	2.43	0.43
15:A:1110:CLA:CED	15:A:1111:CLA:HHC	2.35	0.43
6:B:5:LEU:CD1	6:B:6:PHE:H	2.12	0.43
6:B:662:PHE:CD2	15:B:1022:CLA:HMD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:79:THR:HG23	8:D:80:PRO:HD2	2.00	0.43
10:F:230:LEU:HG	10:F:231:LEU:HD12	1.99	0.43
1:1:83:MET:CE	15:1:601:CLA:CAB	2.96	0.43
15:1:603:CLA:CHD	15:1:615:CLA:HAB	2.49	0.43
2:2:104:GLN:HA	2:2:107:LEU:HD12	2.01	0.43
3:3:143:THR:O	15:3:606:CLA:HED2	2.19	0.43
12:4:501:LUT:H183	15:4:603:CLA:C3B	2.48	0.43
15:4:601:CLA:HBC2	16:4:611:CHL:O1A	2.17	0.43
5:A:598:TRP:CZ3	15:B:1022:CLA:HAB	2.53	0.43
5:A:610:PHE:O	5:A:614:MET:HG2	2.19	0.43
5:A:647:ARG:HA	6:B:633:ILE:HG21	2.00	0.43
5:A:700:ILE:HD13	15:A:1138:CLA:CMD	2.46	0.43
15:A:1012:CLA:C14	14:J:4001:BCR:H14C	2.48	0.43
6:B:118:THR:N	15:B:1205:CLA:OBD	2.47	0.43
6:B:258:PHE:CD1	15:B:1214:CLA:CMB	3.01	0.43
2:2:134:PRO:HB3	2:2:142:GLU:OE2	2.18	0.43
5:A:316:TRP:CZ3	15:A:1118:CLA:HAA1	2.54	0.43
6:B:339:LEU:HD21	15:B:1226:CLA:HAB	2.01	0.43
10:F:230:LEU:HD23	10:F:230:LEU:H	1.84	0.43
14:1:505:BCR:H281	15:4:605:CLA:HAC2	2.01	0.43
2:2:204:ASP:OD1	15:2:601:CLA:HBA2	2.18	0.43
2:2:223:VAL:O	2:2:227:ARG:HG3	2.19	0.43
3:3:186:GLN:HB2	3:3:194:GLN:NE2	2.33	0.43
3:3:282:THR:N	15:3:603:CLA:CED	2.82	0.43
14:3:503:BCR:H402	15:3:606:CLA:NB	2.33	0.43
4:4:285:LEU:HG	12:4:501:LUT:H191	2.00	0.43
15:4:608:CLA:HMB1	15:4:608:CLA:CBB	2.41	0.43
5:A:25:ASN:OD1	5:A:26:PHE:N	2.51	0.43
5:A:371:MET:HE1	15:A:1127:CLA:O1D	2.18	0.43
6:B:175:ARG:HH11	15:B:1221:CLA:CMD	2.32	0.43
11:J:1:MET:O	11:J:5:THR:HG23	2.19	0.43
12:2:501:LUT:H24	15:2:603:CLA:HMA1	2.00	0.43
3:3:250:MET:HG2	13:3:502:XAT:C12	2.34	0.43
4:4:126:LEU:HD12	4:4:145:TYR:O	2.18	0.43
4:4:166:GLU:HG3	15:4:604:CLA:CHB	2.47	0.43
4:4:273:SER:N	4:4:274:PRO:CD	2.82	0.43
4:4:296:THR:O	4:4:298:ALA:N	2.52	0.43
5:A:241:HIS:CE1	5:A:242:GLU:HG3	2.53	0.43
15:B:1229:CLA:HBB1	15:B:1229:CLA:CMB	2.48	0.43
1:1:57:ASP:HB2	15:1:604:CLA:HBA2	2.01	0.43
1:1:218:PHE:HB3	15:1:603:CLA:O2A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:612:CLA:HBA1	19:1:811:SQD:C7	2.49	0.43
12:3:501:LUT:H27	12:3:501:LUT:H381	1.86	0.43
4:4:178:VAL:HG21	12:4:501:LUT:C40	2.49	0.43
5:A:392:THR:HG23	5:A:607:ILE:HG21	1.99	0.43
25:A:2001:PQN:H191	25:A:2001:PQN:H211	1.55	0.43
10:F:163:GLU:HA	11:J:38:VAL:HG23	2.00	0.43
3:3:176:ALA:HB1	14:3:503:BCR:C17	2.48	0.43
14:3:503:BCR:H351	14:3:503:BCR:H15C	1.70	0.43
15:4:615:CLA:HBC1	21:4:811:DGD:C1B	2.49	0.43
5:A:26:PHE:HD2	11:J:4:PHE:HB2	1.84	0.43
5:A:78:PHE:CZ	15:A:1108:CLA:HBB1	2.54	0.43
5:A:119:TRP:CD2	14:J:4002:BCR:HC41	2.53	0.43
5:A:358:ALA:HB2	14:A:4005:BCR:H382	1.99	0.43
15:A:1103:CLA:H61	14:A:4003:BCR:H402	2.00	0.43
15:A:1136:CLA:HMB1	15:A:1136:CLA:CBB	2.45	0.43
11:J:18:TRP:CZ3	11:J:19:ALA:HB2	2.54	0.43
15:1:605:CLA:HED1	15:1:612:CLA:H11	2.01	0.42
2:2:109:HIS:CD2	15:2:612:CLA:CMD	3.01	0.42
2:2:140:GLY:O	16:2:610:CHL:HMD1	2.19	0.42
14:3:503:BCR:C15	15:3:611:CLA:HMB2	2.48	0.42
15:3:612:CLA:H2A	15:3:612:CLA:CED	2.49	0.42
5:A:233:ASP:HB3	5:A:236:GLU:HG2	2.01	0.42
5:A:299:LEU:HD21	15:A:1113:CLA:HMC2	2.00	0.42
5:A:450:PHE:CZ	15:B:1023:CLA:H51	2.54	0.42
5:A:531:SER:O	5:A:535:VAL:HG23	2.18	0.42
5:A:577:GLY:HA2	6:B:563:PRO:HD3	2.00	0.42
15:A:1108:CLA:H2A	15:A:1108:CLA:HED2	2.01	0.42
6:B:129:GLY:O	6:B:130:LEU:HG	2.18	0.42
6:B:453:GLN:NE2	10:F:145:LEU:HD13	2.33	0.42
6:B:460:PHE:HB2	15:B:1235:CLA:OBD	2.19	0.42
6:B:664:PHE:CZ	15:B:1239:CLA:HBC3	2.54	0.42
15:B:1211:CLA:H43	14:B:4003:BCR:C17	2.49	0.42
15:B:1226:CLA:CED	15:B:1226:CLA:H2A	2.49	0.42
15:B:1239:CLA:H141	15:B:1239:CLA:H161	1.63	0.42
8:D:123:MET:HE1	8:D:130:LEU:HD11	1.99	0.42
1:1:47:LEU:HA	1:1:50:LEU:HD12	2.01	0.42
1:1:80:ARG:HB3	15:1:601:CLA:HBC3	1.98	0.42
15:1:601:CLA:HMB2	15:1:601:CLA:H42	2.01	0.42
16:1:609:CHL:HAA1	4:4:228:THR:OG1	2.19	0.42
16:2:613:CHL:OMC	16:2:613:CHL:HAC2	2.18	0.42
4:4:150:LEU:HD22	10:F:213:GLN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:503:BCR:H15C	14:4:503:BCR:H351	1.60	0.42
5:A:427:LEU:O	5:A:431:ILE:HG13	2.19	0.42
5:A:535:VAL:HG11	5:A:609:HIS:CG	2.54	0.42
5:A:561:ARG:NE	8:D:90:GLY:H	2.17	0.42
5:A:670:LEU:HD12	15:A:1107:CLA:HAC1	2.00	0.42
6:B:91:ALA:C	6:B:92:ILE:HD12	2.45	0.42
6:B:345:ILE:O	6:B:349:VAL:HG23	2.19	0.42
6:B:456:ILE:HD13	10:F:148:LEU:HB2	2.01	0.42
8:D:168:HIS:HA	8:D:169:PRO:HA	1.67	0.42
1:1:103:ALA:HA	15:1:606:CLA:CED	2.32	0.42
14:1:505:BCR:H17C	15:4:612:CLA:HMB2	1.99	0.42
2:2:206:MET:O	2:2:208:MET:N	2.52	0.42
15:2:605:CLA:HAC1	15:2:612:CLA:CGA	2.48	0.42
4:4:264:PHE:HD2	4:4:266:PRO:O	2.02	0.42
5:A:494:ALA:HB3	5:A:495:PRO:HD3	2.01	0.42
5:A:598:TRP:HZ2	15:B:1023:CLA:ND	2.16	0.42
5:A:680:ALA:O	15:A:1013:CLA:HAB	2.18	0.42
15:A:1101:CLA:CGA	25:A:2001:PQN:H222	2.49	0.42
15:A:1106:CLA:CAD	15:A:1126:CLA:HAA2	2.50	0.42
6:B:61:TRP:CG	15:B:1203:CLA:HBC1	2.54	0.42
6:B:235:ALA:HB2	6:B:256:LEU:O	2.19	0.42
6:B:581:VAL:O	6:B:585:LEU:HD13	2.19	0.42
8:D:179:ASN:O	8:D:180:ALA:C	2.62	0.42
9:E:90:VAL:HG11	9:E:93:VAL:HG23	2.01	0.42
1:1:183:LEU:HD11	15:1:607:CLA:HHD	2.01	0.42
13:1:502:XAT:H15	13:1:502:XAT:H201	1.71	0.42
2:2:107:LEU:HD13	2:2:198:TYR:HE1	1.83	0.42
3:3:154:PRO:CG	3:3:155:PRO:HD3	2.46	0.42
3:3:243:GLY:O	3:3:247:MET:HG3	2.19	0.42
24:A:1011:CL0:H22	6:B:626:TRP:CD1	2.55	0.42
6:B:316:LEU:O	6:B:411:ARG:NE	2.52	0.42
12:2:501:LUT:H201	12:2:501:LUT:H15	1.69	0.42
3:3:147:TRP:HE1	3:3:264:PRO:HD3	1.84	0.42
3:3:153:ILE:O	3:3:153:ILE:HG22	2.20	0.42
3:3:237:LEU:HD12	3:3:238:ASN:N	2.33	0.42
3:3:271:HIS:HE1	15:3:608:CLA:C2C	2.32	0.42
4:4:172:TRP:CZ2	16:4:613:CHL:HMB3	2.55	0.42
5:A:341:LEU:O	5:A:344:ILE:HB	2.19	0.42
24:A:1011:CL0:H15	24:A:1011:CL0:CMB	2.41	0.42
15:A:1012:CLA:HAA2	15:A:1012:CLA:HBD	2.00	0.42
14:A:4006:BCR:H383	14:J:4001:BCR:H322	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:17:PRO:HD2	7:C:73:SER:HA	2.01	0.42
6:B:118:THR:HA	6:B:368:THR:HG22	2.01	0.42
6:B:175:ARG:HE	15:B:1221:CLA:HMD3	1.85	0.42
6:B:547:LEU:HD22	6:B:571:ILE:CD1	2.48	0.42
15:B:1021:CLA:HMB3	15:B:1022:CLA:OBD	2.19	0.42
15:B:1239:CLA:H162	15:B:1239:CLA:H193	1.73	0.42
14:B:4004:BCR:H15C	14:B:4004:BCR:H351	1.60	0.42
8:D:209:PRO:O	8:D:210:PHE:HB2	2.18	0.42
14:J:4003:BCR:C8	14:J:4003:BCR:H321	2.50	0.42
1:1:153:TYR:CZ	1:1:174:LYS:HE3	2.55	0.42
1:1:183:LEU:HD13	15:1:607:CLA:CMD	2.50	0.42
2:2:104:GLN:NE2	2:2:169:ARG:HD3	2.34	0.42
15:3:608:CLA:HBA2	15:3:608:CLA:O2D	2.20	0.42
5:A:657:VAL:HG13	5:A:658:ILE:HG23	2.00	0.42
25:A:2001:PQN:H302	25:A:2001:PQN:H261	1.83	0.42
6:B:341:SER:O	6:B:344:THR:HG22	2.20	0.42
6:B:577:PHE:O	6:B:581:VAL:HG23	2.19	0.42
16:3:604:CHL:HBB1	16:3:604:CHL:CMB	2.45	0.42
4:4:178:VAL:HG23	12:4:501:LUT:H35	2.01	0.42
5:A:84:ILE:HD13	15:A:1104:CLA:CBC	2.46	0.42
5:A:459:ASN:ND2	5:A:640:ASN:O	2.53	0.42
15:A:1107:CLA:HMB3	15:A:1107:CLA:CBB	2.40	0.42
15:A:1115:CLA:HED2	15:A:1115:CLA:H2A	2.00	0.42
15:A:1139:CLA:HBB1	15:A:1139:CLA:HMB1	2.00	0.42
25:A:2001:PQN:H172	14:B:4006:BCR:H331	2.02	0.42
6:B:258:PHE:CE2	6:B:494:TRP:CE3	3.07	0.42
6:B:453:GLN:NE2	6:B:455:LEU:HD11	2.35	0.42
6:B:586:ASN:ND2	15:B:1021:CLA:H43	2.35	0.42
15:B:1217:CLA:HHC	15:B:1217:CLA:HBB1	2.02	0.42
1:1:120:VAL:HG11	15:1:613:CLA:CMD	2.50	0.42
2:2:119:GLY:O	2:2:123:THR:HG23	2.20	0.42
2:2:198:TYR:HE2	2:2:219:LYS:HB2	1.85	0.42
3:3:120:ALA:CB	3:3:247:MET:HG2	2.49	0.42
14:3:503:BCR:H292	15:3:606:CLA:C1C	2.50	0.42
4:4:296:THR:C	4:4:298:ALA:N	2.76	0.42
5:A:81:LEU:HD11	15:A:1111:CLA:HBA2	2.02	0.42
5:A:341:LEU:HD23	5:A:344:ILE:HG13	2.02	0.42
5:A:474:ASP:H	5:A:637:GLN:HE22	1.67	0.42
6:B:87:PRO:HA	6:B:122:TYR:HE2	1.85	0.42
6:B:545:SER:C	10:F:239:VAL:HG21	2.45	0.42
15:B:1204:CLA:CBB	15:B:1204:CLA:HHC	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1229:CLA:H162	15:B:1229:CLA:H202	1.93	0.42
10:F:204:VAL:N	10:F:205:PRO:HD2	2.34	0.42
15:1:606:CLA:HMB1	15:1:606:CLA:CBB	2.48	0.42
5:A:473:SER:HB3	5:A:637:GLN:NE2	2.35	0.42
5:A:562:LEU:HD11	5:A:580:ARG:HG3	2.02	0.42
15:A:1121:CLA:HHC	15:A:1121:CLA:HBB1	2.02	0.42
15:A:1130:CLA:HBC2	15:A:1137:CLA:HMC2	2.02	0.42
6:B:352:HIS:HB3	15:B:1214:CLA:HED2	2.02	0.42
6:B:586:ASN:C	6:B:586:ASN:HD22	2.28	0.42
6:B:718:TYR:CZ	15:B:1021:CLA:HED1	2.55	0.42
8:D:105:TRP:HE1	8:D:130:LEU:HD13	1.85	0.42
1:1:118:ILE:O	1:1:118:ILE:HG22	2.19	0.42
15:1:605:CLA:HBC1	15:1:612:CLA:CBC	2.49	0.42
16:1:610:CHL:HBD	16:1:610:CHL:CBA	2.50	0.42
3:3:244:ARG:HH11	16:3:604:CHL:CHD	2.33	0.42
3:3:280:LEU:HD22	15:3:603:CLA:C4B	2.50	0.42
5:A:69:ILE:O	5:A:73:VAL:HG23	2.19	0.42
5:A:334:THR:HA	5:A:429:ARG:NE	2.34	0.42
5:A:338:HIS:HE1	15:A:1122:CLA:ND	2.18	0.42
5:A:365:ILE:HG12	5:A:395:MET:HA	2.01	0.42
5:A:436:ALA:HB2	6:B:681:TRP:CH2	2.55	0.42
24:A:1011:CL0:C3B	15:A:1012:CLA:HED2	2.50	0.42
15:A:1138:CLA:H141	15:A:1138:CLA:H162	1.85	0.42
15:A:1138:CLA:H151	15:A:1139:CLA:H43	2.01	0.42
6:B:399:TYR:CD2	6:B:401:PRO:HD3	2.55	0.42
15:B:1222:CLA:HBA2	15:B:1236:CLA:HAA1	2.01	0.42
15:B:1223:CLA:HMA3	14:B:4005:BCR:H312	2.02	0.42
10:F:184:GLN:HE21	10:F:210:LEU:HB3	1.85	0.42
1:1:71:TYR:CB	15:1:604:CLA:CMA	2.98	0.41
15:1:603:CLA:HMA1	15:1:608:CLA:HBC3	2.01	0.41
3:3:225:PHE:CD1	20:3:902:CAC:AS	3.33	0.41
15:3:606:CLA:HBA1	15:3:613:CLA:C2D	2.50	0.41
4:4:311:HIS:HA	4:4:318:VAL:HG21	2.02	0.41
12:4:501:LUT:H401	12:4:501:LUT:H35	1.83	0.41
21:4:811:DGD:HE62	21:4:811:DGD:O3E	2.20	0.41
5:A:95:GLY:HA3	5:A:148:TRP:CZ3	2.55	0.41
5:A:580:ARG:O	5:A:580:ARG:HG2	2.20	0.41
15:A:1110:CLA:HBB1	15:A:1110:CLA:CMB	2.50	0.41
15:A:1140:CLA:H91	11:J:16:LEU:CD2	2.50	0.41
15:A:1140:CLA:HBC1	14:B:4006:BCR:HC7	2.02	0.41
6:B:388:PHE:HA	14:B:4005:BCR:H382	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1228:CLA:H62	15:B:1228:CLA:H92	1.75	0.41
8:D:95:ALA:HA	8:D:99:GLU:O	2.20	0.41
15:3:608:CLA:HHC	15:3:608:CLA:HBB1	2.03	0.41
5:A:516:ALA:HB2	5:A:521:VAL:HG12	2.02	0.41
6:B:395:PHE:HZ	6:B:409:LEU:HD11	1.84	0.41
1:1:185:MET:HE1	15:1:604:CLA:HAB	2.02	0.41
1:1:206:LEU:HD12	12:1:501:LUT:H22	2.02	0.41
2:2:228:LEU:CD2	15:2:602:CLA:HAA1	2.50	0.41
12:2:501:LUT:H393	15:2:602:CLA:HBA2	2.02	0.41
4:4:174:MET:HB2	15:4:601:CLA:CMC	2.47	0.41
15:4:602:CLA:HHD	15:4:602:CLA:HBC3	2.02	0.41
5:A:85:LEU:CB	5:A:170:ALA:HB2	2.50	0.41
6:B:277:HIS:HB2	15:B:1214:CLA:CHB	2.50	0.41
6:B:659:ALA:HB1	15:B:1023:CLA:HAB	2.02	0.41
12:2:501:LUT:H11	12:2:501:LUT:H191	1.67	0.41
4:4:218:ILE:C	4:4:218:ILE:HD12	2.45	0.41
15:4:601:CLA:NA	15:4:601:CLA:HBA1	2.30	0.41
5:A:74:PHE:HB2	5:A:191:PHE:HE1	1.86	0.41
5:A:97:ARG:HA	5:A:160:TYR:HH	1.86	0.41
5:A:129:GLY:N	5:A:137:GLY:O	2.53	0.41
5:A:441:LEU:HB3	5:A:548:LEU:HD13	2.02	0.41
5:A:687:PHE:HE1	6:B:666:ILE:HG13	1.86	0.41
15:A:1139:CLA:H52	15:A:1139:CLA:H11	1.88	0.41
14:A:4007:BCR:HC31	6:B:649:TRP:CZ3	2.55	0.41
6:B:426:VAL:O	6:B:430:LEU:HD23	2.20	0.41
8:D:204:PHE:O	8:D:205:THR:C	2.63	0.41
10:F:148:LEU:HD13	10:F:163:GLU:OE1	2.21	0.41
15:1:615:CLA:HED2	15:1:615:CLA:H2A	2.02	0.41
2:2:199:PRO:HD2	15:2:601:CLA:O2D	2.21	0.41
2:2:203:PHE:HB2	15:2:601:CLA:OBD	2.21	0.41
3:3:110:GLN:O	3:3:113:GLU:HG2	2.19	0.41
3:3:158:VAL:HG13	3:3:158:VAL:O	2.20	0.41
5:A:282:LEU:HA	5:A:290:TRP:CZ3	2.56	0.41
5:A:479:LEU:HB2	5:A:530:THR:HG23	2.01	0.41
15:A:1125:CLA:HBB1	15:A:1125:CLA:CHC	2.41	0.41
15:A:1132:CLA:HMD1	15:B:1206:CLA:CBB	2.50	0.41
14:A:4007:BCR:HC31	6:B:649:TRP:HZ3	1.85	0.41
6:B:175:ARG:HB2	15:B:1210:CLA:CBC	2.50	0.41
6:B:175:ARG:HD3	15:B:1210:CLA:HBC2	2.03	0.41
15:B:1216:CLA:HMB2	15:B:1221:CLA:CED	2.49	0.41
3:3:111:TYR:CD1	3:3:213:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:279:ASN:HB3	3:3:280:LEU:H	1.79	0.41
4:4:205:TYR:N	4:4:206:PRO:CD	2.83	0.41
4:4:272:THR:HG23	4:4:272:THR:O	2.20	0.41
5:A:516:ALA:HA	5:A:522:ALA:H	1.86	0.41
5:A:602:SER:O	5:A:606:VAL:HG23	2.21	0.41
5:A:653:GLN:O	5:A:746:ARG:HD3	2.20	0.41
24:A:1011:CL0:H13	15:A:1012:CLA:HMD3	2.03	0.41
6:B:191:TRP:NE1	6:B:195:LEU:HD11	2.35	0.41
6:B:255:ILE:HG13	6:B:256:LEU:N	2.36	0.41
15:B:1234:CLA:HHC	15:B:1234:CLA:CBB	2.50	0.41
1:1:103:ALA:HB3	1:1:104:PRO:CD	2.51	0.41
1:1:130:VAL:HA	1:1:133:VAL:HG22	2.03	0.41
14:3:504:BCR:H313	15:3:612:CLA:H43	2.02	0.41
4:4:226:VAL:HG11	16:4:611:CHL:C1B	2.51	0.41
5:A:63:THR:HG23	5:A:65:ASP:H	1.86	0.41
5:A:447:PHE:O	5:A:451:HIS:ND1	2.44	0.41
5:A:603:LEU:O	5:A:607:ILE:HG23	2.21	0.41
15:A:1013:CLA:H41	15:A:1013:CLA:H61	1.67	0.41
15:A:1110:CLA:C4D	15:A:1110:CLA:HED2	2.49	0.41
15:A:1124:CLA:H2	15:A:1125:CLA:CED	2.46	0.41
6:B:312:PRO:HG2	17:B:5001:LHG:HC31	2.03	0.41
6:B:404:ASN:OD1	6:B:407:ASN:ND2	2.53	0.41
15:B:1023:CLA:HMB3	15:B:1023:CLA:CBB	2.42	0.41
15:B:1205:CLA:H2A	15:B:1205:CLA:O2D	2.21	0.41
15:B:1211:CLA:H11	14:B:4003:BCR:H21C	2.02	0.41
15:B:1239:CLA:HHC	15:B:1239:CLA:CBB	2.50	0.41
11:J:2:LYS:HE2	11:J:2:LYS:HB3	1.87	0.41
1:1:72:ARG:HE	1:1:152:LEU:CD1	2.34	0.41
16:1:610:CHL:HBC2	15:1:613:CLA:CMC	2.50	0.41
2:2:230:MET:SD	15:2:604:CLA:HMC3	2.61	0.41
16:2:609:CHL:C2D	14:3:503:BCR:H312	2.51	0.41
13:3:502:XAT:H381	13:3:502:XAT:C28	2.31	0.41
12:4:501:LUT:H183	15:4:603:CLA:C4B	2.51	0.41
5:A:39:LEU:C	5:A:48:TRP:HE1	2.26	0.41
24:A:1011:CL0:CMA	24:A:1011:CL0:H10	2.41	0.41
6:B:55:LEU:O	6:B:59:PHE:HD2	2.04	0.41
6:B:196:VAL:HG23	6:B:197:HIS:ND1	2.35	0.41
6:B:388:PHE:CG	6:B:535:LEU:HD13	2.55	0.41
6:B:429:PHE:CD2	15:B:1235:CLA:HAB	2.55	0.41
15:B:1222:CLA:C2	15:B:1234:CLA:HMA3	2.50	0.41
10:F:186:ILE:O	10:F:190:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:502:XAT:H11	13:1:502:XAT:H191	1.92	0.41
13:1:502:XAT:H31	13:1:502:XAT:H391	1.82	0.41
2:2:110:CYS:CB	2:2:226:GLY:HA3	2.49	0.41
2:2:208:MET:HE1	15:2:601:CLA:H43	2.03	0.41
15:4:604:CLA:H3A	15:4:604:CLA:HBA2	1.30	0.41
16:4:613:CHL:OMC	16:4:613:CHL:HAC2	2.19	0.41
15:4:615:CLA:HED3	15:J:1302:CLA:C3	2.51	0.41
5:A:325:ILE:HG23	5:A:329:HIS:HE1	1.85	0.41
5:A:446:ILE:HG23	5:A:450:PHE:CE2	2.56	0.41
5:A:509:THR:HA	5:A:525:PRO:HA	2.03	0.41
5:A:578:PRO:HD3	6:B:562:GLY:HA2	2.03	0.41
5:A:644:GLY:HA2	5:A:647:ARG:HB3	2.03	0.41
5:A:665:LEU:HD22	5:A:668:TYR:CE2	2.56	0.41
5:A:673:LEU:HB3	15:A:1012:CLA:C2	2.50	0.41
5:A:702:TRP:CH2	6:B:418:ALA:HB2	2.56	0.41
15:A:1138:CLA:H143	15:A:1139:CLA:H43	2.03	0.41
14:A:4005:BCR:C8	14:A:4005:BCR:H331	2.51	0.41
14:A:4006:BCR:H15C	14:A:4006:BCR:H351	1.86	0.41
6:B:5:LEU:HD12	6:B:21:ARG:NH1	2.36	0.41
6:B:102:VAL:HA	6:B:113:PRO:HG3	2.03	0.41
6:B:131:ARG:HD2	6:B:207:HIS:ND1	2.35	0.41
6:B:206:GLN:HB3	6:B:208:VAL:HG23	2.02	0.41
6:B:263:HIS:HD1	6:B:266:THR:H	1.68	0.41
15:B:1229:CLA:HAB	15:B:1230:CLA:HMB1	2.01	0.41
15:B:1230:CLA:HBA2	14:B:4006:BCR:H271	2.01	0.41
15:B:1239:CLA:O1A	25:B:2002:PQN:H271	2.20	0.41
7:C:55:GLU:OE2	7:C:66:ARG:HA	2.21	0.41
8:D:129:LEU:C	8:D:130:LEU:HD12	2.45	0.41
11:J:21:PHE:HE1	14:J:4003:BCR:HC21	1.85	0.41
15:J:1302:CLA:HAC1	14:J:4002:BCR:H10C	2.02	0.41
2:2:232:ALA:HB2	12:2:501:LUT:H392	2.02	0.41
16:2:613:CHL:HAA2	16:2:613:CHL:CBD	2.50	0.41
3:3:152:VAL:HG23	15:3:610:CLA:C1D	2.51	0.41
3:3:234:LYS:O	3:3:237:LEU:HG	2.22	0.41
3:3:271:HIS:CE1	15:3:608:CLA:C2C	3.04	0.41
15:4:604:CLA:H43	10:F:219:LEU:HD22	2.03	0.41
15:4:604:CLA:HHC	15:4:604:CLA:CBB	2.51	0.41
5:A:130:ASP:OD2	10:F:105:ARG:HD3	2.21	0.41
5:A:442:ASN:ND2	15:B:1023:CLA:HED1	2.36	0.41
5:A:466:GLY:HA3	6:B:641:MET:HE2	2.02	0.41
5:A:679:TRP:CH2	5:A:683:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1109:CLA:HBA1	15:A:1109:CLA:CBD	2.51	0.41
14:A:4002:BCR:C6	14:A:4002:BCR:C34	2.99	0.41
6:B:341:SER:HA	6:B:344:THR:HG22	2.03	0.41
6:B:422:HIS:CE1	15:B:1227:CLA:HMB2	2.56	0.41
6:B:423:LEU:HD21	15:B:1236:CLA:CMB	2.50	0.41
6:B:441:ASN:CB	6:B:616:TYR:HB3	2.51	0.41
6:B:601:THR:HG21	6:B:610:PHE:HB2	2.03	0.41
15:B:1225:CLA:HBB1	15:B:1225:CLA:CHC	2.42	0.41
15:B:1228:CLA:HBC2	15:B:1236:CLA:HMC3	2.03	0.41
8:D:141:LEU:CD1	8:D:145:LEU:HD11	2.51	0.41
10:F:166:ILE:CD1	10:F:167:PRO:HD3	2.50	0.41
16:2:609:CHL:CED	3:3:182:LEU:HB3	2.52	0.40
3:3:280:LEU:O	15:3:603:CLA:HMA3	2.21	0.40
4:4:158:ARG:NE	10:F:223:GLN:HG3	2.36	0.40
5:A:35:PHE:HB2	5:A:62:HIS:CG	2.56	0.40
5:A:140:ILE:HD12	5:A:140:ILE:C	2.46	0.40
5:A:483:PHE:O	5:A:487:ILE:HG12	2.21	0.40
5:A:526:ILE:HG12	5:A:618:VAL:CG2	2.51	0.40
5:A:669:GLY:O	5:A:672:PHE:HB3	2.21	0.40
5:A:675:ALA:CB	5:A:737:ALA:HB3	2.51	0.40
15:A:1115:CLA:HMB1	15:A:1115:CLA:CBB	2.52	0.40
6:B:30:HIS:HD2	15:B:1202:CLA:CBB	2.33	0.40
6:B:374:THR:HG22	15:B:1224:CLA:CAB	2.51	0.40
15:B:1021:CLA:CAB	15:B:1022:CLA:HED3	2.51	0.40
15:B:1227:CLA:HBC2	14:B:4004:BCR:H393	2.04	0.40
9:E:94:ASP:HB3	9:E:101:PRO:HA	2.03	0.40
15:3:601:CLA:CBB	15:3:601:CLA:HHC	2.51	0.40
14:4:505:BCR:C8	14:4:505:BCR:H321	2.51	0.40
5:A:234:PRO:HA	5:A:237:ILE:HD12	2.04	0.40
5:A:448:LEU:HD21	15:A:1136:CLA:CBB	2.51	0.40
5:A:521:VAL:O	5:A:521:VAL:HG23	2.21	0.40
15:A:1104:CLA:H93	15:A:1104:CLA:H61	1.89	0.40
15:A:1136:CLA:CMA	15:A:1137:CLA:HED2	2.45	0.40
15:B:1205:CLA:HBC2	15:B:1206:CLA:HMD1	2.02	0.40
14:B:4003:BCR:H351	14:B:4003:BCR:H15C	1.72	0.40
11:J:2:LYS:HD2	11:J:2:LYS:C	2.45	0.40
11:J:10:THR:CB	11:J:12:PRO:HD2	2.51	0.40
14:J:4003:BCR:H15C	14:J:4003:BCR:H351	1.91	0.40
1:1:82:ALA:O	1:1:83:MET:C	2.64	0.40
19:1:811:SQD:H102	15:B:1219:CLA:CHB	2.52	0.40
5:A:214:ALA:HB1	5:A:299:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:459:ASN:OD1	5:A:472:PHE:HB2	2.21	0.40
6:B:47:ILE:HG22	6:B:51:HIS:HE1	1.87	0.40
6:B:70:ALA:HB2	6:B:136:LEU:HB2	2.03	0.40
6:B:193:GLY:HA2	6:B:196:VAL:HG22	2.03	0.40
6:B:592:THR:HB	6:B:722:TYR:OH	2.21	0.40
15:J:1302:CLA:CAC	14:J:4002:BCR:H10C	2.51	0.40
1:1:70:ARG:CZ	19:1:811:SQD:O49	2.70	0.40
1:1:218:PHE:O	1:1:224:SER:HB2	2.22	0.40
14:1:505:BCR:H10C	14:4:505:BCR:C20	2.51	0.40
13:4:502:XAT:H31	13:4:502:XAT:H391	1.67	0.40
15:4:607:CLA:HBB1	15:4:607:CLA:HMB3	2.02	0.40
16:4:611:CHL:H2A	16:4:611:CHL:O2D	2.21	0.40
5:A:51:ASN:ND2	17:A:5002:LHG:O2	2.51	0.40
5:A:393:HIS:O	5:A:397:ILE:HG12	2.21	0.40
5:A:526:ILE:HG12	5:A:618:VAL:HG22	2.03	0.40
6:B:160:PRO:C	6:B:162:PHE:H	2.29	0.40
6:B:547:LEU:HD23	6:B:547:LEU:C	2.47	0.40
8:D:142:THR:HG22	8:D:153:PRO:HG2	2.03	0.40
9:E:89:LYS:NZ	9:E:105:ARG:HD3	2.36	0.40
10:F:239:VAL:HG13	10:F:240:SER:N	2.37	0.40
1:1:114:THR:HG22	1:1:119:GLU:HA	2.04	0.40
2:2:271:PRO:HB2	15:A:1114:CLA:O1D	2.22	0.40
3:3:240:ILE:HG22	3:3:244:ARG:NH2	2.37	0.40
4:4:181:LEU:HD22	4:4:305:ILE:HD11	2.03	0.40
5:A:249:ILE:O	5:A:253:LEU:HD23	2.22	0.40
5:A:361:GLY:HA2	5:A:398:GLY:HA2	2.03	0.40
5:A:539:HIS:CG	5:A:606:VAL:HG22	2.57	0.40
5:A:676:HIS:HB3	15:A:1012:CLA:HBD	2.04	0.40
5:A:700:ILE:HG22	5:A:704:HIS:HE1	1.87	0.40
14:A:4002:BCR:H15C	14:A:4002:BCR:H351	1.89	0.40
6:B:77:GLN:O	6:B:85:VAL:HG11	2.21	0.40
6:B:93:TRP:O	6:B:95:PRO:HD3	2.22	0.40
6:B:531:THR:OG1	6:B:583:TRP:HB3	2.22	0.40
6:B:560:CYS:HB2	6:B:568:THR:O	2.21	0.40
15:B:1231:CLA:H11	15:B:1231:CLA:H52	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:168:LYS:NZ	23:4:831:GSH:O31[2_555]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	193/195 (99%)	189 (98%)	4 (2%)	0	100 100
2	2	209/211 (99%)	194 (93%)	15 (7%)	0	100 100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100 100
4	4	209/211 (99%)	184 (88%)	25 (12%)	0	100 100
5	A	737/739 (100%)	702 (95%)	35 (5%)	0	100 100
6	B	732/734 (100%)	695 (95%)	37 (5%)	0	100 100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100 100
8	D	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	9 31
9	E	62/64 (97%)	54 (87%)	8 (13%)	0	100 100
10	F	161/163 (99%)	145 (90%)	16 (10%)	0	100 100
11	J	39/41 (95%)	30 (77%)	9 (23%)	0	100 100
All	All	2768/2790 (99%)	2588 (94%)	178 (6%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	175	PRO
8	D	174	TYR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	151/151 (100%)	151 (100%)	0	100	100
2	2	169/169 (100%)	169 (100%)	0	100	100
3	3	160/160 (100%)	160 (100%)	0	100	100
4	4	169/169 (100%)	169 (100%)	0	100	100
5	A	598/598 (100%)	598 (100%)	0	100	100
6	B	593/593 (100%)	593 (100%)	0	100	100
7	C	68/68 (100%)	68 (100%)	0	100	100
8	D	122/122 (100%)	122 (100%)	0	100	100
9	E	57/57 (100%)	57 (100%)	0	100	100
10	F	136/136 (100%)	136 (100%)	0	100	100
11	J	36/36 (100%)	36 (100%)	0	100	100
All	All	2259/2259 (100%)	2259 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	194	GLN
1	1	221	ASN
2	2	109	HIS
2	2	250	ASN
3	3	178	GLN
3	3	267	ASN
3	3	271	HIS
3	3	279	ASN
4	4	281	GLN
5	A	320	HIS
5	A	433	HIS
5	A	442	ASN
5	A	653	GLN
5	A	714	GLN
6	B	90	HIS
6	B	99	GLN
6	B	159	GLN
6	B	320	HIS
6	B	403	GLN
6	B	445	GLN
6	B	453	GLN

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Mol	Chain	Res	Type
6	B	503	ASN
6	B	673	GLN
9	E	85	ASN
10	F	136	GLN
10	F	159	ASN
10	F	184	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 203 ligands modelled in this entry, 1 is monoatomic - leaving 202 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	B	1236	6	53,57,73	1.52	6 (11%)	62,93,113	2.20	19 (30%)
18	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.19	3 (9%)
14	BCR	1	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.53	16 (28%)
15	CLA	A	1107	5	53,57,73	1.57	6 (11%)	62,93,113	2.12	16 (25%)
15	CLA	B	1235	6	64,68,73	1.42	10 (15%)	77,107,113	1.98	18 (23%)
17	LHG	2	801	-	20,20,48	0.62	0	23,26,54	1.48	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	BCR	1	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.54	21 (37%)
15	CLA	A	1122	-	53,57,73	1.54	7 (13%)	62,93,113	2.12	17 (27%)
15	CLA	2	602	-	53,57,73	1.57	7 (13%)	62,93,113	2.17	17 (27%)
14	BCR	A	4007	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	18 (32%)
15	CLA	1	603	-	49,53,73	1.74	8 (16%)	59,89,113	2.04	16 (27%)
15	CLA	A	1112	-	53,57,73	1.56	7 (13%)	62,93,113	2.13	18 (29%)
15	CLA	2	603	-	50,54,73	1.59	6 (12%)	60,90,113	2.01	14 (23%)
15	CLA	A	1116	-	53,57,73	1.53	8 (15%)	62,93,113	2.14	16 (25%)
14	BCR	3	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.34	17 (30%)
13	XAT	3	502	-	39,47,47	0.67	1 (2%)	54,74,74	1.92	14 (25%)
15	CLA	4	607	-	53,57,73	1.56	8 (15%)	62,93,113	2.07	18 (29%)
21	DGD	2	811	-	48,48,67	0.94	3 (6%)	62,62,81	1.06	3 (4%)
15	CLA	J	1302	-	53,57,73	1.57	6 (11%)	62,93,113	2.07	15 (24%)
17	LHG	1	801	15	22,22,48	0.56	0	25,28,54	1.33	3 (12%)
14	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.29	16 (28%)
15	CLA	4	604	4	53,57,73	1.59	7 (13%)	62,93,113	2.16	17 (27%)
15	CLA	A	1121	-	53,57,73	1.55	7 (13%)	62,93,113	2.12	16 (25%)
15	CLA	1	611	-	53,57,73	1.58	7 (13%)	62,93,113	2.12	18 (29%)
19	SQD	1	811	-	39,40,54	0.89	0	48,51,65	0.99	3 (6%)
15	CLA	1	612	-	63,67,73	1.45	7 (11%)	75,105,113	1.98	16 (21%)
15	CLA	B	1216	-	53,57,73	1.53	8 (15%)	62,93,113	2.12	18 (29%)
14	BCR	B	4004	-	41,41,41	1.78	4 (9%)	56,56,56	4.46	15 (26%)
25	PQN	A	2001	-	34,34,34	0.49	0	42,45,45	1.17	3 (7%)
15	CLA	4	605	-	53,57,73	1.62	8 (15%)	62,93,113	2.15	15 (24%)
14	BCR	A	4002	-	41,41,41	1.88	4 (9%)	56,56,56	4.42	18 (32%)
14	BCR	4	505	-	41,41,41	1.87	4 (9%)	56,56,56	4.52	18 (32%)
12	LUT	1	501	-	42,43,43	2.44	1 (2%)	51,60,60	4.93	27 (52%)
15	CLA	A	1131	-	54,58,73	1.55	7 (12%)	65,95,113	2.11	17 (26%)
16	CHL	4	613	-	54,58,74	0.85	1 (1%)	59,94,114	1.52	12 (20%)
15	CLA	A	1126	5	53,57,73	1.61	5 (9%)	62,93,113	2.19	15 (24%)
20	CAC	4	902	-	1,4,4	3.44	1 (100%)	2,6,6	1.23	0
15	CLA	3	610	-	53,57,73	1.53	7 (13%)	62,93,113	2.05	17 (27%)
23	GSH	B	5031	-	18,19,19	2.11	3 (16%)	23,24,24	1.54	3 (13%)
15	CLA	A	1106	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
14	BCR	B	4005	-	41,41,41	1.87	4 (9%)	56,56,56	4.47	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	A	1130	-	59,63,73	1.49	7 (11%)	71,101,113	2.07	18 (25%)
15	CLA	A	1139	-	56,60,73	1.55	7 (12%)	67,97,113	2.10	20 (29%)
15	CLA	4	612	-	53,57,73	1.60	8 (15%)	62,93,113	2.15	19 (30%)
15	CLA	2	601	-	53,57,73	1.50	7 (13%)	62,93,113	2.03	17 (27%)
15	CLA	B	1221	-	53,57,73	1.58	7 (13%)	62,93,113	2.20	19 (30%)
15	CLA	B	1234	-	53,57,73	1.56	9 (16%)	62,93,113	2.13	18 (29%)
18	LMG	1	802	-	36,36,55	0.73	1 (2%)	44,44,63	1.19	4 (9%)
15	CLA	B	1218	-	53,57,73	1.55	8 (15%)	62,93,113	2.13	17 (27%)
15	CLA	4	606	-	53,57,73	1.57	8 (15%)	62,93,113	2.11	16 (25%)
15	CLA	2	615	2	54,58,73	1.51	8 (14%)	65,95,113	2.10	17 (26%)
15	CLA	3	606	-	49,53,73	1.61	6 (12%)	59,89,113	2.07	16 (27%)
15	CLA	1	602	-	50,54,73	1.58	8 (16%)	60,90,113	2.05	16 (26%)
15	CLA	A	1103	-	59,63,73	1.47	7 (11%)	71,101,113	2.01	18 (25%)
15	CLA	1	604	1	53,57,73	1.56	7 (13%)	62,93,113	2.16	20 (32%)
16	CHL	4	611	-	54,58,74	0.89	1 (1%)	59,94,114	1.48	10 (16%)
15	CLA	A	1135	-	53,57,73	1.54	8 (15%)	62,93,113	2.15	16 (25%)
16	CHL	2	610	-	54,58,74	0.86	1 (1%)	59,94,114	1.40	12 (20%)
15	CLA	2	604	-	53,57,73	1.55	7 (13%)	62,93,113	2.12	18 (29%)
15	CLA	3	601	-	53,57,73	1.60	6 (11%)	62,93,113	2.23	17 (27%)
26	SF4	C	3003	7	0,12,12	-	-	-		
15	CLA	B	1213	-	53,57,73	1.47	7 (13%)	62,93,113	2.09	19 (30%)
15	CLA	A	1134	-	53,57,73	1.54	7 (13%)	62,93,113	2.16	18 (29%)
15	CLA	A	1102	5,15	49,53,73	1.61	8 (16%)	59,89,113	2.08	15 (25%)
15	CLA	3	608	-	52,56,73	1.56	8 (15%)	62,92,113	2.04	16 (25%)
15	CLA	A	1109	15	53,57,73	1.54	8 (15%)	62,93,113	2.16	17 (27%)
15	CLA	B	1217	-	50,54,73	1.60	7 (14%)	60,90,113	2.01	15 (25%)
14	BCR	J	4002	-	41,41,41	1.82	5 (12%)	56,56,56	4.52	21 (37%)
15	CLA	A	1101	5	49,53,73	1.66	7 (14%)	59,89,113	2.12	17 (28%)
15	CLA	A	1137	-	53,57,73	1.54	7 (13%)	62,93,113	2.16	19 (30%)
15	CLA	1	606	-	49,53,73	1.60	7 (14%)	59,89,113	2.11	16 (27%)
14	BCR	4	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.47	18 (32%)
15	CLA	B	1023	-	64,68,73	1.46	8 (12%)	77,107,113	1.88	18 (23%)
15	CLA	F	1302	-	53,57,73	1.53	10 (18%)	62,93,113	2.05	17 (27%)
15	CLA	A	1111	5	53,57,73	1.49	6 (11%)	62,93,113	2.20	20 (32%)
15	CLA	A	1108	-	50,54,73	1.64	7 (14%)	60,90,113	2.09	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	2	606	-	50,54,73	1.65	8 (16%)	60,90,113	2.11	16 (26%)
15	CLA	B	1208	-	53,57,73	1.57	6 (11%)	62,93,113	2.13	18 (29%)
15	CLA	B	1215	-	53,57,73	1.63	6 (11%)	62,93,113	2.29	17 (27%)
15	CLA	4	601	4	53,57,73	1.53	8 (15%)	62,93,113	2.12	20 (32%)
14	BCR	A	4004	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	15 (26%)
15	CLA	2	612	-	53,57,73	1.60	7 (13%)	62,93,113	2.13	16 (25%)
15	CLA	A	1138	5	69,73,73	1.37	7 (10%)	83,113,113	1.90	16 (19%)
15	CLA	B	1206	6	53,57,73	1.56	8 (15%)	62,93,113	2.13	17 (27%)
15	CLA	B	1238	-	54,58,73	1.54	6 (11%)	65,95,113	2.11	17 (26%)
12	LUT	4	501	-	42,43,43	2.39	2 (4%)	51,60,60	1.92	14 (27%)
14	BCR	3	504	-	41,41,41	1.87	4 (9%)	56,56,56	4.57	17 (30%)
15	CLA	B	1219	-	53,57,73	1.52	8 (15%)	62,93,113	2.10	17 (27%)
16	CHL	2	609	2	54,58,74	0.84	1 (1%)	59,94,114	1.38	11 (18%)
15	CLA	2	608	-	53,57,73	1.55	7 (13%)	62,93,113	2.19	18 (29%)
15	CLA	4	602	-	53,57,73	1.54	6 (11%)	62,93,113	2.09	16 (25%)
15	CLA	3	615	-	50,54,73	1.63	7 (14%)	60,90,113	2.04	15 (25%)
15	CLA	A	1128	-	53,57,73	1.59	8 (15%)	62,93,113	2.16	17 (27%)
14	BCR	B	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	17 (30%)
15	CLA	A	1133	-	53,57,73	1.57	7 (13%)	62,93,113	2.09	16 (25%)
16	CHL	1	610	-	51,55,74	0.89	1 (1%)	57,91,114	1.60	12 (21%)
15	CLA	4	603	-	53,57,73	1.59	8 (15%)	62,93,113	2.08	16 (25%)
18	LMG	1	803	-	23,23,55	0.58	0	31,31,63	1.36	2 (6%)
15	CLA	A	1115	-	53,57,73	1.58	7 (13%)	62,93,113	2.18	17 (27%)
15	CLA	B	1237	-	53,57,73	1.56	7 (13%)	62,93,113	2.12	17 (27%)
21	DGD	4	811	-	46,46,67	0.90	2 (4%)	60,60,81	0.98	3 (5%)
15	CLA	3	607	-	54,58,73	1.53	7 (12%)	65,95,113	2.10	18 (27%)
15	CLA	B	1226	-	53,57,73	1.53	8 (15%)	62,93,113	2.19	18 (29%)
15	CLA	B	1231	6	64,68,73	1.43	5 (7%)	77,107,113	1.96	19 (24%)
15	CLA	A	1123	-	52,56,73	1.60	7 (13%)	62,92,113	2.08	17 (27%)
15	CLA	B	1230	6	53,57,73	1.56	8 (15%)	62,93,113	2.20	15 (24%)
15	CLA	3	612	-	59,63,73	1.44	8 (13%)	71,101,113	2.04	19 (26%)
20	CAC	1	901	-	1,4,4	3.49	1 (100%)	2,6,6	1.11	0
15	CLA	3	603	-	49,53,73	1.63	8 (16%)	59,89,113	2.31	20 (33%)
20	CAC	4	901	-	1,4,4	3.54	1 (100%)	2,6,6	1.10	0
15	CLA	B	1228	-	64,68,73	1.39	7 (10%)	77,107,113	1.94	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	B	1222	-	53,57,73	1.61	9 (16%)	62,93,113	2.17	16 (25%)
15	CLA	3	605	-	50,54,73	1.58	9 (18%)	60,90,113	1.96	14 (23%)
15	CLA	A	1105	-	53,57,73	1.56	9 (16%)	62,93,113	2.14	16 (25%)
24	CL0	A	1011	5	54,58,73	2.76	22 (40%)	65,95,113	2.84	24 (36%)
15	CLA	1	607	17	50,54,73	1.58	7 (14%)	60,90,113	2.06	15 (25%)
15	CLA	3	613	-	50,54,73	1.60	6 (12%)	60,90,113	2.04	14 (23%)
15	CLA	4	609	4	53,57,73	1.55	6 (11%)	62,93,113	2.19	17 (27%)
15	CLA	A	1104	-	64,68,73	1.38	7 (10%)	77,107,113	2.06	19 (24%)
15	CLA	A	1114	-	50,54,73	1.58	9 (18%)	60,90,113	2.05	14 (23%)
14	BCR	A	4005	-	41,41,41	4.26	5 (12%)	56,56,56	4.55	21 (37%)
15	CLA	B	1204	-	53,57,73	1.57	7 (13%)	62,93,113	2.10	17 (27%)
15	CLA	B	1214	-	53,57,73	1.57	10 (18%)	62,93,113	2.11	19 (30%)
15	CLA	B	1220	6	59,63,73	1.49	6 (10%)	71,101,113	2.02	19 (26%)
20	CAC	3	901	-	1,4,4	2.83	1 (100%)	2,6,6	1.23	0
15	CLA	2	607	-	53,57,73	1.58	6 (11%)	62,93,113	2.16	17 (27%)
15	CLA	B	1201	-	52,56,73	1.60	8 (15%)	62,92,113	2.07	16 (25%)
15	CLA	A	1120	-	53,57,73	1.55	7 (13%)	62,93,113	2.14	18 (29%)
26	SF4	C	3002	7	0,12,12	-	-	-		
15	CLA	A	1124	-	53,57,73	1.54	7 (13%)	62,93,113	2.15	18 (29%)
15	CLA	F	1301	-	51,55,73	1.64	5 (9%)	61,91,113	2.15	17 (27%)
15	CLA	A	1119	-	53,57,73	1.57	6 (11%)	62,93,113	2.13	17 (27%)
25	PQN	B	2002	-	34,34,34	0.44	0	42,45,45	1.17	3 (7%)
15	CLA	A	1132	5	53,57,73	1.54	8 (15%)	62,93,113	2.16	17 (27%)
14	BCR	B	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.60	20 (35%)
15	CLA	4	608	4	50,54,73	1.57	7 (14%)	60,90,113	2.04	14 (23%)
15	CLA	A	1113	-	49,53,73	1.61	8 (16%)	59,89,113	2.03	15 (25%)
15	CLA	B	1211	6	53,57,73	1.55	8 (15%)	62,93,113	2.12	15 (24%)
16	CHL	1	609	1	54,58,74	0.88	2 (3%)	59,94,114	1.46	12 (20%)
15	CLA	A	1140	5	59,63,73	1.47	11 (18%)	71,101,113	2.00	15 (21%)
15	CLA	A	1129	-	52,56,73	1.57	7 (13%)	62,92,113	2.07	18 (29%)
13	XAT	1	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
15	CLA	B	1212	-	49,53,73	1.61	6 (12%)	59,89,113	2.03	16 (27%)
23	GSH	4	831	-	18,19,19	2.09	4 (22%)	23,24,24	1.57	3 (13%)
26	SF4	A	3001	5,6	0,12,12	-	-	-		
22	LMT	2	821	-	24,24,36	1.34	5 (20%)	35,35,47	1.04	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	A	1141	-	54,58,73	1.54	6 (11%)	65,95,113	2.13	18 (27%)
15	CLA	B	1232	-	53,57,73	1.56	7 (13%)	62,93,113	2.14	16 (25%)
15	CLA	A	1012	-	64,68,73	1.49	9 (14%)	77,107,113	1.95	19 (24%)
15	CLA	1	601	-	53,57,73	1.51	9 (16%)	62,93,113	2.07	17 (27%)
12	LUT	2	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.24	15 (29%)
20	CAC	1	902	-	1,4,4	3.07	1 (100%)	2,6,6	1.18	0
15	CLA	2	605	-	69,73,73	1.40	7 (10%)	83,113,113	1.96	20 (24%)
20	CAC	3	902	-	1,4,4	3.23	1 (100%)	2,6,6	1.17	0
15	CLA	4	615	-	59,63,73	1.45	5 (8%)	71,101,113	2.03	18 (25%)
16	CHL	4	610	-	51,55,74	0.89	1 (1%)	57,91,114	1.44	11 (19%)
21	DGD	B	5002	-	39,39,67	0.93	2 (5%)	53,53,81	1.00	3 (5%)
16	CHL	2	613	-	50,54,74	0.89	1 (2%)	56,90,114	1.46	12 (21%)
14	BCR	A	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.33	17 (30%)
15	CLA	B	1225	-	53,57,73	1.53	7 (13%)	62,93,113	2.14	18 (29%)
15	CLA	B	1021	-	69,73,73	1.40	8 (11%)	83,113,113	1.93	18 (21%)
15	CLA	B	1227	-	49,53,73	1.70	8 (16%)	59,89,113	2.11	15 (25%)
15	CLA	3	611	-	50,54,73	1.59	7 (14%)	60,90,113	2.04	14 (23%)
15	CLA	B	1223	6	54,58,73	1.63	7 (12%)	65,95,113	2.20	18 (27%)
15	CLA	A	1117	-	53,57,73	1.56	8 (15%)	62,93,113	2.16	17 (27%)
15	CLA	B	1207	-	26,32,73	3.28	12 (46%)	34,54,113	2.44	13 (38%)
14	BCR	J	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.42	14 (25%)
13	XAT	4	502	-	39,47,47	0.73	0	54,74,74	1.90	13 (24%)
15	CLA	B	1224	6	53,57,73	1.52	7 (13%)	62,93,113	2.10	17 (27%)
15	CLA	B	1202	-	53,57,73	1.55	6 (11%)	62,93,113	2.15	17 (27%)
21	DGD	J	5001	-	29,29,67	0.61	0	41,41,81	0.60	0
15	CLA	B	1022	-	54,58,73	1.50	8 (14%)	65,95,113	2.15	20 (30%)
15	CLA	B	1210	-	53,57,73	1.51	7 (13%)	62,93,113	2.12	15 (24%)
15	CLA	A	1125	5	53,57,73	1.53	6 (11%)	62,93,113	2.12	17 (27%)
15	CLA	1	615	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	16 (19%)
16	CHL	3	604	-	51,55,74	0.88	1 (1%)	57,91,114	1.49	10 (17%)
16	CHL	2	611	-	52,56,74	0.87	1 (1%)	58,92,114	1.43	13 (22%)
14	BCR	J	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.39	17 (30%)
12	LUT	3	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.13	12 (23%)
17	LHG	A	5002	-	23,23,48	0.52	0	26,29,54	1.44	3 (11%)
15	CLA	A	1110	-	53,57,73	1.52	7 (13%)	62,93,113	2.16	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	B	1239	6	69,73,73	1.38	8 (11%)	83,113,113	1.90	17 (20%)
14	BCR	B	4002	-	41,41,41	1.90	4 (9%)	56,56,56	4.37	17 (30%)
15	CLA	B	1229	6	69,73,73	1.48	9 (13%)	83,113,113	1.91	19 (22%)
14	BCR	B	4006	-	41,41,41	1.89	4 (9%)	56,56,56	4.41	15 (26%)
15	CLA	B	1205	-	53,57,73	1.54	8 (15%)	62,93,113	2.17	16 (25%)
15	CLA	A	1136	-	53,57,73	1.56	6 (11%)	62,93,113	2.12	16 (25%)
15	CLA	B	1209	-	50,54,73	1.61	7 (14%)	60,90,113	2.04	16 (26%)
15	CLA	A	1118	-	53,57,73	1.52	8 (15%)	62,93,113	2.14	16 (25%)
18	LMG	2	803	-	15,16,55	0.51	0	20,22,63	0.54	0
15	CLA	1	605	-	52,56,73	1.53	5 (9%)	62,92,113	2.10	17 (27%)
13	XAT	2	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	14 (25%)
15	CLA	A	1013	-	69,73,73	1.39	9 (13%)	83,113,113	1.89	18 (21%)
15	CLA	B	1240	17	69,73,73	1.39	7 (10%)	83,113,113	1.88	18 (21%)
15	CLA	1	613	-	49,53,73	1.57	8 (16%)	59,89,113	2.05	16 (27%)
17	LHG	A	5001	-	15,15,48	0.75	1 (6%)	16,19,54	0.57	0
14	BCR	2	503	-	41,41,41	1.87	4 (9%)	56,56,56	4.50	17 (30%)
17	LHG	B	5001	15	20,20,48	0.64	0	23,26,54	1.43	2 (8%)
15	CLA	1	608	1	50,54,73	1.59	7 (14%)	60,90,113	2.12	15 (25%)
15	CLA	B	1203	-	53,57,73	1.55	6 (11%)	62,93,113	2.14	15 (24%)
14	BCR	F	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.56	19 (33%)
15	CLA	A	1127	-	53,57,73	1.60	8 (15%)	62,93,113	2.18	18 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1236	6	-	10/20/96/115	-
18	LMG	2	802	-	-	8/20/40/70	0/1/1/1
14	BCR	1	505	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1107	5	-	4/20/96/115	-
15	CLA	B	1235	6	-	20/33/109/115	-
17	LHG	2	801	-	-	10/23/23/53	-
14	BCR	1	503	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1122	-	-	11/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	602	-	-	8/20/96/115	-
14	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
15	CLA	1	603	-	-	8/15/91/115	-
15	CLA	A	1112	-	-	7/20/96/115	-
15	CLA	2	603	-	-	6/17/93/115	-
15	CLA	A	1116	-	-	8/20/96/115	-
14	BCR	3	503	-	-	13/29/63/63	0/2/2/2
13	XAT	3	502	-	1/1/12/26	14/31/93/93	0/4/4/4
15	CLA	4	607	-	-	10/20/96/115	-
21	DGD	2	811	-	-	13/36/76/95	0/2/2/2
15	CLA	J	1302	-	-	12/20/96/115	-
17	LHG	1	801	15	-	11/26/26/53	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
15	CLA	4	604	4	-	11/20/96/115	-
15	CLA	A	1121	-	-	10/20/96/115	-
15	CLA	1	611	-	-	12/20/96/115	-
19	SQD	1	811	-	-	6/34/54/69	0/1/1/1
15	CLA	1	612	-	1/1/14/20	10/29/105/115	-
15	CLA	B	1216	-	-	10/20/96/115	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
25	PQN	A	2001	-	-	12/23/43/43	0/2/2/2
15	CLA	4	605	-	-	11/20/96/115	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
14	BCR	4	505	-	-	19/29/63/63	0/2/2/2
12	LUT	1	501	-	-	8/29/67/67	0/2/2/2
15	CLA	A	1131	-	-	10/21/97/115	-
16	CHL	4	613	-	1/1/11/21	7/22/98/117	-
15	CLA	A	1126	5	-	9/20/96/115	-
15	CLA	3	610	-	-	9/20/96/115	-
23	GSH	B	5031	-	-	13/24/24/24	-
15	CLA	A	1106	-	-	15/39/115/115	-
14	BCR	B	4005	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1130	-	-	16/27/103/115	-
15	CLA	A	1139	-	-	6/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	612	-	-	11/20/96/115	-
15	CLA	2	601	-	-	10/20/96/115	-
15	CLA	B	1221	-	-	7/20/96/115	-
15	CLA	B	1234	-	-	8/20/96/115	-
18	LMG	1	802	-	-	8/31/51/70	0/1/1/1
15	CLA	B	1218	-	-	10/20/96/115	-
15	CLA	4	606	-	-	11/20/96/115	-
15	CLA	2	615	2	-	9/21/97/115	-
15	CLA	3	606	-	-	5/15/91/115	-
15	CLA	1	602	-	-	13/17/93/115	-
15	CLA	A	1103	-	-	16/27/103/115	-
15	CLA	1	604	1	-	7/20/96/115	-
16	CHL	4	611	-	-	6/22/98/117	-
16	CHL	2	610	-	1/1/11/21	9/22/98/117	-
15	CLA	A	1135	-	-	11/20/96/115	-
15	CLA	2	604	-	-	12/20/96/115	-
15	CLA	3	601	-	-	12/20/96/115	-
26	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	B	1213	-	-	9/20/96/115	-
15	CLA	A	1134	-	-	8/20/96/115	-
15	CLA	A	1102	5,15	-	7/15/91/115	-
15	CLA	3	608	-	-	7/19/95/115	-
15	CLA	A	1109	15	-	8/20/96/115	-
15	CLA	B	1217	-	-	11/17/93/115	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	A	1101	5	-	8/15/91/115	-
15	CLA	A	1137	-	-	10/20/96/115	-
15	CLA	1	606	-	-	8/15/91/115	-
14	BCR	4	503	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1023	-	-	15/33/109/115	-
15	CLA	F	1302	-	-	9/20/96/115	-
15	CLA	A	1111	5	-	7/20/96/115	-
15	CLA	A	1108	-	-	10/17/93/115	-
15	CLA	2	606	-	-	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1208	-	-	7/20/96/115	-
15	CLA	B	1215	-	-	9/20/96/115	-
15	CLA	4	601	4	-	9/20/96/115	-
14	BCR	A	4004	-	-	10/29/63/63	0/2/2/2
15	CLA	2	612	-	-	14/20/96/115	-
15	CLA	A	1138	5	-	20/39/115/115	-
15	CLA	B	1206	6	-	9/20/96/115	-
15	CLA	B	1238	-	-	8/21/97/115	-
12	LUT	4	501	-	-	7/29/67/67	0/2/2/2
14	BCR	3	504	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1219	-	-	9/20/96/115	-
16	CHL	2	609	2	-	7/22/98/117	-
15	CLA	2	608	-	-	9/20/96/115	-
15	CLA	4	602	-	-	5/20/96/115	-
15	CLA	3	615	-	-	6/17/93/115	-
15	CLA	A	1128	-	-	10/20/96/115	-
14	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
15	CLA	A	1133	-	-	7/20/96/115	-
16	CHL	1	610	-	-	5/19/95/117	-
15	CLA	4	603	-	-	4/20/96/115	-
18	LMG	1	803	-	-	6/16/36/70	0/1/1/1
15	CLA	A	1115	-	-	10/20/96/115	-
15	CLA	B	1237	-	-	11/20/96/115	-
21	DGD	4	811	-	-	14/34/74/95	0/2/2/2
15	CLA	3	607	-	-	11/21/97/115	-
15	CLA	B	1226	-	-	10/20/96/115	-
15	CLA	B	1231	6	-	11/33/109/115	-
15	CLA	A	1123	-	-	9/19/95/115	-
15	CLA	B	1230	6	-	8/20/96/115	-
15	CLA	3	612	-	-	10/27/103/115	-
15	CLA	3	603	-	-	5/15/91/115	-
15	CLA	B	1228	-	-	9/33/109/115	-
15	CLA	B	1222	-	-	9/20/96/115	-
15	CLA	3	605	-	-	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1105	-	-	10/20/96/115	-
24	CL0	A	1011	5	-	13/21/97/115	-
15	CLA	1	607	17	-	11/17/93/115	-
15	CLA	3	613	-	-	10/17/93/115	-
15	CLA	4	609	4	-	7/20/96/115	-
15	CLA	A	1104	-	-	17/33/109/115	-
15	CLA	A	1114	-	-	6/17/93/115	-
14	BCR	A	4005	-	-	8/29/63/63	0/2/2/2
15	CLA	B	1204	-	-	8/20/96/115	-
15	CLA	B	1214	-	-	12/20/96/115	-
15	CLA	B	1220	6	-	12/27/103/115	-
15	CLA	2	607	-	-	12/20/96/115	-
15	CLA	B	1201	-	-	10/19/95/115	-
15	CLA	A	1120	-	-	10/20/96/115	-
26	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	A	1124	-	-	10/20/96/115	-
15	CLA	F	1301	-	-	11/18/94/115	-
15	CLA	A	1119	-	-	11/20/96/115	-
25	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
15	CLA	A	1132	5	-	12/20/96/115	-
14	BCR	B	4001	-	-	14/29/63/63	0/2/2/2
15	CLA	4	608	4	-	6/17/93/115	-
15	CLA	A	1113	-	-	8/15/91/115	-
15	CLA	B	1211	6	-	9/20/96/115	-
16	CHL	1	609	1	1/1/11/21	7/22/98/117	-
15	CLA	A	1140	5	-	13/27/103/115	-
15	CLA	A	1129	-	-	12/19/95/115	-
13	XAT	1	502	-	-	3/31/93/93	0/4/4/4
15	CLA	B	1212	-	-	8/15/91/115	-
23	GSH	4	831	-	-	5/24/24/24	-
26	SF4	A	3001	5,6	-	-	0/6/5/5
22	LMT	2	821	-	-	1/8/48/61	0/2/2/2
15	CLA	A	1141	-	-	9/21/97/115	-
15	CLA	B	1232	-	-	8/20/96/115	-
15	CLA	A	1012	-	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	1	601	-	-	13/20/96/115	-
12	LUT	2	501	-	-	6/29/67/67	0/2/2/2
15	CLA	2	605	-	-	15/39/115/115	-
15	CLA	4	615	-	-	12/27/103/115	-
16	CHL	4	610	-	1/1/11/21	6/19/95/117	-
21	DGD	B	5002	-	-	9/27/67/95	0/2/2/2
16	CHL	2	613	-	-	3/17/93/117	-
14	BCR	A	4006	-	-	15/29/63/63	0/2/2/2
15	CLA	B	1225	-	-	8/20/96/115	-
15	CLA	B	1021	-	-	17/39/115/115	-
15	CLA	B	1227	-	-	7/15/91/115	-
15	CLA	3	611	-	-	9/17/93/115	-
15	CLA	B	1223	6	-	7/21/97/115	-
15	CLA	A	1117	-	-	7/20/96/115	-
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
13	XAT	4	502	-	1/1/12/26	6/31/93/93	0/4/4/4
15	CLA	B	1224	6	-	11/20/96/115	-
15	CLA	B	1202	-	-	11/20/96/115	-
21	DGD	J	5001	-	-	5/14/54/95	0/2/2/2
15	CLA	B	1022	-	-	9/21/97/115	-
15	CLA	B	1210	-	-	12/20/96/115	-
15	CLA	A	1125	5	-	10/20/96/115	-
15	CLA	1	615	-	-	20/39/115/115	-
16	CHL	3	604	-	-	7/19/95/117	-
16	CHL	2	611	-	1/1/11/21	1/20/96/117	-
14	BCR	J	4003	-	-	14/29/63/63	0/2/2/2
12	LUT	3	501	-	-	4/29/67/67	0/2/2/2
17	LHG	A	5002	-	-	18/28/28/53	-
15	CLA	A	1110	-	-	8/20/96/115	-
15	CLA	B	1239	6	-	17/39/115/115	-
14	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1229	6	-	17/39/115/115	-
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1205	-	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1136	-	-	11/20/96/115	-
15	CLA	B	1209	-	-	8/17/93/115	-
15	CLA	A	1118	-	-	14/20/96/115	-
18	LMG	2	803	-	-	3/7/27/70	0/1/1/1
15	CLA	1	605	-	-	10/19/95/115	-
13	XAT	2	502	-	1/1/12/26	3/31/93/93	0/4/4/4
15	CLA	A	1013	-	-	20/39/115/115	-
15	CLA	B	1240	17	-	19/39/115/115	-
15	CLA	1	613	-	-	4/15/91/115	-
17	LHG	A	5001	-	-	14/18/18/53	-
14	BCR	2	503	-	-	14/29/63/63	0/2/2/2
17	LHG	B	5001	15	-	13/23/23/53	-
15	CLA	1	608	1	-	7/17/93/115	-
15	CLA	B	1203	-	-	8/20/96/115	-
14	BCR	F	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1127	-	-	11/20/96/115	-

All (1129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4005	BCR	C11-C12	19.10	1.83	1.34
14	A	4005	BCR	C11-C10	15.97	1.92	1.43
12	1	501	LUT	C24-C25	14.94	1.51	1.33
12	3	501	LUT	C24-C25	14.66	1.51	1.33
12	4	501	LUT	C24-C25	14.54	1.51	1.33
12	2	501	LUT	C24-C25	14.53	1.51	1.33
24	A	1011	CL0	MG-NA	9.00	2.27	2.06
15	B	1207	CLA	C3D-C2D	8.76	1.54	1.35
14	A	4005	BCR	C12-C13	7.94	1.63	1.45
15	B	1207	CLA	MG-ND	7.82	2.21	2.05
14	B	4002	BCR	C10-C9	7.68	1.46	1.35
14	A	4002	BCR	C10-C9	7.58	1.45	1.35
14	4	505	BCR	C10-C9	7.55	1.45	1.35
14	B	4006	BCR	C10-C9	7.49	1.45	1.35
14	B	4003	BCR	C10-C9	7.46	1.45	1.35
14	A	4007	BCR	C10-C9	7.45	1.45	1.35
14	A	4004	BCR	C10-C9	7.42	1.45	1.35
14	3	503	BCR	C10-C9	7.37	1.45	1.35
14	2	503	BCR	C10-C9	7.35	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	503	BCR	C10-C9	7.33	1.45	1.35
14	1	505	BCR	C10-C9	7.32	1.45	1.35
14	B	4005	BCR	C10-C9	7.24	1.45	1.35
15	B	1229	CLA	MG-NA	7.23	2.23	2.06
14	3	504	BCR	C10-C9	7.23	1.45	1.35
14	A	4003	BCR	C10-C9	7.19	1.45	1.35
14	4	503	BCR	C10-C9	7.18	1.45	1.35
14	J	4003	BCR	C10-C9	7.15	1.45	1.35
15	B	1215	CLA	MG-NA	7.12	2.23	2.06
14	F	4002	BCR	C10-C9	7.06	1.45	1.35
15	B	1223	CLA	MG-NA	7.03	2.23	2.06
14	B	4001	BCR	C10-C9	6.98	1.45	1.35
15	A	1126	CLA	MG-NA	6.93	2.22	2.06
15	B	1227	CLA	MG-NA	6.88	2.22	2.06
15	2	606	CLA	MG-NA	6.87	2.22	2.06
15	3	601	CLA	MG-NA	6.85	2.22	2.06
15	B	1021	CLA	MG-NA	6.85	2.22	2.06
15	B	1230	CLA	MG-NA	6.84	2.22	2.06
15	A	1108	CLA	MG-NA	6.84	2.22	2.06
15	1	603	CLA	MG-NA	6.82	2.22	2.06
14	J	4001	BCR	C10-C9	6.81	1.44	1.35
15	4	604	CLA	MG-NA	6.80	2.22	2.06
14	A	4006	BCR	C10-C9	6.80	1.44	1.35
15	3	615	CLA	MG-NA	6.78	2.22	2.06
15	4	605	CLA	MG-NA	6.74	2.22	2.06
14	J	4002	BCR	C10-C9	6.73	1.44	1.35
15	2	602	CLA	MG-NA	6.71	2.22	2.06
15	A	1101	CLA	MG-NA	6.70	2.22	2.06
15	1	611	CLA	MG-NA	6.67	2.22	2.06
15	2	607	CLA	MG-NA	6.65	2.22	2.06
15	B	1208	CLA	MG-NA	6.62	2.22	2.06
15	A	1115	CLA	MG-NA	6.61	2.22	2.06
15	A	1123	CLA	MG-NA	6.61	2.22	2.06
15	B	1222	CLA	MG-NA	6.60	2.22	2.06
14	B	4004	BCR	C10-C9	6.57	1.44	1.35
15	A	1106	CLA	MG-NA	6.57	2.21	2.06
15	B	1221	CLA	MG-NA	6.55	2.21	2.06
15	2	605	CLA	MG-NA	6.53	2.21	2.06
15	F	1301	CLA	MG-NA	6.52	2.21	2.06
15	4	612	CLA	MG-NA	6.52	2.21	2.06
15	B	1238	CLA	MG-NA	6.51	2.21	2.06
15	B	1239	CLA	MG-NA	6.50	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1214	CLA	MG-NA	6.50	2.21	2.06
15	1	612	CLA	MG-NA	6.50	2.21	2.06
15	B	1204	CLA	MG-NA	6.49	2.21	2.06
15	B	1231	CLA	MG-NA	6.48	2.21	2.06
15	B	1234	CLA	MG-NA	6.48	2.21	2.06
15	A	1127	CLA	MG-NA	6.48	2.21	2.06
15	A	1129	CLA	MG-NA	6.47	2.21	2.06
15	B	1202	CLA	MG-NA	6.47	2.21	2.06
15	B	1237	CLA	MG-NA	6.46	2.21	2.06
15	B	1232	CLA	MG-NA	6.46	2.21	2.06
15	3	607	CLA	MG-NA	6.45	2.21	2.06
15	B	1220	CLA	MG-NA	6.45	2.21	2.06
15	A	1141	CLA	MG-NA	6.45	2.21	2.06
15	B	1240	CLA	MG-NA	6.44	2.21	2.06
15	1	615	CLA	MG-NA	6.43	2.21	2.06
15	B	1201	CLA	MG-NA	6.43	2.21	2.06
15	A	1120	CLA	MG-NA	6.43	2.21	2.06
15	A	1107	CLA	MG-NA	6.43	2.21	2.06
15	4	606	CLA	MG-NA	6.42	2.21	2.06
15	A	1102	CLA	MG-NA	6.41	2.21	2.06
15	A	1128	CLA	MG-NA	6.41	2.21	2.06
15	A	1139	CLA	MG-NA	6.40	2.21	2.06
15	3	608	CLA	MG-NA	6.40	2.21	2.06
15	4	609	CLA	MG-NA	6.39	2.21	2.06
15	3	603	CLA	MG-NA	6.39	2.21	2.06
15	A	1112	CLA	MG-NA	6.38	2.21	2.06
15	A	1136	CLA	MG-NA	6.38	2.21	2.06
15	B	1209	CLA	MG-NA	6.38	2.21	2.06
15	A	1121	CLA	MG-NA	6.38	2.21	2.06
15	A	1130	CLA	MG-NA	6.37	2.21	2.06
15	4	615	CLA	MG-NA	6.37	2.21	2.06
15	A	1119	CLA	MG-NA	6.37	2.21	2.06
15	3	613	CLA	MG-NA	6.37	2.21	2.06
15	3	611	CLA	MG-NA	6.37	2.21	2.06
15	B	1206	CLA	MG-NA	6.37	2.21	2.06
15	3	606	CLA	MG-NA	6.37	2.21	2.06
15	A	1131	CLA	MG-NA	6.36	2.21	2.06
15	A	1125	CLA	MG-NA	6.36	2.21	2.06
15	2	612	CLA	MG-NA	6.36	2.21	2.06
15	A	1133	CLA	MG-NA	6.36	2.21	2.06
15	B	1212	CLA	MG-NA	6.36	2.21	2.06
15	A	1113	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1205	CLA	MG-NA	6.35	2.21	2.06
15	A	1137	CLA	MG-NA	6.33	2.21	2.06
15	B	1023	CLA	MG-NA	6.33	2.21	2.06
15	A	1135	CLA	MG-NA	6.32	2.21	2.06
15	A	1109	CLA	MG-NA	6.32	2.21	2.06
15	A	1134	CLA	MG-NA	6.32	2.21	2.06
15	A	1105	CLA	MG-NA	6.31	2.21	2.06
15	B	1203	CLA	MG-NA	6.31	2.21	2.06
15	1	607	CLA	MG-NA	6.31	2.21	2.06
15	A	1012	CLA	MG-NA	6.31	2.21	2.06
15	A	1114	CLA	MG-NA	6.30	2.21	2.06
15	B	1225	CLA	MG-NA	6.30	2.21	2.06
15	B	1211	CLA	MG-NA	6.30	2.21	2.06
15	J	1302	CLA	MG-NA	6.30	2.21	2.06
15	1	604	CLA	MG-NA	6.30	2.21	2.06
15	1	606	CLA	MG-NA	6.29	2.21	2.06
15	A	1117	CLA	MG-NA	6.29	2.21	2.06
15	A	1103	CLA	MG-NA	6.28	2.21	2.06
15	A	1124	CLA	MG-NA	6.28	2.21	2.06
15	1	608	CLA	MG-NA	6.28	2.21	2.06
15	A	1104	CLA	MG-NA	6.27	2.21	2.06
15	A	1118	CLA	MG-NA	6.26	2.21	2.06
15	4	608	CLA	MG-NA	6.26	2.21	2.06
15	A	1138	CLA	MG-NA	6.25	2.21	2.06
15	B	1218	CLA	MG-NA	6.24	2.21	2.06
15	B	1217	CLA	MG-NA	6.24	2.21	2.06
15	1	602	CLA	MG-NA	6.24	2.21	2.06
15	A	1132	CLA	MG-NA	6.23	2.21	2.06
15	A	1122	CLA	MG-NA	6.23	2.21	2.06
15	2	608	CLA	MG-NA	6.22	2.21	2.06
14	4	503	BCR	C24-C23	6.22	1.51	1.33
15	A	1140	CLA	MG-NA	6.18	2.21	2.06
15	A	1013	CLA	MG-NA	6.18	2.21	2.06
15	3	610	CLA	MG-NA	6.18	2.21	2.06
15	B	1022	CLA	MG-NA	6.16	2.20	2.06
15	B	1228	CLA	MG-NA	6.13	2.20	2.06
15	4	603	CLA	MG-NA	6.12	2.20	2.06
15	A	1116	CLA	MG-NA	6.12	2.20	2.06
15	2	615	CLA	MG-NA	6.10	2.20	2.06
15	3	612	CLA	MG-NA	6.10	2.20	2.06
15	B	1224	CLA	MG-NA	6.07	2.20	2.06
15	B	1226	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	613	CLA	MG-NA	6.05	2.20	2.06
15	2	603	CLA	MG-NA	6.04	2.20	2.06
15	B	1236	CLA	MG-NA	6.02	2.20	2.06
15	1	601	CLA	MG-NA	6.02	2.20	2.06
15	A	1110	CLA	MG-NA	6.02	2.20	2.06
15	B	1235	CLA	MG-NA	6.02	2.20	2.06
15	4	602	CLA	MG-NA	6.01	2.20	2.06
15	2	604	CLA	MG-NA	5.97	2.20	2.06
15	B	1219	CLA	MG-NA	5.94	2.20	2.06
15	B	1210	CLA	MG-NA	5.94	2.20	2.06
14	3	503	BCR	C24-C23	5.93	1.51	1.33
15	A	1111	CLA	MG-NA	5.92	2.20	2.06
15	1	605	CLA	MG-NA	5.90	2.20	2.06
15	4	601	CLA	MG-NA	5.89	2.20	2.06
14	B	4006	BCR	C24-C23	5.89	1.50	1.33
15	3	605	CLA	MG-NA	5.89	2.20	2.06
15	4	607	CLA	MG-NA	5.88	2.20	2.06
15	B	1207	CLA	CHA-C4D	5.86	1.51	1.38
14	1	505	BCR	C24-C23	5.84	1.50	1.33
14	4	505	BCR	C24-C23	5.84	1.50	1.33
15	F	1302	CLA	MG-NA	5.83	2.20	2.06
14	2	503	BCR	C24-C23	5.82	1.50	1.33
14	F	4002	BCR	C24-C23	5.82	1.50	1.33
14	B	4001	BCR	C24-C23	5.80	1.50	1.33
14	A	4004	BCR	C24-C23	5.79	1.50	1.33
14	A	4002	BCR	C24-C23	5.78	1.50	1.33
14	A	4007	BCR	C24-C23	5.78	1.50	1.33
14	J	4002	BCR	C24-C23	5.78	1.50	1.33
14	A	4005	BCR	C24-C23	5.77	1.50	1.33
15	B	1216	CLA	MG-NA	5.76	2.20	2.06
14	B	4002	BCR	C24-C23	5.76	1.50	1.33
14	J	4001	BCR	C24-C23	5.76	1.50	1.33
14	3	504	BCR	C24-C23	5.72	1.50	1.33
14	B	4005	BCR	C24-C23	5.69	1.50	1.33
15	2	601	CLA	MG-NA	5.67	2.19	2.06
14	B	4003	BCR	C24-C23	5.64	1.50	1.33
23	B	5031	GSH	CD1-N2	5.61	1.46	1.34
14	B	4004	BCR	C24-C23	5.60	1.50	1.33
14	J	4003	BCR	C24-C23	5.58	1.49	1.33
15	B	1213	CLA	MG-NA	5.57	2.19	2.06
14	1	503	BCR	C24-C23	5.56	1.49	1.33
14	A	4003	BCR	C24-C23	5.56	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	831	GSH	C2-N3	5.52	1.45	1.33
23	B	5031	GSH	C2-N3	5.50	1.45	1.33
23	4	831	GSH	CD1-N2	5.41	1.45	1.34
14	A	4006	BCR	C24-C23	5.31	1.49	1.33
14	J	4001	BCR	C11-C12	-5.28	1.21	1.34
14	2	503	BCR	C11-C12	-5.20	1.21	1.34
14	1	505	BCR	C11-C12	-5.16	1.21	1.34
14	A	4006	BCR	C11-C12	-5.13	1.21	1.34
24	A	1011	CL0	O2D-CGD	5.12	1.45	1.33
14	J	4003	BCR	C11-C12	-5.11	1.21	1.34
14	3	504	BCR	C11-C12	-5.09	1.21	1.34
14	B	4004	BCR	C11-C12	-5.09	1.21	1.34
14	4	503	BCR	C11-C12	-5.09	1.21	1.34
14	B	4001	BCR	C11-C12	-5.08	1.21	1.34
14	1	503	BCR	C11-C12	-5.07	1.21	1.34
14	B	4002	BCR	C11-C12	-5.05	1.21	1.34
15	B	1207	CLA	C3A-C2A	-5.05	1.39	1.52
14	A	4002	BCR	C11-C12	-5.05	1.21	1.34
14	A	4007	BCR	C11-C12	-5.04	1.21	1.34
14	B	4005	BCR	C11-C12	-5.03	1.21	1.34
24	A	1011	CL0	O2A-C1	5.01	1.60	1.46
14	B	4003	BCR	C11-C12	-5.00	1.21	1.34
14	A	4004	BCR	C11-C12	-4.99	1.21	1.34
14	F	4002	BCR	C11-C12	-4.99	1.21	1.34
14	3	503	BCR	C11-C12	-4.99	1.21	1.34
15	B	1023	CLA	MG-ND	-4.96	1.95	2.05
24	A	1011	CL0	C3C-C2C	4.92	1.47	1.36
14	A	4003	BCR	C11-C12	-4.89	1.22	1.34
14	J	4002	BCR	C11-C12	-4.89	1.22	1.34
14	4	505	BCR	C11-C12	-4.81	1.22	1.34
24	A	1011	CL0	CHD-C1D	4.80	1.47	1.38
14	B	4006	BCR	C11-C12	-4.77	1.22	1.34
15	F	1301	CLA	MG-ND	-4.71	1.96	2.05
24	A	1011	CL0	CHC-C1C	4.69	1.48	1.38
14	B	4005	BCR	C16-C17	-4.57	1.29	1.43
24	A	1011	CL0	CHC-C4B	4.54	1.49	1.39
15	1	613	CLA	CBB-CAB	4.48	1.52	1.30
15	B	1236	CLA	MG-ND	-4.46	1.96	2.05
15	4	606	CLA	CBB-CAB	4.43	1.52	1.30
15	B	1218	CLA	CBB-CAB	4.43	1.52	1.30
21	2	811	DGD	O1G-C1A	4.43	1.46	1.33
15	4	607	CLA	CBB-CAB	4.43	1.52	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	605	CLA	CBB-CAB	4.43	1.52	1.30
15	4	615	CLA	CBB-CAB	4.42	1.52	1.30
14	J	4001	BCR	C16-C17	-4.41	1.29	1.43
15	F	1302	CLA	CBB-CAB	4.40	1.52	1.30
14	A	4006	BCR	C16-C17	-4.40	1.29	1.43
24	A	1011	CL0	C3D-C4D	-4.39	1.34	1.44
15	B	1231	CLA	MG-ND	-4.37	1.97	2.05
14	1	503	BCR	C16-C17	-4.37	1.29	1.43
14	4	503	BCR	C16-C17	-4.37	1.29	1.43
15	B	1208	CLA	CBB-CAB	4.36	1.51	1.30
15	1	615	CLA	CBB-CAB	4.35	1.51	1.30
15	B	1228	CLA	CBB-CAB	4.35	1.51	1.30
21	4	811	DGD	O1G-C1A	4.35	1.46	1.33
15	4	603	CLA	MG-ND	-4.34	1.97	2.05
15	B	1216	CLA	CBB-CAB	4.34	1.51	1.30
14	J	4002	BCR	C16-C17	-4.34	1.30	1.43
15	B	1231	CLA	CBB-CAB	4.33	1.51	1.30
15	A	1135	CLA	CBB-CAB	4.33	1.51	1.30
16	4	610	CHL	CBB-CAB	4.33	1.51	1.30
15	A	1138	CLA	CBB-CAB	4.33	1.51	1.30
15	B	1213	CLA	CBB-CAB	4.33	1.51	1.30
15	A	1127	CLA	CBB-CAB	4.33	1.51	1.30
15	B	1201	CLA	CBB-CAB	4.33	1.51	1.30
14	3	504	BCR	C16-C17	-4.33	1.30	1.43
15	B	1206	CLA	CBB-CAB	4.33	1.51	1.30
15	B	1235	CLA	MG-ND	-4.33	1.97	2.05
15	2	608	CLA	CBB-CAB	4.33	1.51	1.30
15	A	1111	CLA	CBB-CAB	4.32	1.51	1.30
15	A	1133	CLA	CBB-CAB	4.32	1.51	1.30
15	1	603	CLA	MG-ND	-4.32	1.97	2.05
15	1	605	CLA	MG-ND	-4.32	1.97	2.05
21	B	5002	DGD	O1G-C1A	4.32	1.46	1.33
15	4	604	CLA	CBB-CAB	4.32	1.51	1.30
15	B	1212	CLA	CBB-CAB	4.32	1.51	1.30
15	4	602	CLA	CBB-CAB	4.32	1.51	1.30
15	1	605	CLA	CBB-CAB	4.32	1.51	1.30
15	B	1229	CLA	CBB-CAB	4.31	1.51	1.30
16	2	610	CHL	CBB-CAB	4.31	1.51	1.30
15	3	601	CLA	CBB-CAB	4.31	1.51	1.30
15	B	1223	CLA	CBB-CAB	4.31	1.51	1.30
15	B	1237	CLA	CBB-CAB	4.31	1.51	1.30
15	3	603	CLA	CBB-CAB	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	603	CLA	CBB-CAB	4.30	1.51	1.30
15	2	612	CLA	CBB-CAB	4.30	1.51	1.30
15	A	1140	CLA	CBB-CAB	4.30	1.51	1.30
15	1	606	CLA	CBB-CAB	4.30	1.51	1.30
15	B	1204	CLA	CBB-CAB	4.30	1.51	1.30
14	A	4004	BCR	C16-C17	-4.30	1.30	1.43
15	A	1122	CLA	CBB-CAB	4.30	1.51	1.30
15	B	1236	CLA	CBB-CAB	4.30	1.51	1.30
15	A	1139	CLA	CBB-CAB	4.30	1.51	1.30
15	A	1116	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1131	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1119	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1101	CLA	MG-ND	-4.29	1.97	2.05
15	B	1023	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1128	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1110	CLA	CBB-CAB	4.29	1.51	1.30
15	B	1225	CLA	CBB-CAB	4.29	1.51	1.30
15	B	1226	CLA	CBB-CAB	4.29	1.51	1.30
15	F	1301	CLA	CBB-CAB	4.29	1.51	1.30
15	B	1205	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1129	CLA	CBB-CAB	4.29	1.51	1.30
15	B	1203	CLA	CBB-CAB	4.29	1.51	1.30
15	A	1141	CLA	CBB-CAB	4.28	1.51	1.30
15	A	1121	CLA	CBB-CAB	4.28	1.51	1.30
15	A	1137	CLA	CBB-CAB	4.28	1.51	1.30
15	A	1117	CLA	CBB-CAB	4.28	1.51	1.30
15	A	1115	CLA	CBB-CAB	4.28	1.51	1.30
24	A	1011	CL0	CHD-C4C	4.28	1.49	1.39
15	3	605	CLA	CBB-CAB	4.28	1.51	1.30
14	B	4004	BCR	C16-C17	-4.28	1.30	1.43
15	B	1239	CLA	CBB-CAB	4.28	1.51	1.30
16	3	604	CHL	CBB-CAB	4.28	1.51	1.30
15	B	1215	CLA	CBB-CAB	4.28	1.51	1.30
15	1	601	CLA	CBB-CAB	4.27	1.51	1.30
15	B	1221	CLA	CBB-CAB	4.27	1.51	1.30
15	4	601	CLA	CBB-CAB	4.27	1.51	1.30
15	A	1130	CLA	CBB-CAB	4.27	1.51	1.30
15	2	604	CLA	MG-ND	-4.27	1.97	2.05
15	4	612	CLA	CBB-CAB	4.27	1.51	1.30
15	A	1114	CLA	CBB-CAB	4.27	1.51	1.30
15	B	1209	CLA	CBB-CAB	4.27	1.51	1.30
15	3	613	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	608	CLA	CBB-CAB	4.27	1.51	1.30
15	A	1013	CLA	CBB-CAB	4.27	1.51	1.30
15	A	1118	CLA	CBB-CAB	4.26	1.51	1.30
15	1	602	CLA	CBB-CAB	4.26	1.51	1.30
15	2	607	CLA	CBB-CAB	4.26	1.51	1.30
15	3	606	CLA	CBB-CAB	4.26	1.51	1.30
15	A	1132	CLA	CBB-CAB	4.26	1.51	1.30
15	1	608	CLA	CBB-CAB	4.26	1.51	1.30
15	3	610	CLA	CBB-CAB	4.26	1.51	1.30
15	A	1120	CLA	CBB-CAB	4.26	1.51	1.30
15	3	607	CLA	CBB-CAB	4.26	1.51	1.30
15	A	1102	CLA	CBB-CAB	4.25	1.51	1.30
15	B	1210	CLA	CBB-CAB	4.25	1.51	1.30
15	4	609	CLA	CBB-CAB	4.25	1.51	1.30
15	A	1105	CLA	CBB-CAB	4.25	1.51	1.30
15	A	1103	CLA	CBB-CAB	4.25	1.51	1.30
15	B	1021	CLA	CBB-CAB	4.25	1.51	1.30
15	B	1220	CLA	CBB-CAB	4.25	1.51	1.30
15	2	605	CLA	CBB-CAB	4.25	1.51	1.30
15	B	1207	CLA	C3B-C4B	4.25	1.49	1.40
15	A	1107	CLA	CBB-CAB	4.25	1.51	1.30
15	A	1134	CLA	CBB-CAB	4.25	1.51	1.30
16	2	609	CHL	CBB-CAB	4.25	1.51	1.30
15	2	602	CLA	CBB-CAB	4.25	1.51	1.30
16	1	610	CHL	CBB-CAB	4.25	1.51	1.30
15	1	607	CLA	CBB-CAB	4.24	1.51	1.30
15	B	1217	CLA	CBB-CAB	4.24	1.51	1.30
15	2	606	CLA	CBB-CAB	4.24	1.51	1.30
15	B	1222	CLA	CBB-CAB	4.24	1.51	1.30
15	A	1113	CLA	CBB-CAB	4.24	1.51	1.30
15	3	608	CLA	CBB-CAB	4.24	1.51	1.30
15	1	604	CLA	CBB-CAB	4.24	1.51	1.30
15	B	1227	CLA	CBB-CAB	4.23	1.51	1.30
15	B	1234	CLA	CBB-CAB	4.23	1.51	1.30
15	A	1123	CLA	CBB-CAB	4.23	1.51	1.30
15	A	1126	CLA	CBB-CAB	4.23	1.51	1.30
15	1	603	CLA	CBB-CAB	4.22	1.51	1.30
15	2	615	CLA	CBB-CAB	4.22	1.51	1.30
15	A	1104	CLA	CBB-CAB	4.22	1.51	1.30
15	1	612	CLA	CBB-CAB	4.22	1.51	1.30
15	B	1202	CLA	CBB-CAB	4.22	1.51	1.30
15	A	1124	CLA	CBB-CAB	4.22	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	601	CLA	CBB-CAB	4.22	1.51	1.30
15	B	1214	CLA	CBB-CAB	4.22	1.51	1.30
24	A	1011	CL0	C1D-ND	-4.22	1.32	1.37
15	1	611	CLA	CBB-CAB	4.22	1.51	1.30
15	B	1238	CLA	CBB-CAB	4.21	1.51	1.30
16	2	613	CHL	CBB-CAB	4.21	1.51	1.30
14	J	4003	BCR	C16-C17	-4.21	1.30	1.43
15	A	1106	CLA	CBB-CAB	4.21	1.51	1.30
15	A	1109	CLA	CBB-CAB	4.21	1.51	1.30
15	3	615	CLA	MG-ND	-4.21	1.97	2.05
15	3	615	CLA	CBB-CAB	4.21	1.51	1.30
15	A	1136	CLA	CBB-CAB	4.21	1.51	1.30
15	B	1224	CLA	CBB-CAB	4.21	1.51	1.30
15	A	1108	CLA	CBB-CAB	4.20	1.51	1.30
15	B	1232	CLA	CBB-CAB	4.20	1.51	1.30
15	A	1112	CLA	CBB-CAB	4.20	1.51	1.30
15	A	1012	CLA	CBB-CAB	4.20	1.51	1.30
14	3	503	BCR	C16-C17	-4.20	1.30	1.43
16	1	609	CHL	CBB-CAB	4.20	1.51	1.30
14	B	4002	BCR	C16-C17	-4.19	1.30	1.43
15	A	1125	CLA	CBB-CAB	4.19	1.51	1.30
15	2	603	CLA	MG-ND	-4.19	1.97	2.05
15	A	1101	CLA	CBB-CAB	4.19	1.51	1.30
16	2	611	CHL	CBB-CAB	4.19	1.51	1.30
14	A	4002	BCR	C16-C17	-4.19	1.30	1.43
14	A	4005	BCR	C16-C17	-4.19	1.30	1.43
14	2	503	BCR	C16-C17	-4.18	1.30	1.43
15	3	612	CLA	CBB-CAB	4.18	1.51	1.30
14	A	4003	BCR	C16-C17	-4.18	1.30	1.43
14	A	4007	BCR	C16-C17	-4.18	1.30	1.43
15	2	605	CLA	MG-ND	-4.18	1.97	2.05
15	3	611	CLA	CBB-CAB	4.17	1.51	1.30
14	F	4002	BCR	C16-C17	-4.16	1.30	1.43
15	2	604	CLA	CBB-CAB	4.15	1.50	1.30
16	4	611	CHL	CBB-CAB	4.13	1.50	1.30
16	4	613	CHL	CBB-CAB	4.13	1.50	1.30
14	B	4001	BCR	C16-C17	-4.13	1.30	1.43
15	B	1211	CLA	CBB-CAB	4.13	1.50	1.30
15	A	1124	CLA	MG-ND	-4.12	1.97	2.05
15	B	1230	CLA	CBB-CAB	4.11	1.50	1.30
14	4	505	BCR	C16-C17	-4.11	1.30	1.43
15	4	603	CLA	CBB-CAB	4.11	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	1302	CLA	CBB-CAB	4.11	1.50	1.30
15	2	612	CLA	MG-ND	-4.10	1.97	2.05
15	B	1022	CLA	CBB-CAB	4.10	1.50	1.30
15	B	1219	CLA	CBB-CAB	4.09	1.50	1.30
14	1	505	BCR	C16-C17	-4.08	1.30	1.43
15	B	1240	CLA	CBB-CAB	4.07	1.50	1.30
15	1	608	CLA	MG-ND	-4.02	1.97	2.05
15	J	1302	CLA	MG-ND	-4.02	1.97	2.05
14	B	4003	BCR	C16-C17	-4.01	1.31	1.43
15	4	602	CLA	MG-ND	-4.00	1.97	2.05
15	B	1208	CLA	MG-ND	-4.00	1.97	2.05
15	4	615	CLA	MG-ND	-3.98	1.97	2.05
15	B	1228	CLA	MG-ND	-3.96	1.97	2.05
15	A	1107	CLA	MG-ND	-3.96	1.97	2.05
15	B	1232	CLA	MG-ND	-3.96	1.97	2.05
15	A	1103	CLA	MG-ND	-3.96	1.97	2.05
15	1	611	CLA	MG-ND	-3.96	1.97	2.05
15	A	1132	CLA	MG-ND	-3.95	1.97	2.05
24	A	1011	CL0	MG-NC	3.95	2.15	2.06
15	4	609	CLA	MG-ND	-3.94	1.98	2.05
15	B	1235	CLA	CBB-CAB	3.94	1.49	1.30
15	B	1216	CLA	MG-ND	-3.93	1.98	2.05
15	A	1113	CLA	MG-ND	-3.93	1.98	2.05
15	F	1302	CLA	MG-ND	-3.93	1.98	2.05
15	B	1217	CLA	MG-ND	-3.92	1.98	2.05
15	A	1112	CLA	MG-ND	-3.91	1.98	2.05
15	A	1136	CLA	MG-ND	-3.91	1.98	2.05
15	B	1224	CLA	MG-ND	-3.90	1.98	2.05
15	2	601	CLA	MG-ND	-3.90	1.98	2.05
15	B	1240	CLA	MG-ND	-3.89	1.98	2.05
15	3	603	CLA	MG-ND	-3.89	1.98	2.05
15	3	613	CLA	MG-ND	-3.88	1.98	2.05
15	B	1220	CLA	MG-ND	-3.87	1.98	2.05
15	2	608	CLA	MG-ND	-3.87	1.98	2.05
15	2	606	CLA	MG-ND	-3.86	1.98	2.05
14	B	4006	BCR	C16-C17	-3.86	1.31	1.43
15	B	1223	CLA	C4B-NB	-3.84	1.33	1.37
15	B	1213	CLA	MG-ND	-3.84	1.98	2.05
15	3	612	CLA	MG-ND	-3.84	1.98	2.05
15	1	607	CLA	MG-ND	-3.83	1.98	2.05
15	A	1137	CLA	MG-ND	-3.83	1.98	2.05
15	B	1209	CLA	MG-ND	-3.83	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1212	CLA	MG-ND	-3.83	1.98	2.05
15	B	1221	CLA	MG-ND	-3.82	1.98	2.05
15	A	1128	CLA	MG-ND	-3.81	1.98	2.05
15	A	1012	CLA	C1C-NC	-3.81	1.32	1.37
15	A	1012	CLA	MG-ND	-3.81	1.98	2.05
15	A	1110	CLA	MG-ND	-3.80	1.98	2.05
15	A	1116	CLA	MG-ND	-3.80	1.98	2.05
15	B	1022	CLA	MG-ND	-3.79	1.98	2.05
15	A	1125	CLA	MG-ND	-3.79	1.98	2.05
24	A	1011	CL0	OBD-CAD	3.79	1.29	1.22
15	A	1119	CLA	MG-ND	-3.78	1.98	2.05
15	A	1134	CLA	MG-ND	-3.78	1.98	2.05
15	A	1106	CLA	MG-ND	-3.77	1.98	2.05
15	2	607	CLA	MG-ND	-3.77	1.98	2.05
15	B	1211	CLA	MG-ND	-3.76	1.98	2.05
15	B	1021	CLA	MG-ND	-3.76	1.98	2.05
15	B	1238	CLA	MG-ND	-3.75	1.98	2.05
15	3	605	CLA	MG-ND	-3.74	1.98	2.05
15	B	1237	CLA	MG-ND	-3.74	1.98	2.05
15	B	1202	CLA	MG-ND	-3.74	1.98	2.05
15	1	612	CLA	MG-ND	-3.74	1.98	2.05
15	B	1229	CLA	C4B-NB	-3.74	1.33	1.37
15	B	1225	CLA	MG-ND	-3.73	1.98	2.05
24	A	1011	CL0	CHB-C1B	3.72	1.47	1.39
15	3	611	CLA	MG-ND	-3.72	1.98	2.05
15	B	1201	CLA	MG-ND	-3.72	1.98	2.05
15	B	1206	CLA	MG-ND	-3.72	1.98	2.05
15	A	1122	CLA	MG-ND	-3.71	1.98	2.05
15	1	604	CLA	MG-ND	-3.70	1.98	2.05
15	A	1102	CLA	MG-ND	-3.70	1.98	2.05
15	A	1108	CLA	MG-ND	-3.70	1.98	2.05
15	1	601	CLA	MG-ND	-3.70	1.98	2.05
15	4	604	CLA	MG-ND	-3.69	1.98	2.05
15	A	1131	CLA	MG-ND	-3.69	1.98	2.05
15	A	1120	CLA	MG-ND	-3.69	1.98	2.05
15	A	1135	CLA	MG-ND	-3.69	1.98	2.05
15	A	1117	CLA	MG-ND	-3.69	1.98	2.05
15	A	1141	CLA	MG-ND	-3.68	1.98	2.05
15	A	1127	CLA	C1C-NC	-3.68	1.32	1.37
15	A	1133	CLA	MG-ND	-3.67	1.98	2.05
15	1	613	CLA	MG-ND	-3.67	1.98	2.05
15	1	602	CLA	MG-ND	-3.67	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	601	CLA	MG-ND	-3.67	1.98	2.05
15	3	601	CLA	MG-ND	-3.66	1.98	2.05
15	A	1115	CLA	MG-ND	-3.66	1.98	2.05
15	A	1123	CLA	MG-ND	-3.66	1.98	2.05
15	A	1139	CLA	MG-ND	-3.65	1.98	2.05
15	A	1121	CLA	MG-ND	-3.65	1.98	2.05
15	1	615	CLA	MG-ND	-3.65	1.98	2.05
15	B	1239	CLA	MG-ND	-3.65	1.98	2.05
15	4	612	CLA	C1C-NC	-3.64	1.32	1.37
15	A	1109	CLA	MG-ND	-3.63	1.98	2.05
15	B	1222	CLA	MG-ND	-3.62	1.98	2.05
15	B	1226	CLA	MG-ND	-3.62	1.98	2.05
15	B	1214	CLA	MG-ND	-3.62	1.98	2.05
15	3	608	CLA	MG-ND	-3.62	1.98	2.05
15	4	612	CLA	MG-ND	-3.62	1.98	2.05
15	A	1138	CLA	MG-ND	-3.61	1.98	2.05
15	1	603	CLA	C4B-NB	-3.61	1.33	1.37
15	3	606	CLA	MG-ND	-3.60	1.98	2.05
15	2	615	CLA	MG-ND	-3.60	1.98	2.05
15	4	605	CLA	C1C-NC	-3.59	1.32	1.37
24	A	1011	CL0	C1B-NB	-3.59	1.33	1.37
15	B	1205	CLA	MG-ND	-3.58	1.98	2.05
15	3	607	CLA	MG-ND	-3.58	1.98	2.05
15	A	1104	CLA	MG-ND	-3.58	1.98	2.05
15	A	1126	CLA	MG-ND	-3.56	1.98	2.05
15	A	1130	CLA	MG-ND	-3.55	1.98	2.05
15	B	1219	CLA	MG-ND	-3.55	1.98	2.05
20	4	901	CAC	O2-AS	3.54	1.79	1.70
15	B	1227	CLA	C1C-NC	-3.54	1.32	1.37
15	B	1227	CLA	MG-ND	-3.53	1.98	2.05
15	B	1218	CLA	C1C-NC	-3.53	1.32	1.37
15	B	1229	CLA	C1C-NC	-3.53	1.32	1.37
15	A	1127	CLA	MG-ND	-3.52	1.98	2.05
15	A	1129	CLA	MG-ND	-3.51	1.98	2.05
15	B	1215	CLA	C4B-NB	-3.51	1.33	1.37
15	A	1013	CLA	C1C-NC	-3.50	1.32	1.37
15	A	1118	CLA	MG-ND	-3.50	1.98	2.05
15	1	604	CLA	C1C-NC	-3.50	1.32	1.37
20	1	901	CAC	O2-AS	3.49	1.79	1.70
15	1	612	CLA	C1C-NC	-3.48	1.32	1.37
15	1	603	CLA	C1C-NC	-3.48	1.32	1.37
15	J	1302	CLA	C1C-NC	-3.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	606	CLA	MG-ND	-3.46	1.98	2.05
15	4	608	CLA	MG-ND	-3.46	1.98	2.05
15	B	1222	CLA	C4B-NB	-3.45	1.33	1.37
15	A	1105	CLA	MG-ND	-3.45	1.98	2.05
15	A	1012	CLA	C4B-NB	-3.45	1.33	1.37
15	2	602	CLA	MG-ND	-3.45	1.99	2.05
20	4	902	CAC	O2-AS	3.44	1.79	1.70
15	4	605	CLA	MG-ND	-3.43	1.99	2.05
15	A	1013	CLA	C4B-NB	-3.42	1.33	1.37
15	1	606	CLA	MG-ND	-3.42	1.99	2.05
15	B	1203	CLA	MG-ND	-3.42	1.99	2.05
15	B	1222	CLA	C1C-NC	-3.39	1.32	1.37
15	A	1131	CLA	C1C-NC	-3.39	1.32	1.37
15	B	1201	CLA	C1C-NC	-3.39	1.32	1.37
15	B	1227	CLA	C4B-NB	-3.38	1.33	1.37
15	B	1215	CLA	C1C-NC	-3.38	1.32	1.37
15	3	610	CLA	MG-ND	-3.36	1.99	2.05
15	3	605	CLA	C1C-NC	-3.36	1.32	1.37
15	A	1140	CLA	C1C-NC	-3.35	1.32	1.37
15	A	1128	CLA	C1C-NC	-3.34	1.32	1.37
15	1	602	CLA	C1C-NC	-3.34	1.32	1.37
15	B	1204	CLA	MG-ND	-3.34	1.99	2.05
15	2	612	CLA	C1C-NC	-3.34	1.32	1.37
15	B	1204	CLA	C1C-NC	-3.33	1.32	1.37
15	A	1130	CLA	C1C-NC	-3.33	1.32	1.37
15	A	1138	CLA	C1C-NC	-3.32	1.32	1.37
15	4	603	CLA	C4B-NB	-3.32	1.33	1.37
15	4	602	CLA	C1C-NC	-3.32	1.32	1.37
15	4	601	CLA	C1C-NC	-3.31	1.32	1.37
15	A	1133	CLA	C1C-NC	-3.31	1.32	1.37
15	4	606	CLA	C1C-NC	-3.31	1.32	1.37
15	2	601	CLA	C1C-NC	-3.30	1.32	1.37
15	3	606	CLA	C1C-NC	-3.30	1.32	1.37
15	4	609	CLA	C1C-NC	-3.27	1.32	1.37
15	1	601	CLA	C1C-NC	-3.27	1.32	1.37
15	B	1209	CLA	C1C-NC	-3.27	1.32	1.37
15	B	1234	CLA	MG-ND	-3.26	1.99	2.05
15	B	1217	CLA	C1C-NC	-3.26	1.32	1.37
15	B	1226	CLA	C1C-NC	-3.26	1.32	1.37
15	B	1210	CLA	MG-ND	-3.25	1.99	2.05
15	A	1139	CLA	C1C-NC	-3.25	1.33	1.37
15	4	607	CLA	MG-ND	-3.24	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1139	CLA	C4B-NB	-3.24	1.33	1.37
15	B	1223	CLA	C1C-NC	-3.24	1.33	1.37
15	A	1118	CLA	C1C-NC	-3.23	1.33	1.37
15	A	1117	CLA	C1C-NC	-3.23	1.33	1.37
15	1	611	CLA	C1C-NC	-3.23	1.33	1.37
15	2	607	CLA	C1C-NC	-3.23	1.33	1.37
15	A	1108	CLA	C1C-NC	-3.23	1.33	1.37
20	3	902	CAC	O2-AS	3.23	1.78	1.70
15	A	1114	CLA	MG-ND	-3.22	1.99	2.05
15	A	1136	CLA	C1C-NC	-3.22	1.33	1.37
15	3	603	CLA	C1C-NC	-3.22	1.33	1.37
15	1	607	CLA	C1C-NC	-3.22	1.33	1.37
15	A	1116	CLA	C1C-NC	-3.22	1.33	1.37
15	3	615	CLA	C1C-NC	-3.22	1.33	1.37
15	1	615	CLA	C4B-NB	-3.22	1.33	1.37
15	B	1240	CLA	C1C-NC	-3.21	1.33	1.37
15	A	1112	CLA	C1C-NC	-3.21	1.33	1.37
15	A	1114	CLA	C1C-NC	-3.21	1.33	1.37
15	2	603	CLA	C1C-NC	-3.20	1.33	1.37
15	A	1132	CLA	C1C-NC	-3.20	1.33	1.37
15	A	1111	CLA	MG-ND	-3.20	1.99	2.05
15	A	1127	CLA	C4B-NB	-3.19	1.33	1.37
15	A	1107	CLA	C1C-NC	-3.19	1.33	1.37
15	1	608	CLA	C1C-NC	-3.19	1.33	1.37
15	3	613	CLA	C1C-NC	-3.19	1.33	1.37
15	1	606	CLA	C1C-NC	-3.19	1.33	1.37
15	3	608	CLA	C1C-NC	-3.19	1.33	1.37
15	B	1218	CLA	MG-ND	-3.19	1.99	2.05
15	B	1202	CLA	C1C-NC	-3.18	1.33	1.37
15	A	1101	CLA	C1C-NC	-3.17	1.33	1.37
15	4	608	CLA	C1C-NC	-3.17	1.33	1.37
15	B	1224	CLA	C1C-NC	-3.17	1.33	1.37
15	B	1207	CLA	MG-NA	-3.16	1.98	2.06
15	A	1119	CLA	C1C-NC	-3.16	1.33	1.37
15	B	1212	CLA	C1C-NC	-3.16	1.33	1.37
15	2	608	CLA	C1C-NC	-3.16	1.33	1.37
15	B	1021	CLA	C1C-NC	-3.15	1.33	1.37
15	B	1223	CLA	MG-ND	-3.15	1.99	2.05
15	A	1013	CLA	MG-ND	-3.15	1.99	2.05
15	B	1211	CLA	C1C-NC	-3.13	1.33	1.37
15	B	1237	CLA	C1C-NC	-3.13	1.33	1.37
15	A	1109	CLA	C1C-NC	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1135	CLA	C1C-NC	-3.12	1.33	1.37
15	A	1115	CLA	C1C-NC	-3.12	1.33	1.37
15	A	1138	CLA	C4B-NB	-3.12	1.34	1.37
15	B	1219	CLA	C1C-NC	-3.11	1.33	1.37
15	4	615	CLA	C1C-NC	-3.11	1.33	1.37
15	B	1215	CLA	MG-ND	-3.11	1.99	2.05
15	B	1208	CLA	C1C-NC	-3.11	1.33	1.37
15	A	1129	CLA	C1C-NC	-3.11	1.33	1.37
15	B	1230	CLA	C1C-NC	-3.10	1.33	1.37
15	4	603	CLA	C1C-NC	-3.10	1.33	1.37
15	3	610	CLA	C1C-NC	-3.10	1.33	1.37
15	A	1121	CLA	C1C-NC	-3.10	1.33	1.37
15	4	605	CLA	C4B-NB	-3.10	1.34	1.37
15	A	1102	CLA	C1C-NC	-3.10	1.33	1.37
15	B	1207	CLA	C2D-C1D	3.10	1.51	1.44
15	A	1110	CLA	C1C-NC	-3.09	1.33	1.37
15	B	1214	CLA	C1C-NC	-3.09	1.33	1.37
15	B	1216	CLA	C1C-NC	-3.08	1.33	1.37
15	3	612	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1141	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1111	CLA	C1C-NC	-3.08	1.33	1.37
15	B	1022	CLA	C1C-NC	-3.08	1.33	1.37
15	B	1220	CLA	C1C-NC	-3.08	1.33	1.37
18	1	802	LMG	C37-C36	-3.08	1.34	1.51
15	B	1221	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1105	CLA	C1C-NC	-3.07	1.33	1.37
15	A	1119	CLA	C4B-NB	-3.07	1.34	1.37
15	2	615	CLA	C1C-NC	-3.07	1.33	1.37
15	B	1206	CLA	C1C-NC	-3.07	1.33	1.37
20	1	902	CAC	O2-AS	3.07	1.78	1.70
15	A	1130	CLA	C4B-NB	-3.07	1.34	1.37
15	A	1113	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1103	CLA	C1C-NC	-3.06	1.33	1.37
15	B	1239	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1106	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1137	CLA	C1C-NC	-3.05	1.33	1.37
15	B	1232	CLA	C1C-NC	-3.05	1.33	1.37
15	F	1301	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1123	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1126	CLA	C1C-NC	-3.05	1.33	1.37
15	B	1203	CLA	C1C-NC	-3.05	1.33	1.37
15	2	605	CLA	C4B-NB	-3.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1134	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1108	CLA	C4B-NB	-3.04	1.34	1.37
15	2	602	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1238	CLA	C1C-NC	-3.04	1.33	1.37
15	A	1107	CLA	C4B-NB	-3.03	1.34	1.37
15	A	1122	CLA	C1C-NC	-3.02	1.33	1.37
15	3	607	CLA	C1C-NC	-3.02	1.33	1.37
24	A	1011	CL0	C4D-CHA	3.02	1.49	1.38
15	3	611	CLA	C1C-NC	-3.01	1.33	1.37
15	B	1201	CLA	C4B-NB	-3.01	1.34	1.37
15	4	607	CLA	C1C-NC	-3.01	1.33	1.37
15	2	612	CLA	C4B-NB	-3.00	1.34	1.37
15	B	1205	CLA	C1C-NC	-2.98	1.33	1.37
15	A	1120	CLA	C1C-NC	-2.98	1.33	1.37
15	B	1207	CLA	C2B-C1B	2.96	1.46	1.40
15	3	601	CLA	C4B-NB	-2.96	1.34	1.37
15	B	1210	CLA	C1C-NC	-2.96	1.33	1.37
15	1	613	CLA	C1C-NC	-2.96	1.33	1.37
15	1	605	CLA	C1C-NC	-2.95	1.33	1.37
15	A	1126	CLA	C4B-NB	-2.95	1.34	1.37
15	3	601	CLA	C1C-NC	-2.94	1.33	1.37
15	B	1230	CLA	MG-ND	-2.93	2.00	2.05
15	2	604	CLA	C1C-NC	-2.93	1.33	1.37
15	B	1207	CLA	C3D-C4D	2.93	1.50	1.44
15	A	1125	CLA	C1C-NC	-2.93	1.33	1.37
15	A	1129	CLA	C4B-NB	-2.93	1.34	1.37
15	2	606	CLA	C4B-NB	-2.92	1.34	1.37
15	J	1302	CLA	C4B-NB	-2.92	1.34	1.37
15	A	1131	CLA	C4B-NB	-2.91	1.34	1.37
15	B	1209	CLA	C4B-NB	-2.90	1.34	1.37
15	B	1234	CLA	C1C-NC	-2.90	1.33	1.37
24	A	1011	CL0	C4C-C3C	2.89	1.50	1.45
15	1	615	CLA	C1C-NC	-2.89	1.33	1.37
15	A	1104	CLA	C1C-NC	-2.89	1.33	1.37
15	A	1115	CLA	C4B-NB	-2.89	1.34	1.37
15	4	612	CLA	C4B-NB	-2.87	1.34	1.37
15	B	1203	CLA	C4B-NB	-2.87	1.34	1.37
24	A	1011	CL0	C3D-C2D	2.87	1.46	1.39
15	B	1229	CLA	MG-ND	-2.86	2.00	2.05
15	4	607	CLA	C4B-NB	-2.85	1.34	1.37
15	2	605	CLA	C1C-NC	-2.84	1.33	1.37
15	F	1302	CLA	C1C-NC	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	606	CLA	C4B-NB	-2.83	1.34	1.37
15	A	1123	CLA	C4B-NB	-2.83	1.34	1.37
20	3	901	CAC	O2-AS	2.83	1.77	1.70
15	B	1225	CLA	C1C-NC	-2.82	1.33	1.37
15	2	607	CLA	C4B-NB	-2.81	1.34	1.37
15	3	611	CLA	C4B-NB	-2.81	1.34	1.37
24	A	1011	CL0	C1B-C2B	2.78	1.49	1.43
15	2	604	CLA	C4B-NB	-2.78	1.34	1.37
15	B	1213	CLA	C1C-NC	-2.78	1.33	1.37
15	B	1207	CLA	MG-NB	2.78	2.11	2.05
15	3	613	CLA	C4B-NB	-2.77	1.34	1.37
15	B	1235	CLA	C4B-NB	-2.76	1.34	1.37
15	A	1136	CLA	C4B-NB	-2.74	1.34	1.37
15	2	606	CLA	C1C-NC	-2.74	1.33	1.37
15	A	1105	CLA	C4B-NB	-2.73	1.34	1.37
15	B	1217	CLA	C4B-NB	-2.73	1.34	1.37
15	B	1231	CLA	C1C-NC	-2.72	1.33	1.37
15	A	1111	CLA	MG-NC	2.72	2.12	2.06
15	A	1135	CLA	C4B-NB	-2.72	1.34	1.37
15	B	1237	CLA	C4B-NB	-2.70	1.34	1.37
15	B	1214	CLA	C4B-NB	-2.70	1.34	1.37
15	A	1114	CLA	C4B-NB	-2.70	1.34	1.37
15	4	609	CLA	C4B-NB	-2.70	1.34	1.37
15	B	1023	CLA	C4B-NB	-2.70	1.34	1.37
15	4	608	CLA	C4B-NB	-2.68	1.34	1.37
15	B	1206	CLA	C4B-NB	-2.68	1.34	1.37
15	A	1101	CLA	C4B-NB	-2.68	1.34	1.37
15	1	604	CLA	C4B-NB	-2.67	1.34	1.37
15	B	1210	CLA	C4B-NB	-2.66	1.34	1.37
15	2	608	CLA	C4B-NB	-2.66	1.34	1.37
15	3	605	CLA	C4B-NB	-2.65	1.34	1.37
15	B	1240	CLA	C4B-NB	-2.65	1.34	1.37
15	B	1219	CLA	C4B-NB	-2.64	1.34	1.37
15	A	1124	CLA	C1C-NC	-2.64	1.33	1.37
15	A	1141	CLA	C4B-NB	-2.64	1.34	1.37
15	A	1120	CLA	C4B-NB	-2.63	1.34	1.37
15	A	1133	CLA	C4B-NB	-2.63	1.34	1.37
15	A	1112	CLA	C4B-NB	-2.63	1.34	1.37
15	3	610	CLA	C4B-NB	-2.62	1.34	1.37
15	B	1211	CLA	C4B-NB	-2.62	1.34	1.37
15	A	1117	CLA	C4B-NB	-2.61	1.34	1.37
15	4	602	CLA	C4B-NB	-2.61	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1218	CLA	C4B-NB	-2.60	1.34	1.37
15	A	1140	CLA	MG-ND	-2.60	2.00	2.05
15	4	607	CLA	C1C-C2C	2.59	1.49	1.44
15	4	615	CLA	C4B-NB	-2.59	1.34	1.37
15	B	1210	CLA	MG-NC	2.59	2.12	2.06
15	2	603	CLA	C4B-NB	-2.58	1.34	1.37
15	A	1132	CLA	C4B-NB	-2.58	1.34	1.37
15	B	1235	CLA	C1C-NC	-2.58	1.34	1.37
15	2	601	CLA	MG-NC	2.58	2.12	2.06
15	A	1110	CLA	C4B-NB	-2.57	1.34	1.37
15	B	1205	CLA	C4B-NB	-2.57	1.34	1.37
15	1	605	CLA	MG-NC	2.56	2.12	2.06
15	2	615	CLA	C4B-NB	-2.56	1.34	1.37
24	A	1011	CL0	C1C-NC	-2.56	1.34	1.37
15	B	1216	CLA	MG-NC	2.56	2.12	2.06
15	B	1202	CLA	C4B-NB	-2.56	1.34	1.37
15	4	604	CLA	C1C-C2C	2.56	1.49	1.44
15	4	606	CLA	C4B-NB	-2.56	1.34	1.37
15	B	1221	CLA	C4B-NB	-2.55	1.34	1.37
15	A	1106	CLA	C4B-NB	-2.55	1.34	1.37
15	B	1204	CLA	C4B-NB	-2.55	1.34	1.37
15	A	1122	CLA	C4B-NB	-2.55	1.34	1.37
15	B	1236	CLA	C1C-NC	-2.55	1.34	1.37
15	B	1220	CLA	C4B-NB	-2.55	1.34	1.37
15	A	1134	CLA	C4B-NB	-2.54	1.34	1.37
21	2	811	DGD	CAA-C9A	-2.54	1.33	1.51
15	A	1116	CLA	C4B-NB	-2.54	1.34	1.37
15	4	602	CLA	MG-NC	2.54	2.12	2.06
21	4	811	DGD	O5D-C1E	2.54	1.44	1.40
15	3	607	CLA	C4B-NB	-2.54	1.34	1.37
24	A	1011	CL0	C1D-C2D	2.53	1.50	1.45
15	3	603	CLA	C4B-NB	-2.53	1.34	1.37
15	4	604	CLA	C4B-NB	-2.53	1.34	1.37
15	B	1238	CLA	C4B-NB	-2.53	1.34	1.37
15	3	615	CLA	C4B-NB	-2.53	1.34	1.37
15	A	1103	CLA	C4B-NB	-2.53	1.34	1.37
15	B	1224	CLA	C4B-NB	-2.53	1.34	1.37
15	B	1219	CLA	C1C-C2C	2.53	1.49	1.44
15	B	1219	CLA	MG-NC	2.52	2.12	2.06
15	3	608	CLA	C4B-NB	-2.52	1.34	1.37
15	4	604	CLA	C1C-NC	-2.52	1.34	1.37
15	1	606	CLA	C4B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1123	CLA	C1C-C2C	2.52	1.49	1.44
15	B	1212	CLA	C4B-NB	-2.52	1.34	1.37
15	1	611	CLA	C4B-NB	-2.51	1.34	1.37
15	A	1111	CLA	C4B-NB	-2.51	1.34	1.37
15	3	601	CLA	C1C-C2C	2.51	1.49	1.44
15	B	1223	CLA	C1C-C2C	2.50	1.49	1.44
15	A	1113	CLA	C4B-NB	-2.50	1.34	1.37
15	B	1202	CLA	C1C-C2C	2.49	1.49	1.44
15	4	603	CLA	MG-NC	2.49	2.12	2.06
15	A	1104	CLA	C4B-NB	-2.49	1.34	1.37
15	A	1012	CLA	CHD-C1D	2.49	1.43	1.38
15	A	1115	CLA	C1C-C2C	2.48	1.49	1.44
15	4	606	CLA	MG-NC	2.48	2.12	2.06
15	B	1216	CLA	C4B-NB	-2.48	1.34	1.37
15	4	601	CLA	MG-NC	2.48	2.12	2.06
15	B	1228	CLA	C1C-NC	-2.47	1.34	1.37
15	B	1236	CLA	MG-NC	2.47	2.12	2.06
15	B	1226	CLA	C4B-NB	-2.47	1.34	1.37
15	B	1023	CLA	C1C-C2C	2.46	1.49	1.44
15	B	1215	CLA	C1C-C2C	2.46	1.49	1.44
15	A	1140	CLA	C4B-NB	-2.46	1.34	1.37
15	B	1208	CLA	C4B-NB	-2.46	1.34	1.37
13	2	502	XAT	O24-C25	-2.46	1.42	1.46
15	A	1128	CLA	CHD-C1D	2.46	1.43	1.38
15	B	1021	CLA	C4B-NB	-2.45	1.34	1.37
15	A	1128	CLA	MG-NC	2.45	2.12	2.06
13	1	502	XAT	O24-C25	-2.45	1.42	1.46
15	B	1234	CLA	C4B-NB	-2.45	1.34	1.37
15	1	602	CLA	C4B-NB	-2.45	1.34	1.37
15	B	1213	CLA	MG-NC	2.44	2.12	2.06
15	B	1022	CLA	MG-NC	2.44	2.12	2.06
15	1	601	CLA	MG-NC	2.43	2.12	2.06
15	B	1229	CLA	CHD-C1D	2.43	1.43	1.38
15	B	1239	CLA	C4B-NB	-2.43	1.34	1.37
15	A	1108	CLA	C1C-C2C	2.42	1.49	1.44
15	B	1226	CLA	MG-NC	2.42	2.12	2.06
15	A	1121	CLA	C4B-NB	-2.42	1.34	1.37
15	4	612	CLA	MG-NC	2.42	2.12	2.06
15	2	602	CLA	C4B-NB	-2.41	1.34	1.37
15	B	1229	CLA	CHB-C4A	2.41	1.43	1.37
15	A	1128	CLA	C4B-NB	-2.41	1.34	1.37
15	1	608	CLA	C4B-NB	-2.41	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	1302	CLA	MG-NC	2.41	2.12	2.06
15	2	603	CLA	MG-NC	2.39	2.12	2.06
15	2	605	CLA	C1C-C2C	2.39	1.49	1.44
15	3	605	CLA	CHD-C1D	2.39	1.43	1.38
15	2	604	CLA	MG-NC	2.38	2.11	2.06
15	1	612	CLA	C4B-NB	-2.38	1.34	1.37
15	B	1222	CLA	CHD-C1D	2.38	1.43	1.38
15	A	1109	CLA	C4B-NB	-2.37	1.34	1.37
15	A	1110	CLA	C1C-C2C	2.37	1.49	1.44
22	2	821	LMT	O3'-C3'	-2.37	1.37	1.43
15	A	1124	CLA	C4B-NB	-2.37	1.34	1.37
21	2	811	DGD	O3G-C1D	2.36	1.44	1.40
15	3	603	CLA	MG-NC	2.36	2.11	2.06
15	A	1125	CLA	C4B-NB	-2.36	1.34	1.37
15	3	613	CLA	C1C-C2C	2.36	1.49	1.44
15	A	1119	CLA	C1C-C2C	2.36	1.49	1.44
15	A	1012	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1218	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1230	CLA	C4B-NB	-2.35	1.34	1.37
15	A	1120	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1232	CLA	C4B-NB	-2.34	1.34	1.37
15	B	1221	CLA	C1C-C2C	2.34	1.49	1.44
15	A	1013	CLA	MG-NC	2.34	2.11	2.06
15	4	601	CLA	C4B-NB	-2.34	1.34	1.37
15	2	606	CLA	C1C-C2C	2.34	1.49	1.44
15	B	1023	CLA	C1C-NC	-2.33	1.34	1.37
22	2	821	LMT	O2B-C2B	-2.33	1.37	1.43
15	A	1121	CLA	C1C-C2C	2.33	1.49	1.44
15	2	612	CLA	C1C-C2C	2.33	1.49	1.44
15	4	607	CLA	MG-NC	2.32	2.11	2.06
24	A	1011	CL0	C3B-C4B	2.32	1.48	1.42
15	1	615	CLA	C1C-C2C	2.32	1.49	1.44
15	B	1239	CLA	C1C-C2C	2.32	1.49	1.44
15	A	1102	CLA	C4B-NB	-2.31	1.34	1.37
15	3	605	CLA	MG-NC	2.31	2.11	2.06
15	2	607	CLA	C1C-C2C	2.31	1.49	1.44
15	B	1214	CLA	C1A-CHA	2.31	1.52	1.43
15	B	1206	CLA	C1C-C2C	2.31	1.49	1.44
15	2	602	CLA	C1C-C2C	2.31	1.49	1.44
15	B	1240	CLA	C1C-C2C	2.30	1.49	1.44
15	1	603	CLA	CHB-C4A	2.30	1.42	1.37
15	3	612	CLA	MG-NC	2.30	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	603	CLA	C1A-CHA	2.30	1.52	1.43
15	2	615	CLA	C1C-C2C	2.29	1.49	1.44
15	B	1217	CLA	MG-NC	2.29	2.11	2.06
22	2	821	LMT	O3B-C3B	-2.29	1.37	1.43
15	A	1105	CLA	C1C-C2C	2.29	1.49	1.44
15	A	1117	CLA	MG-NC	2.28	2.11	2.06
22	2	821	LMT	O2'-C2'	-2.28	1.37	1.43
15	B	1234	CLA	C3D-C4D	-2.28	1.39	1.44
15	A	1109	CLA	C1C-C2C	2.28	1.49	1.44
15	B	1224	CLA	C1C-C2C	2.27	1.49	1.44
15	3	607	CLA	C1C-C2C	2.27	1.49	1.44
15	B	1226	CLA	CHD-C1D	2.27	1.42	1.38
15	A	1102	CLA	MG-NC	2.27	2.11	2.06
15	B	1022	CLA	CHD-C1D	2.26	1.42	1.38
15	B	1225	CLA	MG-NC	2.26	2.11	2.06
23	B	5031	GSH	O2-C2	-2.26	1.18	1.23
15	A	1114	CLA	C1C-C2C	2.26	1.48	1.44
15	A	1134	CLA	C1C-C2C	2.26	1.48	1.44
15	3	610	CLA	C1C-C2C	2.26	1.48	1.44
15	B	1234	CLA	C1A-CHA	2.25	1.52	1.43
15	4	601	CLA	CHD-C1D	2.25	1.42	1.38
15	1	607	CLA	MG-NC	2.25	2.11	2.06
15	A	1130	CLA	C1C-C2C	2.25	1.48	1.44
15	A	1140	CLA	C1C-C2C	2.24	1.48	1.44
23	4	831	GSH	O2-C2	-2.24	1.18	1.23
15	A	1012	CLA	MG-NC	2.24	2.11	2.06
15	2	608	CLA	C1C-C2C	2.24	1.48	1.44
15	A	1124	CLA	C1C-C2C	2.24	1.48	1.44
15	F	1302	CLA	C4B-NB	-2.24	1.35	1.37
15	F	1301	CLA	C4B-NB	-2.23	1.35	1.37
15	A	1133	CLA	C1C-C2C	2.23	1.48	1.44
15	B	1023	CLA	CHC-C1C	2.23	1.43	1.38
15	A	1118	CLA	C4B-NB	-2.23	1.35	1.37
15	B	1238	CLA	C1C-C2C	2.23	1.48	1.44
15	J	1302	CLA	MG-NC	2.23	2.11	2.06
15	1	613	CLA	C1C-C2C	2.22	1.48	1.44
15	B	1231	CLA	C4B-NB	-2.22	1.35	1.37
15	1	603	CLA	C1A-CHA	2.21	1.52	1.43
14	J	4002	BCR	C1-C6	-2.21	1.50	1.53
15	B	1230	CLA	C3D-C4D	-2.21	1.39	1.44
15	B	1021	CLA	C1C-C2C	2.21	1.48	1.44
15	1	612	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	605	CLA	C1C-C2C	2.21	1.48	1.44
15	4	603	CLA	C1C-C2C	2.20	1.48	1.44
15	B	1232	CLA	C1C-C2C	2.20	1.48	1.44
15	3	612	CLA	C4B-NB	-2.20	1.35	1.37
15	A	1127	CLA	C1C-C2C	2.20	1.48	1.44
15	A	1137	CLA	C4B-NB	-2.20	1.35	1.37
15	A	1103	CLA	C1C-C2C	2.20	1.48	1.44
15	B	1227	CLA	MG-NC	2.20	2.11	2.06
15	B	1205	CLA	MG-NC	2.20	2.11	2.06
15	A	1140	CLA	MG-NB	-2.19	2.01	2.05
15	A	1122	CLA	C1C-C2C	2.19	1.48	1.44
15	4	606	CLA	CHD-C1D	2.19	1.42	1.38
15	A	1106	CLA	C1C-C2C	2.18	1.48	1.44
15	3	608	CLA	C1C-C2C	2.18	1.48	1.44
17	A	5001	LHG	O7-C7	-2.18	1.34	1.42
15	B	1204	CLA	C1C-C2C	2.18	1.48	1.44
15	A	1132	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1222	CLA	C1C-C2C	2.18	1.48	1.44
15	4	608	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1211	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1205	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1116	CLA	C1C-C2C	2.17	1.48	1.44
15	B	1216	CLA	CHD-C1D	2.17	1.42	1.38
15	A	1140	CLA	C3B-C4B	2.17	1.47	1.42
15	A	1104	CLA	C1C-C2C	2.17	1.48	1.44
15	B	1214	CLA	C3D-C4D	-2.17	1.39	1.44
15	A	1141	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1013	CLA	C1A-CHA	2.17	1.52	1.43
15	A	1136	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1131	CLA	MG-NC	2.17	2.11	2.06
15	A	1105	CLA	MG-NC	2.17	2.11	2.06
15	B	1201	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1209	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1235	CLA	MG-NC	2.16	2.11	2.06
15	A	1104	CLA	MG-NC	2.16	2.11	2.06
15	A	1113	CLA	C1C-C2C	2.16	1.48	1.44
15	2	601	CLA	C4B-NB	-2.16	1.35	1.37
15	A	1138	CLA	C1C-C2C	2.16	1.48	1.44
15	1	602	CLA	C1C-C2C	2.16	1.48	1.44
15	4	601	CLA	C1A-CHA	2.16	1.52	1.43
15	1	604	CLA	C1C-C2C	2.16	1.48	1.44
15	1	611	CLA	C1C-C2C	2.16	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1221	CLA	C1A-CHA	2.16	1.52	1.43
15	A	1137	CLA	C1C-C2C	2.15	1.48	1.44
15	A	1139	CLA	C1C-C2C	2.15	1.48	1.44
15	A	1118	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1234	CLA	MG-NC	2.15	2.11	2.06
15	A	1127	CLA	MG-NC	2.15	2.11	2.06
15	B	1023	CLA	MG-NC	2.15	2.11	2.06
15	A	1109	CLA	CHD-C1D	2.15	1.42	1.38
15	B	1214	CLA	CHD-C1D	2.15	1.42	1.38
15	1	602	CLA	MG-NC	2.15	2.11	2.06
15	4	605	CLA	C1C-C2C	2.15	1.48	1.44
15	3	610	CLA	MG-NC	2.15	2.11	2.06
15	A	1117	CLA	CHD-C1D	2.14	1.42	1.38
15	2	606	CLA	C1A-CHA	2.14	1.52	1.43
15	3	615	CLA	C1A-CHA	2.14	1.52	1.43
15	2	615	CLA	MG-NC	2.14	2.11	2.06
15	B	1208	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1213	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1131	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1140	CLA	C1A-CHA	2.13	1.52	1.43
15	A	1129	CLA	C1C-C2C	2.13	1.48	1.44
15	3	606	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1125	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1226	CLA	C1C-C2C	2.13	1.48	1.44
15	4	612	CLA	C1A-CHA	2.13	1.51	1.43
15	B	1230	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1228	CLA	MG-NC	2.13	2.11	2.06
15	A	1112	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1239	CLA	C3D-C4D	-2.13	1.39	1.44
15	F	1302	CLA	C3D-C4D	-2.13	1.39	1.44
15	A	1132	CLA	MG-NC	2.12	2.11	2.06
15	B	1206	CLA	MG-NC	2.12	2.11	2.06
15	A	1135	CLA	MG-NC	2.12	2.11	2.06
15	B	1224	CLA	MG-NC	2.12	2.11	2.06
15	B	1237	CLA	C1C-C2C	2.12	1.48	1.44
15	F	1302	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1212	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1204	CLA	C1A-CHA	2.12	1.51	1.43
15	F	1302	CLA	CHD-C1D	2.12	1.42	1.38
15	B	1235	CLA	C1A-CHA	2.12	1.51	1.43
15	A	1107	CLA	C1C-C2C	2.12	1.48	1.44
15	A	1012	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1225	CLA	C4B-NB	-2.12	1.35	1.37
15	B	1217	CLA	C1C-C2C	2.12	1.48	1.44
15	1	613	CLA	C4B-NB	-2.12	1.35	1.37
15	1	613	CLA	MG-NC	2.11	2.11	2.06
15	A	1101	CLA	C1C-C2C	2.11	1.48	1.44
15	A	1114	CLA	C1A-CHA	2.11	1.51	1.43
12	4	501	LUT	C1-C6	-2.11	1.50	1.53
15	A	1140	CLA	C3D-C4D	-2.11	1.39	1.44
15	4	608	CLA	MG-NC	2.11	2.11	2.06
15	A	1130	CLA	CHD-C1D	2.11	1.42	1.38
15	1	613	CLA	C1A-CHA	2.10	1.51	1.43
15	B	1239	CLA	C1A-CHA	2.10	1.51	1.43
15	1	601	CLA	C1C-C2C	2.10	1.48	1.44
15	A	1138	CLA	C3D-C4D	-2.10	1.39	1.44
15	4	609	CLA	C1A-CHA	2.10	1.51	1.43
15	A	1122	CLA	MG-NC	2.10	2.11	2.06
15	A	1140	CLA	MG-NC	2.10	2.11	2.06
15	2	602	CLA	C3D-C4D	-2.10	1.39	1.44
15	B	1235	CLA	C1C-C2C	2.10	1.48	1.44
15	A	1112	CLA	MG-NC	2.10	2.11	2.06
15	B	1218	CLA	C1A-CHA	2.10	1.51	1.43
15	B	1229	CLA	C3D-C4D	-2.10	1.39	1.44
15	B	1203	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1227	CLA	CHD-C1D	2.09	1.42	1.38
24	A	1011	CL0	C4B-NB	-2.09	1.35	1.37
15	B	1218	CLA	MG-NC	2.09	2.11	2.06
15	A	1108	CLA	C1A-CHA	2.09	1.51	1.43
15	B	1236	CLA	C1A-CHA	2.09	1.51	1.43
15	3	611	CLA	CHD-C1D	2.09	1.42	1.38
15	1	607	CLA	C1A-CHA	2.08	1.51	1.43
15	B	1207	CLA	CHB-C4A	2.08	1.42	1.36
15	4	607	CLA	CHD-C1D	2.08	1.42	1.38
15	4	612	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1113	CLA	MG-NC	2.08	2.11	2.06
15	B	1211	CLA	C1A-CHA	2.08	1.51	1.43
15	A	1127	CLA	CHD-C1D	2.08	1.42	1.38
15	B	1214	CLA	C1C-C2C	2.08	1.48	1.44
15	F	1302	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1103	CLA	C1A-CHA	2.07	1.51	1.43
15	2	612	CLA	MG-NC	2.07	2.11	2.06
15	A	1102	CLA	C1A-CHA	2.07	1.51	1.43
13	3	502	XAT	O24-C25	-2.07	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1222	CLA	C3D-C4D	-2.07	1.39	1.44
15	A	1128	CLA	C1A-CHA	2.07	1.51	1.43
15	B	1021	CLA	C3D-C4D	-2.06	1.39	1.44
15	2	604	CLA	C1A-CHA	2.06	1.51	1.43
15	B	1222	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1116	CLA	MG-NC	2.06	2.11	2.06
16	1	609	CHL	C1B-NB	-2.06	1.35	1.37
15	B	1227	CLA	C1A-CHA	2.06	1.51	1.43
15	B	1220	CLA	MG-NC	2.06	2.11	2.06
15	B	1219	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1134	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1139	CLA	C3D-C4D	-2.06	1.39	1.44
15	A	1135	CLA	C1C-C2C	2.06	1.48	1.44
15	A	1013	CLA	C3D-C4D	-2.06	1.39	1.44
15	1	604	CLA	MG-NC	2.06	2.11	2.06
15	1	606	CLA	C3D-C4D	-2.05	1.39	1.44
15	A	1101	CLA	CHD-C1D	2.05	1.42	1.38
15	A	1118	CLA	MG-NC	2.05	2.11	2.06
15	A	1132	CLA	C1A-CHA	2.05	1.51	1.43
15	1	601	CLA	CHD-C1D	2.05	1.42	1.38
15	A	1117	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1201	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1232	CLA	C1A-CHA	2.05	1.51	1.43
15	4	605	CLA	CHD-C1D	2.05	1.42	1.38
15	B	1022	CLA	C4B-NB	-2.05	1.35	1.37
15	2	605	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1210	CLA	C3D-C4D	-2.05	1.39	1.44
15	A	1106	CLA	C1A-CHA	2.05	1.51	1.43
15	1	606	CLA	C1C-C2C	2.05	1.48	1.44
15	1	615	CLA	C3D-C4D	-2.04	1.39	1.44
15	B	1235	CLA	C3B-C4B	2.04	1.47	1.42
15	B	1229	CLA	C1C-C2C	2.04	1.48	1.44
15	1	607	CLA	C4B-NB	-2.04	1.35	1.37
15	4	603	CLA	CHB-C4A	2.04	1.42	1.37
15	4	606	CLA	C1A-CHA	2.04	1.51	1.43
15	2	608	CLA	MG-NC	2.04	2.11	2.06
15	A	1115	CLA	C1A-CHA	2.04	1.51	1.43
15	1	615	CLA	C1A-CHA	2.04	1.51	1.43
15	3	612	CLA	CHD-C1D	2.03	1.42	1.38
23	4	831	GSH	OE1-CD1	-2.03	1.19	1.23
15	2	606	CLA	C3D-C4D	-2.03	1.39	1.44
15	B	1216	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1209	CLA	MG-NC	2.03	2.11	2.06
15	A	1113	CLA	C1A-CHA	2.03	1.51	1.43
15	A	1120	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1021	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1235	CLA	CHB-C4A	2.03	1.42	1.37
15	A	1105	CLA	C3D-C4D	-2.03	1.39	1.44
15	A	1105	CLA	C1A-CHA	2.03	1.51	1.43
15	A	1109	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1234	CLA	CHD-C1D	2.03	1.42	1.38
15	B	1223	CLA	CHB-C4A	2.03	1.42	1.37
15	1	603	CLA	MG-NC	2.03	2.11	2.06
15	A	1102	CLA	C3D-C4D	-2.03	1.39	1.44
15	A	1135	CLA	C1A-CHA	2.03	1.51	1.43
15	3	603	CLA	C1C-C2C	2.02	1.48	1.44
15	3	608	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1129	CLA	C3D-C4D	-2.02	1.39	1.44
15	1	601	CLA	C1A-CHA	2.02	1.51	1.43
15	3	611	CLA	C1C-C2C	2.02	1.48	1.44
15	A	1118	CLA	C1A-CHA	2.02	1.51	1.43
15	B	1213	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1121	CLA	C1A-CHA	2.02	1.51	1.43
15	B	1225	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1133	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1110	CLA	MG-NC	2.02	2.11	2.06
15	B	1240	CLA	C3D-C4D	-2.02	1.39	1.44
15	3	612	CLA	C1A-CHA	2.02	1.51	1.43
15	B	1214	CLA	MG-NC	2.02	2.11	2.06
15	B	1237	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1123	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1114	CLA	C3D-C4D	-2.02	1.39	1.44
15	3	607	CLA	C1A-CHA	2.01	1.51	1.43
15	A	1114	CLA	MG-NC	2.01	2.11	2.06
15	B	1211	CLA	MG-NC	2.01	2.11	2.06
15	2	615	CLA	C1A-CHA	2.01	1.51	1.43
15	B	1206	CLA	C1A-CHA	2.01	1.51	1.43
15	3	615	CLA	C3D-C4D	-2.01	1.39	1.44
15	1	601	CLA	C4B-NB	-2.01	1.35	1.37
15	B	1205	CLA	C1A-CHA	2.01	1.51	1.43
22	2	821	LMT	O4'-C4B	-2.01	1.38	1.43
15	1	611	CLA	C1A-CHA	2.01	1.51	1.43
15	1	602	CLA	C1A-CHA	2.01	1.51	1.43
15	3	605	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	608	CLA	C3D-C4D	-2.01	1.39	1.44
15	B	1228	CLA	C1A-CHA	2.01	1.51	1.43
21	B	5002	DGD	O5D-C1E	2.01	1.43	1.40
15	1	608	CLA	C1C-C2C	2.01	1.48	1.44
15	1	612	CLA	C1C-C2C	2.01	1.48	1.44
15	B	1201	CLA	MG-NC	2.01	2.11	2.06
15	B	1230	CLA	MG-NC	2.00	2.11	2.06
15	A	1137	CLA	MG-NC	2.00	2.11	2.06
15	2	601	CLA	C1A-CHA	2.00	1.51	1.43
15	B	1228	CLA	C3D-C4D	-2.00	1.39	1.44
15	4	604	CLA	C1A-CHA	2.00	1.51	1.43
15	3	608	CLA	MG-NC	2.00	2.11	2.06
15	4	605	CLA	C3D-C4D	-2.00	1.39	1.44
15	B	1207	CLA	C2A-C1A	-2.00	1.40	1.52
15	B	1022	CLA	C1C-C2C	2.00	1.48	1.44
15	A	1124	CLA	C1A-CHA	2.00	1.51	1.43
15	A	1013	CLA	CHD-C1D	2.00	1.42	1.38
15	A	1116	CLA	CHD-C1D	2.00	1.42	1.38

All (2941) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4001	BCR	C10-C11-C12	17.73	178.54	123.22
14	2	503	BCR	C10-C11-C12	17.71	178.50	123.22
14	3	504	BCR	C10-C11-C12	17.63	178.23	123.22
14	4	503	BCR	C10-C11-C12	17.61	178.18	123.22
14	A	4004	BCR	C10-C11-C12	17.60	178.13	123.22
14	F	4002	BCR	C10-C11-C12	17.57	178.04	123.22
14	A	4007	BCR	C10-C11-C12	17.54	177.94	123.22
14	B	4006	BCR	C10-C11-C12	17.46	177.72	123.22
14	4	505	BCR	C10-C11-C12	17.46	177.70	123.22
14	A	4002	BCR	C10-C11-C12	17.40	177.53	123.22
14	B	4005	BCR	C10-C11-C12	17.39	177.50	123.22
14	3	503	BCR	C10-C11-C12	17.24	177.01	123.22
14	B	4004	BCR	C10-C11-C12	17.23	176.99	123.22
14	1	505	BCR	C10-C11-C12	17.11	176.63	123.22
14	B	4002	BCR	C10-C11-C12	16.84	175.77	123.22
14	B	4003	BCR	C10-C11-C12	16.71	175.38	123.22
14	J	4003	BCR	C10-C11-C12	16.69	175.32	123.22
14	J	4001	BCR	C10-C11-C12	16.64	175.13	123.22
14	A	4006	BCR	C10-C11-C12	16.56	174.90	123.22
14	1	505	BCR	C16-C15-C14	16.50	157.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	503	BCR	C10-C11-C12	16.45	174.55	123.22
14	A	4003	BCR	C10-C11-C12	16.44	174.54	123.22
12	1	501	LUT	C36-C21-C26	-16.44	84.64	109.55
14	J	4002	BCR	C10-C11-C12	16.43	174.48	123.22
14	A	4007	BCR	C16-C15-C14	16.10	156.46	123.47
14	3	504	BCR	C16-C15-C14	15.85	155.94	123.47
12	1	501	LUT	C37-C21-C36	-15.46	85.11	107.89
14	A	4005	BCR	C16-C15-C14	15.36	154.93	123.47
14	B	4001	BCR	C16-C15-C14	15.33	154.87	123.47
14	F	4002	BCR	C16-C15-C14	14.90	154.00	123.47
14	4	505	BCR	C16-C15-C14	14.75	153.69	123.47
14	2	503	BCR	C16-C15-C14	14.69	153.56	123.47
14	J	4002	BCR	C16-C15-C14	14.68	153.55	123.47
14	B	4003	BCR	C11-C10-C9	14.48	147.97	127.31
14	1	503	BCR	C16-C15-C14	14.46	153.09	123.47
14	B	4002	BCR	C16-C15-C14	14.33	152.84	123.47
14	B	4005	BCR	C16-C15-C14	14.33	152.82	123.47
14	A	4003	BCR	C11-C10-C9	14.29	147.70	127.31
14	B	4004	BCR	C11-C10-C9	14.06	147.38	127.31
14	A	4004	BCR	C16-C15-C14	13.94	152.03	123.47
14	A	4007	BCR	C11-C10-C9	13.87	147.11	127.31
14	1	503	BCR	C11-C10-C9	13.80	147.01	127.31
14	3	503	BCR	C11-C10-C9	13.73	146.91	127.31
14	B	4003	BCR	C16-C15-C14	13.65	151.44	123.47
14	4	503	BCR	C16-C15-C14	13.62	151.38	123.47
14	B	4001	BCR	C11-C10-C9	13.62	146.75	127.31
14	B	4006	BCR	C16-C15-C14	13.61	151.36	123.47
14	B	4004	BCR	C16-C15-C14	13.58	151.29	123.47
14	J	4001	BCR	C11-C10-C9	13.48	146.54	127.31
14	A	4006	BCR	C11-C10-C9	13.47	146.54	127.31
14	F	4002	BCR	C11-C10-C9	13.42	146.46	127.31
14	J	4002	BCR	C11-C10-C9	13.40	146.43	127.31
14	4	503	BCR	C11-C10-C9	13.24	146.21	127.31
14	J	4003	BCR	C16-C15-C14	13.23	150.57	123.47
14	B	4005	BCR	C11-C10-C9	13.08	145.97	127.31
14	3	504	BCR	C11-C10-C9	13.01	145.88	127.31
14	2	503	BCR	C11-C10-C9	12.99	145.85	127.31
14	J	4001	BCR	C16-C15-C14	12.95	150.01	123.47
14	A	4002	BCR	C21-C20-C19	12.94	163.61	123.22
14	A	4002	BCR	C16-C15-C14	12.71	149.52	123.47
14	B	4006	BCR	C11-C10-C9	12.67	145.39	127.31
14	4	505	BCR	C21-C20-C19	12.62	162.61	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	503	BCR	C16-C15-C14	12.50	149.07	123.47
14	A	4002	BCR	C11-C10-C9	12.36	144.95	127.31
14	B	4003	BCR	C21-C20-C19	12.29	161.56	123.22
14	F	4002	BCR	C21-C20-C19	12.29	161.56	123.22
14	A	4004	BCR	C21-C20-C19	12.27	161.50	123.22
14	A	4004	BCR	C11-C10-C9	12.16	144.67	127.31
14	A	4003	BCR	C16-C15-C14	12.12	148.31	123.47
14	B	4006	BCR	C21-C20-C19	12.08	160.92	123.22
14	B	4002	BCR	C21-C20-C19	12.05	160.81	123.22
14	J	4003	BCR	C11-C12-C13	11.98	160.08	126.42
14	J	4003	BCR	C11-C10-C9	11.93	144.33	127.31
12	1	501	LUT	C36-C21-C22	-11.89	86.92	109.44
14	1	505	BCR	C11-C10-C9	11.85	144.22	127.31
14	1	505	BCR	C21-C20-C19	11.84	160.16	123.22
14	1	503	BCR	C11-C12-C13	11.78	159.51	126.42
14	J	4001	BCR	C11-C12-C13	11.74	159.39	126.42
14	A	4006	BCR	C16-C15-C14	11.72	147.49	123.47
14	J	4003	BCR	C21-C20-C19	11.72	159.79	123.22
14	A	4003	BCR	C11-C12-C13	11.71	159.32	126.42
14	J	4001	BCR	C21-C20-C19	11.70	159.73	123.22
14	4	505	BCR	C11-C10-C9	11.68	143.98	127.31
14	J	4002	BCR	C21-C20-C19	11.68	159.67	123.22
14	2	503	BCR	C21-C20-C19	11.66	159.62	123.22
14	3	504	BCR	C21-C20-C19	11.60	159.42	123.22
14	A	4005	BCR	C10-C11-C12	-11.59	87.05	123.22
14	4	503	BCR	C21-C20-C19	11.41	158.83	123.22
14	B	4004	BCR	C21-C20-C19	11.40	158.78	123.22
14	B	4003	BCR	C11-C12-C13	11.38	158.39	126.42
14	A	4006	BCR	C11-C12-C13	11.36	158.33	126.42
14	A	4005	BCR	C21-C20-C19	11.36	158.67	123.22
14	B	4002	BCR	C11-C10-C9	11.34	143.50	127.31
14	B	4001	BCR	C21-C20-C19	11.28	158.43	123.22
14	A	4005	BCR	C11-C12-C13	-11.11	95.22	126.42
14	B	4005	BCR	C21-C20-C19	11.09	157.82	123.22
14	B	4006	BCR	C11-C12-C13	11.06	157.49	126.42
14	A	4006	BCR	C21-C20-C19	10.83	157.00	123.22
14	3	503	BCR	C21-C20-C19	10.75	156.75	123.22
14	A	4002	BCR	C11-C12-C13	10.74	156.59	126.42
14	A	4007	BCR	C21-C20-C19	10.69	156.56	123.22
14	1	503	BCR	C21-C20-C19	10.58	156.23	123.22
14	A	4004	BCR	C11-C12-C13	10.57	156.11	126.42
14	A	4005	BCR	C35-C13-C12	10.56	134.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4005	BCR	C11-C12-C13	10.47	155.83	126.42
14	A	4003	BCR	C21-C20-C19	10.40	155.68	123.22
14	B	4002	BCR	C11-C12-C13	10.12	154.85	126.42
14	4	503	BCR	C11-C12-C13	9.98	154.45	126.42
14	B	4004	BCR	C11-C12-C13	9.97	154.44	126.42
14	2	503	BCR	C11-C12-C13	9.88	154.18	126.42
14	A	4007	BCR	C11-C12-C13	9.86	154.12	126.42
14	F	4002	BCR	C11-C12-C13	9.78	153.90	126.42
15	B	1215	CLA	C4A-NA-C1A	9.72	111.08	106.71
14	4	505	BCR	C11-C12-C13	9.67	153.58	126.42
14	A	4006	BCR	C20-C19-C18	9.60	153.38	126.42
14	J	4002	BCR	C11-C12-C13	9.56	153.27	126.42
14	3	503	BCR	C11-C12-C13	9.51	153.13	126.42
15	B	1230	CLA	C4A-NA-C1A	9.45	110.95	106.71
14	1	505	BCR	C11-C12-C13	9.44	152.92	126.42
14	4	505	BCR	C20-C19-C18	9.34	152.66	126.42
15	B	1226	CLA	C4A-NA-C1A	9.28	110.88	106.71
14	3	504	BCR	C11-C12-C13	9.25	152.40	126.42
14	B	4001	BCR	C11-C12-C13	9.25	152.39	126.42
14	B	4005	BCR	C20-C19-C18	9.20	152.27	126.42
15	A	1126	CLA	C4A-NA-C1A	9.12	110.81	106.71
15	3	603	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	B	1021	CLA	C4A-NA-C1A	9.07	110.78	106.71
15	2	606	CLA	C4A-NA-C1A	9.01	110.76	106.71
15	A	1106	CLA	C4A-NA-C1A	9.01	110.75	106.71
12	1	501	LUT	C31-C30-C29	-9.00	114.46	127.31
15	B	1229	CLA	C4A-NA-C1A	8.98	110.74	106.71
15	F	1301	CLA	C4A-NA-C1A	8.93	110.72	106.71
15	A	1104	CLA	C4A-NA-C1A	8.93	110.72	106.71
15	B	1205	CLA	C4A-NA-C1A	8.92	110.72	106.71
15	B	1227	CLA	C4A-NA-C1A	8.84	110.68	106.71
14	A	4004	BCR	C20-C19-C18	8.83	151.23	126.42
15	A	1127	CLA	C4A-NA-C1A	8.82	110.67	106.71
14	A	4005	BCR	C20-C19-C18	8.82	151.19	126.42
15	A	1115	CLA	C4A-NA-C1A	8.80	110.66	106.71
15	2	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
15	B	1202	CLA	C4A-NA-C1A	8.76	110.65	106.71
15	B	1206	CLA	C4A-NA-C1A	8.74	110.64	106.71
15	A	1102	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	A	1134	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	B	1203	CLA	C4A-NA-C1A	8.72	110.63	106.71
15	B	1223	CLA	C4A-NA-C1A	8.71	110.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1221	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	3	601	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	A	1129	CLA	C4A-NA-C1A	8.70	110.62	106.71
14	1	503	BCR	C20-C19-C18	8.69	150.84	126.42
15	1	608	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	2	605	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	2	602	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	2	607	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	4	612	CLA	C4A-NA-C1A	8.67	110.61	106.71
14	3	504	BCR	C20-C19-C18	8.65	150.70	126.42
15	A	1128	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	A	1132	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	4	608	CLA	C4A-NA-C1A	8.62	110.58	106.71
15	A	1130	CLA	C4A-NA-C1A	8.62	110.58	106.71
14	4	503	BCR	C20-C19-C18	8.59	150.56	126.42
15	B	1234	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	1	607	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	4	605	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	A	1118	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	A	1131	CLA	C4A-NA-C1A	8.58	110.56	106.71
15	A	1141	CLA	C4A-NA-C1A	8.58	110.56	106.71
14	B	4003	BCR	C20-C19-C18	8.57	150.50	126.42
14	3	503	BCR	C20-C19-C18	8.57	150.50	126.42
15	A	1135	CLA	C4A-NA-C1A	8.57	110.56	106.71
15	B	1236	CLA	C4A-NA-C1A	8.57	110.56	106.71
15	A	1117	CLA	C4A-NA-C1A	8.56	110.56	106.71
15	B	1218	CLA	C4A-NA-C1A	8.56	110.56	106.71
15	A	1110	CLA	C4A-NA-C1A	8.56	110.56	106.71
14	1	505	BCR	C20-C19-C18	8.55	150.44	126.42
15	A	1116	CLA	C4A-NA-C1A	8.55	110.55	106.71
15	4	606	CLA	C4A-NA-C1A	8.54	110.55	106.71
15	A	1139	CLA	C4A-NA-C1A	8.54	110.55	106.71
15	1	615	CLA	C4A-NA-C1A	8.52	110.54	106.71
15	2	608	CLA	C4A-NA-C1A	8.52	110.54	106.71
15	B	1210	CLA	C4A-NA-C1A	8.52	110.53	106.71
12	1	501	LUT	C15-C35-C34	-8.51	106.05	123.47
15	B	1222	CLA	C4A-NA-C1A	8.46	110.51	106.71
15	A	1123	CLA	C4A-NA-C1A	8.45	110.51	106.71
14	B	4004	BCR	C20-C19-C18	8.45	150.15	126.42
15	A	1109	CLA	C4A-NA-C1A	8.45	110.50	106.71
15	1	606	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	A	1114	CLA	C4A-NA-C1A	8.44	110.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	1302	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	B	1240	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	A	1125	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	3	615	CLA	C4A-NA-C1A	8.43	110.50	106.71
15	A	1108	CLA	C4A-NA-C1A	8.42	110.49	106.71
15	B	1208	CLA	C4A-NA-C1A	8.41	110.48	106.71
15	A	1105	CLA	C4A-NA-C1A	8.40	110.48	106.71
15	B	1238	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	2	503	BCR	C20-C19-C18	8.38	149.97	126.42
15	A	1120	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	1	611	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	B	1219	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	A	1112	CLA	C4A-NA-C1A	8.37	110.47	106.71
15	B	1237	CLA	C4A-NA-C1A	8.37	110.47	106.71
15	2	615	CLA	C4A-NA-C1A	8.36	110.46	106.71
15	A	1121	CLA	C4A-NA-C1A	8.36	110.46	106.71
15	A	1113	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	J	4002	BCR	C20-C19-C18	8.33	149.83	126.42
14	A	4005	BCR	C12-C13-C14	-8.33	106.15	118.94
15	4	609	CLA	C4A-NA-C1A	8.33	110.45	106.71
14	J	4001	BCR	C20-C19-C18	8.33	149.81	126.42
15	A	1124	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	A	1138	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	3	607	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	1	613	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	B	1231	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	A	1122	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	1	612	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	3	608	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	A	1119	CLA	C4A-NA-C1A	8.25	110.41	106.71
15	A	1140	CLA	C4A-NA-C1A	8.24	110.41	106.71
15	1	602	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	B	1214	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	B	1022	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	B	1201	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	B	1212	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	3	613	CLA	C4A-NA-C1A	8.21	110.40	106.71
15	A	1013	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	B	1209	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	3	606	CLA	C4A-NA-C1A	8.19	110.39	106.71
15	3	612	CLA	C4A-NA-C1A	8.19	110.39	106.71
15	A	1101	CLA	C4A-NA-C1A	8.18	110.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	603	CLA	C4A-NA-C1A	8.16	110.37	106.71
15	B	1220	CLA	C4A-NA-C1A	8.15	110.37	106.71
15	3	611	CLA	C4A-NA-C1A	8.13	110.36	106.71
15	A	1107	CLA	C4A-NA-C1A	8.12	110.36	106.71
14	B	4006	BCR	C20-C19-C18	8.12	149.22	126.42
15	B	1239	CLA	C4A-NA-C1A	8.11	110.35	106.71
15	B	1232	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	A	1111	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	B	1217	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	1	601	CLA	C4A-NA-C1A	8.09	110.34	106.71
14	A	4005	BCR	C11-C10-C9	8.08	138.84	127.31
14	B	4002	BCR	C20-C19-C18	8.08	149.11	126.42
15	4	615	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	B	1023	CLA	C4A-NA-C1A	8.06	110.33	106.71
15	B	1224	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	J	4003	BCR	C20-C19-C18	8.06	149.05	126.42
15	B	1211	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	B	1225	CLA	C4A-NA-C1A	8.03	110.31	106.71
15	B	1216	CLA	C4A-NA-C1A	8.02	110.31	106.71
15	A	1136	CLA	C4A-NA-C1A	8.01	110.31	106.71
15	A	1137	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	3	605	CLA	C4A-NA-C1A	7.99	110.30	106.71
15	F	1302	CLA	C4A-NA-C1A	7.98	110.29	106.71
15	1	605	CLA	C4A-NA-C1A	7.95	110.28	106.71
15	4	602	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	2	603	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	A	1133	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	4	603	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	A	1012	CLA	C4A-NA-C1A	7.90	110.26	106.71
14	F	4002	BCR	C20-C19-C18	7.90	148.60	126.42
24	A	1011	CL0	CMD-C2D-C1D	7.89	138.62	124.71
15	3	610	CLA	C4A-NA-C1A	7.87	110.24	106.71
15	B	1204	CLA	C4A-NA-C1A	7.85	110.24	106.71
15	4	604	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	1	604	CLA	C4A-NA-C1A	7.84	110.23	106.71
14	B	4001	BCR	C20-C19-C18	7.78	148.27	126.42
15	A	1103	CLA	C4A-NA-C1A	7.77	110.20	106.71
15	4	601	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	2	601	CLA	C4A-NA-C1A	7.70	110.17	106.71
15	B	1235	CLA	C4A-NA-C1A	7.52	110.09	106.71
12	1	501	LUT	C37-C21-C26	7.51	120.92	109.55
15	B	1228	CLA	C4A-NA-C1A	7.41	110.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1213	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	A	4005	BCR	C8-C9-C10	-7.27	107.79	118.94
15	2	604	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	4	607	CLA	C4A-NA-C1A	7.16	109.93	106.71
14	A	4002	BCR	C20-C19-C18	7.02	146.12	126.42
14	A	4007	BCR	C20-C19-C18	6.73	145.31	126.42
15	B	1207	CLA	C2A-C1A-CHA	-6.68	111.23	122.63
14	A	4007	BCR	C15-C14-C13	-6.60	117.89	127.31
14	A	4003	BCR	C20-C19-C18	6.55	144.81	126.42
15	3	603	CLA	O2D-CGD-CBD	6.52	122.86	111.27
24	A	1011	CL0	C4A-NA-C1A	6.44	109.60	106.71
24	A	1011	CL0	C2C-C1C-NC	6.28	115.86	109.97
12	4	501	LUT	C21-C26-C25	6.16	122.45	111.42
12	1	501	LUT	C21-C26-C27	6.03	120.33	112.70
15	A	1111	CLA	O2D-CGD-CBD	5.94	121.81	111.27
15	B	1211	CLA	O2A-C1-C2	5.93	122.83	108.97
15	4	609	CLA	O2A-C1-C2	5.87	122.71	108.97
15	3	601	CLA	O2A-C1-C2	5.87	122.69	108.97
15	B	1207	CLA	C4D-ND-C1D	5.82	110.47	106.33
15	2	608	CLA	O2A-C1-C2	5.81	122.56	108.97
15	4	615	CLA	CMD-C2D-C1D	5.79	134.93	124.71
13	1	502	XAT	C31-C30-C29	-5.79	119.05	127.31
15	1	606	CLA	O2D-CGD-CBD	5.79	121.55	111.27
15	1	607	CLA	CMD-C2D-C1D	5.79	134.91	124.71
15	A	1101	CLA	O2D-CGD-CBD	5.79	121.55	111.27
15	A	1109	CLA	O2A-C1-C2	5.77	122.46	108.97
15	4	605	CLA	O2D-CGD-CBD	5.75	121.49	111.27
15	4	602	CLA	O2A-C1-C2	5.75	122.42	108.97
12	3	501	LUT	C21-C26-C25	5.74	121.70	111.42
14	B	4001	BCR	C15-C14-C13	-5.73	119.13	127.31
15	A	1124	CLA	O2A-C1-C2	5.72	122.33	108.97
15	4	609	CLA	O2D-CGD-CBD	5.71	121.42	111.27
15	A	1110	CLA	O2A-C1-C2	5.71	122.32	108.97
15	B	1217	CLA	CMD-C2D-C1D	5.70	134.77	124.71
15	B	1221	CLA	CMD-C2D-C1D	5.70	134.75	124.71
15	B	1215	CLA	O2D-CGD-CBD	5.68	121.37	111.27
15	2	607	CLA	CMD-C2D-C1D	5.67	134.70	124.71
15	4	603	CLA	CMD-C2D-C1D	5.65	134.68	124.71
15	A	1117	CLA	CMD-C2D-C1D	5.65	134.67	124.71
15	A	1107	CLA	O2A-C1-C2	5.65	122.18	108.97
15	1	604	CLA	O2D-CGD-CBD	5.64	121.30	111.27
15	4	604	CLA	CMD-C2D-C1D	5.64	134.66	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	604	CLA	O2A-C1-C2	5.64	122.16	108.97
15	4	603	CLA	O2A-C1-C2	5.64	122.15	108.97
15	B	1022	CLA	CMD-C2D-C1D	5.64	134.65	124.71
15	1	603	CLA	CMD-C2D-C1D	5.63	134.63	124.71
12	2	501	LUT	C15-C14-C13	-5.62	119.28	127.31
24	A	1011	CL0	CHD-C1D-ND	-5.62	119.29	124.45
15	2	604	CLA	CMD-C2D-C1D	5.62	134.62	124.71
15	2	603	CLA	CMD-C2D-C1D	5.62	134.61	124.71
15	A	1110	CLA	CMD-C2D-C1D	5.62	134.61	124.71
15	3	601	CLA	O2D-CGD-CBD	5.61	121.24	111.27
15	A	1132	CLA	CMD-C2D-C1D	5.61	134.60	124.71
15	A	1111	CLA	CMD-C2D-C1D	5.61	134.59	124.71
15	A	1111	CLA	O2A-C1-C2	5.60	122.08	108.97
15	B	1226	CLA	O2D-CGD-CBD	5.59	121.20	111.27
15	3	603	CLA	CMD-C2D-C1D	5.59	134.56	124.71
15	2	605	CLA	CMD-C2D-C1D	5.59	134.56	124.71
15	B	1232	CLA	CMD-C2D-C1D	5.59	134.56	124.71
15	A	1137	CLA	O2D-CGD-CBD	5.59	121.19	111.27
15	4	601	CLA	O2A-C1-C2	5.58	122.03	108.97
15	1	606	CLA	CMD-C2D-C1D	5.58	134.55	124.71
15	B	1227	CLA	CMD-C2D-C1D	5.58	134.55	124.71
15	B	1225	CLA	CMD-C2D-C1D	5.58	134.55	124.71
15	B	1236	CLA	O2D-CGD-CBD	5.58	121.18	111.27
15	2	604	CLA	O2D-CGD-CBD	5.58	121.18	111.27
12	2	501	LUT	C11-C10-C9	-5.58	119.35	127.31
15	A	1125	CLA	CMD-C2D-C1D	5.58	134.54	124.71
15	1	608	CLA	O2D-CGD-CBD	5.58	121.18	111.27
15	4	606	CLA	O2A-C1-C2	5.57	122.00	108.97
15	1	611	CLA	CMD-C2D-C1D	5.57	134.53	124.71
15	B	1205	CLA	O2A-C1-C2	5.57	122.00	108.97
15	4	604	CLA	O2D-CGD-CBD	5.57	121.17	111.27
15	B	1216	CLA	CMD-C2D-C1D	5.57	134.53	124.71
15	2	606	CLA	CMD-C2D-C1D	5.57	134.53	124.71
15	B	1219	CLA	CMD-C2D-C1D	5.57	134.53	124.71
15	B	1236	CLA	CMD-C2D-C1D	5.57	134.52	124.71
15	A	1115	CLA	CMD-C2D-C1D	5.56	134.52	124.71
15	A	1107	CLA	CMD-C2D-C1D	5.56	134.51	124.71
15	B	1023	CLA	CMD-C2D-C1D	5.56	134.51	124.71
15	4	606	CLA	CMD-C2D-C1D	5.56	134.51	124.71
15	A	1134	CLA	CMD-C2D-C1D	5.56	134.50	124.71
15	B	1203	CLA	CMD-C2D-C1D	5.55	134.50	124.71
15	B	1234	CLA	CMD-C2D-C1D	5.55	134.50	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1104	CLA	CMD-C2D-C1D	5.55	134.50	124.71
15	A	1119	CLA	CMD-C2D-C1D	5.55	134.50	124.71
15	B	1201	CLA	CMD-C2D-C1D	5.55	134.49	124.71
15	A	1121	CLA	CMD-C2D-C1D	5.55	134.49	124.71
15	3	606	CLA	CMD-C2D-C1D	5.55	134.49	124.71
15	A	1137	CLA	CMD-C2D-C1D	5.55	134.49	124.71
15	B	1208	CLA	CMD-C2D-C1D	5.54	134.49	124.71
15	A	1112	CLA	CMD-C2D-C1D	5.54	134.48	124.71
15	A	1120	CLA	CMD-C2D-C1D	5.54	134.48	124.71
15	A	1129	CLA	CMD-C2D-C1D	5.54	134.48	124.71
15	B	1224	CLA	CMD-C2D-C1D	5.54	134.48	124.71
15	3	613	CLA	CMD-C2D-C1D	5.54	134.47	124.71
15	A	1130	CLA	CMD-C2D-C1D	5.54	134.47	124.71
15	3	605	CLA	CMD-C2D-C1D	5.53	134.47	124.71
15	A	1132	CLA	O2D-CGD-CBD	5.53	121.10	111.27
15	B	1213	CLA	CMD-C2D-C1D	5.53	134.46	124.71
15	A	1109	CLA	CMD-C2D-C1D	5.53	134.46	124.71
15	1	601	CLA	O2A-C1-C2	5.53	121.89	108.97
15	A	1137	CLA	O2A-C1-C2	5.52	121.89	108.97
15	B	1202	CLA	CMD-C2D-C1D	5.52	134.45	124.71
15	1	612	CLA	CMD-C2D-C1D	5.52	134.44	124.71
15	B	1231	CLA	CMD-C2D-C1D	5.52	134.44	124.71
15	B	1226	CLA	CMD-C2D-C1D	5.52	134.44	124.71
15	B	1225	CLA	O2A-C1-C2	5.52	121.87	108.97
15	3	607	CLA	CMD-C2D-C1D	5.52	134.43	124.71
15	A	1140	CLA	CMD-C2D-C1D	5.51	134.43	124.71
15	B	1230	CLA	O2A-C1-C2	5.51	121.86	108.97
15	B	1222	CLA	O2D-CGD-CBD	5.51	121.07	111.27
15	A	1113	CLA	CMD-C2D-C1D	5.51	134.43	124.71
15	1	602	CLA	CMD-C2D-C1D	5.51	134.43	124.71
15	A	1141	CLA	CMD-C2D-C1D	5.51	134.43	124.71
15	B	1232	CLA	O2A-C1-C2	5.51	121.86	108.97
15	B	1228	CLA	CMD-C2D-C1D	5.51	134.42	124.71
15	1	615	CLA	CMD-C2D-C1D	5.50	134.41	124.71
15	A	1133	CLA	CMD-C2D-C1D	5.50	134.41	124.71
15	B	1224	CLA	O2A-C1-C2	5.50	121.83	108.97
15	B	1223	CLA	CMD-C2D-C1D	5.50	134.40	124.71
15	A	1127	CLA	CMD-C2D-C1D	5.50	134.40	124.71
15	2	608	CLA	CMD-C2D-C1D	5.50	134.40	124.71
15	A	1118	CLA	O2A-C1-C2	5.50	121.82	108.97
15	1	615	CLA	O2D-CGD-CBD	5.50	121.03	111.27
15	3	601	CLA	CMD-C2D-C1D	5.50	134.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	611	CLA	CMD-C2D-C1D	5.50	134.40	124.71
15	1	613	CLA	CMD-C2D-C1D	5.50	134.40	124.71
15	B	1237	CLA	CMD-C2D-C1D	5.49	134.40	124.71
15	B	1208	CLA	O2A-C1-C2	5.49	121.81	108.97
15	B	1218	CLA	CMD-C2D-C1D	5.49	134.39	124.71
15	1	605	CLA	CMD-C2D-C1D	5.49	134.39	124.71
12	1	501	LUT	C32-C33-C34	5.49	127.36	118.94
15	3	608	CLA	CMD-C2D-C1D	5.49	134.38	124.71
15	A	1138	CLA	CMD-C2D-C1D	5.49	134.38	124.71
15	2	615	CLA	CMD-C2D-C1D	5.49	134.38	124.71
15	J	1302	CLA	CMD-C2D-C1D	5.49	134.38	124.71
15	B	1215	CLA	CMD-C2D-C1D	5.48	134.38	124.71
15	1	608	CLA	CMD-C2D-C1D	5.48	134.37	124.71
15	B	1230	CLA	CMD-C2D-C1D	5.48	134.37	124.71
15	A	1104	CLA	O2D-CGD-CBD	5.48	121.00	111.27
15	A	1128	CLA	O2D-CGD-CBD	5.48	121.00	111.27
15	B	1220	CLA	CMD-C2D-C1D	5.48	134.37	124.71
15	A	1126	CLA	CMD-C2D-C1D	5.48	134.37	124.71
13	4	502	XAT	C31-C30-C29	-5.48	119.49	127.31
15	A	1118	CLA	CMD-C2D-C1D	5.48	134.37	124.71
12	1	501	LUT	C31-C32-C33	-5.48	111.03	126.42
15	F	1301	CLA	CMD-C2D-C1D	5.48	134.37	124.71
15	A	1135	CLA	CMD-C2D-C1D	5.48	134.36	124.71
15	B	1205	CLA	CMD-C2D-C1D	5.47	134.36	124.71
15	3	610	CLA	CMD-C2D-C1D	5.47	134.36	124.71
15	A	1108	CLA	CMD-C2D-C1D	5.47	134.35	124.71
15	3	612	CLA	O2D-CGD-CBD	5.47	120.99	111.27
15	A	1119	CLA	O2A-C1-C2	5.47	121.75	108.97
15	B	1222	CLA	O2A-C1-C2	5.47	121.75	108.97
15	B	1206	CLA	CMD-C2D-C1D	5.47	134.35	124.71
15	A	1106	CLA	CMD-C2D-C1D	5.46	134.34	124.71
15	B	1209	CLA	CMD-C2D-C1D	5.46	134.34	124.71
15	B	1239	CLA	CMD-C2D-C1D	5.46	134.34	124.71
15	1	604	CLA	CMD-C2D-C1D	5.46	134.33	124.71
15	A	1131	CLA	CMD-C2D-C1D	5.46	134.33	124.71
15	3	612	CLA	CMD-C2D-C1D	5.46	134.33	124.71
15	4	607	CLA	CMD-C2D-C1D	5.46	134.33	124.71
15	B	1212	CLA	CMD-C2D-C1D	5.45	134.32	124.71
15	B	1238	CLA	CMD-C2D-C1D	5.45	134.32	124.71
15	A	1122	CLA	CMD-C2D-C1D	5.45	134.32	124.71
15	A	1115	CLA	O2D-CGD-CBD	5.45	120.95	111.27
15	A	1116	CLA	CMD-C2D-C1D	5.45	134.32	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	601	CLA	CMD-C2D-C1D	5.45	134.31	124.71
15	2	602	CLA	CMD-C2D-C1D	5.45	134.31	124.71
15	2	601	CLA	O2A-C1-C2	5.45	121.70	108.97
24	A	1011	CL0	C2D-C1D-ND	5.44	114.12	110.10
15	3	615	CLA	CMD-C2D-C1D	5.44	134.30	124.71
15	B	1235	CLA	O2D-CGD-CBD	5.44	120.93	111.27
15	A	1125	CLA	O2A-C1-C2	5.44	121.68	108.97
15	A	1139	CLA	CMD-C2D-C1D	5.43	134.29	124.71
15	A	1114	CLA	CMD-C2D-C1D	5.43	134.29	124.71
15	B	1211	CLA	CMD-C2D-C1D	5.43	134.28	124.71
15	B	1223	CLA	O2D-CGD-CBD	5.42	120.90	111.27
15	B	1240	CLA	CMD-C2D-C1D	5.42	134.26	124.71
15	B	1218	CLA	O2A-C1-C2	5.42	121.64	108.97
15	B	1205	CLA	O2D-CGD-CBD	5.42	120.89	111.27
15	B	1234	CLA	O2A-C1-C2	5.41	121.63	108.97
15	A	1102	CLA	O2D-CGD-CBD	5.41	120.88	111.27
15	4	601	CLA	CMD-C2D-C1D	5.41	134.25	124.71
15	B	1204	CLA	CMD-C2D-C1D	5.41	134.25	124.71
15	A	1127	CLA	O2A-C1-C2	5.41	121.62	108.97
15	4	608	CLA	CMD-C2D-C1D	5.41	134.25	124.71
15	A	1112	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1122	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1117	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1134	CLA	O2A-C1-C2	5.39	121.58	108.97
15	A	1135	CLA	O2A-C1-C2	5.39	121.58	108.97
15	B	1210	CLA	O2A-C1-C2	5.39	121.58	108.97
15	A	1105	CLA	CMD-C2D-C1D	5.39	134.21	124.71
15	4	609	CLA	CMD-C2D-C1D	5.39	134.21	124.71
15	1	611	CLA	O2A-C1-C2	5.39	121.57	108.97
15	A	1136	CLA	CMD-C2D-C1D	5.39	134.21	124.71
15	B	1214	CLA	CMD-C2D-C1D	5.39	134.21	124.71
15	1	605	CLA	O2D-CGD-CBD	5.38	120.83	111.27
15	1	601	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	A	1011	CL0	C1-C2-C3	-5.38	118.05	126.75
15	A	1101	CLA	CMD-C2D-C1D	5.38	134.19	124.71
15	B	1215	CLA	O2A-C1-C2	5.38	121.54	108.97
15	4	612	CLA	O2D-CGD-CBD	5.38	120.82	111.27
15	A	1120	CLA	O2A-C1-C2	5.38	121.54	108.97
15	B	1021	CLA	CMD-C2D-C1D	5.37	134.18	124.71
15	A	1123	CLA	CMD-C2D-C1D	5.37	134.18	124.71
12	1	501	LUT	C37-C21-C22	5.37	119.60	109.44
15	A	1140	CLA	O2D-CGD-CBD	5.37	120.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1229	CLA	CMD-C2D-C1D	5.37	134.17	124.71
15	B	1214	CLA	O2A-C1-C2	5.36	121.52	108.97
15	2	607	CLA	O2A-C1-C2	5.35	121.49	108.97
15	B	1206	CLA	O2A-C1-C2	5.35	121.48	108.97
15	2	602	CLA	O2A-C1-C2	5.35	121.48	108.97
15	2	612	CLA	O2A-C1-C2	5.35	121.47	108.97
15	4	612	CLA	O2A-C1-C2	5.34	121.46	108.97
15	B	1204	CLA	O2D-CGD-CBD	5.34	120.76	111.27
15	A	1102	CLA	CMD-C2D-C1D	5.34	134.12	124.71
15	4	604	CLA	O2A-C1-C2	5.33	121.44	108.97
14	3	504	BCR	C15-C14-C13	-5.33	119.70	127.31
15	B	1221	CLA	O2D-CGD-CBD	5.33	120.75	111.27
15	A	1108	CLA	O2D-CGD-CBD	5.33	120.75	111.27
15	4	612	CLA	CMD-C2D-C1D	5.33	134.11	124.71
14	J	4002	BCR	C15-C14-C13	-5.33	119.70	127.31
15	B	1210	CLA	CMD-C2D-C1D	5.33	134.11	124.71
14	A	4005	BCR	C34-C9-C10	5.33	130.39	122.92
15	A	1124	CLA	CMD-C2D-C1D	5.33	134.10	124.71
15	A	1105	CLA	O2A-C1-C2	5.33	121.43	108.97
15	A	1134	CLA	O2D-CGD-CBD	5.33	120.74	111.27
12	2	501	LUT	C21-C26-C27	5.33	119.44	112.70
15	A	1103	CLA	O2D-CGD-CBD	5.32	120.72	111.27
15	A	1116	CLA	O2A-C1-C2	5.32	121.41	108.97
24	A	1011	CL0	C1C-C2C-C3C	-5.32	101.37	106.96
15	A	1128	CLA	O2A-C1-C2	5.31	121.39	108.97
12	1	501	LUT	C35-C15-C14	5.31	134.35	123.47
15	A	1103	CLA	CMD-C2D-C1D	5.30	134.06	124.71
13	1	502	XAT	C7-C8-C9	-5.30	117.31	125.53
15	A	1128	CLA	CMD-C2D-C1D	5.30	134.05	124.71
15	B	1216	CLA	O2A-C1-C2	5.29	121.35	108.97
15	F	1302	CLA	CMD-C2D-C1D	5.29	134.04	124.71
15	B	1213	CLA	O2A-C1-C2	5.29	121.33	108.97
15	B	1021	CLA	O2A-C1-C2	5.28	122.52	108.64
15	3	606	CLA	O2D-CGD-CBD	5.28	120.65	111.27
15	B	1220	CLA	O2A-C1-C2	5.27	122.49	108.64
15	B	1216	CLA	O2D-CGD-CBD	5.27	120.64	111.27
15	1	602	CLA	O2D-CGD-CBD	5.26	120.62	111.27
15	A	1114	CLA	O2D-CGD-CBD	5.26	120.61	111.27
15	A	1136	CLA	O2A-C1-C2	5.26	121.26	108.97
15	4	602	CLA	CMD-C2D-C1D	5.26	133.97	124.71
15	4	605	CLA	CMD-C2D-C1D	5.25	133.97	124.71
15	A	1115	CLA	O2A-C1-C2	5.25	121.24	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1225	CLA	O2D-CGD-CBD	5.24	120.58	111.27
15	B	1236	CLA	O2A-C1-C2	5.24	121.22	108.97
12	2	501	LUT	C21-C26-C25	5.24	120.80	111.42
15	B	1202	CLA	O2A-C1-C2	5.24	121.22	108.97
15	A	1133	CLA	O2A-C1-C2	5.23	121.19	108.97
15	B	1212	CLA	O2D-CGD-CBD	5.22	120.54	111.27
15	4	607	CLA	O2D-CGD-CBD	5.21	120.53	111.27
15	2	612	CLA	O2D-CGD-CBD	5.21	120.53	111.27
15	A	1013	CLA	CMD-C2D-C1D	5.21	133.90	124.71
15	B	1213	CLA	O2D-CGD-CBD	5.20	120.51	111.27
15	B	1214	CLA	O2D-CGD-CBD	5.20	120.50	111.27
15	A	1136	CLA	O2D-CGD-CBD	5.20	120.50	111.27
15	B	1022	CLA	O2A-C1-C2	5.20	122.29	108.64
15	B	1237	CLA	O2A-C1-C2	5.19	121.11	108.97
15	A	1132	CLA	O2A-C1-C2	5.19	121.10	108.97
15	A	1126	CLA	O2A-C1-C2	5.18	121.07	108.97
15	A	1105	CLA	O2D-CGD-CBD	5.17	120.46	111.27
15	B	1239	CLA	O2A-C1-C2	5.17	122.23	108.64
15	B	1227	CLA	O2D-CGD-CBD	5.17	120.46	111.27
15	B	1226	CLA	O2A-C1-C2	5.17	121.06	108.97
15	B	1235	CLA	CMD-C2D-C1D	5.17	133.82	124.71
15	B	1220	CLA	O2D-CGD-CBD	5.16	120.44	111.27
15	B	1240	CLA	O2A-C1-C2	5.16	122.19	108.64
15	B	1219	CLA	O2A-C1-C2	5.15	121.01	108.97
15	3	610	CLA	O2A-C1-C2	5.15	121.01	108.97
12	1	501	LUT	C12-C13-C14	-5.12	111.08	118.94
15	2	606	CLA	O2D-CGD-CBD	5.12	120.37	111.27
14	J	4003	BCR	C33-C5-C6	-5.12	118.78	124.53
15	1	613	CLA	O2D-CGD-CBD	5.12	120.36	111.27
15	A	1106	CLA	O2D-CGD-CBD	5.12	120.36	111.27
13	2	502	XAT	C15-C14-C13	-5.11	120.01	127.31
15	4	607	CLA	O2A-C1-C2	5.11	120.92	108.97
15	A	1121	CLA	O2A-C1-C2	5.11	120.91	108.97
15	B	1221	CLA	O2A-C1-C2	5.11	120.91	108.97
15	2	602	CLA	O2D-CGD-CBD	5.10	120.33	111.27
15	B	1235	CLA	O2A-C1-C2	5.10	122.04	108.64
13	2	502	XAT	C38-C25-C24	5.10	120.01	114.28
15	A	1012	CLA	CMD-C2D-C1D	5.09	133.68	124.71
15	2	608	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1209	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1210	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1229	CLA	O2D-CGD-CBD	5.08	120.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1203	CLA	O2A-C1-C2	5.07	120.83	108.97
15	1	612	CLA	O2A-C1-C2	5.07	121.95	108.64
15	2	607	CLA	O2D-CGD-CBD	5.06	120.26	111.27
15	A	1131	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	A	1012	CLA	O2A-C1-C2	5.05	121.91	108.64
13	3	502	XAT	C31-C30-C29	-5.05	120.10	127.31
15	B	1237	CLA	O2D-CGD-CBD	5.05	120.24	111.27
15	4	605	CLA	O2A-C1-C2	5.05	120.77	108.97
15	A	1141	CLA	O2D-CGD-CBD	5.04	120.23	111.27
15	A	1122	CLA	O2D-CGD-CBD	5.04	120.23	111.27
15	4	602	CLA	O2D-CGD-CBD	5.04	120.22	111.27
15	B	1239	CLA	O2D-CGD-CBD	5.04	120.22	111.27
15	A	1126	CLA	O2D-CGD-CBD	5.03	120.21	111.27
15	B	1201	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	B	1231	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	A	1109	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	A	1116	CLA	O2D-CGD-CBD	5.02	120.19	111.27
15	B	1238	CLA	O2D-CGD-CBD	5.02	120.19	111.27
15	1	603	CLA	O2D-CGD-CBD	5.02	120.19	111.27
13	1	502	XAT	C15-C14-C13	-5.02	120.14	127.31
14	A	4007	BCR	C33-C5-C6	-5.01	118.90	124.53
15	A	1130	CLA	O2A-C1-C2	5.01	121.79	108.64
13	4	502	XAT	C15-C14-C13	-5.01	120.17	127.31
18	1	803	LMG	O7-C10-C11	5.00	120.29	111.09
15	A	1127	CLA	O2D-CGD-CBD	5.00	120.16	111.27
15	1	611	CLA	O2D-CGD-CBD	5.00	120.15	111.27
15	A	1130	CLA	O2D-CGD-CBD	4.99	120.13	111.27
15	A	1120	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	2	603	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	B	1022	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	A	1124	CLA	O2D-CGD-CBD	4.98	120.11	111.27
15	A	1121	CLA	O2D-CGD-CBD	4.97	120.11	111.27
15	4	615	CLA	O2A-C1-C2	4.97	121.69	108.64
15	F	1301	CLA	O2D-CGD-CBD	4.97	120.09	111.27
15	B	1204	CLA	O2A-C1-C2	4.96	120.57	108.97
15	4	608	CLA	O2D-CGD-CBD	4.96	120.08	111.27
15	A	1104	CLA	O2A-C1-C2	4.95	121.66	108.64
15	2	604	CLA	O2A-C1-C2	4.95	120.55	108.97
15	B	1222	CLA	CMD-C2D-C1D	4.95	133.43	124.71
15	A	1123	CLA	O2D-CGD-CBD	4.95	120.06	111.27
15	2	615	CLA	O2A-C1-C2	4.94	121.63	108.64
13	1	502	XAT	C18-C5-C4	4.94	119.84	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	615	CLA	O2D-CGD-CBD	4.94	120.04	111.27
16	1	610	CHL	C4D-CHA-C1A	4.93	127.25	121.25
15	A	1113	CLA	O2D-CGD-CBD	4.93	120.03	111.27
15	B	1232	CLA	O2D-CGD-CBD	4.93	120.03	111.27
15	A	1106	CLA	O2A-C1-C2	4.93	121.58	108.64
15	3	607	CLA	O2D-CGD-CBD	4.92	120.00	111.27
16	1	610	CHL	CHD-C1D-ND	-4.91	119.95	124.45
15	F	1302	CLA	O2A-C1-C2	4.90	120.44	108.97
15	A	1129	CLA	O2D-CGD-CBD	4.89	119.96	111.27
15	3	615	CLA	O2D-CGD-CBD	4.89	119.95	111.27
15	3	608	CLA	O2D-CGD-CBD	4.89	119.95	111.27
15	B	1223	CLA	O2A-C1-C2	4.88	121.47	108.64
15	B	1228	CLA	O2A-C1-C2	4.88	121.46	108.64
15	A	1135	CLA	O2D-CGD-CBD	4.88	119.93	111.27
15	B	1211	CLA	O2D-CGD-CBD	4.88	119.93	111.27
15	A	1112	CLA	O2D-CGD-CBD	4.87	119.92	111.27
13	3	502	XAT	C7-C8-C9	-4.87	117.98	125.53
15	2	605	CLA	O2D-CGD-CBD	4.86	119.90	111.27
17	2	801	LHG	O7-C7-C8	4.86	120.03	111.09
17	B	5001	LHG	O7-C7-C8	4.86	120.03	111.09
15	A	1133	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	A	1139	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	A	1117	CLA	O2D-CGD-CBD	4.85	119.88	111.27
14	J	4001	BCR	C33-C5-C6	-4.85	119.09	124.53
15	A	1118	CLA	O2D-CGD-CBD	4.85	119.88	111.27
15	A	1107	CLA	O2D-CGD-CBD	4.84	119.88	111.27
15	B	1228	CLA	O2D-CGD-CBD	4.84	119.88	111.27
15	2	605	CLA	O2A-C1-C2	4.84	121.34	108.64
15	A	1012	CLA	O2D-CGD-CBD	4.83	119.85	111.27
15	B	1234	CLA	O2D-CGD-CBD	4.83	119.84	111.27
14	F	4002	BCR	C15-C14-C13	-4.82	120.43	127.31
15	4	606	CLA	O2D-CGD-CBD	4.82	119.83	111.27
15	A	1119	CLA	O2D-CGD-CBD	4.81	119.82	111.27
15	3	613	CLA	O2D-CGD-CBD	4.81	119.81	111.27
13	2	502	XAT	C31-C30-C29	-4.80	120.46	127.31
15	3	612	CLA	O2A-C1-C2	4.80	121.25	108.64
12	1	501	LUT	C15-C14-C13	4.79	134.14	127.31
15	J	1302	CLA	O2A-C1-C2	4.79	120.17	108.97
15	A	1139	CLA	O2A-C1-C2	4.78	121.21	108.64
15	2	612	CLA	CMD-C2D-C1D	4.78	133.13	124.71
15	F	1302	CLA	O2D-CGD-CBD	4.77	119.75	111.27
15	B	1023	CLA	O2A-C1-C2	4.77	121.18	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	502	XAT	C38-C25-C24	4.77	119.65	114.28
15	A	1138	CLA	O2A-C1-C2	4.77	121.17	108.64
15	B	1230	CLA	O2D-CGD-CBD	4.76	119.72	111.27
24	A	1011	CL0	C2B-C1B-NB	4.75	113.42	110.23
15	B	1219	CLA	O2D-CGD-CBD	4.75	119.71	111.27
15	1	607	CLA	O2D-CGD-CBD	4.75	119.71	111.27
15	A	1103	CLA	O2A-C1-C2	4.75	121.11	108.64
15	B	1208	CLA	O2D-CGD-CBD	4.74	119.69	111.27
24	A	1011	CL0	O2A-CGA-O1A	-4.71	111.70	123.59
24	A	1011	CL0	C3B-C2B-C1B	-4.71	101.47	107.16
15	J	1302	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	A	1138	CLA	O2D-CGD-CBD	4.71	119.63	111.27
15	B	1224	CLA	O2D-CGD-CBD	4.70	119.62	111.27
15	B	1217	CLA	O2D-CGD-CBD	4.70	119.62	111.27
16	4	611	CHL	CHD-C1D-ND	-4.69	120.14	124.45
15	A	1141	CLA	O2A-C1-C2	4.69	120.97	108.64
15	3	610	CLA	O2D-CGD-CBD	4.69	119.60	111.27
12	1	501	LUT	C40-C33-C34	-4.68	116.36	122.92
15	1	615	CLA	O2A-C1-C2	4.67	120.91	108.64
15	A	1140	CLA	O2A-C1-C2	4.66	120.89	108.64
15	3	607	CLA	O2A-C1-C2	4.66	120.89	108.64
15	B	1206	CLA	O2D-CGD-CBD	4.66	119.55	111.27
15	A	1125	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	A	1011	CL0	O2A-C1-C2	4.63	120.81	108.64
15	3	611	CLA	O2D-CGD-CBD	4.63	119.50	111.27
15	B	1238	CLA	O2A-C1-C2	4.63	120.80	108.64
15	B	1218	CLA	O2D-CGD-CBD	4.63	119.49	111.27
15	B	1202	CLA	O2D-CGD-CBD	4.63	119.49	111.27
12	1	501	LUT	C18-C5-C6	-4.63	119.33	124.53
12	3	501	LUT	C11-C10-C9	-4.62	120.71	127.31
24	A	1011	CL0	C3D-C2D-C1D	-4.62	99.53	105.83
15	B	1203	CLA	O2D-CGD-CBD	4.61	119.47	111.27
14	F	4002	BCR	C33-C5-C6	-4.61	119.35	124.53
15	A	1131	CLA	O2A-C1-C2	4.61	120.74	108.64
15	A	1013	CLA	O2D-CGD-CBD	4.61	119.45	111.27
12	1	501	LUT	C21-C26-C25	4.60	119.67	111.42
15	B	1231	CLA	O2A-C1-C2	4.57	120.64	108.64
12	3	501	LUT	C18-C5-C6	-4.57	119.40	124.53
13	2	502	XAT	C18-C5-C4	4.56	119.42	114.28
14	2	503	BCR	C33-C5-C6	-4.55	119.42	124.53
15	4	603	CLA	O2D-CGD-CBD	4.54	119.34	111.27
15	B	1021	CLA	O2D-CGD-CBD	4.54	119.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	601	CLA	O2D-CGD-CBD	4.52	119.30	111.27
17	A	5002	LHG	O7-C7-C8	4.51	121.22	111.50
12	3	501	LUT	C7-C8-C9	-4.49	119.44	126.23
14	B	4004	BCR	C33-C5-C6	-4.48	119.49	124.53
18	1	802	LMG	O7-C10-C11	4.47	121.14	111.50
15	3	605	CLA	O2D-CGD-CBD	4.47	119.21	111.27
14	B	4002	BCR	C15-C14-C13	-4.47	120.93	127.31
14	J	4002	BCR	C4-C5-C6	-4.46	116.25	122.73
12	3	501	LUT	C21-C26-C27	4.46	118.34	112.70
13	3	502	XAT	C18-C5-C4	4.45	119.29	114.28
12	4	501	LUT	C18-C5-C6	-4.45	119.53	124.53
14	A	4004	BCR	C33-C5-C6	-4.44	119.54	124.53
14	B	4005	BCR	C33-C5-C6	-4.43	119.55	124.53
15	1	601	CLA	O2D-CGD-CBD	4.41	119.10	111.27
13	4	502	XAT	C18-C5-C4	4.39	119.22	114.28
15	1	612	CLA	C1-C2-C3	-4.39	118.45	126.04
13	1	502	XAT	C38-C25-C24	4.38	119.21	114.28
15	A	1110	CLA	O2D-CGD-CBD	4.34	118.98	111.27
24	A	1011	CL0	O2D-CGD-CBD	4.34	118.98	111.27
14	3	504	BCR	C33-C5-C6	-4.34	119.66	124.53
15	B	1207	CLA	C2D-C3D-C4D	-4.34	102.48	107.28
16	2	613	CHL	CHD-C1D-ND	-4.32	120.49	124.45
13	3	502	XAT	C38-C25-C24	4.31	119.13	114.28
14	A	4002	BCR	C33-C5-C6	-4.29	119.71	124.53
15	B	1207	CLA	C1C-NC-C4C	4.29	108.64	106.71
15	B	1229	CLA	O2A-C1-C2	4.28	119.89	108.64
12	2	501	LUT	C7-C8-C9	-4.28	119.77	126.23
14	1	505	BCR	C33-C5-C6	-4.28	119.72	124.53
12	2	501	LUT	C18-C5-C6	-4.26	119.74	124.53
14	B	4002	BCR	C33-C5-C6	-4.24	119.76	124.53
17	1	801	LHG	O7-C7-C8	4.23	120.62	111.50
12	3	501	LUT	C35-C34-C33	-4.22	121.29	127.31
14	4	503	BCR	C33-C5-C6	-4.20	119.81	124.53
16	1	609	CHL	CHD-C1D-ND	-4.19	120.61	124.45
12	1	501	LUT	C20-C13-C12	4.18	124.66	118.08
15	1	612	CLA	O2D-CGD-CBD	4.18	118.69	111.27
16	4	610	CHL	CHD-C1D-ND	-4.17	120.63	124.45
15	A	1013	CLA	O2A-C1-C2	4.15	119.55	108.64
15	B	1223	CLA	C1-C2-C3	-4.15	120.05	126.75
21	2	811	DGD	O2G-C1B-C2B	4.13	120.39	111.50
15	4	615	CLA	O2D-CGD-CBD	4.12	118.59	111.27
15	B	1240	CLA	O2D-CGD-CBD	4.10	118.56	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	4002	BCR	C33-C5-C4	4.10	121.50	113.62
16	3	604	CHL	CHD-C1D-ND	-4.10	120.68	124.45
23	4	831	GSH	CA2-CB2-SG2	-4.10	109.58	114.19
14	B	4003	BCR	C33-C5-C6	-4.09	119.94	124.53
12	1	501	LUT	C10-C11-C12	-4.08	110.47	123.22
23	B	5031	GSH	CA2-CB2-SG2	-4.07	109.62	114.19
16	4	613	CHL	CHD-C1D-ND	-4.06	120.72	124.45
16	2	611	CHL	CHD-C1D-ND	-4.04	120.75	124.45
15	2	601	CLA	O2D-CGD-CBD	4.02	118.42	111.27
15	4	615	CLA	C1-C2-C3	-4.02	119.09	126.04
14	A	4006	BCR	C33-C5-C6	-4.02	120.01	124.53
15	B	1023	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	4	811	DGD	O2G-C1B-C2B	3.99	120.09	111.50
16	2	609	CHL	CHD-C1D-ND	-3.98	120.80	124.45
12	4	501	LUT	C15-C14-C13	-3.96	121.66	127.31
15	B	1022	CLA	C1-C2-C3	-3.95	120.36	126.75
14	J	4002	BCR	C1-C6-C5	-3.94	117.06	122.61
14	A	4005	BCR	C15-C14-C13	-3.94	121.69	127.31
14	3	503	BCR	C33-C5-C6	-3.92	120.13	124.53
12	4	501	LUT	C22-C23-C24	-3.91	107.29	111.74
14	2	503	BCR	C15-C14-C13	-3.88	121.77	127.31
21	B	5002	DGD	O2G-C1B-C2B	3.88	119.85	111.50
14	A	4003	BCR	C33-C5-C6	-3.87	120.18	124.53
15	A	1141	CLA	C1-C2-C3	-3.87	120.49	126.75
14	B	4001	BCR	C33-C5-C4	3.86	121.03	113.62
12	3	501	LUT	C15-C14-C13	-3.83	121.84	127.31
15	B	1238	CLA	C1-C2-C3	-3.82	120.56	126.75
15	A	1013	CLA	CHD-C1D-ND	-3.81	120.95	124.45
16	2	610	CHL	CHD-C1D-ND	-3.80	120.96	124.45
15	B	1207	CLA	C3D-C2D-C1D	-3.80	103.07	107.28
14	1	503	BCR	C33-C5-C6	-3.79	120.27	124.53
14	2	503	BCR	C33-C5-C4	3.77	120.86	113.62
15	A	1012	CLA	C1-C2-C3	-3.75	119.55	126.04
12	1	501	LUT	C35-C34-C33	3.74	132.65	127.31
15	B	1235	CLA	CHD-C1D-ND	-3.74	121.02	124.45
15	1	605	CLA	O2A-C1-C2	3.73	122.11	109.49
14	4	503	BCR	C15-C14-C13	-3.73	121.98	127.31
15	B	1021	CLA	C1-C2-C3	-3.73	119.59	126.04
15	3	603	CLA	CAC-C3C-C4C	3.73	129.65	124.81
15	B	1222	CLA	CHD-C1D-ND	-3.72	121.03	124.45
15	A	1131	CLA	C1-C2-C3	-3.71	120.74	126.75
13	2	502	XAT	C7-C8-C9	-3.69	119.80	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	503	BCR	C33-C5-C4	3.69	120.70	113.62
15	3	607	CLA	C1-C2-C3	-3.68	120.80	126.75
15	A	1126	CLA	C2C-C1C-NC	3.68	113.42	109.97
25	B	2002	PQN	C11-C12-C13	-3.67	120.68	126.79
15	4	604	CLA	CHD-C1D-ND	-3.67	121.08	124.45
15	B	1215	CLA	CHD-C1D-ND	-3.66	121.09	124.45
14	1	503	BCR	C33-C5-C4	3.64	120.61	113.62
15	1	608	CLA	CHD-C1D-ND	-3.63	121.12	124.45
14	B	4004	BCR	C15-C14-C13	-3.63	122.13	127.31
15	4	615	CLA	CHD-C1D-ND	-3.63	121.12	124.45
14	4	505	BCR	C33-C5-C4	3.63	120.58	113.62
15	B	1231	CLA	CHD-C1D-ND	-3.63	121.12	124.45
15	B	1235	CLA	C1-C2-C3	-3.61	119.80	126.04
17	A	5002	LHG	O8-C23-C24	3.61	120.84	111.38
15	B	1207	CLA	C4A-NA-C1A	-3.61	105.08	106.71
15	A	1111	CLA	CHD-C1D-ND	-3.61	121.14	124.45
15	2	607	CLA	CHD-C1D-ND	-3.60	121.15	124.45
15	A	1110	CLA	CHD-C1D-ND	-3.59	121.16	124.45
15	2	605	CLA	C1-C2-C3	-3.59	119.84	126.04
15	B	1221	CLA	CHD-C1D-ND	-3.58	121.16	124.45
15	F	1301	CLA	O2A-C1-C2	3.58	121.58	108.42
16	4	610	CHL	C3C-C4C-NC	-3.58	106.56	110.57
14	A	4002	BCR	C34-C9-C10	-3.57	117.92	122.92
15	B	1201	CLA	O2A-C1-C2	3.57	121.56	109.49
15	2	615	CLA	C1-C2-C3	-3.57	120.98	126.75
13	2	502	XAT	O24-C25-C24	3.57	116.06	113.38
15	1	607	CLA	CHD-C1D-ND	-3.57	121.18	124.45
15	A	1101	CLA	CHD-C1D-ND	-3.56	121.18	124.45
15	B	1203	CLA	CHD-C1D-ND	-3.55	121.19	124.45
15	B	1228	CLA	C1-C2-C3	-3.55	119.91	126.04
15	3	606	CLA	CHD-C1D-ND	-3.55	121.20	124.45
15	A	1126	CLA	CHD-C1D-ND	-3.54	121.20	124.45
15	3	615	CLA	C2C-C1C-NC	3.54	113.29	109.97
15	1	606	CLA	CHD-C1D-ND	-3.54	121.20	124.45
15	A	1137	CLA	CHD-C1D-ND	-3.54	121.20	124.45
15	A	1138	CLA	C1-C2-C3	-3.54	119.92	126.04
15	3	611	CLA	CHD-C1D-ND	-3.53	121.21	124.45
15	B	1204	CLA	CHD-C1D-ND	-3.52	121.22	124.45
15	3	613	CLA	CHD-C1D-ND	-3.52	121.22	124.45
15	B	1213	CLA	CHD-C1D-ND	-3.51	121.23	124.45
14	J	4002	BCR	C34-C9-C10	-3.50	118.01	122.92
15	A	1104	CLA	C1-C2-C3	-3.50	119.99	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4006	BCR	C33-C5-C6	-3.50	120.60	124.53
15	4	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
15	3	603	CLA	C2C-C1C-NC	3.50	113.25	109.97
15	3	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
15	B	1232	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	2	802	LMG	O8-C28-C29	3.49	120.53	111.38
24	A	1011	CL0	O2A-CGA-CBA	3.49	122.86	111.91
15	A	1123	CLA	O2A-C1-C2	3.49	121.29	109.49
15	B	1227	CLA	CHD-C1D-ND	-3.49	121.25	124.45
15	4	609	CLA	CHD-C1D-ND	-3.48	121.25	124.45
15	A	1129	CLA	O2A-C1-C2	3.48	121.24	109.49
15	B	1228	CLA	CHD-C1D-ND	-3.47	121.26	124.45
15	A	1104	CLA	CHD-C1D-ND	-3.46	121.27	124.45
15	2	603	CLA	CHD-C1D-ND	-3.45	121.28	124.45
15	A	1130	CLA	C1-C2-C3	-3.45	120.07	126.04
15	B	1209	CLA	CHD-C1D-ND	-3.45	121.28	124.45
15	1	612	CLA	CHD-C1D-ND	-3.45	121.28	124.45
14	A	4005	BCR	C33-C5-C4	3.44	120.23	113.62
15	A	1117	CLA	CHD-C1D-ND	-3.43	121.30	124.45
14	B	4003	BCR	C33-C5-C4	3.43	120.21	113.62
25	A	2001	PQN	C11-C12-C13	-3.43	121.08	126.79
15	B	1202	CLA	CHD-C1D-ND	-3.43	121.30	124.45
16	1	610	CHL	C4B-CHC-C1C	3.43	134.46	126.34
15	2	606	CLA	C2C-C1C-NC	3.42	113.18	109.97
15	B	1201	CLA	CHD-C1D-ND	-3.42	121.31	124.45
15	A	1130	CLA	CHD-C1D-ND	-3.42	121.31	124.45
15	2	606	CLA	CHD-C1D-ND	-3.42	121.31	124.45
15	2	602	CLA	CHD-C1D-ND	-3.41	121.32	124.45
14	A	4005	BCR	C33-C5-C6	-3.41	120.70	124.53
15	A	1109	CLA	CHD-C1D-ND	-3.41	121.32	124.45
15	A	1136	CLA	CHD-C1D-ND	-3.41	121.32	124.45
13	4	502	XAT	C7-C8-C9	-3.41	120.24	125.53
15	4	609	CLA	C2C-C1C-NC	3.41	113.17	109.97
15	2	608	CLA	CHD-C1D-ND	-3.41	121.32	124.45
15	B	1223	CLA	C2C-C1C-NC	3.41	113.16	109.97
15	A	1124	CLA	CHD-C1D-ND	-3.40	121.33	124.45
14	B	4006	BCR	C27-C26-C25	-3.40	117.79	122.73
15	2	604	CLA	C2C-C1C-NC	3.40	113.16	109.97
15	3	607	CLA	CHD-C1D-ND	-3.40	121.33	124.45
15	3	608	CLA	O2A-C1-C2	3.39	120.97	109.49
15	B	1216	CLA	CHD-C1D-ND	-3.39	121.34	124.45
16	2	613	CHL	C3C-C4C-NC	-3.39	106.77	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	1301	CLA	CHD-C1D-ND	-3.38	121.34	124.45
14	4	505	BCR	C33-C5-C6	-3.38	120.73	124.53
13	2	502	XAT	O4-C5-C4	-3.38	110.84	113.38
15	B	1212	CLA	CHD-C1D-ND	-3.38	121.34	124.45
15	A	1139	CLA	C1-C2-C3	-3.38	120.19	126.04
15	A	1128	CLA	CHD-C1D-ND	-3.38	121.35	124.45
15	1	602	CLA	CHD-C1D-ND	-3.38	121.35	124.45
15	B	1231	CLA	C1-C2-C3	-3.38	120.20	126.04
14	A	4005	BCR	C27-C26-C25	-3.38	117.83	122.73
15	B	1218	CLA	CHD-C1D-ND	-3.38	121.35	124.45
15	A	1103	CLA	C2C-C1C-NC	3.38	113.13	109.97
16	3	604	CHL	C3C-C4C-NC	-3.37	106.79	110.57
16	4	613	CHL	CMA-C3A-C4A	3.37	120.83	111.77
14	B	4001	BCR	C33-C5-C6	-3.37	120.74	124.53
16	4	613	CHL	C2C-C3C-C4C	3.37	108.89	106.49
15	B	1229	CLA	CHD-C1D-ND	-3.37	121.36	124.45
14	B	4002	BCR	C33-C5-C4	3.36	120.08	113.62
15	B	1225	CLA	CHD-C1D-ND	-3.36	121.36	124.45
15	B	1022	CLA	CHD-C1D-ND	-3.36	121.36	124.45
15	1	604	CLA	CHD-C1D-ND	-3.36	121.36	124.45
15	A	1133	CLA	CHD-C1D-ND	-3.36	121.36	124.45
15	B	1208	CLA	CHD-C1D-ND	-3.36	121.37	124.45
15	A	1140	CLA	C1-C2-C3	-3.36	120.24	126.04
15	B	1224	CLA	CHD-C1D-ND	-3.35	121.37	124.45
14	A	4003	BCR	C36-C18-C17	-3.35	118.23	122.92
16	4	613	CHL	C2B-C1B-NB	-3.35	107.99	110.23
15	B	1236	CLA	C2D-C1D-ND	3.35	112.57	110.10
15	F	1301	CLA	C2C-C1C-NC	3.35	113.11	109.97
15	A	1115	CLA	CHD-C1D-ND	-3.34	121.38	124.45
15	A	1119	CLA	CHD-C1D-ND	-3.34	121.38	124.45
15	1	613	CLA	CHD-C1D-ND	-3.34	121.38	124.45
15	A	1118	CLA	CHD-C1D-ND	-3.34	121.39	124.45
15	A	1120	CLA	CHD-C1D-ND	-3.34	121.39	124.45
12	2	501	LUT	C35-C34-C33	-3.33	122.55	127.31
15	A	1125	CLA	CHD-C1D-ND	-3.33	121.39	124.45
15	A	1141	CLA	CHD-C1D-ND	-3.33	121.39	124.45
15	2	612	CLA	C2D-C1D-ND	3.33	112.56	110.10
15	B	1237	CLA	CHD-C1D-ND	-3.32	121.40	124.45
17	2	801	LHG	C5-O7-C7	-3.32	111.71	117.90
16	1	609	CHL	CMA-C3A-C4A	3.32	120.70	111.77
15	A	1121	CLA	CHD-C1D-ND	-3.32	121.41	124.45
15	A	1123	CLA	CHD-C1D-ND	-3.31	121.41	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4005	BCR	C33-C5-C4	3.31	119.98	113.62
15	1	608	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	3	612	CLA	C1-C2-C3	-3.31	120.32	126.04
15	B	1221	CLA	C2C-C1C-NC	3.30	113.07	109.97
14	A	4004	BCR	C15-C14-C13	-3.30	122.59	127.31
15	3	611	CLA	C2C-C1C-NC	3.30	113.07	109.97
15	B	1226	CLA	CHD-C1D-ND	-3.30	121.42	124.45
15	1	605	CLA	CHD-C1D-ND	-3.30	121.42	124.45
13	2	502	XAT	C26-C27-C28	-3.30	119.02	125.99
15	4	608	CLA	CHD-C1D-ND	-3.30	121.42	124.45
15	A	1105	CLA	CHD-C1D-ND	-3.30	121.42	124.45
15	2	601	CLA	CHD-C1D-ND	-3.30	121.42	124.45
15	A	1113	CLA	CHD-C1D-ND	-3.29	121.43	124.45
15	B	1202	CLA	C2C-C1C-NC	3.29	113.06	109.97
15	2	615	CLA	CHD-C1D-ND	-3.29	121.43	124.45
15	1	615	CLA	C2C-C1C-NC	3.29	113.05	109.97
16	3	604	CHL	C4D-CHA-C1A	3.29	125.25	121.25
15	3	608	CLA	CHD-C1D-ND	-3.29	121.43	124.45
15	A	1134	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	1	803	LMG	C8-O7-C10	-3.29	111.77	117.90
15	A	1129	CLA	CHD-C1D-ND	-3.29	121.43	124.45
12	4	501	LUT	C35-C34-C33	-3.29	122.62	127.31
14	1	505	BCR	C33-C5-C4	3.29	119.93	113.62
15	A	1127	CLA	CHD-C1D-ND	-3.29	121.43	124.45
15	B	1223	CLA	CHD-C1D-ND	-3.28	121.44	124.45
15	A	1114	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	1	811	SQD	O7-S-C6	-3.28	103.04	106.94
15	J	1302	CLA	CHD-C1D-ND	-3.28	121.44	124.45
16	2	613	CHL	C2C-C3C-C4C	3.28	108.82	106.49
14	A	4002	BCR	C27-C26-C25	-3.27	117.98	122.73
15	A	1112	CLA	CHD-C1D-ND	-3.27	121.45	124.45
15	B	1211	CLA	C2C-C1C-NC	3.27	113.04	109.97
15	1	602	CLA	C2D-C1D-ND	3.27	112.52	110.10
15	B	1230	CLA	CHD-C1D-ND	-3.27	121.45	124.45
15	A	1112	CLA	C2C-C1C-NC	3.27	113.03	109.97
18	2	802	LMG	O7-C10-C11	3.27	119.91	110.80
15	1	611	CLA	CHD-C1D-ND	-3.27	121.45	124.45
14	J	4002	BCR	C8-C9-C10	3.26	123.95	118.94
15	B	1205	CLA	CHD-C1D-ND	-3.26	121.45	124.45
15	A	1135	CLA	C2C-C1C-NC	3.26	113.03	109.97
14	B	4001	BCR	C27-C26-C25	-3.26	117.99	122.73
15	B	1238	CLA	CHD-C1D-ND	-3.26	121.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	610	CHL	CMA-C3A-C4A	3.26	120.54	111.77
15	3	612	CLA	CHD-C1D-ND	-3.26	121.46	124.45
14	J	4001	BCR	C27-C26-C25	-3.26	118.00	122.73
15	A	1127	CLA	C2C-C1C-NC	3.26	113.02	109.97
15	A	1104	CLA	C2C-C1C-NC	3.25	113.02	109.97
15	A	1136	CLA	C2C-C1C-NC	3.25	113.02	109.97
16	1	609	CHL	C4D-CHA-C1A	3.24	125.20	121.25
15	3	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
15	B	1210	CLA	CHD-C1D-ND	-3.24	121.47	124.45
15	4	608	CLA	C2C-C1C-NC	3.24	113.01	109.97
15	B	1021	CLA	CHD-C1D-ND	-3.24	121.48	124.45
15	A	1135	CLA	CHD-C1D-ND	-3.24	121.48	124.45
16	4	613	CHL	C4A-NA-C1A	3.24	108.16	106.71
24	A	1011	CL0	C1D-ND-C4D	-3.24	104.04	106.33
15	B	1220	CLA	CHD-C1D-ND	-3.24	121.48	124.45
15	1	613	CLA	C2C-C1C-NC	3.23	113.00	109.97
15	B	1211	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	2	821	LMT	C1'-O5'-C5'	-3.23	107.56	113.66
15	A	1012	CLA	CHD-C1D-ND	-3.23	121.48	124.45
15	4	605	CLA	CHD-C1D-ND	-3.23	121.49	124.45
15	A	1115	CLA	C2C-C1C-NC	3.23	113.00	109.97
14	4	505	BCR	C34-C9-C10	-3.22	118.41	122.92
15	A	1107	CLA	CMA-C3A-C4A	3.22	120.43	111.77
15	A	1122	CLA	CHD-C1D-ND	-3.22	121.49	124.45
15	3	606	CLA	C2C-C1C-NC	3.22	112.99	109.97
15	1	601	CLA	CHD-C1D-ND	-3.22	121.50	124.45
15	1	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
16	2	611	CHL	CMA-C3A-C4A	3.22	120.42	111.77
15	A	1107	CLA	C2C-C1C-NC	3.22	112.98	109.97
15	B	1204	CLA	C2C-C1C-NC	3.22	112.98	109.97
15	B	1214	CLA	C2C-C1C-NC	3.21	112.98	109.97
15	4	615	CLA	CMA-C3A-C4A	3.21	120.41	111.77
15	A	1102	CLA	CHD-C1D-ND	-3.21	121.50	124.45
16	4	610	CHL	CMA-C3A-C4A	3.21	120.40	111.77
15	A	1013	CLA	C2C-C1C-NC	3.21	112.98	109.97
15	4	602	CLA	CHD-C1D-ND	-3.21	121.51	124.45
16	2	610	CHL	CMA-C3A-C4A	3.21	120.39	111.77
15	A	1101	CLA	C2C-C1C-NC	3.20	112.97	109.97
15	4	615	CLA	C2C-C1C-NC	3.20	112.97	109.97
16	2	609	CHL	CMA-C3A-C4A	3.20	120.38	111.77
15	B	1239	CLA	CHD-C1D-ND	-3.20	121.52	124.45
13	3	502	XAT	C15-C14-C13	-3.20	122.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	3	501	LUT	C31-C30-C29	-3.20	122.75	127.31
16	2	610	CHL	C3C-C4C-NC	-3.19	106.99	110.57
16	2	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57
15	A	1106	CLA	C2C-C1C-NC	3.19	112.96	109.97
15	B	1240	CLA	C2C-C1C-NC	3.19	112.96	109.97
15	4	609	CLA	CMA-C3A-C4A	3.19	120.34	111.77
15	B	1217	CLA	CHD-C1D-ND	-3.19	121.53	124.45
14	A	4003	BCR	C34-C9-C10	-3.19	118.46	122.92
15	B	1210	CLA	C2C-C1C-NC	3.18	112.95	109.97
15	4	606	CLA	CHD-C1D-ND	-3.18	121.53	124.45
15	B	1240	CLA	CHD-C1D-ND	-3.18	121.53	124.45
15	3	615	CLA	CHD-C1D-ND	-3.18	121.53	124.45
14	3	504	BCR	C33-C5-C4	3.18	119.72	113.62
14	B	4005	BCR	C15-C14-C13	-3.17	122.78	127.31
15	A	1131	CLA	CHD-C1D-ND	-3.17	121.54	124.45
16	2	610	CHL	C4D-CHA-C1A	3.17	125.11	121.25
16	3	604	CHL	CHD-C4C-C3C	3.17	129.50	124.84
14	A	4004	BCR	C33-C5-C4	3.17	119.71	113.62
15	2	605	CLA	CMA-C3A-C4A	3.17	120.29	111.77
14	B	4001	BCR	C1-C6-C5	-3.17	118.15	122.61
15	3	605	CLA	CHD-C1D-ND	-3.17	121.54	124.45
16	4	613	CHL	C3C-C4C-NC	-3.17	107.02	110.57
15	2	607	CLA	C2C-C1C-NC	3.16	112.94	109.97
15	3	601	CLA	CMA-C3A-C4A	3.16	120.27	111.77
14	4	503	BCR	C27-C26-C25	-3.16	118.14	122.73
15	A	1123	CLA	C2C-C1C-NC	3.16	112.93	109.97
15	A	1103	CLA	CHD-C1D-ND	-3.16	121.55	124.45
14	B	4004	BCR	C27-C26-C25	-3.16	118.14	122.73
15	B	1209	CLA	C2C-C1C-NC	3.16	112.93	109.97
16	4	611	CHL	C4D-CHA-C1A	3.16	125.09	121.25
15	A	1138	CLA	CHD-C1D-ND	-3.16	121.55	124.45
15	A	1137	CLA	CMA-C3A-C4A	3.16	120.26	111.77
14	J	4003	BCR	C27-C26-C25	-3.16	118.15	122.73
15	1	608	CLA	CMA-C3A-C4A	3.16	120.26	111.77
15	B	1230	CLA	C2C-C1C-NC	3.16	112.93	109.97
16	1	609	CHL	C3C-C4C-NC	-3.16	107.03	110.57
14	B	4004	BCR	C33-C5-C4	3.15	119.67	113.62
16	4	611	CHL	C2C-C3C-C4C	3.15	108.74	106.49
14	A	4002	BCR	C33-C5-C4	3.15	119.67	113.62
15	B	1222	CLA	C2D-C1D-ND	3.15	112.43	110.10
15	A	1106	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	B	5002	DGD	O1G-C1A-C2A	3.15	119.64	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1217	CLA	CMA-C3A-C4A	3.15	120.23	111.77
15	A	1124	CLA	C2C-C1C-NC	3.15	112.92	109.97
16	2	611	CHL	C3C-C4C-NC	-3.15	107.04	110.57
15	3	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
15	2	602	CLA	C2C-C1C-NC	3.14	112.92	109.97
14	4	503	BCR	C38-C26-C27	3.14	119.65	113.62
15	A	1132	CLA	CHD-C1D-ND	-3.14	121.57	124.45
15	B	1224	CLA	C2C-C1C-NC	3.14	112.92	109.97
15	A	1139	CLA	CHD-C1D-ND	-3.14	121.57	124.45
15	4	615	CLA	C2D-C1D-ND	3.14	112.42	110.10
15	A	1012	CLA	C2C-C1C-NC	3.14	112.91	109.97
15	B	1231	CLA	C2C-C1C-NC	3.14	112.91	109.97
14	3	503	BCR	C27-C26-C25	-3.14	118.18	122.73
15	3	603	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
15	A	1140	CLA	CMA-C3A-C4A	3.14	120.20	111.77
15	B	1021	CLA	C2C-C1C-NC	3.13	112.91	109.97
15	A	1116	CLA	CHD-C1D-ND	-3.13	121.57	124.45
15	A	1103	CLA	C1-C2-C3	-3.13	120.62	126.04
15	A	1130	CLA	C2C-C1C-NC	3.13	112.91	109.97
14	3	503	BCR	C36-C18-C17	-3.13	118.54	122.92
16	3	604	CHL	CMA-C3A-C4A	3.13	120.19	111.77
15	B	1023	CLA	CHD-C1D-ND	-3.13	121.58	124.45
14	J	4002	BCR	C27-C26-C25	-3.13	118.19	122.73
15	2	604	CLA	CHD-C1D-ND	-3.13	121.58	124.45
15	B	1219	CLA	C2C-C1C-NC	3.13	112.90	109.97
13	3	502	XAT	O4-C5-C18	-3.13	111.31	115.06
15	4	612	CLA	CHD-C1D-ND	-3.13	121.58	124.45
15	B	1226	CLA	CMA-C3A-C4A	3.12	120.17	111.77
15	F	1302	CLA	C2C-C1C-NC	3.12	112.90	109.97
15	A	1140	CLA	CHD-C1D-ND	-3.12	121.58	124.45
15	B	1239	CLA	C1-C2-C3	-3.12	120.64	126.04
12	2	501	LUT	C22-C23-C24	-3.12	108.19	111.74
15	A	1114	CLA	C2C-C1C-NC	3.12	112.89	109.97
15	B	1206	CLA	CHD-C1D-ND	-3.12	121.59	124.45
15	2	605	CLA	CHD-C1D-ND	-3.12	121.59	124.45
15	A	1121	CLA	C2C-C1C-NC	3.11	112.89	109.97
15	A	1116	CLA	C2C-C1C-NC	3.11	112.89	109.97
15	F	1302	CLA	CHD-C1D-ND	-3.11	121.59	124.45
15	4	602	CLA	C2D-C1D-ND	3.11	112.40	110.10
14	F	4002	BCR	C33-C5-C4	3.11	119.59	113.62
15	4	605	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	A	1107	CLA	CHD-C1D-ND	-3.11	121.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1211	CLA	CMA-C3A-C4A	3.11	120.12	111.77
15	2	603	CLA	CMA-C3A-C4A	3.11	120.12	111.77
15	1	611	CLA	C2C-C1C-NC	3.10	112.88	109.97
14	B	4001	BCR	C4-C5-C6	-3.10	118.23	122.73
15	2	605	CLA	C2C-C1C-NC	3.10	112.88	109.97
15	B	1222	CLA	C2C-C1C-NC	3.10	112.88	109.97
15	A	1135	CLA	CMA-C3A-C4A	3.10	120.11	111.77
15	4	607	CLA	CHD-C1D-ND	-3.10	121.61	124.45
15	A	1141	CLA	C2C-C1C-NC	3.10	112.87	109.97
15	A	1139	CLA	CMA-C3A-C4A	3.09	120.09	111.77
15	A	1132	CLA	C2C-C1C-NC	3.09	112.87	109.97
14	A	4007	BCR	C27-C26-C25	-3.09	118.24	122.73
14	A	4007	BCR	C36-C18-C17	-3.09	118.59	122.92
14	1	503	BCR	C38-C26-C27	3.09	119.55	113.62
15	A	1108	CLA	CHD-C1D-ND	-3.09	121.62	124.45
15	B	1210	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	B	1237	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	B	1205	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	3	607	CLA	C2C-C1C-NC	3.09	112.86	109.97
16	2	613	CHL	CMA-C3A-C4A	3.08	120.06	111.77
14	B	4005	BCR	C38-C26-C25	-3.08	121.06	124.53
15	A	1110	CLA	C2D-C1D-ND	3.08	112.38	110.10
15	B	1221	CLA	C2D-C1D-ND	3.08	112.38	110.10
15	B	1212	CLA	C2C-C1C-NC	3.08	112.86	109.97
15	B	1237	CLA	C2C-C1C-NC	3.08	112.86	109.97
15	2	608	CLA	CMA-C3A-C4A	3.08	120.05	111.77
15	3	603	CLA	CHD-C1D-ND	-3.08	121.62	124.45
15	2	604	CLA	C2D-C1D-ND	3.08	112.37	110.10
14	A	4003	BCR	C33-C5-C4	3.08	119.53	113.62
14	1	503	BCR	C34-C9-C10	-3.07	118.62	122.92
15	A	1119	CLA	C2C-C1C-NC	3.07	112.85	109.97
15	B	1219	CLA	CHD-C1D-ND	-3.07	121.63	124.45
15	B	1220	CLA	CMA-C3A-C4A	3.07	120.03	111.77
15	A	1129	CLA	C2C-C1C-NC	3.07	112.85	109.97
14	B	4003	BCR	C34-C9-C10	-3.07	118.63	122.92
14	1	503	BCR	C28-C27-C26	-3.07	108.60	114.08
15	1	607	CLA	C2C-C1C-NC	3.07	112.84	109.97
15	B	1215	CLA	C2C-C1C-NC	3.07	112.84	109.97
15	B	1209	CLA	C2D-C1D-ND	3.06	112.36	110.10
15	F	1301	CLA	C2D-C1D-ND	3.06	112.36	110.10
15	B	1235	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	B	1238	CLA	CMA-C3A-C4A	3.06	120.00	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1234	CLA	CHD-C1D-ND	-3.06	121.64	124.45
15	3	611	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	B	1230	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	B	1207	CLA	C2B-C3B-C4B	-3.06	103.44	106.75
15	A	1134	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	B	1238	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	4	608	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	B	1206	CLA	CMA-C3A-C4A	3.06	119.98	111.77
15	B	1202	CLA	C2D-C1D-ND	3.05	112.36	110.10
15	A	1137	CLA	C2C-C1C-NC	3.05	112.83	109.97
15	A	1101	CLA	CMA-C3A-C4A	3.05	119.98	111.77
15	B	1232	CLA	C2C-C1C-NC	3.05	112.83	109.97
15	B	1235	CLA	CMA-C3A-C4A	3.05	119.98	111.77
14	1	503	BCR	C27-C26-C25	-3.05	118.30	122.73
15	2	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
14	F	4002	BCR	C27-C26-C25	-3.05	118.30	122.73
16	1	610	CHL	C3C-C4C-NC	-3.05	107.15	110.57
15	B	1204	CLA	CMA-C3A-C4A	3.05	119.97	111.77
15	1	605	CLA	CMA-C3A-C4A	3.05	119.96	111.77
14	4	503	BCR	C33-C5-C4	3.05	119.47	113.62
14	J	4001	BCR	C33-C5-C4	3.05	119.47	113.62
15	B	1218	CLA	CMA-C3A-C4A	3.04	119.96	111.77
15	1	615	CLA	CHD-C1D-ND	-3.04	121.66	124.45
15	2	615	CLA	C2C-C1C-NC	3.04	112.82	109.97
12	1	501	LUT	C39-C29-C30	-3.04	118.66	122.92
15	B	1218	CLA	C2C-C1C-NC	3.04	112.82	109.97
15	B	1206	CLA	C2C-C1C-NC	3.04	112.82	109.97
14	B	4002	BCR	C27-C26-C25	-3.04	118.32	122.73
15	A	1125	CLA	CMA-C3A-C4A	3.04	119.95	111.77
15	3	603	CLA	CMA-C3A-C4A	3.04	119.94	111.77
15	A	1139	CLA	C6-C5-C3	-3.04	109.65	114.62
15	3	607	CLA	CMA-C3A-C4A	3.04	119.94	111.77
16	4	611	CHL	C3C-C4C-NC	-3.04	107.16	110.57
15	A	1112	CLA	CMA-C3A-C4A	3.04	119.94	111.77
15	A	1117	CLA	C2C-C1C-NC	3.04	112.82	109.97
15	B	1232	CLA	CMA-C3A-C4A	3.04	119.93	111.77
15	1	608	CLA	C2C-C1C-NC	3.03	112.81	109.97
14	A	4002	BCR	C36-C18-C17	-3.03	118.67	122.92
15	1	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	A	1120	CLA	CMA-C3A-C4A	3.03	119.92	111.77
15	B	1236	CLA	CHD-C1D-ND	-3.03	121.67	124.45
14	B	4001	BCR	C23-C24-C25	-3.03	118.69	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	608	CLA	CMA-C3A-C4A	3.03	119.91	111.77
14	B	4005	BCR	C23-C24-C25	-3.03	118.70	127.20
15	A	1130	CLA	CMA-C3A-C4A	3.03	119.91	111.77
15	A	1106	CLA	C1-C2-C3	-3.03	120.81	126.04
15	B	1239	CLA	CMA-C3A-C4A	3.03	119.91	111.77
15	B	1216	CLA	C2D-C1D-ND	3.02	112.33	110.10
15	A	1111	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	A	1123	CLA	CMA-C3A-C4A	3.02	119.89	111.77
15	2	612	CLA	CHD-C1D-ND	-3.02	121.68	124.45
15	B	1228	CLA	C2C-C1C-NC	3.02	112.80	109.97
15	B	1234	CLA	C2C-C1C-NC	3.02	112.80	109.97
15	1	605	CLA	C3B-C4B-NB	-3.02	107.72	110.52
25	B	2002	PQN	C14-C13-C15	3.02	120.34	115.27
14	J	4003	BCR	C30-C25-C26	-3.02	118.37	122.61
15	B	1227	CLA	CMA-C3A-C4A	3.02	119.88	111.77
15	B	1222	CLA	CMA-C3A-C4A	3.01	119.88	111.77
15	A	1126	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
15	A	1116	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	A	1131	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	J	1302	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	B	1240	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	A	1136	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	B	1221	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1115	CLA	CMA-C3A-C4A	3.01	119.86	111.77
14	1	505	BCR	C30-C25-C26	-3.01	118.38	122.61
15	B	1219	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1141	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1121	CLA	CMA-C3A-C4A	3.01	119.85	111.77
15	3	603	CLA	C2D-C1D-ND	3.00	112.32	110.10
15	A	1125	CLA	C2C-C1C-NC	3.00	112.79	109.97
15	B	1220	CLA	C2C-C1C-NC	3.00	112.79	109.97
14	1	505	BCR	C35-C13-C14	-3.00	118.72	122.92
14	A	4006	BCR	C23-C24-C25	-3.00	118.77	127.20
15	1	604	CLA	C2D-C1D-ND	3.00	112.31	110.10
15	4	603	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	B	1203	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	A	1113	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	1	612	CLA	C2D-C1D-ND	3.00	112.31	110.10
15	A	1102	CLA	C2D-C1D-ND	3.00	112.31	110.10
15	A	1109	CLA	C2C-C1C-NC	3.00	112.78	109.97
15	B	1203	CLA	C2C-C1C-NC	2.99	112.78	109.97
15	A	1105	CLA	C2C-C1C-NC	2.99	112.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1120	CLA	C2C-C1C-NC	2.99	112.78	109.97
15	A	1129	CLA	CMA-C3A-C4A	2.99	119.81	111.77
15	3	610	CLA	C2C-C1C-NC	2.99	112.77	109.97
15	B	1208	CLA	C2D-C1D-ND	2.99	112.31	110.10
15	A	1104	CLA	CMA-C3A-C4A	2.99	119.81	111.77
15	B	1227	CLA	C2C-C1C-NC	2.99	112.77	109.97
15	3	612	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	3	605	CLA	C2C-C1C-NC	2.99	112.77	109.97
15	A	1138	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	B	1223	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	A	1118	CLA	CMA-C3A-C4A	2.99	119.80	111.77
16	3	604	CHL	C4B-CHC-C1C	2.98	133.42	126.34
15	A	1139	CLA	C2C-C1C-NC	2.98	112.77	109.97
15	A	1132	CLA	CMA-C3A-C4A	2.98	119.79	111.77
15	B	1201	CLA	C2C-C1C-NC	2.98	112.77	109.97
15	A	1122	CLA	CMA-C3A-C4A	2.98	119.78	111.77
15	B	1217	CLA	C2C-C1C-NC	2.98	112.76	109.97
14	4	505	BCR	C27-C26-C25	-2.98	118.41	122.73
12	2	501	LUT	C31-C30-C29	-2.98	123.06	127.31
15	3	605	CLA	CMA-C3A-C4A	2.97	119.77	111.77
15	4	603	CLA	CHD-C1D-ND	-2.97	121.72	124.45
25	A	2001	PQN	C14-C13-C15	2.97	120.27	115.27
14	B	4003	BCR	C27-C26-C25	-2.97	118.42	122.73
15	B	1209	CLA	CMA-C3A-C4A	2.97	119.76	111.77
15	A	1128	CLA	C2D-C1D-ND	2.97	112.29	110.10
15	1	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
15	A	1138	CLA	C2C-C1C-NC	2.97	112.75	109.97
15	2	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	A	1117	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	A	1122	CLA	C2C-C1C-NC	2.97	112.75	109.97
14	3	504	BCR	C27-C26-C25	-2.97	118.42	122.73
15	3	610	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	A	1124	CLA	CMA-C3A-C4A	2.96	119.74	111.77
15	B	1231	CLA	C2D-C1D-ND	2.96	112.29	110.10
15	B	1228	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	A	1108	CLA	C2C-C1C-NC	2.96	112.75	109.97
15	1	615	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	A	1111	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	A	1101	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
14	A	4007	BCR	C34-C9-C10	-2.96	118.78	122.92
15	J	1302	CLA	C2C-C1C-NC	2.96	112.74	109.97
15	B	1201	CLA	CMA-C3A-C4A	2.96	119.72	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1022	CLA	C2C-C1C-NC	2.96	112.74	109.97
15	B	1229	CLA	CMA-C3A-C4A	2.96	119.72	111.77
14	A	4006	BCR	C27-C26-C25	-2.96	118.44	122.73
15	B	1225	CLA	CMA-C3A-C4A	2.96	119.72	111.77
15	B	1224	CLA	CMA-C3A-C4A	2.95	119.71	111.77
15	1	615	CLA	C1-C2-C3	-2.95	120.94	126.04
15	A	1127	CLA	CMA-C3A-C4A	2.95	119.71	111.77
12	4	501	LUT	C31-C30-C29	-2.95	123.10	127.31
12	2	501	LUT	C18-C5-C4	2.95	119.82	114.36
15	A	1117	CLA	C2D-C1D-ND	2.94	112.27	110.10
15	B	1205	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	A	1011	CL0	CAA-C2A-C3A	-2.94	104.72	112.78
15	2	607	CLA	C2D-C1D-ND	2.94	112.27	110.10
14	A	4005	BCR	C23-C24-C25	-2.94	118.94	127.20
15	4	607	CLA	CMA-C3A-C4A	2.94	119.68	111.77
15	B	1240	CLA	C1-C2-C3	-2.94	120.96	126.04
15	A	1113	CLA	C2C-C1C-NC	2.94	112.72	109.97
15	A	1110	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	B	1215	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	B	1202	CLA	CMA-C3A-C4A	2.93	119.66	111.77
15	1	608	CLA	C2D-C1D-ND	2.93	112.27	110.10
15	B	1213	CLA	C2C-C1C-NC	2.93	112.72	109.97
15	1	611	CLA	CMA-C3A-C4A	2.93	119.65	111.77
12	4	501	LUT	C21-C26-C27	2.93	116.41	112.70
15	1	601	CLA	C3B-C4B-NB	-2.93	107.80	110.52
15	A	1134	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	A	1105	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	A	1126	CLA	CMA-C3A-C4A	2.93	119.64	111.77
16	4	611	CHL	C4B-CHC-C1C	2.92	133.27	126.34
15	4	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	2	615	CLA	CMA-C3A-C4A	2.92	119.63	111.77
15	1	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	3	613	CLA	CMA-C3A-C4A	2.92	119.62	111.77
14	B	4004	BCR	C30-C25-C26	-2.92	118.50	122.61
15	2	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	B	1236	CLA	C2C-C1C-NC	2.92	112.71	109.97
16	4	610	CHL	C4B-CHC-C1C	2.92	133.26	126.34
15	A	1108	CLA	CMA-C3A-C4A	2.91	119.60	111.77
15	B	1212	CLA	CMA-C3A-C4A	2.91	119.60	111.77
15	B	1203	CLA	C2D-C1D-ND	2.91	112.25	110.10
15	1	612	CLA	CMA-C3A-C4A	2.91	119.59	111.77
15	1	602	CLA	C2C-C1C-NC	2.91	112.70	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	607	CLA	CMA-C3A-C4A	2.91	119.59	111.77
15	1	607	CLA	CMA-C3A-C4A	2.91	119.59	111.77
14	A	4003	BCR	C19-C18-C17	2.91	123.40	118.94
15	B	1208	CLA	C2C-C1C-NC	2.91	112.70	109.97
15	3	601	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1101	CLA	C2D-C1D-ND	2.90	112.24	110.10
15	A	1102	CLA	C2C-C1C-NC	2.90	112.69	109.97
14	B	4006	BCR	C33-C5-C4	2.90	119.19	113.62
15	B	1213	CLA	C2D-C1D-ND	2.90	112.24	110.10
16	2	611	CHL	C2C-C3C-C4C	2.90	108.56	106.49
15	4	601	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	4	602	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	F	1301	CLA	CMA-C3A-C4A	2.90	119.57	111.77
14	1	505	BCR	C27-C26-C25	-2.90	118.52	122.73
15	4	607	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1128	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	4	612	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	B	1235	CLA	C2D-C1D-ND	2.90	112.24	110.10
15	2	604	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	A	1133	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1133	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	A	1119	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	B	1234	CLA	CMA-C3A-C4A	2.89	119.55	111.77
15	4	604	CLA	C2C-C1C-NC	2.89	112.68	109.97
14	A	4005	BCR	C30-C25-C26	-2.89	118.54	122.61
15	A	1118	CLA	C2C-C1C-NC	2.89	112.68	109.97
15	A	1131	CLA	C2C-C1C-NC	2.89	112.68	109.97
15	B	1208	CLA	C3B-C4B-NB	-2.89	107.83	110.52
15	B	1229	CLA	C2C-C1C-NC	2.89	112.68	109.97
15	A	1120	CLA	C2D-C1D-ND	2.89	112.23	110.10
16	1	609	CHL	C2C-C3C-C4C	2.89	108.55	106.49
15	4	601	CLA	C2D-C1D-ND	2.88	112.23	110.10
16	4	611	CHL	C3B-C4B-NB	-2.88	107.84	110.52
15	3	608	CLA	C2C-C1C-NC	2.88	112.67	109.97
15	4	612	CLA	C2D-C1D-ND	2.88	112.23	110.10
15	A	1114	CLA	CMA-C3A-C4A	2.88	119.52	111.77
15	3	615	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
15	B	1223	CLA	C2D-C1D-ND	2.88	112.23	110.10
15	A	1109	CLA	CMA-C3A-C4A	2.88	119.52	111.77
16	2	610	CHL	C4B-CHC-C1C	2.88	133.17	126.34
15	3	607	CLA	C2D-C1D-ND	2.88	112.23	110.10
15	1	601	CLA	CMA-C3A-C4A	2.88	119.52	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	607	CLA	C2D-C1D-ND	2.88	112.23	110.10
15	B	1236	CLA	CMA-C3A-C4A	2.88	119.51	111.77
15	A	1013	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
16	4	611	CHL	CMA-C3A-C4A	2.88	119.51	111.77
14	J	4003	BCR	C33-C5-C4	2.88	119.14	113.62
15	1	603	CLA	CMA-C3A-C4A	2.87	119.50	111.77
15	1	601	CLA	C2C-C1C-NC	2.87	112.67	109.97
15	B	1235	CLA	C1D-ND-C4D	-2.87	104.29	106.33
15	2	605	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
15	2	606	CLA	C2D-C1D-ND	2.87	112.22	110.10
15	1	613	CLA	CMA-C3A-C4A	2.87	119.49	111.77
14	A	4007	BCR	C33-C5-C4	2.87	119.13	113.62
16	4	613	CHL	C3B-C4B-NB	-2.87	107.86	110.52
15	A	1125	CLA	C2D-C1D-ND	2.87	112.22	110.10
15	1	602	CLA	CMA-C3A-C4A	2.87	119.48	111.77
15	B	1214	CLA	CHD-C1D-ND	-2.87	121.82	124.45
15	B	1022	CLA	CMA-C3A-C4A	2.87	119.47	111.77
16	2	611	CHL	C4D-CHA-C1A	2.86	124.73	121.25
14	4	505	BCR	C38-C26-C27	2.86	119.12	113.62
16	2	609	CHL	C2C-C3C-C4C	2.86	108.53	106.49
15	2	603	CLA	C2C-C1C-NC	2.86	112.65	109.97
15	1	605	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	B	1213	CLA	C3B-C4B-NB	-2.86	107.86	110.52
15	3	612	CLA	C2C-C1C-NC	2.86	112.65	109.97
15	3	612	CLA	C2D-C1D-ND	2.86	112.21	110.10
15	B	1215	CLA	C2D-C1D-ND	2.86	112.21	110.10
14	4	505	BCR	C35-C13-C14	-2.86	118.92	122.92
15	1	606	CLA	C2D-C1D-ND	2.86	112.21	110.10
15	B	1228	CLA	C2D-C1D-ND	2.86	112.21	110.10
15	B	1235	CLA	C3B-C4B-NB	-2.85	107.87	110.52
14	A	4007	BCR	C23-C24-C25	-2.85	119.19	127.20
14	J	4003	BCR	C38-C26-C27	2.85	119.10	113.62
15	A	1103	CLA	CMA-C3A-C4A	2.85	119.44	111.77
15	1	613	CLA	C2D-C1D-ND	2.85	112.21	110.10
15	B	1227	CLA	C3B-C4B-NB	-2.85	107.87	110.52
15	A	1105	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	B	1226	CLA	C2C-C1C-NC	2.85	112.64	109.97
15	B	1219	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
15	A	1102	CLA	CMA-C3A-C4A	2.85	119.43	111.77
16	2	613	CHL	C4D-CHA-C1A	2.85	124.72	121.25
15	B	1208	CLA	CMA-C3A-C4A	2.85	119.42	111.77
15	A	1130	CLA	C1C-C2C-C3C	-2.85	103.96	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	4002	BCR	C34-C9-C10	-2.84	118.94	122.92
15	B	1213	CLA	CMA-C3A-C4A	2.84	119.41	111.77
15	4	601	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
15	3	615	CLA	CMA-C3A-C4A	2.84	119.41	111.77
14	B	4001	BCR	C34-C9-C10	-2.84	118.94	122.92
15	A	1104	CLA	C2D-C1D-ND	2.84	112.20	110.10
14	B	4002	BCR	C38-C26-C27	2.84	119.07	113.62
15	F	1301	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
15	B	1225	CLA	C2D-C1D-ND	2.84	112.19	110.10
15	B	1210	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
15	1	603	CLA	C2C-C1C-NC	2.83	112.62	109.97
14	A	4005	BCR	C38-C26-C27	2.83	119.05	113.62
15	3	611	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
15	2	601	CLA	C2C-C1C-NC	2.83	112.62	109.97
14	J	4001	BCR	C38-C26-C27	2.83	119.05	113.62
15	B	1023	CLA	CMA-C3A-C4A	2.83	119.37	111.77
15	B	1223	CLA	C1C-C2C-C3C	-2.83	103.99	106.96
15	B	1216	CLA	C2C-C1C-NC	2.82	112.62	109.97
14	3	503	BCR	C38-C26-C27	2.82	119.04	113.62
15	4	605	CLA	CMA-C3A-C4A	2.82	119.36	111.77
15	1	603	CLA	C2D-C1D-ND	2.82	112.19	110.10
15	B	1232	CLA	C2D-C1D-ND	2.82	112.19	110.10
16	2	613	CHL	C4B-CHC-C1C	2.82	133.03	126.34
13	4	502	XAT	C6-C7-C8	-2.82	120.03	125.99
14	A	4002	BCR	C38-C26-C27	2.82	119.04	113.62
15	4	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
15	A	1141	CLA	C2D-C1D-ND	2.82	112.18	110.10
15	A	1108	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
15	2	603	CLA	C2D-C1D-ND	2.82	112.18	110.10
15	4	603	CLA	C2C-C1C-NC	2.82	112.61	109.97
15	B	1202	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
13	3	502	XAT	C26-C27-C28	-2.82	120.04	125.99
15	A	1109	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
15	A	1104	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	B	1214	CLA	CMA-C3A-C4A	2.81	119.33	111.77
15	B	1229	CLA	O2A-CGA-CBA	2.81	120.73	111.91
15	B	1239	CLA	C2C-C1C-NC	2.81	112.61	109.97
16	2	609	CHL	C3B-C4B-NB	-2.81	107.91	110.52
15	B	1021	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
16	3	604	CHL	C2C-C3C-C4C	2.81	108.49	106.49
13	4	502	XAT	C26-C27-C28	-2.81	120.06	125.99
12	3	501	LUT	C22-C23-C24	-2.80	108.55	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1235	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
14	1	505	BCR	C15-C14-C13	-2.80	123.31	127.31
15	B	1225	CLA	C2C-C1C-NC	2.80	112.60	109.97
15	A	1134	CLA	C2D-C1D-ND	2.80	112.17	110.10
15	4	604	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
14	B	4002	BCR	C23-C24-C25	-2.80	119.34	127.20
16	1	609	CHL	C4B-CHC-C1C	2.80	132.98	126.34
15	A	1101	CLA	C1D-ND-C4D	-2.80	104.35	106.33
15	4	605	CLA	C2C-C1C-NC	2.80	112.59	109.97
15	A	1128	CLA	CMA-C3A-C4A	2.79	119.28	111.77
15	A	1127	CLA	C2D-C1D-ND	2.79	112.16	110.10
16	4	610	CHL	C2C-C3C-C4C	2.79	108.48	106.49
15	4	609	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
14	4	505	BCR	C4-C5-C6	-2.79	118.68	122.73
15	A	1108	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
15	3	613	CLA	C2D-C1D-ND	2.79	112.16	110.10
15	A	1103	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
16	2	611	CHL	C3B-C4B-NB	-2.79	107.93	110.52
15	1	608	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
15	3	601	CLA	C2D-C1D-ND	2.79	112.16	110.10
15	B	1216	CLA	CMA-C3A-C4A	2.78	119.25	111.77
15	A	1137	CLA	C2D-C1D-ND	2.78	112.15	110.10
15	A	1110	CLA	C2C-C1C-NC	2.78	112.58	109.97
15	1	606	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
15	4	602	CLA	C2C-C1C-NC	2.78	112.58	109.97
15	A	1111	CLA	C3B-C4B-NB	-2.78	107.94	110.52
13	2	502	XAT	O24-C25-C38	-2.78	111.73	115.06
15	B	1236	CLA	C3B-C4B-NB	-2.78	107.94	110.52
14	B	4001	BCR	C38-C26-C27	2.78	118.95	113.62
16	4	611	CHL	C2B-C1B-NB	-2.77	108.37	110.23
14	B	4004	BCR	C38-C26-C27	2.77	118.94	113.62
14	3	503	BCR	C30-C25-C26	-2.77	118.71	122.61
15	2	601	CLA	CMA-C3A-C4A	2.77	119.23	111.77
13	4	502	XAT	C38-C25-C26	-2.77	117.62	122.26
15	B	1023	CLA	O2A-CGA-CBA	2.77	120.60	111.91
15	A	1124	CLA	C2D-C1D-ND	2.77	112.15	110.10
14	A	4007	BCR	C38-C26-C27	2.77	118.94	113.62
15	A	1106	CLA	CMA-C3A-C4A	2.77	119.22	111.77
13	3	502	XAT	C35-C15-C14	-2.77	117.80	123.47
15	3	608	CLA	C2D-C1D-ND	2.77	112.14	110.10
15	4	608	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
15	A	1135	CLA	C1C-C2C-C3C	-2.77	104.05	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	601	CLA	C2D-C1D-ND	2.77	112.14	110.10
14	A	4006	BCR	C33-C5-C4	2.77	118.93	113.62
15	2	606	CLA	CMA-C3A-C4A	2.77	119.21	111.77
15	4	602	CLA	C3B-C4B-NB	-2.76	107.95	110.52
15	A	1118	CLA	C2D-C1D-ND	2.76	112.14	110.10
15	A	1107	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
15	A	1121	CLA	C2D-C1D-ND	2.76	112.14	110.10
14	A	4005	BCR	C35-C13-C14	-2.76	119.06	122.92
15	2	612	CLA	CMA-C3A-C4A	2.76	119.19	111.77
15	B	1238	CLA	C2D-C1D-ND	2.76	112.14	110.10
15	B	1207	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	2	603	CLA	C3B-C4B-NB	-2.76	107.96	110.52
14	3	504	BCR	C38-C26-C27	2.75	118.91	113.62
13	1	502	XAT	C38-C25-C26	-2.75	117.64	122.26
15	B	1230	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	B	1212	CLA	C2D-C1D-ND	2.75	112.13	110.10
15	1	615	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
15	1	606	CLA	CAA-C2A-C1A	-2.75	102.96	111.97
14	J	4001	BCR	C23-C24-C25	-2.75	119.48	127.20
15	A	1140	CLA	C2C-C1C-NC	2.75	112.55	109.97
15	3	612	CLA	C3B-C4B-NB	-2.75	107.97	110.52
15	3	613	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
14	A	4007	BCR	C8-C9-C10	2.74	123.15	118.94
15	4	615	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	B	1214	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
15	4	606	CLA	C3B-C4B-NB	-2.74	107.97	110.52
15	J	1302	CLA	C2D-C1D-ND	2.74	112.12	110.10
12	4	501	LUT	C8-C7-C6	-2.74	119.50	127.20
15	1	613	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
15	B	1023	CLA	C3B-C4B-NB	-2.74	107.97	110.52
15	A	1113	CLA	C2D-C1D-ND	2.74	112.12	110.10
14	B	4004	BCR	C23-C24-C25	-2.73	119.52	127.20
15	A	1133	CLA	C2D-C1D-ND	2.73	112.12	110.10
15	3	605	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
15	1	611	CLA	C2D-C1D-ND	2.73	112.12	110.10
15	3	601	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	J	4002	BCR	C38-C26-C27	2.73	118.86	113.62
15	A	1119	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
15	A	1141	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
14	1	505	BCR	C38-C26-C27	2.73	118.86	113.62
15	B	1225	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	A	4002	BCR	C37-C22-C21	-2.73	119.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1206	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
15	B	1217	CLA	C3B-C4B-NB	-2.72	107.99	110.52
14	2	503	BCR	C27-C26-C25	-2.72	118.78	122.73
14	1	503	BCR	C37-C22-C23	2.72	122.37	118.08
14	A	4002	BCR	C30-C25-C26	-2.72	118.78	122.61
24	A	1011	CL0	CMC-C2C-C1C	2.72	129.19	125.04
15	B	1228	CLA	C1D-ND-C4D	-2.72	104.40	106.33
14	4	503	BCR	C30-C25-C26	-2.72	118.78	122.61
14	J	4002	BCR	C30-C25-C26	-2.72	118.78	122.61
15	A	1122	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	3	606	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	A	1131	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	B	1203	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
15	A	1103	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	4	604	CLA	CMA-C3A-C4A	2.72	119.08	111.77
15	1	607	CLA	C3B-C4B-NB	-2.72	107.99	110.52
15	A	1112	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	B	1224	CLA	C3B-C4B-NB	-2.72	108.00	110.52
15	B	1240	CLA	C2D-C1D-ND	2.72	112.11	110.10
15	A	1115	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
16	1	609	CHL	C1-O2A-CGA	2.71	123.56	116.44
15	A	1124	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
21	2	811	DGD	O1G-C1A-C2A	2.71	120.42	111.91
15	2	608	CLA	C2D-C1D-ND	2.71	112.10	110.10
15	2	612	CLA	C3B-C4B-NB	-2.71	108.00	110.52
21	4	811	DGD	C2G-O2G-C1B	-2.71	111.12	117.79
15	A	1012	CLA	C2D-C1D-ND	2.71	112.10	110.10
18	1	802	LMG	C8-O7-C10	-2.71	111.12	117.79
16	4	610	CHL	C2B-C1B-NB	-2.71	108.42	110.23
15	A	1131	CLA	C3B-C4B-NB	-2.71	108.00	110.52
16	1	610	CHL	CHC-C1C-NC	2.71	128.31	124.20
13	2	502	XAT	C6-C7-C8	-2.71	120.27	125.99
16	4	610	CHL	C3B-C4B-NB	-2.71	108.00	110.52
21	B	5002	DGD	C2G-O2G-C1B	-2.70	111.13	117.79
16	2	610	CHL	C3B-C4B-NB	-2.70	108.01	110.52
15	B	1211	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
15	B	1223	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	F	1302	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	A	1115	CLA	C2D-C1D-ND	2.70	112.10	110.10
15	B	1231	CLA	CMA-C3A-C4A	2.70	119.03	111.77
15	4	608	CLA	C2D-C1D-ND	2.70	112.09	110.10
14	B	4003	BCR	C38-C26-C27	2.70	118.80	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1130	CLA	C2D-C1D-ND	2.70	112.09	110.10
14	J	4003	BCR	C23-C24-C25	-2.70	119.63	127.20
15	B	1218	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
15	B	1222	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
14	4	505	BCR	C1-C6-C5	-2.70	118.81	122.61
15	A	1104	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
14	A	4007	BCR	C19-C18-C17	2.70	123.08	118.94
21	4	811	DGD	O1G-C1A-C2A	2.70	120.37	111.91
15	A	1136	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
15	A	1133	CLA	C3B-C4B-NB	-2.69	108.02	110.52
15	B	1228	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	B	4001	BCR	C30-C25-C26	-2.69	118.82	122.61
14	1	503	BCR	C36-C18-C17	-2.69	119.15	122.92
15	B	1216	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	B	1240	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	A	1140	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	A	1112	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
14	J	4001	BCR	C30-C25-C26	-2.69	118.83	122.61
15	A	1128	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	1	503	BCR	C35-C13-C12	2.69	122.31	118.08
15	A	1123	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	A	1106	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	B	1224	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	2	605	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	4	503	BCR	C34-C9-C10	-2.69	119.16	122.92
15	2	602	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
15	A	1116	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
15	B	1222	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	A	1011	CL0	CAC-C3C-C4C	2.68	128.29	124.81
15	2	607	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	B	1217	CLA	C2D-C1D-ND	2.68	112.08	110.10
15	B	1237	CLA	C2D-C1D-ND	2.68	112.08	110.10
15	B	1226	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	B	1205	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	3	606	CLA	CMA-C3A-C4A	2.68	118.98	111.77
14	A	4006	BCR	C35-C13-C12	2.68	122.30	118.08
15	B	1215	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	A	1118	CLA	C3B-C4B-NB	-2.68	108.03	110.52
15	3	601	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	F	1302	CLA	CMA-C3A-C4A	2.68	118.97	111.77
15	A	1105	CLA	C3B-C4B-NB	-2.68	108.03	110.52
15	1	605	CLA	C2D-C1D-ND	2.68	112.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1103	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
17	B	5001	LHG	C5-O7-C7	-2.68	112.91	117.90
13	1	502	XAT	C19-C9-C10	-2.67	119.18	122.92
15	2	606	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
15	B	1229	CLA	C3B-C4B-NB	-2.67	108.03	110.52
13	3	502	XAT	C40-C33-C34	-2.67	119.18	122.92
15	4	604	CLA	C2D-C1D-ND	2.67	112.07	110.10
15	B	1023	CLA	C2D-C1D-ND	2.67	112.07	110.10
15	B	1214	CLA	C2D-C1D-ND	2.67	112.07	110.10
15	A	1132	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	3	612	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	3	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
15	B	1022	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
15	B	1201	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	2	503	BCR	C38-C26-C27	2.67	118.74	113.62
15	A	1119	CLA	C2D-C1D-ND	2.67	112.07	110.10
15	1	602	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
16	2	611	CHL	C4B-CHC-C1C	2.67	132.66	126.34
15	A	1121	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
15	A	1137	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	A	1132	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
15	3	613	CLA	C1D-ND-C4D	-2.66	104.44	106.33
15	B	1211	CLA	C2D-C1D-ND	2.66	112.06	110.10
24	A	1011	CL0	C5-C3-C4	2.66	120.48	114.60
16	1	609	CHL	C3B-C4B-NB	-2.66	108.05	110.52
14	3	504	BCR	C8-C7-C6	-2.66	119.74	127.20
15	1	602	CLA	C3B-C4B-NB	-2.66	108.05	110.52
15	B	1204	CLA	C2D-C1D-ND	2.66	112.06	110.10
15	B	1226	CLA	C2D-C1D-ND	2.66	112.06	110.10
15	4	604	CLA	C1D-ND-C4D	-2.65	104.45	106.33
15	A	1117	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
15	1	611	CLA	C3B-C4B-NB	-2.65	108.05	110.52
15	3	603	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
15	A	1012	CLA	CMA-C3A-C4A	2.65	118.90	111.77
15	3	601	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
14	B	4003	BCR	C30-C25-C26	-2.65	118.88	122.61
14	A	4003	BCR	C8-C9-C10	2.65	123.01	118.94
15	4	603	CLA	C2D-C1D-ND	2.65	112.05	110.10
15	A	1132	CLA	C2D-C1D-ND	2.65	112.05	110.10
15	B	1201	CLA	C2D-C1D-ND	2.65	112.05	110.10
15	B	1220	CLA	C1-C2-C3	-2.65	121.47	126.04
13	3	502	XAT	C38-C25-C26	-2.64	117.83	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1126	CLA	C2D-C1D-ND	2.64	112.05	110.10
15	B	1021	CLA	C3B-C4B-NB	-2.64	108.06	110.52
15	4	607	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
15	A	1126	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	3	607	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
15	A	1123	CLA	C2D-C1D-ND	2.64	112.05	110.10
15	B	1023	CLA	C1-C2-C3	-2.64	121.48	126.04
16	1	609	CHL	C2B-C1B-NB	-2.64	108.46	110.23
15	1	606	CLA	C3B-C4B-NB	-2.64	108.07	110.52
15	A	1122	CLA	C3B-C4B-NB	-2.64	108.07	110.52
16	2	611	CHL	C4A-NA-C1A	2.64	107.89	106.71
15	B	1222	CLA	C1D-ND-C4D	-2.64	104.46	106.33
14	F	4002	BCR	C38-C26-C27	2.64	118.68	113.62
15	B	1206	CLA	C2D-C1D-ND	2.64	112.05	110.10
14	B	4001	BCR	C1-C6-C7	2.64	123.23	115.78
15	2	612	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
14	A	4006	BCR	C30-C25-C26	-2.63	118.91	122.61
16	2	609	CHL	C4B-CHC-C1C	2.63	132.58	126.34
15	B	1220	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
15	B	1023	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
25	A	2001	PQN	C2M-C2-C3	-2.63	120.11	124.40
16	4	613	CHL	C1-O2A-CGA	2.63	123.34	116.44
15	1	605	CLA	C4B-CHC-C1C	2.63	132.57	126.34
15	4	607	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	A	1012	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
15	B	1238	CLA	C3B-C4B-NB	-2.63	108.08	110.52
15	4	606	CLA	C2C-C1C-NC	2.62	112.43	109.97
15	B	1234	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
15	B	1235	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	1	802	LMG	O8-C28-C29	2.62	120.13	111.91
16	3	604	CHL	CHC-C1C-NC	2.62	128.18	124.20
15	4	609	CLA	C2D-C1D-ND	2.62	112.03	110.10
15	A	1134	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
15	B	1222	CLA	C3B-C4B-NB	-2.62	108.09	110.52
15	1	604	CLA	CMA-C3A-C4A	2.62	118.81	111.77
17	1	801	LHG	C5-O7-C7	-2.62	111.35	117.79
15	A	1125	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	B	4006	BCR	C36-C18-C17	-2.62	119.26	122.92
15	2	604	CLA	O2A-CGA-CBA	2.61	120.11	111.91
12	4	501	LUT	C31-C32-C33	-2.61	119.08	126.42
15	B	1237	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
15	A	1138	CLA	O2A-CGA-CBA	2.61	120.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	608	CLA	C3B-C4B-NB	-2.61	108.09	110.52
15	4	605	CLA	C2D-C1D-ND	2.61	112.03	110.10
15	2	608	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
15	2	615	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
24	A	1011	CL0	CMB-C2B-C1B	2.61	129.34	125.37
15	1	615	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	B	4004	BCR	C34-C9-C10	-2.61	119.27	122.92
15	A	1135	CLA	C2D-C1D-ND	2.61	112.03	110.10
15	A	1141	CLA	C3B-C4B-NB	-2.61	108.10	110.52
14	J	4003	BCR	C34-C9-C10	-2.61	119.27	122.92
15	A	1114	CLA	C2D-C1D-ND	2.61	112.02	110.10
15	B	1221	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
15	A	1012	CLA	O2A-CGA-CBA	2.60	120.08	111.91
16	2	611	CHL	C2B-C1B-NB	-2.60	108.49	110.23
15	1	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
15	A	1013	CLA	C3B-C4B-NB	-2.60	108.10	110.52
15	A	1136	CLA	C2D-C1D-ND	2.60	112.02	110.10
15	B	1234	CLA	C2D-C1D-ND	2.60	112.02	110.10
15	A	1115	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
15	1	608	CLA	C3B-C4B-NB	-2.60	108.10	110.52
15	B	1022	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	4	505	BCR	C37-C22-C21	-2.60	119.28	122.92
15	A	1109	CLA	C3B-C4B-NB	-2.60	108.10	110.52
15	B	1207	CLA	CHA-C4D-ND	-2.60	122.00	124.52
15	A	1127	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
15	A	1137	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
15	A	1111	CLA	C2D-C1D-ND	2.60	112.02	110.10
12	3	501	LUT	C18-C5-C4	2.60	119.17	114.36
15	A	1012	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	B	1239	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	B	4002	BCR	C34-C9-C10	-2.59	119.29	122.92
15	B	1236	CLA	CHA-C4D-ND	2.59	137.93	132.50
15	B	1215	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
15	A	1127	CLA	C4B-CHC-C1C	2.59	132.49	126.34
16	1	610	CHL	CHD-C4C-C3C	2.59	128.65	124.84
14	A	4006	BCR	C38-C26-C27	2.59	118.59	113.62
15	A	1108	CLA	C2D-C1D-ND	2.59	112.01	110.10
15	A	1012	CLA	C3B-C4B-NB	-2.59	108.11	110.52
15	1	601	CLA	C2D-C1D-ND	2.59	112.01	110.10
15	B	1204	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
15	A	1139	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
15	A	1113	CLA	C3B-C4B-NB	-2.59	108.11	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1139	CLA	C2D-C1D-ND	2.59	112.01	110.10
14	2	503	BCR	C36-C18-C17	-2.59	119.30	122.92
15	B	1227	CLA	C2D-C1D-ND	2.58	112.01	110.10
15	B	1239	CLA	C2D-C1D-ND	2.58	112.01	110.10
15	A	1138	CLA	C2D-C1D-ND	2.58	112.01	110.10
15	2	604	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
15	2	602	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
15	B	1226	CLA	C3B-C4B-NB	-2.58	108.12	110.52
15	4	603	CLA	C4B-CHC-C1C	2.58	132.45	126.34
15	B	1022	CLA	C2D-C1D-ND	2.58	112.00	110.10
16	2	610	CHL	C2C-C3C-C4C	2.57	108.32	106.49
15	A	1127	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	B	1228	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	B	4001	BCR	C35-C13-C14	-2.57	119.32	122.92
15	A	1104	CLA	O2A-CGA-CBA	2.57	119.98	111.91
13	1	502	XAT	C18-C5-C6	-2.57	117.95	122.26
15	A	1101	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	B	1238	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
14	A	4004	BCR	C37-C22-C21	-2.57	119.32	122.92
15	4	601	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	1	601	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
15	B	1215	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	4	606	CLA	CMA-C3A-C4A	2.57	118.67	111.77
15	A	1114	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
14	3	504	BCR	C30-C25-C26	-2.57	119.00	122.61
15	A	1131	CLA	C4B-CHC-C1C	2.56	132.42	126.34
15	3	615	CLA	C2D-C1D-ND	2.56	111.99	110.10
15	2	604	CLA	CHA-C4D-ND	2.56	137.86	132.50
15	4	615	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
15	A	1129	CLA	C2D-C1D-ND	2.56	111.99	110.10
15	2	605	CLA	C2D-C1D-ND	2.56	111.99	110.10
14	J	4001	BCR	C35-C13-C12	2.56	122.11	118.08
15	B	1221	CLA	C1D-ND-C4D	-2.56	104.52	106.33
25	B	2002	PQN	C2M-C2-C3	-2.56	120.23	124.40
15	B	1204	CLA	C3B-C4B-NB	-2.55	108.15	110.52
15	A	1116	CLA	C2D-C1D-ND	2.55	111.98	110.10
15	1	605	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	A	1117	CLA	O2A-CGA-CBA	2.55	119.92	111.91
15	A	1139	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
15	3	608	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
15	A	1128	CLA	C1D-ND-C4D	-2.55	104.52	106.33
12	1	501	LUT	C7-C8-C9	-2.55	122.38	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1220	CLA	C2D-C1D-ND	2.55	111.98	110.10
15	4	605	CLA	C3B-C4B-NB	-2.55	108.15	110.52
15	A	1129	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
15	A	1138	CLA	C3B-C4B-NB	-2.55	108.15	110.52
15	A	1110	CLA	C1D-ND-C4D	-2.55	104.53	106.33
15	2	608	CLA	O2A-CGA-CBA	2.54	119.89	111.91
15	4	602	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
15	F	1302	CLA	C2D-C1D-ND	2.54	111.98	110.10
14	J	4003	BCR	C35-C13-C12	2.54	122.08	118.08
14	4	505	BCR	C30-C25-C26	-2.54	119.03	122.61
15	4	604	CLA	O2A-CGA-CBA	2.54	119.89	111.91
15	2	602	CLA	C2D-C1D-ND	2.54	111.98	110.10
14	3	503	BCR	C8-C7-C6	-2.54	120.07	127.20
15	1	611	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
15	4	603	CLA	C3B-C4B-NB	-2.54	108.16	110.52
15	3	603	CLA	CHA-C4D-ND	2.54	137.81	132.50
15	A	1125	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
15	A	1107	CLA	C2D-C1D-ND	2.53	111.97	110.10
15	3	607	CLA	C3B-C4B-NB	-2.53	108.16	110.52
15	A	1120	CLA	C3B-C4B-NB	-2.53	108.16	110.52
15	B	1201	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
15	4	609	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
15	4	605	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
15	B	1203	CLA	C1D-ND-C4D	-2.53	104.54	106.33
15	4	607	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	A	1117	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	A	1127	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	F	1301	CLA	C1D-ND-C4D	-2.53	104.54	106.33
15	B	1236	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	A	1102	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	A	1121	CLA	C3B-C4B-NB	-2.52	108.17	110.52
15	2	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
16	3	604	CHL	C3B-C4B-NB	-2.52	108.17	110.52
14	A	4002	BCR	C34-C9-C8	2.52	122.05	118.08
15	B	1021	CLA	CMA-C3A-C4A	2.52	118.55	111.77
15	2	601	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
15	B	1205	CLA	C2D-C1D-ND	2.52	111.96	110.10
15	A	1136	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	4	602	CLA	C4B-CHC-C1C	2.52	132.31	126.34
14	A	4005	BCR	C4-C5-C6	-2.52	119.08	122.73
15	A	1133	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
15	F	1302	CLA	C3B-C4B-NB	-2.52	108.18	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1111	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	4	606	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	A	1113	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
14	1	505	BCR	C37-C22-C21	-2.51	119.40	122.92
15	B	1240	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
15	1	606	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
15	4	607	CLA	C2D-C1D-ND	2.51	111.96	110.10
15	3	610	CLA	C2D-C1D-ND	2.51	111.95	110.10
15	B	1023	CLA	CHA-C4D-ND	2.51	137.75	132.50
15	A	1109	CLA	C2D-C1D-ND	2.51	111.95	110.10
15	1	607	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
24	A	1011	CL0	CMD-C2D-C3D	-2.51	121.85	127.61
15	1	604	CLA	C3B-C4B-NB	-2.50	108.19	110.52
15	A	1137	CLA	C3B-C4B-NB	-2.50	108.19	110.52
15	B	1209	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
15	3	611	CLA	C2D-C1D-ND	2.50	111.95	110.10
15	A	1012	CLA	OBD-CAD-C3D	-2.50	122.50	128.52
15	B	1229	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
14	A	4002	BCR	C19-C18-C17	2.50	122.78	118.94
15	B	1239	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
16	4	613	CHL	C4B-CHC-C1C	2.50	132.26	126.34
15	2	605	CLA	CHA-C4D-ND	2.50	137.72	132.50
15	B	1235	CLA	O2A-CGA-CBA	2.50	119.74	111.91
15	B	1232	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
15	2	601	CLA	C3B-C4B-NB	-2.50	108.20	110.52
15	3	610	CLA	C3B-C4B-NB	-2.50	108.20	110.52
15	B	1232	CLA	C3B-C4B-NB	-2.49	108.20	110.52
15	B	1211	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	A	1120	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
15	4	604	CLA	C3B-C4B-NB	-2.49	108.20	110.52
15	2	603	CLA	C4B-CHC-C1C	2.49	132.25	126.34
15	A	1114	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	1	503	BCR	C4-C5-C6	-2.49	119.11	122.73
15	B	1021	CLA	C2D-C1D-ND	2.49	111.94	110.10
15	1	612	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	B	5031	GSH	CG1-CD1-N2	2.49	120.15	115.83
15	1	608	CLA	C4B-CHC-C1C	2.49	132.24	126.34
15	1	602	CLA	CHA-C4D-ND	2.49	137.71	132.50
15	A	1123	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	B	1023	CLA	C2C-C1C-NC	2.49	112.30	109.97
14	F	4002	BCR	C36-C18-C17	-2.49	119.44	122.92
15	4	605	CLA	C4B-CHC-C1C	2.48	132.23	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1219	CLA	C4B-CHC-C1C	2.48	132.23	126.34
15	4	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	A	1122	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
15	A	1109	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	A	1140	CLA	CHA-C4D-ND	2.48	137.69	132.50
15	4	603	CLA	CHA-C4D-ND	2.48	137.69	132.50
15	A	1130	CLA	C3B-C4B-NB	-2.48	108.21	110.52
15	A	1110	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	B	1216	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	B	1229	CLA	C1-C2-C3	-2.48	121.76	126.04
15	B	1225	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
16	1	610	CHL	C2C-C3C-C4C	2.48	108.25	106.49
15	A	1111	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
15	B	1239	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	A	1105	CLA	C2D-C1D-ND	2.48	111.93	110.10
15	2	607	CLA	CHA-C4D-ND	2.48	137.68	132.50
21	2	811	DGD	C2G-O2G-C1B	-2.48	111.70	117.79
15	B	1205	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
15	A	1119	CLA	C4B-CHC-C1C	2.47	132.21	126.34
15	3	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	J	1302	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1110	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1118	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
14	1	505	BCR	C34-C9-C10	-2.47	119.46	122.92
15	B	1220	CLA	O2A-CGA-CBA	2.47	119.66	111.91
15	B	1205	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	F	4002	BCR	C30-C25-C26	-2.47	119.13	122.61
15	B	1208	CLA	CHA-C4D-ND	2.47	137.66	132.50
15	3	603	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
15	4	615	CLA	C3B-C4B-NB	-2.47	108.22	110.52
15	1	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	F	1302	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1134	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
15	B	1230	CLA	C3B-C4B-NB	-2.47	108.23	110.52
15	A	1132	CLA	CHA-C4D-ND	2.47	137.66	132.50
15	1	612	CLA	CHA-C4D-ND	2.46	137.66	132.50
15	1	603	CLA	C3B-C4B-NB	-2.46	108.23	110.52
15	A	1124	CLA	C3B-C4B-NB	-2.46	108.23	110.52
15	3	612	CLA	CHA-C4D-ND	2.46	137.65	132.50
15	A	1104	CLA	CHA-C4D-ND	2.46	137.65	132.50
15	1	615	CLA	C2D-C1D-ND	2.46	111.92	110.10
13	1	502	XAT	C26-C27-C28	-2.46	120.79	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4003	BCR	C35-C13-C12	2.46	121.95	118.08
18	2	802	LMG	C8-O7-C10	-2.46	111.73	117.79
15	B	1209	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	1	608	CLA	C1D-ND-C4D	-2.46	104.59	106.33
12	1	501	LUT	C8-C7-C6	-2.46	120.30	127.20
15	1	606	CLA	C1D-ND-C4D	-2.46	104.59	106.33
15	B	1231	CLA	C1D-ND-C4D	-2.46	104.59	106.33
14	1	503	BCR	C3-C4-C5	-2.46	109.69	114.08
15	A	1121	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
15	A	1125	CLA	C4B-CHC-C1C	2.46	132.16	126.34
15	B	1022	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
14	B	4003	BCR	C8-C9-C10	2.45	122.71	118.94
15	1	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
15	B	1217	CLA	CHA-C4D-ND	2.45	137.63	132.50
15	B	1225	CLA	C1D-ND-C4D	-2.45	104.59	106.33
15	B	1227	CLA	C4B-CHC-C1C	2.45	132.16	126.34
15	1	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
15	A	1101	CLA	C4B-CHC-C1C	2.45	132.16	126.34
15	A	1137	CLA	C4B-CHC-C1C	2.45	132.16	126.34
15	B	1219	CLA	C3B-C4B-NB	-2.45	108.24	110.52
16	4	611	CHL	C4A-NA-C1A	2.45	107.81	106.71
15	B	1235	CLA	C4B-CHC-C1C	2.45	132.15	126.34
15	B	1216	CLA	C1D-ND-C4D	-2.45	104.59	106.33
14	3	503	BCR	C4-C5-C6	-2.45	119.17	122.73
14	A	4006	BCR	C34-C9-C10	-2.45	119.49	122.92
15	B	1240	CLA	C3B-C4B-NB	-2.45	108.24	110.52
15	A	1138	CLA	C4B-CHC-C1C	2.45	132.14	126.34
14	3	504	BCR	C37-C22-C21	-2.45	119.49	122.92
15	F	1301	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
15	A	1126	CLA	CHA-C4D-ND	2.44	137.61	132.50
15	2	615	CLA	C2D-C1D-ND	2.44	111.91	110.10
15	4	601	CLA	C1D-ND-C4D	-2.44	104.60	106.33
15	B	1218	CLA	C2D-C1D-ND	2.44	111.90	110.10
16	4	610	CHL	CHD-C4C-C3C	2.44	128.43	124.84
15	B	1212	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
12	1	501	LUT	C28-C29-C30	2.44	122.69	118.94
15	A	1131	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	1	612	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	B	1230	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	B	1214	CLA	C4B-CHC-C1C	2.44	132.12	126.34
15	B	1217	CLA	C4B-CHC-C1C	2.44	132.12	126.34
15	B	1208	CLA	C1C-C2C-C3C	-2.44	104.39	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	4003	BCR	C36-C18-C17	-2.44	119.51	122.92
15	B	1217	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	4	604	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
15	B	1210	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
15	1	607	CLA	C1D-ND-C4D	-2.44	104.61	106.33
14	B	4005	BCR	C34-C9-C10	-2.44	119.51	122.92
15	B	1230	CLA	O2A-CGA-CBA	2.43	119.55	111.91
15	A	1013	CLA	C2D-C1D-ND	2.43	111.90	110.10
14	4	503	BCR	C36-C18-C17	-2.43	119.51	122.92
15	3	607	CLA	O2A-CGA-CBA	2.43	119.55	111.91
15	B	1220	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	B	1204	CLA	C4B-CHC-C1C	2.43	132.11	126.34
15	4	601	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	B	1226	CLA	C4B-CHC-C1C	2.43	132.11	126.34
15	A	1108	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	B	1227	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
15	2	601	CLA	CHA-C4D-ND	2.43	137.59	132.50
15	A	1137	CLA	C1D-ND-C4D	-2.43	104.61	106.33
15	A	1126	CLA	C4B-CHC-C1C	2.43	132.10	126.34
15	J	1302	CLA	C4B-CHC-C1C	2.43	132.10	126.34
15	A	1138	CLA	CHA-C4D-ND	2.43	137.58	132.50
16	2	609	CHL	C2B-C1B-NB	-2.43	108.60	110.23
15	2	603	CLA	C1D-ND-C4D	-2.43	104.61	106.33
15	A	1123	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	A	4007	BCR	C30-C25-C26	-2.43	119.19	122.61
15	A	1113	CLA	CHA-C4D-ND	2.43	137.58	132.50
15	1	603	CLA	C4B-CHC-C1C	2.43	132.10	126.34
15	4	612	CLA	CHA-C4D-ND	2.43	137.58	132.50
23	4	831	GSH	CG1-CD1-N2	2.43	120.04	115.83
15	A	1124	CLA	C1D-ND-C4D	-2.43	104.61	106.33
15	B	1212	CLA	C1D-ND-C4D	-2.43	104.61	106.33
15	B	1232	CLA	C1D-ND-C4D	-2.43	104.61	106.33
15	2	605	CLA	C4B-CHC-C1C	2.43	132.09	126.34
15	4	601	CLA	O2A-CGA-CBA	2.43	119.52	111.91
15	3	615	CLA	C3B-C4B-NB	-2.43	108.27	110.52
15	B	1205	CLA	CHA-C4D-ND	2.43	137.57	132.50
14	B	4003	BCR	C15-C14-C13	-2.43	123.85	127.31
15	1	611	CLA	CHA-C4D-ND	2.42	137.57	132.50
15	3	615	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
15	B	1220	CLA	CHA-C4D-ND	2.42	137.57	132.50
15	1	604	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
15	A	1124	CLA	C4B-CHC-C1C	2.42	132.09	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	606	CLA	CHA-C4D-ND	2.42	137.57	132.50
15	A	1108	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	A	4007	BCR	C35-C13-C14	-2.42	119.53	122.92
15	A	1106	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	A	1131	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
15	B	1213	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
14	J	4002	BCR	C35-C13-C14	-2.42	119.53	122.92
15	B	1209	CLA	CHA-C4D-ND	2.42	137.56	132.50
15	3	613	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	A	1012	CLA	C4B-CHC-C1C	2.42	132.07	126.34
15	A	1117	CLA	C1D-ND-C4D	-2.42	104.62	106.33
16	2	613	CHL	C3B-C4B-NB	-2.42	108.27	110.52
15	4	601	CLA	C2C-C1C-NC	2.42	112.24	109.97
15	A	1105	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
15	1	604	CLA	O2A-CGA-CBA	2.42	119.49	111.91
15	4	612	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	3	605	CLA	C4B-CHC-C1C	2.42	132.07	126.34
15	A	1116	CLA	C3B-C4B-NB	-2.42	108.27	110.52
14	A	4006	BCR	C36-C18-C19	2.42	121.88	118.08
15	A	1120	CLA	C1D-ND-C4D	-2.42	104.62	106.33
15	1	607	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
15	3	615	CLA	CHA-C4D-ND	2.41	137.55	132.50
15	1	613	CLA	CHA-C4D-ND	2.41	137.55	132.50
15	4	612	CLA	O2A-CGA-CBA	2.41	119.48	111.91
15	1	604	CLA	CHA-C4D-ND	2.41	137.54	132.50
15	A	1118	CLA	CHA-C4D-ND	2.41	137.54	132.50
16	2	610	CHL	C4A-NA-C1A	2.41	107.79	106.71
15	B	1206	CLA	CHA-C4D-ND	2.41	137.54	132.50
15	B	1223	CLA	CHA-C4D-ND	2.41	137.54	132.50
15	A	1103	CLA	C3B-C4B-NB	-2.41	108.28	110.52
15	A	1124	CLA	O2A-CGA-CBA	2.41	119.47	111.91
15	1	613	CLA	C3B-C4B-NB	-2.41	108.28	110.52
15	3	601	CLA	C4B-CHC-C1C	2.41	132.05	126.34
15	A	1106	CLA	C2D-C1D-ND	2.41	111.88	110.10
15	B	1218	CLA	C1D-ND-C4D	-2.41	104.62	106.33
15	B	1209	CLA	C4B-CHC-C1C	2.41	132.05	126.34
15	A	1140	CLA	C2D-C1D-ND	2.40	111.88	110.10
15	A	1107	CLA	CHA-C4D-ND	2.40	137.53	132.50
15	B	1022	CLA	CHA-C4D-ND	2.40	137.53	132.50
15	B	1221	CLA	CHA-C4D-ND	2.40	137.53	132.50
15	A	1112	CLA	CHA-C4D-ND	2.40	137.53	132.50
15	A	1013	CLA	C4B-CHC-C1C	2.40	132.04	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1127	CLA	O2A-CGA-CBA	2.40	119.45	111.91
15	B	1236	CLA	C4B-CHC-C1C	2.40	132.04	126.34
15	4	607	CLA	C4B-CHC-C1C	2.40	132.04	126.34
15	A	1013	CLA	CBA-CAA-C2A	-2.40	106.77	113.86
15	B	1219	CLA	C2D-C1D-ND	2.40	111.87	110.10
15	A	1129	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	4	602	CLA	CHA-C4D-ND	2.40	137.52	132.50
15	A	1141	CLA	C4B-CHC-C1C	2.40	132.03	126.34
15	B	1211	CLA	C4B-CHC-C1C	2.40	132.03	126.34
15	A	1111	CLA	CHA-C4D-ND	2.40	137.52	132.50
15	1	606	CLA	C4B-CHC-C1C	2.40	132.03	126.34
15	3	608	CLA	CHA-C4D-ND	2.40	137.52	132.50
15	B	1239	CLA	CHA-C4D-ND	2.40	137.52	132.50
14	A	4003	BCR	C38-C26-C25	-2.40	121.83	124.53
15	B	1240	CLA	O2A-CGA-CBA	2.40	119.43	111.91
15	3	607	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	B	1227	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	A	1108	CLA	CHA-C4D-ND	2.40	137.51	132.50
15	B	1217	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
15	A	1141	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
14	4	503	BCR	C30-C25-C24	2.40	122.55	115.78
15	B	1210	CLA	C2D-C1D-ND	2.40	111.87	110.10
15	1	615	CLA	CHA-C4D-ND	2.39	137.51	132.50
15	A	1134	CLA	CHA-C4D-ND	2.39	137.51	132.50
15	B	1231	CLA	C3B-C4B-NB	-2.39	108.29	110.52
15	B	1225	CLA	C4B-CHC-C1C	2.39	132.02	126.34
15	F	1301	CLA	C4B-CHC-C1C	2.39	132.01	126.34
15	2	603	CLA	CHA-C4D-ND	2.39	137.50	132.50
16	4	611	CHL	C1-O2A-CGA	2.39	122.72	116.44
15	A	1135	CLA	CHA-C4D-ND	2.39	137.50	132.50
15	A	1108	CLA	C4B-CHC-C1C	2.39	132.01	126.34
15	A	1119	CLA	CHA-C4D-ND	2.39	137.50	132.50
15	A	1135	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	1	606	CLA	C2C-C1C-NC	2.39	112.21	109.97
15	A	1140	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	B	1234	CLA	C4B-CHC-C1C	2.39	132.01	126.34
15	1	602	CLA	C4B-CHC-C1C	2.39	132.00	126.34
15	4	607	CLA	C1D-ND-C4D	-2.39	104.64	106.33
15	A	1123	CLA	CHA-C4D-ND	2.39	137.50	132.50
15	B	1221	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	3	605	CLA	C2D-C1D-ND	2.39	111.86	110.10
15	A	1107	CLA	C4B-CHC-C1C	2.39	132.00	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1226	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
15	B	1201	CLA	C4B-CHC-C1C	2.39	132.00	126.34
15	1	605	CLA	CHA-C4D-ND	2.39	137.49	132.50
15	A	1122	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	A	1131	CLA	CHA-C4D-ND	2.39	137.49	132.50
15	B	1231	CLA	O2A-CGA-CBA	2.39	119.40	111.91
15	B	1204	CLA	C1D-ND-C4D	-2.39	104.64	106.33
15	B	1021	CLA	C4B-CHC-C1C	2.39	132.00	126.34
15	B	1224	CLA	C4B-CHC-C1C	2.39	132.00	126.34
15	A	1113	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
14	3	503	BCR	C15-C14-C13	-2.38	123.91	127.31
15	A	1123	CLA	C4B-CHC-C1C	2.38	131.99	126.34
15	A	1114	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	1	604	CLA	C4B-CHC-C1C	2.38	131.99	126.34
15	B	1234	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	A	1106	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	3	603	CLA	C4B-CHC-C1C	2.38	131.99	126.34
15	A	1115	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	A	1133	CLA	C4B-CHC-C1C	2.38	131.99	126.34
15	B	1215	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	4	612	CLA	C4B-CHC-C1C	2.38	131.98	126.34
15	4	615	CLA	C4B-CHC-C1C	2.38	131.98	126.34
15	3	605	CLA	C3B-C4B-NB	-2.38	108.31	110.52
16	2	613	CHL	CHD-C4C-C3C	2.38	128.34	124.84
15	B	1238	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	A	1110	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
15	4	603	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
15	B	1203	CLA	C3B-C4B-NB	-2.38	108.31	110.52
16	2	613	CHL	C2B-C1B-NB	-2.38	108.64	110.23
15	A	1117	CLA	CHA-C4D-ND	2.38	137.47	132.50
15	B	1202	CLA	CHA-C4D-ND	2.38	137.47	132.50
15	B	1237	CLA	CHA-C4D-ND	2.38	137.47	132.50
15	B	1232	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	B	1237	CLA	O2A-CGA-CBA	2.38	119.37	111.91
15	4	606	CLA	C4B-CHC-C1C	2.38	131.97	126.34
24	A	1011	CL0	C3D-C4D-ND	2.38	114.08	110.24
15	A	1102	CLA	CHA-C4D-ND	2.38	137.47	132.50
15	4	605	CLA	CHA-C4D-ND	2.38	137.47	132.50
15	A	1128	CLA	C3B-C4B-NB	-2.38	108.31	110.52
15	B	1206	CLA	C3B-C4B-NB	-2.38	108.31	110.52
15	3	608	CLA	C4B-CHC-C1C	2.38	131.97	126.34
15	A	1114	CLA	C3B-C4B-NB	-2.37	108.31	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1240	CLA	C4B-CHC-C1C	2.37	131.97	126.34
14	B	4006	BCR	C38-C26-C27	2.37	118.18	113.62
15	B	1219	CLA	CHA-C4D-ND	2.37	137.47	132.50
12	2	501	LUT	C8-C7-C6	-2.37	120.53	127.20
15	1	612	CLA	C4B-CHC-C1C	2.37	131.97	126.34
15	2	602	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	B	1209	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	B	1201	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	3	615	CLA	C4B-CHC-C1C	2.37	131.97	126.34
15	A	1139	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	2	612	CLA	C4B-CHC-C1C	2.37	131.97	126.34
15	A	1121	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	4	602	CLA	C1D-ND-C4D	-2.37	104.65	106.33
15	A	1130	CLA	C4B-CHC-C1C	2.37	131.96	126.34
15	B	1021	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	A	1141	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	A	1101	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
15	3	607	CLA	CHA-C4D-ND	2.37	137.46	132.50
15	F	1302	CLA	C1D-ND-C4D	-2.37	104.65	106.33
15	3	611	CLA	C4B-CHC-C1C	2.37	131.96	126.34
15	4	605	CLA	O2A-CGA-CBA	2.37	119.34	111.91
15	A	1105	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	B	1210	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	3	606	CLA	C4B-CHC-C1C	2.37	131.96	126.34
13	4	502	XAT	C18-C5-C6	-2.37	118.29	122.26
15	A	1127	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	1	604	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
15	B	1211	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	B	1238	CLA	C4B-CHC-C1C	2.37	131.95	126.34
15	A	1139	CLA	C1-O2A-CGA	2.37	122.65	116.44
15	A	1116	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	A	1120	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
15	B	1230	CLA	C4B-CHC-C1C	2.36	131.94	126.34
15	1	607	CLA	CHA-C4D-ND	2.36	137.44	132.50
13	1	502	XAT	C40-C33-C34	-2.36	119.61	122.92
15	B	1210	CLA	O2A-CGA-CBA	2.36	119.33	111.91
15	A	1116	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
15	B	1211	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	B	1220	CLA	C4B-CHC-C1C	2.36	131.94	126.34
15	B	1231	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
15	A	1126	CLA	O2A-CGA-CBA	2.36	119.32	111.91
15	2	603	CLA	CMD-C2D-C3D	-2.36	122.18	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1218	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
14	2	503	BCR	C30-C25-C26	-2.36	119.29	122.61
15	A	1105	CLA	C4B-CHC-C1C	2.36	131.94	126.34
15	3	612	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
15	3	603	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	F	1301	CLA	C3B-C4B-NB	-2.36	108.33	110.52
15	A	1122	CLA	CHA-C4D-ND	2.36	137.44	132.50
15	F	1301	CLA	CHA-C4D-ND	2.36	137.44	132.50
15	A	1126	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
15	A	1133	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	B	1216	CLA	CHA-C4D-ND	2.36	137.43	132.50
15	B	1216	CLA	C4B-CHC-C1C	2.36	131.93	126.34
15	2	607	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
15	B	1213	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
15	4	615	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
15	2	608	CLA	C3B-C4B-NB	-2.36	108.33	110.52
16	4	610	CHL	CHB-C4A-NA	2.36	127.77	124.51
15	A	1109	CLA	C1D-ND-C4D	-2.36	104.66	106.33
13	4	502	XAT	O4-C5-C18	-2.36	112.23	115.06
15	B	1222	CLA	C4B-CHC-C1C	2.36	131.93	126.34
15	B	1230	CLA	CHA-C4D-ND	2.36	137.43	132.50
15	A	1125	CLA	CHA-C4D-ND	2.36	137.43	132.50
15	2	601	CLA	C4B-CHC-C1C	2.36	131.92	126.34
15	3	606	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	A	1129	CLA	CHA-C4D-ND	2.35	137.43	132.50
13	3	502	XAT	C19-C9-C10	-2.35	119.62	122.92
15	3	611	CLA	CHA-C4D-ND	2.35	137.42	132.50
15	1	611	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
15	A	1122	CLA	C4B-CHC-C1C	2.35	131.92	126.34
15	A	1103	CLA	CHA-C4D-ND	2.35	137.42	132.50
15	4	608	CLA	C4B-CHC-C1C	2.35	131.92	126.34
15	3	610	CLA	C4B-CHC-C1C	2.35	131.92	126.34
14	A	4004	BCR	C38-C26-C27	2.35	118.13	113.62
15	3	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	A	1106	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	B	1216	CLA	O2A-CGA-CBA	2.35	119.29	111.91
15	B	1225	CLA	CHA-C4D-ND	2.35	137.42	132.50
15	3	601	CLA	C1D-ND-C4D	-2.35	104.67	106.33
15	A	1113	CLA	C4B-CHC-C1C	2.35	131.91	126.34
15	4	609	CLA	C4B-CHC-C1C	2.35	131.91	126.34
15	B	1226	CLA	CHA-C4D-ND	2.35	137.41	132.50
22	2	821	LMT	C3'-C4'-C5'	-2.35	105.54	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1214	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	3	607	CLA	C1D-ND-C4D	-2.35	104.67	106.33
15	4	609	CLA	C1D-ND-C4D	-2.35	104.67	106.33
15	B	1218	CLA	O2A-CGA-CBA	2.35	119.28	111.91
15	2	615	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	B	1224	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	B	1231	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	A	1135	CLA	C4B-CHC-C1C	2.35	131.91	126.34
15	2	608	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	B	1221	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
15	A	1120	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	2	612	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	B	1204	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	2	608	CLA	C4B-CHC-C1C	2.35	131.91	126.34
15	B	1215	CLA	C4B-CHC-C1C	2.35	131.91	126.34
15	B	1224	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	B	1234	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	4	606	CLA	CHA-C4D-ND	2.35	137.41	132.50
14	F	4002	BCR	C35-C13-C14	-2.35	119.64	122.92
15	B	1223	CLA	C4B-CHC-C1C	2.35	131.90	126.34
15	A	1118	CLA	C4B-CHC-C1C	2.34	131.90	126.34
15	B	1239	CLA	O2A-CGA-CBA	2.34	119.26	111.91
12	2	501	LUT	C15-C35-C34	-2.34	118.67	123.47
15	B	1240	CLA	CHA-C4D-ND	2.34	137.40	132.50
15	A	1121	CLA	C4B-CHC-C1C	2.34	131.90	126.34
15	B	1210	CLA	C4B-CHC-C1C	2.34	131.90	126.34
15	2	603	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
14	B	4006	BCR	C34-C9-C10	-2.34	119.64	122.92
15	A	1141	CLA	C1D-ND-C4D	-2.34	104.67	106.33
15	B	1202	CLA	C1D-ND-C4D	-2.34	104.67	106.33
15	A	1118	CLA	O2A-CGA-CBA	2.34	119.26	111.91
16	4	610	CHL	C4D-CHA-C1A	2.34	124.10	121.25
15	1	601	CLA	C4B-CHC-C1C	2.34	131.89	126.34
15	3	608	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
15	B	1229	CLA	CHA-C4D-ND	2.34	137.40	132.50
15	A	1125	CLA	C1D-ND-C4D	-2.34	104.67	106.33
14	3	503	BCR	C19-C18-C17	2.34	122.53	118.94
15	B	1215	CLA	O2A-CGA-CBA	2.34	119.25	111.91
15	3	613	CLA	C4B-CHC-C1C	2.34	131.89	126.34
15	A	1136	CLA	C4B-CHC-C1C	2.34	131.89	126.34
15	2	604	CLA	C3B-C4B-NB	-2.34	108.35	110.52
15	2	607	CLA	C4B-CHC-C1C	2.34	131.88	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1110	CLA	C4B-CHC-C1C	2.34	131.88	126.34
15	B	1237	CLA	C4B-CHC-C1C	2.34	131.88	126.34
15	A	1124	CLA	CHA-C4D-ND	2.34	137.39	132.50
15	A	1116	CLA	C4B-CHC-C1C	2.34	131.88	126.34
15	B	1213	CLA	CHA-C4D-ND	2.34	137.38	132.50
15	B	1232	CLA	CHA-C4D-ND	2.34	137.38	132.50
13	1	502	XAT	C20-C13-C14	-2.33	119.65	122.92
15	2	604	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
15	3	611	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
15	A	1128	CLA	C4B-CHC-C1C	2.33	131.87	126.34
15	A	1117	CLA	C4B-CHC-C1C	2.33	131.87	126.34
15	B	1212	CLA	CHA-C4D-ND	2.33	137.38	132.50
15	2	605	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
15	4	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	3	607	CLA	C4B-CHC-C1C	2.33	131.87	126.34
15	B	1238	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	4	604	CLA	CHA-C4D-ND	2.33	137.38	132.50
15	A	1111	CLA	C4B-CHC-C1C	2.33	131.87	126.34
15	A	1133	CLA	CHA-C4D-ND	2.33	137.38	132.50
15	A	1102	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
15	B	1225	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
15	A	1124	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	2	605	CLA	CHA-C1A-NA	-2.33	121.06	126.40
15	B	1023	CLA	CHA-C1A-NA	-2.33	121.06	126.40
15	B	1227	CLA	CHA-C4D-ND	2.33	137.37	132.50
14	B	4003	BCR	C36-C18-C17	-2.33	119.66	122.92
15	A	1132	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
15	A	1139	CLA	C4B-CHC-C1C	2.33	131.86	126.34
15	2	602	CLA	CHA-C4D-ND	2.33	137.37	132.50
15	1	601	CLA	CHA-C4D-ND	2.33	137.37	132.50
15	B	1208	CLA	C4B-CHC-C1C	2.33	131.86	126.34
15	B	1220	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
15	A	1101	CLA	C3B-C4B-NB	-2.33	108.36	110.52
15	B	1218	CLA	C4B-CHC-C1C	2.33	131.85	126.34
12	3	501	LUT	C19-C9-C10	-2.33	119.67	122.92
15	2	606	CLA	C3B-C4B-NB	-2.33	108.36	110.52
15	2	607	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
15	A	1109	CLA	CHA-C4D-ND	2.32	137.36	132.50
15	2	615	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
15	A	1136	CLA	CHA-C4D-ND	2.32	137.36	132.50
12	1	501	LUT	C18-C5-C4	2.32	118.66	114.36
15	B	1234	CLA	C3B-C4B-NB	-2.32	108.36	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1115	CLA	C4B-CHC-C1C	2.32	131.85	126.34
15	B	1203	CLA	C4B-CHC-C1C	2.32	131.85	126.34
15	B	1224	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
15	1	602	CLA	C1D-ND-C4D	-2.32	104.69	106.33
15	B	1201	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
15	A	1102	CLA	C3B-C4B-NB	-2.32	108.36	110.52
15	A	1130	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
16	1	609	CHL	CHC-C1C-NC	2.32	127.72	124.20
15	4	612	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
15	3	610	CLA	CHA-C4D-ND	2.32	137.35	132.50
15	2	607	CLA	C3B-C4B-NB	-2.32	108.36	110.52
15	A	1120	CLA	C4B-CHC-C1C	2.32	131.84	126.34
15	A	1120	CLA	O2A-CGA-CBA	2.32	119.18	111.91
14	A	4002	BCR	C23-C24-C25	-2.32	120.69	127.20
15	B	1229	CLA	C2D-C1D-ND	2.32	111.81	110.10
15	J	1302	CLA	CHA-C4D-ND	2.32	137.35	132.50
15	B	1212	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
15	3	605	CLA	CHA-C4D-ND	2.32	137.35	132.50
15	A	1140	CLA	C4B-CHC-C1C	2.32	131.83	126.34
15	A	1106	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
15	B	1205	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
15	B	1229	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
15	A	1112	CLA	C4B-CHC-C1C	2.31	131.83	126.34
15	A	1138	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
15	B	1206	CLA	C4B-CHC-C1C	2.31	131.82	126.34
15	4	603	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
15	A	1135	CLA	C3B-C4B-NB	-2.31	108.37	110.52
15	B	1226	CLA	O2A-CGA-CBA	2.31	119.16	111.91
15	B	1218	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	1	612	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
15	A	1129	CLA	C4B-CHC-C1C	2.31	131.82	126.34
15	B	1221	CLA	C4B-CHC-C1C	2.31	131.82	126.34
15	B	1214	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	2	615	CLA	O2A-CGA-CBA	2.31	119.16	111.91
15	A	1107	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	B	1232	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
15	A	1119	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	2	615	CLA	C4B-CHC-C1C	2.31	131.81	126.34
15	A	1134	CLA	C4B-CHC-C1C	2.31	131.81	126.34
15	A	1130	CLA	CHA-C4D-ND	2.31	137.32	132.50
15	B	1201	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
15	4	608	CLA	C3B-C4B-NB	-2.31	108.38	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1	501	LUT	C22-C23-C24	-2.31	109.12	111.74
15	B	1204	CLA	CHA-C4D-ND	2.31	137.32	132.50
15	A	1013	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
15	A	1132	CLA	C3B-C4B-NB	-2.31	108.38	110.52
15	A	1137	CLA	CHA-C4D-ND	2.30	137.32	132.50
15	A	1139	CLA	O2A-CGA-CBA	2.30	119.14	111.91
15	A	1107	CLA	C3B-C4B-NB	-2.30	108.38	110.52
15	1	613	CLA	C1D-ND-C4D	-2.30	104.70	106.33
15	B	1202	CLA	C4B-CHC-C1C	2.30	131.80	126.34
15	2	608	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	A	1130	CLA	C1D-ND-C4D	-2.30	104.70	106.33
15	4	608	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	B	1237	CLA	C3B-C4B-NB	-2.30	108.38	110.52
15	B	1227	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
15	4	607	CLA	CHA-C4D-ND	2.30	137.31	132.50
15	A	1119	CLA	O2A-CGA-CBA	2.30	119.13	111.91
15	A	1112	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	1	606	CLA	CHA-C4D-ND	2.30	137.31	132.50
15	2	602	CLA	C4B-CHC-C1C	2.30	131.79	126.34
15	3	610	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
15	1	611	CLA	C4B-CHC-C1C	2.30	131.79	126.34
15	A	1109	CLA	C4B-CHC-C1C	2.30	131.79	126.34
15	A	1114	CLA	C4B-CHC-C1C	2.30	131.79	126.34
15	3	610	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	B	1230	CLA	C2D-C1D-ND	2.30	111.80	110.10
15	A	1123	CLA	O2A-CGA-CBA	2.30	119.12	111.91
15	B	1207	CLA	C1C-CHC-C4B	2.30	131.86	126.13
15	A	1107	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
15	4	606	CLA	C2D-C1D-ND	2.30	111.80	110.10
14	4	505	BCR	C8-C9-C10	2.30	122.46	118.94
15	A	1115	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
16	2	610	CHL	CHD-C4C-C3C	2.29	128.21	124.84
15	3	601	CLA	CHA-C4D-ND	2.29	137.30	132.50
15	4	604	CLA	C4B-CHC-C1C	2.29	131.78	126.34
15	B	1023	CLA	C4B-CHC-C1C	2.29	131.78	126.34
14	4	505	BCR	C15-C14-C13	-2.29	124.04	127.31
15	A	1110	CLA	CHA-C4D-ND	2.29	137.29	132.50
15	A	1134	CLA	C1D-ND-C4D	-2.29	104.71	106.33
15	4	607	CLA	O2A-CGA-CBA	2.29	119.10	111.91
15	1	603	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
15	A	1111	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
15	A	1013	CLA	O2A-CGA-CBA	2.29	119.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4001	BCR	C3-C4-C5	-2.29	109.99	114.08
15	B	1022	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
15	B	1203	CLA	O2A-CGA-CBA	2.29	119.09	111.91
15	B	1209	CLA	C1D-ND-C4D	-2.29	104.71	106.33
15	A	1106	CLA	C4B-CHC-C1C	2.29	131.77	126.34
15	B	1228	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
15	A	1118	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
15	A	1132	CLA	C4B-CHC-C1C	2.29	131.77	126.34
15	B	1228	CLA	CHA-C4D-ND	2.29	137.29	132.50
15	B	1239	CLA	C4B-CHC-C1C	2.29	131.76	126.34
19	1	811	SQD	O3-C3-C2	-2.29	105.06	110.35
15	2	615	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
15	3	613	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
15	1	605	CLA	C1D-ND-C4D	-2.29	104.71	106.33
15	B	1214	CLA	C1D-ND-C4D	-2.29	104.71	106.33
15	3	611	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
15	3	612	CLA	C4B-CHC-C1C	2.29	131.76	126.34
15	A	1134	CLA	C3B-C4B-NB	-2.29	108.39	110.52
15	3	606	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
15	2	608	CLA	C1D-ND-C4D	-2.28	104.71	106.33
15	4	608	CLA	C1D-ND-C4D	-2.28	104.71	106.33
12	2	501	LUT	C19-C9-C10	-2.28	119.72	122.92
13	4	502	XAT	O24-C25-C24	2.28	115.10	113.38
15	B	1232	CLA	C4B-CHC-C1C	2.28	131.76	126.34
15	A	1117	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
14	J	4002	BCR	C23-C24-C25	-2.28	120.79	127.20
12	2	501	LUT	C11-C12-C13	-2.28	120.00	126.42
15	A	1104	CLA	C3B-C4B-NB	-2.28	108.40	110.52
15	A	1117	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
15	3	613	CLA	CHA-C4D-ND	2.28	137.27	132.50
15	B	1203	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
15	3	601	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
15	3	606	CLA	CHA-C4D-ND	2.28	137.27	132.50
15	4	608	CLA	CHA-C4D-ND	2.28	137.27	132.50
14	B	4006	BCR	C15-C14-C13	-2.28	124.06	127.31
15	1	613	CLA	C4B-CHC-C1C	2.28	131.74	126.34
15	A	1136	CLA	C1D-ND-C4D	-2.28	104.72	106.33
15	A	1128	CLA	O2A-CGA-CBA	2.28	119.05	111.91
15	B	1225	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
15	A	1103	CLA	C1D-ND-C4D	-2.28	104.72	106.33
15	2	602	CLA	O2A-CGA-CBA	2.28	119.05	111.91
16	1	609	CHL	C4A-NA-C1A	2.28	107.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1205	CLA	C4B-CHC-C1C	2.28	131.74	126.34
15	B	1201	CLA	C1D-ND-C4D	-2.27	104.72	106.33
15	2	606	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
15	A	1109	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
15	B	1213	CLA	C1D-ND-C4D	-2.27	104.72	106.33
15	2	603	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
15	3	606	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
15	A	1119	CLA	C3B-C4B-NB	-2.27	108.41	110.52
15	B	1203	CLA	CHA-C4D-ND	2.27	137.25	132.50
15	A	1121	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
15	A	1012	CLA	CHA-C4D-ND	2.27	137.25	132.50
13	2	502	XAT	C38-C25-C26	-2.27	118.46	122.26
15	4	606	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
16	2	610	CHL	C1-O2A-CGA	2.27	122.39	116.44
15	2	604	CLA	C1D-ND-C4D	-2.27	104.72	106.33
15	1	605	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
15	A	1128	CLA	CHA-C4D-ND	2.27	137.24	132.50
15	B	1202	CLA	C3B-C4B-NB	-2.27	108.41	110.52
15	B	1206	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
15	A	1121	CLA	C1D-ND-C4D	-2.27	104.72	106.33
15	A	1119	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
15	2	612	CLA	O2A-CGA-CBA	2.26	119.01	111.91
15	A	1132	CLA	O2A-CGA-CBA	2.26	119.01	111.91
15	1	615	CLA	C4B-CHC-C1C	2.26	131.71	126.34
15	A	1111	CLA	CHA-C1A-NA	-2.26	121.21	126.40
15	2	608	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
15	A	1134	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
15	B	1237	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	J	4001	BCR	C36-C18-C17	-2.26	119.75	122.92
15	A	1012	CLA	C1D-ND-C4D	-2.26	104.73	106.33
15	1	615	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
16	2	609	CHL	C4D-CHA-C1A	2.26	124.00	121.25
15	A	1133	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	B	1231	CLA	C4B-CHC-C1C	2.26	131.70	126.34
14	4	503	BCR	C37-C22-C21	-2.26	119.76	122.92
14	1	505	BCR	C12-C13-C14	2.26	122.41	118.94
15	1	611	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	B	1204	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	1	612	CLA	C1D-ND-C4D	-2.26	104.73	106.33
15	2	602	CLA	C1D-ND-C4D	-2.26	104.73	106.33
14	1	503	BCR	C23-C22-C21	-2.26	115.48	118.94
15	B	1212	CLA	C4B-CHC-C1C	2.26	131.69	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1218	CLA	CHA-C4D-ND	2.26	137.22	132.50
15	3	605	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	A	1120	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
15	B	1236	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
14	B	4006	BCR	C28-C27-C26	-2.26	110.05	114.08
15	B	1228	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
15	A	1013	CLA	CMA-C3A-C4A	2.25	117.83	111.77
15	B	1206	CLA	O2A-CGA-CBA	2.25	118.98	111.91
15	B	1212	CLA	C3B-C4B-NB	-2.25	108.42	110.52
15	A	1102	CLA	C4B-CHC-C1C	2.25	131.68	126.34
15	B	1208	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
15	B	1230	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
15	B	1221	CLA	C3B-C4B-NB	-2.25	108.43	110.52
14	B	4002	BCR	C36-C18-C17	-2.25	119.77	122.92
15	1	608	CLA	CHA-C4D-ND	2.25	137.21	132.50
12	4	501	LUT	C10-C11-C12	-2.25	116.20	123.22
15	A	1123	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	1	607	CLA	C4B-CHC-C1C	2.25	131.67	126.34
15	3	607	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	A	1135	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	B	1223	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	A	1140	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	A	1114	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
15	4	606	CLA	O2A-CGA-CBA	2.25	118.96	111.91
15	4	603	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	3	601	CLA	O2A-CGA-CBA	2.25	118.96	111.91
15	A	1129	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	2	606	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
15	B	1021	CLA	O2A-CGA-CBA	2.24	118.95	111.91
15	A	1122	CLA	C1D-ND-C4D	-2.24	104.74	106.33
15	A	1103	CLA	C4B-CHC-C1C	2.24	131.66	126.34
15	A	1125	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
15	F	1302	CLA	C4B-CHC-C1C	2.24	131.66	126.34
15	3	605	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	B	1231	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	A	1113	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
15	1	606	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
14	A	4004	BCR	C8-C7-C6	-2.24	120.91	127.20
15	2	615	CLA	C3B-C4B-NB	-2.24	108.44	110.52
15	B	1231	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
15	B	1023	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
15	B	1211	CLA	CMD-C2D-C3D	-2.24	122.46	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	604	CLA	C4B-CHC-C1C	2.24	131.65	126.34
15	B	1228	CLA	C4B-CHC-C1C	2.24	131.65	126.34
15	1	605	CLA	O2A-CGA-CBA	2.24	118.93	111.91
15	3	605	CLA	C1D-ND-C4D	-2.24	104.75	106.33
15	A	1137	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
14	F	4002	BCR	C23-C24-C25	-2.24	120.92	127.20
15	A	1104	CLA	C4B-CHC-C1C	2.24	131.64	126.34
15	A	1114	CLA	C1D-ND-C4D	-2.24	104.75	106.33
15	A	1115	CLA	C1D-ND-C4D	-2.24	104.75	106.33
15	A	1122	CLA	O2A-CGA-CBA	2.24	118.92	111.91
14	B	4001	BCR	C36-C18-C17	-2.23	119.79	122.92
15	J	1302	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
15	B	1236	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
13	4	502	XAT	C40-C33-C34	-2.23	119.79	122.92
15	B	1211	CLA	C3B-C4B-NB	-2.23	108.44	110.52
15	2	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
15	2	604	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
16	1	610	CHL	C1-O2A-CGA	2.23	123.47	116.11
15	B	1221	CLA	O2A-CGA-CBA	2.23	118.91	111.91
15	B	1218	CLA	C3B-C4B-NB	-2.23	108.44	110.52
15	A	1129	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
15	J	1302	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
15	A	1112	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
15	B	1224	CLA	C2D-C1D-ND	2.23	111.75	110.10
15	B	1229	CLA	C4B-CHC-C1C	2.23	131.63	126.34
15	A	1128	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	3	606	CLA	C3B-C4B-NB	-2.23	108.45	110.52
15	1	603	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	B	1214	CLA	O2A-CGA-CBA	2.23	118.91	111.91
15	B	1220	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
15	4	609	CLA	CHA-C4D-ND	2.23	137.16	132.50
15	F	1302	CLA	CHA-C4D-ND	2.23	137.16	132.50
15	A	1138	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
15	A	1121	CLA	O2A-CGA-CBA	2.23	118.90	111.91
15	A	1123	CLA	C1D-ND-C4D	-2.23	104.75	106.33
15	4	615	CLA	CHA-C4D-ND	2.23	137.16	132.50
15	B	1237	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
15	1	603	CLA	C1D-ND-C4D	-2.23	104.75	106.33
15	B	1222	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
15	A	1141	CLA	CMD-C2D-C3D	-2.23	122.50	127.61
15	2	612	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
15	A	1130	CLA	CMD-C2D-C3D	-2.22	122.50	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1208	CLA	O2A-CGA-CBA	2.22	118.89	111.91
15	B	1228	CLA	O2A-CGA-CBA	2.22	118.89	111.91
15	A	1104	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	A	1118	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	1	607	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
15	3	606	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
15	3	608	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	1	613	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	3	615	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	B	1219	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
15	3	603	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
15	A	1013	CLA	CHA-C4D-ND	2.22	137.14	132.50
14	B	4002	BCR	C30-C25-C26	-2.22	119.49	122.61
15	B	1202	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
15	B	1240	CLA	C1D-ND-C4D	-2.22	104.76	106.33
15	A	1112	CLA	C3B-C4B-NB	-2.22	108.46	110.52
15	A	1139	CLA	C3B-C4B-NB	-2.22	108.46	110.52
15	4	601	CLA	C4B-CHC-C1C	2.22	131.60	126.34
15	1	611	CLA	O2A-CGA-CBA	2.22	118.87	111.91
15	4	607	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
15	A	1140	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
15	3	610	CLA	O2A-CGA-CBA	2.22	118.87	111.91
15	A	1134	CLA	O2A-CGA-CBA	2.22	118.86	111.91
13	2	502	XAT	O4-C5-C18	-2.22	112.40	115.06
15	A	1108	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
15	2	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	A	1133	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
15	B	1207	CLA	C2C-C3C-C4C	-2.21	104.56	107.21
15	3	608	CLA	C1D-ND-C4D	-2.21	104.76	106.33
15	A	1103	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	2	615	CLA	C1D-ND-C4D	-2.21	104.76	106.33
15	B	1216	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
14	3	504	BCR	C23-C24-C25	-2.21	120.99	127.20
15	4	609	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
15	B	1239	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
14	2	503	BCR	C34-C9-C10	-2.21	119.83	122.92
15	B	1022	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	B	1212	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
15	B	1206	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
15	B	1213	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
15	A	1136	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
15	B	1238	CLA	C1D-ND-C4D	-2.21	104.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1022	CLA	C4B-CHC-C1C	2.21	131.57	126.34
15	J	1302	CLA	C3B-C4B-NB	-2.21	108.47	110.52
15	A	1135	CLA	O2A-CGA-CBA	2.21	118.83	111.91
15	1	611	CLA	C1D-ND-C4D	-2.21	104.77	106.33
15	A	1105	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
14	F	4002	BCR	C37-C22-C21	-2.20	119.83	122.92
15	A	1110	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
15	B	1021	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
16	1	610	CHL	C3B-C4B-NB	-2.20	108.47	110.52
15	1	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
15	4	601	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
15	B	1202	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
14	A	4005	BCR	C8-C7-C6	-2.20	121.02	127.20
15	A	1124	CLA	C1-O2A-CGA	2.20	122.21	116.44
15	B	1234	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
15	B	1216	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	B	1238	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	A	1131	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	B	1204	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
15	A	1115	CLA	C3B-C4B-NB	-2.20	108.48	110.52
15	4	607	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	A	1110	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	A	1012	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	4	608	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	2	601	CLA	O2A-CGA-CBA	2.20	118.80	111.91
15	3	611	CLA	C1D-ND-C4D	-2.20	104.78	106.33
15	B	1210	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
15	4	601	CLA	CHA-C4D-ND	2.20	137.09	132.50
15	B	1202	CLA	O2A-CGA-CBA	2.19	118.80	111.91
15	A	1118	CLA	C1D-ND-C4D	-2.19	104.78	106.33
14	B	4005	BCR	C38-C26-C27	2.19	117.83	113.62
15	B	1222	CLA	CHA-C4D-ND	2.19	137.09	132.50
16	2	610	CHL	C2B-C1B-NB	-2.19	108.76	110.23
15	A	1116	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
12	2	501	LUT	C20-C13-C14	-2.19	119.85	122.92
15	B	1236	CLA	O2A-CGA-CBA	2.19	118.78	111.91
15	B	1022	CLA	C1D-ND-C4D	-2.19	104.78	106.33
12	4	501	LUT	C38-C25-C24	-2.19	118.88	123.56
15	F	1302	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	A	1141	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	3	606	CLA	CHA-C1A-NA	-2.19	121.39	126.40
15	3	603	CLA	C1C-C2C-C3C	-2.19	104.66	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	811	SQD	O8-S-C6	-2.19	102.25	105.74
14	B	4003	BCR	C23-C24-C25	-2.19	121.06	127.20
15	A	1131	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	F	1301	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	3	603	CLA	C3B-C4B-NB	-2.18	108.49	110.52
15	2	606	CLA	C1D-ND-C4D	-2.18	104.78	106.33
15	1	613	CLA	CHA-C1A-NA	-2.18	121.40	126.40
13	3	502	XAT	C27-C28-C29	2.18	128.92	125.53
15	4	609	CLA	CHA-C1A-NA	-2.18	121.40	126.40
15	A	1112	CLA	O2A-CGA-CBA	2.18	118.75	111.91
15	A	1130	CLA	O2A-CGA-CBA	2.18	118.75	111.91
15	A	1101	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
15	B	1236	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
15	B	1240	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
15	B	1204	CLA	O2A-CGA-CBA	2.18	118.74	111.91
15	B	1215	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
15	A	1116	CLA	O2A-CGA-CBA	2.18	118.73	111.91
15	B	1213	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B	1217	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
15	3	608	CLA	O2A-CGA-CBA	2.17	118.72	111.91
17	A	5002	LHG	O7-C7-O9	-2.17	118.45	123.70
15	1	612	CLA	O2A-CGA-CBA	2.17	118.72	111.91
15	A	1122	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
15	1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
15	A	1101	CLA	CHA-C1A-NA	-2.17	121.43	126.40
15	1	606	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
15	B	1201	CLA	O2A-CGA-CBA	2.17	118.72	111.91
15	B	1208	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
14	A	4003	BCR	C38-C26-C27	2.17	117.78	113.62
15	A	1131	CLA	C1D-ND-C4D	-2.17	104.80	106.33
15	3	603	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
15	A	1113	CLA	C1D-ND-C4D	-2.17	104.80	106.33
15	2	601	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
15	B	1235	CLA	CHA-C4D-ND	2.16	137.03	132.50
15	3	612	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
13	3	502	XAT	O24-C25-C24	2.16	115.01	113.38
15	B	1236	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
15	2	607	CLA	O2A-CGA-CBA	2.16	118.69	111.91
15	1	608	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
15	A	1136	CLA	O2A-CGA-CBA	2.16	118.69	111.91
14	1	503	BCR	C12-C13-C14	-2.16	115.63	118.94
15	A	1139	CLA	CMD-C2D-C3D	-2.16	122.65	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	502	XAT	C39-C29-C30	-2.16	119.90	122.92
15	4	615	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
15	B	1209	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
15	B	1226	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
15	A	1119	CLA	C1D-ND-C4D	-2.16	104.80	106.33
15	2	601	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	B	1214	CLA	C3B-C4B-NB	-2.16	108.52	110.52
15	A	1127	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
15	A	1137	CLA	O2A-CGA-CBA	2.16	118.67	111.91
14	A	4003	BCR	C37-C22-C21	-2.16	119.90	122.92
14	4	503	BCR	C3-C4-C5	-2.16	110.23	114.08
15	B	1223	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	1	602	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
16	3	604	CHL	CHB-C4A-NA	2.15	127.49	124.51
14	B	4002	BCR	C37-C22-C21	-2.15	119.91	122.92
15	B	1221	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
15	A	1133	CLA	O2A-CGA-CBA	2.15	118.66	111.91
15	B	1219	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
15	B	1023	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
15	A	1129	CLA	O2A-CGA-CBA	2.15	118.66	111.91
15	B	1234	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
14	B	4005	BCR	C28-C27-C26	-2.15	110.24	114.08
15	B	1215	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
15	A	1102	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
14	A	4006	BCR	C12-C13-C14	-2.15	115.64	118.94
15	3	612	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	A	1111	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	A	1110	CLA	CHA-C1A-NA	-2.15	121.48	126.40
14	1	503	BCR	C8-C7-C6	-2.15	121.18	127.20
15	2	612	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
16	2	611	CHL	C1-O2A-CGA	2.15	122.96	116.73
15	A	1103	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	B	1229	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
15	1	615	CLA	C1D-ND-C4D	-2.14	104.81	106.33
15	2	605	CLA	C1D-ND-C4D	-2.14	104.81	106.33
15	B	1213	CLA	O2A-CGA-CBA	2.14	118.63	111.91
15	B	1226	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
15	3	610	CLA	C1D-ND-C4D	-2.14	104.81	106.33
15	B	1223	CLA	C3B-C4B-NB	-2.14	108.53	110.52
15	B	1205	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
15	B	1228	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	A	1115	CLA	O2A-CGA-CBA	2.14	118.62	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	2	611	CHL	CHC-C1C-NC	2.14	127.45	124.20
15	1	602	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
15	A	1101	CLA	CHA-C4D-ND	2.14	136.97	132.50
15	3	601	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
24	A	1011	CL0	O2D-CGD-O1D	-2.14	119.66	123.84
15	1	601	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
15	B	1216	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
16	4	613	CHL	CHB-C4A-NA	2.14	127.47	124.51
15	B	1227	CLA	C1D-ND-C4D	-2.14	104.82	106.33
15	B	1239	CLA	C1D-ND-C4D	-2.14	104.82	106.33
14	A	4004	BCR	C38-C26-C25	-2.14	122.13	124.53
15	F	1301	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
18	1	802	LMG	O7-C10-O9	-2.14	118.54	123.70
14	J	4003	BCR	C7-C6-C5	-2.14	116.29	121.46
15	A	1106	CLA	O2A-CGA-CBA	2.14	118.61	111.91
15	A	1136	CLA	C3B-C4B-NB	-2.14	108.53	110.52
13	3	502	XAT	C18-C5-C6	-2.13	118.69	122.26
15	A	1127	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
14	F	4002	BCR	C8-C9-C10	2.13	122.21	118.94
15	B	1225	CLA	O2A-CGA-CBA	2.13	118.60	111.91
15	A	1116	CLA	C1D-ND-C4D	-2.13	104.82	106.33
15	B	1219	CLA	O2A-CGA-CBA	2.13	118.59	111.91
15	A	1012	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
15	B	1223	CLA	O2A-CGA-CBA	2.13	118.59	111.91
15	4	601	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
15	F	1301	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
14	1	503	BCR	C38-C26-C25	-2.13	122.14	124.53
15	1	601	CLA	C1D-ND-C4D	-2.13	104.82	106.33
15	4	601	CLA	C1-O2A-CGA	2.13	122.02	116.44
15	2	606	CLA	C4B-CHC-C1C	2.13	131.38	126.34
16	2	609	CHL	CHC-C1C-NC	2.13	127.43	124.20
16	2	611	CHL	CHB-C4A-NA	2.12	127.45	124.51
15	4	602	CLA	O2A-CGA-CBA	2.12	118.57	111.91
15	A	1112	CLA	C1D-ND-C4D	-2.12	104.83	106.33
15	B	1226	CLA	C1D-ND-C4D	-2.12	104.83	106.33
14	B	4004	BCR	C36-C18-C17	-2.12	119.95	122.92
15	4	601	CLA	CHA-C1A-NA	-2.12	121.54	126.40
14	A	4004	BCR	C28-C27-C26	-2.12	110.29	114.08
15	B	1237	CLA	C1D-ND-C4D	-2.12	104.83	106.33
14	A	4006	BCR	C8-C7-C6	-2.12	121.25	127.20
15	A	1107	CLA	C1D-ND-C4D	-2.12	104.83	106.33
15	2	608	CLA	C1-O2A-CGA	2.12	122.00	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1021	CLA	C1-O2A-CGA	2.12	122.00	116.44
15	B	1212	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
15	1	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
15	3	615	CLA	C1D-ND-C4D	-2.12	104.83	106.33
15	A	1103	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
15	B	1208	CLA	C1D-ND-C4D	-2.12	104.83	106.33
14	A	4002	BCR	C35-C13-C12	2.12	121.41	118.08
15	B	1224	CLA	O2A-CGA-CBA	2.12	118.55	111.91
15	A	1135	CLA	C1D-ND-C4D	-2.12	104.83	106.33
15	A	1107	CLA	O2A-CGA-CBA	2.12	118.55	111.91
15	A	1137	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
14	J	4002	BCR	C36-C18-C17	-2.11	119.96	122.92
15	A	1109	CLA	CHA-C1A-NA	-2.11	121.56	126.40
15	A	1126	CLA	C3B-C4B-NB	-2.11	108.56	110.52
15	A	1101	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
16	2	609	CHL	CHD-C4C-C3C	2.11	127.94	124.84
12	1	501	LUT	C38-C25-C24	-2.11	119.04	123.56
14	J	4003	BCR	C37-C22-C21	-2.11	119.97	122.92
15	3	611	CLA	C3B-C4B-NB	-2.11	108.56	110.52
15	A	1108	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
15	B	1213	CLA	C4B-CHC-C1C	2.11	131.34	126.34
15	B	1234	CLA	O2A-CGA-CBA	2.11	118.53	111.91
15	B	1215	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
16	4	613	CHL	C4D-CHA-C1A	2.11	123.81	121.25
15	A	1124	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
15	B	1214	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
15	2	605	CLA	O2A-CGA-CBA	2.10	118.51	111.91
15	4	612	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
15	A	1112	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	4	615	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	3	612	CLA	C1D-ND-C4D	-2.10	104.84	106.33
15	B	1236	CLA	C1D-ND-C4D	-2.10	104.84	106.33
15	B	1214	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
15	B	1229	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
16	4	613	CHL	CHD-C4C-C3C	2.10	127.93	124.84
15	A	1124	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	1	601	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
15	B	1236	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	A	1117	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
15	B	1219	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
15	B	1220	CLA	C1D-ND-C4D	-2.10	104.85	106.33
15	1	601	CLA	CHA-C1A-NA	-2.10	121.60	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	612	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
15	2	605	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
15	A	1137	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B	1226	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
15	3	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B	1223	CLA	C1D-ND-C4D	-2.09	104.85	106.33
15	B	1022	CLA	C1-O2A-CGA	2.09	121.93	116.44
12	4	501	LUT	C7-C8-C9	-2.09	123.08	126.23
15	A	1111	CLA	C1D-ND-C4D	-2.09	104.85	106.33
15	2	601	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
16	2	613	CHL	C4A-NA-C1A	2.09	107.64	106.71
15	A	1139	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	4	612	CLA	CHA-C1A-NA	-2.09	121.62	126.40
14	J	4002	BCR	C3-C4-C5	-2.09	110.35	114.08
15	A	1102	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
15	1	608	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
15	A	1105	CLA	C1D-ND-C4D	-2.08	104.85	106.33
15	B	1238	CLA	CHA-C1A-NA	-2.08	121.62	126.40
15	2	606	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
15	B	1240	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	A	1125	CLA	O2A-CGA-CBA	2.08	118.44	111.91
15	1	606	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
15	B	1209	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	4	601	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
15	B	1216	CLA	CHA-C1A-NA	-2.08	121.63	126.40
14	F	4002	BCR	C31-C1-C6	-2.08	106.92	110.30
15	F	1302	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	A	1013	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
15	1	615	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
15	B	1214	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
14	B	4006	BCR	C19-C18-C17	2.08	122.13	118.94
15	A	1104	CLA	C1D-ND-C4D	-2.08	104.86	106.33
15	4	605	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
14	2	503	BCR	C4-C5-C6	-2.08	119.72	122.73
15	B	1202	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
15	B	1217	CLA	CHA-C1A-NA	-2.07	121.65	126.40
14	4	503	BCR	C38-C26-C25	-2.07	122.20	124.53
15	A	1105	CLA	O2A-CGA-CBA	2.07	118.42	111.91
15	A	1104	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
15	A	1134	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
15	F	1302	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
15	2	605	CLA	O2D-CGD-O1D	-2.07	119.78	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	610	CHL	C1D-CHD-C4C	-2.07	121.59	126.06
14	A	4004	BCR	C27-C26-C25	-2.07	119.72	122.73
15	A	1125	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
15	2	612	CLA	C1D-ND-C4D	-2.07	104.86	106.33
15	B	1022	CLA	O2A-CGA-CBA	2.07	118.41	111.91
15	A	1111	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
15	1	602	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	B	1022	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
15	1	604	CLA	C1-O2A-CGA	2.07	121.88	116.44
15	B	1210	CLA	C3B-C4B-NB	-2.07	108.59	110.52
13	2	502	XAT	C19-C9-C10	-2.07	120.02	122.92
15	B	1214	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	B	1209	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
15	B	1213	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
15	3	603	CLA	C1D-ND-C4D	-2.07	104.87	106.33
15	A	1106	CLA	C1D-ND-C4D	-2.07	104.87	106.33
13	4	502	XAT	C39-C29-C30	-2.07	120.03	122.92
15	J	1302	CLA	C1D-ND-C4D	-2.07	104.87	106.33
23	B	5031	GSH	O32-C3-CA3	2.07	119.92	112.74
14	3	504	BCR	C35-C13-C14	-2.07	120.03	122.92
23	4	831	GSH	O32-C3-CA3	2.06	119.91	112.74
15	A	1110	CLA	C1-O2A-CGA	2.06	121.86	116.44
15	B	1220	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	B	1220	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
15	A	1128	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
14	3	503	BCR	C34-C9-C10	-2.06	120.03	122.92
15	B	1213	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
15	1	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	2	601	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
15	2	606	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
15	1	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
24	A	1011	CL0	C4D-C3D-CAD	2.06	110.52	108.10
15	1	607	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
15	B	1023	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
15	A	1132	CLA	C1D-ND-C4D	-2.06	104.88	106.33
15	A	1108	CLA	CHA-C1A-NA	-2.05	121.69	126.40
15	A	1132	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
14	2	503	BCR	C1-C6-C7	2.05	121.59	115.78
15	B	1219	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	B	1205	CLA	O2A-CGA-CBA	2.05	118.35	111.91
16	4	610	CHL	C1-O2A-CGA	2.05	122.87	116.11
13	1	502	XAT	O4-C5-C4	-2.05	111.84	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	4	501	LUT	C18-C5-C4	2.05	118.16	114.36
15	A	1130	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
15	B	1221	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
14	J	4002	BCR	C37-C22-C21	-2.05	120.05	122.92
16	2	610	CHL	CHC-C1C-NC	2.05	127.31	124.20
15	1	605	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
15	A	1112	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
15	1	605	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
15	2	607	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
15	4	603	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	A	1123	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	3	612	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
15	B	1224	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	A	1109	CLA	O2A-CGA-CBA	2.05	118.33	111.91
15	A	1115	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
15	A	1125	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
15	B	1212	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	4	602	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
15	A	1013	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A	1129	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
15	B	1207	CLA	C3D-C4D-ND	2.04	112.55	109.46
15	A	1127	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	4	603	CLA	O2A-CGA-CBA	2.04	118.32	111.91
15	3	607	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A	1013	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
15	A	1137	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
15	A	1120	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	B	1229	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	3	603	CLA	CAC-C3C-C2C	-2.04	124.04	127.53
15	B	1229	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
15	2	605	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
15	1	604	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
15	A	1129	CLA	C1D-ND-C4D	-2.04	104.89	106.33
14	B	4003	BCR	C37-C22-C21	-2.04	120.07	122.92
15	B	1234	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	B	1021	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
15	B	1225	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	1	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
15	4	612	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
16	1	609	CHL	CHD-C4C-C3C	2.04	127.83	124.84
15	B	1234	CLA	C1-O2A-CGA	2.03	121.78	116.44
14	3	504	BCR	C34-C9-C10	-2.03	120.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	4002	BCR	C33-C5-C6	-2.03	122.25	124.53
15	4	606	CLA	CHA-C1A-NA	-2.03	121.74	126.40
16	2	609	CHL	C1-O2A-CGA	2.03	121.78	116.44
15	A	1108	CLA	C1D-ND-C4D	-2.03	104.89	106.33
15	A	1119	CLA	CHA-C1A-NA	-2.03	121.75	126.40
14	2	503	BCR	C23-C24-C25	-2.03	121.50	127.20
15	A	1111	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
15	A	1122	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
15	B	1021	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	A	1139	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
12	3	501	LUT	C40-C33-C34	-2.03	120.08	122.92
15	2	607	CLA	C1D-ND-C4D	-2.03	104.89	106.33
15	3	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40
15	2	602	CLA	CHA-C1A-NA	-2.03	121.76	126.40
15	3	615	CLA	CHA-C1A-NA	-2.02	121.76	126.40
15	A	1104	CLA	C1-O2A-CGA	2.02	121.75	116.44
15	B	1222	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
15	B	1231	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
15	B	1237	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
14	B	4002	BCR	C35-C13-C14	-2.02	120.09	122.92
15	A	1127	CLA	C1-O2A-CGA	2.02	121.75	116.44
15	4	604	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	4	602	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	B	1224	CLA	C1D-ND-C4D	-2.02	104.90	106.33
15	B	1225	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
15	4	615	CLA	O2A-CGA-CBA	2.02	118.24	111.91
15	B	1235	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
15	B	1235	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
15	A	1113	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	A	1141	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
15	A	1129	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	1	601	CLA	O2A-CGA-CBA	2.02	118.23	111.91
15	A	1102	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
15	B	1232	CLA	O2A-CGA-CBA	2.02	118.23	111.91
16	1	610	CHL	C4A-NA-C1A	2.02	107.61	106.71
15	B	1208	CLA	CHA-C1A-NA	-2.01	121.78	126.40
12	1	501	LUT	C19-C9-C8	2.01	121.25	118.08
15	A	1128	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
15	B	1208	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
15	B	1221	CLA	CHA-C1A-NA	-2.01	121.78	126.40
15	2	608	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
15	4	609	CLA	O2A-CGA-CBA	2.01	118.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	2	502	XAT	C18-C5-C6	-2.01	118.89	122.26
15	A	1134	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
15	B	1218	CLA	CHA-C1A-NA	-2.01	121.80	126.40
12	4	501	LUT	C19-C9-C8	2.01	121.24	118.08
15	B	1206	CLA	C1D-ND-C4D	-2.01	104.91	106.33
16	2	613	CHL	CHB-C4A-NA	2.01	127.29	124.51
15	B	1206	CLA	CHA-C1A-NA	-2.01	121.80	126.40
15	A	1111	CLA	CMC-C2C-C1C	2.01	128.09	125.04
16	2	613	CHL	CHC-C1C-NC	2.01	127.25	124.20
16	2	611	CHL	CHD-C4C-C3C	2.01	127.79	124.84
15	4	612	CLA	C1D-ND-C4D	-2.01	104.91	106.33
15	B	1217	CLA	C1D-ND-C4D	-2.01	104.91	106.33
15	A	1120	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
15	B	1231	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
15	B	1207	CLA	CHC-C4B-NB	-2.00	122.24	124.27
15	1	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
15	1	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	4	607	CLA	C3B-C2B-C1B	-2.00	104.74	107.16
15	4	606	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
15	B	1227	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
14	A	4005	BCR	C37-C22-C21	-2.00	120.12	122.92
15	A	1138	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
17	1	801	LHG	O7-C7-O9	-2.00	118.87	123.70

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	2	502	XAT	C26
13	3	502	XAT	C6
13	4	502	XAT	C6
15	1	612	CLA	C13
16	1	609	CHL	C3A
16	2	610	CHL	C3A
16	2	611	CHL	C3A
16	4	610	CHL	C3A
16	4	613	CHL	C3A

All (1915) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C13-C14-C15-C35
12	1	501	LUT	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
12	2	501	LUT	C7-C8-C9-C19
12	2	501	LUT	C21-C26-C27-C28
12	3	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C1-C6-C7-C8
12	4	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C27-C28-C29-C39
13	1	502	XAT	C30-C31-C32-C33
13	2	502	XAT	O24-C26-C27-C28
13	3	502	XAT	C14-C15-C35-C34
13	3	502	XAT	C26-C27-C28-C29
13	3	502	XAT	C27-C28-C29-C30
13	3	502	XAT	C27-C28-C29-C39
13	3	502	XAT	C30-C31-C32-C33
13	3	502	XAT	C32-C33-C34-C35
13	3	502	XAT	C40-C33-C34-C35
13	4	502	XAT	C27-C28-C29-C39
14	1	503	BCR	C10-C11-C12-C13
14	1	503	BCR	C17-C18-C19-C20
14	1	503	BCR	C36-C18-C19-C20
14	1	503	BCR	C23-C24-C25-C26
14	1	505	BCR	C5-C6-C7-C8
14	1	505	BCR	C11-C10-C9-C8
14	1	505	BCR	C11-C10-C9-C34
14	1	505	BCR	C13-C14-C15-C16
14	1	505	BCR	C19-C20-C21-C22
14	1	505	BCR	C23-C24-C25-C26
14	2	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C5-C6-C7-C8
14	2	503	BCR	C7-C8-C9-C34
14	2	503	BCR	C11-C10-C9-C8
14	2	503	BCR	C11-C10-C9-C34
14	2	503	BCR	C9-C10-C11-C12
14	2	503	BCR	C10-C11-C12-C13
14	2	503	BCR	C37-C22-C23-C24
14	2	503	BCR	C23-C24-C25-C26
14	2	503	BCR	C23-C24-C25-C30
14	3	503	BCR	C5-C6-C7-C8
14	3	503	BCR	C11-C10-C9-C8
14	3	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C10-C11-C12-C13
14	3	503	BCR	C17-C18-C19-C20
14	3	503	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
14	3	503	BCR	C21-C22-C23-C24
14	3	503	BCR	C37-C22-C23-C24
14	3	504	BCR	C5-C6-C7-C8
14	3	504	BCR	C11-C10-C9-C8
14	3	504	BCR	C11-C10-C9-C34
14	3	504	BCR	C10-C11-C12-C13
14	3	504	BCR	C11-C12-C13-C35
14	4	503	BCR	C1-C6-C7-C8
14	4	503	BCR	C5-C6-C7-C8
14	4	503	BCR	C11-C10-C9-C8
14	4	503	BCR	C11-C10-C9-C34
14	4	503	BCR	C10-C11-C12-C13
14	4	503	BCR	C36-C18-C19-C20
14	4	503	BCR	C21-C22-C23-C24
14	4	503	BCR	C37-C22-C23-C24
14	4	505	BCR	C1-C6-C7-C8
14	4	505	BCR	C5-C6-C7-C8
14	4	505	BCR	C11-C10-C9-C8
14	4	505	BCR	C11-C10-C9-C34
14	4	505	BCR	C11-C12-C13-C35
14	A	4002	BCR	C1-C6-C7-C8
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	C11-C12-C13-C14
14	A	4002	BCR	C11-C12-C13-C35
14	A	4002	BCR	C17-C18-C19-C20
14	A	4002	BCR	C36-C18-C19-C20
14	A	4003	BCR	C19-C20-C21-C22
14	A	4003	BCR	C21-C22-C23-C24
14	A	4003	BCR	C37-C22-C23-C24
14	A	4003	BCR	C23-C24-C25-C26
14	A	4004	BCR	C23-C24-C25-C26
14	A	4004	BCR	C23-C24-C25-C30
14	A	4005	BCR	C7-C8-C9-C10
14	A	4006	BCR	C7-C8-C9-C10
14	A	4006	BCR	C7-C8-C9-C34
14	A	4006	BCR	C11-C12-C13-C35
14	A	4006	BCR	C21-C22-C23-C24
14	A	4006	BCR	C37-C22-C23-C24
14	A	4007	BCR	C5-C6-C7-C8
14	A	4007	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	A	4007	BCR	C11-C10-C9-C34
14	A	4007	BCR	C23-C24-C25-C30
14	B	4001	BCR	C1-C6-C7-C8
14	B	4001	BCR	C5-C6-C7-C8
14	B	4001	BCR	C11-C10-C9-C8
14	B	4001	BCR	C11-C10-C9-C34
14	B	4001	BCR	C10-C11-C12-C13
14	B	4002	BCR	C1-C6-C7-C8
14	B	4002	BCR	C5-C6-C7-C8
14	B	4002	BCR	C11-C10-C9-C8
14	B	4002	BCR	C11-C10-C9-C34
14	B	4002	BCR	C10-C11-C12-C13
14	B	4002	BCR	C11-C12-C13-C35
14	B	4002	BCR	C17-C18-C19-C20
14	B	4002	BCR	C36-C18-C19-C20
14	B	4002	BCR	C21-C22-C23-C24
14	B	4002	BCR	C37-C22-C23-C24
14	B	4003	BCR	C11-C10-C9-C8
14	B	4003	BCR	C11-C10-C9-C34
14	B	4003	BCR	C23-C24-C25-C26
14	B	4003	BCR	C23-C24-C25-C30
14	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C11-C10-C9-C34
14	B	4004	BCR	C10-C11-C12-C13
14	B	4004	BCR	C23-C24-C25-C30
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C7-C8-C9-C10
14	B	4005	BCR	C7-C8-C9-C34
14	B	4005	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C34
14	B	4005	BCR	C10-C11-C12-C13
14	B	4005	BCR	C36-C18-C19-C20
14	B	4006	BCR	C7-C8-C9-C10
14	B	4006	BCR	C7-C8-C9-C34
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C10-C11-C12-C13
14	B	4006	BCR	C17-C18-C19-C20
14	B	4006	BCR	C36-C18-C19-C20
14	F	4002	BCR	C11-C10-C9-C8
14	F	4002	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
14	F	4002	BCR	C10-C11-C12-C13
14	F	4002	BCR	C21-C22-C23-C24
14	F	4002	BCR	C37-C22-C23-C24
14	J	4001	BCR	C5-C6-C7-C8
14	J	4001	BCR	C17-C18-C19-C20
14	J	4001	BCR	C36-C18-C19-C20
14	J	4001	BCR	C23-C24-C25-C26
14	J	4001	BCR	C23-C24-C25-C30
14	J	4002	BCR	C1-C6-C7-C8
14	J	4002	BCR	C5-C6-C7-C8
14	J	4002	BCR	C7-C8-C9-C10
14	J	4002	BCR	C7-C8-C9-C34
14	J	4002	BCR	C11-C10-C9-C8
14	J	4002	BCR	C11-C10-C9-C34
14	J	4002	BCR	C10-C11-C12-C13
14	J	4002	BCR	C17-C18-C19-C20
14	J	4002	BCR	C36-C18-C19-C20
14	J	4002	BCR	C19-C20-C21-C22
14	J	4002	BCR	C37-C22-C23-C24
14	J	4002	BCR	C23-C24-C25-C26
14	J	4002	BCR	C23-C24-C25-C30
14	J	4003	BCR	C5-C6-C7-C8
14	J	4003	BCR	C11-C10-C9-C8
14	J	4003	BCR	C11-C10-C9-C34
14	J	4003	BCR	C11-C12-C13-C14
14	J	4003	BCR	C11-C12-C13-C35
14	J	4003	BCR	C19-C20-C21-C22
14	J	4003	BCR	C23-C24-C25-C26
15	1	601	CLA	C3A-C2A-CAA-CBA
15	1	601	CLA	CHA-CBD-CGD-O1D
15	1	601	CLA	CHA-CBD-CGD-O2D
15	1	601	CLA	CBD-CGD-O2D-CED
15	1	602	CLA	CBD-CGD-O2D-CED
15	1	603	CLA	C1A-C2A-CAA-CBA
15	1	603	CLA	CHA-CBD-CGD-O1D
15	1	603	CLA	CHA-CBD-CGD-O2D
15	1	604	CLA	CAD-CBD-CGD-O1D
15	1	605	CLA	CBA-CGA-O2A-C1
15	1	608	CLA	C1A-C2A-CAA-CBA
15	1	608	CLA	C3A-C2A-CAA-CBA
15	1	612	CLA	C3A-C2A-CAA-CBA
15	1	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	1	613	CLA	C3A-C2A-CAA-CBA
15	1	613	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	C3A-C2A-CAA-CBA
15	1	615	CLA	CHA-CBD-CGD-O1D
15	1	615	CLA	CHA-CBD-CGD-O2D
15	2	601	CLA	CHA-CBD-CGD-O1D
15	2	601	CLA	CHA-CBD-CGD-O2D
15	2	601	CLA	CAD-CBD-CGD-O1D
15	2	601	CLA	CBD-CGD-O2D-CED
15	2	602	CLA	CBD-CGD-O2D-CED
15	2	603	CLA	CHA-CBD-CGD-O1D
15	2	603	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	C2-C1-O2A-CGA
15	2	604	CLA	CBD-CGD-O2D-CED
15	2	605	CLA	C1A-C2A-CAA-CBA
15	2	605	CLA	C3A-C2A-CAA-CBA
15	2	606	CLA	C3A-C2A-CAA-CBA
15	2	606	CLA	C2A-CAA-CBA-CGA
15	2	606	CLA	CBD-CGD-O2D-CED
15	2	607	CLA	C1A-C2A-CAA-CBA
15	2	607	CLA	C3A-C2A-CAA-CBA
15	2	607	CLA	CHA-CBD-CGD-O1D
15	2	607	CLA	CHA-CBD-CGD-O2D
15	2	607	CLA	CBD-CGD-O2D-CED
15	2	608	CLA	CBA-CGA-O2A-C1
15	2	608	CLA	O1A-CGA-O2A-C1
15	2	608	CLA	CHA-CBD-CGD-O1D
15	2	608	CLA	CHA-CBD-CGD-O2D
15	2	612	CLA	C1A-C2A-CAA-CBA
15	2	612	CLA	C3A-C2A-CAA-CBA
15	2	612	CLA	CBD-CGD-O2D-CED
15	3	601	CLA	C1A-C2A-CAA-CBA
15	3	603	CLA	C2C-C3C-CAC-CBC
15	3	603	CLA	C4C-C3C-CAC-CBC
15	3	603	CLA	CHA-CBD-CGD-O1D
15	3	603	CLA	CHA-CBD-CGD-O2D
15	3	606	CLA	CHA-CBD-CGD-O1D
15	3	606	CLA	CHA-CBD-CGD-O2D
15	3	607	CLA	C1A-C2A-CAA-CBA
15	3	607	CLA	C3A-C2A-CAA-CBA
15	3	610	CLA	C3A-C2A-CAA-CBA
15	3	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	3	611	CLA	CHA-CBD-CGD-O1D
15	3	611	CLA	CHA-CBD-CGD-O2D
15	3	612	CLA	CHA-CBD-CGD-O1D
15	3	612	CLA	CHA-CBD-CGD-O2D
15	3	613	CLA	C1A-C2A-CAA-CBA
15	3	613	CLA	C3A-C2A-CAA-CBA
15	3	613	CLA	CBA-CGA-O2A-C1
15	3	613	CLA	CHA-CBD-CGD-O1D
15	3	613	CLA	CBD-CGD-O2D-CED
15	3	615	CLA	CBA-CGA-O2A-C1
15	3	615	CLA	CBD-CGD-O2D-CED
15	4	602	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	C1A-C2A-CAA-CBA
15	4	604	CLA	C3A-C2A-CAA-CBA
15	4	604	CLA	C2-C1-O2A-CGA
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D
15	4	604	CLA	CAD-CBD-CGD-O1D
15	4	605	CLA	C1A-C2A-CAA-CBA
15	4	605	CLA	C2-C1-O2A-CGA
15	4	606	CLA	CHA-CBD-CGD-O1D
15	4	606	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O1D
15	4	607	CLA	C1A-C2A-CAA-CBA
15	4	607	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	CHA-CBD-CGD-O1D
15	4	608	CLA	CHA-CBD-CGD-O2D
15	4	615	CLA	C1A-C2A-CAA-CBA
15	4	615	CLA	C3A-C2A-CAA-CBA
15	4	615	CLA	CBD-CGD-O2D-CED
15	A	1012	CLA	CBD-CGD-O2D-CED
15	A	1013	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	A	1101	CLA	CHA-CBD-CGD-O1D
15	A	1101	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1102	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	CBD-CGD-O2D-CED
15	A	1103	CLA	C2-C1-O2A-CGA
15	A	1103	CLA	CHA-CBD-CGD-O1D
15	A	1103	CLA	CHA-CBD-CGD-O2D
15	A	1103	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	A	1103	CLA	CBD-CGD-O2D-CED
15	A	1104	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	CHA-CBD-CGD-O1D
15	A	1104	CLA	CHA-CBD-CGD-O2D
15	A	1105	CLA	C1A-C2A-CAA-CBA
15	A	1105	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1108	CLA	C1A-C2A-CAA-CBA
15	A	1108	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	C1A-C2A-CAA-CBA
15	A	1109	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C1A-C2A-CAA-CBA
15	A	1110	CLA	CBD-CGD-O2D-CED
15	A	1111	CLA	C1A-C2A-CAA-CBA
15	A	1111	CLA	C3A-C2A-CAA-CBA
15	A	1111	CLA	CHA-CBD-CGD-O1D
15	A	1111	CLA	CHA-CBD-CGD-O2D
15	A	1113	CLA	C1A-C2A-CAA-CBA
15	A	1114	CLA	CBA-CGA-O2A-C1
15	A	1114	CLA	CHA-CBD-CGD-O2D
15	A	1115	CLA	C3A-C2A-CAA-CBA
15	A	1115	CLA	CHA-CBD-CGD-O1D
15	A	1115	CLA	CHA-CBD-CGD-O2D
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1116	CLA	C2A-CAA-CBA-CGA
15	A	1116	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	CHA-CBD-CGD-O1D
15	A	1118	CLA	CHA-CBD-CGD-O2D
15	A	1118	CLA	CAD-CBD-CGD-O1D
15	A	1118	CLA	CAD-CBD-CGD-O2D
15	A	1119	CLA	CHA-CBD-CGD-O1D
15	A	1119	CLA	CHA-CBD-CGD-O2D
15	A	1120	CLA	CBD-CGD-O2D-CED
15	A	1122	CLA	C1A-C2A-CAA-CBA
15	A	1122	CLA	C3A-C2A-CAA-CBA
15	A	1122	CLA	CBD-CGD-O2D-CED
15	A	1123	CLA	C1A-C2A-CAA-CBA
15	A	1123	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	A	1124	CLA	C1A-C2A-CAA-CBA
15	A	1124	CLA	CBA-CGA-O2A-C1
15	A	1124	CLA	O1A-CGA-O2A-C1
15	A	1124	CLA	CHA-CBD-CGD-O1D
15	A	1124	CLA	CHA-CBD-CGD-O2D
15	A	1125	CLA	C1A-C2A-CAA-CBA
15	A	1125	CLA	CHA-CBD-CGD-O1D
15	A	1125	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	C2-C1-O2A-CGA
15	A	1127	CLA	C1A-C2A-CAA-CBA
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	C1A-C2A-CAA-CBA
15	A	1129	CLA	C3A-C2A-CAA-CBA
15	A	1130	CLA	CHA-CBD-CGD-O1D
15	A	1130	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	C1A-C2A-CAA-CBA
15	A	1131	CLA	C3A-C2A-CAA-CBA
15	A	1131	CLA	C2-C1-O2A-CGA
15	A	1134	CLA	C1A-C2A-CAA-CBA
15	A	1135	CLA	CBD-CGD-O2D-CED
15	A	1137	CLA	C1A-C2A-CAA-CBA
15	A	1137	CLA	C3A-C2A-CAA-CBA
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D
15	A	1138	CLA	C1A-C2A-CAA-CBA
15	A	1138	CLA	C3A-C2A-CAA-CBA
15	A	1139	CLA	C2-C3-C5-C6
15	A	1139	CLA	C4-C3-C5-C6
15	A	1140	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	C2-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	A	1141	CLA	C1A-C2A-CAA-CBA
15	A	1141	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	CHA-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O2D
15	B	1023	CLA	C2-C1-O2A-CGA
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	B	1204	CLA	C2-C1-O2A-CGA
15	B	1204	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1205	CLA	C1A-C2A-CAA-CBA
15	B	1205	CLA	C3A-C2A-CAA-CBA
15	B	1205	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CHA-CBD-CGD-O1D
15	B	1209	CLA	CHA-CBD-CGD-O2D
15	B	1210	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	C1A-C2A-CAA-CBA
15	B	1211	CLA	C3A-C2A-CAA-CBA
15	B	1211	CLA	CBD-CGD-O2D-CED
15	B	1212	CLA	C1A-C2A-CAA-CBA
15	B	1212	CLA	CBD-CGD-O2D-CED
15	B	1213	CLA	CBD-CGD-O2D-CED
15	B	1214	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	CBD-CGD-O2D-CED
15	B	1215	CLA	C1A-C2A-CAA-CBA
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1215	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	C3A-C2A-CAA-CBA
15	B	1217	CLA	CAD-CBD-CGD-O1D
15	B	1217	CLA	CAD-CBD-CGD-O2D
15	B	1218	CLA	C1A-C2A-CAA-CBA
15	B	1218	CLA	CHA-CBD-CGD-O1D
15	B	1218	CLA	CHA-CBD-CGD-O2D
15	B	1218	CLA	CBD-CGD-O2D-CED
15	B	1220	CLA	C1A-C2A-CAA-CBA
15	B	1220	CLA	C3A-C2A-CAA-CBA
15	B	1220	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	C3A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1225	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	C1A-C2A-CAA-CBA
15	B	1226	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	CHA-CBD-CGD-O1D
15	B	1226	CLA	CHA-CBD-CGD-O2D
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	CHA-CBD-CGD-O1D
15	B	1229	CLA	CHA-CBD-CGD-O2D
15	B	1229	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	B	1230	CLA	C2-C1-O2A-CGA
15	B	1230	CLA	CBD-CGD-O2D-CED
15	B	1231	CLA	CHA-CBD-CGD-O1D
15	B	1231	CLA	CBD-CGD-O2D-CED
15	B	1235	CLA	CHA-CBD-CGD-O1D
15	B	1235	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C2-C1-O2A-CGA
15	B	1239	CLA	CBD-CGD-O2D-CED
15	B	1240	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	C3A-C2A-CAA-CBA
15	F	1301	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	C2-C1-O2A-CGA
15	F	1302	CLA	CHA-CBD-CGD-O1D
15	F	1302	CLA	CHA-CBD-CGD-O2D
15	J	1302	CLA	C3A-C2A-CAA-CBA
15	J	1302	CLA	CHA-CBD-CGD-O1D
15	J	1302	CLA	CHA-CBD-CGD-O2D
16	1	609	CHL	C1A-C2A-CAA-CBA
16	1	610	CHL	C1A-C2A-CAA-CBA
16	1	610	CHL	C3A-C2A-CAA-CBA
16	4	610	CHL	CHA-CBD-CGD-O1D
16	4	610	CHL	CHA-CBD-CGD-O2D
16	4	610	CHL	CAD-CBD-CGD-O1D
16	4	611	CHL	CHA-CBD-CGD-O1D
16	4	611	CHL	CHA-CBD-CGD-O2D
16	4	613	CHL	CHA-CBD-CGD-O1D
16	4	613	CHL	CHA-CBD-CGD-O2D
16	4	613	CHL	CAD-CBD-CGD-O1D
17	1	801	LHG	O2-C2-C3-O3
17	1	801	LHG	C3-O3-P-O5
17	1	801	LHG	C3-O3-P-O6
17	1	801	LHG	C8-C7-O7-C5
17	2	801	LHG	C4-O6-P-O5
17	2	801	LHG	C8-C7-O7-C5
17	A	5001	LHG	O1-C1-C2-C3
17	A	5001	LHG	C1-C2-C3-O3
17	A	5001	LHG	C4-O6-P-O5
17	A	5001	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	O7-C5-C6-O8
17	A	5002	LHG	O1-C1-C2-C3
17	A	5002	LHG	C1-C2-C3-O3
17	A	5002	LHG	O2-C2-C3-O3
17	A	5002	LHG	C8-C7-O7-C5
17	B	5001	LHG	O1-C1-C2-C3
17	B	5001	LHG	C1-C2-C3-O3
17	B	5001	LHG	C3-O3-P-O4
17	B	5001	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O6
17	B	5001	LHG	O6-C4-C5-O7
17	B	5001	LHG	C8-C7-O7-C5
18	1	803	LMG	C2-C1-O1-C7
18	1	803	LMG	O6-C1-O1-C7
18	2	802	LMG	C2-C1-O1-C7
18	2	802	LMG	O6-C1-O1-C7
18	2	802	LMG	C11-C10-O7-C8
18	2	803	LMG	C2-C1-O1-C7
18	2	803	LMG	O6-C1-O1-C7
19	1	811	SQD	O5-C5-C6-S
21	2	811	DGD	O6D-C1D-O3G-C3G
21	4	811	DGD	C2A-C1A-O1G-C1G
21	4	811	DGD	O1A-C1A-O1G-C1G
21	4	811	DGD	C2E-C1E-O5D-C6D
21	4	811	DGD	O6E-C1E-O5D-C6D
21	B	5002	DGD	C2B-C1B-O2G-C2G
21	B	5002	DGD	O2G-C2G-C3G-O3G
21	J	5001	DGD	C2D-C1D-O3G-C3G
21	J	5001	DGD	O6D-C1D-O3G-C3G
23	4	831	GSH	C1-CA1-CB1-CG1
23	B	5031	GSH	O11-C1-CA1-N1
23	B	5031	GSH	N1-CA1-CB1-CG1
23	B	5031	GSH	CA1-CB1-CG1-CD1
23	B	5031	GSH	N2-CA2-CB2-SG2
23	B	5031	GSH	C2-CA2-CB2-SG2
24	A	1011	CL0	C1A-C2A-CAA-CBA
24	A	1011	CL0	CBD-CGD-O2D-CED
16	3	604	CHL	C2C-C3C-CAC-CBC
18	1	803	LMG	C11-C10-O7-C8
15	1	601	CLA	O1D-CGD-O2D-CED
15	1	612	CLA	O1D-CGD-O2D-CED
15	2	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	4	603	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	O1D-CGD-O2D-CED
15	4	615	CLA	O1D-CGD-O2D-CED
15	A	1139	CLA	O1D-CGD-O2D-CED
15	B	1021	CLA	O1D-CGD-O2D-CED
15	B	1218	CLA	O1D-CGD-O2D-CED
17	2	801	LHG	O9-C7-O7-C5
17	B	5001	LHG	O9-C7-O7-C5
18	1	803	LMG	O9-C10-O7-C8
15	1	607	CLA	O1D-CGD-O2D-CED
15	2	601	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	O1D-CGD-O2D-CED
15	B	1202	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED
15	B	1240	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	1	603	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CBD-CGD-O2D-CED
15	1	605	CLA	CBD-CGD-O2D-CED
15	1	606	CLA	CBD-CGD-O2D-CED
15	1	607	CLA	CBD-CGD-O2D-CED
15	1	608	CLA	CBD-CGD-O2D-CED
15	1	611	CLA	CBD-CGD-O2D-CED
15	1	612	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	CBD-CGD-O2D-CED
15	2	605	CLA	CBD-CGD-O2D-CED
15	2	608	CLA	CBD-CGD-O2D-CED
15	2	615	CLA	CBD-CGD-O2D-CED
15	3	605	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	CBD-CGD-O2D-CED
15	3	608	CLA	CBD-CGD-O2D-CED
15	3	610	CLA	CBD-CGD-O2D-CED
15	3	611	CLA	CBD-CGD-O2D-CED
15	3	612	CLA	CBD-CGD-O2D-CED
15	4	603	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	CBD-CGD-O2D-CED
15	4	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	4	606	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	CBD-CGD-O2D-CED
15	4	612	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	A	1104	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
15	A	1106	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	CBD-CGD-O2D-CED
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1113	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	A	1118	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1123	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	CBD-CGD-O2D-CED
15	A	1136	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1139	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	CBD-CGD-O2D-CED
15	B	1022	CLA	CBD-CGD-O2D-CED
15	B	1201	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	CBD-CGD-O2D-CED
15	B	1203	CLA	CBD-CGD-O2D-CED
15	B	1206	CLA	CBD-CGD-O2D-CED
15	B	1208	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	CBD-CGD-O2D-CED
15	B	1219	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1221	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1223	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	B	1234	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	CBD-CGD-O2D-CED
15	1	605	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	O1A-CGA-O2A-C1
15	A	1133	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	B	1218	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	F	1302	CLA	O1A-CGA-O2A-C1
15	1	608	CLA	O1A-CGA-O2A-C1
15	4	608	CLA	O1A-CGA-O2A-C1
16	3	604	CHL	C4C-C3C-CAC-CBC
15	1	603	CLA	O1D-CGD-O2D-CED
15	1	611	CLA	O1D-CGD-O2D-CED
15	3	607	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	O1D-CGD-O2D-CED
15	3	610	CLA	O1D-CGD-O2D-CED
15	3	611	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	A	1116	CLA	O1D-CGD-O2D-CED
15	A	1117	CLA	O1D-CGD-O2D-CED
15	A	1118	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	O1D-CGD-O2D-CED
15	A	1124	CLA	O1D-CGD-O2D-CED
15	A	1129	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	O1D-CGD-O2D-CED
15	A	1131	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	O1D-CGD-O2D-CED
15	A	1141	CLA	O1D-CGD-O2D-CED
15	B	1022	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1208	CLA	O1D-CGD-O2D-CED
15	B	1217	CLA	O1D-CGD-O2D-CED
15	B	1225	CLA	O1D-CGD-O2D-CED
15	B	1230	CLA	O1D-CGD-O2D-CED
15	B	1232	CLA	O1D-CGD-O2D-CED
15	B	1234	CLA	O1D-CGD-O2D-CED
24	A	1011	CL0	O1D-CGD-O2D-CED
15	1	608	CLA	CBA-CGA-O2A-C1
15	4	608	CLA	CBA-CGA-O2A-C1
15	B	1209	CLA	CBA-CGA-O2A-C1
15	1	602	CLA	O1D-CGD-O2D-CED
15	2	602	CLA	O1D-CGD-O2D-CED
15	2	603	CLA	O1D-CGD-O2D-CED
15	2	606	CLA	O1D-CGD-O2D-CED
15	2	612	CLA	O1D-CGD-O2D-CED
15	2	615	CLA	O1D-CGD-O2D-CED
15	3	613	CLA	O1D-CGD-O2D-CED
15	3	615	CLA	O1D-CGD-O2D-CED
15	4	602	CLA	O1D-CGD-O2D-CED
15	4	607	CLA	O1D-CGD-O2D-CED
15	4	608	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	O1D-CGD-O2D-CED
15	A	1109	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1127	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	O1D-CGD-O2D-CED
15	B	1201	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	B	1210	CLA	O1D-CGD-O2D-CED
15	B	1211	CLA	O1D-CGD-O2D-CED
15	B	1213	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	B	1220	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	B	1229	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1231	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	B	1238	CLA	O1D-CGD-O2D-CED
15	B	1239	CLA	O1D-CGD-O2D-CED
15	F	1302	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	CBA-CGA-O2A-C1
15	A	1116	CLA	CBA-CGA-O2A-C1
15	A	1133	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	F	1302	CLA	CBA-CGA-O2A-C1
24	A	1011	CL0	CBA-CGA-O2A-C1
15	4	609	CLA	CBD-CGD-O2D-CED
15	B	1235	CLA	CBD-CGD-O2D-CED
15	1	606	CLA	C2C-C3C-CAC-CBC
15	1	615	CLA	O1A-CGA-O2A-C1
15	A	1117	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	O1A-CGA-O2A-C1
15	A	1127	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
15	A	1140	CLA	O1A-CGA-O2A-C1
15	A	1141	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	O1A-CGA-O2A-C1
15	B	1206	CLA	O1A-CGA-O2A-C1
18	2	802	LMG	O10-C28-O8-C9
24	A	1011	CL0	O1A-CGA-O2A-C1
15	A	1114	CLA	O1A-CGA-O2A-C1
15	2	607	CLA	O1D-CGD-O2D-CED
15	A	1120	CLA	O1D-CGD-O2D-CED
15	A	1122	CLA	O1D-CGD-O2D-CED
15	B	1204	CLA	O1D-CGD-O2D-CED
15	B	1236	CLA	O1D-CGD-O2D-CED
15	1	611	CLA	C4C-C3C-CAC-CBC
15	1	613	CLA	O1D-CGD-O2D-CED
15	2	604	CLA	O1D-CGD-O2D-CED
15	A	1108	CLA	O1D-CGD-O2D-CED
15	A	1136	CLA	O1D-CGD-O2D-CED
15	B	1212	CLA	O1D-CGD-O2D-CED
15	B	1215	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	O1D-CGD-O2D-CED
15	3	601	CLA	CBD-CGD-O2D-CED
15	2	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	4	604	CLA	O1D-CGD-O2D-CED
15	4	612	CLA	O1D-CGD-O2D-CED
15	A	1102	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	O1D-CGD-O2D-CED
17	1	801	LHG	O9-C7-O7-C5
17	A	5002	LHG	O9-C7-O7-C5
18	2	802	LMG	O9-C10-O7-C8
21	B	5002	DGD	O1B-C1B-O2G-C2G
15	B	1217	CLA	CBA-CGA-O2A-C1
15	1	611	CLA	C2C-C3C-CAC-CBC
15	A	1108	CLA	O1A-CGA-O2A-C1
15	B	1209	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	O1A-CGA-O2A-C1
15	4	615	CLA	C3-C5-C6-C7
15	A	1013	CLA	C3-C5-C6-C7
15	A	1106	CLA	C3-C5-C6-C7
15	A	1130	CLA	C3-C5-C6-C7
15	B	1220	CLA	C3-C5-C6-C7
15	B	1229	CLA	C3-C5-C6-C7
25	A	2001	PQN	C13-C15-C16-C17
25	B	2002	PQN	C13-C15-C16-C17
15	1	615	CLA	CBA-CGA-O2A-C1
15	A	1120	CLA	CBA-CGA-O2A-C1
15	A	1126	CLA	CBA-CGA-O2A-C1
15	A	1127	CLA	CBA-CGA-O2A-C1
15	A	1141	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	CBA-CGA-O2A-C1
15	B	1218	CLA	CBA-CGA-O2A-C1
15	B	1219	CLA	CBA-CGA-O2A-C1
15	B	1226	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	C29-C28-O8-C9
19	1	811	SQD	O10-C23-O48-C46
15	A	1128	CLA	O1D-CGD-O2D-CED
15	B	1222	CLA	O1D-CGD-O2D-CED
15	B	1223	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	C2-C1-O2A-CGA
15	4	612	CLA	O1A-CGA-O2A-C1
15	B	1201	CLA	O1A-CGA-O2A-C1
15	3	615	CLA	O1A-CGA-O2A-C1
15	1	606	CLA	C4C-C3C-CAC-CBC
15	A	1108	CLA	CBA-CGA-O2A-C1
15	3	605	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	A	1013	CLA	C4-C3-C5-C6
15	2	608	CLA	C2A-CAA-CBA-CGA
15	3	606	CLA	C2A-CAA-CBA-CGA
15	4	607	CLA	C2A-CAA-CBA-CGA
15	4	612	CLA	C2A-CAA-CBA-CGA
15	B	1201	CLA	C2A-CAA-CBA-CGA
15	B	1213	CLA	C2A-CAA-CBA-CGA
16	2	610	CHL	C2A-CAA-CBA-CGA
16	2	613	CHL	C2A-CAA-CBA-CGA
15	3	612	CLA	O1D-CGD-O2D-CED
15	A	1115	CLA	O1D-CGD-O2D-CED
15	B	1221	CLA	O1D-CGD-O2D-CED
15	2	604	CLA	CBA-CGA-O2A-C1
15	3	601	CLA	CBA-CGA-O2A-C1
15	4	601	CLA	CBA-CGA-O2A-C1
15	4	604	CLA	CBA-CGA-O2A-C1
15	4	606	CLA	CBA-CGA-O2A-C1
15	A	1117	CLA	CBA-CGA-O2A-C1
15	A	1118	CLA	CBA-CGA-O2A-C1
15	A	1130	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
15	A	1140	CLA	CBA-CGA-O2A-C1
15	B	1204	CLA	CBA-CGA-O2A-C1
15	B	1206	CLA	CBA-CGA-O2A-C1
15	B	1211	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	B	1232	CLA	CBA-CGA-O2A-C1
21	B	5002	DGD	C2A-C1A-O1G-C1G
19	1	811	SQD	C24-C23-O48-C46
15	1	604	CLA	O1D-CGD-O2D-CED
15	1	608	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	O1D-CGD-O2D-CED
15	4	601	CLA	CBD-CGD-O2D-CED
24	A	1011	CL0	C2C-C3C-CAC-CBC
15	1	606	CLA	O1D-CGD-O2D-CED
15	1	615	CLA	O1D-CGD-O2D-CED
15	3	605	CLA	O1D-CGD-O2D-CED
15	A	1101	CLA	O1D-CGD-O2D-CED
15	A	1104	CLA	O1D-CGD-O2D-CED
15	A	1106	CLA	O1D-CGD-O2D-CED
15	B	1226	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	3	601	CLA	O1A-CGA-O2A-C1
15	3	612	CLA	O1A-CGA-O2A-C1
15	4	601	CLA	O1A-CGA-O2A-C1
15	A	1120	CLA	O1A-CGA-O2A-C1
15	B	1204	CLA	O1A-CGA-O2A-C1
15	B	1208	CLA	O1A-CGA-O2A-C1
15	B	1216	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	O1A-CGA-O2A-C1
21	B	5002	DGD	O1A-C1A-O1G-C1G
18	1	803	LMG	O10-C28-O8-C9
18	1	803	LMG	C29-C28-O8-C9
15	3	613	CLA	O1A-CGA-O2A-C1
13	3	502	XAT	C33-C34-C35-C15
14	3	503	BCR	C9-C10-C11-C12
14	A	4005	BCR	C13-C14-C15-C16
14	F	4002	BCR	C9-C10-C11-C12
17	A	5001	LHG	O2-C2-C3-O3
17	B	5001	LHG	O2-C2-C3-O3
15	2	615	CLA	CBA-CGA-O2A-C1
15	3	612	CLA	CBA-CGA-O2A-C1
15	4	612	CLA	CBA-CGA-O2A-C1
15	4	615	CLA	CBA-CGA-O2A-C1
15	A	1119	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	CBA-CGA-O2A-C1
15	A	1132	CLA	CBA-CGA-O2A-C1
15	B	1201	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	CBA-CGA-O2A-C1
15	B	1215	CLA	CBA-CGA-O2A-C1
15	B	1216	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	O1A-CGA-O2A-C1
15	A	1126	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	O1D-CGD-O2D-CED
15	A	1134	CLA	O1D-CGD-O2D-CED
15	1	607	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	C3-C5-C6-C7
15	B	1208	CLA	CBA-CGA-O2A-C1
15	2	604	CLA	O1A-CGA-O2A-C1
15	4	604	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1A-CGA-O2A-C1
15	B	1202	CLA	O1A-CGA-O2A-C1
15	B	1230	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1240	CLA	C4-C3-C5-C6
25	A	2001	PQN	C14-C13-C15-C16
15	B	1240	CLA	C2-C3-C5-C6
25	A	2001	PQN	C12-C13-C15-C16
15	1	611	CLA	C2A-CAA-CBA-CGA
15	2	612	CLA	C2A-CAA-CBA-CGA
15	4	606	CLA	C2A-CAA-CBA-CGA
15	F	1302	CLA	C2A-CAA-CBA-CGA
15	J	1302	CLA	C2A-CAA-CBA-CGA
15	4	605	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	O1A-CGA-O2A-C1
15	A	1132	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1A-CGA-O2A-C1
19	1	811	SQD	O5-C1-O6-C44
15	A	1107	CLA	CBA-CGA-O2A-C1
15	B	1220	CLA	CBA-CGA-O2A-C1
15	B	1231	CLA	CBA-CGA-O2A-C1
15	3	611	CLA	CBA-CGA-O2A-C1
15	3	605	CLA	C4C-C3C-CAC-CBC
15	B	1235	CLA	O1D-CGD-O2D-CED
15	2	615	CLA	O1A-CGA-O2A-C1
15	4	615	CLA	O1A-CGA-O2A-C1
15	B	1215	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C1-C2-C3-O3
15	B	1231	CLA	O1A-CGA-O2A-C1
15	2	605	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	A	1112	CLA	CBA-CGA-O2A-C1
15	A	1122	CLA	CBA-CGA-O2A-C1
15	A	1131	CLA	CBA-CGA-O2A-C1
15	A	1135	CLA	CBA-CGA-O2A-C1
15	B	1210	CLA	CBA-CGA-O2A-C1
15	B	1222	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1
15	B	1229	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	CBA-CGA-O2A-C1
15	B	1238	CLA	CBA-CGA-O2A-C1
15	B	1239	CLA	CBA-CGA-O2A-C1
14	1	503	BCR	C13-C14-C15-C16
14	4	503	BCR	C9-C10-C11-C12
14	A	4007	BCR	C19-C20-C21-C22
14	B	4001	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	B	4003	BCR	C19-C20-C21-C22
14	J	4001	BCR	C19-C20-C21-C22
14	J	4002	BCR	C9-C10-C11-C12
16	4	611	CHL	C2C-C3C-CAC-CBC
15	2	605	CLA	C5-C6-C7-C8
25	A	2001	PQN	C20-C21-C22-C23
21	4	811	DGD	C2D-C1D-O3G-C3G
15	A	1135	CLA	O1A-CGA-O2A-C1
15	B	1222	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	O1A-CGA-O2A-C1
15	B	1239	CLA	O1A-CGA-O2A-C1
15	A	1012	CLA	C11-C10-C8-C9
15	A	1013	CLA	C11-C12-C13-C14
15	A	1106	CLA	C11-C12-C13-C14
25	A	2001	PQN	C19-C18-C20-C21
25	B	2002	PQN	C19-C18-C20-C21
15	4	609	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	C5-C6-C7-C8
15	2	604	CLA	C2A-CAA-CBA-CGA
15	A	1105	CLA	C2A-CAA-CBA-CGA
16	3	604	CHL	C2A-CAA-CBA-CGA
13	2	502	XAT	C7-C8-C9-C19
14	1	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C11-C12-C13-C35
14	4	505	BCR	C36-C18-C19-C20
14	A	4003	BCR	C36-C18-C19-C20
14	A	4004	BCR	C36-C18-C19-C20
14	A	4006	BCR	C36-C18-C19-C20
14	B	4001	BCR	C7-C8-C9-C34
14	B	4001	BCR	C36-C18-C19-C20
14	B	4004	BCR	C36-C18-C19-C20
14	B	4005	BCR	C37-C22-C23-C24
14	B	4006	BCR	C37-C22-C23-C24
14	F	4002	BCR	C36-C18-C19-C20
14	J	4001	BCR	C7-C8-C9-C34
14	J	4003	BCR	C7-C8-C9-C34
14	2	503	BCR	C7-C8-C9-C10
14	4	505	BCR	C17-C18-C19-C20
14	A	4004	BCR	C17-C18-C19-C20
14	A	4006	BCR	C17-C18-C19-C20
14	B	4001	BCR	C17-C18-C19-C20
14	B	4006	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	F	4002	BCR	C17-C18-C19-C20
14	J	4001	BCR	C7-C8-C9-C10
14	J	4002	BCR	C21-C22-C23-C24
18	1	802	LMG	C11-C10-O7-C8
15	2	605	CLA	O1A-CGA-O2A-C1
15	A	1122	CLA	O1A-CGA-O2A-C1
15	B	1210	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	C13-C15-C16-C17
24	A	1011	CL0	C4C-C3C-CAC-CBC
15	F	1301	CLA	CBA-CGA-O2A-C1
15	J	1302	CLA	CBA-CGA-O2A-C1
21	2	811	DGD	C2A-C1A-O1G-C1G
15	1	612	CLA	C5-C6-C7-C8
15	2	605	CLA	C13-C15-C16-C17
15	A	1013	CLA	C5-C6-C7-C8
15	A	1106	CLA	C5-C6-C7-C8
15	A	1106	CLA	C8-C10-C11-C12
15	B	1021	CLA	C8-C10-C11-C12
15	B	1021	CLA	C13-C15-C16-C17
15	B	1238	CLA	O1A-CGA-O2A-C1
23	B	5031	GSH	O12-C1-CA1-N1
25	A	2001	PQN	C15-C16-C17-C18
15	B	1225	CLA	CBA-CGA-O2A-C1
15	2	602	CLA	C2-C1-O2A-CGA
15	2	607	CLA	C2-C1-O2A-CGA
15	2	612	CLA	C2-C1-O2A-CGA
15	2	615	CLA	C2-C1-O2A-CGA
15	3	607	CLA	C2-C1-O2A-CGA
15	3	608	CLA	C2-C1-O2A-CGA
15	3	610	CLA	C2-C1-O2A-CGA
15	3	612	CLA	C2-C1-O2A-CGA
15	4	606	CLA	C2-C1-O2A-CGA
15	4	607	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	C2-C1-O2A-CGA
15	A	1109	CLA	C2-C1-O2A-CGA
15	A	1112	CLA	C2-C1-O2A-CGA
15	A	1115	CLA	C2-C1-O2A-CGA
15	A	1119	CLA	C2-C1-O2A-CGA
15	A	1121	CLA	C2-C1-O2A-CGA
15	A	1122	CLA	C2-C1-O2A-CGA
15	A	1125	CLA	C2-C1-O2A-CGA
15	A	1128	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	C2-C1-O2A-CGA
15	A	1132	CLA	C2-C1-O2A-CGA
15	A	1133	CLA	C2-C1-O2A-CGA
15	A	1134	CLA	C2-C1-O2A-CGA
15	A	1135	CLA	C2-C1-O2A-CGA
15	A	1136	CLA	C2-C1-O2A-CGA
15	A	1139	CLA	C2-C1-O2A-CGA
15	A	1141	CLA	C2-C1-O2A-CGA
15	B	1021	CLA	C2-C1-O2A-CGA
15	B	1201	CLA	C2-C1-O2A-CGA
15	B	1202	CLA	C2-C1-O2A-CGA
15	B	1203	CLA	C2-C1-O2A-CGA
15	B	1205	CLA	C2-C1-O2A-CGA
15	B	1206	CLA	C2-C1-O2A-CGA
15	B	1210	CLA	C2-C1-O2A-CGA
15	B	1220	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
15	B	1224	CLA	C2-C1-O2A-CGA
15	B	1225	CLA	C2-C1-O2A-CGA
15	B	1226	CLA	C2-C1-O2A-CGA
15	B	1231	CLA	C2-C1-O2A-CGA
15	B	1234	CLA	C2-C1-O2A-CGA
15	B	1236	CLA	C2-C1-O2A-CGA
15	B	1237	CLA	C2-C1-O2A-CGA
15	B	1239	CLA	C2-C1-O2A-CGA
15	J	1302	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	C12-C13-C15-C16
15	A	1106	CLA	C11-C12-C13-C15
15	3	612	CLA	C3-C5-C6-C7
15	A	1112	CLA	O1A-CGA-O2A-C1
15	A	1131	CLA	O1A-CGA-O2A-C1
15	B	1235	CLA	O1A-CGA-O2A-C1
13	3	502	XAT	C29-C30-C31-C32
14	1	503	BCR	C15-C16-C17-C18
14	4	505	BCR	C13-C14-C15-C16
14	A	4005	BCR	C19-C20-C21-C22
14	B	4004	BCR	C9-C10-C11-C12
14	J	4002	BCR	C13-C14-C15-C16
15	A	1102	CLA	C2A-CAA-CBA-CGA
15	A	1121	CLA	C2A-CAA-CBA-CGA
15	A	1129	CLA	C2A-CAA-CBA-CGA
15	A	1130	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1022	CLA	C2A-CAA-CBA-CGA
15	B	1234	CLA	C2A-CAA-CBA-CGA
15	3	601	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	C5-C6-C7-C8
15	A	1111	CLA	O1A-CGA-O2A-C1
15	B	1220	CLA	O1A-CGA-O2A-C1
21	4	811	DGD	O6D-C1D-O3G-C3G
25	A	2001	PQN	C23-C25-C26-C27
13	1	502	XAT	C10-C11-C12-C13
13	4	502	XAT	C10-C11-C12-C13
14	A	4003	BCR	C10-C11-C12-C13
14	A	4006	BCR	C10-C11-C12-C13
14	A	4007	BCR	C10-C11-C12-C13
21	2	811	DGD	C8A-C9A-CAA-CBA
17	2	801	LHG	O2-C2-C3-O3
15	1	607	CLA	O1A-CGA-O2A-C1
25	A	2001	PQN	C25-C26-C27-C28
15	A	1107	CLA	O1A-CGA-O2A-C1
15	B	1228	CLA	O1A-CGA-O2A-C1
15	F	1301	CLA	O1A-CGA-O2A-C1
15	J	1302	CLA	O1A-CGA-O2A-C1
21	J	5001	DGD	C4D-C5D-C6D-O5D
15	A	1013	CLA	C15-C16-C17-C18
25	A	2001	PQN	C18-C20-C21-C22
15	B	1225	CLA	O1A-CGA-O2A-C1
16	4	611	CHL	C4C-C3C-CAC-CBC
17	2	801	LHG	C1-C2-C3-O3
18	1	802	LMG	O9-C10-O7-C8
15	A	1013	CLA	C2-C3-C5-C6
15	B	1240	CLA	C13-C15-C16-C17
15	3	601	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	A	1117	CLA	C2A-CAA-CBA-CGA
15	B	1208	CLA	C2A-CAA-CBA-CGA
15	B	1215	CLA	C2A-CAA-CBA-CGA
15	F	1301	CLA	C2A-CAA-CBA-CGA
15	3	608	CLA	CBA-CGA-O2A-C1
15	4	605	CLA	CBA-CGA-O2A-C1
15	A	1128	CLA	CBA-CGA-O2A-C1
13	3	502	XAT	C20-C13-C14-C15
13	4	502	XAT	C20-C13-C14-C15
14	1	503	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
14	A	4003	BCR	C11-C10-C9-C34
14	A	4005	BCR	C11-C10-C9-C34
14	A	4006	BCR	C11-C10-C9-C34
14	J	4001	BCR	C11-C10-C9-C34
21	2	811	DGD	O1A-C1A-O1G-C1G
15	2	605	CLA	C16-C17-C18-C19
15	3	612	CLA	C6-C7-C8-C10
15	B	1235	CLA	C11-C12-C13-C15
15	3	607	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C6-C5-O7-C7
15	4	601	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	C2C-C3C-CAC-CBC
13	3	502	XAT	C12-C13-C14-C15
13	4	502	XAT	C12-C13-C14-C15
14	1	503	BCR	C11-C10-C9-C8
14	A	4003	BCR	C11-C10-C9-C8
14	A	4006	BCR	C11-C10-C9-C8
14	J	4001	BCR	C11-C10-C9-C8
21	2	811	DGD	C2D-C1D-O3G-C3G
15	A	1103	CLA	C6-C7-C8-C9
15	A	1138	CLA	C16-C17-C18-C19
15	A	1138	CLA	C11-C10-C8-C9
15	1	615	CLA	C8-C10-C11-C12
15	A	1104	CLA	C5-C6-C7-C8
15	1	602	CLA	C2A-CAA-CBA-CGA
15	1	605	CLA	C2A-CAA-CBA-CGA
15	A	1013	CLA	C2A-CAA-CBA-CGA
15	A	1118	CLA	C2A-CAA-CBA-CGA
15	A	1136	CLA	C2A-CAA-CBA-CGA
15	A	1138	CLA	C2A-CAA-CBA-CGA
16	1	610	CHL	C2A-CAA-CBA-CGA
24	A	1011	CL0	C2A-CAA-CBA-CGA
14	3	504	BCR	C7-C8-C9-C34
14	3	504	BCR	C36-C18-C19-C20
16	1	610	CHL	C2C-C3C-CAC-CBC
17	1	801	LHG	O1-C1-C2-C3
17	2	801	LHG	O1-C1-C2-C3
12	2	501	LUT	C7-C8-C9-C10
14	2	503	BCR	C21-C22-C23-C24
14	3	504	BCR	C11-C12-C13-C14
14	4	505	BCR	C11-C12-C13-C14
14	A	4006	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	B	4001	BCR	C7-C8-C9-C10
14	B	4005	BCR	C17-C18-C19-C20
15	B	1022	CLA	C4B-C3B-CAB-CBB
15	A	1103	CLA	C6-C7-C8-C10
15	B	1023	CLA	C11-C12-C13-C14
15	B	1023	CLA	C11-C12-C13-C15
15	B	1240	CLA	C16-C17-C18-C19
15	B	1240	CLA	C16-C17-C18-C20
15	1	602	CLA	CBA-CGA-O2A-C1
15	3	608	CLA	O1A-CGA-O2A-C1
15	A	1128	CLA	O1A-CGA-O2A-C1
15	3	611	CLA	O1A-CGA-O2A-C1
21	J	5001	DGD	O6D-C5D-C6D-O5D
15	1	602	CLA	C3A-C2A-CAA-CBA
15	1	603	CLA	C3A-C2A-CAA-CBA
15	2	615	CLA	C3A-C2A-CAA-CBA
15	3	601	CLA	C3A-C2A-CAA-CBA
15	3	608	CLA	C3A-C2A-CAA-CBA
15	4	607	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C3A-C2A-CAA-CBA
15	A	1123	CLA	C3A-C2A-CAA-CBA
15	A	1124	CLA	C3A-C2A-CAA-CBA
15	A	1135	CLA	C3A-C2A-CAA-CBA
15	B	1206	CLA	C3A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	B	1221	CLA	C3A-C2A-CAA-CBA
15	B	1223	CLA	C3A-C2A-CAA-CBA
15	B	1234	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
16	1	609	CHL	C3A-C2A-CAA-CBA
15	2	605	CLA	C16-C17-C18-C20
15	A	1104	CLA	C11-C12-C13-C15
15	A	1138	CLA	C16-C17-C18-C20
15	A	1130	CLA	C4-C3-C5-C6
15	A	1130	CLA	C2-C3-C5-C6
21	2	811	DGD	C2G-C1G-O1G-C1A
17	1	801	LHG	O1-C1-C2-O2
17	2	801	LHG	O1-C1-C2-O2
17	A	5001	LHG	O1-C1-C2-O2
22	2	821	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
15	B	1235	CLA	C11-C12-C13-C14
16	2	609	CHL	C2C-C3C-CAC-CBC
15	B	1022	CLA	C2B-C3B-CAB-CBB
18	1	802	LMG	C33-C34-C35-C36
15	1	611	CLA	C2-C1-O2A-CGA
15	1	615	CLA	C2-C1-O2A-CGA
15	2	605	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	C2-C1-O2A-CGA
15	A	1111	CLA	C2-C1-O2A-CGA
15	A	1116	CLA	C2-C1-O2A-CGA
15	A	1120	CLA	C2-C1-O2A-CGA
15	A	1123	CLA	C2-C1-O2A-CGA
15	A	1130	CLA	C2-C1-O2A-CGA
15	A	1137	CLA	C2-C1-O2A-CGA
15	A	1140	CLA	C2-C1-O2A-CGA
15	B	1022	CLA	C2-C1-O2A-CGA
15	B	1208	CLA	C2-C1-O2A-CGA
15	B	1213	CLA	C2-C1-O2A-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1216	CLA	C2-C1-O2A-CGA
15	B	1219	CLA	C2-C1-O2A-CGA
15	B	1222	CLA	C2-C1-O2A-CGA
15	B	1223	CLA	C2-C1-O2A-CGA
15	B	1228	CLA	C2-C1-O2A-CGA
15	4	605	CLA	O1A-CGA-O2A-C1
12	4	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C1-C6-C7-C8
14	1	503	BCR	C5-C6-C7-C8
14	1	503	BCR	C23-C24-C25-C30
14	1	505	BCR	C1-C6-C7-C8
14	1	505	BCR	C23-C24-C25-C30
14	3	503	BCR	C1-C6-C7-C8
14	3	504	BCR	C1-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C26
14	3	504	BCR	C23-C24-C25-C30
14	4	505	BCR	C23-C24-C25-C26
14	4	505	BCR	C23-C24-C25-C30
14	A	4002	BCR	C5-C6-C7-C8
14	A	4003	BCR	C23-C24-C25-C30
14	A	4007	BCR	C1-C6-C7-C8
14	A	4007	BCR	C23-C24-C25-C26
14	B	4001	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
14	B	4003	BCR	C1-C6-C7-C8
14	B	4003	BCR	C5-C6-C7-C8
14	B	4004	BCR	C23-C24-C25-C26
14	B	4005	BCR	C23-C24-C25-C26
14	B	4005	BCR	C23-C24-C25-C30
14	J	4001	BCR	C1-C6-C7-C8
14	J	4003	BCR	C1-C6-C7-C8
14	J	4003	BCR	C23-C24-C25-C30
15	B	1021	CLA	C3-C5-C6-C7
15	1	604	CLA	CBA-CGA-O2A-C1
15	2	612	CLA	CBA-CGA-O2A-C1
15	4	609	CLA	CBA-CGA-O2A-C1
15	B	1205	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	C10-C11-C12-C13
15	3	607	CLA	O1A-CGA-O2A-C1
15	B	1235	CLA	C4-C3-C5-C6
15	A	1138	CLA	C11-C10-C8-C7
15	4	609	CLA	O1A-CGA-O2A-C1
18	2	802	LMG	O7-C10-C11-C12
15	B	1229	CLA	C10-C11-C12-C13
14	3	503	BCR	C19-C20-C21-C22
14	4	503	BCR	C19-C20-C21-C22
14	A	4005	BCR	C9-C10-C11-C12
14	B	4004	BCR	C19-C20-C21-C22
15	A	1121	CLA	CBA-CGA-O2A-C1
15	1	607	CLA	C2A-CAA-CBA-CGA
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	A	1140	CLA	C2A-CAA-CBA-CGA
15	B	1211	CLA	C2A-CAA-CBA-CGA
16	2	609	CHL	C2A-CAA-CBA-CGA
15	A	1013	CLA	C13-C15-C16-C17
19	1	811	SQD	C14-C15-C16-C17
15	2	605	CLA	C15-C16-C17-C18
15	B	1220	CLA	C5-C6-C7-C8
15	A	1012	CLA	C3-C5-C6-C7
15	B	1239	CLA	C3-C5-C6-C7
15	A	1134	CLA	CBA-CGA-O2A-C1
15	2	612	CLA	O1A-CGA-O2A-C1
15	B	1205	CLA	O1A-CGA-O2A-C1
15	A	1138	CLA	C13-C15-C16-C17
15	B	1235	CLA	C2-C3-C5-C6
15	A	1013	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	1	612	CLA	C2A-CAA-CBA-CGA
15	A	1135	CLA	C2A-CAA-CBA-CGA
15	B	1235	CLA	C2A-CAA-CBA-CGA
18	2	803	LMG	O6-C5-C6-O5
12	2	501	LUT	C31-C32-C33-C40
14	1	503	BCR	C37-C22-C23-C24
15	1	604	CLA	O1A-CGA-O2A-C1
15	1	601	CLA	C1A-C2A-CAA-CBA
15	1	602	CLA	C1A-C2A-CAA-CBA
15	1	606	CLA	C1A-C2A-CAA-CBA
15	1	612	CLA	C1A-C2A-CAA-CBA
15	1	615	CLA	C1A-C2A-CAA-CBA
15	2	601	CLA	C1A-C2A-CAA-CBA
15	2	604	CLA	C1A-C2A-CAA-CBA
15	2	606	CLA	C1A-C2A-CAA-CBA
15	2	608	CLA	C1A-C2A-CAA-CBA
15	2	615	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C1A-C2A-CAA-CBA
15	3	610	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1115	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	A	1135	CLA	C1A-C2A-CAA-CBA
15	B	1021	CLA	C1A-C2A-CAA-CBA
15	B	1204	CLA	C1A-C2A-CAA-CBA
15	B	1208	CLA	C1A-C2A-CAA-CBA
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	B	1217	CLA	C1A-C2A-CAA-CBA
15	B	1219	CLA	C1A-C2A-CAA-CBA
15	B	1221	CLA	C1A-C2A-CAA-CBA
15	B	1222	CLA	C1A-C2A-CAA-CBA
15	B	1223	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	B	1239	CLA	C1A-C2A-CAA-CBA
15	F	1301	CLA	C1A-C2A-CAA-CBA
15	J	1302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1104	CLA	C11-C12-C13-C14
25	B	2002	PQN	C26-C27-C28-C30
14	2	503	BCR	C19-C20-C21-C22
14	3	504	BCR	C9-C10-C11-C12
14	4	505	BCR	C19-C20-C21-C22
14	A	4004	BCR	C19-C20-C21-C22
17	A	5001	LHG	C4-O6-P-O3
15	B	1240	CLA	C3-C5-C6-C7
15	B	1239	CLA	C13-C15-C16-C17
15	3	612	CLA	C6-C7-C8-C9
15	A	1104	CLA	C8-C10-C11-C12
15	A	1121	CLA	O1A-CGA-O2A-C1
21	B	5002	DGD	C1G-C2G-C3G-O3G
15	A	1103	CLA	CBA-CGA-O2A-C1
21	2	811	DGD	C2G-C3G-O3G-C1D
21	4	811	DGD	C5D-C6D-O5D-C1E
21	4	811	DGD	O6E-C5E-C6E-O5E
15	B	1220	CLA	CAA-CBA-CGA-O2A
18	1	802	LMG	O6-C5-C6-O5
17	A	5002	LHG	O1-C1-C2-O2
17	B	5001	LHG	O1-C1-C2-O2
14	B	4005	BCR	C13-C14-C15-C16
21	J	5001	DGD	O6E-C5E-C6E-O5E
15	A	1104	CLA	C4-C3-C5-C6
15	3	601	CLA	C2C-C3C-CAC-CBC
15	A	1126	CLA	C2A-CAA-CBA-CGA
15	B	1224	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	C15-C16-C17-C18
15	2	608	CLA	C2-C1-O2A-CGA
15	4	601	CLA	C2-C1-O2A-CGA
15	4	609	CLA	C2-C1-O2A-CGA
15	4	612	CLA	C2-C1-O2A-CGA
15	A	1118	CLA	C2-C1-O2A-CGA
15	A	1127	CLA	C2-C1-O2A-CGA
15	B	1214	CLA	C2-C1-O2A-CGA
15	B	1232	CLA	C2-C1-O2A-CGA
15	1	601	CLA	CBA-CGA-O2A-C1
15	A	1134	CLA	O1A-CGA-O2A-C1
18	1	802	LMG	C2-C1-O1-C7
18	1	802	LMG	O1-C7-C8-O7
15	B	1229	CLA	C4-C3-C5-C6
15	1	615	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	A	1012	CLA	C6-C7-C8-C10
15	A	1104	CLA	C2-C3-C5-C6
15	B	1240	CLA	C12-C13-C15-C16
25	A	2001	PQN	C21-C22-C23-C25
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	B	1023	CLA	C11-C10-C8-C9
15	B	1229	CLA	C5-C6-C7-C8
15	3	606	CLA	C2C-C3C-CAC-CBC
13	4	502	XAT	C27-C28-C29-C30
14	1	503	BCR	C7-C8-C9-C10
14	1	503	BCR	C21-C22-C23-C24
14	3	503	BCR	C11-C12-C13-C14
14	A	4002	BCR	C7-C8-C9-C10
15	B	1023	CLA	CBA-CGA-O2A-C1
15	B	1236	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C26-C27-C28-C29
17	A	5002	LHG	O6-C4-C5-C6
17	B	5001	LHG	O6-C4-C5-C6
15	B	1203	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C20-C21-C22-C23
15	2	607	CLA	CBA-CGA-O2A-C1
15	A	1012	CLA	CBA-CGA-O2A-C1
15	B	1237	CLA	CAA-CBA-CGA-O2A
21	4	811	DGD	C2B-C3B-C4B-C5B
15	1	607	CLA	C3A-C2A-CAA-CBA
15	A	1118	CLA	C3A-C2A-CAA-CBA
15	A	1125	CLA	C3A-C2A-CAA-CBA
15	A	1140	CLA	C3A-C2A-CAA-CBA
15	B	1239	CLA	C3A-C2A-CAA-CBA
24	A	1011	CL0	C3A-C2A-CAA-CBA
14	A	4006	BCR	C19-C20-C21-C22
14	B	4005	BCR	C9-C10-C11-C12
23	B	5031	GSH	OE1-CD1-CG1-CB1
18	1	802	LMG	O1-C7-C8-C9
21	2	811	DGD	O1G-C1G-C2G-C3G
15	A	1103	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	C2-C3-C5-C6
17	B	5001	LHG	C4-O6-P-O3
15	1	602	CLA	O1A-CGA-O2A-C1
15	4	615	CLA	C5-C6-C7-C8
17	A	5001	LHG	O6-C4-C5-O7
17	A	5002	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
15	1	601	CLA	O1A-CGA-O2A-C1
15	2	604	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	O1A-CGA-O2A-C1
21	4	811	DGD	O2G-C2G-C3G-O3G
15	A	1129	CLA	CBA-CGA-O2A-C1
15	A	1108	CLA	C2C-C3C-CAC-CBC
23	4	831	GSH	O12-C1-CA1-CB1
15	A	1013	CLA	C14-C13-C15-C16
15	B	1235	CLA	C11-C10-C8-C9
15	B	1239	CLA	C14-C13-C15-C16
25	A	2001	PQN	C21-C22-C23-C24
15	B	1231	CLA	C10-C11-C12-C13
17	1	801	LHG	C2-C3-O3-P
12	1	501	LUT	C1-C6-C7-C8
12	1	501	LUT	C5-C6-C7-C8
14	A	4002	BCR	C23-C24-C25-C26
14	A	4002	BCR	C23-C24-C25-C30
14	A	4005	BCR	C1-C6-C7-C8
14	A	4005	BCR	C5-C6-C7-C8
14	F	4002	BCR	C1-C6-C7-C8
15	1	615	CLA	C3-C5-C6-C7
15	1	607	CLA	CAA-CBA-CGA-O2A
21	2	811	DGD	O1G-C1A-C2A-C3A
12	2	501	LUT	C31-C32-C33-C34
12	4	501	LUT	C27-C28-C29-C30
14	4	503	BCR	C17-C18-C19-C20
14	A	4003	BCR	C17-C18-C19-C20
14	B	4002	BCR	C11-C12-C13-C14
14	B	4004	BCR	C17-C18-C19-C20
14	B	4005	BCR	C21-C22-C23-C24
14	J	4003	BCR	C7-C8-C9-C10
15	B	1240	CLA	C10-C11-C12-C13
15	A	1110	CLA	C4C-C3C-CAC-CBC
17	A	5001	LHG	C4-C5-O7-C7
17	A	5001	LHG	C6-C5-O7-C7
15	A	1104	CLA	C11-C10-C8-C7
15	B	1023	CLA	C11-C10-C8-C7
15	B	1229	CLA	C12-C13-C15-C16
15	B	1235	CLA	C11-C10-C8-C7
12	4	501	LUT	C29-C30-C31-C32
14	3	504	BCR	C19-C20-C21-C22
14	B	4005	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	B	4006	BCR	C9-C10-C11-C12
15	2	601	CLA	CBA-CGA-O2A-C1
23	B	5031	GSH	N2-CD1-CG1-CB1
15	B	1239	CLA	C10-C11-C12-C13
15	A	1106	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C18-C20-C21-C22
15	1	604	CLA	CAD-CBD-CGD-O2D
15	2	601	CLA	CAD-CBD-CGD-O2D
15	4	607	CLA	CAD-CBD-CGD-O2D
15	A	1121	CLA	CAD-CBD-CGD-O2D
15	B	1204	CLA	CAD-CBD-CGD-O2D
15	B	1224	CLA	CAD-CBD-CGD-O2D
15	B	1227	CLA	CAD-CBD-CGD-O2D
16	4	610	CHL	CAD-CBD-CGD-O2D
16	4	613	CHL	CAD-CBD-CGD-O2D
15	B	1239	CLA	C15-C16-C17-C18
15	1	612	CLA	C14-C13-C15-C16
17	A	5002	LHG	C4-C5-C6-O8
21	4	811	DGD	O1G-C1G-C2G-C3G
21	4	811	DGD	C1G-C2G-C3G-O3G
15	A	1129	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	C5-C6-C7-C8
14	B	4003	BCR	C18-C19-C20-C21
15	4	602	CLA	O2A-C1-C2-C3
15	B	1214	CLA	O2A-C1-C2-C3
23	B	5031	GSH	O32-C3-CA3-N3
15	2	603	CLA	CHA-CBD-CGD-O2D
15	2	615	CLA	CHA-CBD-CGD-O1D
15	3	613	CLA	CHA-CBD-CGD-O2D
15	4	612	CLA	CHA-CBD-CGD-O1D
15	4	612	CLA	CHA-CBD-CGD-O2D
15	A	1108	CLA	CHA-CBD-CGD-O1D
15	A	1108	CLA	CHA-CBD-CGD-O2D
15	A	1114	CLA	CHA-CBD-CGD-O1D
15	A	1122	CLA	CHA-CBD-CGD-O1D
15	A	1125	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CHA-CBD-CGD-O1D
15	A	1129	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	CHA-CBD-CGD-O1D
15	A	1131	CLA	CHA-CBD-CGD-O2D
15	A	1132	CLA	CHA-CBD-CGD-O1D
15	A	1132	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	1138	CLA	CHA-CBD-CGD-O1D
15	A	1138	CLA	CHA-CBD-CGD-O2D
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	B	1210	CLA	CHA-CBD-CGD-O1D
15	B	1210	CLA	CHA-CBD-CGD-O2D
15	B	1231	CLA	CHA-CBD-CGD-O2D
23	B	5031	GSH	C1-CA1-CB1-CG1
16	1	610	CHL	C4C-C3C-CAC-CBC
15	2	601	CLA	O1A-CGA-O2A-C1
15	2	607	CLA	O1A-CGA-O2A-C1
15	A	1012	CLA	O1A-CGA-O2A-C1
15	B	1023	CLA	O1A-CGA-O2A-C1
21	2	811	DGD	O1G-C1G-C2G-O2G
21	4	811	DGD	O1G-C1G-C2G-O2G
15	A	1138	CLA	C4-C3-C5-C6
15	B	1203	CLA	O1A-CGA-O2A-C1
15	1	615	CLA	C11-C12-C13-C14
15	B	1229	CLA	C14-C13-C15-C16
19	1	811	SQD	C4-C5-C6-S
15	3	615	CLA	C2A-CAA-CBA-CGA
15	4	601	CLA	C2A-CAA-CBA-CGA
15	4	615	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	CAA-CBA-CGA-O2A
13	3	502	XAT	C31-C32-C33-C40
14	1	505	BCR	C36-C18-C19-C20
13	2	502	XAT	C7-C8-C9-C10
13	3	502	XAT	C31-C32-C33-C34
14	3	504	BCR	C7-C8-C9-C10
15	1	607	CLA	C1A-C2A-CAA-CBA
15	B	1206	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	B	1229	CLA	C1A-C2A-CAA-CBA
23	4	831	GSH	O11-C1-CA1-CB1
23	B	5031	GSH	O11-C1-CA1-CB1
15	2	601	CLA	C2-C1-O2A-CGA
15	4	615	CLA	C2-C1-O2A-CGA
13	1	502	XAT	C29-C30-C31-C32
14	1	503	BCR	C9-C10-C11-C12
14	4	505	BCR	C15-C16-C17-C18
15	B	1239	CLA	C8-C10-C11-C12
17	2	801	LHG	C4-O6-P-O3
17	A	5001	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	C2-C3-O3-P
15	1	602	CLA	C4B-C3B-CAB-CBB
15	1	607	CLA	C4B-C3B-CAB-CBB
15	1	612	CLA	C4B-C3B-CAB-CBB
15	3	610	CLA	C4B-C3B-CAB-CBB
15	A	1120	CLA	C4B-C3B-CAB-CBB
15	B	1214	CLA	C4B-C3B-CAB-CBB
15	B	1227	CLA	C4B-C3B-CAB-CBB
15	1	601	CLA	O2A-C1-C2-C3
16	2	609	CHL	O2A-C1-C2-C3
17	A	5001	LHG	O6-C4-C5-C6
15	1	605	CLA	CAD-CBD-CGD-O1D
15	2	605	CLA	CAD-CBD-CGD-O1D
15	A	1110	CLA	CAD-CBD-CGD-O1D
15	A	1112	CLA	CAD-CBD-CGD-O1D
15	A	1122	CLA	CAD-CBD-CGD-O1D
15	A	1131	CLA	CAD-CBD-CGD-O1D
15	A	1135	CLA	CAD-CBD-CGD-O1D
15	B	1210	CLA	CAD-CBD-CGD-O1D
16	1	609	CHL	CAD-CBD-CGD-O1D
23	4	831	GSH	N1-CA1-CB1-CG1
15	3	615	CLA	CAA-CBA-CGA-O2A
15	A	1103	CLA	C5-C6-C7-C8
12	1	501	LUT	C25-C26-C27-C28
12	3	501	LUT	C25-C26-C27-C28
15	1	615	CLA	C11-C12-C13-C15
15	A	1012	CLA	C11-C10-C8-C7
15	A	1013	CLA	C11-C12-C13-C15
15	A	1138	CLA	C11-C12-C13-C15
15	B	1021	CLA	C11-C10-C8-C7
15	B	1212	CLA	C3A-C2A-CAA-CBA
15	B	1231	CLA	C11-C10-C8-C7
14	J	4002	BCR	C15-C16-C17-C18
15	A	1013	CLA	C2C-C3C-CAC-CBC
15	A	1106	CLA	O1A-CGA-O2A-C1
23	B	5031	GSH	O12-C1-CA1-CB1
17	A	5002	LHG	O7-C5-C6-O8
15	B	1228	CLA	C3-C5-C6-C7
15	B	1224	CLA	CBA-CGA-O2A-C1
15	A	1138	CLA	C2-C3-C5-C6
15	1	615	CLA	C11-C10-C8-C9
15	A	1104	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	1240	CLA	C14-C13-C15-C16
15	B	1224	CLA	O1A-CGA-O2A-C1
16	4	613	CHL	C2A-CAA-CBA-CGA
15	3	610	CLA	CAA-CBA-CGA-O2A
14	4	505	BCR	C18-C19-C20-C21
14	A	4003	BCR	C18-C19-C20-C21
14	A	4004	BCR	C18-C19-C20-C21
14	A	4007	BCR	C18-C19-C20-C21
14	B	4001	BCR	C18-C19-C20-C21
14	J	4003	BCR	C18-C19-C20-C21
12	2	501	LUT	C29-C30-C31-C32
14	J	4001	BCR	C37-C22-C23-C24
15	1	612	CLA	C2B-C3B-CAB-CBB
15	A	1120	CLA	C2B-C3B-CAB-CBB
15	B	1214	CLA	C2B-C3B-CAB-CBB
15	B	1227	CLA	C2B-C3B-CAB-CBB
15	4	607	CLA	CAA-CBA-CGA-O2A
15	1	601	CLA	C1-C2-C3-C4
15	1	611	CLA	C1-C2-C3-C4
15	2	602	CLA	C1-C2-C3-C4
15	2	612	CLA	C1-C2-C3-C4
15	3	610	CLA	C1-C2-C3-C4
15	4	601	CLA	C1-C2-C3-C4
15	4	602	CLA	C1-C2-C3-C4
15	4	604	CLA	C1-C2-C3-C4
15	4	605	CLA	C1-C2-C3-C4
15	4	607	CLA	C1-C2-C3-C4
15	A	1105	CLA	C1-C2-C3-C4
15	A	1117	CLA	C1-C2-C3-C4
15	A	1119	CLA	C1-C2-C3-C4
15	A	1121	CLA	C1-C2-C3-C4
15	A	1125	CLA	C1-C2-C3-C4
15	A	1126	CLA	C1-C2-C3-C4
15	A	1127	CLA	C1-C2-C3-C4
15	A	1128	CLA	C1-C2-C3-C4
15	A	1132	CLA	C1-C2-C3-C4
15	A	1134	CLA	C1-C2-C3-C4
15	A	1135	CLA	C1-C2-C3-C4
15	A	1136	CLA	C1-C2-C3-C4
15	A	1137	CLA	C1-C2-C3-C4
15	B	1202	CLA	C1-C2-C3-C4
15	B	1203	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
15	B	1205	CLA	C1-C2-C3-C4
15	B	1206	CLA	C1-C2-C3-C4
15	B	1210	CLA	C1-C2-C3-C4
15	B	1213	CLA	C1-C2-C3-C4
15	B	1214	CLA	C1-C2-C3-C4
15	B	1215	CLA	C1-C2-C3-C4
15	B	1216	CLA	C1-C2-C3-C4
15	B	1218	CLA	C1-C2-C3-C4
15	B	1219	CLA	C1-C2-C3-C4
15	B	1222	CLA	C1-C2-C3-C4
15	B	1224	CLA	C1-C2-C3-C4
15	B	1225	CLA	C1-C2-C3-C4
15	B	1226	CLA	C1-C2-C3-C4
15	B	1230	CLA	C1-C2-C3-C4
15	B	1232	CLA	C1-C2-C3-C4
15	B	1234	CLA	C1-C2-C3-C4
15	B	1236	CLA	C1-C2-C3-C4
15	B	1237	CLA	C1-C2-C3-C4
15	J	1302	CLA	C1-C2-C3-C4
16	1	609	CHL	C1-C2-C3-C4
16	2	609	CHL	C1-C2-C3-C4
16	2	610	CHL	C1-C2-C3-C4
16	4	613	CHL	C1-C2-C3-C4
15	A	1119	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C2A-CAA-CBA-CGA
15	B	1212	CLA	C2A-CAA-CBA-CGA
15	B	1237	CLA	C2A-CAA-CBA-CGA
15	1	605	CLA	C2-C1-O2A-CGA
15	B	1218	CLA	C2-C1-O2A-CGA
16	4	611	CHL	C2-C1-O2A-CGA
24	A	1011	CL0	C2-C1-O2A-CGA
14	B	4001	BCR	C23-C24-C25-C26
14	F	4002	BCR	C5-C6-C7-C8
21	2	811	DGD	O1B-C1B-O2G-C2G
15	4	605	CLA	CAA-CBA-CGA-O2A
16	2	609	CHL	C4C-C3C-CAC-CBC
15	1	615	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	C4C-C3C-CAC-CBC
17	1	801	LHG	C4-O6-P-O3
17	2	801	LHG	C3-O3-P-O6
17	A	5001	LHG	C3-O3-P-O6
17	A	5002	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	C4-O6-P-O3
15	A	1012	CLA	C6-C7-C8-C9
12	3	501	LUT	C29-C30-C31-C32
13	3	502	XAT	C13-C14-C15-C35
14	2	503	BCR	C13-C14-C15-C16
14	A	4002	BCR	C13-C14-C15-C16
15	A	1137	CLA	CBA-CGA-O2A-C1
15	1	612	CLA	C12-C13-C15-C16
18	1	802	LMG	O7-C10-C11-C12
15	B	1239	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C10-C11-C12-C13
15	2	602	CLA	CBA-CGA-O2A-C1
14	1	505	BCR	C17-C18-C19-C20
15	J	1302	CLA	O2A-C1-C2-C3
16	1	609	CHL	O2A-C1-C2-C3
15	B	1237	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C7-C8-C9-C10
15	A	1137	CLA	O1A-CGA-O2A-C1
15	2	604	CLA	C4B-C3B-CAB-CBB
15	A	1130	CLA	C4B-C3B-CAB-CBB
15	B	1220	CLA	CAA-CBA-CGA-O1A
14	B	4003	BCR	C15-C16-C17-C18
15	B	1237	CLA	O1A-CGA-O2A-C1
13	4	502	XAT	C30-C31-C32-C33
16	2	610	CHL	CAA-CBA-CGA-O2A
15	B	1224	CLA	CAA-CBA-CGA-O2A
24	A	1011	CL0	CAA-CBA-CGA-O2A
16	2	610	CHL	C2-C1-O2A-CGA
15	B	1240	CLA	C8-C10-C11-C12
15	2	607	CLA	C2A-CAA-CBA-CGA
21	B	5002	DGD	O1A-C1A-C2A-C3A
15	3	611	CLA	C3A-C2A-CAA-CBA
15	4	605	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C3A-C2A-CAA-CBA
12	1	501	LUT	C29-C30-C31-C32
14	J	4003	BCR	C13-C14-C15-C16
15	A	1102	CLA	CAA-CBA-CGA-O1A
15	B	1231	CLA	C11-C10-C8-C9
12	1	501	LUT	C40-C33-C34-C35
14	1	505	BCR	C35-C13-C14-C15
14	4	505	BCR	C35-C13-C14-C15
14	4	505	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
14	A	4004	BCR	C16-C17-C18-C36
14	A	4006	BCR	C16-C17-C18-C36
14	A	4007	BCR	C16-C17-C18-C36
14	F	4002	BCR	C16-C17-C18-C36
15	B	1225	CLA	C2A-CAA-CBA-CGA
14	3	504	BCR	C17-C18-C19-C20
15	A	1132	CLA	C1A-C2A-CAA-CBA
15	A	1140	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	C6-C7-C8-C10
17	A	5002	LHG	O8-C23-C24-C25
21	B	5002	DGD	O1G-C1A-C2A-C3A
17	2	801	LHG	C2-C3-O3-P
15	B	1240	CLA	C2A-CAA-CBA-CGA
16	1	609	CHL	C2A-CAA-CBA-CGA
15	2	602	CLA	O1A-CGA-O2A-C1
15	B	1212	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	C15-C16-C17-C18
23	B	5031	GSH	O31-C3-CA3-N3
15	1	602	CLA	C2B-C3B-CAB-CBB
15	1	607	CLA	C2B-C3B-CAB-CBB
15	3	610	CLA	C2B-C3B-CAB-CBB
15	A	1102	CLA	CAA-CBA-CGA-O2A
15	A	1138	CLA	C10-C11-C12-C13
12	1	501	LUT	C32-C33-C34-C35
14	1	505	BCR	C12-C13-C14-C15
14	4	505	BCR	C12-C13-C14-C15
14	4	505	BCR	C16-C17-C18-C19
14	A	4004	BCR	C16-C17-C18-C19
14	A	4006	BCR	C16-C17-C18-C19
14	A	4007	BCR	C16-C17-C18-C19
14	F	4002	BCR	C16-C17-C18-C19
14	3	504	BCR	C15-C16-C17-C18
14	4	505	BCR	C9-C10-C11-C12
14	A	4006	BCR	C9-C10-C11-C12
15	A	1138	CLA	C8-C10-C11-C12
15	1	606	CLA	CAA-CBA-CGA-O1A
15	3	601	CLA	C4C-C3C-CAC-CBC
15	B	1235	CLA	C2-C1-O2A-CGA
21	2	811	DGD	C2B-C1B-O2G-C2G
15	B	1240	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	B	1219	CLA	C2A-CAA-CBA-CGA
15	B	1212	CLA	CAA-CBA-CGA-O2A
16	2	610	CHL	C2C-C3C-CAC-CBC
12	3	501	LUT	C1-C6-C7-C8
14	A	4004	BCR	C1-C6-C7-C8
14	A	4005	BCR	C23-C24-C25-C30
14	B	4004	BCR	C1-C6-C7-C8
15	A	1103	CLA	C4-C3-C5-C6
18	2	802	LMG	C8-C7-O1-C1
21	B	5002	DGD	C5D-C6D-O5D-C1E
15	1	606	CLA	CAA-CBA-CGA-O2A
15	A	1121	CLA	CAA-CBA-CGA-O1A
15	1	603	CLA	CAA-CBA-CGA-O2A
15	B	1216	CLA	C2A-CAA-CBA-CGA
16	4	610	CHL	C2A-CAA-CBA-CGA
15	2	602	CLA	C4B-C3B-CAB-CBB
15	A	1105	CLA	C4B-C3B-CAB-CBB
15	B	1023	CLA	C4-C3-C5-C6
15	A	1103	CLA	C2-C3-C5-C6
14	3	504	BCR	C13-C14-C15-C16
14	A	4003	BCR	C9-C10-C11-C12
14	J	4003	BCR	C9-C10-C11-C12
17	1	801	LHG	C7-C8-C9-C10
17	A	5002	LHG	C2-C3-O3-P
16	2	610	CHL	O2A-C1-C2-C3
15	A	1105	CLA	CAA-CBA-CGA-O2A
15	A	1138	CLA	CAA-CBA-CGA-O2A
15	B	1202	CLA	CAA-CBA-CGA-O2A
25	B	2002	PQN	C25-C26-C27-C28
17	A	5002	LHG	O10-C23-C24-C25
15	A	1138	CLA	C11-C12-C13-C14
15	B	1021	CLA	C11-C10-C8-C9
15	B	1235	CLA	C6-C7-C8-C9
15	B	1240	CLA	C6-C7-C8-C9
15	B	1237	CLA	CAA-CBA-CGA-O1A
15	3	603	CLA	C3A-C2A-CAA-CBA
15	4	612	CLA	C3A-C2A-CAA-CBA
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	A	1119	CLA	CAA-CBA-CGA-O2A
15	B	1213	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	1	608	CLA	CAD-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O2D
15	A	1134	CLA	CAD-CBD-CGD-O2D
15	B	1205	CLA	CAD-CBD-CGD-O2D
16	2	609	CHL	CAD-CBD-CGD-O2D
16	2	613	CHL	CAD-CBD-CGD-O2D
14	B	4001	BCR	C15-C16-C17-C18
15	B	1217	CLA	C2A-CAA-CBA-CGA
15	4	609	CLA	CAA-CBA-CGA-O2A
15	B	1201	CLA	CAA-CBA-CGA-O2A
15	A	1013	CLA	C4C-C3C-CAC-CBC
15	B	1220	CLA	C4-C3-C5-C6
15	1	603	CLA	CAA-CBA-CGA-O1A
15	2	604	CLA	CAA-CBA-CGA-O1A
15	3	601	CLA	CAA-CBA-CGA-O2A
15	3	613	CLA	CAA-CBA-CGA-O2A
15	4	603	CLA	CAA-CBA-CGA-O2A
15	A	1132	CLA	CAA-CBA-CGA-O2A
12	4	501	LUT	C31-C32-C33-C34
14	J	4001	BCR	C21-C22-C23-C24
15	2	612	CLA	CAA-CBA-CGA-O2A
15	4	601	CLA	CAA-CBA-CGA-O2A
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	A	1133	CLA	CAA-CBA-CGA-O2A
15	A	1141	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	CAA-CBA-CGA-O2A
15	2	603	CLA	C2A-CAA-CBA-CGA
15	A	1137	CLA	CAA-CBA-CGA-O2A
15	1	602	CLA	CHA-CBD-CGD-O1D
15	1	602	CLA	CHA-CBD-CGD-O2D
15	1	606	CLA	CHA-CBD-CGD-O1D
15	1	611	CLA	CHA-CBD-CGD-O1D
15	1	611	CLA	CHA-CBD-CGD-O2D
15	2	604	CLA	CHA-CBD-CGD-O1D
15	2	604	CLA	CHA-CBD-CGD-O2D
15	2	606	CLA	CHA-CBD-CGD-O1D
15	2	612	CLA	CHA-CBD-CGD-O1D
15	2	612	CLA	CHA-CBD-CGD-O2D
15	2	615	CLA	CHA-CBD-CGD-O2D
15	3	607	CLA	CHA-CBD-CGD-O1D
15	3	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	4	605	CLA	CHA-CBD-CGD-O1D
15	4	605	CLA	CHA-CBD-CGD-O2D
15	4	615	CLA	CHA-CBD-CGD-O1D
15	4	615	CLA	CHA-CBD-CGD-O2D
15	A	1013	CLA	CHA-CBD-CGD-O2D
15	A	1110	CLA	CHA-CBD-CGD-O1D
15	A	1113	CLA	CHA-CBD-CGD-O1D
15	A	1113	CLA	CHA-CBD-CGD-O2D
15	A	1120	CLA	CHA-CBD-CGD-O2D
15	A	1122	CLA	CHA-CBD-CGD-O2D
15	A	1126	CLA	CHA-CBD-CGD-O1D
15	A	1126	CLA	CHA-CBD-CGD-O2D
15	A	1127	CLA	CHA-CBD-CGD-O1D
15	A	1127	CLA	CHA-CBD-CGD-O2D
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1136	CLA	CHA-CBD-CGD-O1D
15	A	1136	CLA	CHA-CBD-CGD-O2D
15	A	1139	CLA	CHA-CBD-CGD-O2D
15	B	1022	CLA	CHA-CBD-CGD-O1D
15	B	1022	CLA	CHA-CBD-CGD-O2D
15	B	1023	CLA	CHA-CBD-CGD-O1D
15	B	1023	CLA	CHA-CBD-CGD-O2D
15	B	1201	CLA	CHA-CBD-CGD-O1D
15	B	1201	CLA	CHA-CBD-CGD-O2D
15	B	1203	CLA	CHA-CBD-CGD-O1D
15	B	1203	CLA	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O1D
15	B	1213	CLA	CHA-CBD-CGD-O1D
15	B	1213	CLA	CHA-CBD-CGD-O2D
15	B	1214	CLA	CHA-CBD-CGD-O1D
15	B	1214	CLA	CHA-CBD-CGD-O2D
15	B	1217	CLA	CHA-CBD-CGD-O1D
15	B	1217	CLA	CHA-CBD-CGD-O2D
15	B	1221	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	CHA-CBD-CGD-O2D
15	B	1222	CLA	CHA-CBD-CGD-O1D
15	B	1225	CLA	CHA-CBD-CGD-O2D
15	B	1228	CLA	CHA-CBD-CGD-O1D
15	B	1228	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	CHA-CBD-CGD-O1D
15	B	1236	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1239	CLA	CHA-CBD-CGD-O1D
15	B	1239	CLA	CHA-CBD-CGD-O2D
15	F	1301	CLA	CHA-CBD-CGD-O1D
15	F	1301	CLA	CHA-CBD-CGD-O2D
16	2	609	CHL	CHA-CBD-CGD-O2D
16	2	610	CHL	CHA-CBD-CGD-O1D
16	2	610	CHL	CHA-CBD-CGD-O2D
16	3	604	CHL	CHA-CBD-CGD-O1D
16	3	604	CHL	CHA-CBD-CGD-O2D
24	A	1011	CL0	CHA-CBD-CGD-O1D
24	A	1011	CL0	CHA-CBD-CGD-O2D
15	A	1113	CLA	CAA-CBA-CGA-O2A
15	1	602	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	CAA-CBA-CGA-O2A
15	1	611	CLA	CAA-CBA-CGA-O2A
15	A	1118	CLA	CAA-CBA-CGA-O2A
15	A	1128	CLA	CAA-CBA-CGA-O2A
15	B	1223	CLA	CAA-CBA-CGA-O2A
15	2	602	CLA	C2A-CAA-CBA-CGA
15	3	605	CLA	CBA-CGA-O2A-C1
15	B	1240	CLA	CBA-CGA-O2A-C1
15	1	607	CLA	CAA-CBA-CGA-O1A
15	A	1124	CLA	CAA-CBA-CGA-O2A
15	A	1127	CLA	CAA-CBA-CGA-O2A
15	1	615	CLA	CAA-CBA-CGA-O2A
15	A	1136	CLA	CAA-CBA-CGA-O2A
15	2	605	CLA	C11-C10-C8-C9
16	2	610	CHL	C2B-C3B-CAB-CBB
16	3	604	CHL	C2B-C3B-CAB-CBB
15	1	611	CLA	O2A-C1-C2-C3
15	4	607	CLA	O2A-C1-C2-C3
15	B	1219	CLA	O2A-C1-C2-C3
15	4	602	CLA	C2C-C3C-CAC-CBC
15	B	1231	CLA	C8-C10-C11-C12
16	4	613	CHL	CAA-CBA-CGA-O2A
15	B	1239	CLA	C16-C17-C18-C19
15	1	604	CLA	C2A-CAA-CBA-CGA
15	A	1109	CLA	C2A-CAA-CBA-CGA
21	2	811	DGD	O1A-C1A-C2A-C3A
15	A	1105	CLA	CAA-CBA-CGA-O1A
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	A	1138	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	1202	CLA	CAA-CBA-CGA-O1A
15	1	605	CLA	O2A-C1-C2-C3
16	2	611	CHL	C2-C1-O2A-CGA
15	1	605	CLA	C1A-C2A-CAA-CBA
15	3	611	CLA	C1A-C2A-CAA-CBA
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	C1A-C2A-CAA-CBA
15	B	1022	CLA	C1A-C2A-CAA-CBA
23	4	831	GSH	OE1-CD1-CG1-CB1
15	A	1136	CLA	CAA-CBA-CGA-O1A
15	1	602	CLA	CAA-CBA-CGA-O1A
15	4	601	CLA	CAA-CBA-CGA-O1A
15	4	603	CLA	CAA-CBA-CGA-O1A
15	A	1133	CLA	CAA-CBA-CGA-O1A
15	B	1201	CLA	CAA-CBA-CGA-O1A
15	B	1236	CLA	CAA-CBA-CGA-O1A
15	1	601	CLA	C2A-CAA-CBA-CGA
15	3	606	CLA	C4C-C3C-CAC-CBC
15	1	615	CLA	C16-C17-C18-C20
15	3	601	CLA	CAA-CBA-CGA-O1A
15	3	613	CLA	CAA-CBA-CGA-O1A
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	A	1140	CLA	CAA-CBA-CGA-O1A
15	A	1106	CLA	C13-C15-C16-C17
15	2	612	CLA	CAA-CBA-CGA-O1A
15	B	1213	CLA	CAA-CBA-CGA-O1A
15	B	1235	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	O1A-CGA-O2A-C1
15	A	1113	CLA	C4B-C3B-CAB-CBB
15	F	1301	CLA	C4B-C3B-CAB-CBB
16	1	609	CHL	C4B-C3B-CAB-CBB
16	2	613	CHL	C4B-C3B-CAB-CBB
16	4	610	CHL	C4B-C3B-CAB-CBB
16	4	611	CHL	C4B-C3B-CAB-CBB
17	A	5002	LHG	C3-O3-P-O5
15	1	611	CLA	CAA-CBA-CGA-O1A
15	A	1119	CLA	CAA-CBA-CGA-O1A
15	A	1124	CLA	CAA-CBA-CGA-O1A
15	A	1127	CLA	CAA-CBA-CGA-O1A
15	A	1117	CLA	O2A-C1-C2-C3
14	4	503	BCR	C23-C24-C25-C26
14	4	503	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
14	A	4004	BCR	C5-C6-C7-C8
14	B	4002	BCR	C23-C24-C25-C30
15	1	615	CLA	CAA-CBA-CGA-O1A
15	A	1141	CLA	CAA-CBA-CGA-O1A
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	A	1113	CLA	CAA-CBA-CGA-O1A
15	2	612	CLA	C2C-C3C-CAC-CBC
15	B	1227	CLA	CAA-CBA-CGA-O2A
15	A	1120	CLA	CAD-CBD-CGD-O1D
15	A	1132	CLA	CAD-CBD-CGD-O1D
15	B	1202	CLA	CAD-CBD-CGD-O1D
15	B	1216	CLA	CAD-CBD-CGD-O1D
15	4	609	CLA	CAA-CBA-CGA-O1A
15	A	1118	CLA	CAA-CBA-CGA-O1A
15	A	1137	CLA	CAA-CBA-CGA-O1A
15	B	1023	CLA	C6-C7-C8-C9
15	B	1240	CLA	C11-C12-C13-C14
25	A	2001	PQN	C16-C17-C18-C19
15	1	601	CLA	CAA-CBA-CGA-O2A
15	2	607	CLA	CAA-CBA-CGA-O2A
15	4	612	CLA	CAA-CBA-CGA-O2A
15	A	1109	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	2	603	CLA	CAA-CBA-CGA-O2A
15	A	1135	CLA	CAA-CBA-CGA-O2A
15	B	1211	CLA	CAA-CBA-CGA-O2A
15	B	1234	CLA	CAA-CBA-CGA-O2A
16	3	604	CHL	CAA-CBA-CGA-O2A
15	B	1235	CLA	C5-C6-C7-C8
15	1	605	CLA	C3A-C2A-CAA-CBA
15	2	605	CLA	C11-C10-C8-C7
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	A	1108	CLA	C3A-C2A-CAA-CBA
25	B	2002	PQN	C22-C23-C25-C26
15	A	1109	CLA	CAA-CBA-CGA-O1A
15	A	1128	CLA	CAA-CBA-CGA-O1A
15	B	1209	CLA	CAA-CBA-CGA-O2A
15	B	1232	CLA	CAA-CBA-CGA-O2A
15	F	1302	CLA	CAA-CBA-CGA-O2A
15	3	601	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	A	1140	CLA	C3-C5-C6-C7
15	1	601	CLA	CAA-CBA-CGA-O1A
15	4	612	CLA	CAA-CBA-CGA-O1A
15	B	1209	CLA	CAA-CBA-CGA-O1A
15	B	1223	CLA	CAA-CBA-CGA-O1A
15	A	1101	CLA	CAA-CBA-CGA-O2A
15	3	607	CLA	CAA-CBA-CGA-O2A
15	2	607	CLA	CAA-CBA-CGA-O1A
15	A	1125	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	B	1211	CLA	CAA-CBA-CGA-O1A
15	B	1232	CLA	CAA-CBA-CGA-O1A
15	B	1227	CLA	CAA-CBA-CGA-O1A
15	4	606	CLA	CAA-CBA-CGA-O2A
15	B	1238	CLA	CAA-CBA-CGA-O2A
15	A	1012	CLA	C10-C11-C12-C13
15	1	615	CLA	C15-C16-C17-C18
15	3	607	CLA	CAA-CBA-CGA-O1A
15	A	1129	CLA	CAA-CBA-CGA-O1A
15	B	1216	CLA	CAA-CBA-CGA-O2A
15	B	1228	CLA	CAA-CBA-CGA-O2A
21	4	811	DGD	O1G-C1A-C2A-C3A
15	A	1101	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

188 monomers are involved in 1127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1236	CLA	6	0
18	2	802	LMG	1	0
14	1	505	BCR	7	0
15	A	1107	CLA	6	0
15	B	1235	CLA	11	0
17	2	801	LHG	2	0
14	1	503	BCR	8	0
15	A	1122	CLA	3	0
15	2	602	CLA	6	0
14	A	4007	BCR	9	0
15	1	603	CLA	9	0
15	A	1112	CLA	1	0
15	2	603	CLA	4	0
15	A	1116	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	3	503	BCR	20	0
13	3	502	XAT	21	0
15	4	607	CLA	4	0
21	2	811	DGD	2	0
15	J	1302	CLA	9	0
17	1	801	LHG	2	0
14	A	4003	BCR	2	0
15	4	604	CLA	14	0
15	A	1121	CLA	3	0
15	1	611	CLA	7	0
19	1	811	SQD	4	0
15	1	612	CLA	3	0
15	B	1216	CLA	8	0
14	B	4004	BCR	5	0
25	A	2001	PQN	9	0
15	4	605	CLA	9	0
14	A	4002	BCR	6	0
14	4	505	BCR	4	0
12	1	501	LUT	10	0
15	A	1131	CLA	2	0
16	4	613	CHL	7	0
15	A	1126	CLA	6	0
20	4	902	CAC	1	0
15	3	610	CLA	4	0
23	B	5031	GSH	2	0
15	A	1106	CLA	8	0
14	B	4005	BCR	5	0
15	A	1130	CLA	4	0
15	A	1139	CLA	9	0
15	4	612	CLA	9	0
15	2	601	CLA	15	0
15	B	1221	CLA	5	0
15	B	1234	CLA	7	0
18	1	802	LMG	1	0
15	B	1218	CLA	4	0
15	4	606	CLA	7	0
15	2	615	CLA	1	0
15	3	606	CLA	18	0
15	1	602	CLA	1	0
15	A	1103	CLA	8	0
15	1	604	CLA	16	0
16	4	611	CHL	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1135	CLA	3	0
16	2	610	CHL	4	0
15	2	604	CLA	5	0
15	3	601	CLA	15	0
26	C	3003	SF4	2	0
15	B	1213	CLA	2	0
15	A	1134	CLA	2	0
15	A	1102	CLA	6	0
15	3	608	CLA	5	0
15	A	1109	CLA	14	0
15	B	1217	CLA	2	0
14	J	4002	BCR	16	0
15	A	1101	CLA	5	0
15	A	1137	CLA	6	0
15	1	606	CLA	17	0
14	4	503	BCR	8	0
15	B	1023	CLA	20	0
15	F	1302	CLA	2	0
15	A	1111	CLA	23	0
15	A	1108	CLA	6	0
15	2	606	CLA	4	0
15	B	1215	CLA	4	0
15	4	601	CLA	12	0
14	A	4004	BCR	4	0
15	2	612	CLA	11	0
15	A	1138	CLA	10	0
15	B	1206	CLA	4	0
15	B	1238	CLA	1	0
12	4	501	LUT	18	0
14	3	504	BCR	5	0
15	B	1219	CLA	5	0
16	2	609	CHL	12	0
15	2	608	CLA	3	0
15	4	602	CLA	6	0
15	A	1128	CLA	10	0
14	B	4003	BCR	9	0
15	A	1133	CLA	4	0
16	1	610	CHL	15	0
15	4	603	CLA	3	0
15	A	1115	CLA	7	0
15	B	1237	CLA	2	0
21	4	811	DGD	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	607	CLA	1	0
15	B	1226	CLA	9	0
15	B	1231	CLA	10	0
15	A	1123	CLA	9	0
15	B	1230	CLA	13	0
15	3	612	CLA	10	0
15	3	603	CLA	22	0
15	B	1228	CLA	8	0
15	B	1222	CLA	6	0
15	3	605	CLA	11	0
15	A	1105	CLA	2	0
24	A	1011	CL0	19	0
15	1	607	CLA	4	0
15	3	613	CLA	14	0
15	4	609	CLA	9	0
15	A	1104	CLA	6	0
15	A	1114	CLA	6	0
14	A	4005	BCR	11	0
15	B	1204	CLA	5	0
15	B	1214	CLA	9	0
15	B	1220	CLA	6	0
15	2	607	CLA	8	0
15	B	1201	CLA	2	0
15	A	1124	CLA	12	0
15	F	1301	CLA	5	0
15	A	1119	CLA	3	0
25	B	2002	PQN	8	0
15	A	1132	CLA	3	0
14	B	4001	BCR	2	0
15	4	608	CLA	4	0
15	A	1113	CLA	6	0
15	B	1211	CLA	8	0
16	1	609	CHL	11	0
15	A	1140	CLA	7	0
15	A	1129	CLA	2	0
13	1	502	XAT	11	0
15	B	1212	CLA	8	0
23	4	831	GSH	0	1
15	A	1141	CLA	3	0
15	B	1232	CLA	3	0
15	A	1012	CLA	24	0
15	1	601	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	2	501	LUT	13	0
15	2	605	CLA	6	0
20	3	902	CAC	1	0
15	4	615	CLA	7	0
16	4	610	CHL	5	0
21	B	5002	DGD	5	0
16	2	613	CHL	6	0
14	A	4006	BCR	7	0
15	B	1225	CLA	6	0
15	B	1021	CLA	21	0
15	B	1227	CLA	7	0
15	3	611	CLA	8	0
15	B	1223	CLA	5	0
15	A	1117	CLA	5	0
14	J	4001	BCR	7	0
13	4	502	XAT	5	0
15	B	1224	CLA	4	0
15	B	1202	CLA	4	0
15	B	1022	CLA	7	0
15	B	1210	CLA	7	0
15	A	1125	CLA	10	0
15	1	615	CLA	4	0
16	3	604	CHL	15	0
16	2	611	CHL	3	0
14	J	4003	BCR	4	0
12	3	501	LUT	11	0
17	A	5002	LHG	4	0
15	A	1110	CLA	16	0
15	B	1239	CLA	12	0
14	B	4002	BCR	2	0
15	B	1229	CLA	6	0
14	B	4006	BCR	11	0
15	B	1205	CLA	4	0
15	A	1136	CLA	9	0
15	B	1209	CLA	2	0
15	A	1118	CLA	3	0
15	1	605	CLA	9	0
13	2	502	XAT	13	0
15	A	1013	CLA	28	0
15	B	1240	CLA	4	0
15	1	613	CLA	23	0
17	A	5001	LHG	1	0

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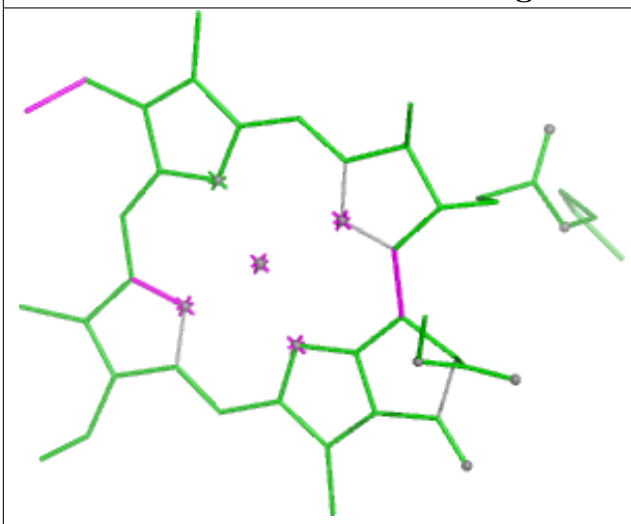
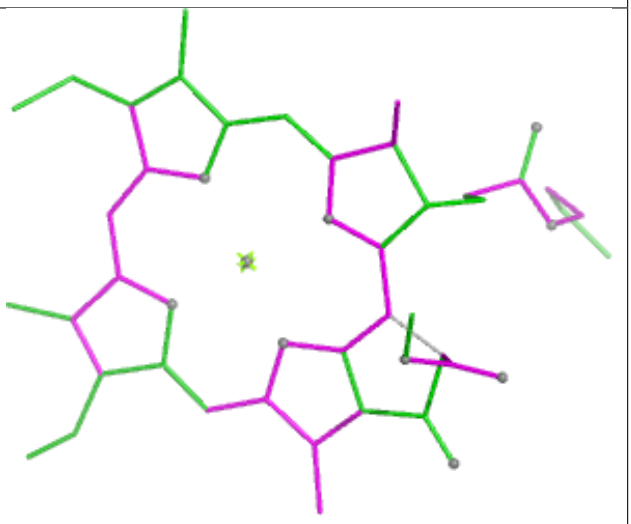
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	503	BCR	8	0
17	B	5001	LHG	2	0
15	1	608	CLA	11	0
15	B	1203	CLA	2	0
14	F	4002	BCR	5	0
15	A	1127	CLA	8	0

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.

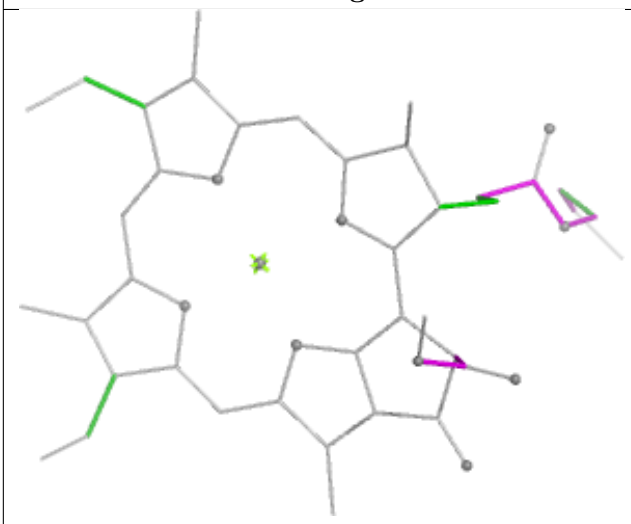
Ligand CLA B 1236



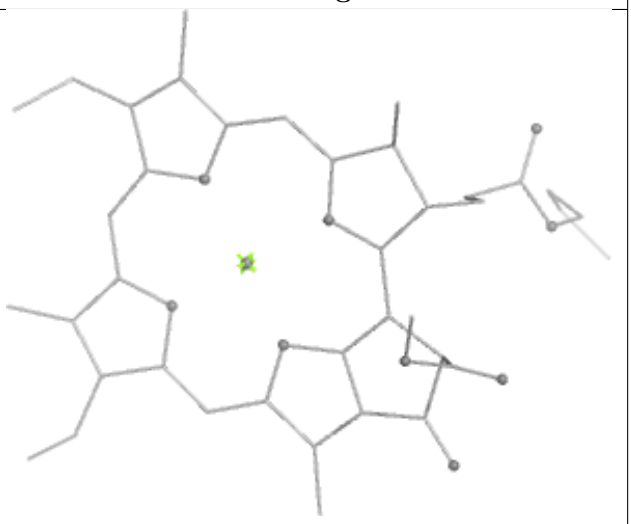
Bond lengths



Bond angles

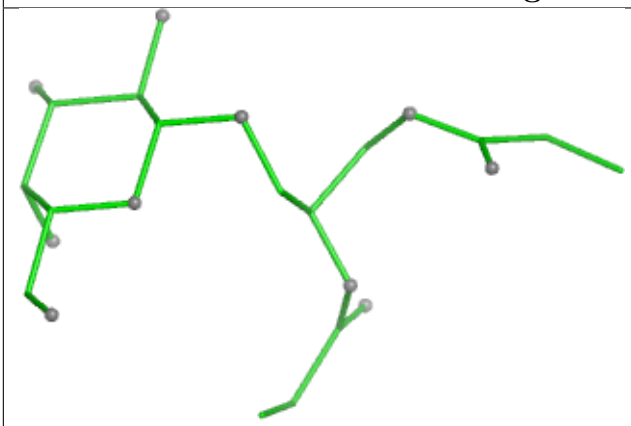


Torsions

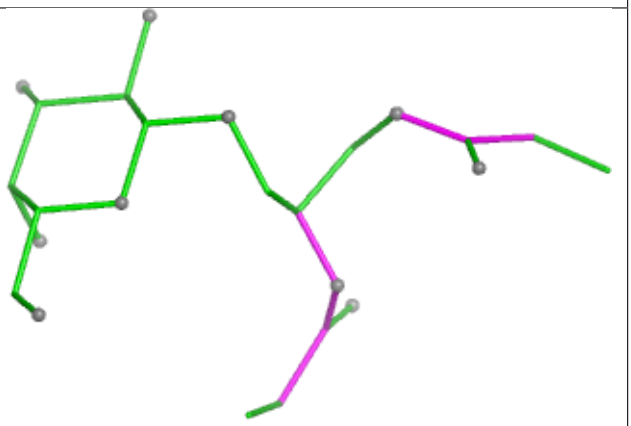


Rings

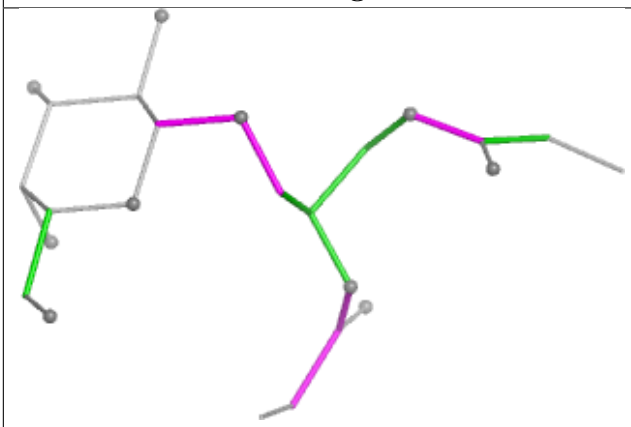
Ligand LMG 2 802



Bond lengths



Bond angles



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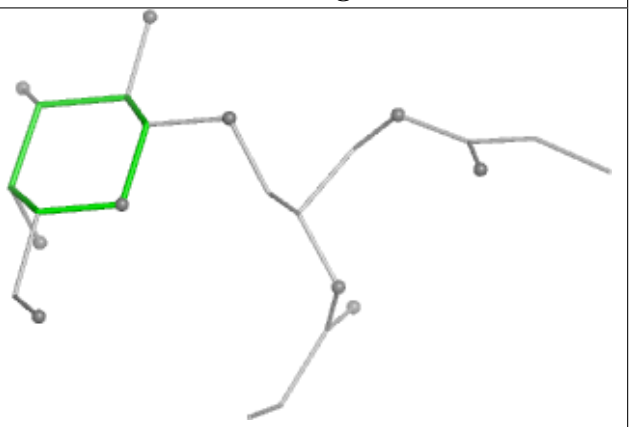
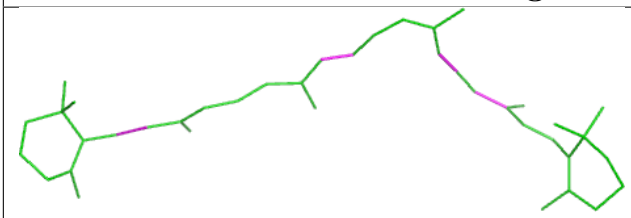
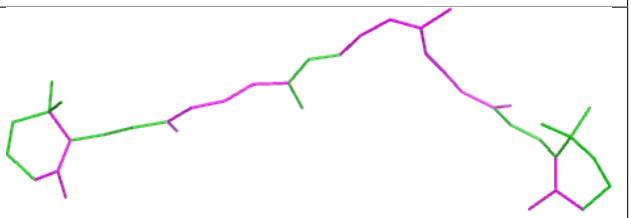


Rings

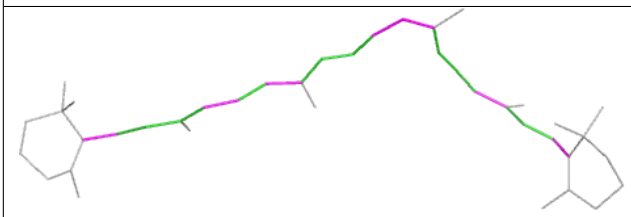
Ligand BCR 1 505



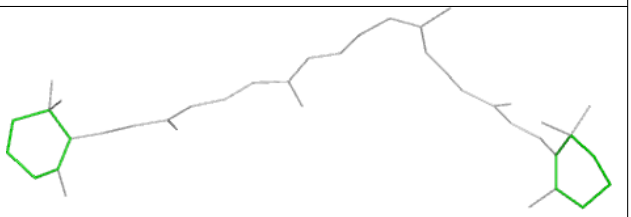
Bond lengths



Bond angles

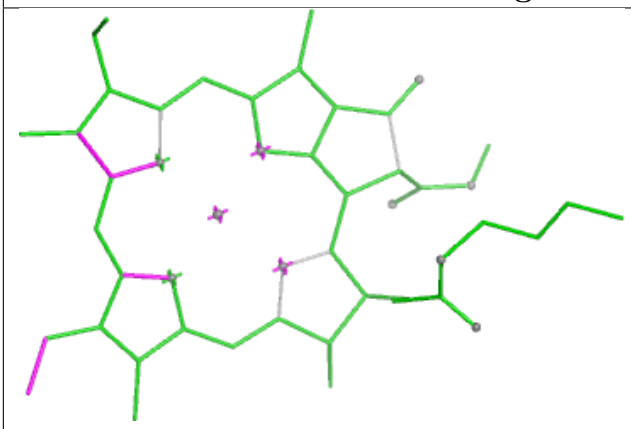


Torsions

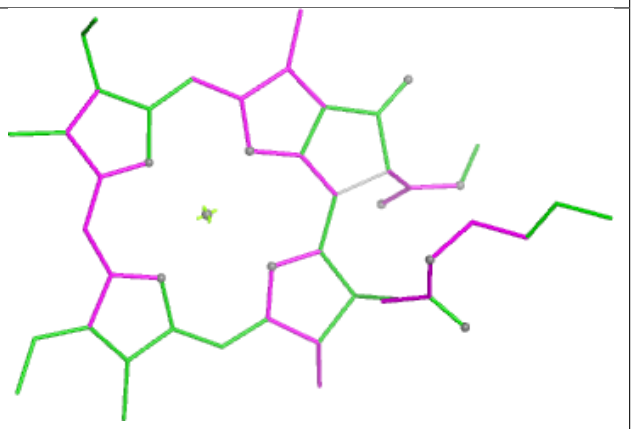


Rings

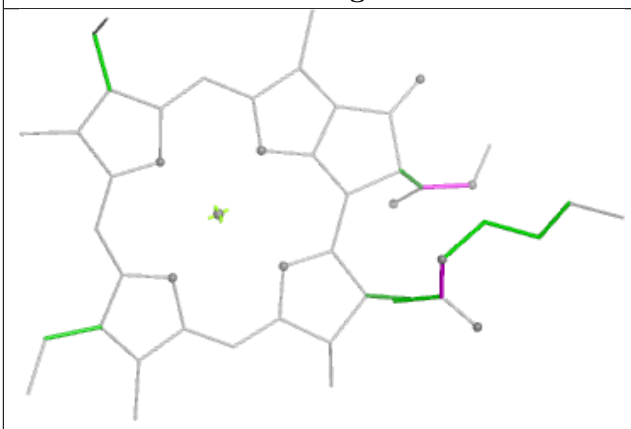
Ligand CLA A 1107



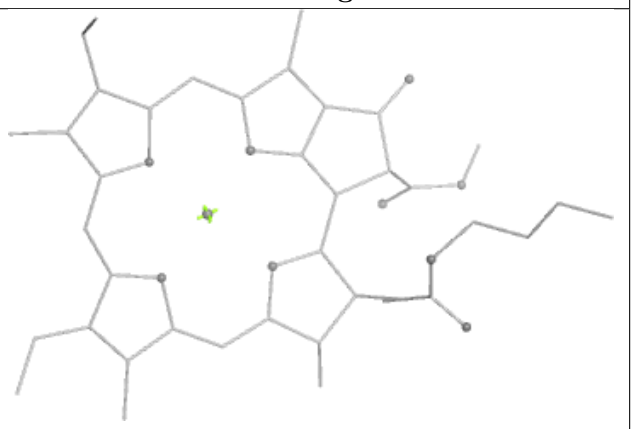
Bond lengths



Bond angles

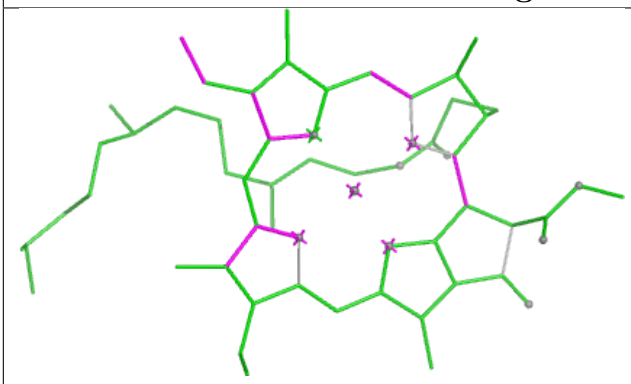


Torsions



Rings

Ligand CLA B 1235



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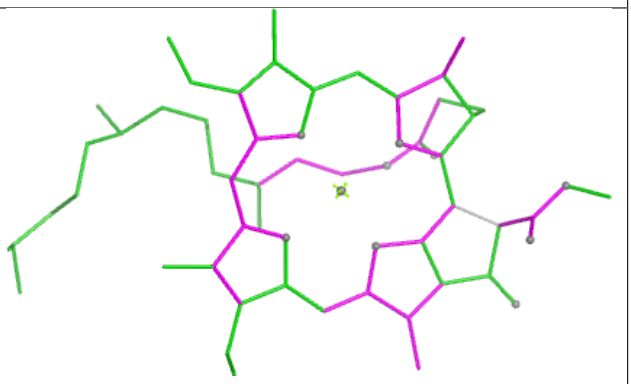
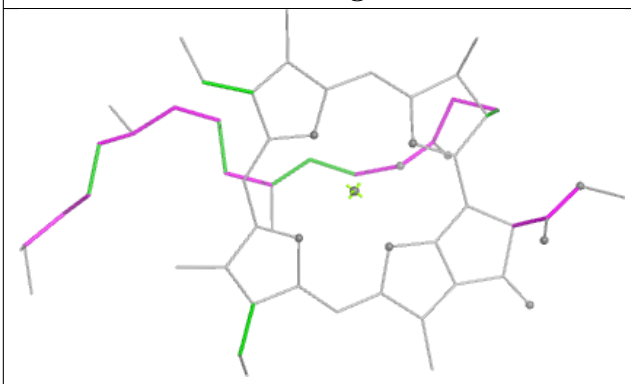


Bond angles



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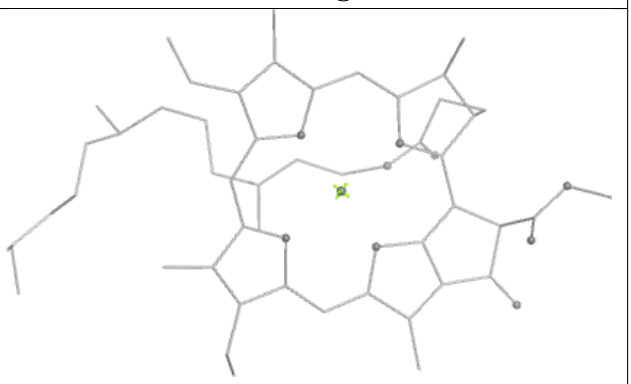
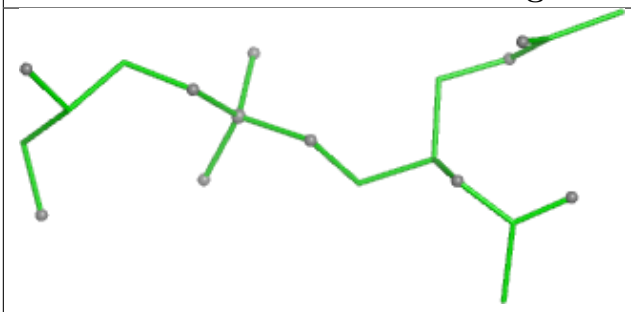


Rings

Ligand LHG 2 801



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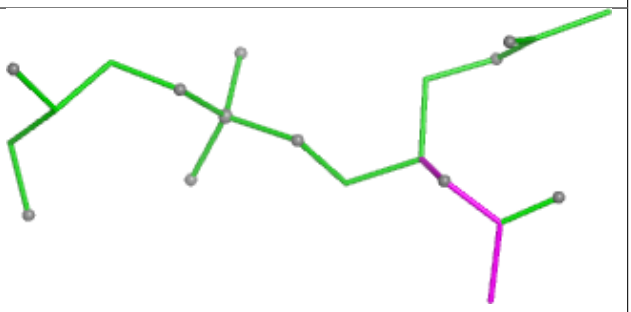

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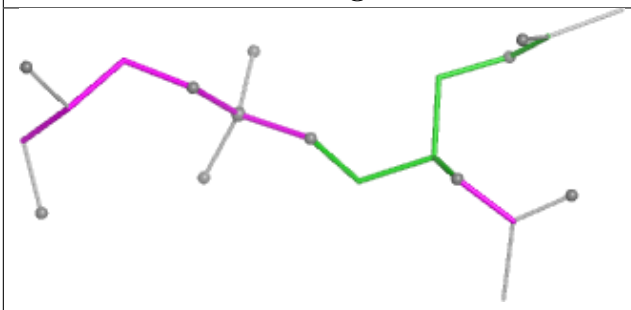

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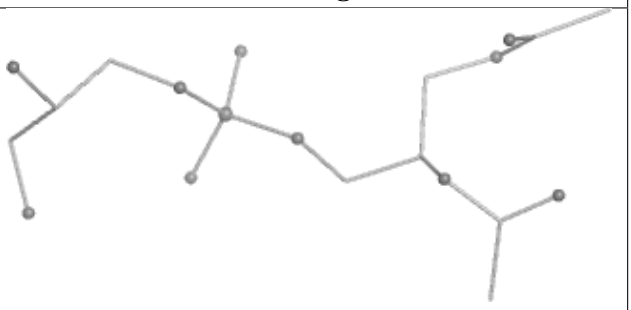
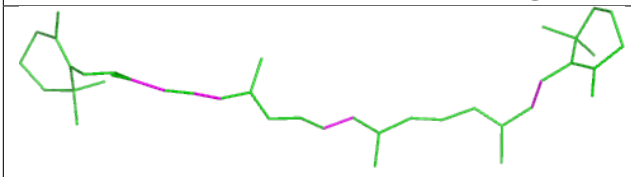


Rings

Ligand BCR 1 503



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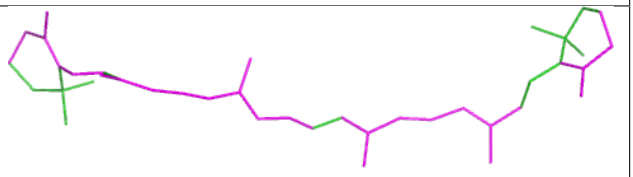

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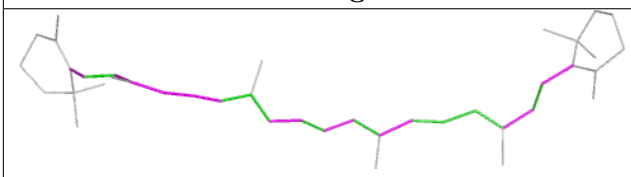

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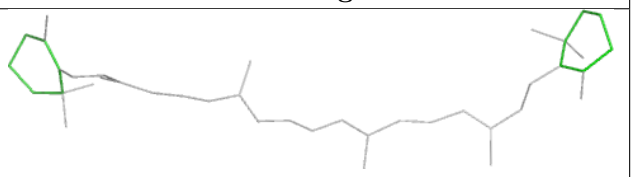
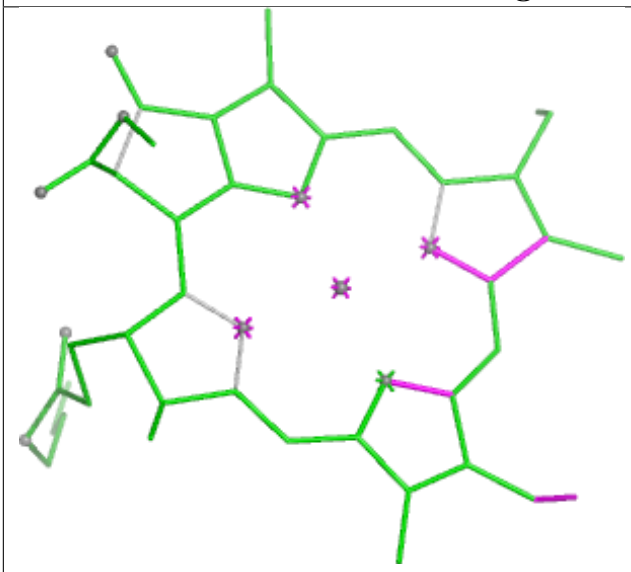


Rings

Ligand CLA A 1122



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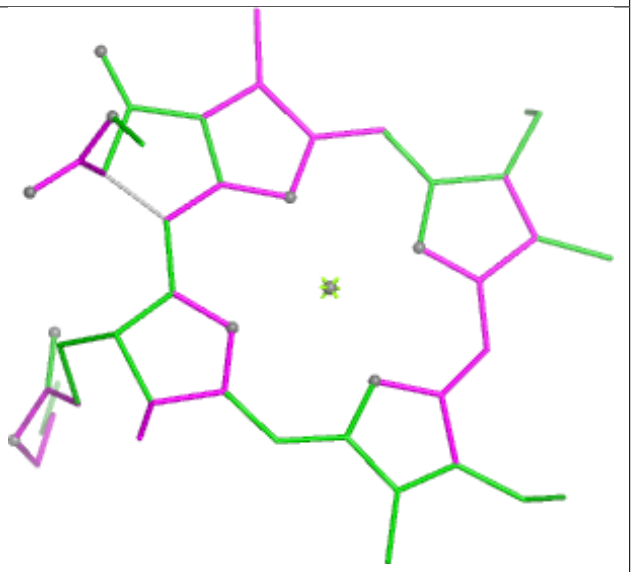

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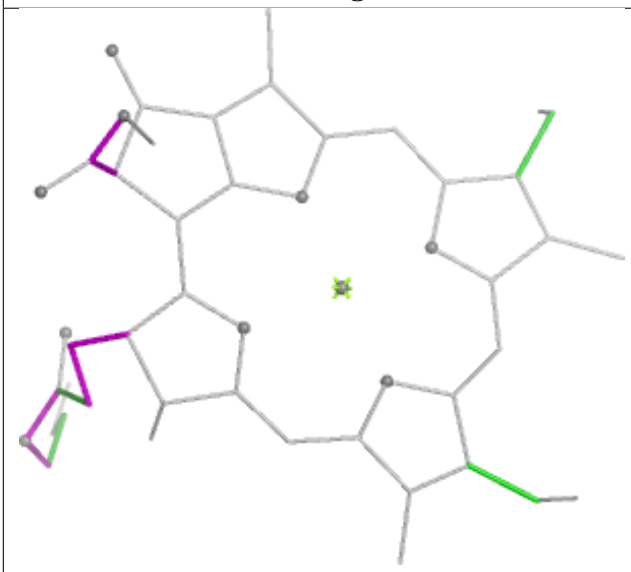

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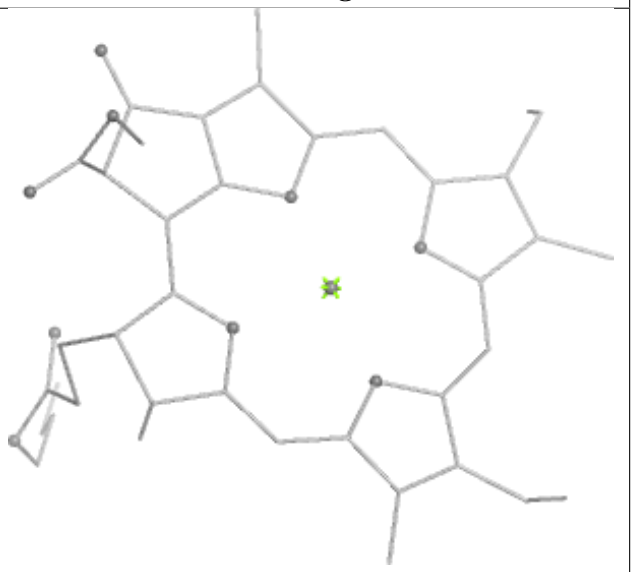
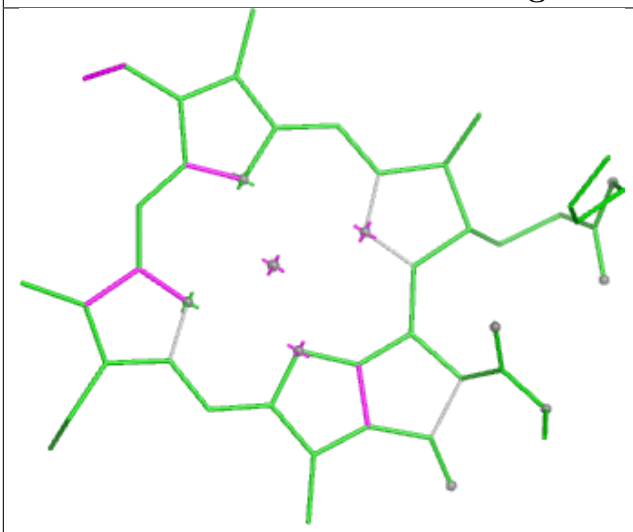


Rings

Ligand CLA 2 602



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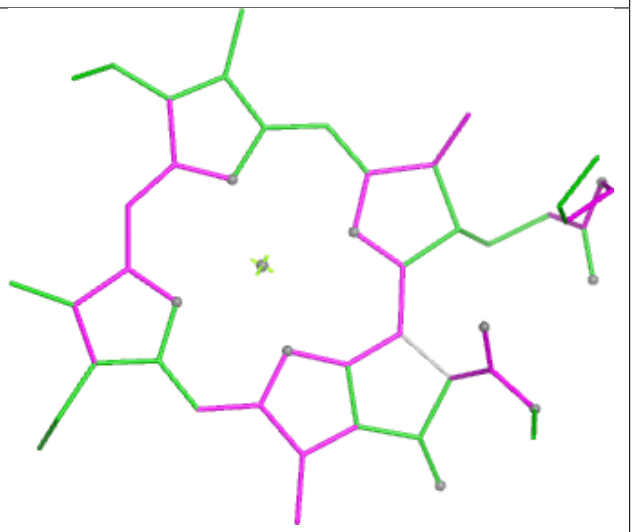

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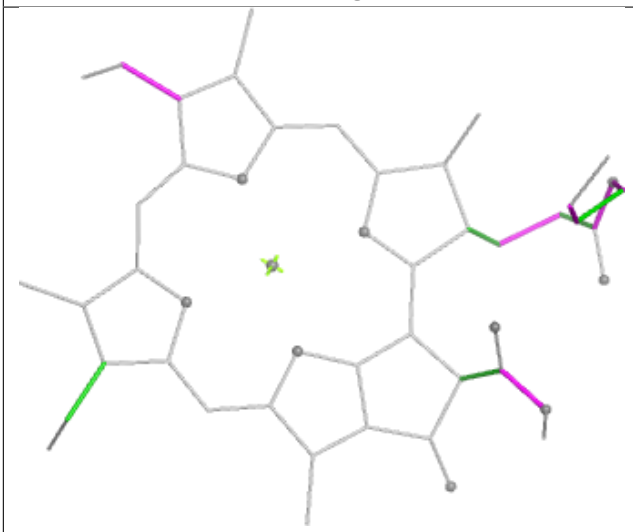

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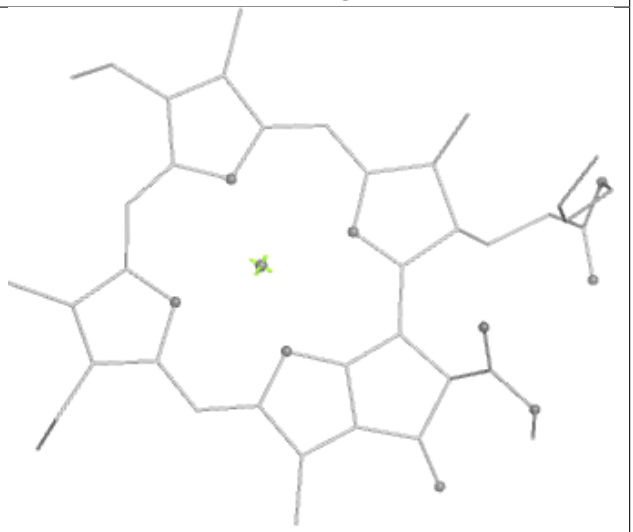
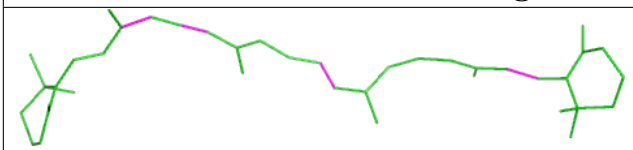


Rings

Ligand BCR A 4007



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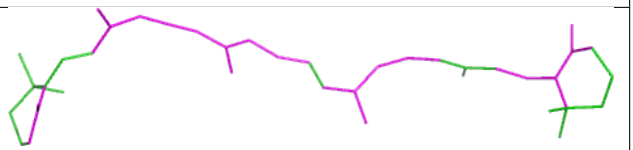
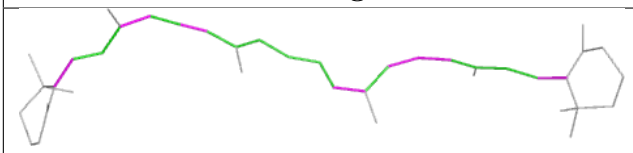


Bond angles



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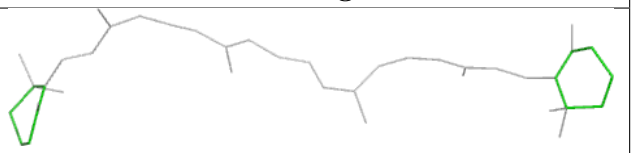
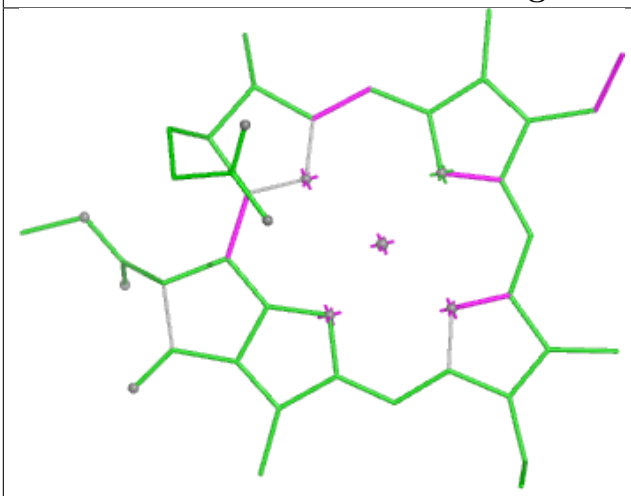


Rings

Ligand CLA 1 603



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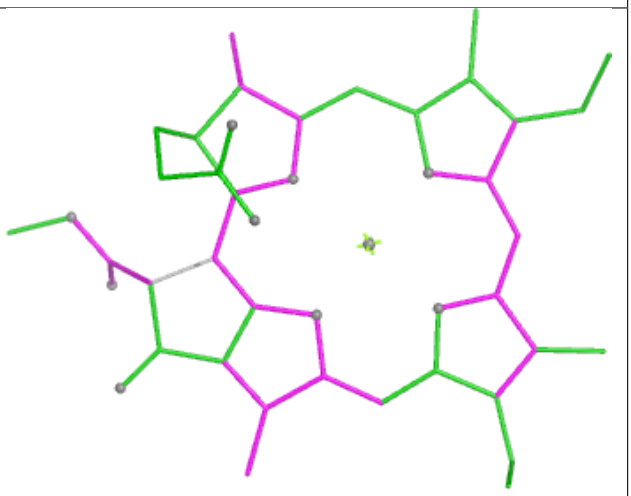

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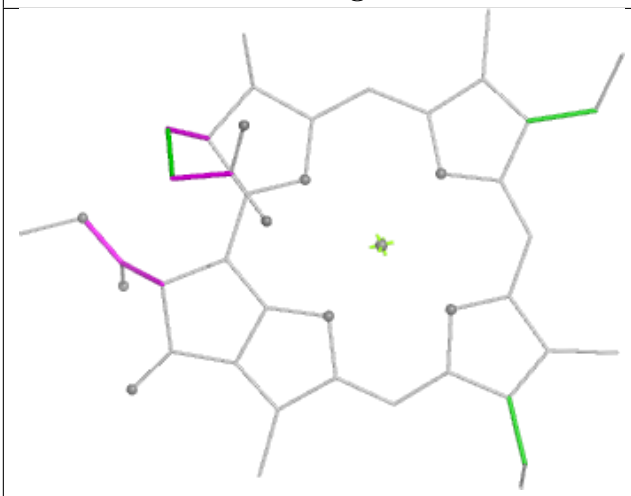

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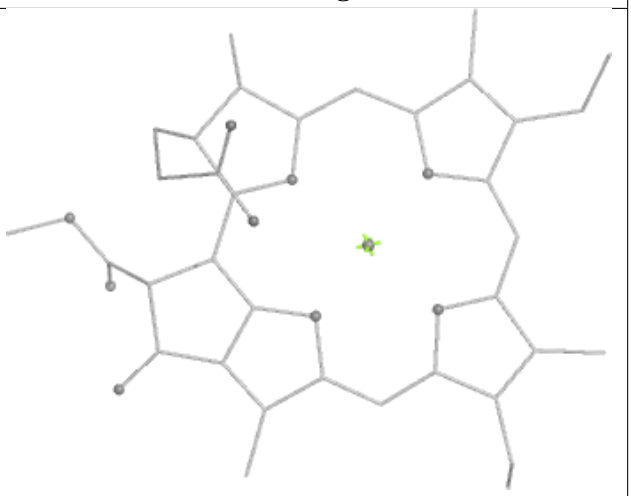
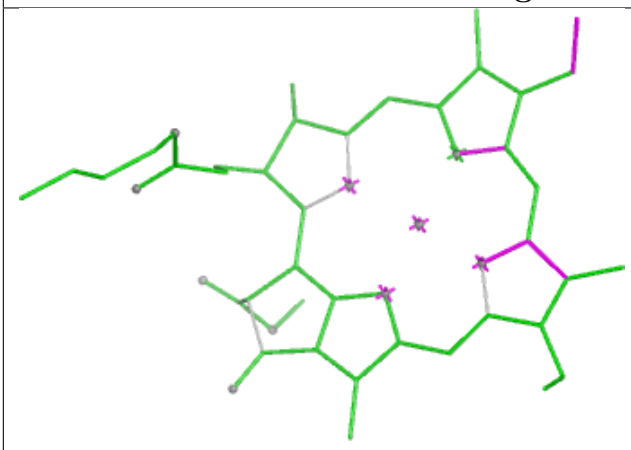


Rings

Ligand CLA A 1112



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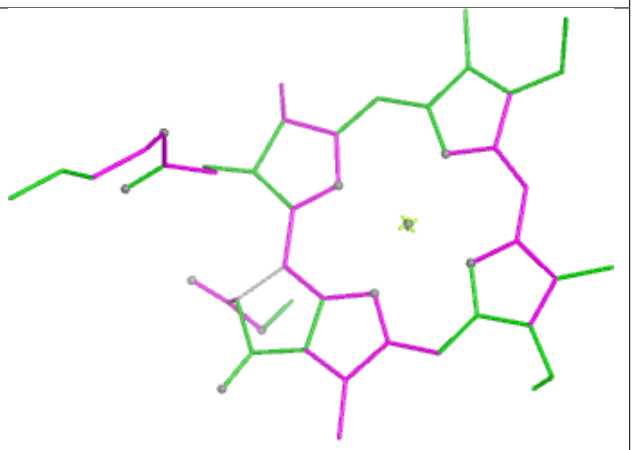

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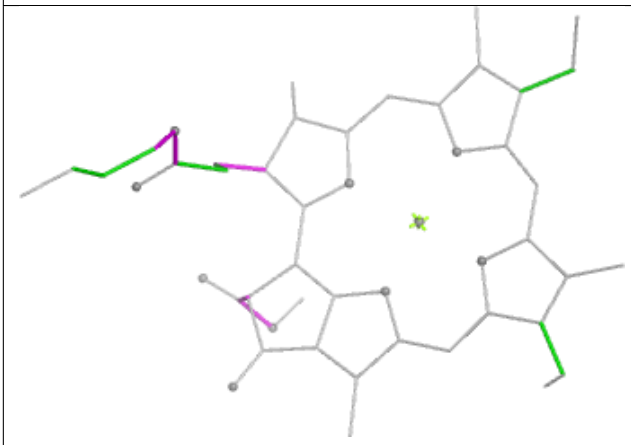

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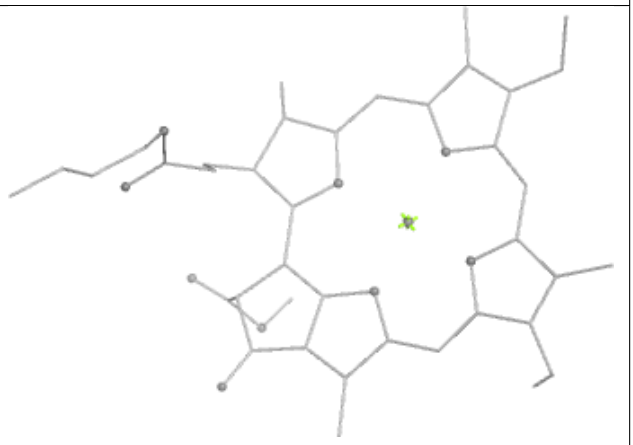
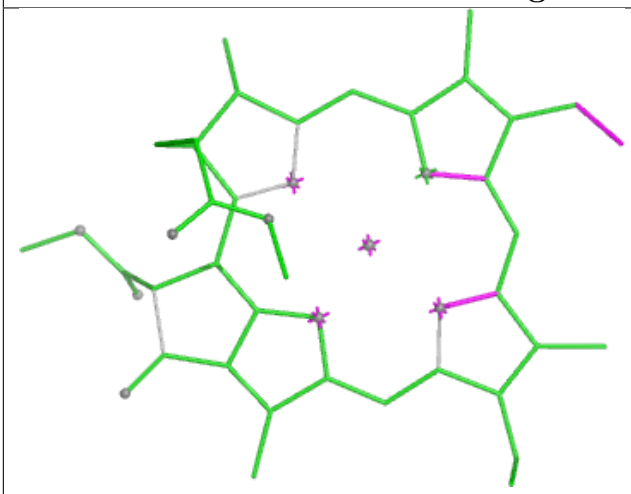


Rings

Ligand CLA 2 603



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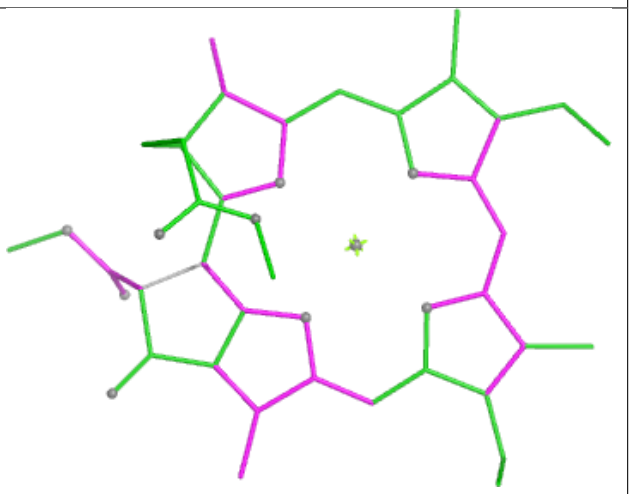
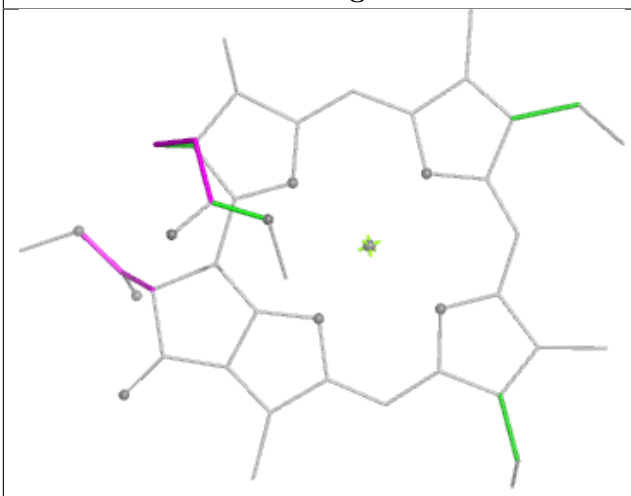


Bond angles



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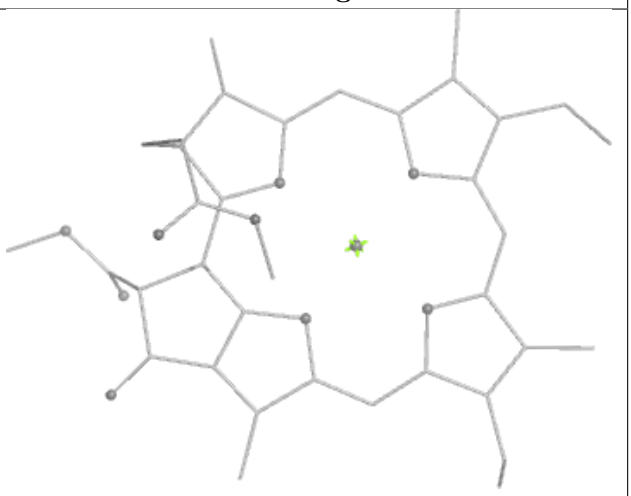
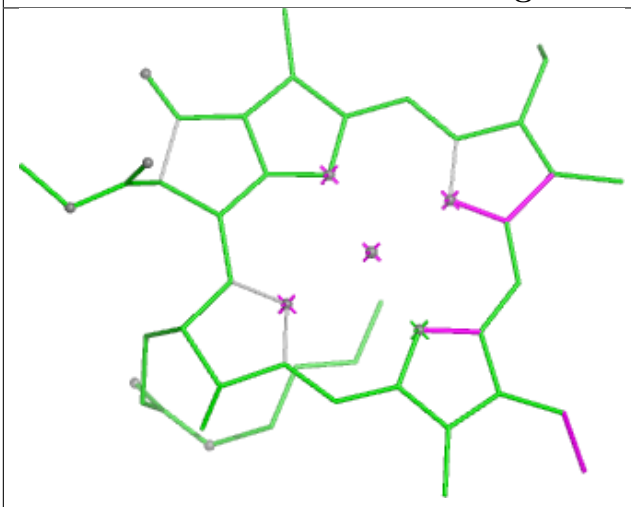


Rings

Ligand CLA A 1116



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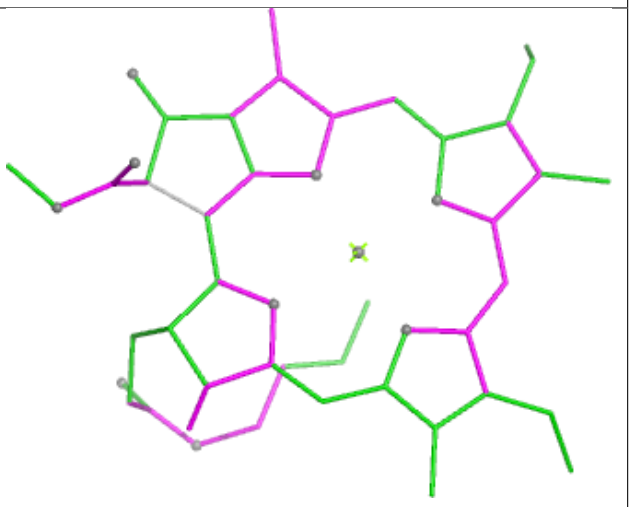

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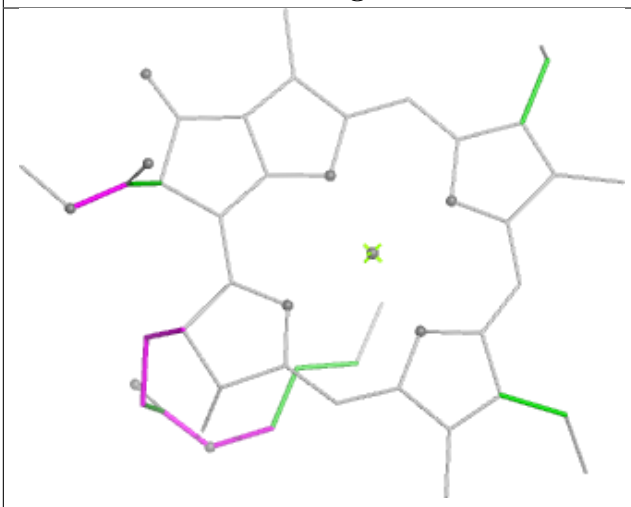

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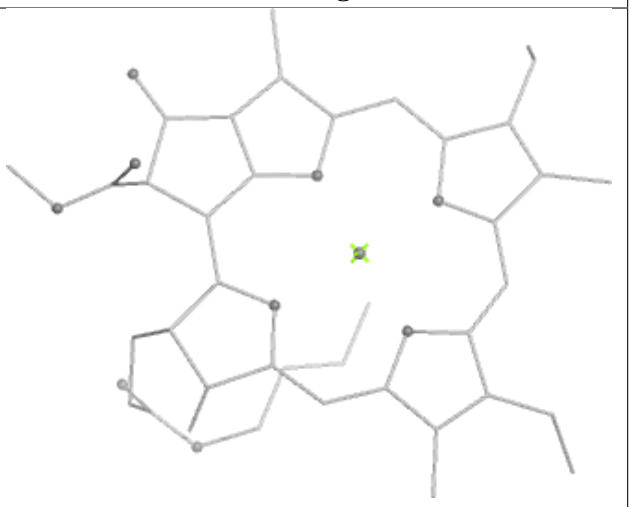
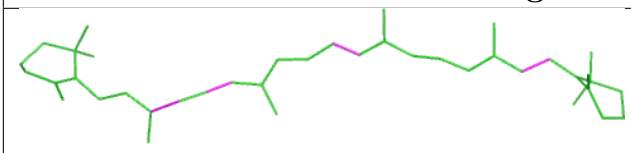


Rings

Ligand BCR 3 503



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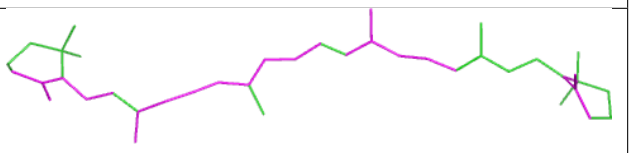

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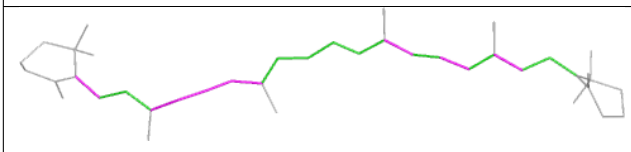

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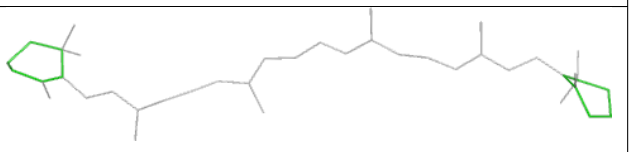
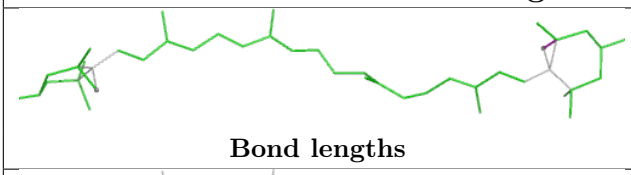


Rings

Ligand XAT 3 502



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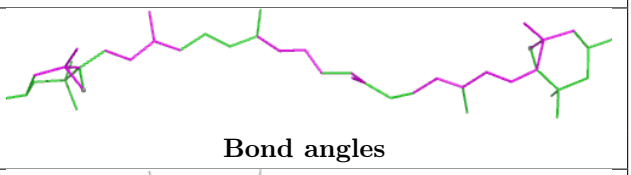
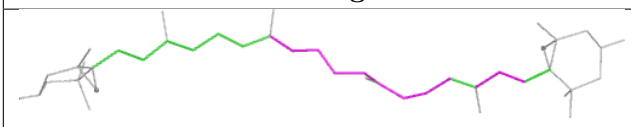


Bond angles



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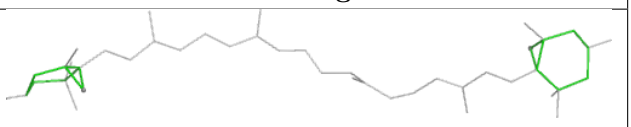
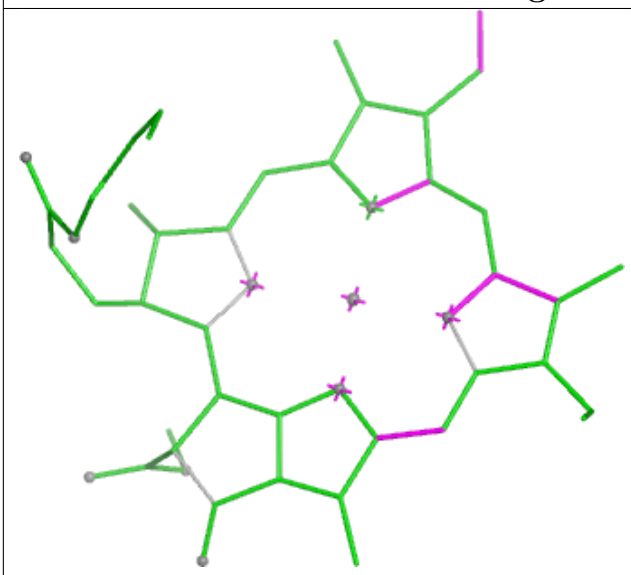


Rings

Ligand CLA 4 607



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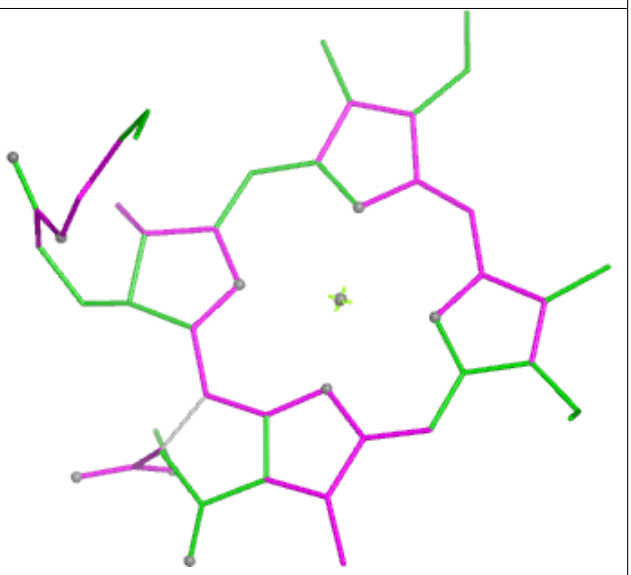
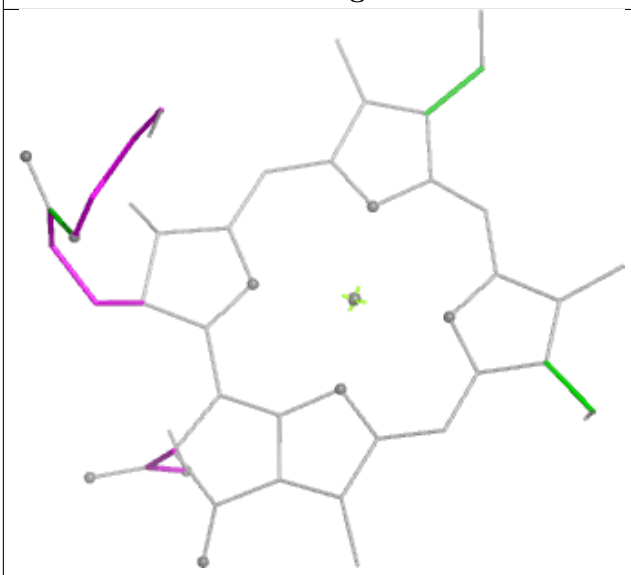


Bond angles



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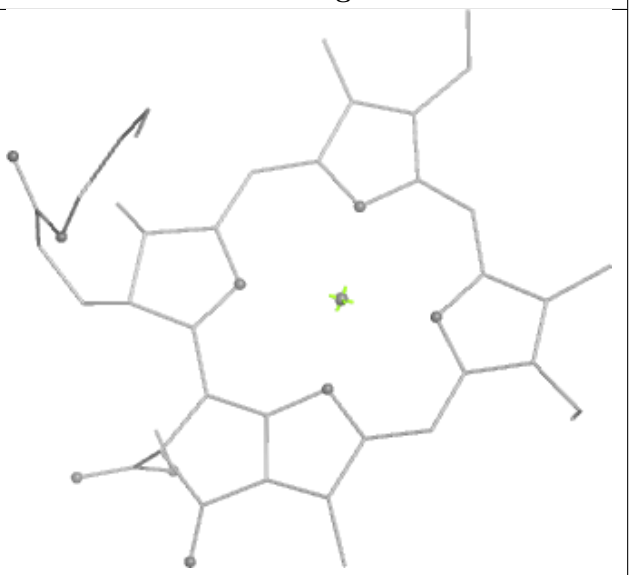
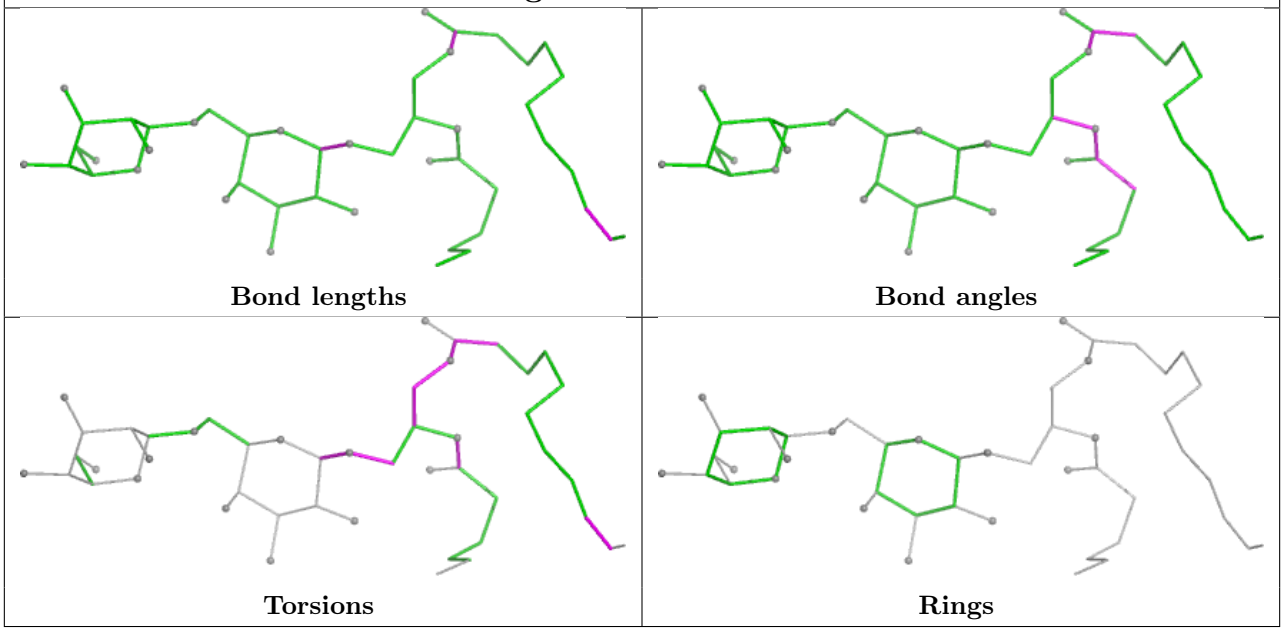
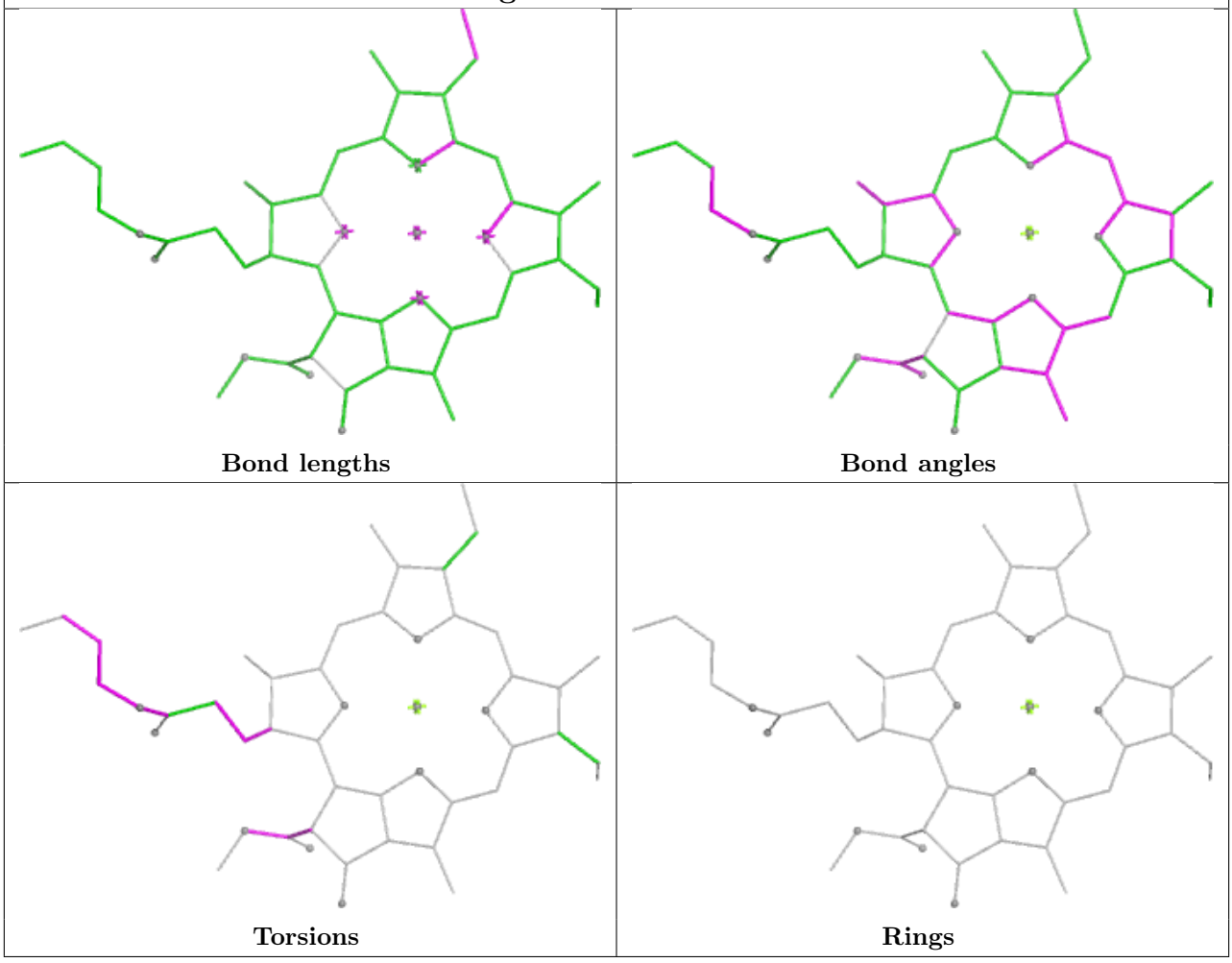


Rings

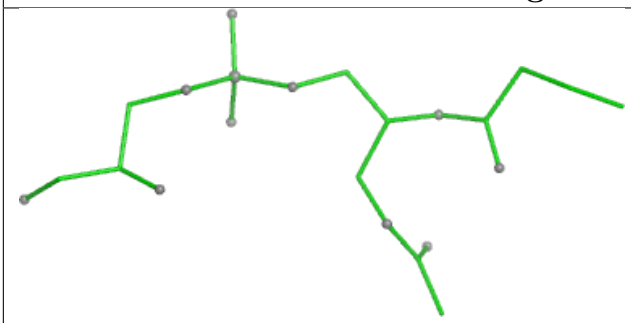
Ligand DGD 2 811



Ligand CLA J 1302



Ligand LHG 1 801



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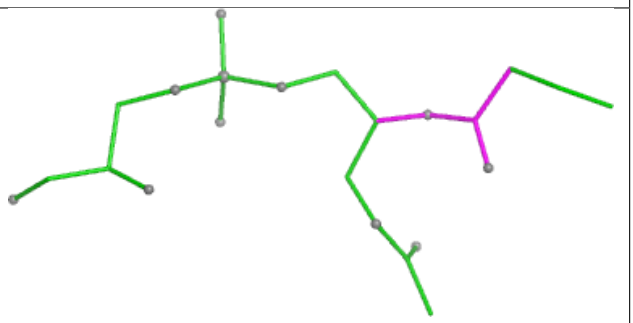
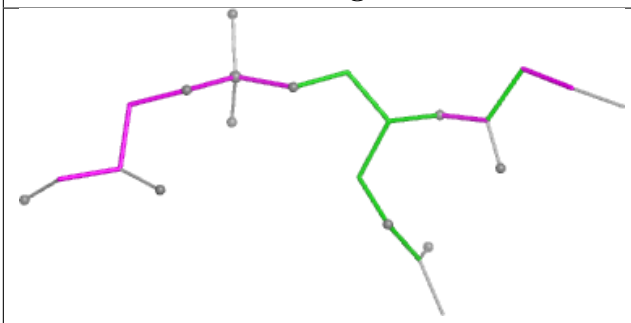
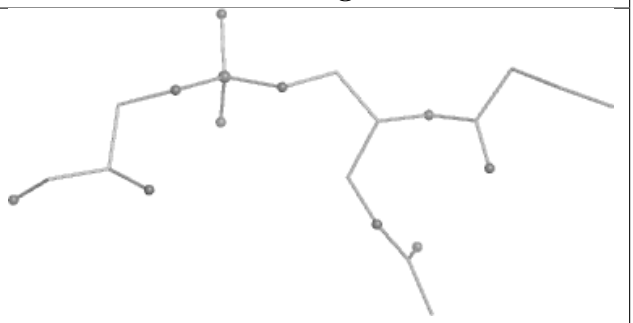


Bond angles

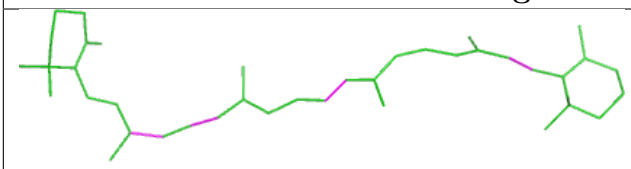


Torsions

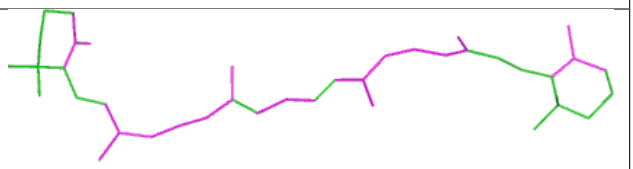


Rings

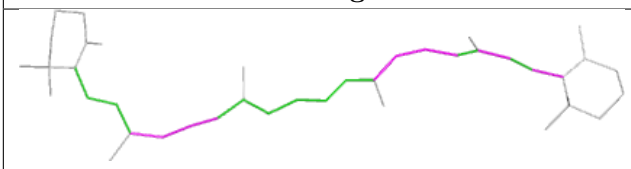
Ligand BCR A 4003



Bond lengths



Bond angles



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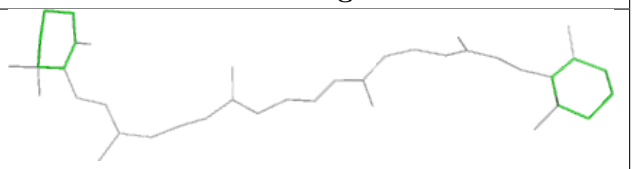
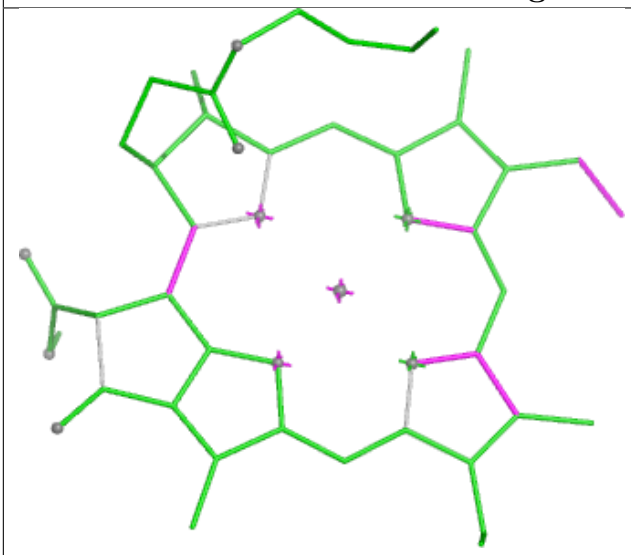


Rings

Ligand CLA 4 604



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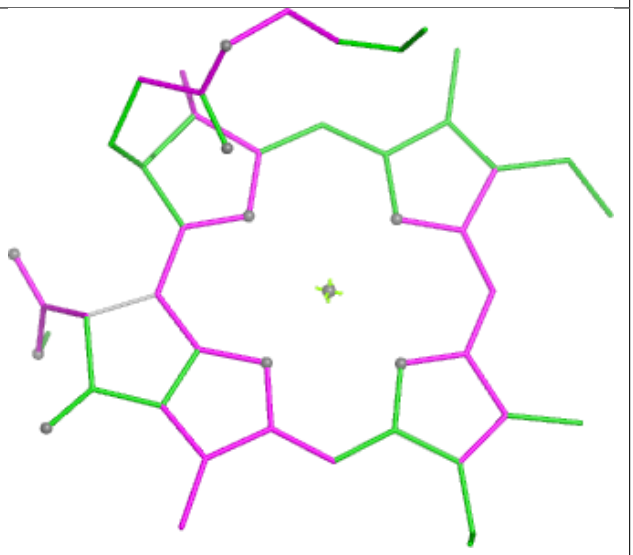

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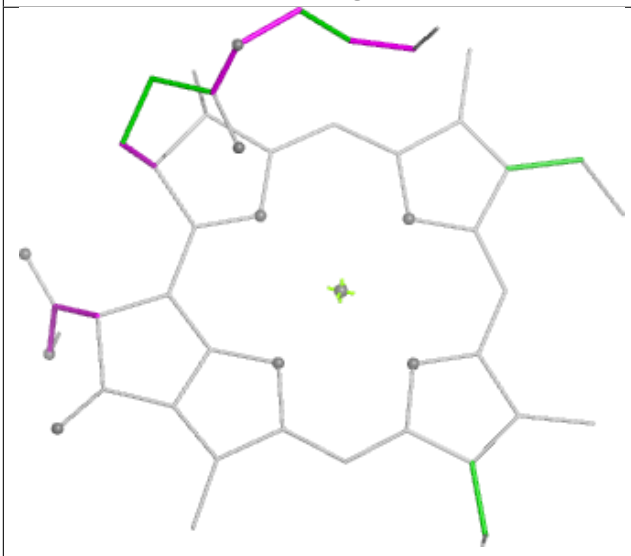

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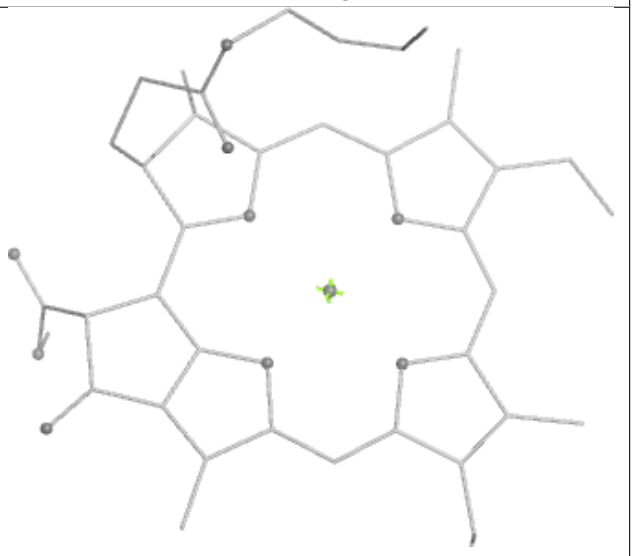
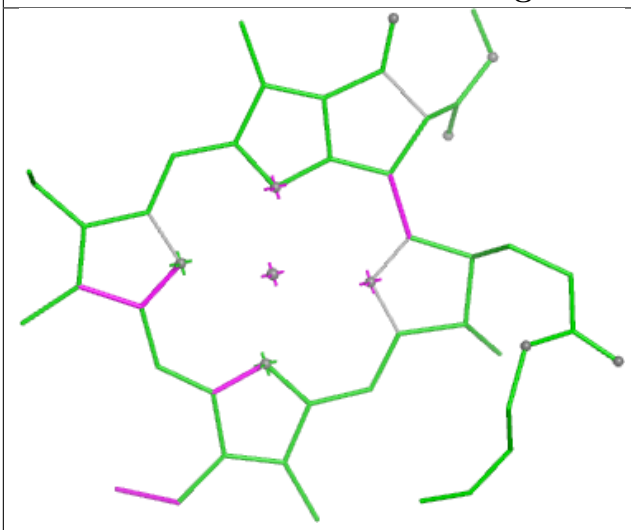


Rings

Ligand CLA A 1121



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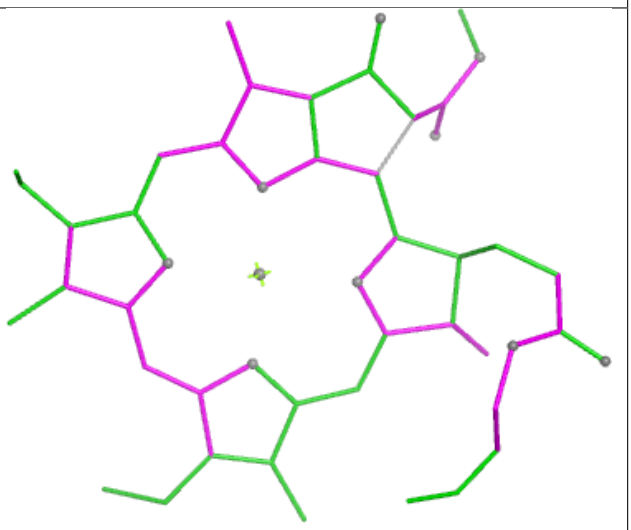

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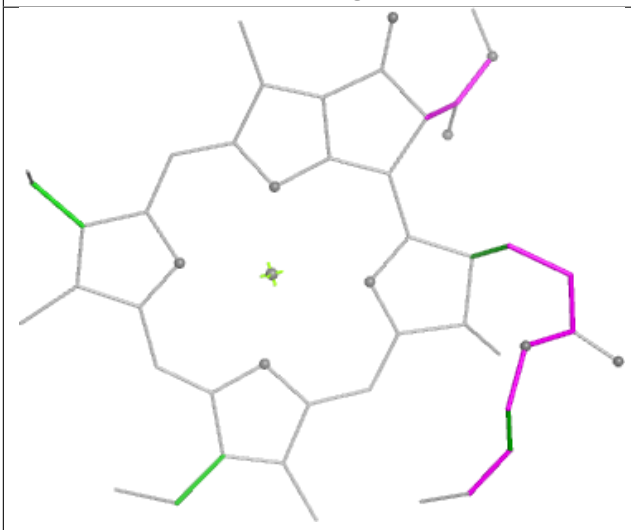

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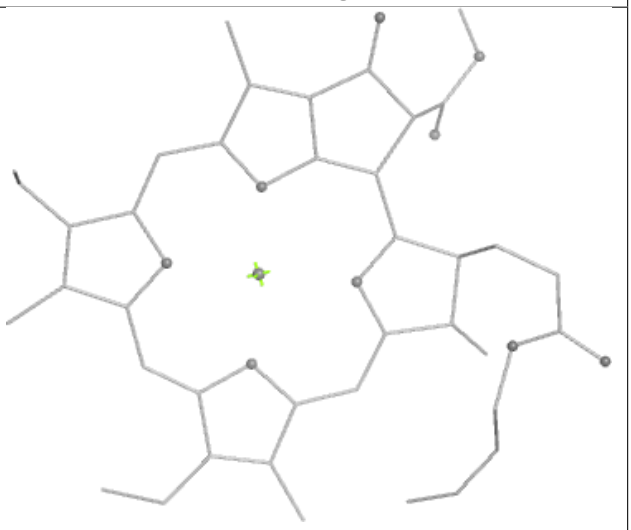
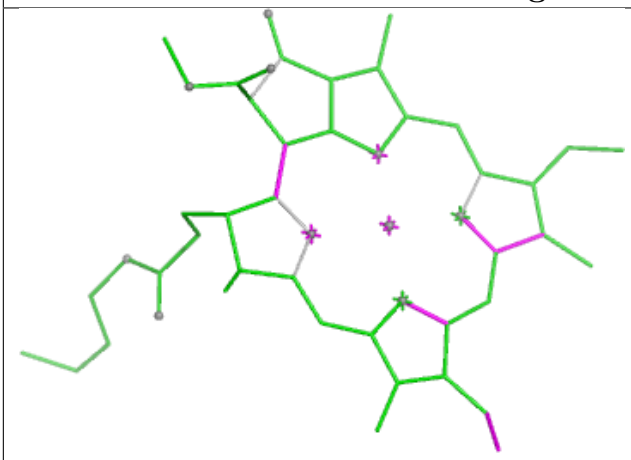


Rings

Ligand CLA 1 611



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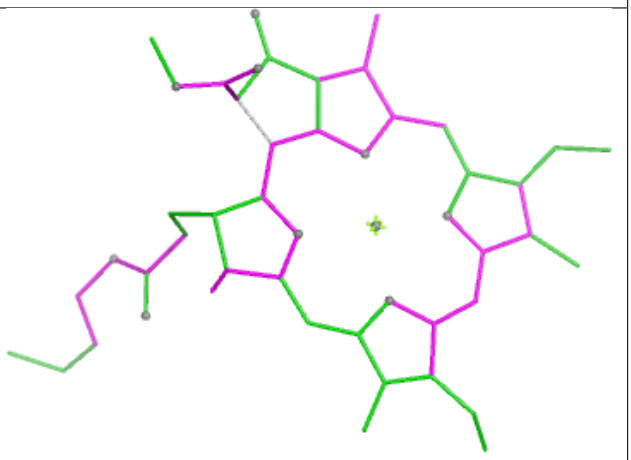
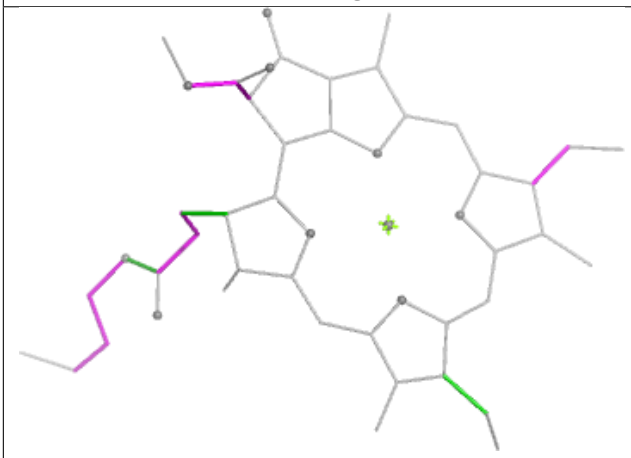


Bond angles



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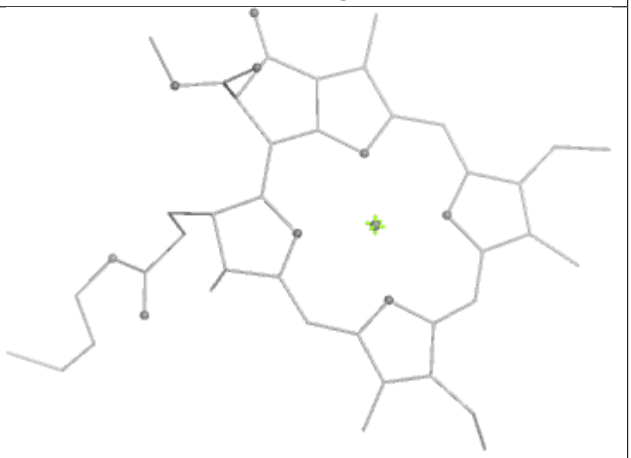
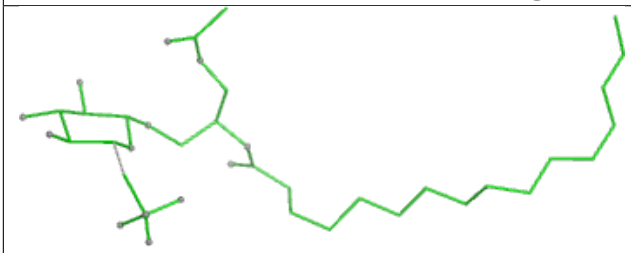


Rings

Ligand SQD 1 811



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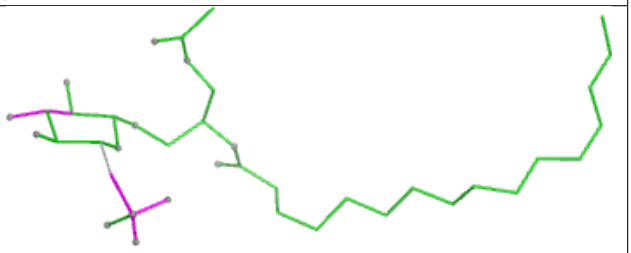
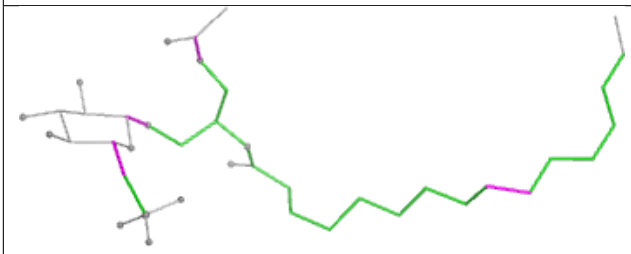


Bond angles



Torsions

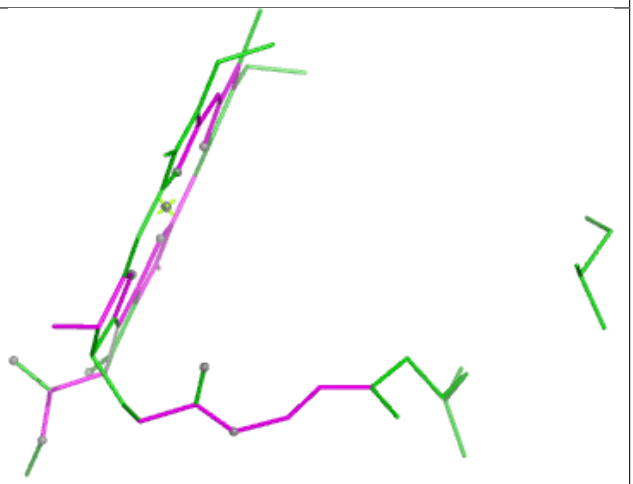


Rings

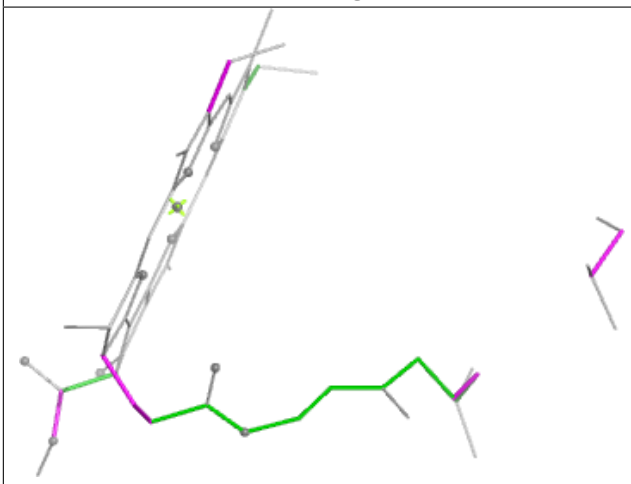
Ligand CLA 1 612



Bond lengths



Bond angles



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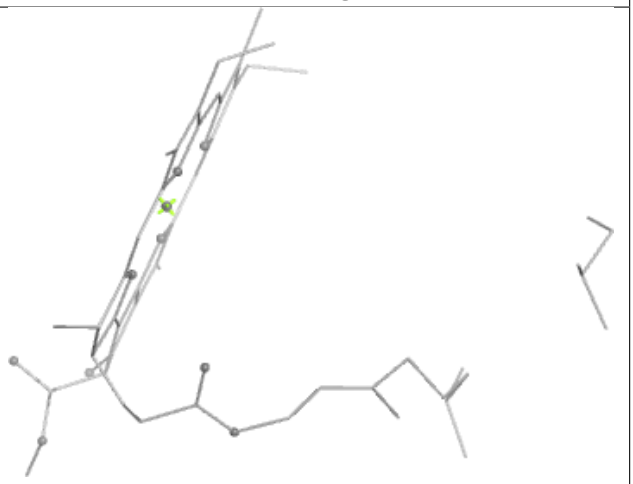
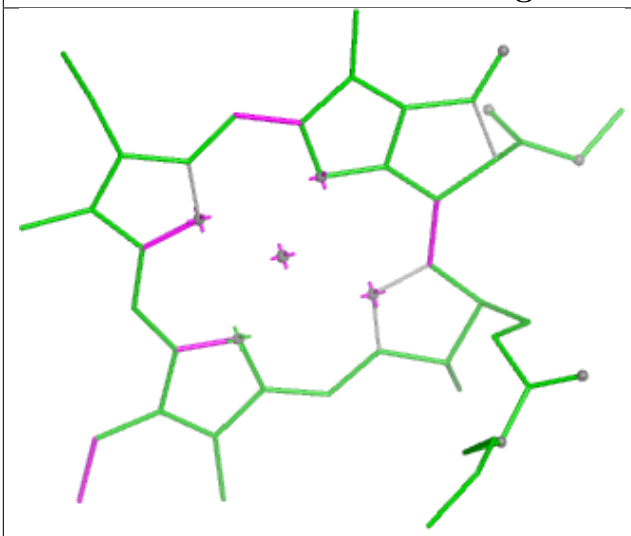


Rings

Ligand CLA B 1216



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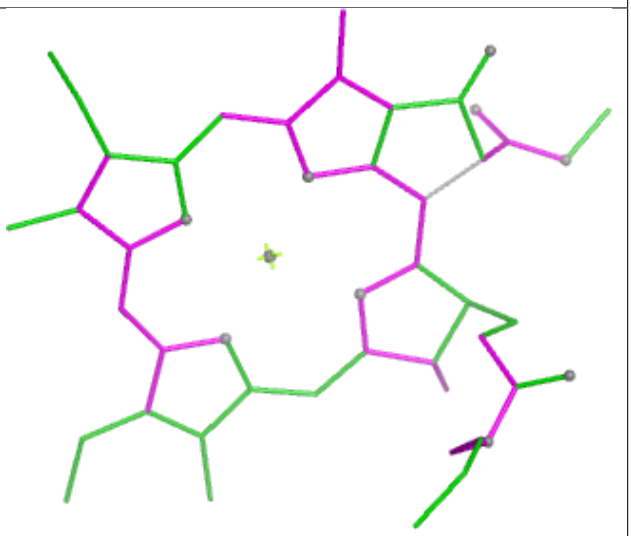

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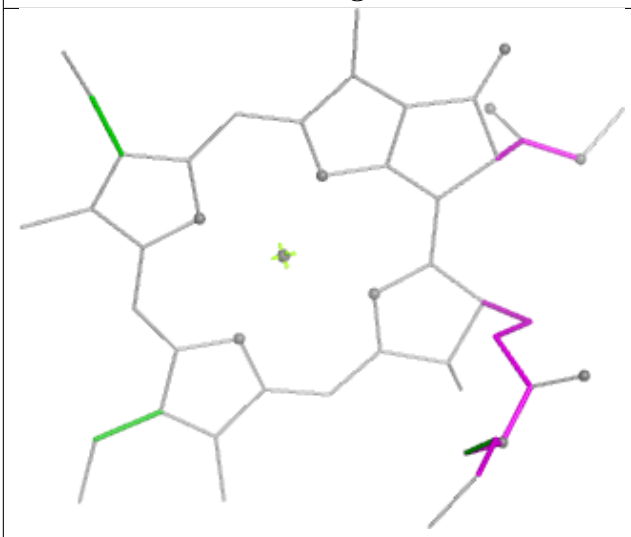

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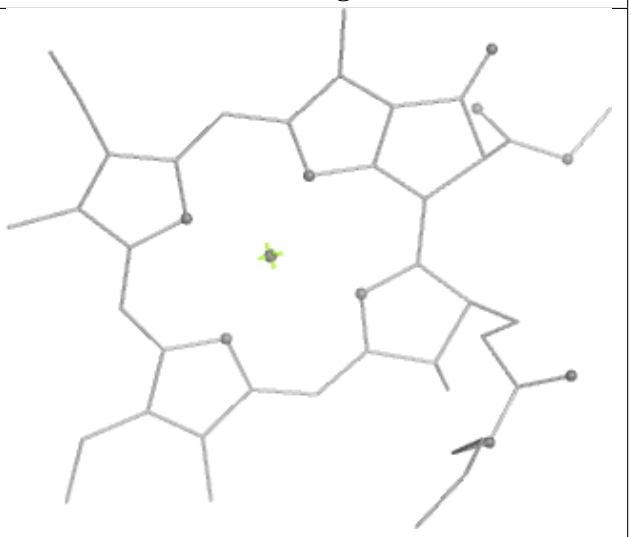
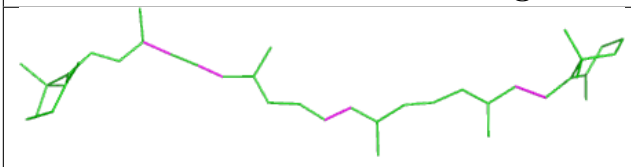


Rings

Ligand BCR B 4004



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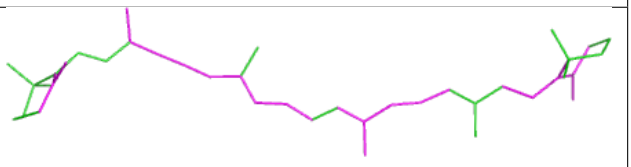
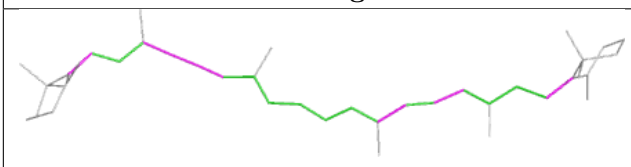


Bond angles



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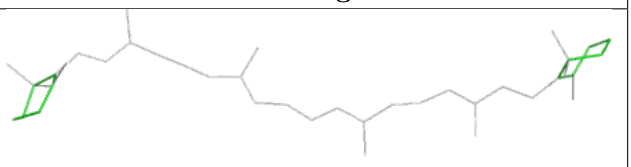
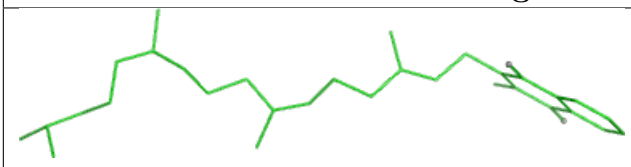


Rings

Ligand PQN A 2001



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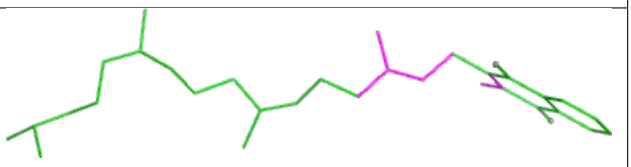
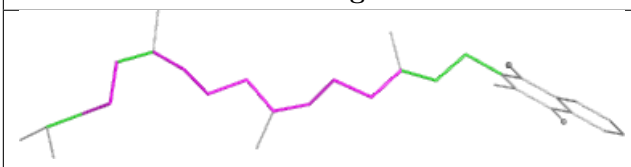


Bond angles



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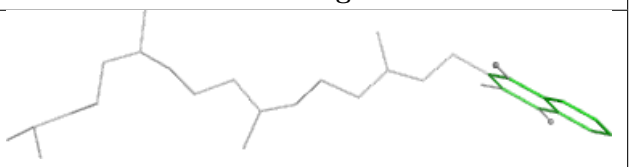
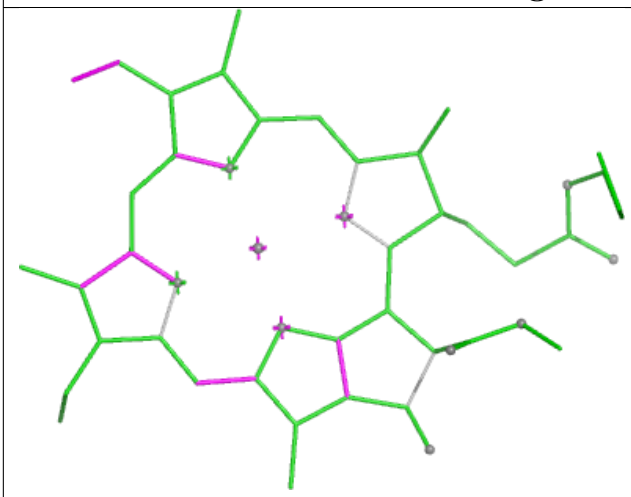


Rings

Ligand CLA 4 605



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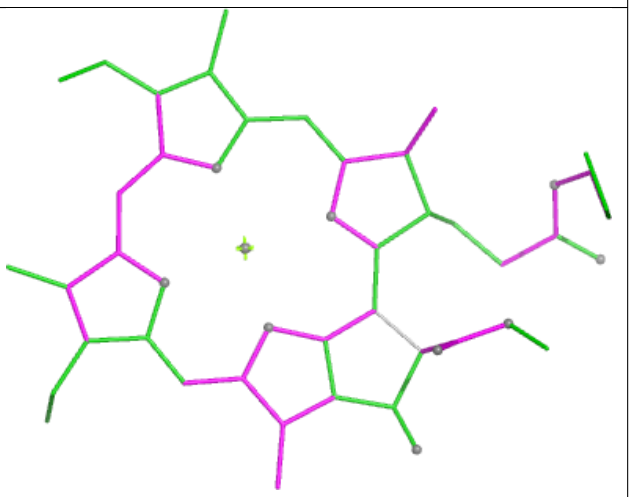
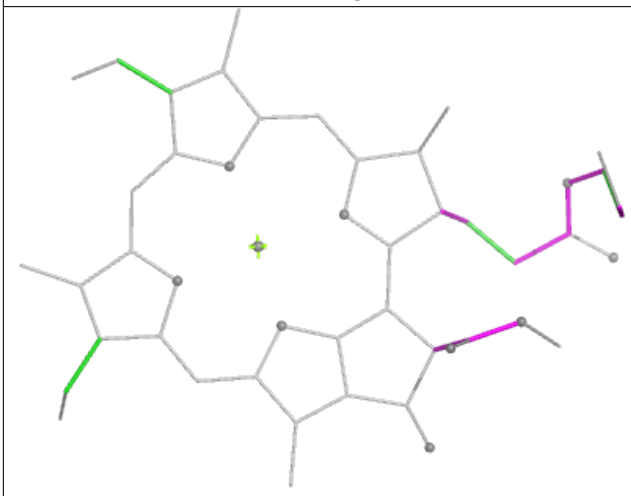


Bond angles



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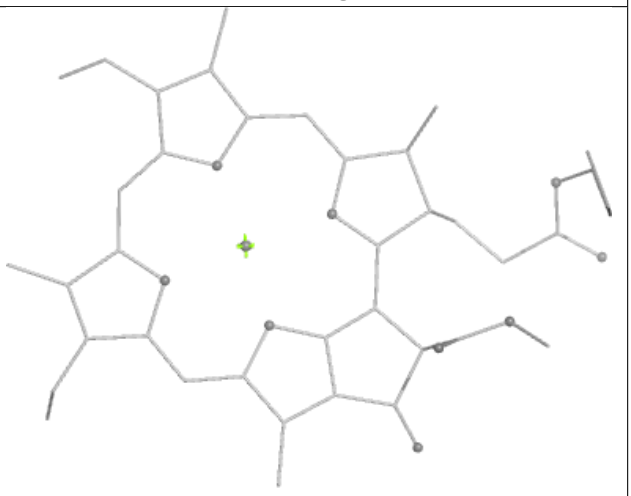
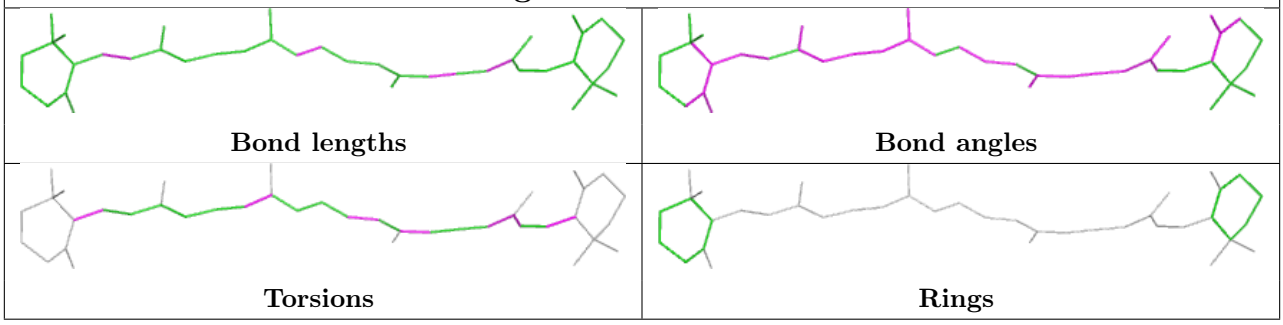
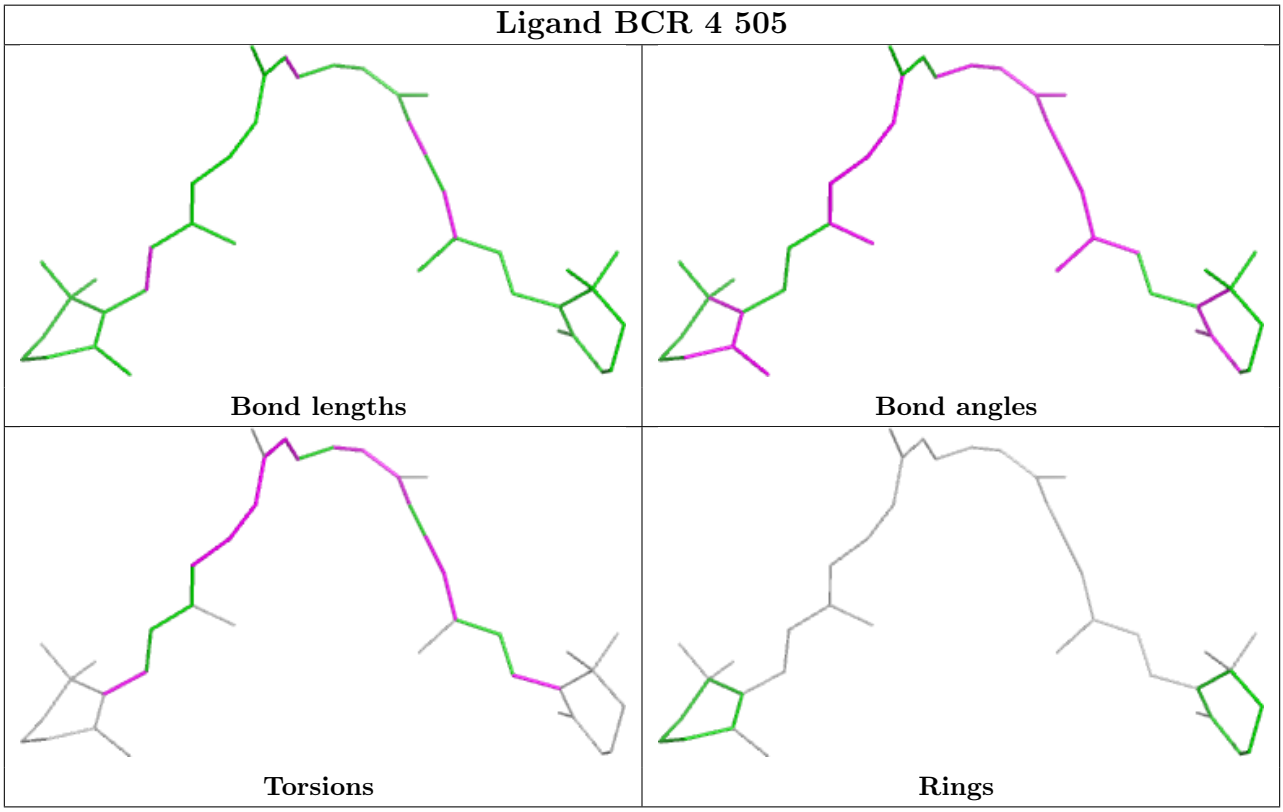


Rings

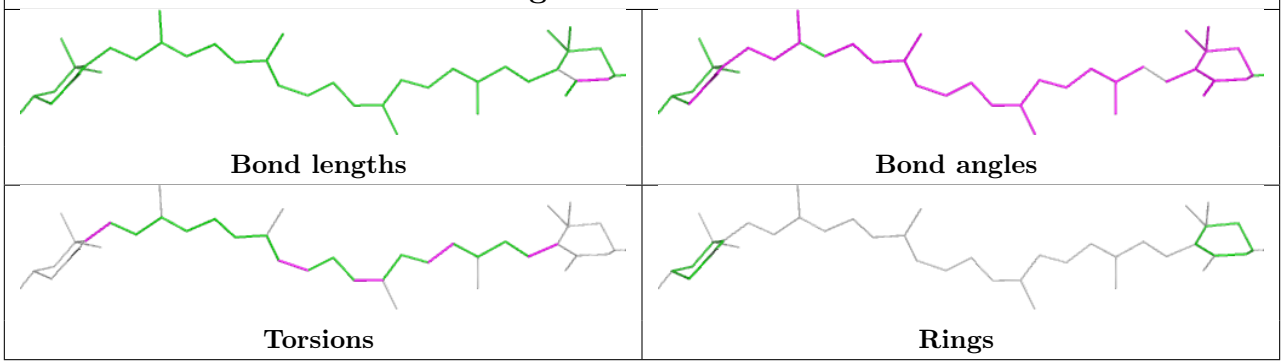
Ligand BCR A 4002



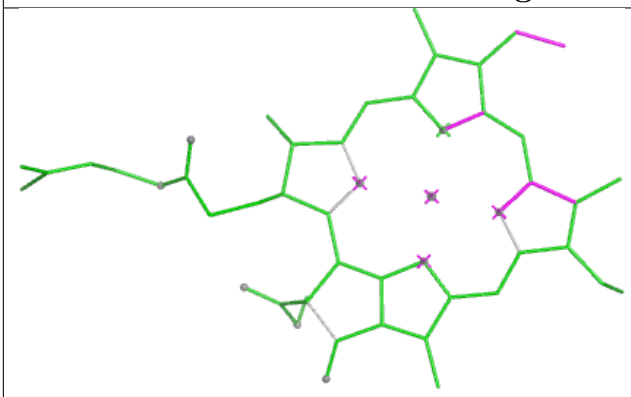
Ligand BCR 4 505



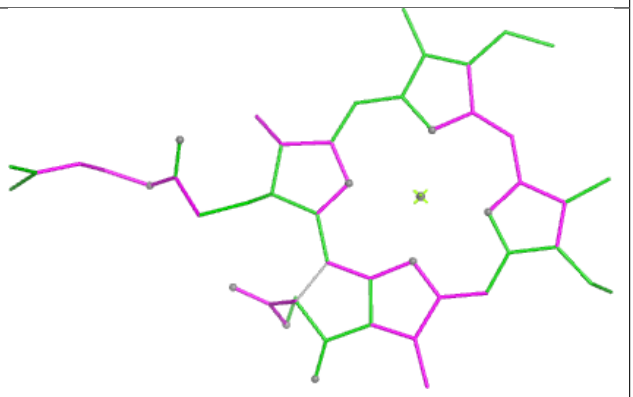
Ligand LUT 1 501



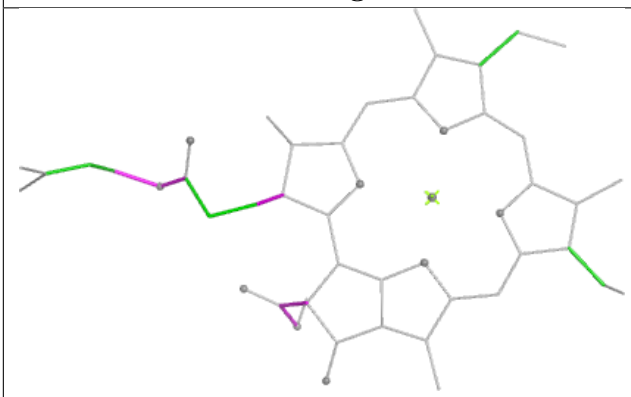
Ligand CLA A 1131



Bond lengths



Bond angles



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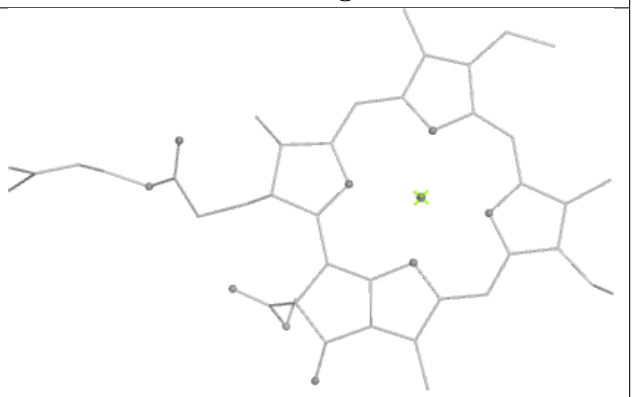
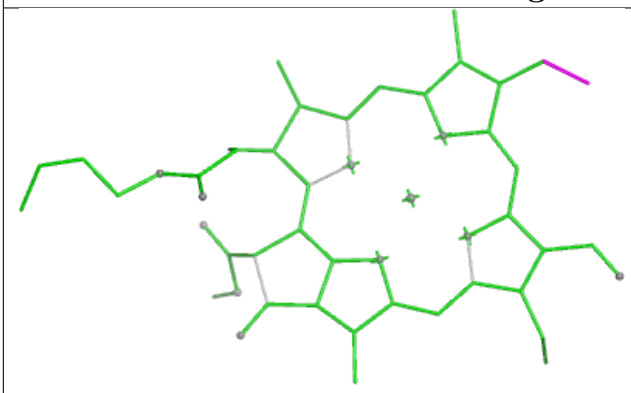


Rings

Ligand CHL 4 613



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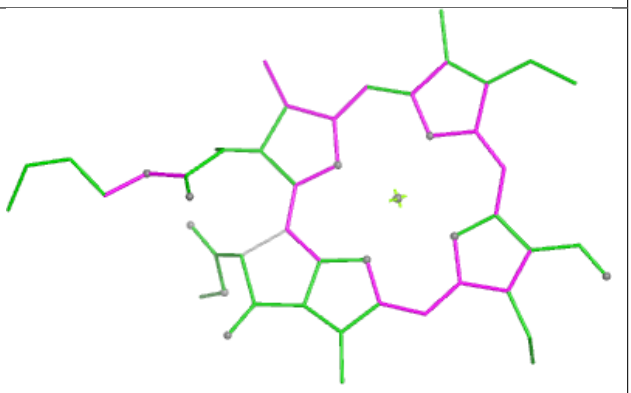
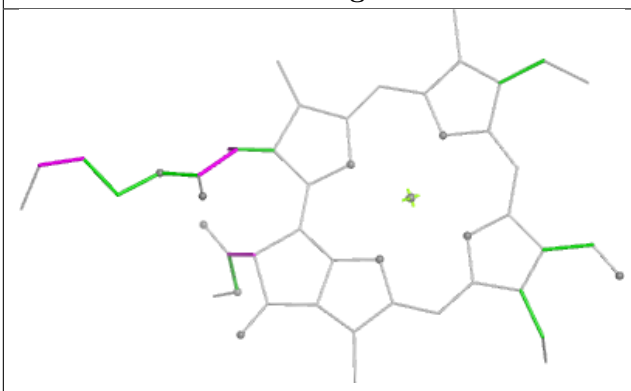


Bond angles



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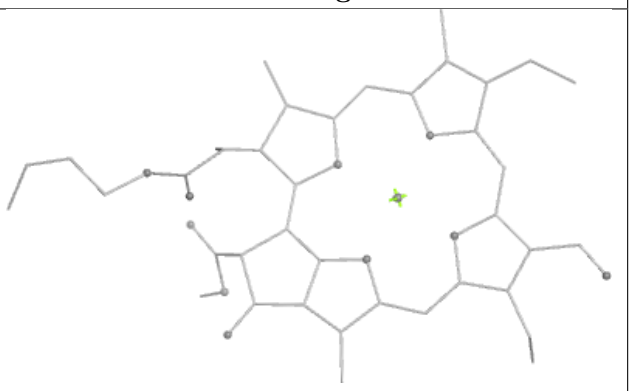
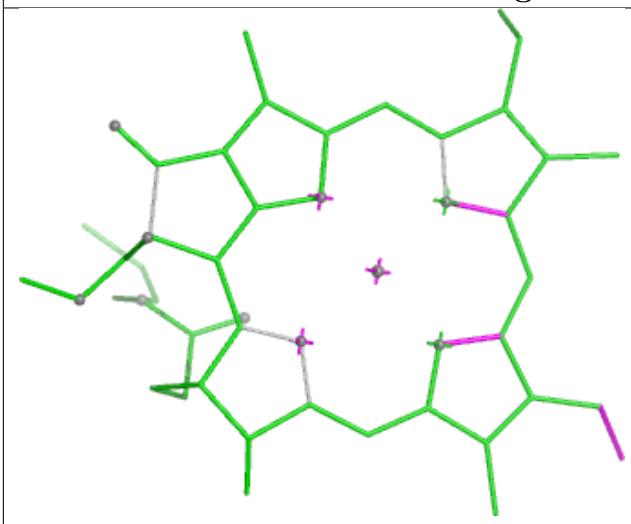


Rings

Ligand CLA A 1126



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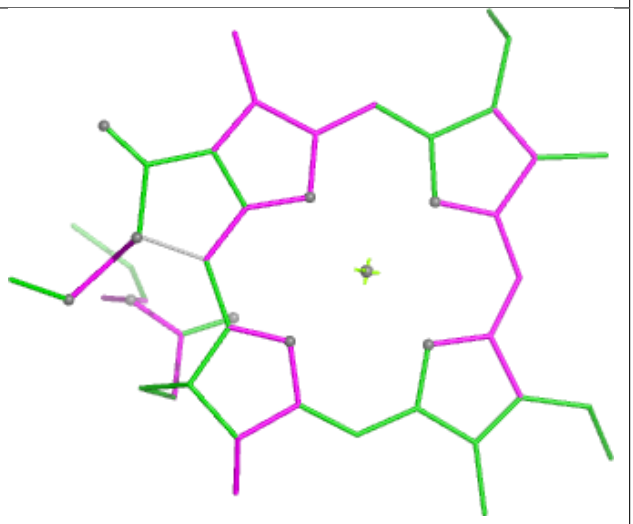
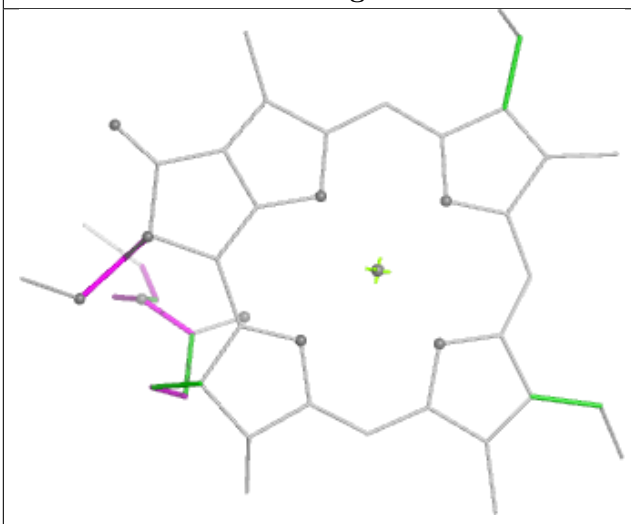


Bond angles



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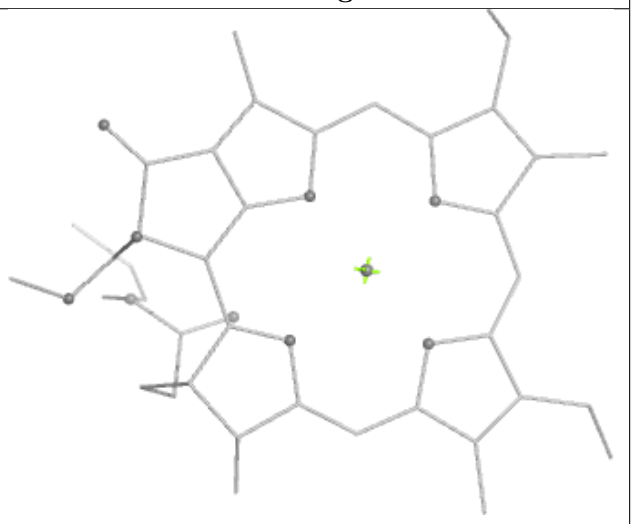
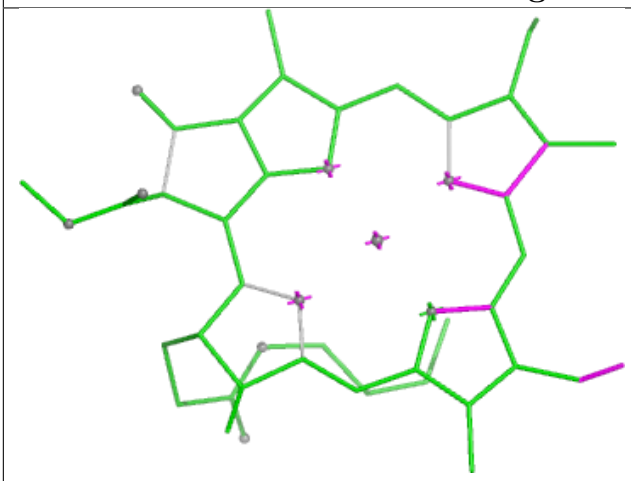
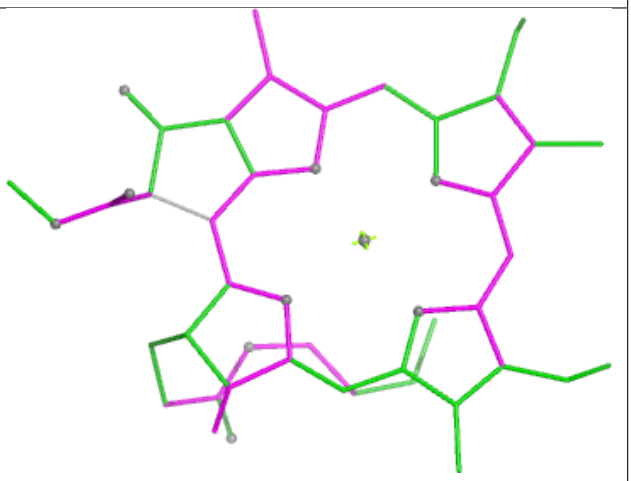


Rings

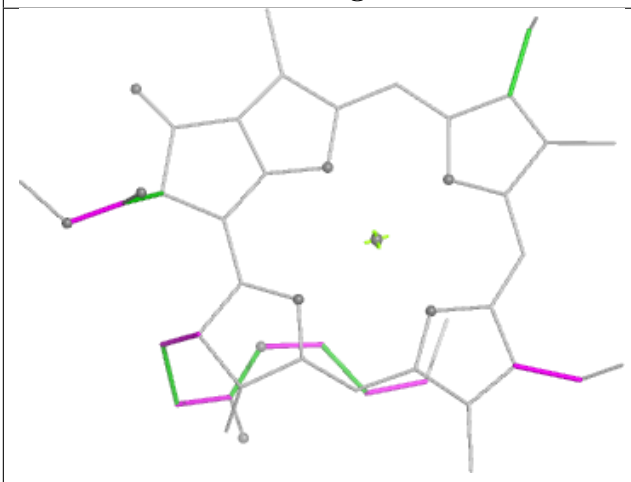
Ligand CLA 3 610



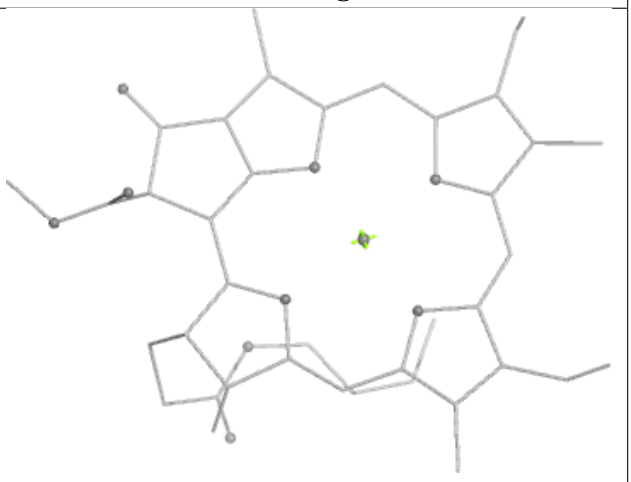
Bond lengths



Bond angles

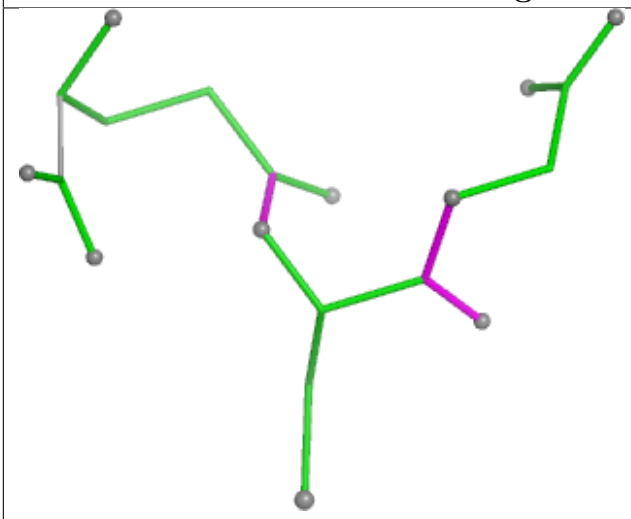


Torsions

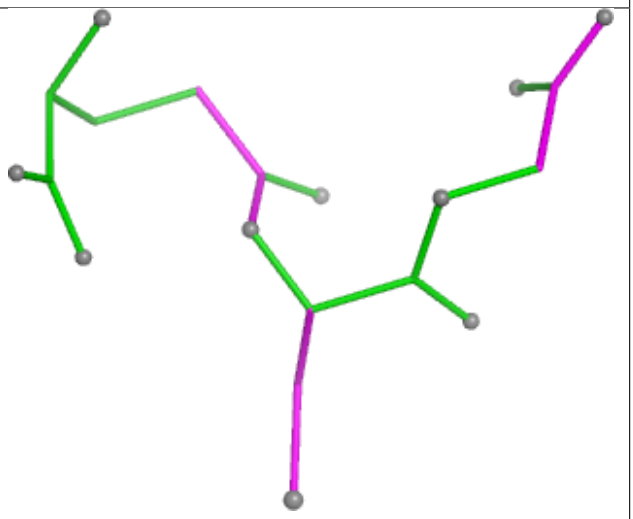


Rings

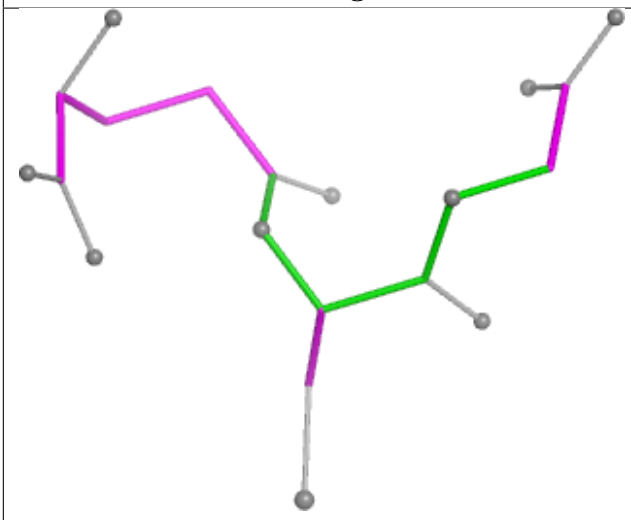
Ligand GSH B 5031



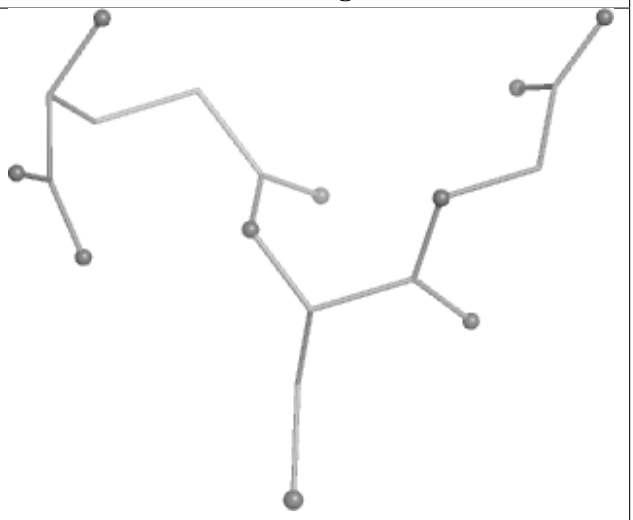
Bond lengths



Bond angles

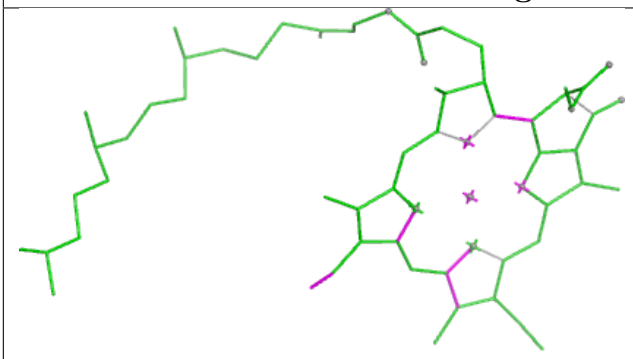


Torsions



Rings

Ligand CLA A 1106



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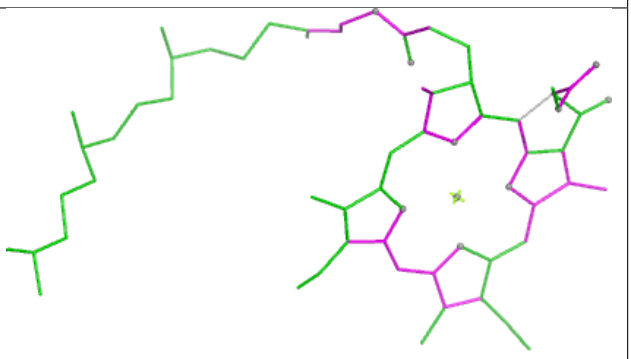
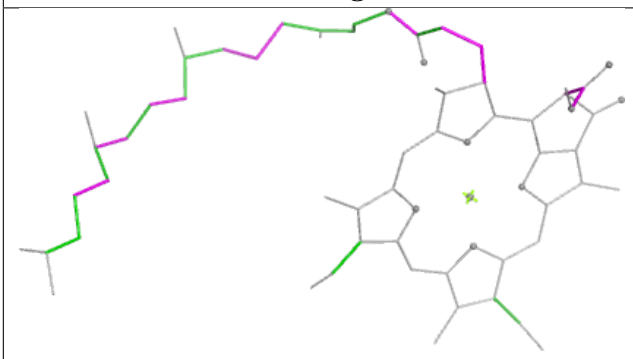


Bond angles

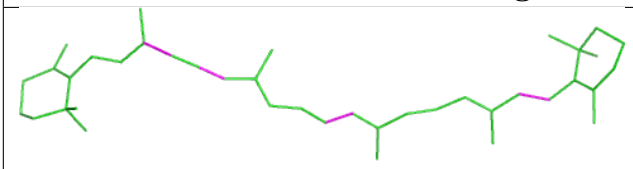


Torsions



Rings

Ligand BCR B 4005



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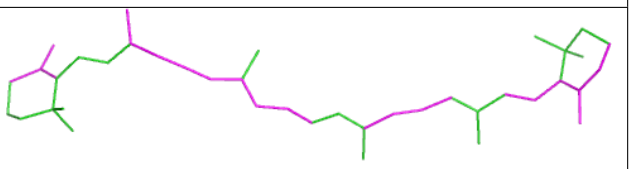
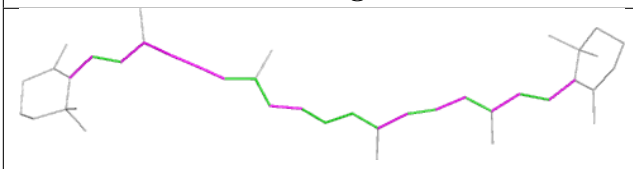


Bond angles



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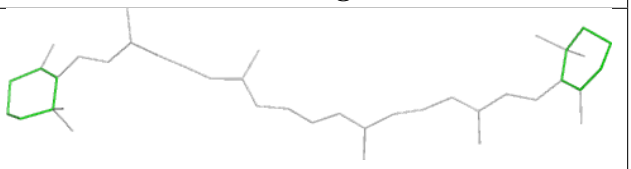
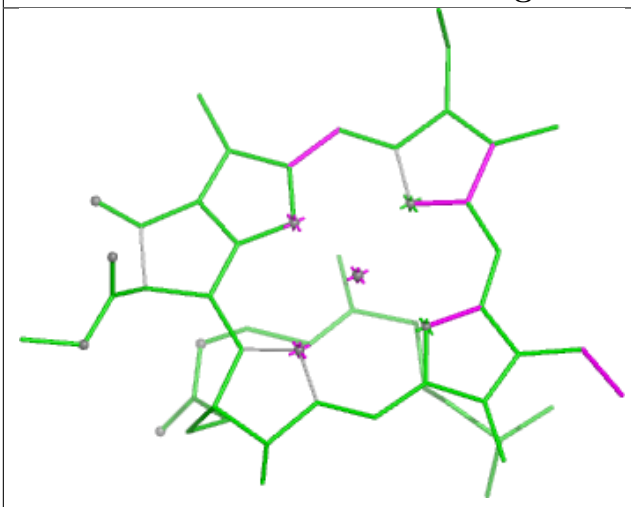


Rings

Ligand CLA A 1130



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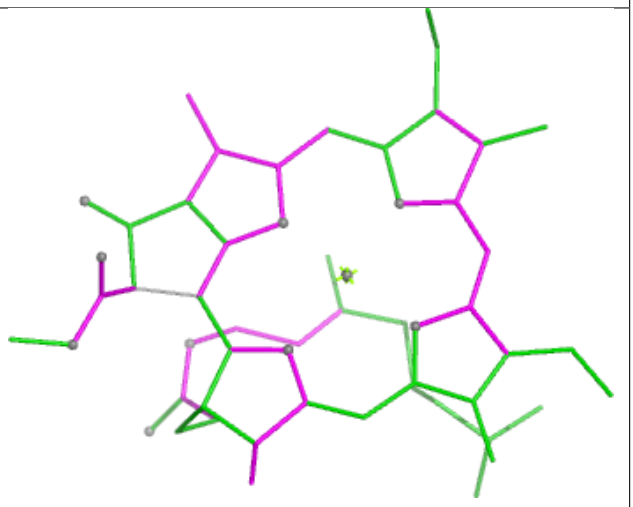

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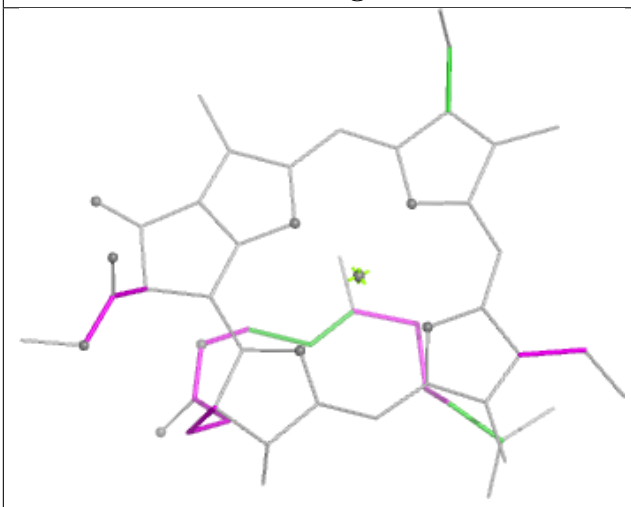

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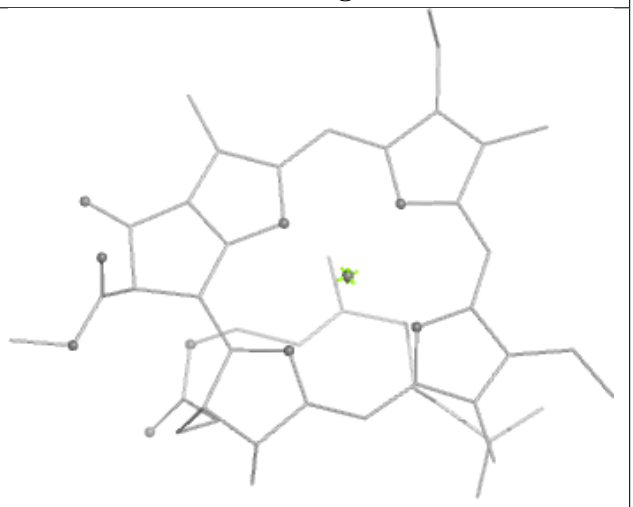
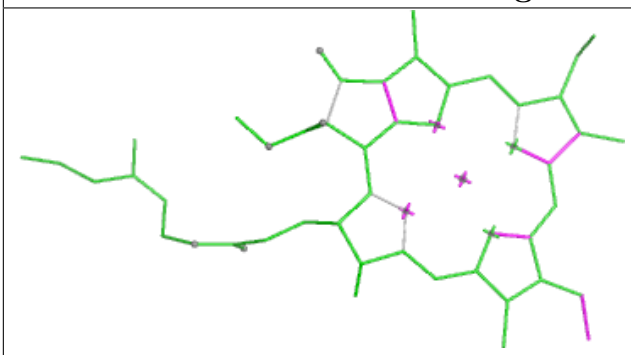


Rings

Ligand CLA A 1139



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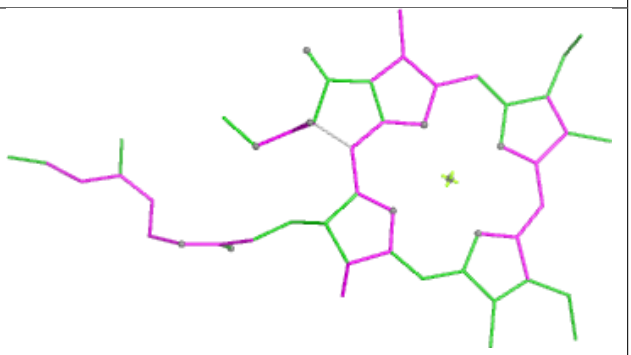
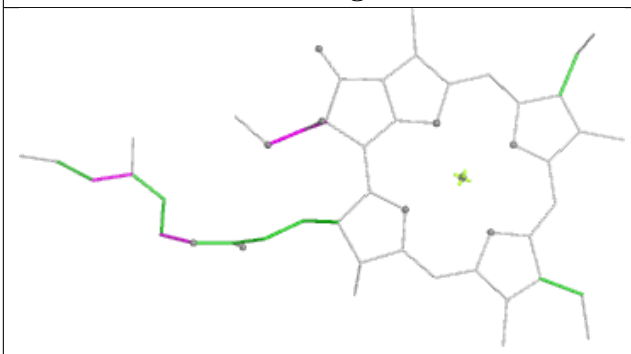


Bond angles



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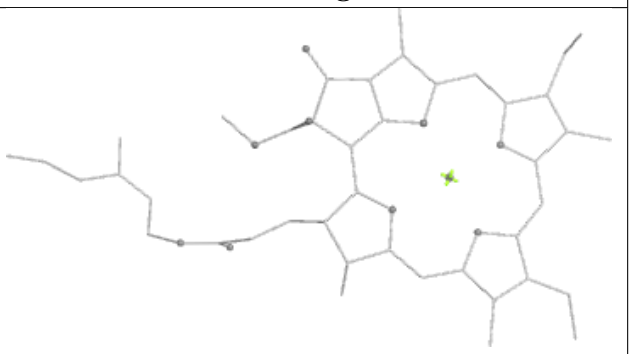
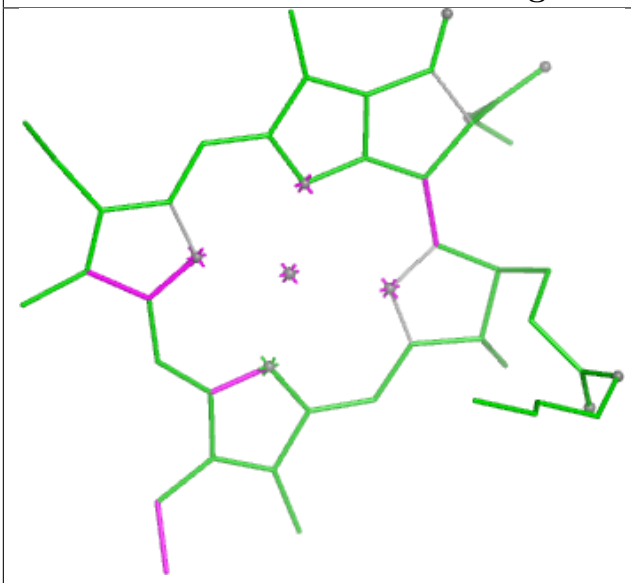


Rings

Ligand CLA 4 612



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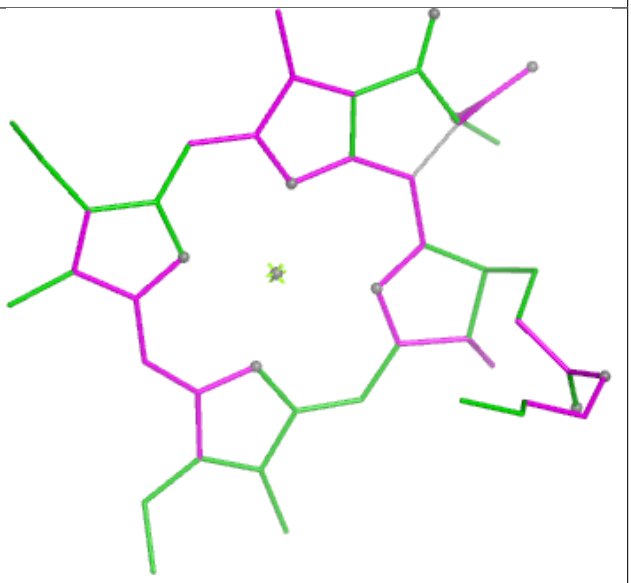

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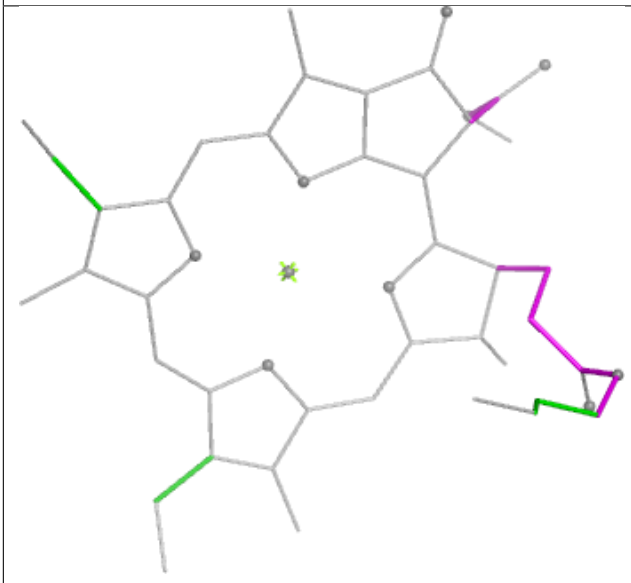

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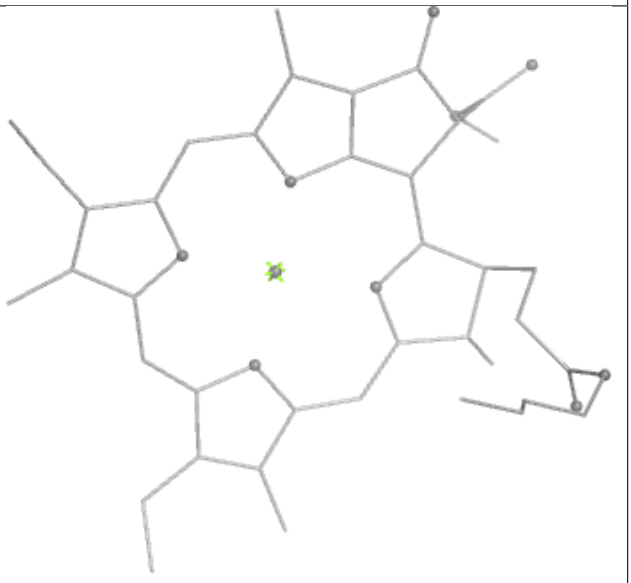
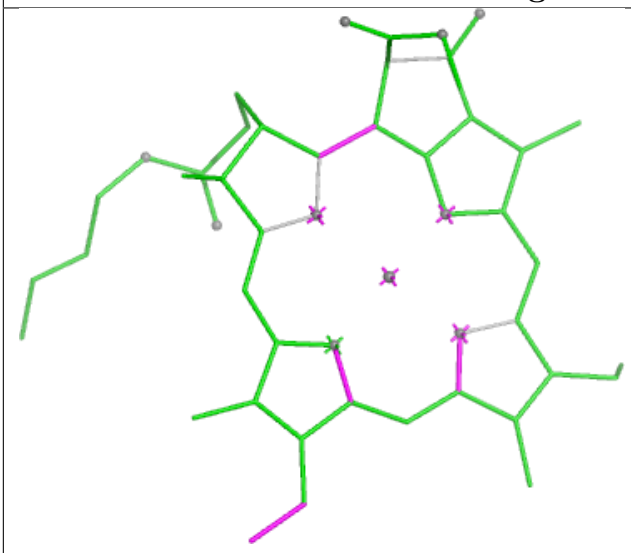


Rings

Ligand CLA 2 601



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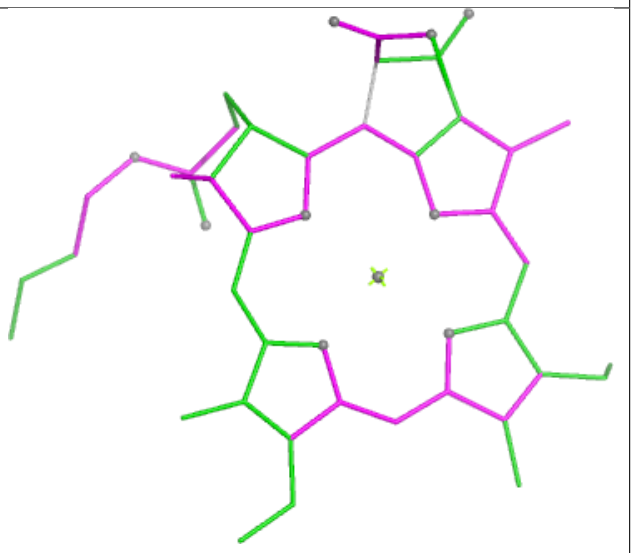
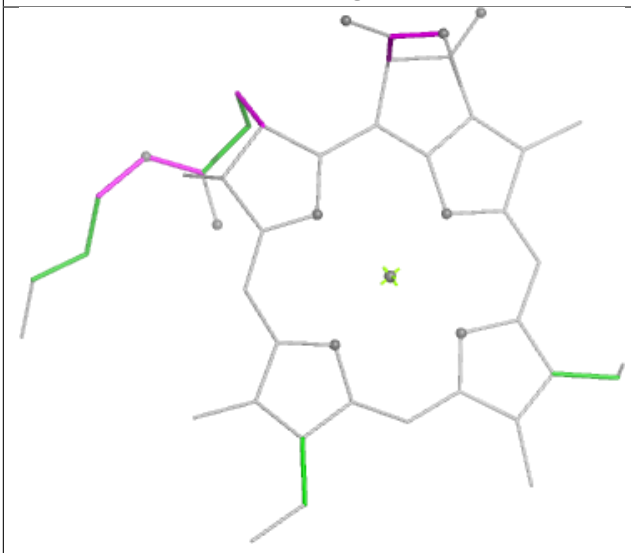


Bond angles



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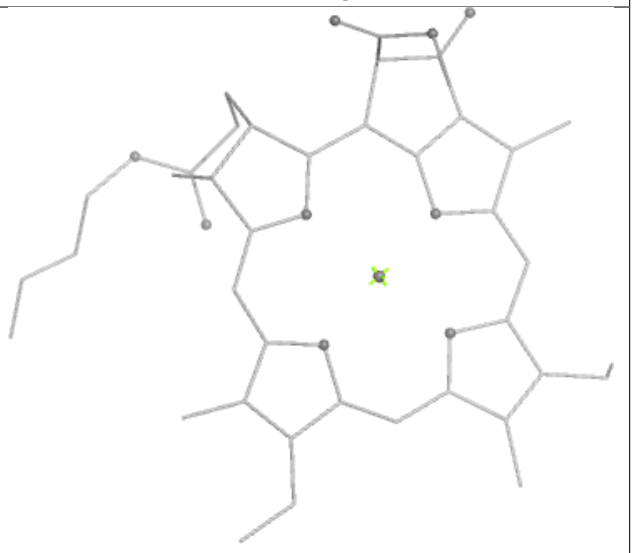
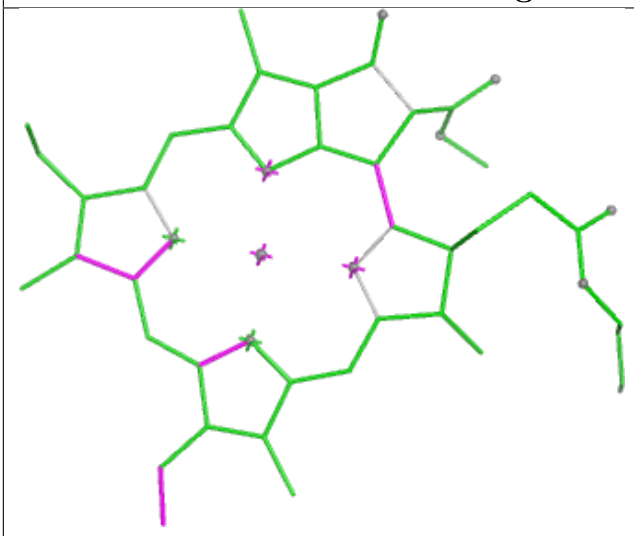


Rings

Ligand CLA B 1221



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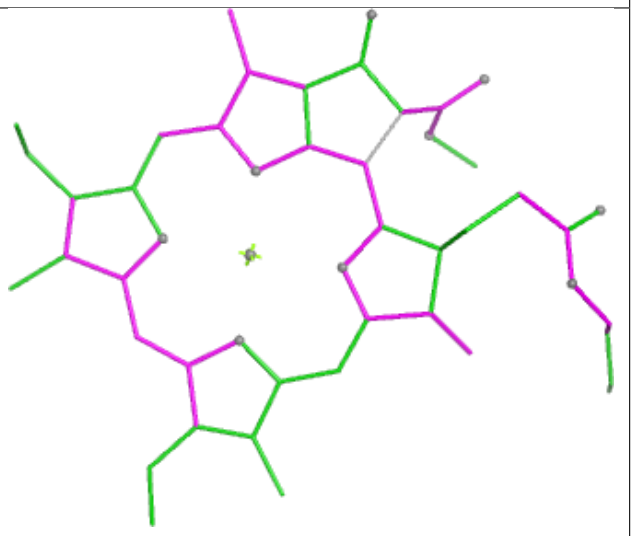

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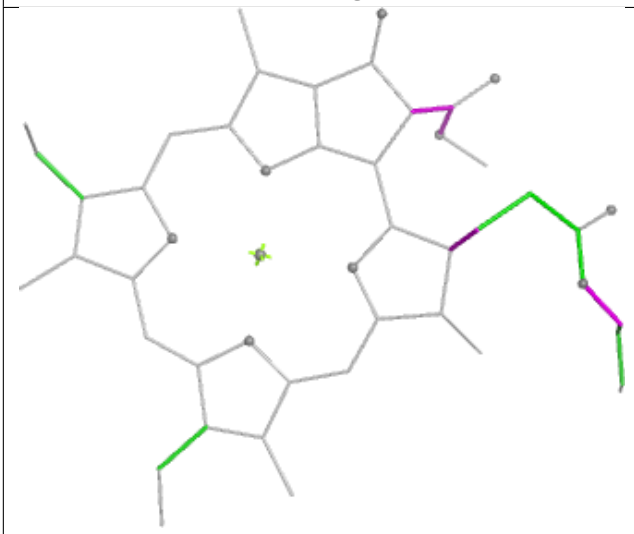

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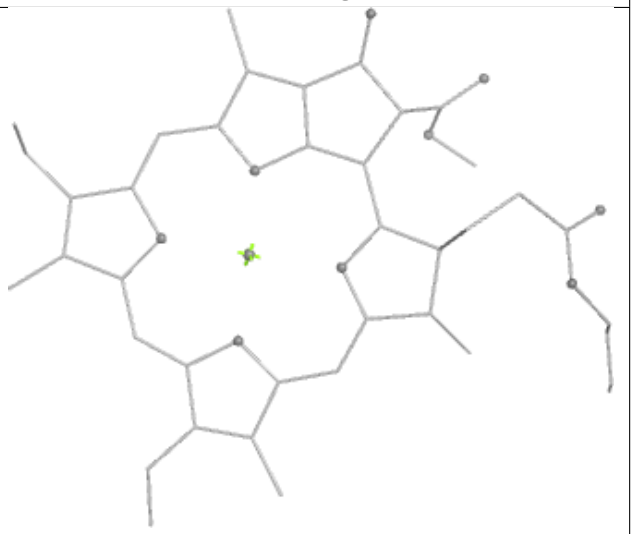
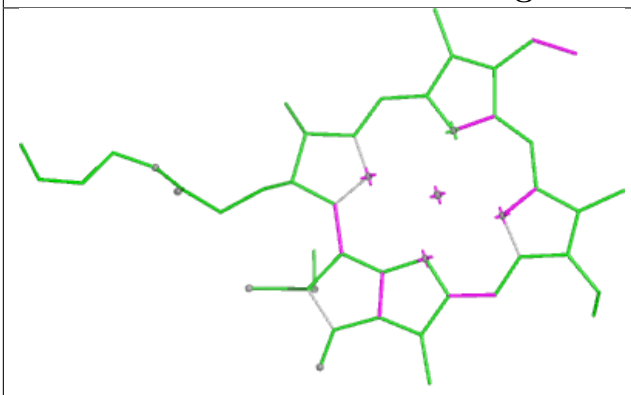


Rings

Ligand CLA B 1234



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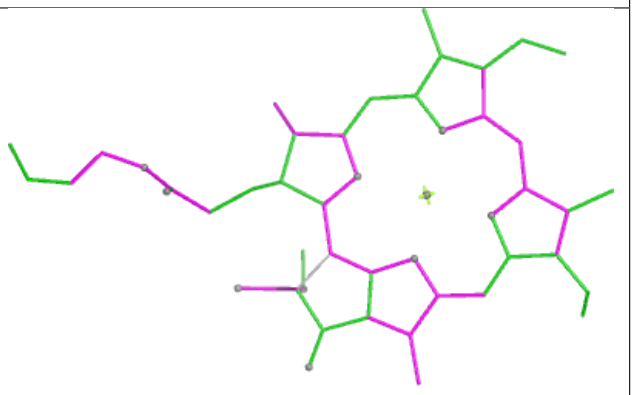
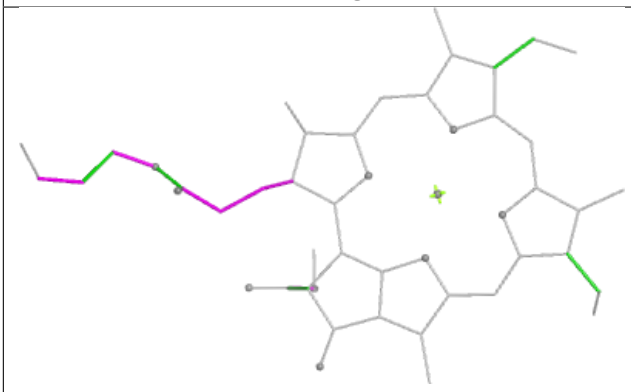


Bond angles

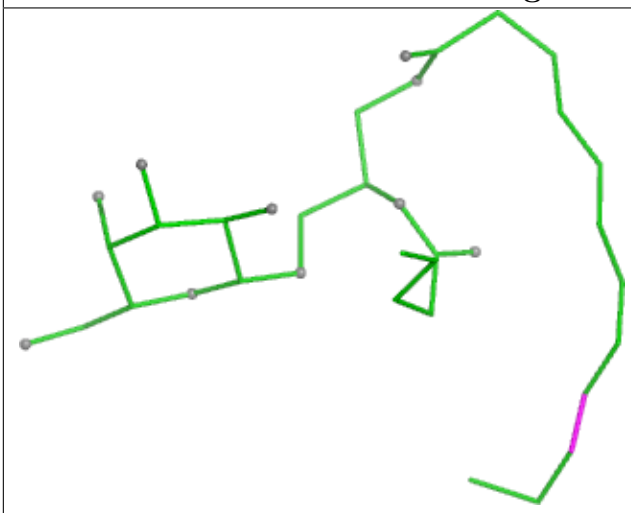


Torsions



Rings

Ligand LMG 1 802



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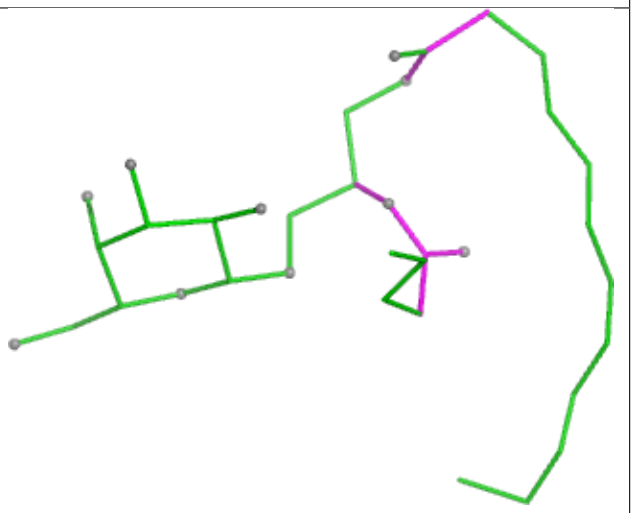
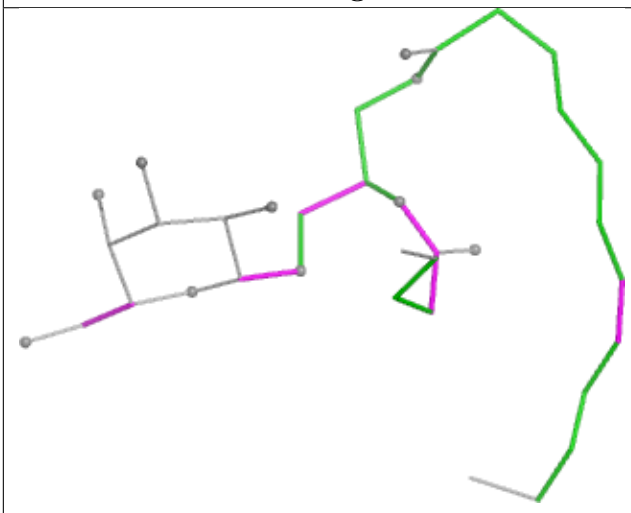


Bond angles



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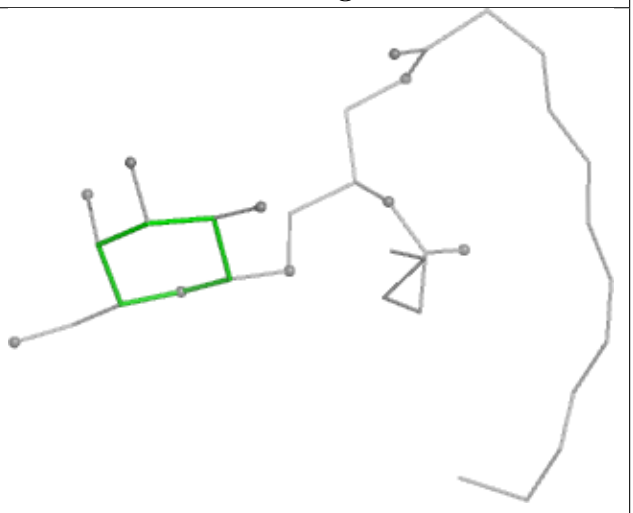
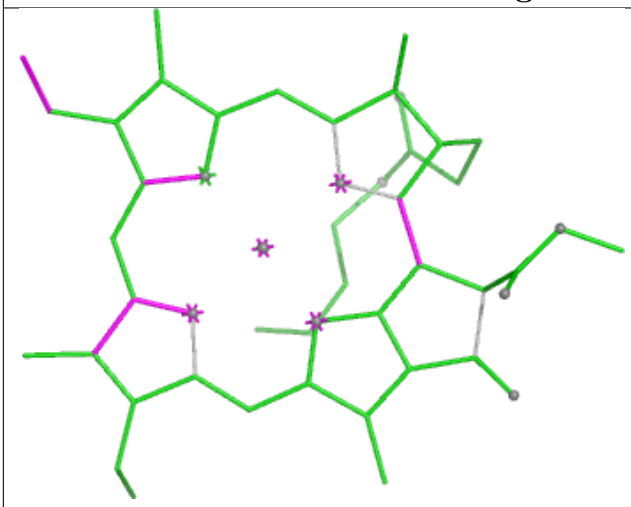


Rings

Ligand CLA B 1218



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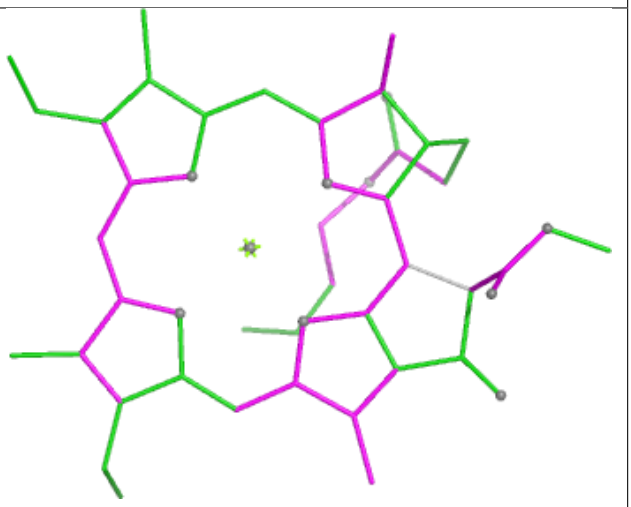

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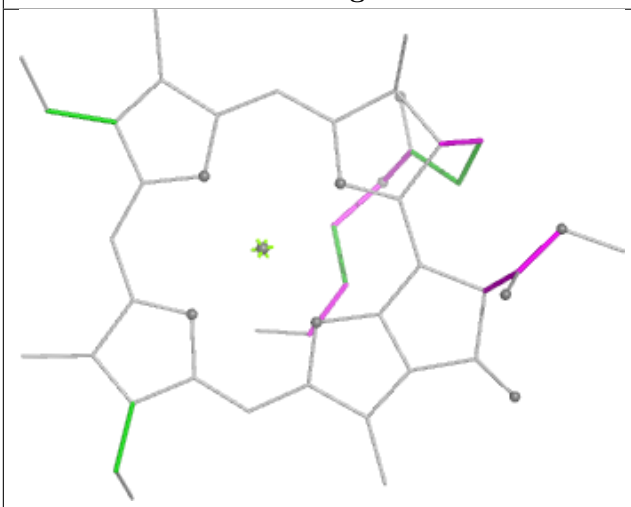

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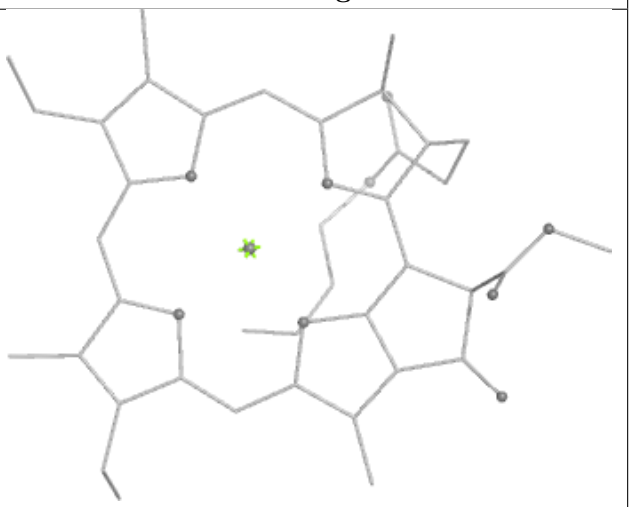
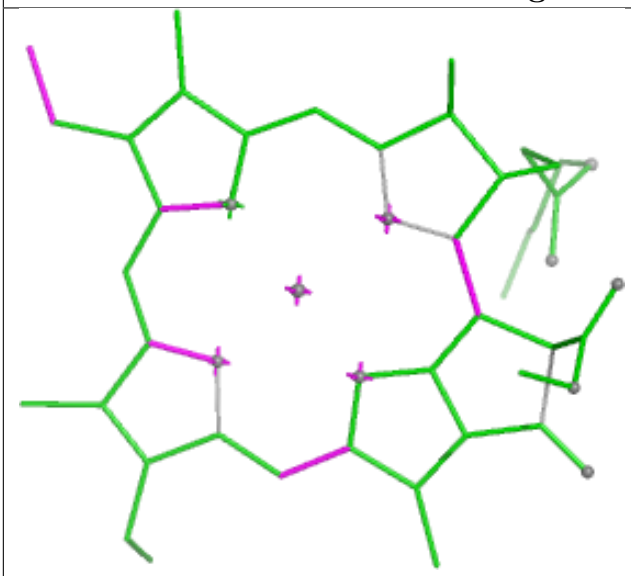


Rings

Ligand CLA 4 606



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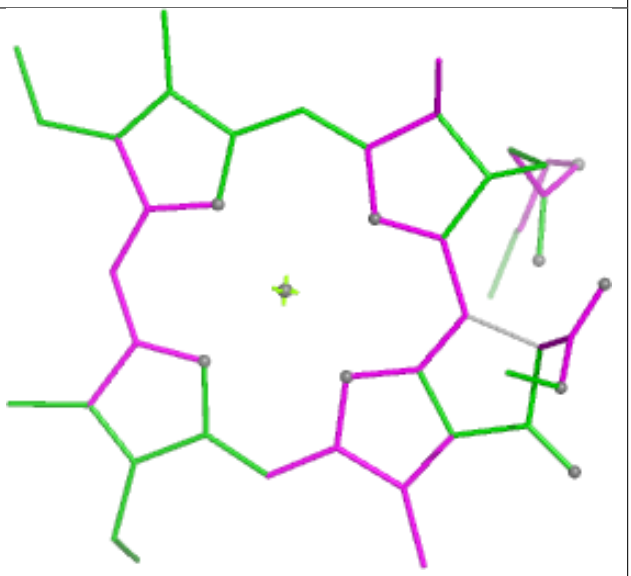
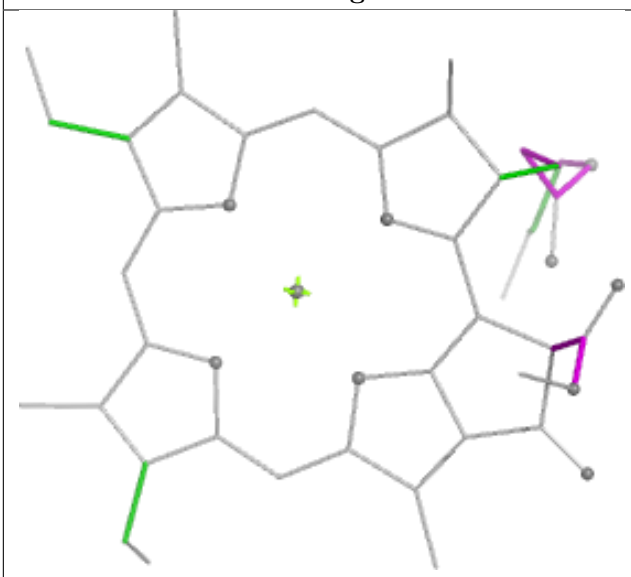


Bond angles



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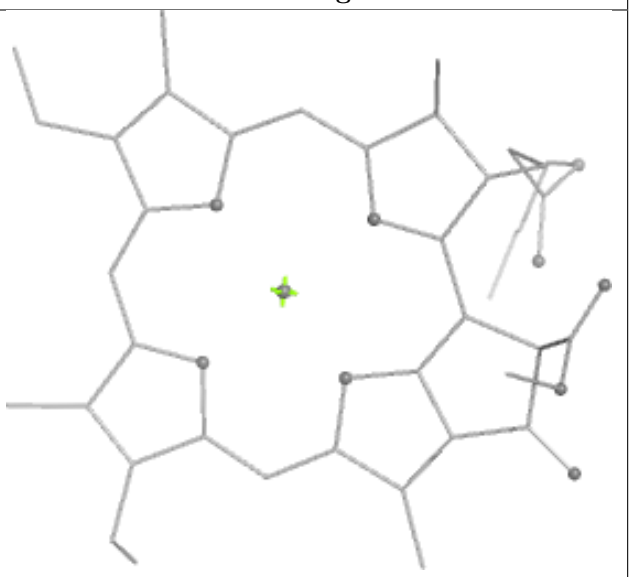
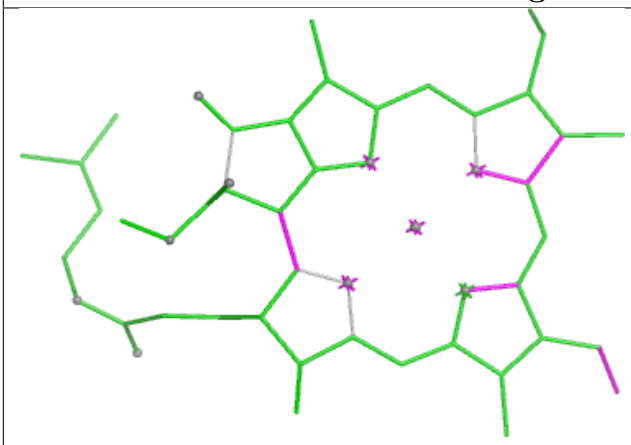


Rings

Ligand CLA 2 615



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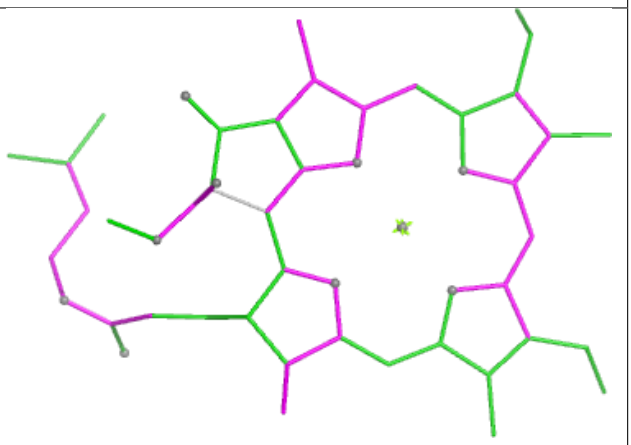
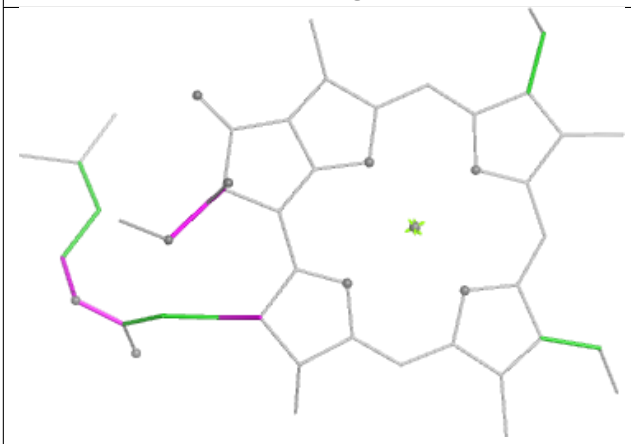


Bond angles



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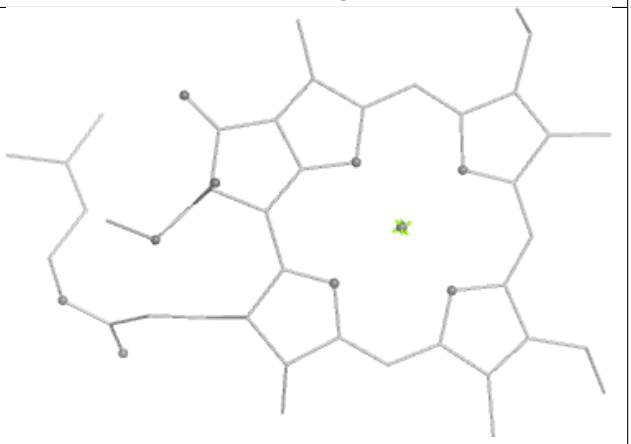
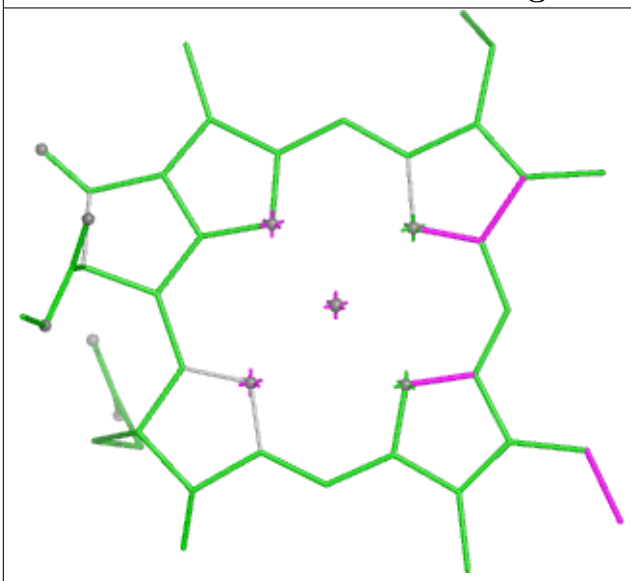


Rings

Ligand CLA 3 606



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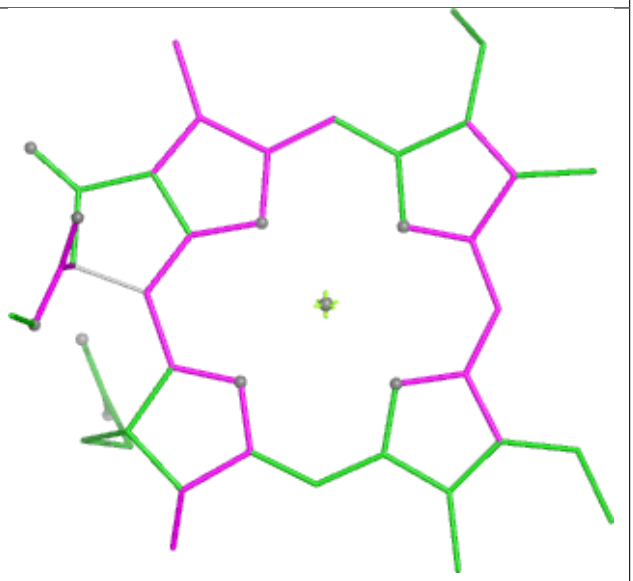
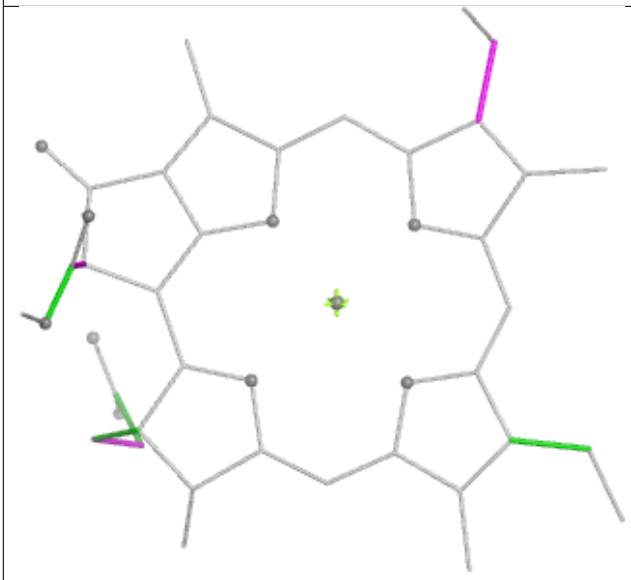


Bond angles



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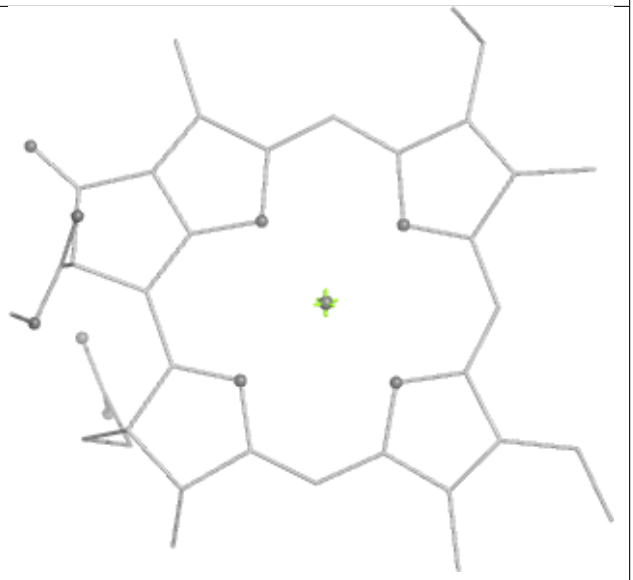
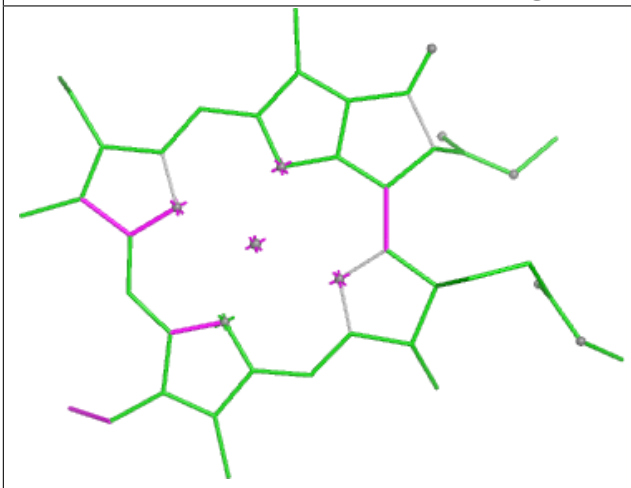


Rings

Ligand CLA 1 602



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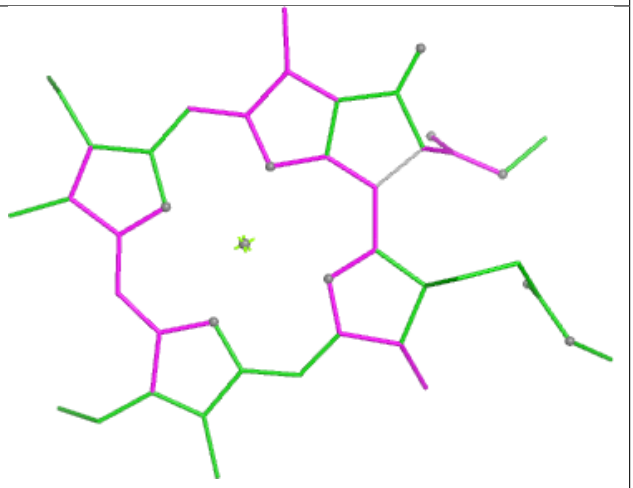
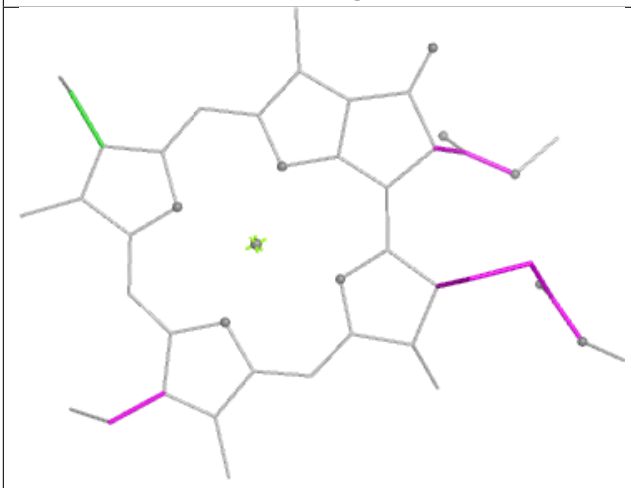


Bond angles



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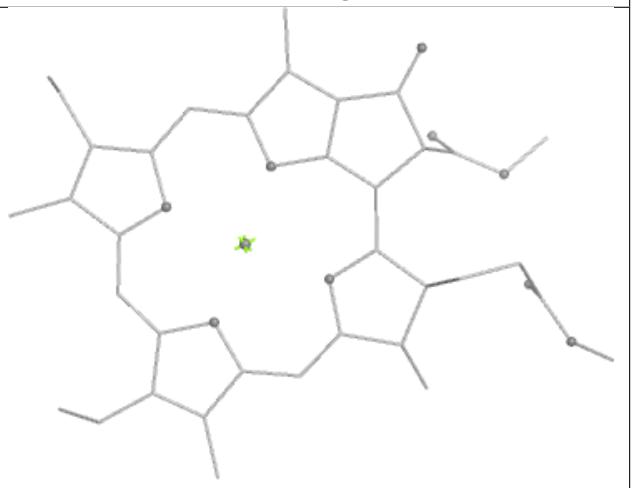
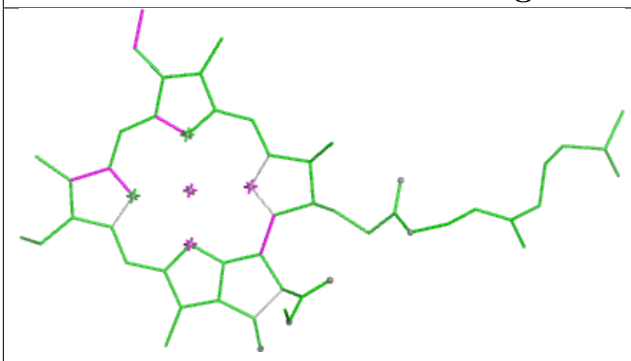
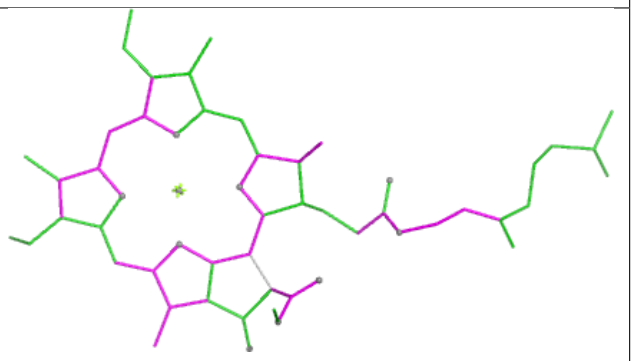


Rings

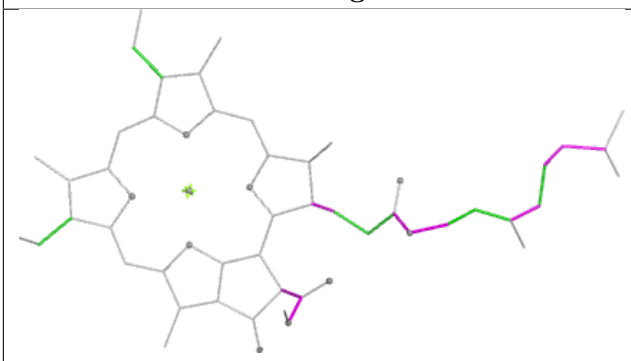
Ligand CLA A 1103



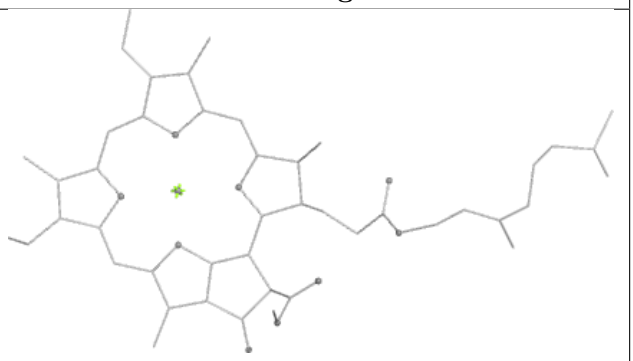
Bond lengths



Bond angles

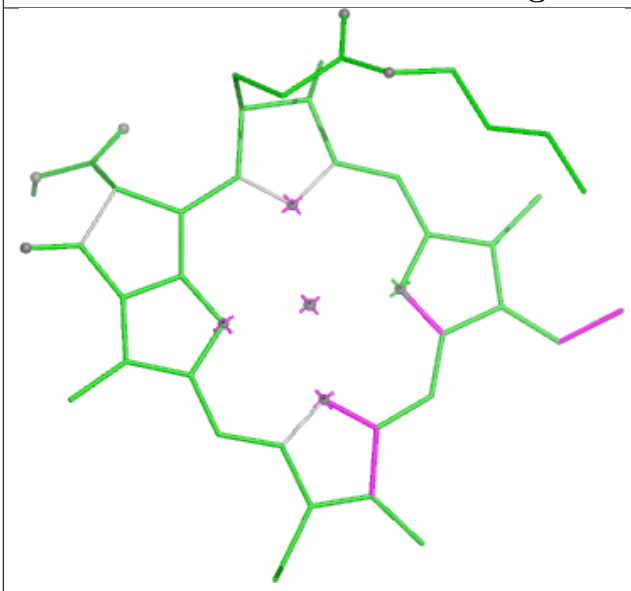


Torsions



Rings

Ligand CLA 1 604



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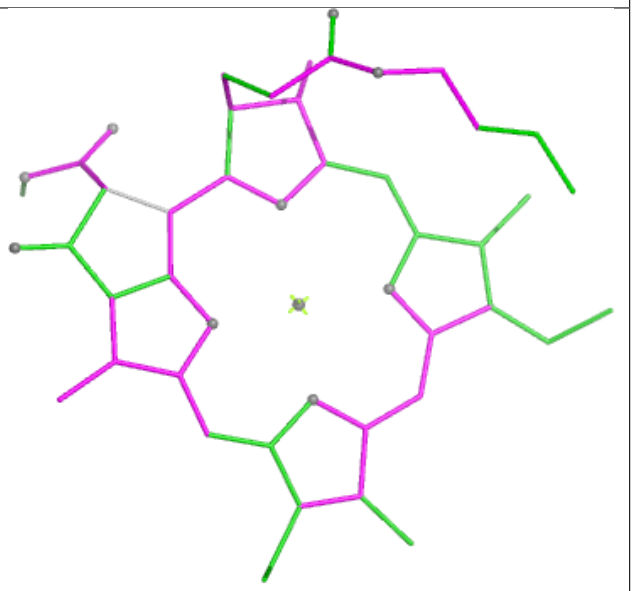

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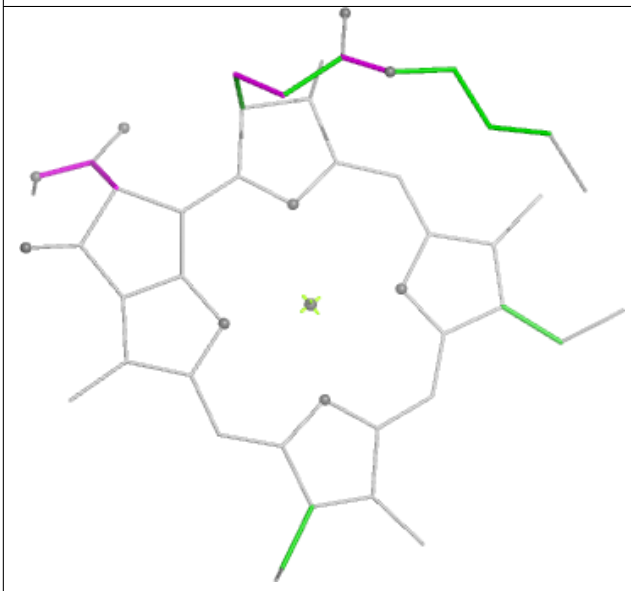

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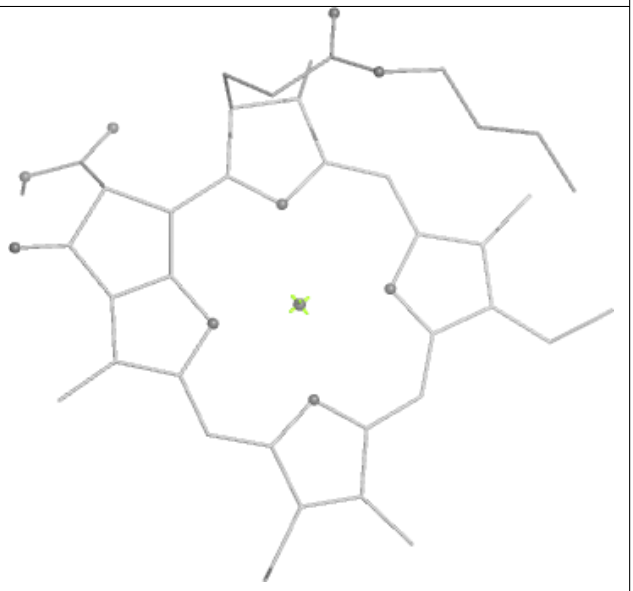
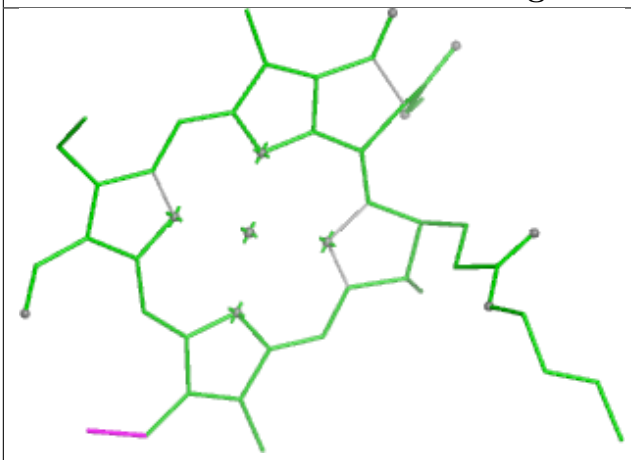


Rings

Ligand CHL 4 611



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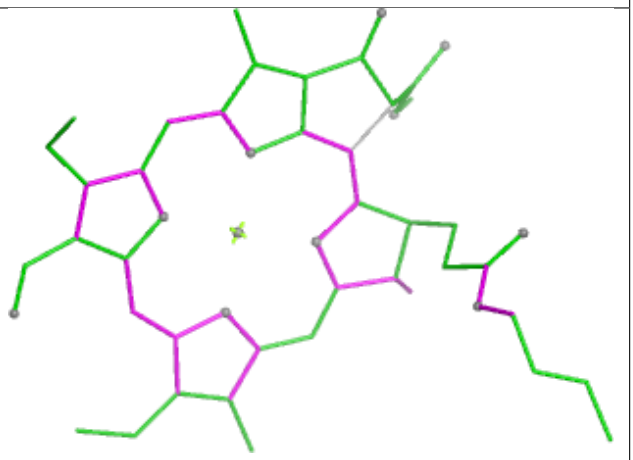

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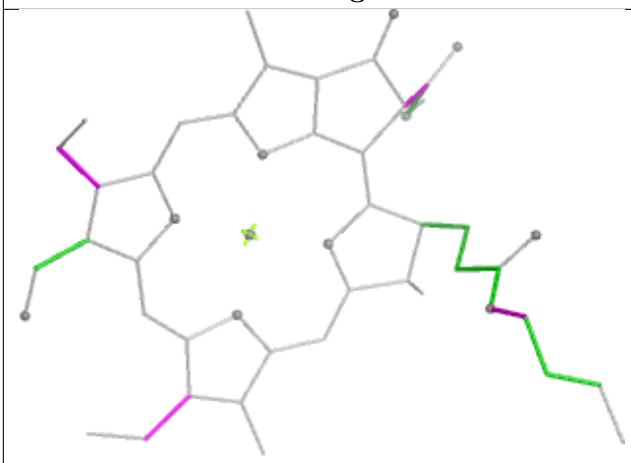

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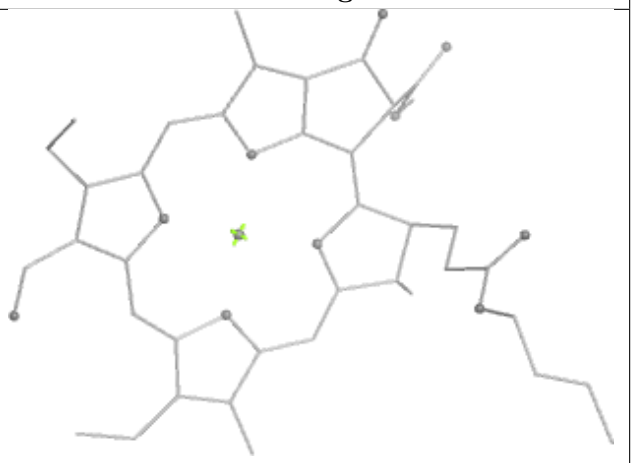
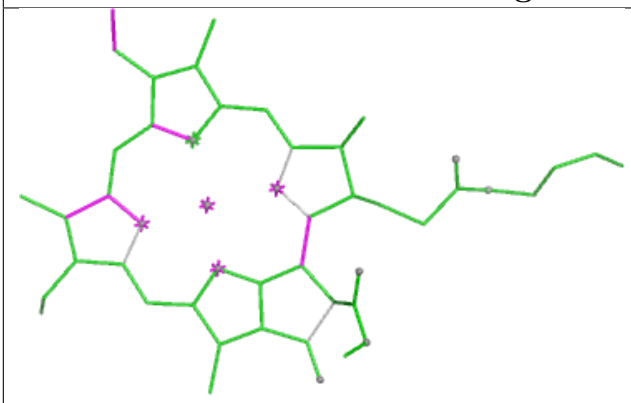


Rings

Ligand CLA A 1135



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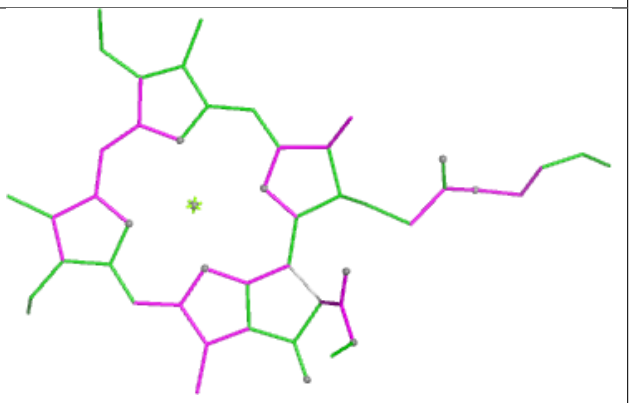
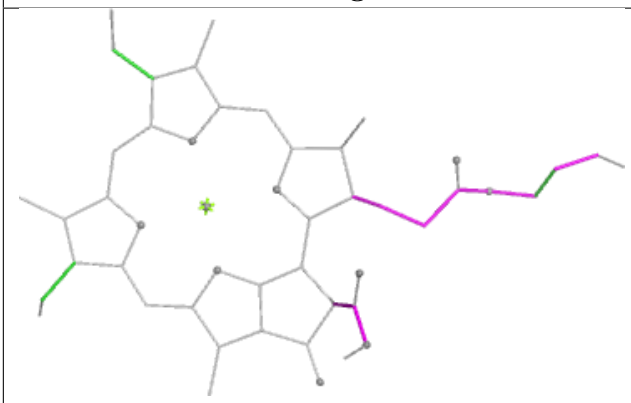


Bond angles



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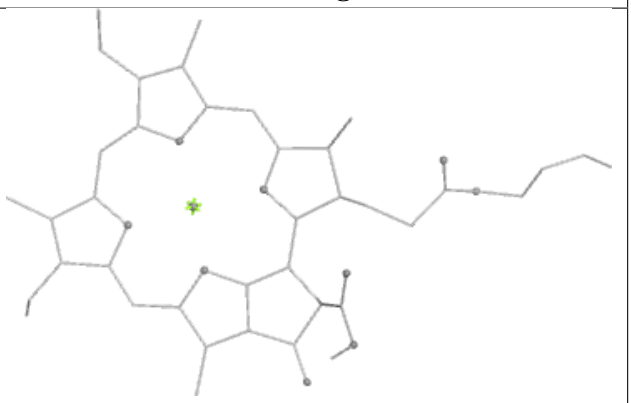
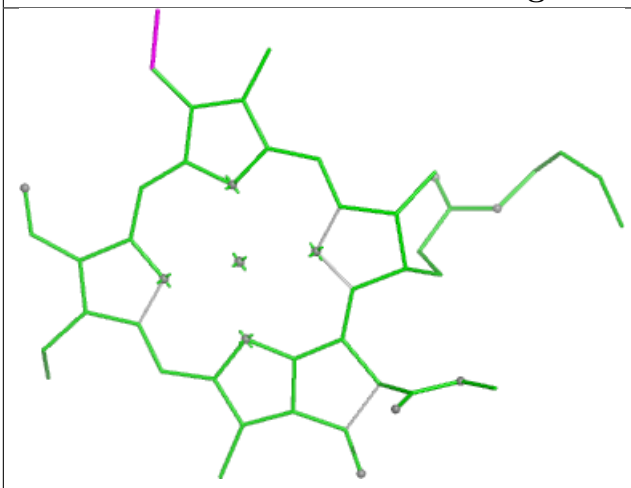


Rings

Ligand CHL 2 610



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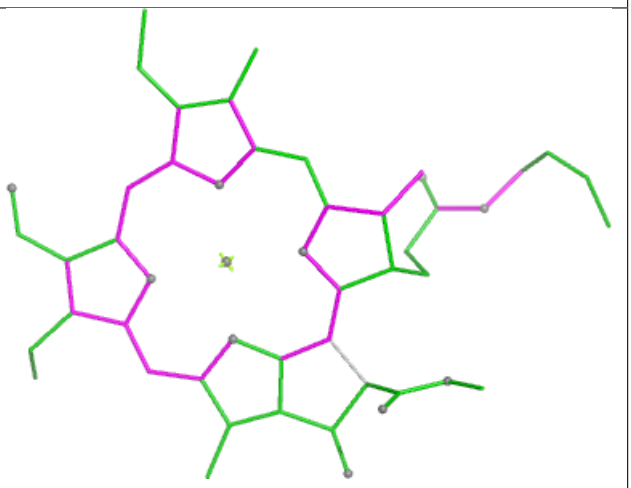

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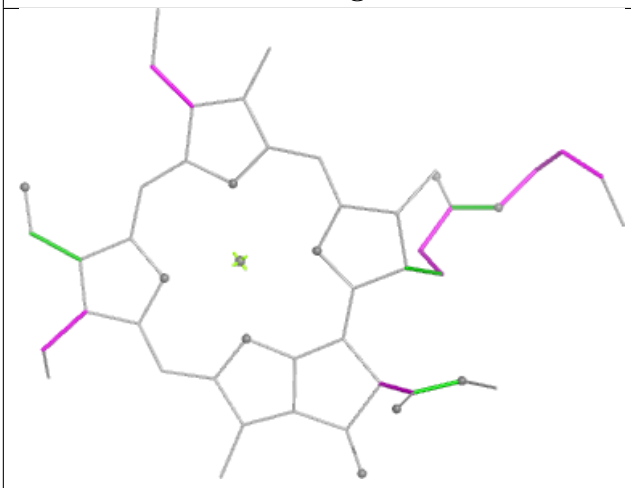

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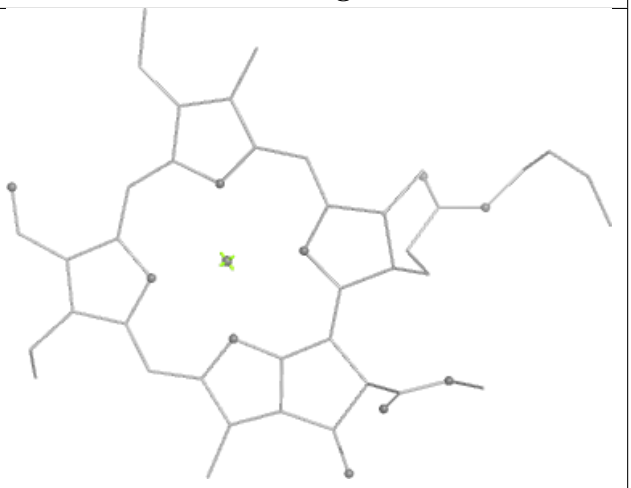
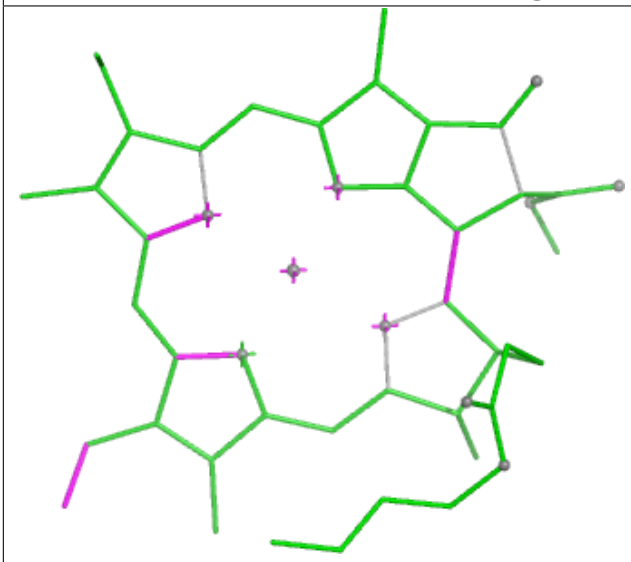


Rings

Ligand CLA 2 604



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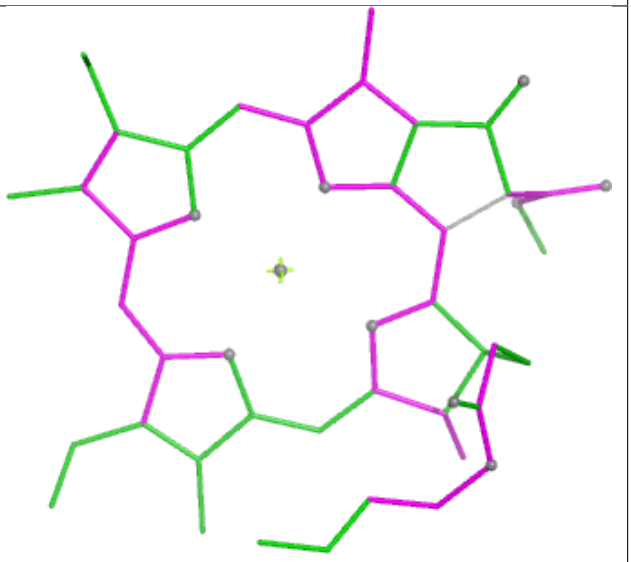

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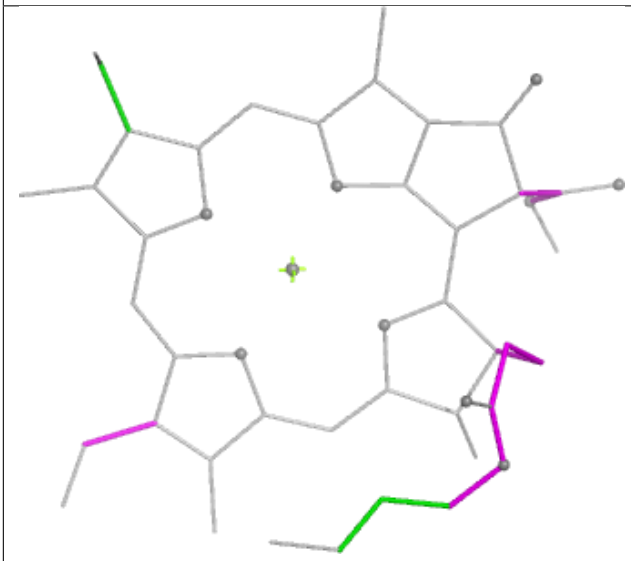

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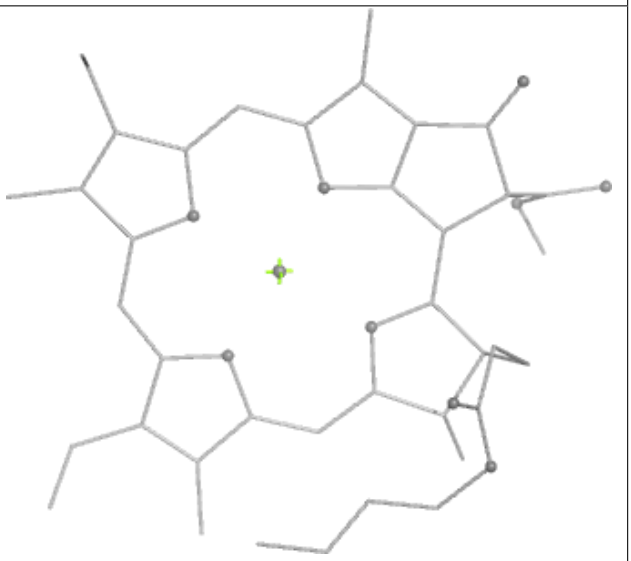

Rings

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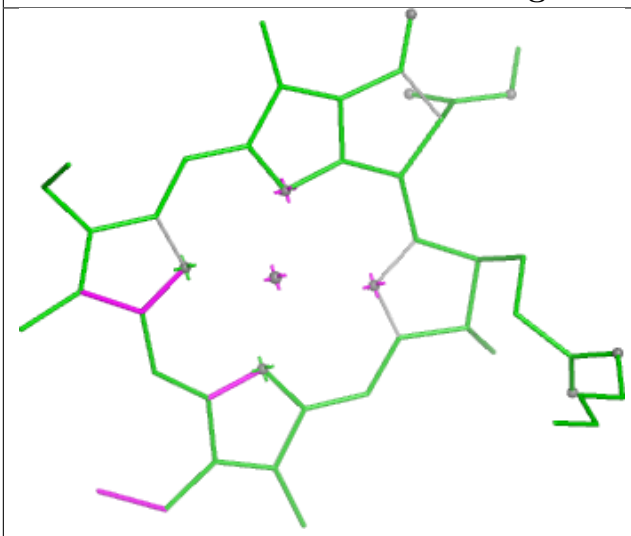

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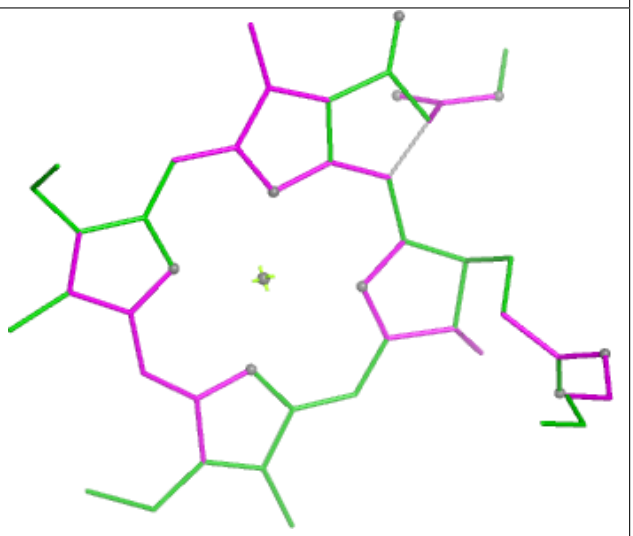
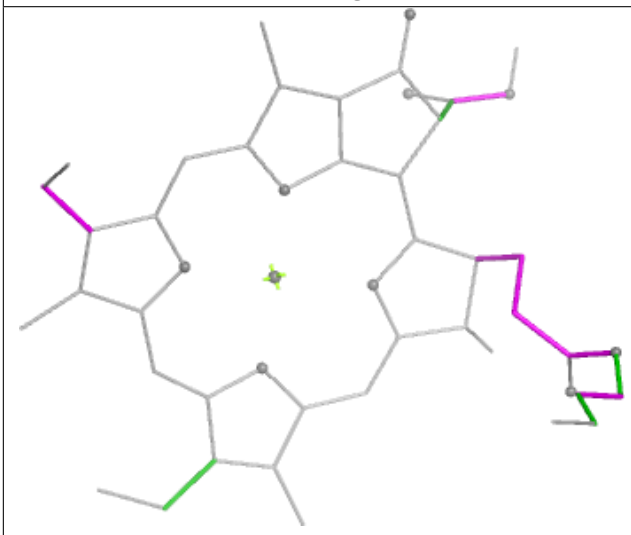


Bond angles



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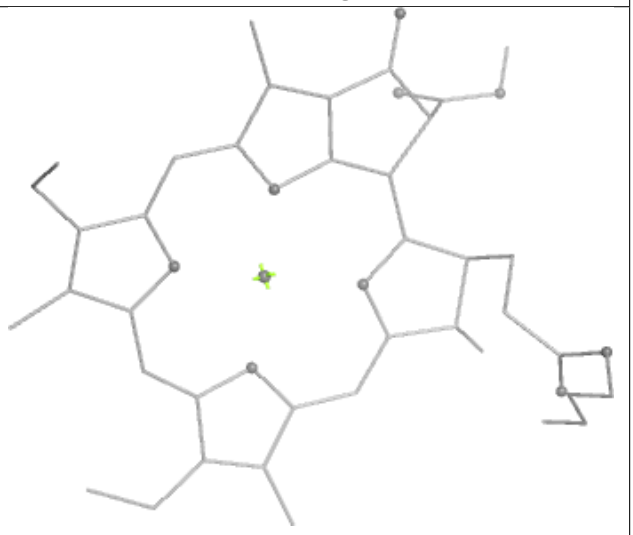
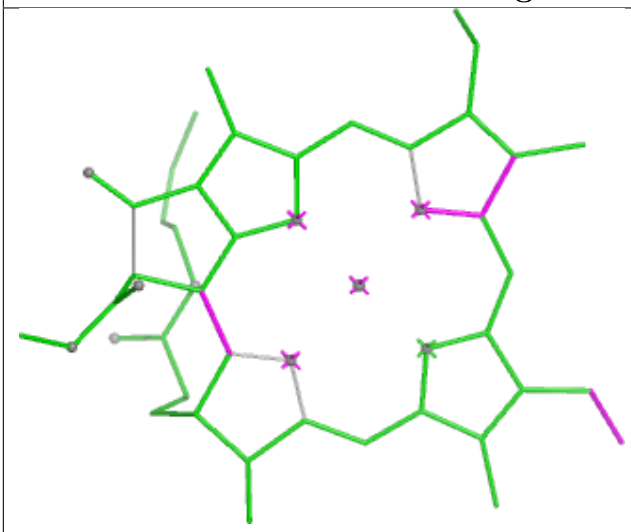


Rings

Ligand CLA B 1213



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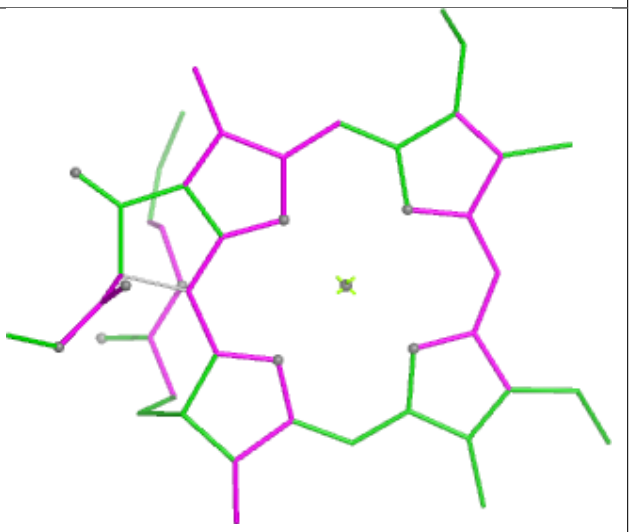

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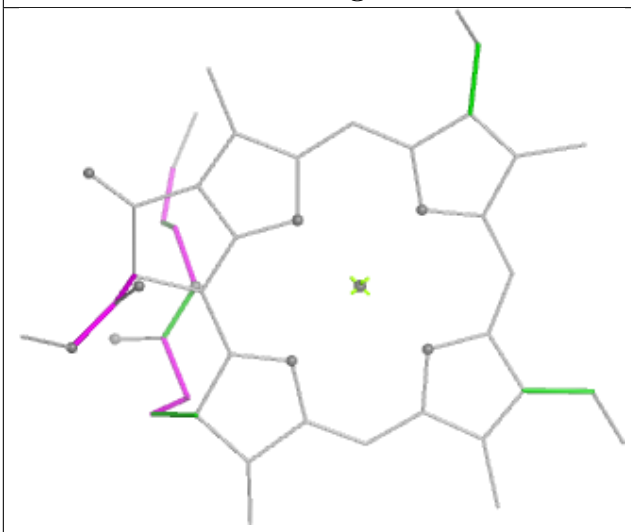

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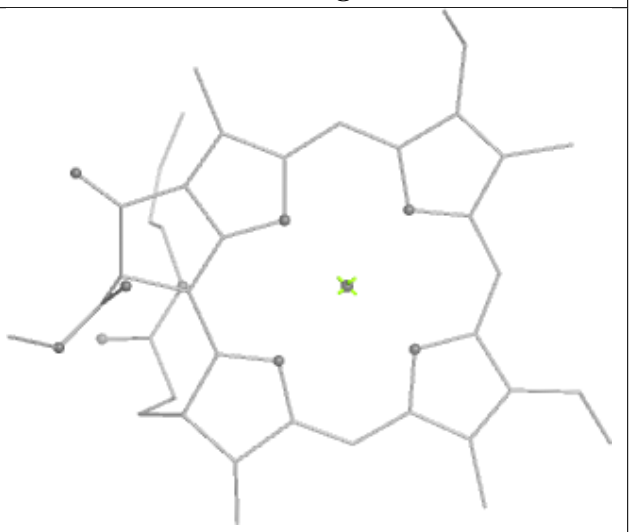
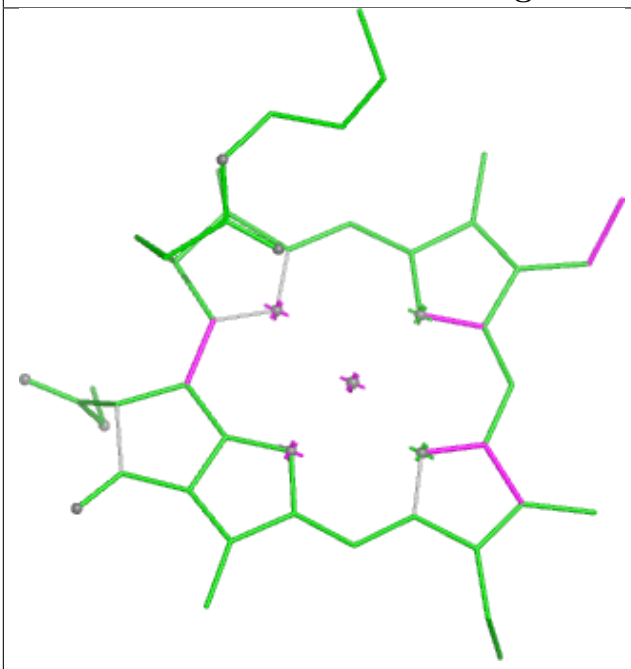


Rings

Ligand CLA A 1134



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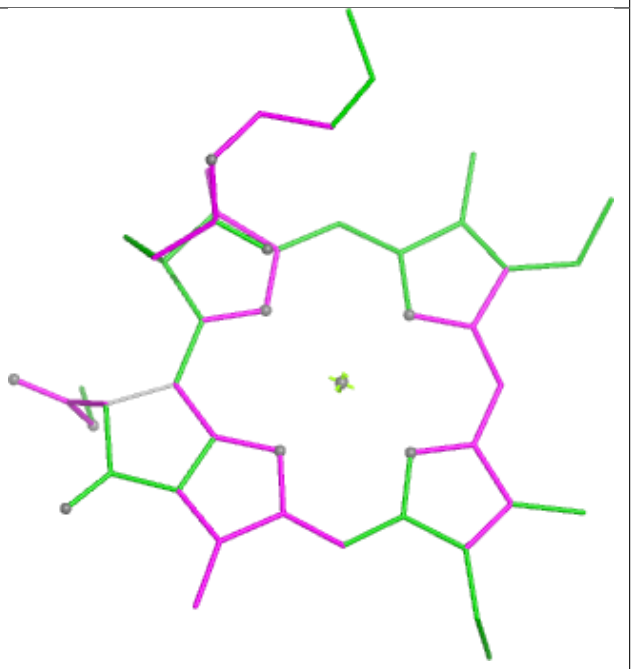
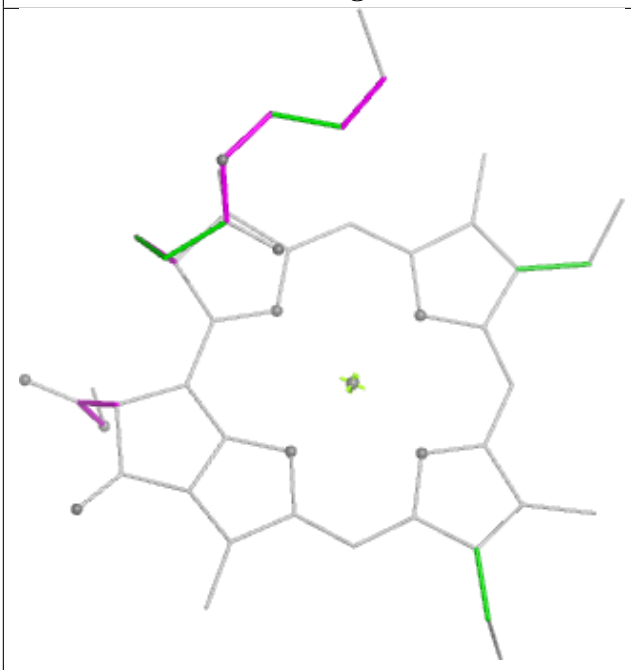


Bond angles



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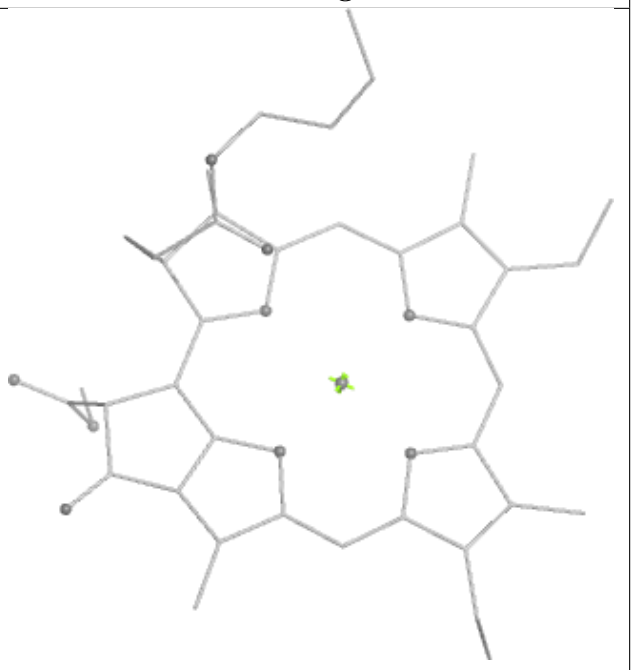
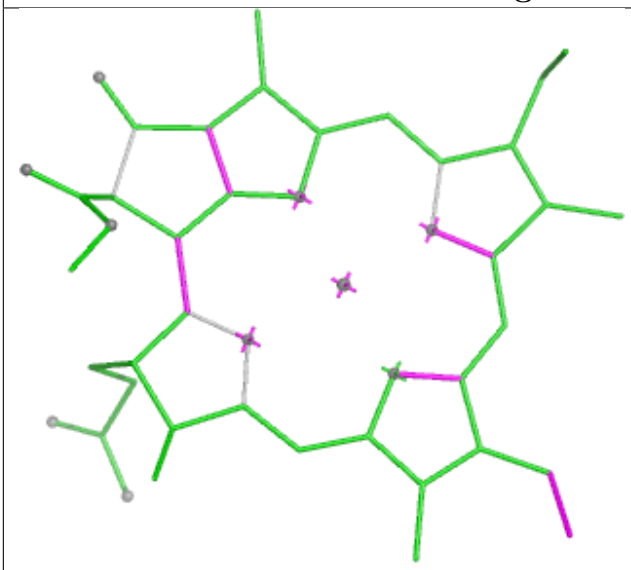


Rings

Ligand CLA A 1102



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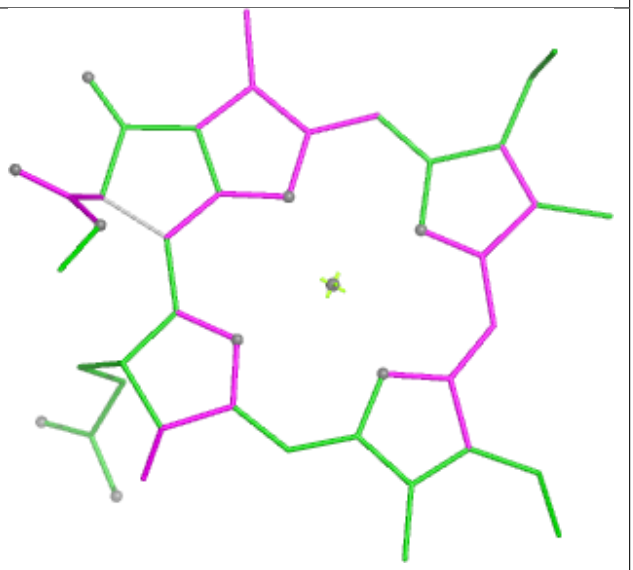
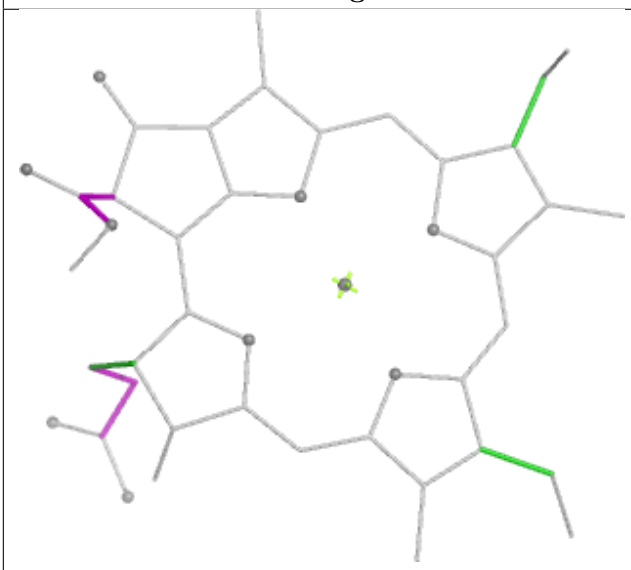


Bond angles



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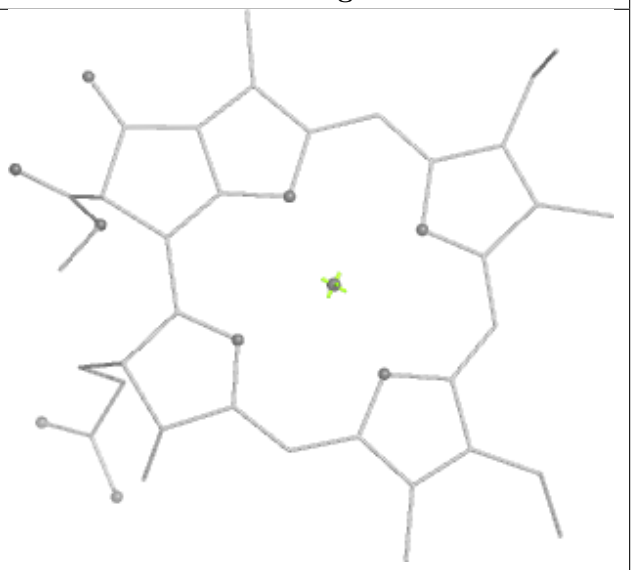
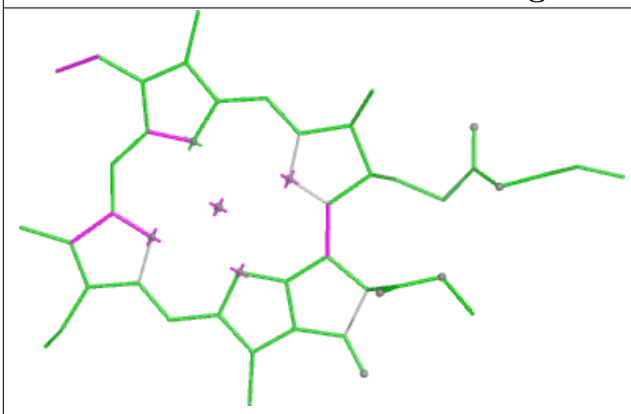


Rings

Ligand CLA 3 608



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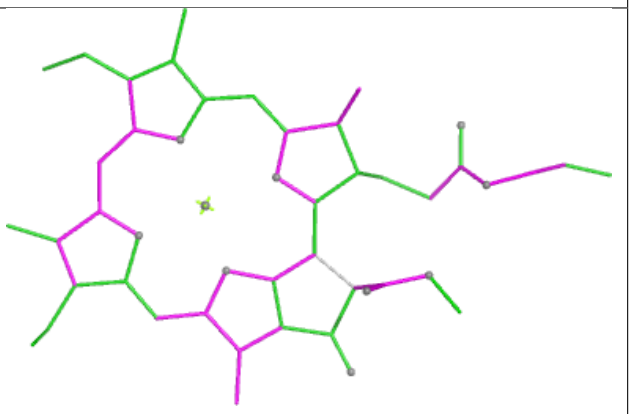

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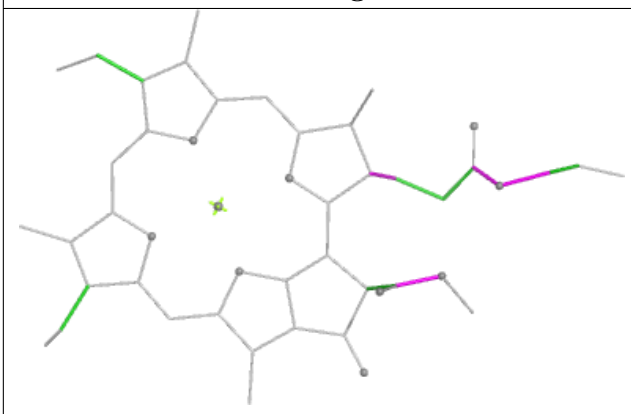

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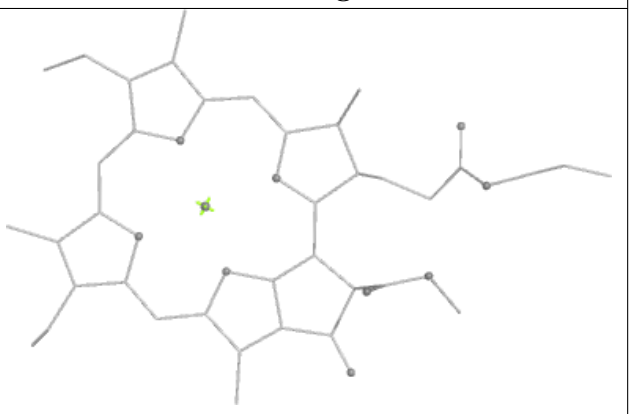
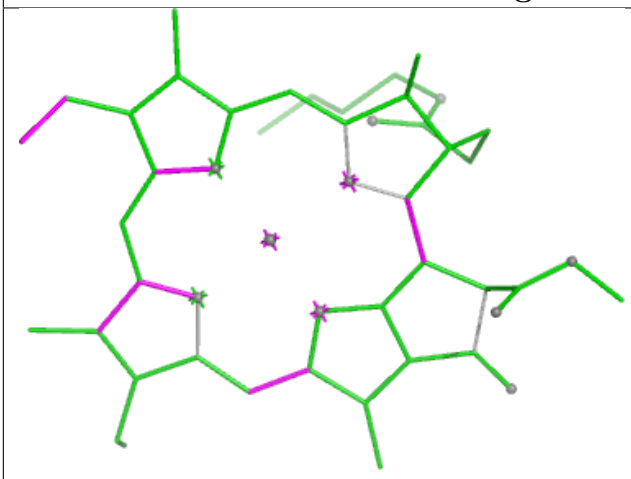


Rings

Ligand CLA A 1109



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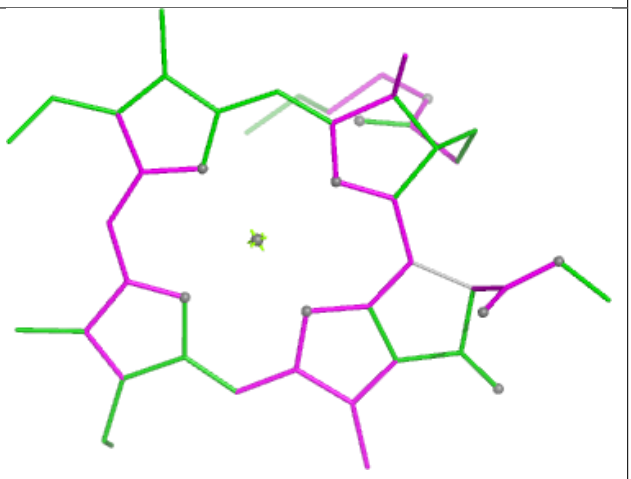
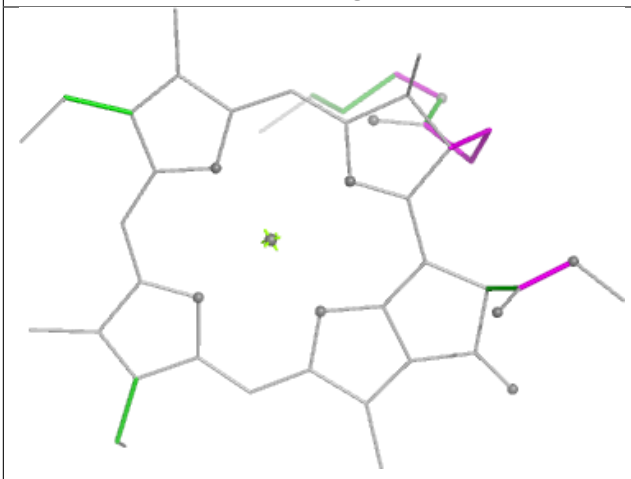


Bond angles



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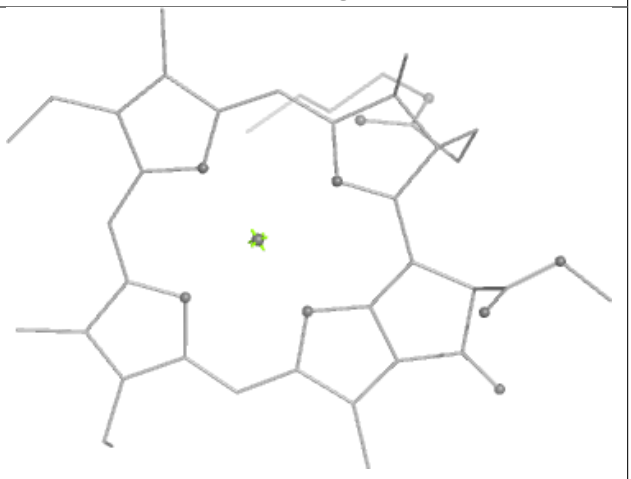
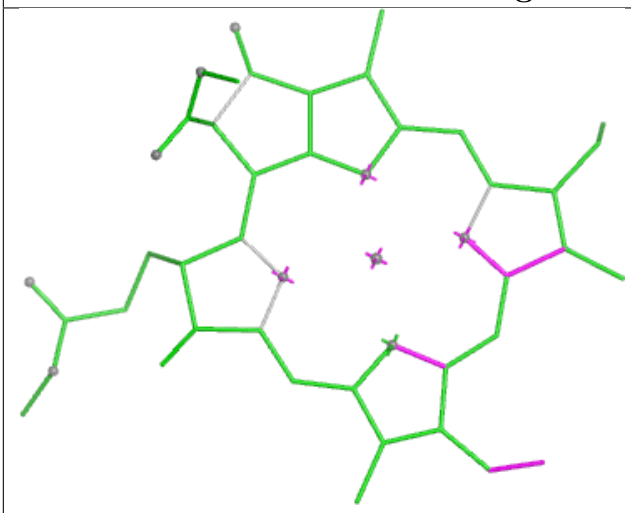


Rings

Ligand CLA B 1217



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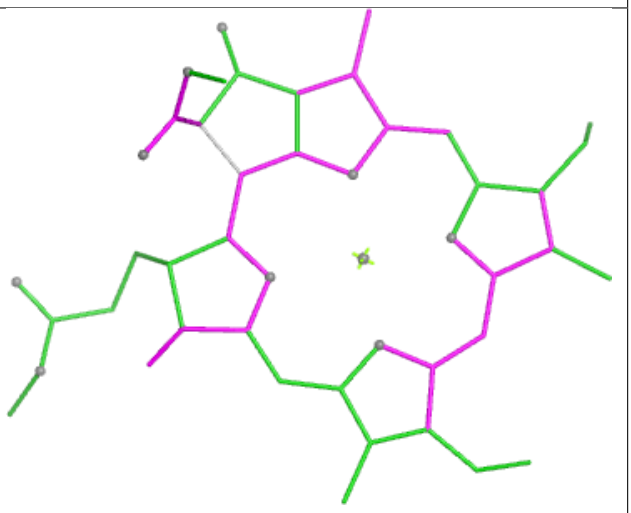
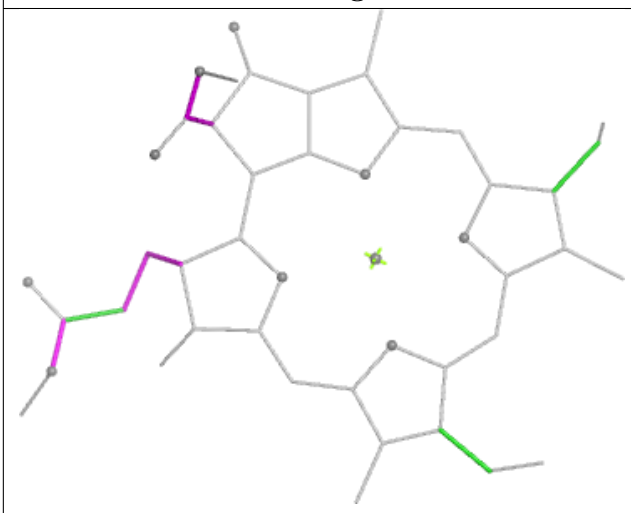


Bond angles



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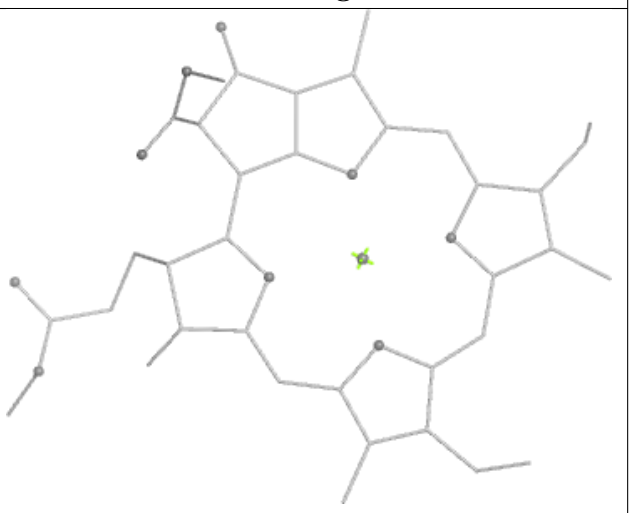
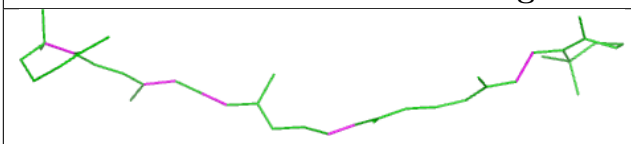


Rings

Ligand BCR J 4002



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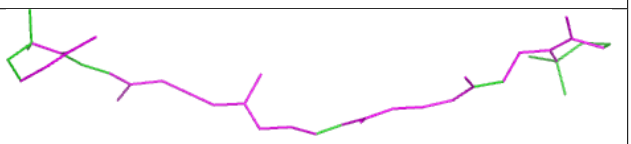
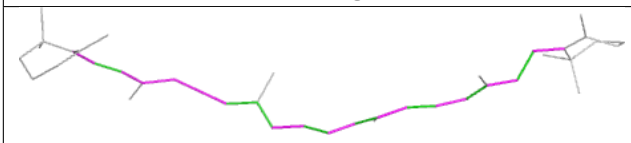


Bond angles



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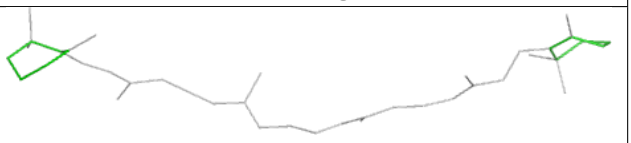
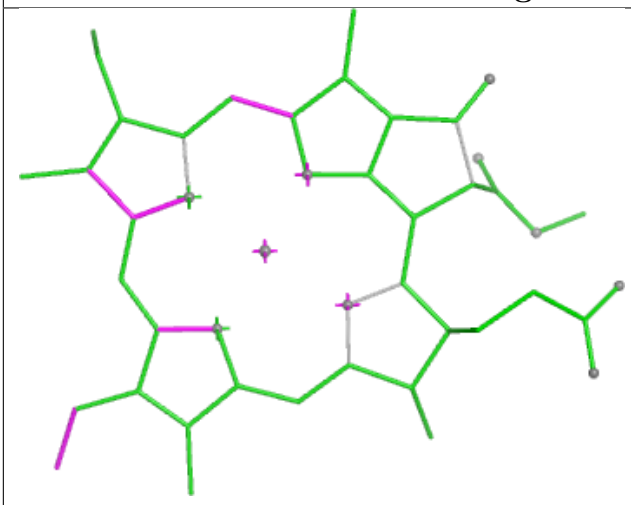
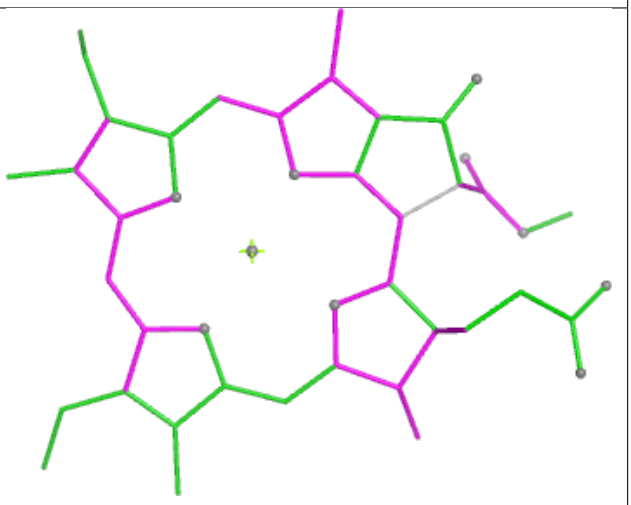


Rings

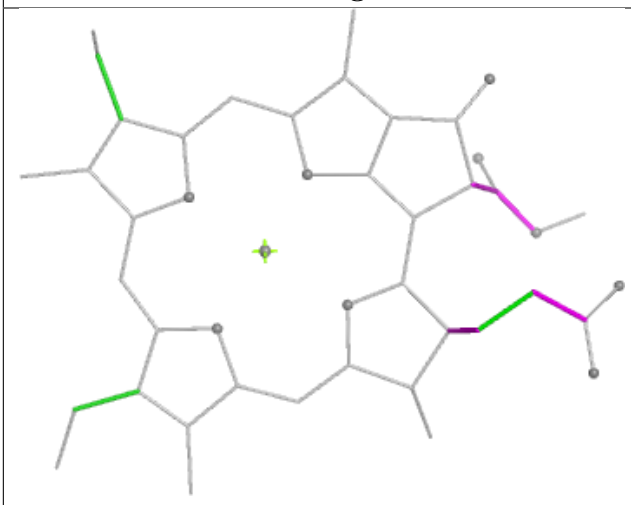
Ligand CLA A 1101



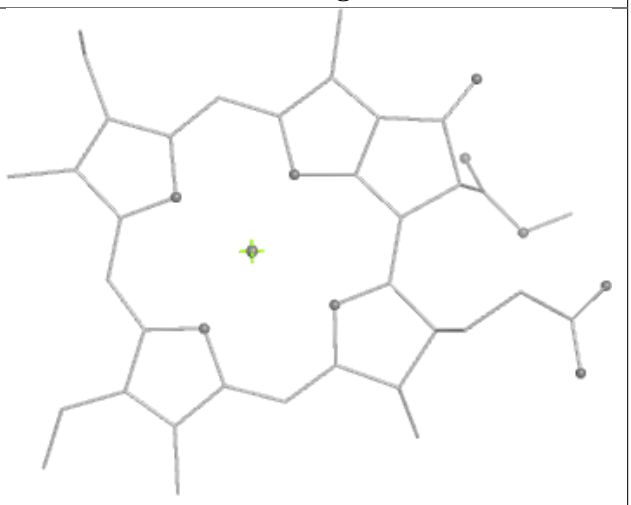
Bond lengths



Bond angles

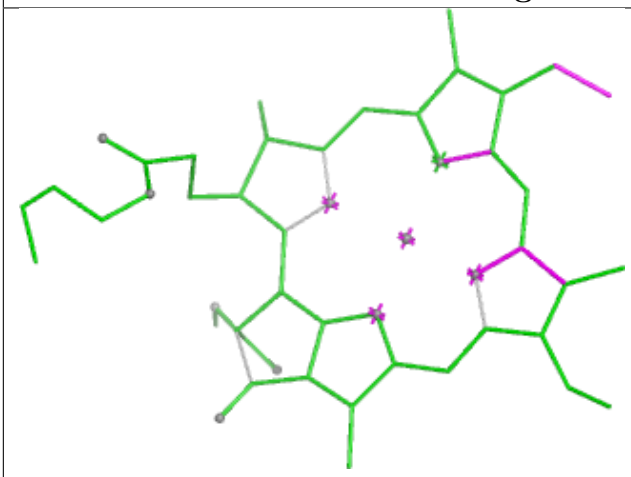


Torsions

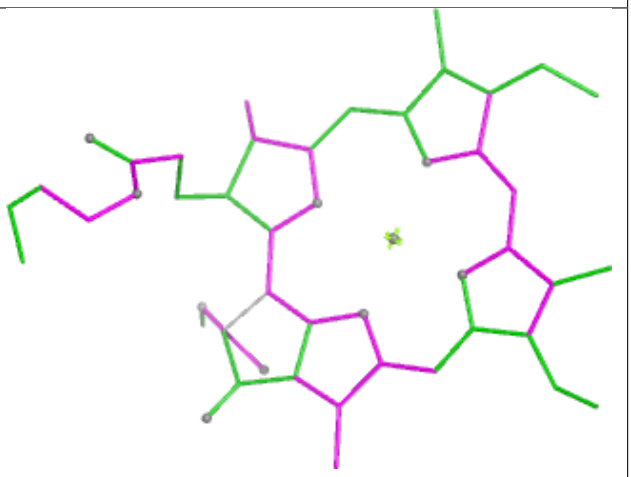


Rings

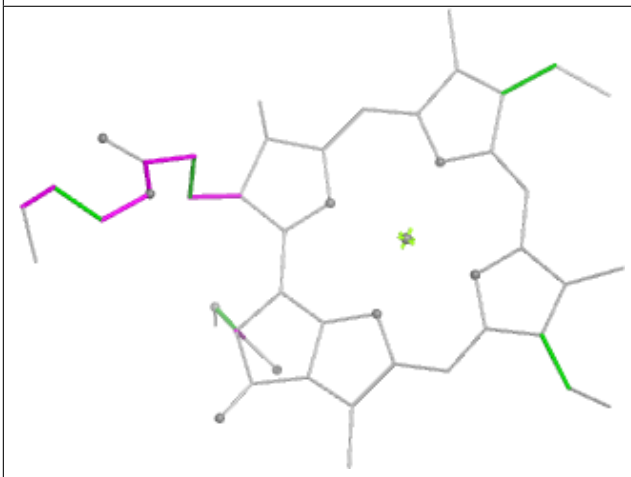
Ligand CLA A 1137



Bond lengths



Bond angles

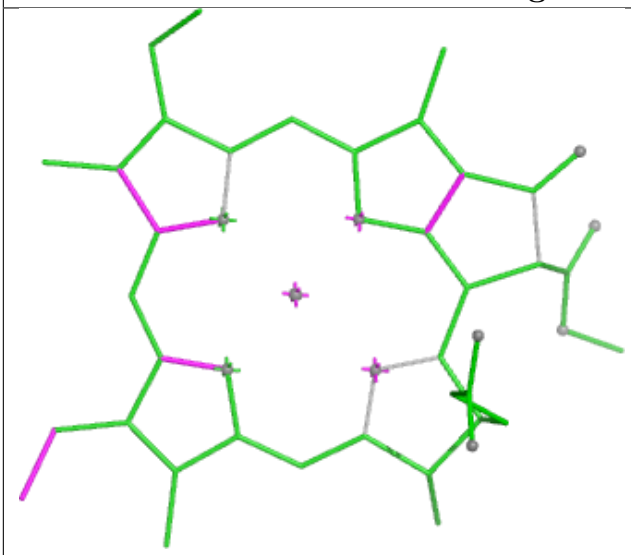


Torsions



Rings

Ligand CLA 1 606



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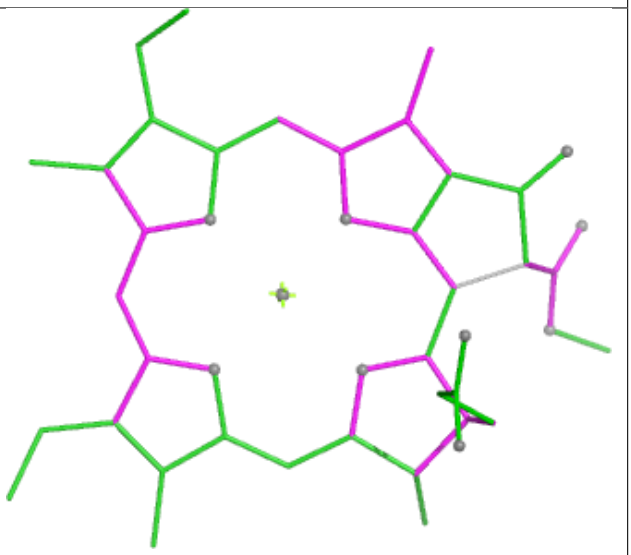
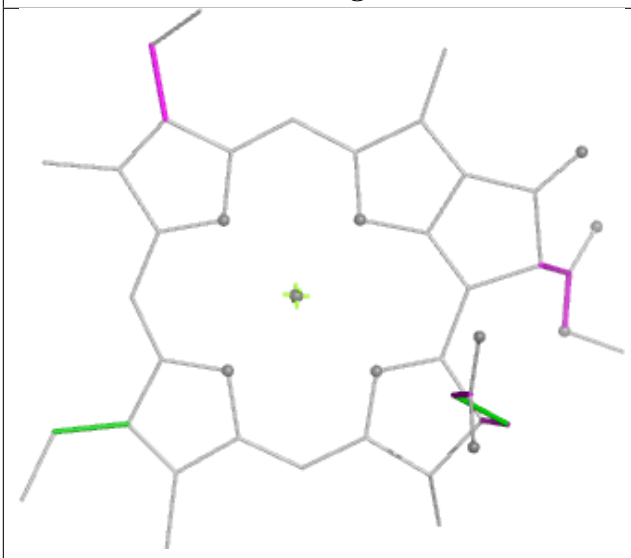


Bond angles



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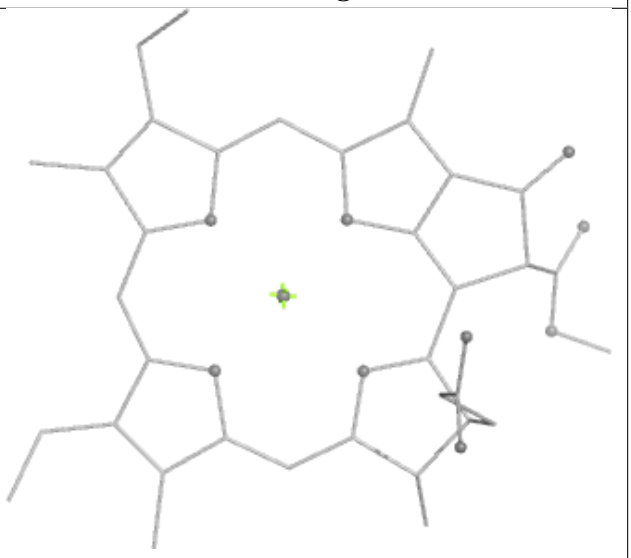
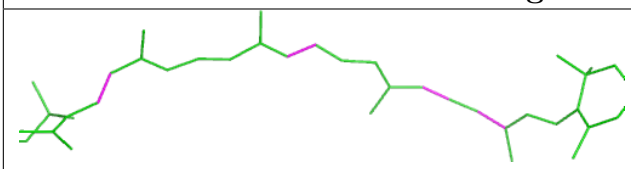


Rings

Ligand BCR 4 503



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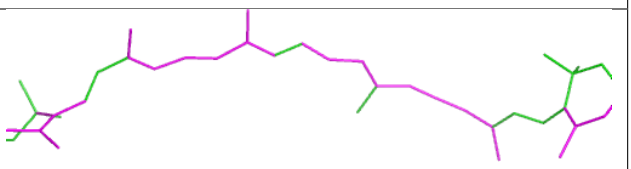
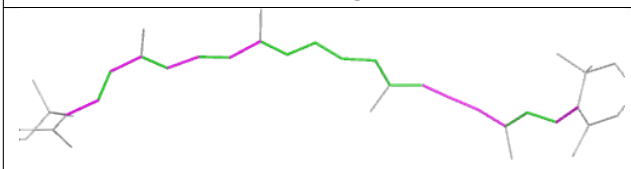


Bond angles



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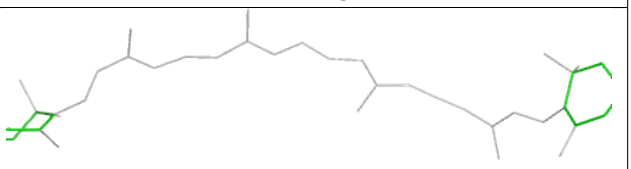
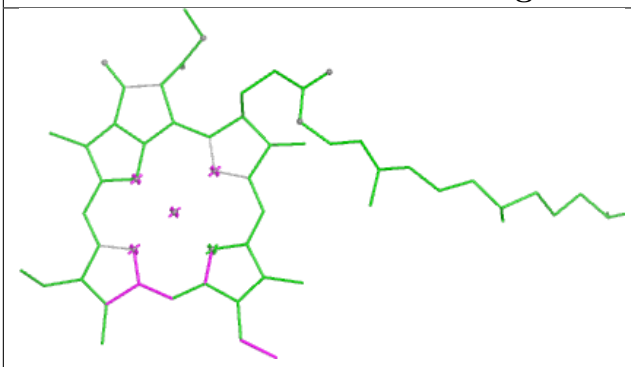


Rings

Ligand CLA B 1023



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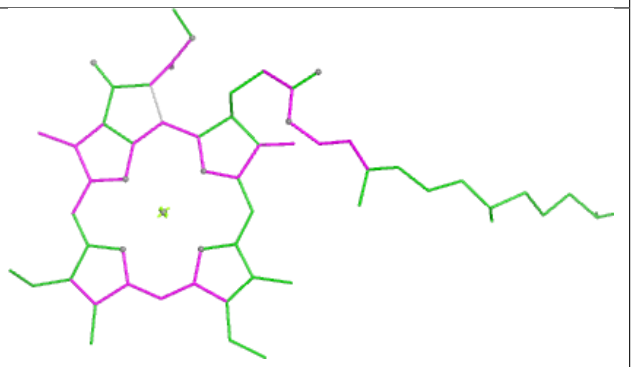

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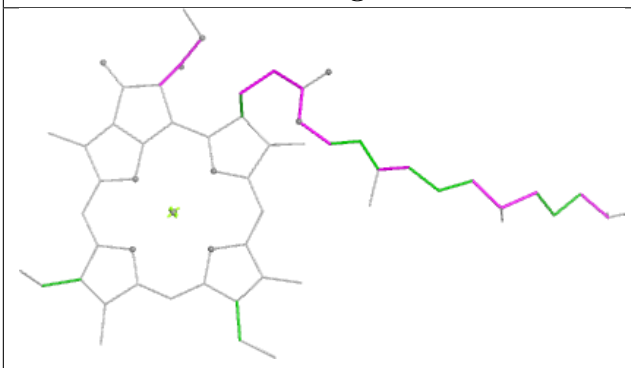

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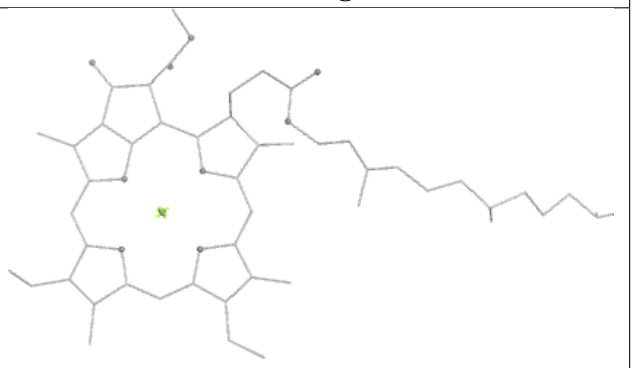
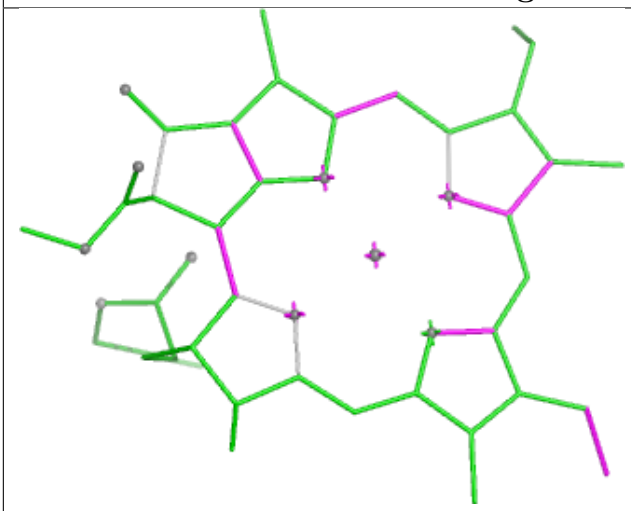


Rings

Ligand CLA F 1302



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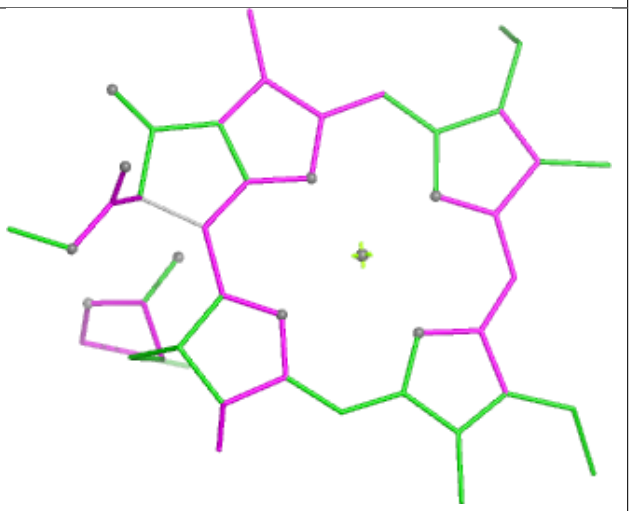

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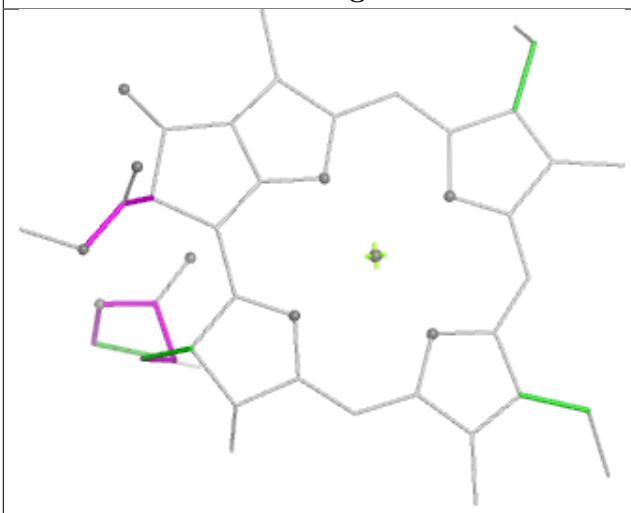

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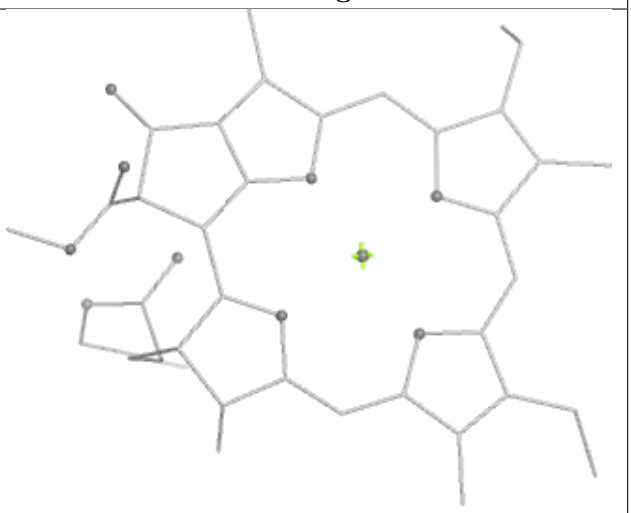
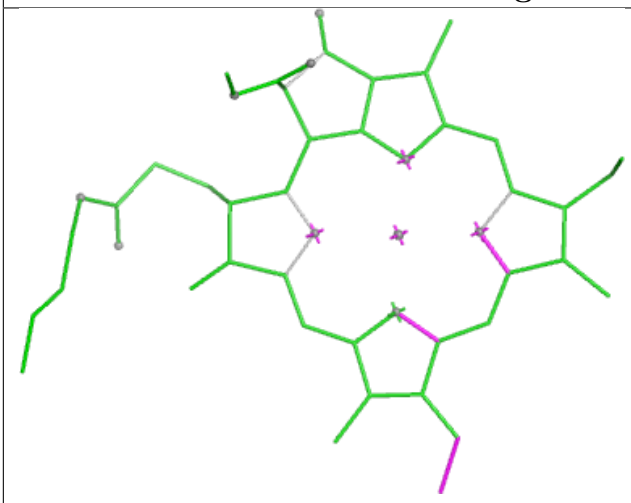


Rings

Ligand CLA A 1111



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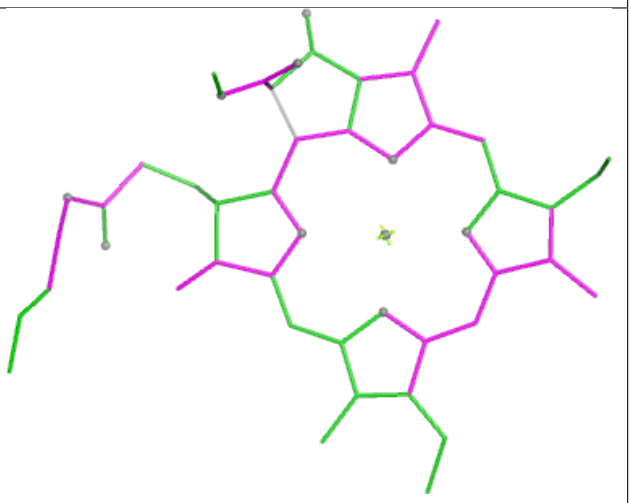
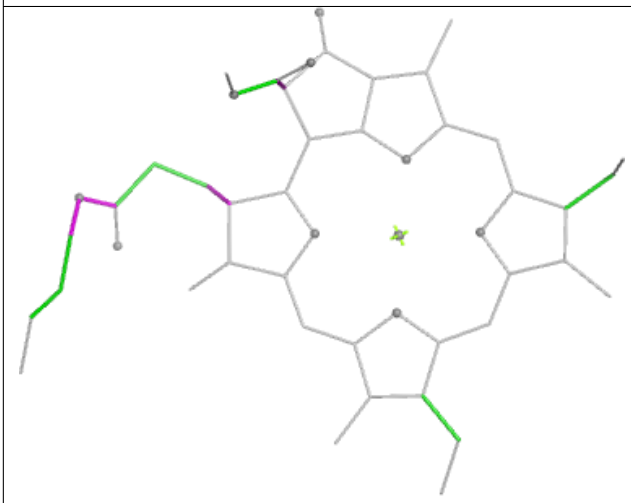


Bond angles



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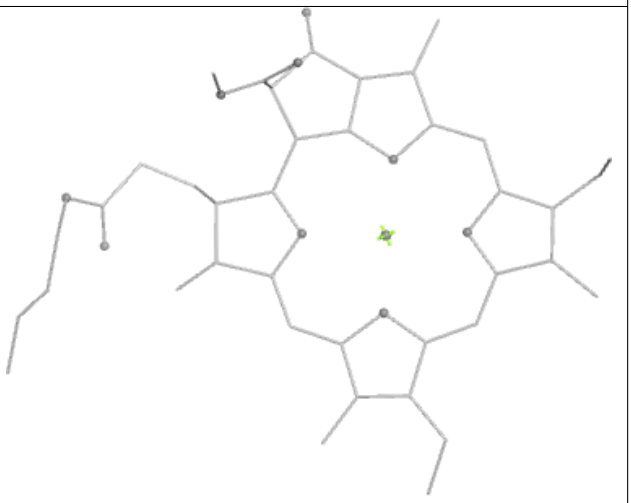
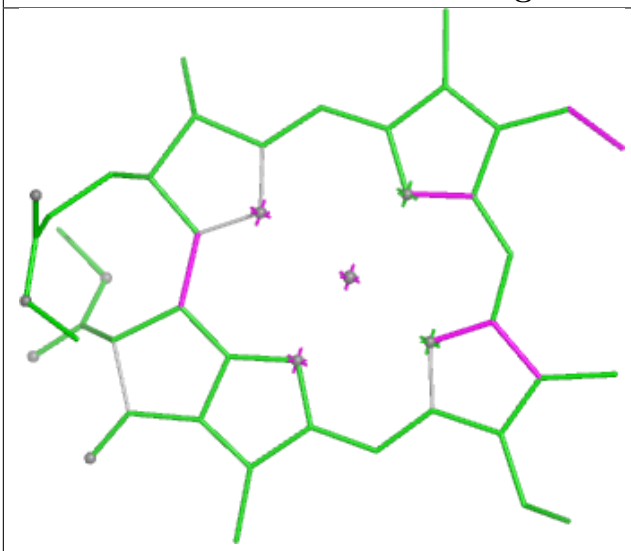


Rings

Ligand CLA A 1108



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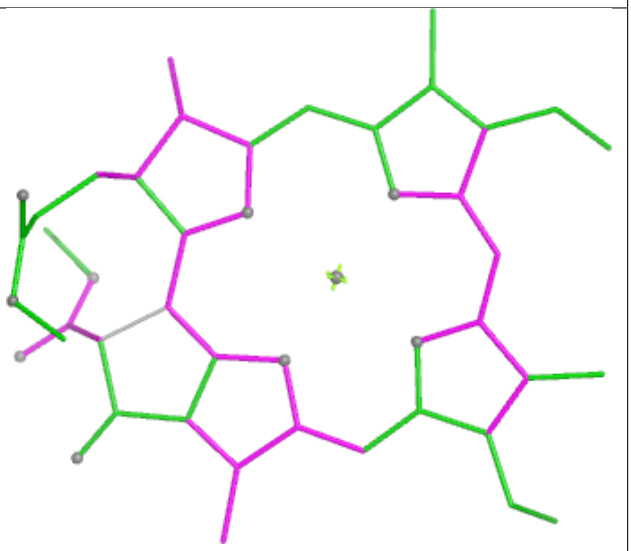
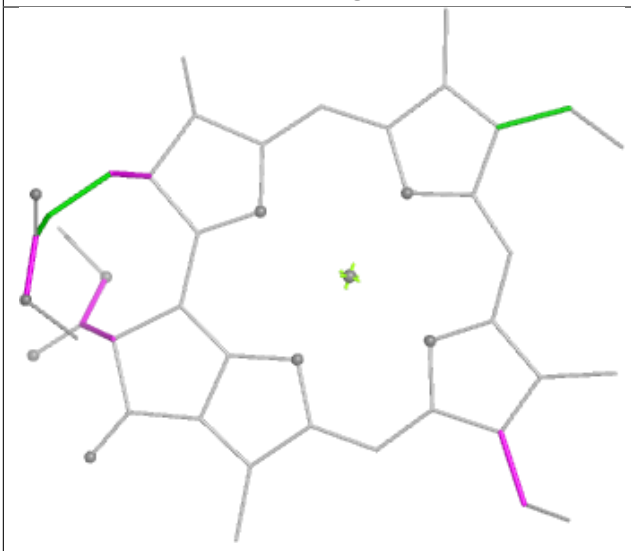


Bond angles



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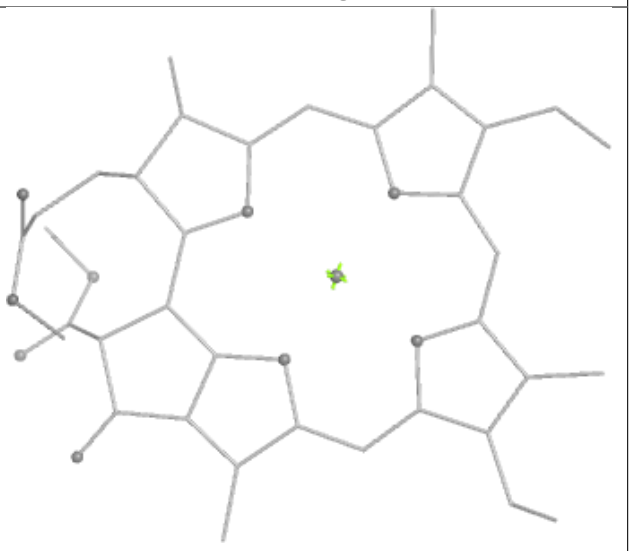
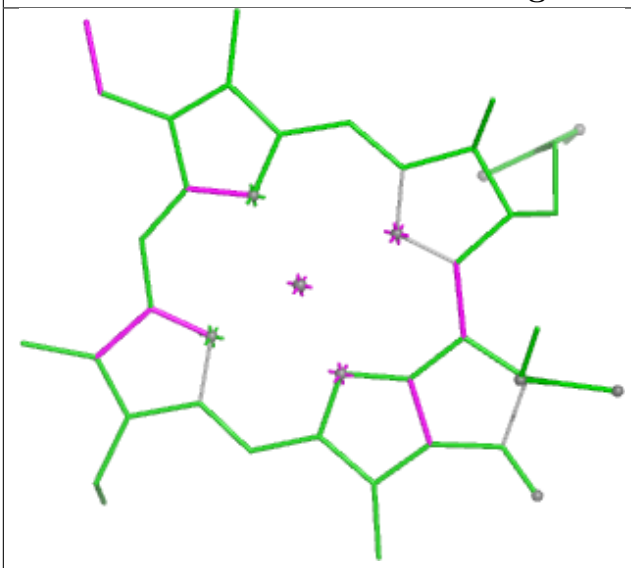


Rings

Ligand CLA 2 606



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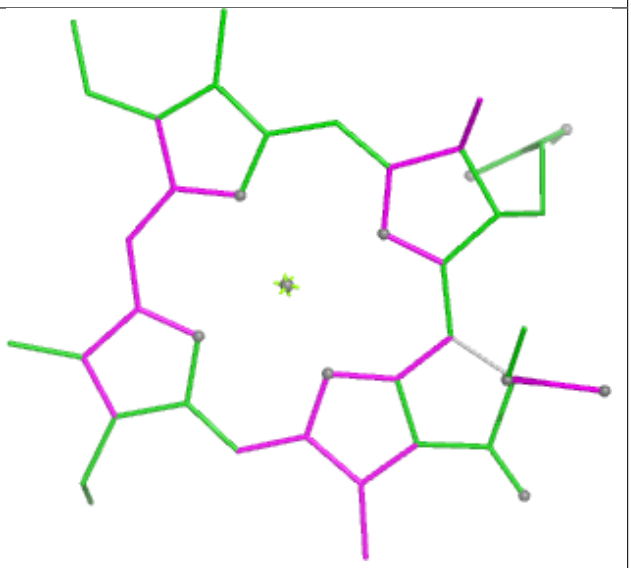
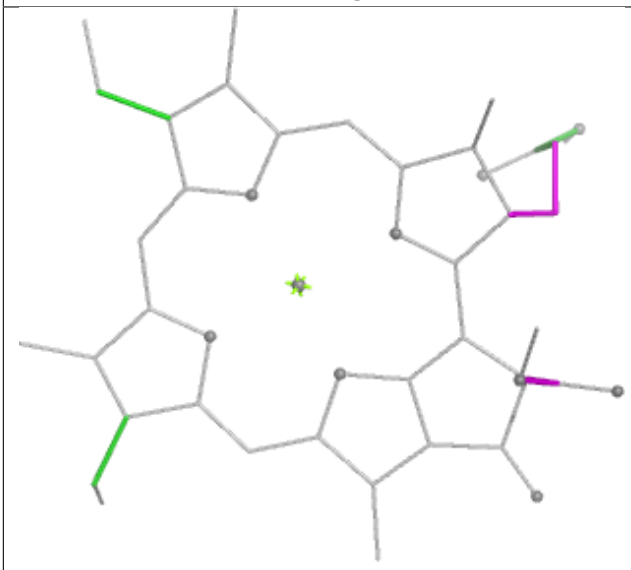


Bond angles



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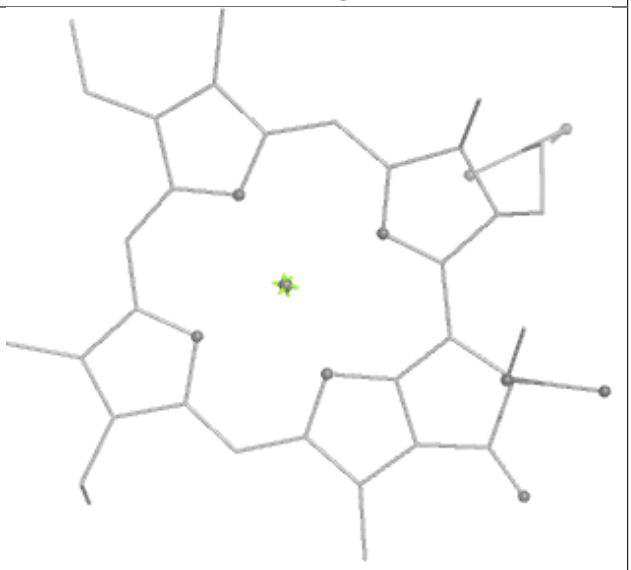
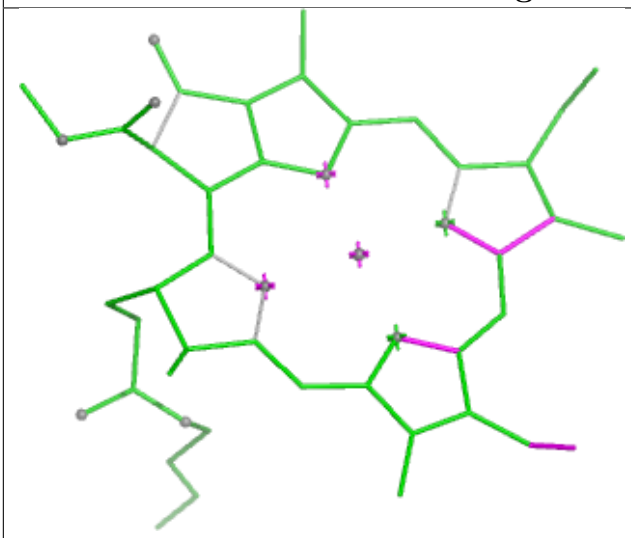


Rings

Ligand CLA B 1208



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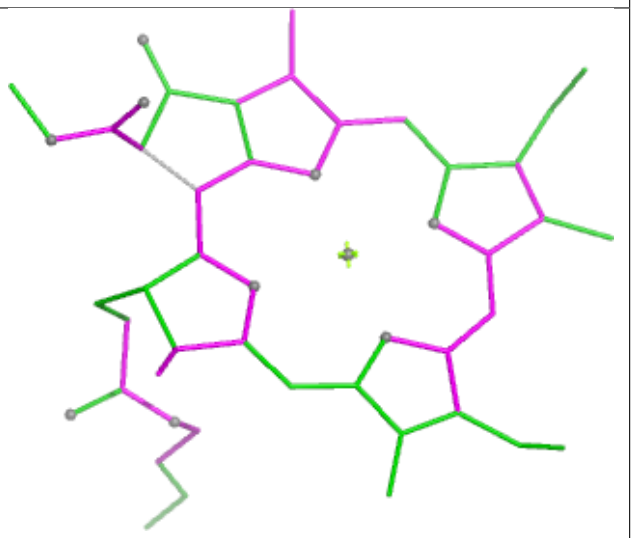
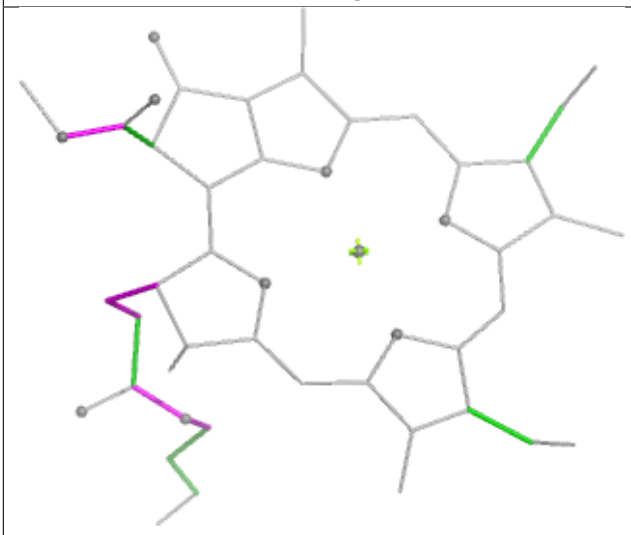


Bond angles



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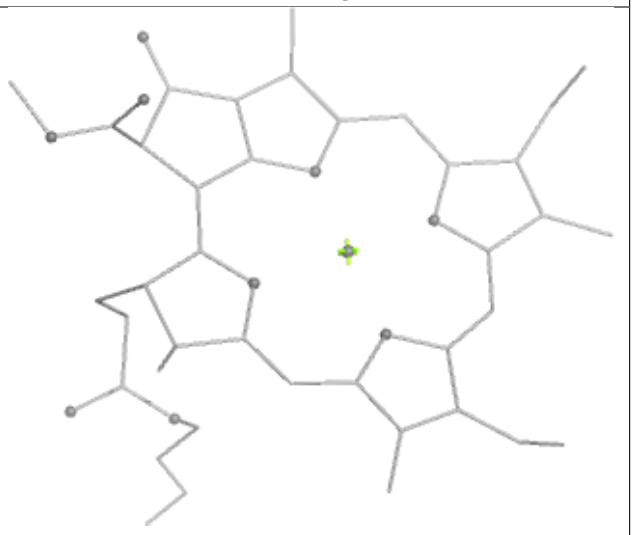
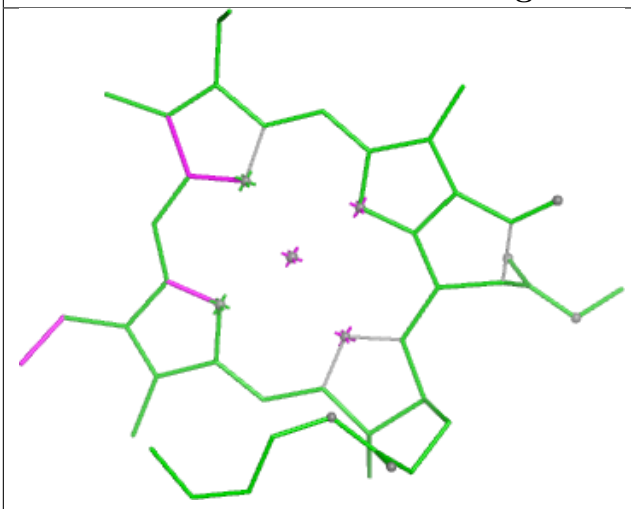


Rings

Ligand CLA B 1215



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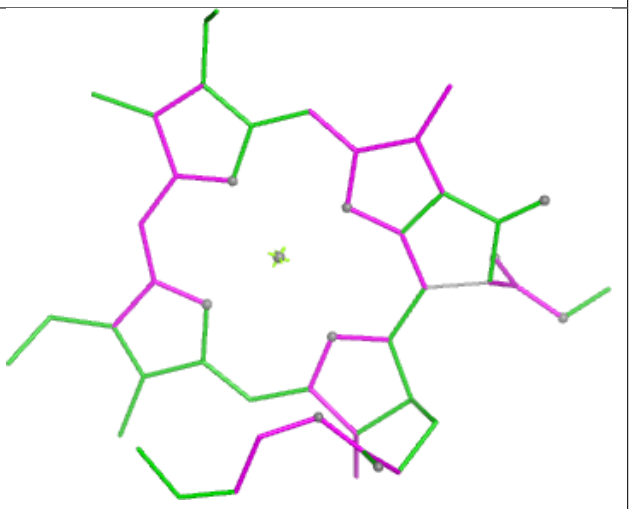
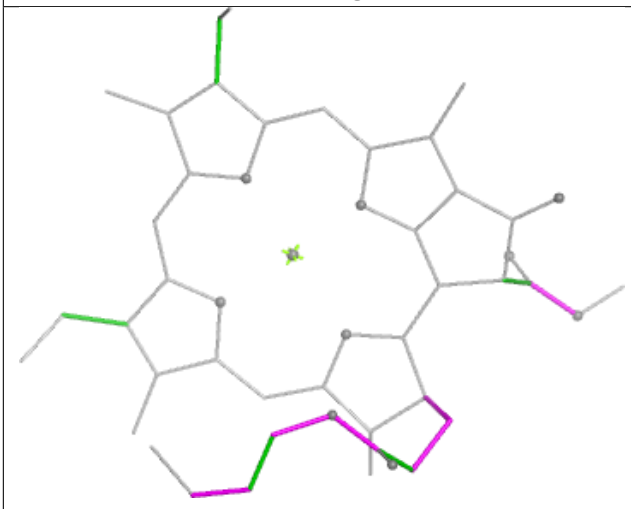


Bond angles



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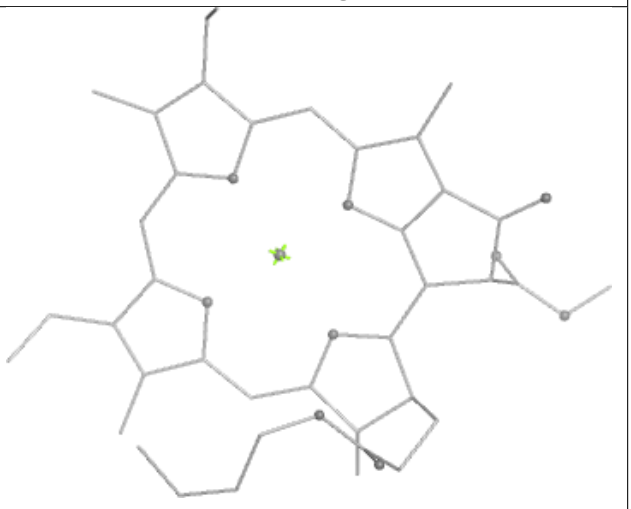
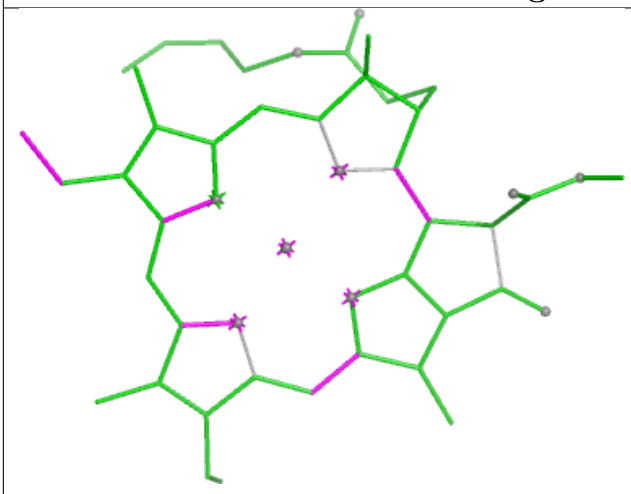


Rings

Ligand CLA 4 601



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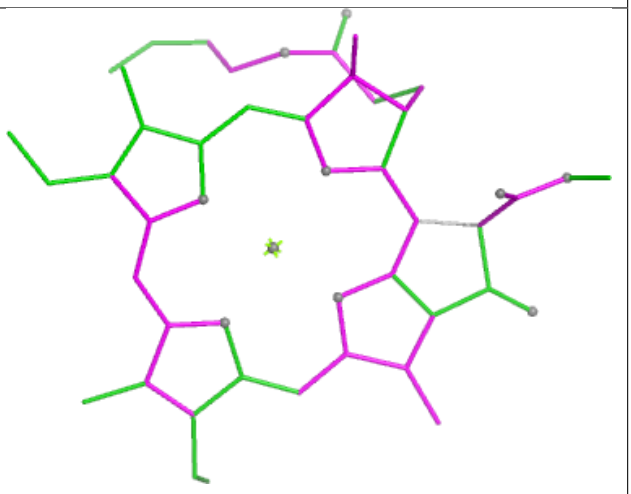
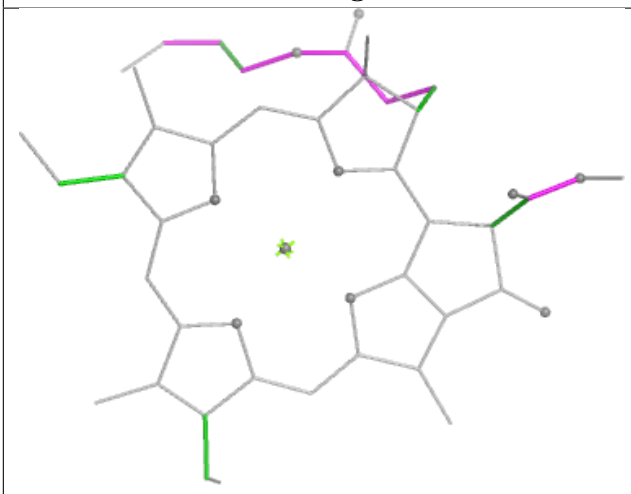


Bond angles



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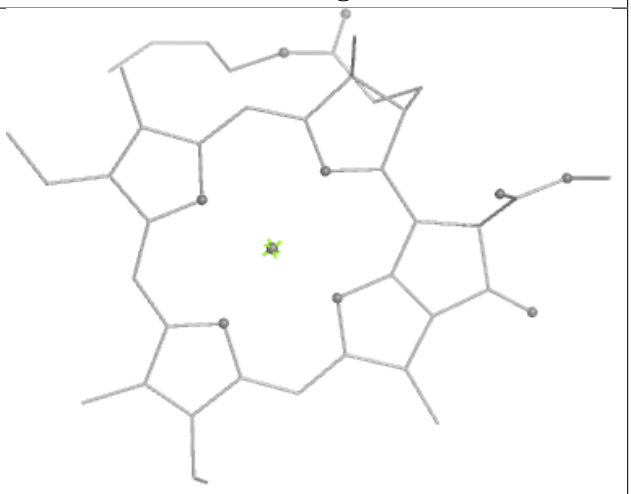
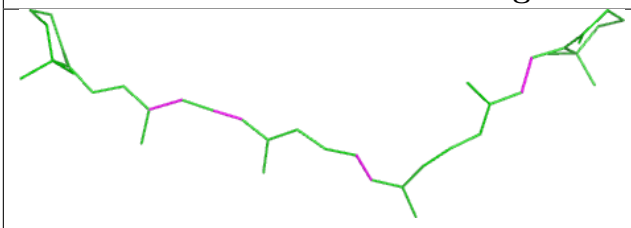


Rings

Ligand BCR A 4004



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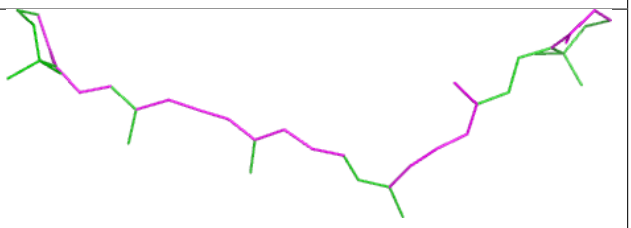
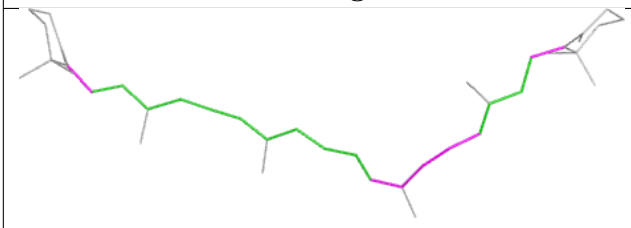


Bond angles



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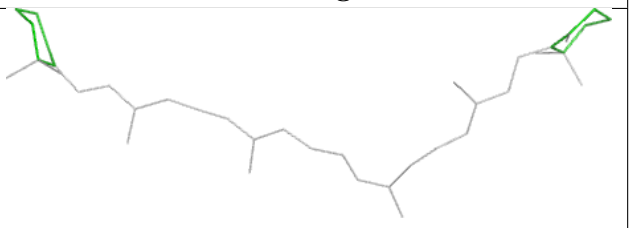
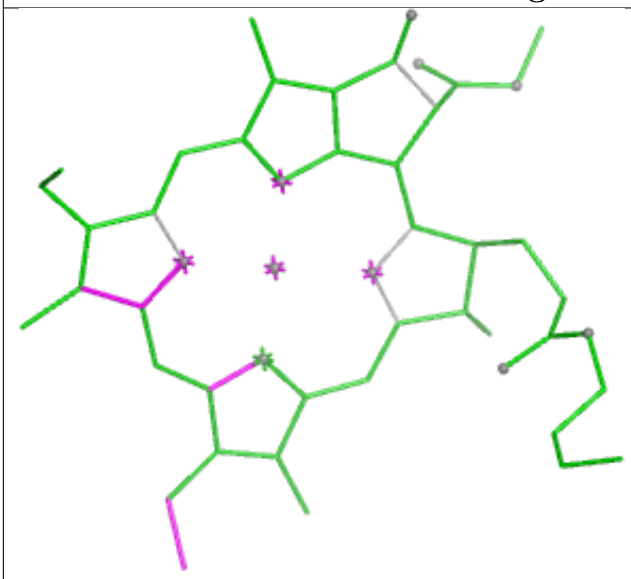
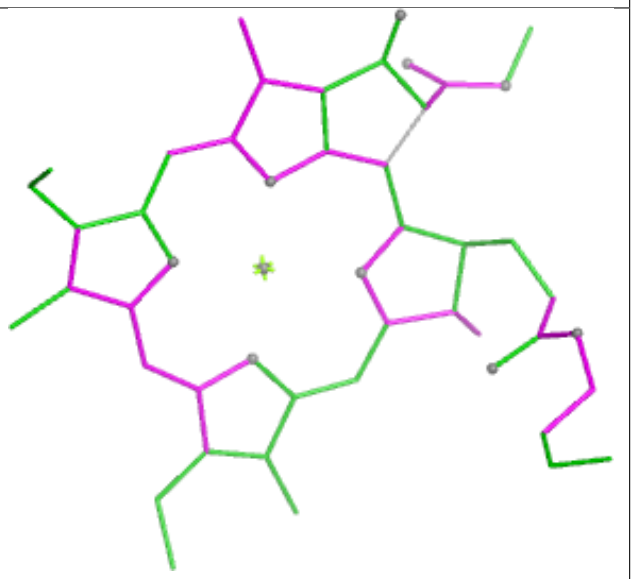


Rings

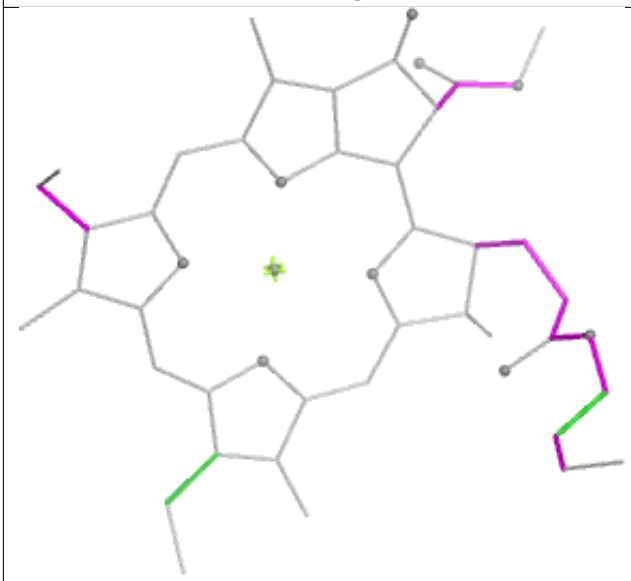
Ligand CLA 2 612



Bond lengths



Bond angles



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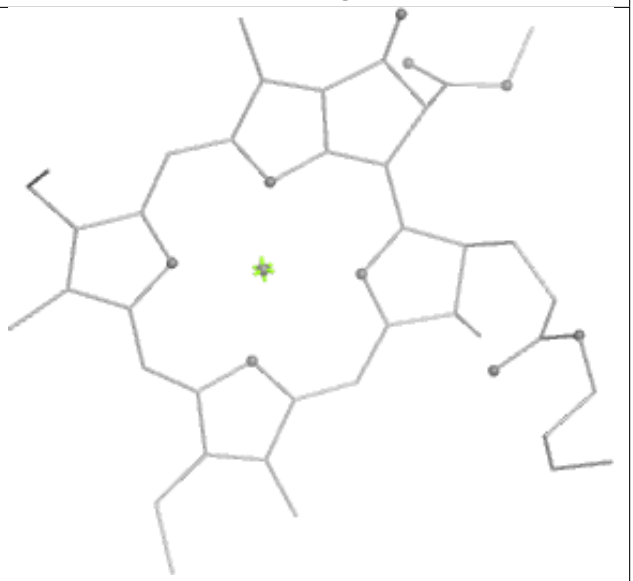
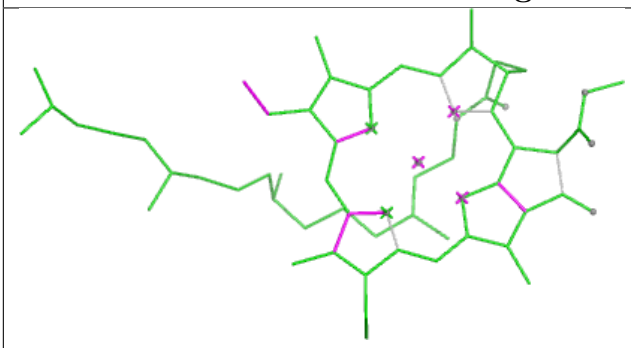
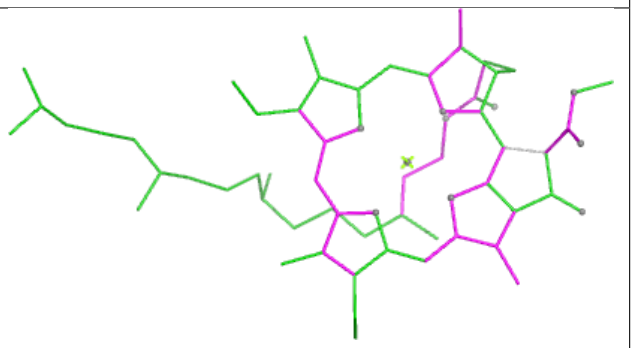


Rings

Ligand CLA A 1138



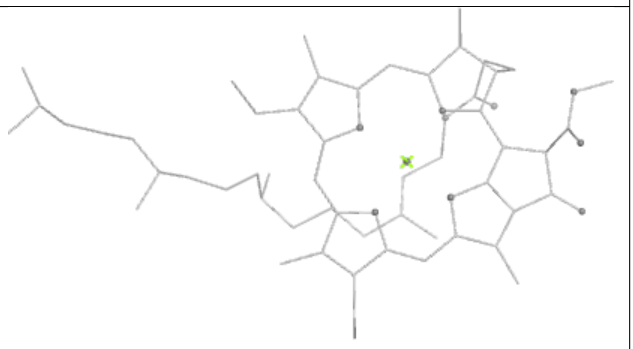
Bond lengths



Bond angles

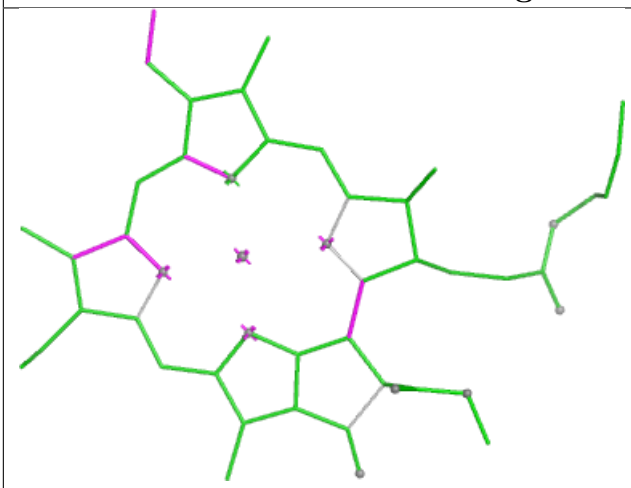


Torsions



Rings

Ligand CLA B 1206



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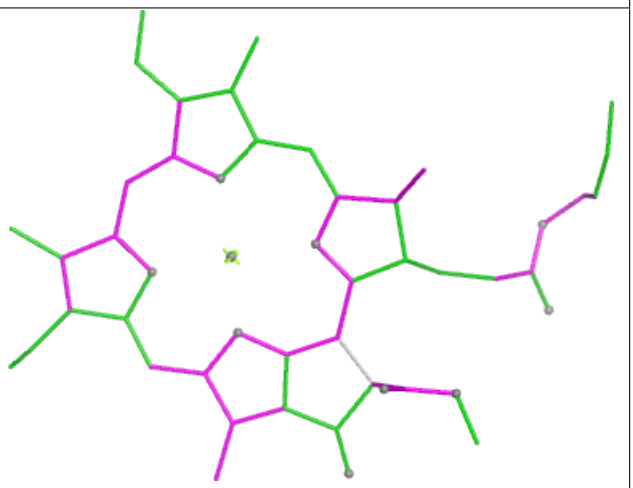
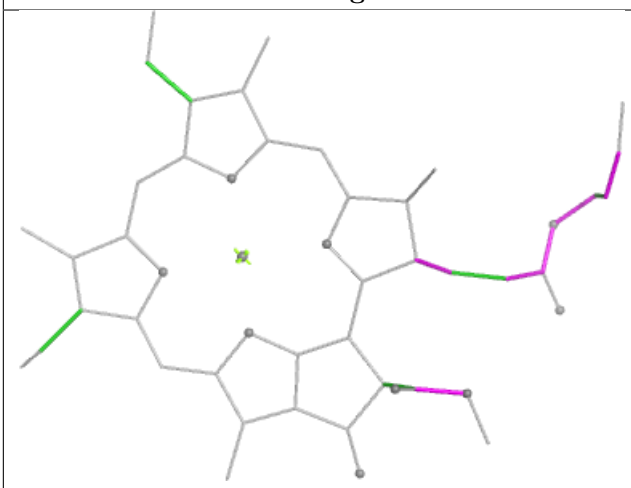
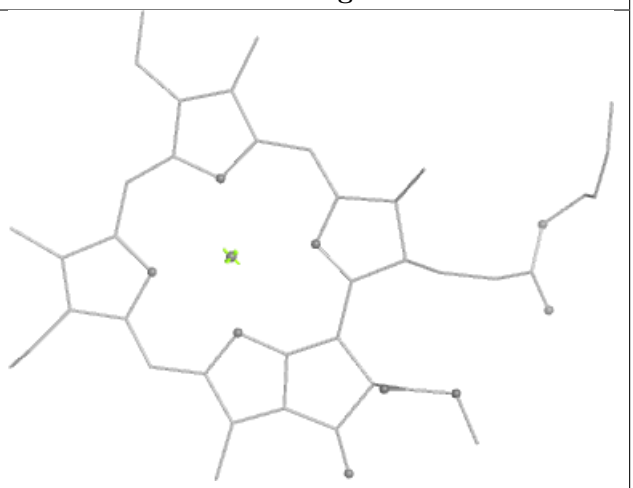


Bond angles

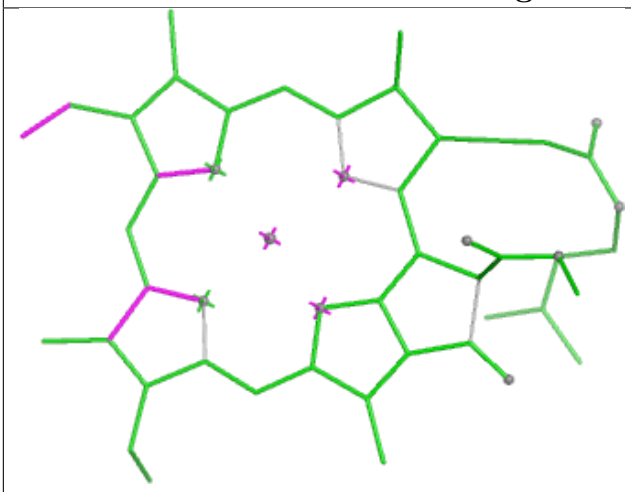


Torsions

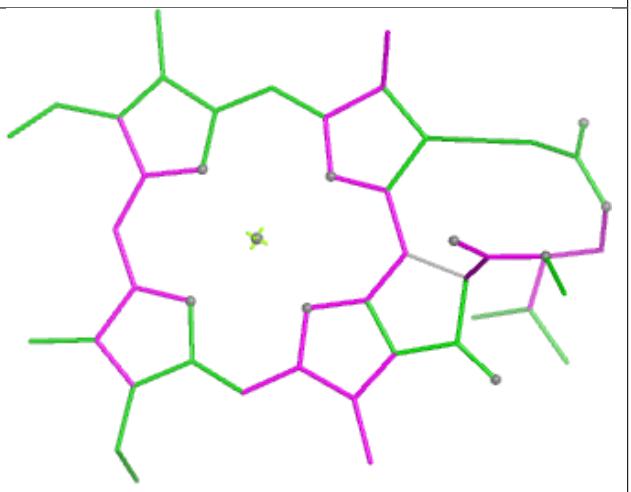


Rings

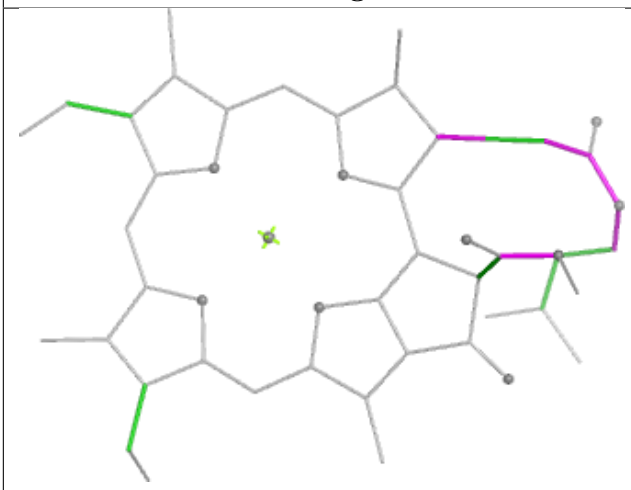
Ligand CLA B 1238



Bond lengths



Bond angles



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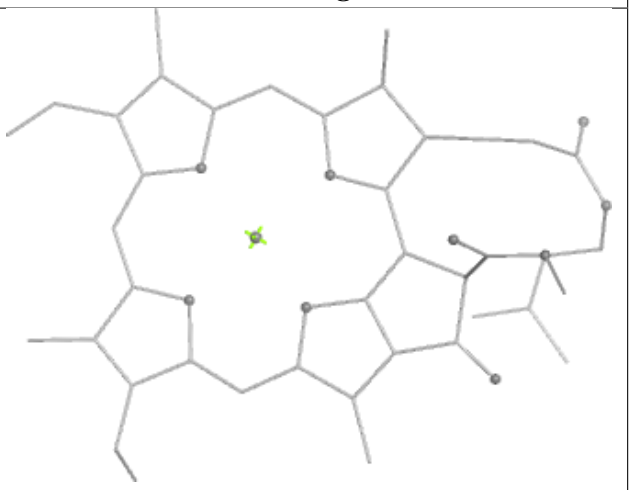
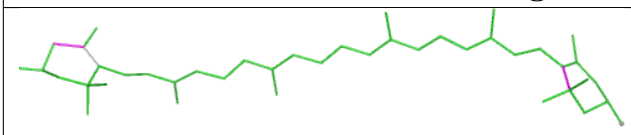


Rings

Ligand LUT 4 501



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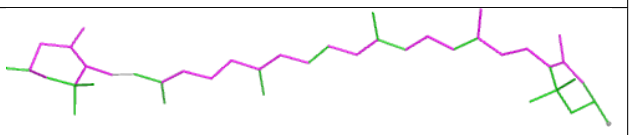

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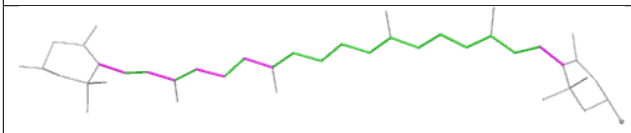

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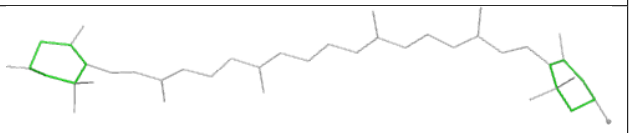
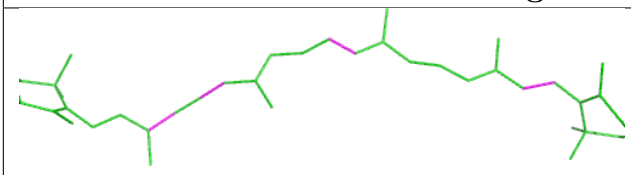


Rings

Ligand BCR 3 504



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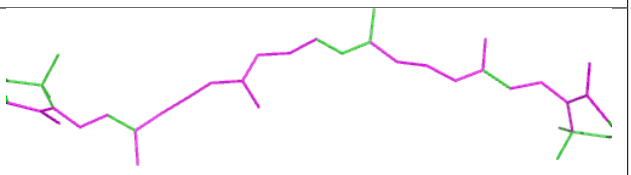
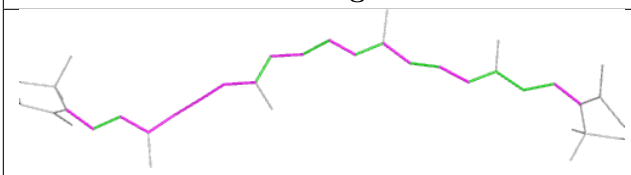


Bond angles



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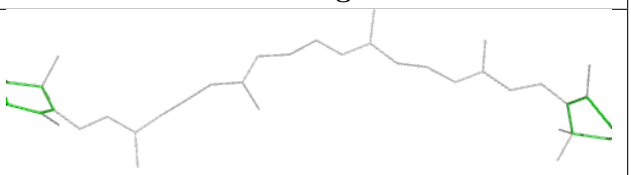
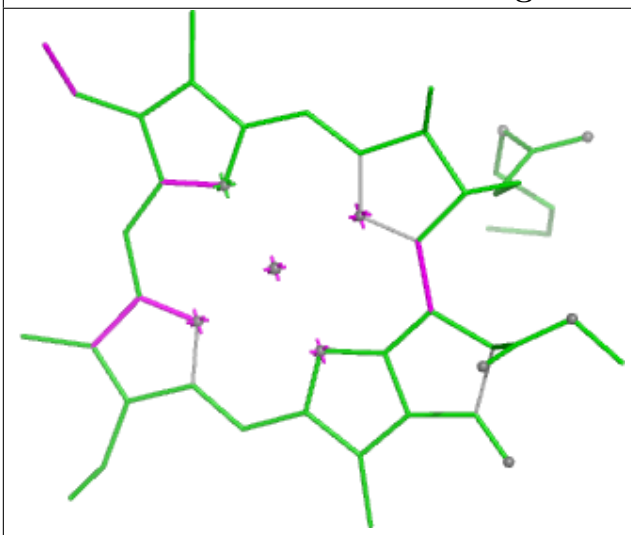


Rings

Ligand CLA B 1219



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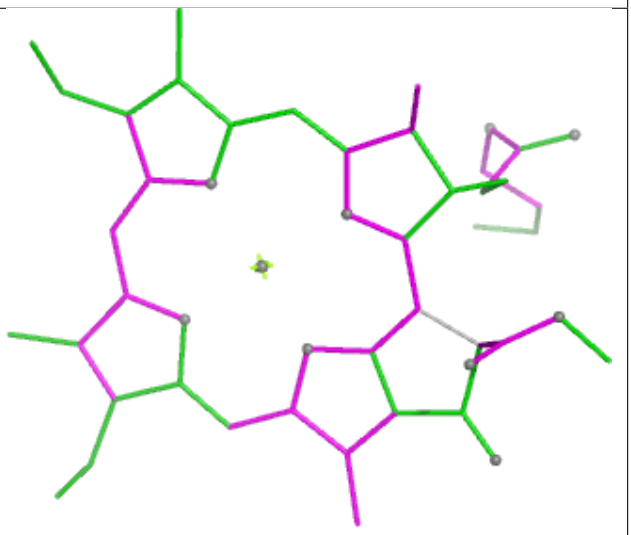
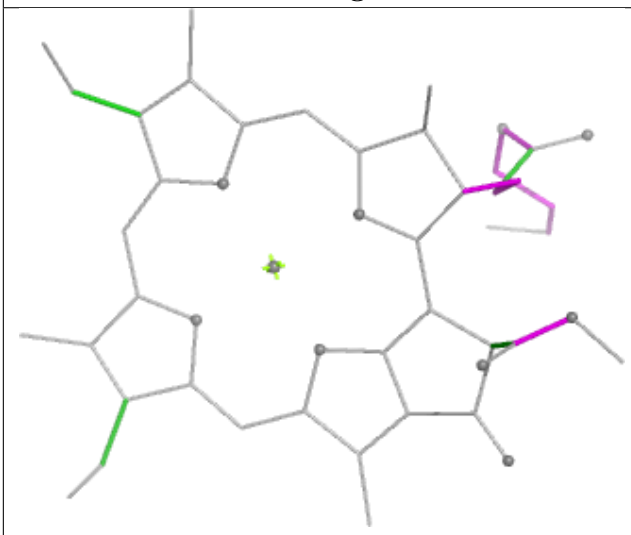


Bond angles



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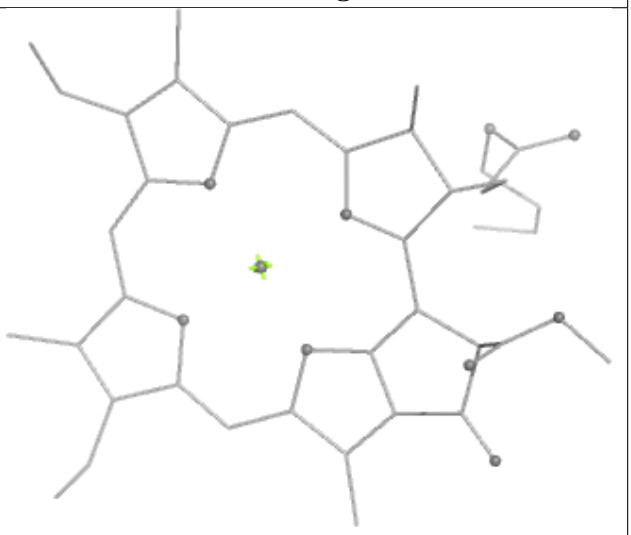
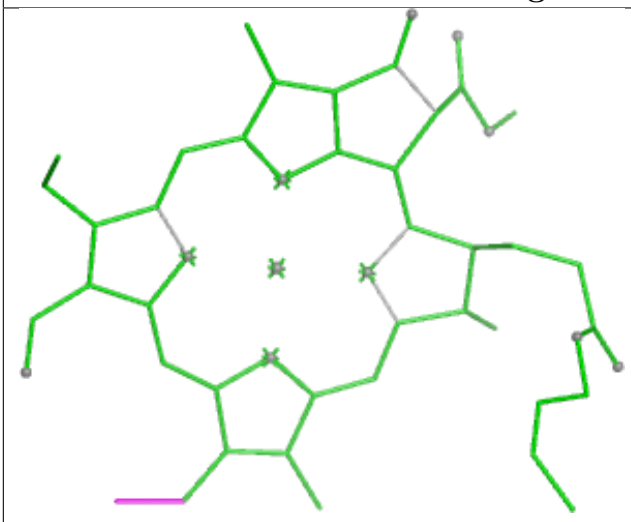


Rings

Ligand CHL 2 609



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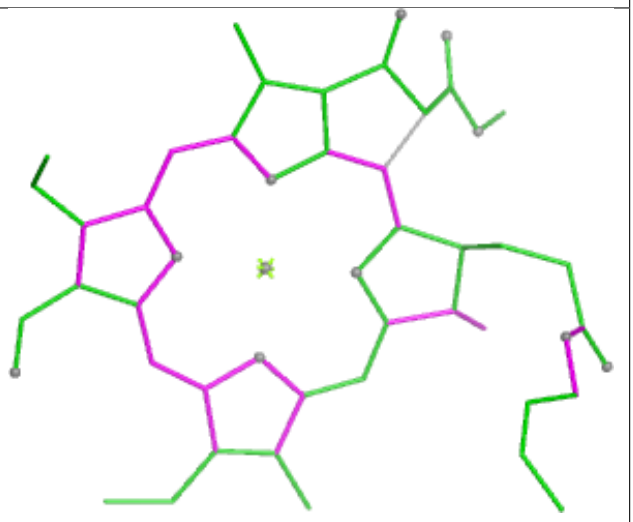
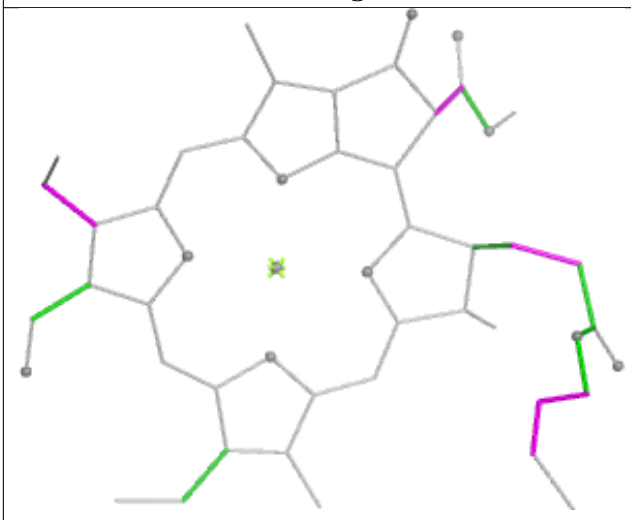


Bond angles



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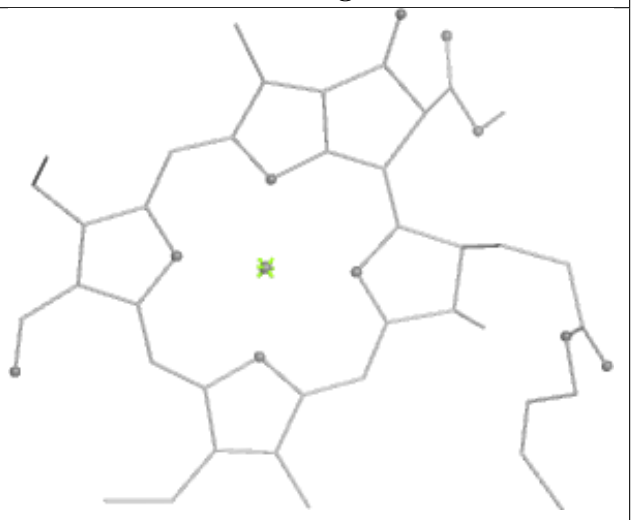
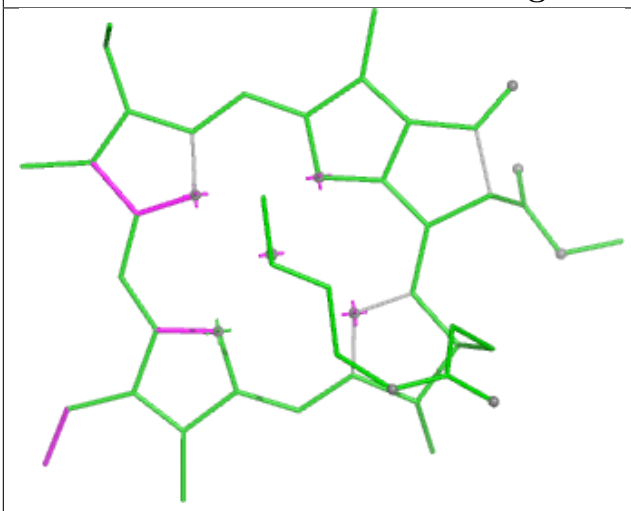


Rings

Ligand CLA 2 608



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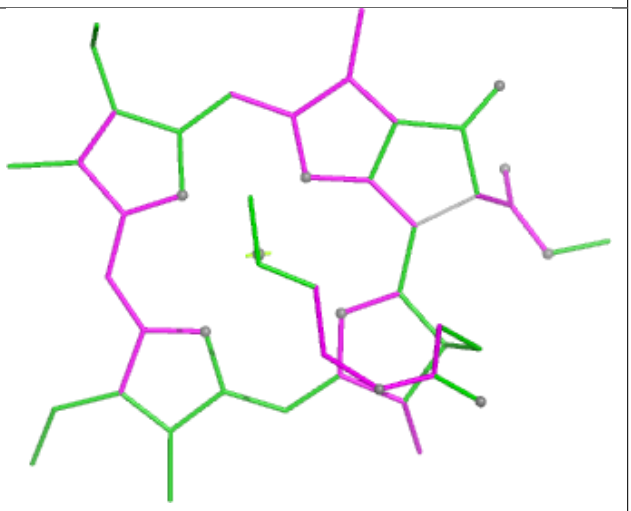
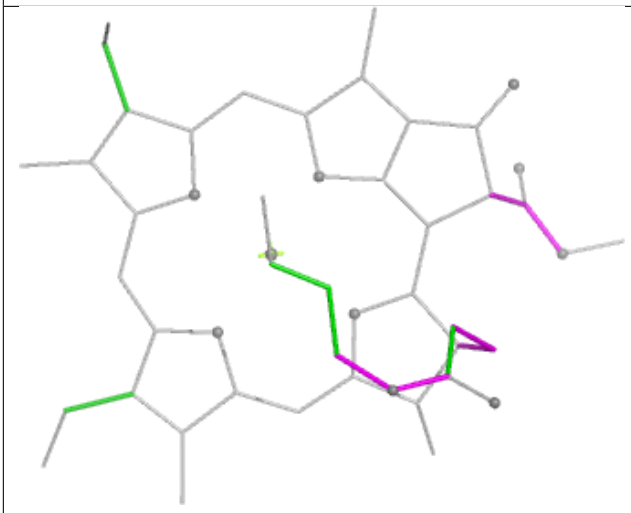


Bond angles



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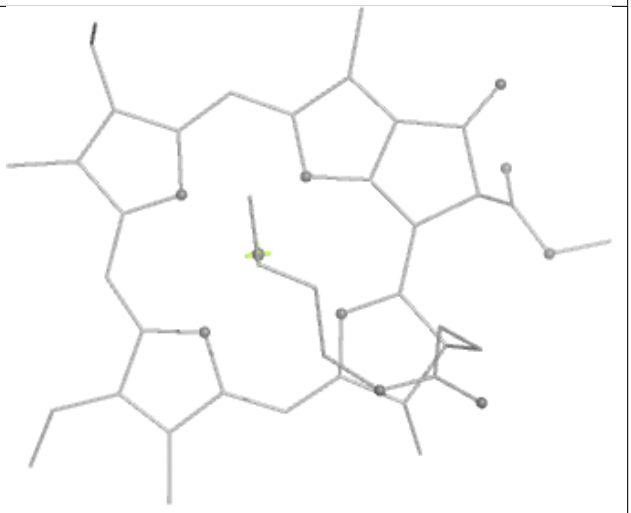
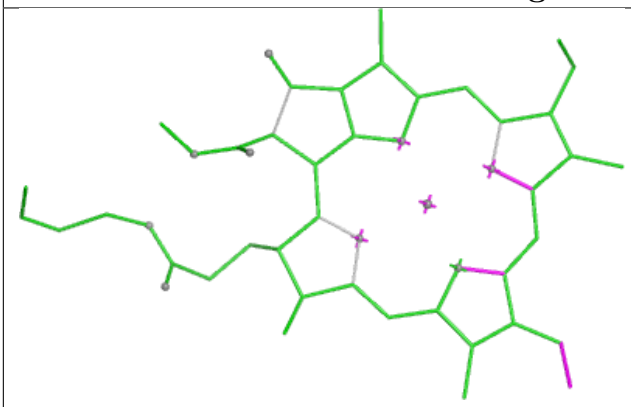


Rings

Ligand CLA 4 602



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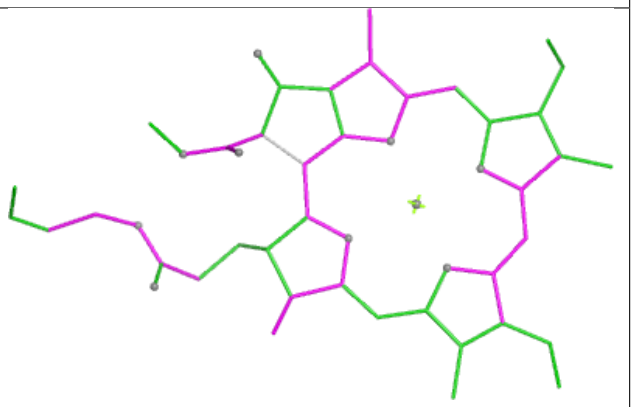
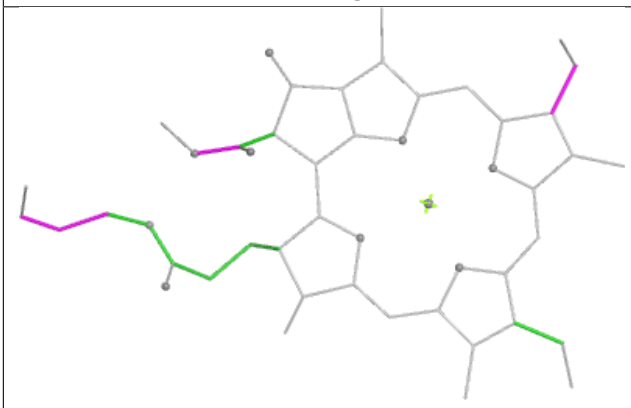


Bond angles



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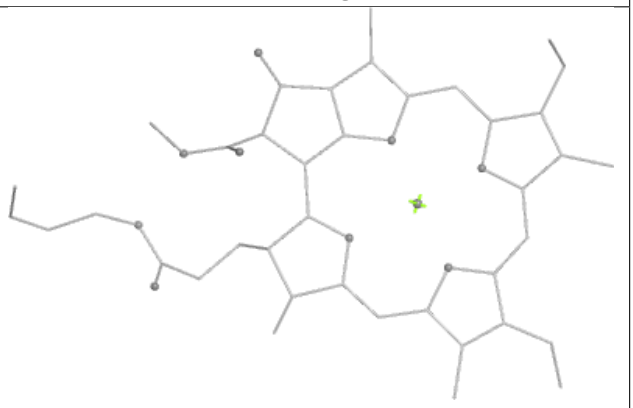
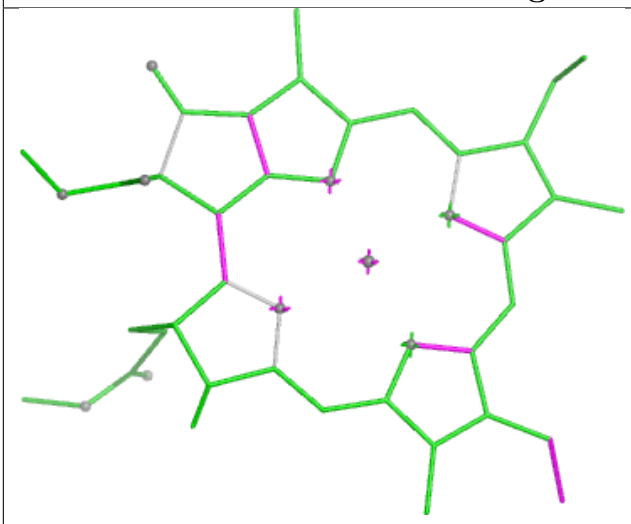


Rings

Ligand CLA 3 615



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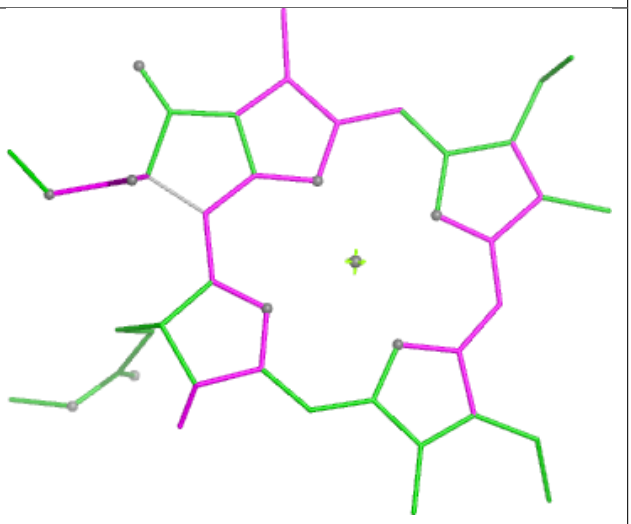
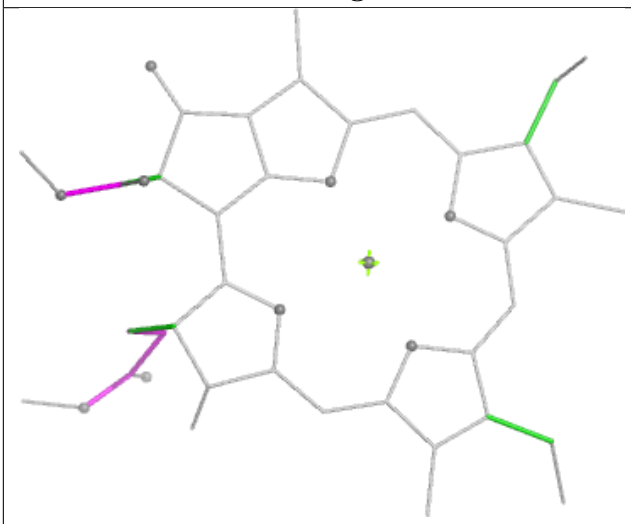


Bond angles



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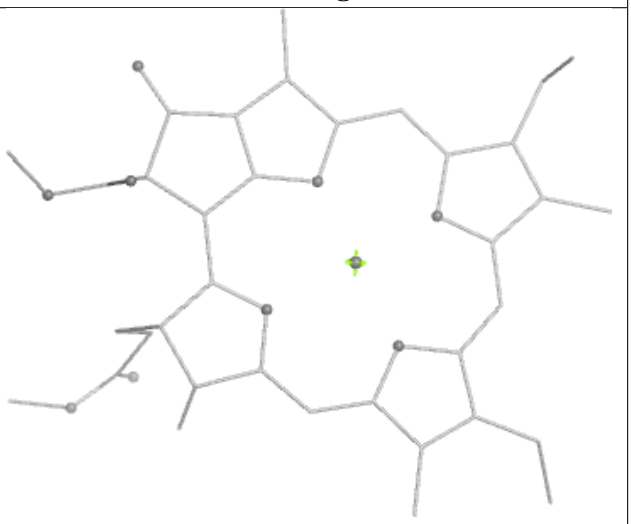
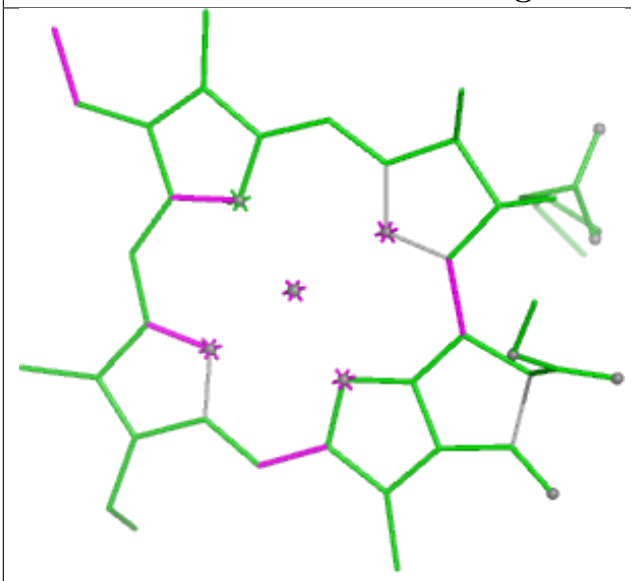


Rings

Ligand CLA A 1128



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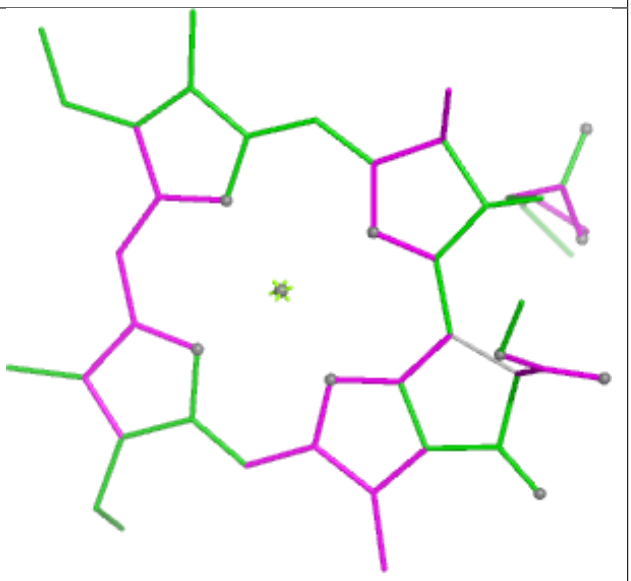
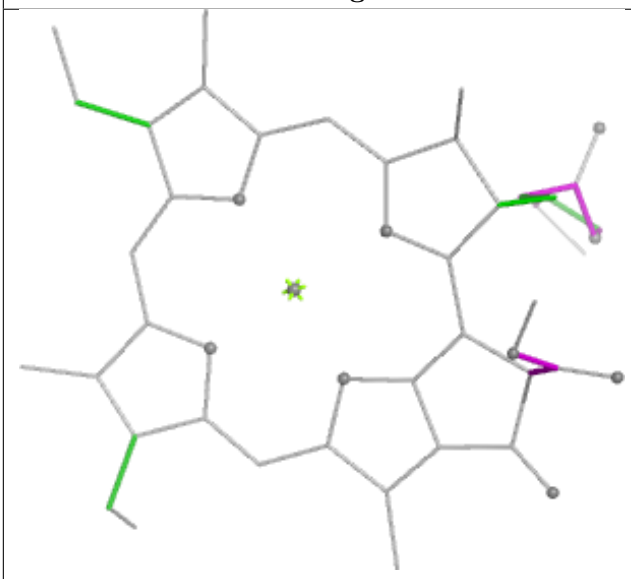


Bond angles



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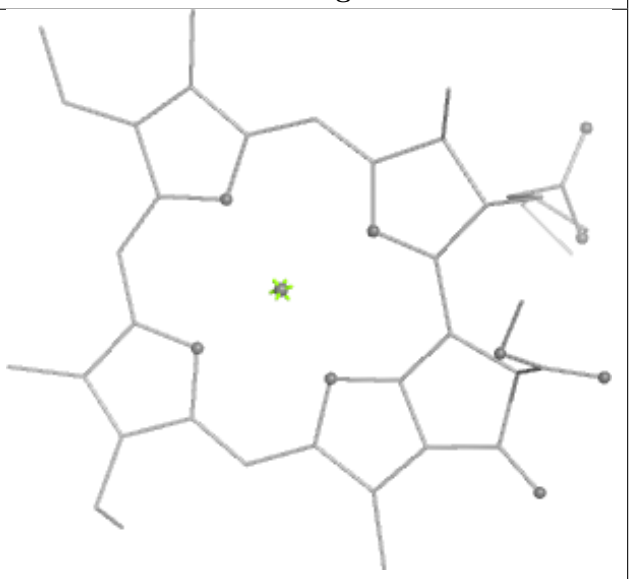
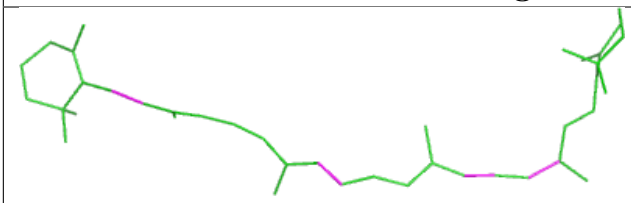


Rings

Ligand BCR B 4003



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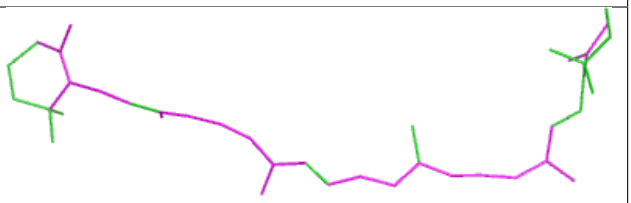
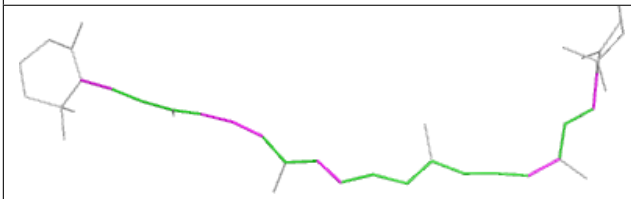


Bond angles



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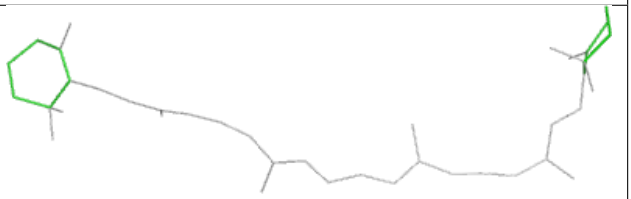
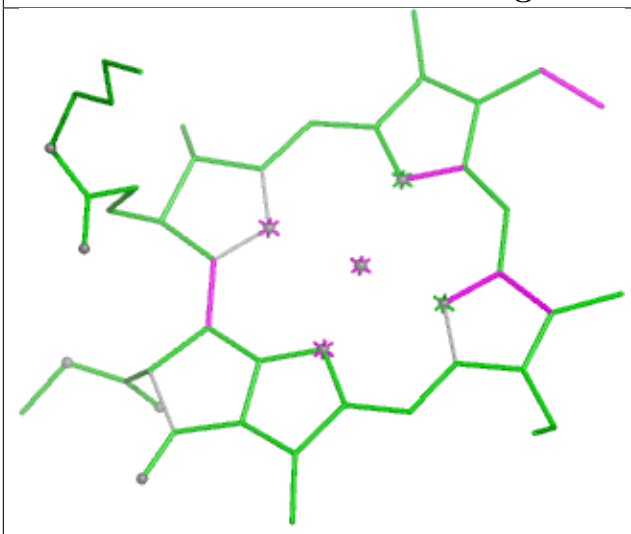


Rings

Ligand CLA A 1133



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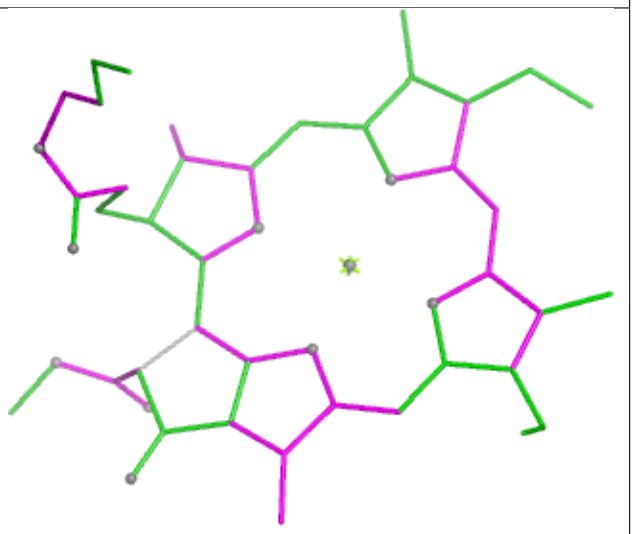
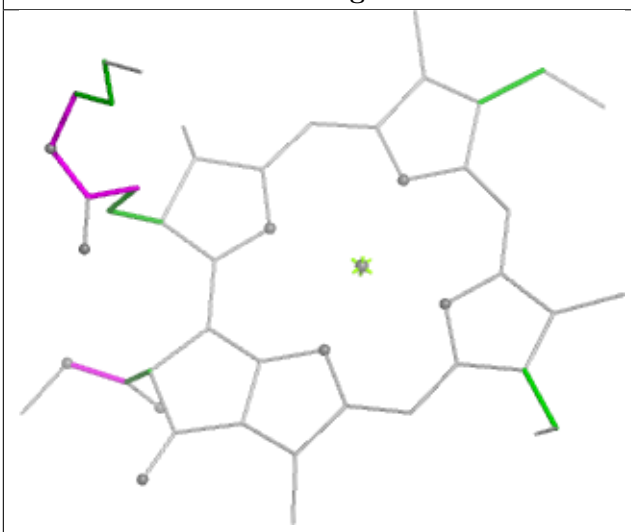


Bond angles



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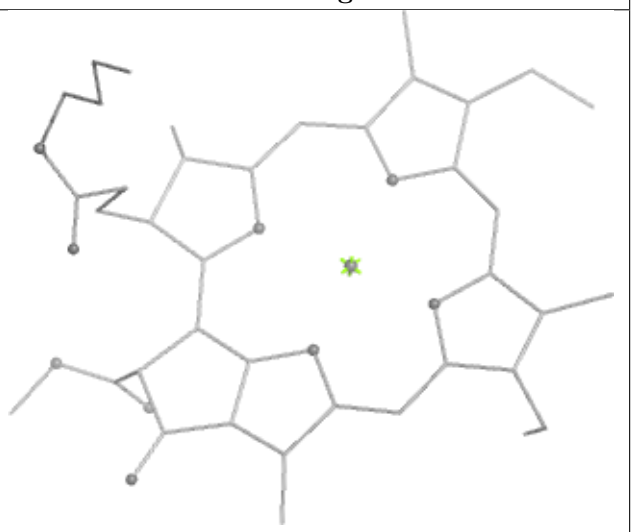
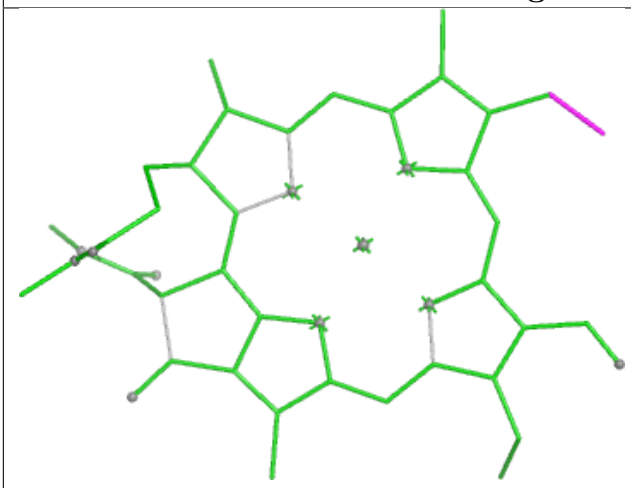


Rings

Ligand CHL 1 610



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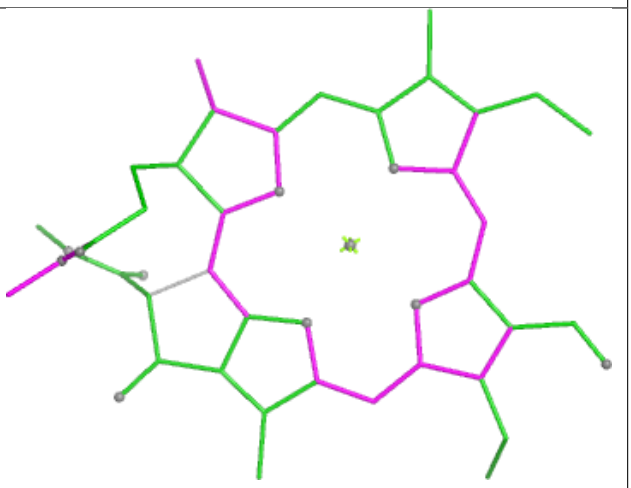
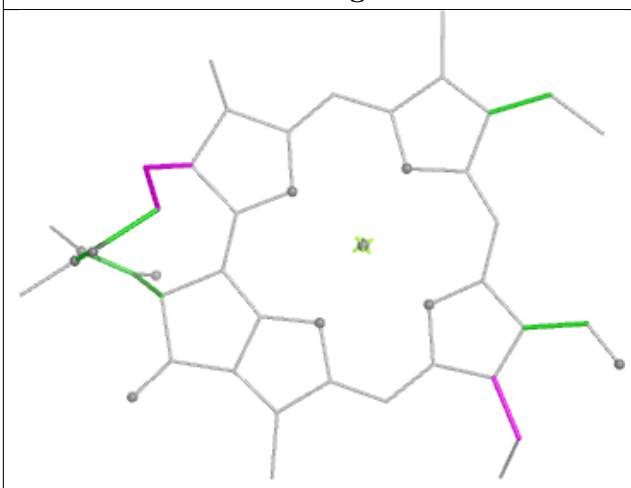


Bond angles



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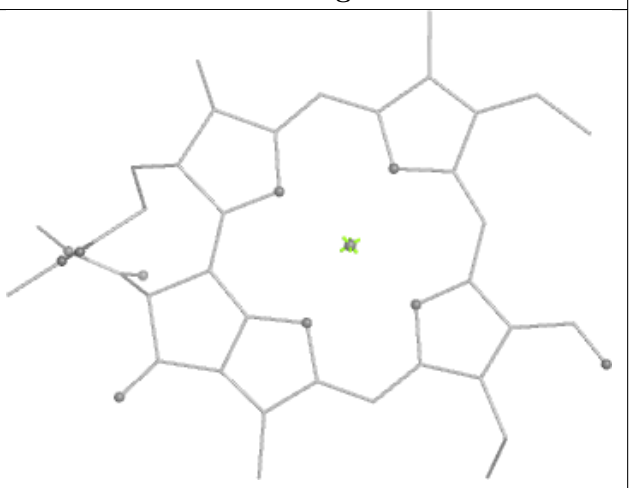
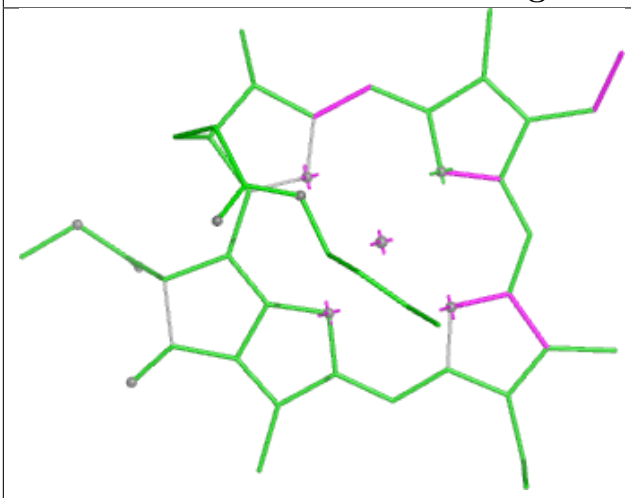
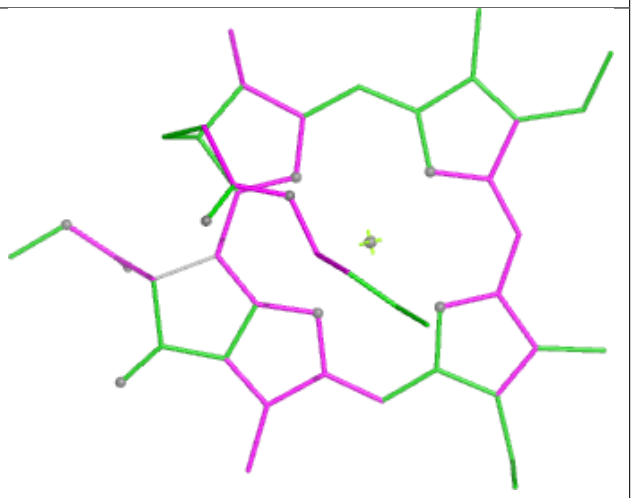


Rings

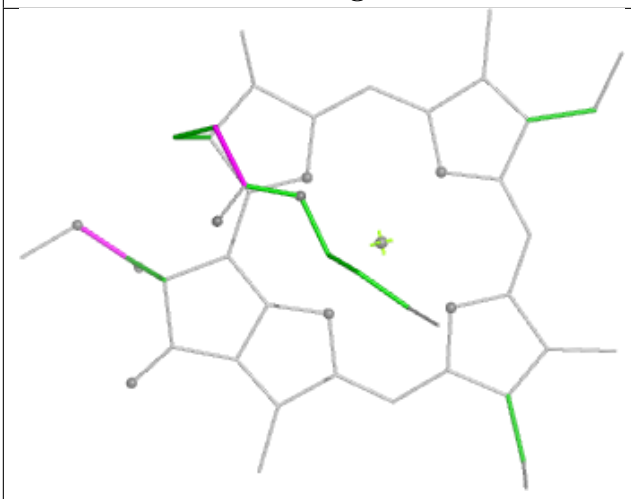
Ligand CLA 4 603



Bond lengths



Bond angles



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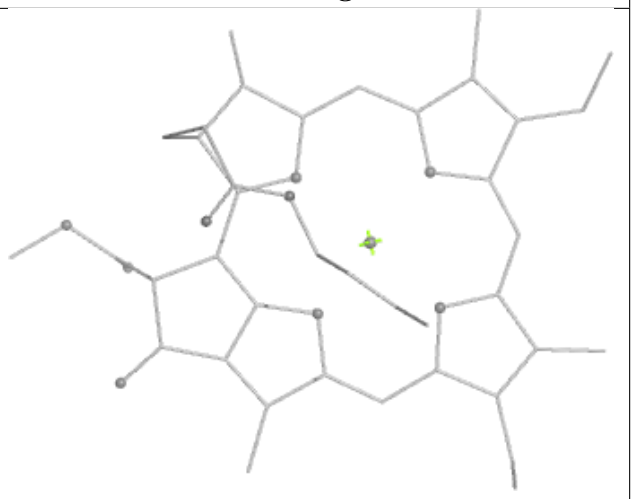
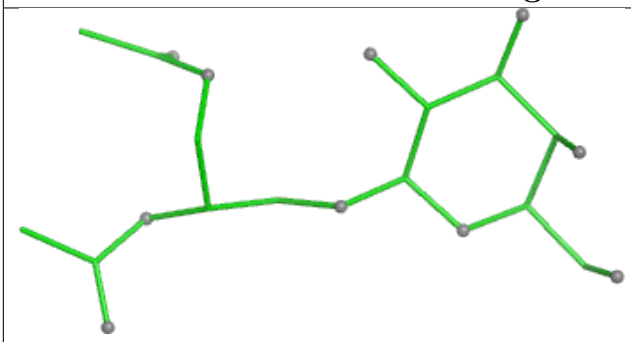
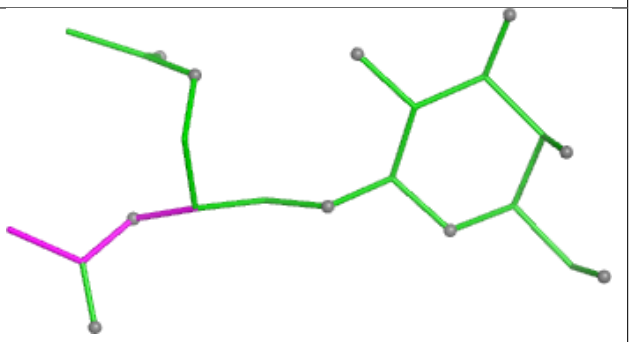


Rings

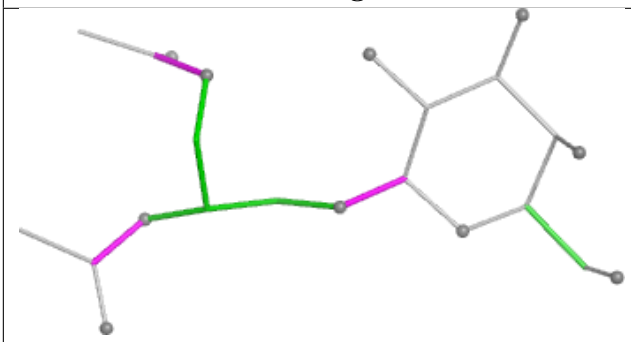
Ligand LMG 1 803



Bond lengths



Bond angles



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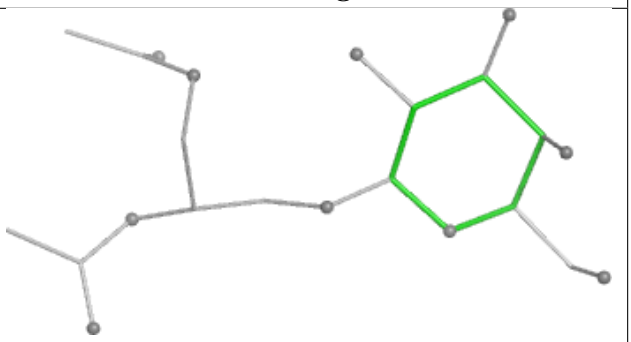
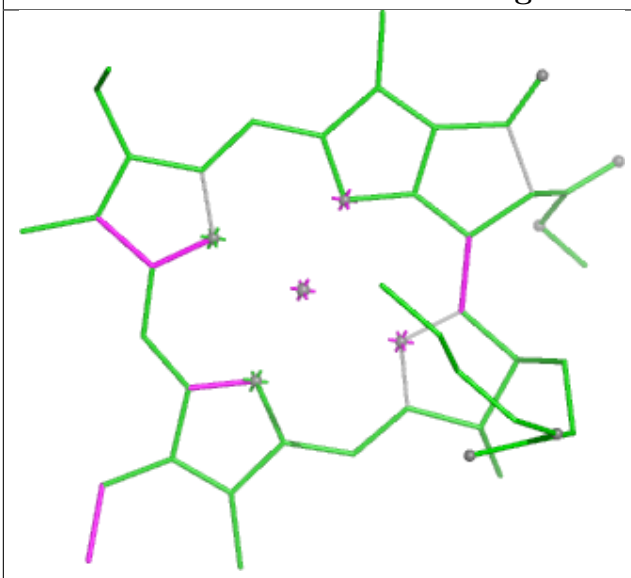
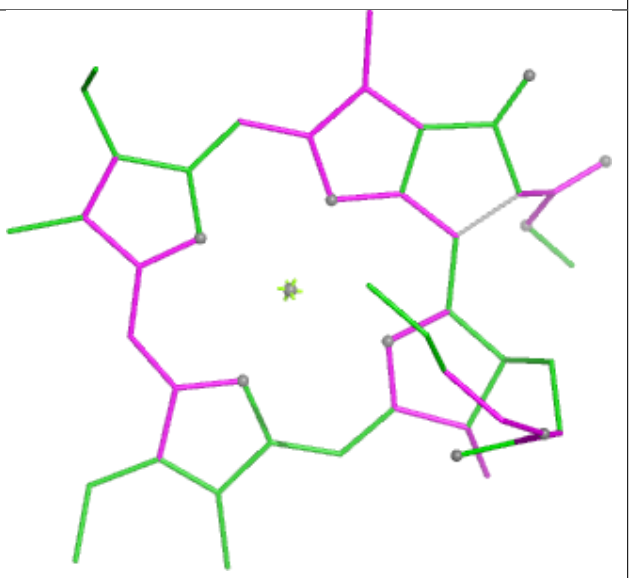


Rings

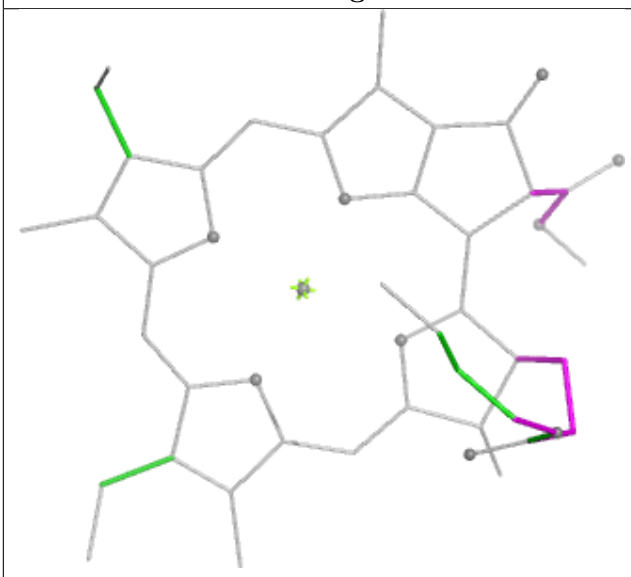
Ligand CLA A 1115



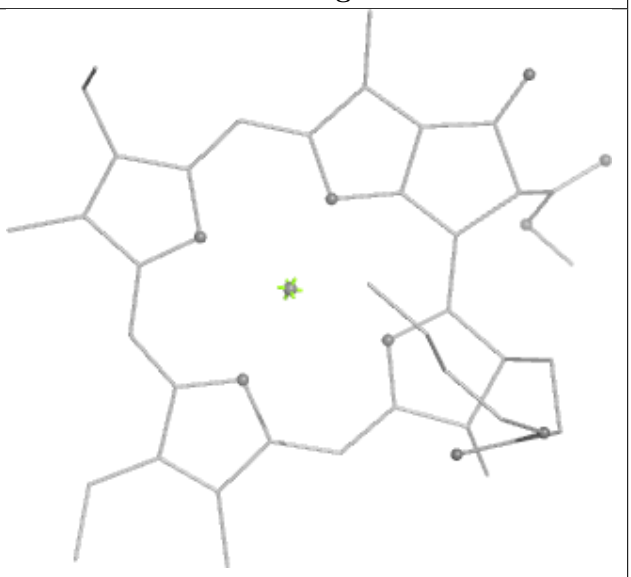
Bond lengths



Bond angles

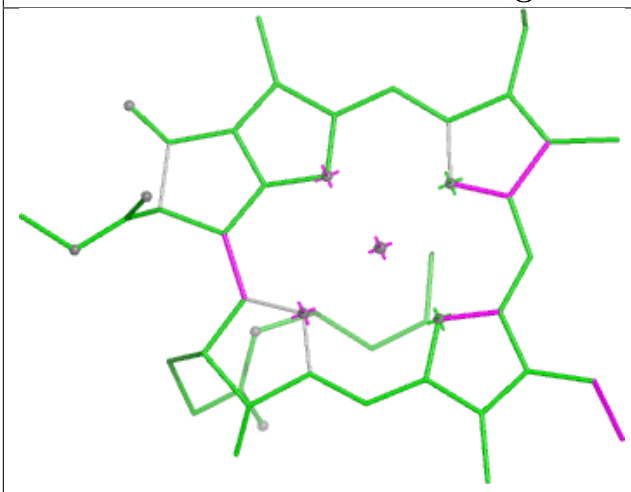


Torsions



Rings

Ligand CLA B 1237



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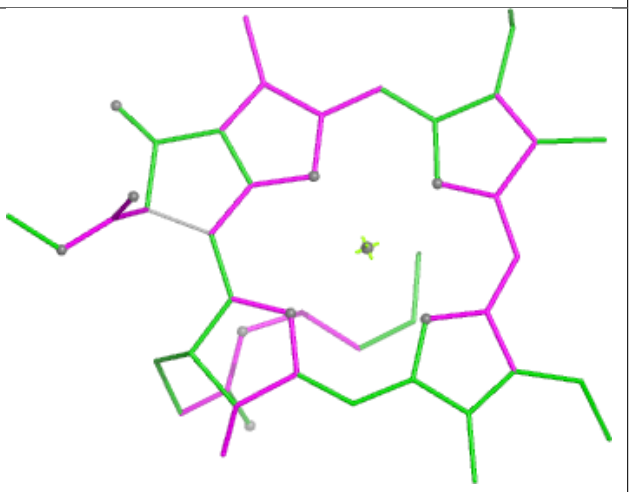
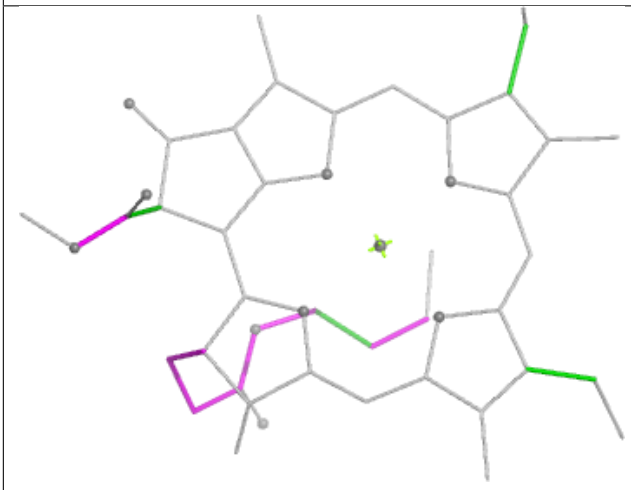


Bond angles



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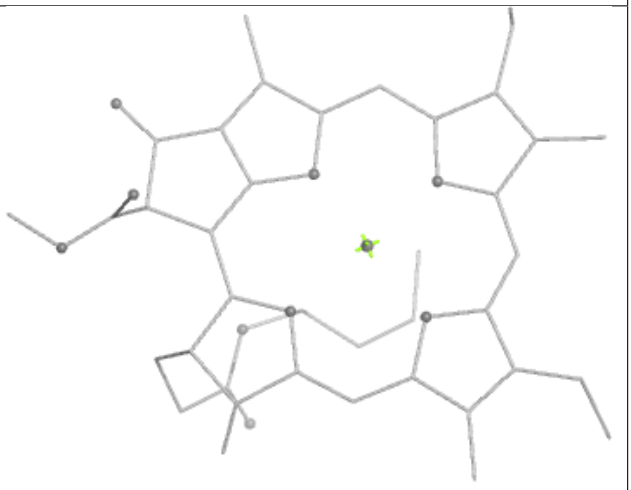
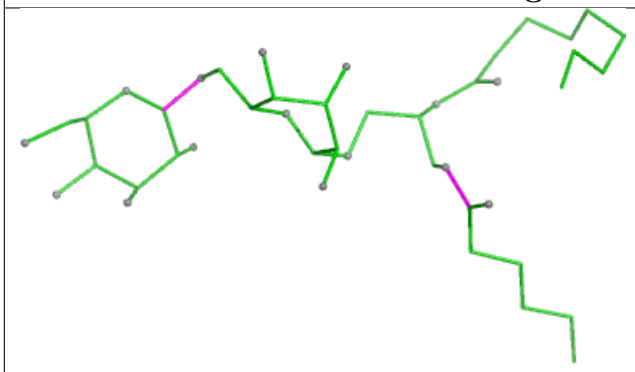
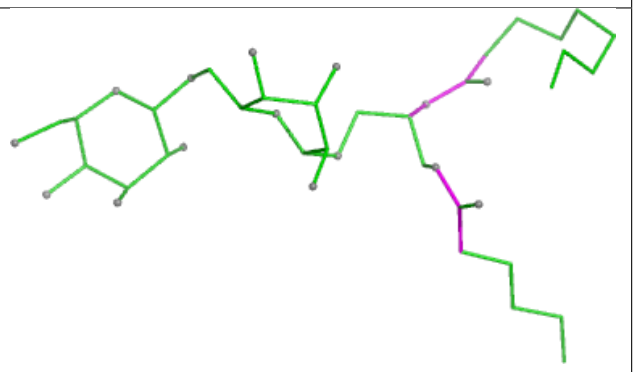


Rings

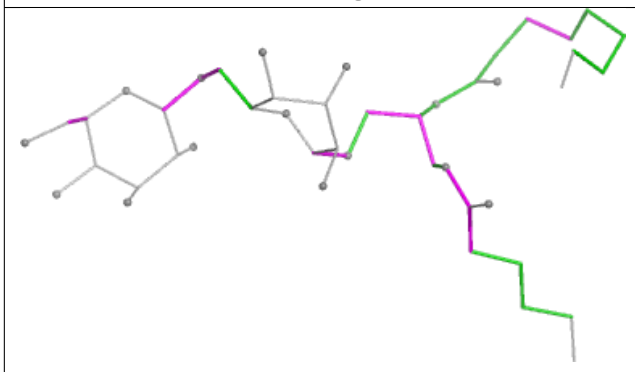
Ligand DGD 4 811



Bond lengths



Bond angles



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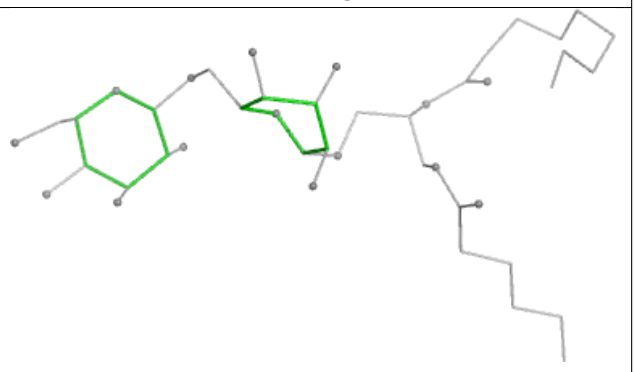
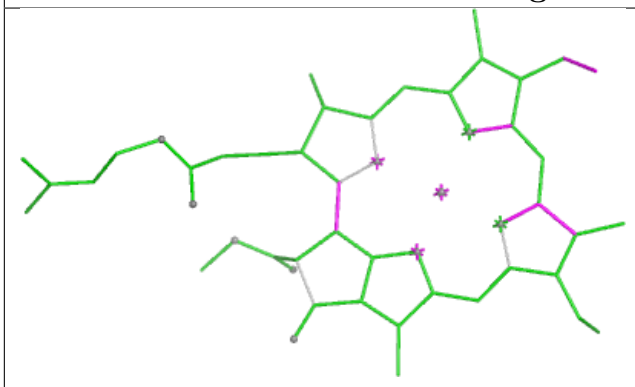


Rings

Ligand CLA 3 607



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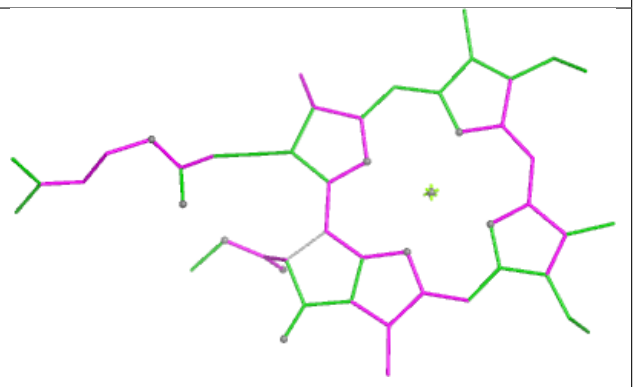
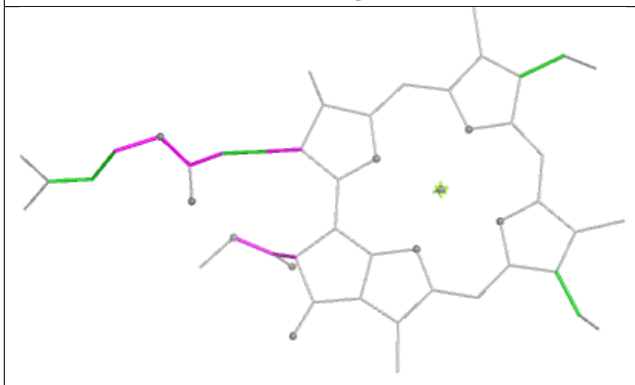


Bond angles



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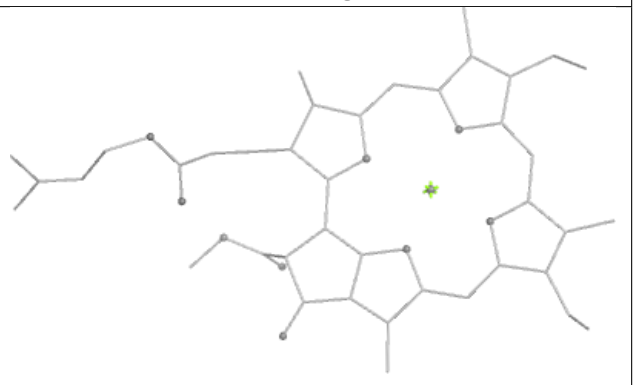
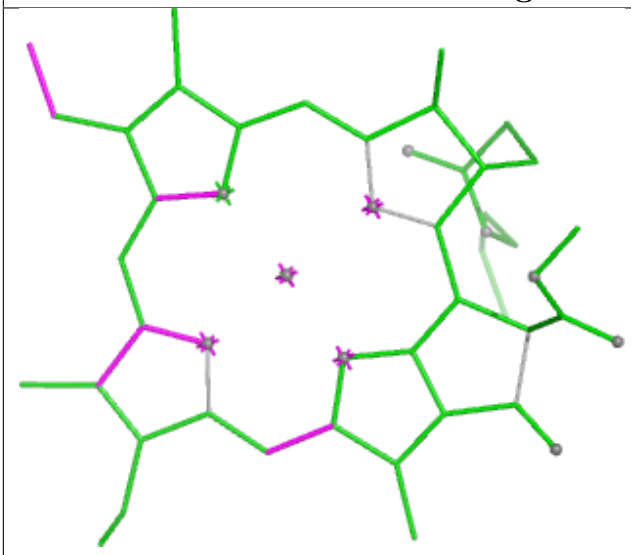


Rings

Ligand CLA B 1226



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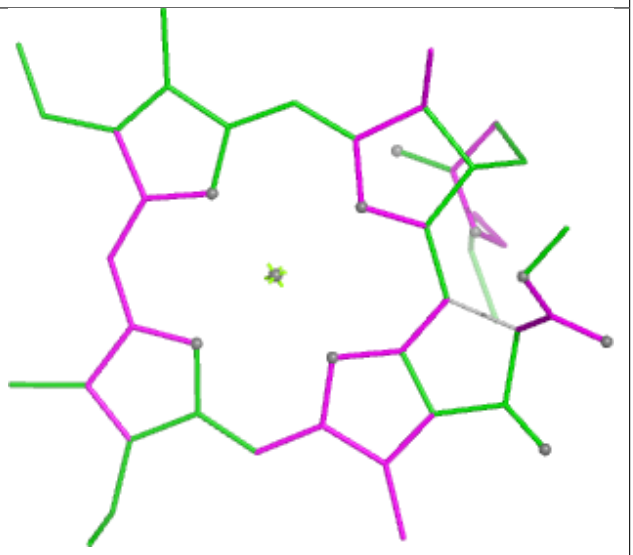
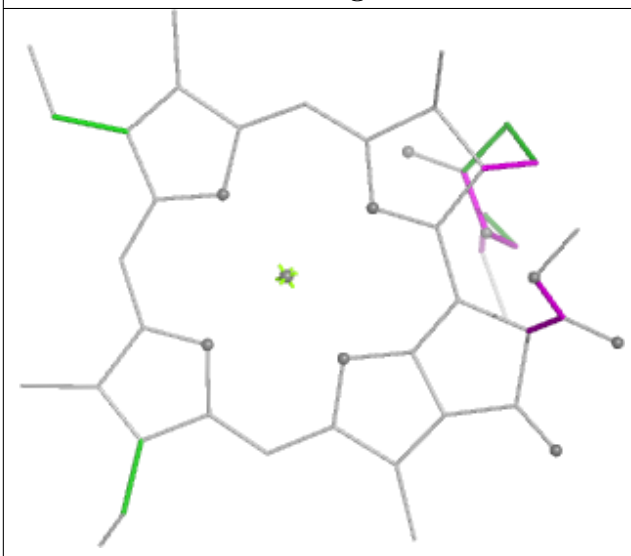


Bond angles



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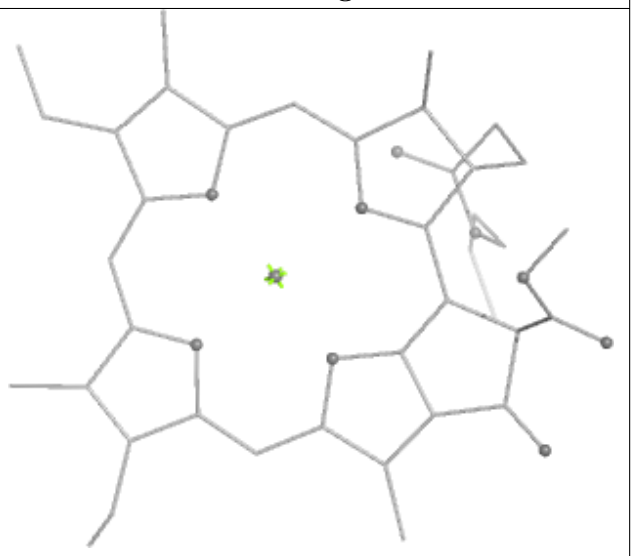
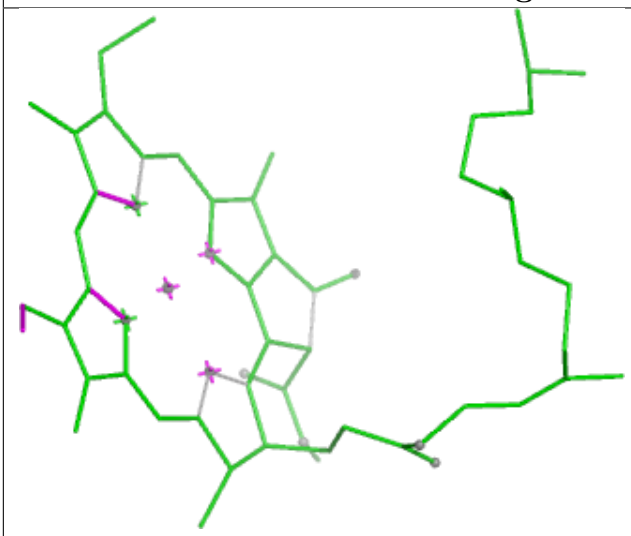


Rings

Ligand CLA B 1231



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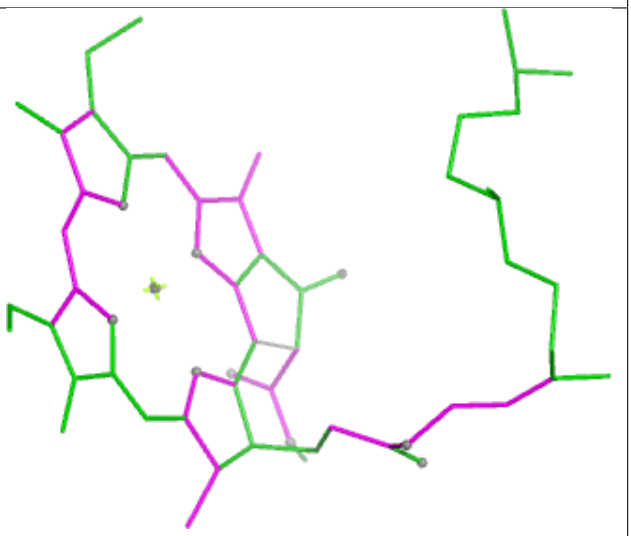
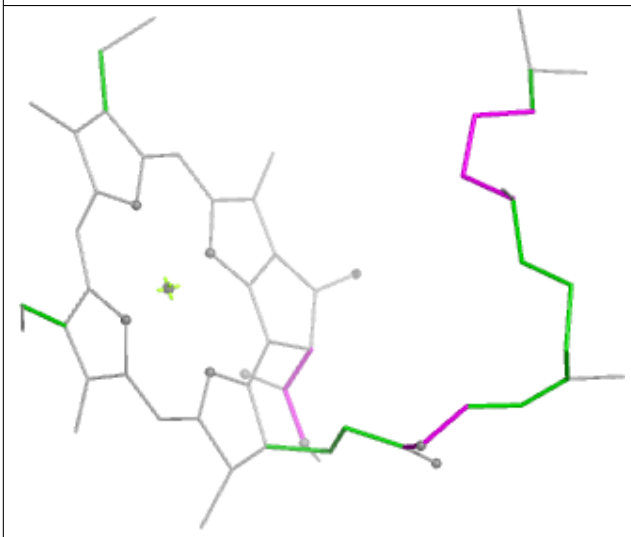


Bond angles

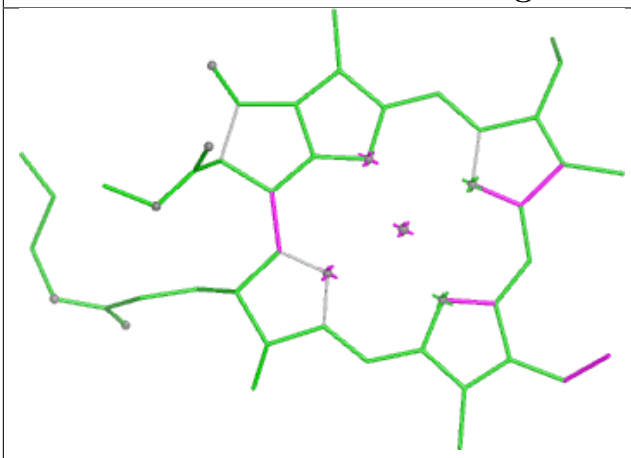


Torsions



Rings

Ligand CLA A 1123



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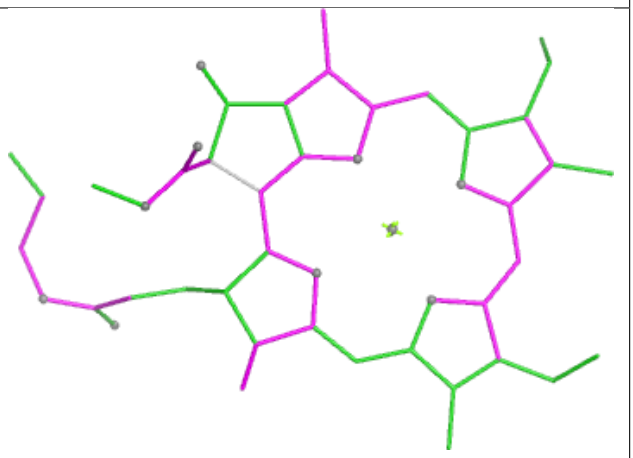
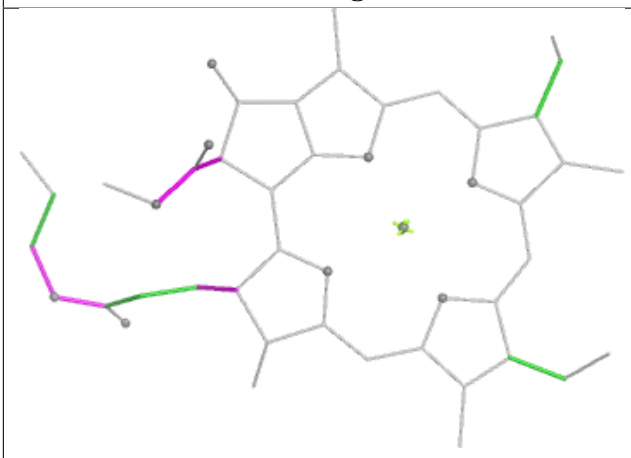


Bond angles



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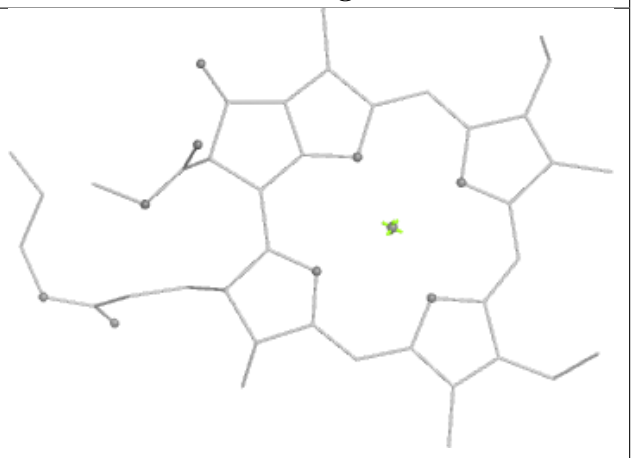
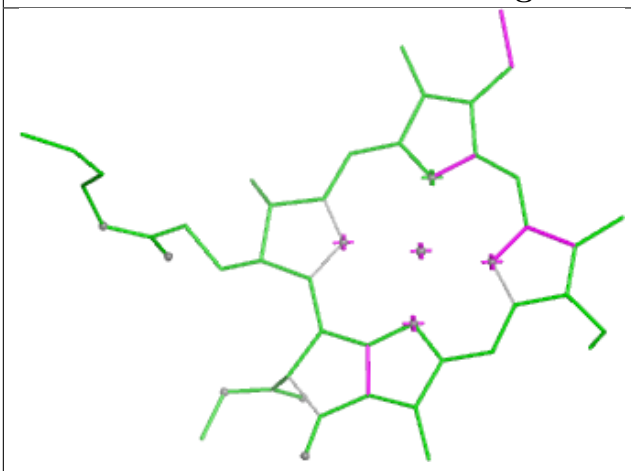


Rings

Ligand CLA B 1230



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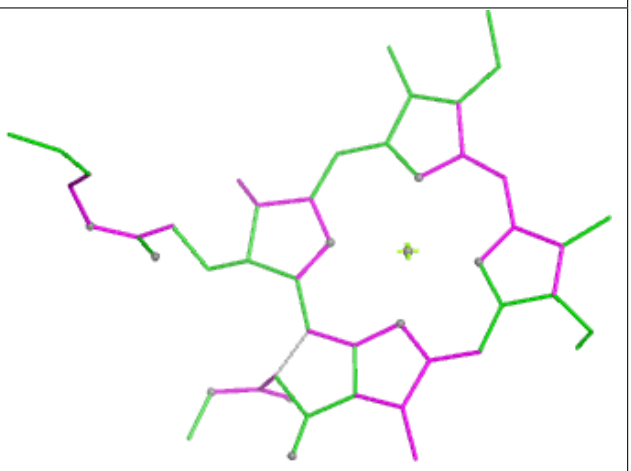
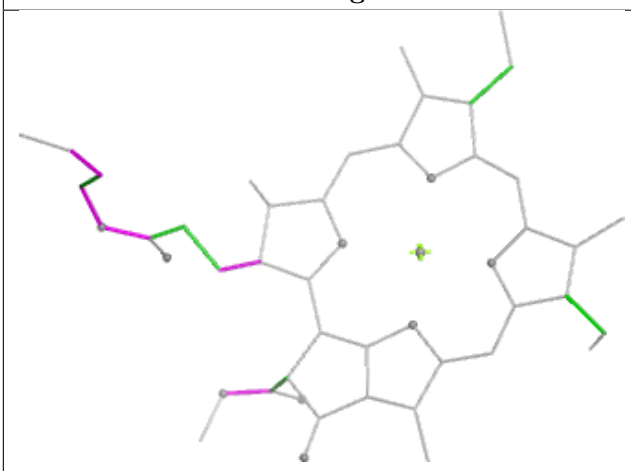


Bond angles



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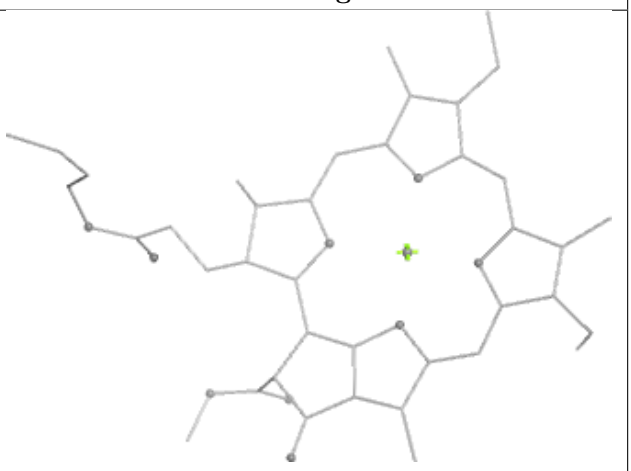
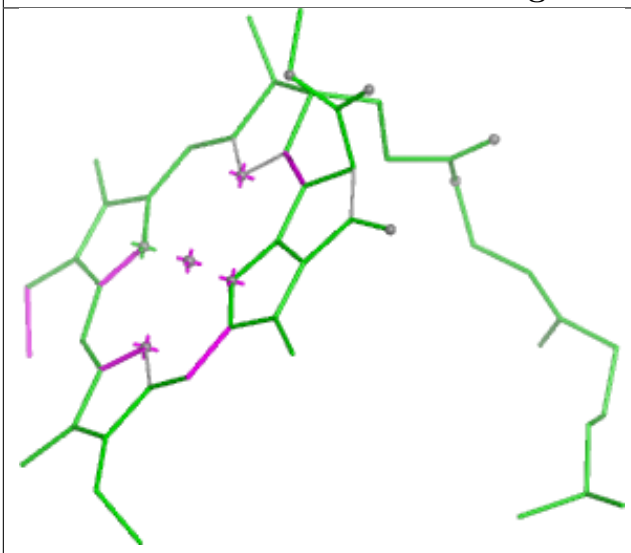


Rings

Ligand CLA 3 612



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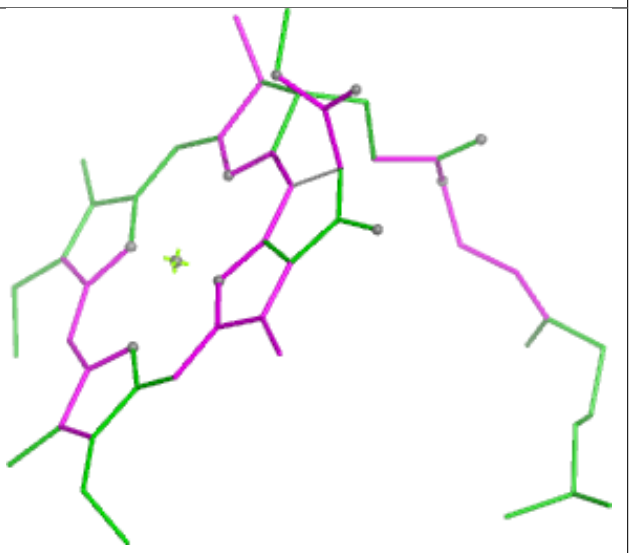
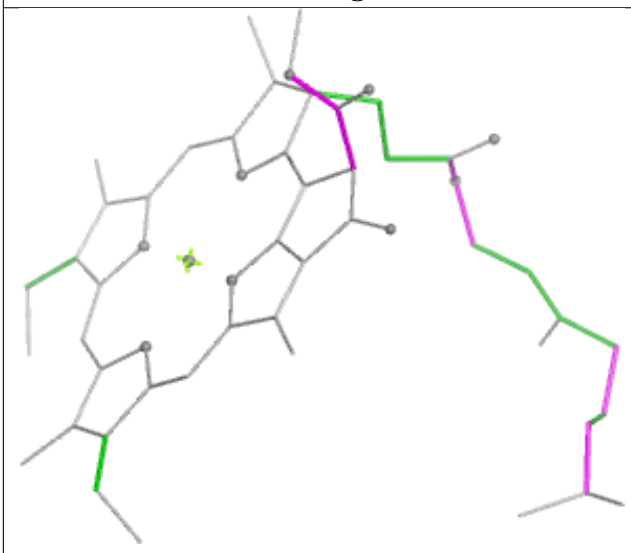


Bond angles



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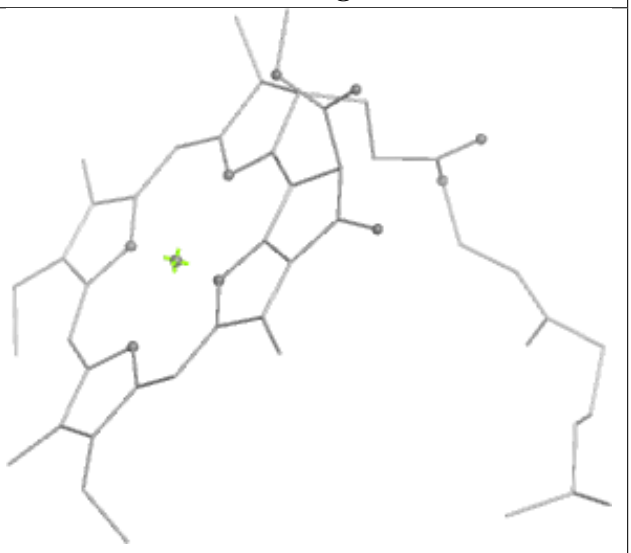
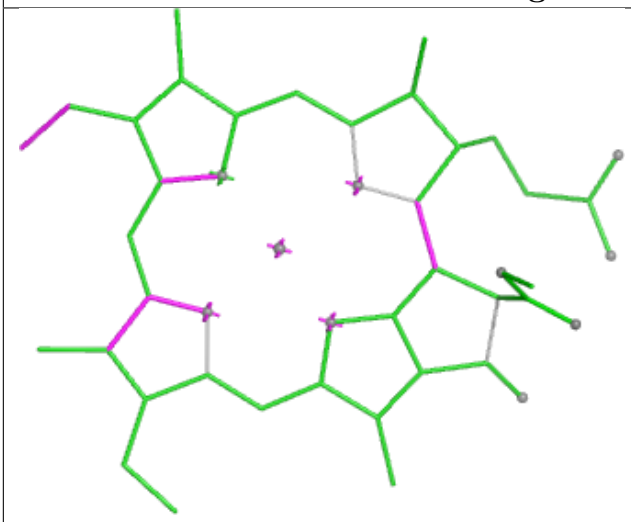


Rings

Ligand CLA 3 603



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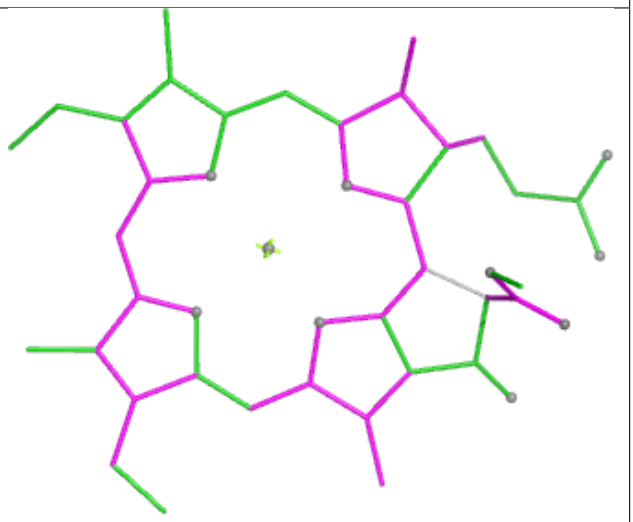
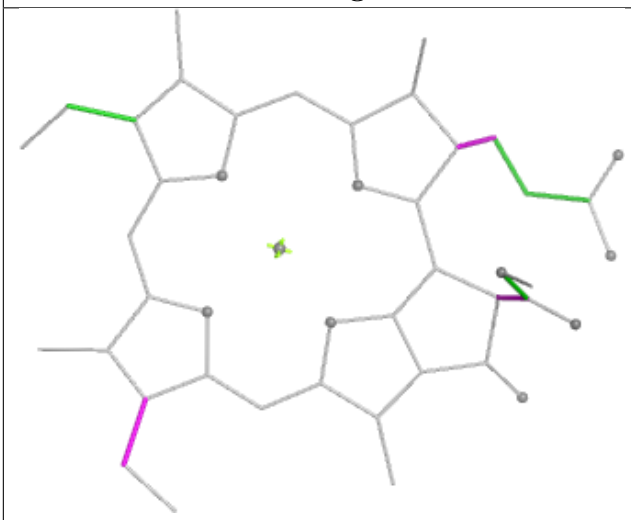


Bond angles



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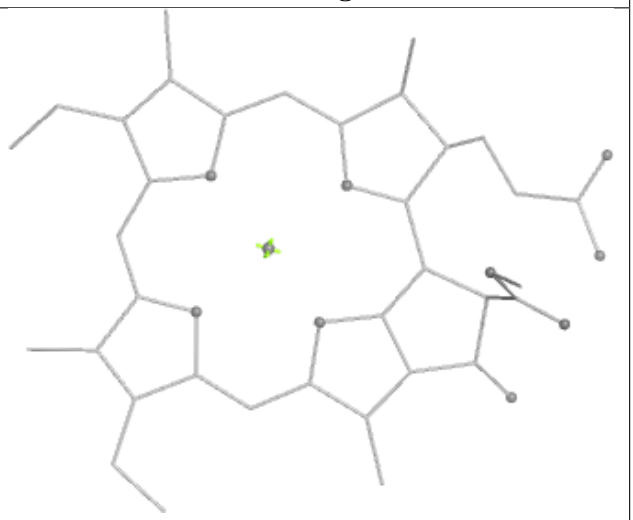


Rings

Ligand CLA B 1228



Bond lengths



Bond angles

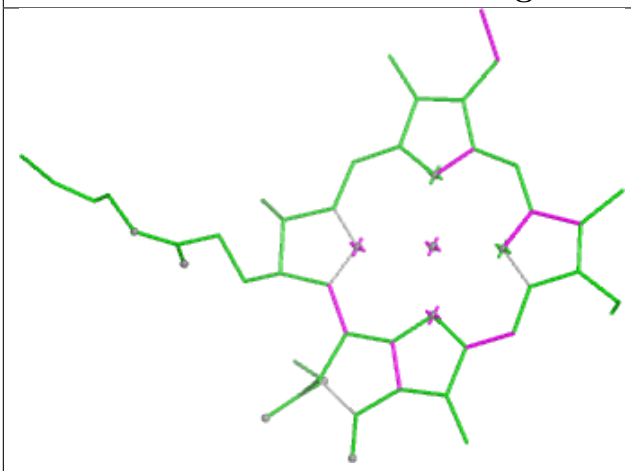


Torsions

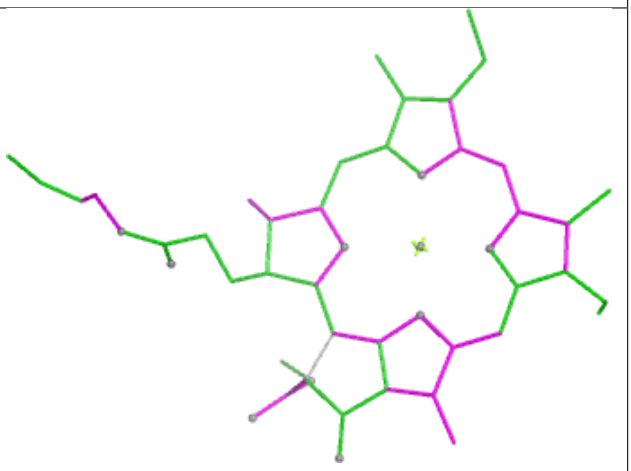


Rings

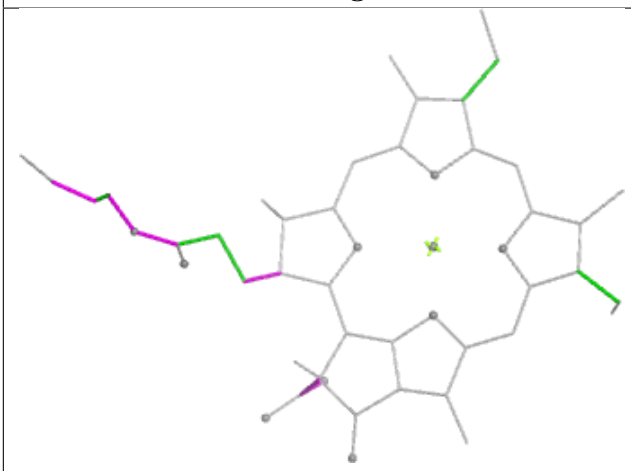
Ligand CLA B 1222



Bond lengths



Bond angles



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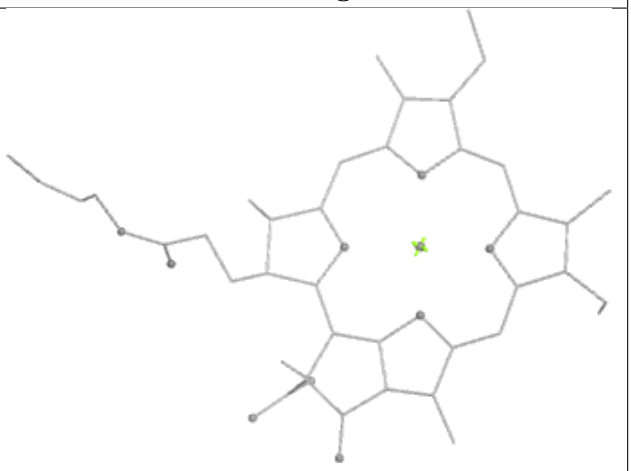
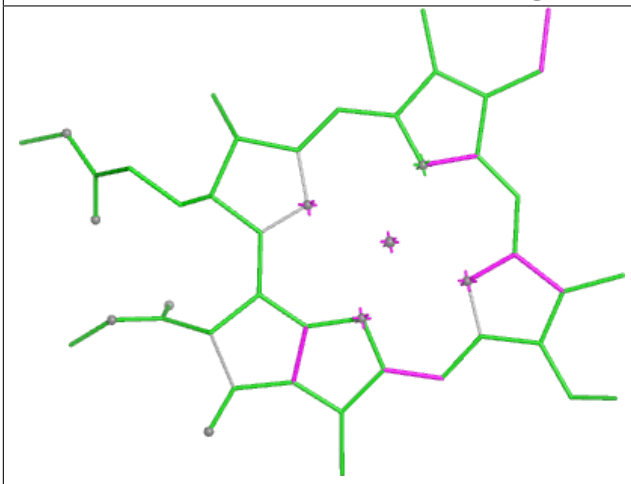


Rings

Ligand CLA 3 605



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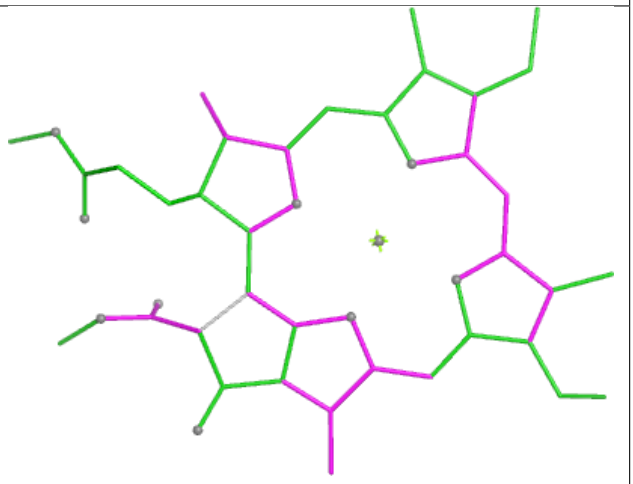
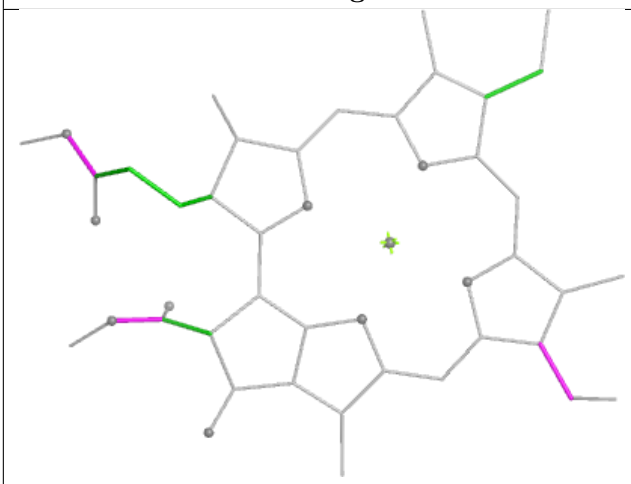


Bond angles

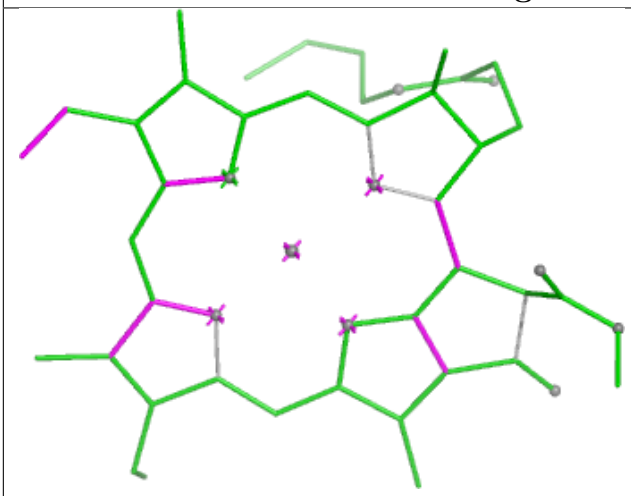


Torsions



Rings

Ligand CLA A 1105



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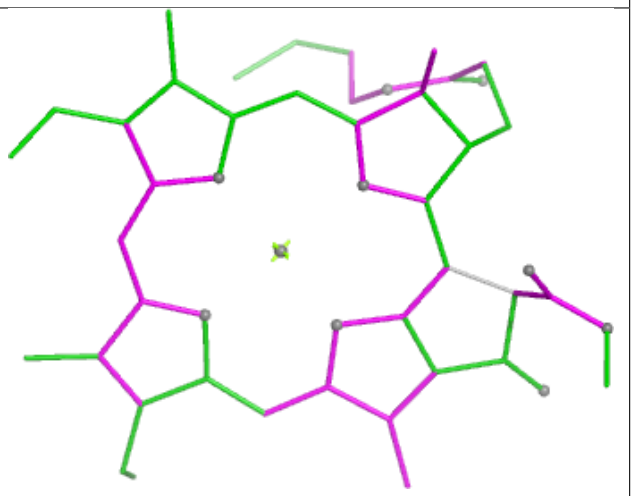
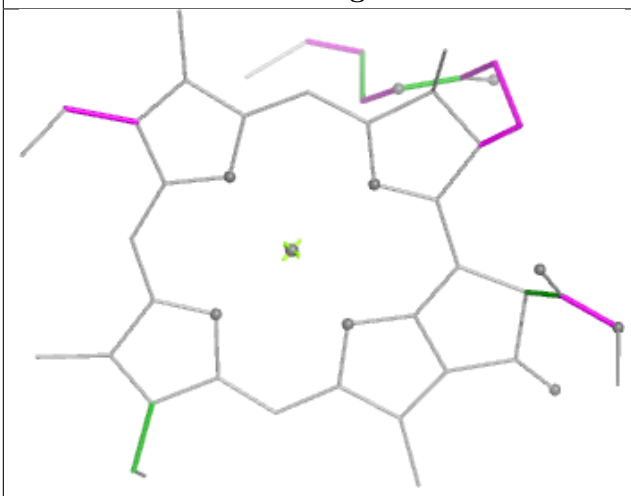


Bond angles



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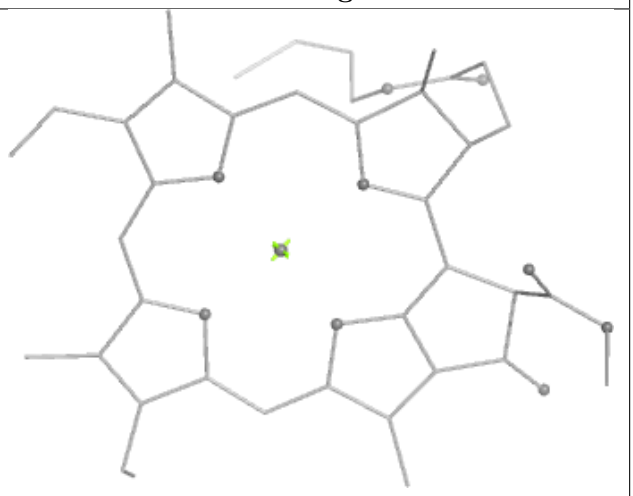
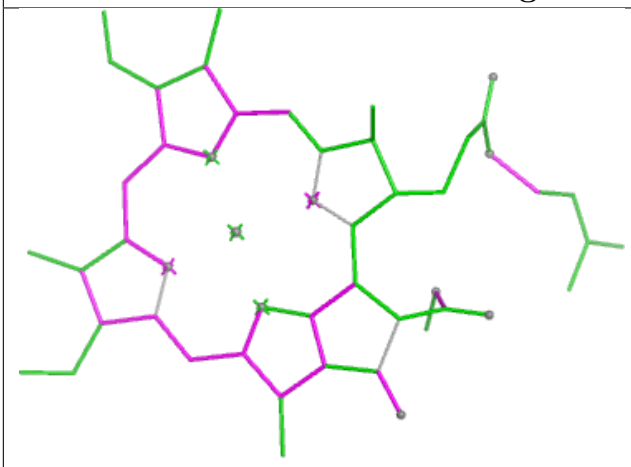
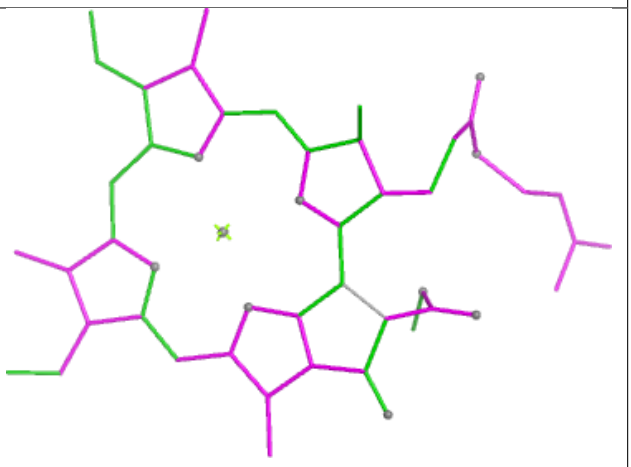


Rings

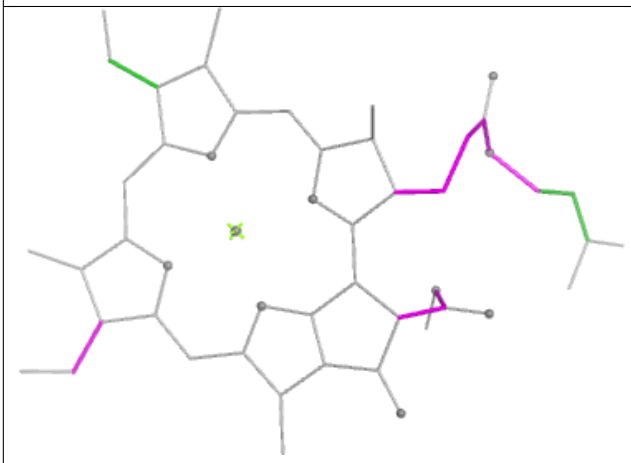
Ligand CL0 A 1011



Bond lengths



Bond angles



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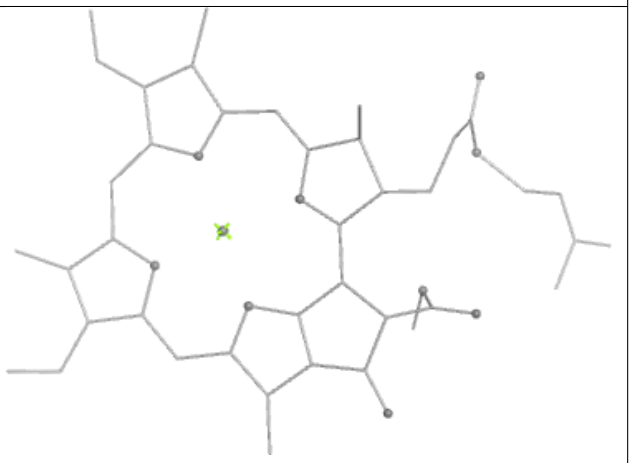
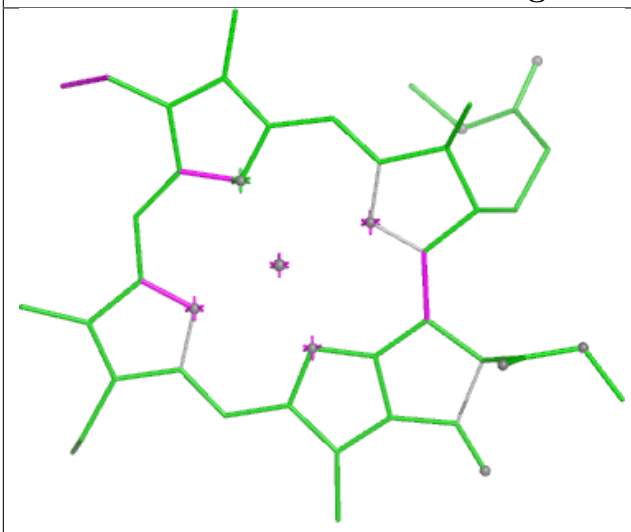


Rings

Ligand CLA 1 607



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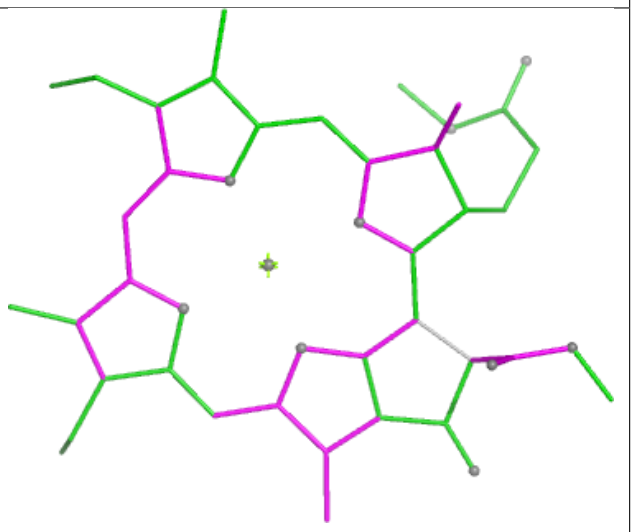
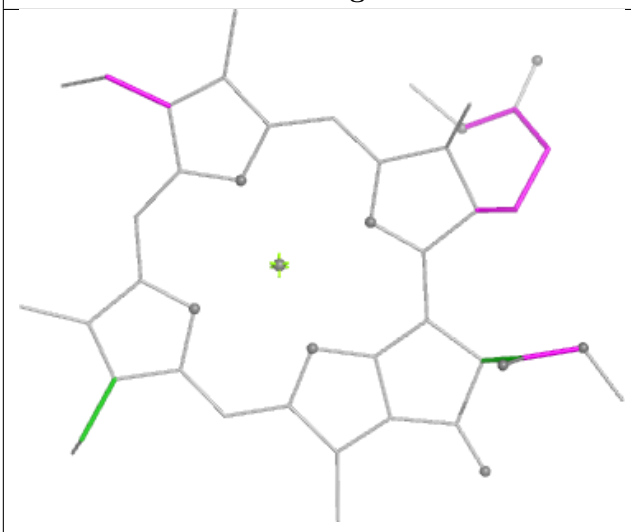
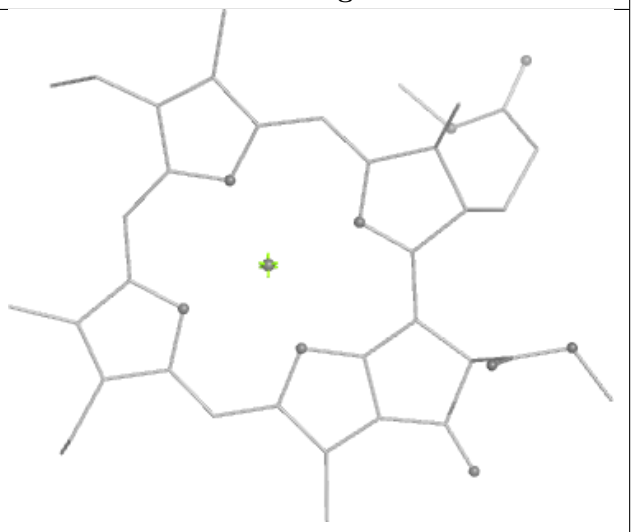


Bond angles

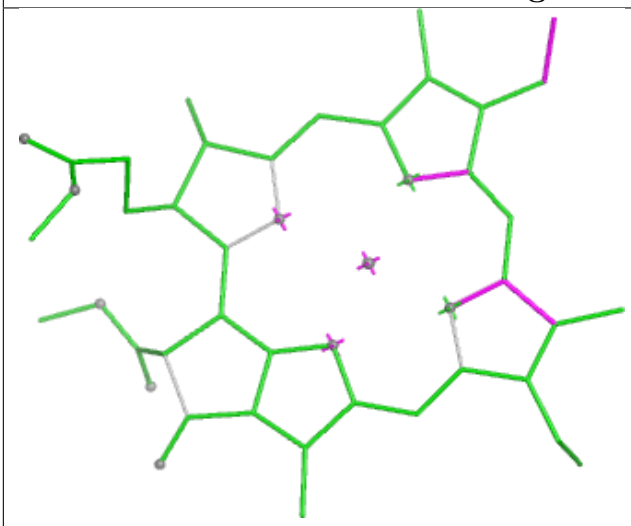


Torsions

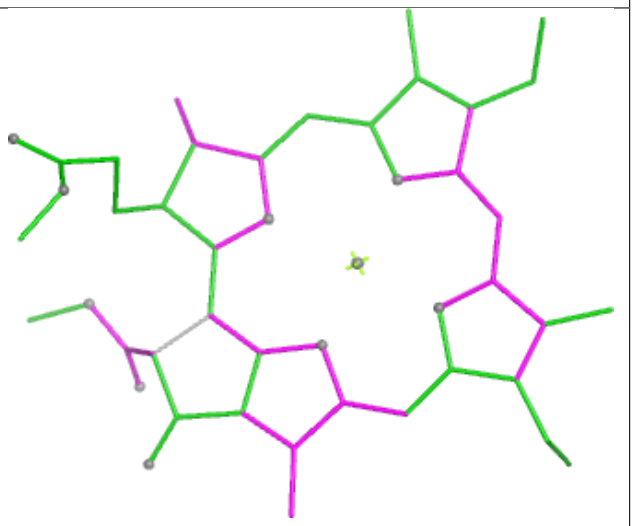


Rings

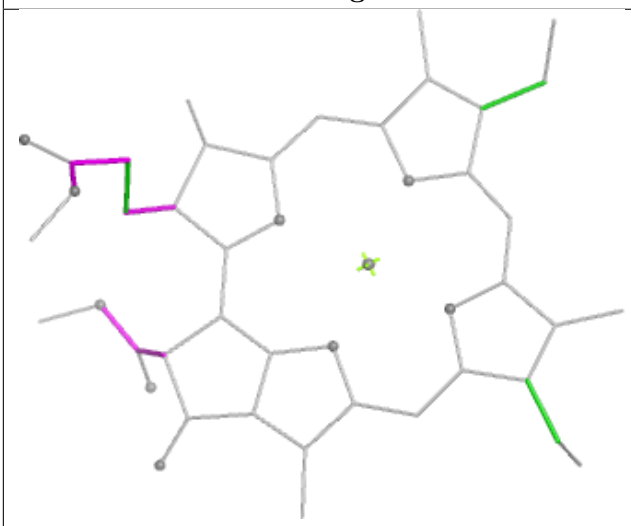
Ligand CLA 3 613



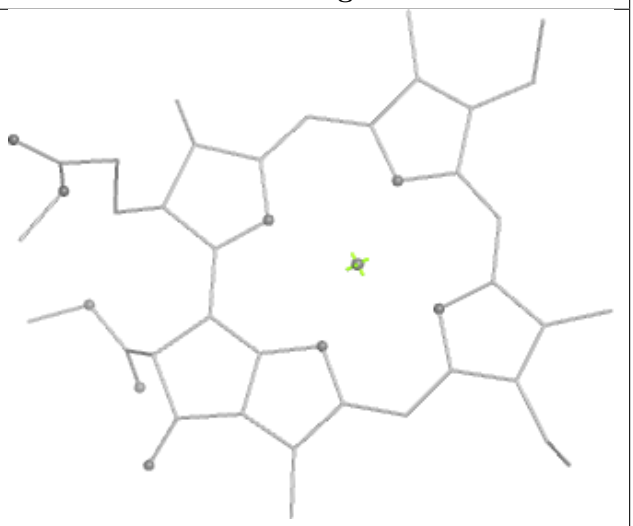
Bond lengths



Bond angles

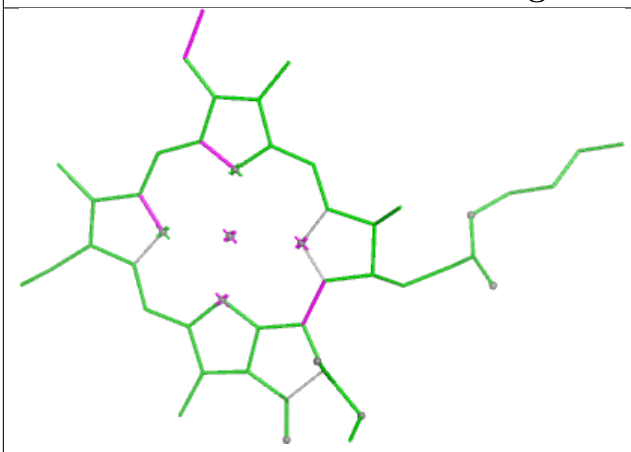


Torsions



Rings

Ligand CLA 4 609



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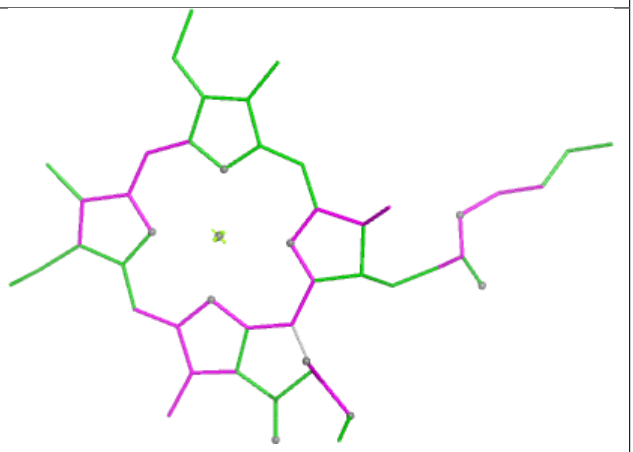

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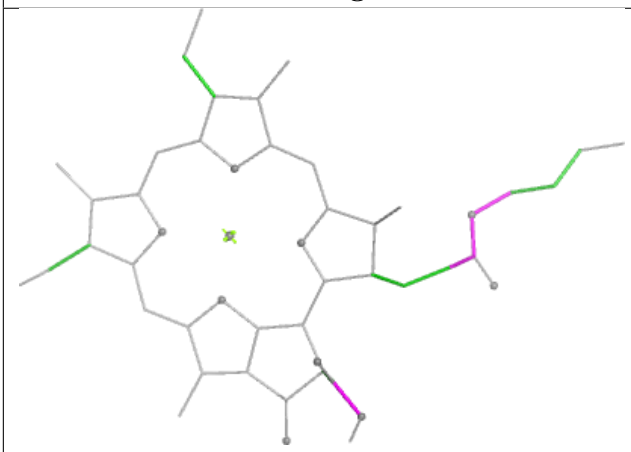

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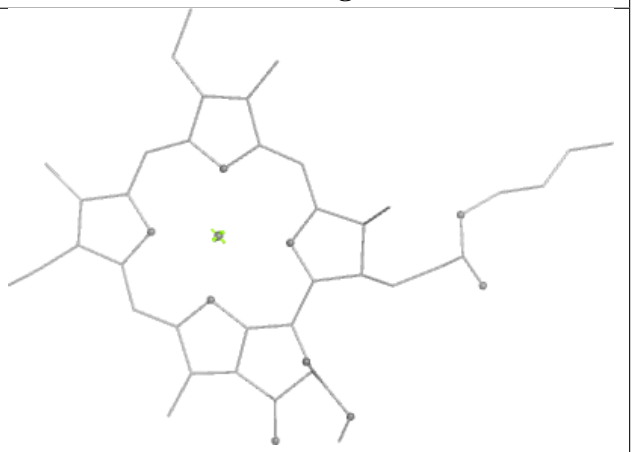
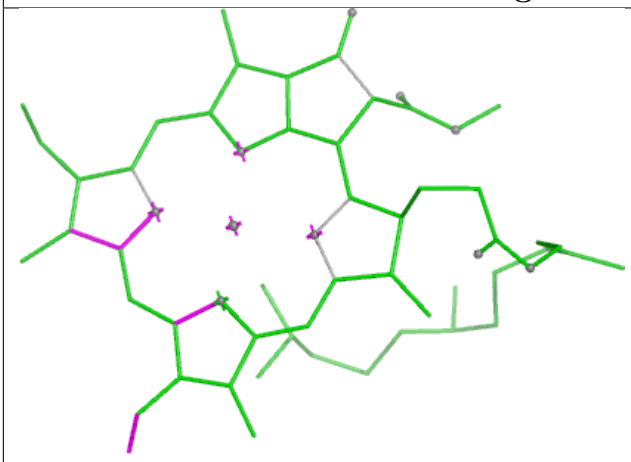


Rings

Ligand CLA A 1104



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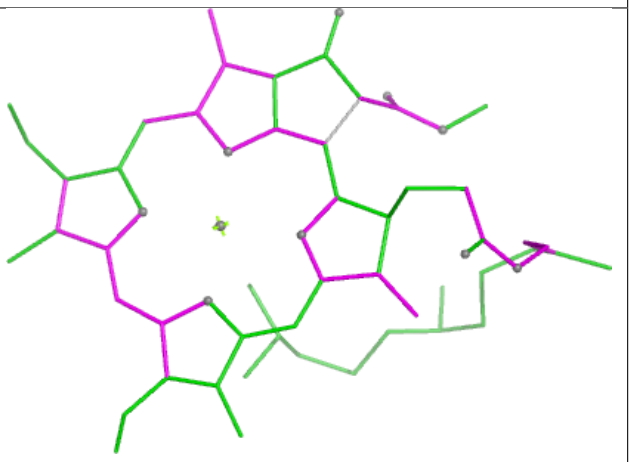

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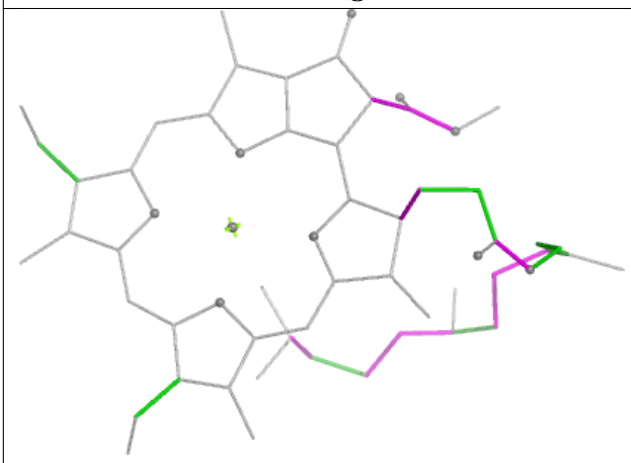

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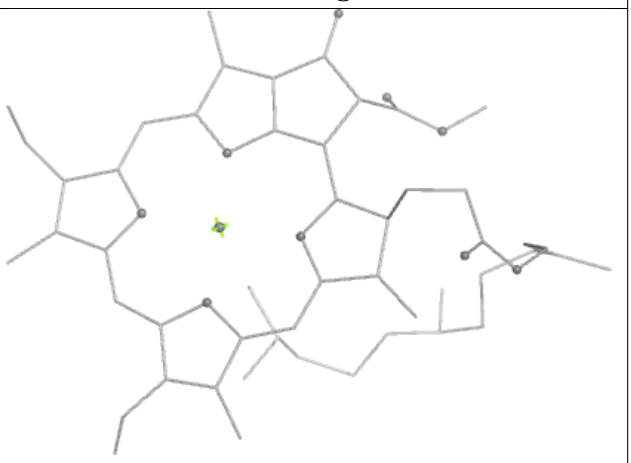
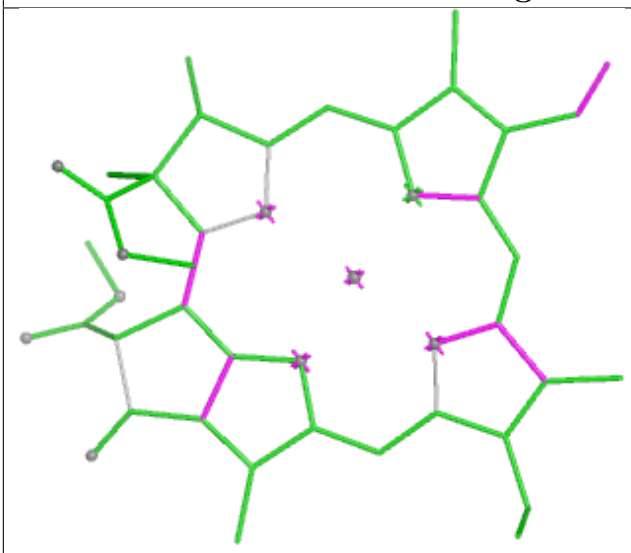


Rings

Ligand CLA A 1114



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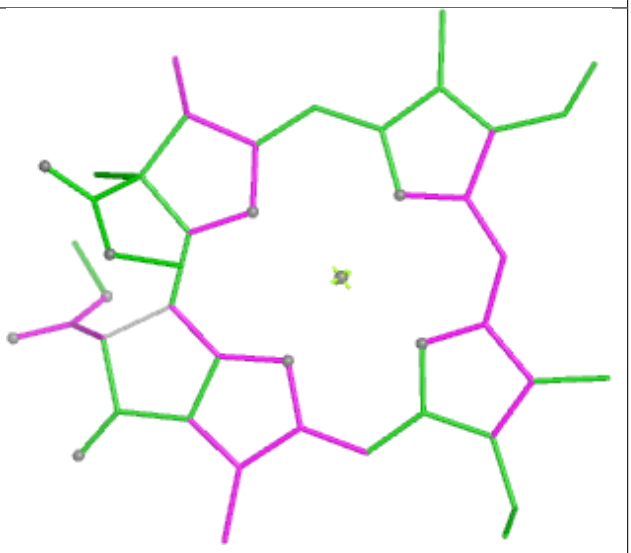
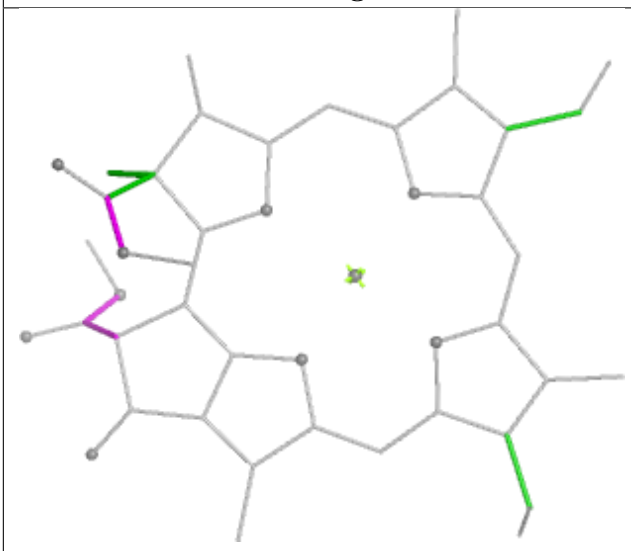


Bond angles



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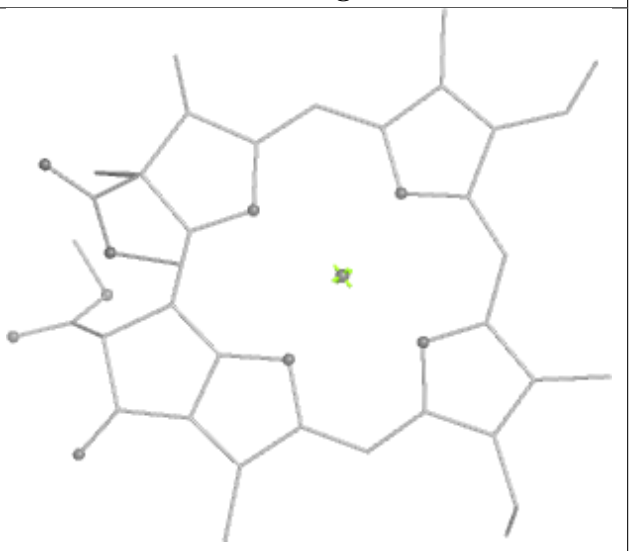
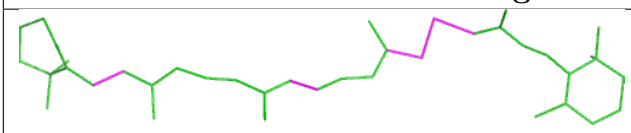


Rings

Ligand BCR A 4005



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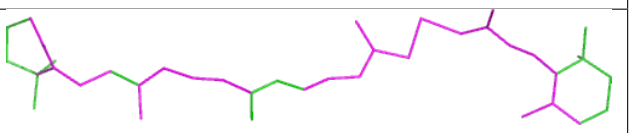
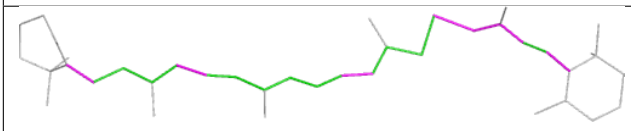


Bond angles



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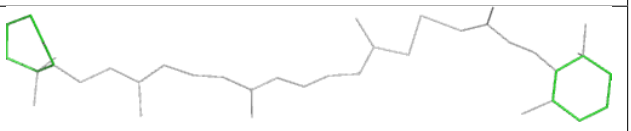
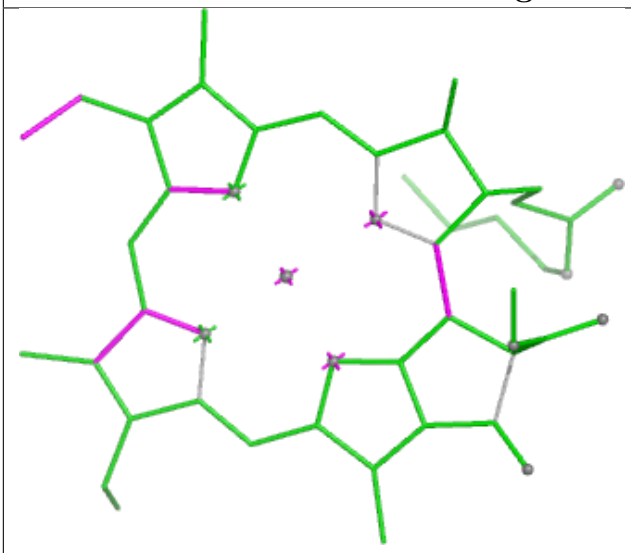


Rings

Ligand CLA B 1204



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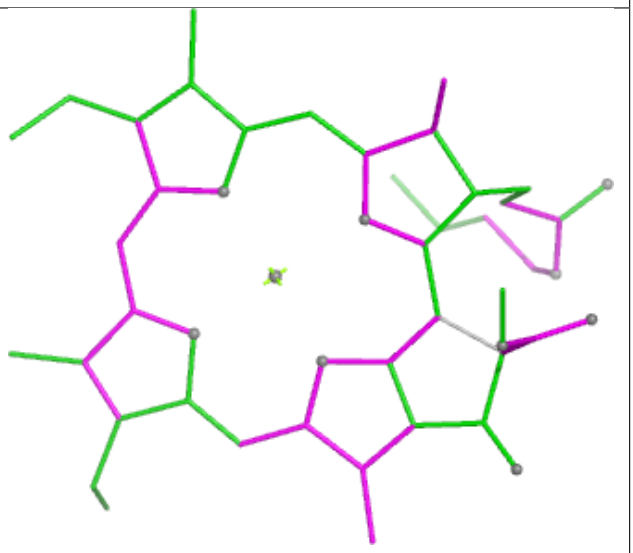

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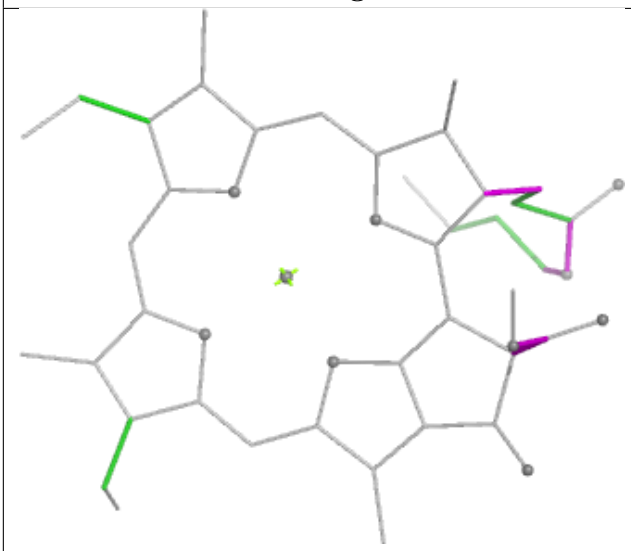

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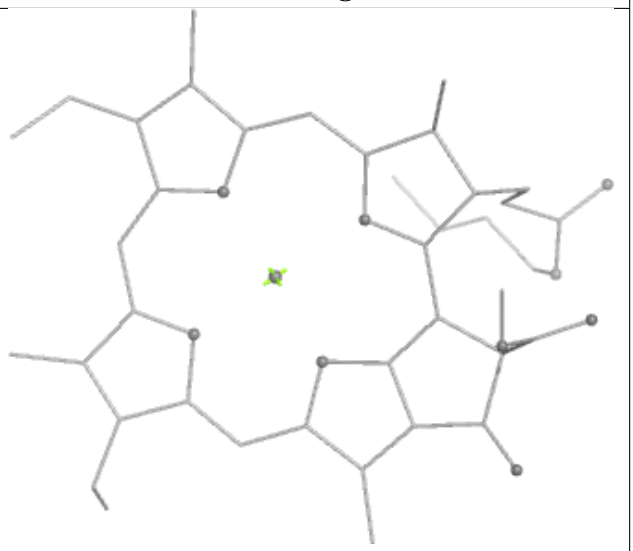
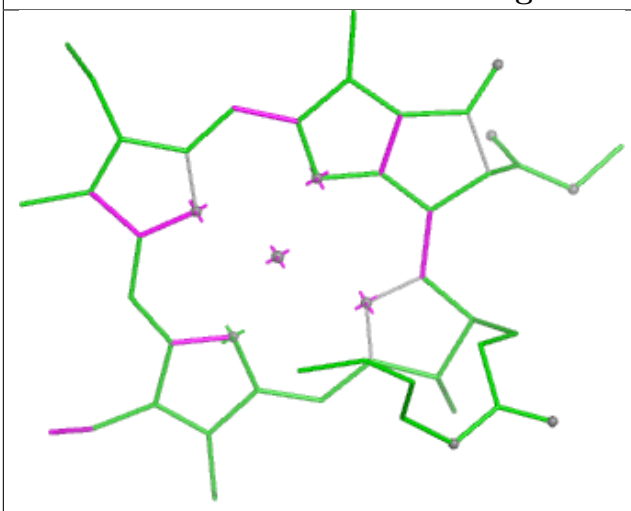


Rings

Ligand CLA B 1214



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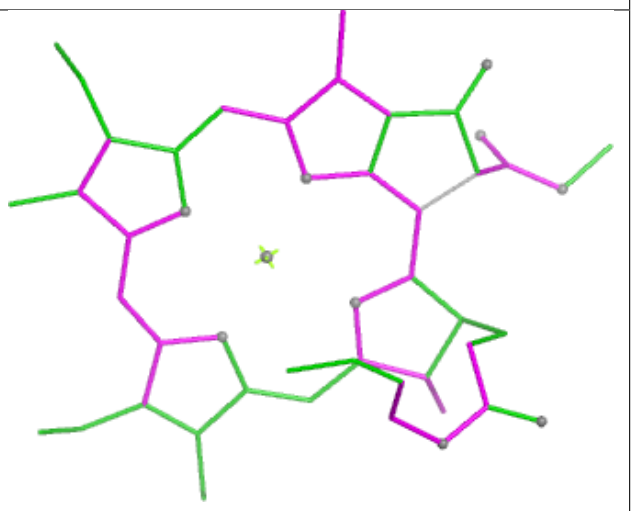
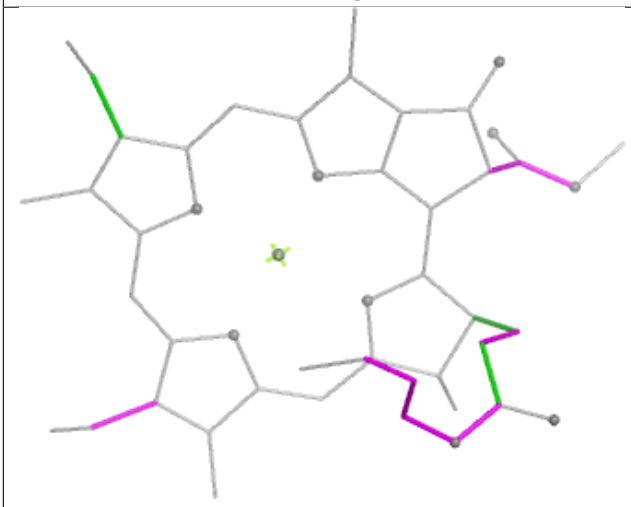


Bond angles



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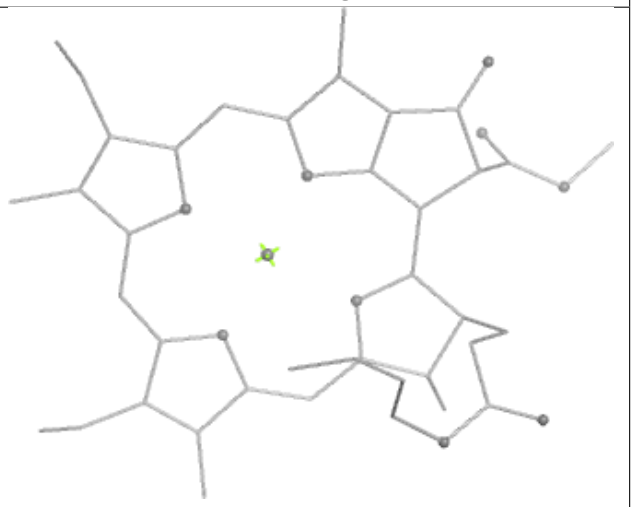
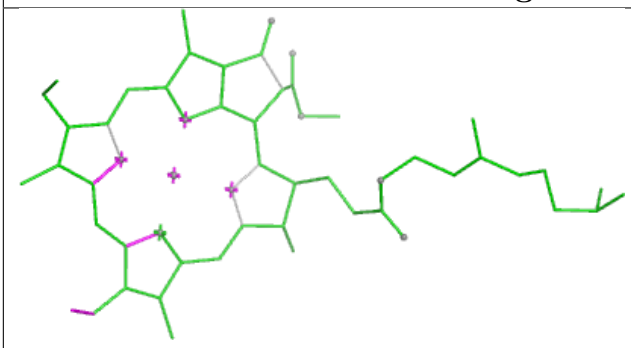


Rings

Ligand CLA B 1220



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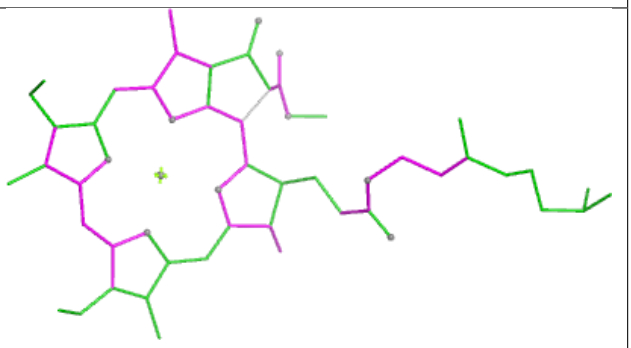

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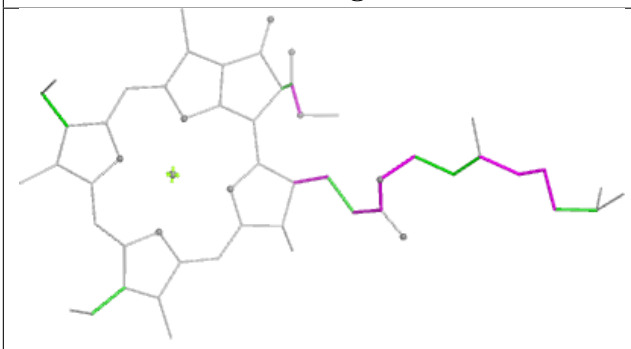

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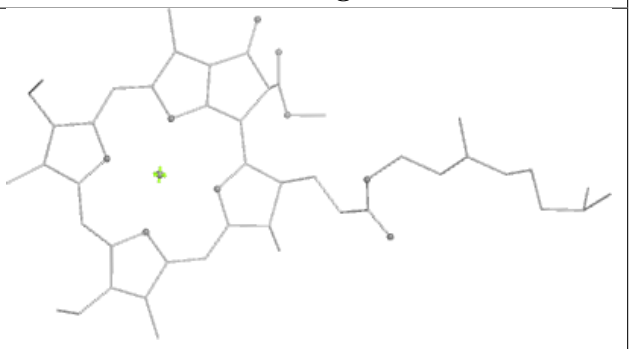
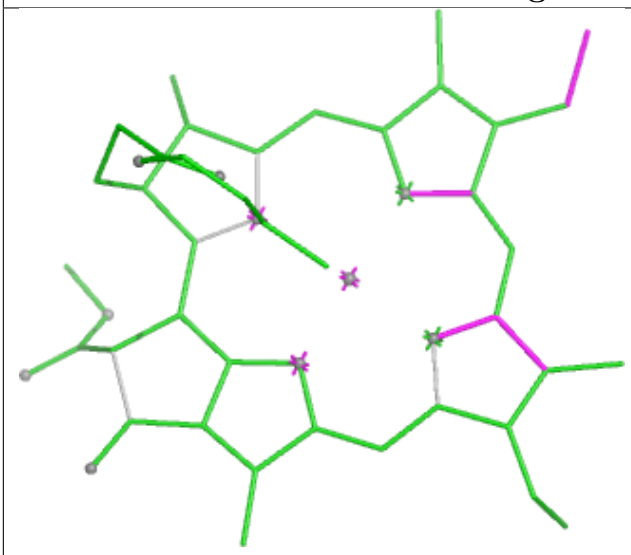


Rings

Ligand CLA 2 607



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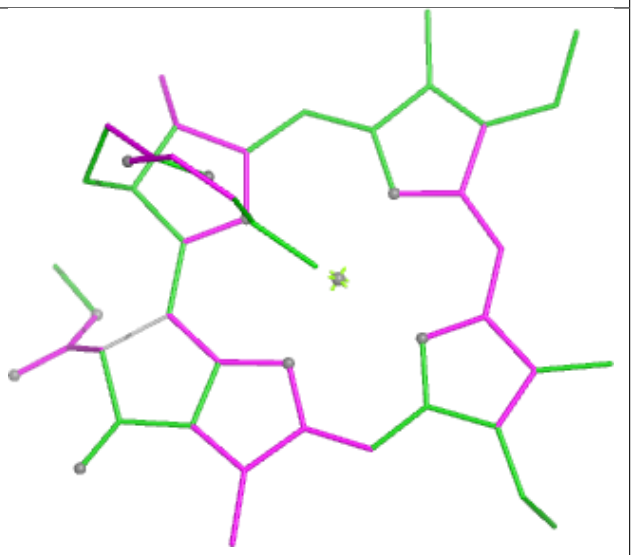
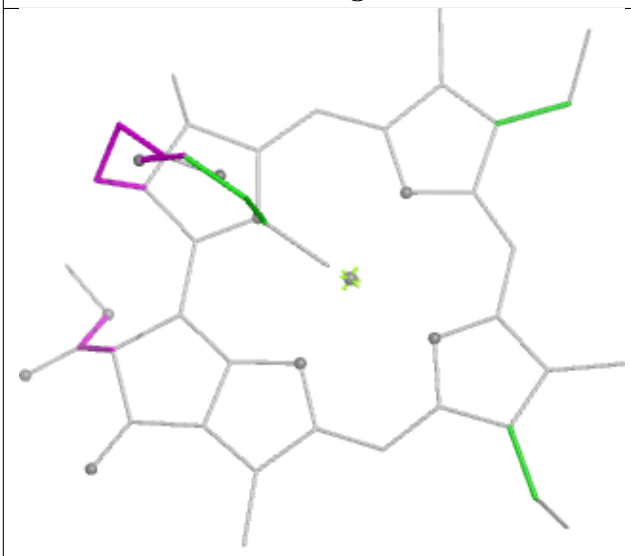


Bond angles



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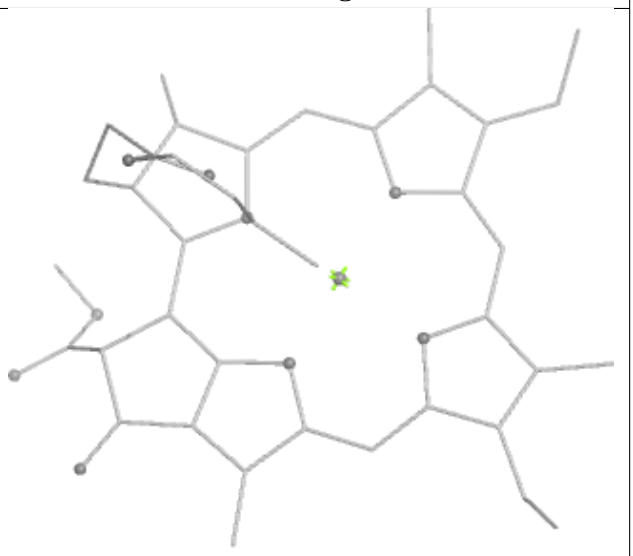
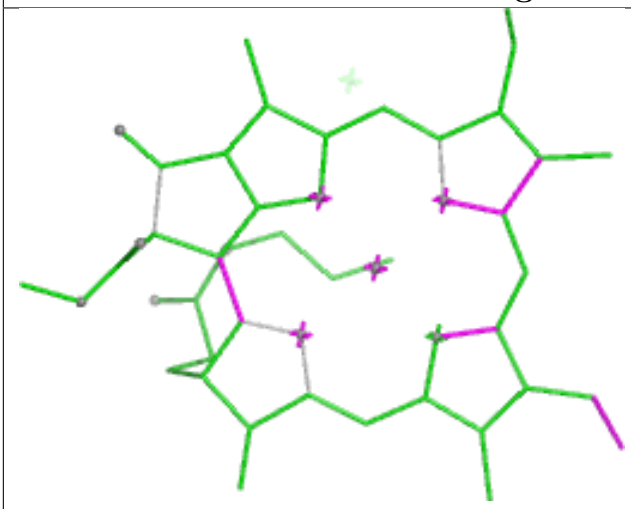


Rings

Ligand CLA B 1201



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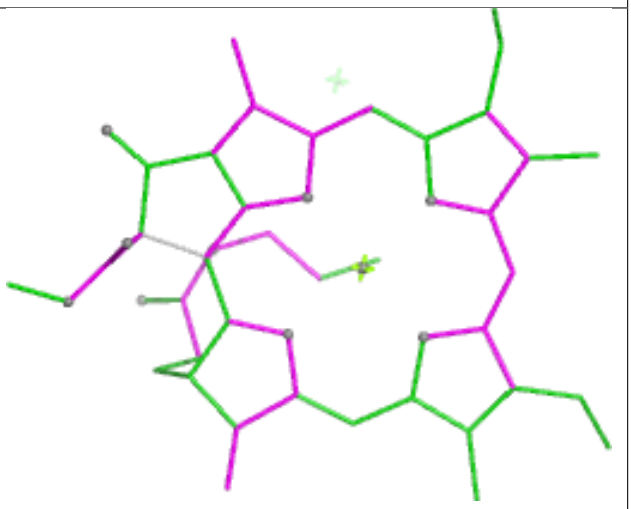
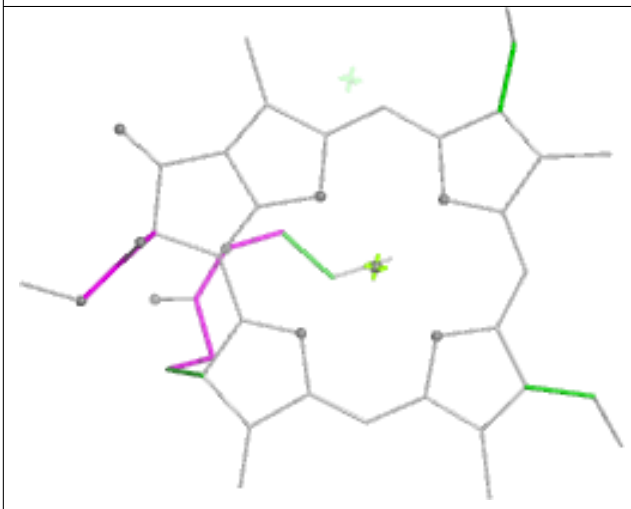


Bond angles



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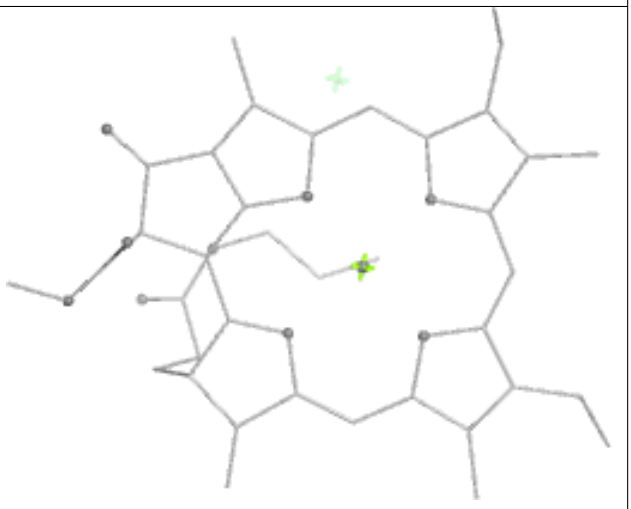
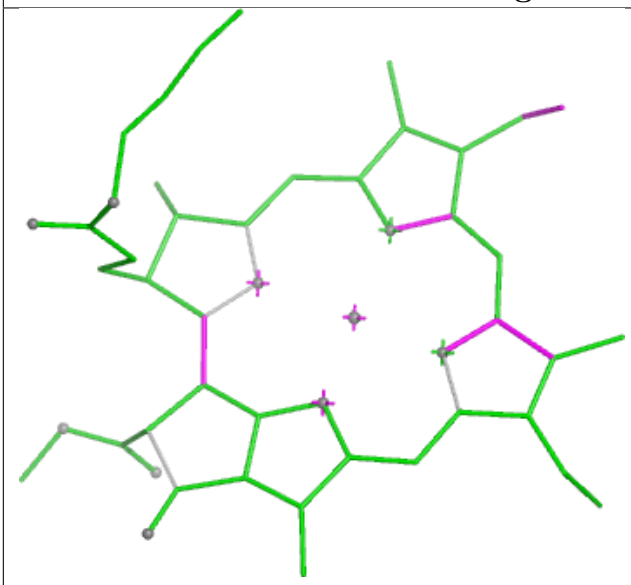


Rings

Ligand CLA A 1120



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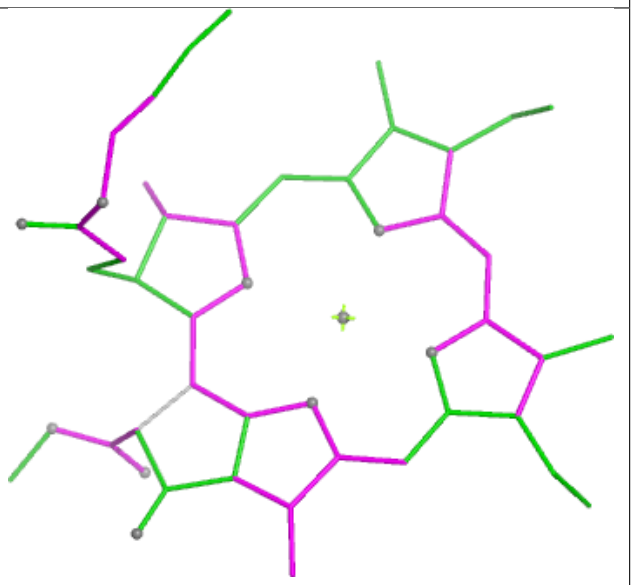
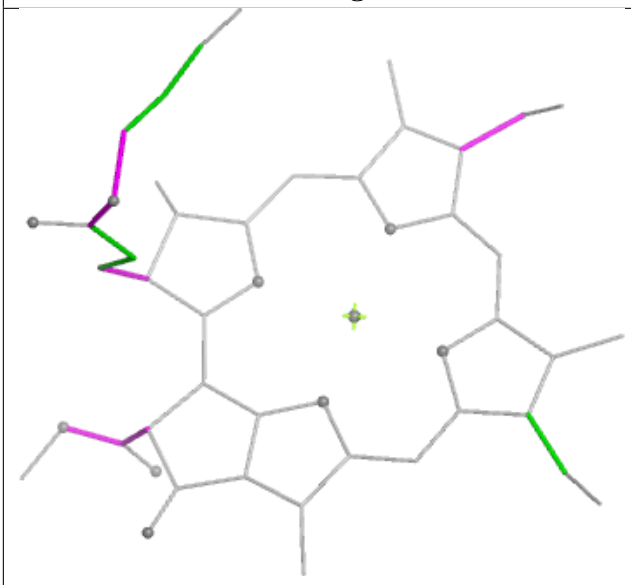


Bond angles



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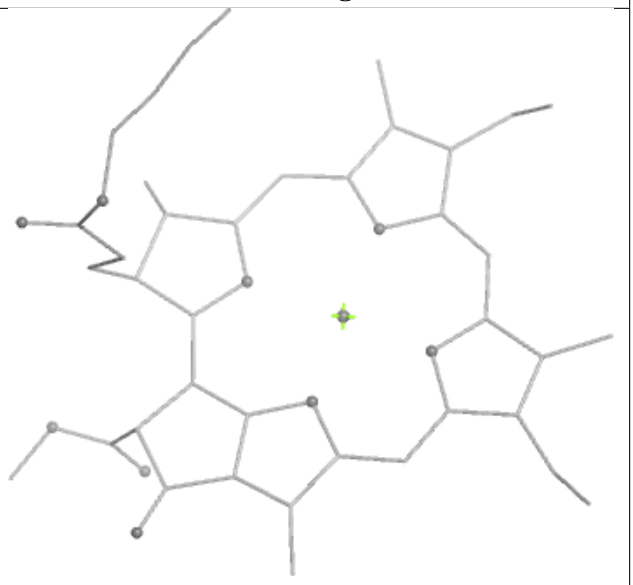
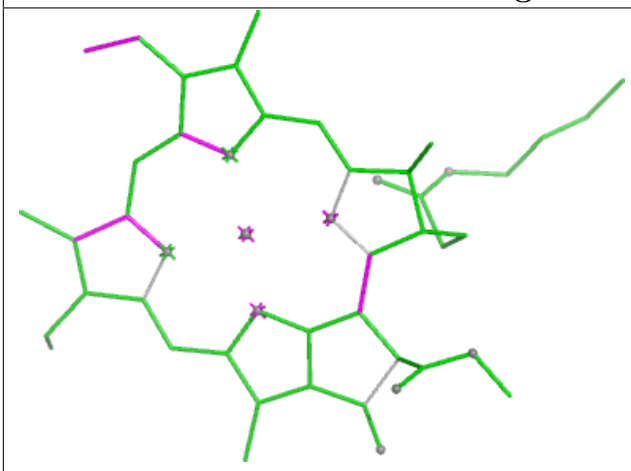


Rings

Ligand CLA A 1124



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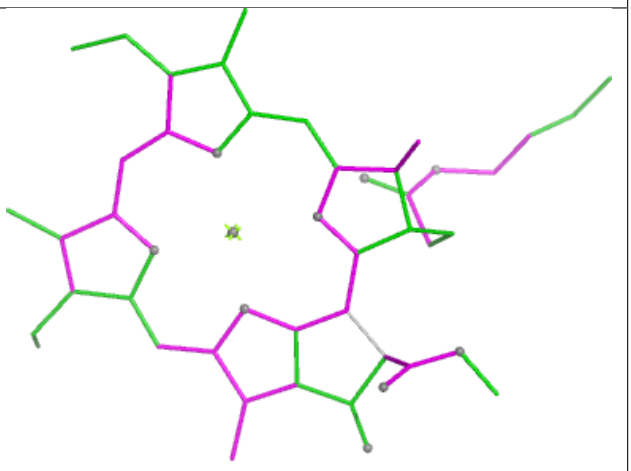
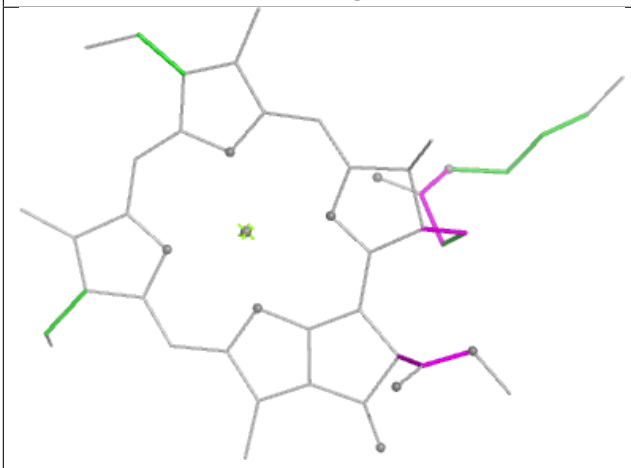


Bond angles

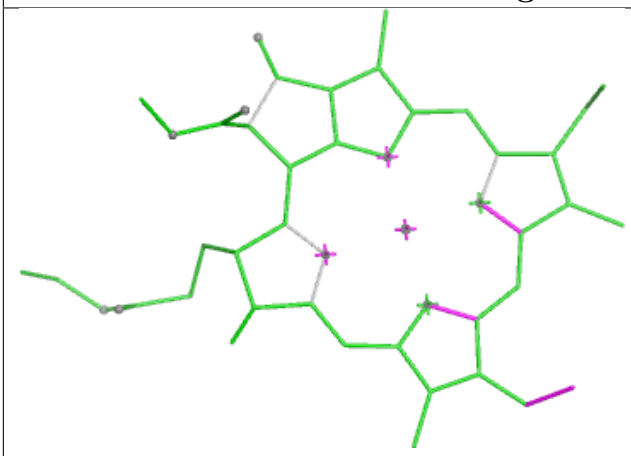


Torsions



Rings

Ligand CLA F 1301



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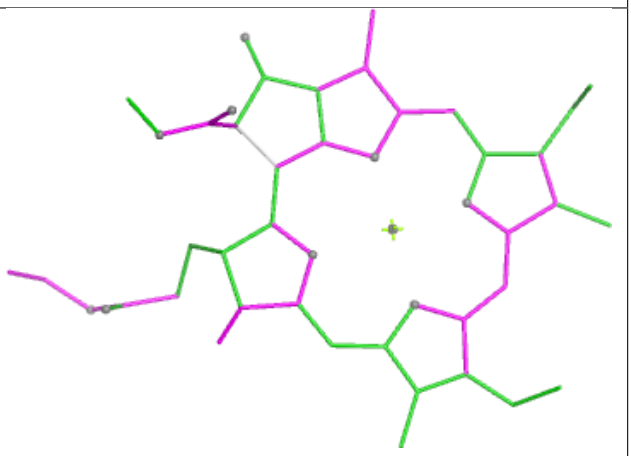
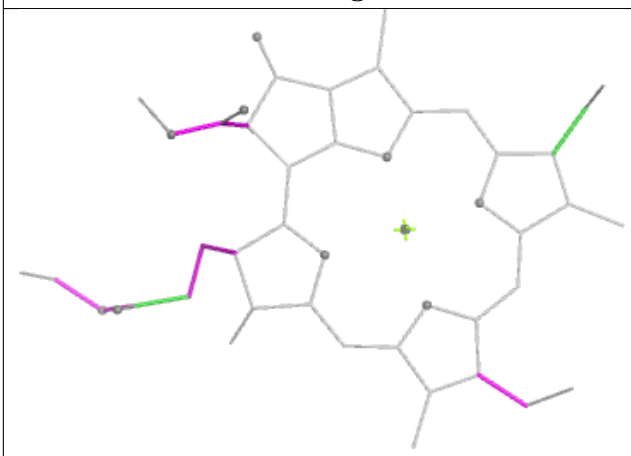


Bond angles



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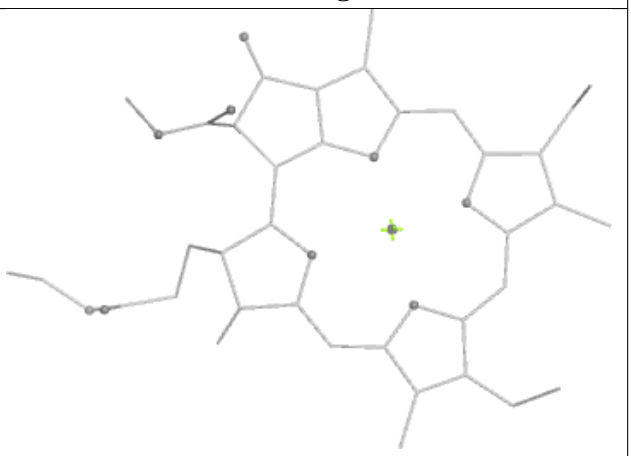
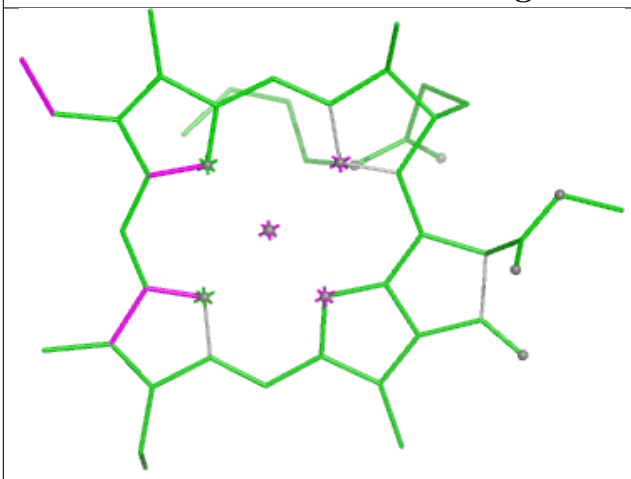


Rings

Ligand CLA A 1119



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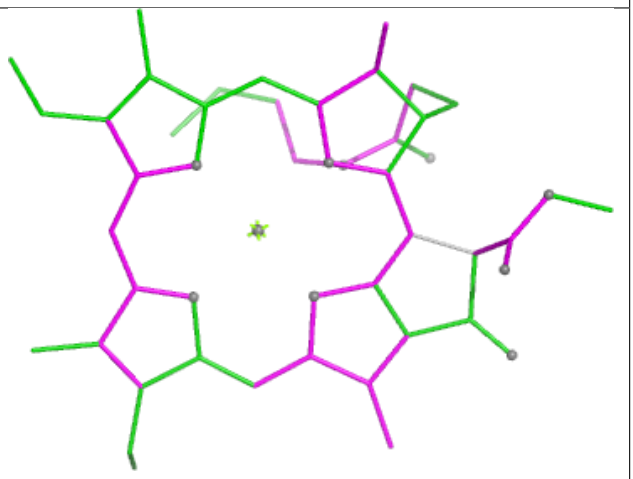
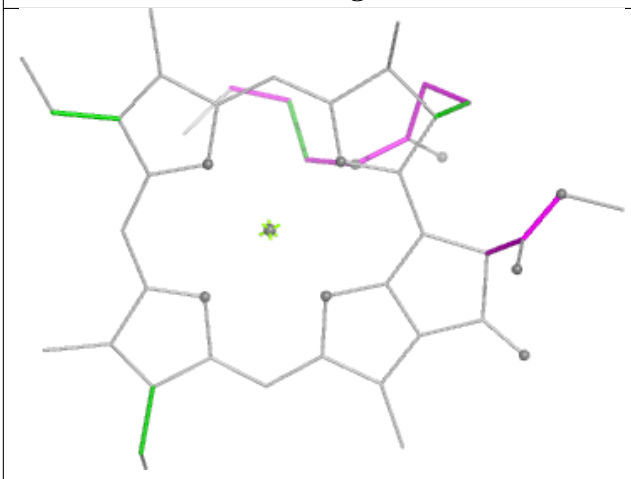


Bond angles



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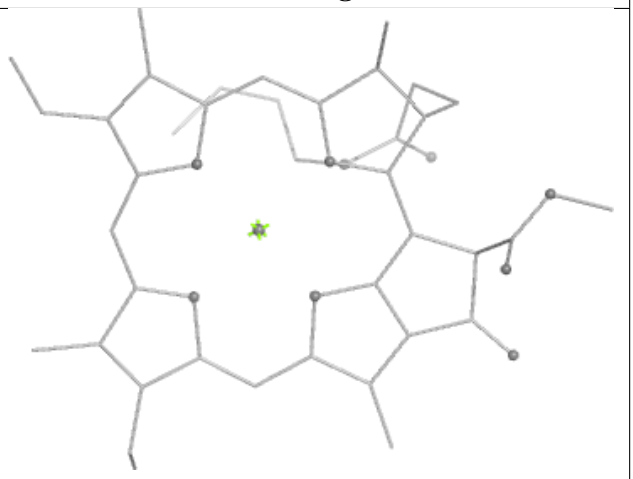


Rings

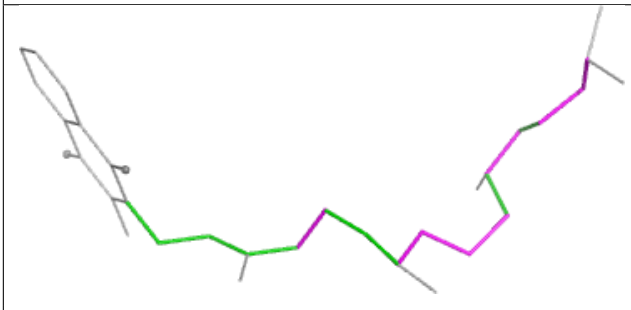
Ligand PQN B 2002



Bond lengths



Bond angles

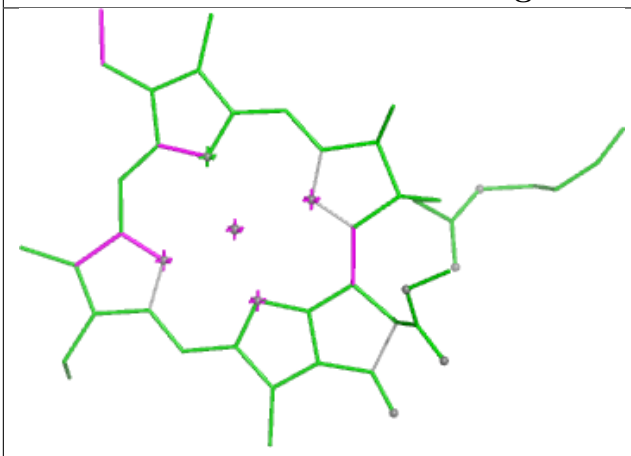


Torsions

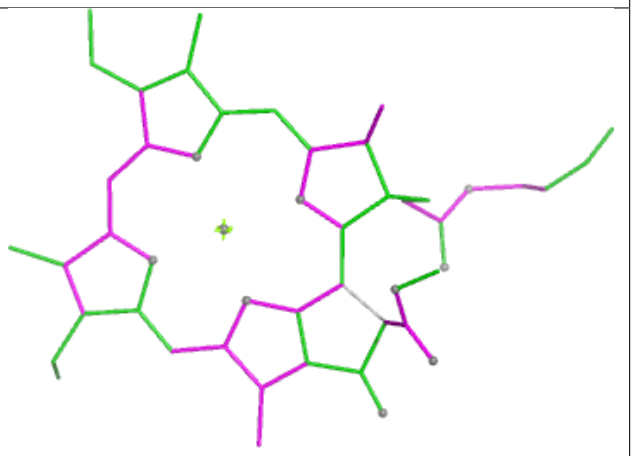


Rings

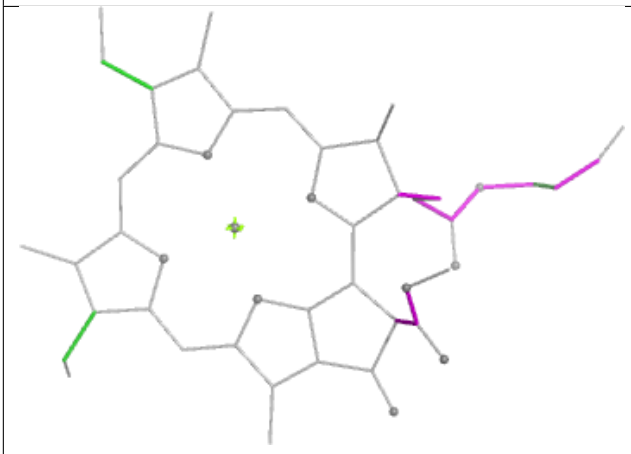
Ligand CLA A 1132



Bond lengths



Bond angles

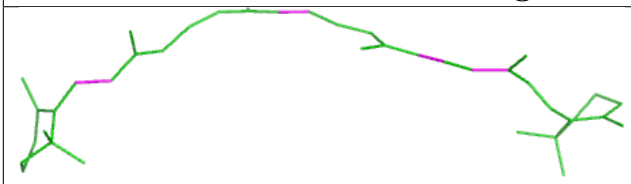


Torsions

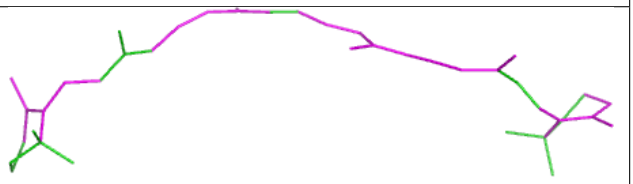


Rings

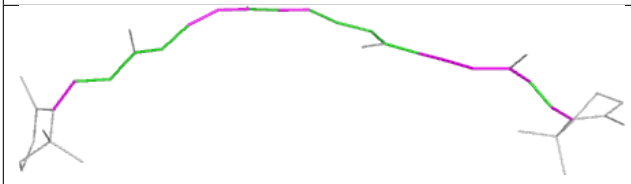
Ligand BCR B 4001



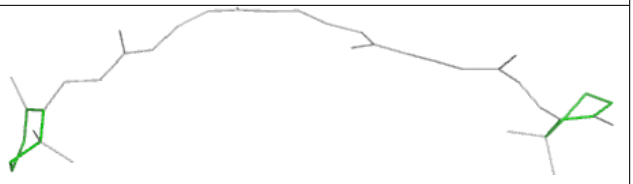
Bond lengths



Bond angles

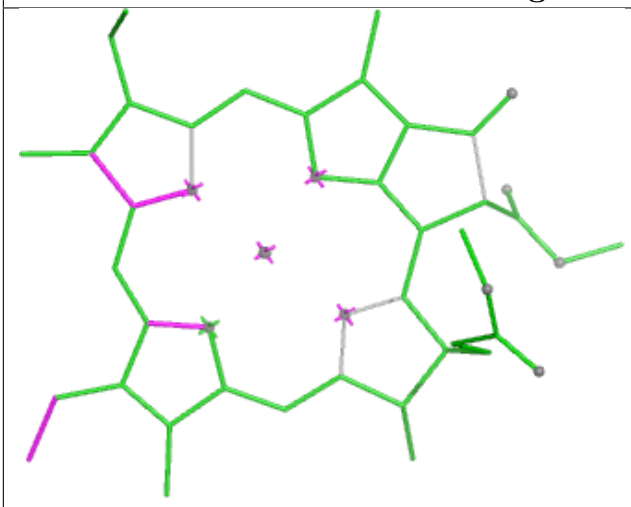


Torsions



Rings

Ligand CLA 4 608



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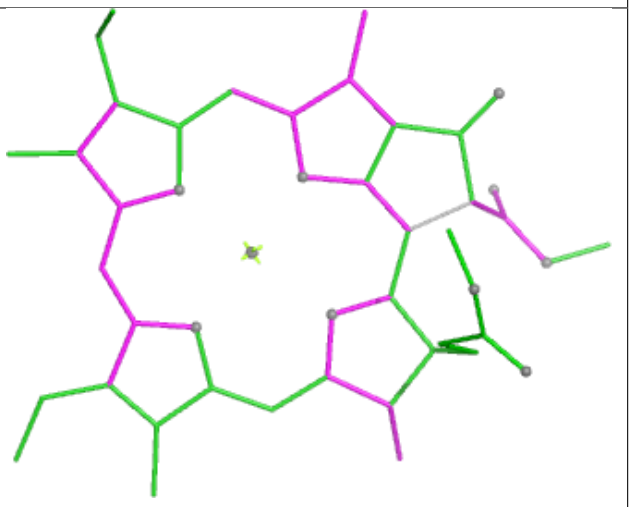

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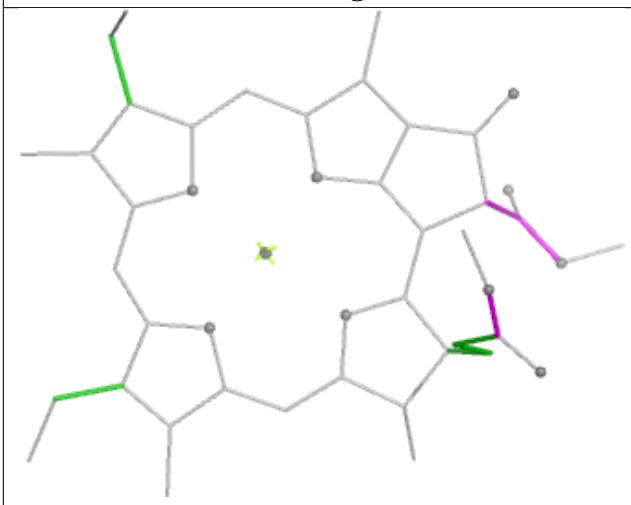

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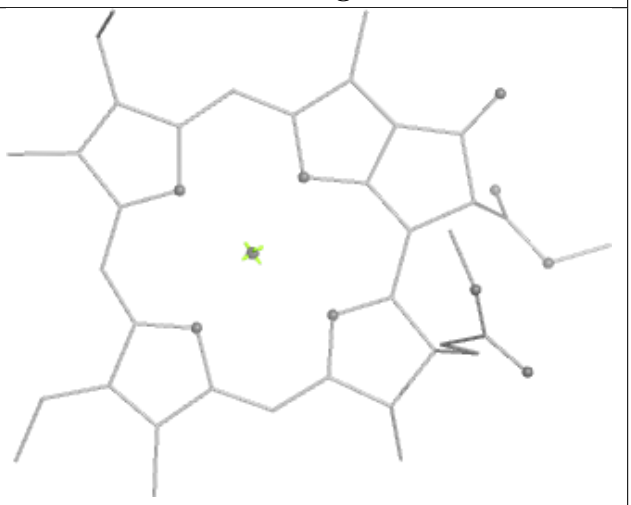
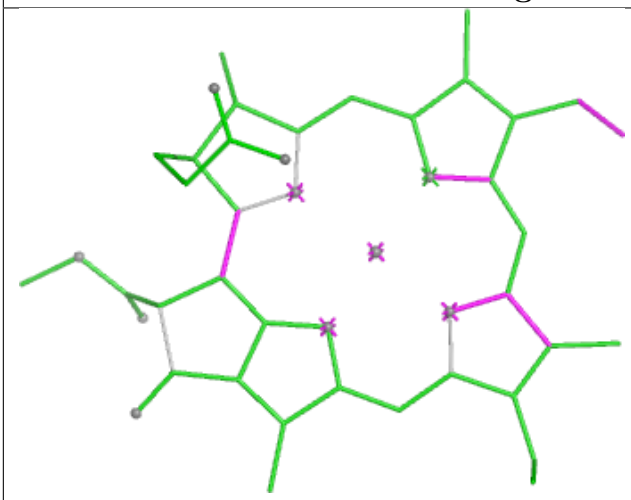


Rings

Ligand CLA A 1113



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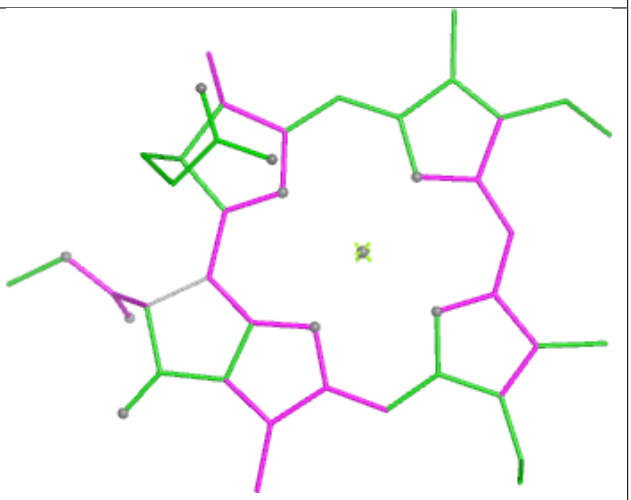

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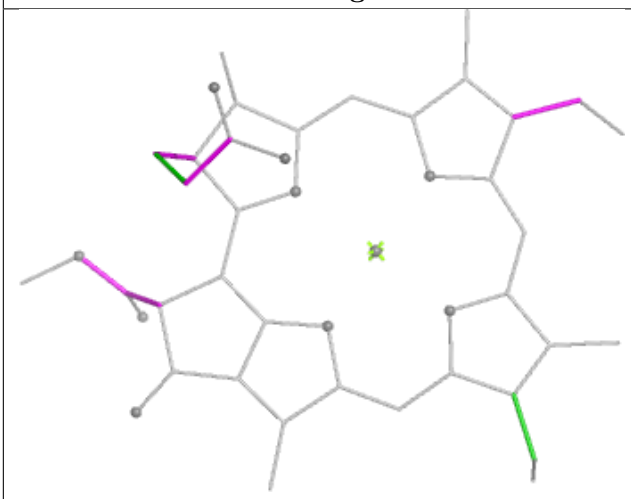

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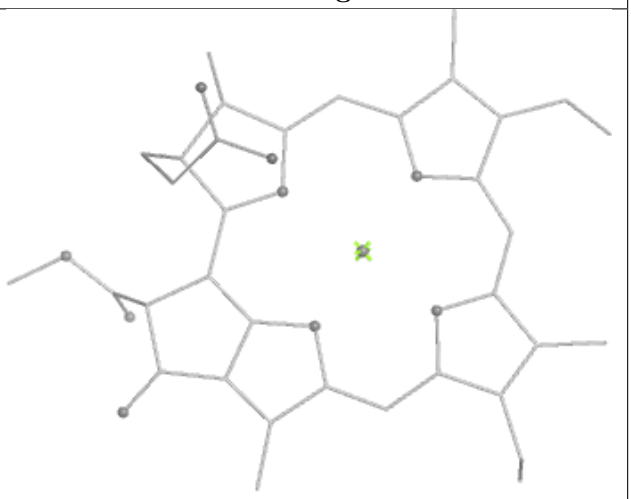
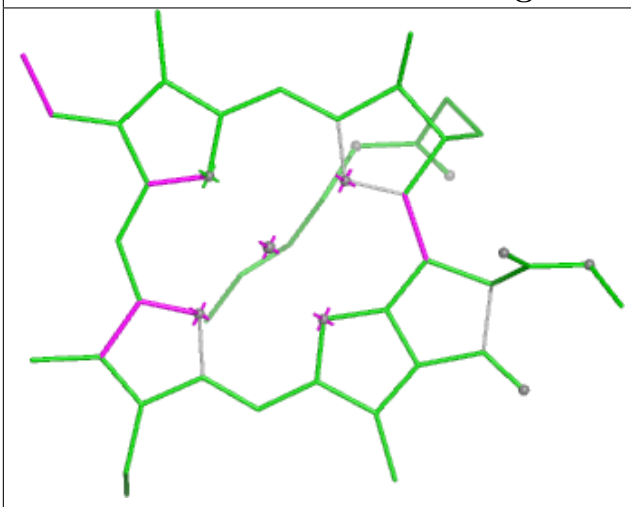


Rings

Ligand CLA B 1211



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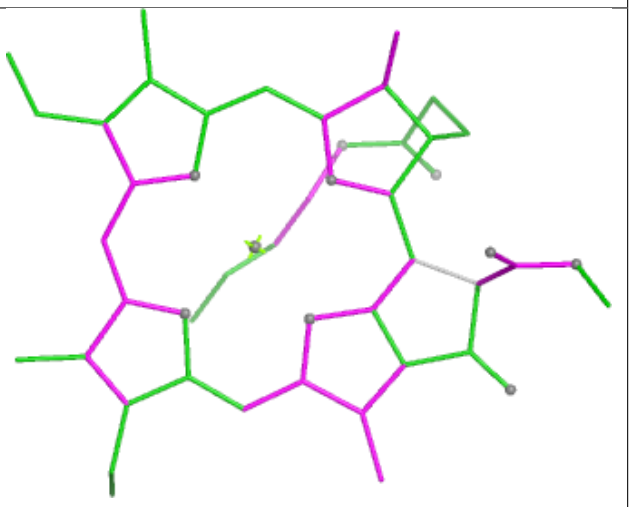

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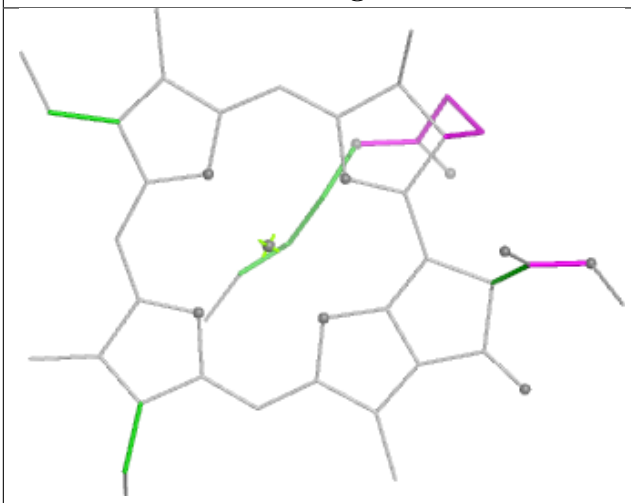

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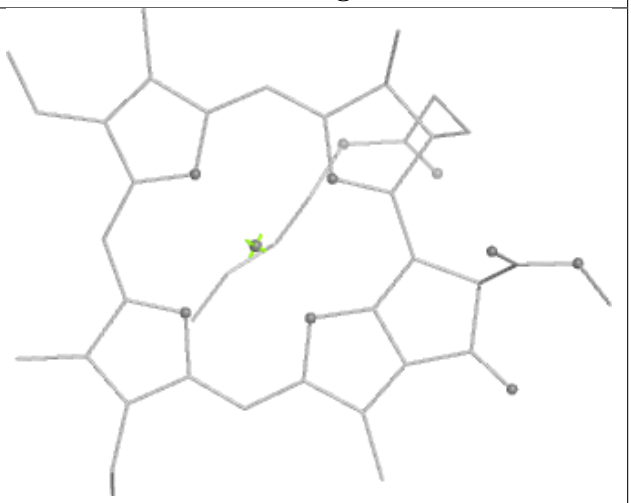
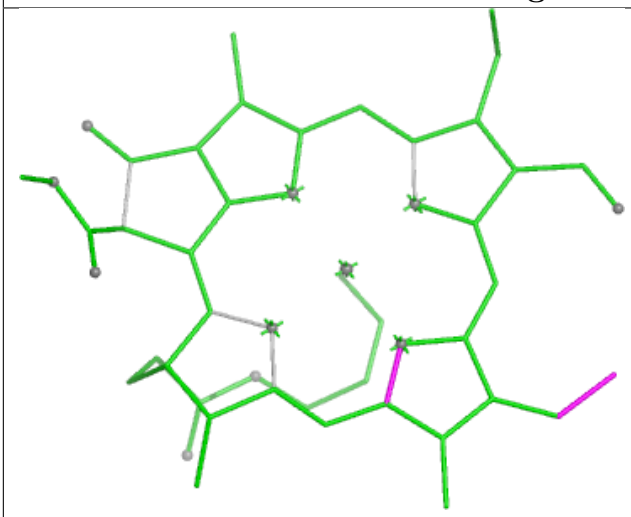


Rings

Ligand CHL 1 609



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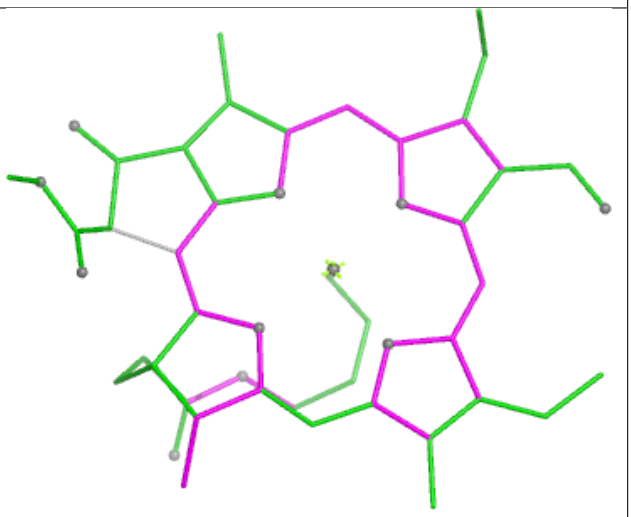

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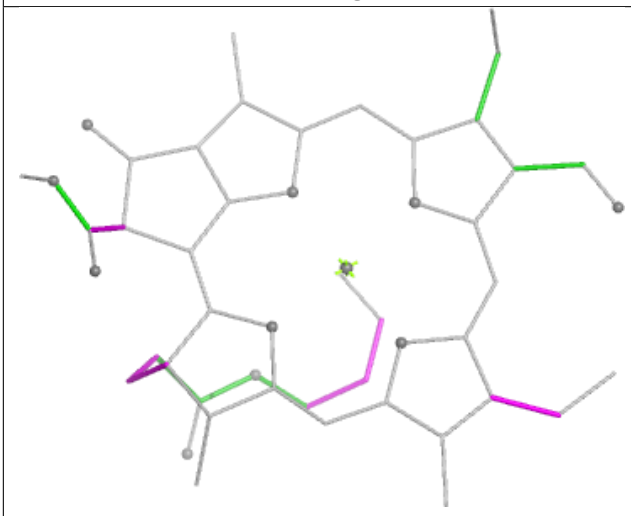

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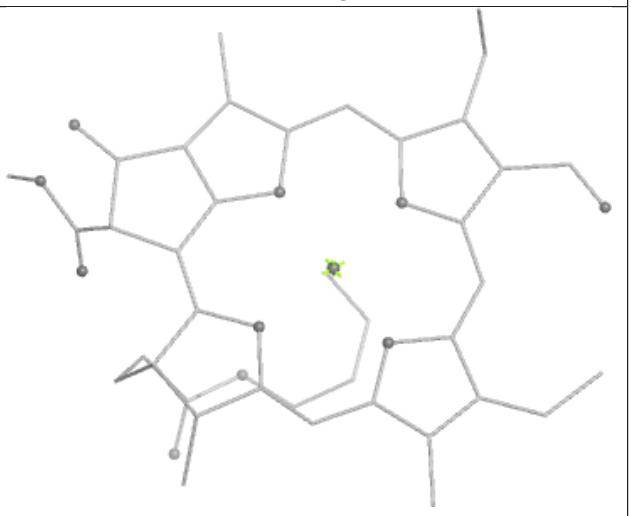
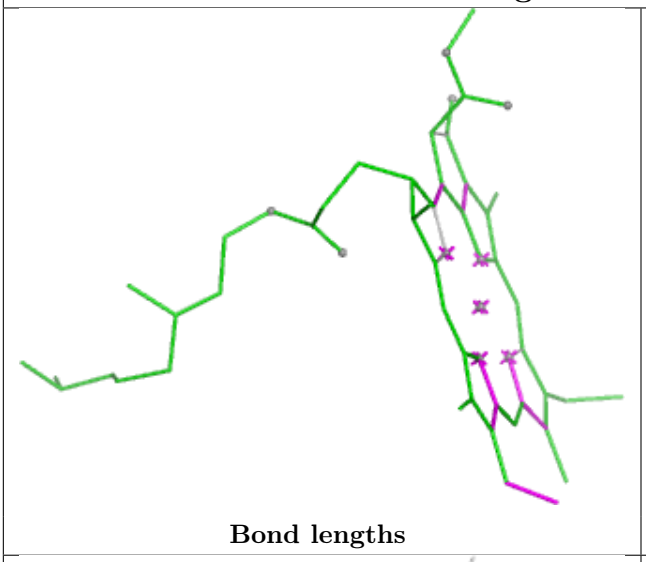


Rings

Ligand CLA A 1140



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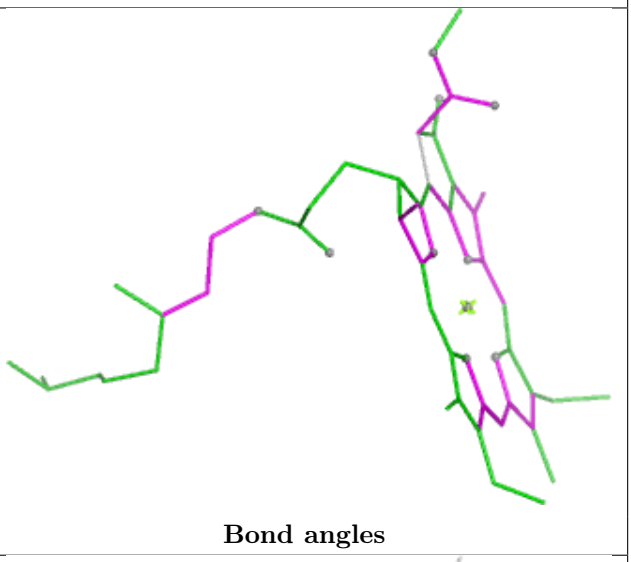

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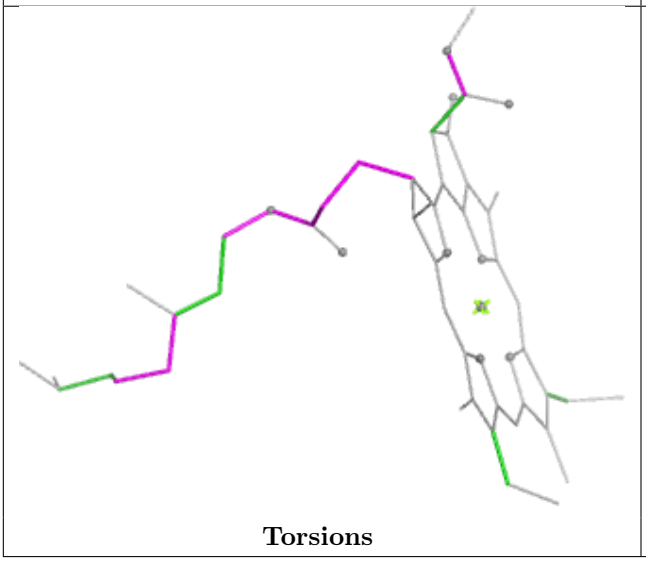

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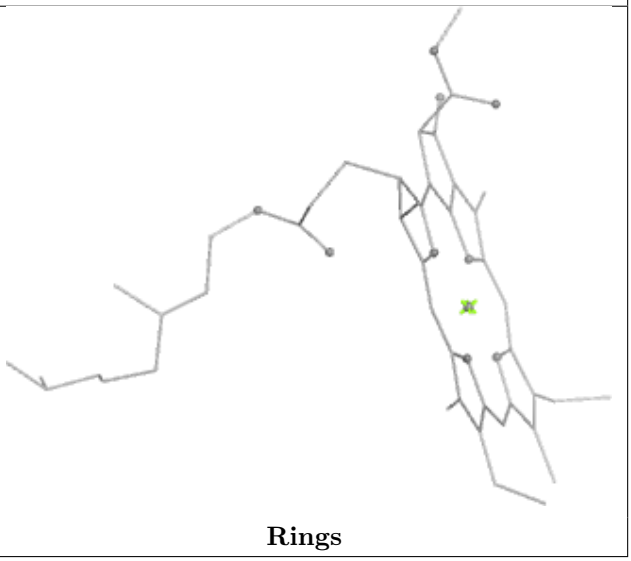
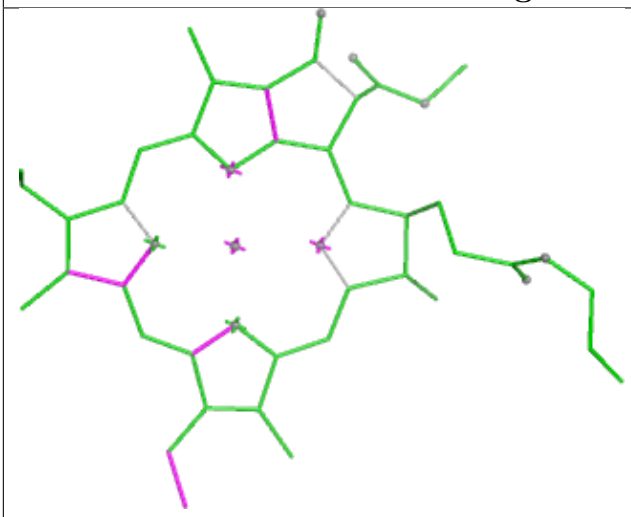


Rings

Ligand CLA A 1129



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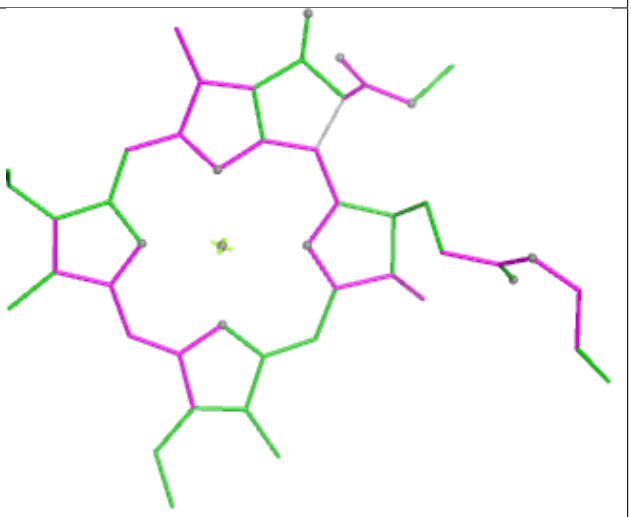

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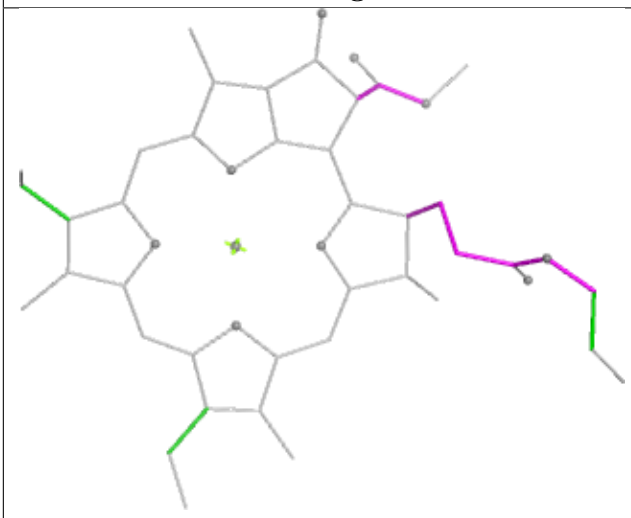

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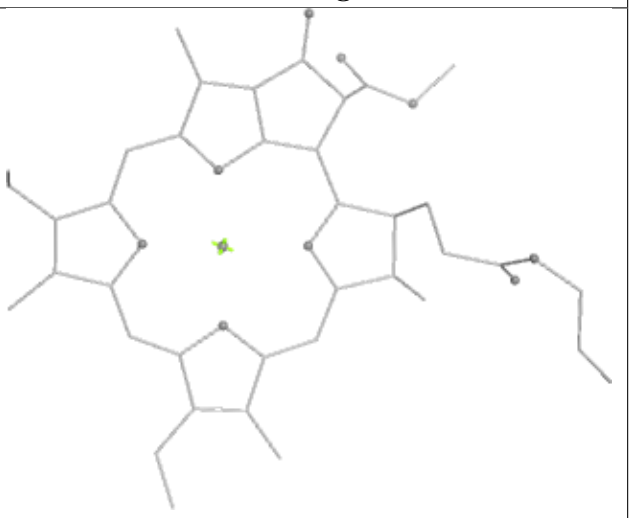
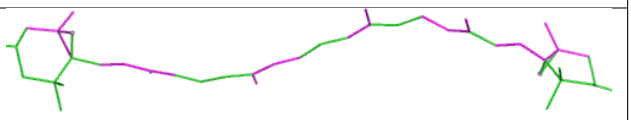


Rings

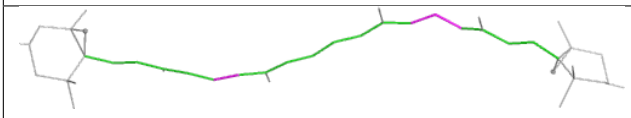
Ligand XAT 1 502



Bond lengths



Bond angles

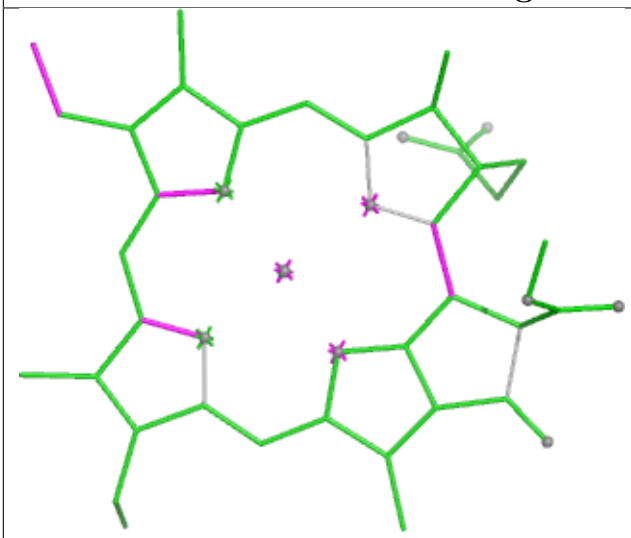


Torsions



Rings

Ligand CLA B 1212



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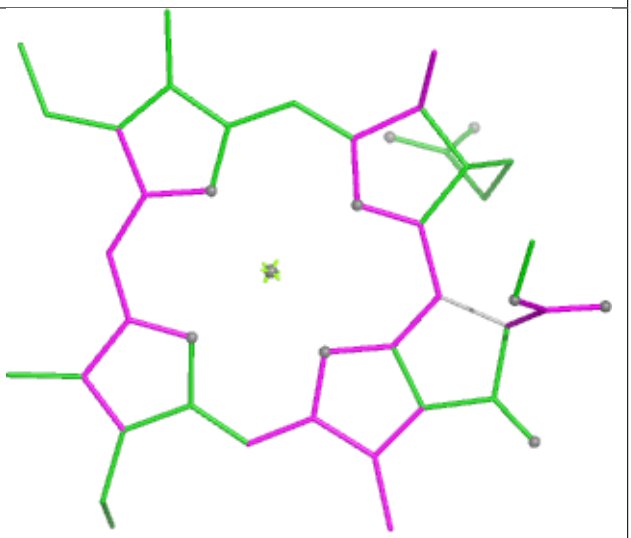

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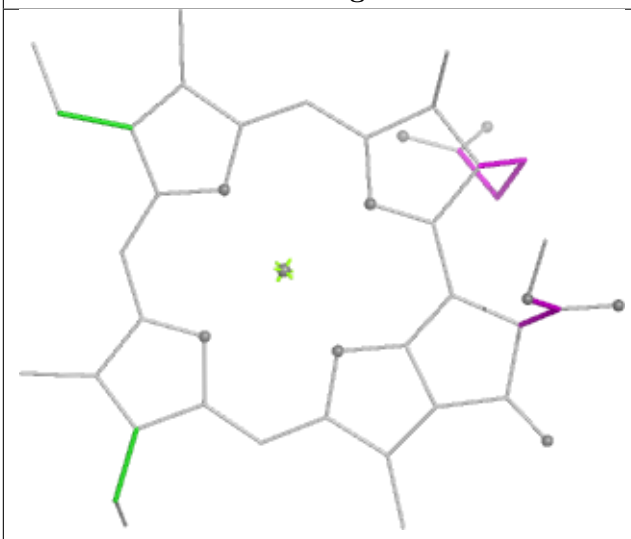

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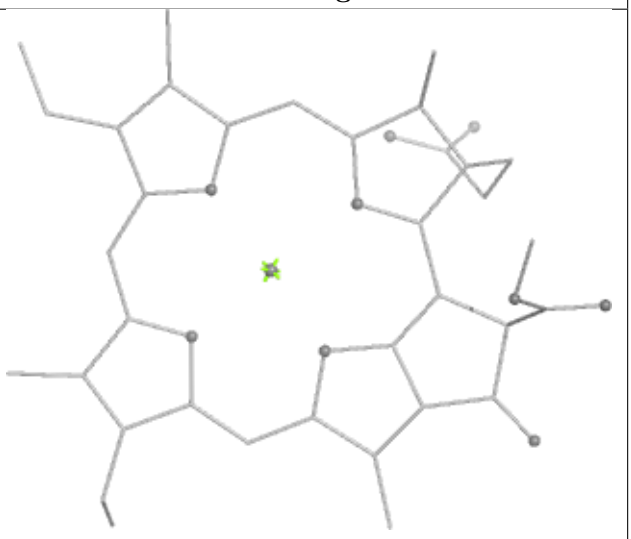
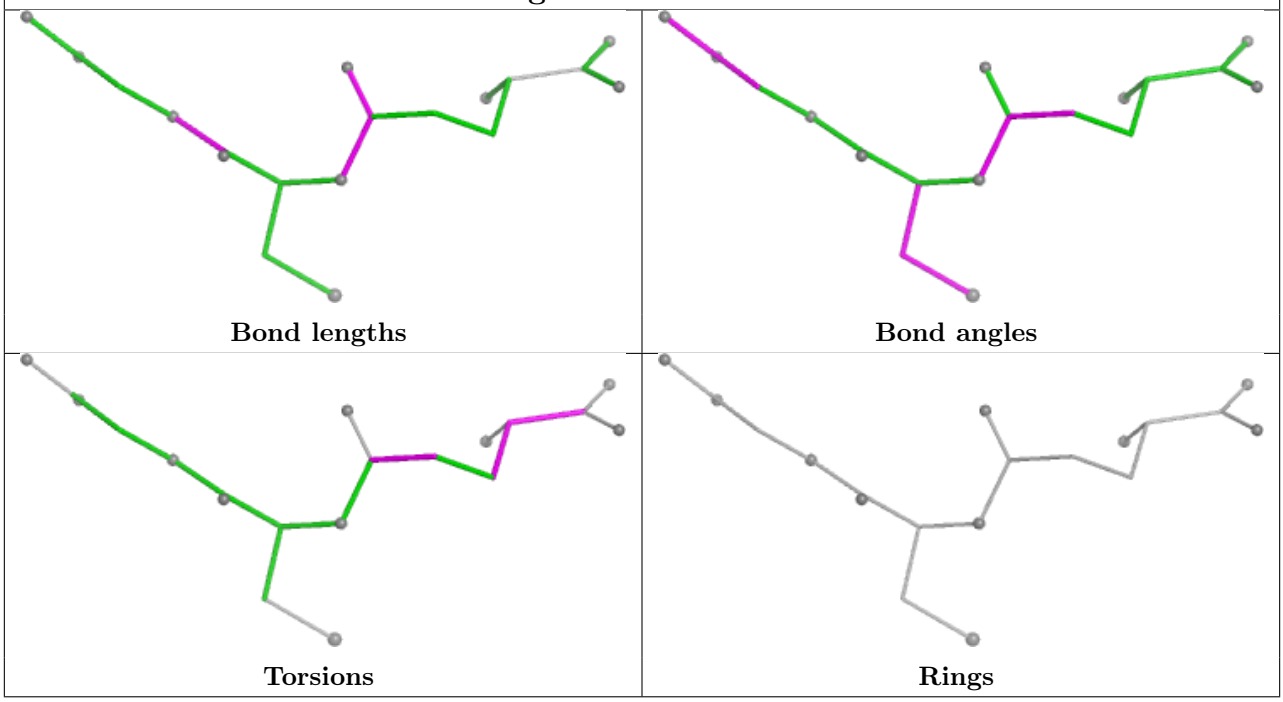
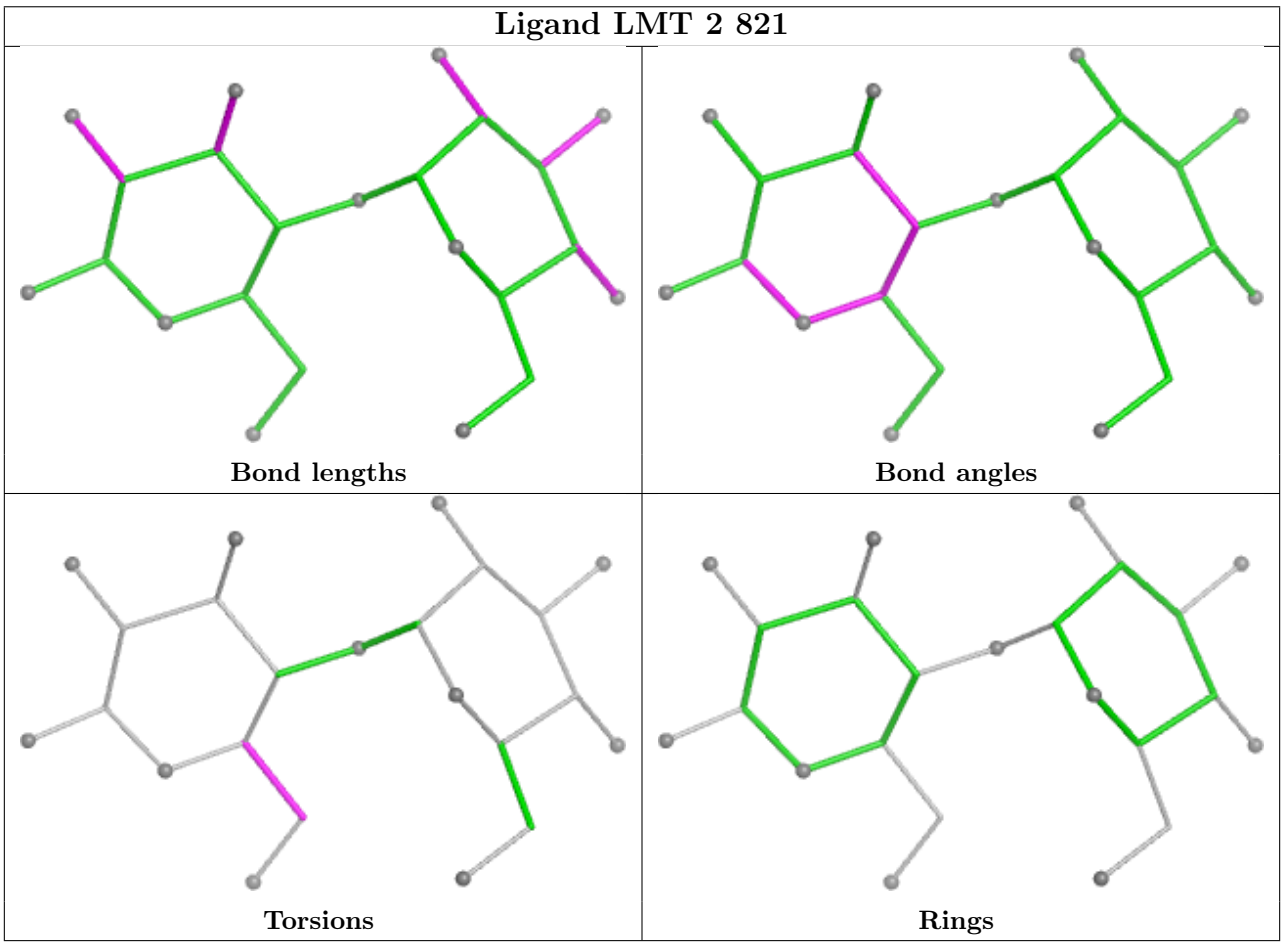


Rings

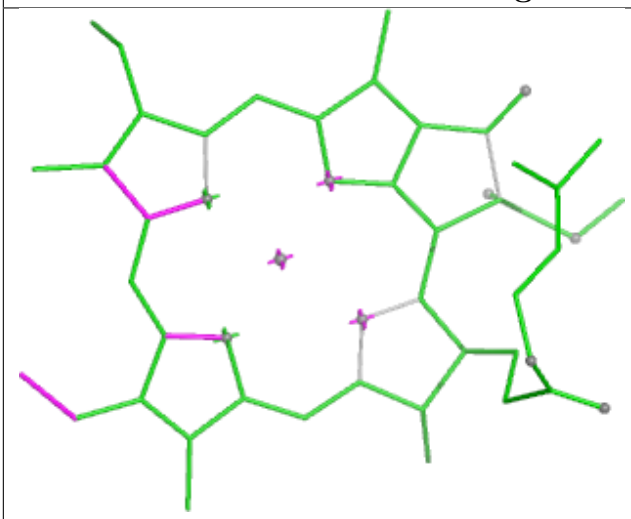
Ligand GSH 4 831



Ligand LMT 2 821



Ligand CLA A 1141



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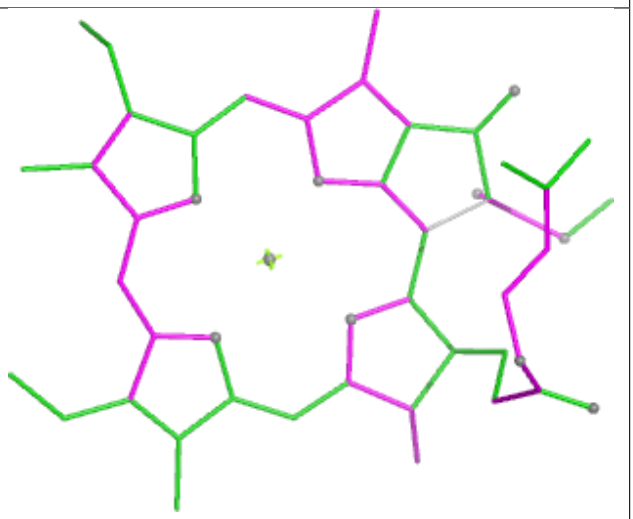

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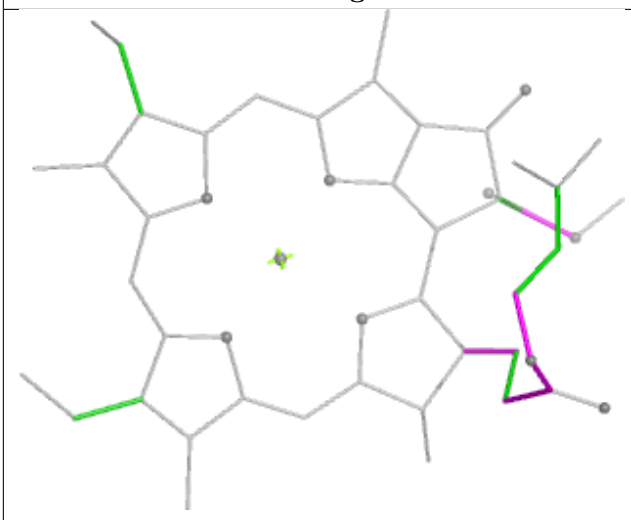

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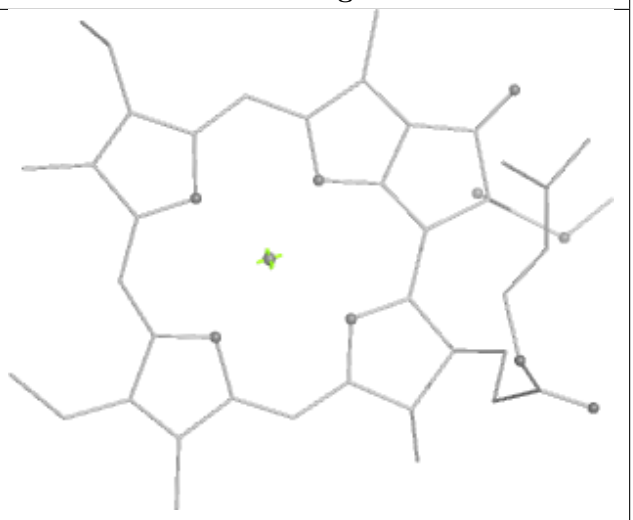
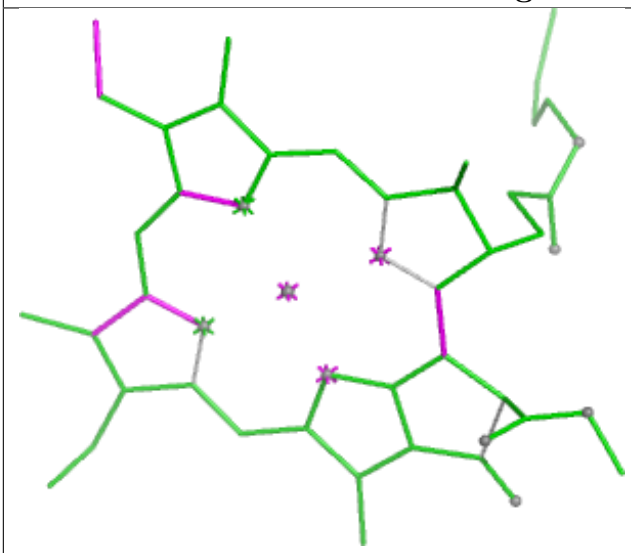


Rings

Ligand CLA B 1232



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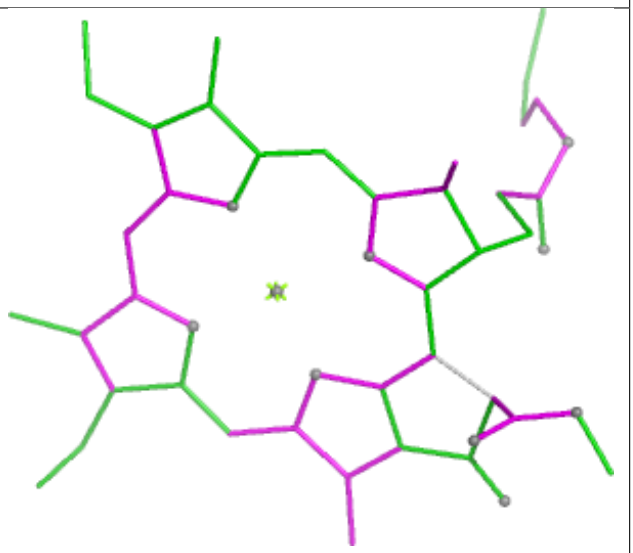

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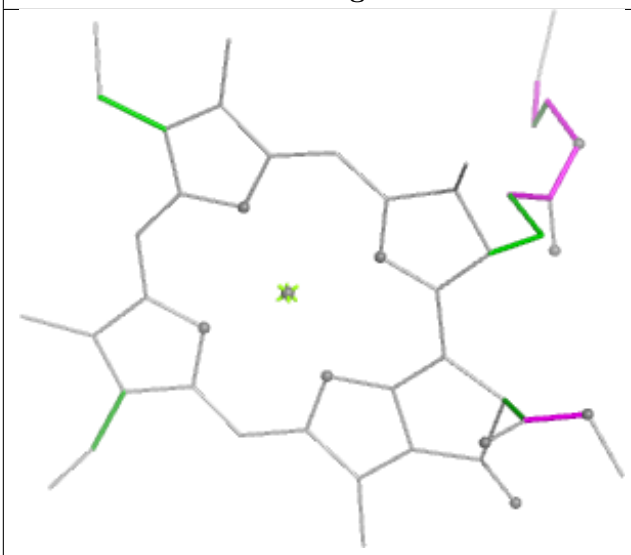
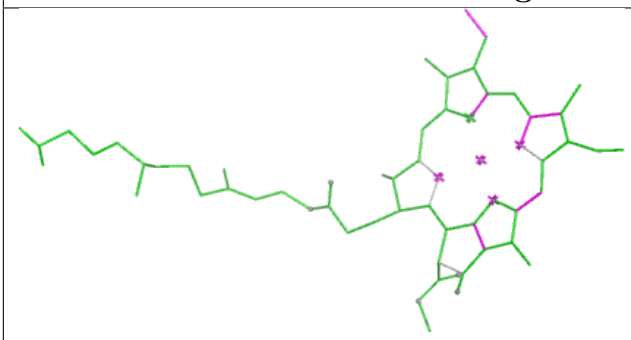


Torsions



Rings

Ligand CLA A 1012



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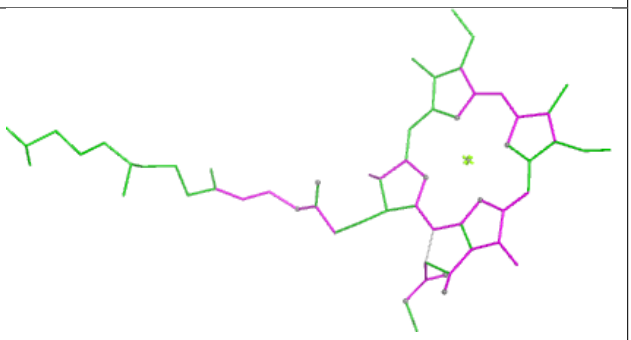

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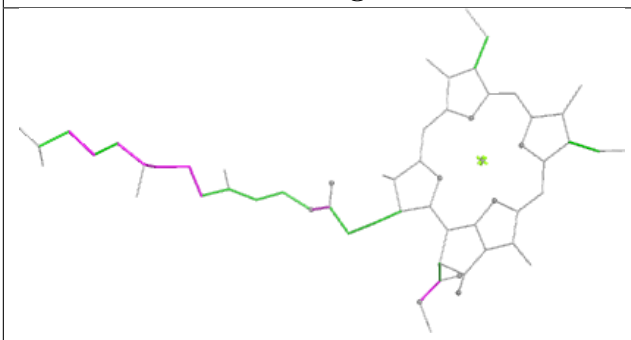

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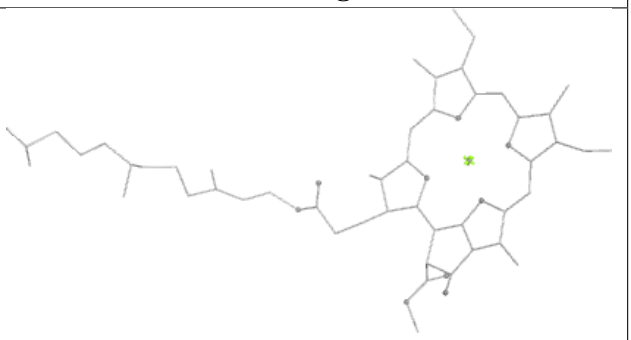
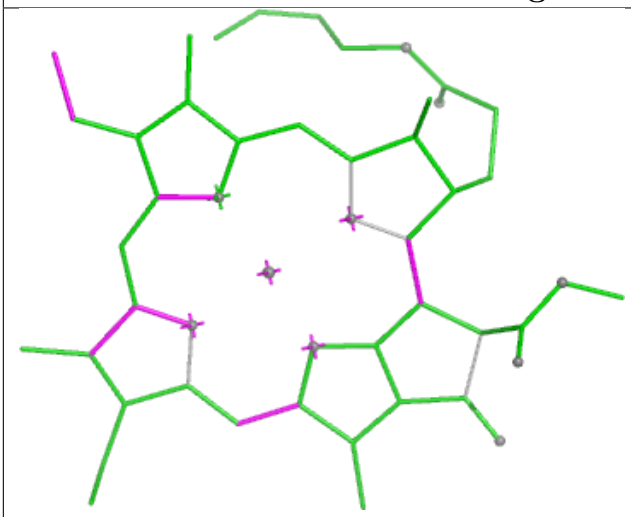


Rings

Ligand CLA 1 601



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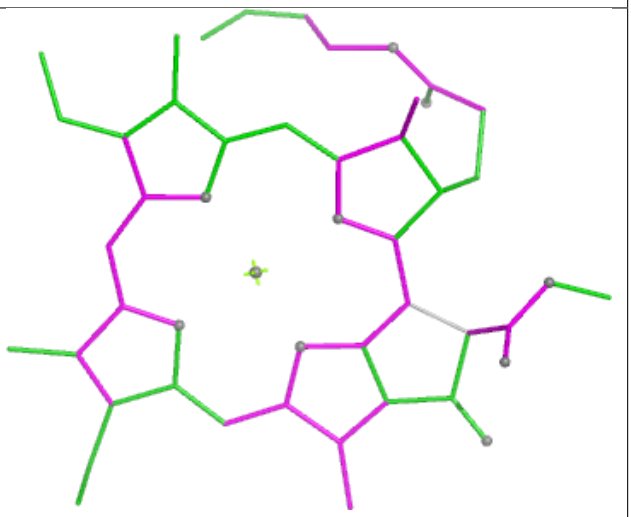
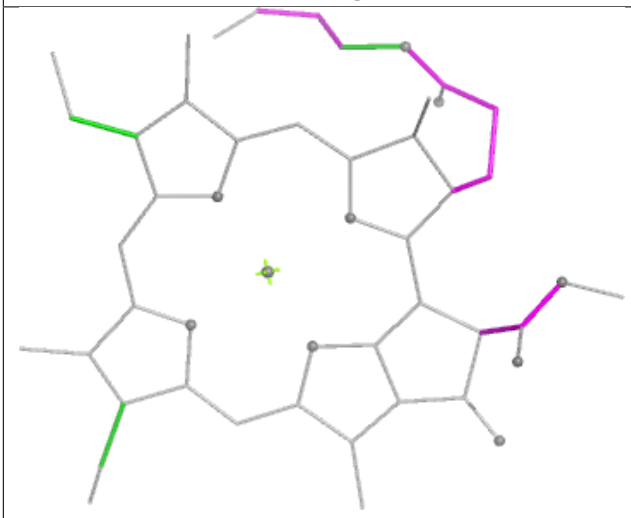


Bond angles



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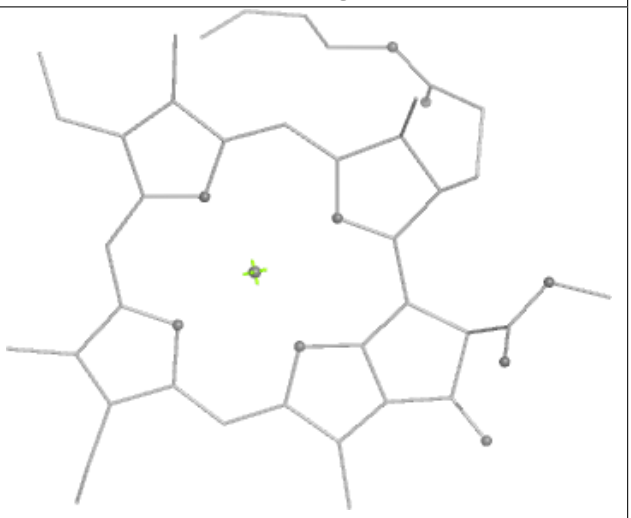
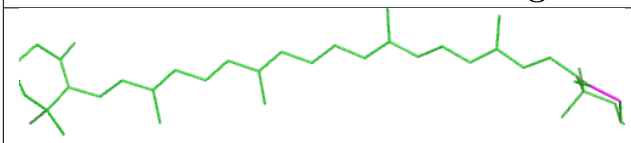


Rings

Ligand LUT 2 501



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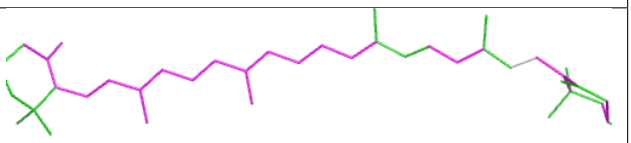
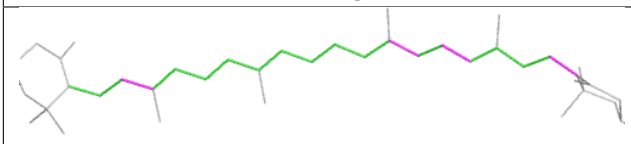


Bond angles



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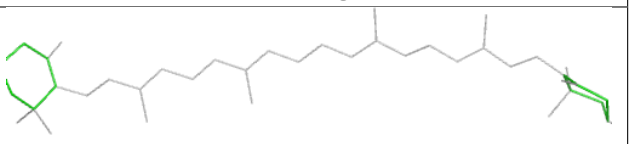
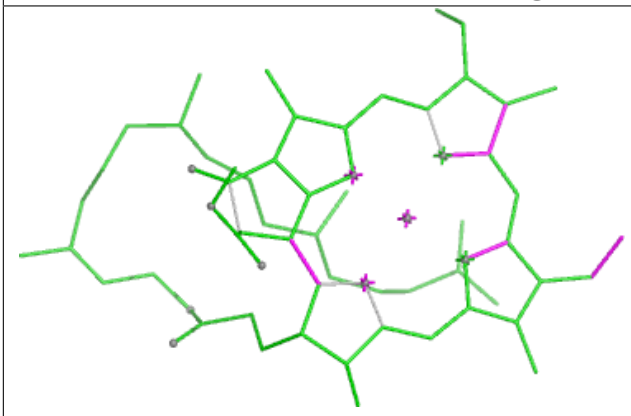


Rings

Ligand CLA 2 605



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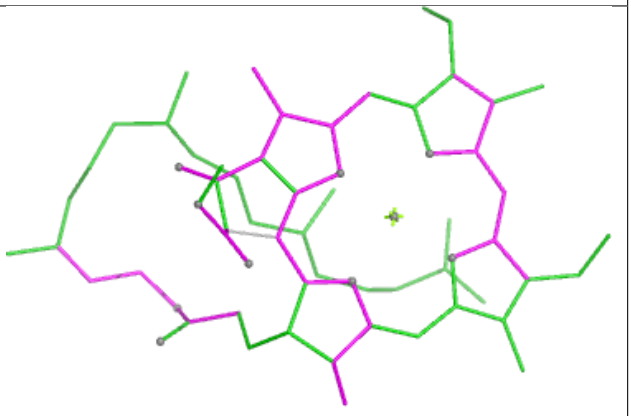
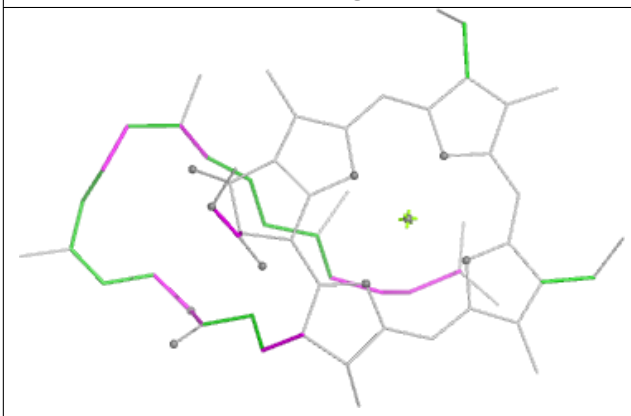


Bond angles



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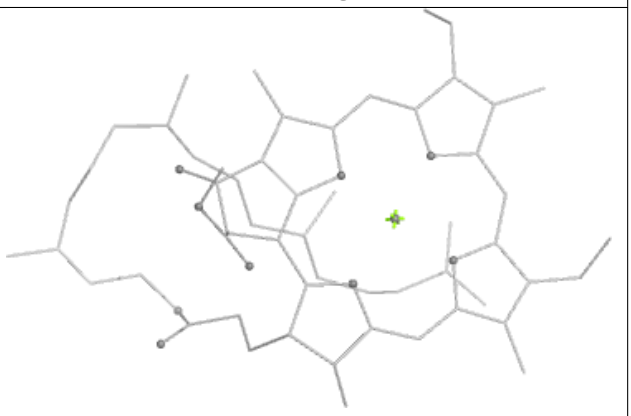
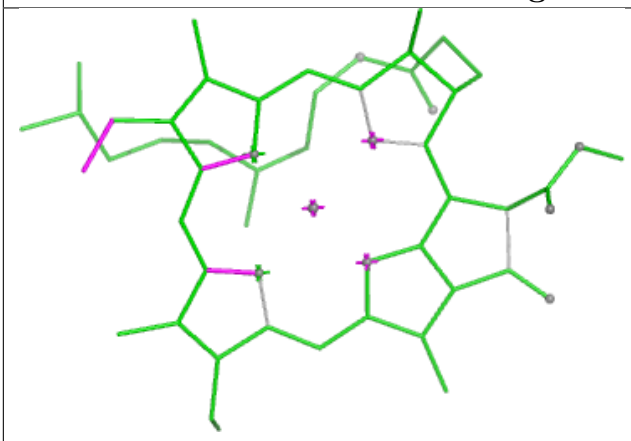


Rings

Ligand CLA 4 615



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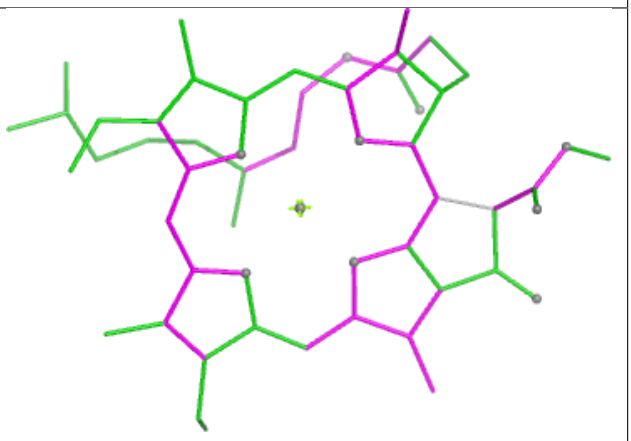
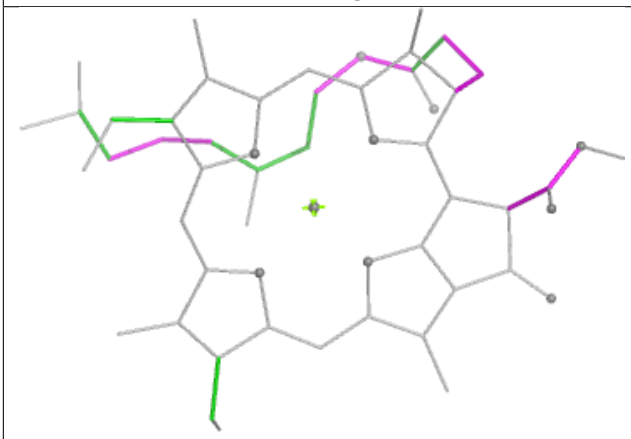
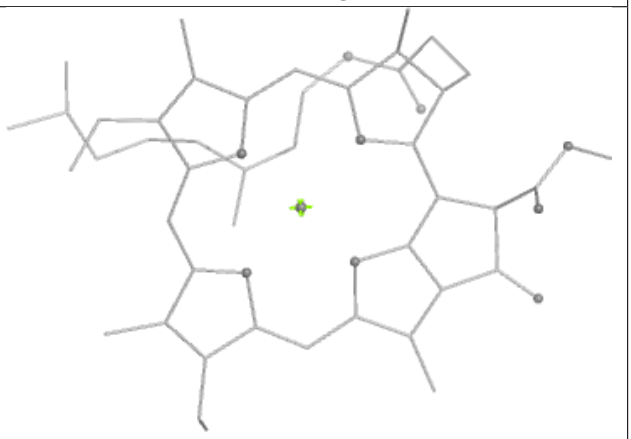


Bond angles

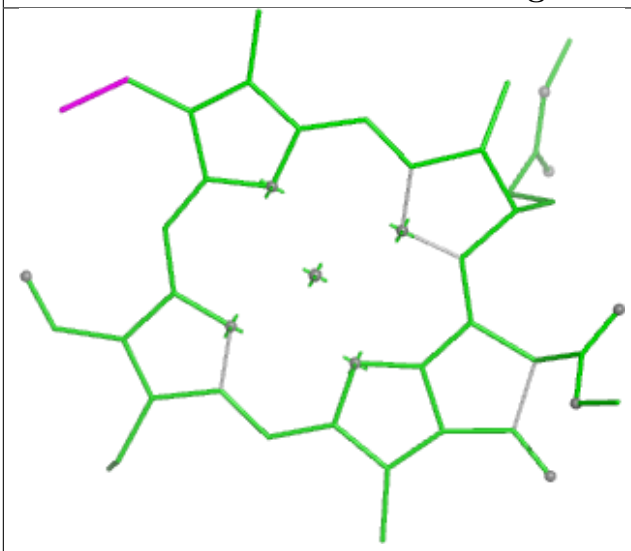


Torsions



Rings

Ligand CHL 4 610



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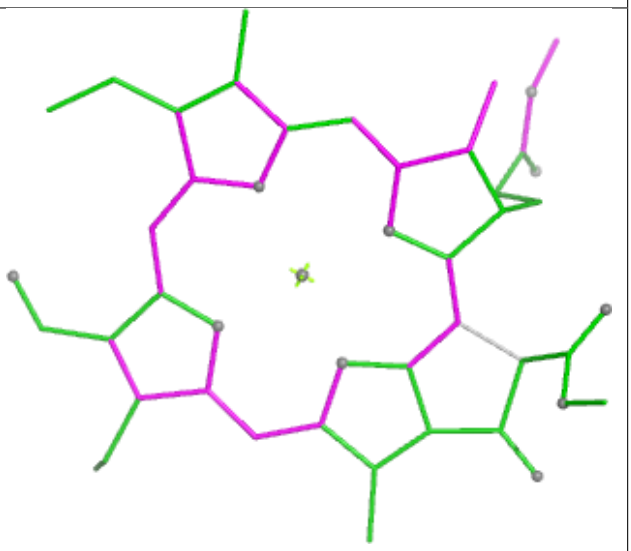

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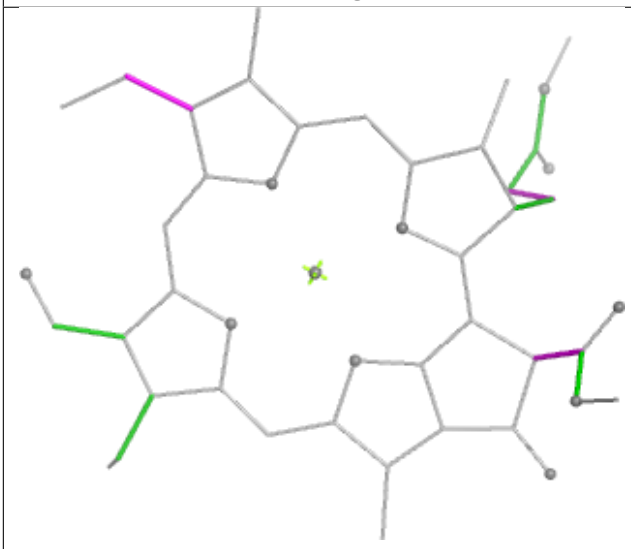

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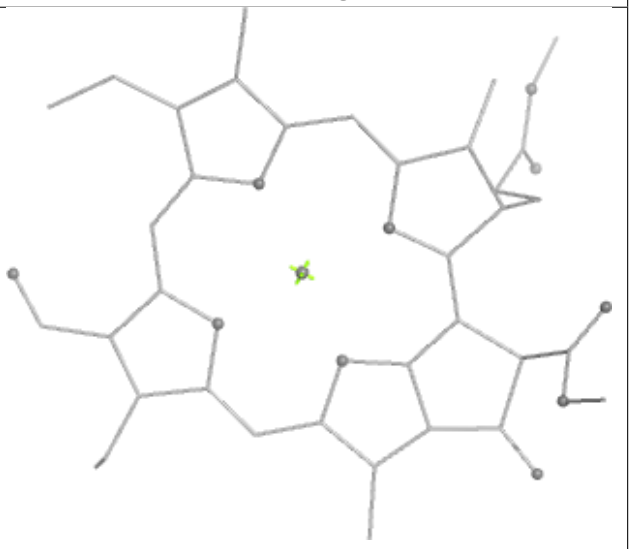
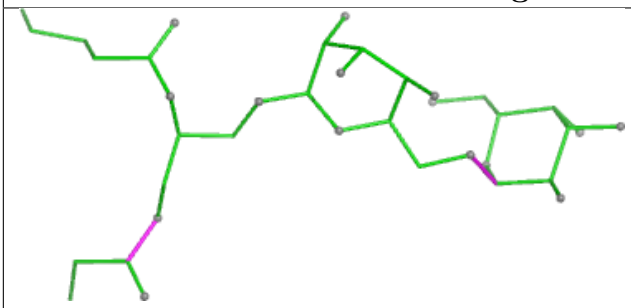


Rings

Ligand DGD B 5002



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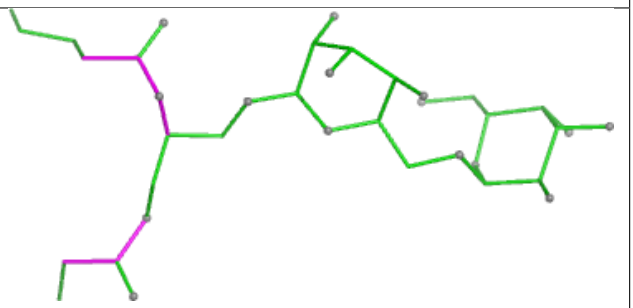

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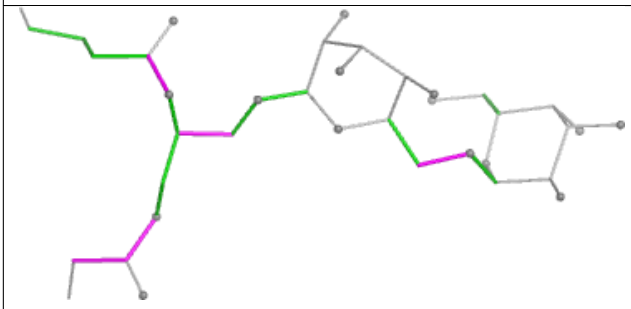

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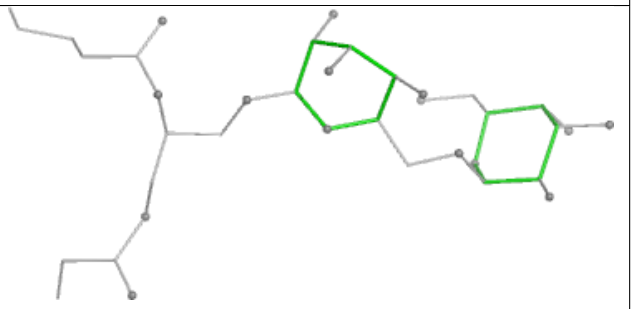
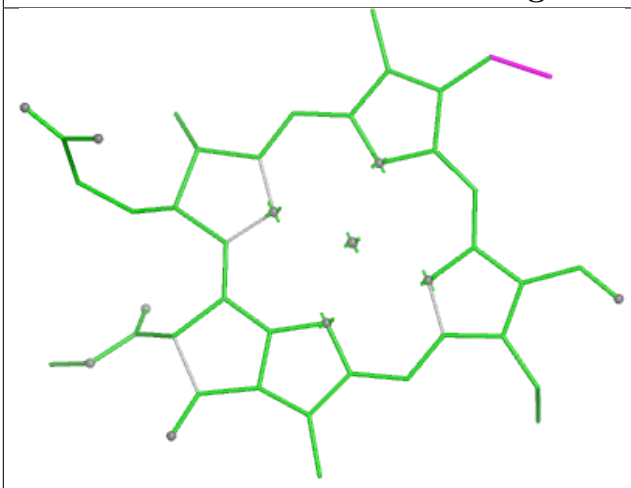


Rings

Ligand CHL 2 613



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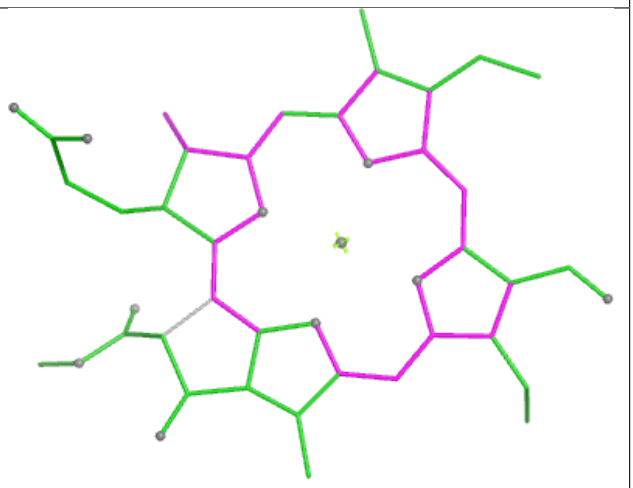

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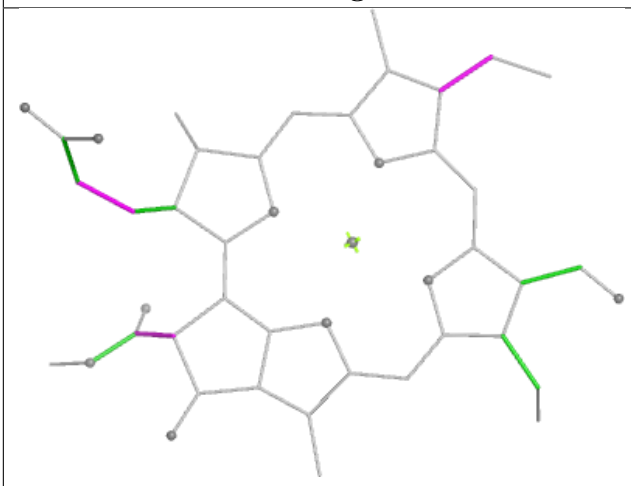

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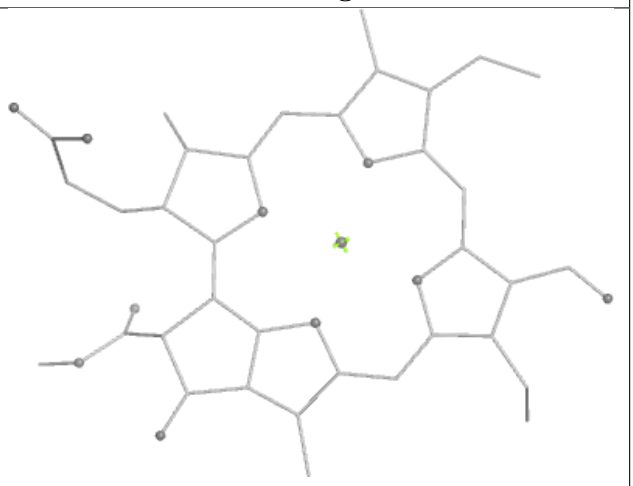
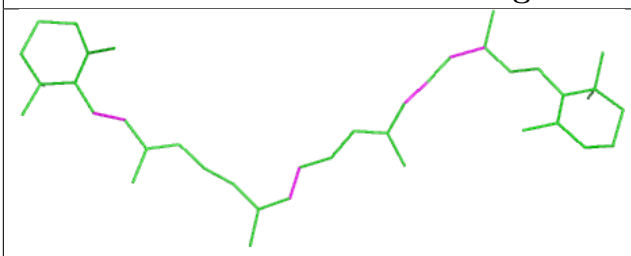


Rings

Ligand BCR A 4006



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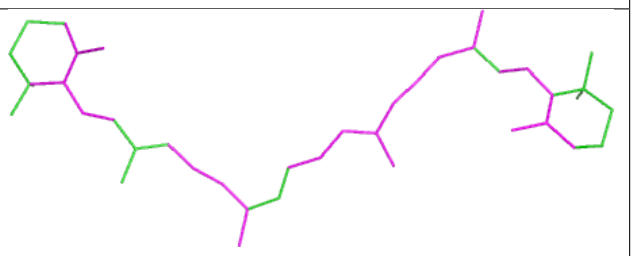

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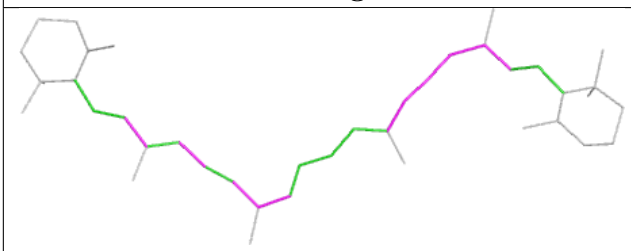

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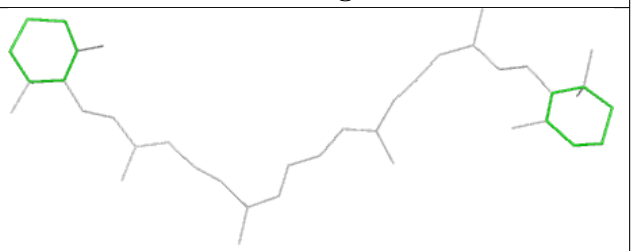
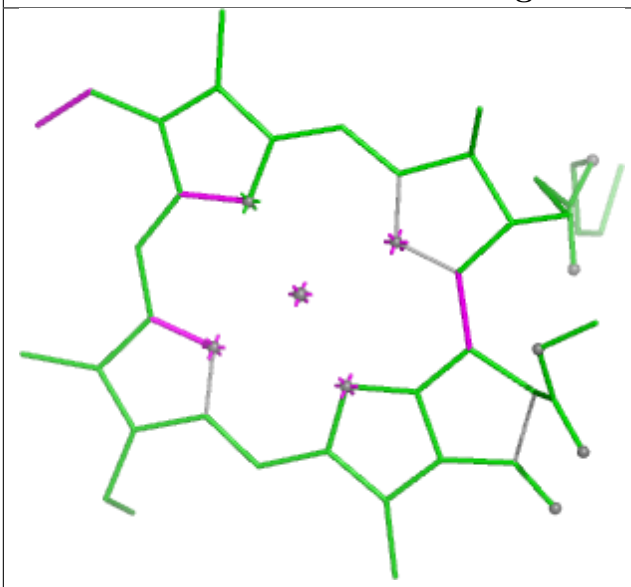


Rings

Ligand CLA B 1225



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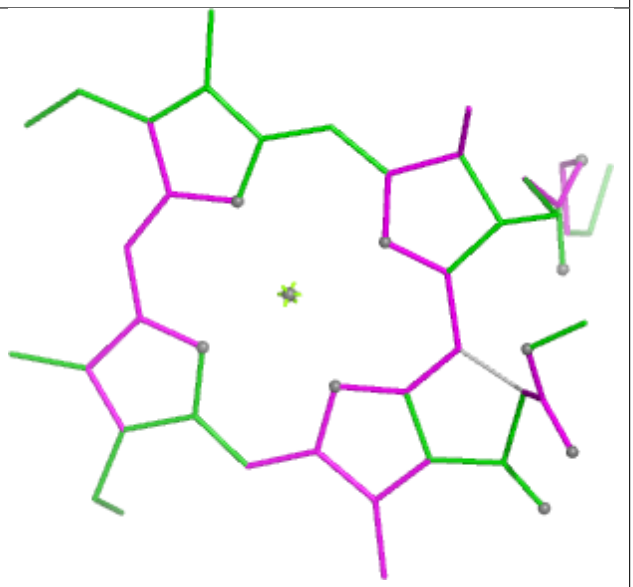

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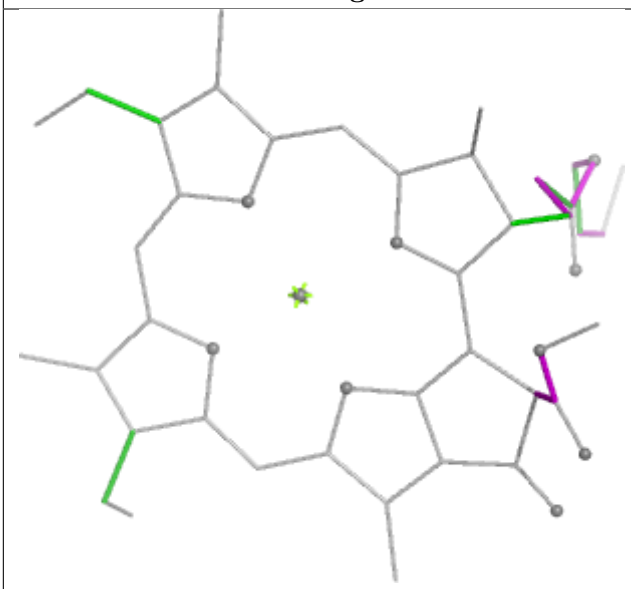

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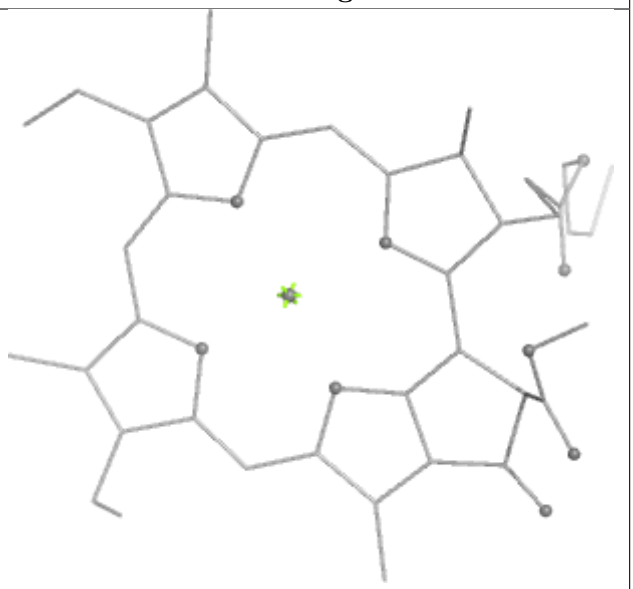
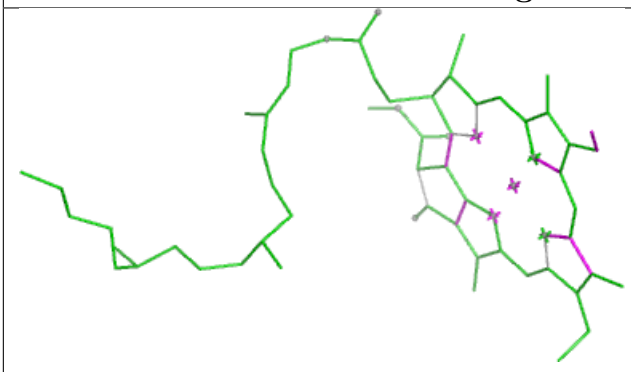


Rings

Ligand CLA B 1021



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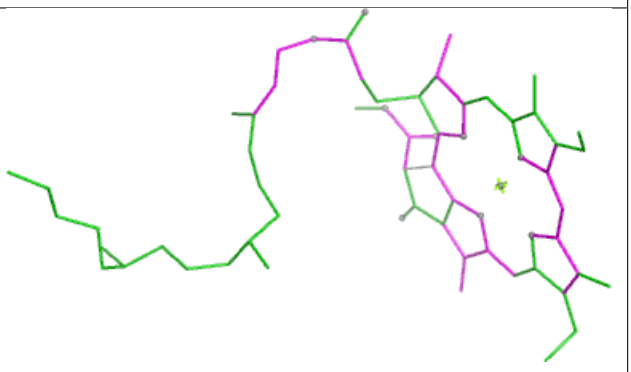

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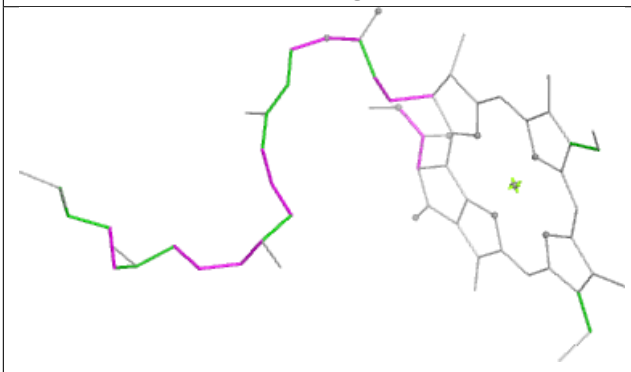
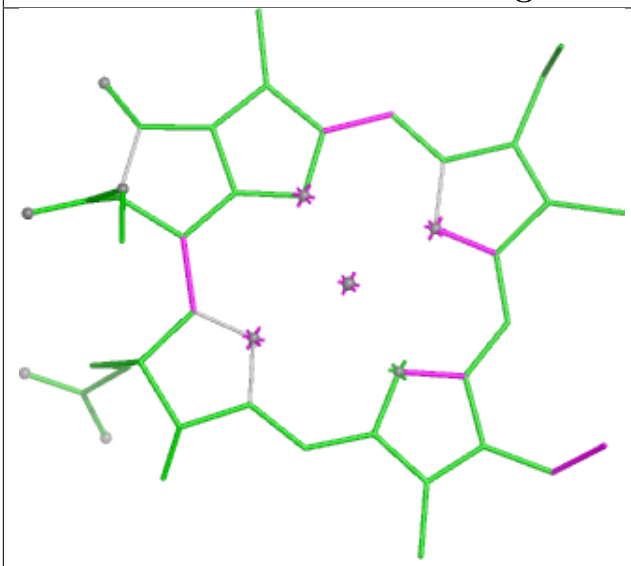


Torsions



Rings

Ligand CLA B 1227



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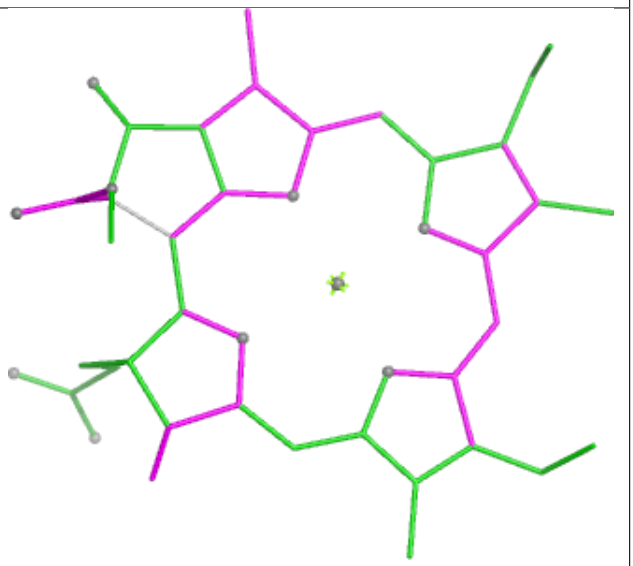

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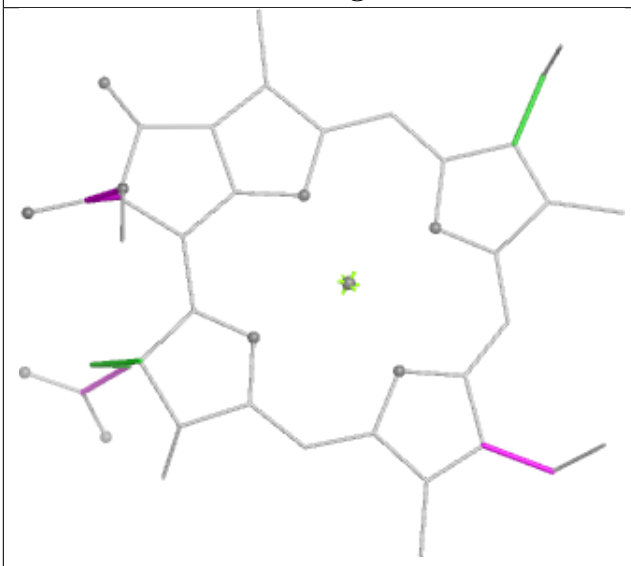

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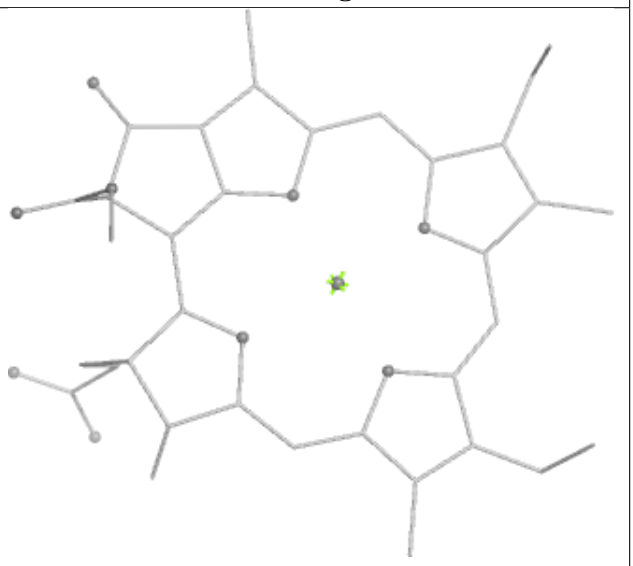
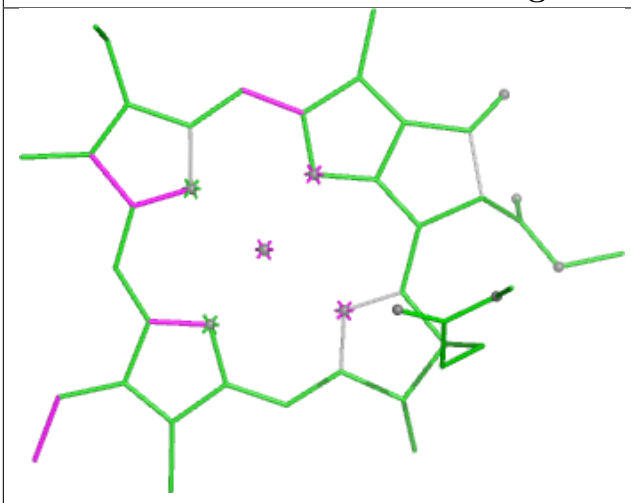


Rings

Ligand CLA 3 611



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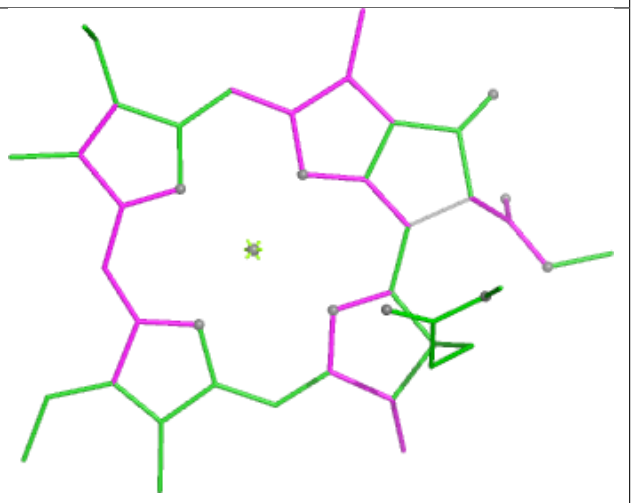

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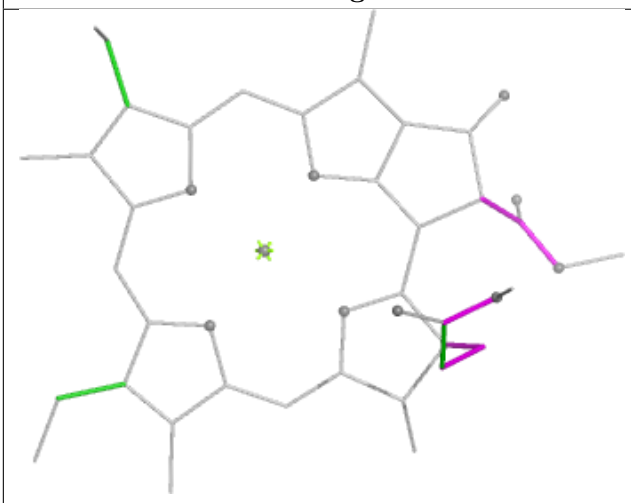

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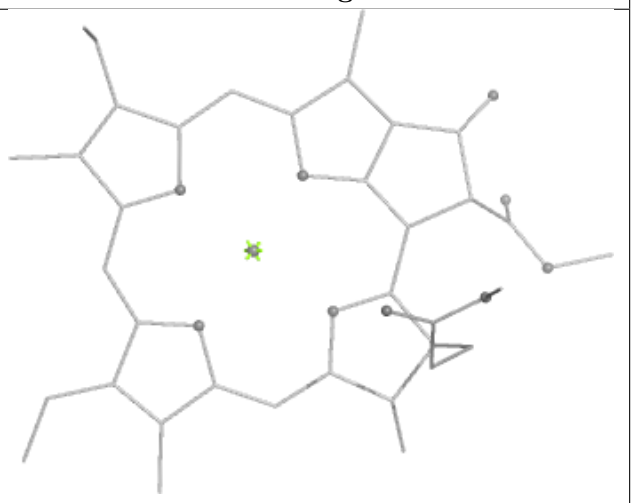
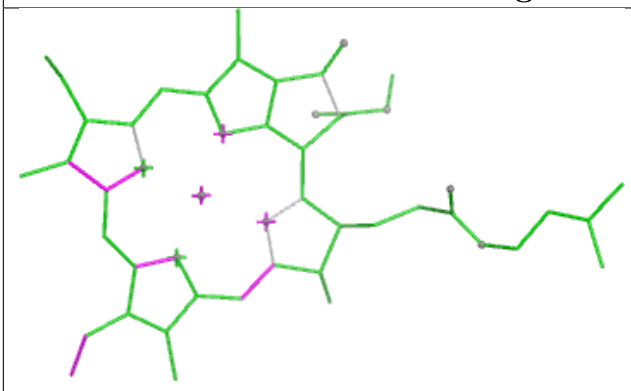


Rings

Ligand CLA B 1223



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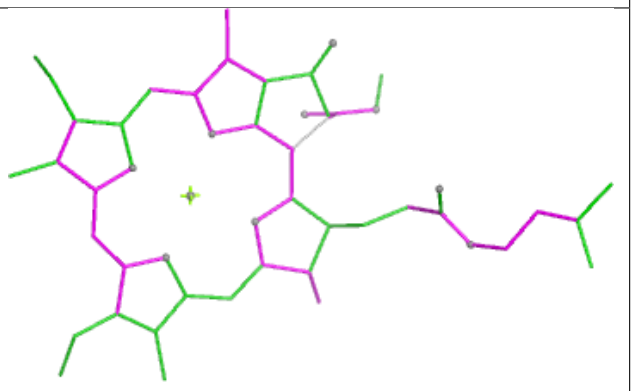

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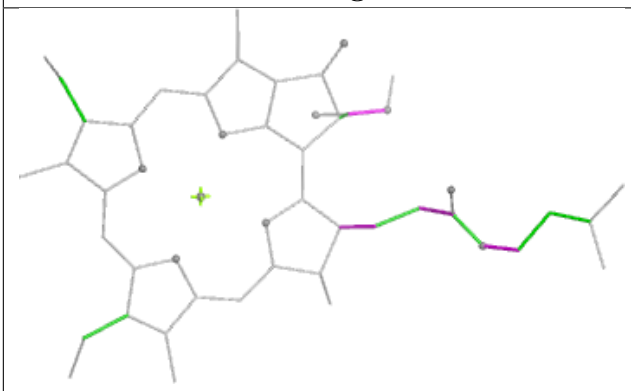

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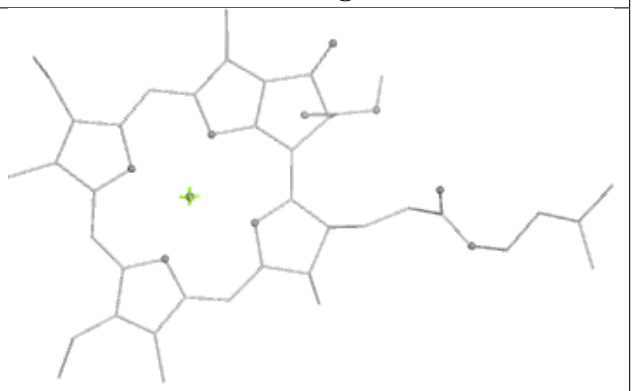
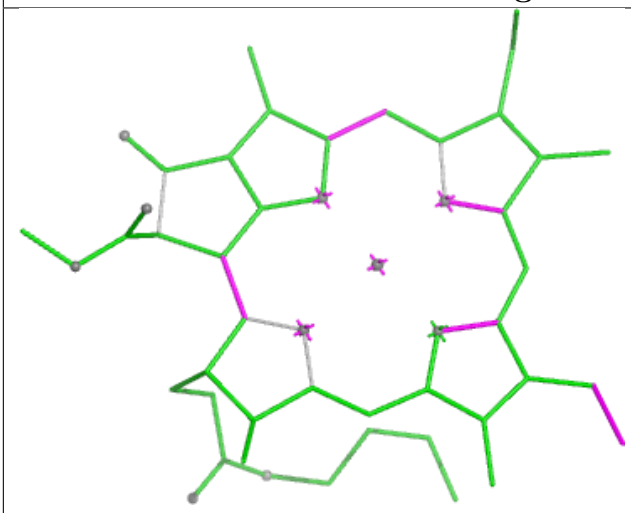


Rings

Ligand CLA A 1117



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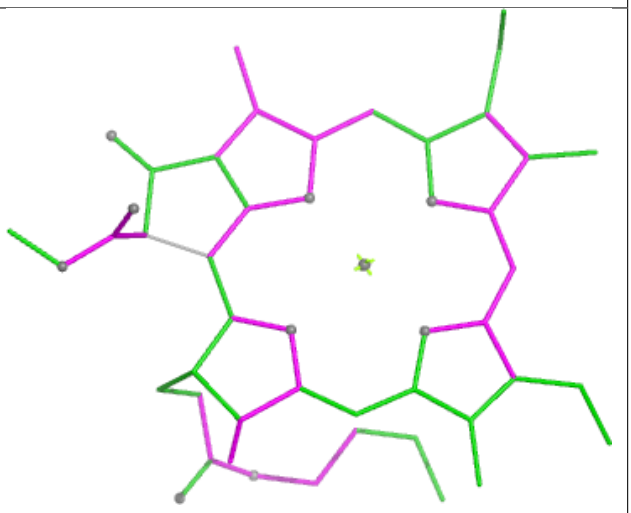

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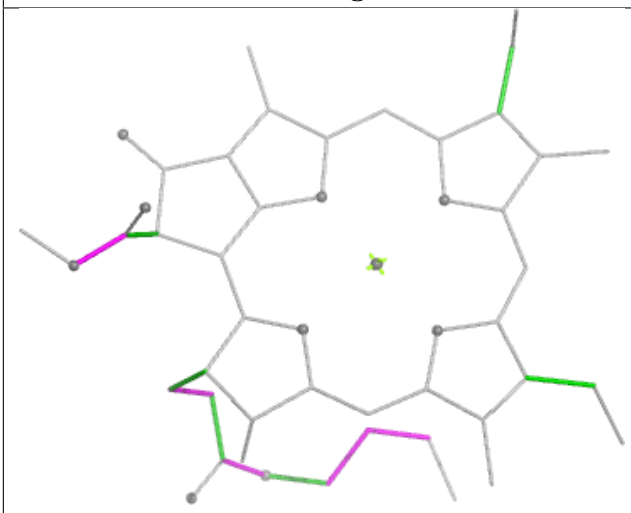

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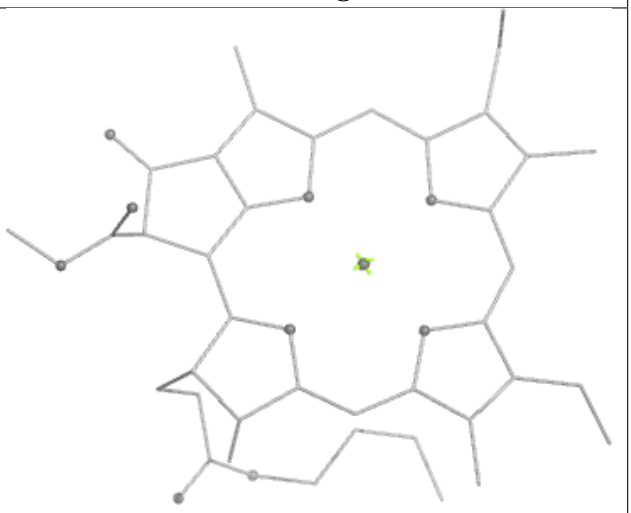
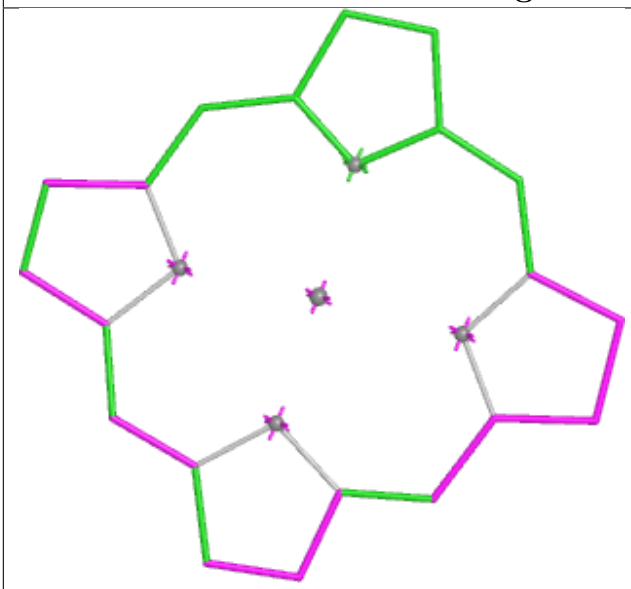


Rings

Ligand CLA B 1207



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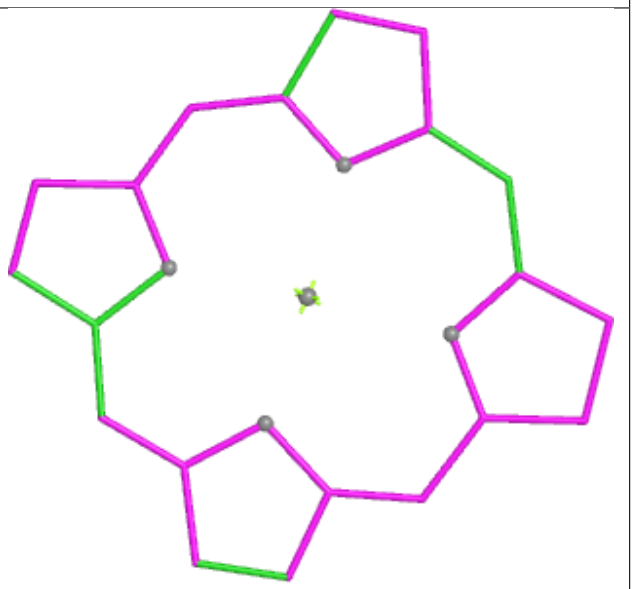
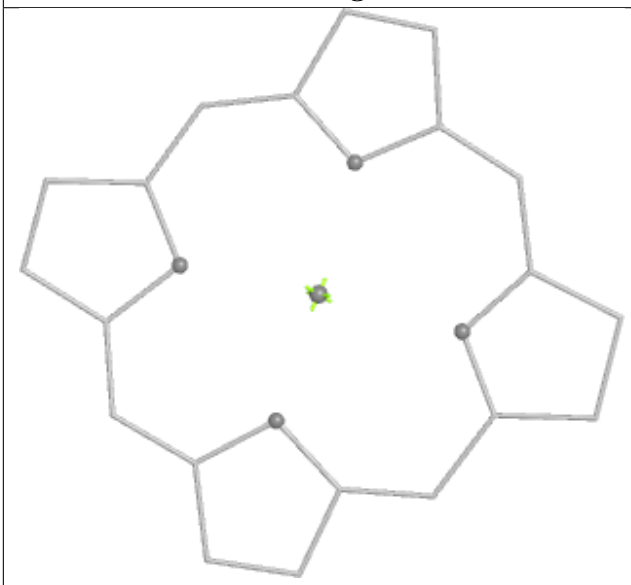


Bond angles



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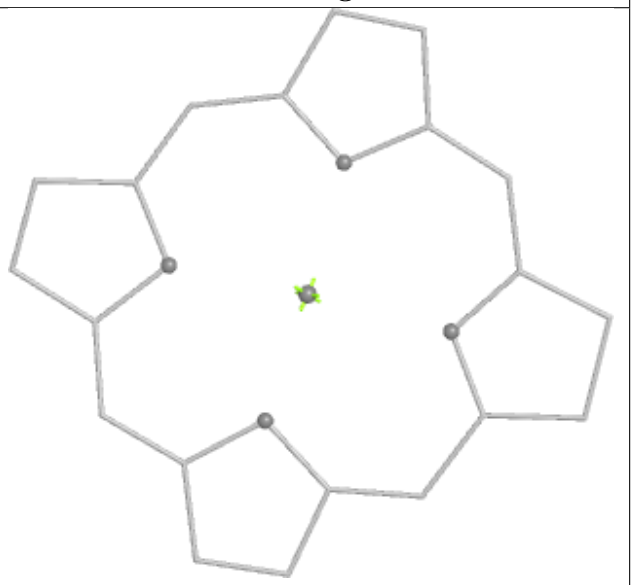
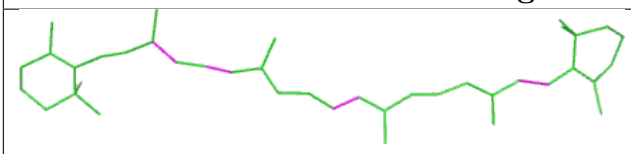


Rings

Ligand BCR J 4001



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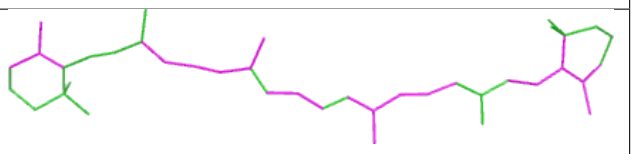
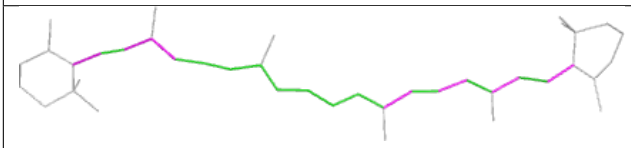


Bond angles



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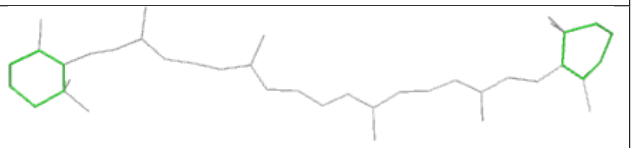
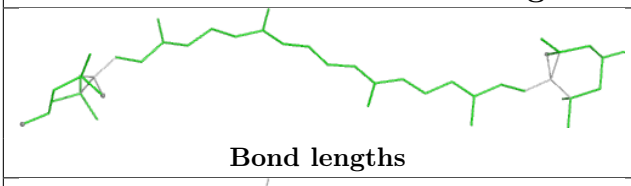


Rings

Ligand XAT 4 502



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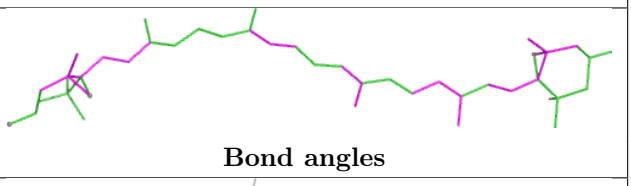
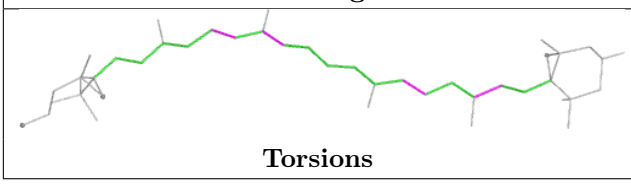


Bond angles



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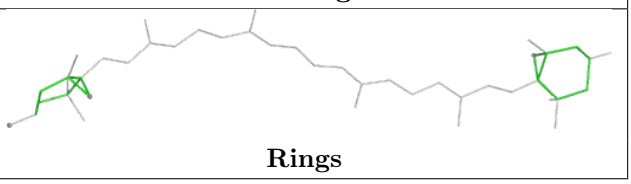
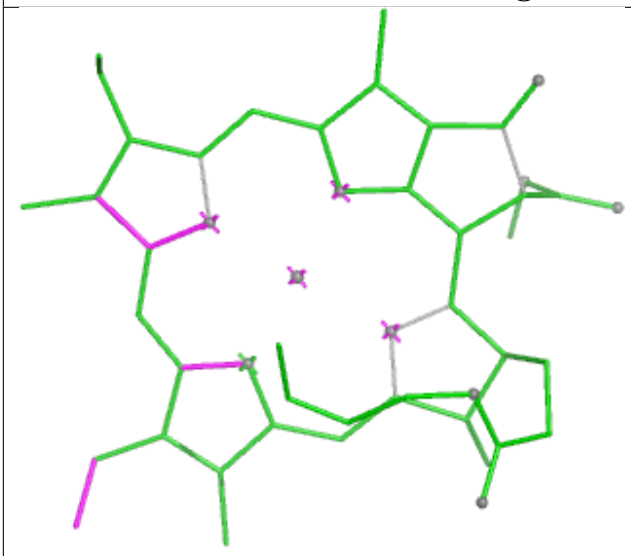


Rings

Ligand CLA B 1224



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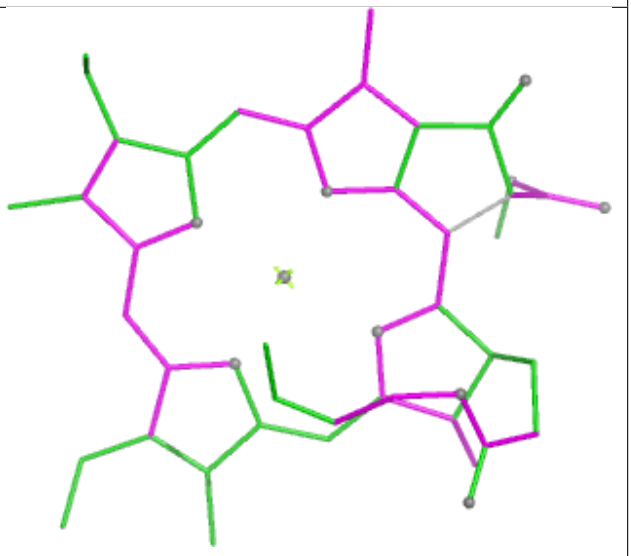
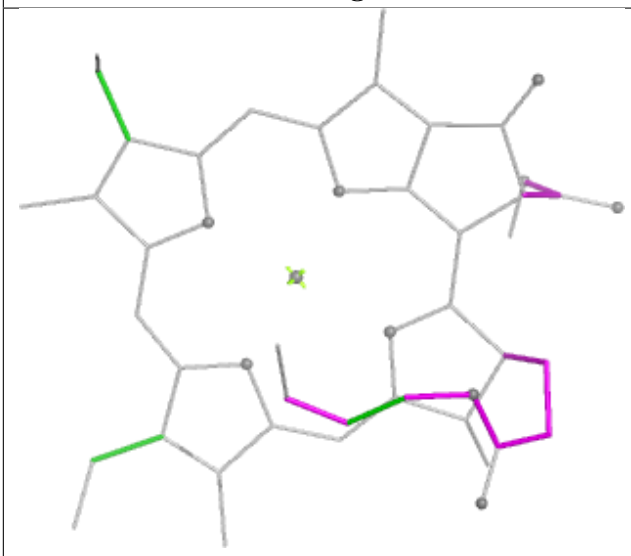


Bond angles



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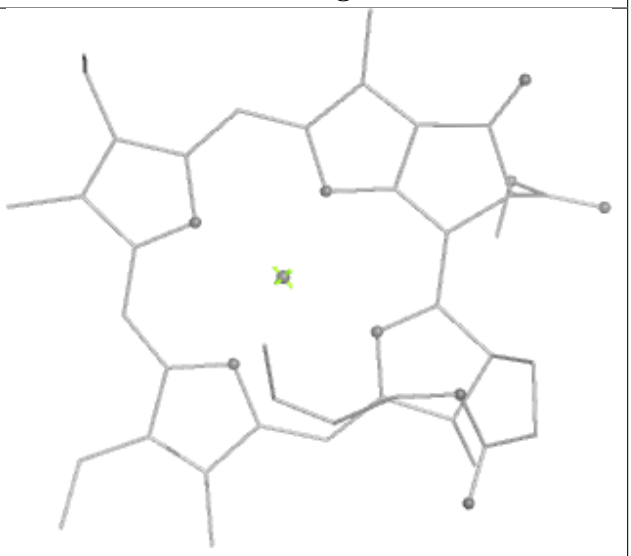
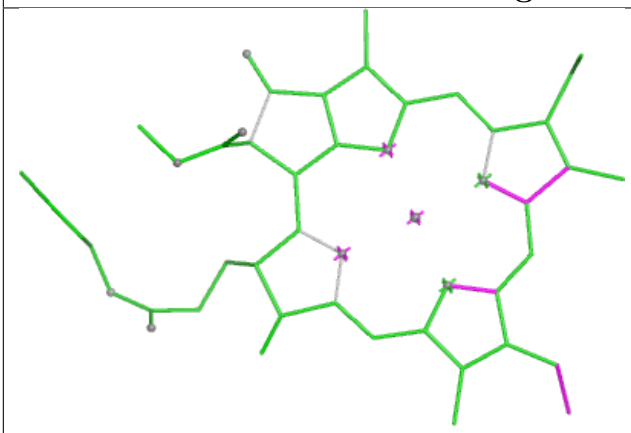
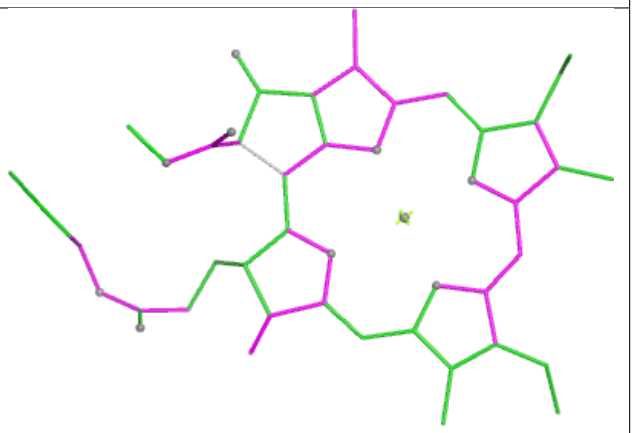


Rings

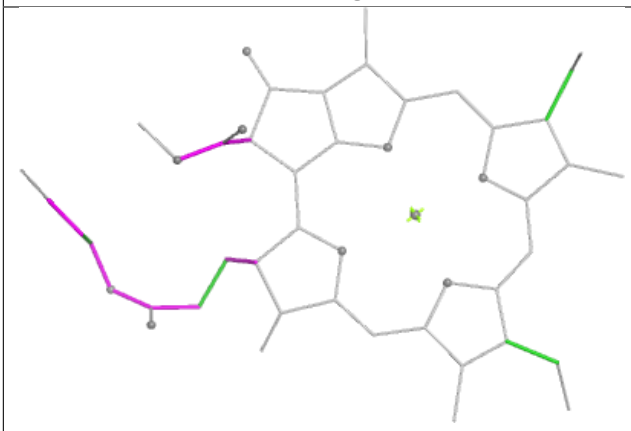
Ligand CLA B 1202



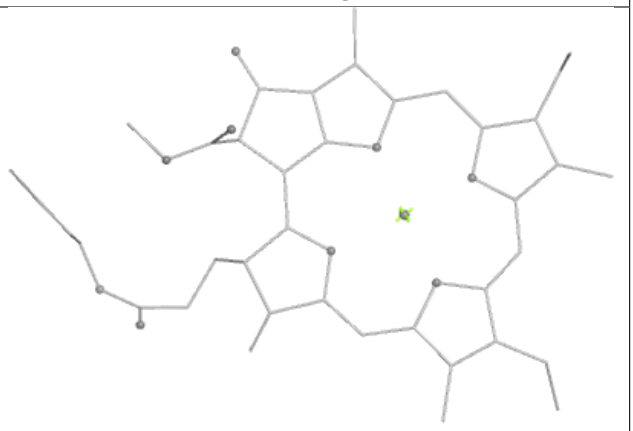
Bond lengths



Bond angles

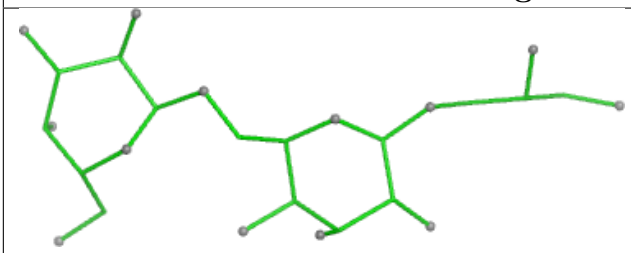


Torsions



Rings

Ligand DGD J 5001



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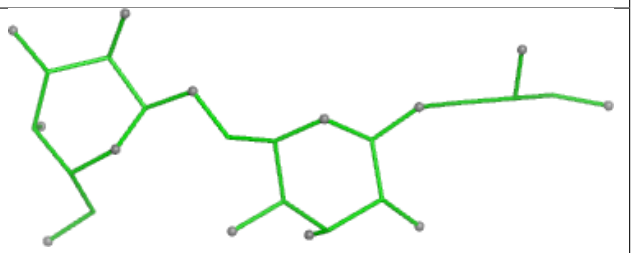

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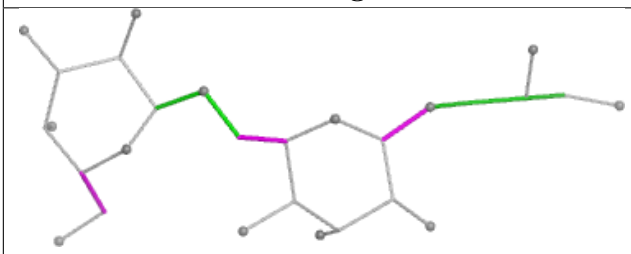

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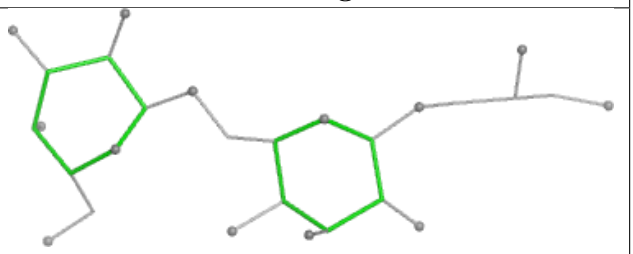
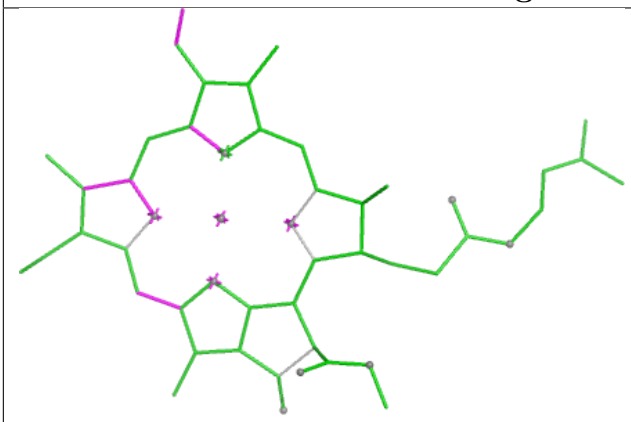


Rings

Ligand CLA B 1022



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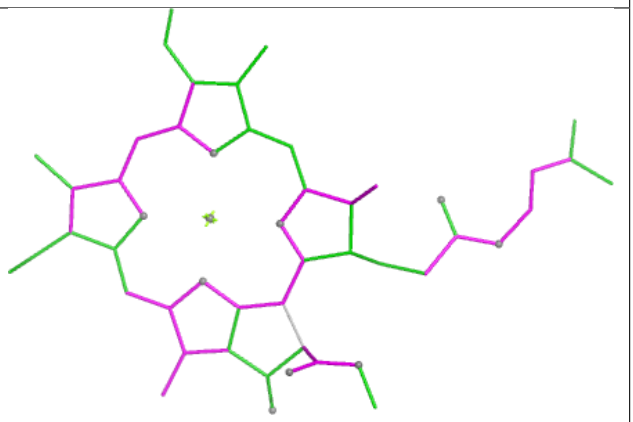

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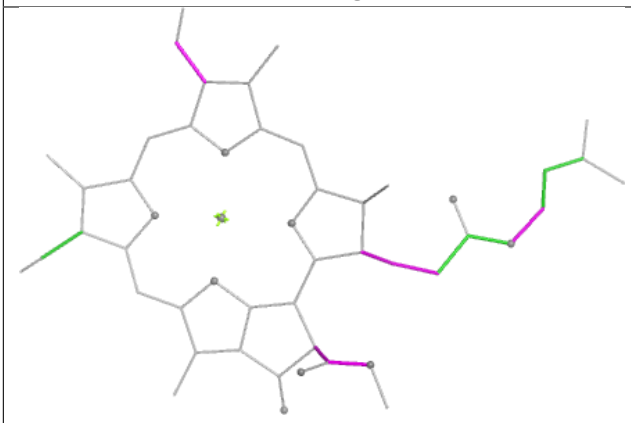

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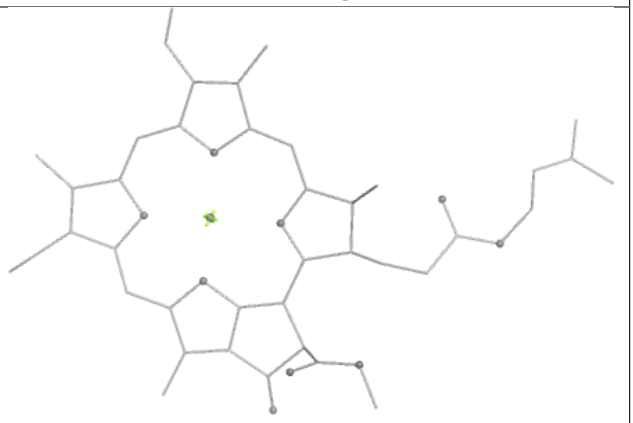
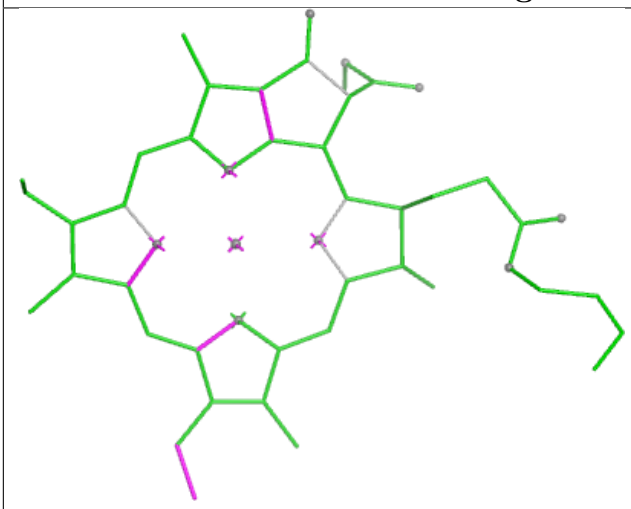


Rings

Ligand CLA B 1210



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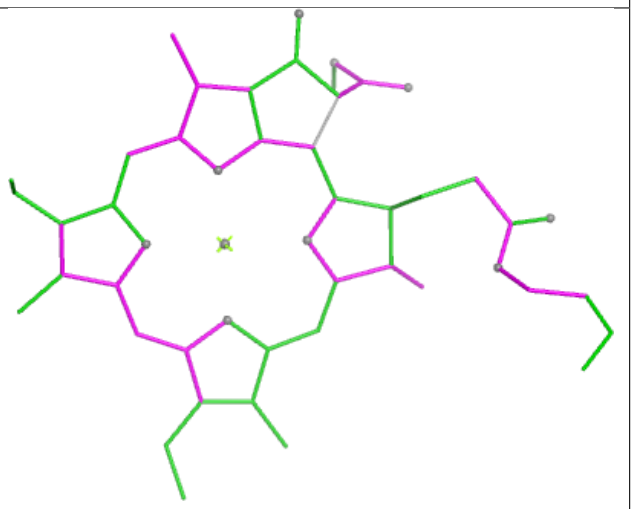

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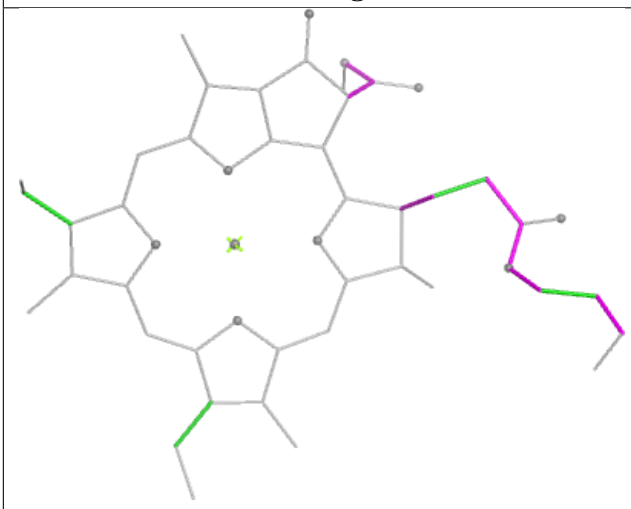

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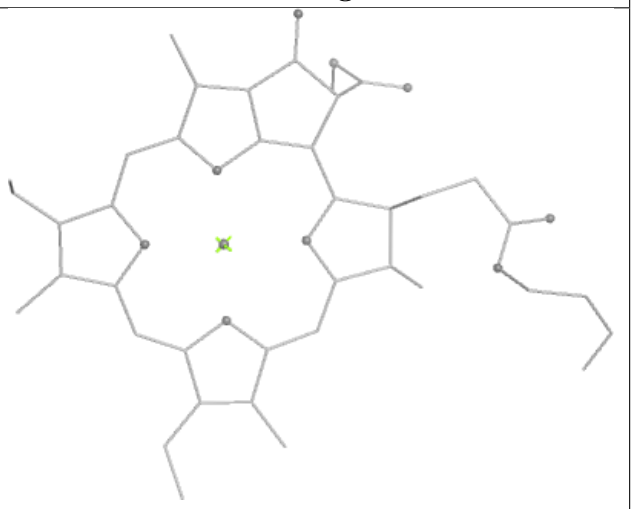
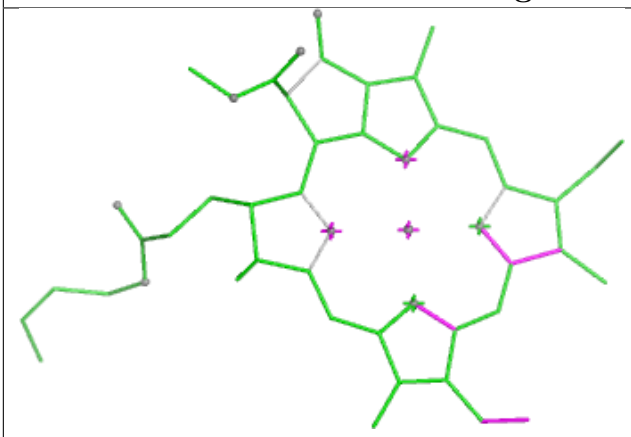


Rings

Ligand CLA A 1125



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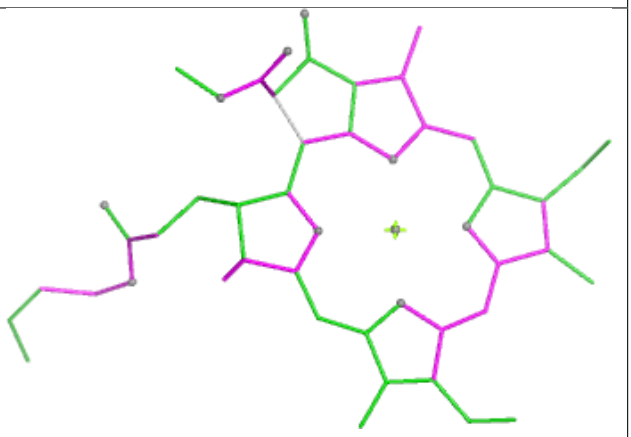

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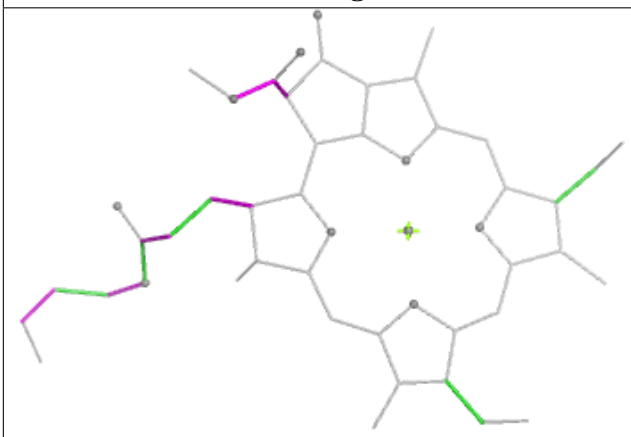

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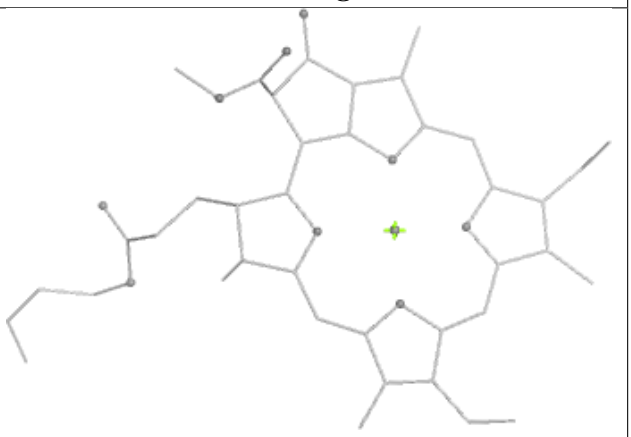
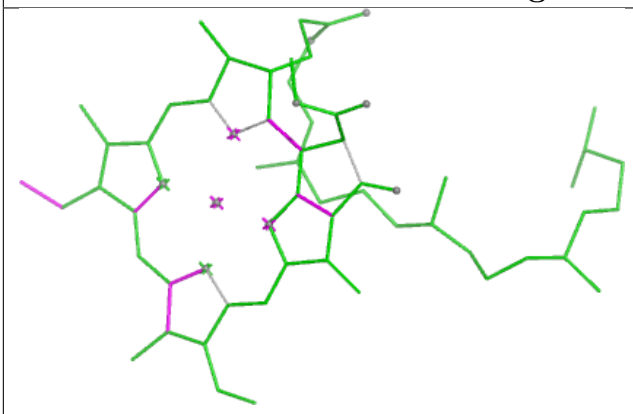


Rings

Ligand CLA 1 615



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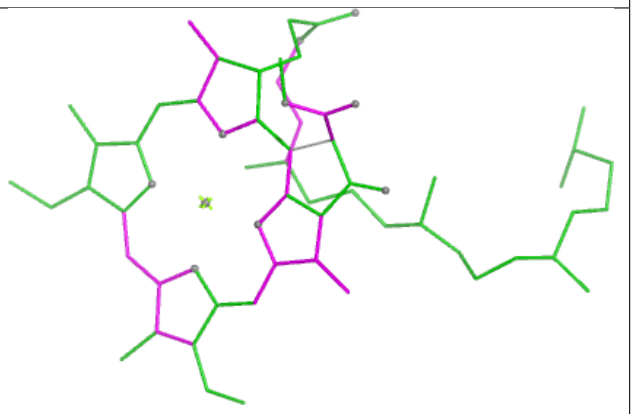

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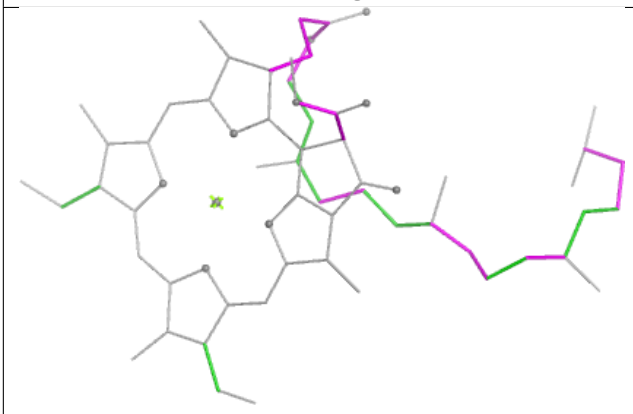

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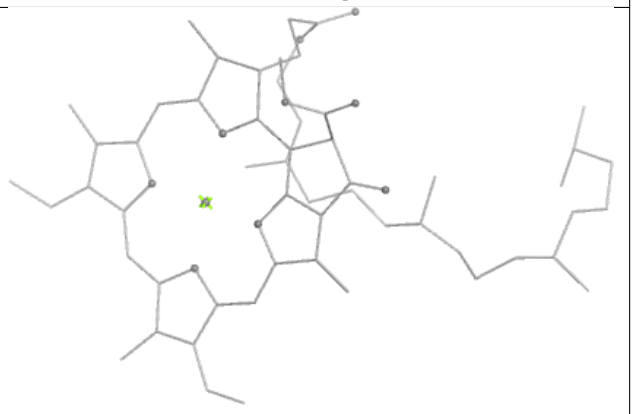
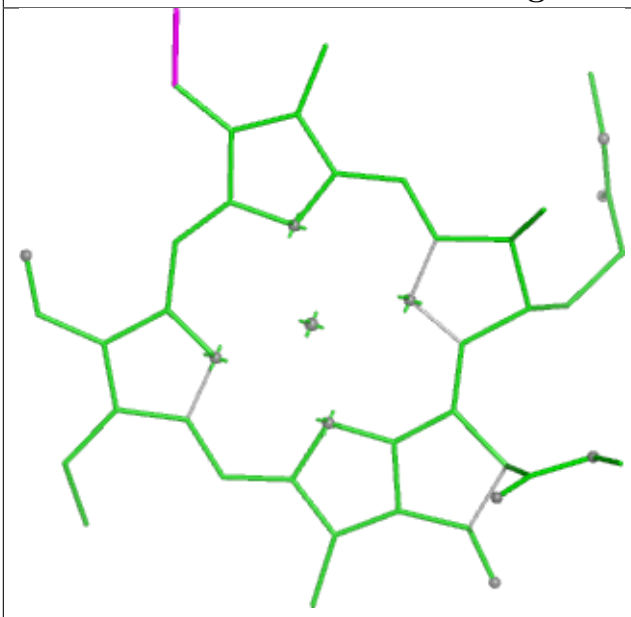


Rings

Ligand CHL 3 604



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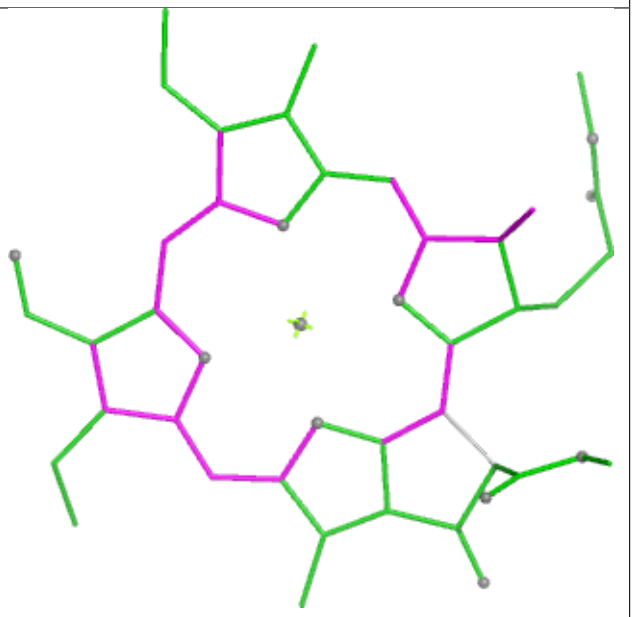

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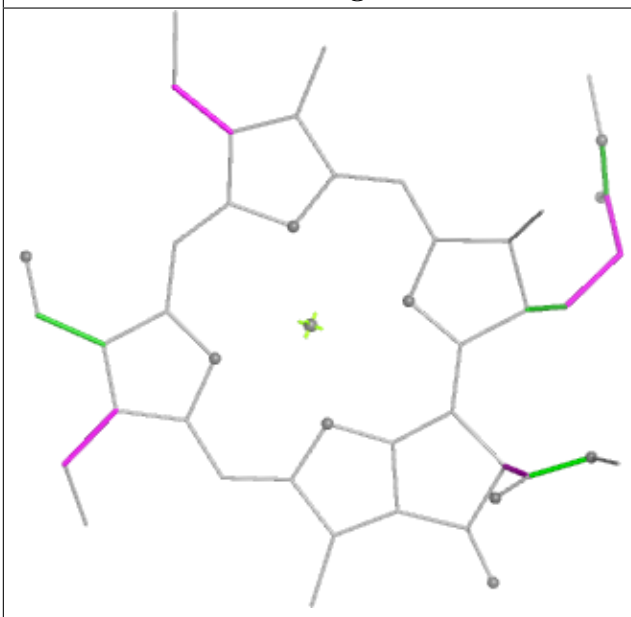

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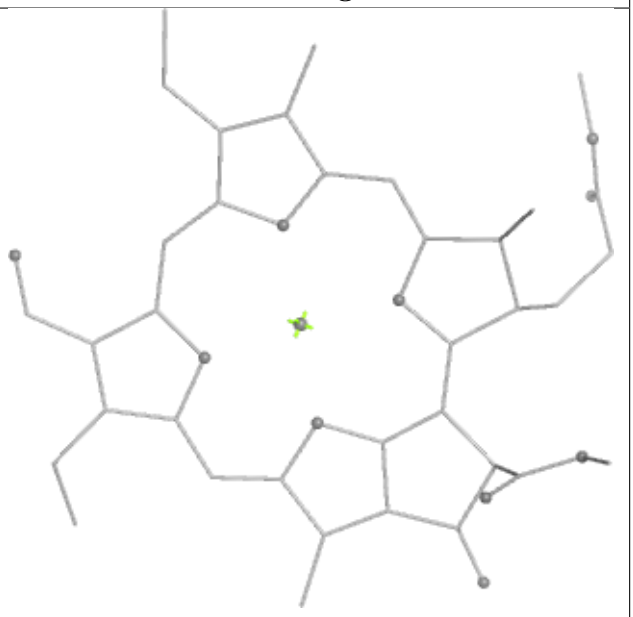

Rings

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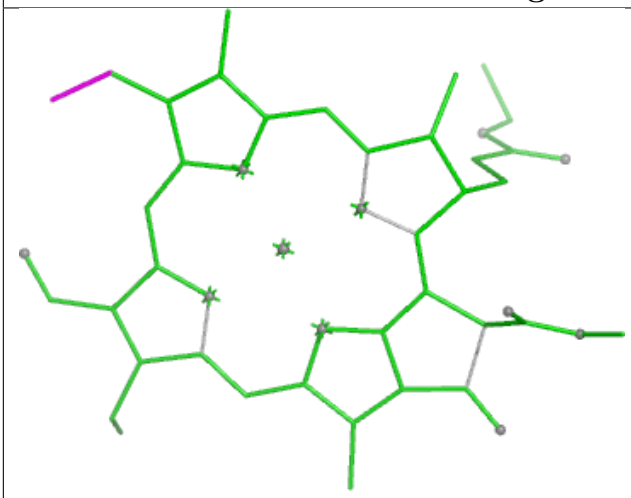

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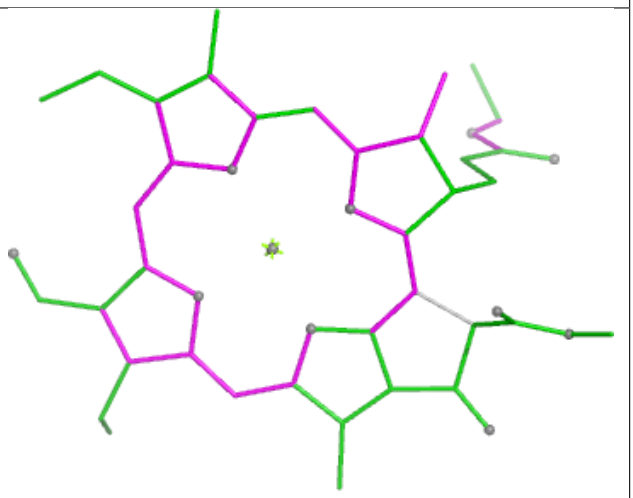

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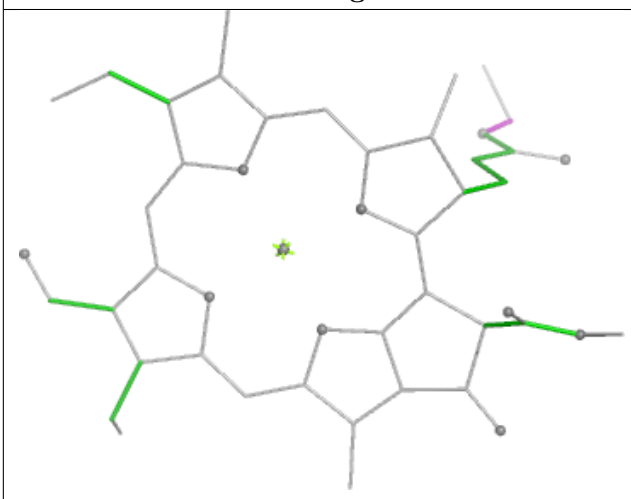

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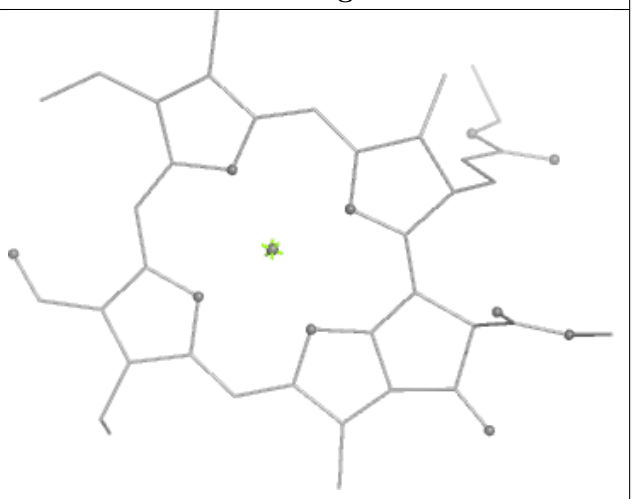
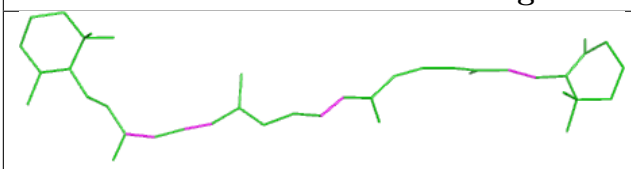


Rings

Ligand BCR J 4003



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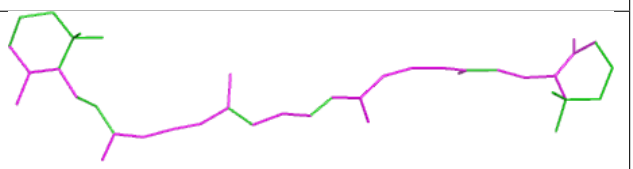
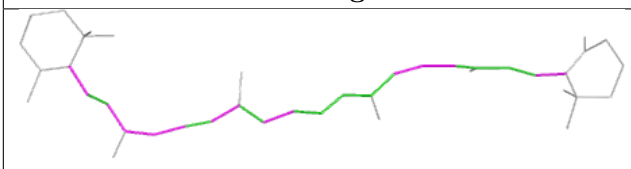


Bond angles



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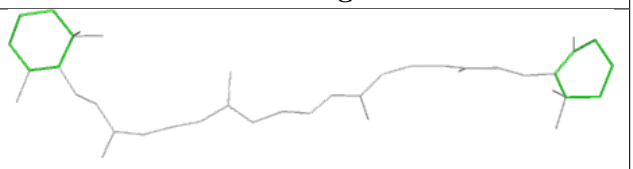
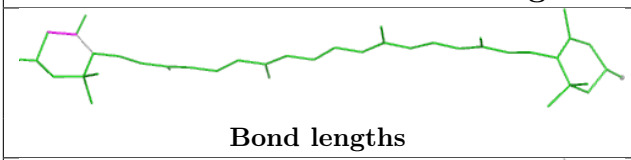


Rings

Ligand LUT 3 501



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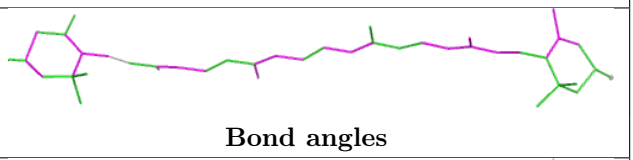

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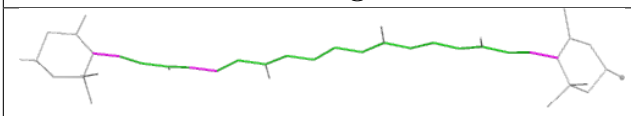

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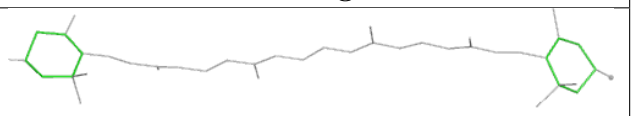
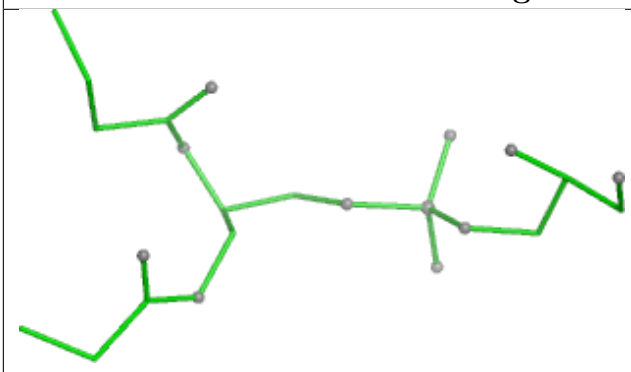


Rings

Ligand LHG A 5002



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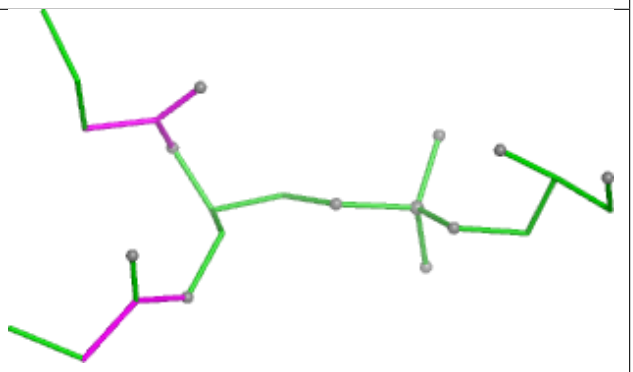

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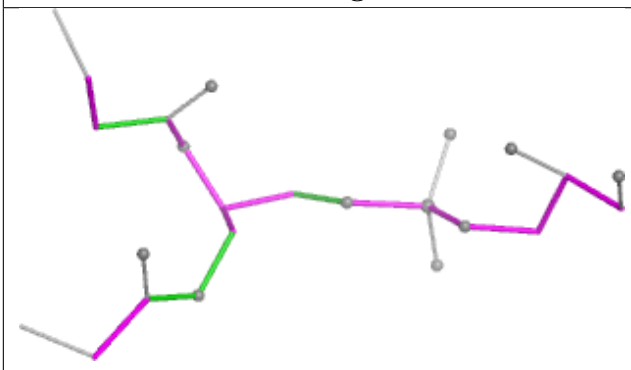

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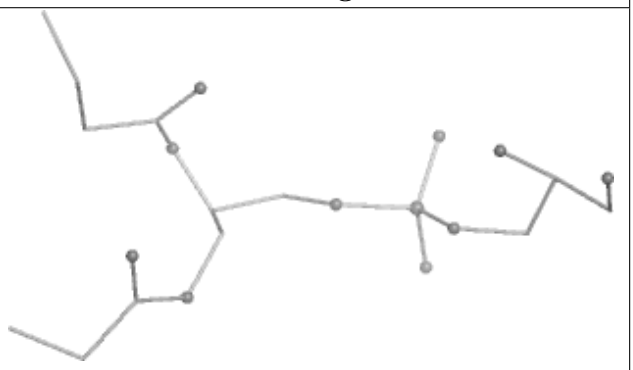
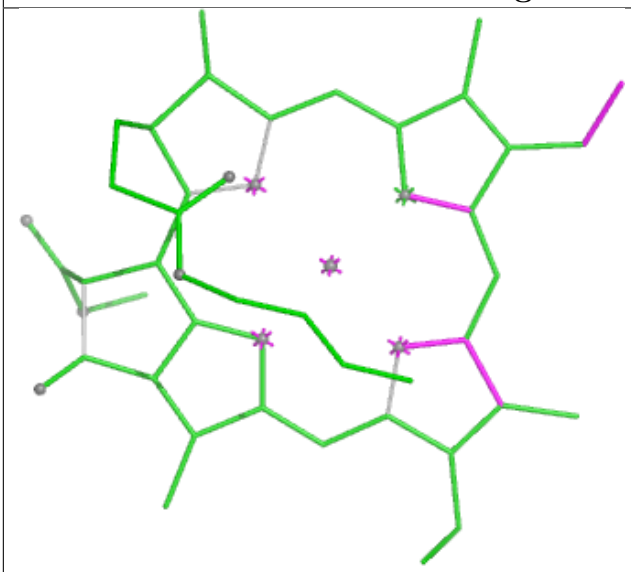


Rings

Ligand CLA A 1110



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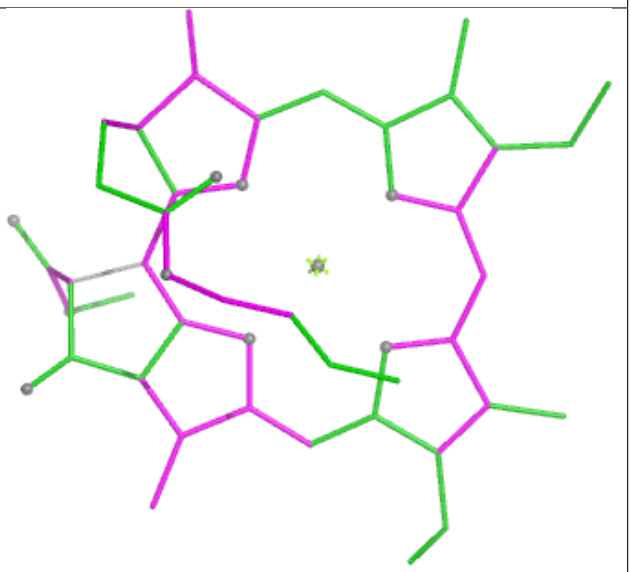
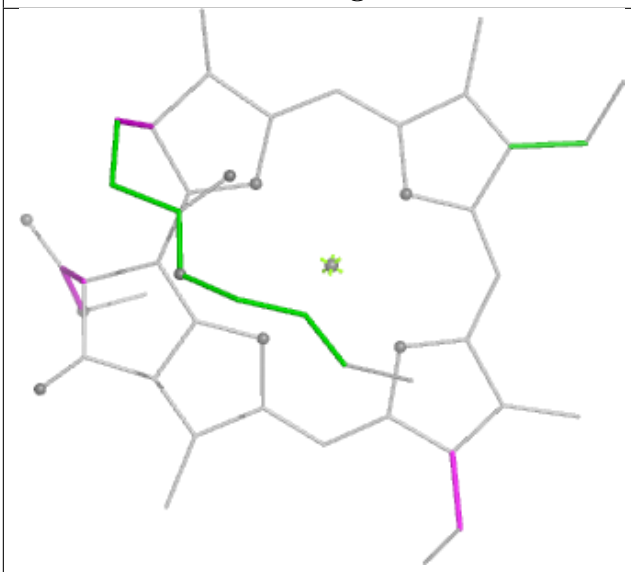


Bond angles



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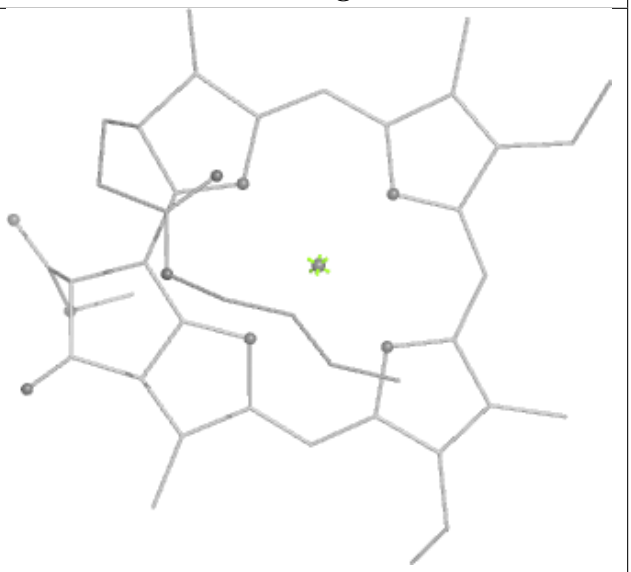
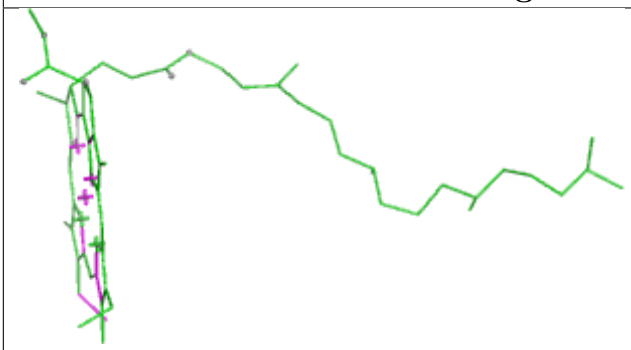


Rings

Ligand CLA B 1239



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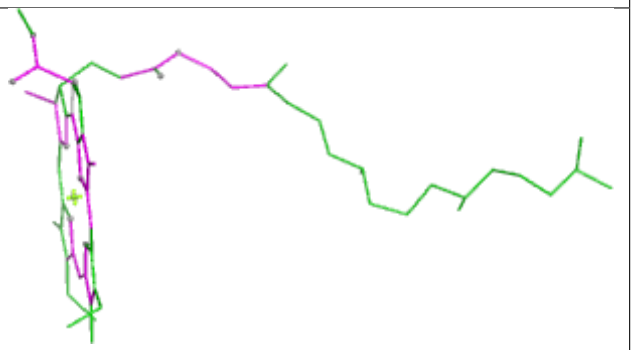
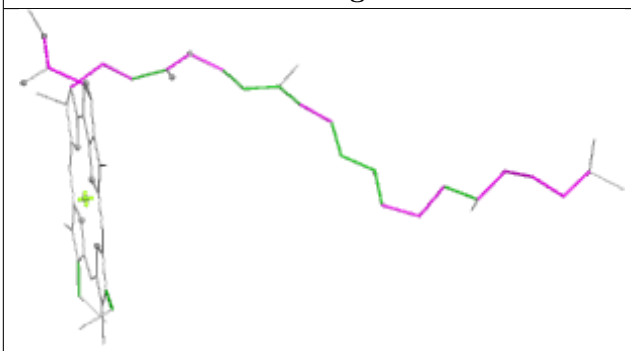


Bond angles



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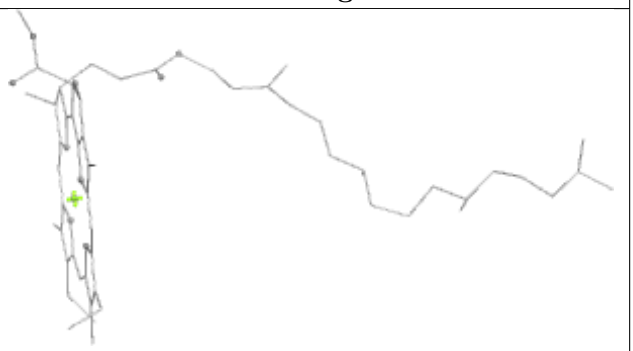
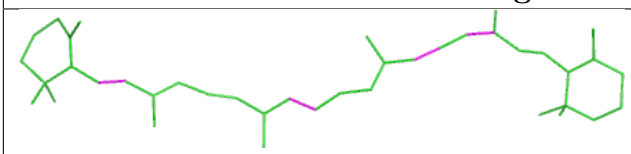


Rings

Ligand BCR B 4002



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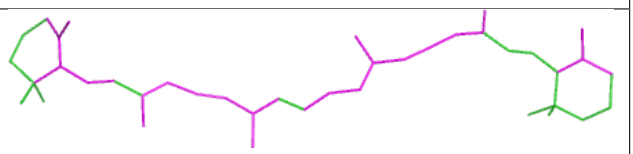
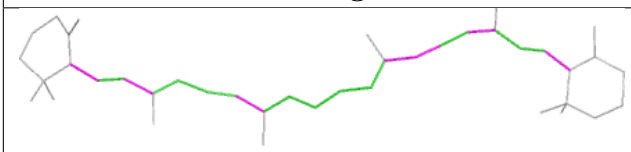


Bond angles



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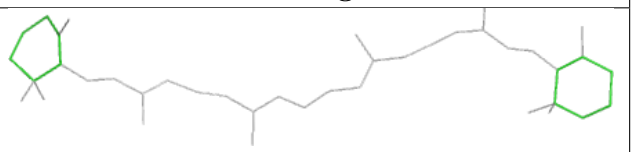
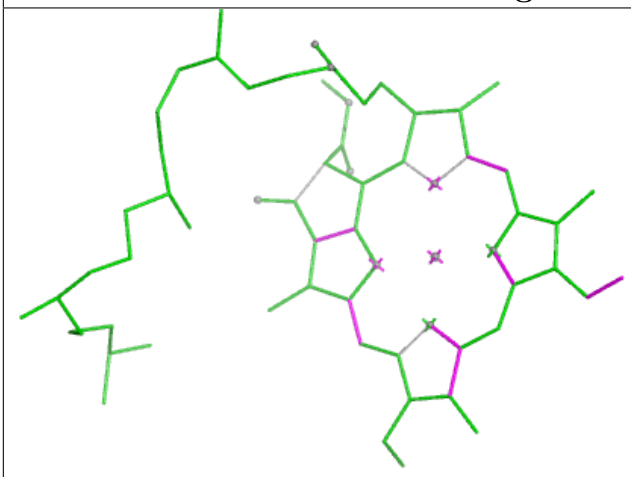
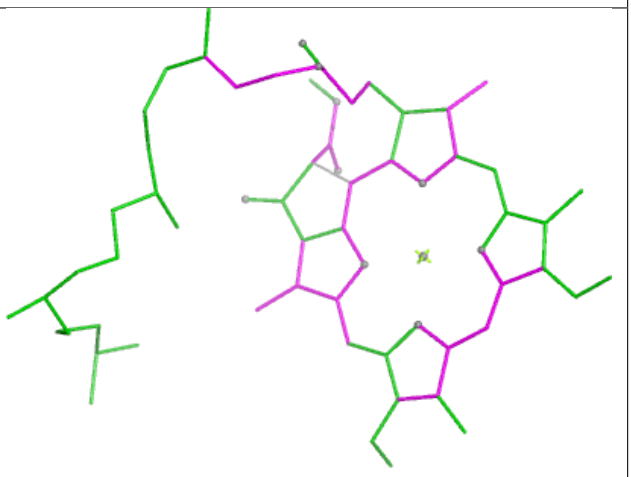


Rings

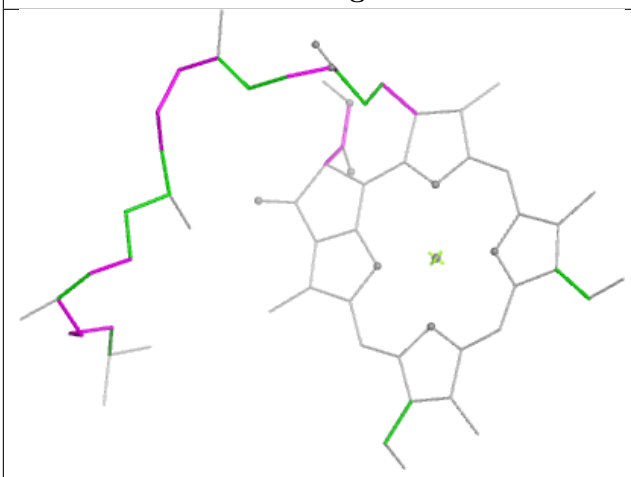
Ligand CLA B 1229



Bond lengths



Bond angles

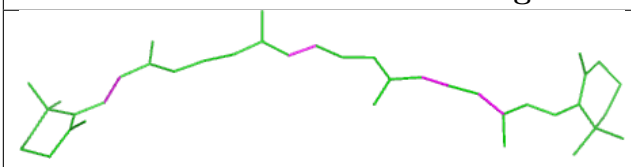


Torsions



Rings

Ligand BCR B 4006



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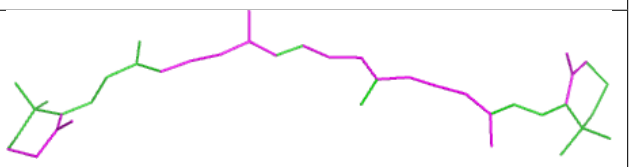
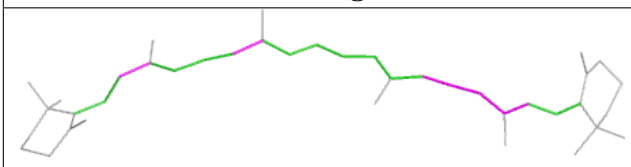
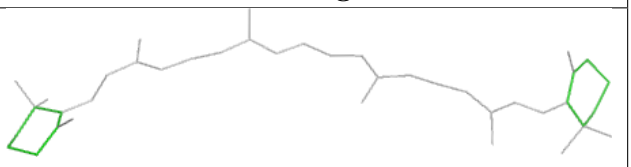


Bond angles

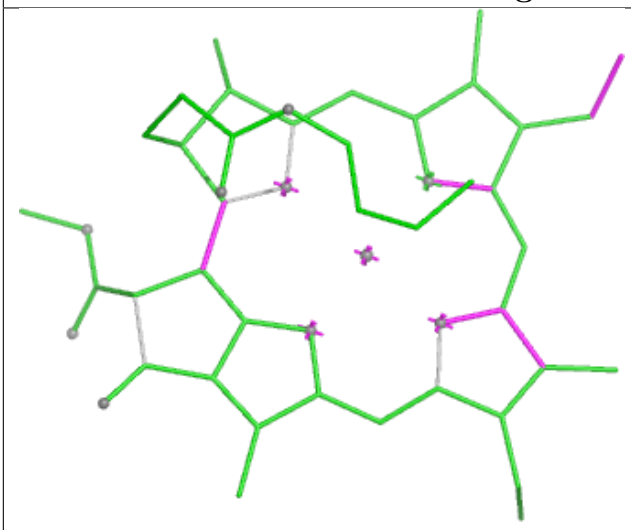


Torsions



Rings

Ligand CLA B 1205



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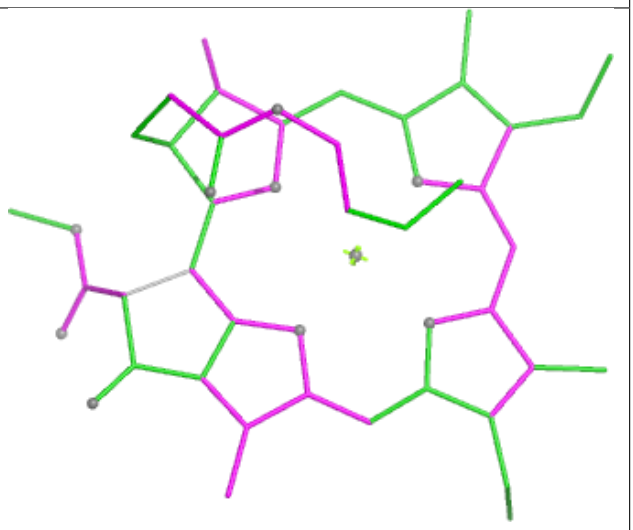

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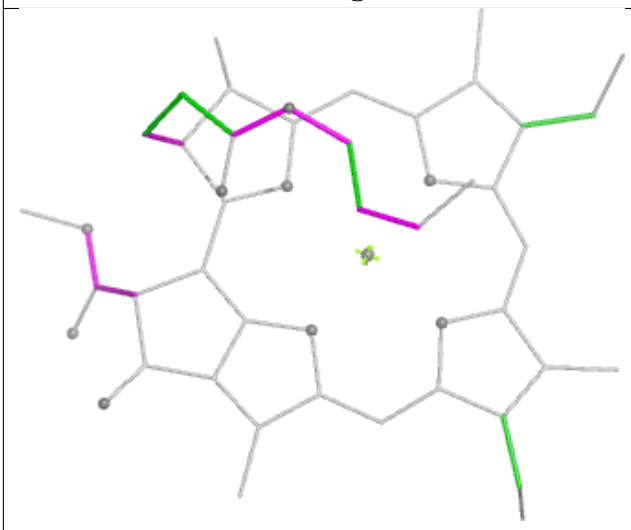

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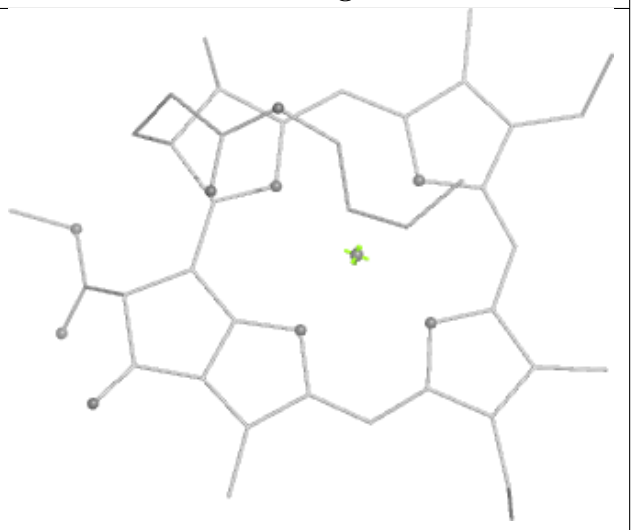
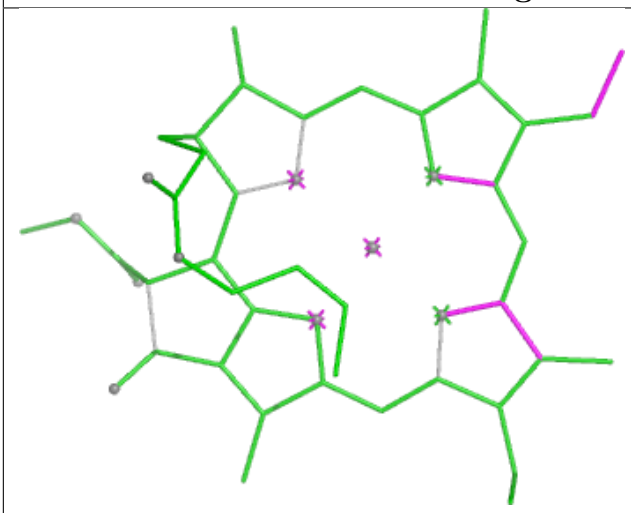


Rings

Ligand CLA A 1136



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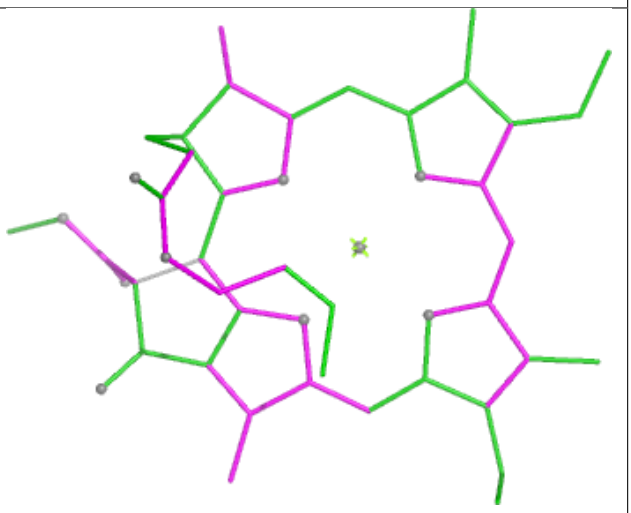

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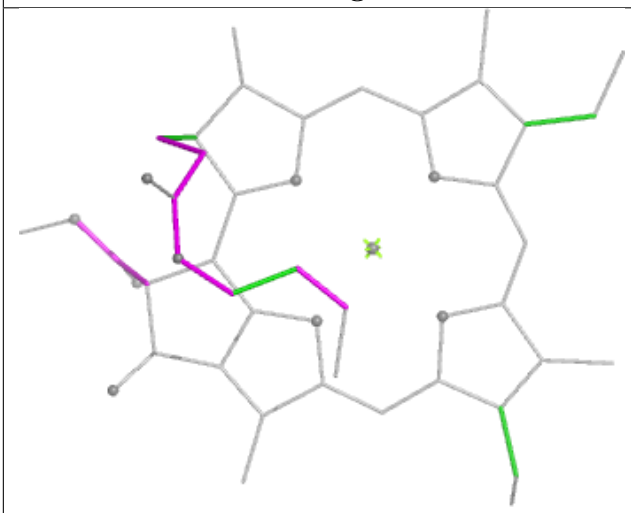

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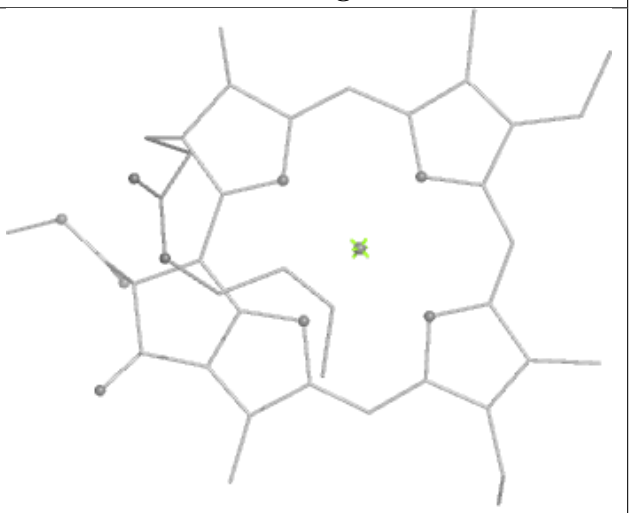
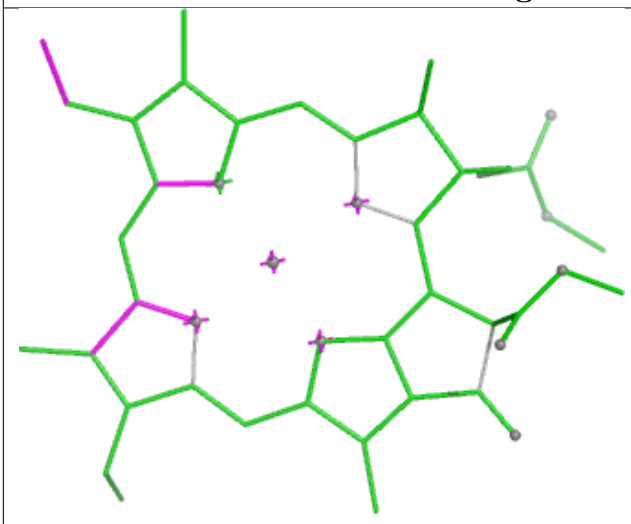


Rings

Ligand CLA B 1209



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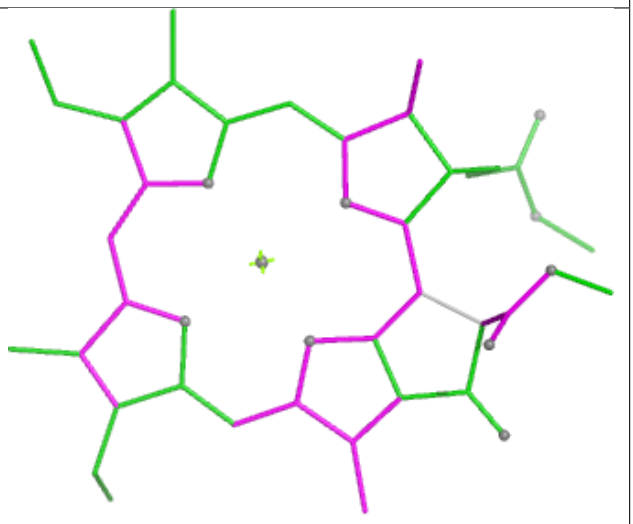

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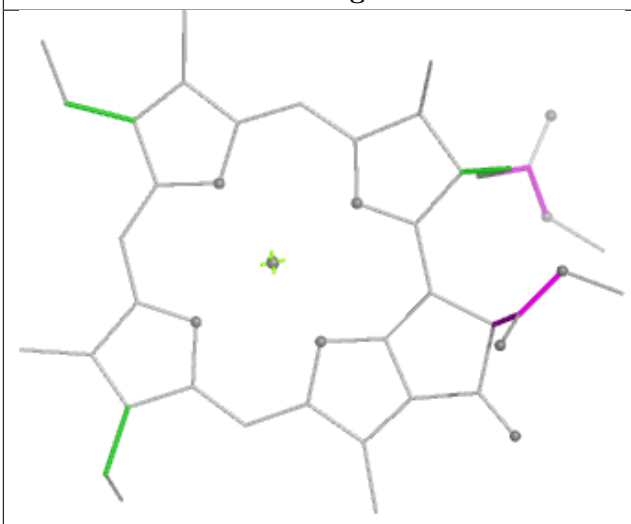

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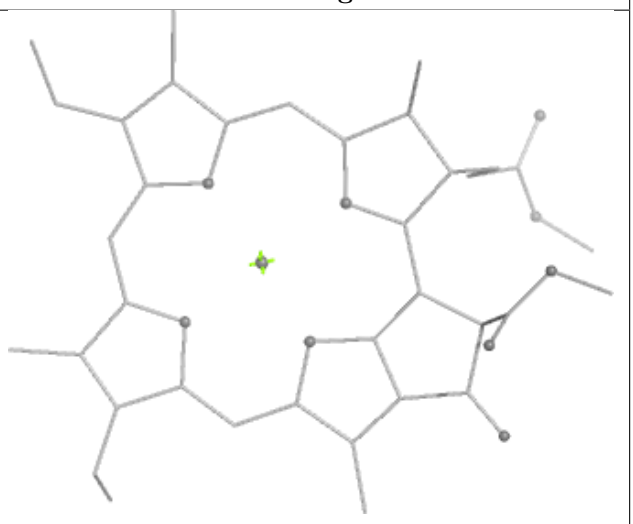
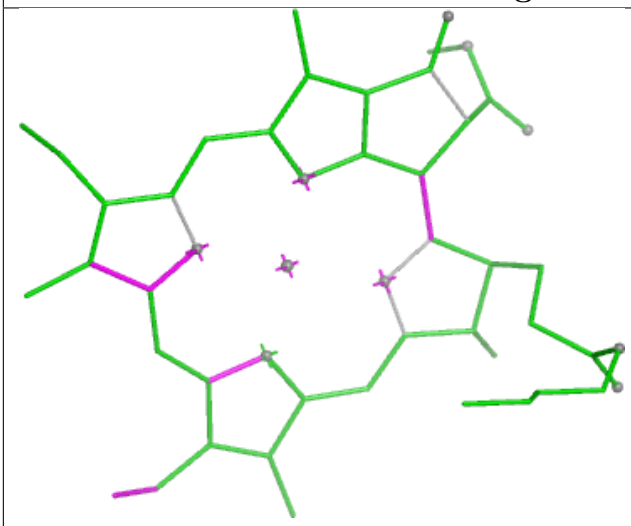


Rings

Ligand CLA A 1118



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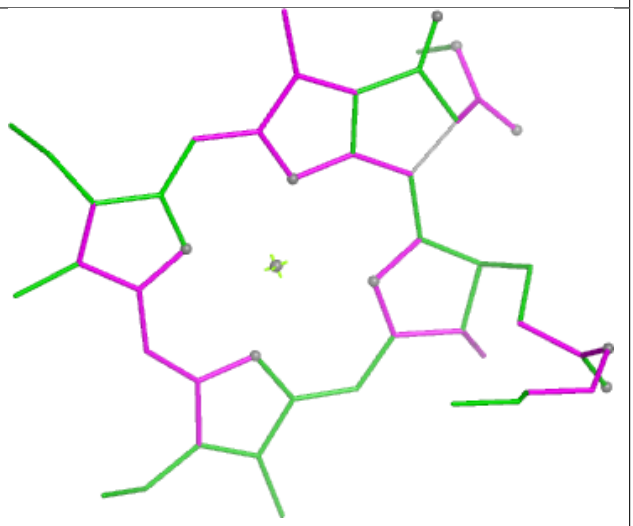

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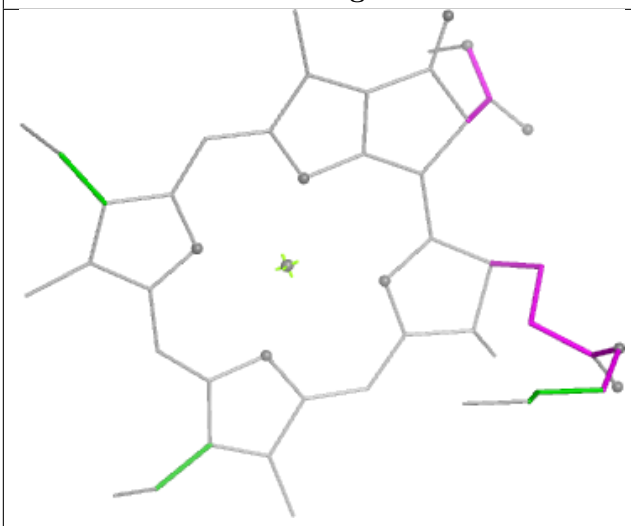
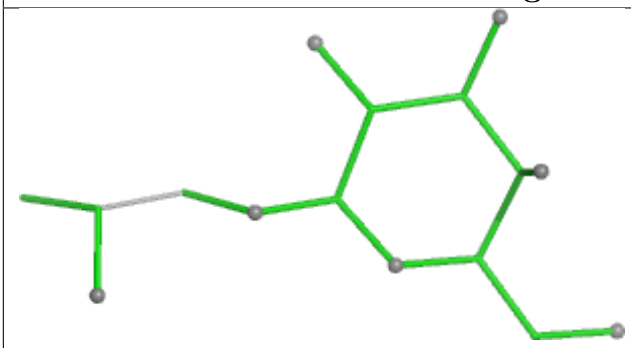


Torsions



Rings

Ligand LMG 2 803



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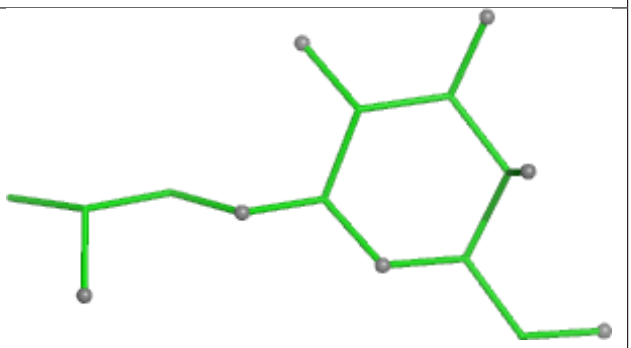

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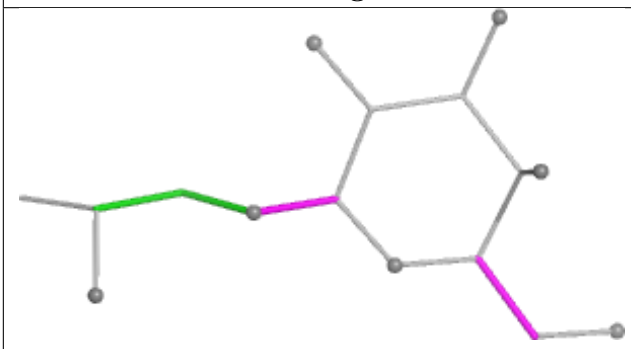

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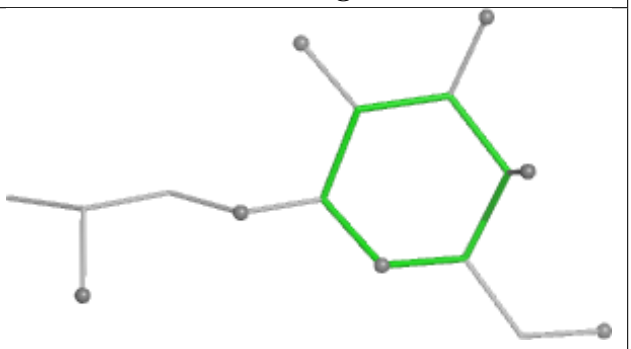
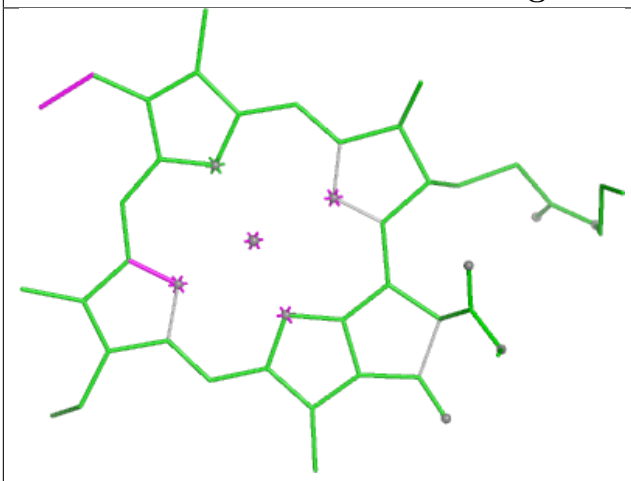


Rings

Ligand CLA 1 605



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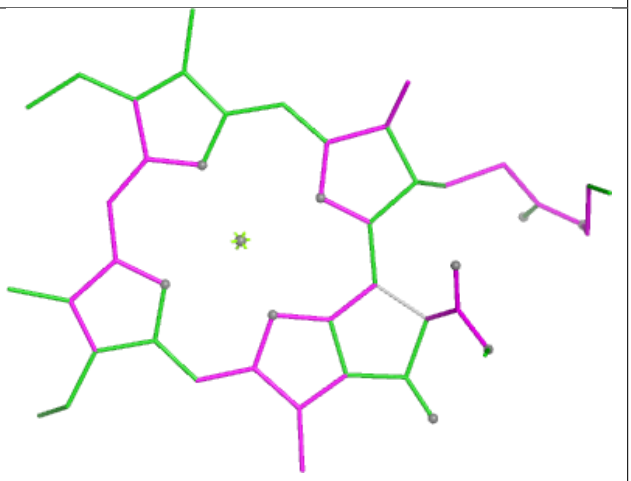
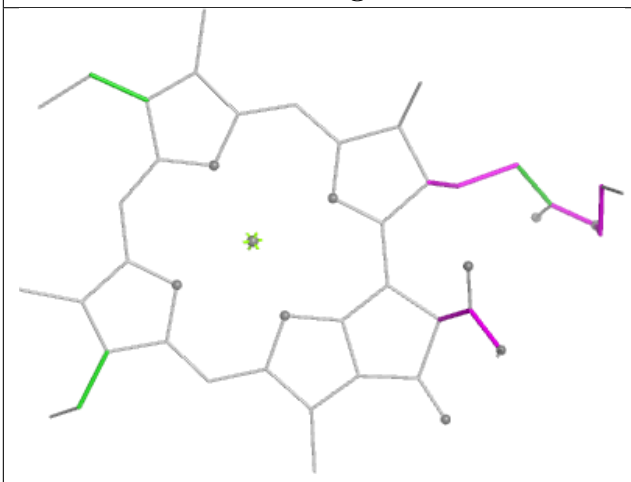


Bond angles



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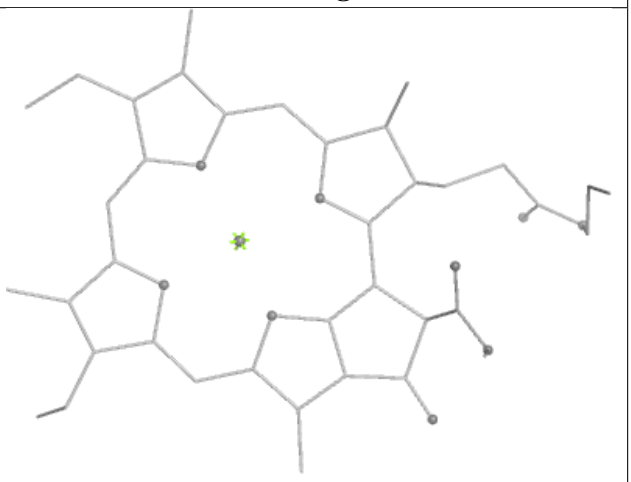
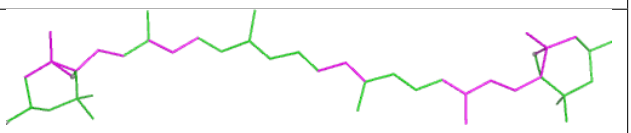


Rings

Ligand XAT 2 502



Bond lengths



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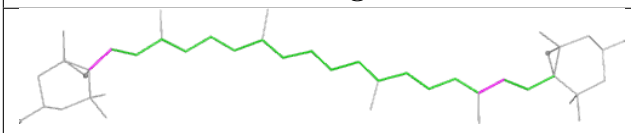

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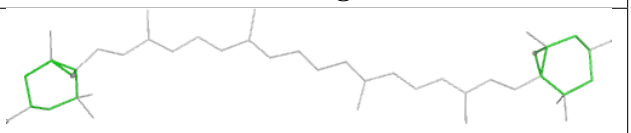
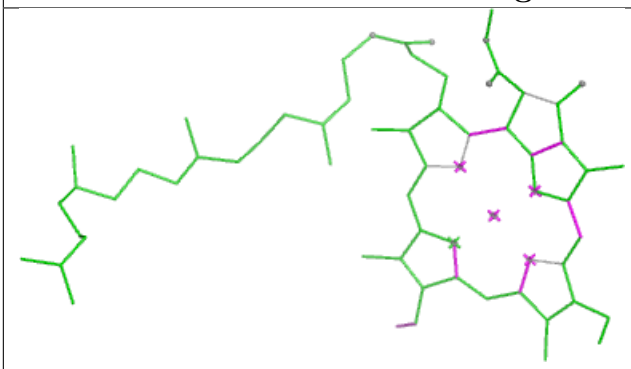


Rings

Ligand CLA A 1013



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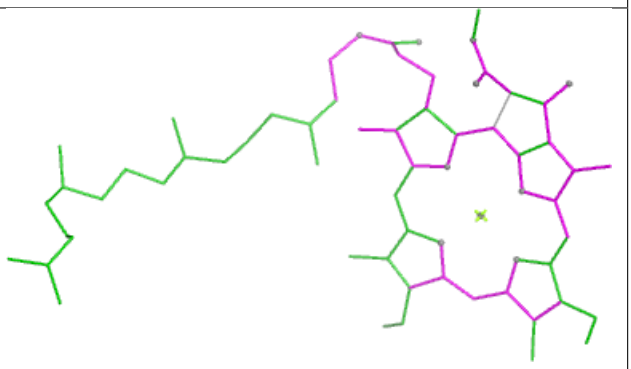
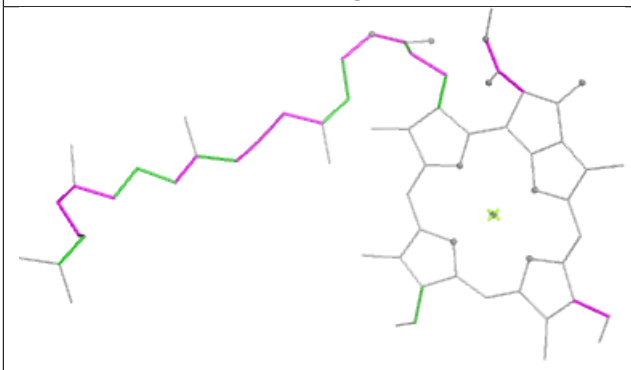


Bond angles

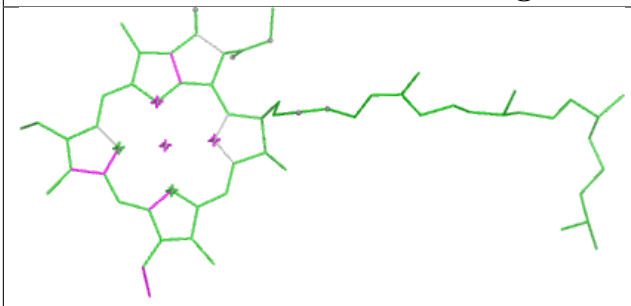


Torsions



Rings

Ligand CLA B 1240



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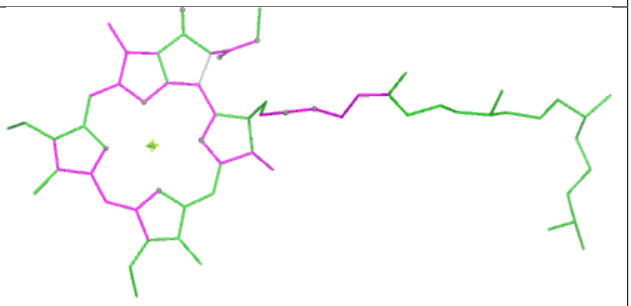
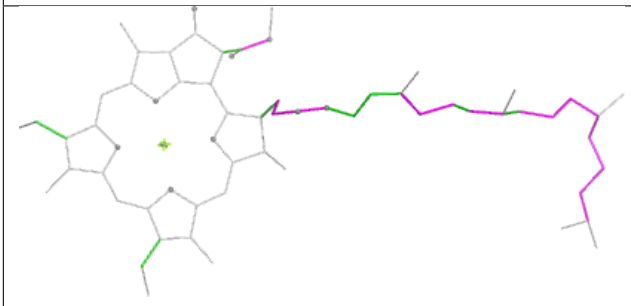


Bond angles



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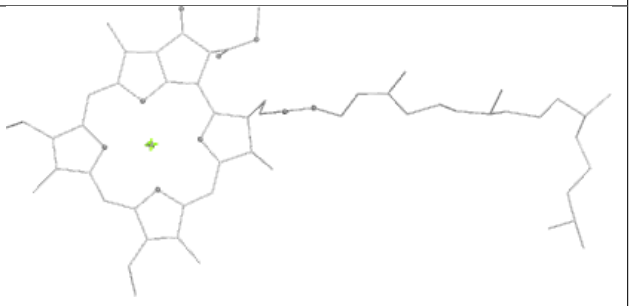
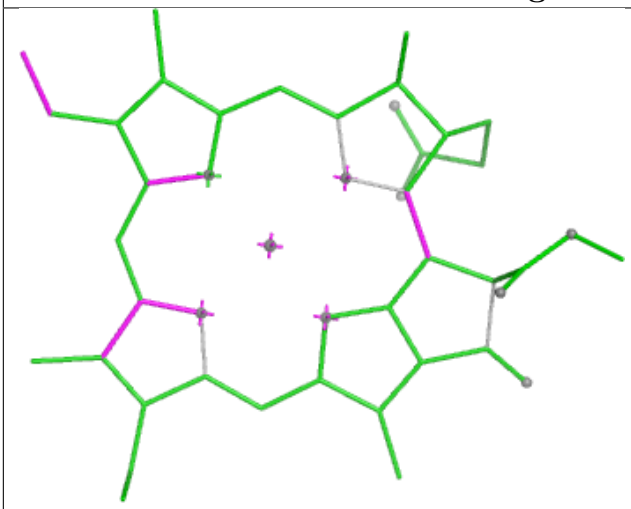


Rings

Ligand CLA 1 613



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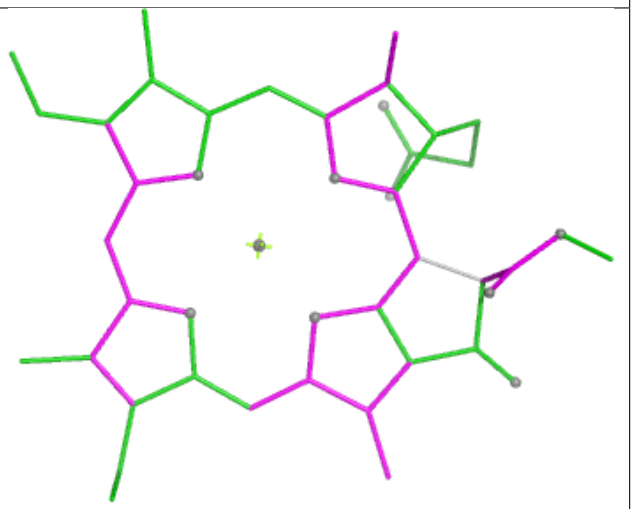

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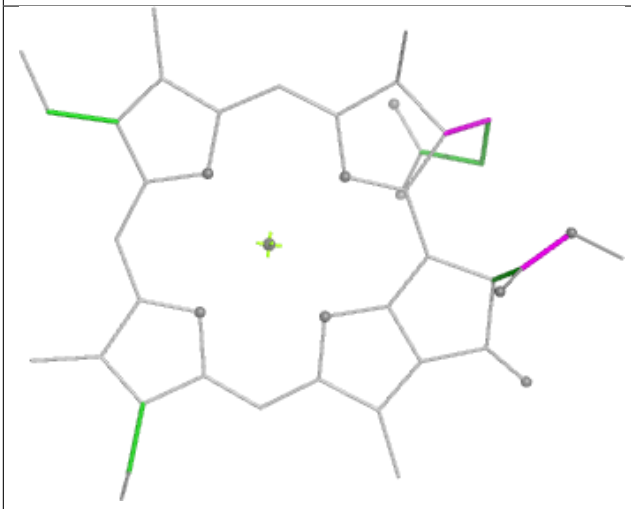

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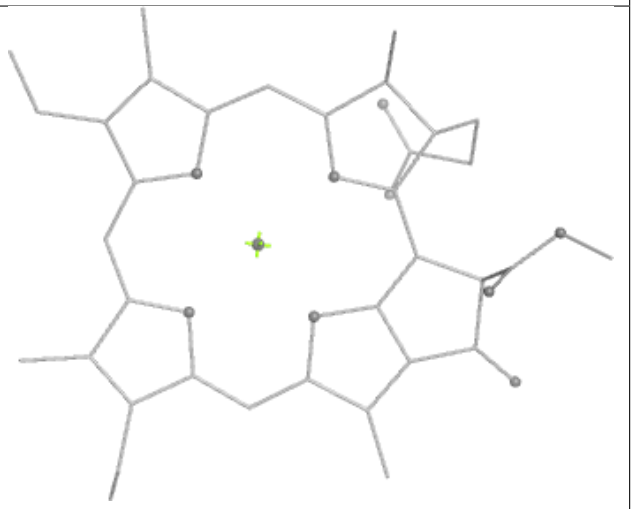
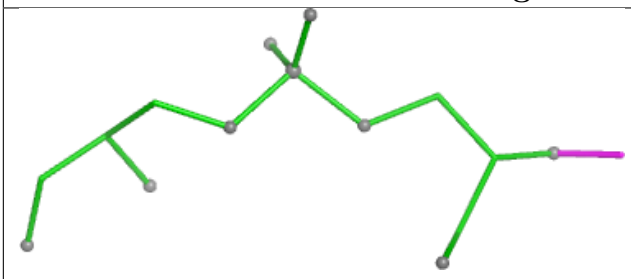


Rings

Ligand LHG A 5001



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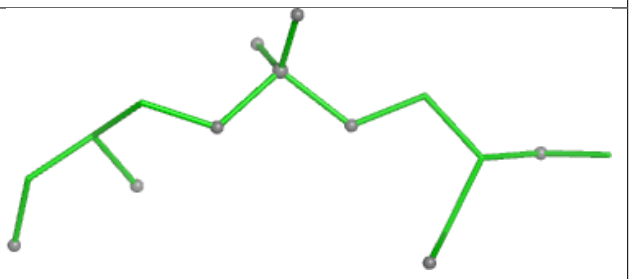
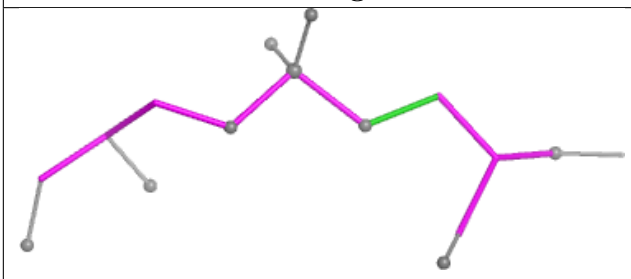


Bond angles



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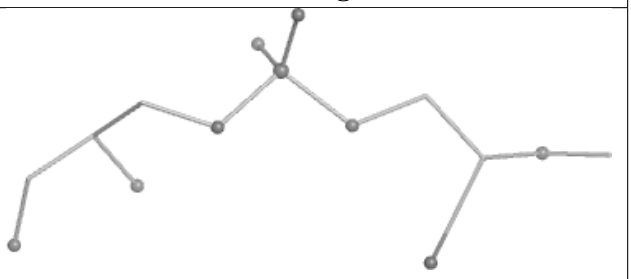
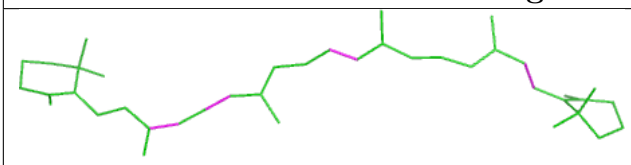


Rings

Ligand BCR 2 503



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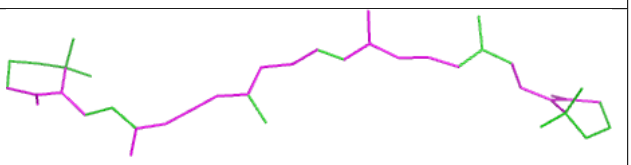
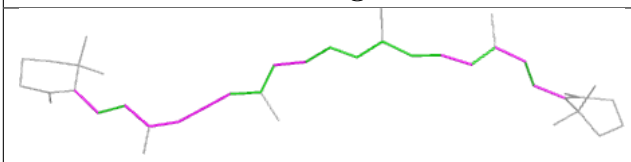


Bond angles



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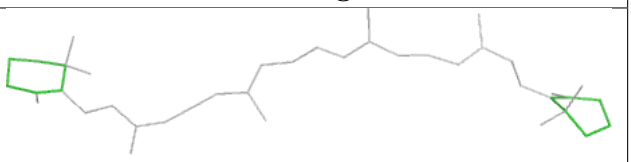
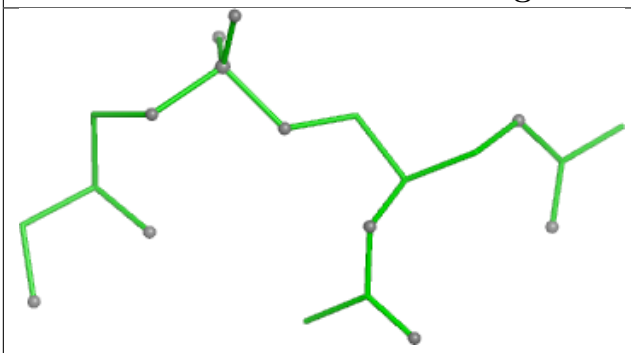


Rings

Ligand LHG B 5001



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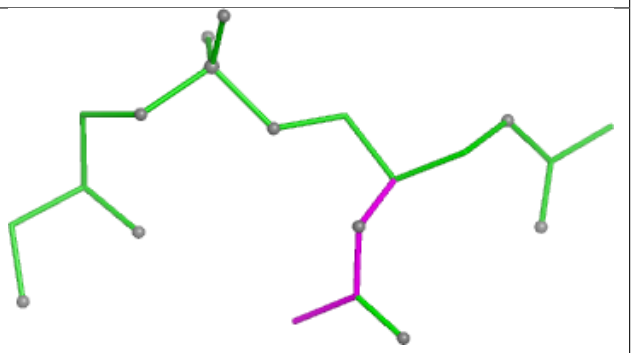

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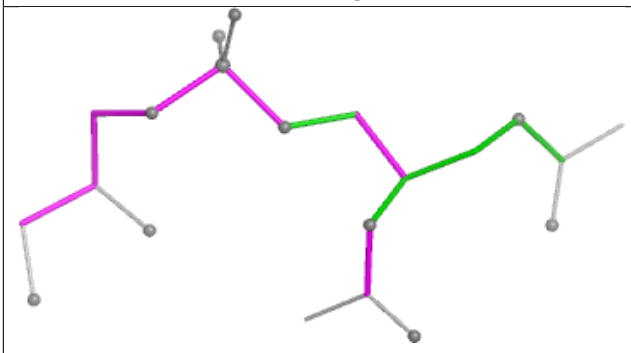

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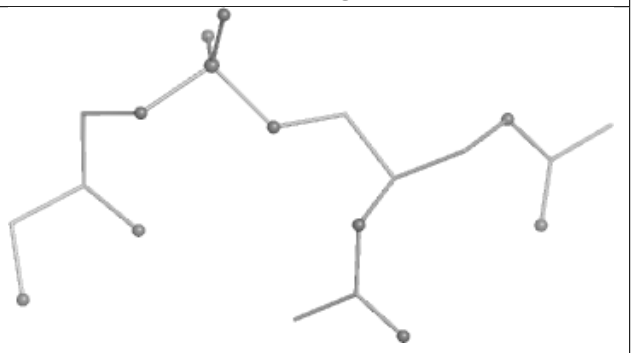
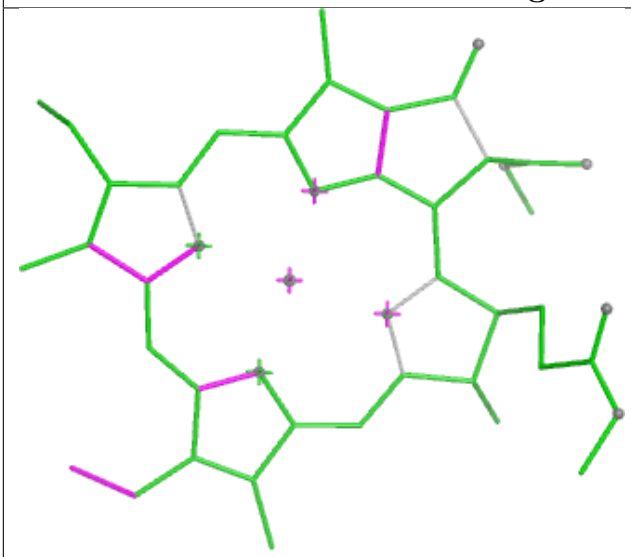
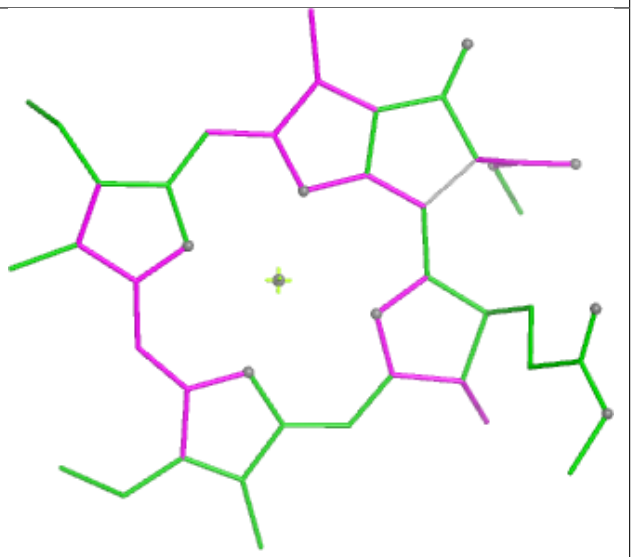


Rings

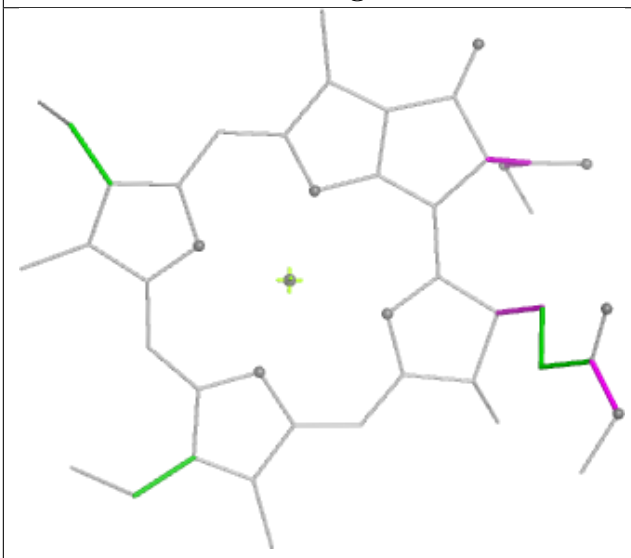
Ligand CLA 1 608



Bond lengths



Bond angles



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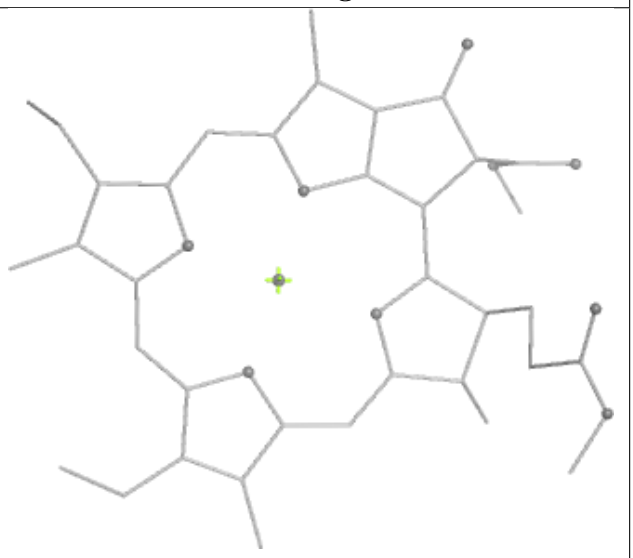
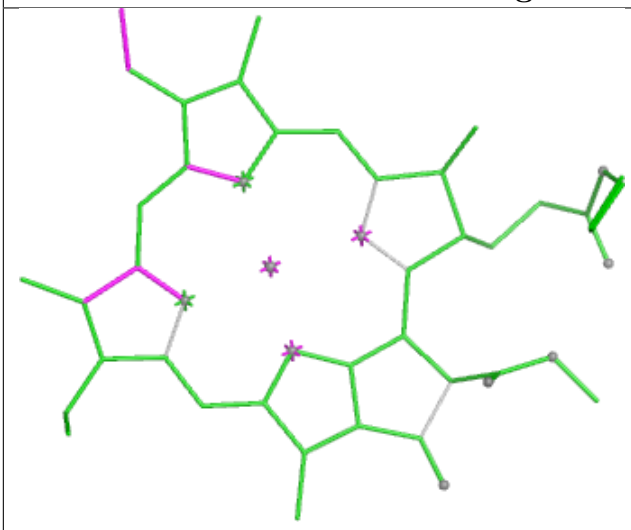
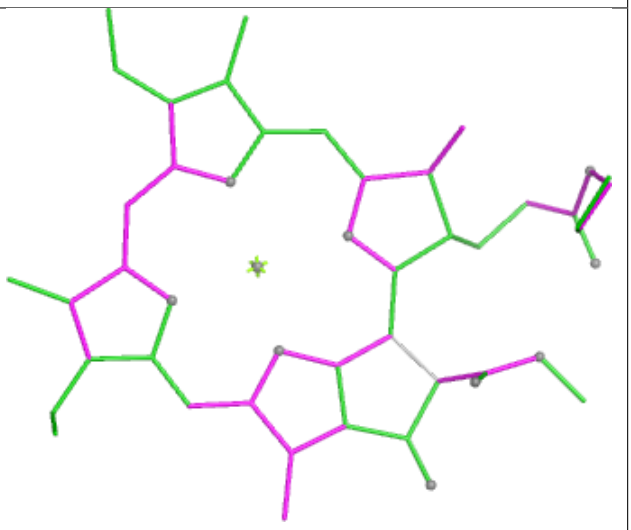


Rings

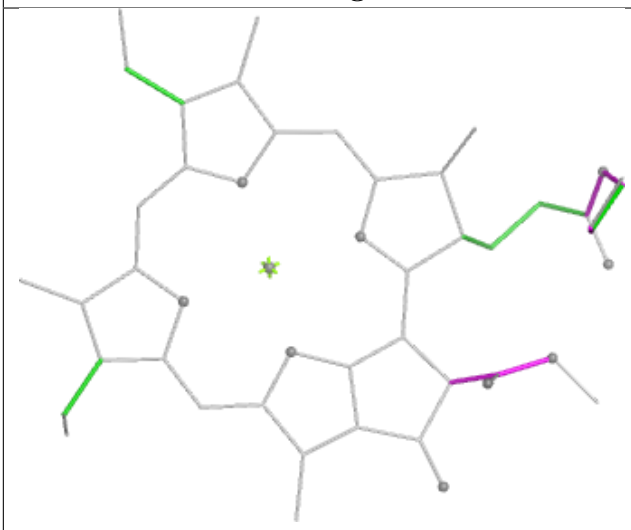
Ligand CLA B 1203



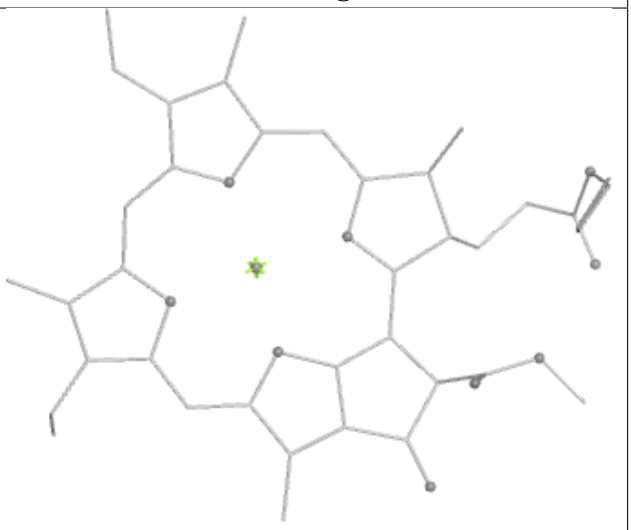
Bond lengths



Bond angles

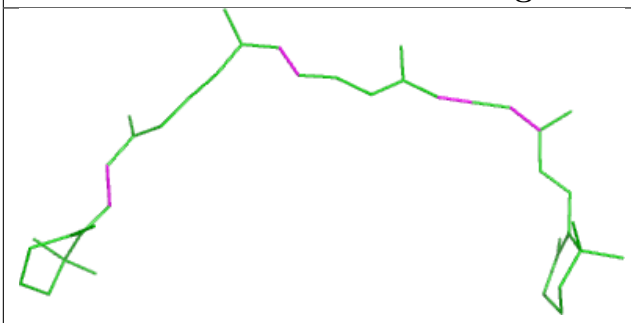


Torsions

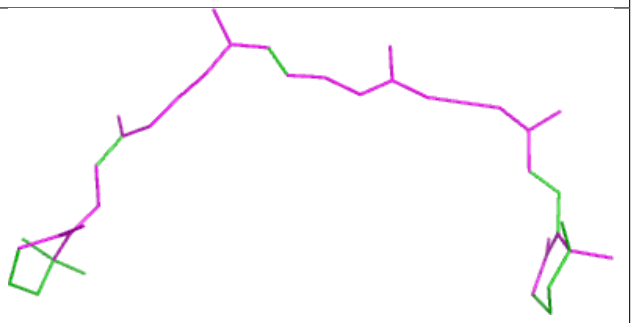


Rings

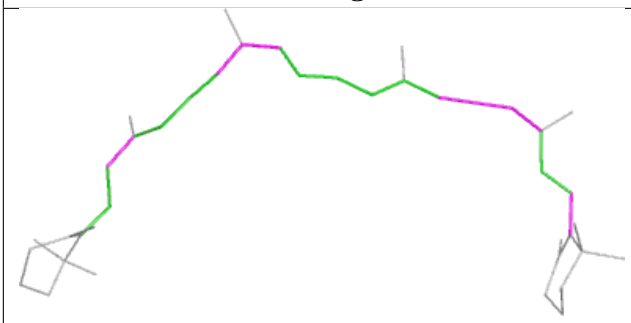
Ligand BCR F 4002



Bond lengths



Bond angles

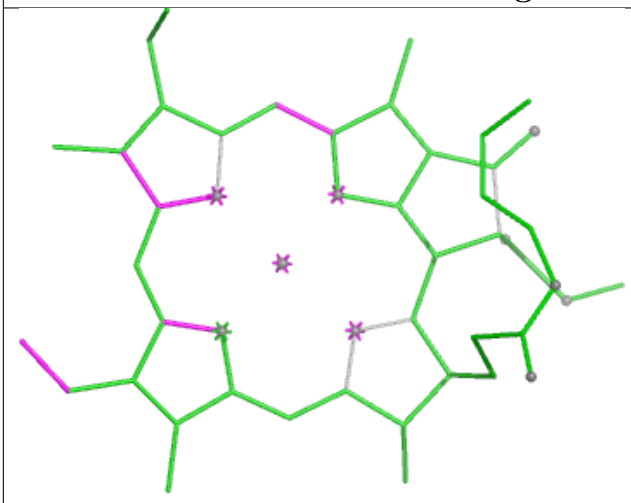


Torsions

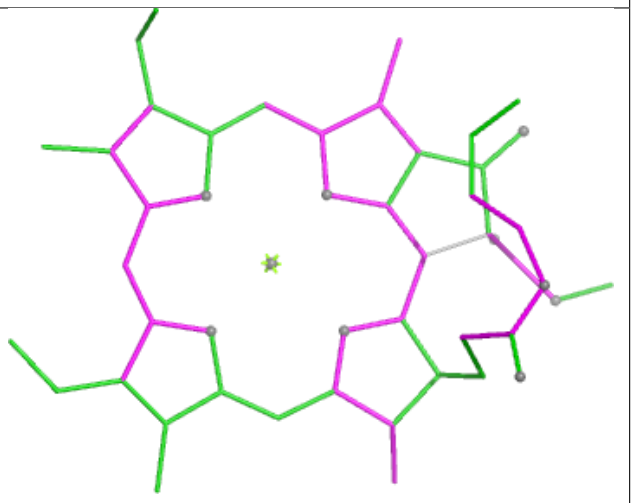


Rings

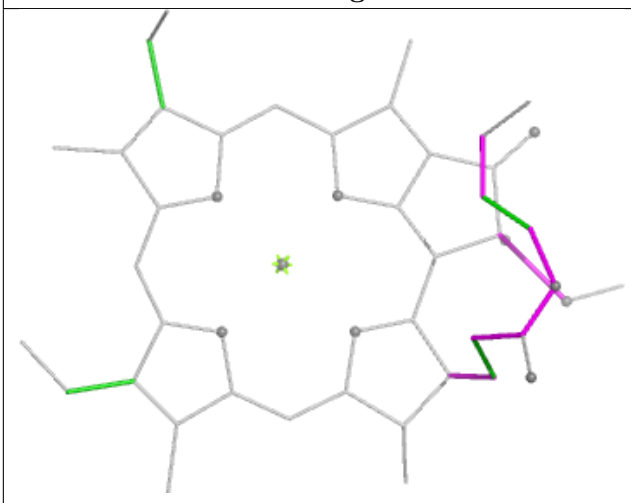
Ligand CLA A 1127



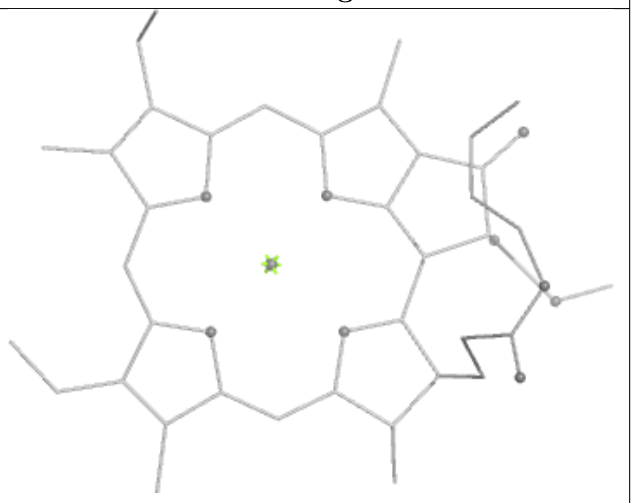
Bond lengths



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	195/195 (100%)	1.26	40 (20%) 2 4	85, 106, 128, 134	0
2	2	211/211 (100%)	1.30	48 (22%) 2 4	91, 115, 139, 155	0
3	3	210/210 (100%)	1.95	70 (33%) 1 1	134, 167, 199, 210	0
4	4	211/211 (100%)	1.48	50 (23%) 2 3	84, 93, 107, 125	0
5	A	739/739 (100%)	1.58	186 (25%) 1 3	84, 127, 168, 187	0
6	B	734/734 (100%)	1.39	174 (23%) 2 3	83, 114, 149, 180	0
7	C	80/80 (100%)	1.30	15 (18%) 3 4	104, 128, 142, 146	0
8	D	142/142 (100%)	1.15	29 (20%) 3 4	108, 153, 174, 189	0
9	E	64/64 (100%)	0.33	2 (3%) 51 38	93, 103, 115, 120	0
10	F	163/163 (100%)	0.55	13 (7%) 18 16	80, 87, 99, 105	0
11	J	41/41 (100%)	0.79	5 (12%) 8 9	82, 87, 103, 105	0
All	All	2790/2790 (100%)	1.37	632 (22%) 2 4	80, 117, 171, 210	0

All (632) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	506	THR	19.0
5	A	280	GLY	16.5
5	A	377	TYR	16.2
5	A	375	PRO	15.1
6	B	735	GLY	13.1
3	3	103	PHE	13.0
5	A	373	ALA	12.9
5	A	507	SER	12.8
3	3	84	PHE	12.5
5	A	289	LEU	11.8
3	3	89	LEU	11.8
6	B	368	THR	11.5

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Mol	Chain	Res	Type	RSRZ
5	A	374	MET	11.2
5	A	359	LEU	11.2
2	2	217	GLU	10.6
3	3	96	ASN	10.4
5	A	376	PRO	10.4
5	A	281	GLY	10.4
5	A	294	THR	10.3
2	2	210	LYS	10.3
6	B	357	PRO	10.1
6	B	369	GLN	9.8
2	2	216	LYS	9.8
3	3	91	ASP	9.6
10	F	236	ASN	9.6
2	2	212	GLU	9.5
6	B	733	ARG	9.4
2	2	207	GLY	9.4
4	4	182	PHE	9.4
5	A	293	ASP	9.2
6	B	354	TYR	9.1
6	B	508	SER	9.1
6	B	331	LEU	9.1
6	B	653	PHE	8.9
6	B	333	PHE	8.7
3	3	111	TYR	8.7
3	3	141	ALA	8.6
6	B	355	SER	8.5
5	A	292	SER	8.3
5	A	291	LEU	8.3
5	A	505	ALA	8.2
5	A	705	ASN	8.2
4	4	194	LEU	8.2
3	3	88	GLY	8.1
5	A	420	THR	7.9
5	A	143	GLY	7.9
3	3	104	VAL	7.8
6	B	394	PHE	7.7
5	A	565	ASP	7.7
6	B	731	ALA	7.6
2	2	215	PHE	7.6
6	B	727	ILE	7.5
5	A	151	SER	7.4
4	4	128	TYR	7.4

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Mol	Chain	Res	Type	RSRZ
8	D	98	GLU	7.4
1	1	94	VAL	7.4
5	A	551	LEU	7.4
8	D	85	GLY	7.3
3	3	85	ASP	7.3
6	B	332	HIS	7.3
4	4	178	VAL	7.2
5	A	282	LEU	7.1
3	3	86	PRO	7.1
5	A	508	LEU	7.0
7	C	76	SER	7.0
6	B	393	ILE	7.0
3	3	114	VAL	7.0
6	B	599	HIS	6.9
5	A	566	LYS	6.8
5	A	564	PRO	6.7
5	A	547	VAL	6.7
2	2	244	HIS	6.6
5	A	245	LEU	6.6
6	B	41	GLU	6.6
3	3	108	TRP	6.5
6	B	334	GLN	6.5
5	A	707	LEU	6.3
3	3	98	GLN	6.3
3	3	87	LEU	6.3
8	D	132	PHE	6.3
5	A	511	GLY	6.2
8	D	99	GLU	6.2
9	E	111	TYR	6.2
5	A	503	LEU	6.2
5	A	557	ALA	6.2
5	A	706	LYS	6.1
6	B	391	GLY	6.1
1	1	214	PHE	6.1
8	D	138	CYS	6.1
5	A	581	GLY	6.1
6	B	666	ILE	6.1
7	C	75	ARG	6.0
6	B	356	LEU	5.9
5	A	387	GLN	5.9
3	3	90	LEU	5.9
2	2	213	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
4	4	172	TRP	5.8
5	A	244	LEU	5.8
10	F	238	THR	5.8
2	2	220	GLN	5.8
6	B	359	TYR	5.7
6	B	44	TYR	5.7
5	A	504	ALA	5.7
1	1	91	ALA	5.7
6	B	362	LEU	5.6
6	B	142	PHE	5.6
6	B	603	TRP	5.6
5	A	692	TYR	5.6
5	A	279	LYS	5.6
5	A	510	TRP	5.6
6	B	730	THR	5.5
5	A	372	TYR	5.5
5	A	509	THR	5.4
6	B	570	ASP	5.4
3	3	160	LYS	5.4
6	B	358	PRO	5.4
5	A	747	ILE	5.3
5	A	147	LEU	5.3
3	3	137	GLY	5.3
5	A	550	LEU	5.3
5	A	709	VAL	5.3
3	3	106	PRO	5.3
3	3	94	VAL	5.2
5	A	749	ALA	5.2
2	2	208	MET	5.2
2	2	183	SER	5.2
6	B	365	ASP	5.1
4	4	275	GLU	5.1
5	A	363	LEU	5.1
6	B	675	LEU	5.1
6	B	601	THR	5.1
5	A	152	GLY	5.1
4	4	211	THR	5.1
6	B	650	THR	5.0
5	A	358	ALA	5.0
5	A	219	HIS	5.0
6	B	509	LEU	5.0
6	B	556	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
5	A	14	LYS	5.0
6	B	304	ALA	4.9
5	A	750	VAL	4.9
11	J	12	PRO	4.9
4	4	269	TYR	4.9
5	A	698	GLU	4.8
6	B	188	SER	4.8
6	B	396	ILE	4.8
3	3	155	PRO	4.8
3	3	93	THR	4.8
5	A	241	HIS	4.8
7	C	43	PRO	4.8
5	A	384	TYR	4.7
3	3	109	LEU	4.7
3	3	92	PRO	4.7
1	1	210	LEU	4.7
6	B	557	SER	4.7
6	B	370	ALA	4.7
1	1	188	CYS	4.7
3	3	156	ALA	4.7
6	B	714	PHE	4.7
3	3	140	PRO	4.7
6	B	595	TRP	4.7
6	B	327	VAL	4.7
8	D	137	GLN	4.6
6	B	574	TYR	4.6
1	1	164	SER	4.6
6	B	734	PHE	4.6
7	C	46	GLU	4.6
1	1	54	PHE	4.6
2	2	171	TYR	4.5
5	A	555	LEU	4.5
5	A	559	SER	4.5
10	F	232	GLU	4.5
6	B	392	ALA	4.5
4	4	272	THR	4.5
6	B	367	THR	4.5
6	B	390	HIS	4.5
5	A	17	VAL	4.5
5	A	751	GLY	4.4
6	B	330	SER	4.4
5	A	554	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
6	B	517	ASP	4.4
3	3	112	SER	4.4
5	A	689	GLY	4.4
6	B	23	TRP	4.4
11	J	4	PHE	4.3
5	A	16	ALA	4.3
5	A	567	ALA	4.3
5	A	144	PHE	4.3
4	4	273	SER	4.3
6	B	594	TYR	4.3
6	B	284	LEU	4.3
5	A	701	VAL	4.3
7	C	47	ASP	4.3
8	D	116	PRO	4.3
6	B	26	LEU	4.2
1	1	35	GLY	4.2
2	2	245	LYS	4.2
6	B	397	ARG	4.2
6	B	596	HIS	4.2
6	B	438	TYR	4.2
3	3	167	PHE	4.1
2	2	189	ASP	4.1
5	A	220	VAL	4.1
4	4	316	PHE	4.1
5	A	278	PHE	4.1
1	1	111	ASP	4.1
1	1	186	VAL	4.1
6	B	189	LEU	4.1
6	B	372	LEU	4.1
6	B	87	PRO	4.1
4	4	215	LEU	4.0
5	A	686	LEU	4.0
2	2	211	ASN	4.0
6	B	382	PHE	4.0
7	C	72	GLU	4.0
6	B	15	GLN	4.0
5	A	687	PHE	4.0
4	4	242	ASP	4.0
2	2	214	SER	3.9
5	A	401	CYS	3.9
6	B	668	TRP	3.9
4	4	200	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
6	B	582	PHE	3.9
5	A	614	MET	3.9
6	B	539	ALA	3.9
1	1	143	ASN	3.8
5	A	748	ILE	3.8
6	B	395	PHE	3.8
5	A	710	ALA	3.8
6	B	353	MET	3.8
4	4	218	ILE	3.8
5	A	383	ASP	3.8
1	1	213	PRO	3.8
5	A	158	GLN	3.8
8	D	101	TYR	3.7
3	3	242	ASN	3.7
5	A	496	GLN	3.7
3	3	105	ASN	3.7
3	3	80	GLY	3.7
5	A	275	PHE	3.7
8	D	94	LYS	3.7
6	B	519	LEU	3.7
6	B	139	SER	3.6
5	A	18	ASP	3.6
3	3	110	GLN	3.6
4	4	203	GLN	3.6
5	A	438	ILE	3.6
6	B	437	LEU	3.6
5	A	657	VAL	3.6
10	F	222	ILE	3.6
6	B	210	TRP	3.6
6	B	728	ALA	3.6
3	3	95	SER	3.6
5	A	15	ILE	3.6
8	D	112	ILE	3.6
6	B	491	GLN	3.6
3	3	142	GLU	3.6
6	B	371	SER	3.6
6	B	186	VAL	3.5
6	B	360	ALA	3.5
5	A	437	ILE	3.5
3	3	127	CYS	3.5
5	A	560	SER	3.5
7	C	2	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	2	206	MET	3.5
1	1	149	GLU	3.5
5	A	628	SER	3.5
6	B	344	THR	3.5
6	B	576	ALA	3.5
2	2	101	TRP	3.5
5	A	421	ASN	3.4
3	3	197	GLN	3.4
5	A	50	TRP	3.4
3	3	115	ILE	3.4
6	B	575	ASP	3.4
1	1	178	LEU	3.4
5	A	157	LEU	3.4
5	A	570	GLY	3.4
6	B	573	ALA	3.4
6	B	373	TYR	3.4
4	4	193	GLY	3.4
5	A	517	VAL	3.3
6	B	711	LEU	3.3
6	B	703	ILE	3.3
6	B	521	HIS	3.3
4	4	213	ARG	3.3
3	3	238	ASN	3.3
5	A	548	LEU	3.3
3	3	134	GLY	3.3
5	A	398	GLY	3.3
6	B	389	ALA	3.3
1	1	209	HIS	3.3
1	1	95	LEU	3.3
4	4	188	SER	3.3
1	1	99	ASN	3.3
5	A	703	ALA	3.3
4	4	324	GLY	3.3
5	A	662	GLY	3.3
3	3	83	GLY	3.2
5	A	304	LEU	3.2
3	3	215	PRO	3.2
5	A	574	PRO	3.2
4	4	232	TYR	3.2
5	A	417	TYR	3.2
2	2	162	PHE	3.2
6	B	138	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
6	B	398	ASP	3.2
4	4	267	LEU	3.2
6	B	143	LEU	3.2
5	A	482	VAL	3.2
2	2	174	ARG	3.2
2	2	218	ALA	3.2
5	A	711	PRO	3.1
5	A	217	GLN	3.1
5	A	13	VAL	3.1
3	3	166	PRO	3.1
8	D	95	ALA	3.1
1	1	206	LEU	3.1
6	B	585	LEU	3.1
6	B	120	GLY	3.1
3	3	119	TRP	3.1
4	4	250	ASP	3.1
6	B	464	ILE	3.1
6	B	656	LEU	3.1
3	3	185	LEU	3.1
2	2	268	VAL	3.1
8	D	114	GLU	3.1
2	2	170	LEU	3.0
6	B	547	LEU	3.0
3	3	184	ARG	3.0
5	A	492	PHE	3.0
5	A	623	THR	3.0
6	B	246	GLY	3.0
1	1	37	PHE	3.0
4	4	186	PHE	3.0
5	A	702	TRP	3.0
6	B	38	MET	3.0
5	A	718	LEU	3.0
4	4	123	ASP	3.0
4	4	208	ASP	3.0
2	2	179	GLN	3.0
8	D	86	GLY	3.0
3	3	152	VAL	3.0
4	4	327	ILE	3.0
1	1	167	PRO	2.9
8	D	87	SER	2.9
8	D	84	PHE	2.9
9	E	85	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
5	A	290	TRP	2.9
4	4	270	SER	2.9
6	B	720	PHE	2.9
8	D	91	LEU	2.9
6	B	684	GLU	2.9
2	2	267	GLY	2.9
6	B	615	THR	2.9
11	J	30	ASN	2.9
6	B	124	TRP	2.9
3	3	151	GLY	2.9
7	C	44	ARG	2.9
1	1	90	LEU	2.9
3	3	139	ILE	2.9
5	A	155	SER	2.9
6	B	655	HIS	2.9
3	3	194	GLN	2.9
5	A	622	VAL	2.9
4	4	254	GLY	2.9
6	B	436	GLY	2.9
3	3	132	ILE	2.9
4	4	231	LEU	2.8
5	A	646	LEU	2.8
6	B	566	GLY	2.8
2	2	62	ALA	2.8
8	D	205	THR	2.8
10	F	87	GLU	2.8
7	C	50	GLY	2.8
8	D	115	MET	2.8
6	B	565	ARG	2.8
5	A	546	THR	2.8
4	4	222	LEU	2.8
4	4	280	LEU	2.8
1	1	96	GLY	2.8
5	A	49	ILE	2.8
6	B	184	PHE	2.8
5	A	512	GLY	2.8
6	B	145	LEU	2.8
6	B	500	GLU	2.8
5	A	418	ASP	2.8
6	B	231	TRP	2.8
5	A	132	GLY	2.8
2	2	269	SER	2.8

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Mol	Chain	Res	Type	RSRZ
6	B	625	LEU	2.8
6	B	665	LEU	2.8
5	A	355	ILE	2.8
5	A	526	ILE	2.8
5	A	582	GLY	2.7
5	A	601	ASN	2.7
6	B	614	SER	2.7
5	A	693	TRP	2.7
4	4	240	GLN	2.7
1	1	202	ILE	2.7
4	4	199	GLU	2.7
6	B	40	GLU	2.7
7	C	73	SER	2.7
2	2	249	ASP	2.7
5	A	295	ALA	2.7
3	3	200	LEU	2.7
6	B	195	LEU	2.7
5	A	694	GLN	2.7
5	A	523	MET	2.7
3	3	135	LYS	2.7
7	C	45	THR	2.7
6	B	693	TYR	2.7
5	A	528	LEU	2.7
6	B	22	ILE	2.7
3	3	157	GLY	2.7
6	B	712	ALA	2.7
6	B	617	LEU	2.7
4	4	209	ASN	2.7
6	B	383	ILE	2.6
6	B	662	PHE	2.6
6	B	546	LYS	2.6
1	1	155	GLY	2.6
6	B	154	GLY	2.6
10	F	98	GLU	2.6
6	B	227	TRP	2.6
3	3	145	VAL	2.6
5	A	720	ILE	2.6
5	A	578	PRO	2.6
5	A	593	PHE	2.6
6	B	690	ASN	2.6
7	C	27	GLU	2.6
7	C	74	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	1	41	SER	2.6
6	B	718	TYR	2.6
6	B	379	ILE	2.6
8	D	96	GLN	2.6
4	4	228	THR	2.6
5	A	736	ILE	2.6
2	2	241	HIS	2.6
5	A	576	ASP	2.6
3	3	97	GLY	2.6
6	B	42	ASN	2.6
1	1	203	LEU	2.6
5	A	81	LEU	2.6
5	A	76	ALA	2.6
6	B	571	ILE	2.6
4	4	205	TYR	2.6
3	3	149	ARG	2.6
4	4	165	ALA	2.6
10	F	149	ILE	2.5
6	B	433	HIS	2.5
6	B	658	TYR	2.5
1	1	62	GLY	2.5
6	B	710	GLY	2.5
5	A	380	LEU	2.5
5	A	650	LEU	2.5
6	B	269	LEU	2.5
5	A	558	ARG	2.5
5	A	716	ARG	2.5
6	B	587	THR	2.5
6	B	725	PHE	2.5
2	2	260	HIS	2.5
3	3	74	LEU	2.5
10	F	240	SER	2.5
6	B	45	GLN	2.5
1	1	36	ASN	2.5
4	4	204	THR	2.5
6	B	510	PHE	2.5
5	A	715	PRO	2.5
2	2	182	GLY	2.5
1	1	205	ALA	2.5
1	1	171	GLU	2.5
5	A	189	GLU	2.5
5	A	621	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	3	126	GLY	2.5
6	B	36	ASP	2.5
4	4	296	THR	2.5
5	A	277	THR	2.5
3	3	158	VAL	2.5
5	A	422	ASN	2.4
4	4	234	LEU	2.4
5	A	386	THR	2.4
2	2	177	GLY	2.4
10	F	134	ALA	2.4
2	2	257	ASP	2.4
2	2	265	THR	2.4
6	B	563	PRO	2.4
2	2	193	GLY	2.4
6	B	287	VAL	2.4
6	B	484	SER	2.4
4	4	277	LEU	2.4
6	B	271	LEU	2.4
5	A	148	TRP	2.4
4	4	195	PRO	2.4
5	A	100	ASN	2.4
5	A	378	PRO	2.4
6	B	441	ASN	2.4
3	3	240	ILE	2.4
2	2	191	LEU	2.4
3	3	133	LEU	2.4
4	4	142	LEU	2.4
6	B	701	LEU	2.4
3	3	212	PRO	2.4
6	B	37	GLY	2.4
6	B	206	GLN	2.4
5	A	603	LEU	2.4
8	D	167	LEU	2.4
8	D	136	GLU	2.4
5	A	240	PRO	2.4
6	B	672	TRP	2.4
6	B	567	GLY	2.3
3	3	136	ALA	2.3
3	3	213	ALA	2.3
5	A	218	ILE	2.3
2	2	184	PHE	2.3
5	A	146	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
6	B	691	LEU	2.3
5	A	72	LYS	2.3
5	A	141	THR	2.3
10	F	214	GLY	2.3
6	B	618	MET	2.3
5	A	538	ILE	2.3
8	D	83	ILE	2.3
8	D	130	LEU	2.3
5	A	453	PHE	2.3
6	B	33	GLU	2.3
10	F	235	GLU	2.3
2	2	219	LYS	2.3
6	B	208	VAL	2.3
1	1	66	GLY	2.3
4	4	216	ALA	2.3
8	D	121	ALA	2.3
7	C	79	LEU	2.3
2	2	253	ASP	2.3
5	A	590	ASP	2.3
8	D	135	LYS	2.3
2	2	161	LEU	2.3
5	A	296	HIS	2.3
5	A	688	SER	2.3
6	B	578	TYR	2.3
1	1	73	GLU	2.2
1	1	204	ALA	2.2
5	A	385	GLY	2.2
6	B	59	PHE	2.2
11	J	10	THR	2.2
6	B	18	SER	2.2
5	A	149	ARG	2.2
4	4	192	VAL	2.2
4	4	302	GLN	2.2
10	F	174	VAL	2.2
1	1	40	GLY	2.2
3	3	264	PRO	2.2
5	A	740	TRP	2.2
6	B	512	THR	2.2
8	D	157	ARG	2.2
5	A	563	ILE	2.2
2	2	138	ASP	2.2
8	D	177	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	A	26	PHE	2.2
5	A	59	PHE	2.2
5	A	619	TRP	2.2
8	D	149	PHE	2.2
5	A	430	VAL	2.2
3	3	209	SER	2.2
5	A	205	LEU	2.2
6	B	602	LEU	2.2
5	A	288	GLY	2.2
5	A	735	GLY	2.2
5	A	597	PHE	2.2
2	2	272	HIS	2.2
8	D	212	ILE	2.2
5	A	436	ALA	2.2
3	3	216	GLY	2.2
5	A	133	GLY	2.2
2	2	87	PHE	2.2
5	A	360	PHE	2.2
6	B	226	PHE	2.2
6	B	620	TRP	2.2
6	B	520	VAL	2.1
5	A	69	ILE	2.1
5	A	665	LEU	2.1
1	1	107	ALA	2.1
3	3	79	PRO	2.1
5	A	305	PHE	2.1
6	B	245	PHE	2.1
1	1	102	ASP	2.1
2	2	181	ASP	2.1
6	B	478	LEU	2.1
6	B	485	PRO	2.1
5	A	315	ASN	2.1
11	J	41	PHE	2.1
4	4	144	ASP	2.1
6	B	463	TRP	2.1
1	1	165	LYS	2.1
6	B	627	LEU	2.1
6	B	707	ARG	2.1
5	A	74	PHE	2.1
5	A	75	SER	2.1
6	B	558	PHE	2.1
1	1	217	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
5	A	58	ASP	2.1
6	B	35	HIS	2.1
6	B	211	ASP	2.1
6	B	440	HIS	2.1
5	A	115	ALA	2.1
2	2	190	GLY	2.1
5	A	586	VAL	2.1
2	2	194	LYS	2.1
4	4	169	ASN	2.1
6	B	8	LYS	2.1
5	A	349	TRP	2.1
5	A	658	ILE	2.1
6	B	676	ILE	2.1
3	3	82	TYR	2.1
5	A	721	THR	2.1
2	2	201	GLY	2.1
5	A	134	GLY	2.1
5	A	525	PRO	2.1
6	B	518	PHE	2.1
5	A	592	VAL	2.0
1	1	55	ASN	2.0
5	A	479	LEU	2.0
6	B	474	GLY	2.0
4	4	125	PRO	2.0
7	C	67	VAL	2.0
5	A	744	LEU	2.0
2	2	178	SER	2.0
6	B	203	SER	2.0
6	B	153	ALA	2.0
3	3	188	TYR	2.0
10	F	192	ASP	2.0
1	1	39	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CAC	3	901	5/5	0.16	0.19	190,190,194,197	0
15	CLA	A	1121	49/65	0.31	0.13	177,193,206,211	0
15	CLA	3	607	50/65	0.37	0.22	195,209,223,228	0
15	CLA	3	608	48/65	0.41	0.12	196,222,240,247	0
20	CAC	1	902	5/5	0.42	0.21	136,142,150,152	0
23	GSH	4	831	20/20	0.42	0.12	136,138,145,146	0
18	LMG	2	802	25/55	0.47	0.18	92,104,127,134	0
18	LMG	1	802	36/55	0.47	0.15	88,102,125,128	0
20	CAC	1	901	5/5	0.48	0.25	130,132,142,147	0
21	DGD	4	811	45/66	0.49	0.19	83,91,111,119	0
21	DGD	J	5001	28/66	0.50	0.12	92,95,97,97	0
14	BCR	4	505	40/40	0.50	0.25	83,85,118,119	0
20	CAC	3	902	5/5	0.53	0.17	200,204,206,207	0
14	BCR	1	505	40/40	0.55	0.33	83,86,98,110	0
14	BCR	J	4003	40/40	0.57	0.21	89,99,105,106	0
18	LMG	1	803	23/55	0.57	0.16	114,119,150,154	0
15	CLA	A	1120	49/65	0.57	0.17	162,176,190,191	0
14	BCR	4	503	40/40	0.57	0.21	90,93,98,99	0
15	CLA	A	1141	50/65	0.57	0.12	170,186,196,199	0
15	CLA	A	1131	50/65	0.58	0.17	145,153,157,158	0
15	CLA	B	1218	49/65	0.59	0.16	104,112,117,137	0
23	GSH	B	5031	20/20	0.59	0.10	151,157,163,166	0
14	BCR	B	4003	40/40	0.61	0.30	125,141,149,153	0
18	LMG	2	803	16/55	0.63	0.12	121,129,134,134	0
15	CLA	3	603	45/65	0.65	0.12	179,187,200,210	0
22	LMT	2	821	23/35	0.66	0.08	109,113,132,138	0
15	CLA	B	1207	25/65	0.66	0.13	145,151,156,158	0
15	CLA	1	615	65/65	0.66	0.19	83,85,89,91	0
15	CLA	A	1114	46/65	0.67	0.20	127,141,157,160	0
14	BCR	A	4002	40/40	0.68	0.31	120,140,167,169	0
15	CLA	2	602	49/65	0.69	0.18	123,128,133,137	0
14	BCR	1	503	40/40	0.70	0.15	115,121,136,138	0
14	BCR	J	4001	40/40	0.70	0.26	83,90,102,103	0
20	CAC	4	902	5/5	0.70	0.21	85,105,119,122	0
14	BCR	B	4001	40/40	0.70	0.20	121,129,137,138	0
12	LUT	4	501	42/42	0.71	0.16	90,93,101,102	0
15	CLA	B	1238	50/65	0.71	0.15	134,148,155,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	BCR	2	503	40/40	0.72	0.22	96,102,110,110	0
15	CLA	B	1201	49/65	0.73	0.14	127,132,139,152	0
14	BCR	3	503	40/40	0.73	0.20	134,148,166,169	0
12	LUT	1	501	42/42	0.74	0.22	100,109,122,125	0
16	CHL	1	610	47/66	0.74	0.15	101,105,111,114	0
12	LUT	2	501	42/42	0.75	0.16	117,120,125,127	0
19	SQD	1	811	40/54	0.75	0.15	100,104,109,109	0
14	BCR	A	4004	40/40	0.75	0.29	136,156,183,186	0
15	CLA	A	1111	49/65	0.76	0.18	122,129,139,142	0
15	CLA	B	1203	49/65	0.76	0.20	112,118,123,126	0
17	LHG	2	801	21/49	0.76	0.14	121,128,134,137	0
14	BCR	A	4007	40/40	0.76	0.29	125,132,135,137	0
15	CLA	4	607	49/65	0.76	0.16	92,98,104,105	0
15	CLA	B	1224	49/65	0.76	0.24	106,114,119,121	0
15	CLA	A	1108	46/65	0.77	0.21	123,132,140,143	0
15	CLA	2	605	65/65	0.77	0.18	95,100,104,108	0
12	LUT	3	501	42/42	0.77	0.18	173,180,186,189	0
16	CHL	3	604	47/66	0.77	0.19	157,171,179,185	0
15	CLA	3	611	46/65	0.77	0.18	147,154,162,167	0
21	DGD	2	811	47/66	0.77	0.15	122,126,134,137	0
15	CLA	3	606	45/65	0.77	0.14	156,165,173,177	0
15	CLA	B	1208	49/65	0.77	0.14	131,141,150,152	0
15	CLA	B	1211	49/65	0.77	0.18	127,137,141,143	0
15	CLA	A	1130	55/65	0.77	0.14	157,163,172,174	0
15	CLA	B	1219	49/65	0.77	0.13	95,103,107,108	0
15	CLA	B	1230	49/65	0.78	0.17	81,83,85,86	0
15	CLA	3	601	49/65	0.78	0.15	165,175,188,190	0
20	CAC	4	901	5/5	0.78	0.17	133,136,139,139	0
15	CLA	4	615	55/65	0.78	0.20	82,84,86,87	0
14	BCR	J	4002	40/40	0.78	0.20	88,91,99,100	0
13	XAT	2	502	44/44	0.79	0.21	103,107,110,110	0
14	BCR	A	4003	40/40	0.79	0.31	116,130,150,152	0
17	LHG	A	5001	16/49	0.79	0.14	165,168,172,175	0
15	CLA	2	608	49/65	0.79	0.17	128,136,143,146	0
25	PQN	B	2002	33/33	0.79	0.19	117,129,134,136	0
15	CLA	A	1115	49/65	0.80	0.14	160,166,178,179	0
15	CLA	B	1239	65/65	0.80	0.19	120,125,155,163	0
15	CLA	3	613	46/65	0.80	0.16	150,153,186,194	0
15	CLA	B	1215	49/65	0.80	0.25	105,112,119,121	0
15	CLA	2	606	46/65	0.80	0.16	105,111,116,119	0
15	CLA	A	1124	49/65	0.80	0.17	123,133,142,148	0
15	CLA	B	1205	49/65	0.80	0.22	122,126,132,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CLA	1	601	49/65	0.80	0.14	111,114,118,119	0
15	CLA	1	607	46/65	0.81	0.17	99,104,109,111	0
15	CLA	A	1132	49/65	0.81	0.12	137,148,163,168	0
15	CLA	A	1134	49/65	0.81	0.15	162,171,183,186	0
15	CLA	B	1240	65/65	0.81	0.18	84,92,97,99	0
15	CLA	F	1302	49/65	0.81	0.15	81,83,86,86	0
15	CLA	A	1101	45/65	0.81	0.20	90,95,99,100	0
14	BCR	B	4002	40/40	0.81	0.25	114,129,145,146	0
13	XAT	3	502	44/44	0.81	0.31	154,161,165,166	0
25	PQN	A	2001	33/33	0.81	0.27	87,91,98,99	0
15	CLA	2	615	50/65	0.81	0.18	112,124,141,146	0
15	CLA	2	604	49/65	0.82	0.13	104,111,117,119	0
16	CHL	2	610	50/66	0.82	0.14	97,100,102,103	0
15	CLA	3	612	55/65	0.82	0.22	135,143,151,153	0
15	CLA	A	1113	45/65	0.82	0.16	147,155,160,161	0
15	CLA	1	605	48/65	0.82	0.15	93,97,101,103	0
15	CLA	4	606	49/65	0.82	0.13	89,94,97,98	0
15	CLA	A	1116	49/65	0.82	0.20	136,151,156,161	0
15	CLA	B	1237	49/65	0.82	0.12	140,150,158,161	0
14	BCR	A	4005	40/40	0.82	0.33	129,142,162,163	0
14	BCR	3	504	40/40	0.82	0.25	137,152,173,173	0
13	XAT	4	502	44/44	0.82	0.21	83,84,88,89	0
15	CLA	A	1129	48/65	0.82	0.18	147,160,175,178	0
15	CLA	4	601	49/65	0.83	0.12	92,95,100,101	0
14	BCR	F	4002	40/40	0.83	0.18	80,81,81,82	0
15	CLA	3	610	49/65	0.83	0.18	134,143,160,173	0
15	CLA	4	612	49/65	0.83	0.15	81,84,85,86	0
13	XAT	1	502	44/44	0.83	0.19	89,97,109,110	0
15	CLA	A	1136	49/65	0.83	0.12	140,148,154,159	0
15	CLA	1	603	45/65	0.83	0.15	91,95,97,99	0
14	BCR	B	4005	40/40	0.83	0.29	92,95,99,101	0
16	CHL	4	613	50/66	0.83	0.13	86,91,96,98	0
15	CLA	A	1109	49/65	0.83	0.13	103,111,114,115	0
15	CLA	B	1229	65/65	0.84	0.16	80,81,82,83	0
15	CLA	B	1209	46/65	0.84	0.13	130,133,140,141	0
15	CLA	B	1232	49/65	0.84	0.18	92,99,103,105	0
15	CLA	A	1126	49/65	0.84	0.23	98,106,108,108	0
17	LHG	B	5001	21/49	0.84	0.12	88,89,92,93	0
14	BCR	B	4006	40/40	0.84	0.26	80,83,89,90	0
21	DGD	B	5002	38/66	0.84	0.14	114,119,125,127	0
14	BCR	A	4006	40/40	0.84	0.28	83,91,102,103	0
15	CLA	A	1137	49/65	0.84	0.16	137,144,151,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CLA	B	1220	55/65	0.84	0.16	91,98,102,103	0
15	CLA	4	604	49/65	0.84	0.17	82,86,89,89	0
15	CLA	B	1226	49/65	0.84	0.17	105,112,118,120	0
16	CHL	2	613	46/66	0.84	0.14	100,102,103,105	0
15	CLA	2	607	49/65	0.85	0.14	125,132,139,141	0
15	CLA	B	1023	60/65	0.85	0.19	113,126,138,141	0
15	CLA	A	1119	49/65	0.85	0.15	140,151,159,162	0
15	CLA	A	1112	49/65	0.85	0.16	124,131,141,144	0
15	CLA	A	1102	45/65	0.85	0.19	100,106,109,111	0
15	CLA	B	1221	49/65	0.85	0.17	99,108,113,115	0
15	CLA	J	1302	49/65	0.85	0.13	86,89,91,92	0
15	CLA	B	1206	49/65	0.85	0.15	131,139,145,148	0
15	CLA	A	1122	49/65	0.85	0.15	144,154,161,164	0
15	CLA	1	612	60/65	0.85	0.15	97,105,110,112	0
15	CLA	2	601	49/65	0.85	0.14	110,116,125,129	0
16	CHL	4	610	47/66	0.85	0.14	82,85,87,87	0
17	LHG	1	801	23/49	0.86	0.15	95,99,101,103	0
15	CLA	B	1022	50/65	0.86	0.20	108,116,124,126	0
15	CLA	4	609	49/65	0.86	0.17	87,92,96,97	0
15	CLA	A	1133	49/65	0.86	0.18	147,157,165,169	0
15	CLA	B	1228	60/65	0.86	0.16	79,82,84,85	0
15	CLA	A	1128	49/65	0.86	0.23	102,113,116,117	0
15	CLA	B	1216	49/65	0.86	0.15	97,105,108,108	0
15	CLA	4	602	49/65	0.86	0.11	95,99,104,107	0
15	CLA	B	1234	49/65	0.86	0.16	86,91,94,95	0
15	CLA	A	1123	48/65	0.86	0.20	128,139,146,148	0
16	CHL	4	611	50/66	0.86	0.14	88,92,96,99	0
15	CLA	1	602	46/65	0.86	0.13	106,110,115,118	0
15	CLA	B	1227	45/65	0.87	0.13	85,88,91,92	0
15	CLA	4	605	49/65	0.87	0.14	80,82,83,84	0
16	CHL	2	611	48/66	0.87	0.17	103,104,111,114	0
15	CLA	A	1140	55/65	0.87	0.20	89,93,98,100	0
15	CLA	1	613	45/65	0.87	0.11	109,119,126,129	0
15	CLA	F	1301	47/65	0.87	0.16	81,82,83,85	0
15	CLA	B	1217	46/65	0.87	0.10	121,128,132,134	0
15	CLA	A	1125	49/65	0.87	0.22	137,141,146,148	0
15	CLA	4	608	46/65	0.88	0.11	92,96,101,103	0
16	CHL	2	609	50/66	0.88	0.13	119,129,136,138	0
15	CLA	A	1135	49/65	0.88	0.15	126,139,154,160	0
15	CLA	A	1118	49/65	0.88	0.16	151,164,172,175	0
15	CLA	1	608	46/65	0.88	0.12	91,96,101,103	0
15	CLA	2	603	46/65	0.88	0.14	115,122,128,129	0

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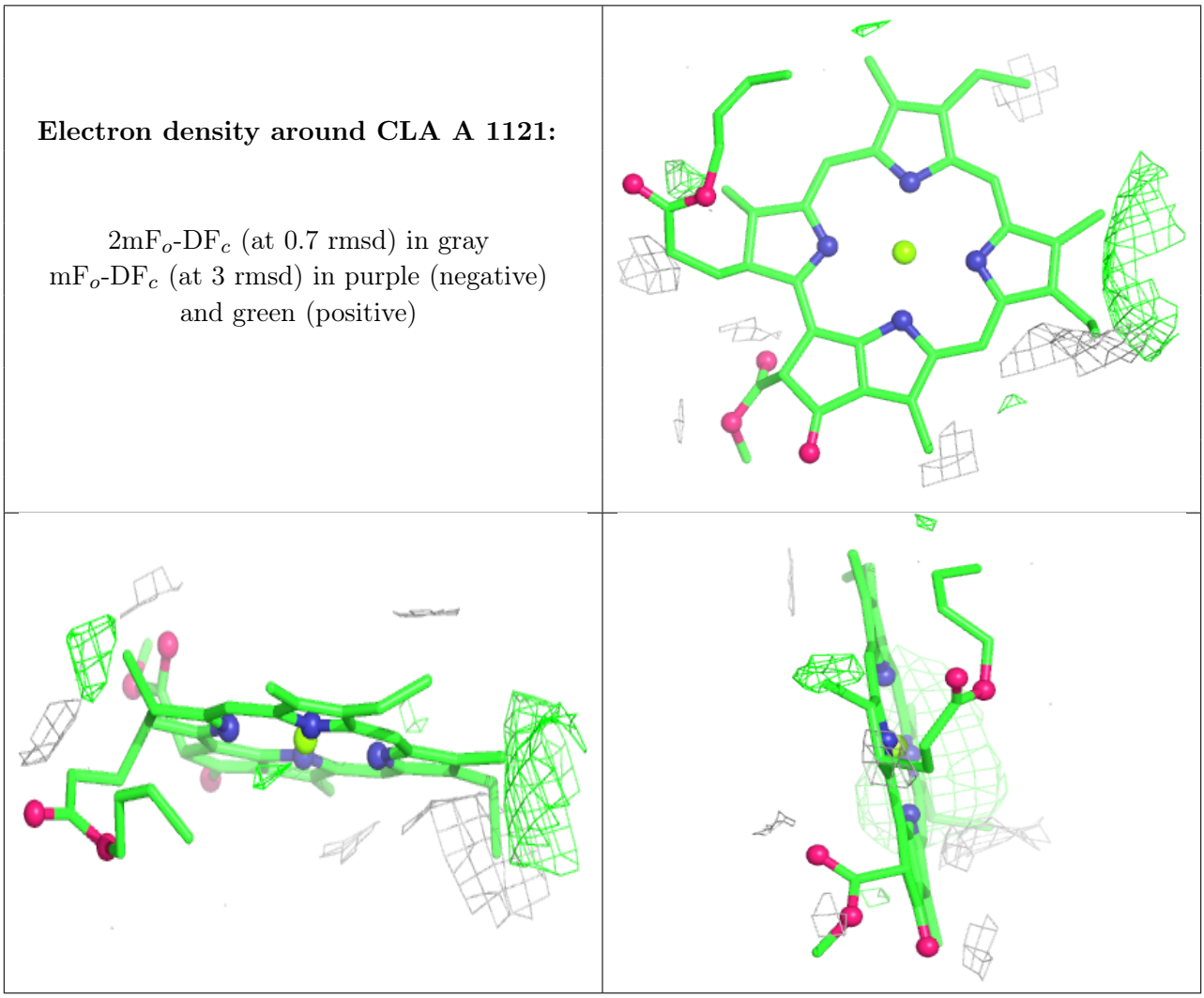
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CLA	1	611	49/65	0.88	0.13	110,118,124,126	0
15	CLA	2	612	49/65	0.88	0.16	91,97,100,102	0
15	CLA	B	1213	49/65	0.88	0.17	111,117,123,125	0
15	CLA	1	606	45/65	0.88	0.12	110,116,120,122	0
15	CLA	A	1105	49/65	0.88	0.12	94,98,104,105	0
15	CLA	A	1117	49/65	0.89	0.20	132,136,143,147	0
14	BCR	B	4004	40/40	0.89	0.20	92,94,97,98	0
15	CLA	B	1212	45/65	0.89	0.16	128,138,147,148	0
15	CLA	A	1106	65/65	0.89	0.21	89,98,104,105	0
15	CLA	A	1110	49/65	0.89	0.14	140,149,157,161	0
15	CLA	B	1223	50/65	0.89	0.18	91,97,99,101	0
16	CHL	1	609	50/66	0.89	0.13	88,91,96,97	0
15	CLA	A	1139	52/65	0.89	0.18	85,88,91,92	0
15	CLA	B	1236	49/65	0.89	0.15	83,87,90,90	0
15	CLA	B	1225	49/65	0.89	0.23	108,114,122,126	0
15	CLA	B	1021	65/65	0.90	0.19	89,103,107,108	0
15	CLA	B	1204	49/65	0.90	0.14	134,146,151,153	0
15	CLA	A	1104	60/65	0.90	0.20	103,109,115,118	0
15	CLA	B	1214	49/65	0.91	0.20	102,105,111,112	0
15	CLA	3	615	46/65	0.91	0.15	118,127,131,133	0
15	CLA	B	1235	60/65	0.91	0.12	80,83,86,87	0
15	CLA	A	1012	60/65	0.91	0.19	89,92,98,100	0
15	CLA	A	1013	65/65	0.91	0.17	86,90,97,99	0
15	CLA	A	1138	65/65	0.91	0.15	82,84,86,87	0
15	CLA	A	1107	49/65	0.91	0.17	85,91,94,96	0
24	CL0	A	1011	50/65	0.91	0.18	100,104,112,115	0
15	CLA	4	603	49/65	0.91	0.14	85,89,92,93	0
15	CLA	1	604	49/65	0.91	0.15	93,95,97,98	0
15	CLA	B	1202	49/65	0.92	0.17	111,117,121,125	0
15	CLA	A	1103	55/65	0.92	0.17	111,121,125,128	0
15	CLA	B	1210	49/65	0.92	0.12	116,124,127,128	0
15	CLA	A	1127	49/65	0.92	0.18	109,118,123,125	0
27	CA	B	6000	1/1	0.92	0.14	97,97,97,97	0
17	LHG	A	5002	24/49	0.93	0.18	99,105,107,108	0
15	CLA	3	605	46/65	0.93	0.16	142,151,156,159	0
15	CLA	B	1231	60/65	0.93	0.16	88,95,99,101	0
15	CLA	B	1222	49/65	0.94	0.12	87,93,96,96	0
26	SF4	C	3003	8/8	0.96	0.09	115,117,119,120	0
26	SF4	A	3001	8/8	0.98	0.07	108,110,111,113	0
26	SF4	C	3002	8/8	0.98	0.06	121,123,127,198	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.

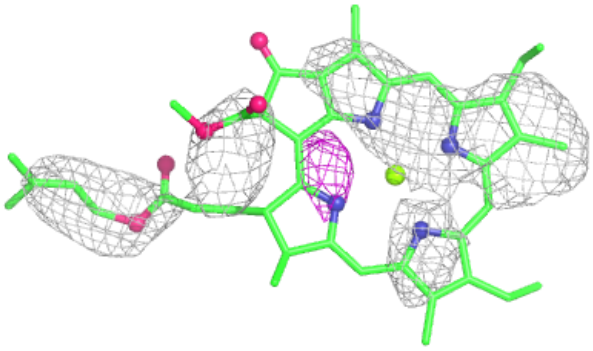
Electron density around CLA A 1121:

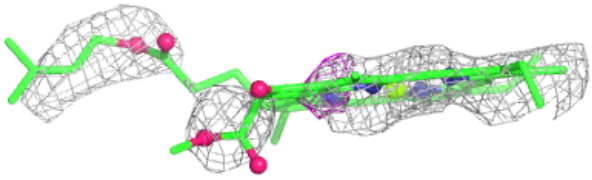
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

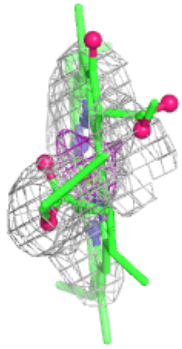


Electron density around CLA 3 607:

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

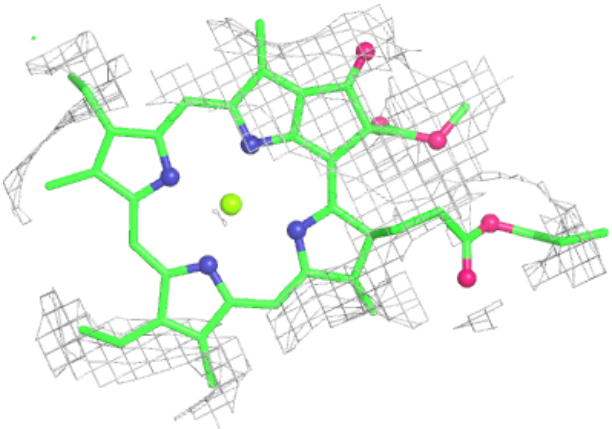


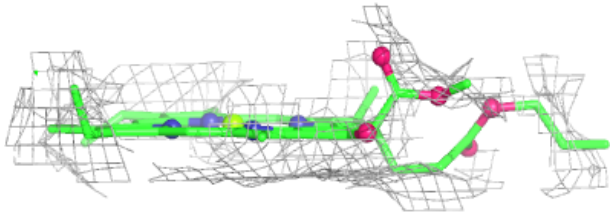


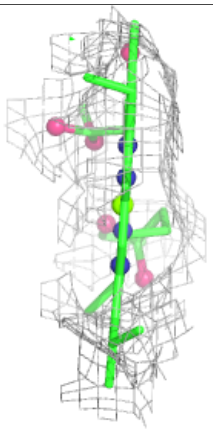


Electron density around CLA 3 608:

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

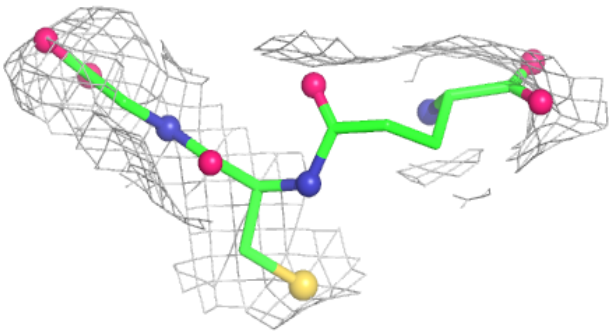


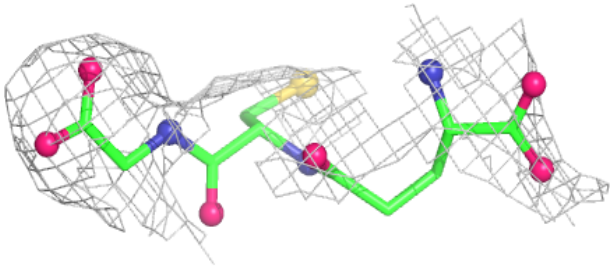


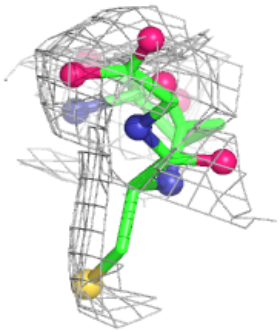


Electron density around GSH 4 831:

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

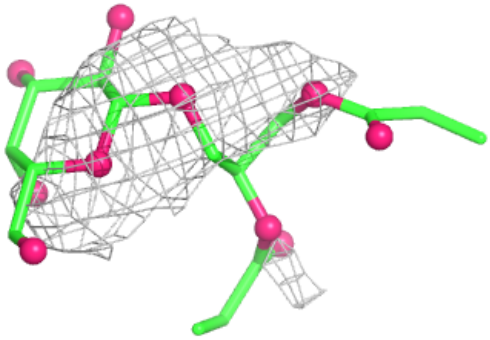


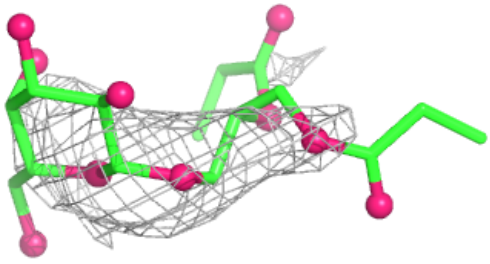


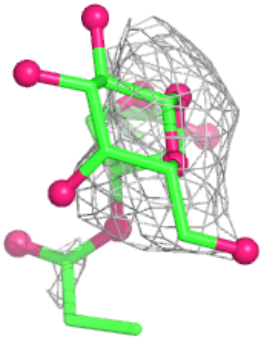


Electron density around LMG 2 802:

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

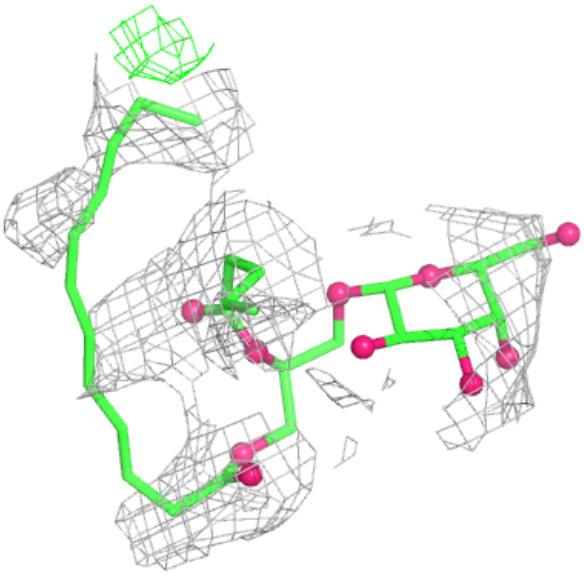


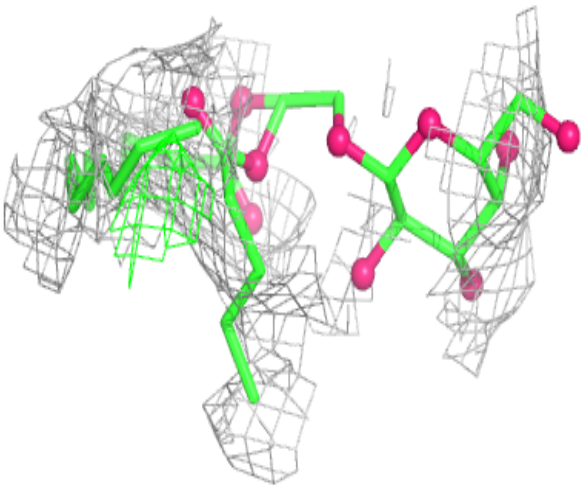




Electron density around LMG 1 802:

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

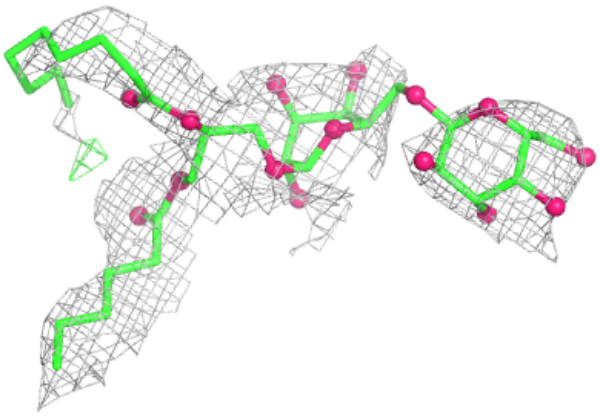


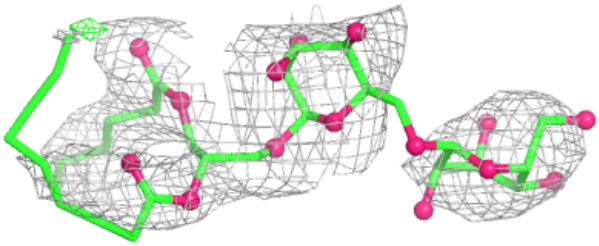


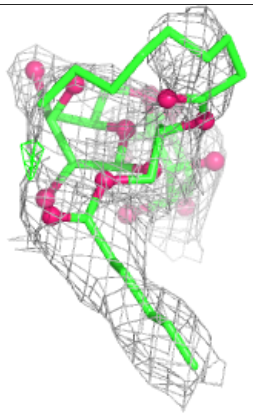


Electron density around DGD 4 811:

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

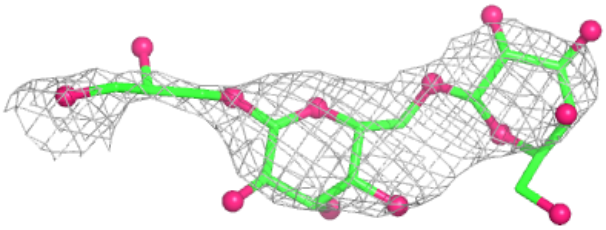


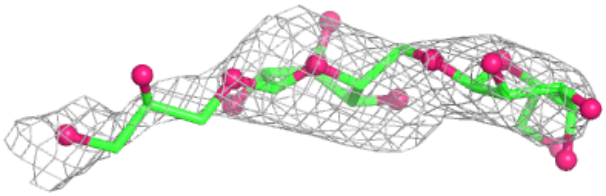


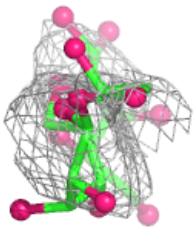


Electron density around DGD J 5001:

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

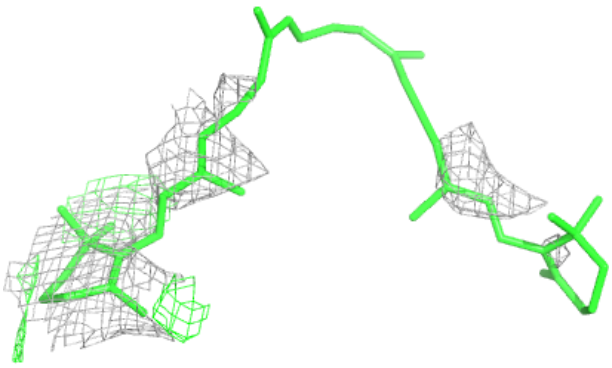


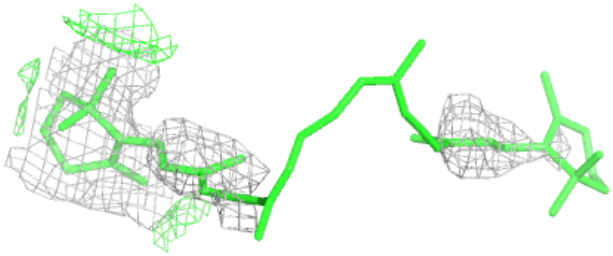


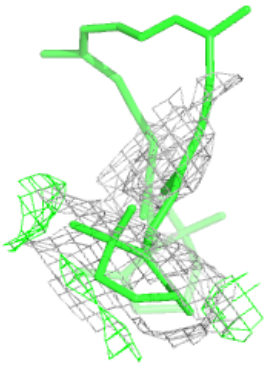


Electron density around BCR 4 505:

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

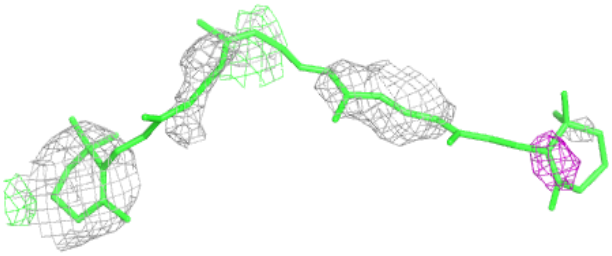


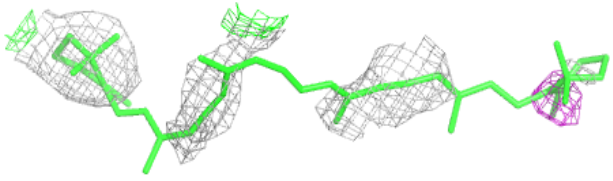


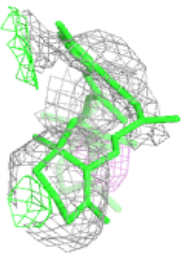


Electron density around BCR 1 505:

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

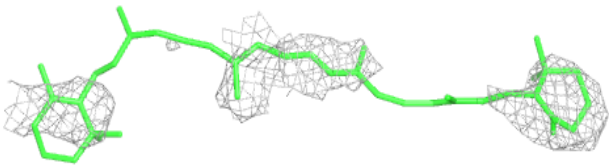


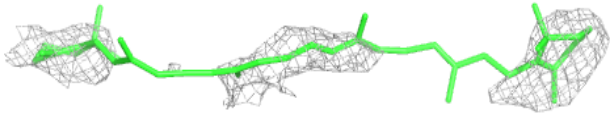


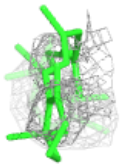


Electron density around BCR J 4003:

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

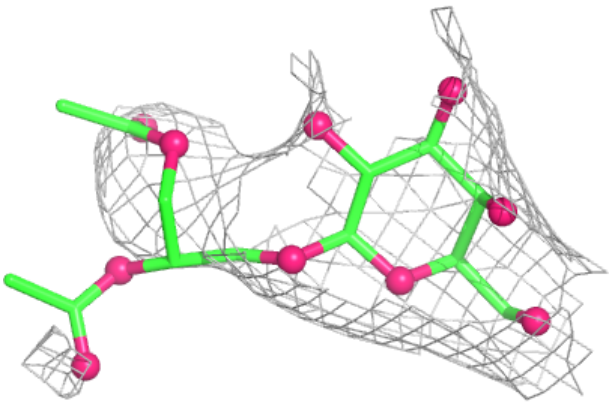


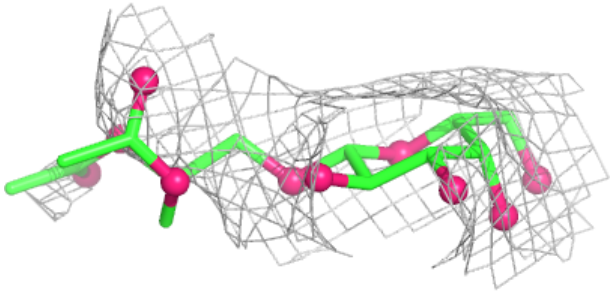


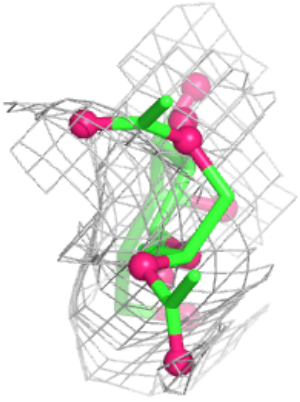


Electron density around LMG 1 803:

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

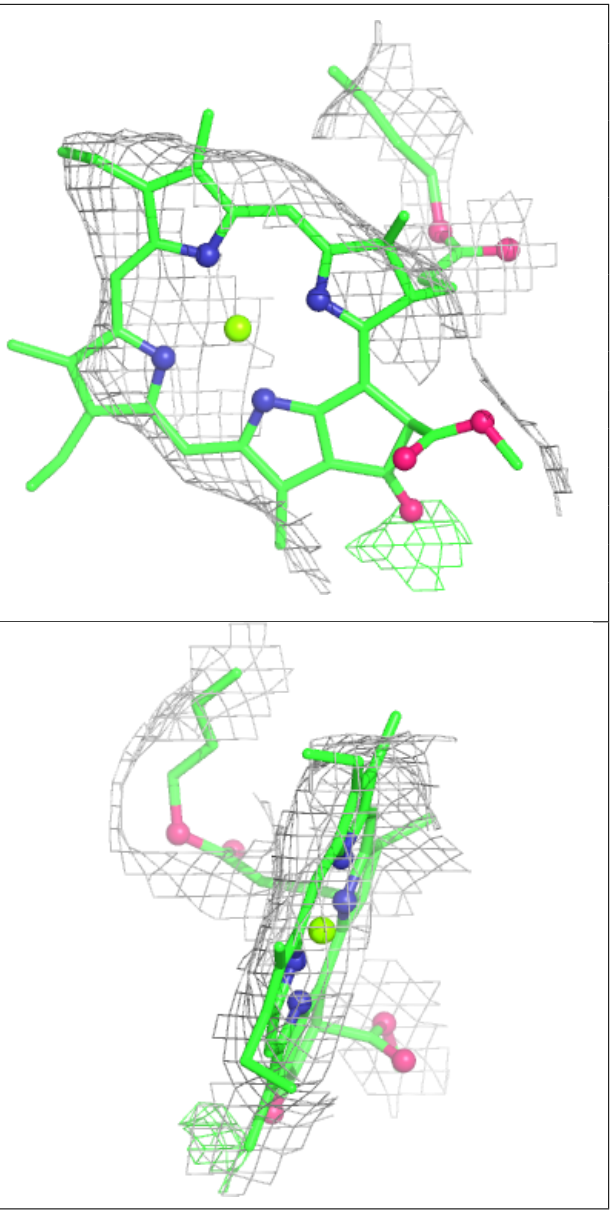


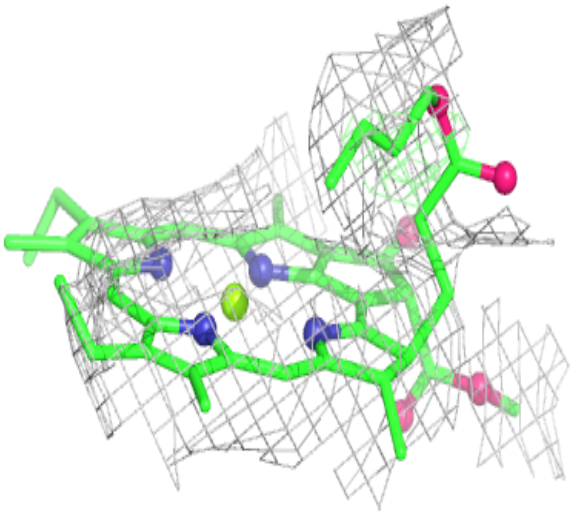




Electron density around CLA A 1120:

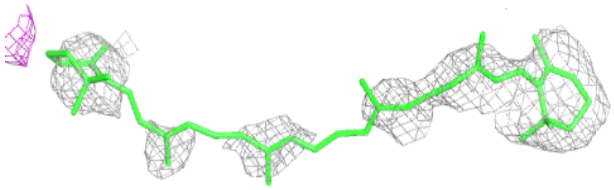
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

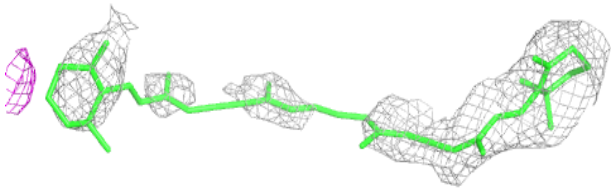


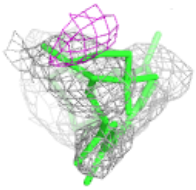


Electron density around BCR 4 503:

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

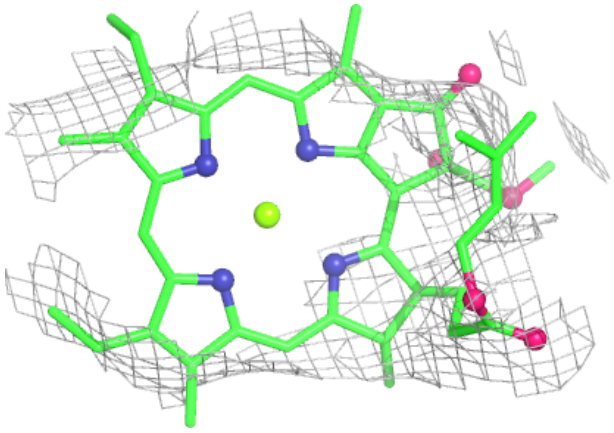


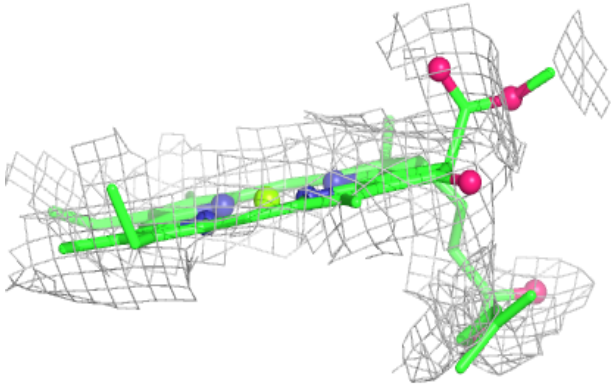


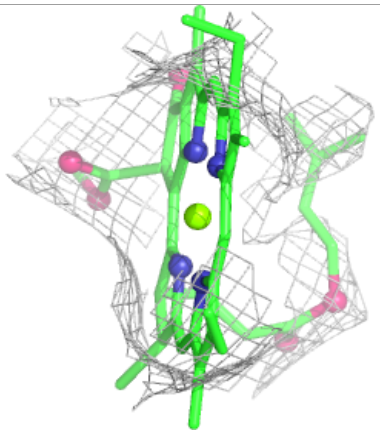


Electron density around CLA A 1141:

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

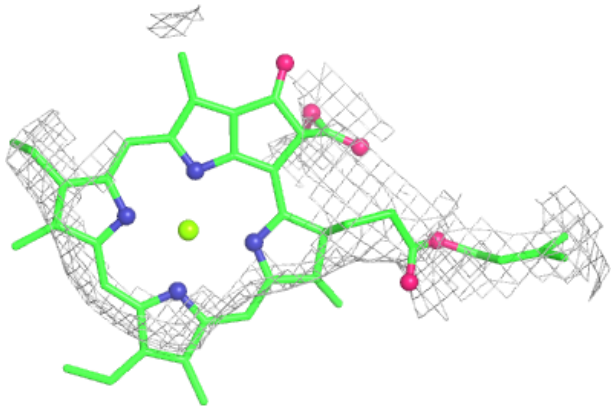


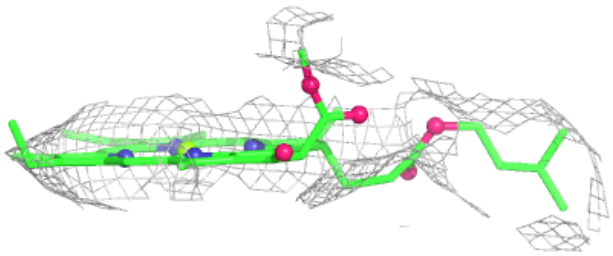


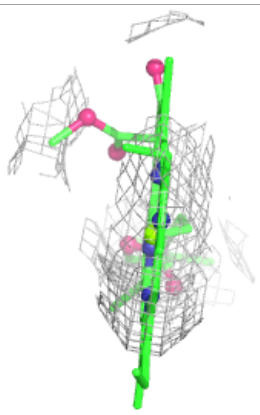


Electron density around CLA A 1131:

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

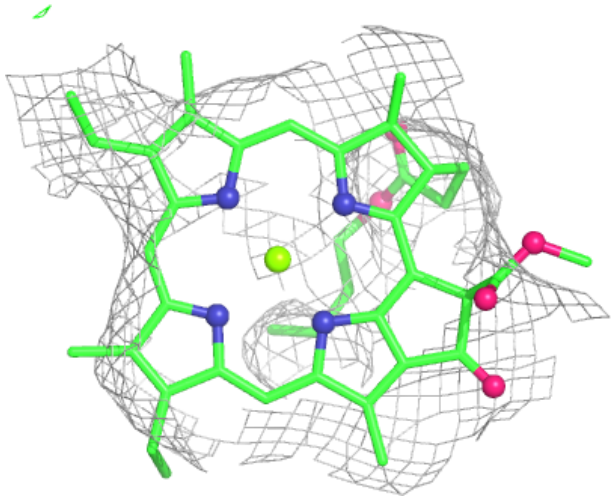


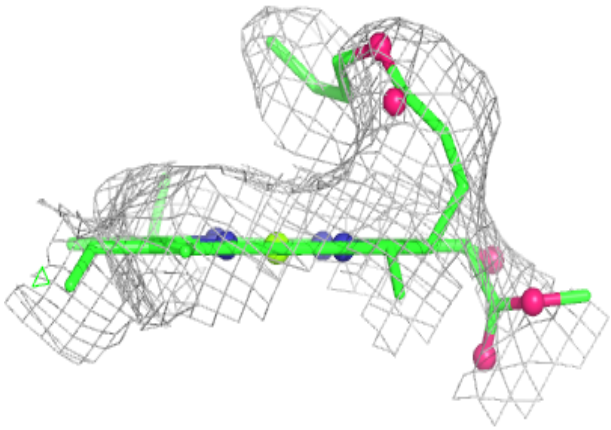


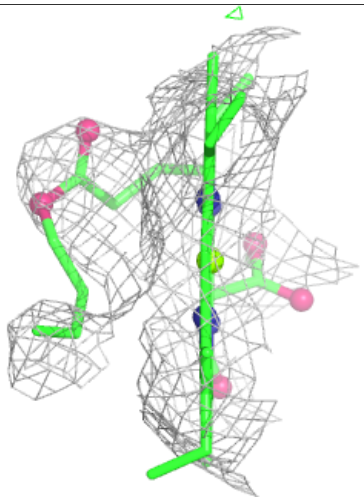


Electron density around CLA B 1218:

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

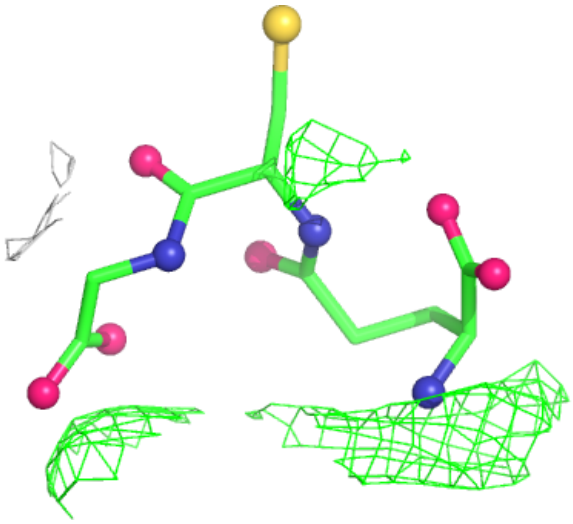


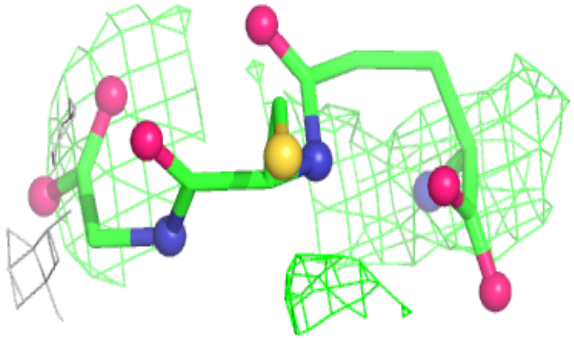


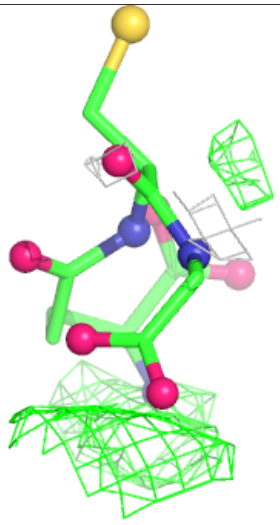


Electron density around GSH B 5031:

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

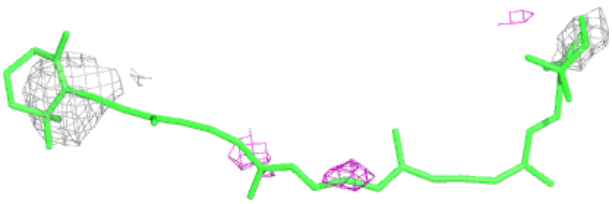


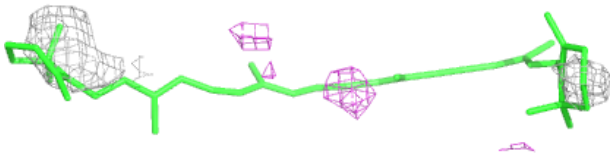


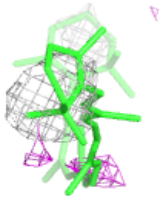


Electron density around BCR B 4003:

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

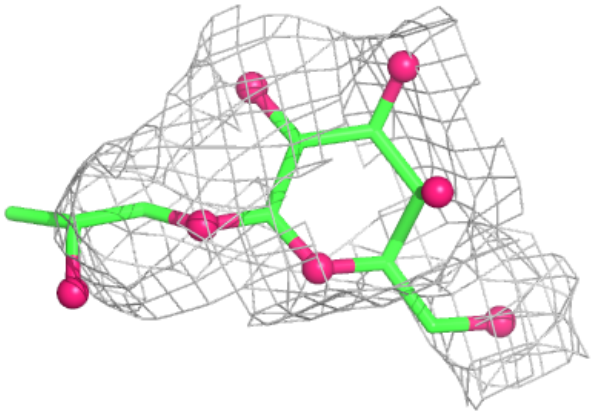


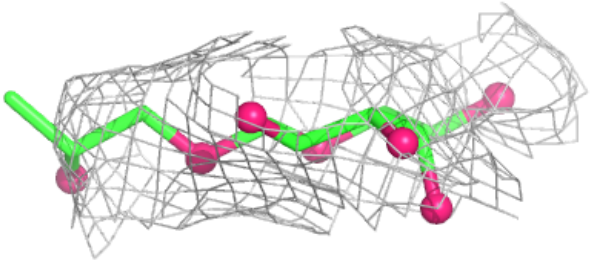


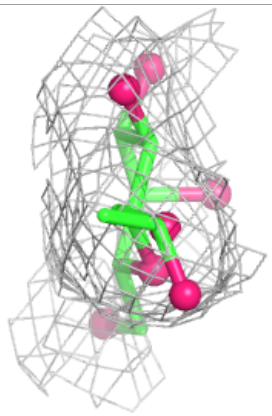


Electron density around LMG 2 803:

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

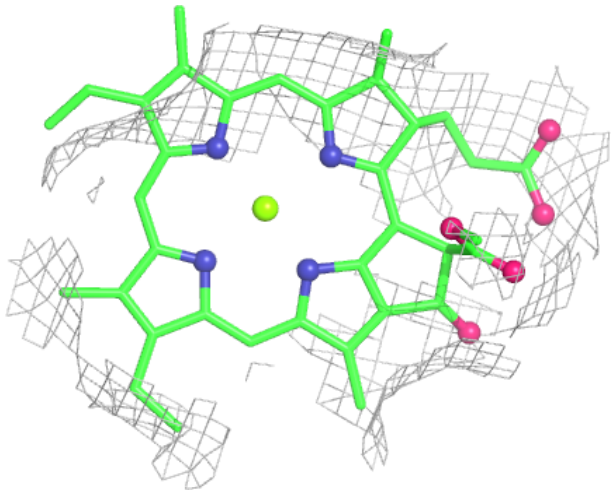


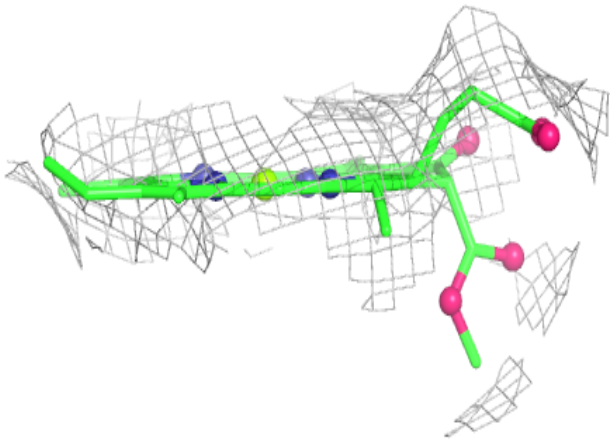


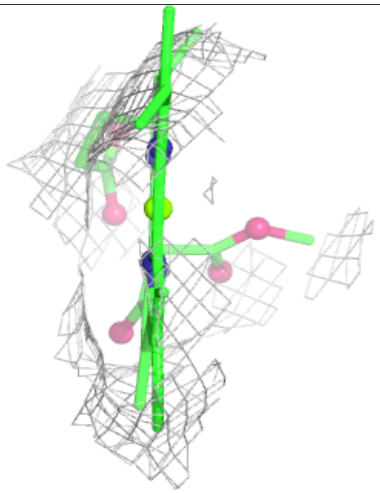


Electron density around CLA 3 603:

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

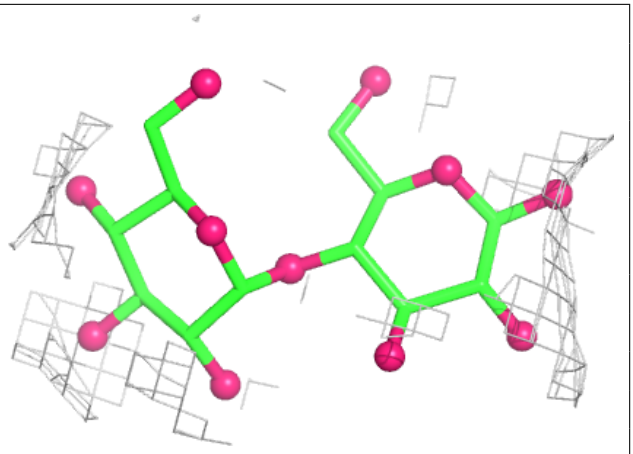


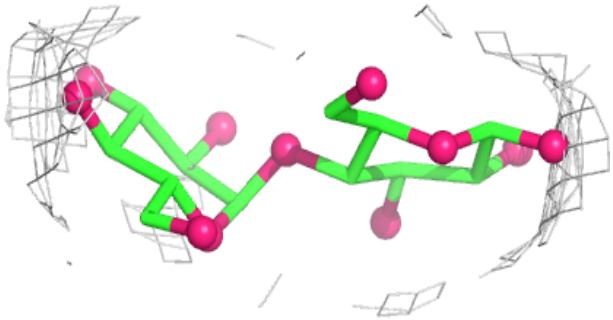


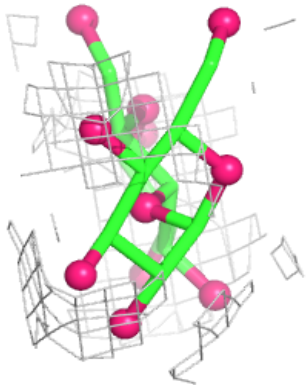


Electron density around LMT 2 821:

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

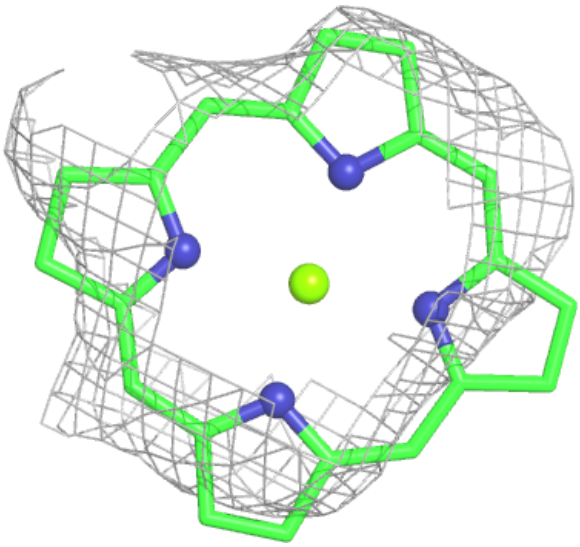


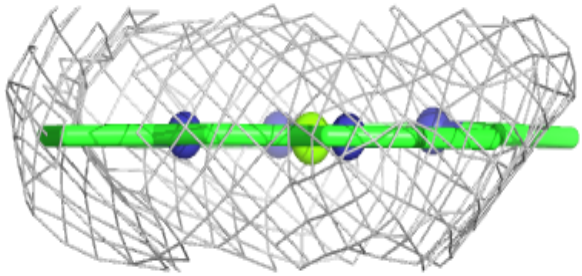


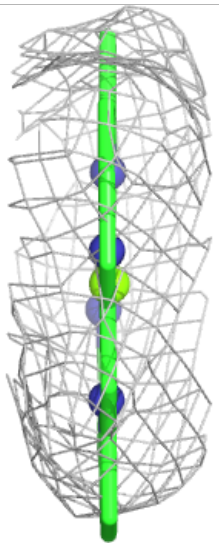


Electron density around CLA B 1207:

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

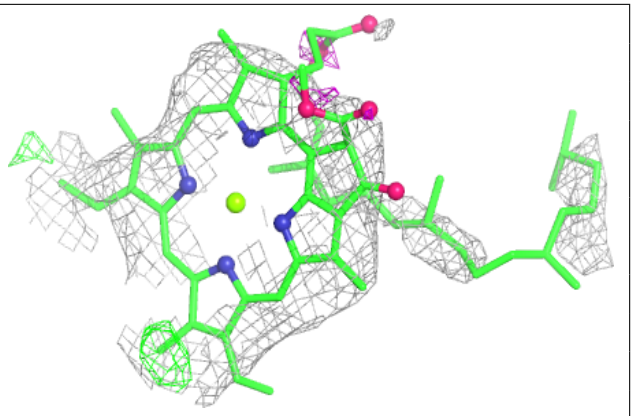


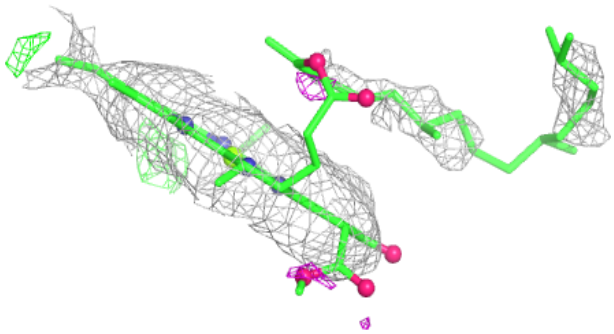


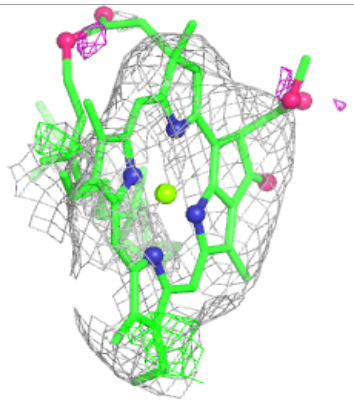


Electron density around CLA 1 615:

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

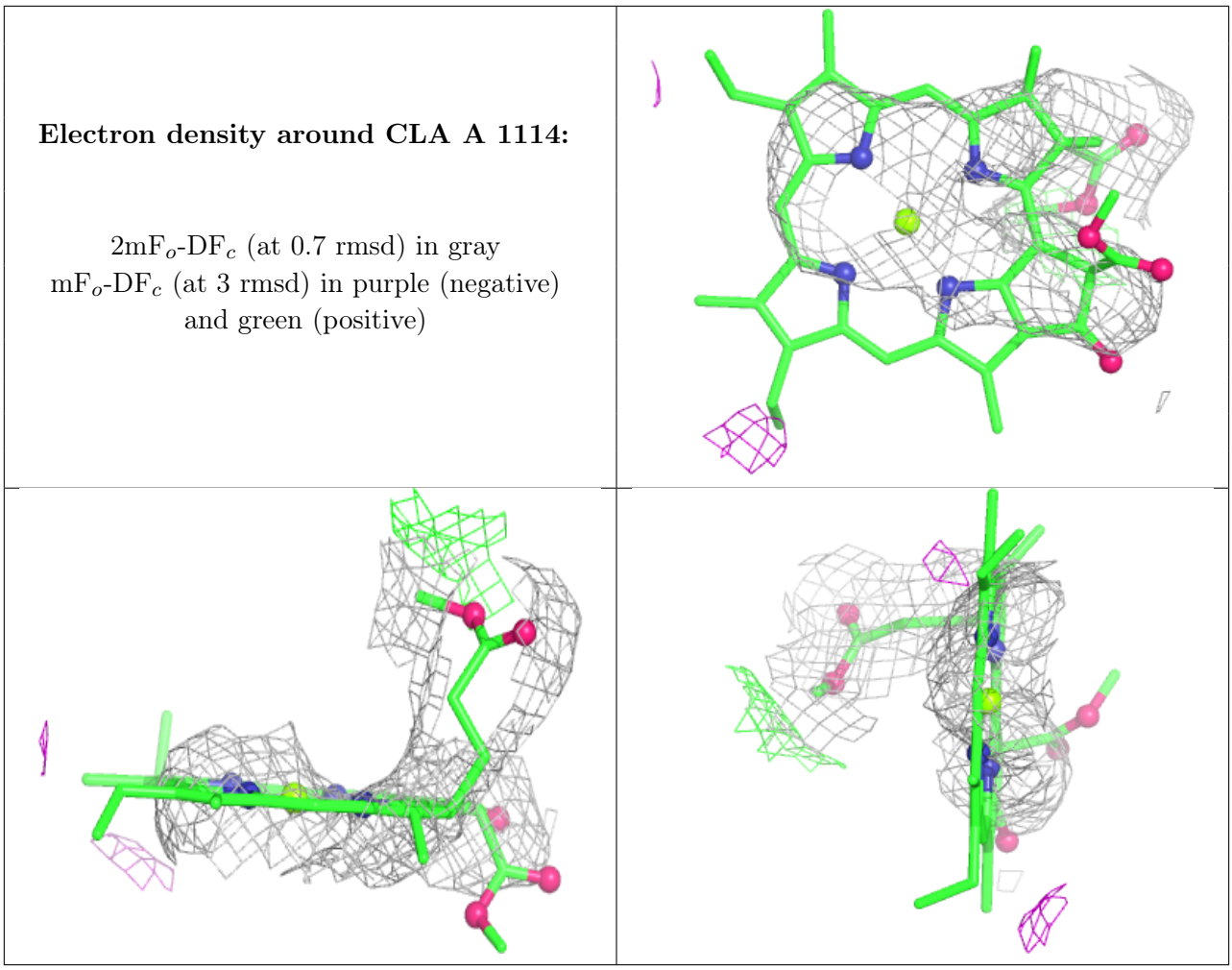






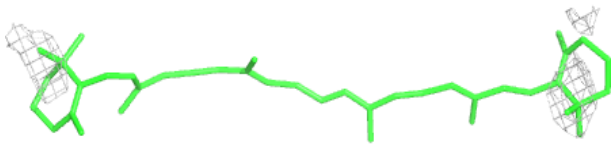
Electron density around CLA A 1114:

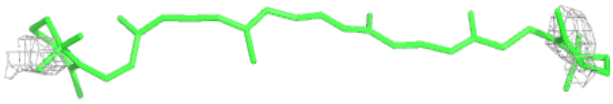
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

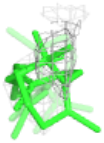


Electron density around BCR A 4002:

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

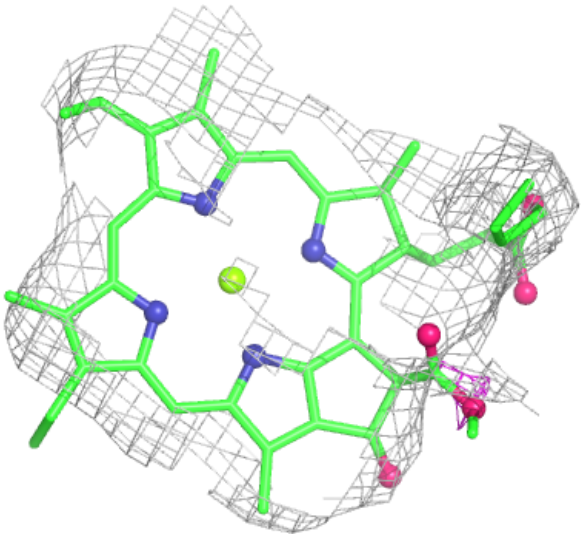


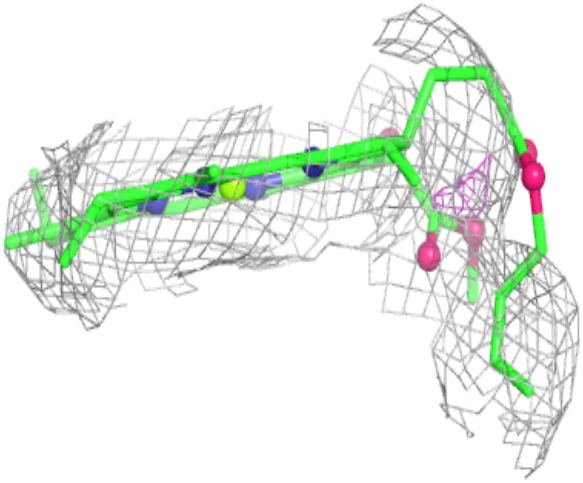


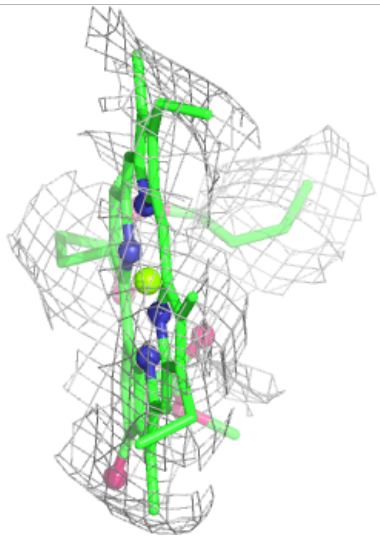


Electron density around CLA 2 602:

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

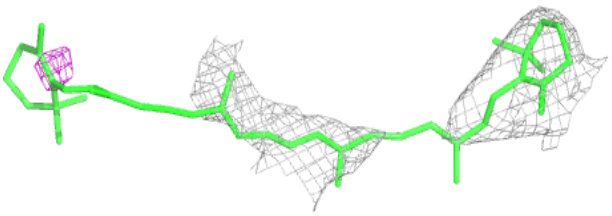


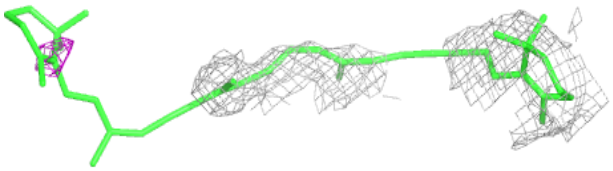


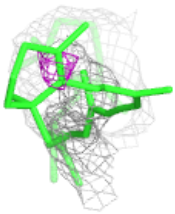


Electron density around BCR 1 503:

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

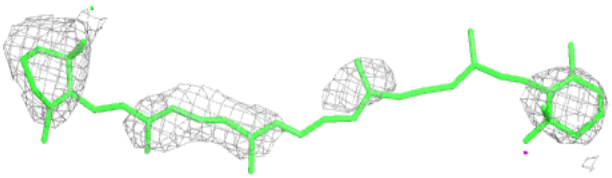


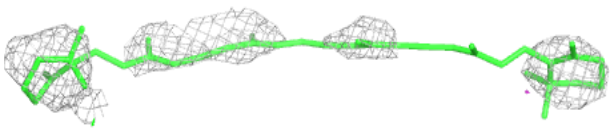


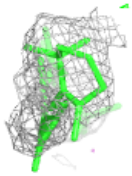


Electron density around BCR J 4001:

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

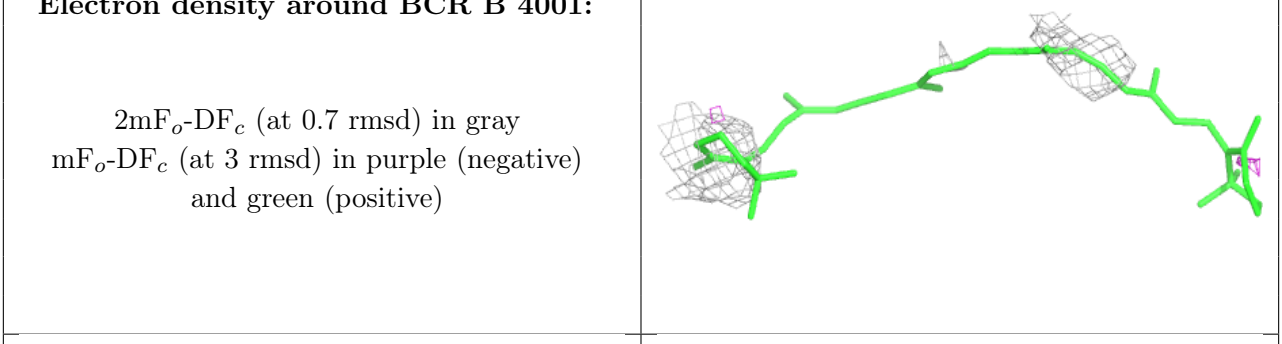






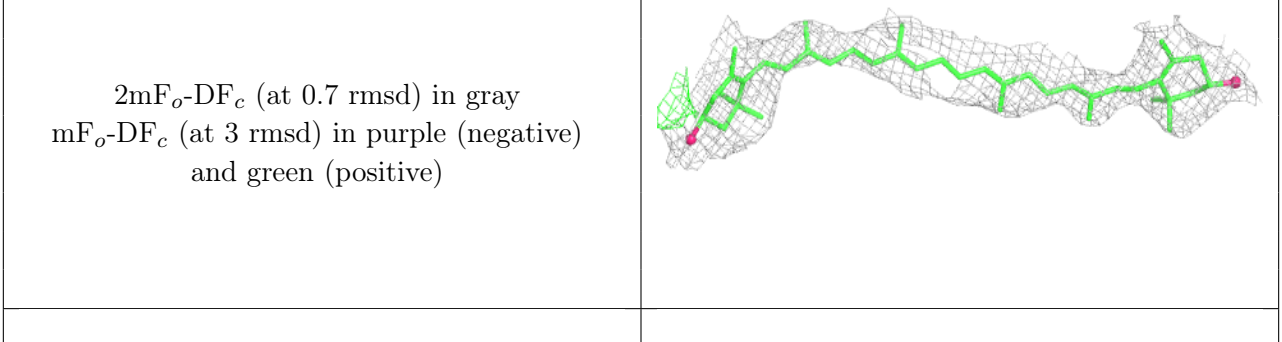
Electron density around BCR B 4001:

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



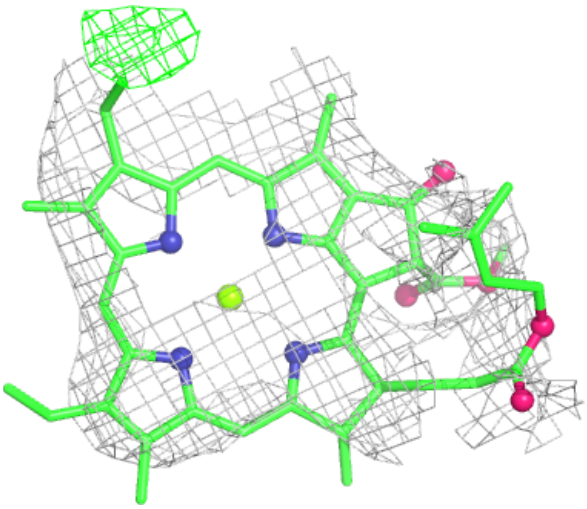
Electron density around LUT 4 501:

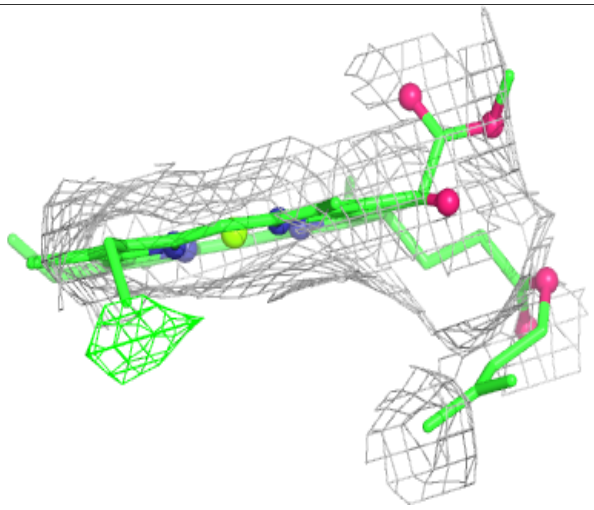
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

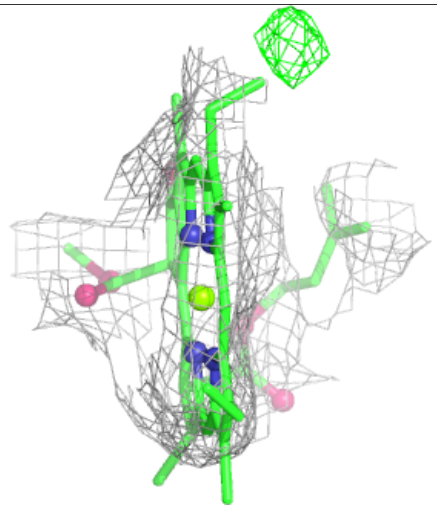


Electron density around CLA B 1238:

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

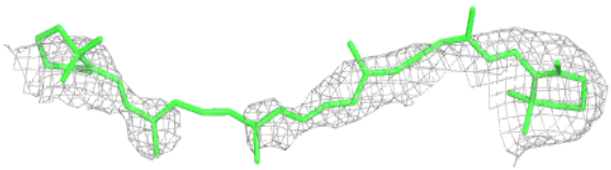


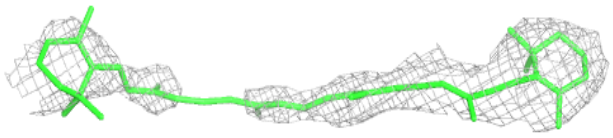


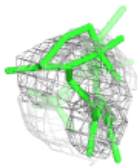


Electron density around BCR 2 503:

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

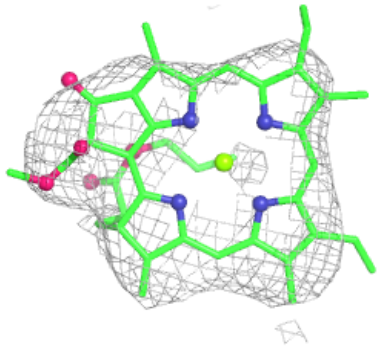


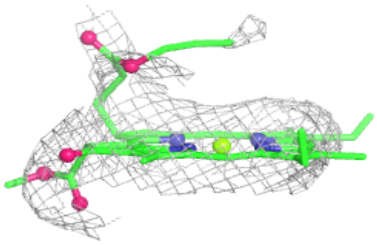


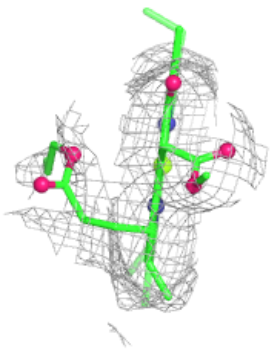


Electron density around CLA B 1201:

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

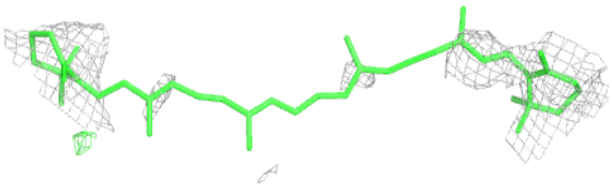


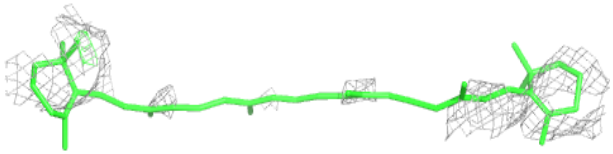


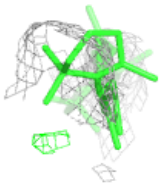


Electron density around BCR 3 503:

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

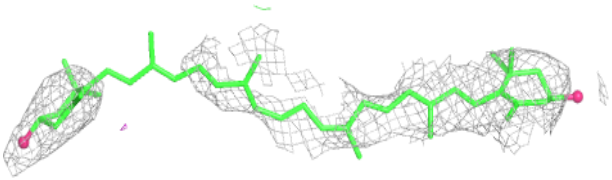


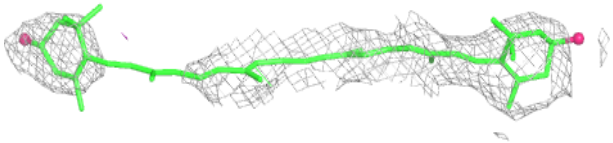


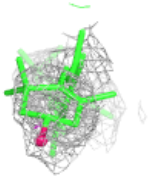


Electron density around LUT 1 501:

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

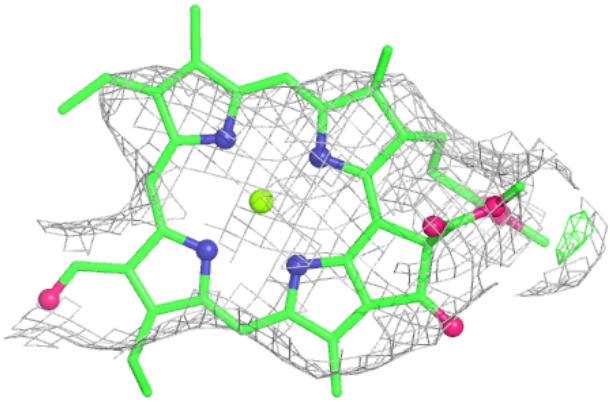


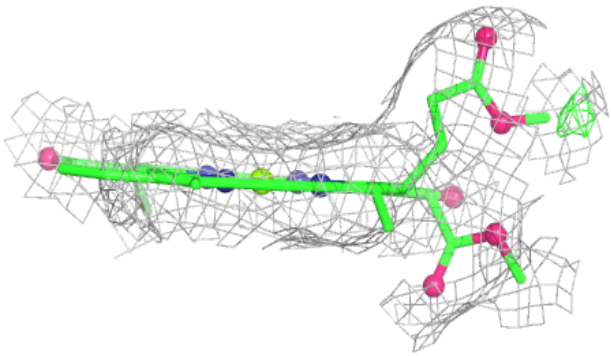


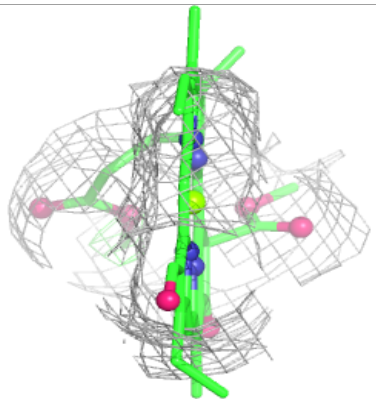


Electron density around CHL 1 610:

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

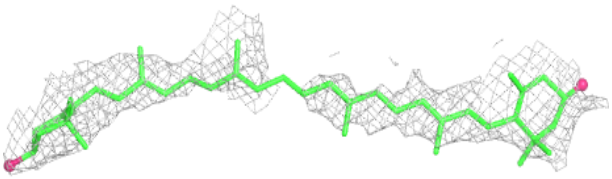


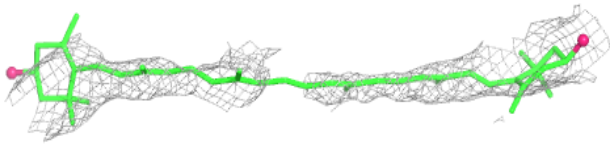


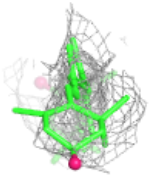


Electron density around LUT 2 501:

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

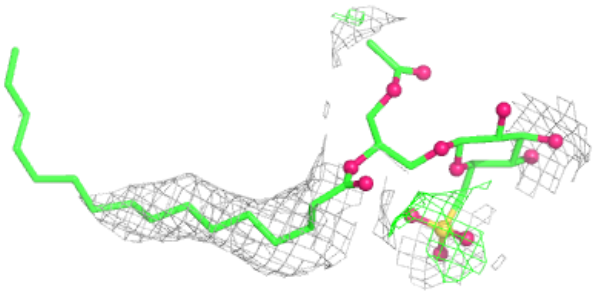


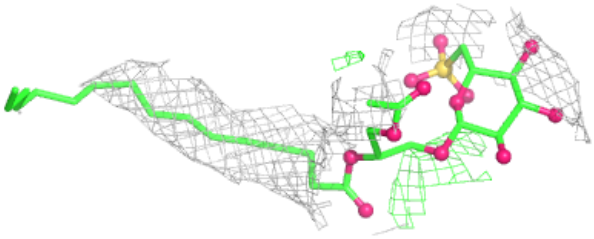


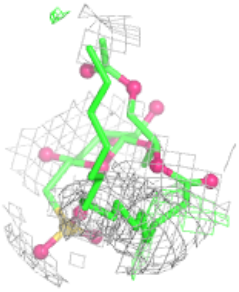


Electron density around SQD 1 811:

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

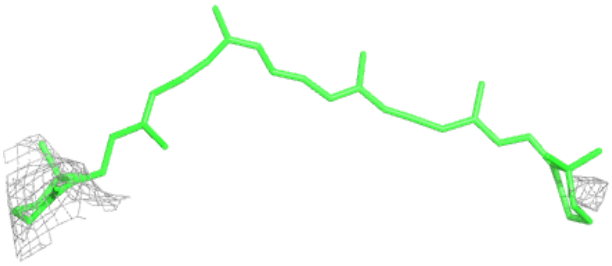


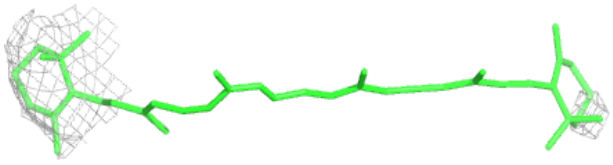


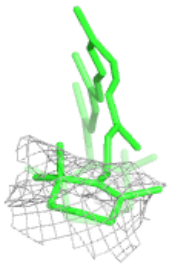


Electron density around BCR A 4004:

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

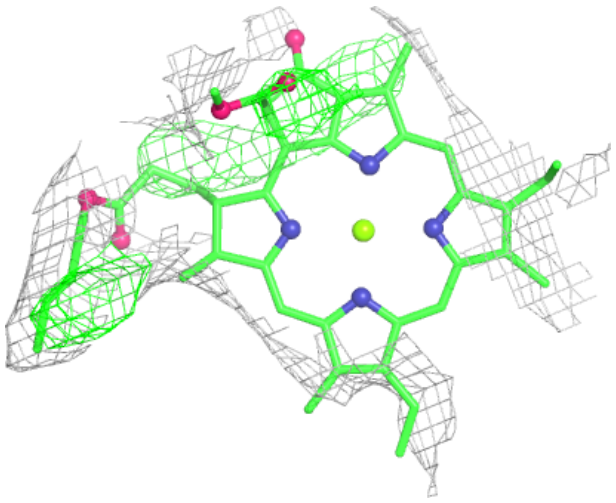


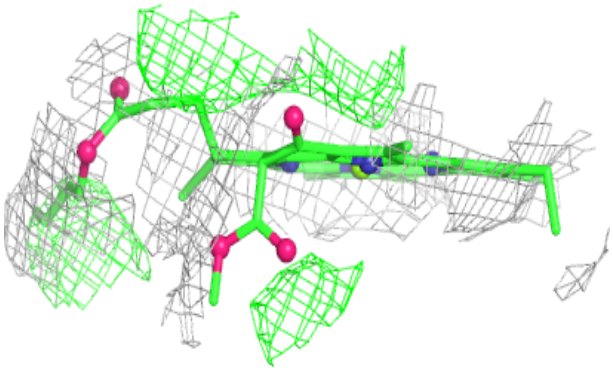


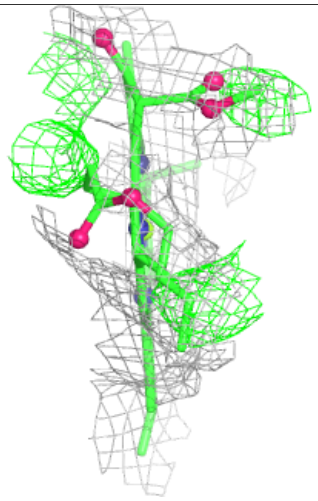


Electron density around CLA A 1111:

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

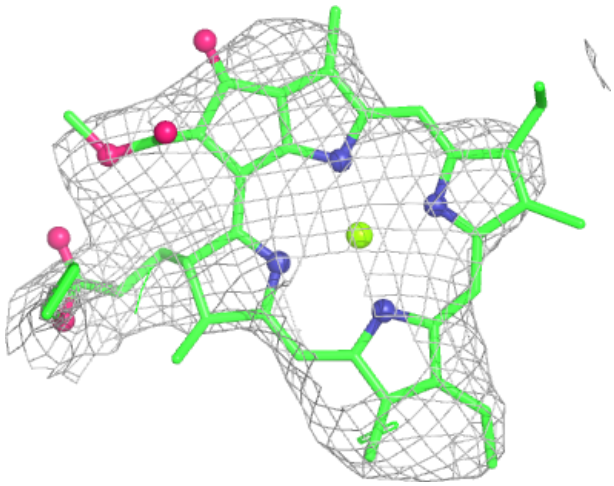


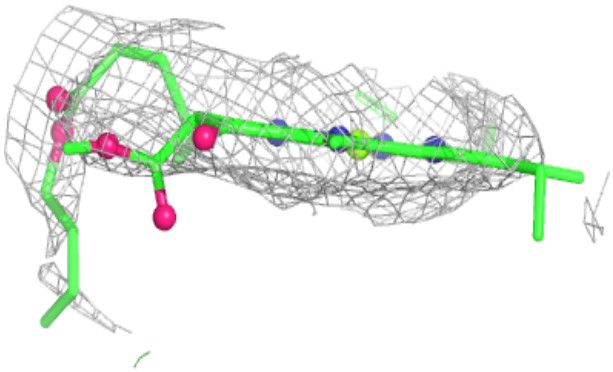


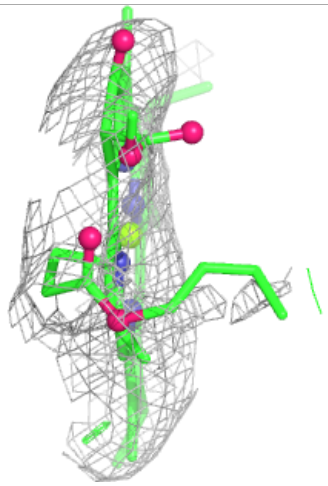


Electron density around CLA B 1203:

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

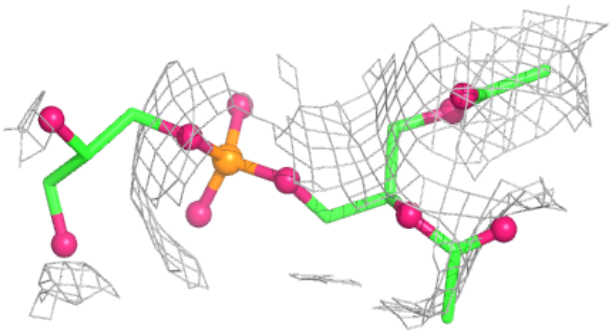


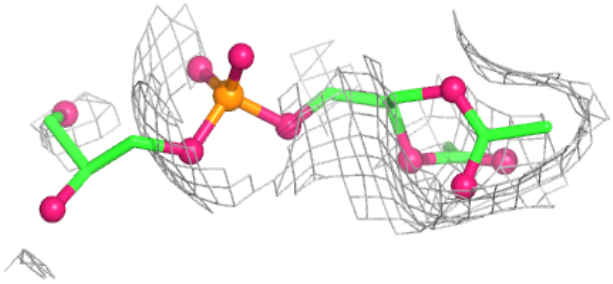


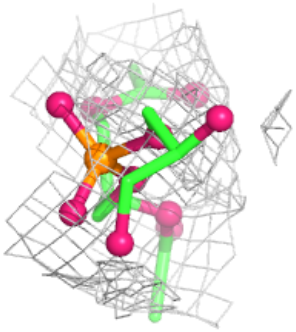


Electron density around LHG 2 801:

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

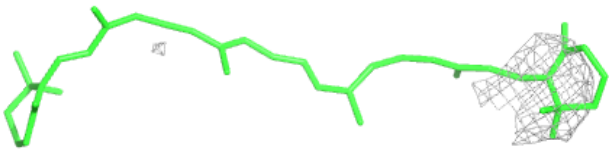


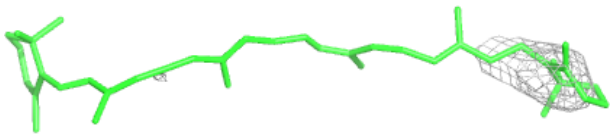


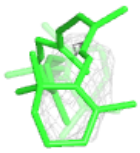


Electron density around BCR A 4007:

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

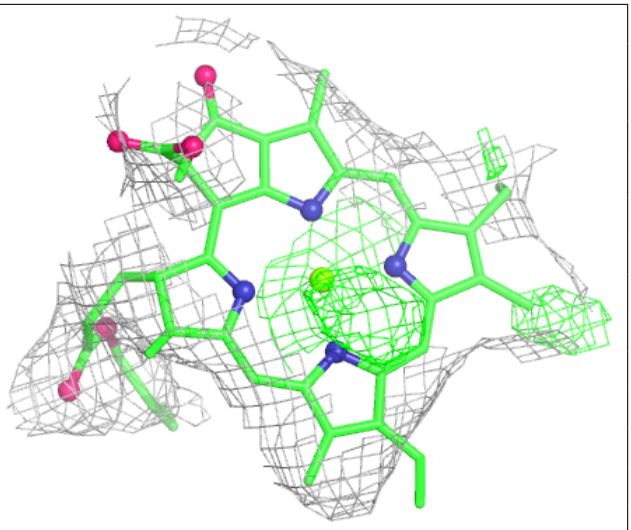


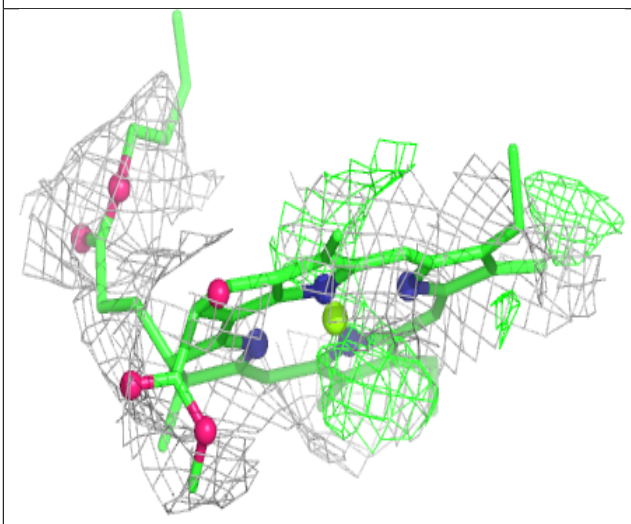


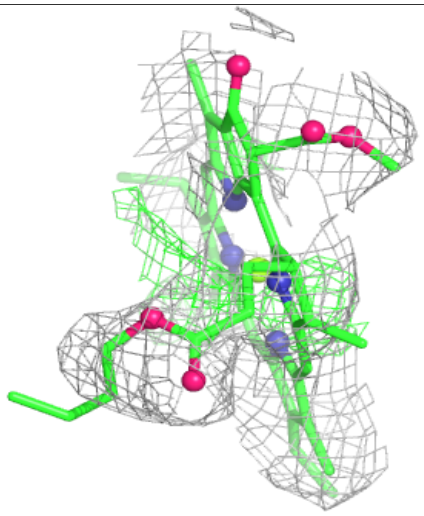


Electron density around CLA 4 607:

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

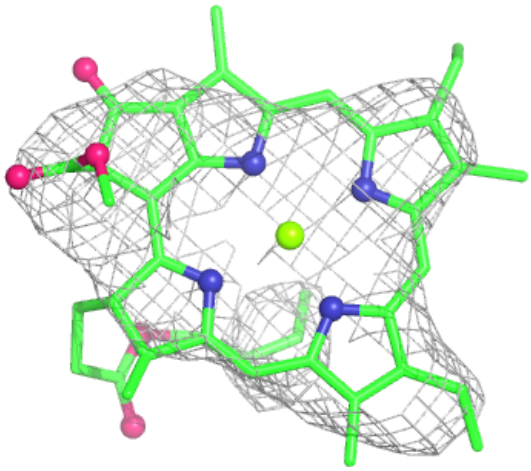


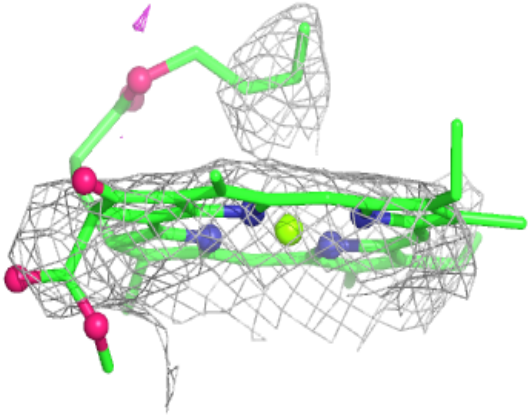


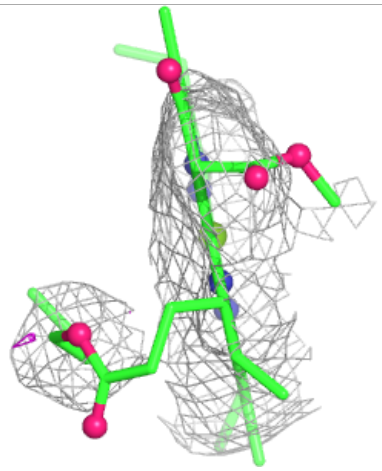


Electron density around CLA B 1224:

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

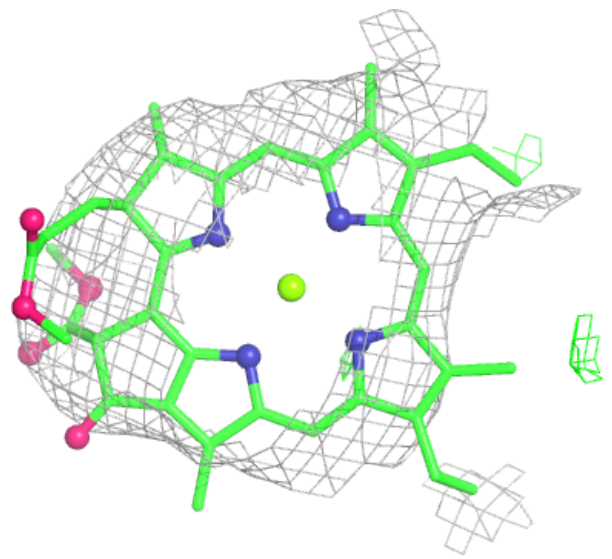


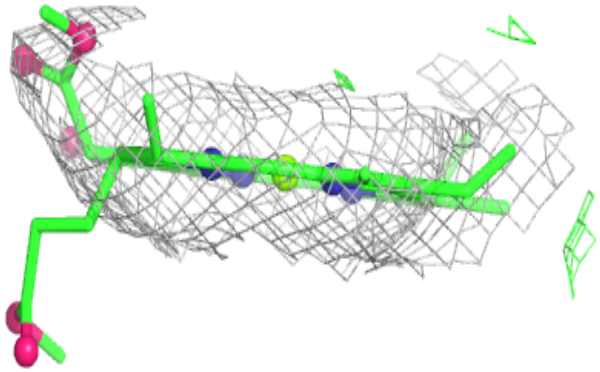


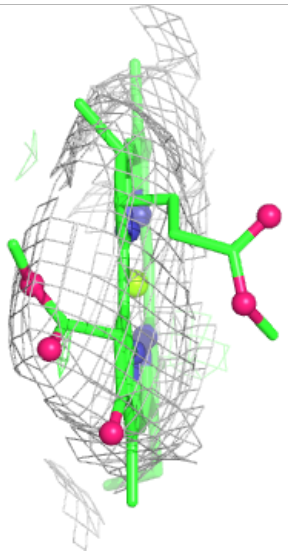


Electron density around CLA A 1108:

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

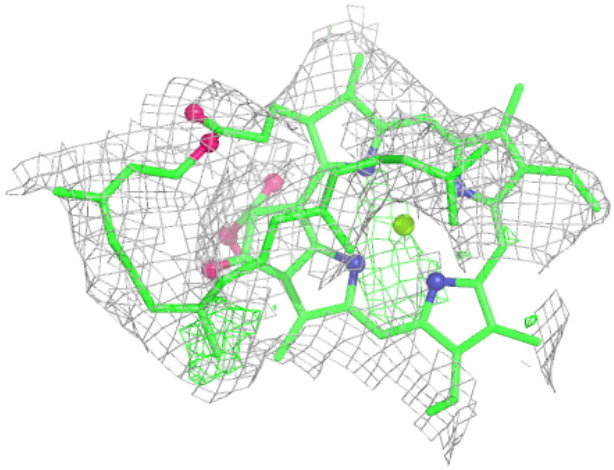


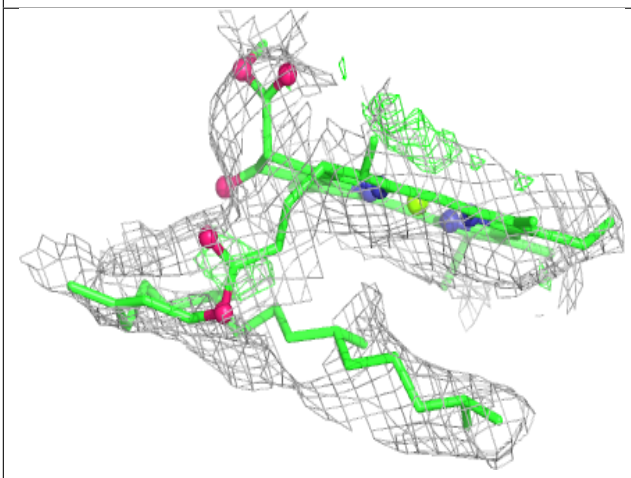


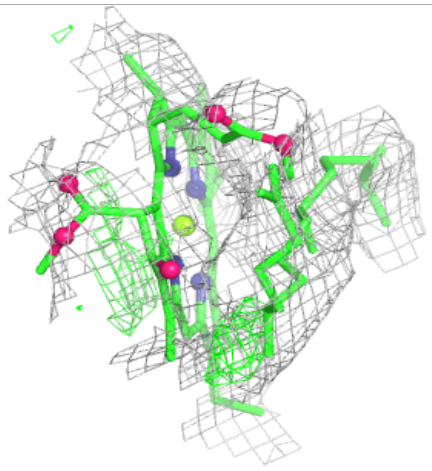


Electron density around CLA 2 605:

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

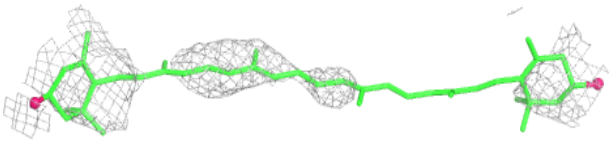


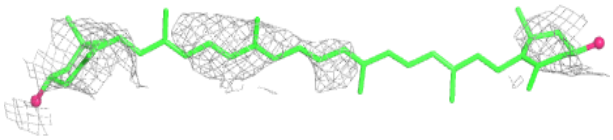


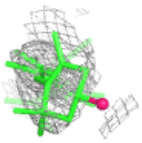


Electron density around LUT 3 501:

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

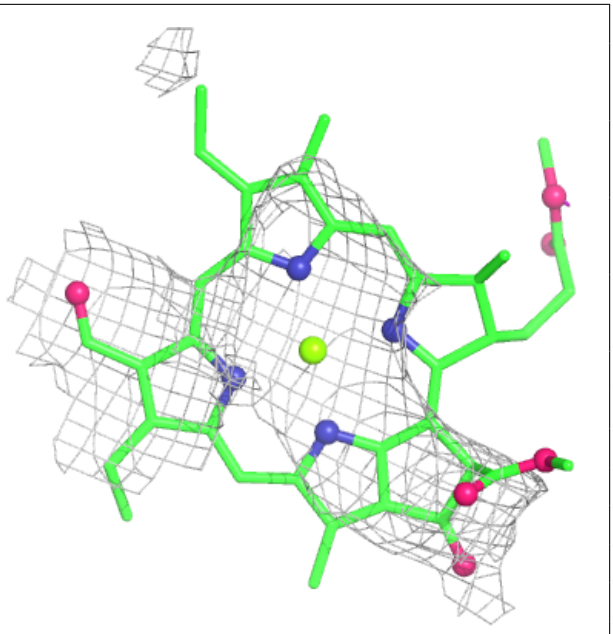


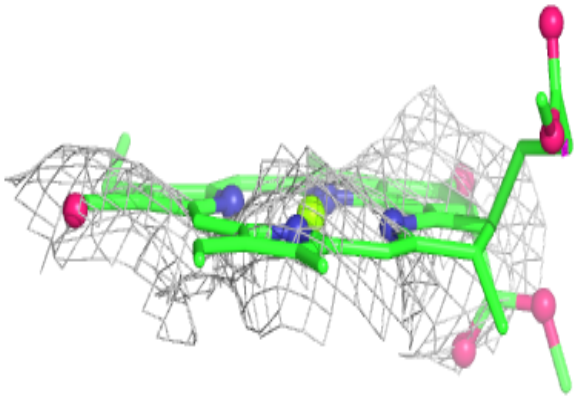


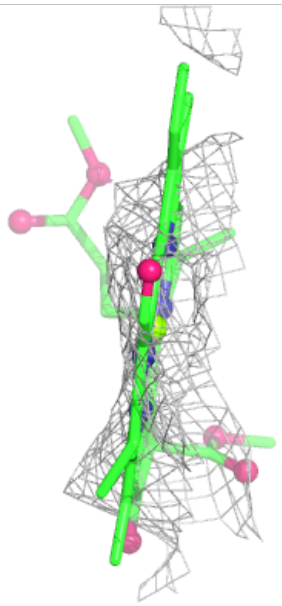


Electron density around CHL 3 604:

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

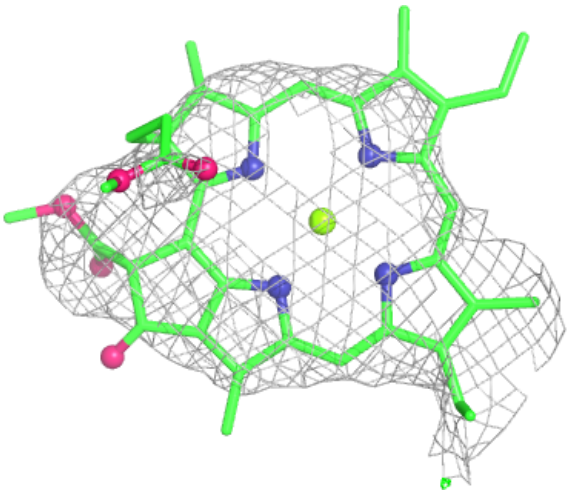


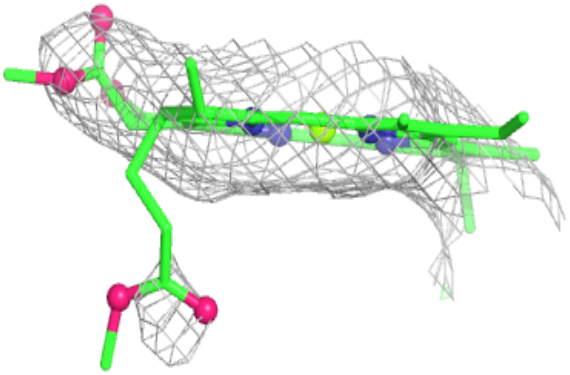


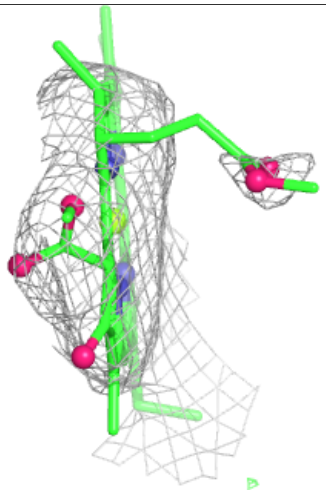


Electron density around CLA 3 611:

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

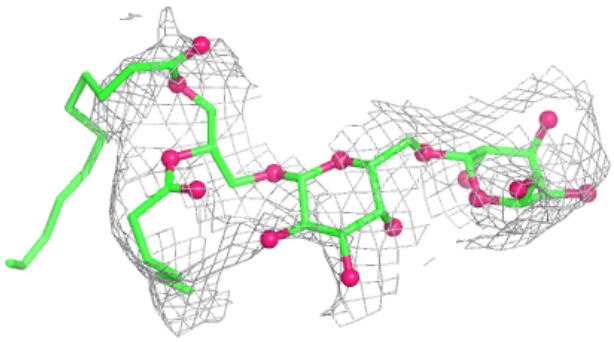


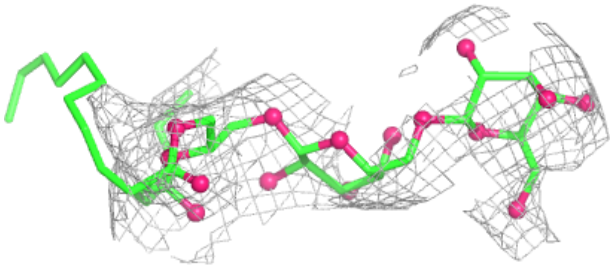


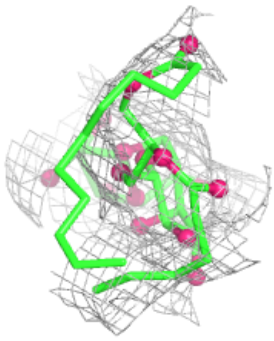


Electron density around DGD 2 811:

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

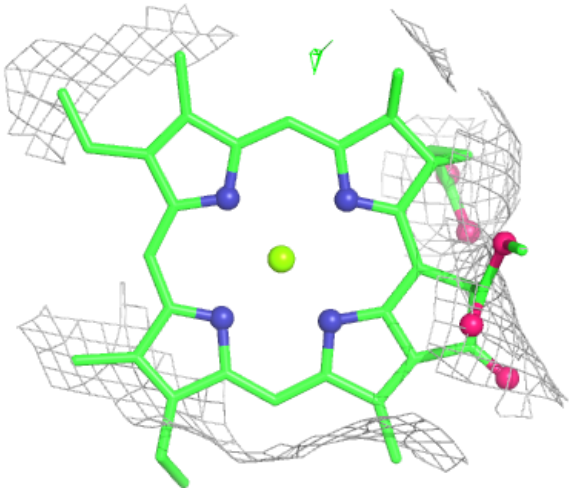


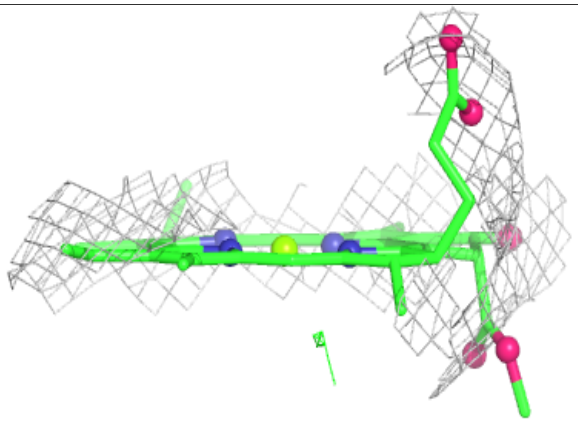


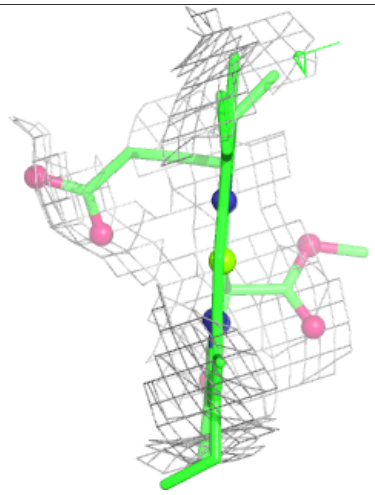


Electron density around CLA 3 606:

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

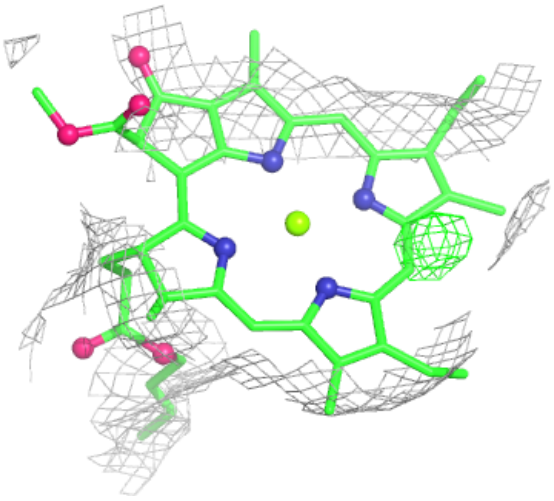


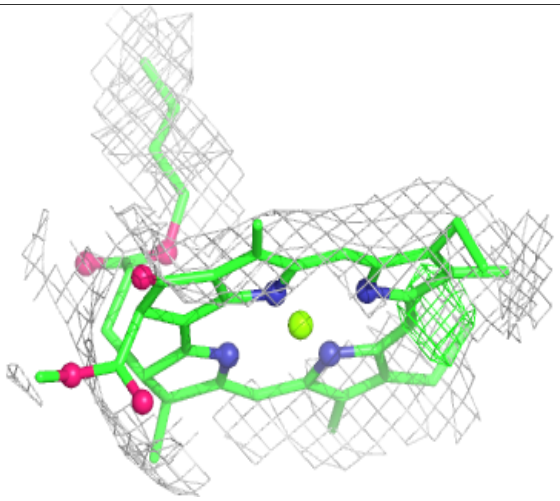


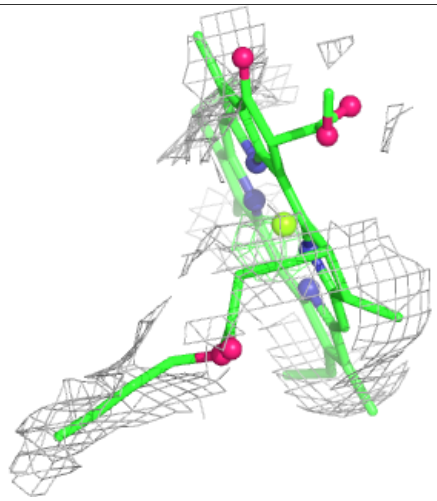


Electron density around CLA B 1208:

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

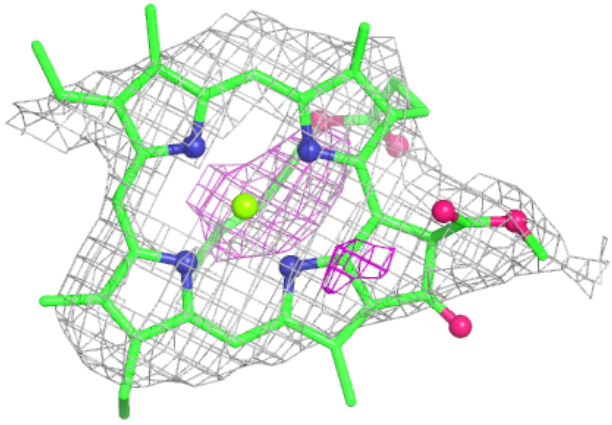


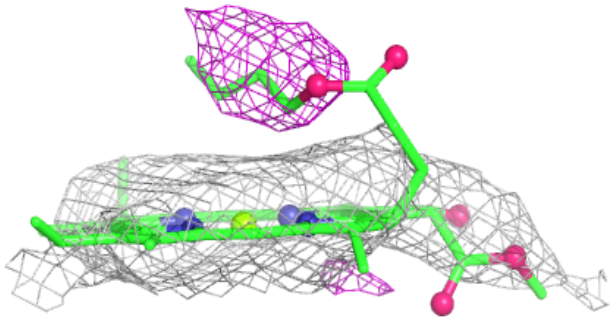


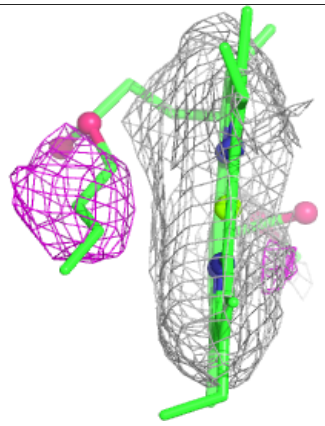


Electron density around CLA B 1211:

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

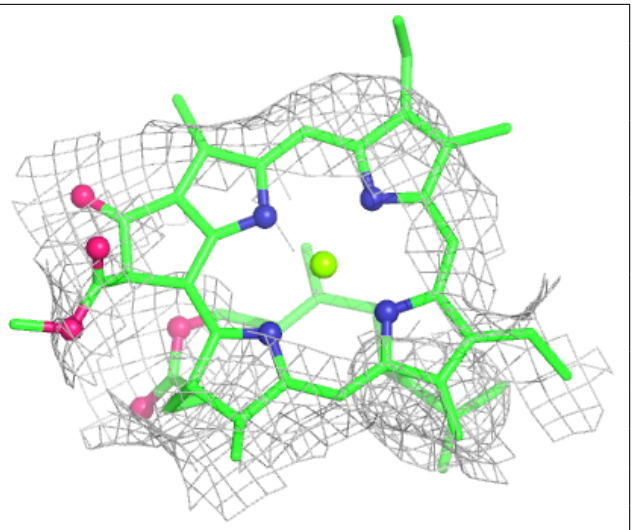


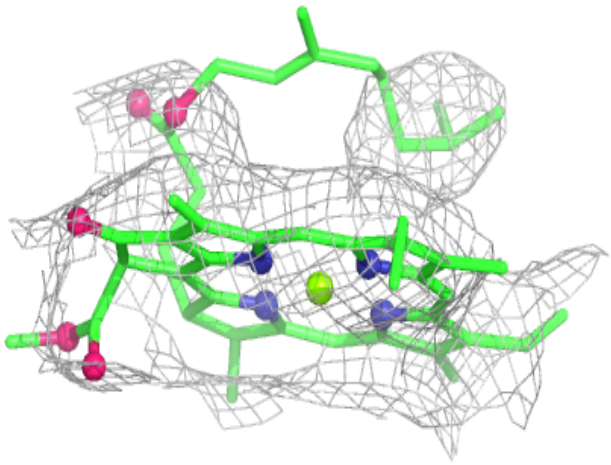


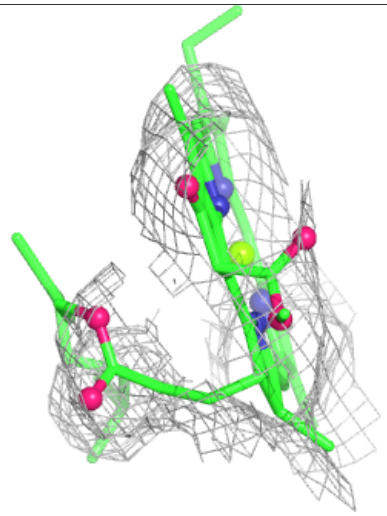


Electron density around CLA A 1130:

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

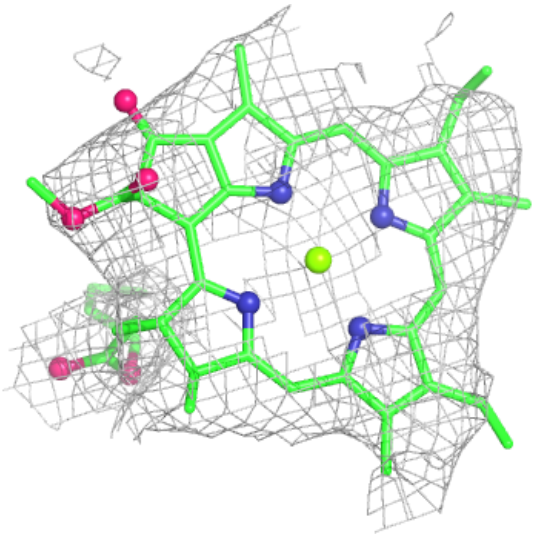


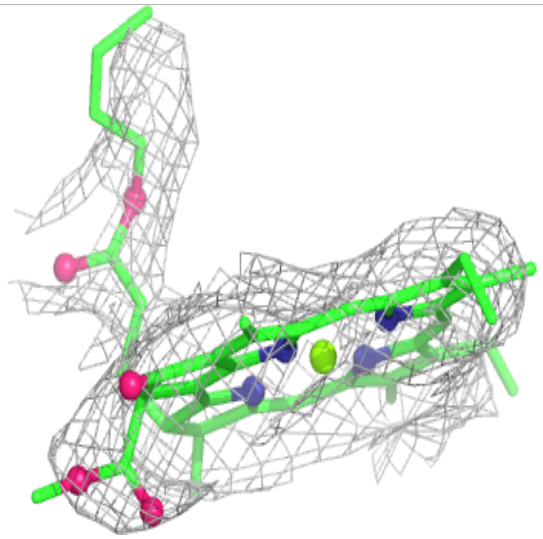


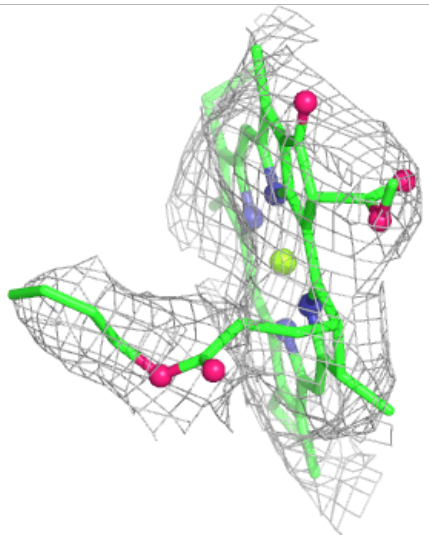


Electron density around CLA B 1219:

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

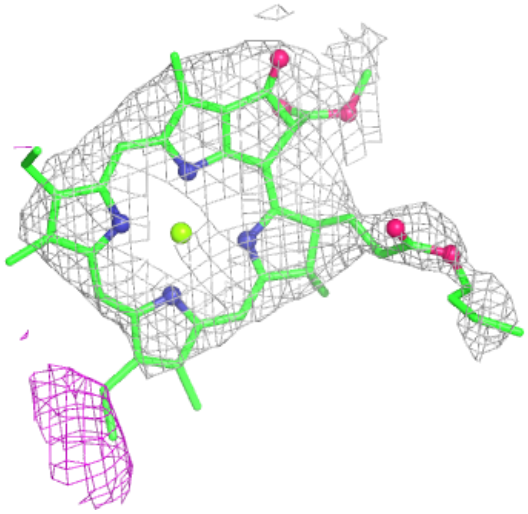


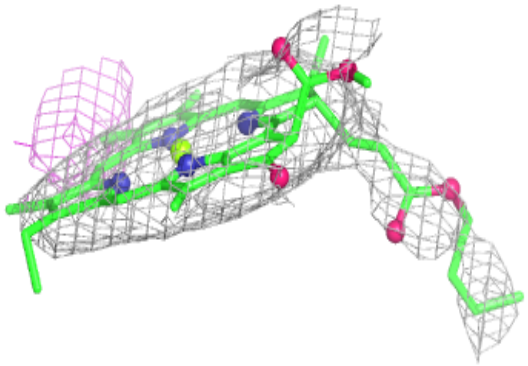


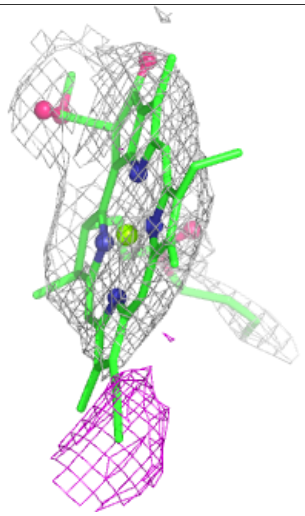


Electron density around CLA B 1230:

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

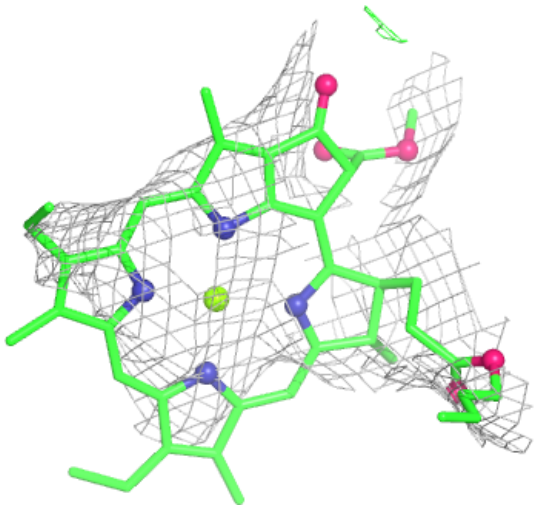




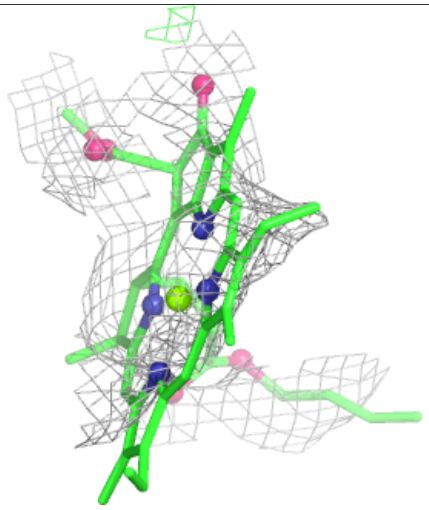


Electron density around CLA 3 601:

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

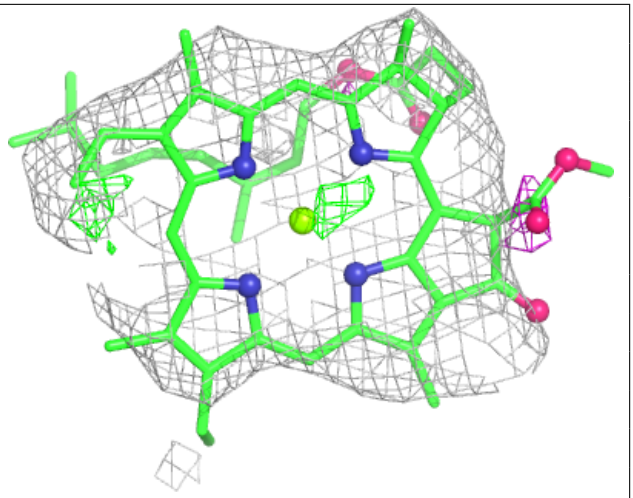


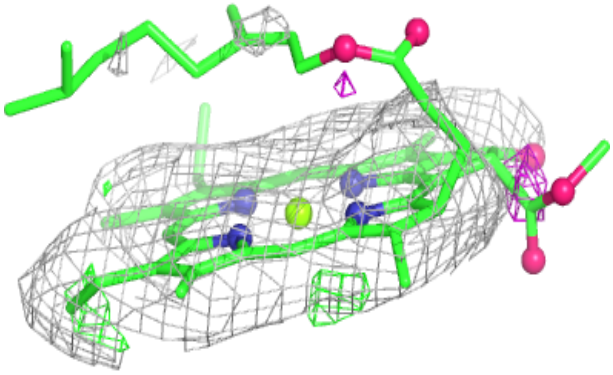


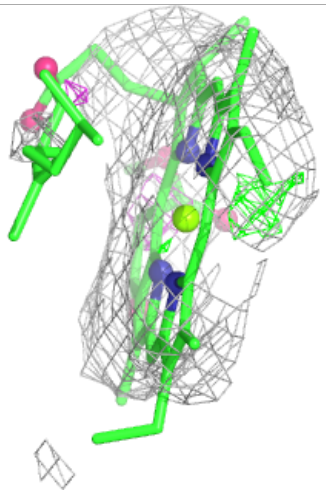


Electron density around CLA 4 615:

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

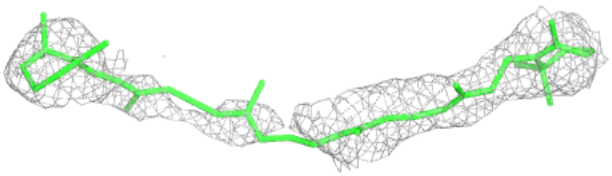


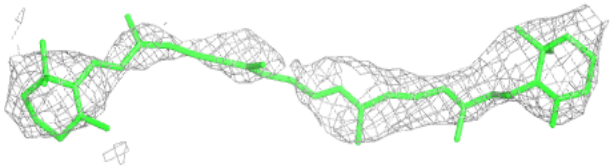


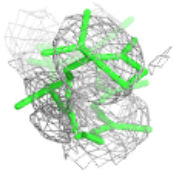


Electron density around BCR J 4002:

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

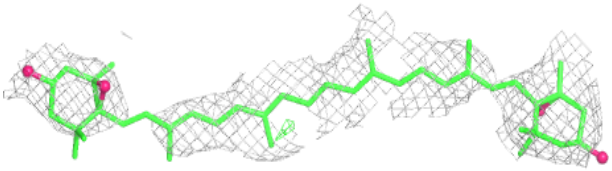


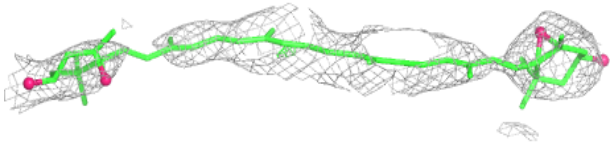


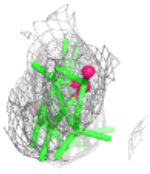


Electron density around XAT 2 502:

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

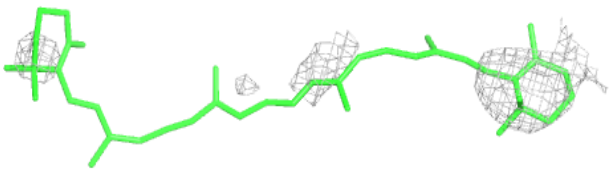


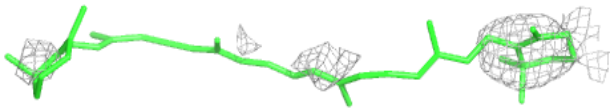


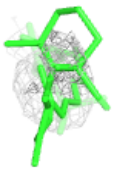


Electron density around BCR A 4003:

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

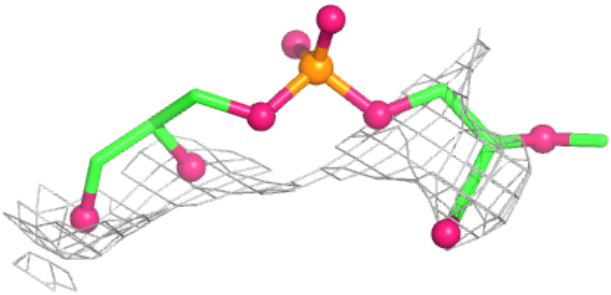


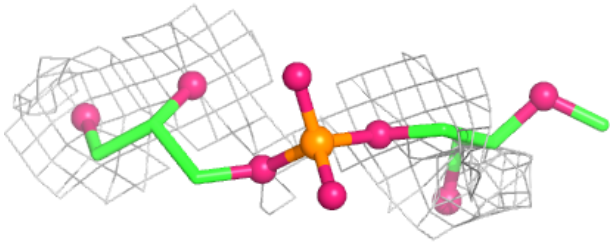


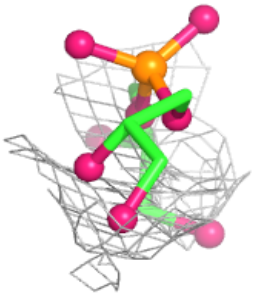


Electron density around LHG A 5001:

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

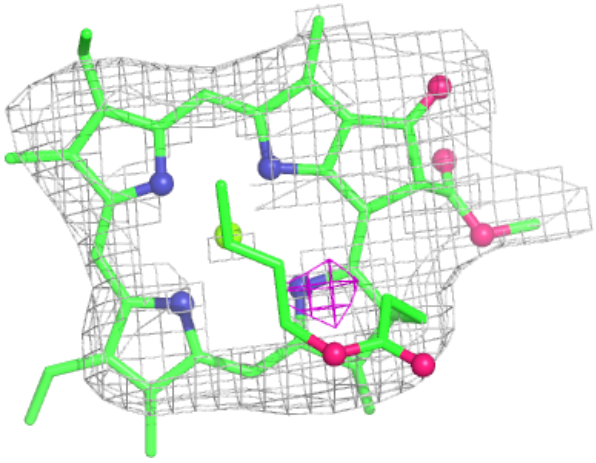


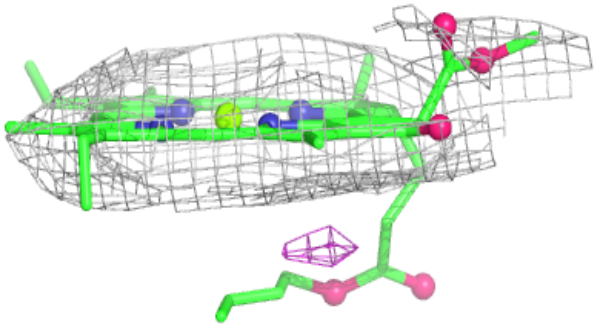


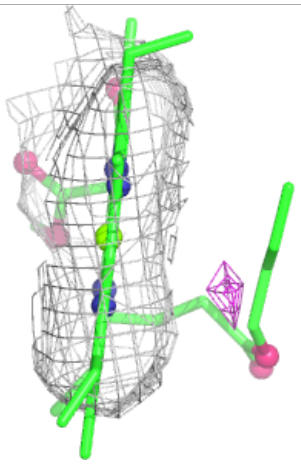


Electron density around CLA 2 608:

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

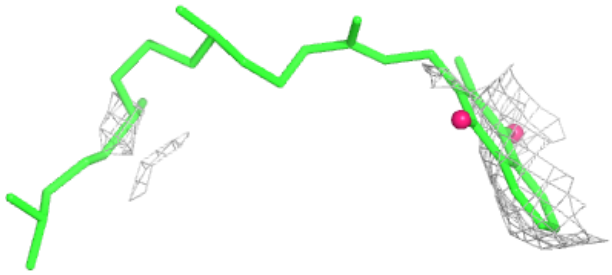


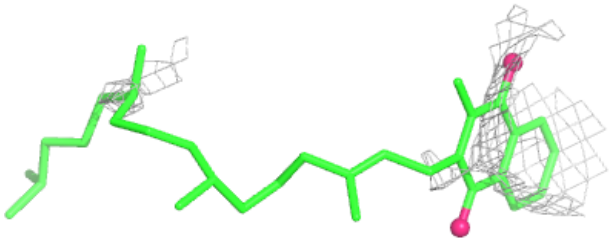




Electron density around PQN B 2002:

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

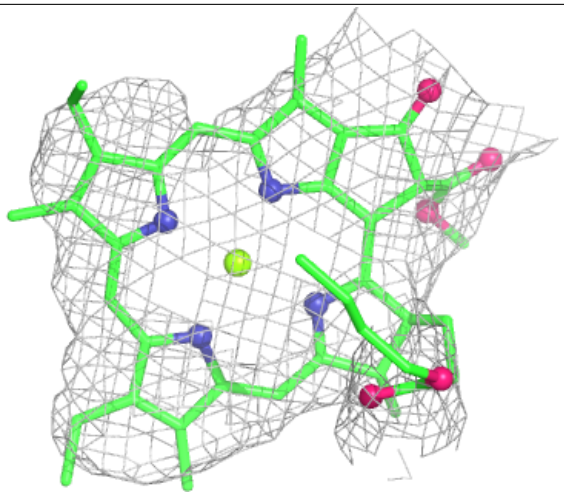


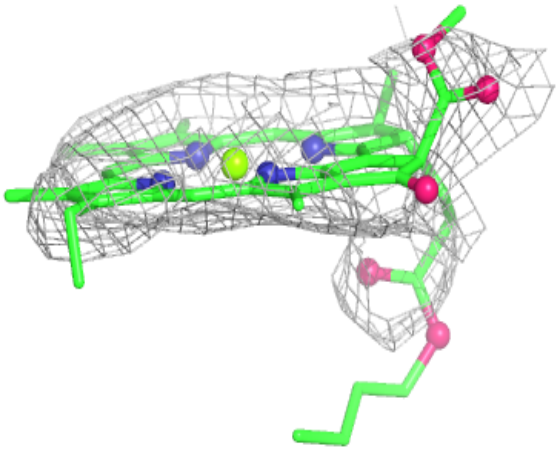


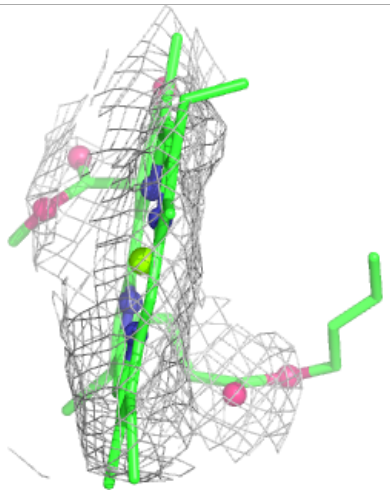


Electron density around CLA A 1115:

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

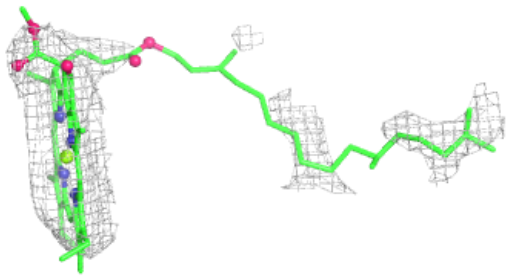


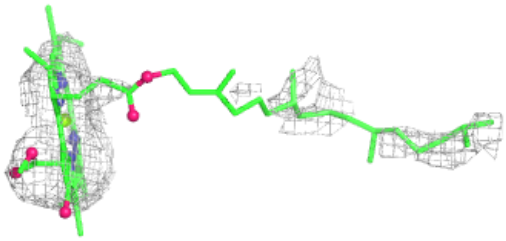


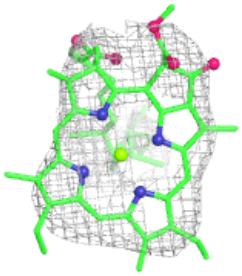


Electron density around CLA B 1239:

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

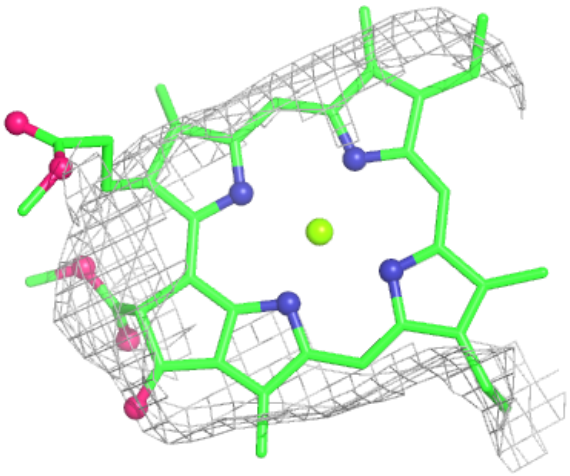


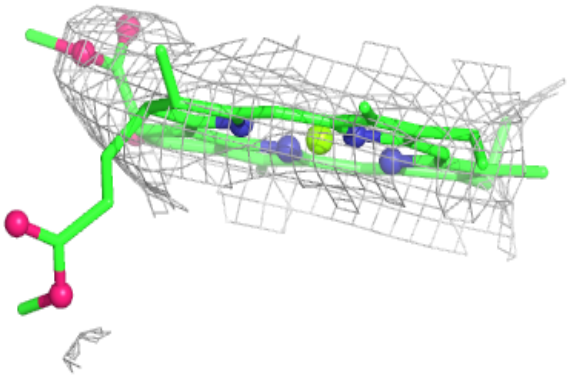




Electron density around CLA 3 613:

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

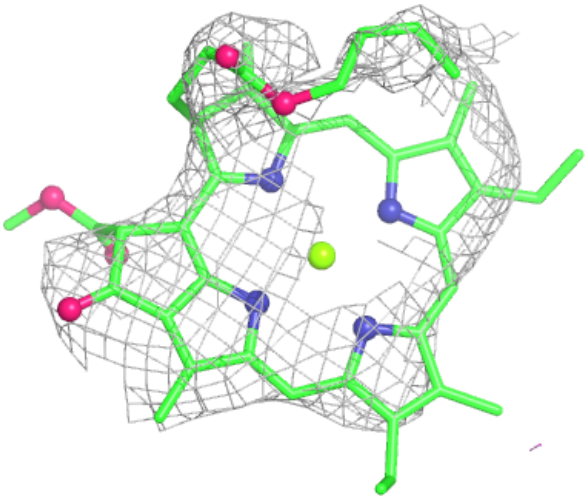


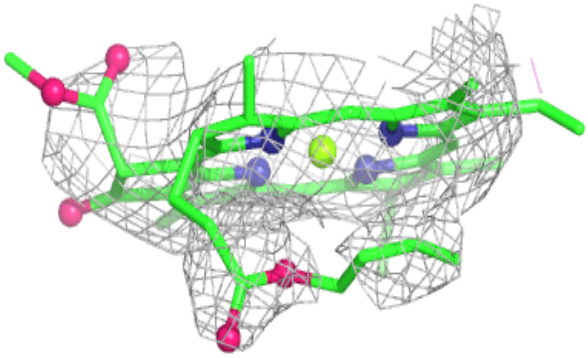


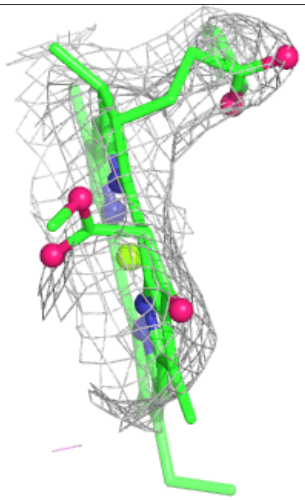


Electron density around CLA B 1215:

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

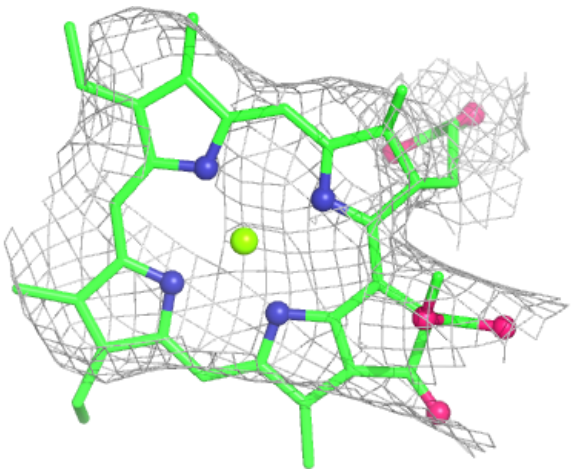


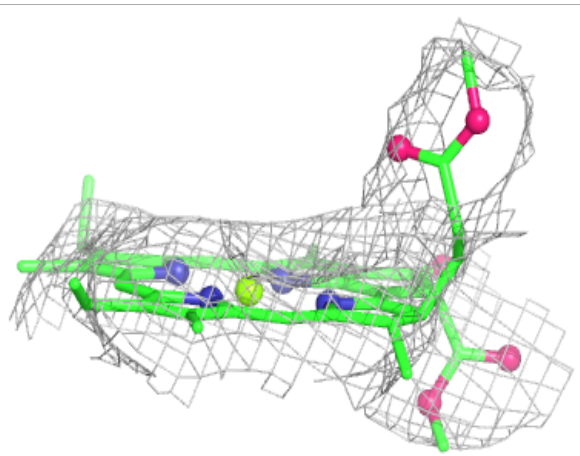


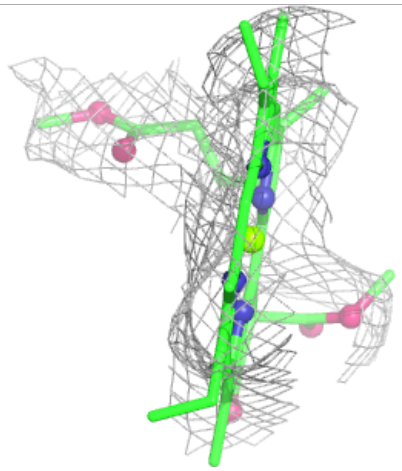


Electron density around CLA 2 606:

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

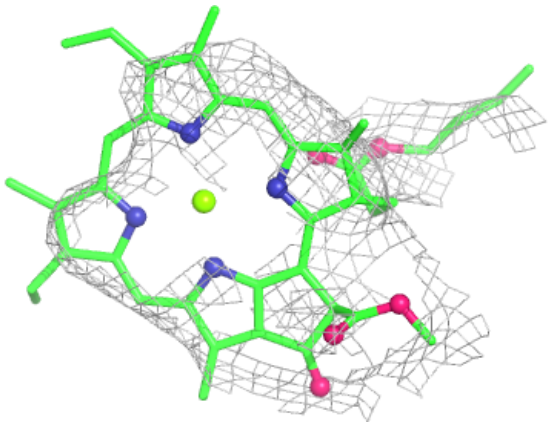


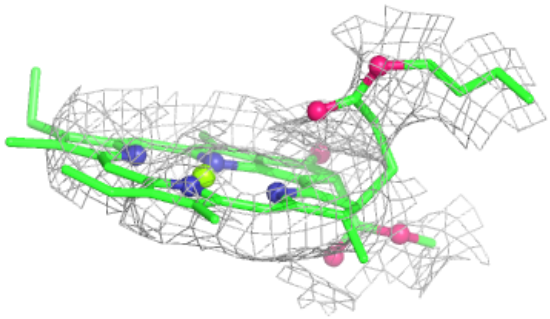


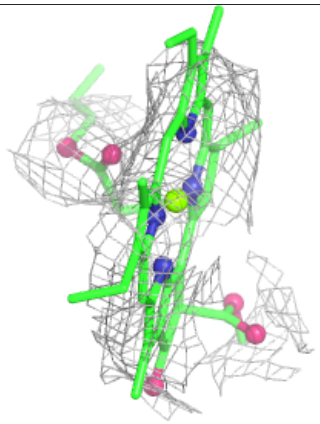


Electron density around CLA A 1124:

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

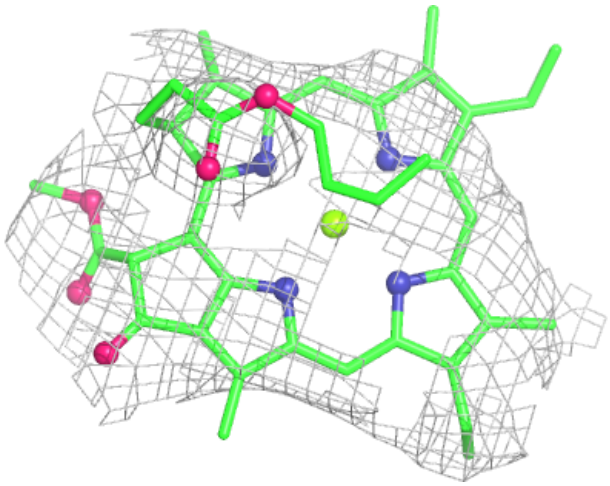


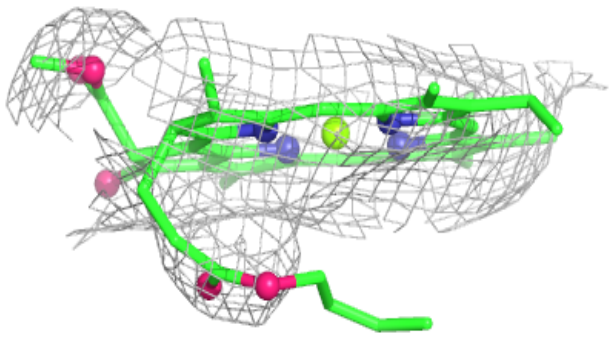


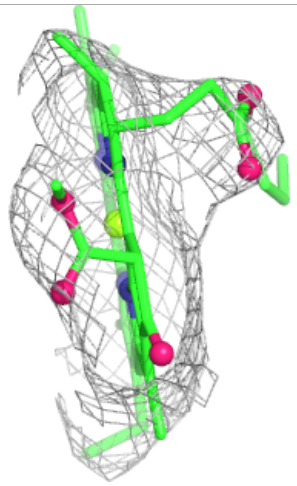


Electron density around CLA B 1205:

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

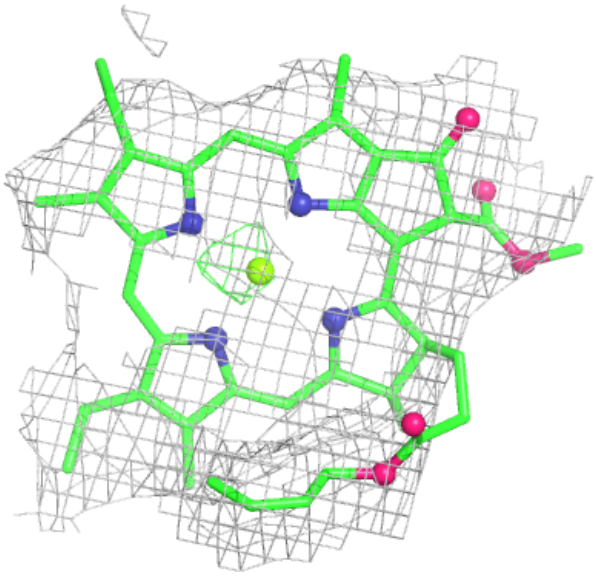


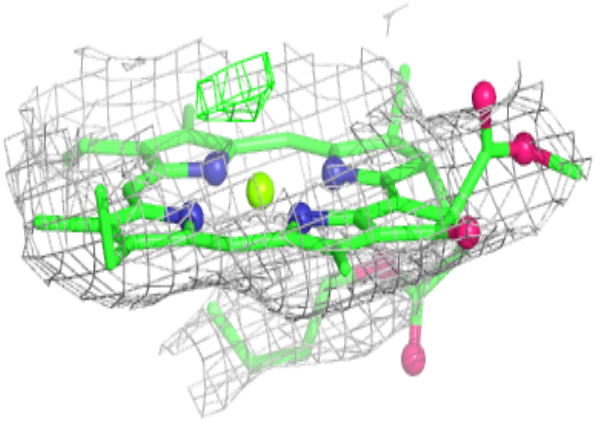


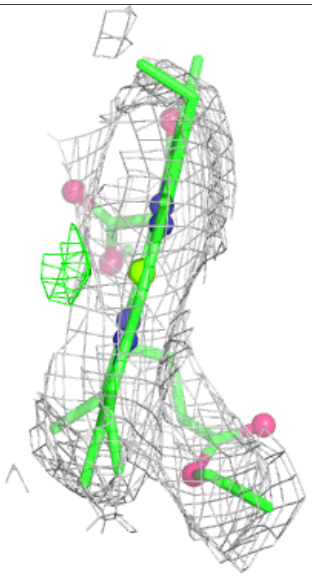


Electron density around CLA 1 601:

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

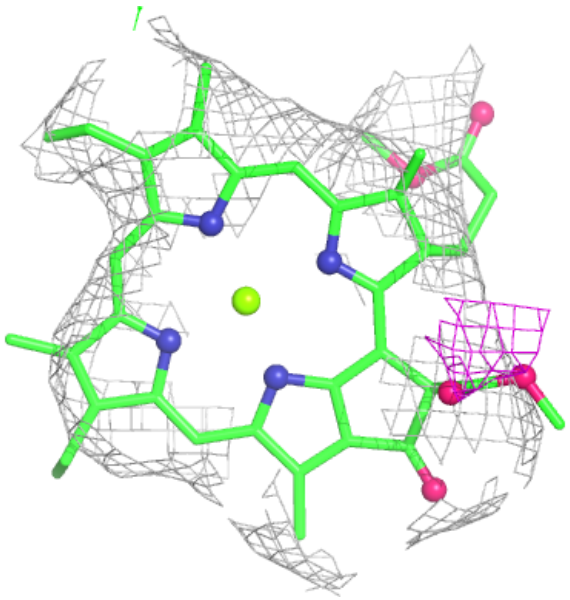


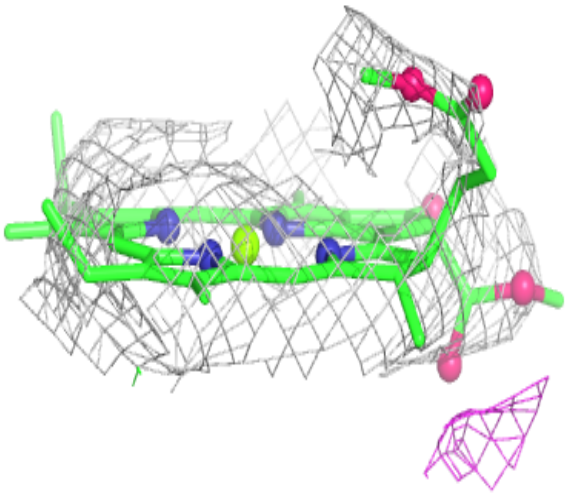


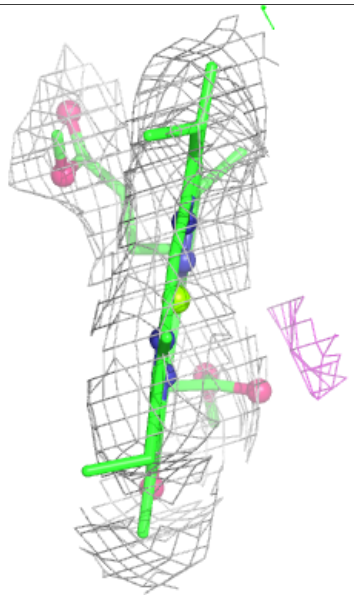


Electron density around CLA 1 607:

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

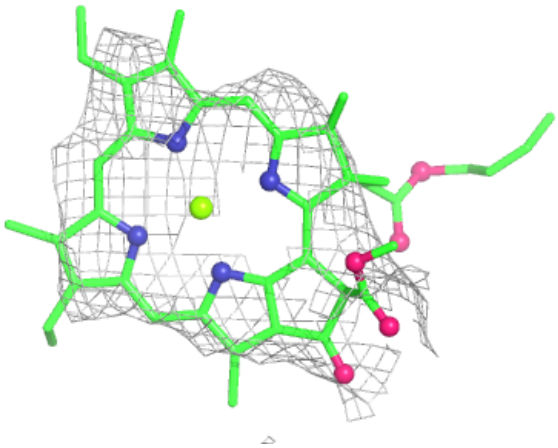


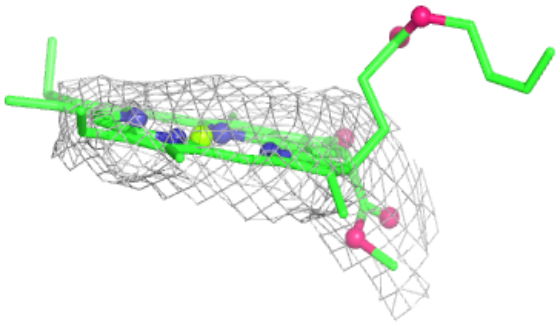


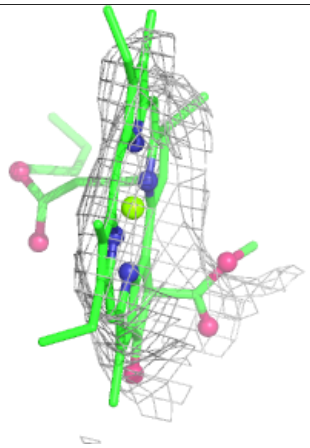


Electron density around CLA A 1132:

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

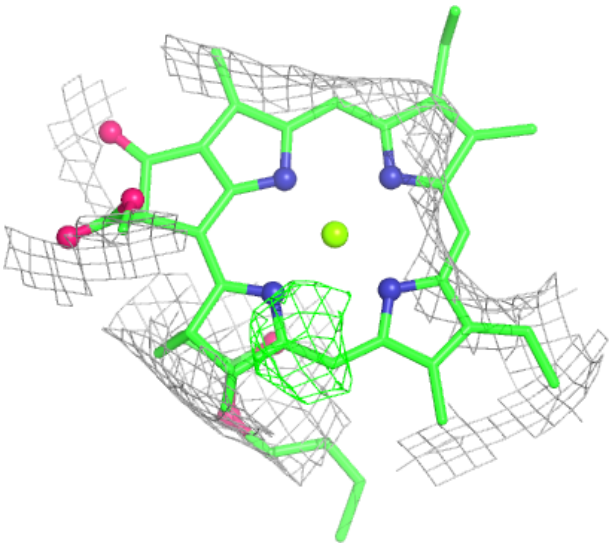


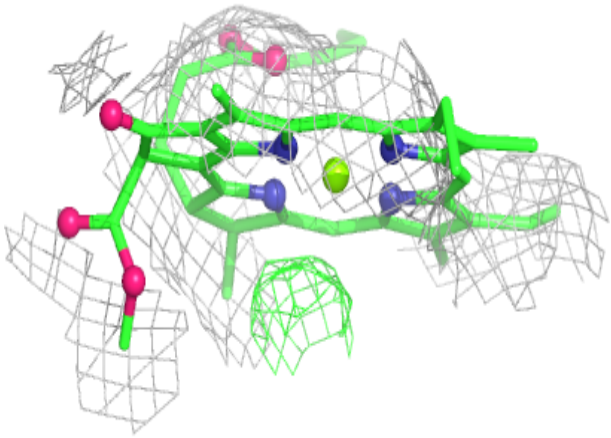


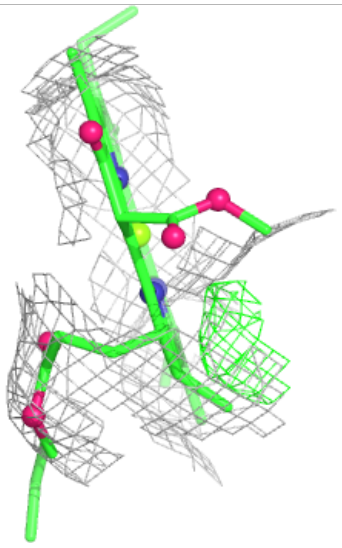


Electron density around CLA A 1134:

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

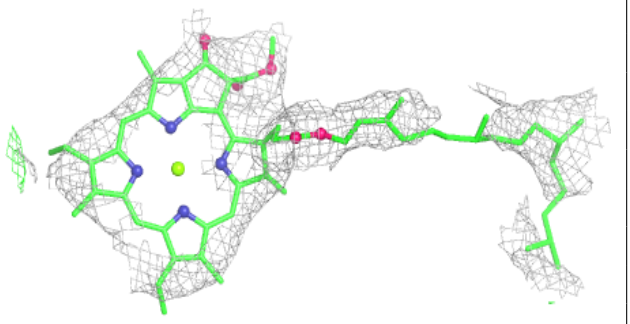






Electron density around CLA B 1240:

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

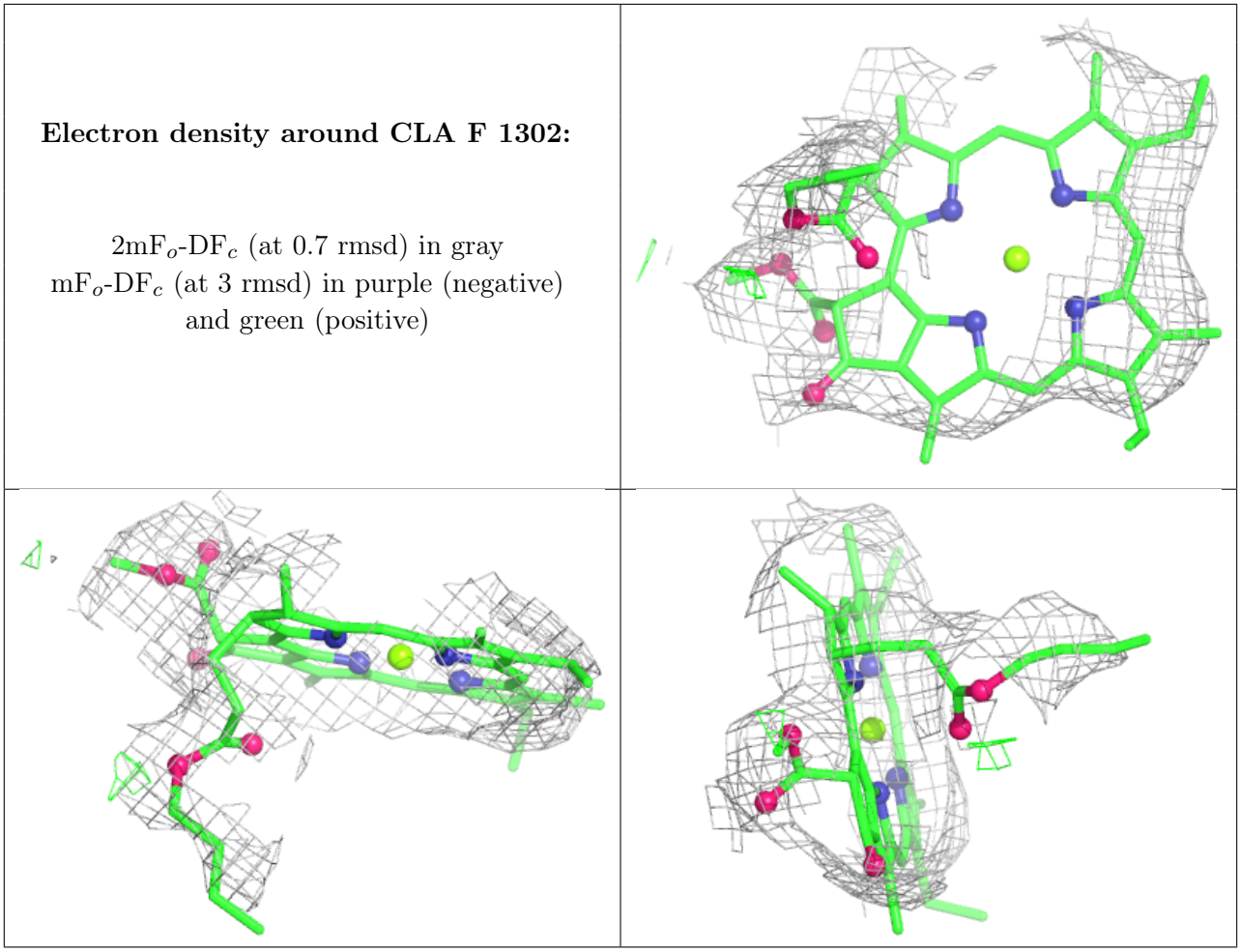






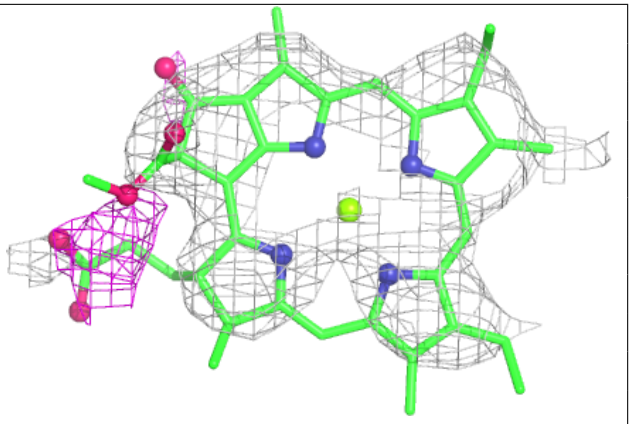
Electron density around CLA F 1302:

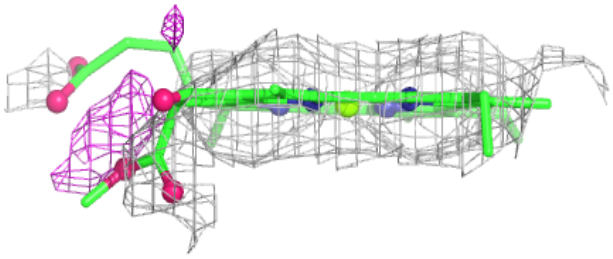
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

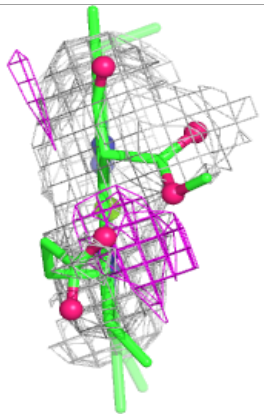


Electron density around CLA A 1101:

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

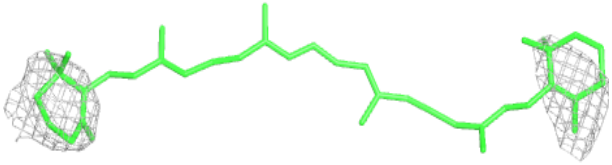






Electron density around BCR B 4002:

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

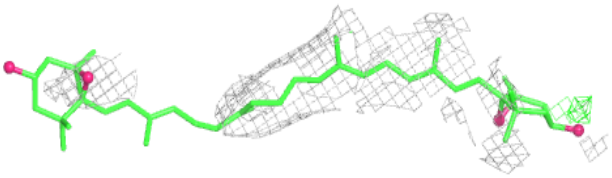




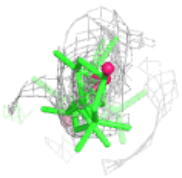


Electron density around XAT 3 502:

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

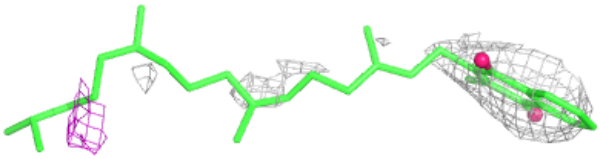


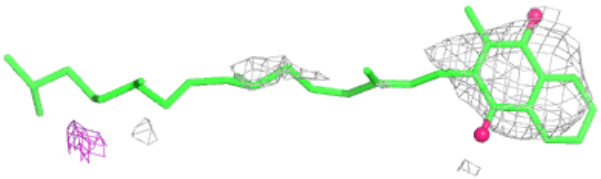


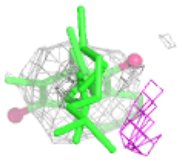


Electron density around PQN A 2001:

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

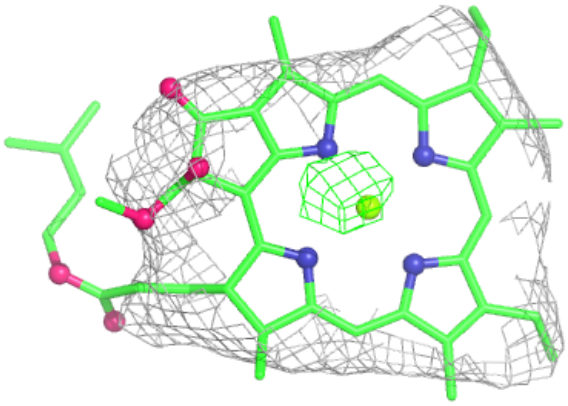


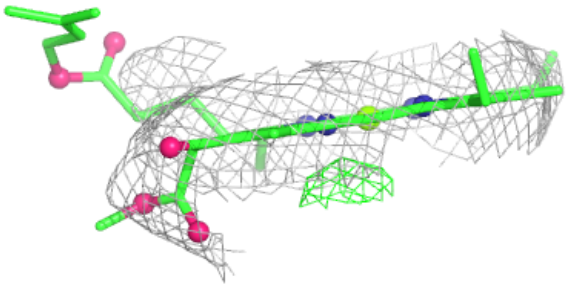


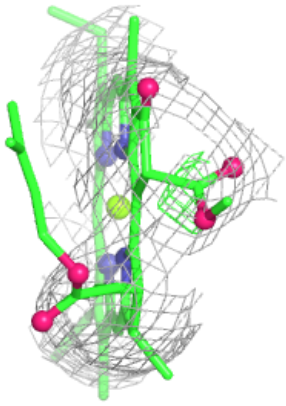


Electron density around CLA 2 615:

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

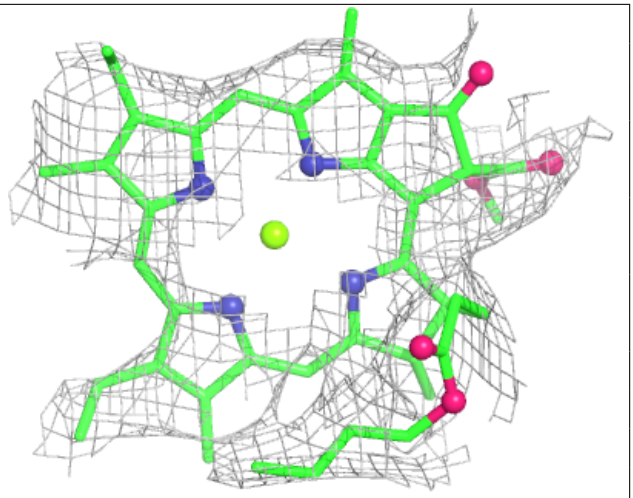


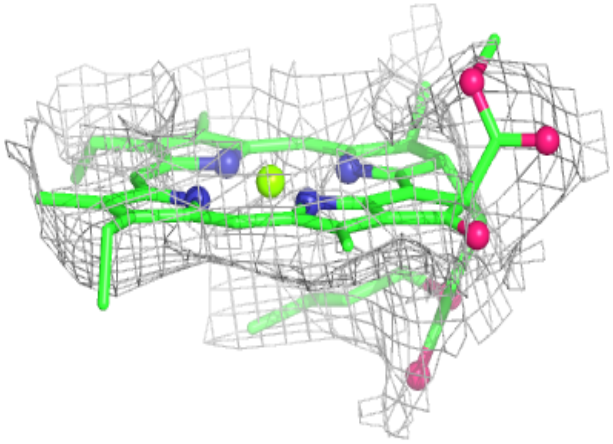




Electron density around CLA 2 604:

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

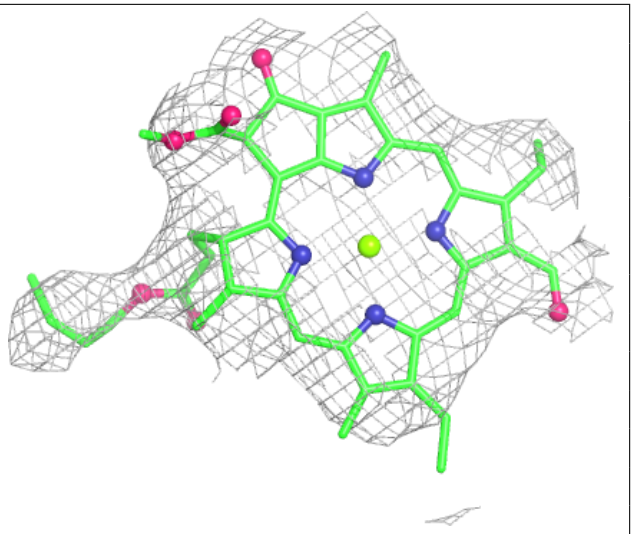


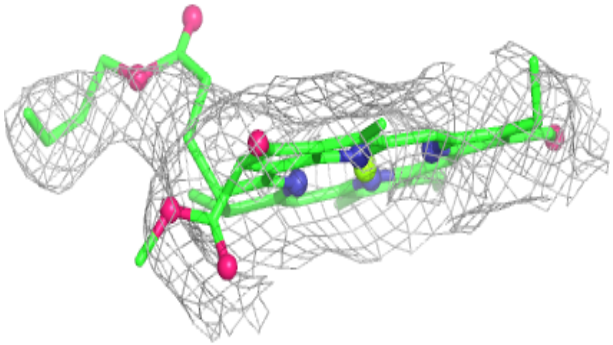


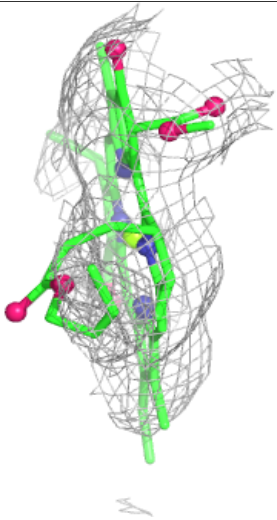


Electron density around CHL 2 610:

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

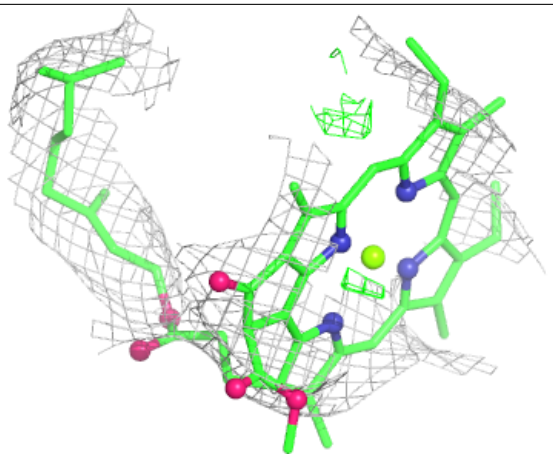


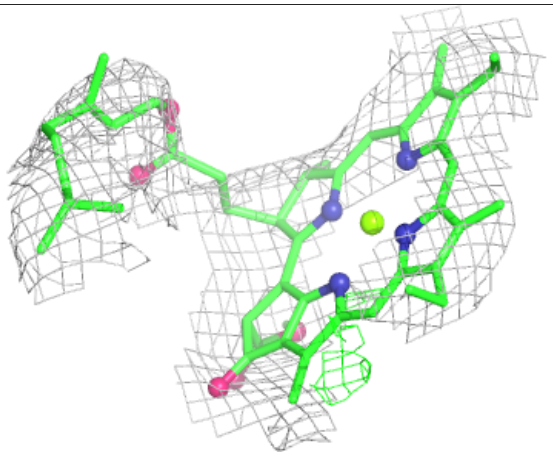


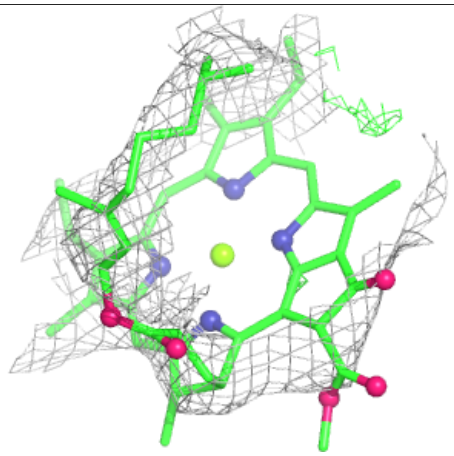


Electron density around CLA 3 612:

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

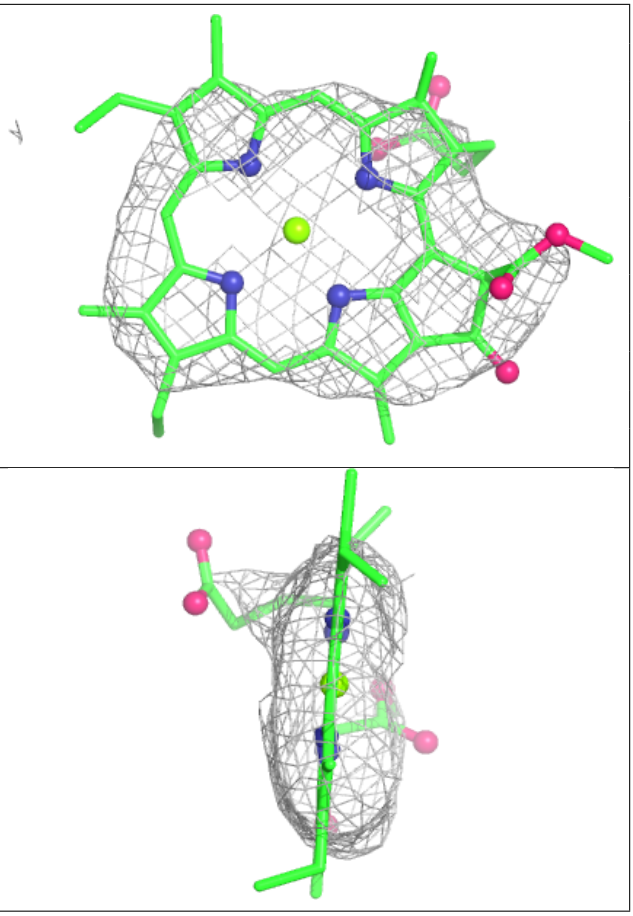






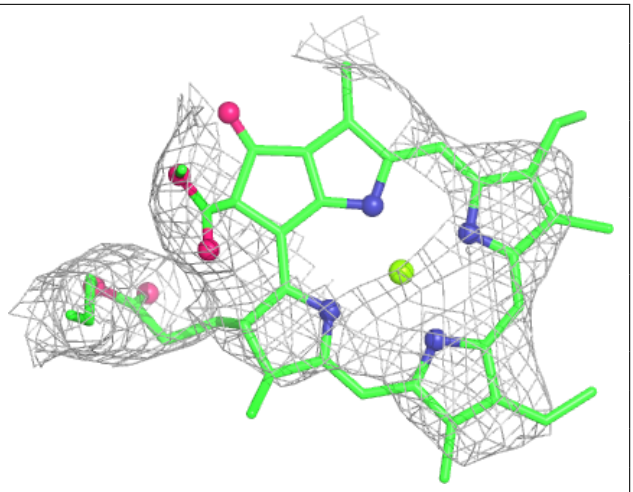
Electron density around CLA A 1113:

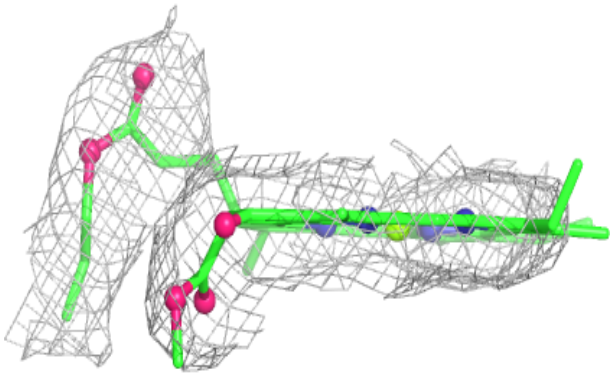
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

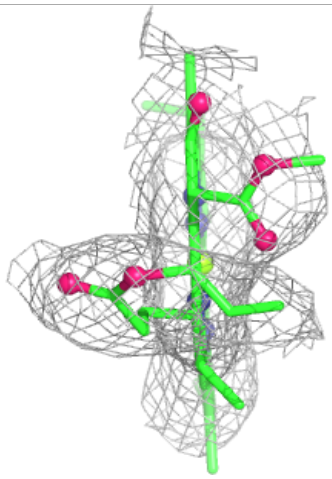


Electron density around CLA 1 605:

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

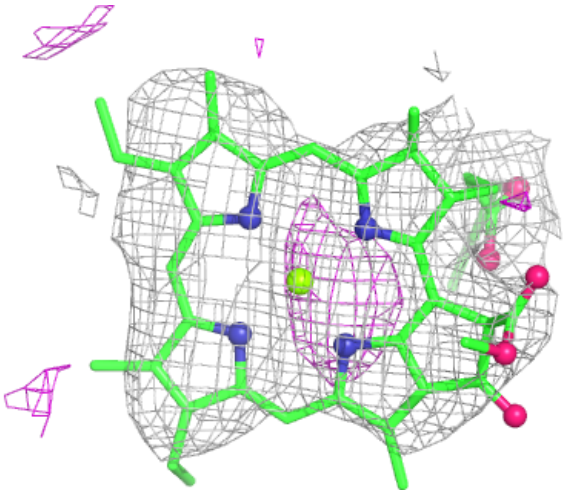


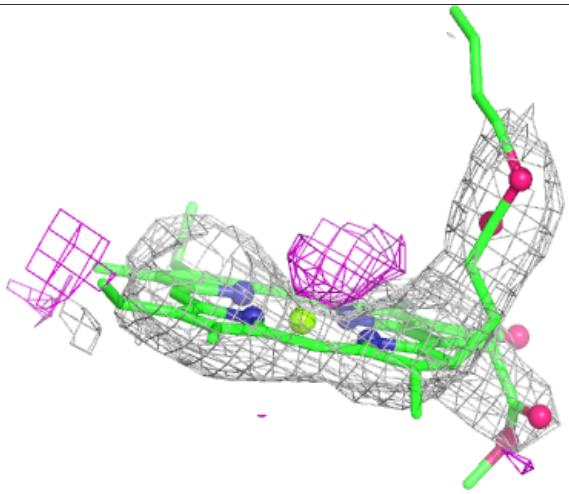


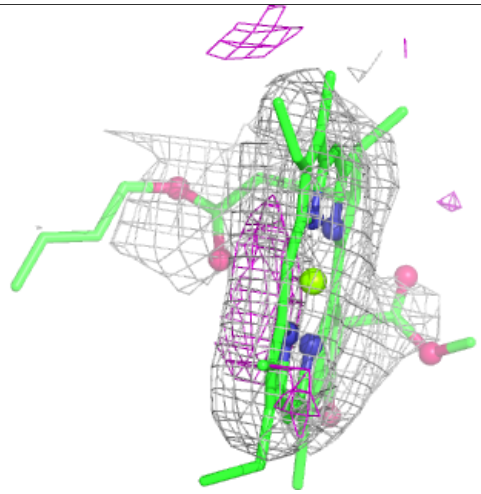


Electron density around CLA 4 606:

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

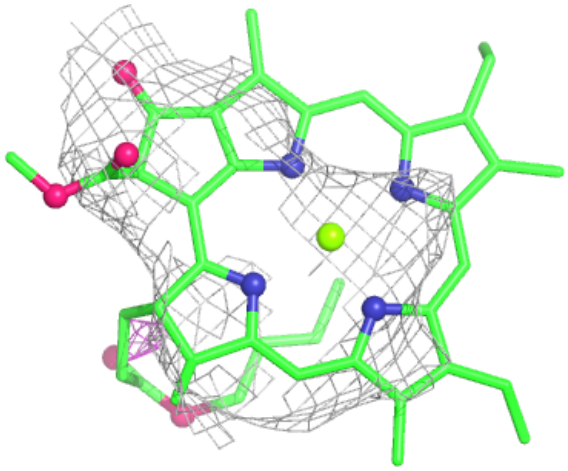


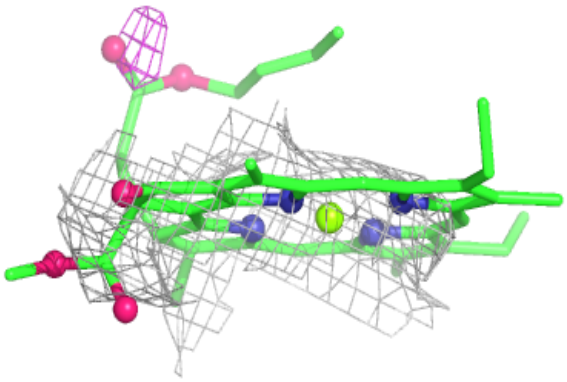


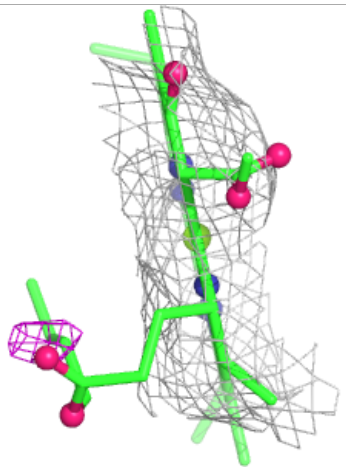


Electron density around CLA A 1116:

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

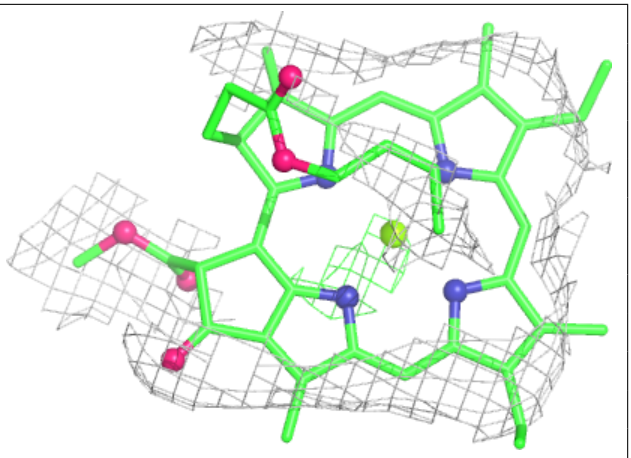


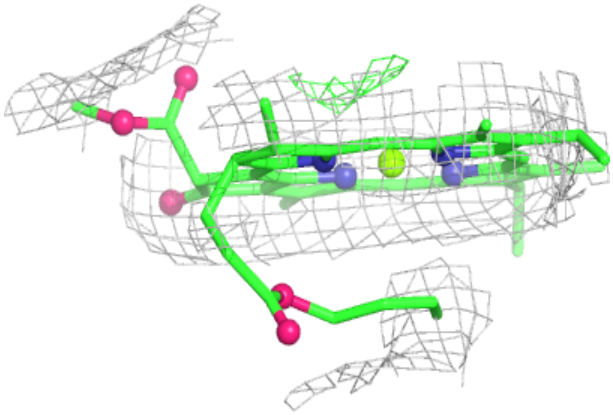


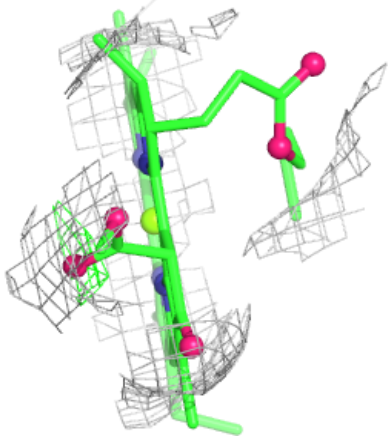


Electron density around CLA B 1237:

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

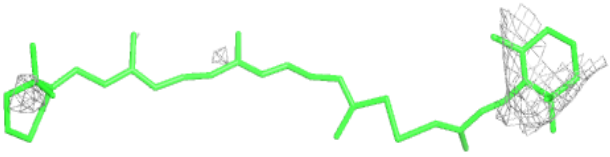


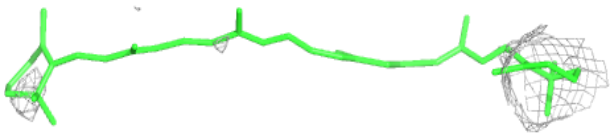


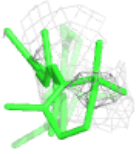


Electron density around BCR A 4005:

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

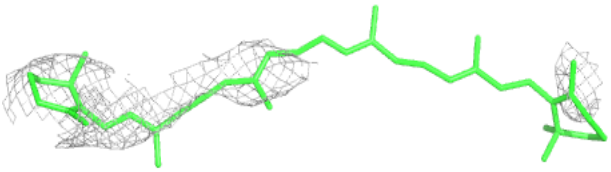


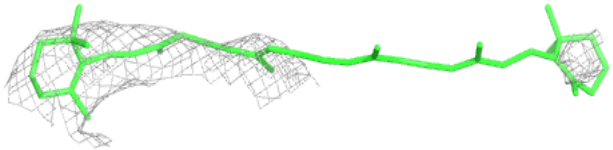


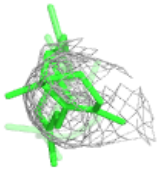


Electron density around BCR 3 504:

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

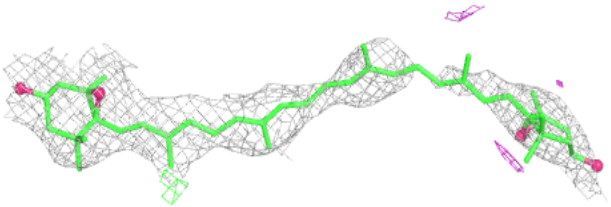


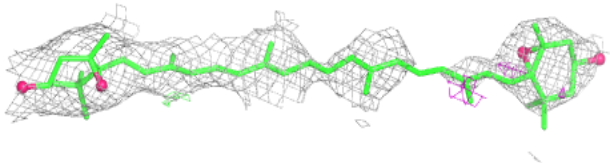




Electron density around XAT 4 502:

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

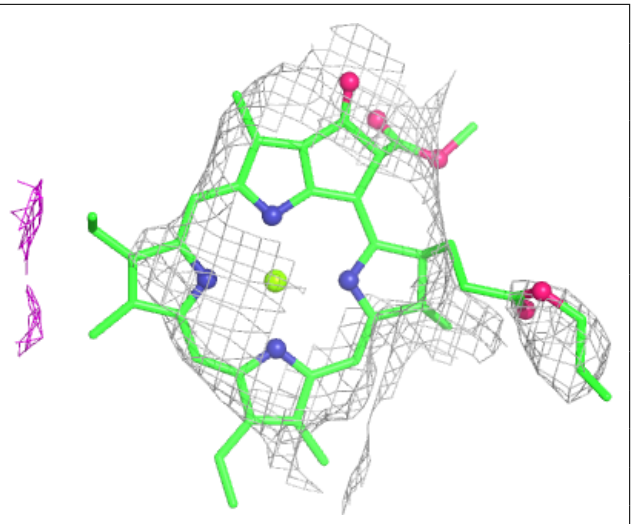


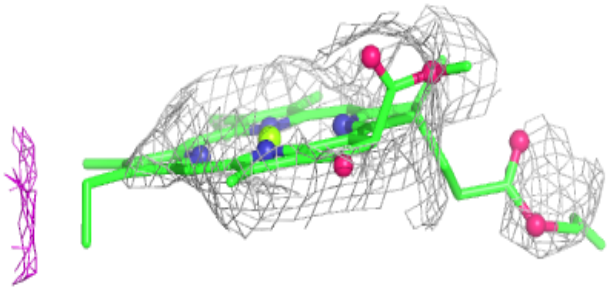




Electron density around CLA A 1129:

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

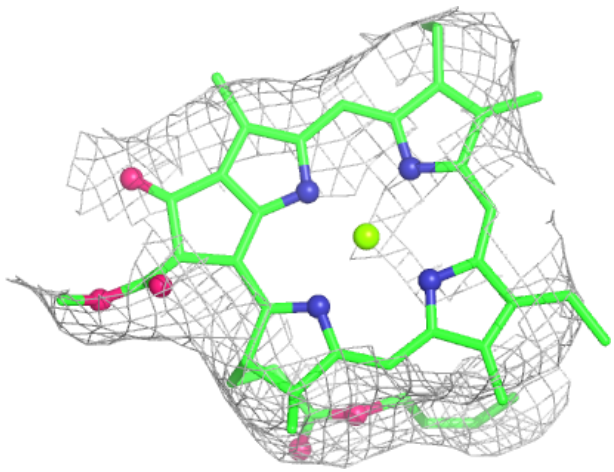


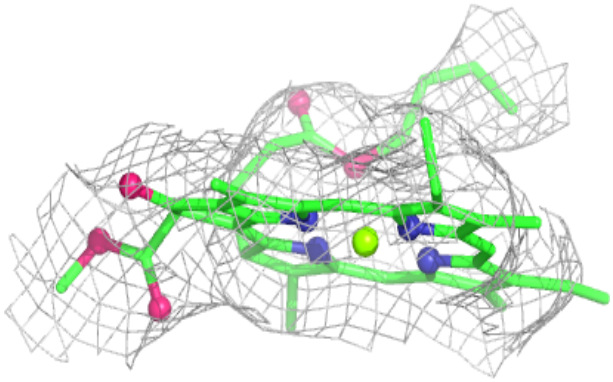


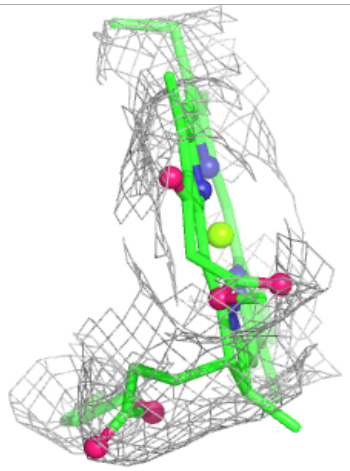


Electron density around CLA 4 601:

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

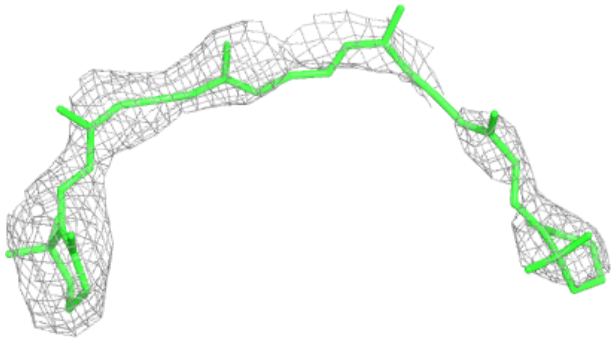


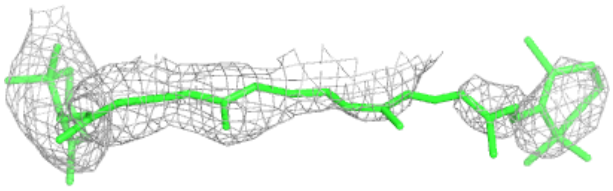


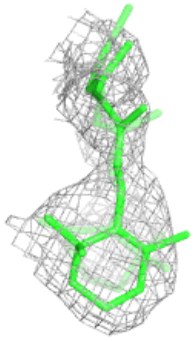


Electron density around BCR F 4002:

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

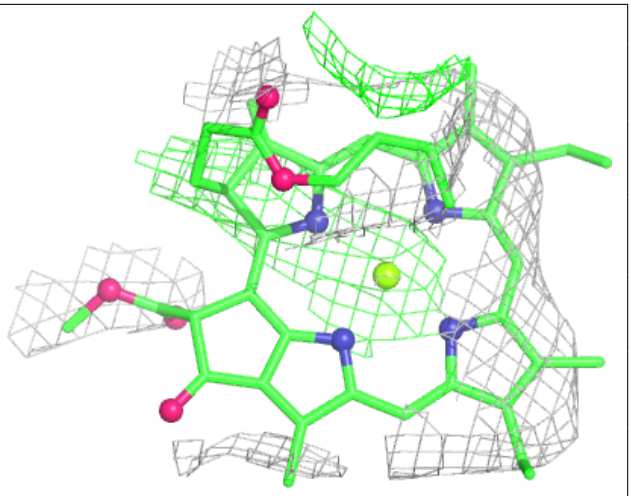


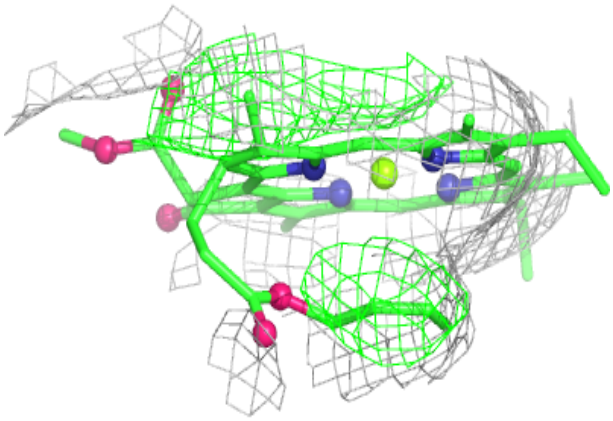


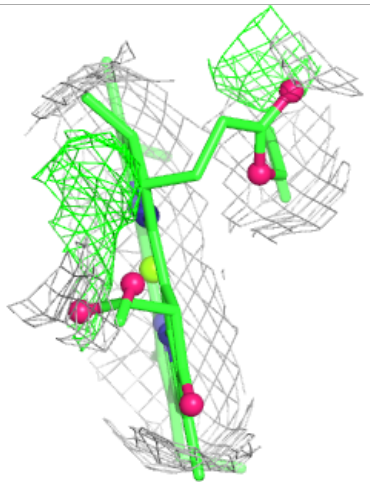


Electron density around CLA 3 610:

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

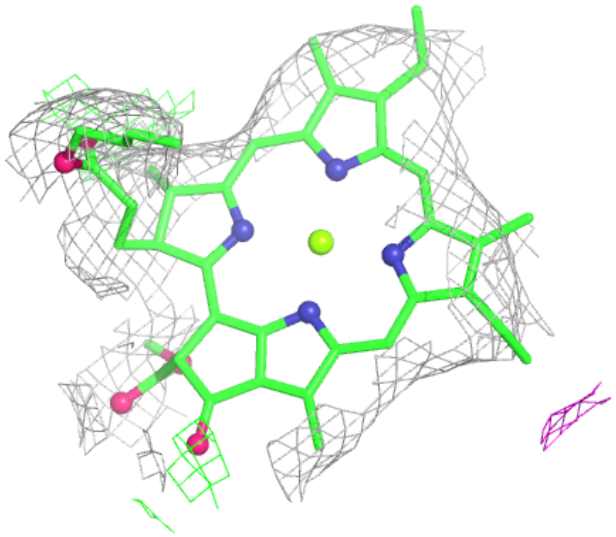


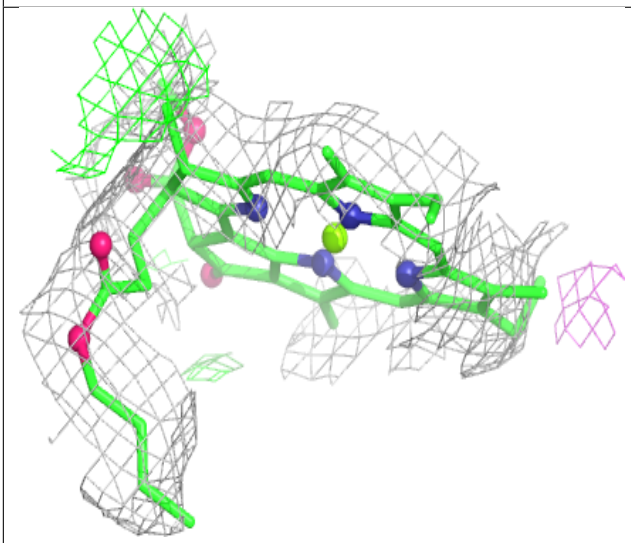


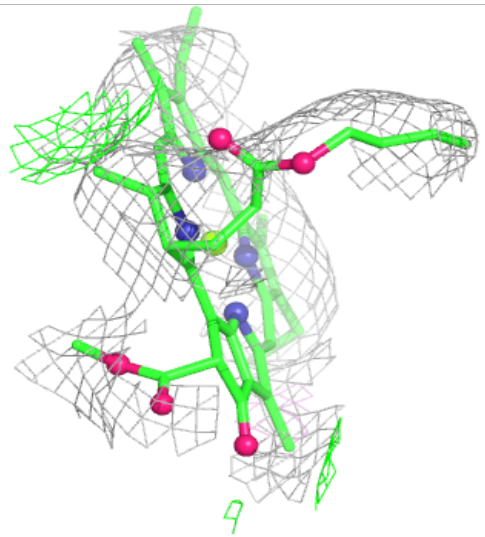


Electron density around CLA 4 612:

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

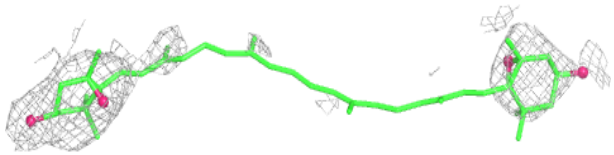


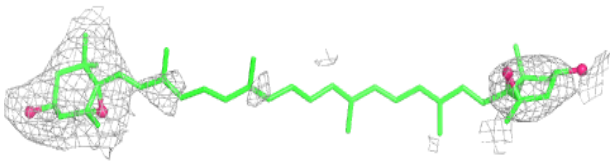


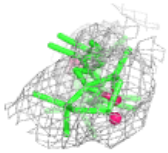


Electron density around XAT 1 502:

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

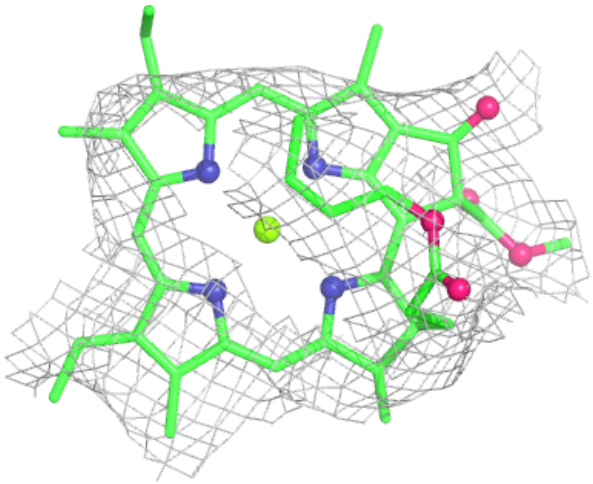


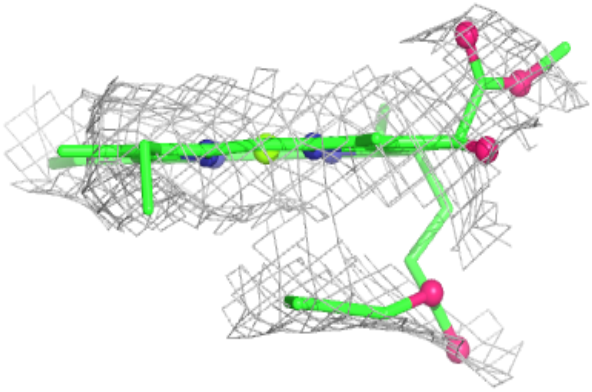


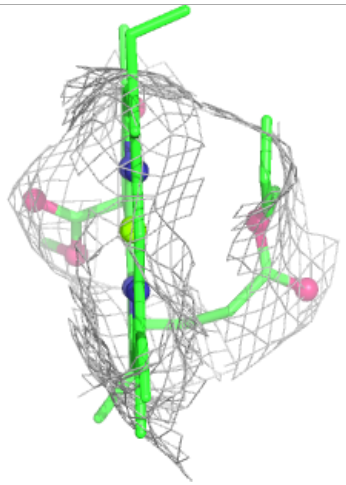


Electron density around CLA A 1136:

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

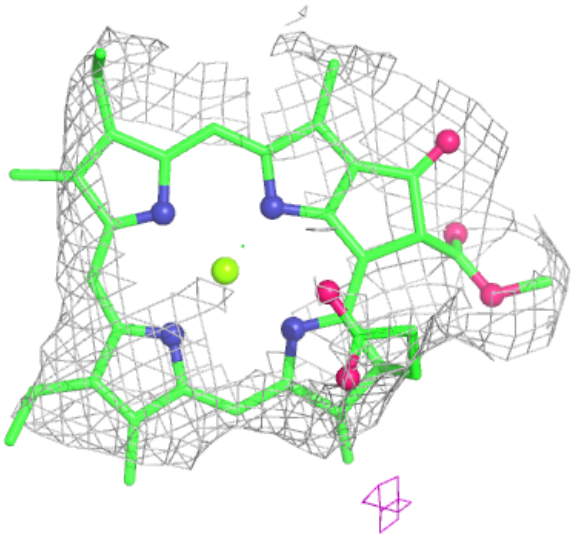


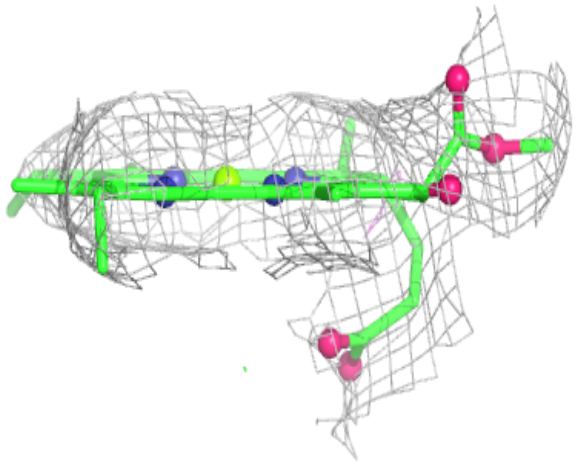


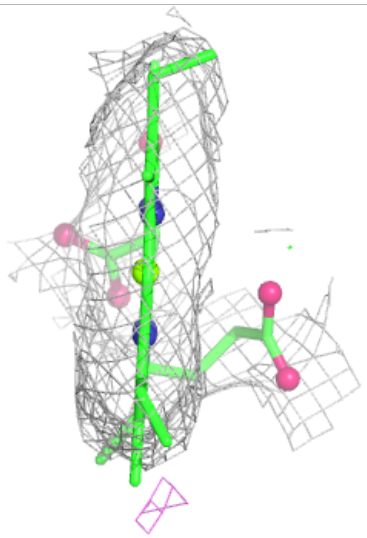


Electron density around CLA 1 603:

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

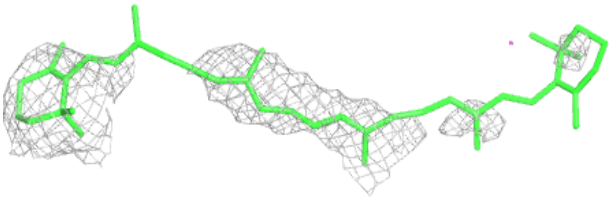


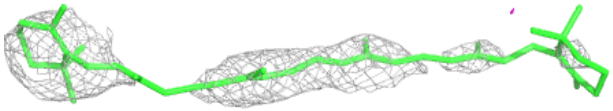


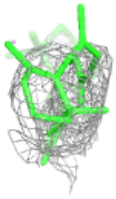


Electron density around BCR B 4005:

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

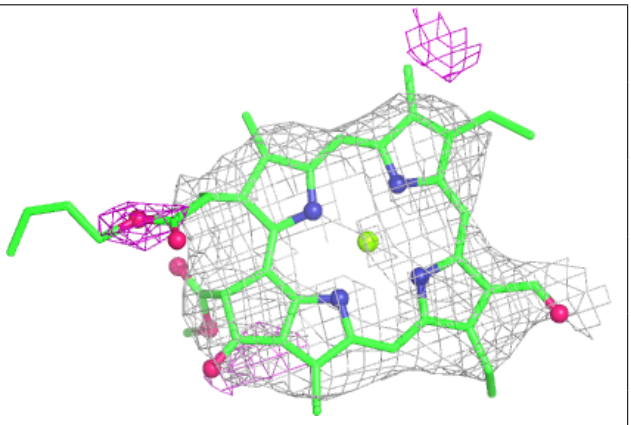


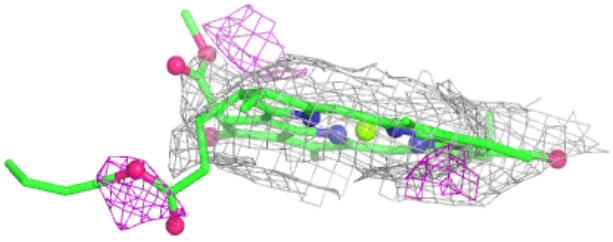


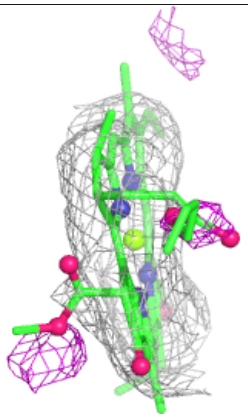


Electron density around CHL 4 613:

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

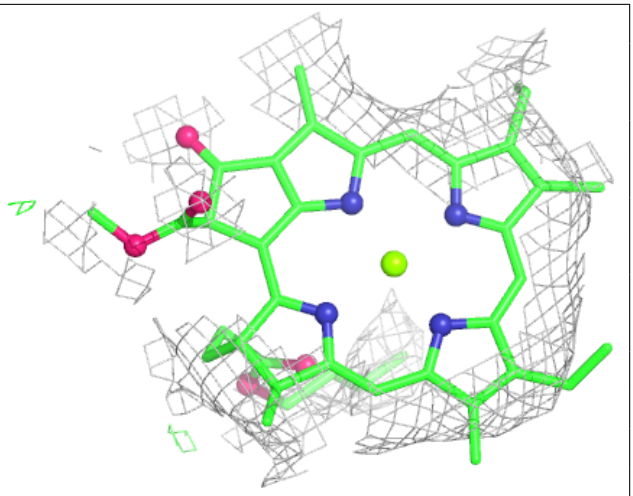


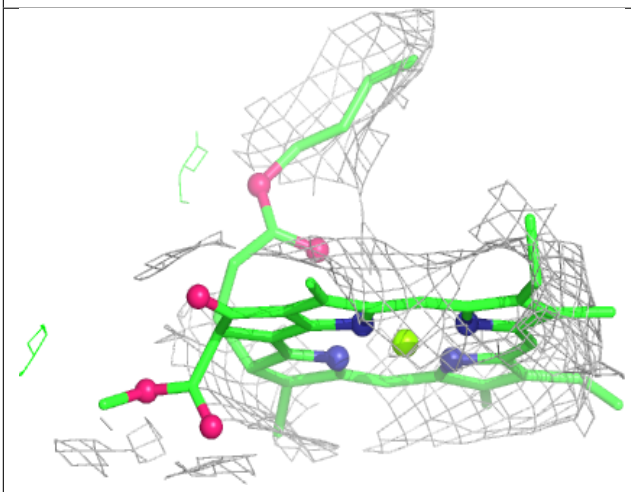


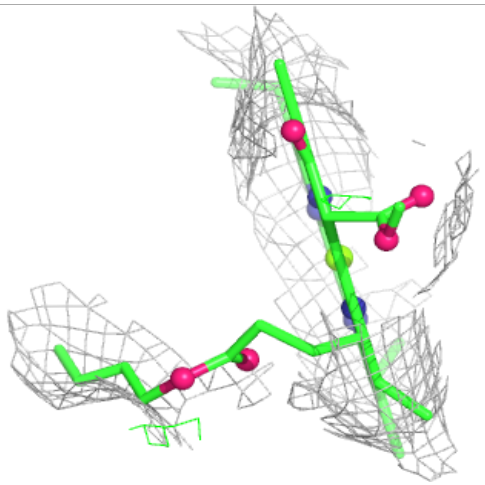


Electron density around CLA A 1109:

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

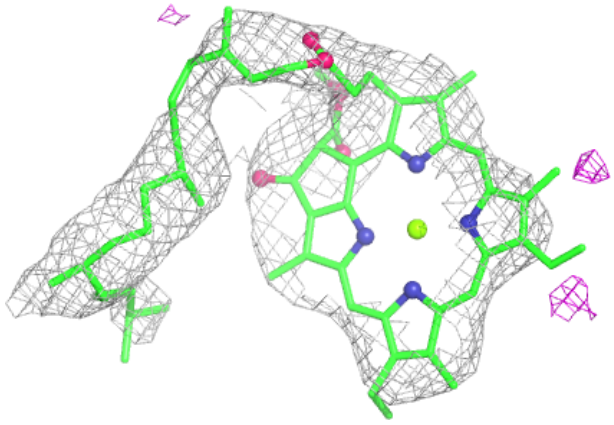


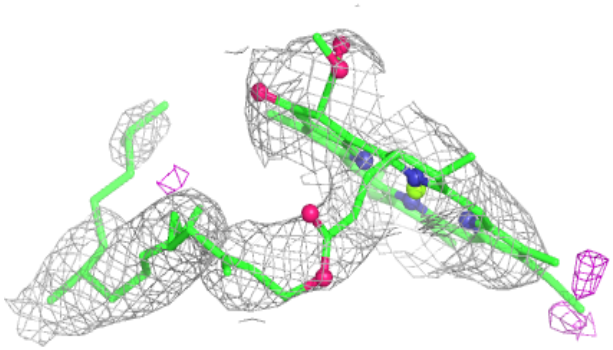


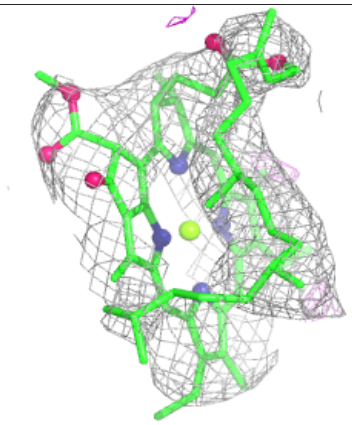


Electron density around CLA B 1229:

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

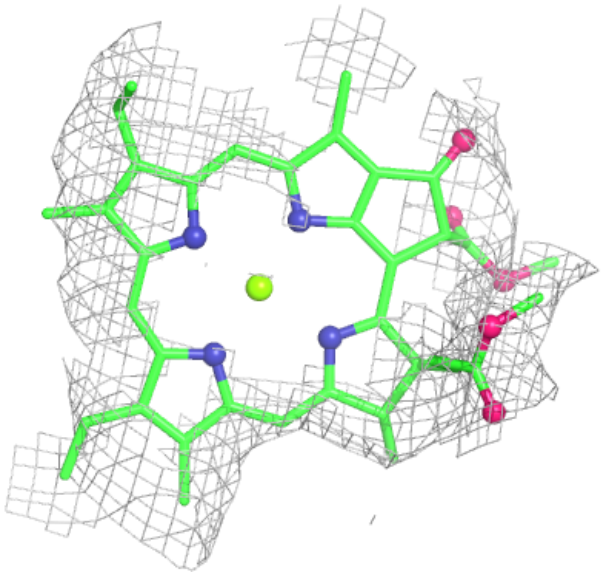


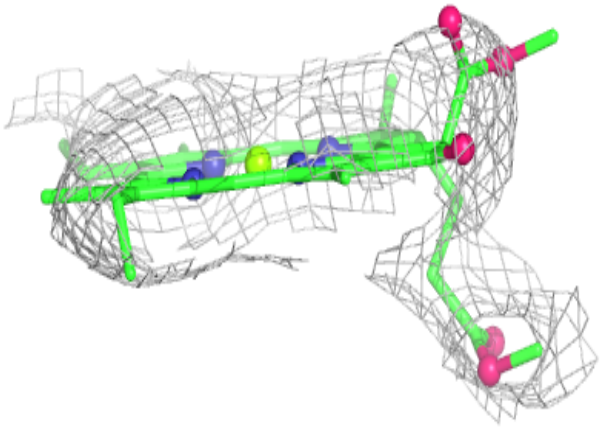


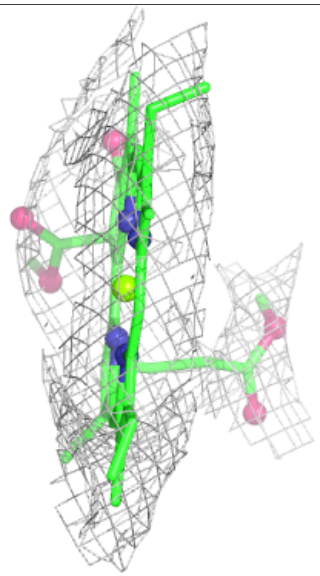


Electron density around CLA B 1209:

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

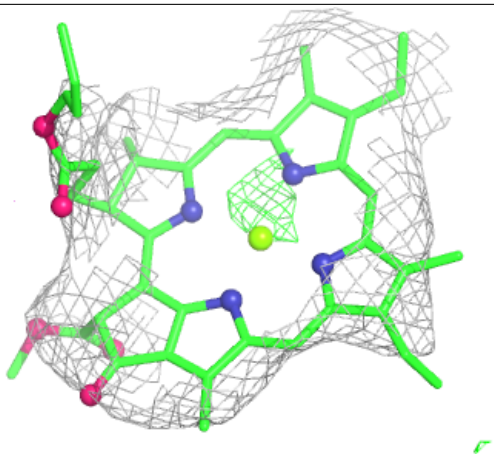


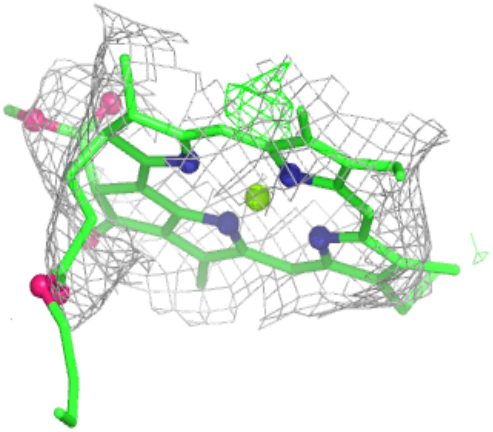


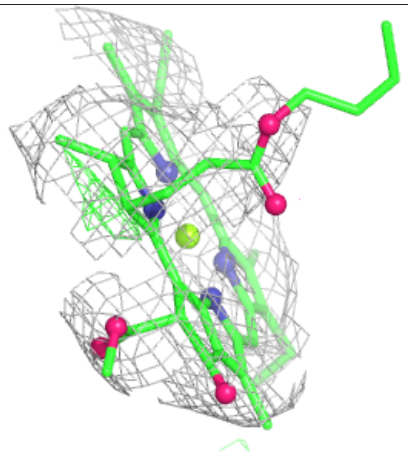


Electron density around CLA B 1232:

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

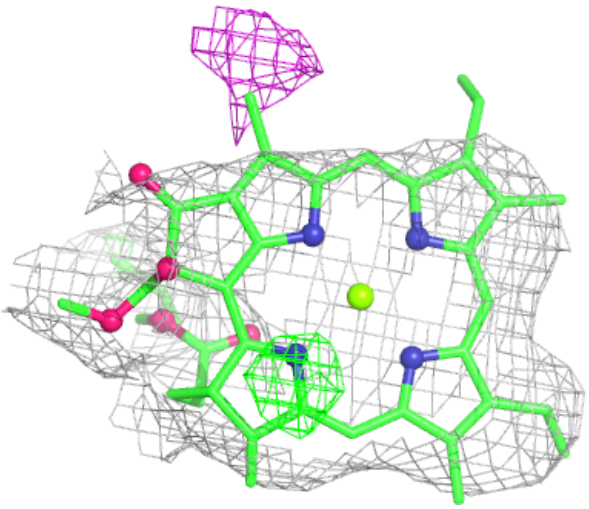


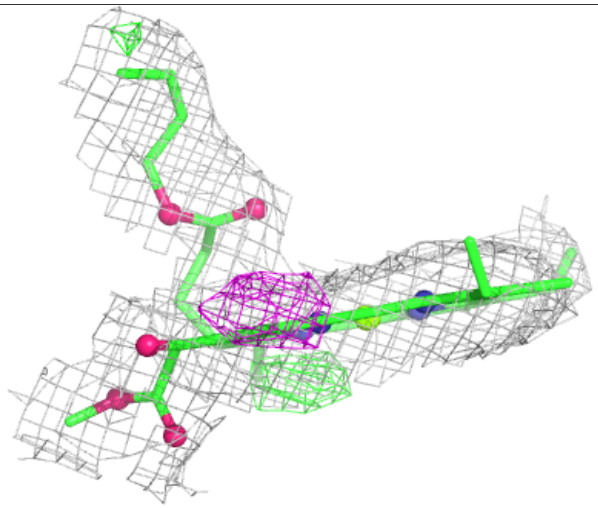


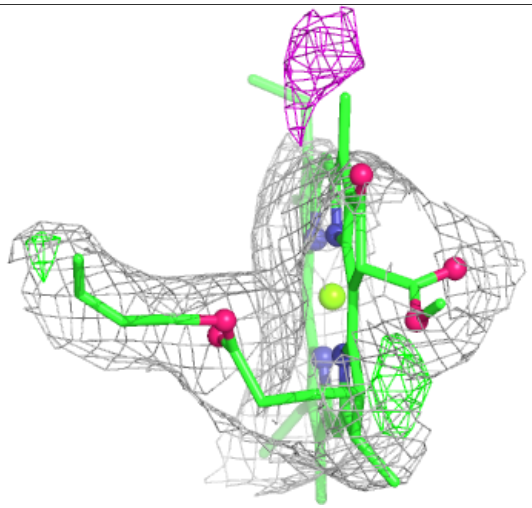


Electron density around CLA A 1126:

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

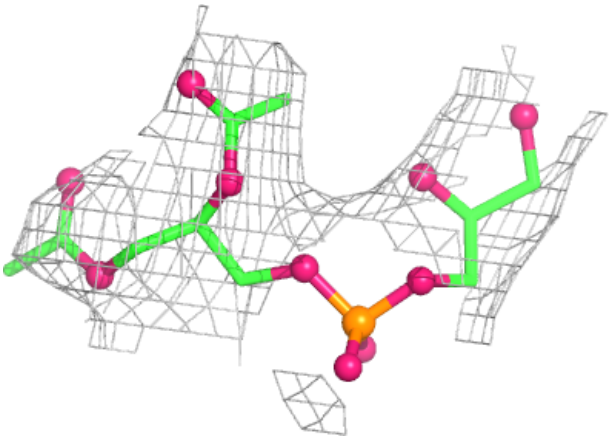


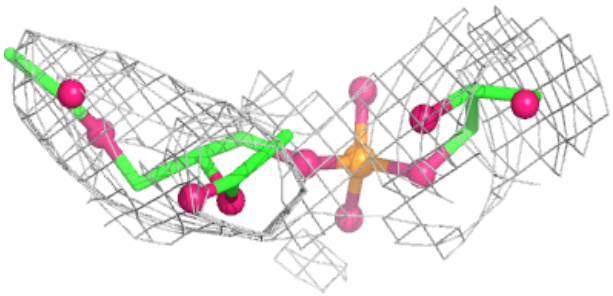


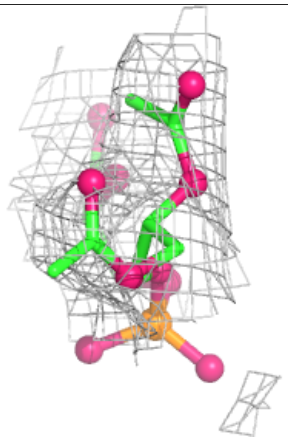


Electron density around LHG B 5001:

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

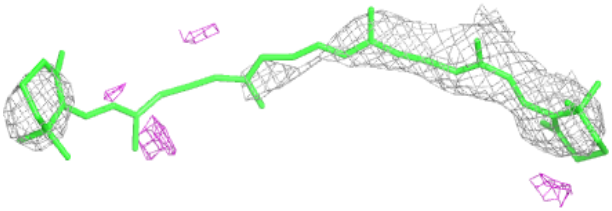


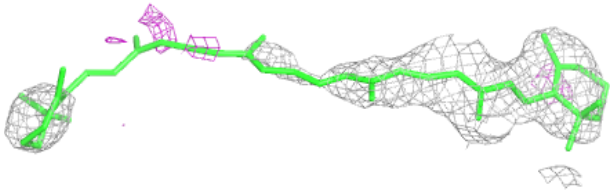


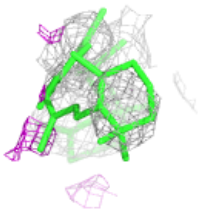


Electron density around BCR B 4006:

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

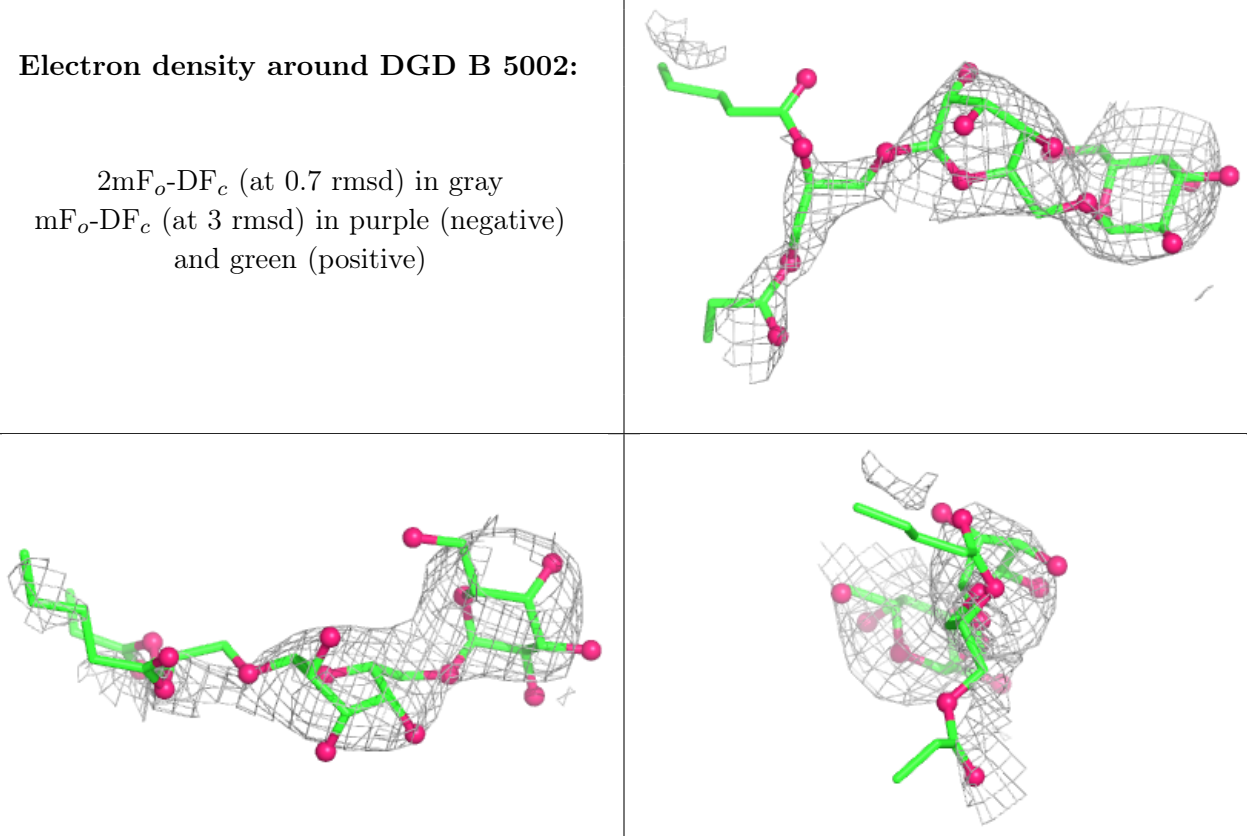






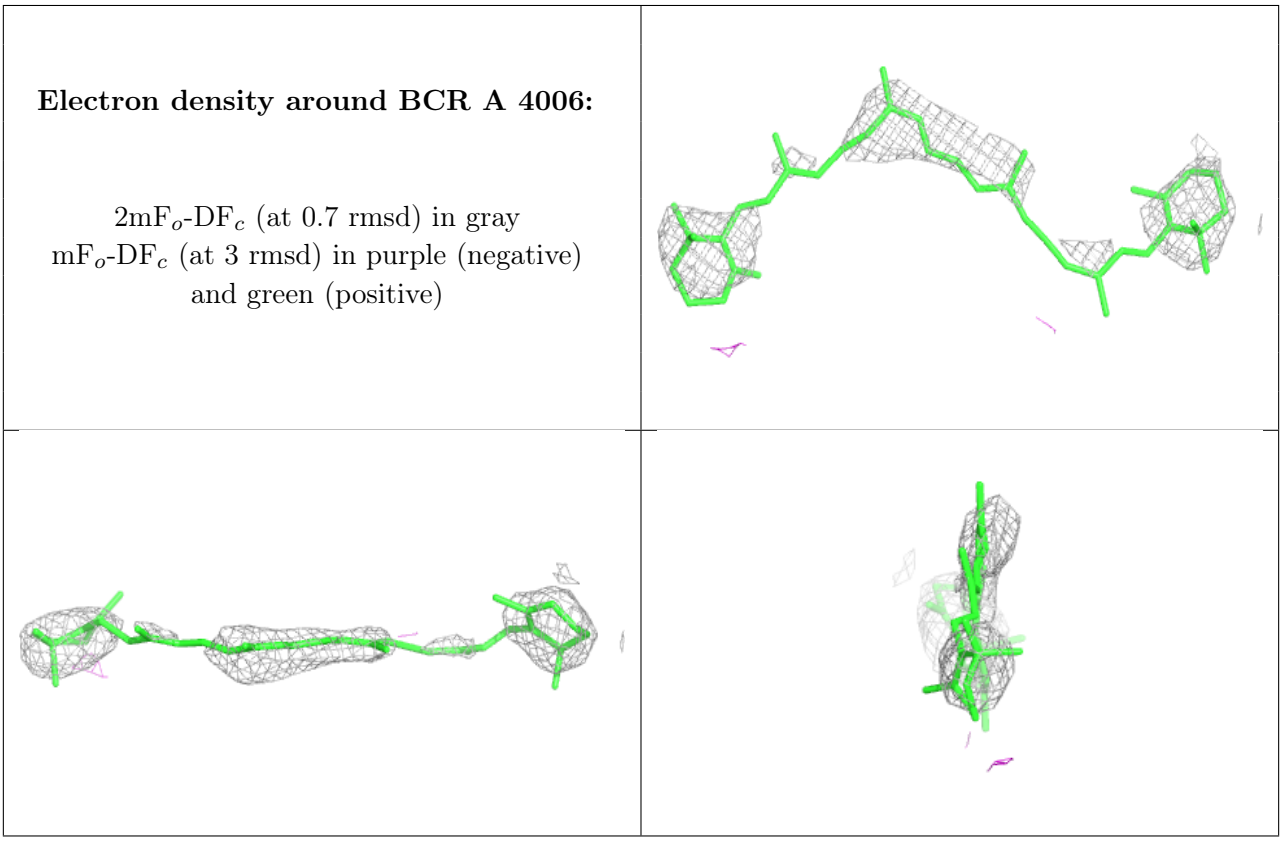
Electron density around DGD B 5002:

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



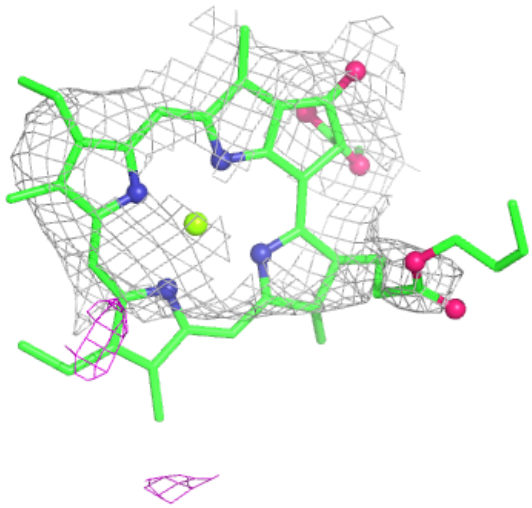
Electron density around BCR A 4006:

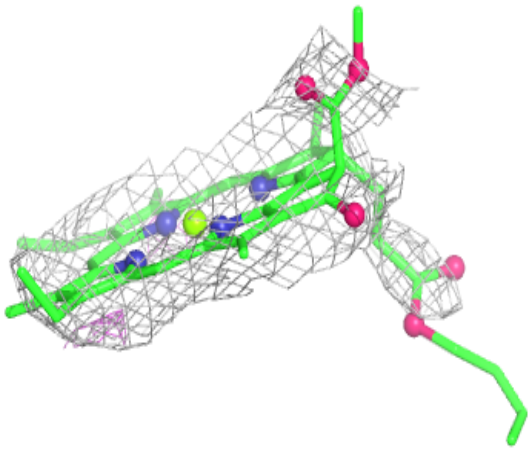
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 1137:

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

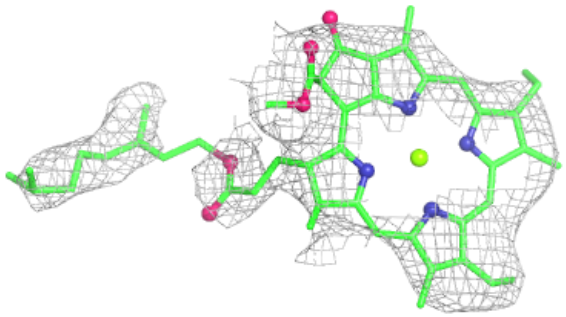


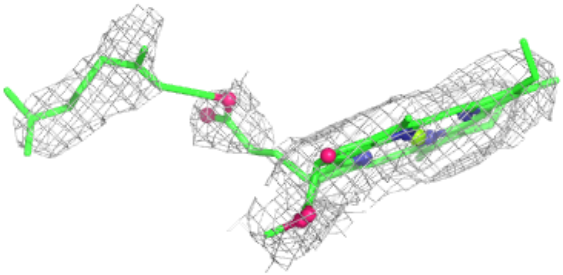


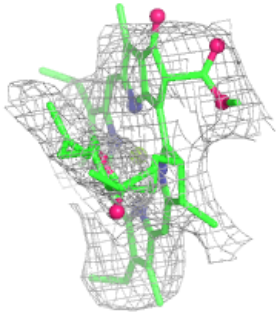


Electron density around CLA B 1220:

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

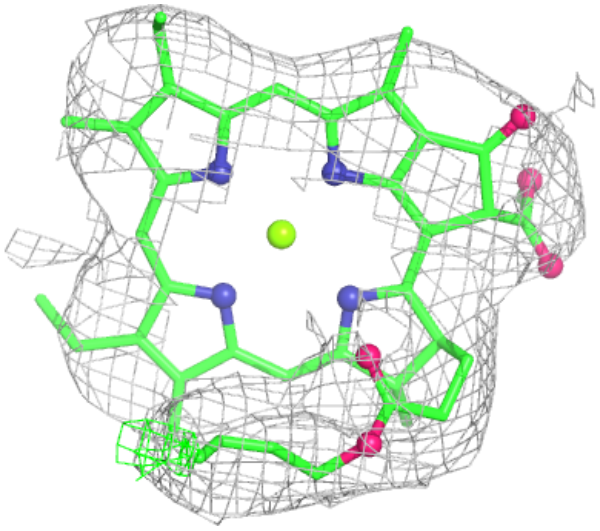


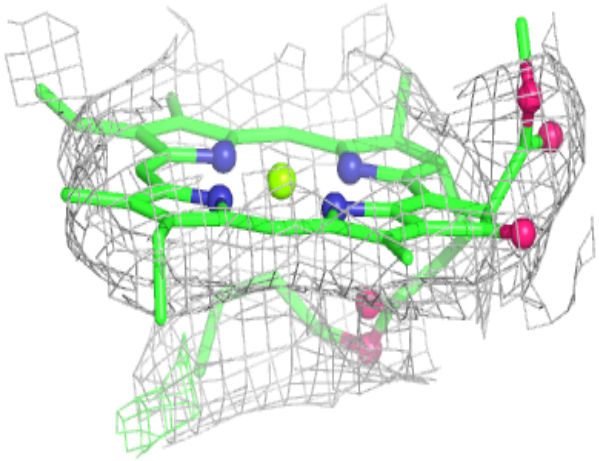




Electron density around CLA 4 604:

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

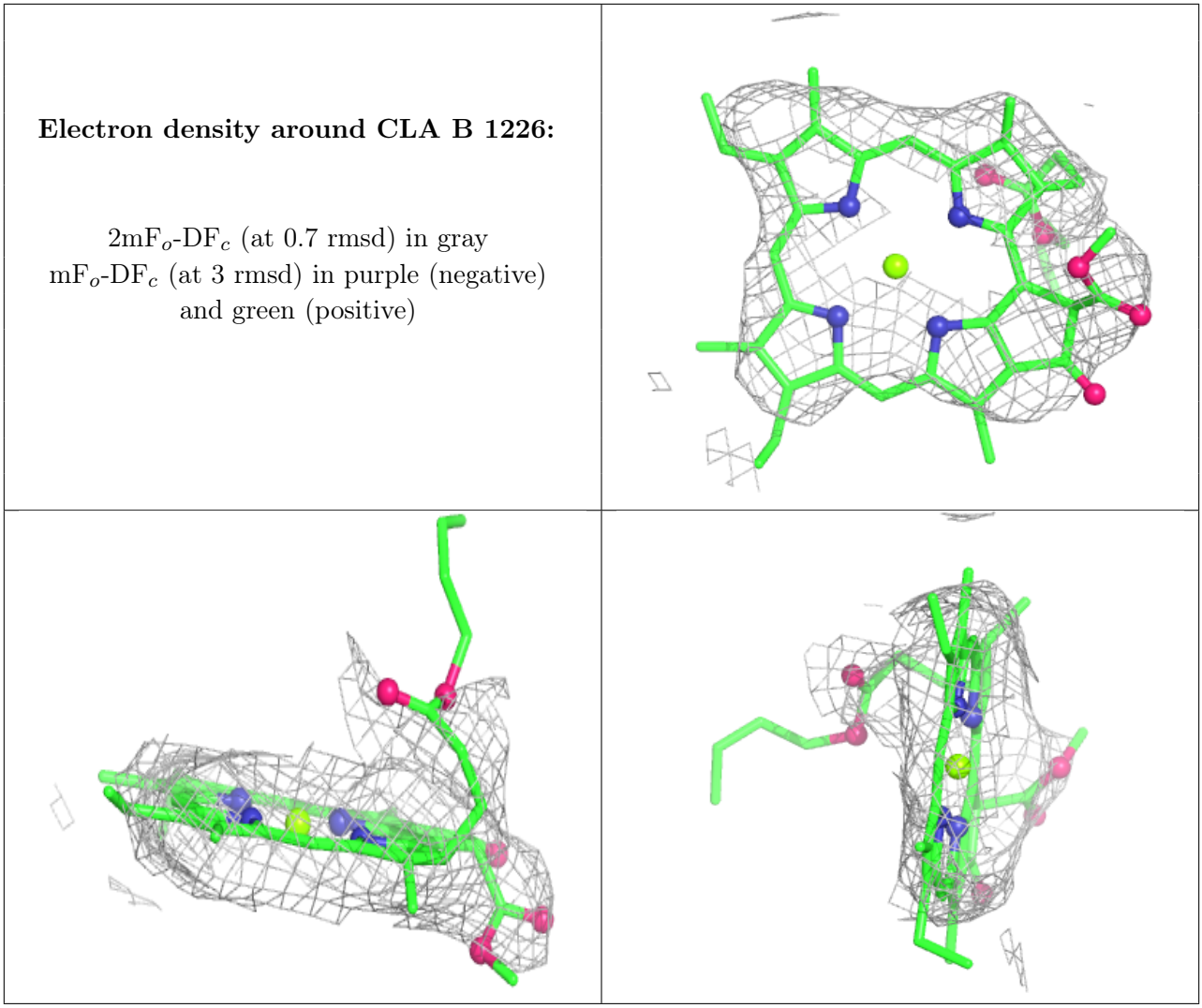






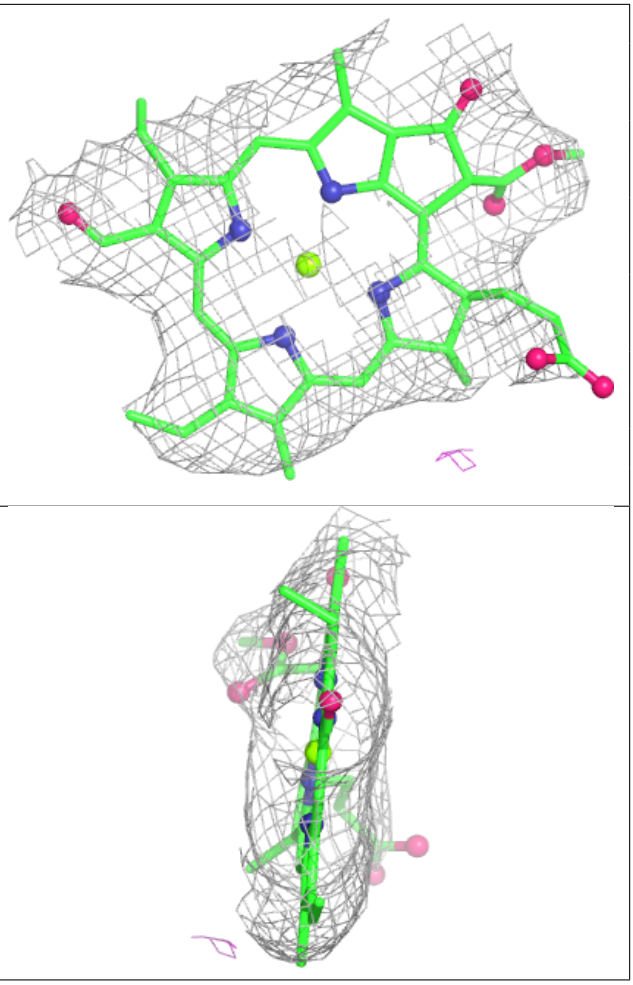
Electron density around CLA B 1226:

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



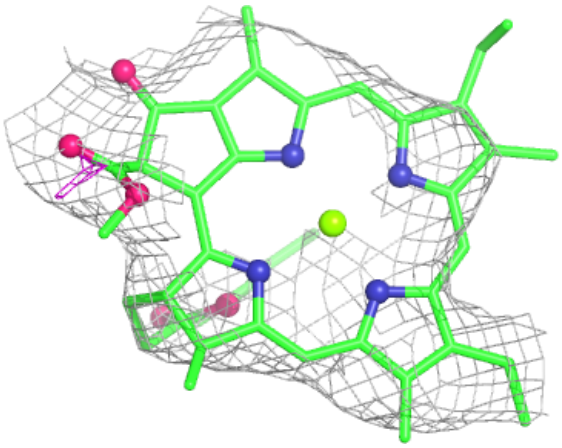
Electron density around CHL 2 613:

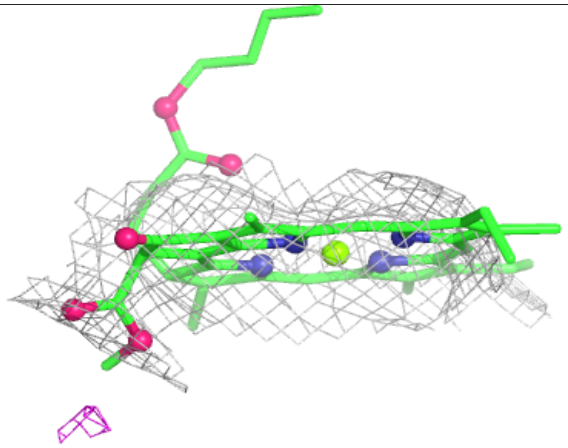
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

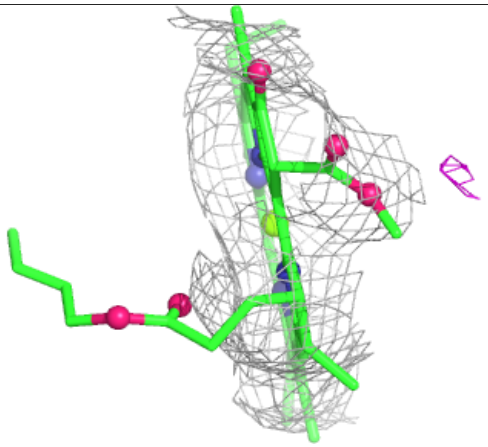


Electron density around CLA 2 607:

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

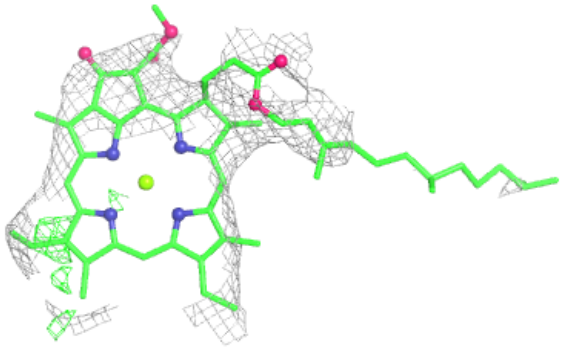


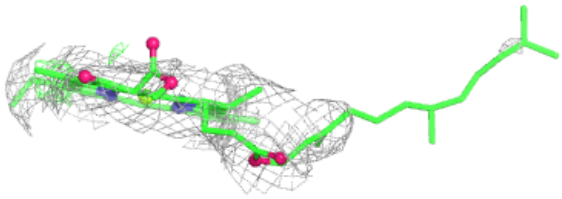




Electron density around CLA B 1023:

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

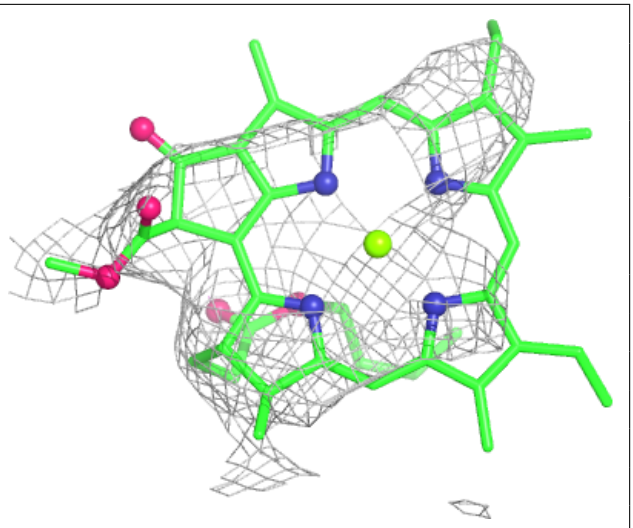


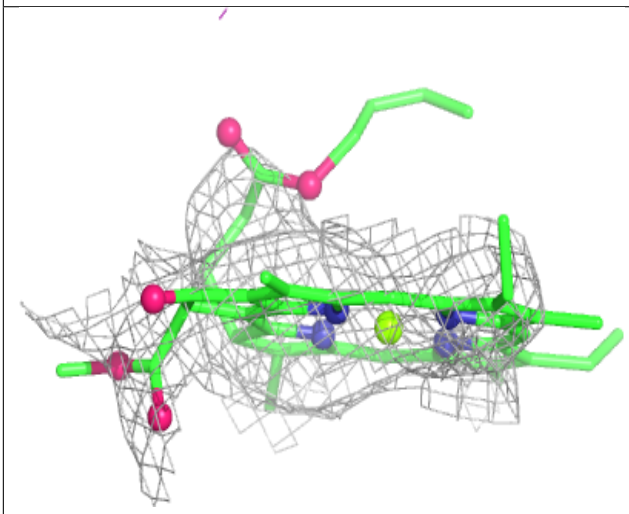


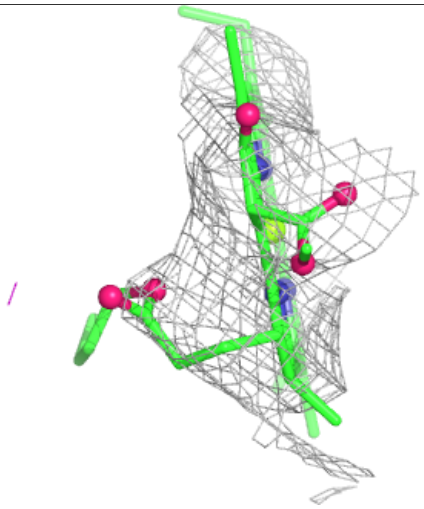


Electron density around CLA A 1119:

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

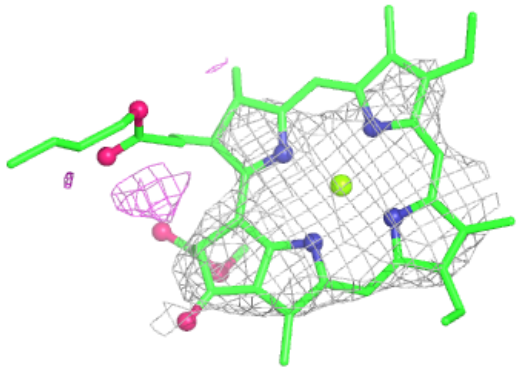


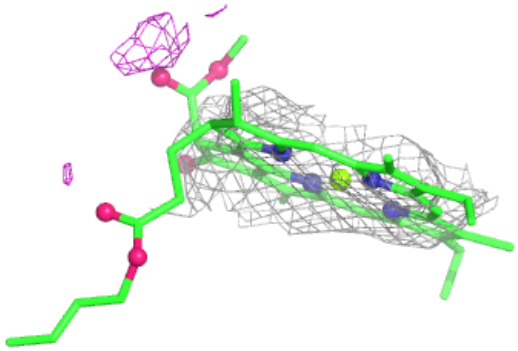


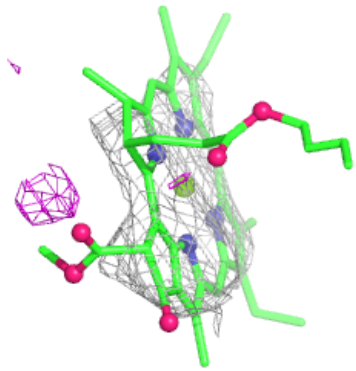


Electron density around CLA A 1112:

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

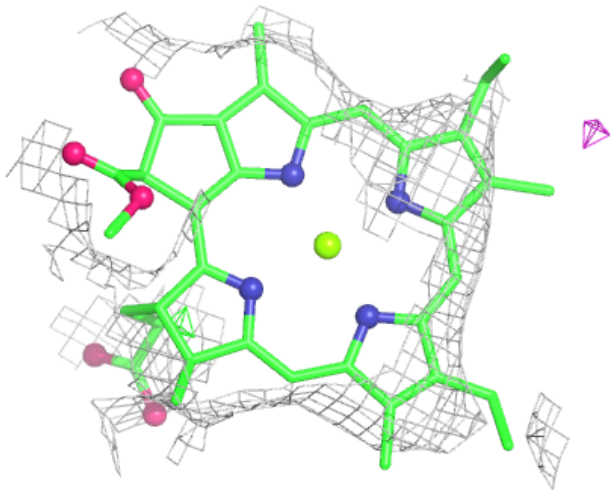


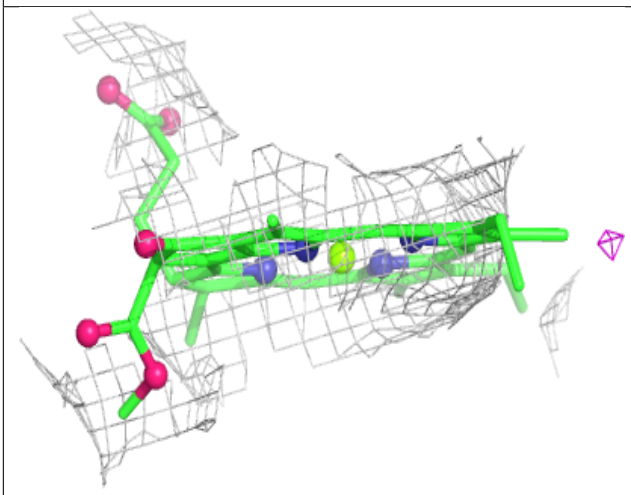


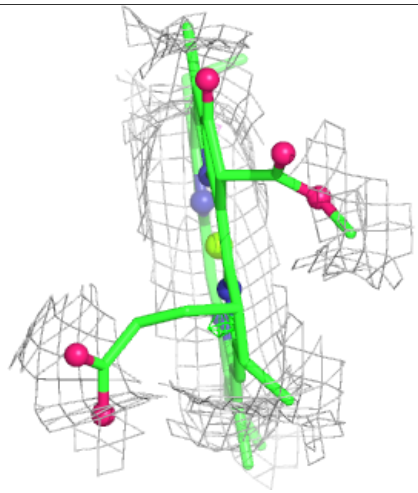


Electron density around CLA A 1102:

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

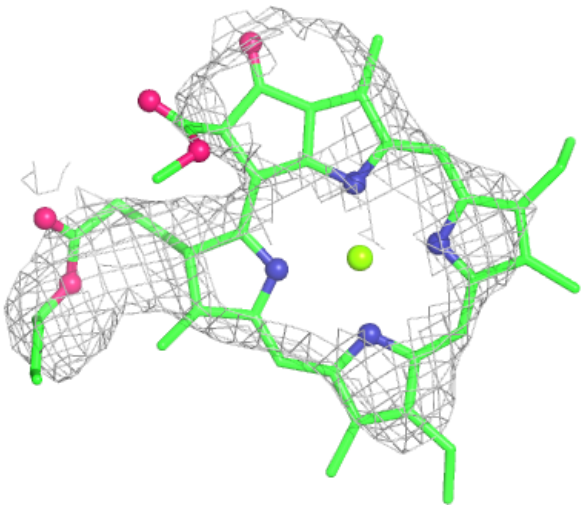


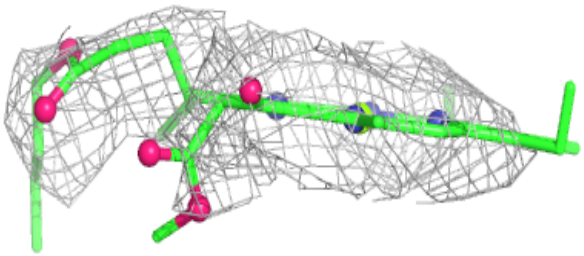


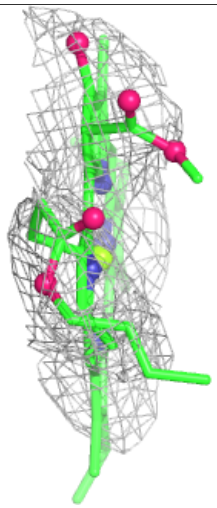


Electron density around CLA B 1221:

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

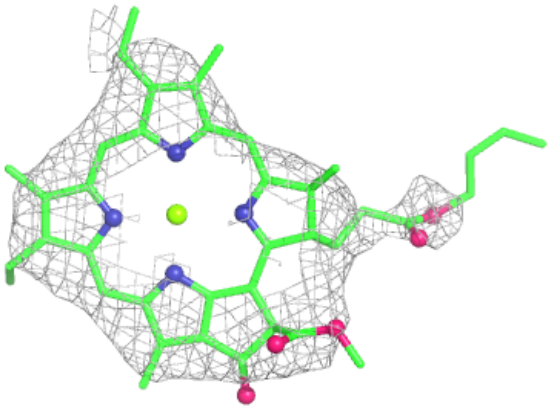


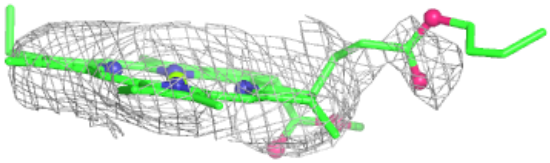


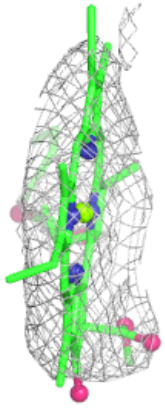


Electron density around CLA J 1302:

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

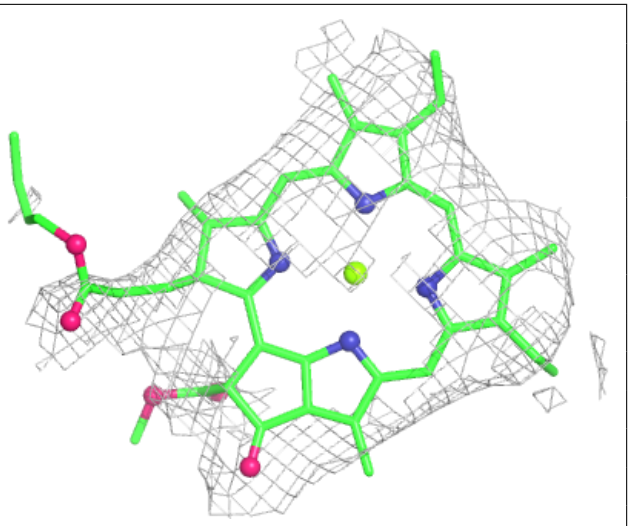


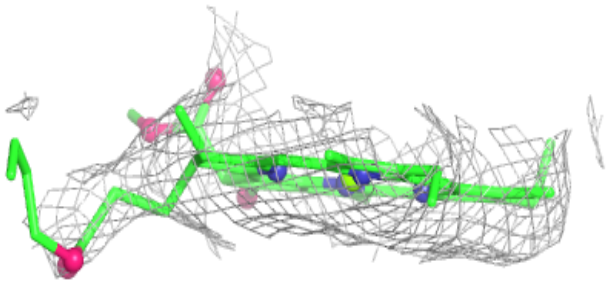


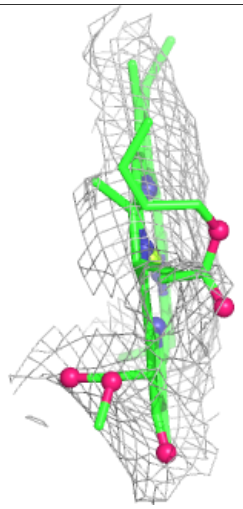


Electron density around CLA B 1206:

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

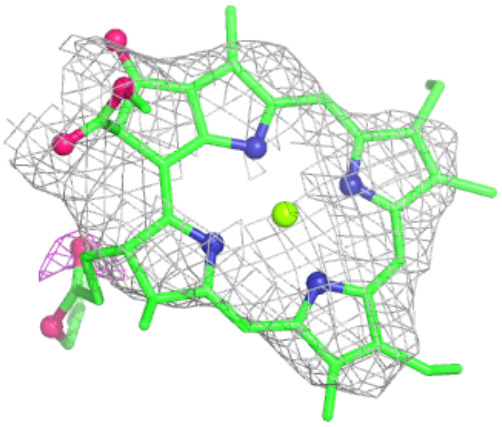


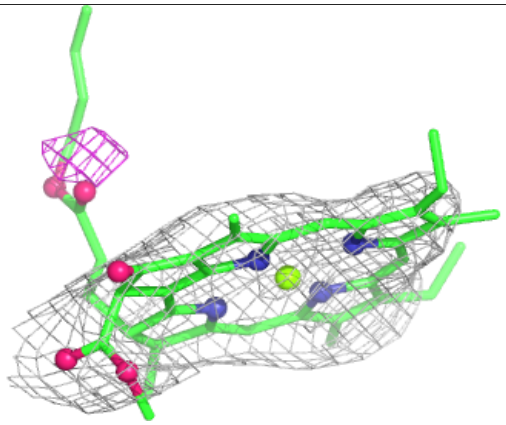


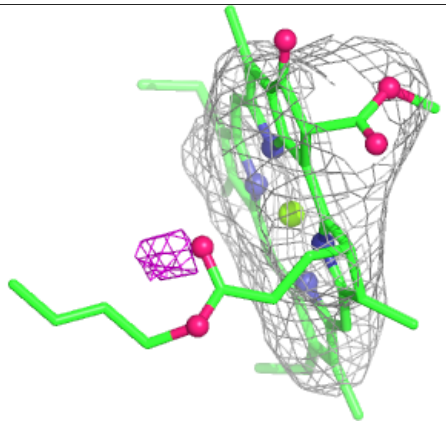


Electron density around CLA A 1122:

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

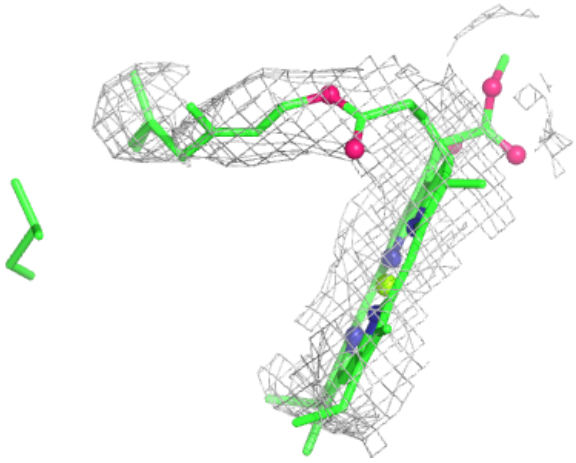


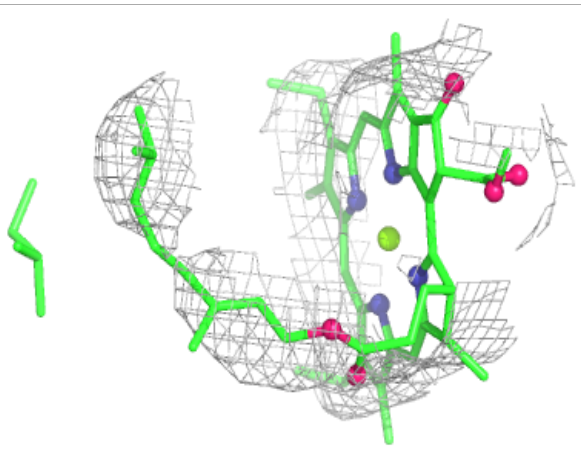


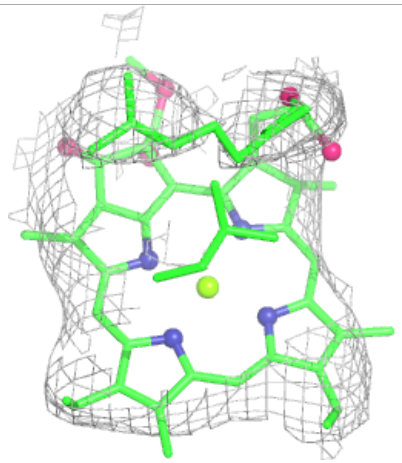


Electron density around CLA 1 612:

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

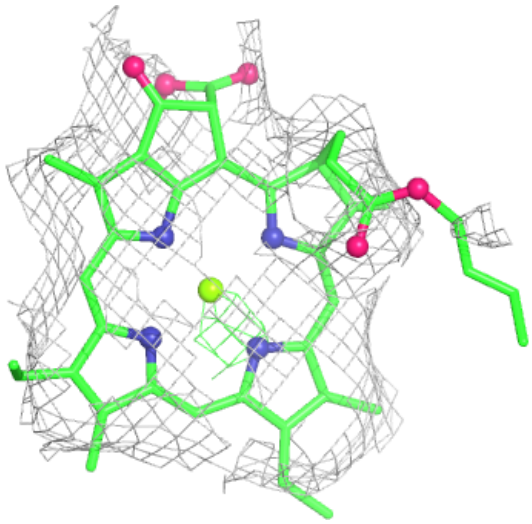


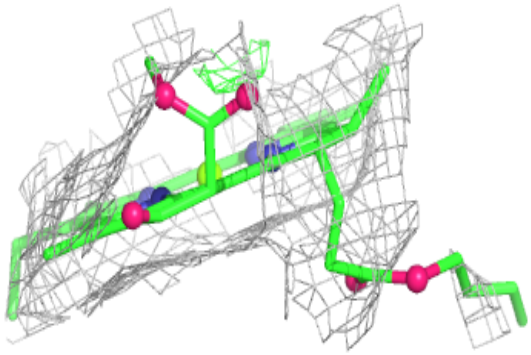


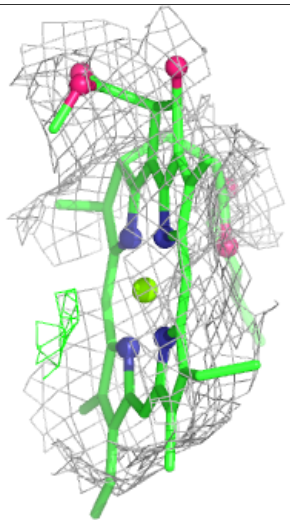


Electron density around CLA 2 601:

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

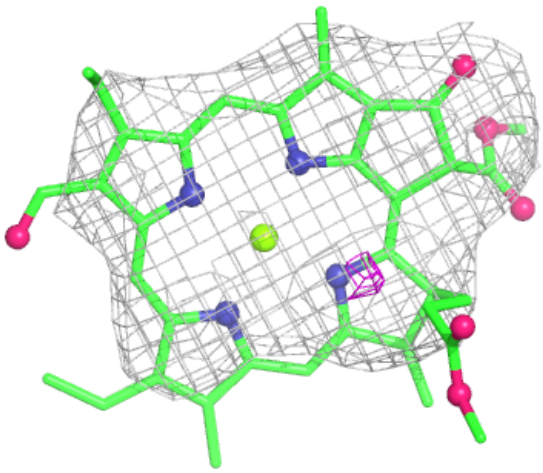


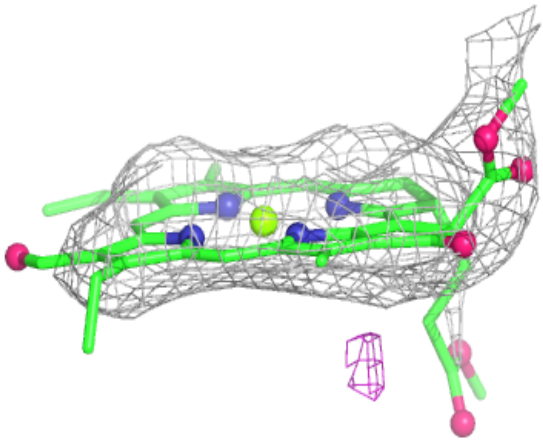


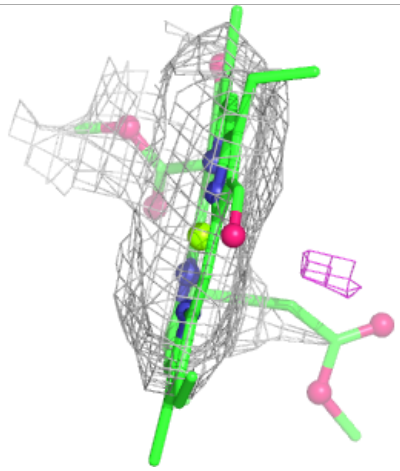


Electron density around CHL 4 610:

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

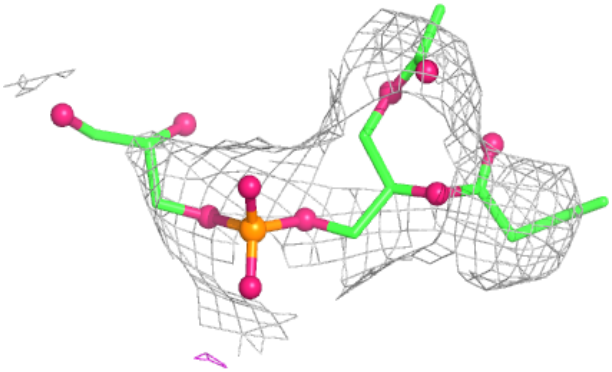


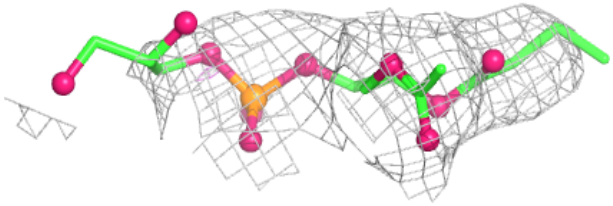


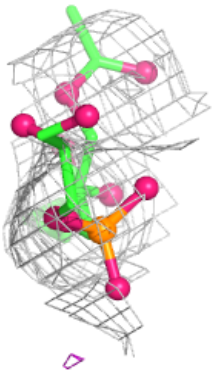


Electron density around LHG 1 801:

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

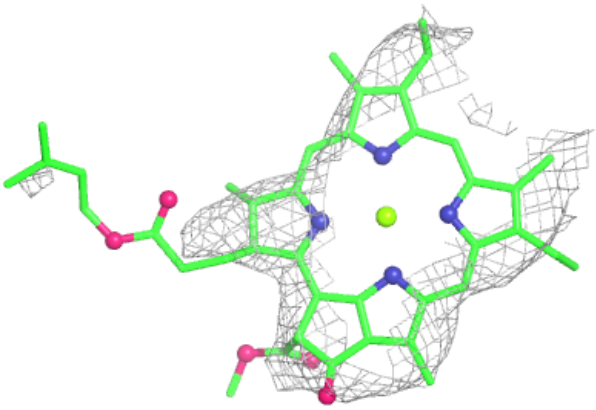


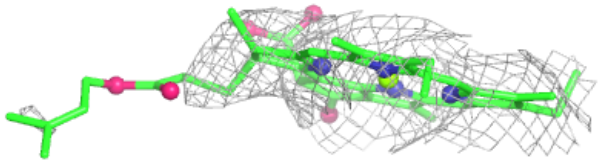


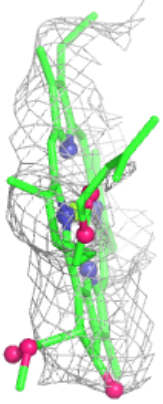


Electron density around CLA B 1022:

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

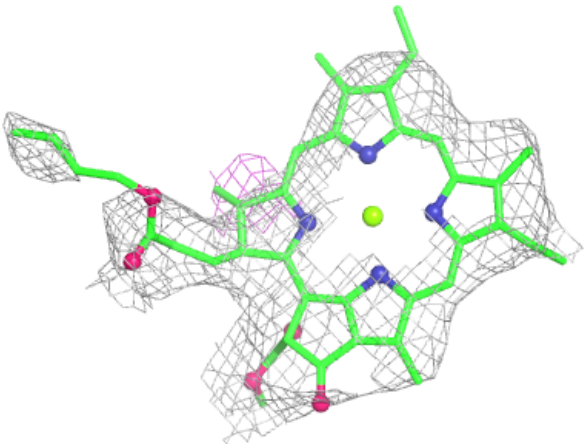


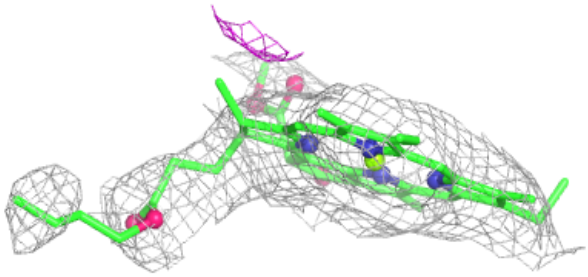


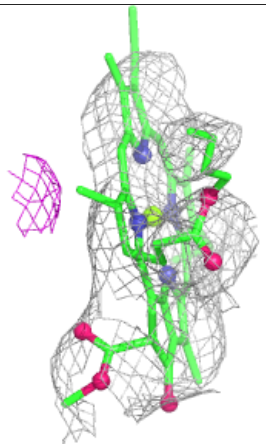


Electron density around CLA 4 609:

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

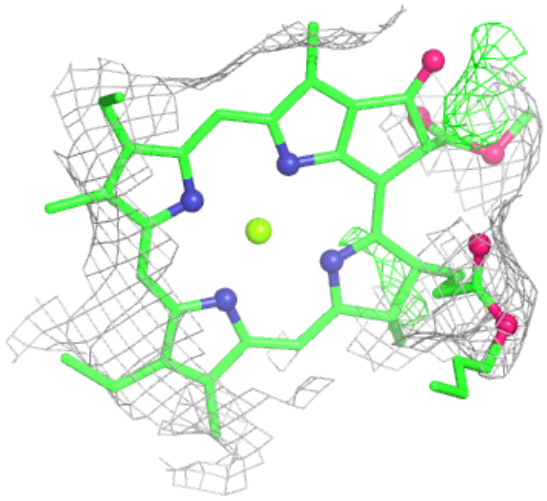


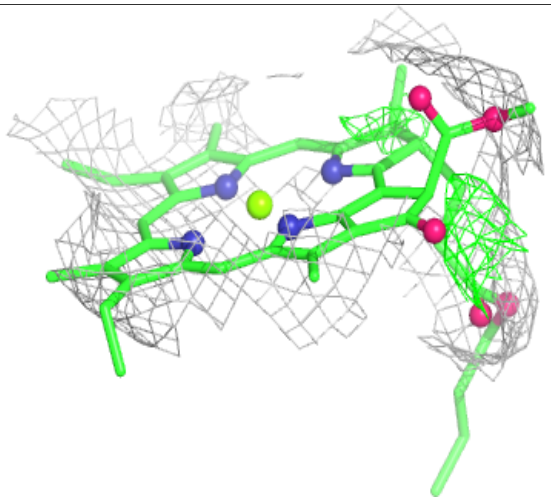


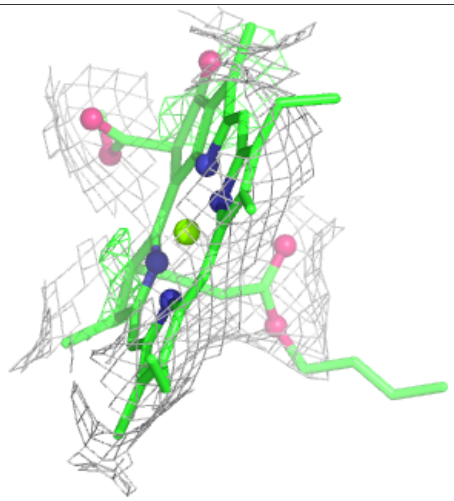


Electron density around CLA A 1133:

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

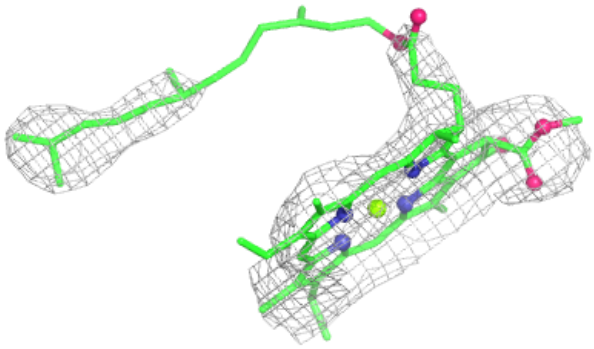


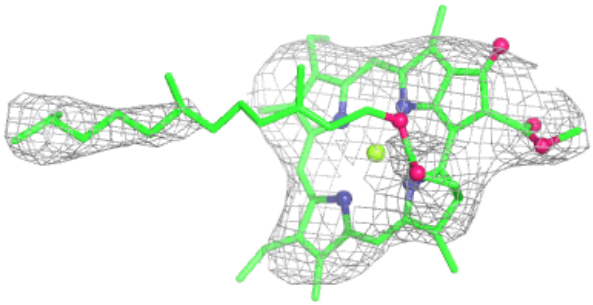


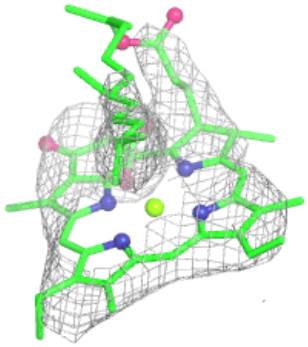


Electron density around CLA B 1228:

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

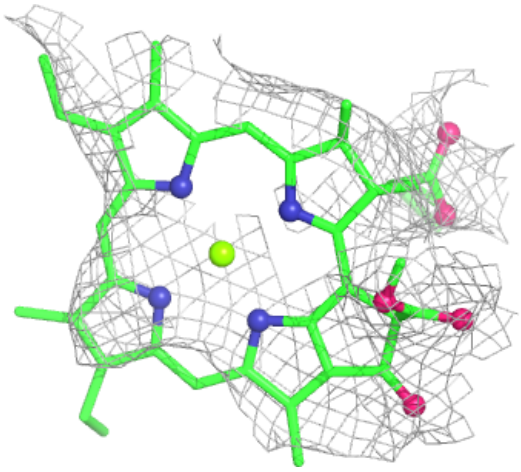


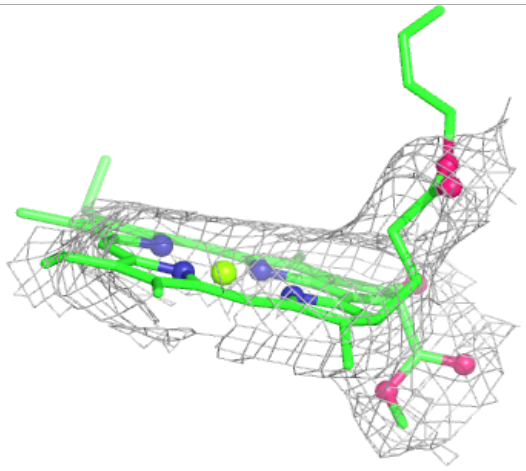


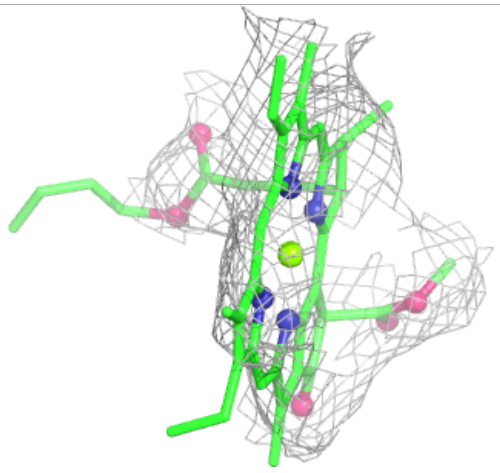


Electron density around CLA A 1128:

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

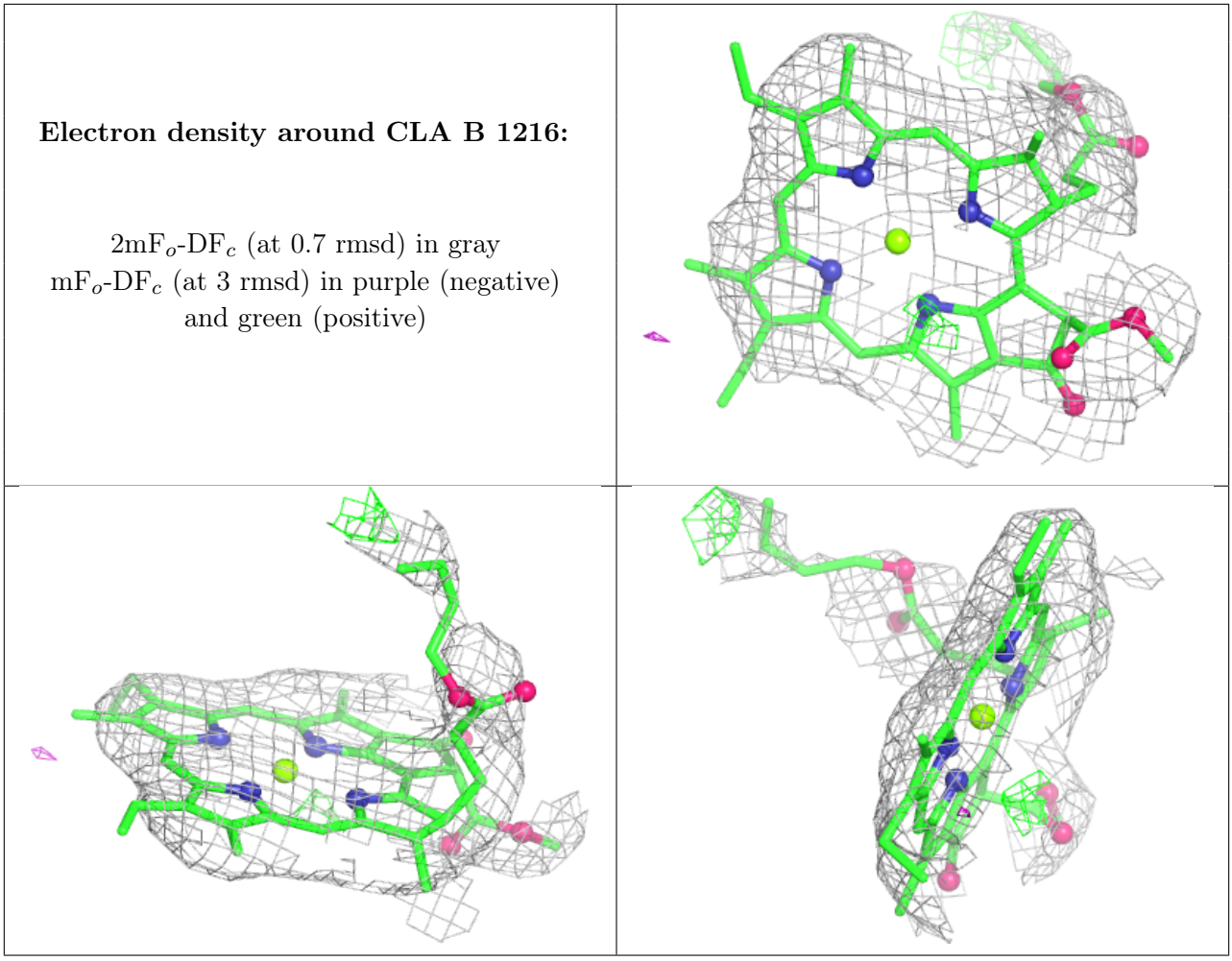






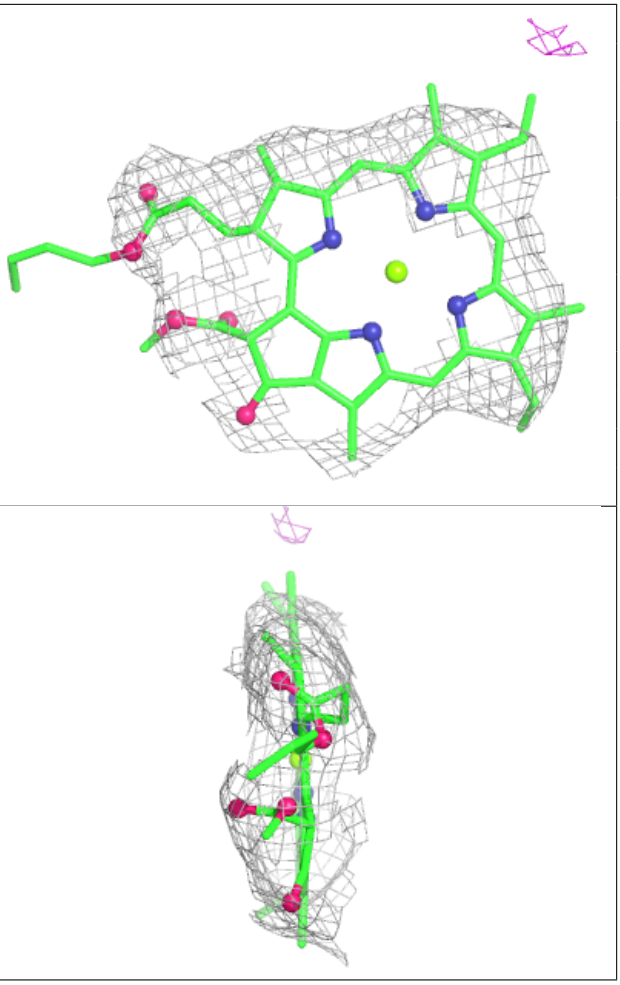
Electron density around CLA B 1216:

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



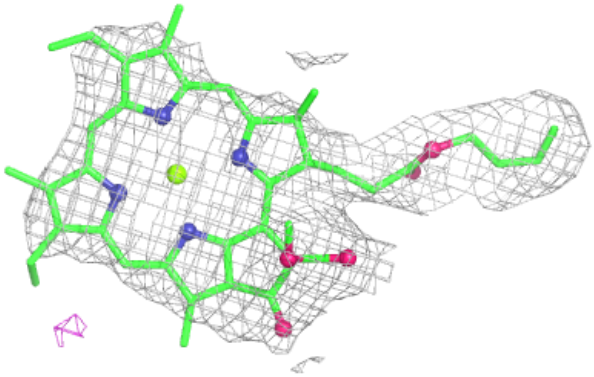
Electron density around CLA 4 602:

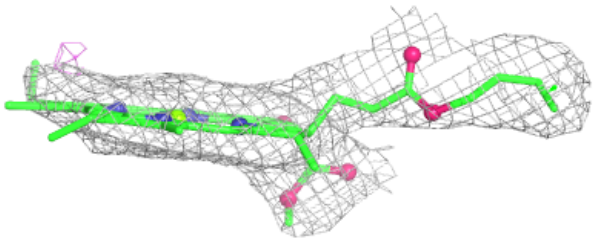
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

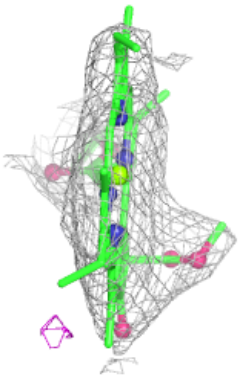


Electron density around CLA B 1234:

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

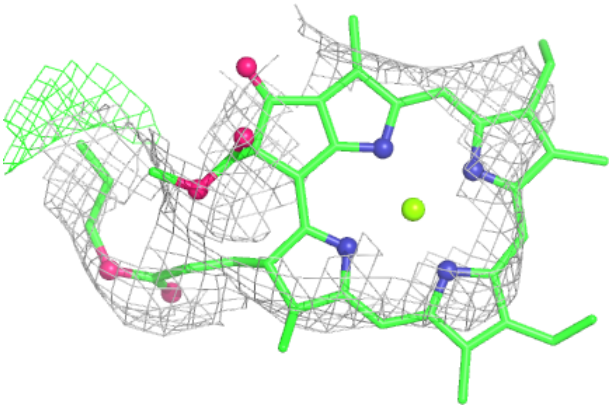


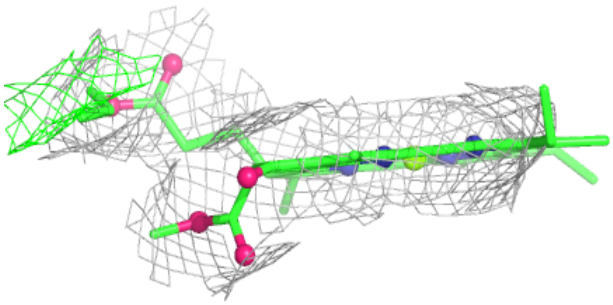


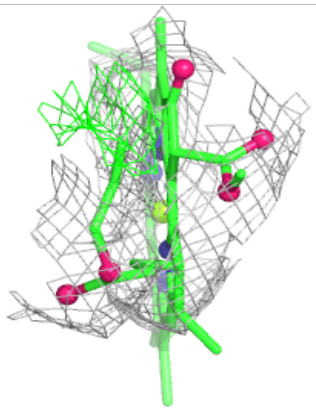


Electron density around CLA A 1123:

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

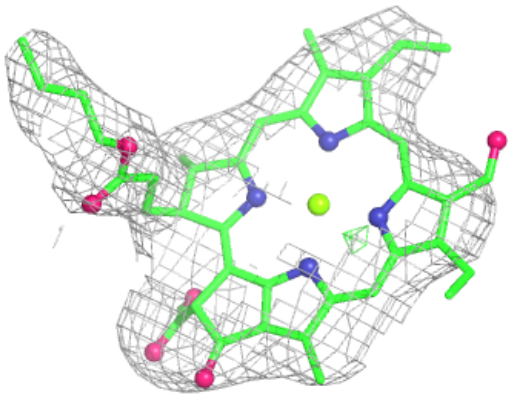


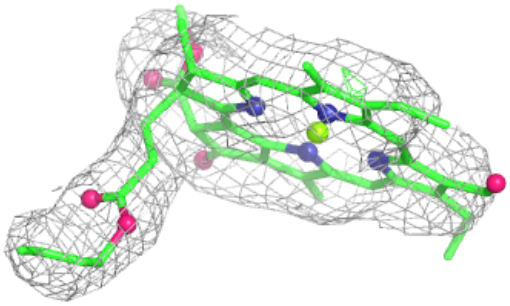


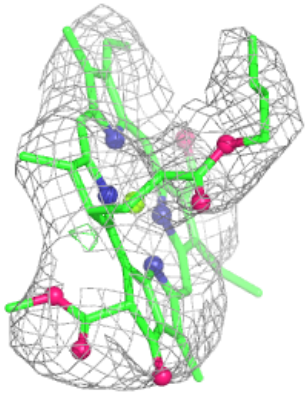


Electron density around CHL 4 611:

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

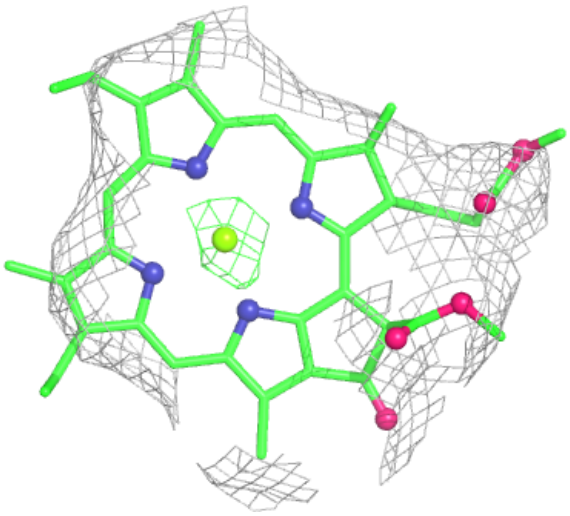


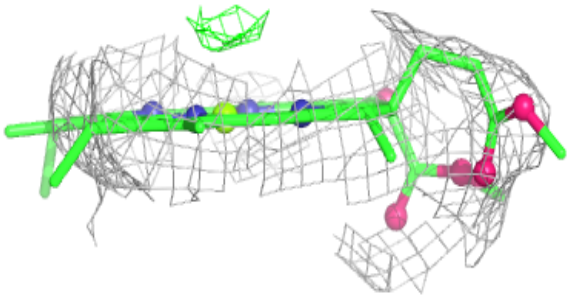


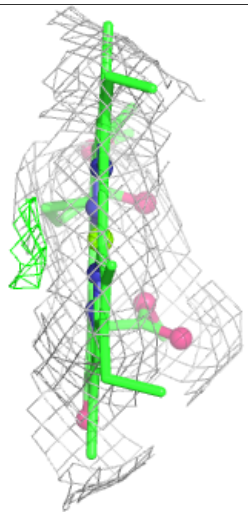


Electron density around CLA 1 602:

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

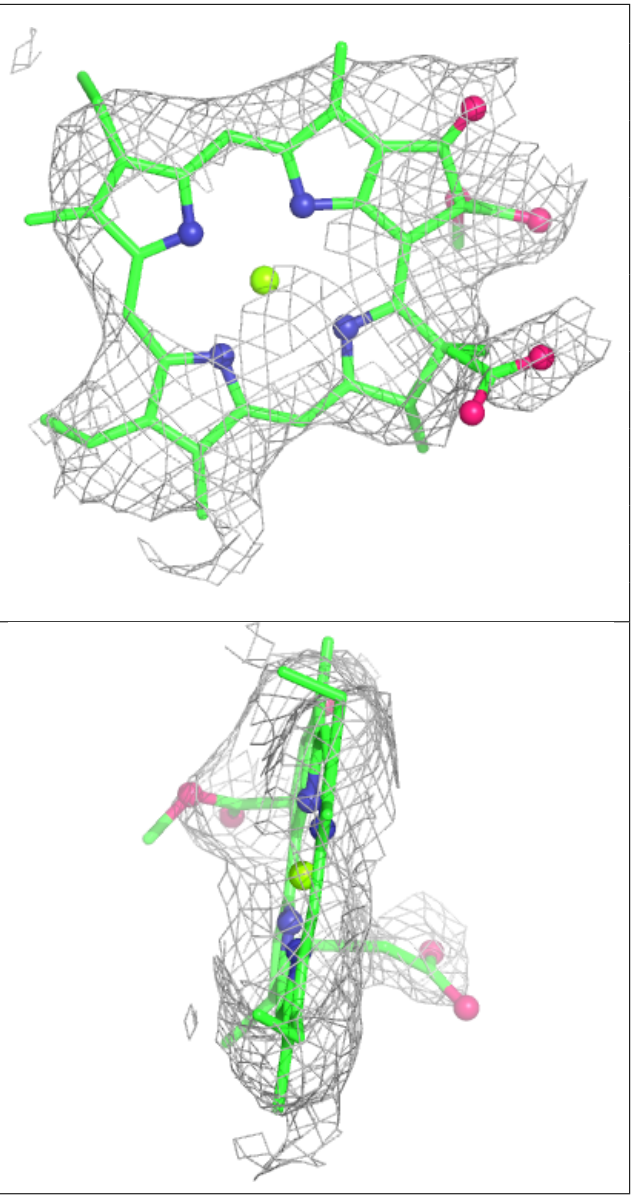






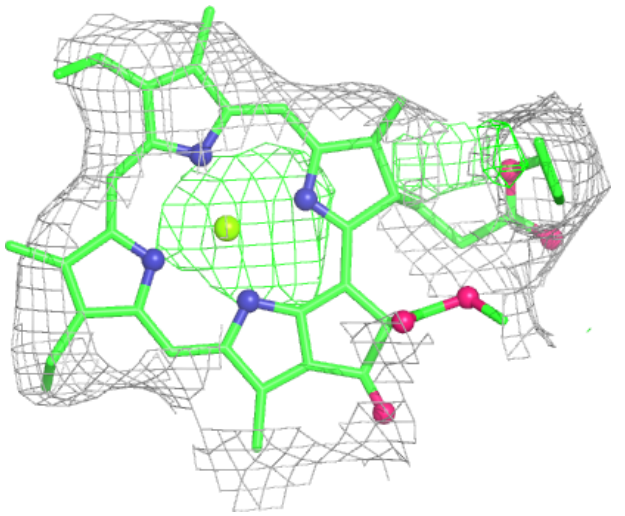
Electron density around CLA B 1227:

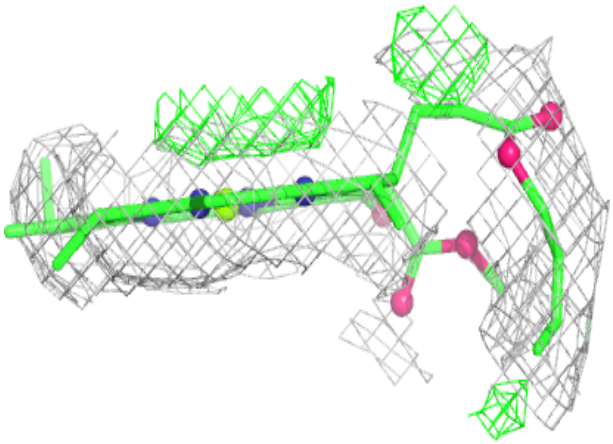
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

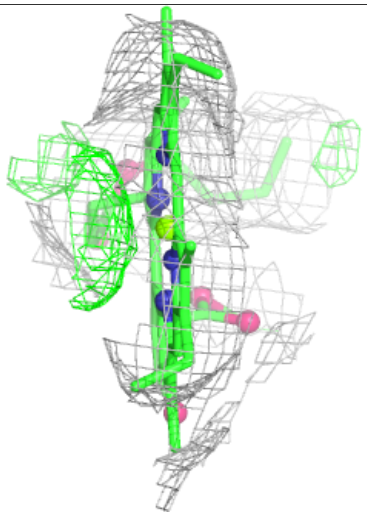


Electron density around CLA 4 605:

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

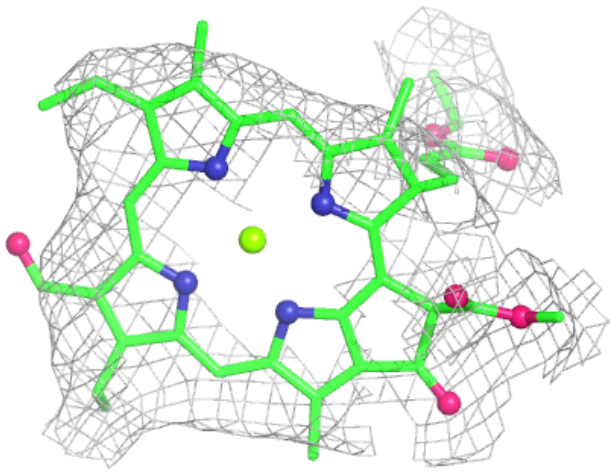


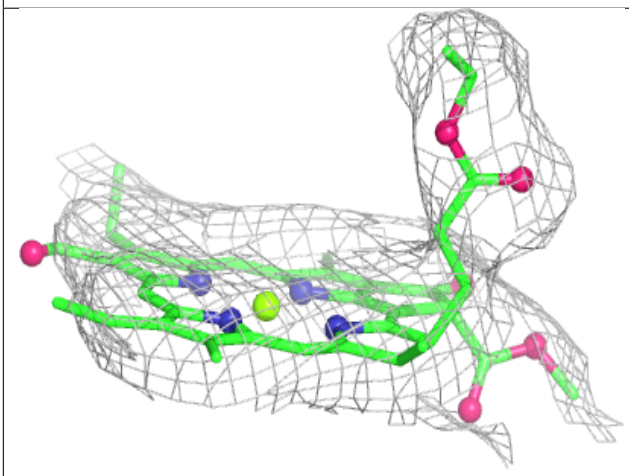


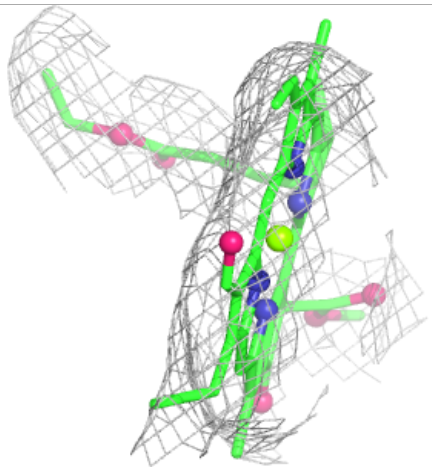


Electron density around CHL 2 611:

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

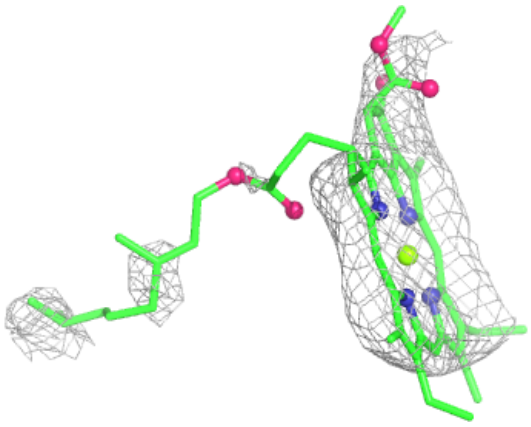


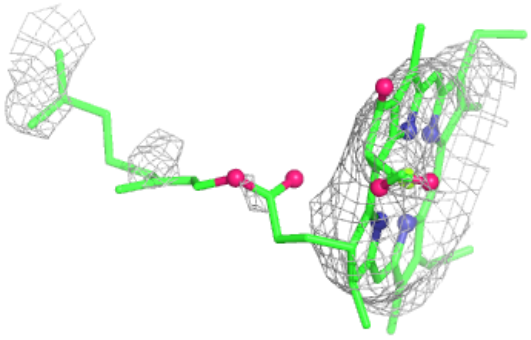


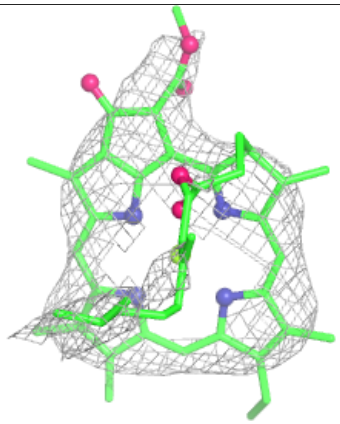


Electron density around CLA A 1140:

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

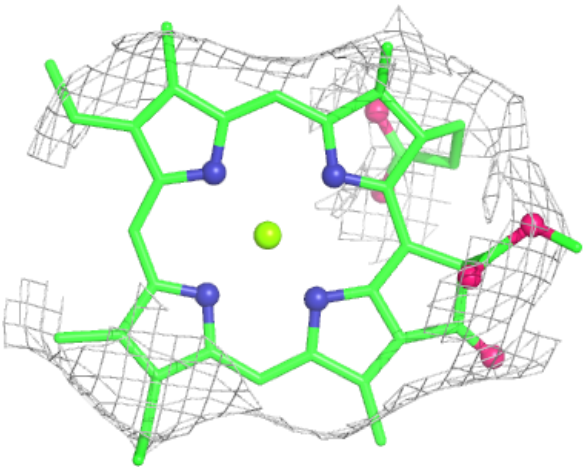


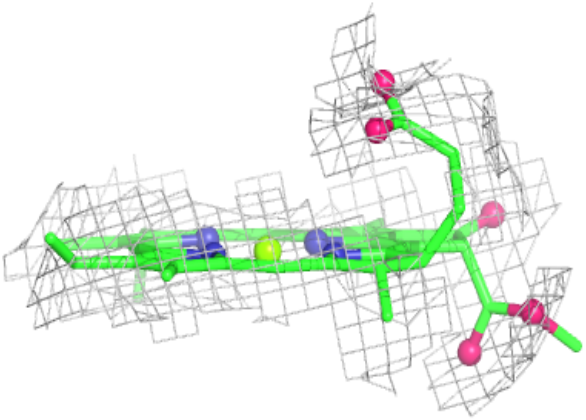


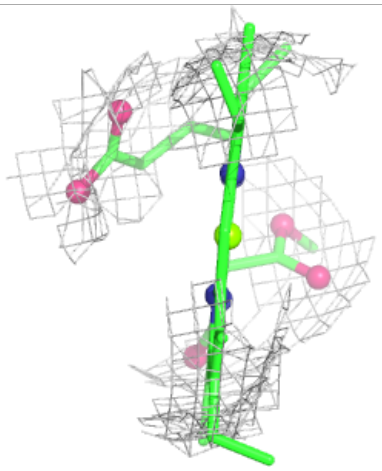


Electron density around CLA 1 613:

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

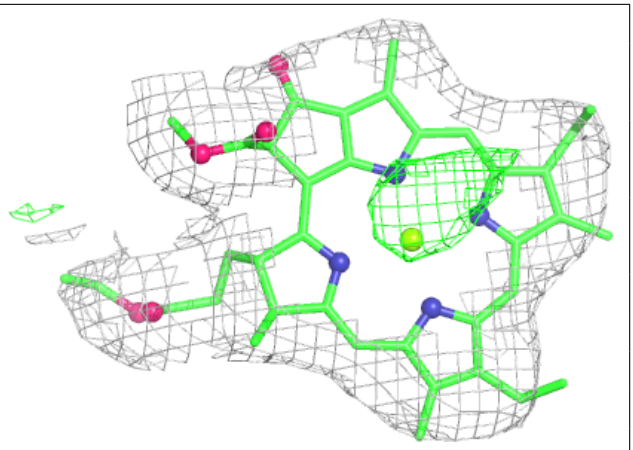


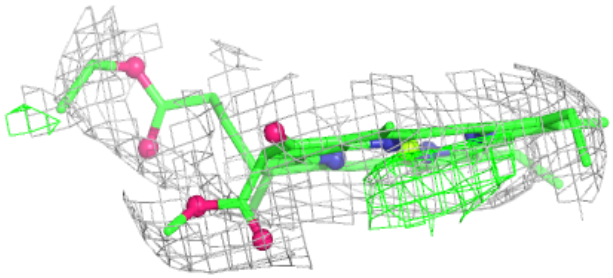


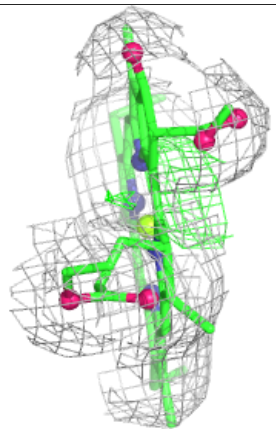


Electron density around CLA F 1301:

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

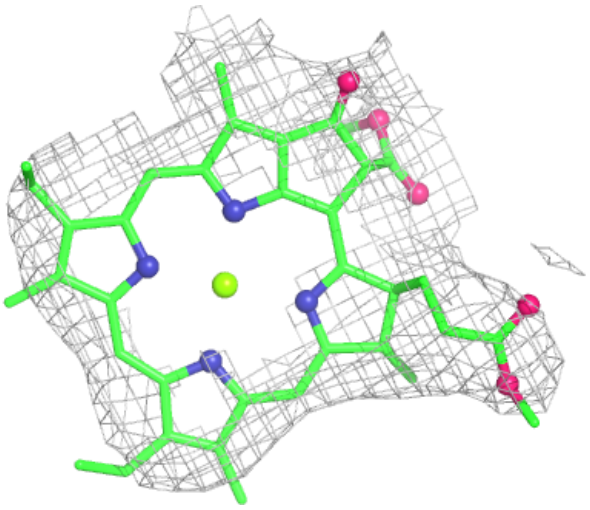


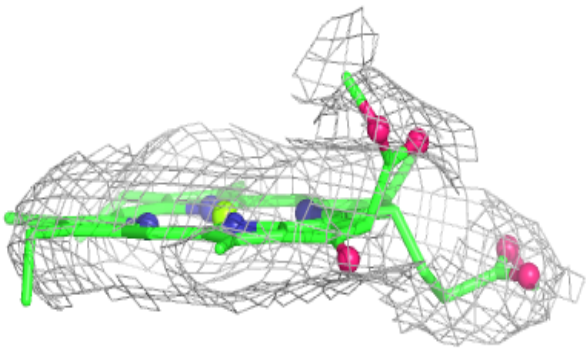


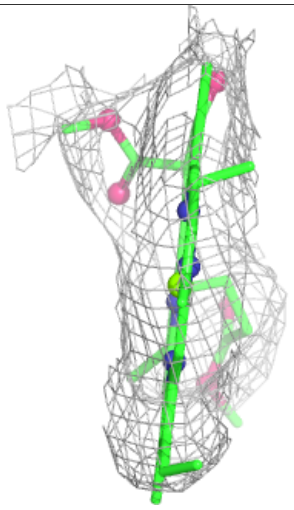


Electron density around CLA B 1217:

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

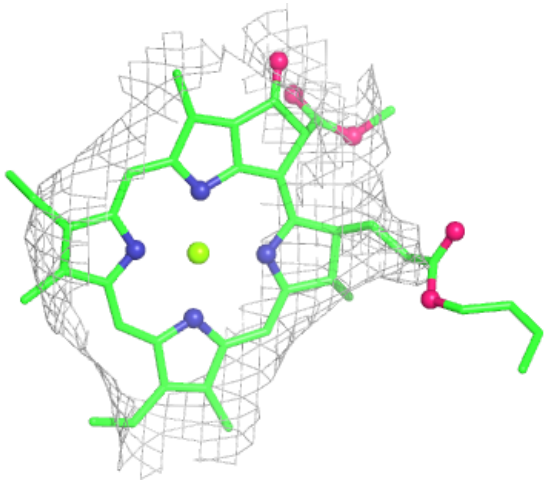


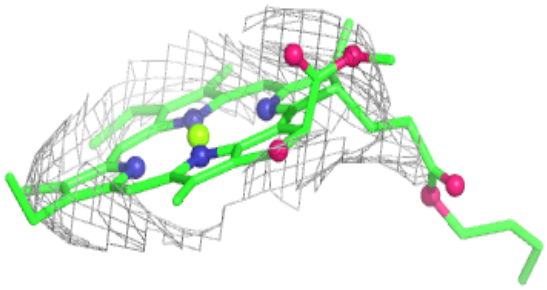


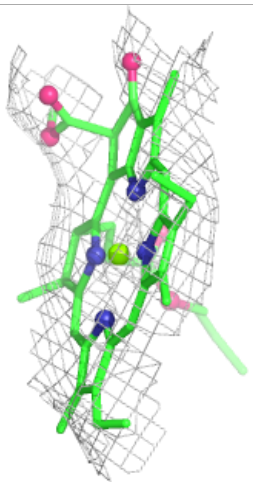


Electron density around CLA A 1125:

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

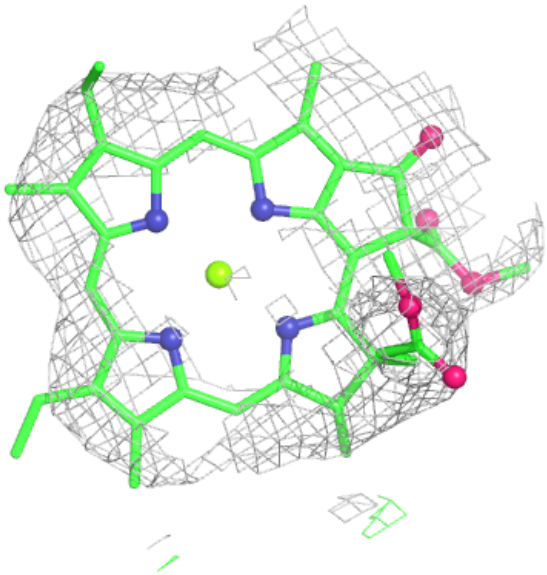


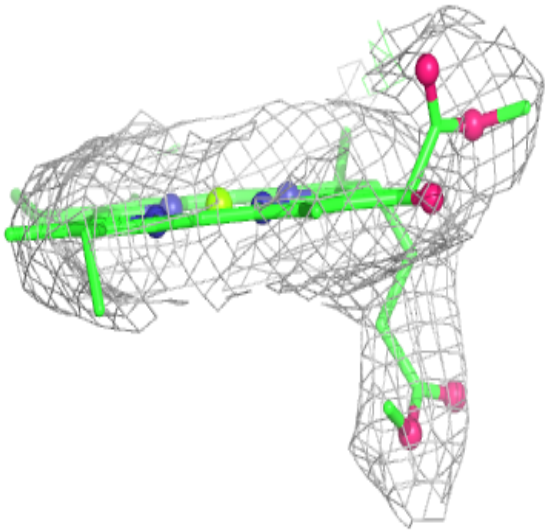


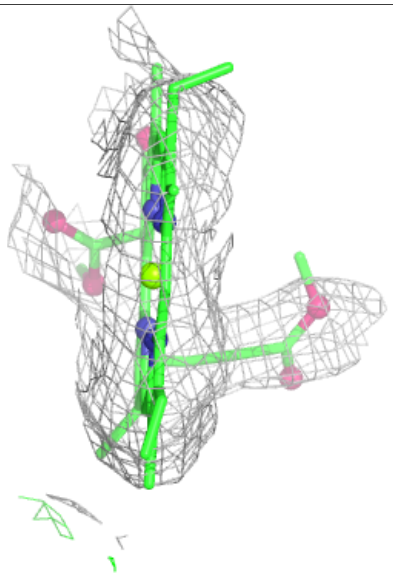


Electron density around CLA 4 608:

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

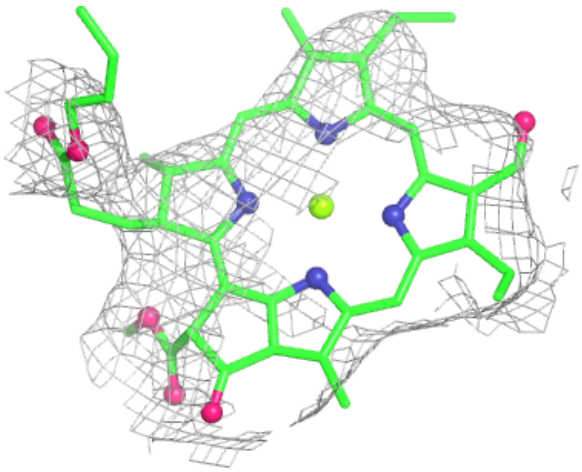


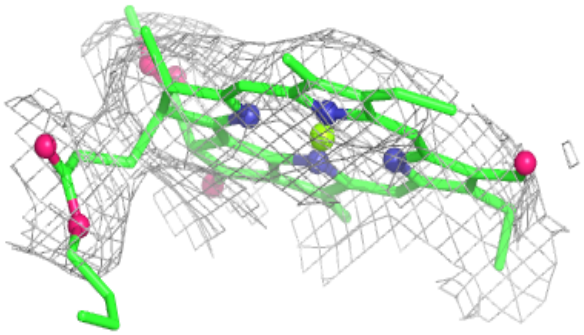


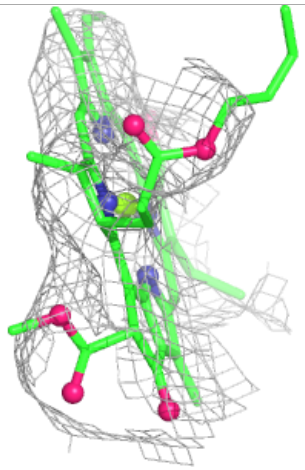


Electron density around CHL 2 609:

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

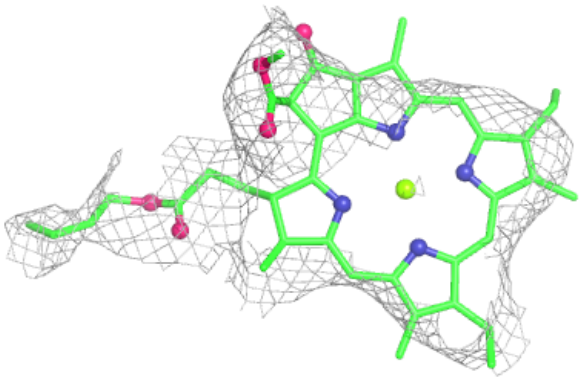


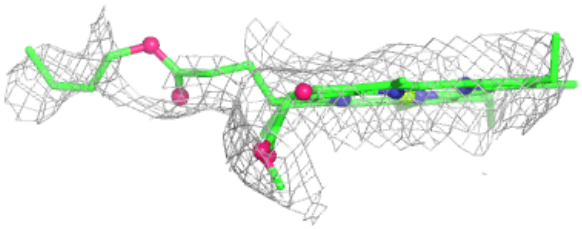


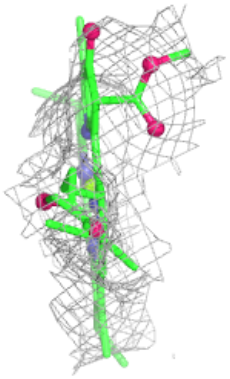


Electron density around CLA A 1135:

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

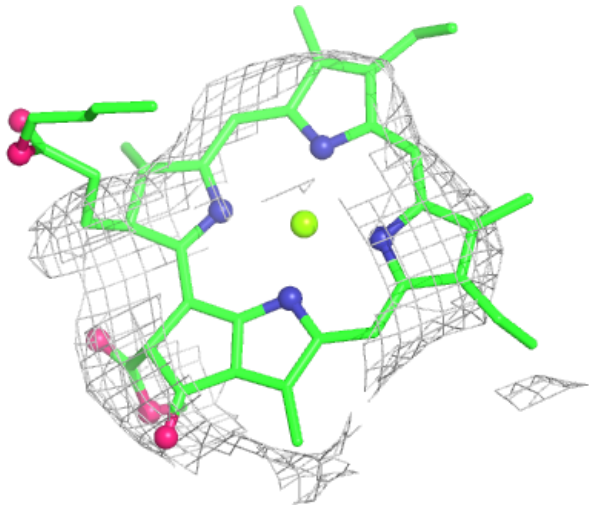


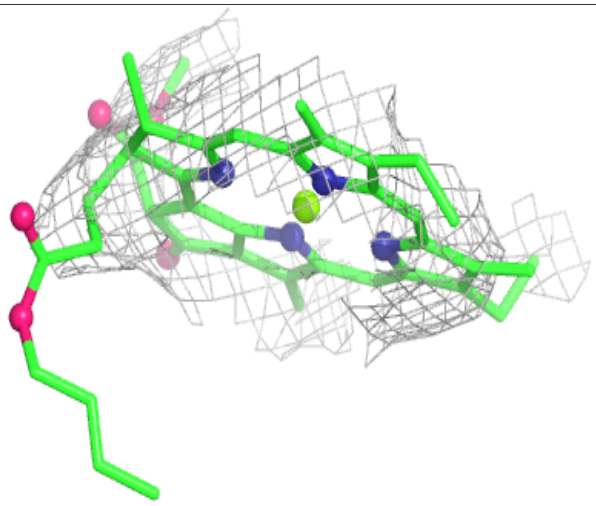


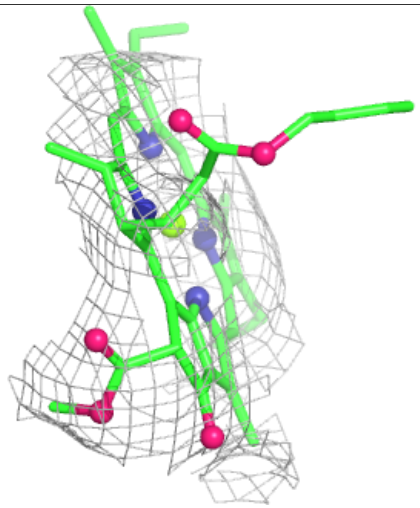


Electron density around CLA A 1118:

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

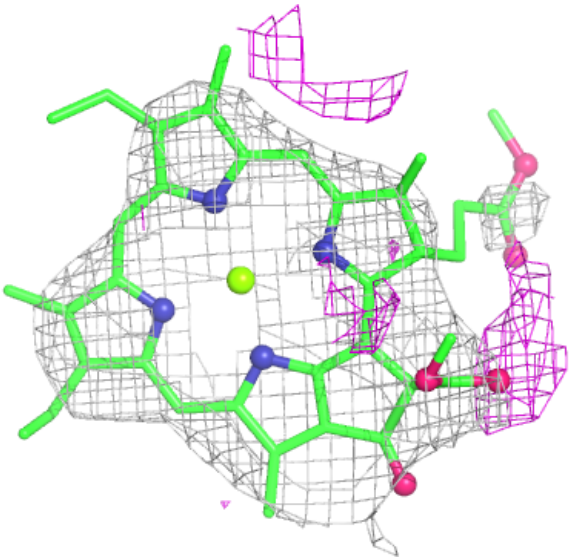


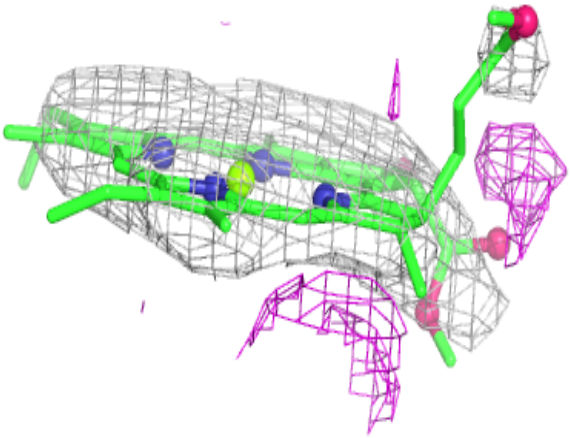


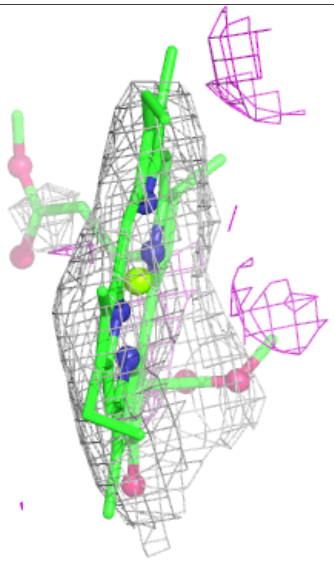


Electron density around CLA 1 608:

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

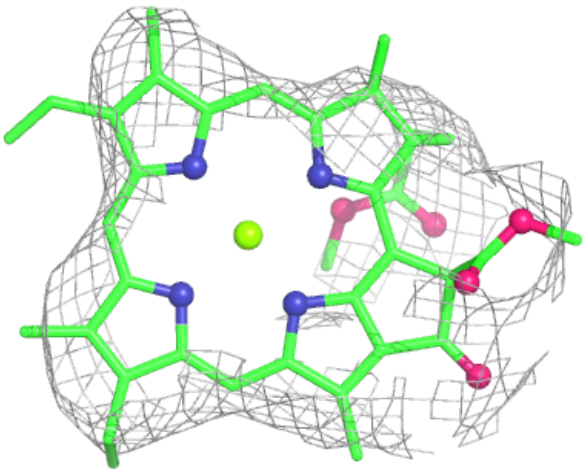


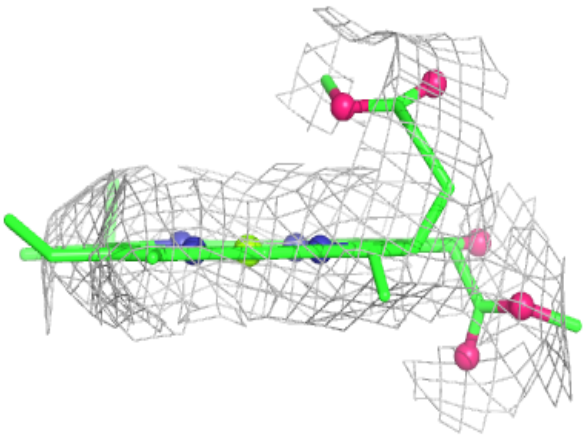


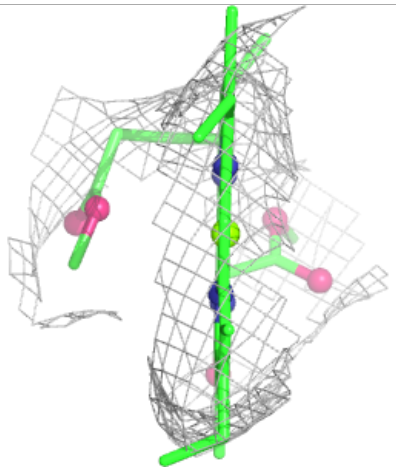


Electron density around CLA 2 603:

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

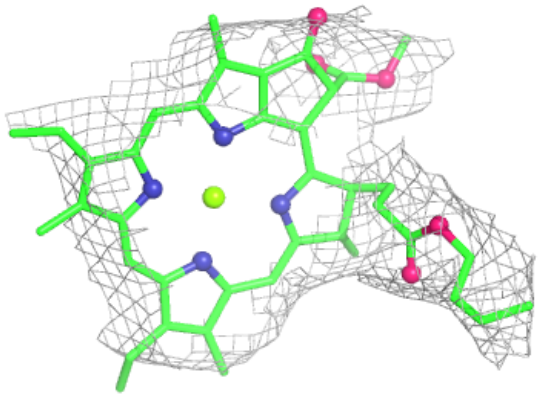


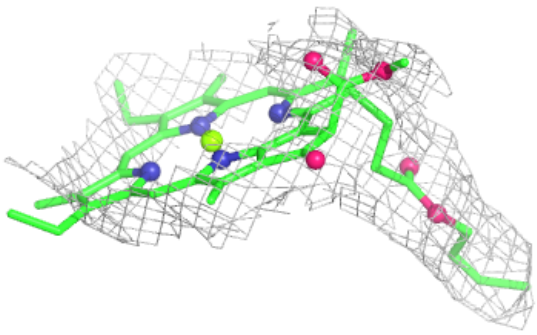


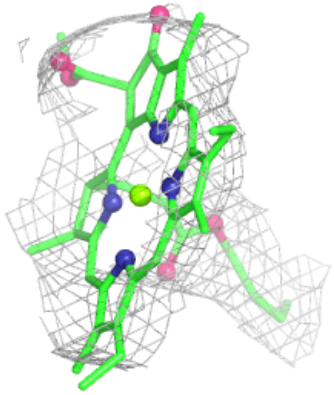


Electron density around CLA 1 611:

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

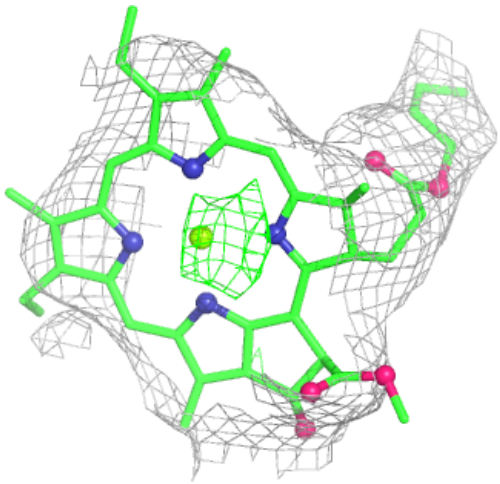


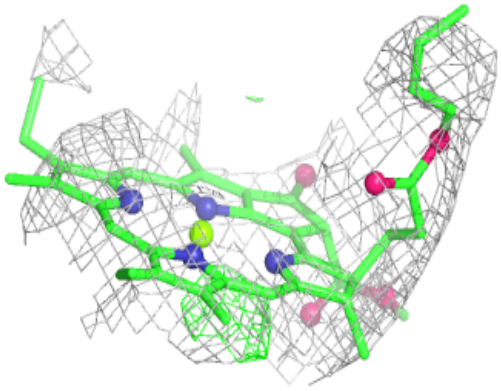


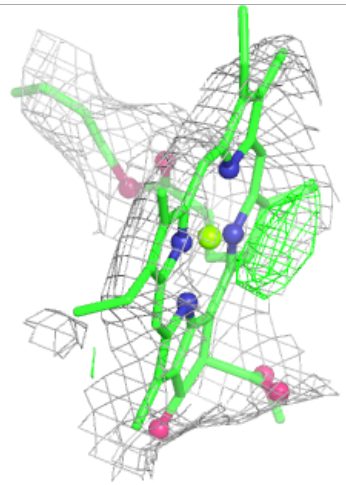


Electron density around CLA 2 612:

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

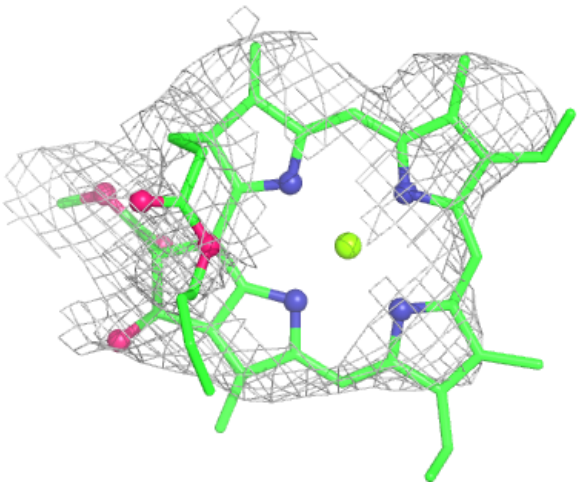


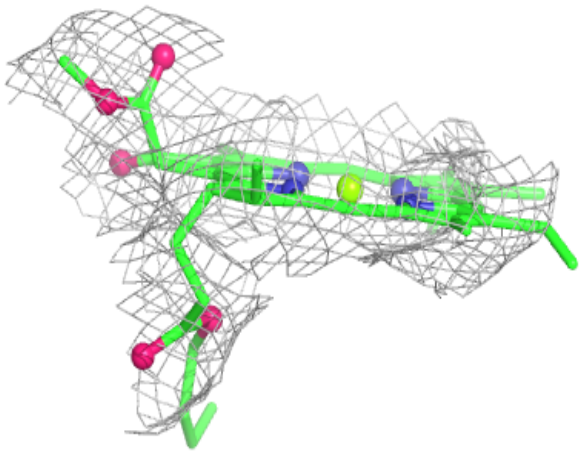


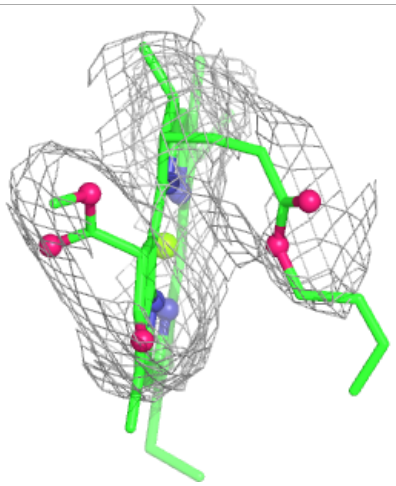


Electron density around CLA B 1213:

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

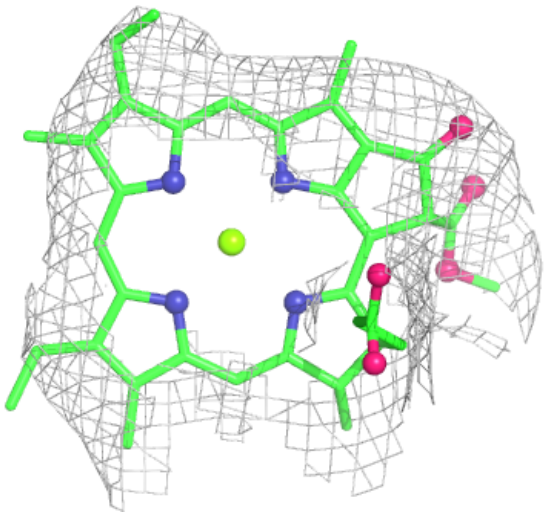


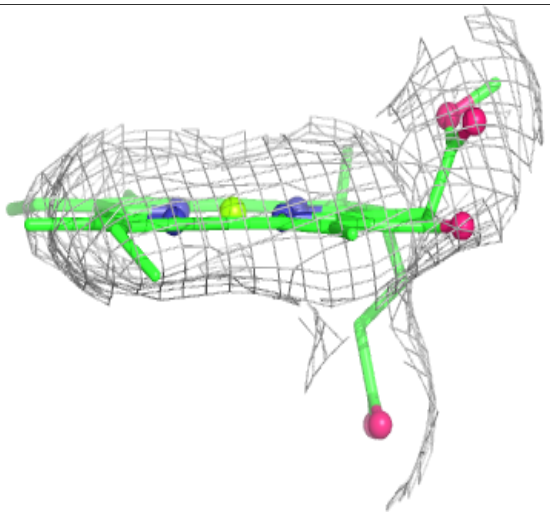


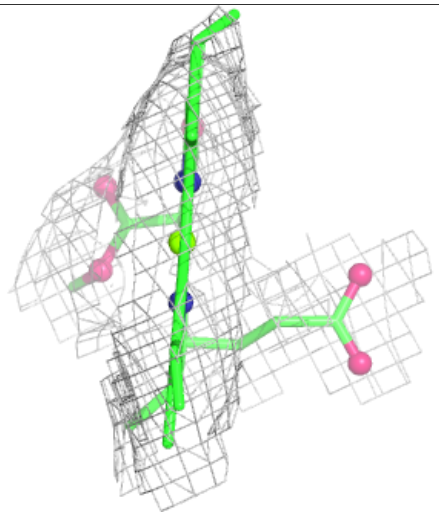


Electron density around CLA 1 606:

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

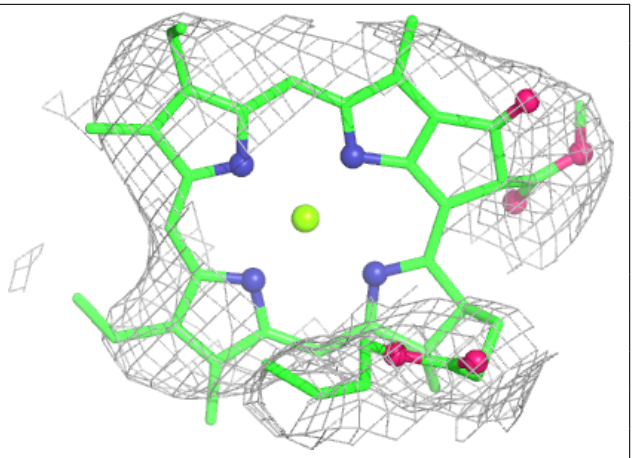


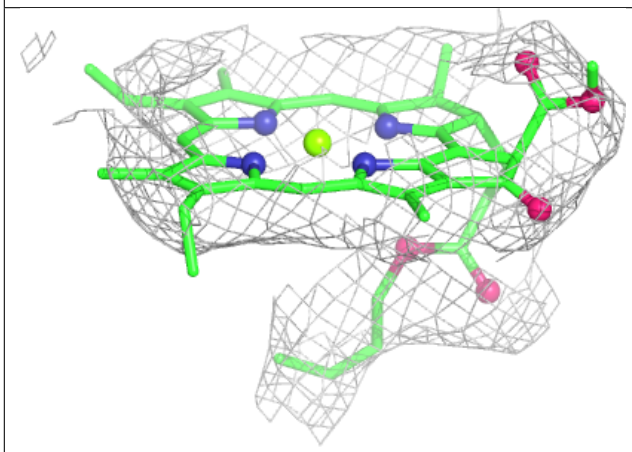


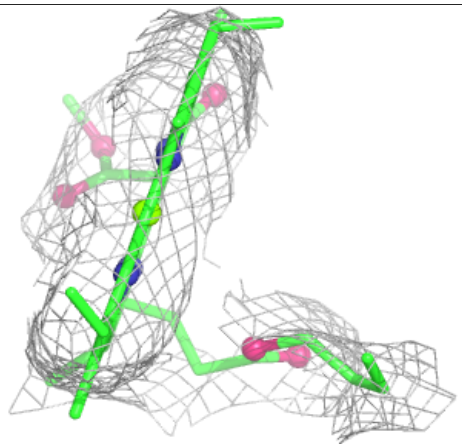


Electron density around CLA A 1105:

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

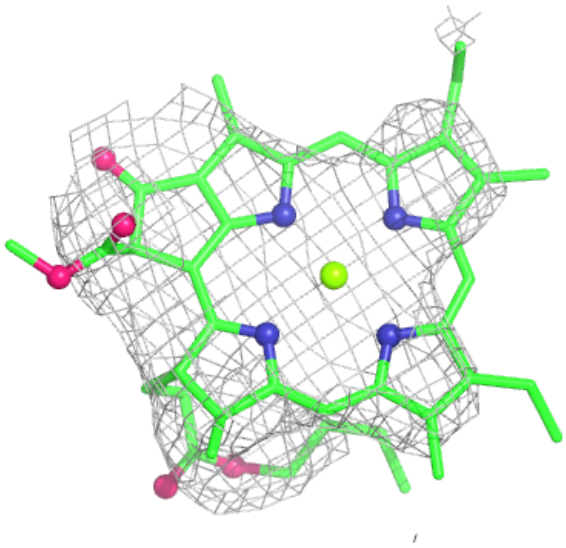


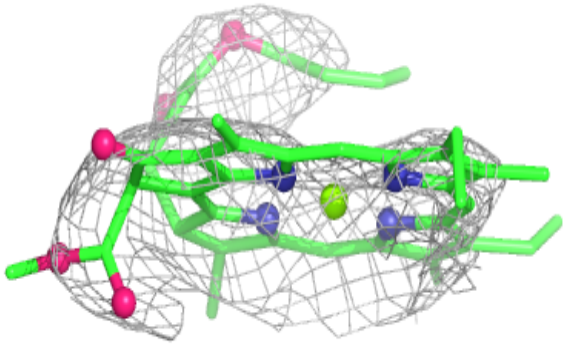


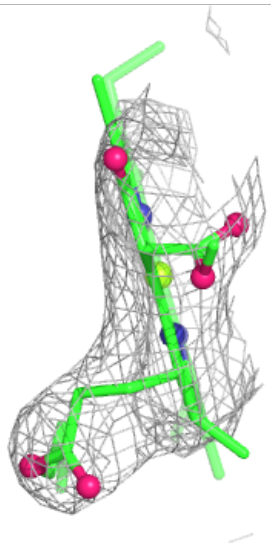


Electron density around CLA A 1117:

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

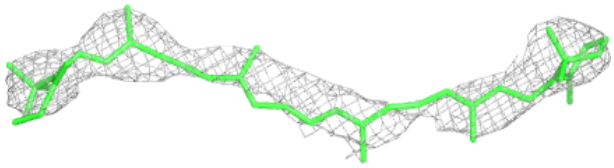


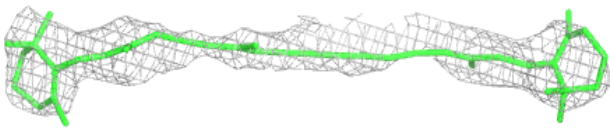


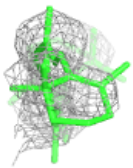


Electron density around BCR B 4004:

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

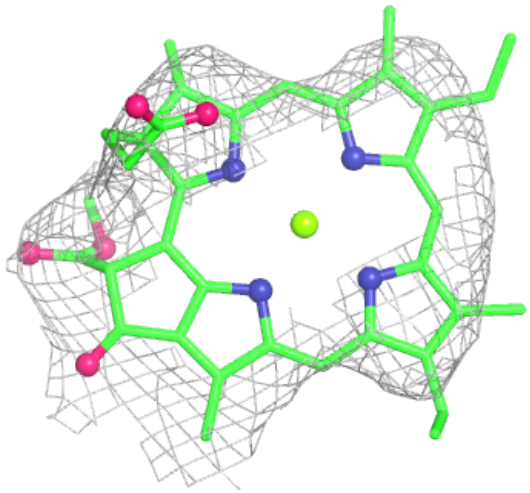


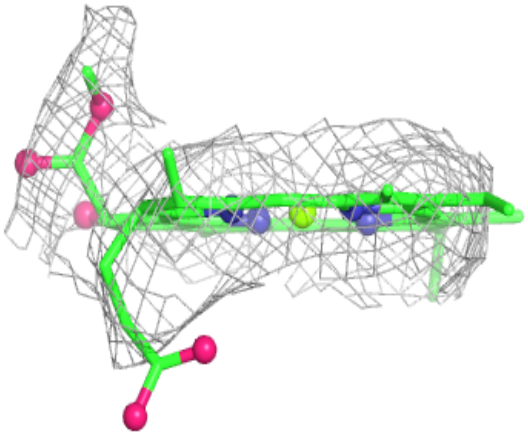


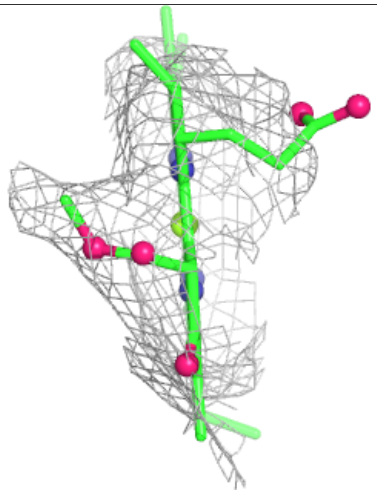


Electron density around CLA B 1212:

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

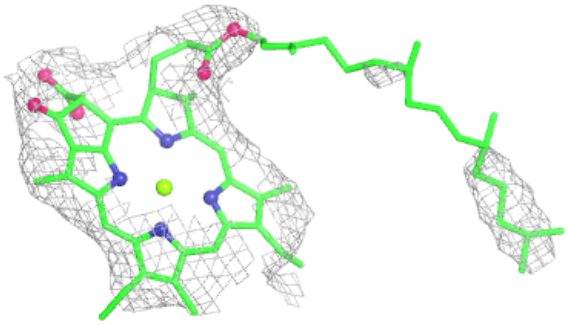


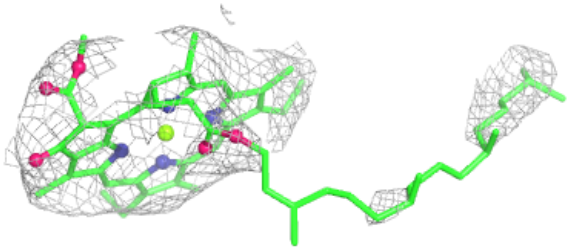


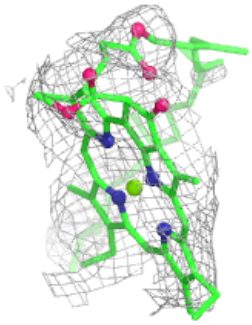


Electron density around CLA A 1106:

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

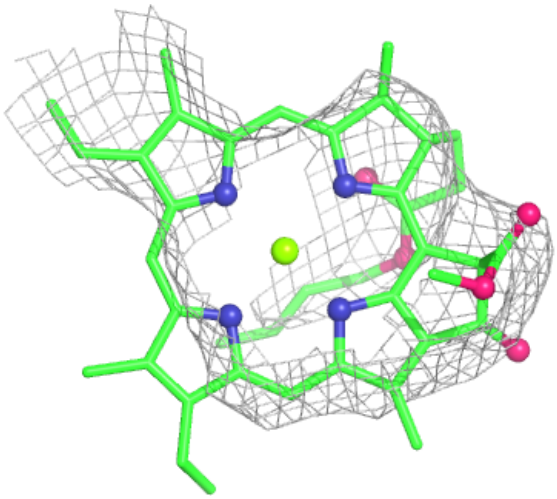


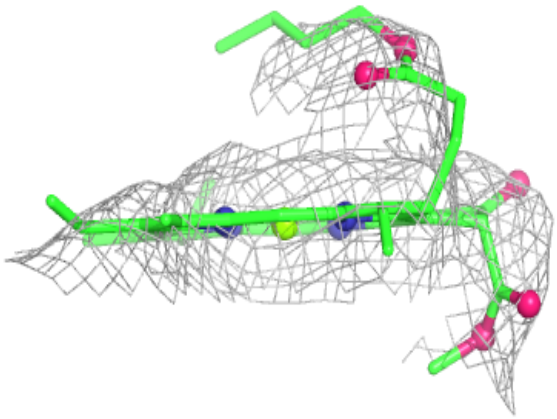


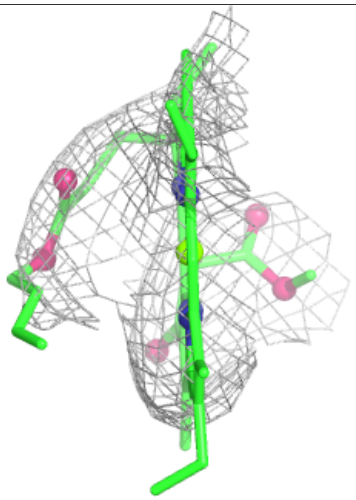


Electron density around CLA A 1110:

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

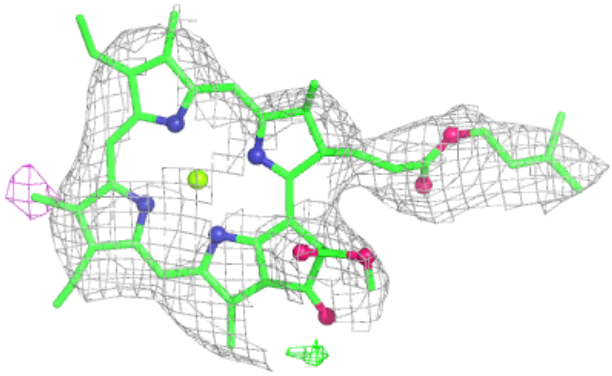


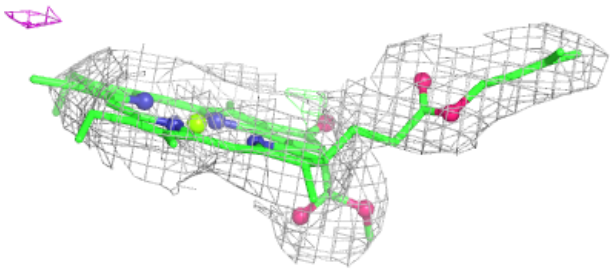


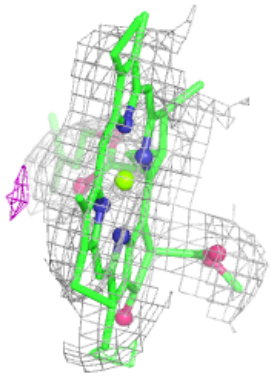


Electron density around CLA B 1223:

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

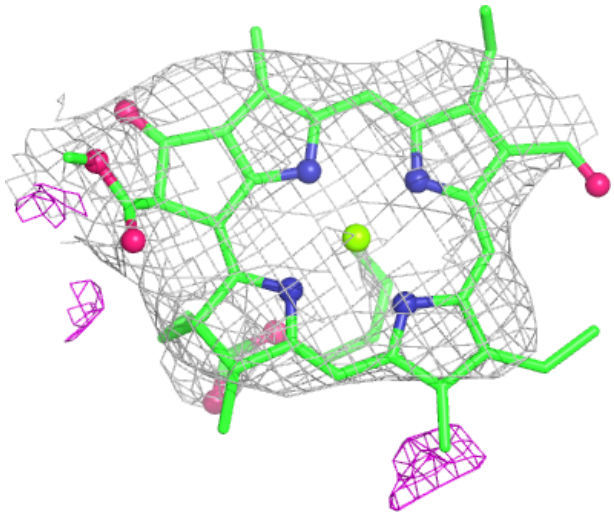


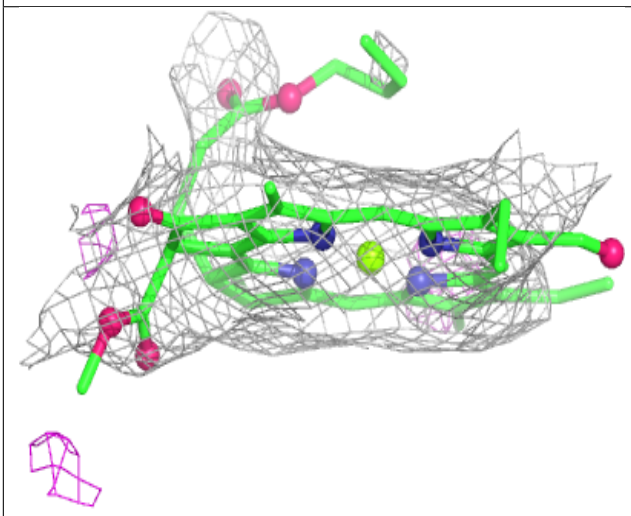


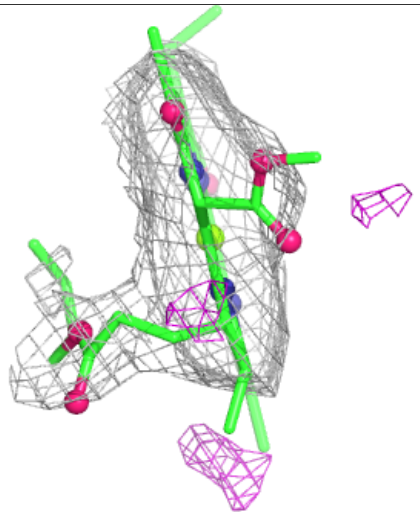


Electron density around CHL 1 609:

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

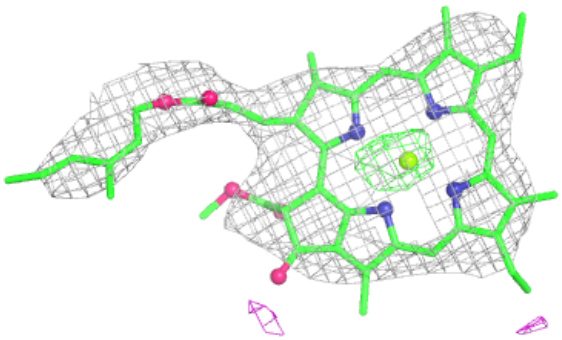


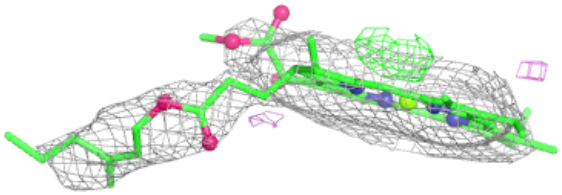


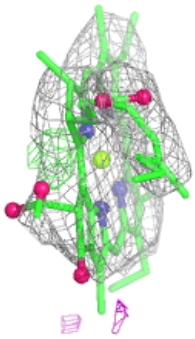


Electron density around CLA A 1139:

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

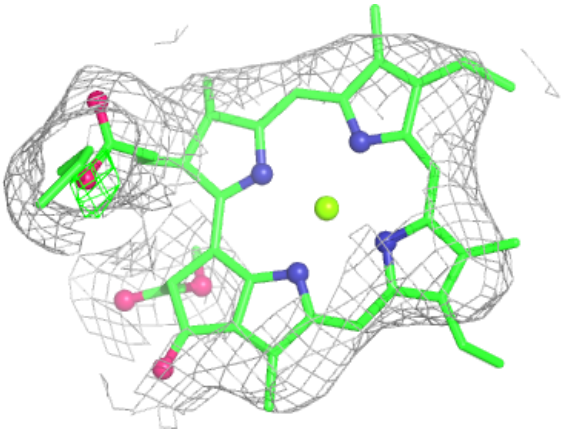


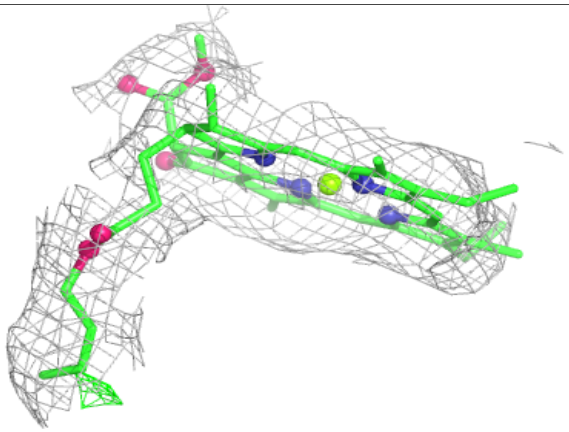


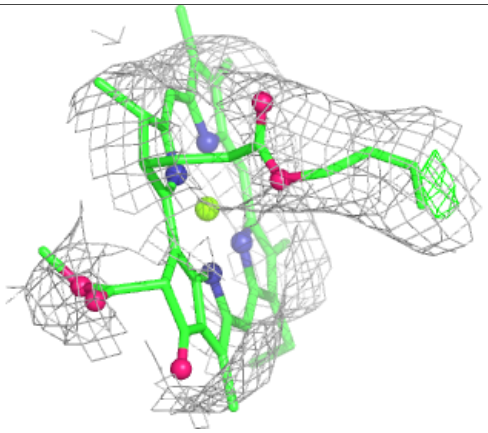


Electron density around CLA B 1236:

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

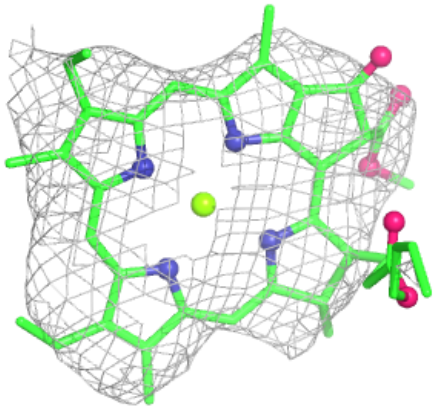


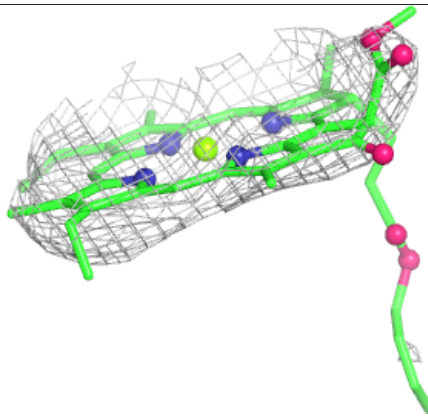


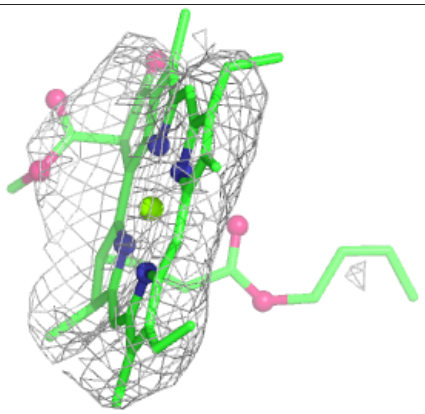


Electron density around CLA B 1225:

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

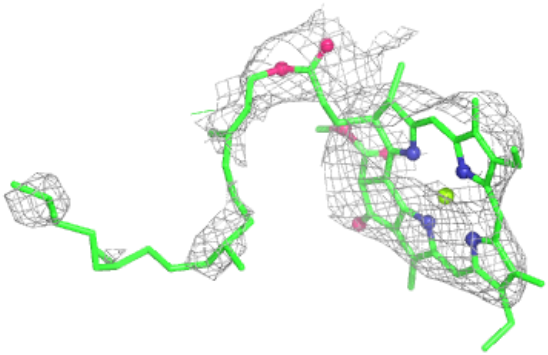


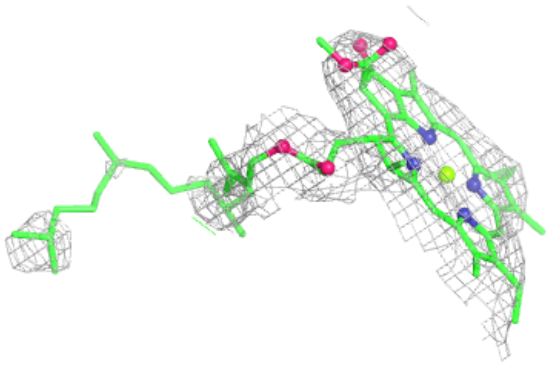


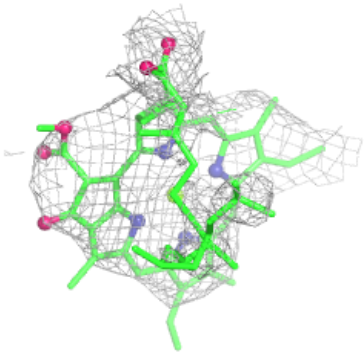


Electron density around CLA B 1021:

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

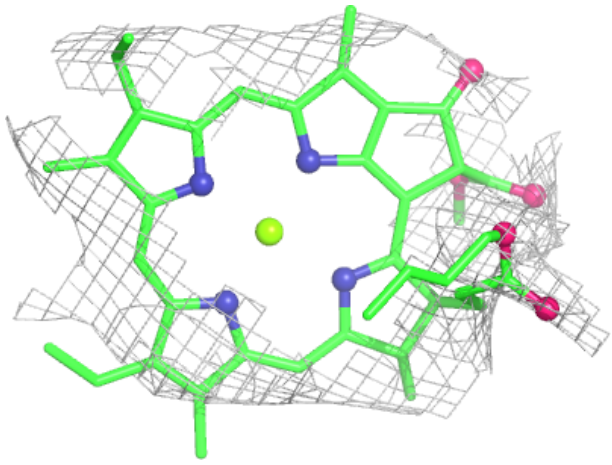


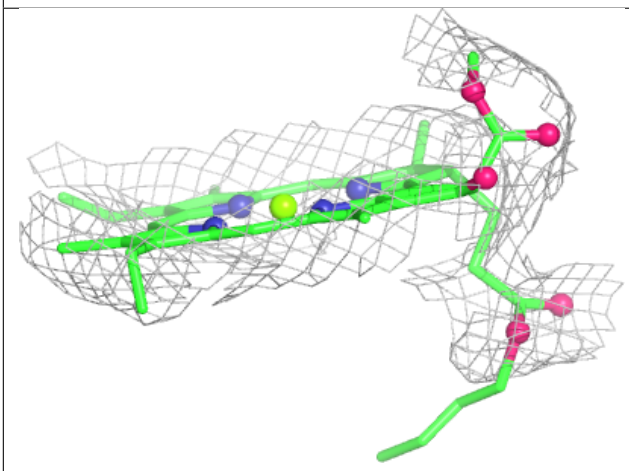


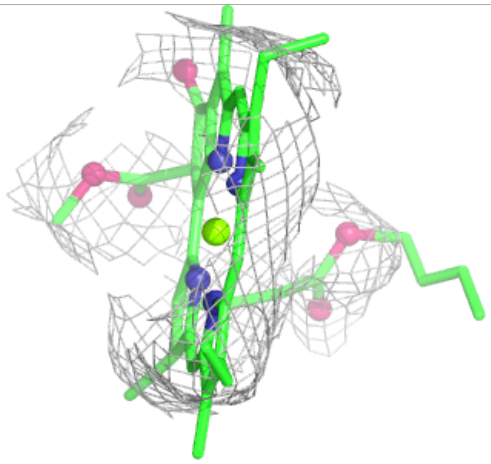


Electron density around CLA B 1204:

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

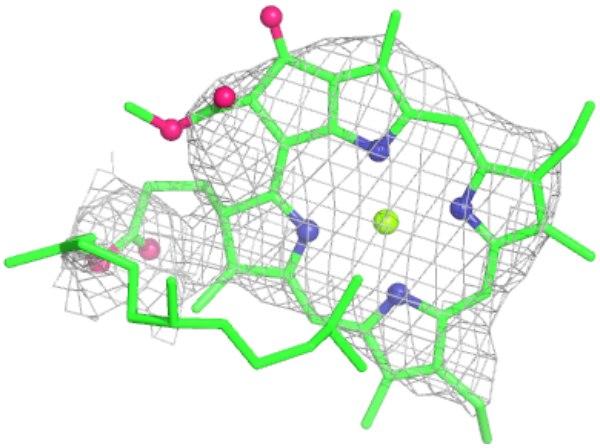


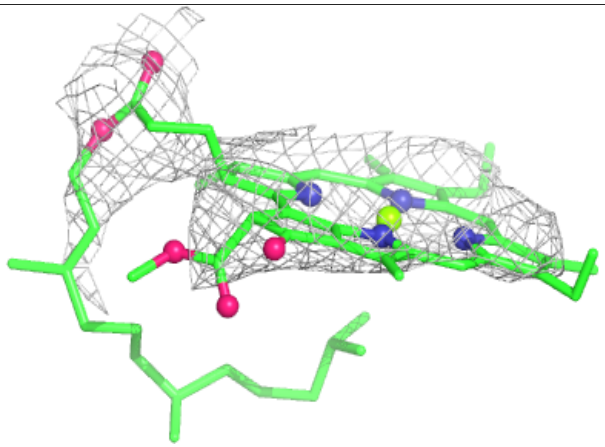


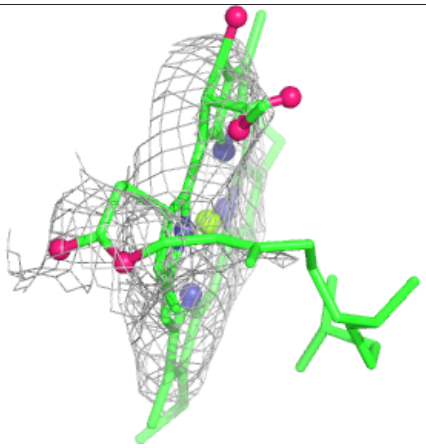


Electron density around CLA A 1104:

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

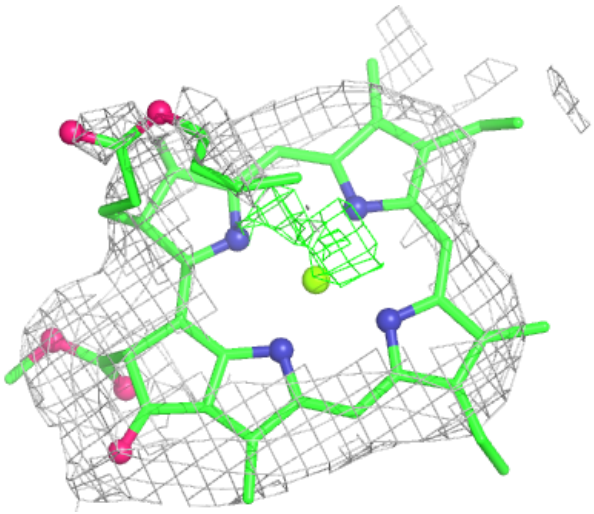


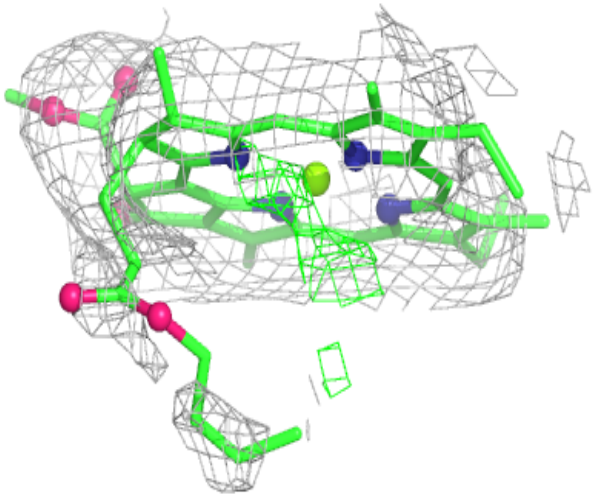


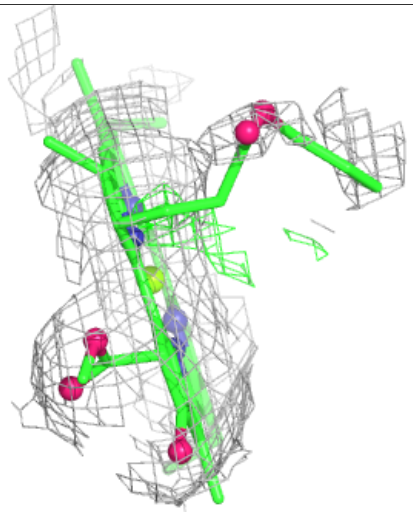


Electron density around CLA B 1214:

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

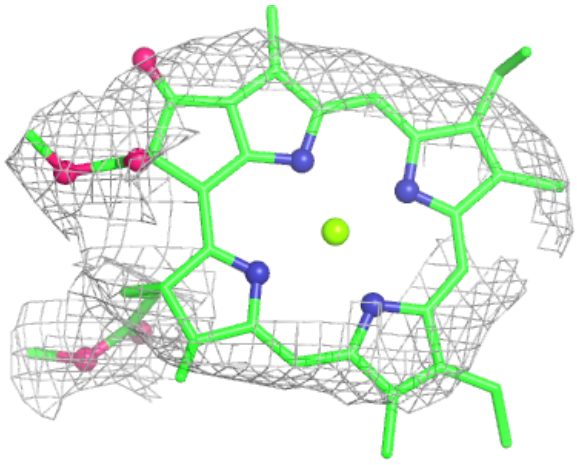


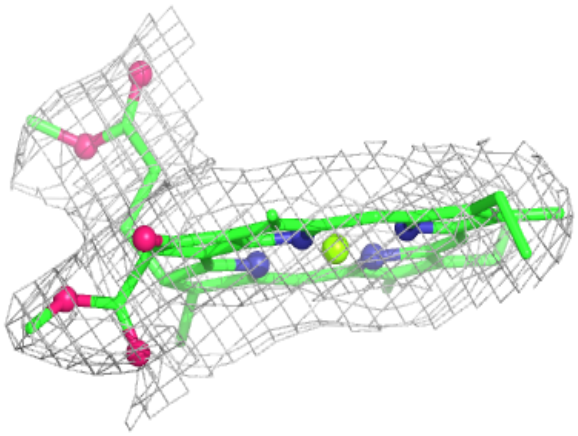


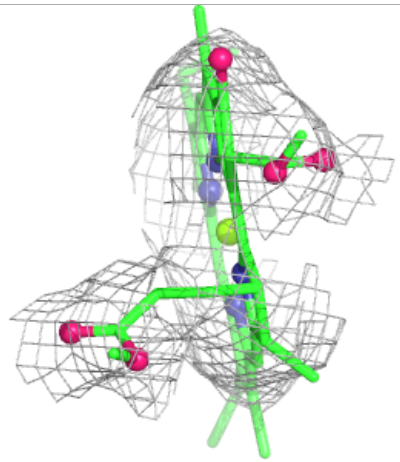


Electron density around CLA 3 615:

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

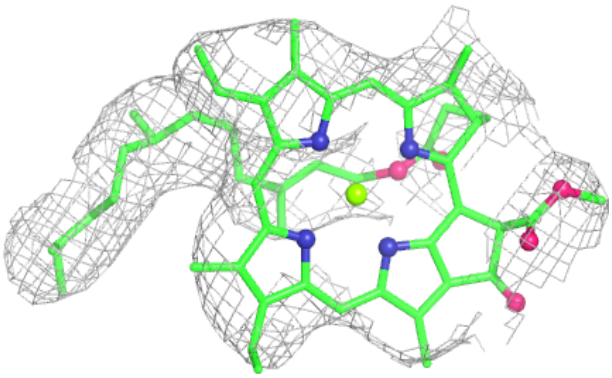


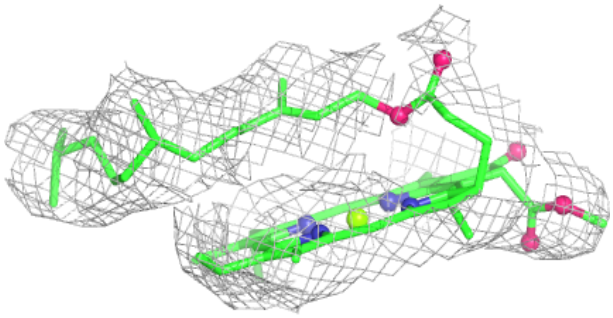


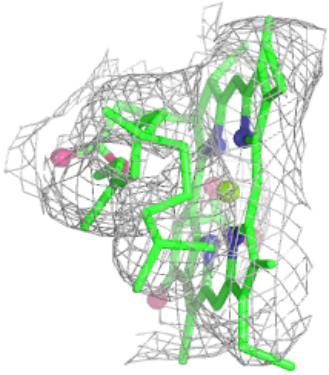


Electron density around CLA B 1235:

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

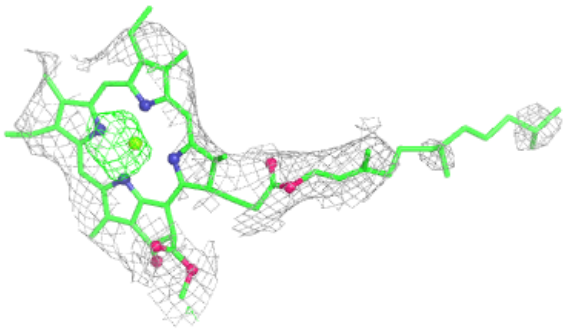


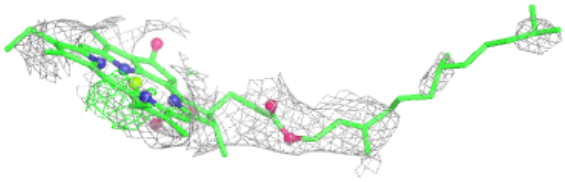


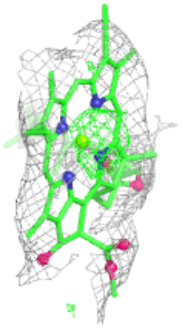


Electron density around CLA A 1012:

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

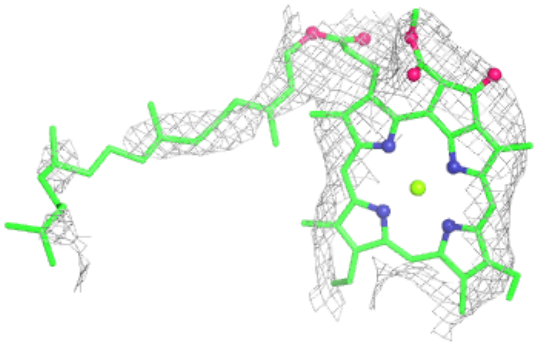


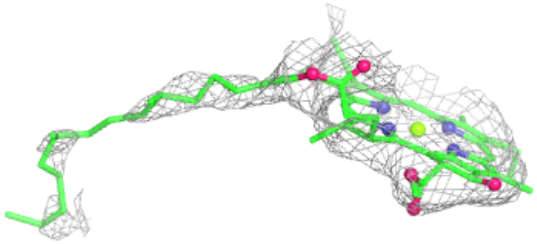


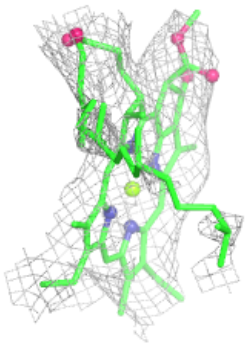


Electron density around CLA A 1013:

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

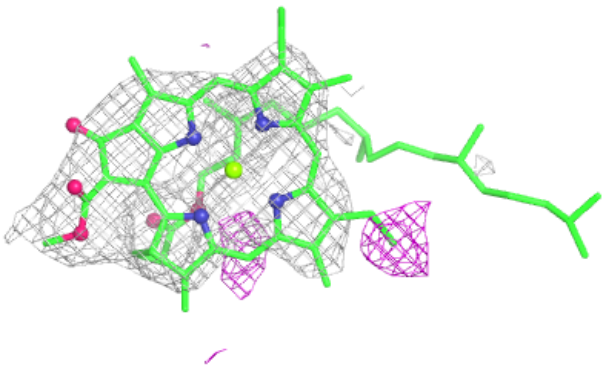


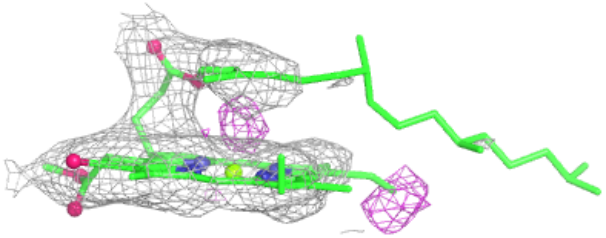


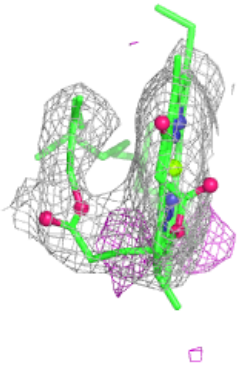


Electron density around CLA A 1138:

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

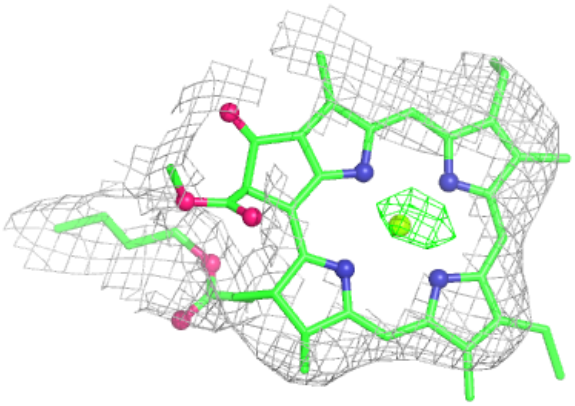


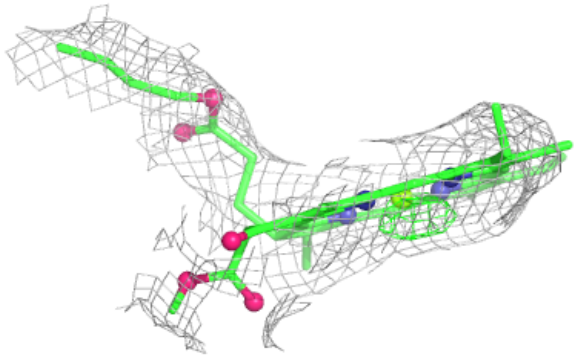


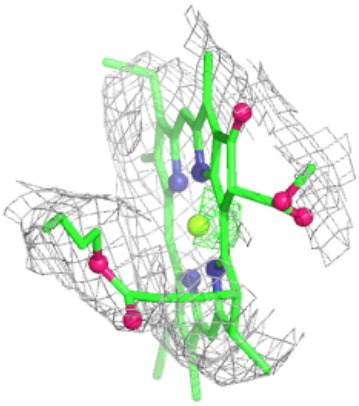


Electron density around CLA A 1107:

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

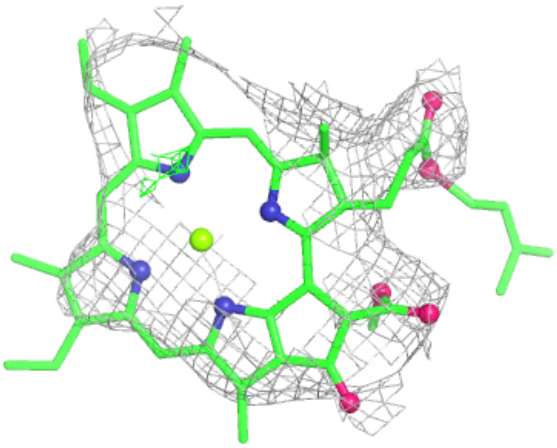


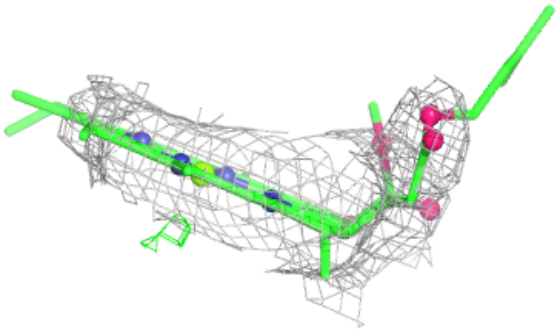


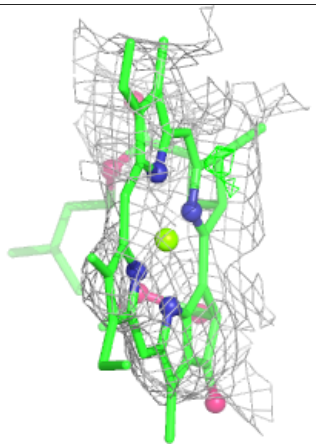


Electron density around CL0 A 1011:

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

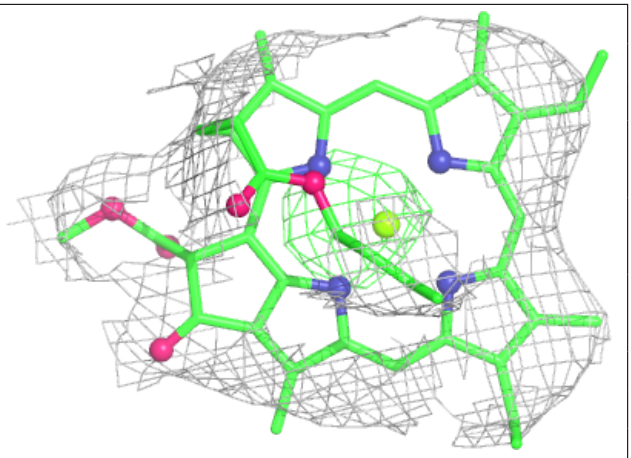


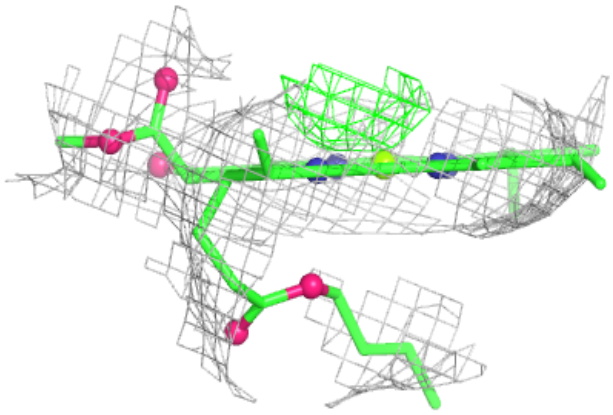


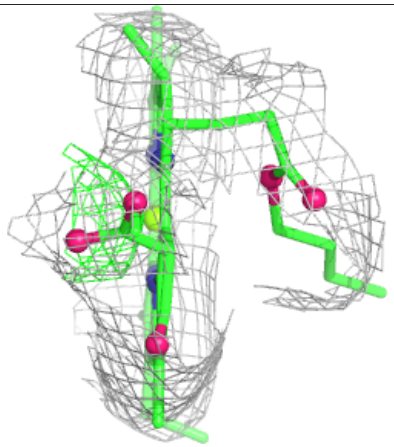


Electron density around CLA 4 603:

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

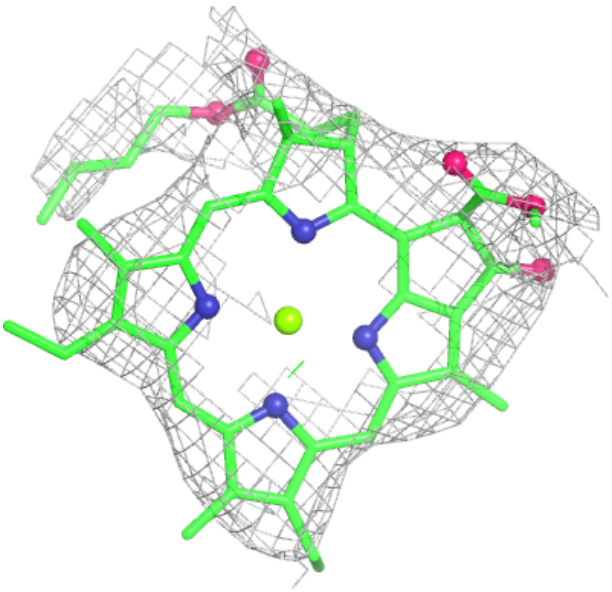


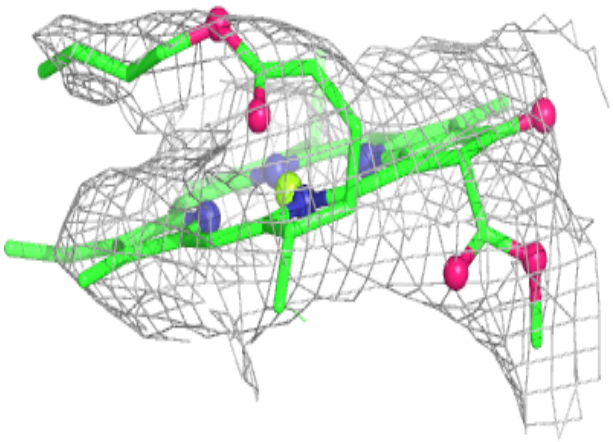


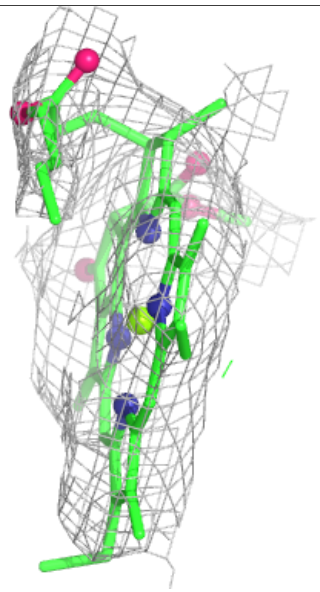


Electron density around CLA 1 604:

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

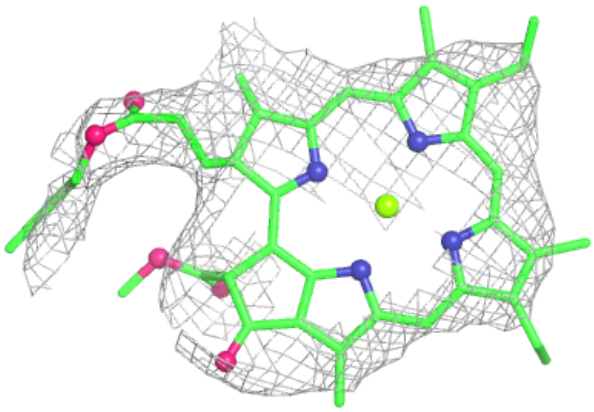


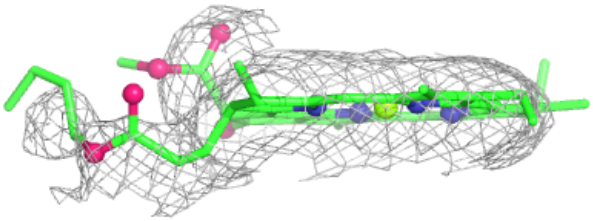


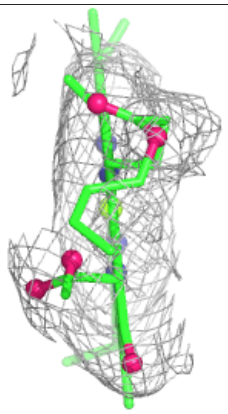


Electron density around CLA B 1202:

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

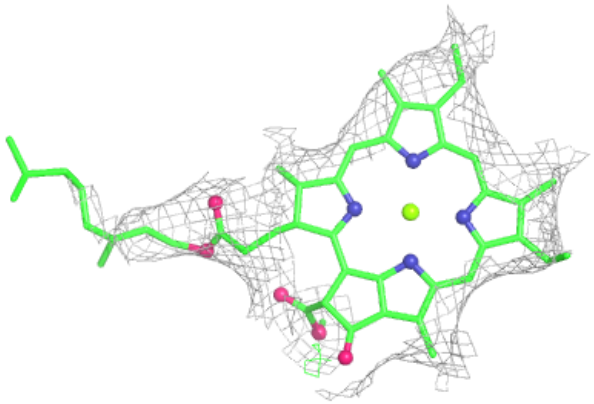


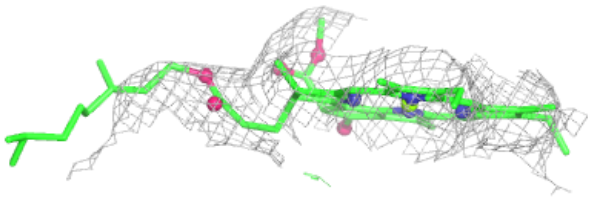




Electron density around CLA A 1103:

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

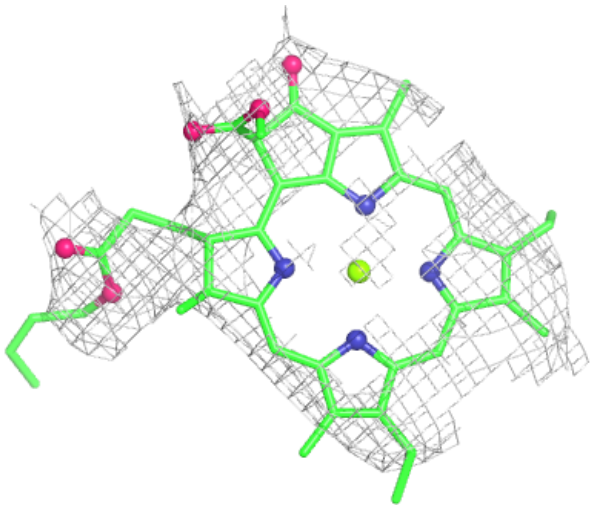


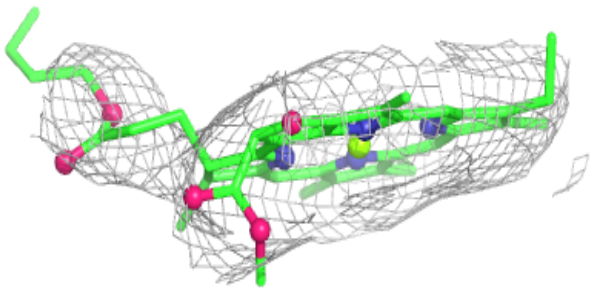


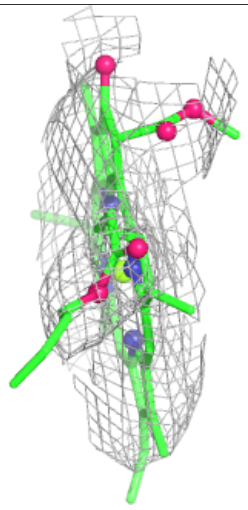


Electron density around CLA B 1210:

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

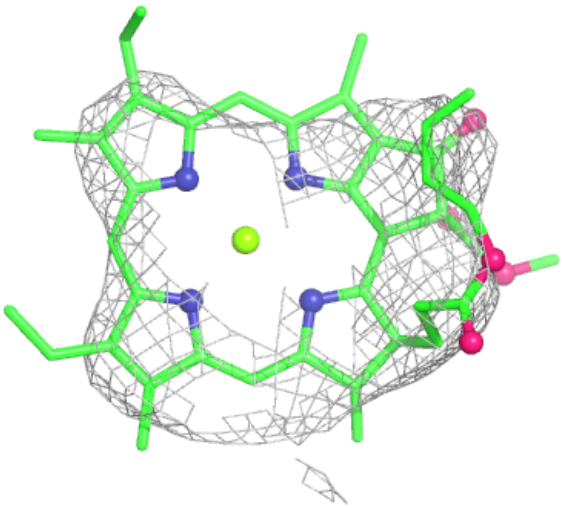


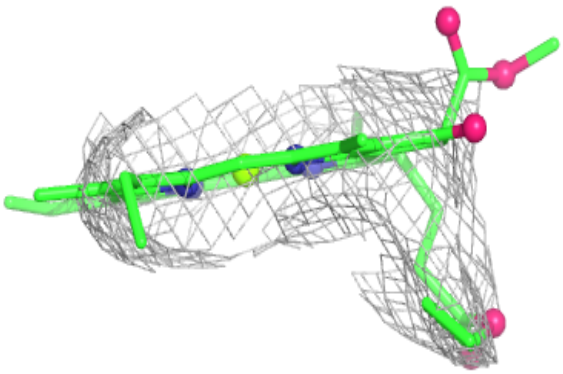


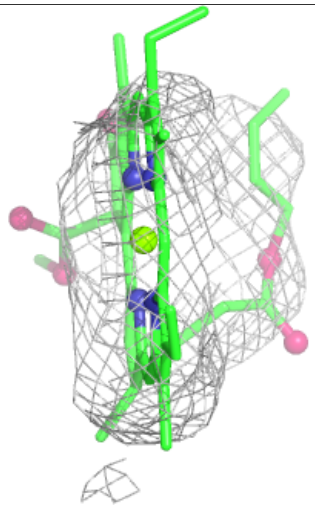


Electron density around CLA A 1127:

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

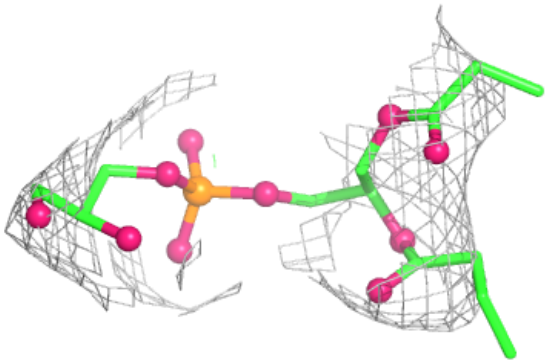


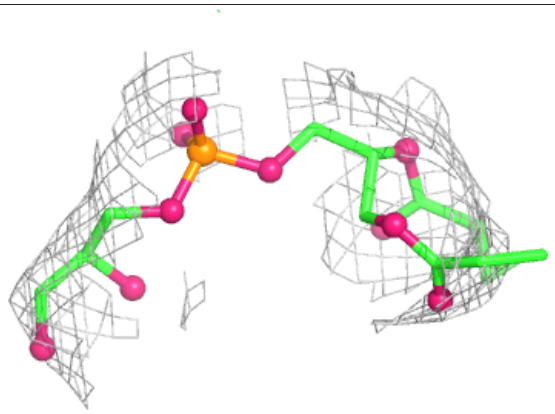


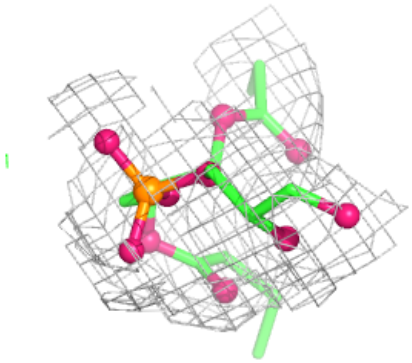


Electron density around LHG A 5002:

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

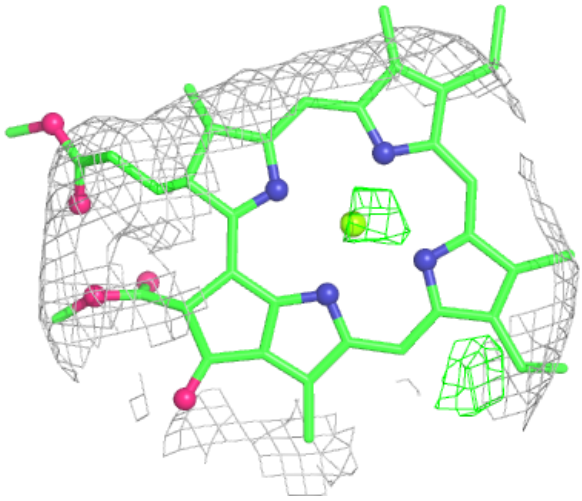


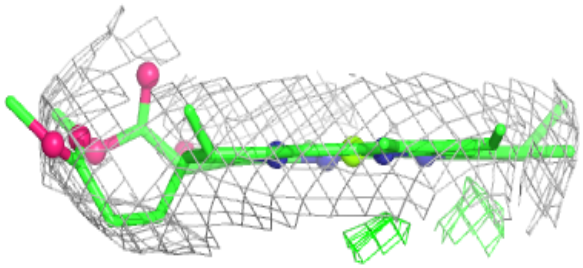




Electron density around CLA 3 605:

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

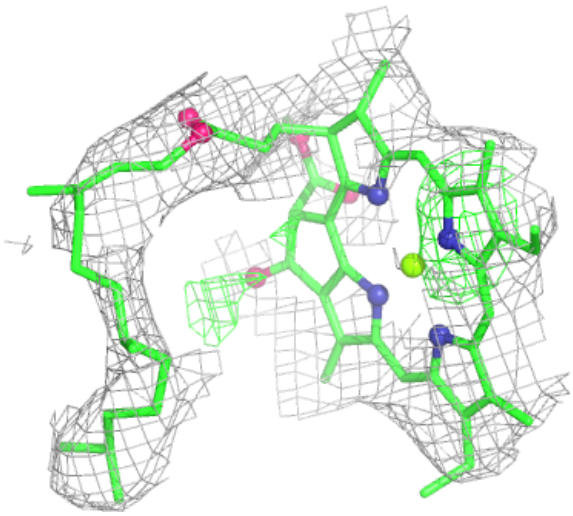


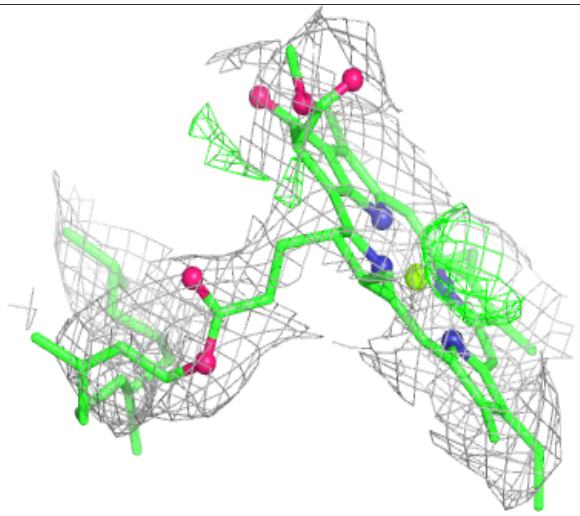


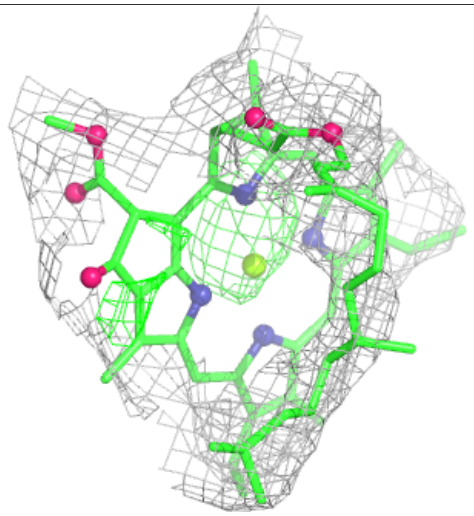


Electron density around CLA B 1231:

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

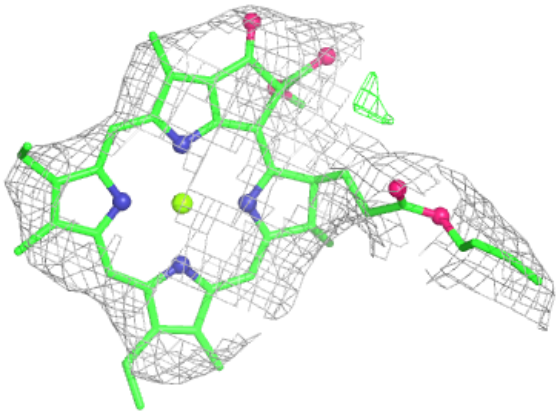


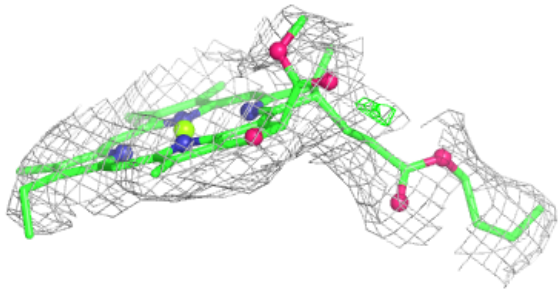




Electron density around CLA B 1222:

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







6.5 Other polymers

There are no such residues in this entry.